# Full wwPDB EM Validation Report (i)

Dec 27, 2024 – 12:44 AM EST

| | | |
|---|---|---|
| PDB ID | : | 6U42 |
| EMDB ID | : | EMD-20631 |
| Title | : | Natively decorated ciliary doublet microtubule |
| Authors | : | Ma, M.; Stoyanova, M.; Rademacher, G.; Dutcher, S.K.; Brown, A.; Zhang, R. |
| Deposited on | : | 2019-08-22 |
| Resolution | : | 3.40 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

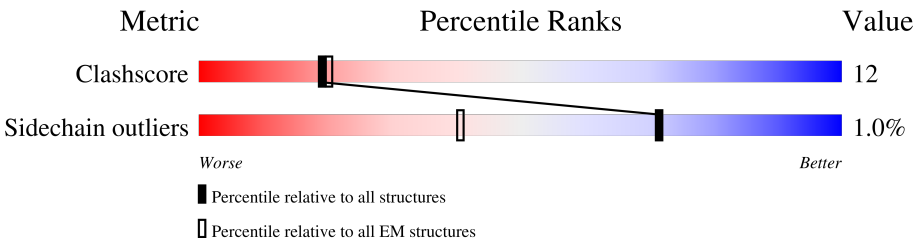
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.40 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0A | 443 | • 63% 33% • |
| 1 | 0C | 443 | 19% 64% 32% • |
| 1 | 0E | 443 | 17% 57% 39% • |
| 1 | 0G | 443 | 5% 63% 33% • |
| 1 | 0I | 443 | 5% 63% 33% • |
| 1 | 0K | 443 | • 62% 34% • |
| 1 | 0M | 443 | • 62% 34% • |
| 1 | 0O | 443 | 6% 61% 35% • |
| 1 | 0Q | 443 | • 64% 33% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0S | 443 | 49% 62% 34% |
| 1 | 0U | 443 | 15% 61% 35% |
| 1 | 0W | 443 | 6% 63% 33% |
| 1 | 0Y | 443 | 7% 65% 31% |
| 1 | 1 | 443 | 29% 69% |
| 1 | 1A | 443 | 5% 70% 26% |
| 1 | 1C | 443 | 5% 65% 31% |
| 1 | 1E | 443 | 7% 60% 36% |
| 1 | 1G | 443 | 8% 65% 31% |
| 1 | 1K | 443 | 64% 32% |
| 1 | 1M | 443 | 66% 30% |
| 1 | 1O | 443 | 68% 28% |
| 1 | 1Q | 443 | 66% 30% |
| 1 | 1S | 443 | 69% 28% |
| 1 | 1U | 443 | 65% 31% |
| 1 | 1W | 443 | 65% 31% |
| 1 | 2A | 443 | 67% 28% |
| 1 | 2C | 443 | 67% 29% |
| 1 | 2E | 443 | 66% 30% |
| 1 | 2G | 443 | 71% 25% |
| 1 | 2I | 443 | 68% 28% |
| 1 | 2K | 443 | 73% 23% |
| 1 | 2M | 443 | 64% 32% |
| 1 | 2Q | 443 | 67% 29% |
| 1 | 2S | 443 | 71% 25% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 2U | 443 | 68% 28% |
| 1 | 2W | 443 | 73% 23% |
| 1 | 2Y | 443 | 67% 28% |
| 1 | 3 | 443 | 95% |
| 1 | 3A | 443 | 66% 30% |
| 1 | 3C | 443 | 61% 34% |
| 1 | 3G | 443 | 70% 26% |
| 1 | 3I | 443 | 70% 26% |
| 1 | 3K | 443 | 66% 30% |
| 1 | 3M | 443 | 71% 25% |
| 1 | 3O | 443 | 69% 27% |
| 1 | 3Q | 443 | 67% 30% |
| 1 | 3S | 443 | 59% 37% |
| 1 | 5 | 443 | 93% 5% |
| 1 | 7 | 443 | 95% |
| 1 | 9 | 443 | 94% |
| 1 | A1 | 443 | 95% |
| 1 | A3 | 443 | 92% 6% |
| 1 | A5 | 443 | 96% |
| 1 | A7 | 443 | 95% |
| 1 | A9 | 443 | 94% |
| 1 | B1 | 443 | 94% |
| 1 | B3 | 443 | 94% |
| 1 | B5 | 443 | 94% |
| 1 | B8 | 443 | 93% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | C0 | 443 | 95% |
| 1 | C2 | 443 | 95% |
| 1 | C4 | 443 | 95% |
| 1 | C6 | 443 | 95% |
| 1 | C8 | 443 | 95% |
| 1 | D0 | 443 | 95% |
| 1 | D2 | 443 | 95% |
| 1 | D4 | 443 | 93% |
| 1 | D6 | 443 | 94% |
| 1 | D8 | 443 | 23% 95% |
| 1 | E0 | 443 | 94% |
| 1 | E2 | 443 | 94% |
| 1 | E4 | 443 | 95% |
| 1 | E6 | 443 | 94% |
| 1 | E8 | 443 | 94% |
| 1 | F0 | 443 | 95% |
| 1 | F2 | 443 | 94% |
| 1 | F6 | 443 | 94% |
| 1 | F8 | 443 | 94% |
| 1 | G0 | 443 | 93% |
| 1 | G2 | 443 | 65% 31% |
| 1 | G4 | 443 | 67% 29% |
| 1 | G6 | 443 | 63% 33% |
| 1 | G8 | 443 | 63% 33% |
| 1 | H2 | 443 | 65% 31% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | H4 | 443 | 67% 29% |
| 1 | H6 | 443 | 69% 27% |
| 1 | H8 | 443 | 74% 21% |
| 1 | I0 | 443 | 72% 24% |
| 1 | I2 | 443 | 69% 27% |
| 1 | I4 | 443 | 64% 32% |
| 1 | I8 | 443 | 66% 30% |
| 1 | J0 | 443 | 69% 27% |
| 1 | J2 | 443 | 73% 23% |
| 1 | J4 | 443 | 70% 26% |
| 1 | J6 | 443 | 71% 25% |
| 1 | J8 | 443 | 74% 22% |
| 1 | K0 | 443 | 74% 22% |
| 1 | K4 | 443 | 70% 26% |
| 1 | K6 | 443 | 73% 23% |
| 1 | K8 | 443 | 71% 25% |
| 1 | L0 | 443 | 72% 24% |
| 1 | L2 | 443 | 70% 26% |
| 1 | L4 | 443 | 70% 26% |
| 1 | L6 | 443 | 68% 28% |
| 1 | M0 | 443 | 69% 27% |
| 1 | M2 | 443 | 72% 24% |
| 1 | M4 | 443 | 72% 24% |
| 1 | M6 | 443 | 69% 27% |
| 1 | M8 | 443 | 72% 24% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | N0 | 443 | 71% 25% |
| 1 | N2 | 443 | 70% 27% |
| 1 | N6 | 443 | 73% 23% |
| 1 | N8 | 443 | 72% 24% |
| 1 | O0 | 443 | 75% 21% |
| 1 | O2 | 443 | 72% 24% |
| 1 | O4 | 443 | 69% 27% |
| 1 | O6 | 443 | 75% 21% |
| 1 | O8 | 443 | 75% 21% |
| 1 | P4 | 443 | 65% 31% |
| 1 | P6 | 443 | 71% 25% |
| 1 | P8 | 443 | 70% 26% |
| 1 | Q0 | 443 | 74% 23% |
| 1 | Q2 | 443 | 70% 27% |
| 1 | Q4 | 443 | 70% 26% |
| 1 | Q6 | 443 | 70% 26% |
| 1 | Q8 | 443 | 37% 61% 33% 5% |
| 1 | R0 | 443 | 72% 26% |
| 1 | R2 | 443 | 71% 25% |
| 1 | R4 | 443 | 67% 29% |
| 1 | R6 | 443 | 69% 27% |
| 1 | R8 | 443 | 70% 27% |
| 1 | S0 | 443 | 69% 26% |
| 1 | S2 | 443 | 70% 27% |
| 1 | S4 | 443 | 14% 60% 36% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | S6 | 443 | 68% 28% |
| 1 | S8 | 443 | 67% 29% |
| 1 | T0 | 443 | 69% 28% |
| 1 | T2 | 443 | 65% 31% |
| 1 | T4 | 443 | 68% 28% |
| 1 | T6 | 443 | 59% 37% |
| 1 | T8 | 443 | 68% 28% |
| 1 | U2 | 443 | 68% 28% |
| 1 | U4 | 443 | 69% 27% |
| 1 | U6 | 443 | 5% 66% 30% |
| 1 | U8 | 443 | 69% 28% |
| 1 | V0 | 443 | 73% 23% |
| 1 | V2 | 443 | 68% 28% |
| 1 | V4 | 443 | 74% 22% |
| 1 | V6 | 443 | 31% 57% 39% |
| 1 | V8 | 443 | 67% 29% |
| 1 | W0 | 443 | 68% 28% |
| 1 | W2 | 443 | 71% 25% |
| 1 | W4 | 443 | 66% 30% |
| 1 | W6 | 443 | 69% 27% |
| 1 | W8 | 443 | 70% 26% |
| 1 | X0 | 443 | 68% 28% |
| 1 | X2 | 443 | 21% 61% 35% |
| 1 | X4 | 443 | 63% 33% |
| 1 | X6 | 443 | 66% 30% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | X8 | 443 | 70% 26% |
| 1 | Y0 | 443 | 66% 30% |
| 1 | Y2 | 443 | 71% 25% |
| 1 | Y4 | 443 | 70% 27% |
| 1 | Y6 | 443 | 73% 23% |
| 1 | Y8 | 443 | 24% 59% 37% |
| 1 | Z0 | 443 | 6% 59% 37% |
| 1 | Z2 | 443 | 9% 59% 37% |
| 1 | Z4 | 443 | 61% 35% |
| 1 | Z6 | 443 | 61% 35% |
| 1 | Z8 | 443 | 6% 56% 40% |
| 2 | 0B | 451 | 62% 33% 5% |
| 2 | 0F | 451 | 59% 35% 5% |
| 2 | 0H | 451 | 61% 33% 5% |
| 2 | 0J | 451 | 6% 60% 35% 5% |
| 2 | 0L | 451 | 59% 36% 5% |
| 2 | 0N | 451 | 6% 57% 37% 5% |
| 2 | 0P | 451 | 65% 30% 5% |
| 2 | 0R | 451 | 5% 59% 36% 5% |
| 2 | 0V | 451 | 8% 59% 35% 5% |
| 2 | 0X | 451 | 7% 61% 33% 5% |
| 2 | 0Z | 451 | 64% 30% 5% |
| 2 | 1B | 451 | 5% 65% 29% 5% |
| 2 | 1D | 451 | 7% 62% 32% 5% |
| 2 | 1F | 451 | 6% 58% 36% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | 1H | 451 | 16% 59% 35% 5% |
| 2 | 1L | 451 | 66% 29% 5% |
| 2 | 1N | 451 | 64% 30% 5% |
| 2 | 1P | 451 | 68% 26% 5% |
| 2 | 1R | 451 | 63% 30% 5% |
| 2 | 1T | 451 | 65% 29% 5% |
| 2 | 1V | 451 | 63% 31% 5% |
| 2 | 1X | 451 | 16% 60% 34% 5% |
| 2 | 1Z | 451 | 24% 65% 29% 5% |
| 2 | 2 | 451 | 94% |
| 2 | 2B | 451 | 69% 26% 5% |
| 2 | 2D | 451 | 70% 24% 5% |
| 2 | 2F | 451 | 67% 28% 5% |
| 2 | 2H | 451 | 67% 27% 5% |
| 2 | 2J | 451 | 68% 26% 5% |
| 2 | 2L | 451 | 69% 26% 5% |
| 2 | 2N | 451 | 13% 61% 33% 5% |
| 2 | 2P | 451 | 64% 30% 5% |
| 2 | 2R | 451 | 70% 25% 5% |
| 2 | 2T | 451 | 67% 27% 5% |
| 2 | 2V | 451 | 69% 25% 5% |
| 2 | 2X | 451 | 67% 30% |
| 2 | 2Z | 451 | 64% 30% 5% |
| 2 | 3B | 451 | 63% 33% |
| 2 | 3D | 451 | 10% 62% 33% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | 3F | 451 | 67% 28% 5% |
| 2 | 3H | 451 | 67% 27% 5% |
| 2 | 3J | 451 | 70% 25% 5% |
| 2 | 3L | 451 | 71% 24% 5% |
| 2 | 3N | 451 | 69% 25% 5% |
| 2 | 3P | 451 | 67% 28% 5% |
| 2 | 3R | 451 | 63% 34% |
| 2 | 3T | 451 | 16% 58% 36% 5% |
| 2 | 4 | 451 | 93% |
| 2 | 6 | 451 | 95% |
| 2 | 8 | 451 | 91% 5% |
| 2 | A0 | 451 | 95% |
| 2 | A2 | 451 | 91% 5% |
| 2 | A4 | 451 | 93% |
| 2 | A8 | 451 | 93% 5% |
| 2 | B0 | 451 | 93% 5% |
| 2 | B2 | 451 | 93% 5% |
| 2 | B4 | 451 | 93% 5% |
| 2 | B7 | 451 | 92% 5% |
| 2 | B9 | 451 | 93% 5% |
| 2 | C1 | 451 | 93% 5% |
| 2 | C5 | 451 | 94% |
| 2 | C7 | 451 | 95% |
| 2 | C9 | 451 | 93% 5% |
| 2 | D1 | 451 | 93% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | D3 | 451 | 94% • 5% |
| 2 | D5 | 451 | 93% • 5% |
| 2 | D7 | 451 | 94% • 5% |
| 2 | E1 | 451 | 93% • 5% |
| 2 | E3 | 451 | 93% • 5% |
| 2 | E5 | 451 | 92% • 5% |
| 2 | E7 | 451 | 92% • 5% |
| 2 | E9 | 451 | 92% • 5% |
| 2 | F1 | 451 | 92% • 5% |
| 2 | F3 | 451 | 8% 92% • 5% |
| 2 | F5 | 451 | 51% 92% • 5% |
| 2 | F7 | 451 | 92% • 5% |
| 2 | F9 | 451 | 94% • • |
| 2 | G1 | 451 | 76% 20% • • |
| 2 | G3 | 451 | 65% 31% • • |
| 2 | G5 | 451 | 66% 29% 5% |
| 2 | G7 | 451 | 61% 33% 5% |
| 2 | G9 | 451 | 20% 56% 39% 5% |
| 2 | H1 | 451 | 29% 62% 33% 5% |
| 2 | H3 | 451 | 65% 29% 5% |
| 2 | H5 | 451 | 68% 27% 5% |
| 2 | H7 | 451 | 69% 25% 5% |
| 2 | H9 | 451 | 68% 27% 5% |
| 2 | I1 | 451 | 66% 28% 5% |
| 2 | I3 | 451 | 67% 27% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | I5 | 451 | 33% 59% 35% 5% |
| 2 | I7 | 451 | 8% 68% 27% 5% |
| 2 | I9 | 451 | 63% 31% • 5% |
| 2 | J1 | 451 | • 63% 32% 5% |
| 2 | J3 | 451 | 68% 27% 5% |
| 2 | J5 | 451 | • 68% 29% • |
| 2 | J7 | 451 | • 65% 29% • 5% |
| 2 | J9 | 451 | • 64% 33% • |
| 2 | K1 | 451 | 41% 62% 32% 5% |
| 2 | K3 | 451 | • 65% 29% 5% |
| 2 | K5 | 451 | 70% 24% 5% |
| 2 | K7 | 451 | • 70% 25% 5% |
| 2 | K9 | 451 | 71% 24% 5% |
| 2 | L1 | 451 | • 72% 22% 5% |
| 2 | L3 | 451 | 67% 27% • 5% |
| 2 | L5 | 451 | • 67% 28% 5% |
| 2 | L7 | 451 | 40% 59% 35% 5% |
| 2 | L9 | 451 | 70% 25% 5% |
| 2 | M1 | 451 | • 71% 24% 5% |
| 2 | M3 | 451 | • 67% 29% • • |
| 2 | M5 | 451 | 69% 26% 5% |
| 2 | M7 | 451 | • 71% 25% • |
| 2 | M9 | 451 | • 67% 30% • |
| 2 | N1 | 451 | • 68% 27% 5% |
| 2 | N3 | 451 | 42% 61% 33% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | N5 | 451 | 66% 28% 5% |
| 2 | N7 | 451 | 64% 30% • 5% |
| 2 | N9 | 451 | 65% 30% 5% |
| 2 | O1 | 451 | 70% 24% 5% |
| 2 | O3 | 451 | 65% 30% 5% |
| 2 | O5 | 451 | 65% 29% 5% |
| 2 | O7 | 451 | 67% 28% • |
| 2 | O9 | 451 | 71% 24% 5% |
| 2 | P3 | 451 | 70% 25% 5% |
| 2 | P5 | 451 | 69% 27% • |
| 2 | P7 | 451 | 71% 24% 5% |
| 2 | P9 | 451 | 69% 28% • |
| 2 | Q1 | 451 | 72% 23% 5% |
| 2 | Q3 | 451 | 69% 26% 5% |
| 2 | Q5 | 451 | 69% 26% 5% |
| 2 | Q9 | 451 | 64% 31% 5% |
| 2 | R1 | 451 | 65% 29% 5% |
| 2 | R3 | 451 | 68% 27% 5% |
| 2 | R5 | 451 | 69% 27% • |
| 2 | R7 | 451 | 70% 24% 5% |
| 2 | R9 | 451 | 68% 29% • |
| 2 | S1 | 451 | 68% 26% 5% |
| 2 | S5 | 451 | 69% 25% 5% |
| 2 | S7 | 451 | 66% 30% • |
| 2 | S9 | 451 | 65% 29% • 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | T1 | 451 | 65% 29% 5% |
| 2 | T3 | 451 | 70% 23% • 5% |
| 2 | T5 | 451 | 66% 29% 5% |
| 2 | T7 | 451 | 68% 26% 5% |
| 2 | U1 | 451 | 70% 25% 5% |
| 2 | U3 | 451 | 71% 24% 5% |
| 2 | U5 | 451 | 68% 27% 5% |
| 2 | U7 | 451 | 69% 25% 5% |
| 2 | U9 | 451 | 65% 29% 5% |
| 2 | V1 | 451 | 65% 29% 5% |
| 2 | V3 | 451 | 65% 29% • 5% |
| 2 | V7 | 451 | 64% 31% 5% |
| 2 | V9 | 451 | 69% 26% 5% |
| 2 | W1 | 451 | 69% 25% 5% |
| 2 | W3 | 451 | 71% 24% 5% |
| 2 | W5 | 451 | 73% 22% 5% |
| 2 | W7 | 451 | 63% 32% 5% |
| 2 | W9 | 451 | 61% 32% • 5% |
| 2 | X3 | 451 | 58% 37% 5% |
| 2 | X5 | 451 | 62% 32% 5% |
| 2 | X7 | 451 | 64% 30% 5% |
| 2 | X9 | 451 | 67% 27% • 5% |
| 2 | Y1 | 451 | 66% 29% 5% |
| 2 | Y3 | 451 | 65% 29% 5% |
| 2 | Y5 | 451 | 66% 28% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | Y9 | 451 | 9% 58% 36% 5% |
| 2 | Z1 | 451 | 10% 64% 31% 5% |
| 2 | Z3 | 451 | 8% 60% 35% 5% |
| 2 | Z5 | 451 | 6% 59% 35% 5% |
| 2 | Z7 | 451 | 7% 61% 33% 5% |
| 2 | Z9 | 451 | 5% 64% 30% 5% |
| 3 | 3V | 307 | 7% 66% 27% |
| 3 | 3X | 307 | 40% 64% 29% |
| 3 | 3Z | 307 | 7% 65% 29% |
| 3 | 4B | 307 | 18% 66% 27% |
| 3 | 4D | 307 | 6% 65% 28% |
| 3 | 4F | 307 | 16% 64% 29% |
| 3 | 4H | 307 | 8% 64% 29% |
| 3 | 4J | 307 | 26% 46% 21% 34% |
| 4 | 3W | 190 | 59% 35% |
| 4 | 3Y | 190 | 61% 34% |
| 4 | 4A | 190 | 61% 34% |
| 4 | 4C | 190 | 59% 35% |
| 4 | 4E | 190 | 62% 33% |
| 4 | 4G | 190 | 61% 34% |
| 4 | 4I | 190 | 61% 34% |
| 5 | 4L | 482 | 5% 34% 16% 51% |
| 5 | 4M | 482 | 47% 18% 34% |
| 6 | 4N | 505 | 7% 90% |
| 6 | 4O | 505 | 17% 67% 28% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | 4P | 505 | 30% 8% 62% |
| 7 | 4Q | 367 | 15% 83% |
| 7 | 4R | 367 | 74% 25% |
| 7 | 4S | 367 | 9% 88% |
| 7 | 4T | 367 | 42% 11% 47% |
| 7 | 4U | 367 | 59% 18% 23% |
| 8 | 4V | 475 | 13% 83% |
| 8 | 4W | 475 | 28% 51% 23% 26% |
| 8 | 4X | 475 | 9% 88% |
| 9 | 4Y | 462 | 18% 9% 73% |
| 9 | 4Z | 462 | 23% 55% 29% 16% |
| 10 | 5A | 501 | 10% 31% 15% 54% |
| 10 | 5B | 501 | 12% 33% 17% 50% |
| 10 | 5C | 501 | 11% 51% 23% 26% |
| 10 | 5D | 501 | 14% 7% 79% |
| 11 | 5E | 274 | 43% 69% 24% 6% |
| 12 | 5F | 391 | 5% 70% 26% |
| 12 | 5G | 391 | 24% 12% 64% |
| 12 | 7B | 391 | 17% 8% 75% |
| 13 | 5H | 137 | 61% 30% 8% |
| 13 | 5I | 137 | 57% 34% 7% |
| 13 | 5J | 137 | 60% 31% 8% |
| 13 | 5K | 137 | 58% 33% 8% |
| 14 | 5L | 633 | 50% 44% 5% |
| 14 | 5M | 633 | 51% 43% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 14 | 5N | 633 | 51% 43% 5% |
| 15 | 5O | 380 | 8% 45% 46% 8% |
| 15 | 5P | 380 | 57% 40% |
| 16 | 5Q | 197 | 6% 63% 32% |
| 17 | 5R | 240 | 7% 91% |
| 17 | 5S | 240 | 15% 50% 29% 5% 17% |
| 17 | 5T | 240 | 14% 51% 25% 6% 18% |
| 17 | 5U | 240 | 18% 50% 28% 17% |
| 17 | 5V | 240 | 7% 32% 13% 55% |
| 18 | 5X | 230 | 52% 37% 8% |
| 18 | 5Y | 230 | 5% 53% 36% 7% |
| 18 | 5Z | 230 | 21% 53% 37% 6% |
| 18 | 6A | 230 | 7% 54% 35% 7% |
| 18 | 6B | 230 | 31% 53% 37% 6% |
| 18 | 6C | 230 | 20% 54% 36% 7% |
| 18 | 6D | 230 | 12% 54% 36% 7% |
| 19 | 6E | 268 | 62% 33% 5% |
| 20 | 6F | 403 | 70% 28% |
| 21 | 6G | 214 | 17% 68% 18% 14% |
| 21 | 6H | 214 | 23% 60% 30% 10% |
| 22 | 6I | 352 | 11% 68% 26% 7% |
| 22 | 6J | 352 | 12% 70% 23% 7% |
| 22 | 6K | 352 | 14% 70% 23% 7% |
| 22 | 6L | 352 | 14% 66% 28% 7% |
| 22 | 6M | 352 | 15% 68% 25% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 22 | 6N | 352 | 20% 67% 26% 7% |
| 22 | 6O | 352 | 16% 68% 25% 7% |
| 22 | 6P | 352 | 28% 55% 28% • 16% |
| 23 | 6Q | 87 | 7% 61% 29% 8% • |
| 23 | 6R | 87 | • 63% 26% 8% • |
| 23 | 6S | 87 | 14% 68% 24% 6% • |
| 24 | 6T | 635 | 7% 57% 31% 11% |
| 24 | 6U | 635 | 9% 57% 32% • 10% |
| 24 | 6V | 635 | 9% 57% 31% 12% |
| 24 | 6W | 635 | 7% 62% 26% • 11% |
| 24 | 6X | 635 | 8% 55% 33% • 10% |
| 24 | 6Y | 635 | 10% 56% 32% • 11% |
| 24 | 6Z | 635 | 8% 57% 31% 11% |
| 24 | 7A | 635 | • 20% 10% 70% |
| 25 | 7C | 111 | 14% 65% 23% 12% |
| 26 | 7D | 146 | • 53% 33% 5% 10% |
| 26 | 7E | 146 | • 52% 34% 5% 10% |
| 26 | 7F | 146 | 21% 47% 37% 6% 10% |
| 27 | 7G | 235 | 9% 63% 32% 5% |
| 28 | 7H | 471 | • 19% 9% • 71% |
| 28 | 7X | 471 | • 18% 9% • 71% |
| 29 | 7I | 483 | 6% 34% 13% 53% |
| 29 | 7J | 483 | • 54% 21% 25% |
| 30 | 7K | 458 | 8% 64% 28% 8% |
| 30 | 7L | 458 | • 30% 9% 62% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 31 | 7M | 139 | 6% 36% 24% • 39% |
| 31 | 7N | 139 | 22% 57% 33% • 9% |
| 32 | 7O | 238 | • 17% 8% 75% |
| 32 | 7P | 238 | 7% 60% 17% 24% |
| 33 | 7Q | 189 | 6% 24% 14% 62% |
| 34 | 7R | 749 | 9% 19% 7% 74% |
| 34 | 7S | 749 | 5% 16% 5% 79% |
| 35 | 7T | 552 | 13% 28% 10% 61% |
| 35 | 7U | 552 | 9% 25% 7% 67% |
| 36 | 7V | 184 | 20% 26% 18% • 52% |
| 36 | 7W | 184 | 31% 24% 20% • 52% |
| 37 | 7Y | 312 | 26% 46% 32% • 21% |
| 38 | 7Z | 242 | • 7% 10% 84% |
| 38 | 8A | 242 | 16% 45% 39% • 14% |
| 38 | 8B | 242 | 19% 44% 41% • 12% |
| 38 | 8C | 242 | 9% 46% 39% • 12% |
| 38 | 8D | 242 | 17% 34% 28% • 35% |

# 2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 1358547 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 1 | 138 | 1120 | 701 | 192 | 214 | 13 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 3 | 433 | 3397 | 2131 | 581 | 655 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 5 | 436 | 3421 | 2147 | 584 | 660 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 7 | 437 | 3430 | 2152 | 585 | 663 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 9 | 436 | 3421 | 2147 | 584 | 660 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | A1 | 432 | 3388 | 2126 | 580 | 652 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | A3 | 435 | 3410 | 2138 | 583 | 659 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | A5 | 430 | 3370 | 2116 | 578 | 646 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | A7 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | A9 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | B1 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | B3 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | B5 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | B8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | C0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | C2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | C4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | C6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | C8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | D0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | D2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | D4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | D6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | D8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | E0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | E2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | E4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | E6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | E8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | F0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | F2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | F6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | F8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | G0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | G2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | G4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | G6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | G8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | H2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | H4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | H6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | H8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | I0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | I2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | I4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | I8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | J0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | J2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | J4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | J6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | J8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | K0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | K4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | K6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | K8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | L0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | L2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | L4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | L6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | M0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | M2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | M4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | M6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | M8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | N0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | N2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | N6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | N8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | O0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | O2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | O4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | O6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | O8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | P4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | P6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | P8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Q0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Q2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Q4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Q6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | Q8 | 420 | 3293 | 2070 | 563 | 631 | 29 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | R0 | 434 | 3401 | 2133 | 582 | 656 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | R2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | R4 | 430 | 3370 | 2116 | 578 | 646 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | R6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | R8 | 431 | 3379 | 2121 | 579 | 649 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | S0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | S2 | 431 | 3379 | 2121 | 579 | 649 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | S4 | 427 | 3354 | 2107 | 575 | 642 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | S6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | S8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | T0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | T2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | T4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | T6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | T8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | U2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | U4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | U6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | U8 | 430 | 3370 | 2116 | 578 | 646 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | V0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | V2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | V4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | V6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | V8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | W0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | W2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | W4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | W6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | W8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | X0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | X2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | X4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | X6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | X8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Y0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Y2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Y4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Y6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Y8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Z0 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | Z2 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | Z4 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | Z6 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | Z8 | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0A | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0C | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0E | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0G | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0I | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0K | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0M | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0O | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0Q | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0S | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0U | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0W | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 0Y | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1A | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1C | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1E | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1G | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1K | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 1M | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1O | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1Q | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1S | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1U | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 1W | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2A | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2C | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2E | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2G | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2I | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2K | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2M | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2Q | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2S | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2U | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2W | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 2Y | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 3A | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 3C | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 1 | 3G | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 3I | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | 3K | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | 3M | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | 3O | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | 3Q | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |
| 1 | 3S | 426 | 3346 | 2103 | 574 | 639 | 30 | 0 | 0 |

- Molecule 2 is a protein called Tubulin alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 2 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | 4 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | 6 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | 8 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | A0 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | A2 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | A4 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | A8 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | B0 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | B2 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | B4 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | B7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | B9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | C1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | C5 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | C7 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | C9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | D1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | D3 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| 2 | D5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | D7 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| 2 | E1 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| 2 | E3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | E5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | E7 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| 2 | E9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | F1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | F3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | F5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | F7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | F9 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | G1 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | G3 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| 2 | G5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | G7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | G9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | H1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | H3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | H5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | H7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | H9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | I1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | I3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | I5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | I7 | 429 | 3332 | 2110 | 567 | 634 | 21 | 0 | 0 |
| 2 | I9 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| 2 | J1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | J3 | 428 | 3326 | 2107 | 566 | 632 | 21 | 0 | 0 |
| 2 | J5 | 437 | 3385 | 2141 | 576 | 647 | 21 | 0 | 0 |
| 2 | J7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | J9 | 437 | 3385 | 2141 | 576 | 647 | 21 | 0 | 0 |
| 2 | K1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | K3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | K5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | K7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | K9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | L1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | L3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | L5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | L7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | L9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | M1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | M3 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | M5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | M7 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | M9 | 437 | 3385 | 2141 | 576 | 647 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | N1 | 428 | 3324 | 2106 | 566 | 631 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | N3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | N5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | N7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | N9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | O1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | O3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | O5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | O7 | 431 | 3340 | 2114 | 569 | 636 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | O9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | P3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | P5 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | P7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | P9 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Q1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Q3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Q5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Q9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | R1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | R3 | 428 | 3327 | 2108 | 566 | 632 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | R5 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | R7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | R9 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | S1 | 429 | 3333 | 2111 | 567 | 634 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | S5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | S7 | 436 | 3376 | 2136 | 575 | 644 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | S9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | T1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | T3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | T5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | T7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | U1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | U3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | U5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | U7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | U9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | V1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | V3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | V7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | V9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | W1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | W3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | W5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | W7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | W9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | X3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | X5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | X7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | X9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | Y1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | Y3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | Y5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | Y9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Z1 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Z3 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Z5 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Z7 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | Z9 | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0B | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0F | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0H | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0J | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0L | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0N | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0P | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0R | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0V | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0X | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 0Z | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1B | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1D | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1F | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1H | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 1L | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1N | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1P | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1R | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1T | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1V | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1X | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 1Z | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2B | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2D | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2F | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2H | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2J | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2L | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2N | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2P | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2R | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2T | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2V | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2X | 437 | 3385 | 2141 | 576 | 647 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | 2Z | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 3B | 437 | 3383 | 2140 | 576 | 646 | 21 | 0 | 0 |
| 2 | 3D | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3F | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3H | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3J | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3L | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3N | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3P | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |
| 2 | 3R | 437 | 3385 | 2141 | 576 | 647 | 21 | 0 | 0 |
| 2 | 3T | 427 | 3318 | 2103 | 565 | 629 | 21 | 0 | 0 |

- Molecule 3 is a protein called PACRG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 3V | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 3X | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 3Z | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 4B | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 4D | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 4F | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 4H | 297 | 2329 | 1491 | 401 | 428 | 9 | 0 | 0 |
| 3 | 4J | 204 | 1643 | 1060 | 281 | 296 | 6 | 0 | 0 |

- Molecule 4 is a protein called FAP20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 3W | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 3Y | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 4A | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 4C | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 4E | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 4G | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |
| 4 | 4I | 184 | 1515 | 971 | 264 | 273 | 7 | 0 | 0 |

- Molecule 5 is a protein called FAP53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 4L | 238 | 1921 | 1164 | 366 | 381 | 10 | 0 | 0 |
| 5 | 4M | 316 | 2622 | 1589 | 514 | 503 | 16 | 0 | 0 |

- Molecule 6 is a protein called FAP127.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 4N | 52 | 422 | 260 | 76 | 85 | 1 | 0 | 0 |
| 6 | 4O | 478 | 3995 | 2407 | 778 | 791 | 19 | 0 | 0 |
| 6 | 4P | 194 | 1588 | 956 | 313 | 315 | 4 | 0 | 0 |

- Molecule 7 is a protein called RIB43a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | 4Q | 63 | 525 | 324 | 101 | 98 | 2 | 0 | 0 |
| 7 | 4R | 366 | 2982 | 1819 | 561 | 589 | 13 | 0 | 0 |
| 7 | 4S | 45 | Total | C | N | O | | 0 | 0 |
| | | | 371 | 228 | 71 | 72 | | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | 4T | 194 | 1574 | 961 | 295 | 307 | 11 | 0 | 0 |
| 7 | 4U | 283 | 2285 | 1392 | 423 | 461 | 9 | 0 | 0 |

- Molecule 8 is a protein called FAP112.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | 4V | 83 | 653 | 396 | 129 | 124 | 4 | 0 | 0 |
| 8 | 4W | 353 | 2750 | 1649 | 552 | 538 | 11 | 0 | 0 |
| 8 | 4X | 59 | 462 | 284 | 85 | 90 | 3 | 0 | 0 |

- Molecule 9 is a protein called FAP210.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | 4Y | 126 | 1004 | 625 | 187 | 189 | 3 | 0 | 0 |
| 9 | 4Z | 389 | 3158 | 1908 | 627 | 615 | 8 | 0 | 0 |

- Molecule 10 is a protein called FAP45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | 5A | 228 | 1902 | 1154 | 367 | 372 | 9 | 0 | 0 |
| 10 | 5B | 249 | 2074 | 1257 | 391 | 410 | 16 | 0 | 0 |
| 10 | 5C | 370 | 3103 | 1881 | 597 | 604 | 21 | 0 | 0 |
| 10 | 5D | 106 | 901 | 542 | 176 | 174 | 9 | 0 | 0 |

- Molecule 11 is a protein called RIB30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | 5E | 258 | 1981 | 1245 | 352 | 380 | 4 | 0 | 0 |

- Molecule 12 is a protein called FAP363.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | 5F | 381 | 3020 | 1921 | 520 | 569 | 10 | 0 | 0 |
| 12 | 5G | 141 | 1123 | 711 | 203 | 206 | 3 | 0 | 0 |
| 12 | 7B | 97 | 753 | 476 | 125 | 148 | 4 | 0 | 0 |

- Molecule 13 is a protein called FAP126.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | 5H | 135 | 1069 | 674 | 190 | 202 | 3 | 0 | 0 |
| 13 | 5I | 135 | 1069 | 674 | 190 | 202 | 3 | 0 | 0 |
| 13 | 5J | 135 | 1069 | 674 | 190 | 202 | 3 | 0 | 0 |
| 13 | 5K | 135 | 1069 | 674 | 190 | 202 | 3 | 0 | 0 |

- Molecule 14 is a protein called FAP52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | 5L | 626 | 4757 | 2992 | 827 | 912 | 26 | 0 | 0 |
| 14 | 5M | 626 | 4757 | 2992 | 827 | 912 | 26 | 0 | 0 |
| 14 | 5N | 626 | 4757 | 2992 | 827 | 912 | 26 | 0 | 0 |

- Molecule 15 is a protein called FAP67.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | 5O | 376 | 2927 | 1862 | 503 | 547 | 15 | 0 | 0 |
| 15 | 5P | 376 | 2927 | 1862 | 503 | 547 | 15 | 0 | 0 |

- Molecule 16 is a protein called FAP85.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | 5Q | 191 | 1523 | 961 | 267 | 293 | 2 | 0 | 0 |

- Molecule 17 is a protein called FAP106.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | 5R | 22 | 162 | 100 | 33 | 28 | 1 | 0 | 0 |
| 17 | 5S | 199 | 1572 | 989 | 291 | 288 | 4 | 0 | 0 |
| 17 | 5T | 198 | 1563 | 984 | 290 | 285 | 4 | 0 | 0 |
| 17 | 5U | 199 | 1572 | 989 | 291 | 288 | 4 | 0 | 0 |
| 17 | 5V | 109 | 879 | 551 | 164 | 162 | 2 | 0 | 0 |

- Molecule 18 is a protein called FAP115.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | 5X | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 5Y | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 5Z | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 6A | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 6B | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 6C | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |
| 18 | 6D | 221 | 1793 | 1153 | 302 | 330 | 8 | 0 | 0 |

- Molecule 19 is a protein called FAP143.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | 6E | 255 | 1952 | 1208 | 345 | 390 | 9 | 0 | 0 |

- Molecule 20 is a protein called FAP161.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | 6F | 394 | 2950 | 1852 | 518 | 566 | 14 | 0 | 0 |

- Molecule 21 is a protein called FAP166.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | 6G | 183 | 1420 | 891 | 251 | 269 | 9 | 0 | 0 |
| 21 | 6H | 193 | 1493 | 937 | 265 | 282 | 9 | 0 | 0 |

- Molecule 22 is a protein called FAP252.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | 6I | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6J | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6K | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6L | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6M | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6N | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6O | 329 | 2617 | 1660 | 442 | 501 | 14 | 0 | 0 |
| 22 | 6P | 297 | 2366 | 1499 | 399 | 454 | 14 | 0 | 0 |

- Molecule 23 is a protein called FAP276.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | 6Q | 85 | 694 | 434 | 130 | 127 | 3 | 0 | 0 |
| 23 | 6R | 85 | 694 | 434 | 130 | 127 | 3 | 0 | 0 |
| 23 | 6S | 85 | 694 | 434 | 130 | 127 | 3 | 0 | 0 |

- Molecule 24 is a protein called RIB72.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | 6T | 564 | 4590 | 2928 | 792 | 854 | 16 | 0 | 0 |
| 24 | 6U | 569 | 4623 | 2949 | 798 | 860 | 16 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | 6V | 561 | 4569 | 2915 | 789 | 849 | 16 | 0 | 0 |
| 24 | 6W | 566 | 4606 | 2938 | 795 | 857 | 16 | 0 | 0 |
| 24 | 6X | 569 | 4631 | 2954 | 799 | 862 | 16 | 0 | 0 |
| 24 | 6Y | 562 | 4579 | 2923 | 791 | 849 | 16 | 0 | 0 |
| 24 | 6Z | 563 | 4585 | 2925 | 791 | 853 | 16 | 0 | 0 |
| 24 | 7A | 189 | 1518 | 962 | 267 | 284 | 5 | 0 | 0 |

- Molecule 25 is a protein called FAP141.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | 7C | 98 | 794 | 486 | 157 | 149 | 2 | 0 | 0 |

- Molecule 26 is a protein called FAP222.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | 7D | 132 | 1016 | 637 | 183 | 189 | 7 | 0 | 0 |
| 26 | 7E | 132 | 1016 | 637 | 183 | 189 | 7 | 0 | 0 |
| 26 | 7F | 132 | 1016 | 637 | 183 | 189 | 7 | 0 | 0 |

- Molecule 27 is a protein called FAP95.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | 7G | 224 | 1728 | 1083 | 305 | 336 | 4 | 0 | 0 |

- Molecule 28 is a protein called FAP182.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | 7H | 138 | 1046 | 651 | 194 | 196 | 5 | 0 | 0 |
| 28 | 7X | 138 | 1046 | 651 | 194 | 196 | 5 | 0 | 0 |

- Molecule 29 is a protein called FAP129.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | 7I | 228 | 1716 | 1065 | 311 | 334 | 6 | 0 | 0 |
| 29 | 7J | 362 | 2741 | 1691 | 505 | 535 | 10 | 0 | 0 |

- Molecule 30 is a protein called FAP21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | 7K | 423 | 3276 | 2026 | 620 | 625 | 5 | 0 | 0 |
| 30 | 7L | 176 | 1333 | 819 | 254 | 257 | 3 | 0 | 0 |

- Molecule 31 is a protein called FAP273.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | 7M | 85 | 662 | 411 | 123 | 125 | 3 | 0 | 0 |
| 31 | 7N | 126 | 977 | 607 | 179 | 186 | 5 | 0 | 0 |

- Molecule 32 is a protein called FAP107.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 32 | 7O | 59 | 443 | 270 | 81 | 92 | | 0 | 0 |
| 32 | 7P | 182 | 1398 | 865 | 257 | 273 | 3 | 0 | 0 |

- Molecule 33 is a protein called RIB21.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 33 | 7Q | 71 | 567 | 352 | 98 | 117 | 0 | 0 |

- Molecule 34 is a protein called DC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | 7R | 195 | 1619 | 988 | 308 | 317 | 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | 7S | 160 | 1347 | 818 | 260 | 263 | 6 | 0 | 0 |

- Molecule 35 is a protein called DC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | 7T | 213 | 1738 | 1068 | 326 | 335 | 9 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 35 | 7U | 181 | 1476 | 904 | 278 | 285 | 9 | 0 | 0 |

- Molecule 36 is a protein called DC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | 7V | 89 | 735 | 457 | 123 | 150 | 5 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 36 | 7W | 89 | 735 | 457 | 123 | 150 | 5 | 0 | 0 |

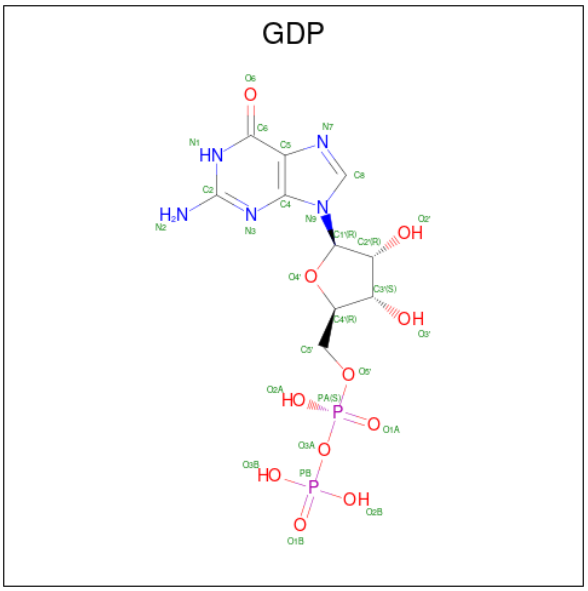
- Molecule 37 is a protein called FAP68.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | 7Y | 247 | 1971 | 1221 | 372 | 370 | 8 | 0 | 0 |

- Molecule 38 is a protein called FAP90.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | 7Z | 39 | 298 | 184 | 50 | 62 | 2 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 38 | 8A | 207 | 1691 | 1058 | 305 | 322 | 6 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 38 | 8B | 213 | 1728 | 1078 | 311 | 332 | 7 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 38 | 8C | 213 | 1728 | 1078 | 311 | 332 | 7 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 38 | 8D | 157 | 1311 | 820 | 236 | 250 | 5 | 0 | 0 |

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 39 | 2 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | 3 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | 7 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | 9 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | A1 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | A3 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | A5 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | A7 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | A9 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | B1 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | B3 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | B5 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 39 | B8 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | C0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | C2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | C4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | C6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | C8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | D0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | D2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | D4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | D6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | D8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | E0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | E2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | E4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | E6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | E8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | F0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | F2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | F6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | F8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | G0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | G2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | G4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | G6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | G8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | H2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | H4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | H6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | H8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | I0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | I2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | I4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | I8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | J0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | J2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | J4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | J6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | J8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | K0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | K4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | K6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | K8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | L0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | L2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | L4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | L6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | M0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | M2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | M4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | M6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | M8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | N0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | N2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | N6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | N8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | O0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | O2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | O4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | O6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | O8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | P4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | P6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | P8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Q0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | Q2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Q4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Q6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Q8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | R0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | R2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | R4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | R6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | R8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | S0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | S2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | S4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | S6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | S8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | T0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | T2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | T4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | T6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | T8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | U2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | U4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | U6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | U8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | V0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | V2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | V4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | V6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | V8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | W0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | W2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | W4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | W6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | W8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | X0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | X2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | X4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | X6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | X8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Y0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Y2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Y4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Y6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | Y8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Z0 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Z2 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Z4 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Z6 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | Z8 | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0A | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0C | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0E | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0G | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0I | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0K | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0M | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0O | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0Q | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0S | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0U | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0W | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 0Y | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1A | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1C | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | 1E | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1G | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1K | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1M | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1O | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1Q | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1S | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1U | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 1W | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2A | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2C | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2E | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2G | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2I | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2K | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2M | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2Q | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2S | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2U | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2W | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 2Y | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 39 | 3A | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3C | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3G | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3I | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3K | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3M | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3O | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3Q | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 39 | 3S | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | 2 | 1 | 1 | 1 | 0 |
| 40 | 4 | 1 | 1 | 1 | 0 |
| 40 | 6 | 1 | 1 | 1 | 0 |
| 40 | 8 | 1 | 1 | 1 | 0 |
| 40 | A0 | 1 | 1 | 1 | 0 |
| 40 | A2 | 1 | 1 | 1 | 0 |
| 40 | A4 | 1 | 1 | 1 | 0 |
| 40 | A8 | 1 | 1 | 1 | 0 |
| 40 | B0 | 1 | 1 | 1 | 0 |
| 40 | B2 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | B4 | 1 | 1 | 1 | 0 |
| 40 | B7 | 1 | 1 | 1 | 0 |
| 40 | B9 | 1 | 1 | 1 | 0 |
| 40 | C1 | 1 | 1 | 1 | 0 |
| 40 | C5 | 1 | 1 | 1 | 0 |
| 40 | C7 | 1 | 1 | 1 | 0 |
| 40 | C9 | 1 | 1 | 1 | 0 |
| 40 | D1 | 1 | 1 | 1 | 0 |
| 40 | D3 | 1 | 1 | 1 | 0 |
| 40 | D5 | 1 | 1 | 1 | 0 |
| 40 | D7 | 1 | 1 | 1 | 0 |
| 40 | E1 | 1 | 1 | 1 | 0 |
| 40 | E3 | 1 | 1 | 1 | 0 |
| 40 | E5 | 1 | 1 | 1 | 0 |
| 40 | E7 | 1 | 1 | 1 | 0 |
| 40 | E9 | 1 | 1 | 1 | 0 |
| 40 | F1 | 1 | 1 | 1 | 0 |
| 40 | F3 | 1 | 1 | 1 | 0 |
| 40 | F5 | 1 | 1 | 1 | 0 |
| 40 | F7 | 1 | 1 | 1 | 0 |
| 40 | F9 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | G1 | 1 | 1 | 1 | 0 |
| 40 | G3 | 1 | 1 | 1 | 0 |
| 40 | G5 | 1 | 1 | 1 | 0 |
| 40 | G7 | 1 | 1 | 1 | 0 |
| 40 | G9 | 1 | 1 | 1 | 0 |
| 40 | H2 | 1 | 1 | 1 | 0 |
| 40 | H3 | 1 | 1 | 1 | 0 |
| 40 | H5 | 1 | 1 | 1 | 0 |
| 40 | H8 | 1 | 1 | 1 | 0 |
| 40 | H9 | 1 | 1 | 1 | 0 |
| 40 | I1 | 1 | 1 | 1 | 0 |
| 40 | I3 | 1 | 1 | 1 | 0 |
| 40 | I5 | 1 | 1 | 1 | 0 |
| 40 | I7 | 1 | 1 | 1 | 0 |
| 40 | I9 | 1 | 1 | 1 | 0 |
| 40 | J1 | 1 | 1 | 1 | 0 |
| 40 | J4 | 1 | 1 | 1 | 0 |
| 40 | J5 | 1 | 1 | 1 | 0 |
| 40 | J7 | 1 | 1 | 1 | 0 |
| 40 | J9 | 1 | 1 | 1 | 0 |
| 40 | K1 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | K3 | 1 | 1 | 1 | 0 |
| 40 | K5 | 1 | 1 | 1 | 0 |
| 40 | K7 | 1 | 1 | 1 | 0 |
| 40 | K9 | 1 | 1 | 1 | 0 |
| 40 | L1 | 1 | 1 | 1 | 0 |
| 40 | L3 | 1 | 1 | 1 | 0 |
| 40 | L5 | 1 | 1 | 1 | 0 |
| 40 | L7 | 1 | 1 | 1 | 0 |
| 40 | L9 | 1 | 1 | 1 | 0 |
| 40 | M1 | 1 | 1 | 1 | 0 |
| 40 | M3 | 1 | 1 | 1 | 0 |
| 40 | M5 | 1 | 1 | 1 | 0 |
| 40 | M7 | 1 | 1 | 1 | 0 |
| 40 | M9 | 1 | 1 | 1 | 0 |
| 40 | N1 | 1 | 1 | 1 | 0 |
| 40 | N3 | 1 | 1 | 1 | 0 |
| 40 | N6 | 1 | 1 | 1 | 0 |
| 40 | N7 | 1 | 1 | 1 | 0 |
| 40 | O0 | 1 | 1 | 1 | 0 |
| 40 | O1 | 1 | 1 | 1 | 0 |
| 40 | O3 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | O5 | 1 | 1 | 1 | 0 |
| 40 | O8 | 1 | 1 | 1 | 0 |
| 40 | O9 | 1 | 1 | 1 | 0 |
| 40 | P4 | 1 | 1 | 1 | 0 |
| 40 | P6 | 1 | 1 | 1 | 0 |
| 40 | P7 | 1 | 1 | 1 | 0 |
| 40 | P9 | 1 | 1 | 1 | 0 |
| 40 | Q1 | 1 | 1 | 1 | 0 |
| 40 | Q3 | 1 | 1 | 1 | 0 |
| 40 | Q5 | 1 | 1 | 1 | 0 |
| 40 | Q9 | 1 | 1 | 1 | 0 |
| 40 | R1 | 1 | 1 | 1 | 0 |
| 40 | R3 | 1 | 1 | 1 | 0 |
| 40 | R6 | 1 | 1 | 1 | 0 |
| 40 | R7 | 1 | 1 | 1 | 0 |
| 40 | R9 | 1 | 1 | 1 | 0 |
| 40 | S1 | 1 | 1 | 1 | 0 |
| 40 | S5 | 1 | 1 | 1 | 0 |
| 40 | S7 | 1 | 1 | 1 | 0 |
| 40 | S9 | 1 | 1 | 1 | 0 |
| 40 | T1 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | T3 | 1 | 1 | 1 | 0 |
| 40 | T5 | 1 | 1 | 1 | 0 |
| 40 | T7 | 1 | 1 | 1 | 0 |
| 40 | U1 | 1 | 1 | 1 | 0 |
| 40 | U3 | 1 | 1 | 1 | 0 |
| 40 | U5 | 1 | 1 | 1 | 0 |
| 40 | U7 | 1 | 1 | 1 | 0 |
| 40 | U9 | 1 | 1 | 1 | 0 |
| 40 | V2 | 1 | 1 | 1 | 0 |
| 40 | V3 | 1 | 1 | 1 | 0 |
| 40 | V7 | 1 | 1 | 1 | 0 |
| 40 | V9 | 1 | 1 | 1 | 0 |
| 40 | W2 | 1 | 1 | 1 | 0 |
| 40 | W3 | 1 | 1 | 1 | 0 |
| 40 | W5 | 1 | 1 | 1 | 0 |
| 40 | W8 | 1 | 1 | 1 | 0 |
| 40 | W9 | 1 | 1 | 1 | 0 |
| 40 | X3 | 1 | 1 | 1 | 0 |
| 40 | X5 | 1 | 1 | 1 | 0 |
| 40 | X7 | 1 | 1 | 1 | 0 |
| 40 | X9 | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | Y1 | 1 | 1 | 1 | 0 |
| 40 | Y3 | 1 | 1 | 1 | 0 |
| 40 | Y5 | 1 | 1 | 1 | 0 |
| 40 | Y9 | 1 | 1 | 1 | 0 |
| 40 | Z2 | 1 | 1 | 1 | 0 |
| 40 | Z3 | 1 | 1 | 1 | 0 |
| 40 | Z5 | 1 | 1 | 1 | 0 |
| 40 | Z7 | 1 | 1 | 1 | 0 |
| 40 | 0A | 1 | 1 | 1 | 0 |
| 40 | 0B | 1 | 1 | 1 | 0 |
| 40 | 0F | 1 | 1 | 1 | 0 |
| 40 | 0H | 1 | 1 | 1 | 0 |
| 40 | 0J | 1 | 1 | 1 | 0 |
| 40 | 0L | 1 | 1 | 1 | 0 |
| 40 | 0N | 1 | 1 | 1 | 0 |
| 40 | 0P | 1 | 1 | 1 | 0 |
| 40 | 0R | 1 | 1 | 1 | 0 |
| 40 | 0W | 1 | 1 | 1 | 0 |
| 40 | 0X | 1 | 1 | 1 | 0 |
| 40 | 1A | 1 | 1 | 1 | 0 |
| 40 | 1B | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | 1D | 1 | 1 | 1 | 0 |
| 40 | 1F | 1 | 1 | 1 | 0 |
| 40 | 1H | 1 | 1 | 1 | 0 |
| 40 | 1L | 1 | 1 | 1 | 0 |
| 40 | 1N | 1 | 1 | 1 | 0 |
| 40 | 1P | 1 | 1 | 1 | 0 |
| 40 | 1R | 1 | 1 | 1 | 0 |
| 40 | 1T | 1 | 1 | 1 | 0 |
| 40 | 1V | 1 | 1 | 1 | 0 |
| 40 | 1X | 1 | 1 | 1 | 0 |
| 40 | 1Z | 1 | 1 | 1 | 0 |
| 40 | 2B | 1 | 1 | 1 | 0 |
| 40 | 2D | 1 | 1 | 1 | 0 |
| 40 | 2F | 1 | 1 | 1 | 0 |
| 40 | 2H | 1 | 1 | 1 | 0 |
| 40 | 2J | 1 | 1 | 1 | 0 |
| 40 | 2L | 1 | 1 | 1 | 0 |
| 40 | 2N | 1 | 1 | 1 | 0 |
| 40 | 2P | 1 | 1 | 1 | 0 |
| 40 | 2R | 1 | 1 | 1 | 0 |
| 40 | 2T | 1 | 1 | 1 | 0 |

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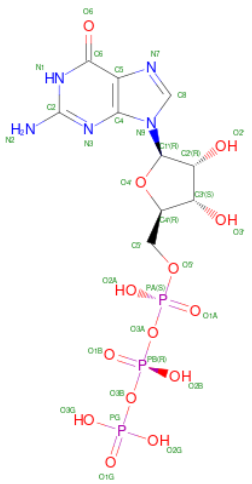
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 40 | 2V | 1 | 1 | 1 | 0 |
| 40 | 2X | 1 | 1 | 1 | 0 |
| 40 | 2Z | 1 | 1 | 1 | 0 |
| 40 | 3B | 1 | 1 | 1 | 0 |
| 40 | 3D | 1 | 1 | 1 | 0 |
| 40 | 3F | 1 | 1 | 1 | 0 |
| 40 | 3H | 1 | 1 | 1 | 0 |
| 40 | 3K | 1 | 1 | 1 | 0 |
| 40 | 3L | 1 | 1 | 1 | 0 |
| 40 | 3N | 1 | 1 | 1 | 0 |
| 40 | 3P | 1 | 1 | 1 | 0 |
| 40 | 3R | 1 | 1 | 1 | 0 |
| 40 | 3T | 1 | 1 | 1 | 0 |

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 41 | 3 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | 4 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | 7 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | 8 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | A1 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | A2 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | A4 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | A9 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | B0 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | B2 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | B5 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | B7 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | C0 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |
| 41 | C1 | 1 | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | C5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | C8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | C9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | D1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | D3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | D5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | D7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | E1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | E4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | E6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | E8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | F0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | F1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | F3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | F5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | F8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | G0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | G1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | G4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | G5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | G7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | G9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | H2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | H3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | H6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | H8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | I0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | I1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | I4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | I5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | I8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | J0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | J2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | J4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | J6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | J8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | K9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | L2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | L4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | L6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | L7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | M0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | M2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | M4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | M6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | M7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | N0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | N1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | N3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | N6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | N8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | O9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | P4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | P6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | P8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | P9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Q2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Q4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Q6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | R0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | R2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | R4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | R6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | R8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | S0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | S2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | S5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | S8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | S9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | T2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | T4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | T6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | T8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | U2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | U4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | U6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | U7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | U9 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | V2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | V3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | V8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | W0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | W2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | W4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | W5 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | W8 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | X0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | X4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | X6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | X7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Y0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Y1 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Y4 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Y6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Z0 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | Z2 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Z3 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Z6 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | Z7 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0A | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0C | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0F | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0I | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0K | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0M | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0O | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0Q | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0S | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0V | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 0Y | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1A | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1C | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1D | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1G | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1H | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 41 | 1L | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | 1N | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 1Q | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 1S | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 1T | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 1W | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 1X | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2A | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2C | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2E | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2G | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2I | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2K | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2L | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2N | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2Q | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2S | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2U | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2W | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 2Y | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3A | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3C | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 41 | 3D | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3G | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3I | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3K | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3M | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3O | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3P | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3S | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 41 | 3T | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

# 3 Residue-property plots (i)

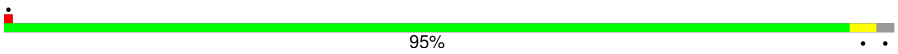
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

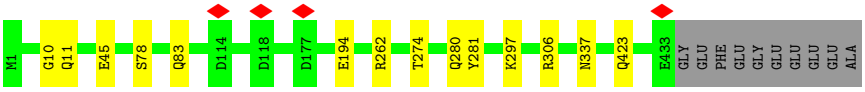
• Molecule 1: Tubulin beta

Chain 1:

• Molecule 1: Tubulin beta

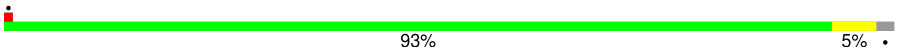
Chain 3:

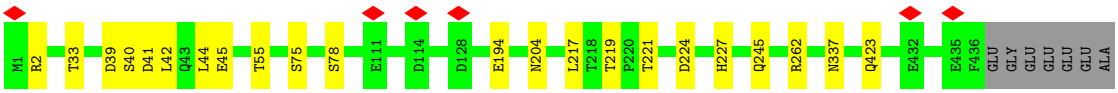



• Molecule 1: Tubulin beta

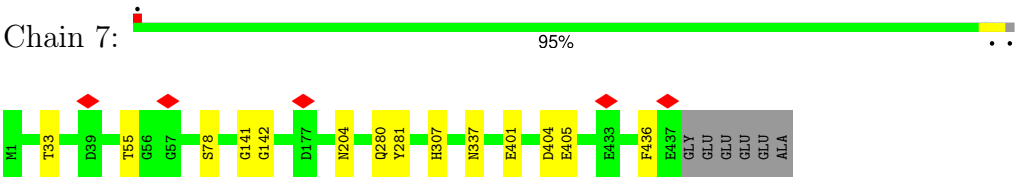
Chain 5:



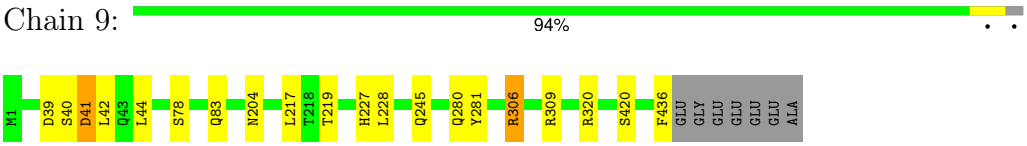

• Molecule 1: Tubulin beta

Chain 7:



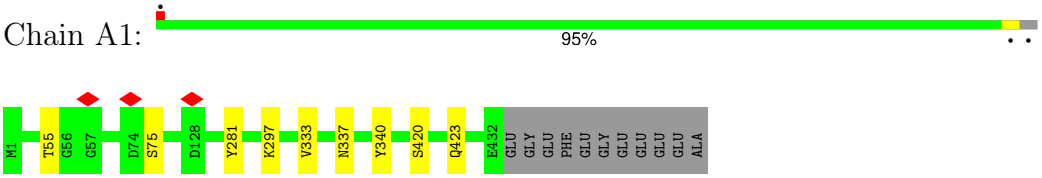

• Molecule 1: Tubulin beta

Chain 9:



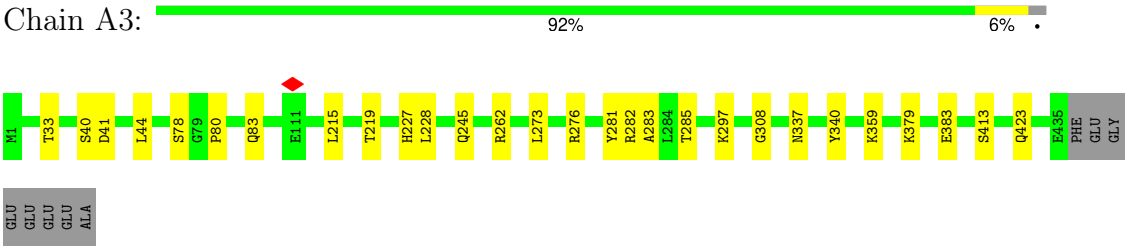

• Molecule 1: Tubulin beta

Chain A1:



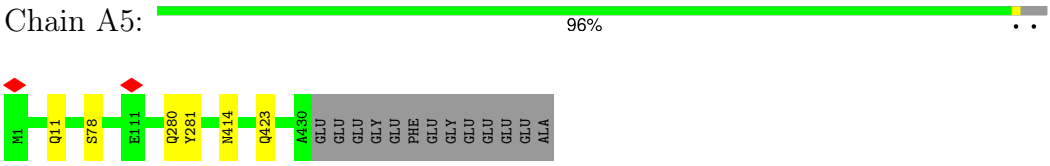

• Molecule 1: Tubulin beta

Chain A3:



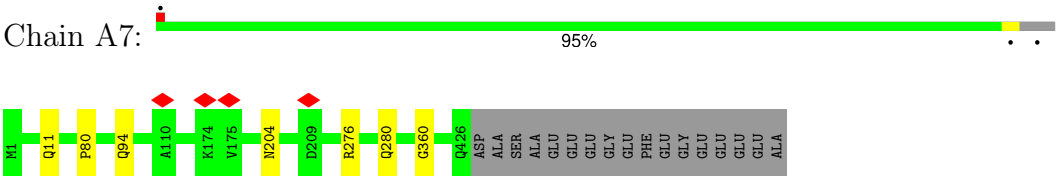

• Molecule 1: Tubulin beta

Chain A5:




• Molecule 1: Tubulin beta

Chain A7:

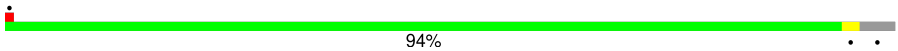


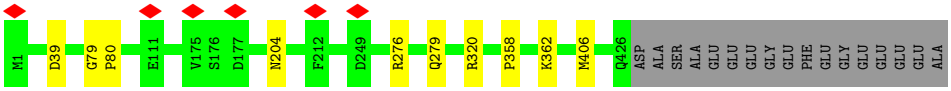

• Molecule 1: Tubulin beta

Chain A9:

• Molecule 1: Tubulin beta

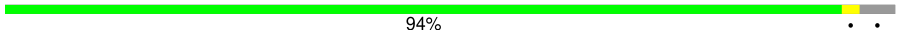
Chain B1:

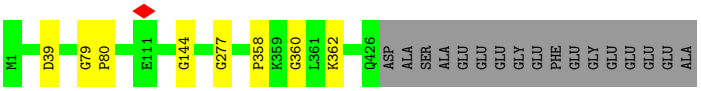



• Molecule 1: Tubulin beta

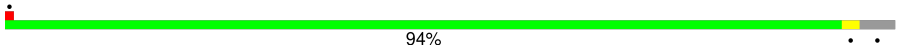
Chain B3:

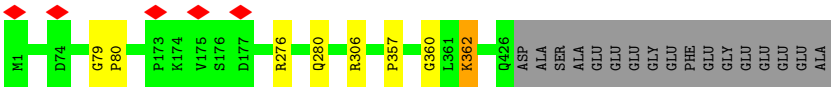



• Molecule 1: Tubulin beta

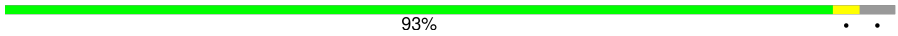
Chain B5:

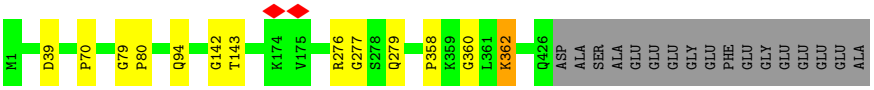



• Molecule 1: Tubulin beta

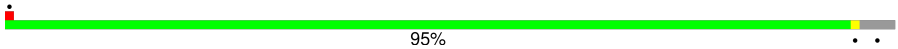
Chain B8:

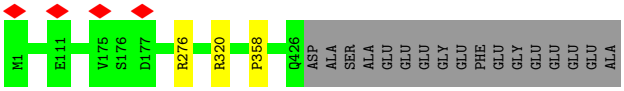



• Molecule 1: Tubulin beta

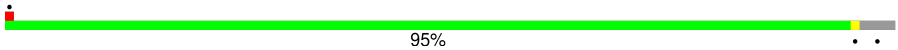
Chain C0:

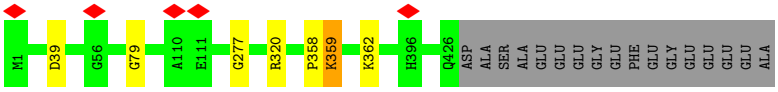



• Molecule 1: Tubulin beta

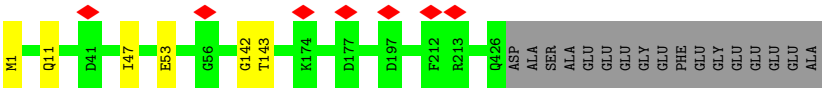
Chain C2:



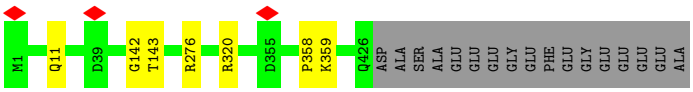

• Molecule 1: Tubulin beta

Chain C4: 95%



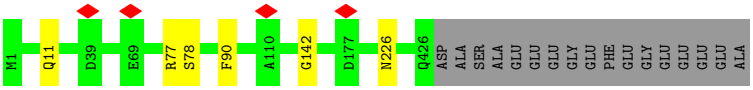

• Molecule 1: Tubulin beta

Chain C6: 95%



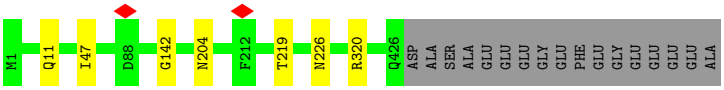

• Molecule 1: Tubulin beta

Chain C8: 95%



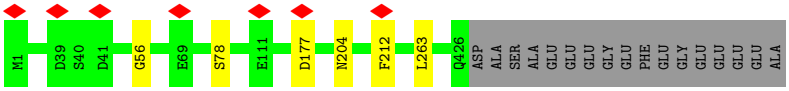

• Molecule 1: Tubulin beta

Chain D0: 95%



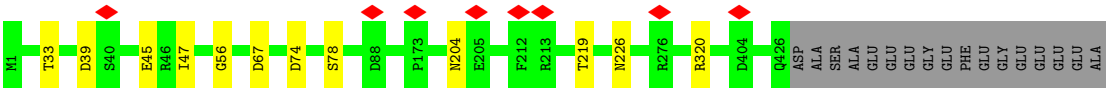

• Molecule 1: Tubulin beta

Chain D2: 95%



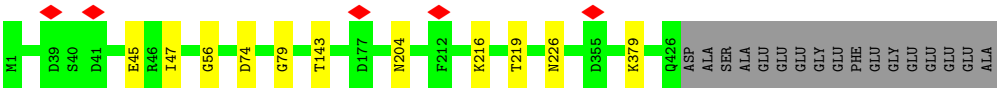

• Molecule 1: Tubulin beta

Chain D4: 93%



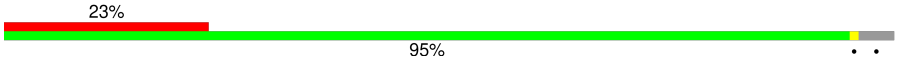

• Molecule 1: Tubulin beta

Chain D6: 94%



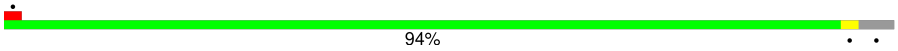
• Molecule 1: Tubulin beta

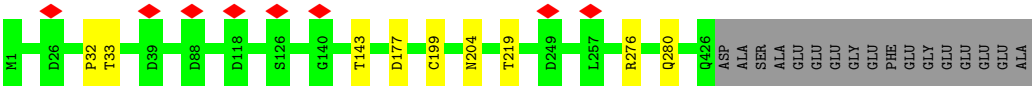
Chain D8:



• Molecule 1: Tubulin beta

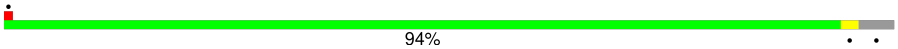
Chain E0:

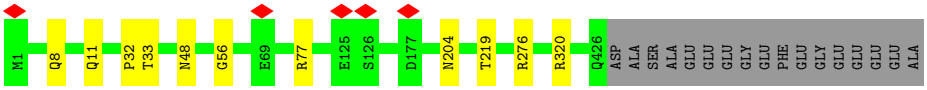



• Molecule 1: Tubulin beta

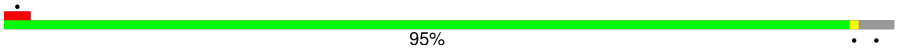
Chain E2:

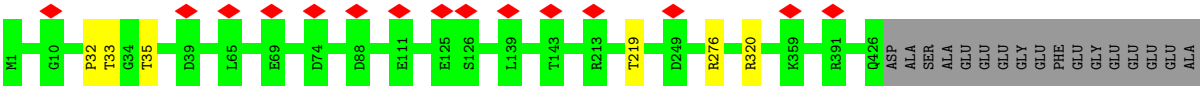



• Molecule 1: Tubulin beta

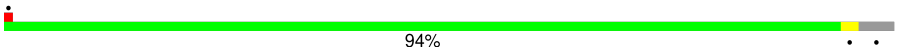
Chain E4:



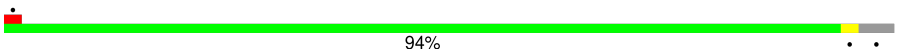

• Molecule 1: Tubulin beta

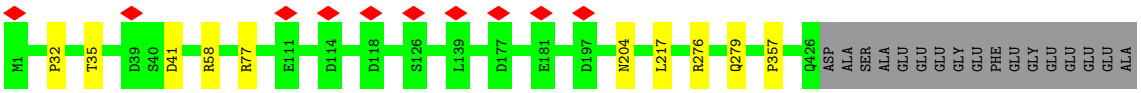
Chain E6:



• Molecule 1: Tubulin beta

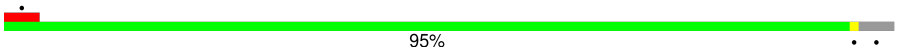
Chain E8:

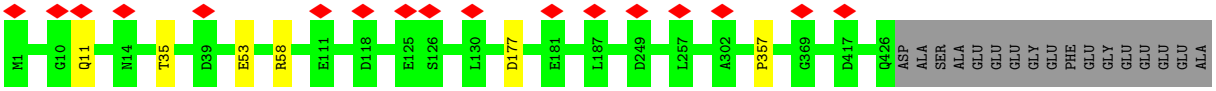





• Molecule 1: Tubulin beta

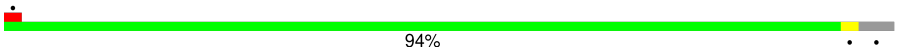
Chain F0:

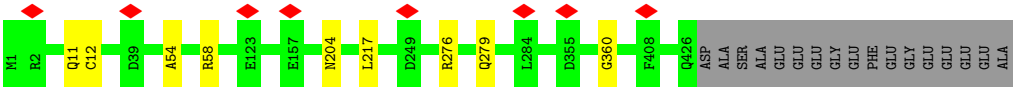



• Molecule 1: Tubulin beta

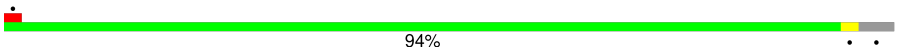
Chain F2:

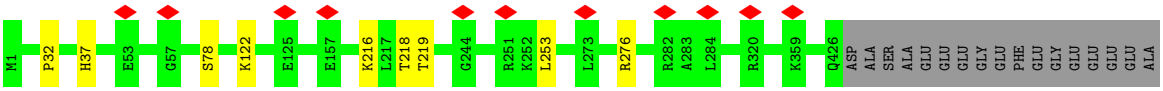



• Molecule 1: Tubulin beta

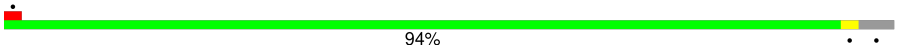
Chain F6:

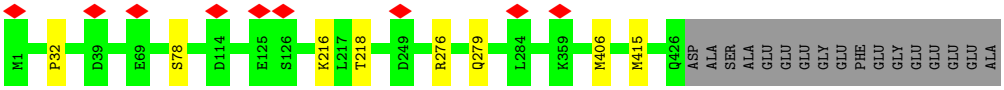



• Molecule 1: Tubulin beta

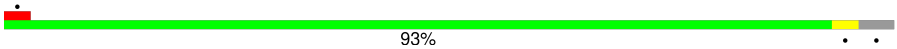
Chain F8:

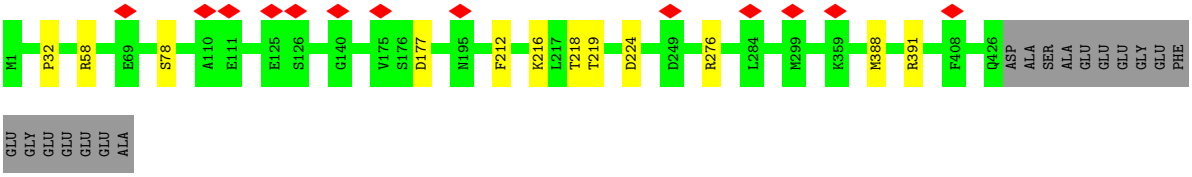



• Molecule 1: Tubulin beta

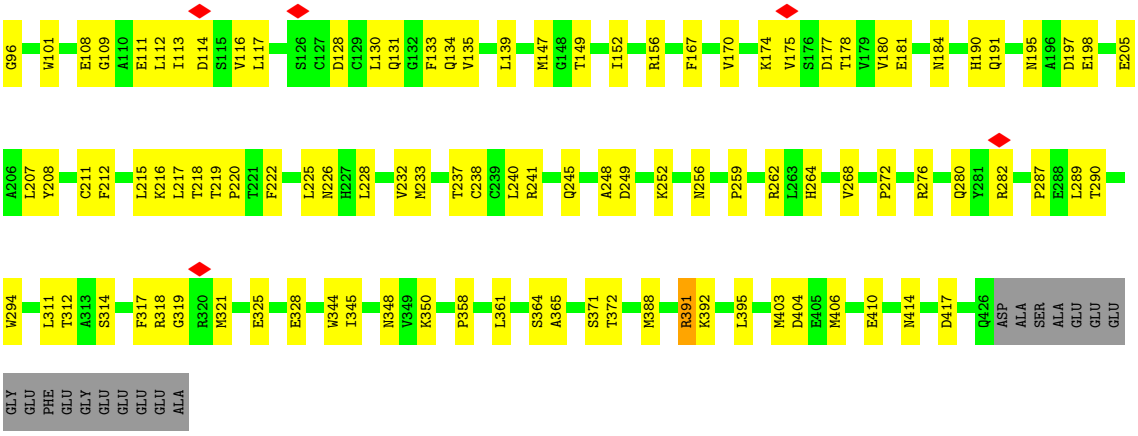
Chain G0:



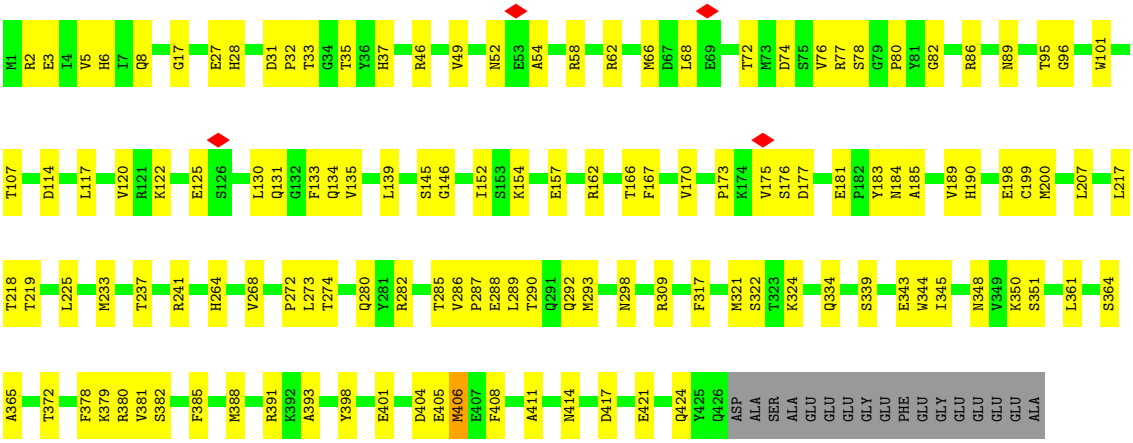

• Molecule 1: Tubulin beta

Chain G2:



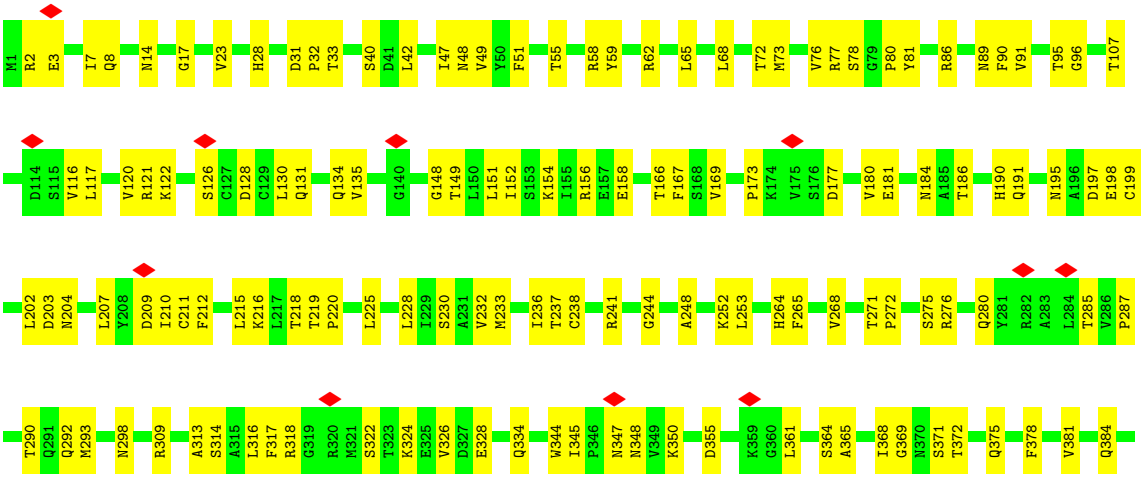

• Molecule 1: Tubulin beta

Chain G4:




• Molecule 1: Tubulin beta

Chain G6:



F389 R390 R391 K392 H396 E401 D404 E405 M406 A411 N414 D417 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

• Molecule 1: Tubulin beta

Chain G8:

M1 R2 E3 I7 Q8 G9 G17 D26 D31 P32 T33 G34 T35 E45 R46 V49 N52 T55 R58 P61 R62 A63 I64 L65 M66 D67 L68 P80 Y81 F85 V91 G96 N100 K103 T107 L112 I113 D114 S115 V116 L117 D118

V119 V120 R121 E125 S126 C127 D128 C129 L130 Q131 V135 C136 H137 S138 L139 G140 S145 G146 M147 L151 I152 R156 E157 E158 Y159 P160 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 Y183 N184 A185 T186 H190 E194 C199 L202

L207 C211 F212 R213 T214 L215 K216 T219 P220 D224 L225 N226 H227 S230 A231 V232 M233 S234 G235 C239 L240 R241 A248 D249 K252 L253 N256 F260 P261 R262 L263 V268 P272 L273 T274 S275 Q280 Y281 R282 A283 L284 T285 V286 P287 T290

M293 M300 R309 Y310 L311 T312 A313 S314 A315 L316 F317 K324 Q334 N335 S338 I345 P346 N347 N348 V349 K350 S351 S352 K359 G360 L361 S364 A365 T366 F367 I368 G369 N370 S371 T372 R380 Q384 F385 M388 K392 L395 H396 W397 E401 D404

E405 M406 E407 E410 A411 N414 D417 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

• Molecule 1: Tubulin beta

Chain H2:

M1 R2 H6 I7 Q8 Q11 F20 V24 S25 D26 T33 G34 T35 Y36 H37 D41 L42 Q43 L44 E45 R46 V49 Y50 F51 N52 E53 R58 R62 M66 D67 L68 T72 V76 R77 D88 N89 F90 V91 G96 A97 K103 T107 E108

E111 L112 I113 D114 S115 V116 L117 V120 R121 K122 E125 D128 Q131 Q134 V135 L139 G140 G141 G142 T143 M147 L151 I152 S153 K154 I155 R156 T166 F167 S168 P173 K174 V175 S176 D177 T178 V179 V180 E181 N184 A185 T186 H190 Q191 L192 N195 A196

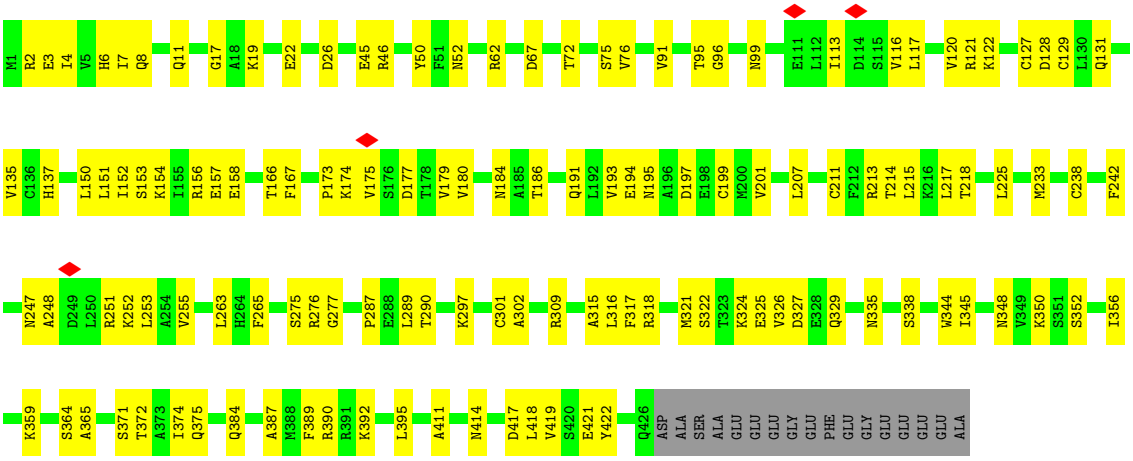
D197 E198 C199 M200 L207 Y208 D209 I210 C211 L215 T218 L225 L228 M233 L240 G244 N247 A248 D249 L250 R251 K252 L257 F265 V268 P272 R276 R282 A283 L284 T285 V286 P287 E288 L289 T290 Q291 K297 C301 A302 A303 D304

H307 G308 R309 S314 F317 M321 S322 E325 M330 Q334 N335 K336 N337 S338 S339 Y340 W344 I345 N348 V349 K359 S364 A365 T372 A373 I374 F378 K379 R380 V381 S382 T386 A387 R390 D404 E405 M406 E410 A411 N414 M415 M416 D417

L418 V419 S420 E421 Y422 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

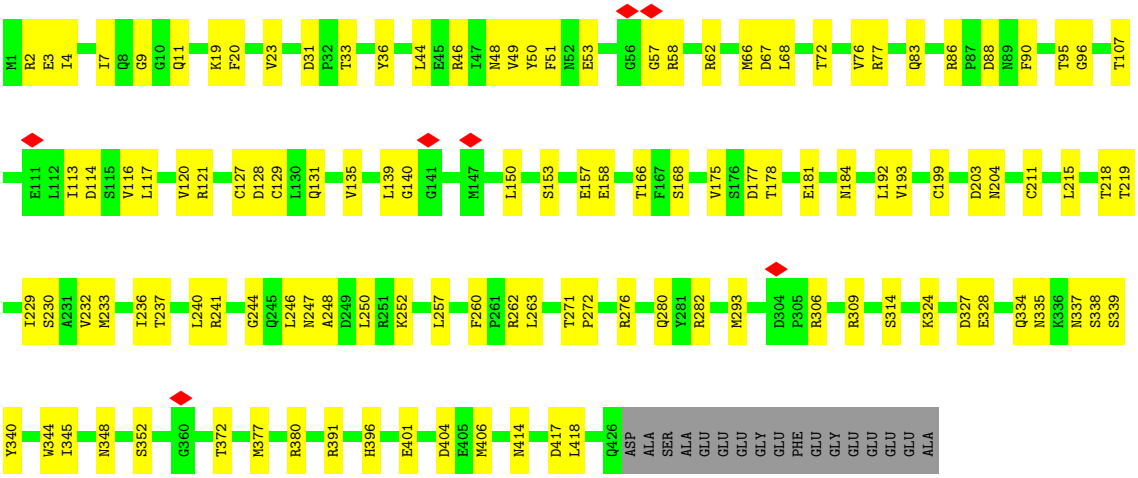
• Molecule 1: Tubulin beta

Chain H4:



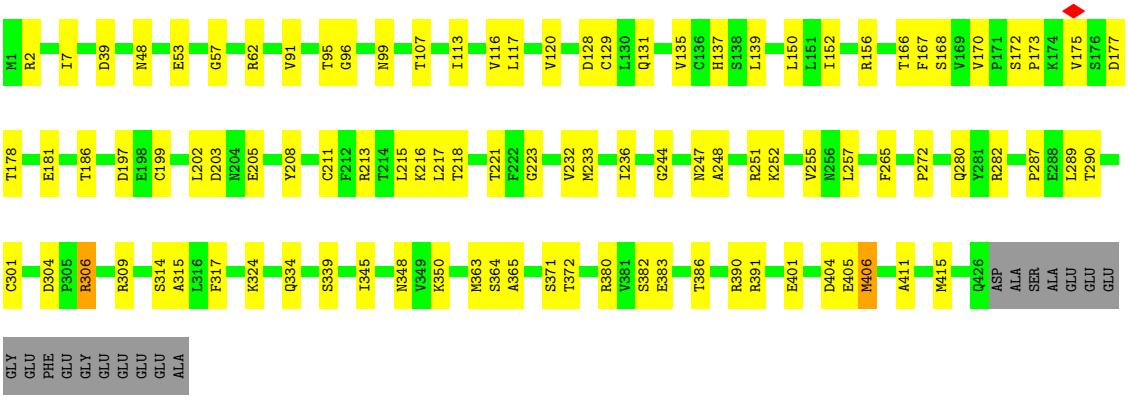

- Molecule 1: Tubulin beta

Chain H6:



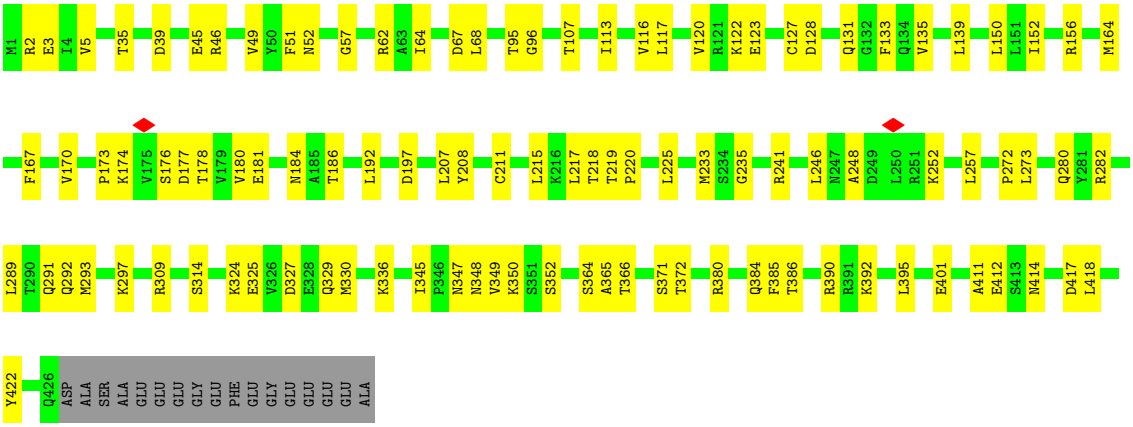

- Molecule 1: Tubulin beta

Chain H8:



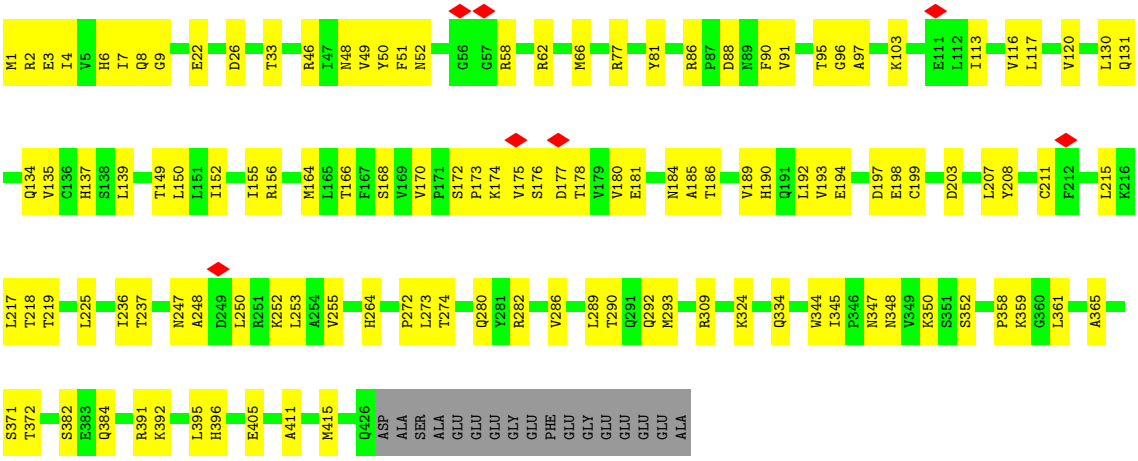

- Molecule 1: Tubulin beta

Chain I0:



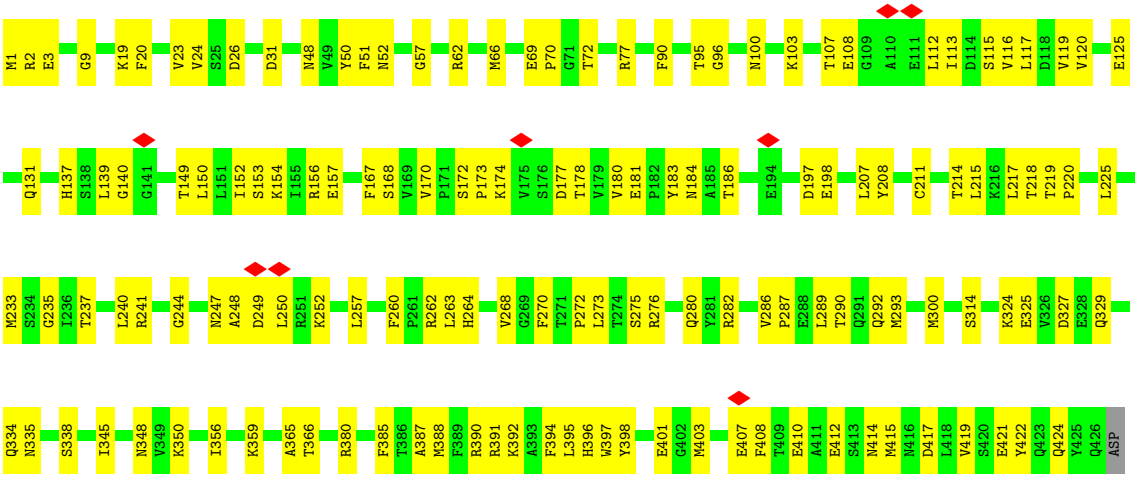

- Molecule 1: Tubulin beta

Chain I2:




- Molecule 1: Tubulin beta

Chain I4:



ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain I8:

M1 R2 E3 I7 G17 A18 K19 F20 W21 E22 V23 V24 D39 S40 D41 E45 R46 I47 N48 V49 Y50 F51 R58 R62 L68 E69 P70 D74 R77 Q83 V91 F92 T95 G96 A97 K103 T107 I113 D114 S115 V116 L117 D118 V119 V120

C127 D128 C129 L130 Q131 V135 C136 H137 S138 L139 G140 S145 G146 M147 L150 L151 I152 S153 K154 E157 M164 L165 T166 V170 P171 S172 V175 S176 D177 T178 V179 N184 A185 S188 V189 L192 D203 L207 Y208 D209 I210 C211 L215 K216 L217

P220 L225 I236 T237 L240 R241 L246 W247 A248 D249 K252 F260 L263 V268 T271 P272 L273 T274 S275 R276 Q279 T285 E288 Q291 Q292 M293 M300 C301 A302 A303 R309 F317 M321 S322 T323 K324 Q334 F941 I345 P346

N347 N348 Y349 K350 S351 S352 D355 I356 K359 G360 S364 A365 T372 A373 I374 Q375 E376 K379 F389 R390 R391 K392 H396 W397 Y398 T399 G400 E401 G402 M403 D404 E405 M406 N414 D417 L418 V419 S420 E421 Q424 Y425 Q426 ASP ALA SER ALA GLU GLU GLU GLY

GLU PHE GLU GLY GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain J0:

M1 R2 E3 I4 I7 W21 S25 I30 D39 S40 Q43 V49 Y50 F51 N52 G56 G57 R58 Y59 V60 P61 R62 A63 E69 P70 R77 I84 F85 R86 P87 D88 N89 F90 V91 F92 T95 G96 N100 K103 T107 E111 L112 I113 D114

S115 V116 K122 E125 S126 C129 L130 Q131 V135 C136 H137 S138 L139 G140 I152 S153 E157 M164 L165 T166 V170 P173 K174 V175 S176 D177 T178 V179 V180 N184 Q191 L192 V193 E194 C199 L207 C211 L215 K216 L217 T218 T219 P220 T221 F222

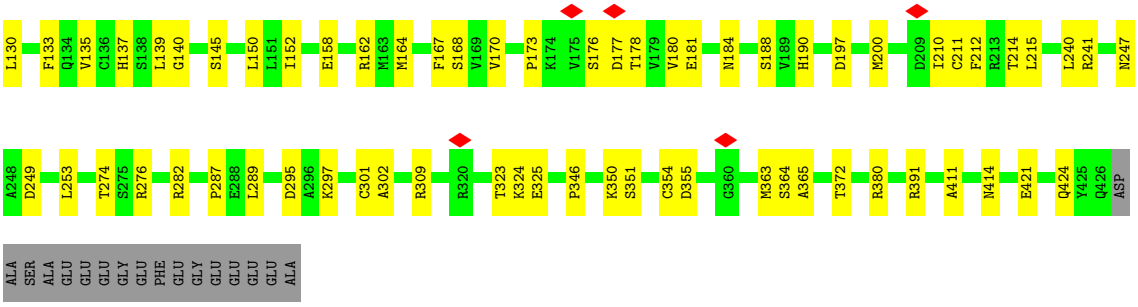
L225 V232 R241 A248 D249 L250 R251 K252 F260 L263 H264 F265 F270 T271 P272 R282 V286 L289 T290 Q291 Q292 M293 R309 F317 R320 M321 K324 Q334 S339 W344 I345 P346 N347 N348 Y349 K350 S351 A365 S371 T372

Q375 E376 M377 R380 V381 S382 T386 R390 E401 D404 E405 M406 M415 M416 D417 L418 V419 S420 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

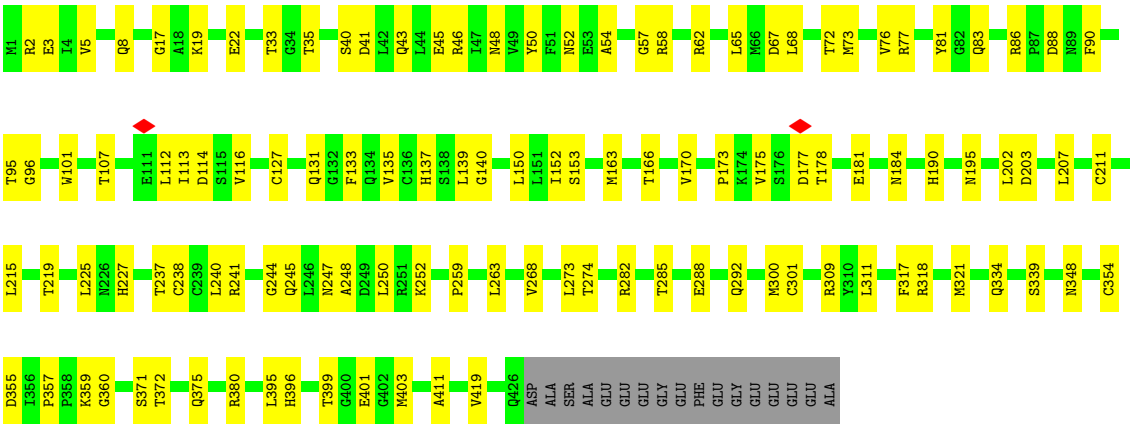
Chain J2:

M1 R2 V5 H6 I7 G10 Q11 D41 L44 E45 R46 V49 N52 V60 P61 R62 D67 L68 E69 P70 G71 D74 R77 I84 F85 R86 P87 D88 F92 A97 G98 N99 N100 K103 E111 L112 I113 D114 S115 V116 R121 K122 E123



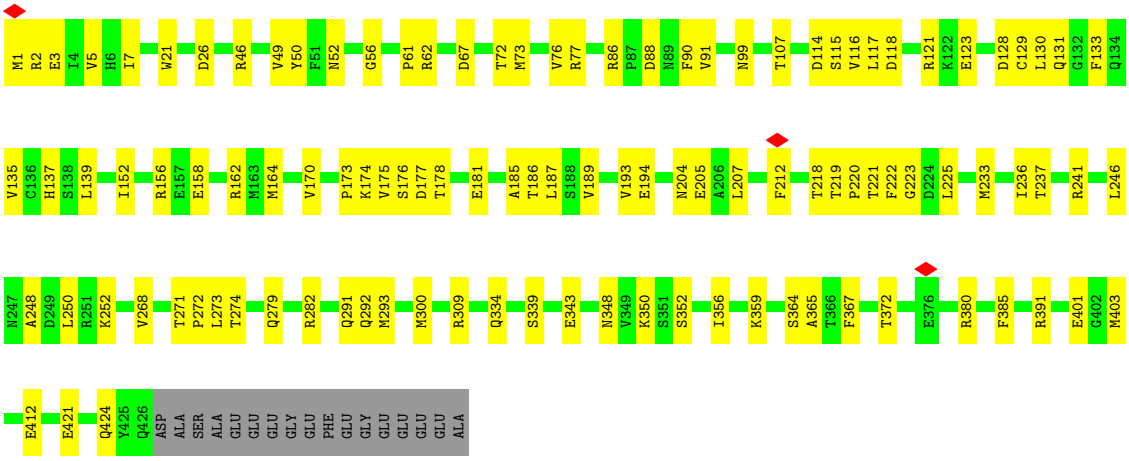

• Molecule 1: Tubulin beta

Chain J4:



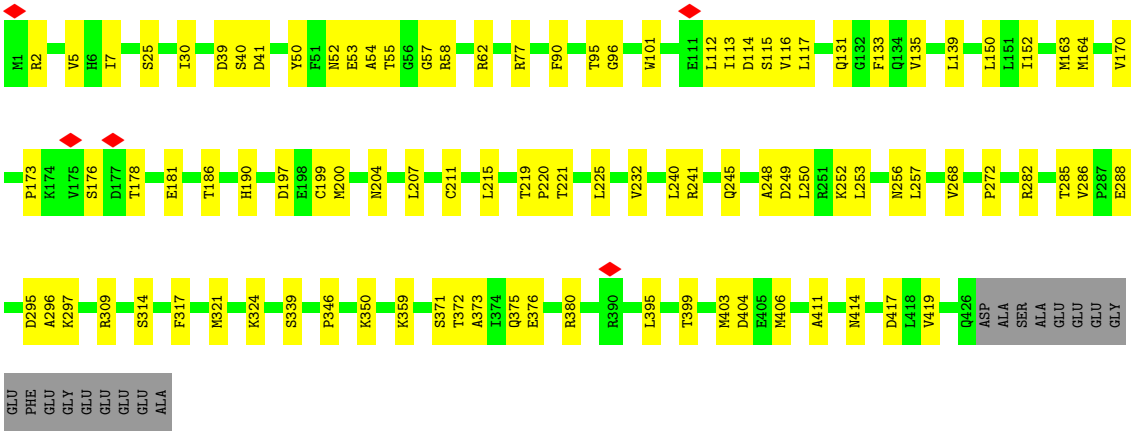

• Molecule 1: Tubulin beta

Chain J6:



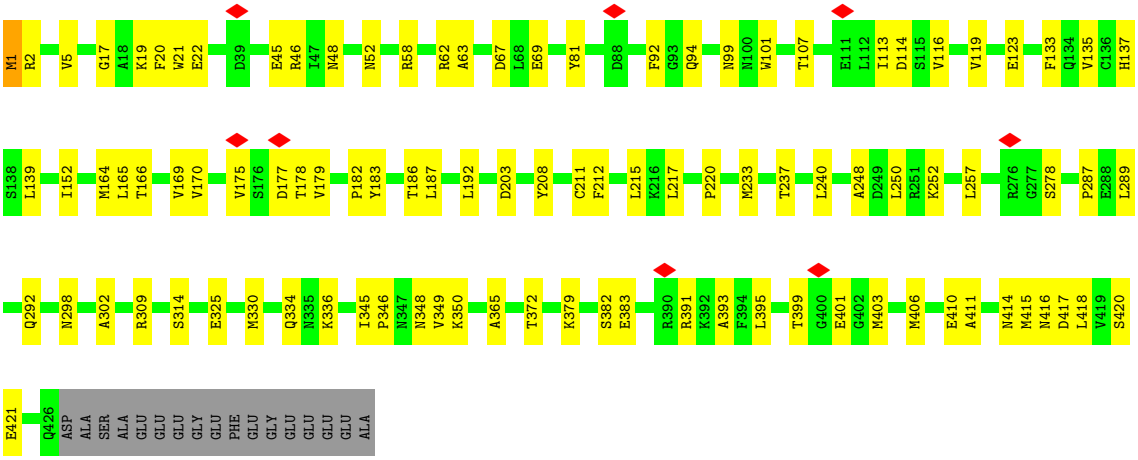

• Molecule 1: Tubulin beta

Chain J8:



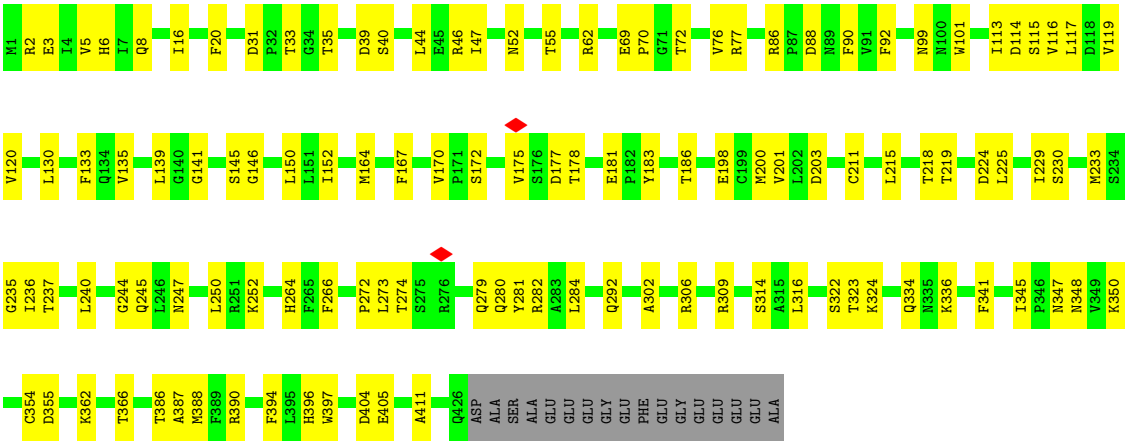

• Molecule 1: Tubulin beta

Chain K0:



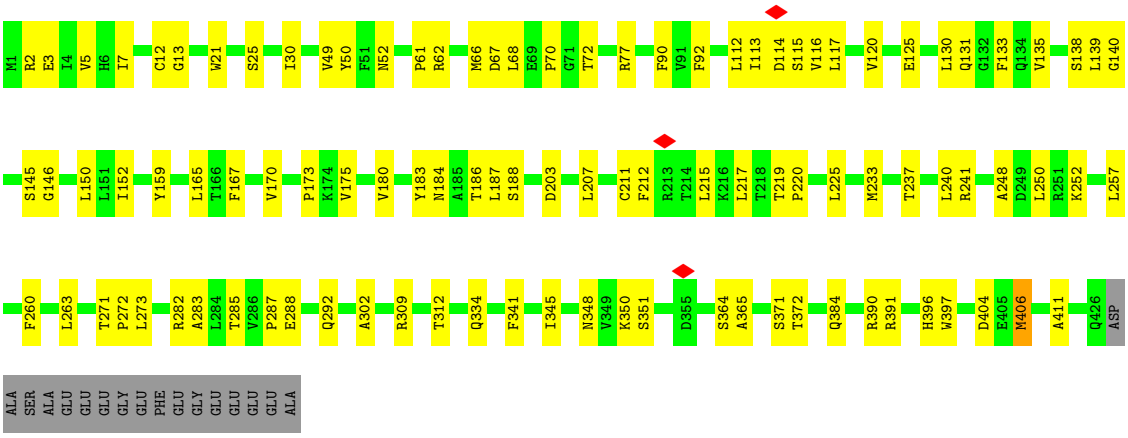

• Molecule 1: Tubulin beta

Chain K4:



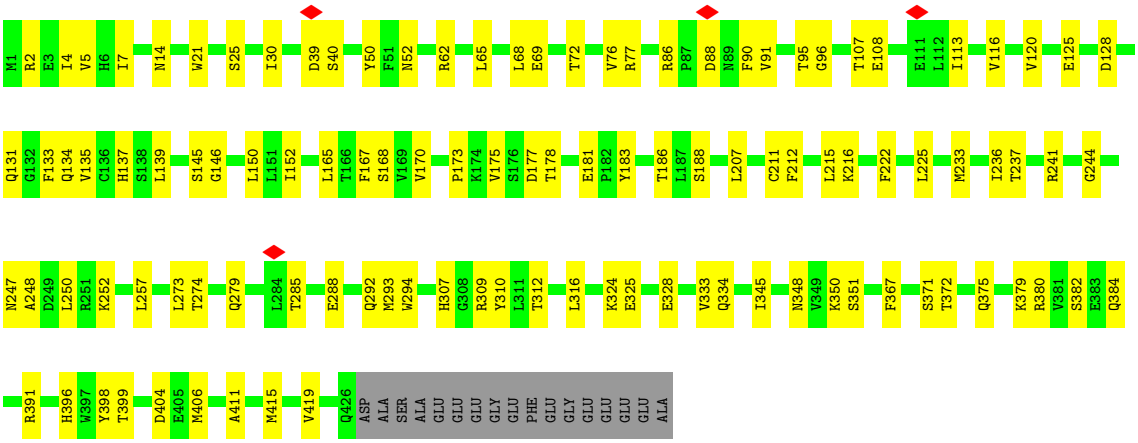

• Molecule 1: Tubulin beta

Chain K6:



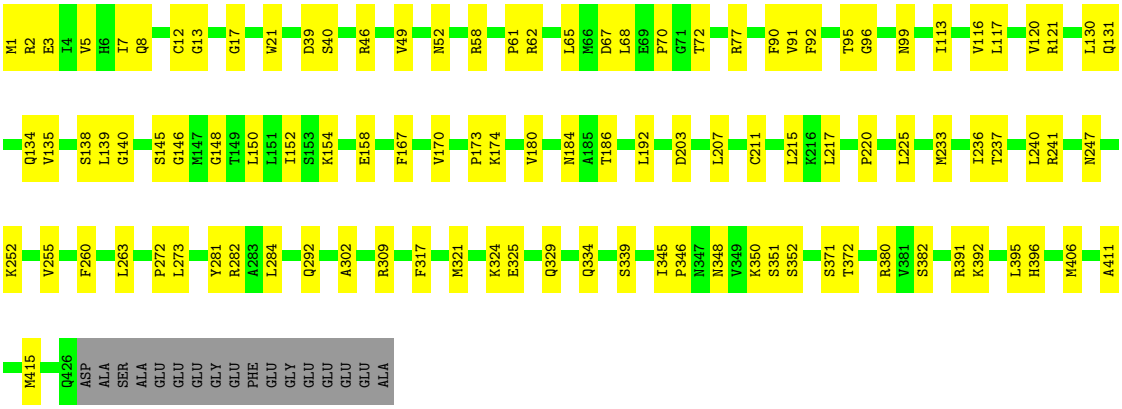

- Molecule 1: Tubulin beta

Chain K8:



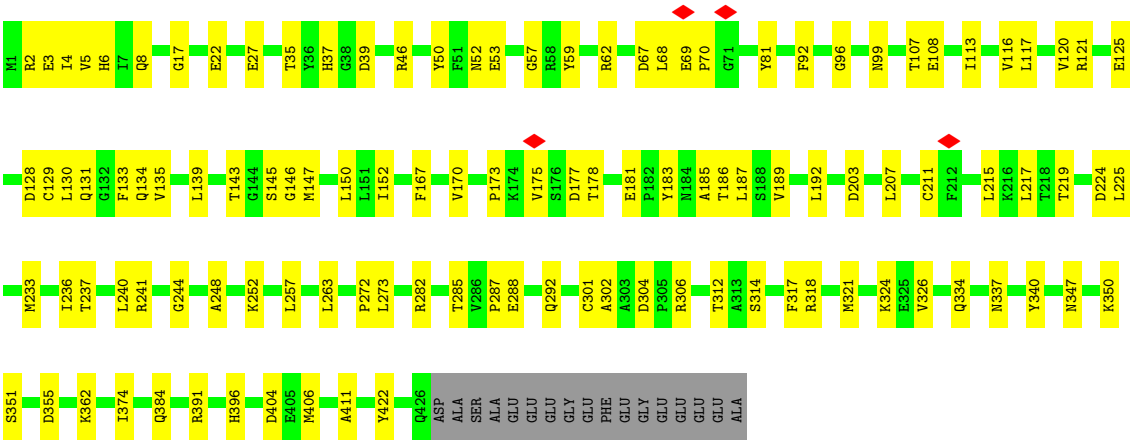

- Molecule 1: Tubulin beta

Chain L0:



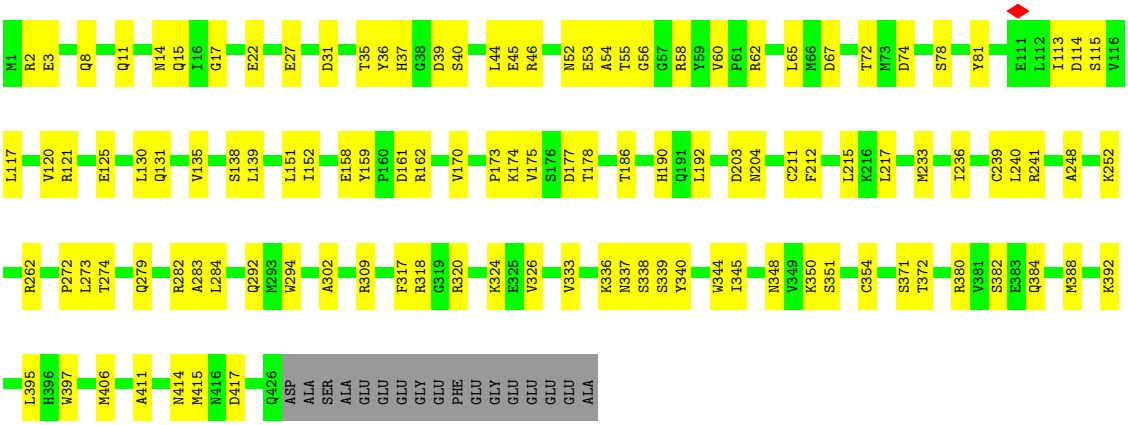

- Molecule 1: Tubulin beta

Chain L2:



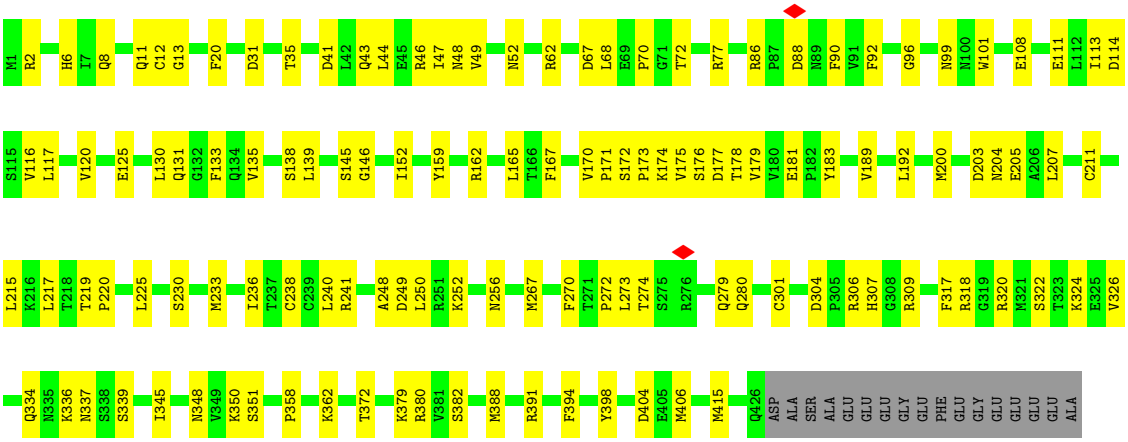

• Molecule 1: Tubulin beta

Chain L4:



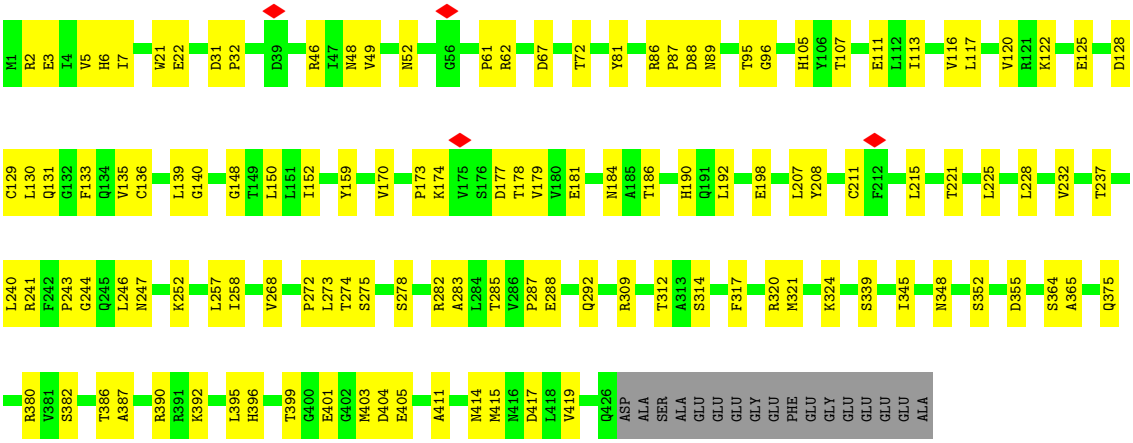

• Molecule 1: Tubulin beta

Chain L6:



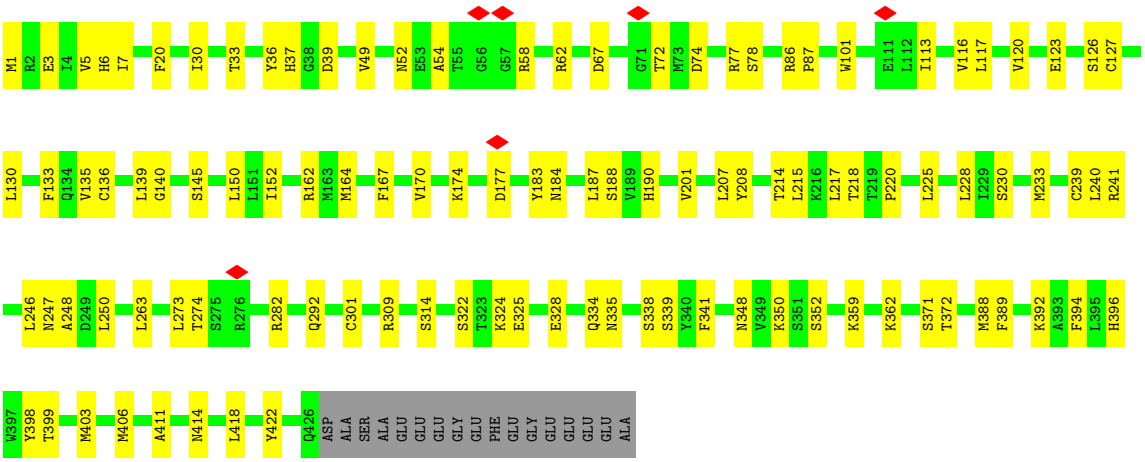
- Molecule 1: Tubulin beta

Chain M0:



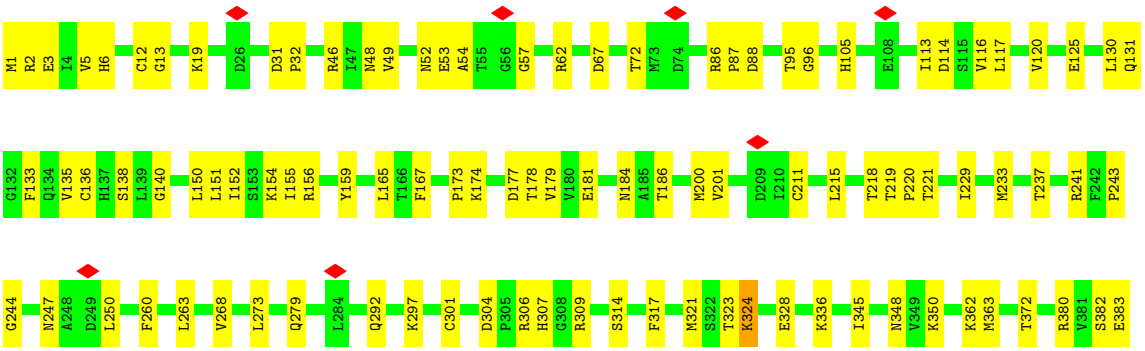

- Molecule 1: Tubulin beta

Chain M2:



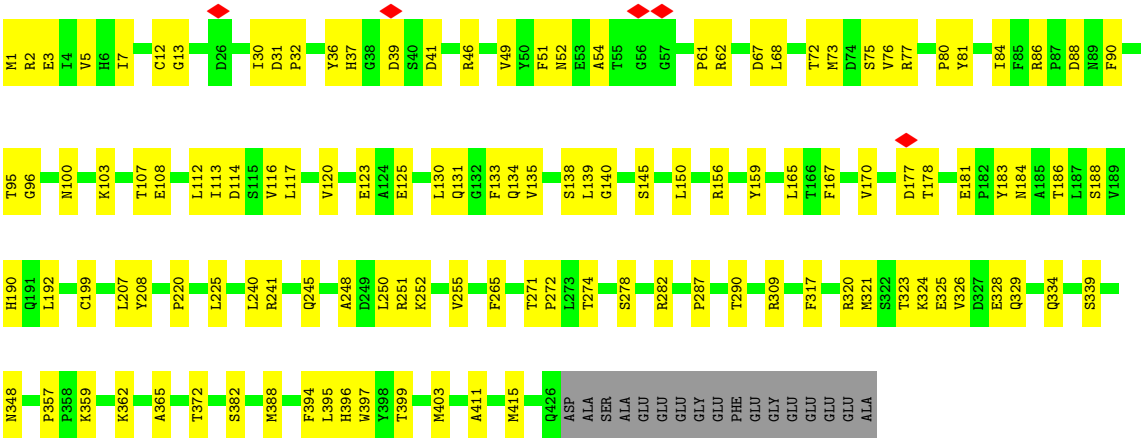

- Molecule 1: Tubulin beta

Chain M4:



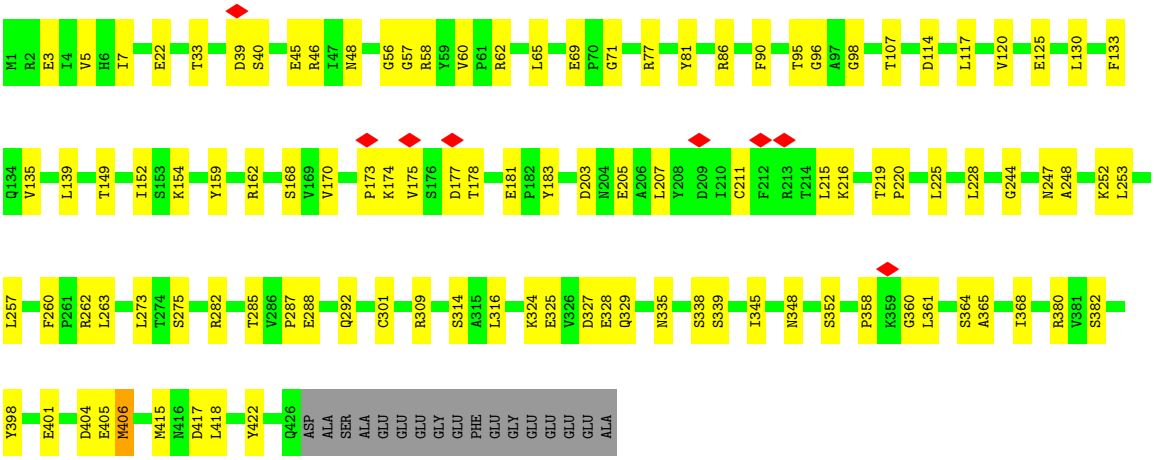
• Molecule 1: Tubulin beta

Chain M6:



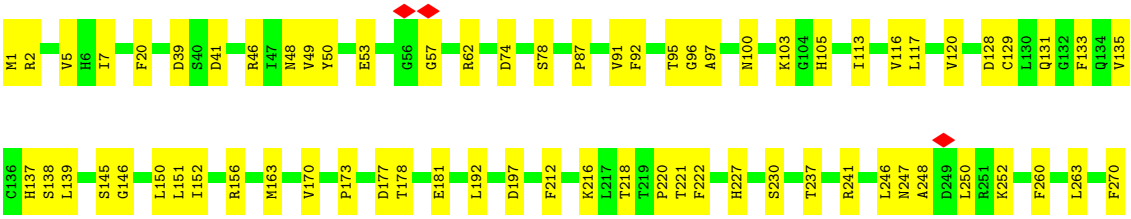

• Molecule 1: Tubulin beta

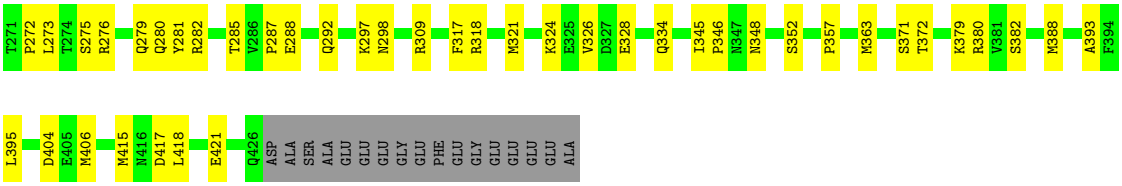
Chain M8:




• Molecule 1: Tubulin beta

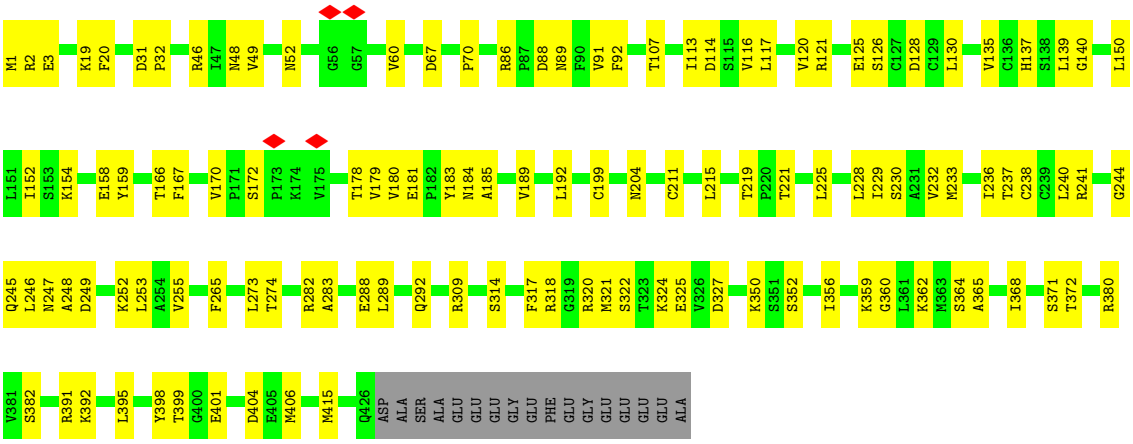
Chain N0:





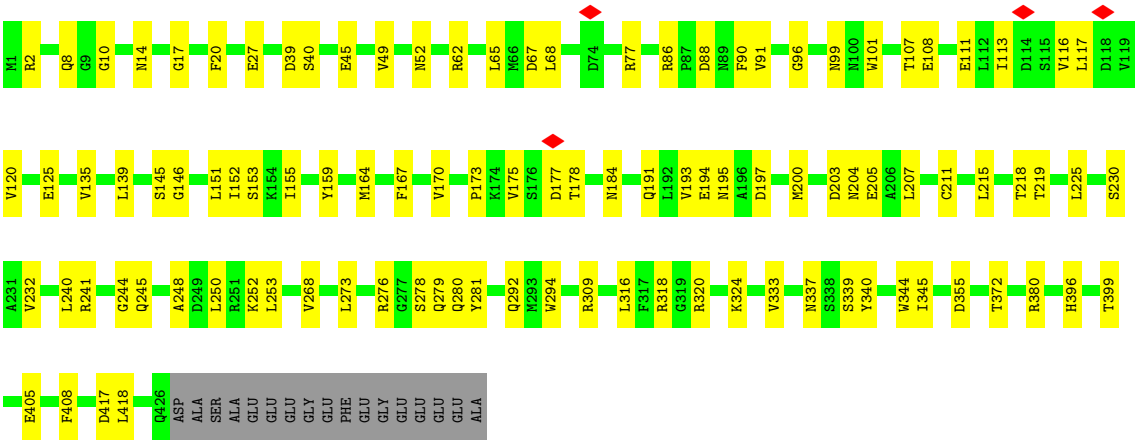

• Molecule 1: Tubulin beta

Chain N2:



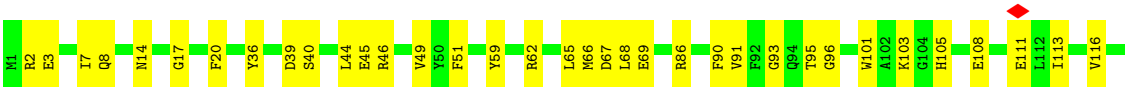

• Molecule 1: Tubulin beta

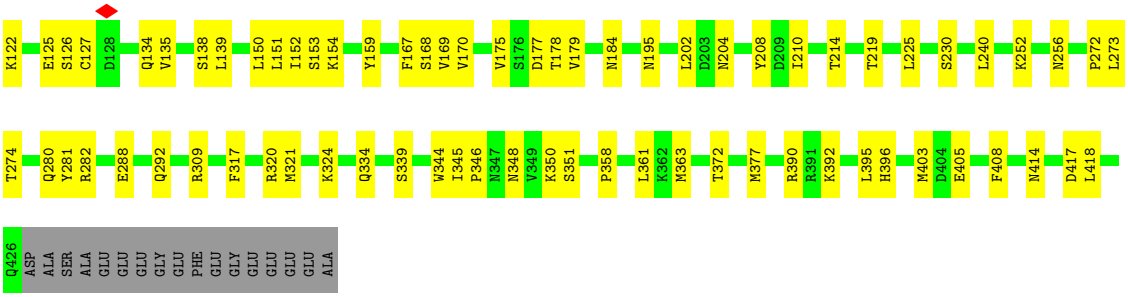
Chain N6:




• Molecule 1: Tubulin beta

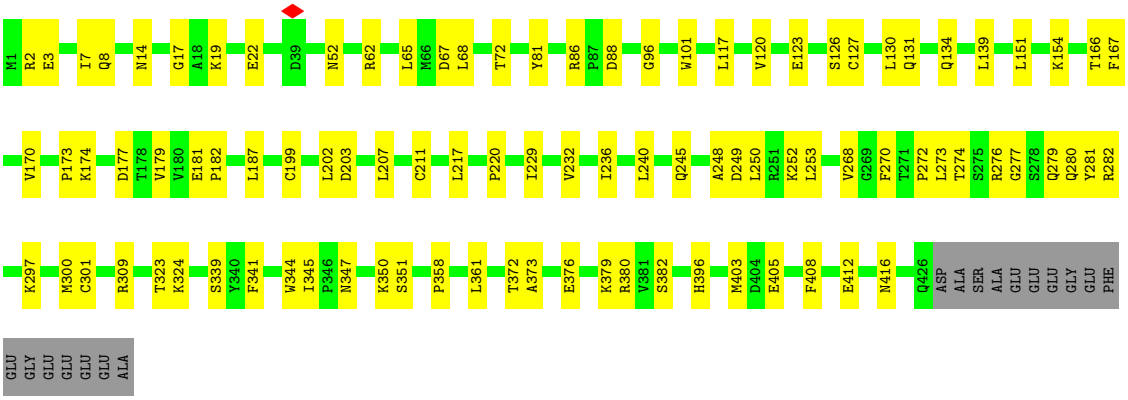
Chain N8:





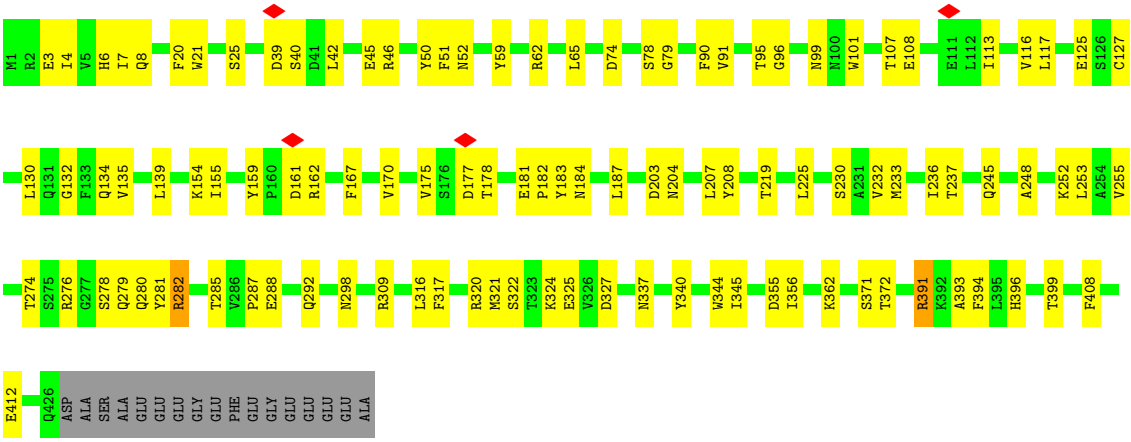

• Molecule 1: Tubulin beta

Chain O0:



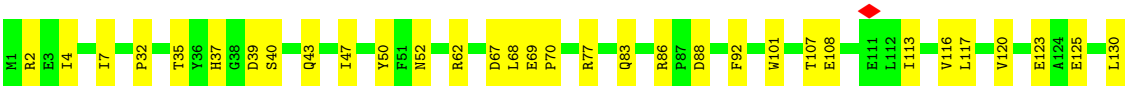

• Molecule 1: Tubulin beta

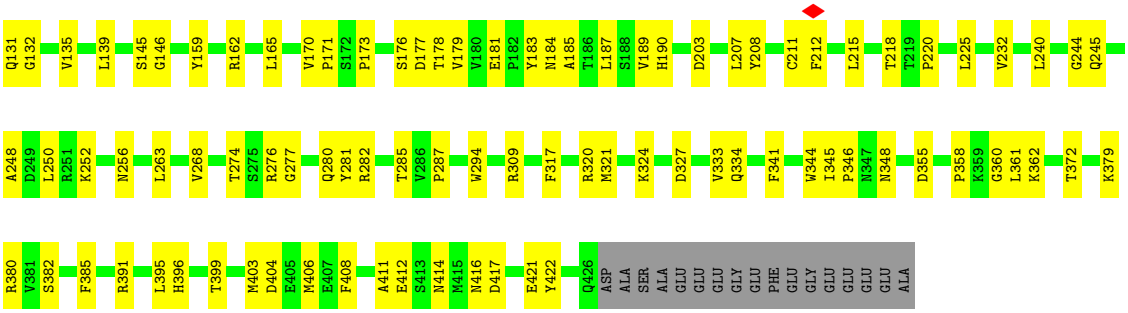
Chain O2:




• Molecule 1: Tubulin beta

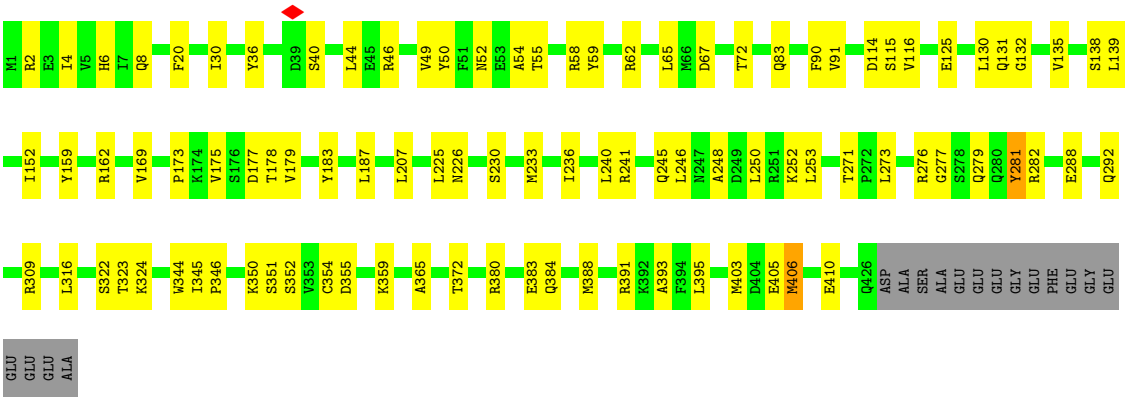
Chain O4:





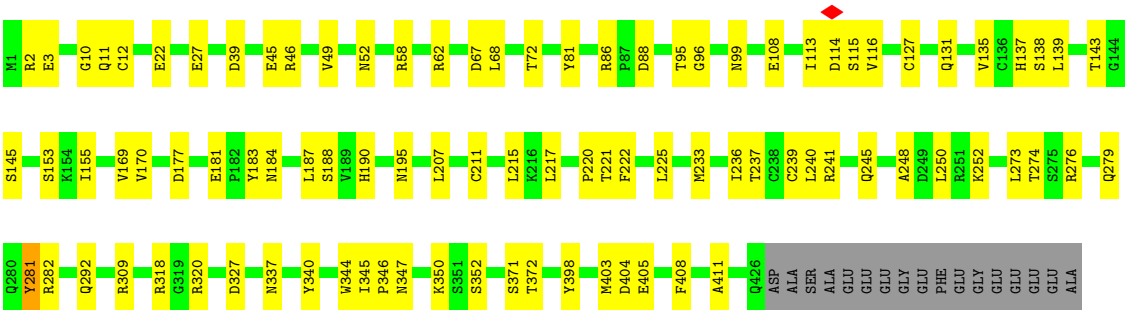

- Molecule 1: Tubulin beta

Chain O6:



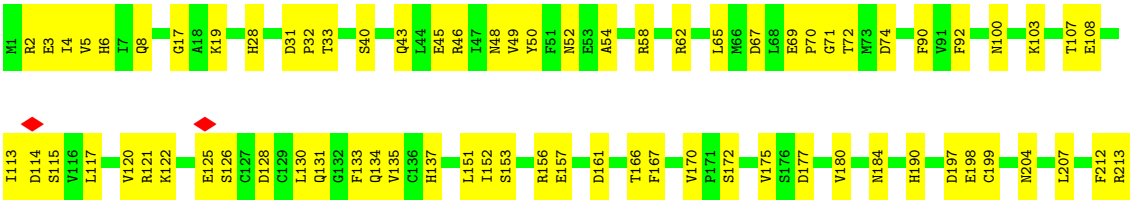

- Molecule 1: Tubulin beta

Chain O8:



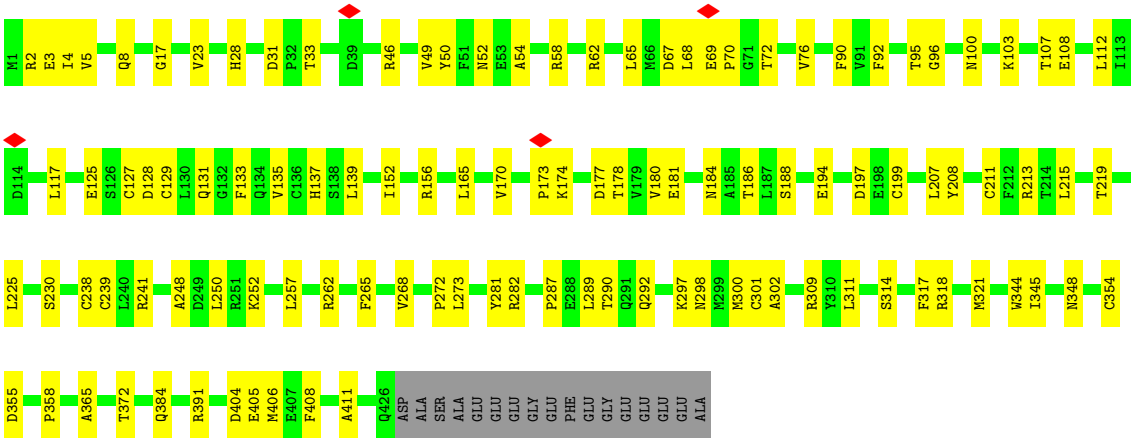

- Molecule 1: Tubulin beta

Chain P4:



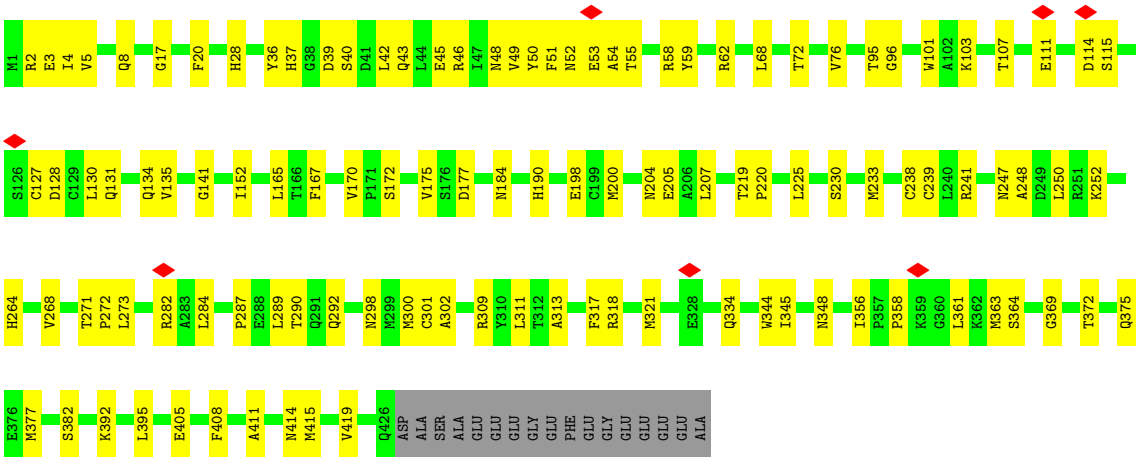
• Molecule 1: Tubulin beta

Chain P6:



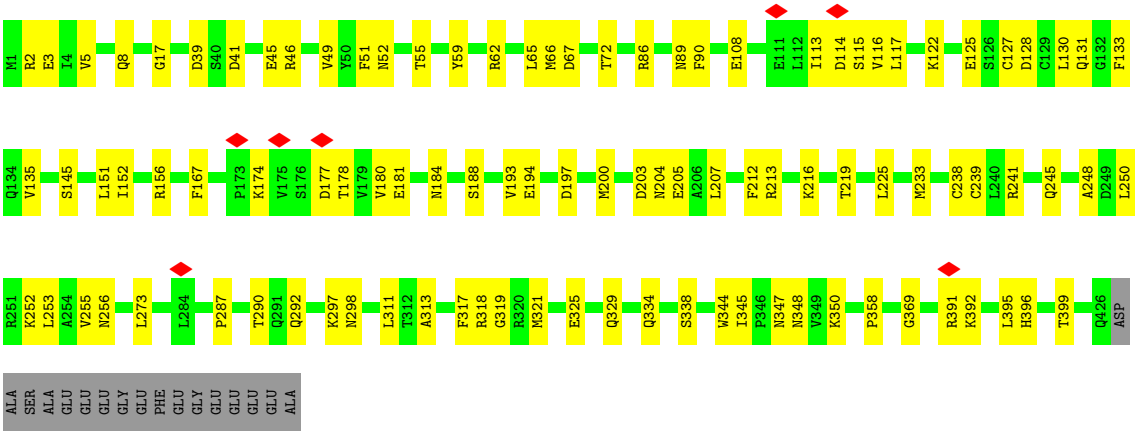

• Molecule 1: Tubulin beta

Chain P8:



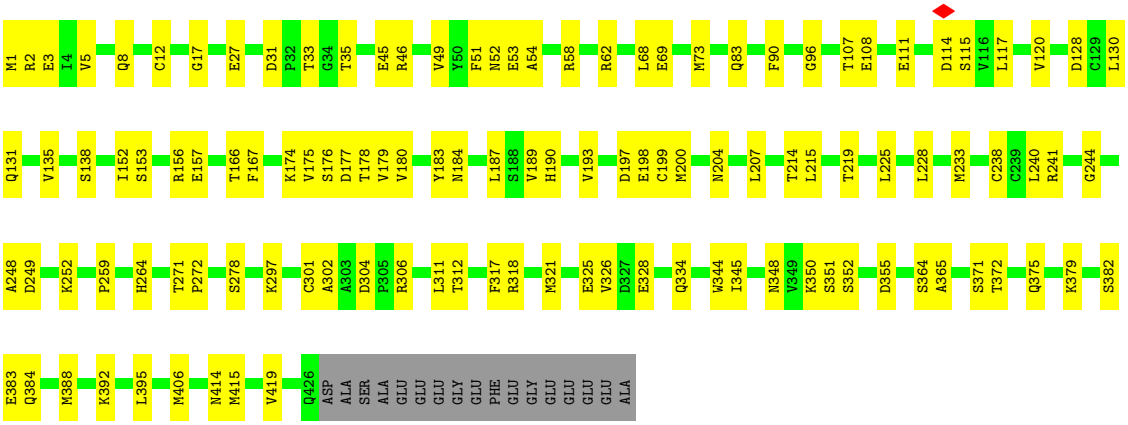

• Molecule 1: Tubulin beta

Chain Q0:



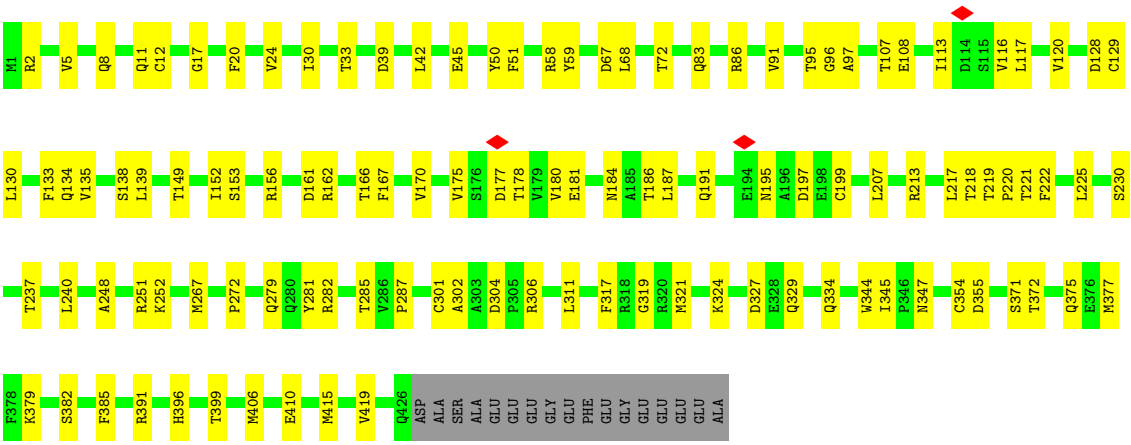

- Molecule 1: Tubulin beta

Chain Q2:



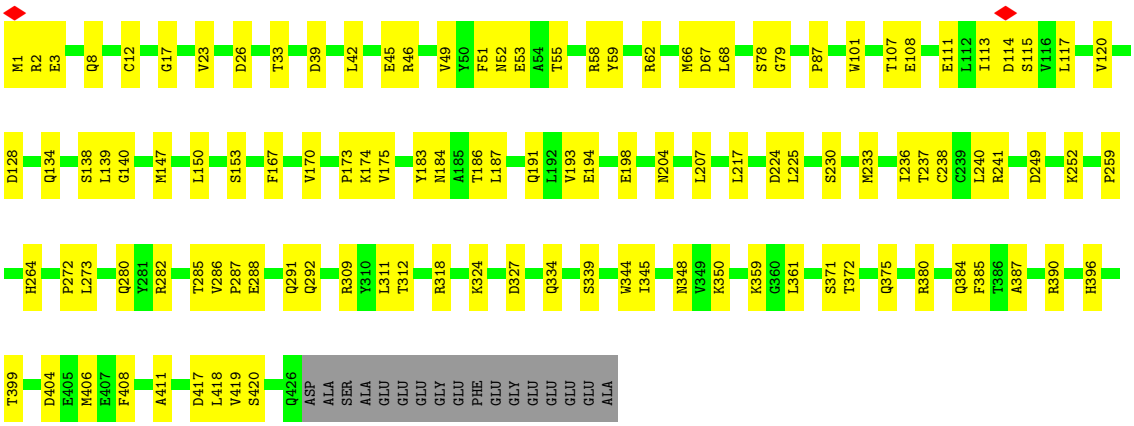

- Molecule 1: Tubulin beta

Chain Q4:



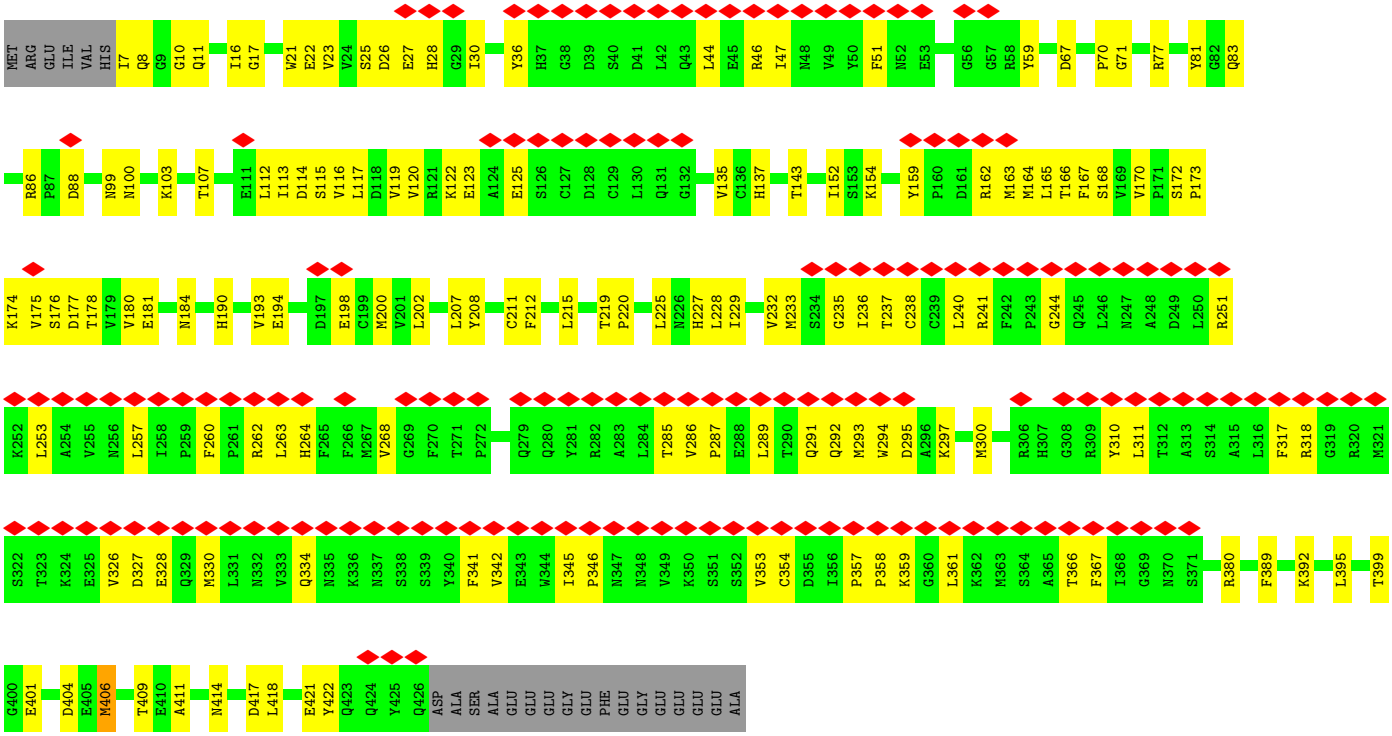

- Molecule 1: Tubulin beta

Chain Q6:



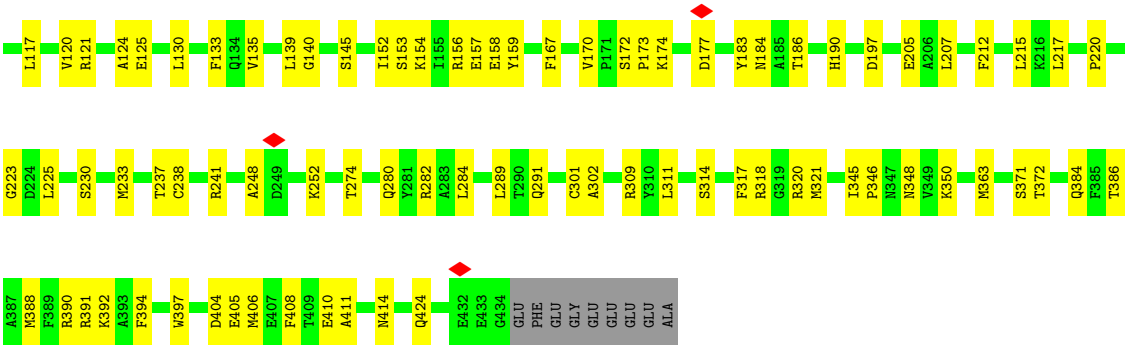

- Molecule 1: Tubulin beta

Chain Q8:



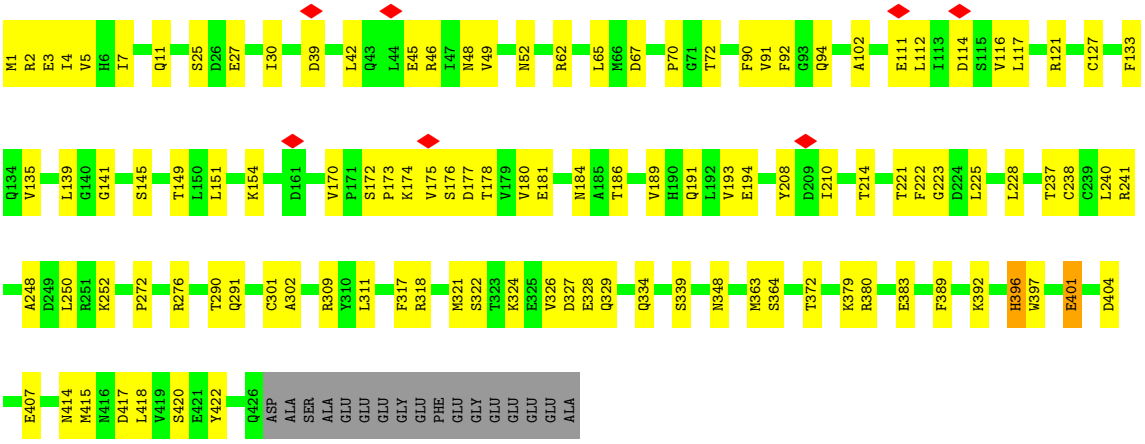

- Molecule 1: Tubulin beta

Chain R0:



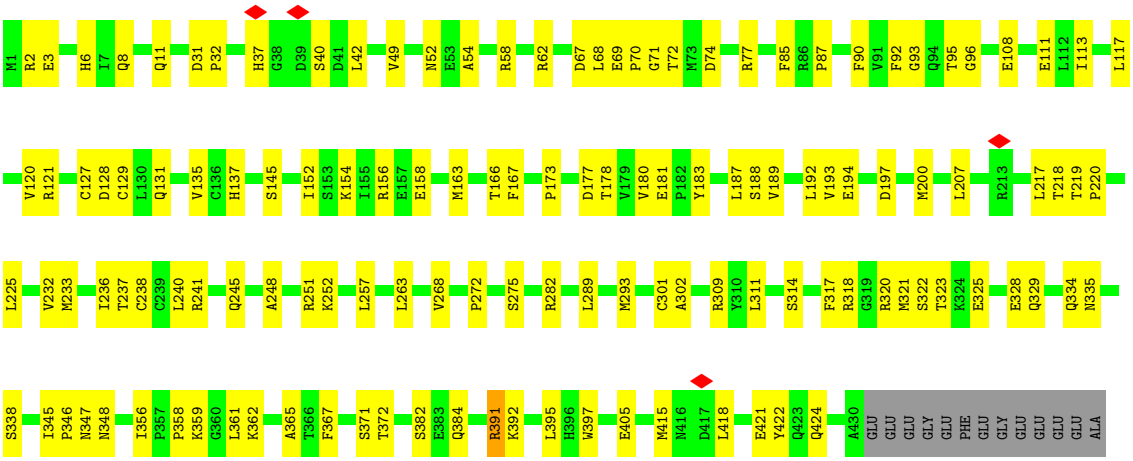

- Molecule 1: Tubulin beta

Chain R2:



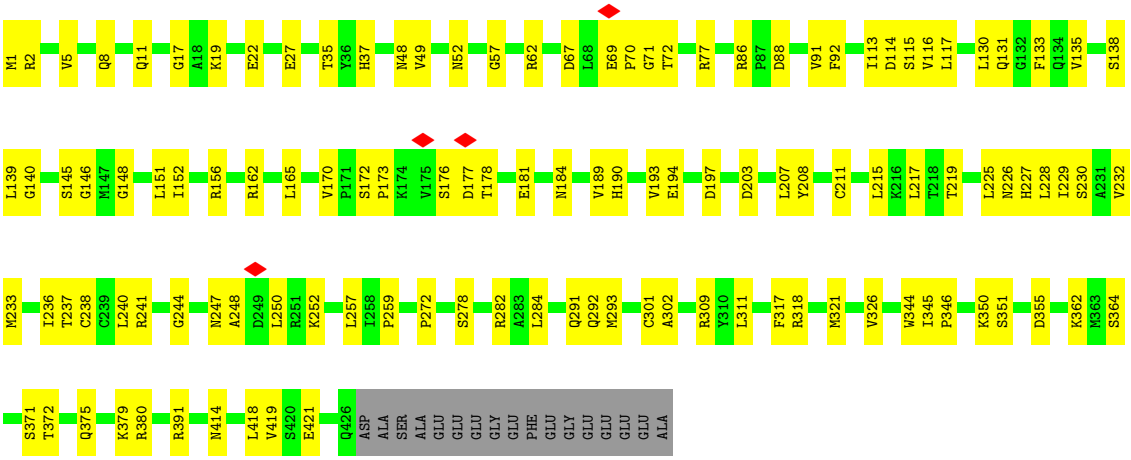

- Molecule 1: Tubulin beta

Chain R4:



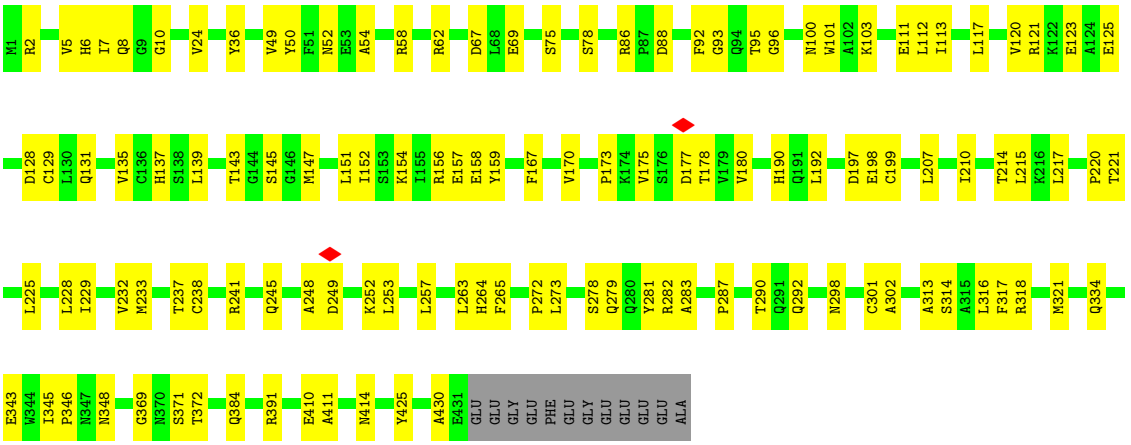

- Molecule 1: Tubulin beta

Chain R6:



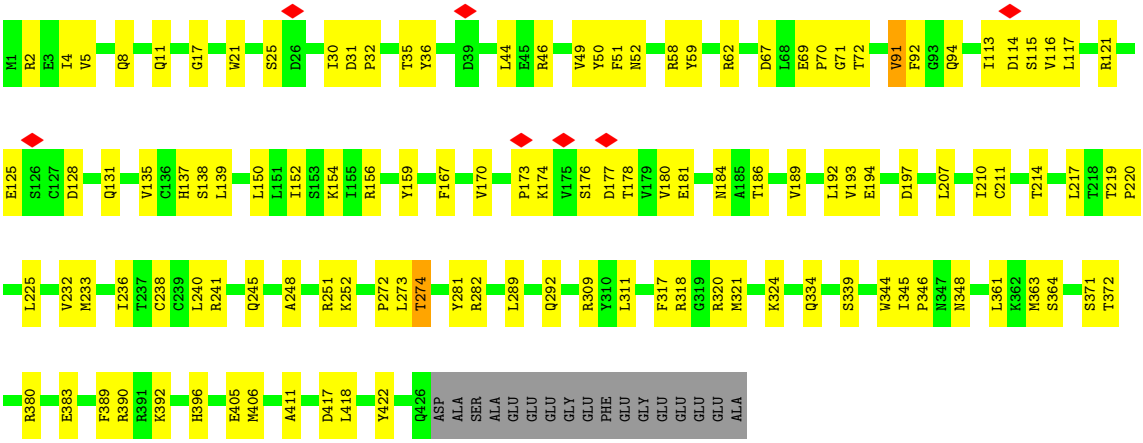

- Molecule 1: Tubulin beta

Chain R8:




- Molecule 1: Tubulin beta

Chain S0:




- Molecule 1: Tubulin beta

Chain S2: 70% 27% •

M1 R2 Q8 Q11 Q15 I16 G17 A18 K19 H28 D31 P32 T33 H37 E45 R46 V49 Y50 F51 N52 E53 A54 R58 Y59 R62 E69 P80 Q83 N89 Q94 T95 G96 N100 K103 E108 I113 V116 L117 D118 V119

V120 R121 K122 E123 A124 E125 Q131 Q134 V135 L139 I152 S153 R156 E157 E158 Y159 M164 F167 V170 P173 K174 V175 E181 P182 Y183 V189 H190 Q191 L192 V193 E194 D197 L207 T219 F222 L225 V232 M233 I236 T237 C238 C239

L240 R241 A248 K252 L253 L263 V268 L273 T274 Q280 Y281 R282 A283 L284 T285 V286 Q292 M300 R309 Y310 L311 S314 A315 L316 F317 R318 G319 R320 M321 E328 Q329 N332 I345 N348 V349 K350 K359 K362 M363 T372 M377 F378

K379 R380 E383 Q384 F385 T386 A387 R390 L395 E405 F408 T409 E410 N414 Q424 Y425 E431 GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

• Molecule 1: Tubulin beta

Chain S4: 14% 60% 36% •

M1 R2 E3 I4 V5 H6 I7 Q11 W21 D26 E27 S40 D41 L42 E45 R46 V49 Y50 F51 N52 P61 R62 D67 G71 T72 M73 D74 R77 R86 P87 D88 V91 N100 K103 T107 L112 I113 V116 V120 E125

D128 C129 L130 Q131 G132 F133 Q134 V135 L139 M147 L150 L151 I152 M163 M164 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 L192 V193 E194 N195 A196 D197 E198 V201 L202 D203 N204 E205 I210 C211 F212

R213 T214 L215 K216 T219 P220 T221 F222 G223 D224 L225 N226 H227 L228 V232 M233 T237 C238 C239 L240 R241 F242 P243 G244 Q245 L246 N247 A248 D249 L250 R251 K252 V255 N256 L257 I258 P259 F260 L263 M267 V268 T271 P272 L273 T274 S275 Q280 Y281 R282 A283 L284 T285

V286 P287 E288 L289 T290 Q291 Q292 M293 K297 C301 A302 A303 R309 Y310 L311 T312 A313 S314 F317 R318 G319 R320 M321 S322 T323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 N337 S338 S339 V342 E343 W344 I345 P346 M347 N348 V349 K350 S351 S352 V353 C354 D355

I356 K359 K362 M363 S364 A365 I368 S371 T372 A373 I374 Q375 E376 R380 F385 R391 K392 H396 T399 G400 E401 D404 E405 M406 E407 F408 T409 N414 Y422 D427 ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

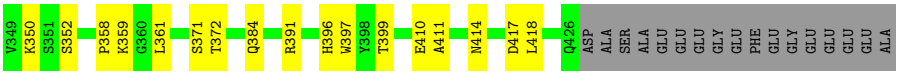
• Molecule 1: Tubulin beta

Chain S6: 68% 28% •

M1 R2 E3 I4 V5 Q8 G17 F20 D39 S40 E45 V49 Y50 F51 N52 R58 Y59 V60 P61 R62 L65 M66 D67 L68 E69 T72 Q83 R86 F90 V91 F92 G96 N100 W101 A102 K103 T107 E108 I113 D114 S115 V116 L117

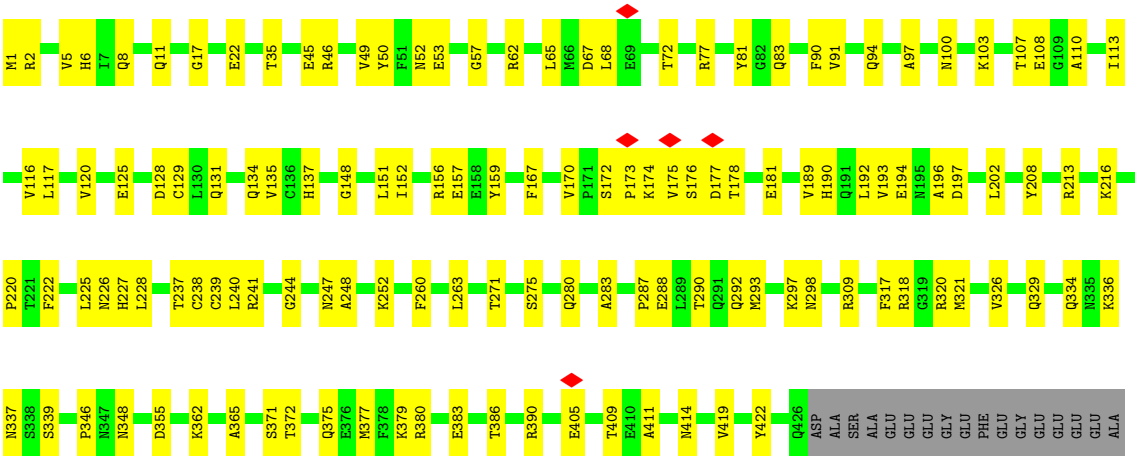
R121 K122 E125 D128 C129 L130 Q131 G132 V135 S138 L139 T149 L150 L151 I152 S153 K154 I155 R156 R162 M163 M164 F167 V170 P173 T178 E181 T186 L187 H190 Q191 L192 D197 E198 L207 Y208 D209 R213 L225 N226 H227 S230

M233 L240 R241 G244 Q245 L246 N247 A248 D249 L250 R251 K252 L257 I258 P259 L263 S275 R276 Q279 Q280 Y281 P287 E288 L289 Q292 D295 A296 K297 N298 R309 S314 R320 E325 V326 D327 E328 Q329 Q334 E343 W344 I345 P346 N347 N348



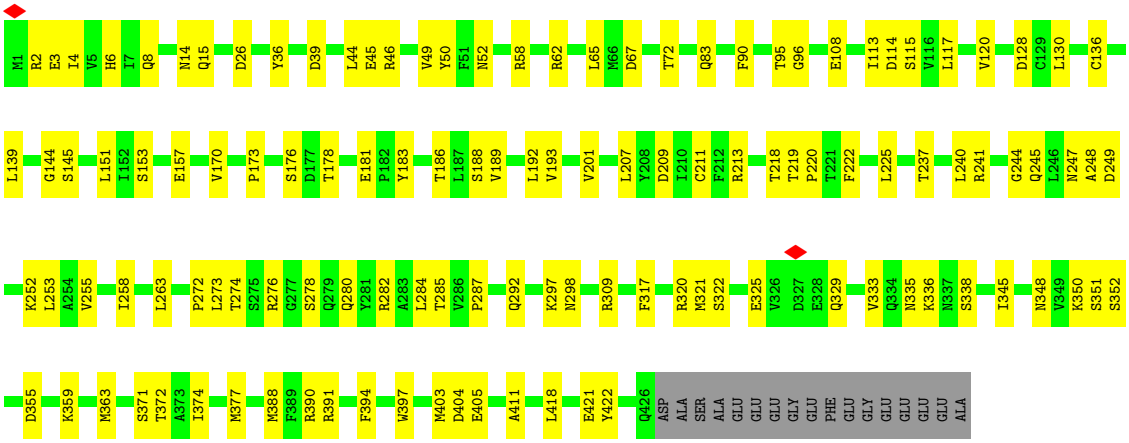

• Molecule 1: Tubulin beta

Chain S8:



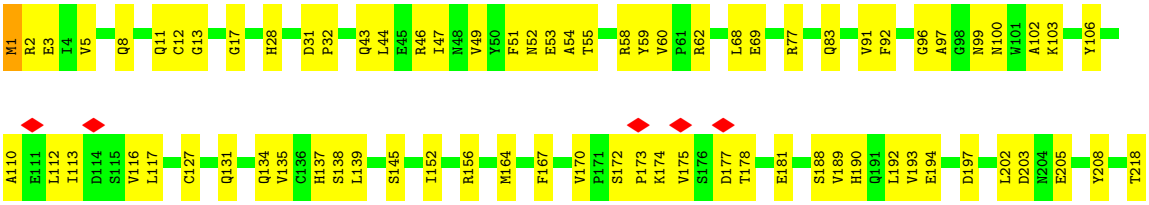

• Molecule 1: Tubulin beta

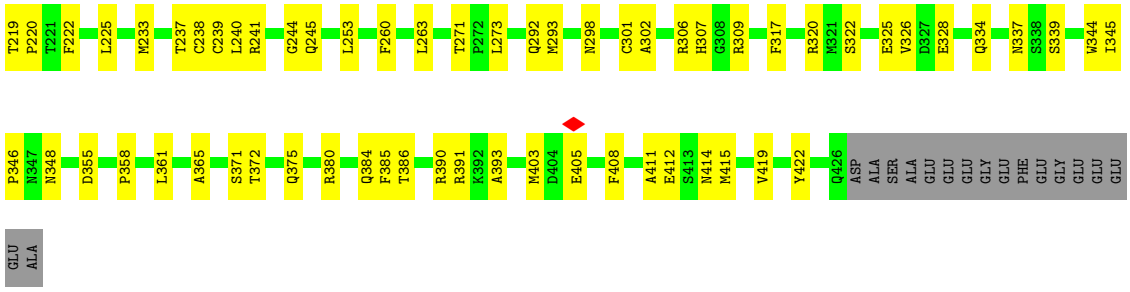
Chain T0:




• Molecule 1: Tubulin beta

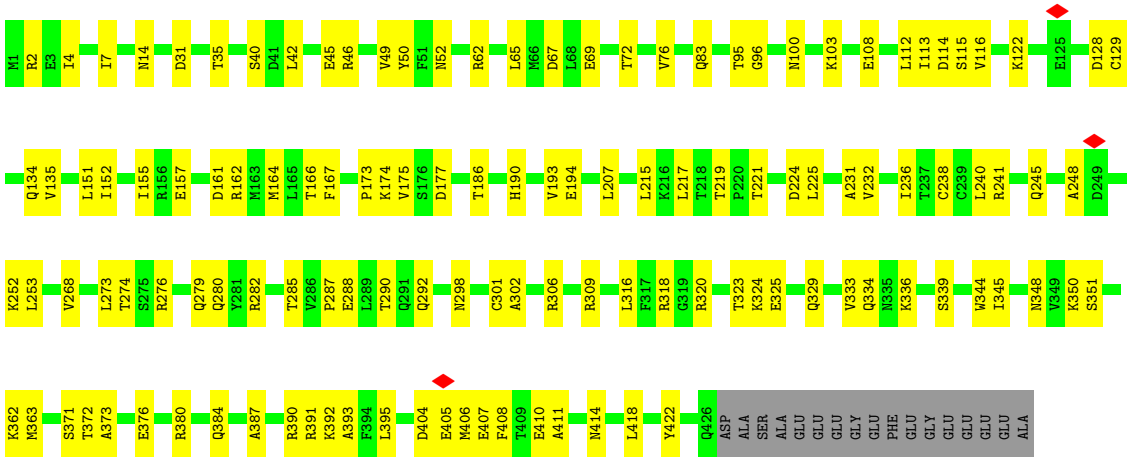
Chain T2:





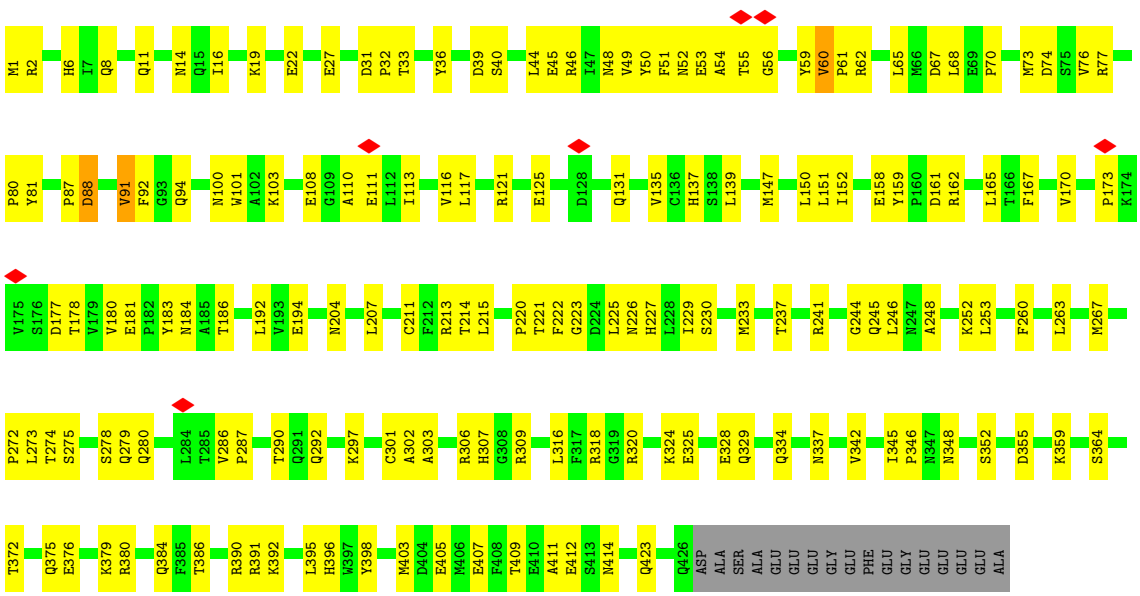

• Molecule 1: Tubulin beta

Chain T4:



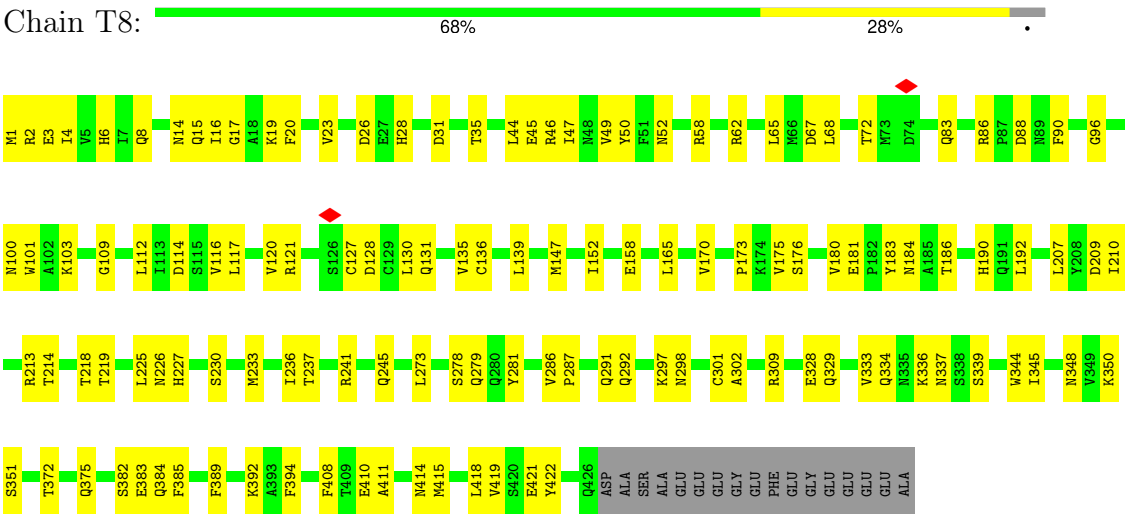

• Molecule 1: Tubulin beta

Chain T6:



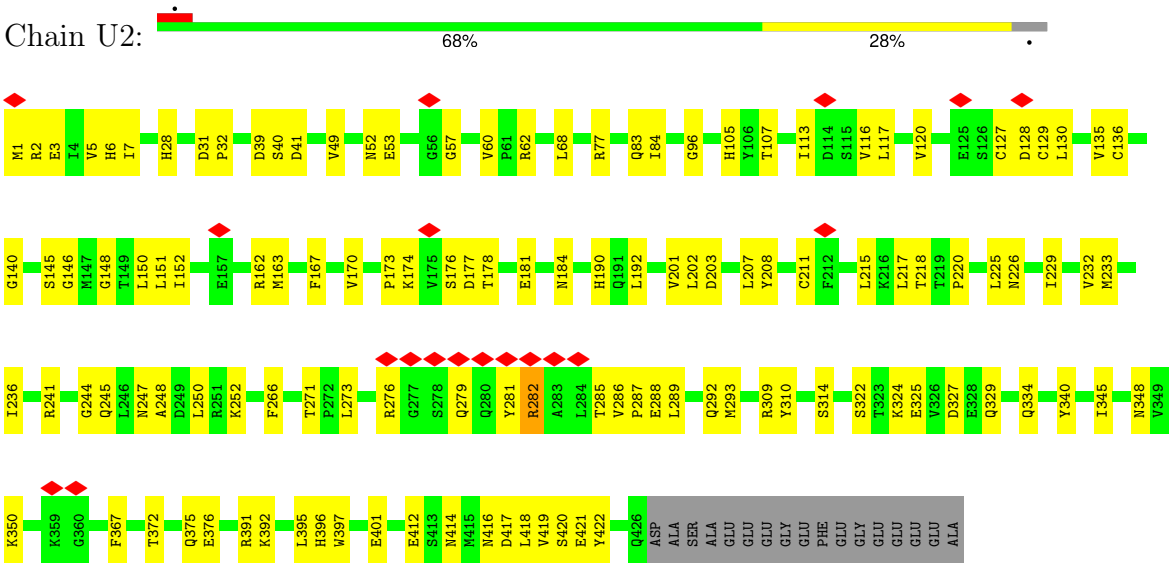

• Molecule 1: Tubulin beta

Chain T8:



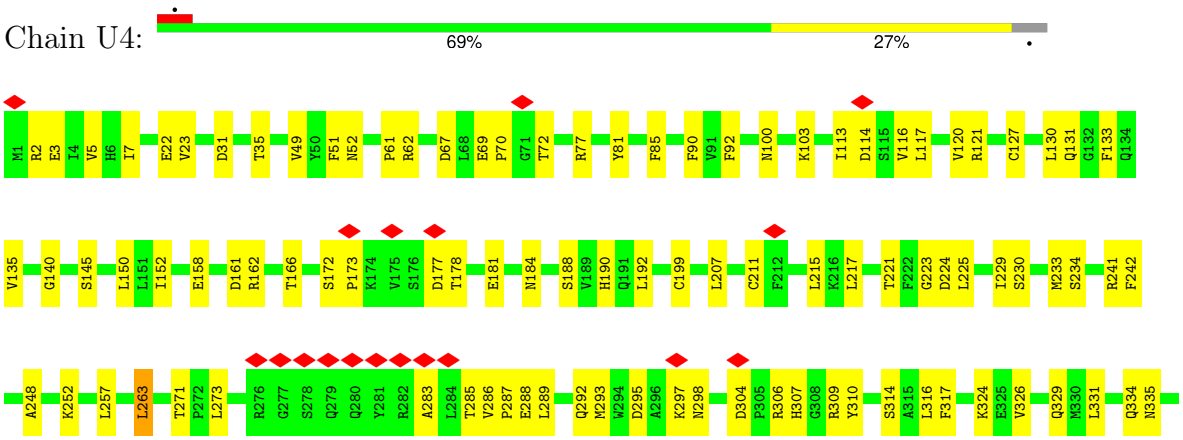

- Molecule 1: Tubulin beta

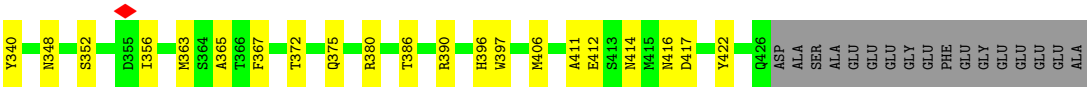
Chain U2:




- Molecule 1: Tubulin beta

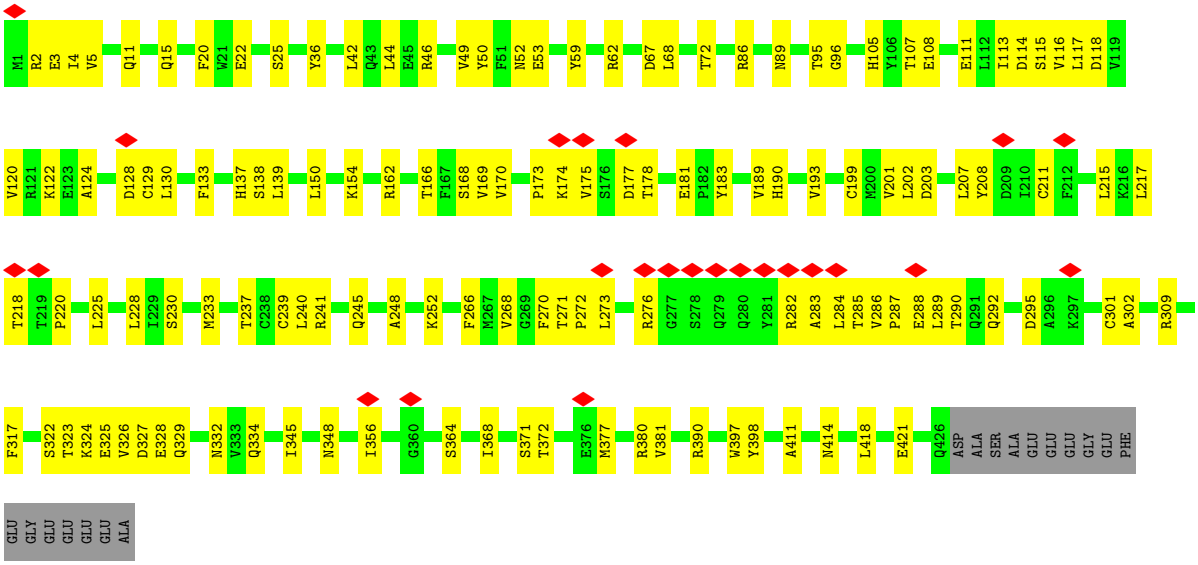
Chain U4:





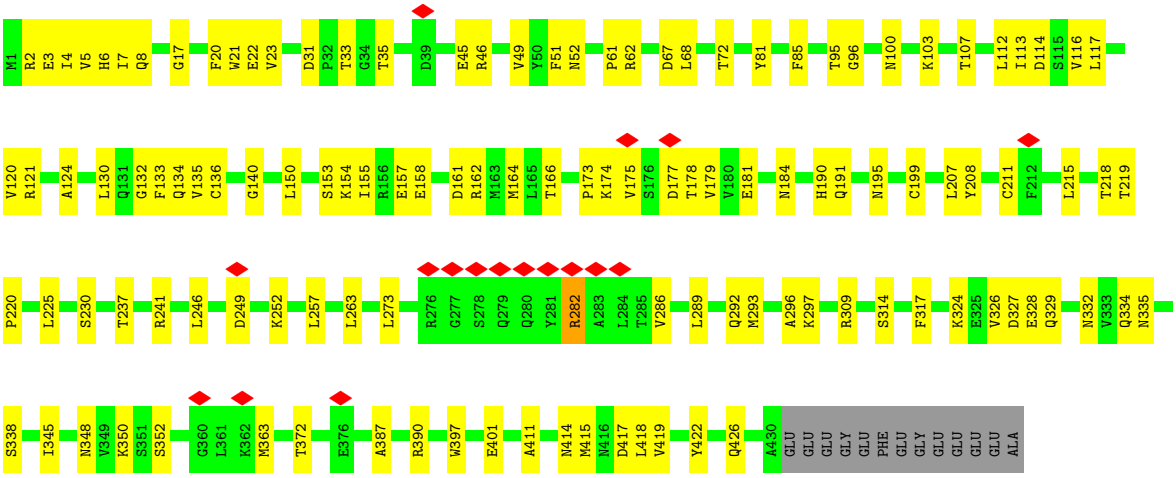

- Molecule 1: Tubulin beta

Chain U6:



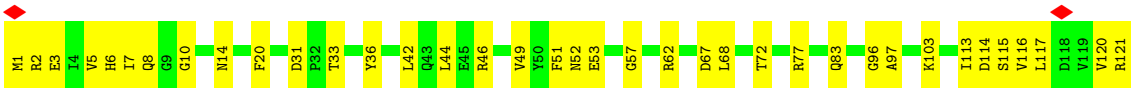

- Molecule 1: Tubulin beta

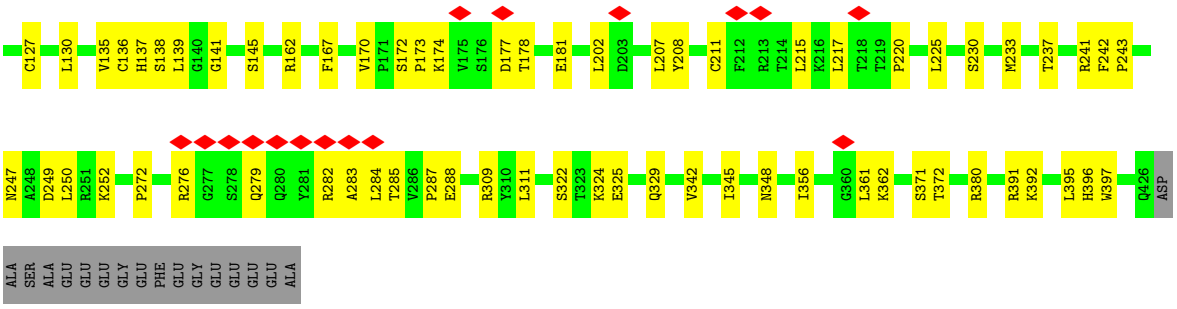
Chain U8:




- Molecule 1: Tubulin beta

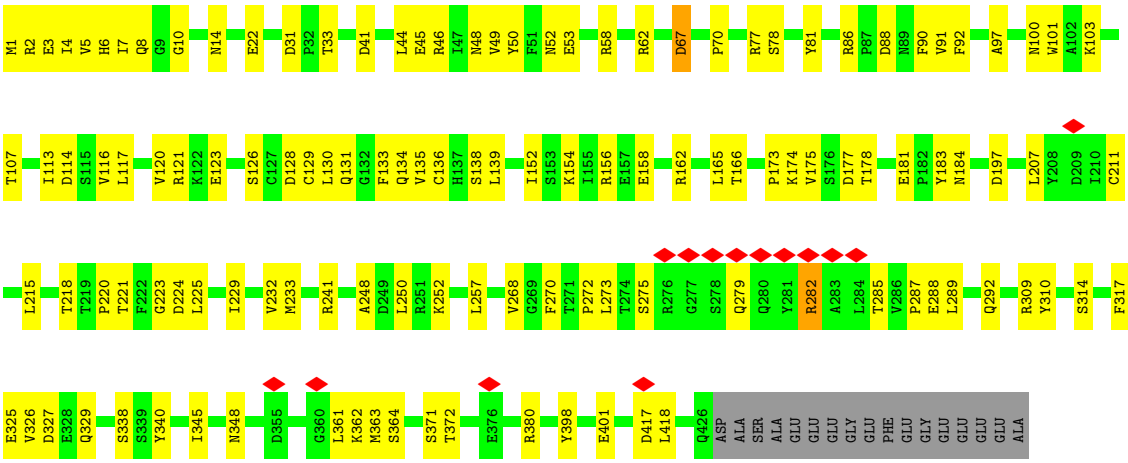
Chain V0:





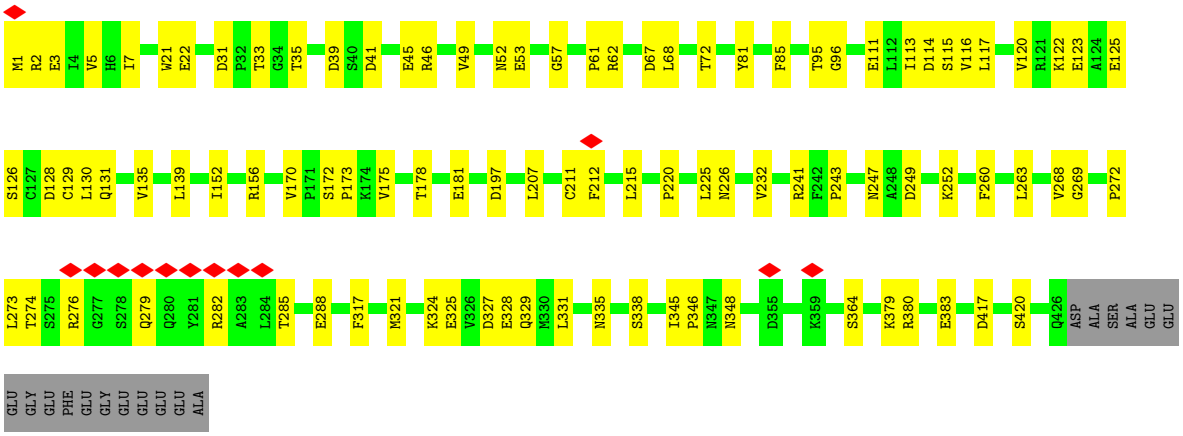

- Molecule 1: Tubulin beta

Chain V2:



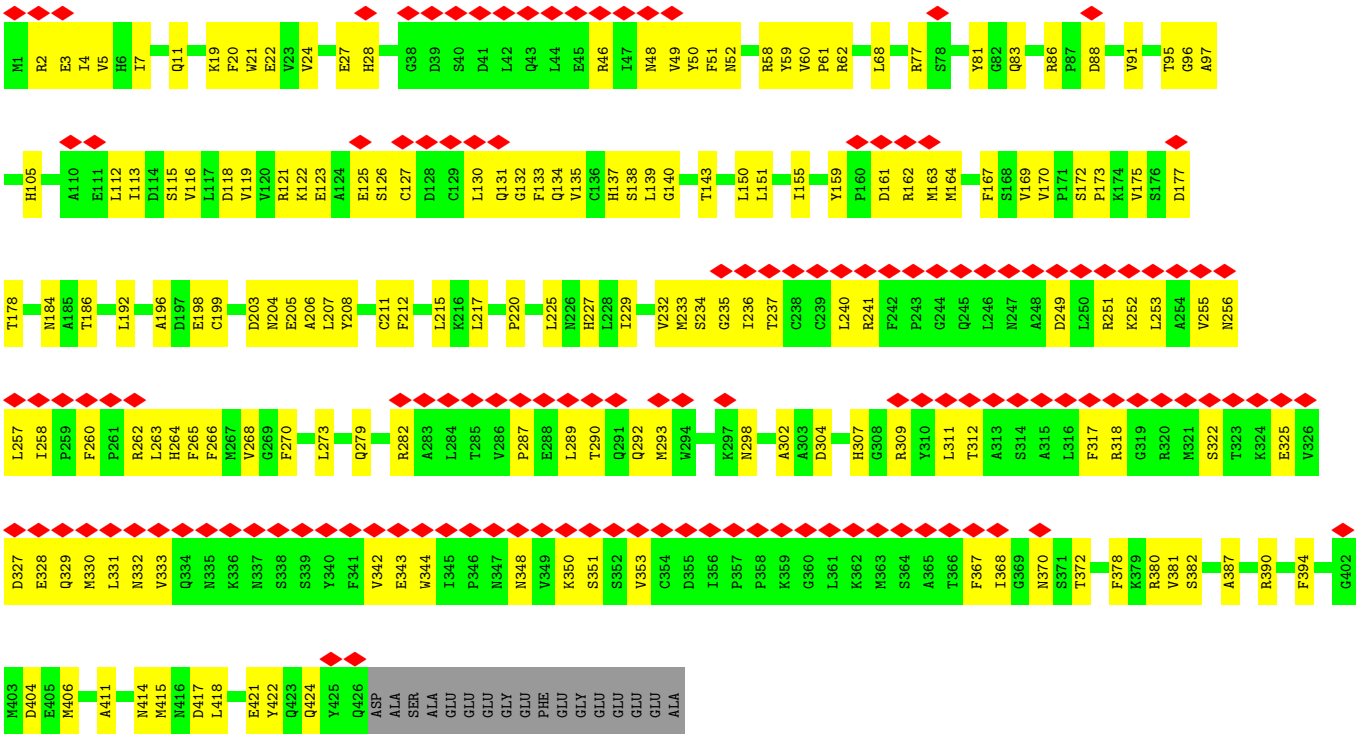

- Molecule 1: Tubulin beta

Chain V4:



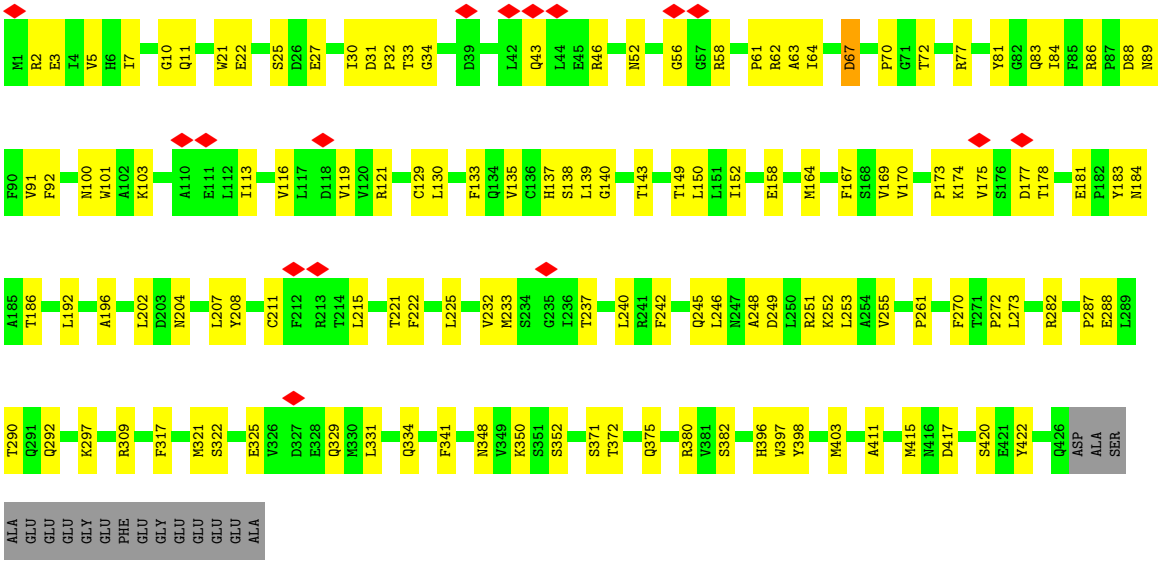

- Molecule 1: Tubulin beta

Chain V6:



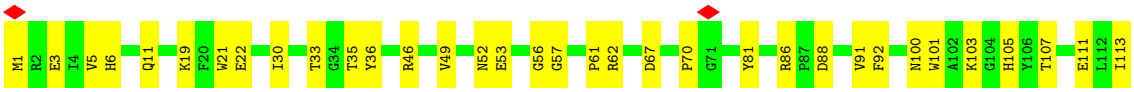

- Molecule 1: Tubulin beta

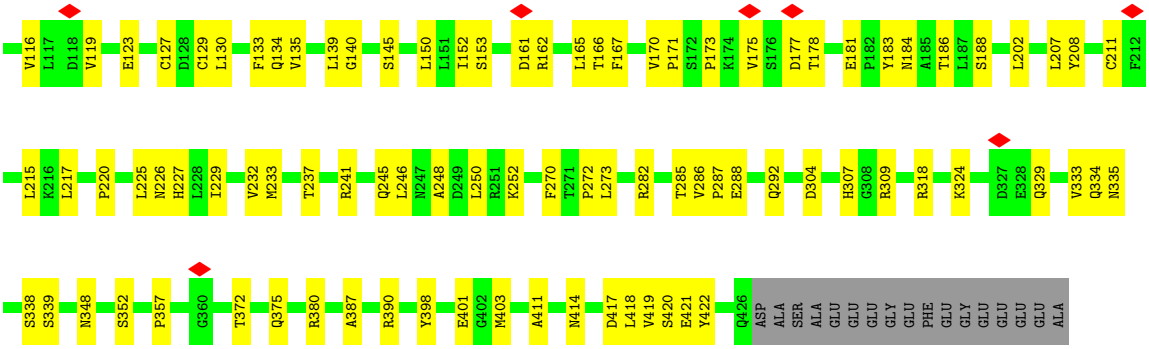
Chain V8:




- Molecule 1: Tubulin beta

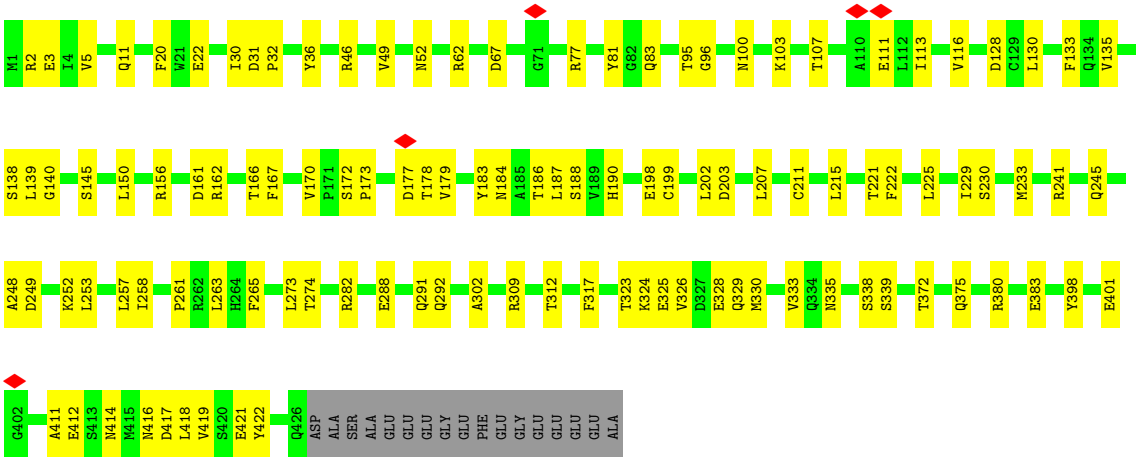
Chain W0:





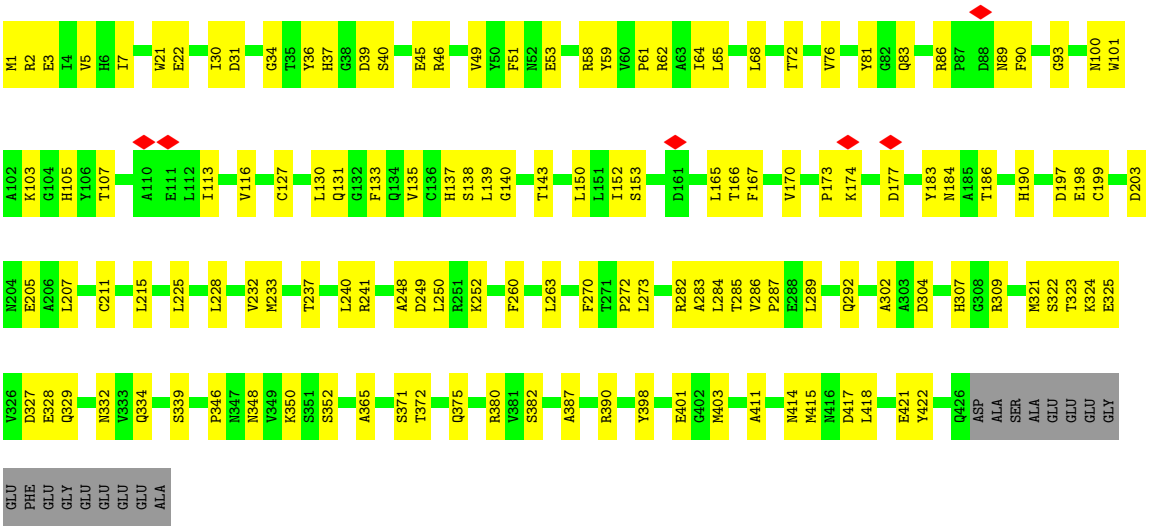

- Molecule 1: Tubulin beta

Chain W2:



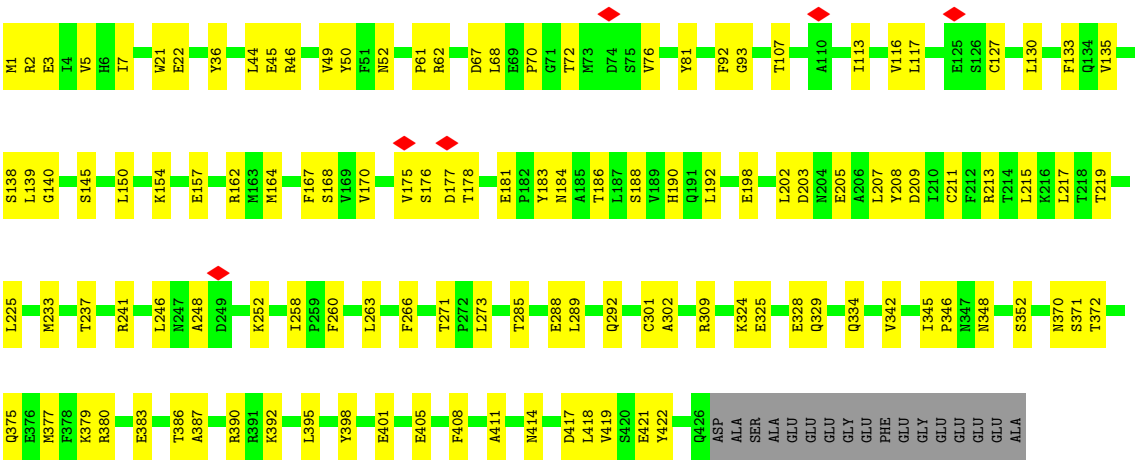

- Molecule 1: Tubulin beta

Chain W4:



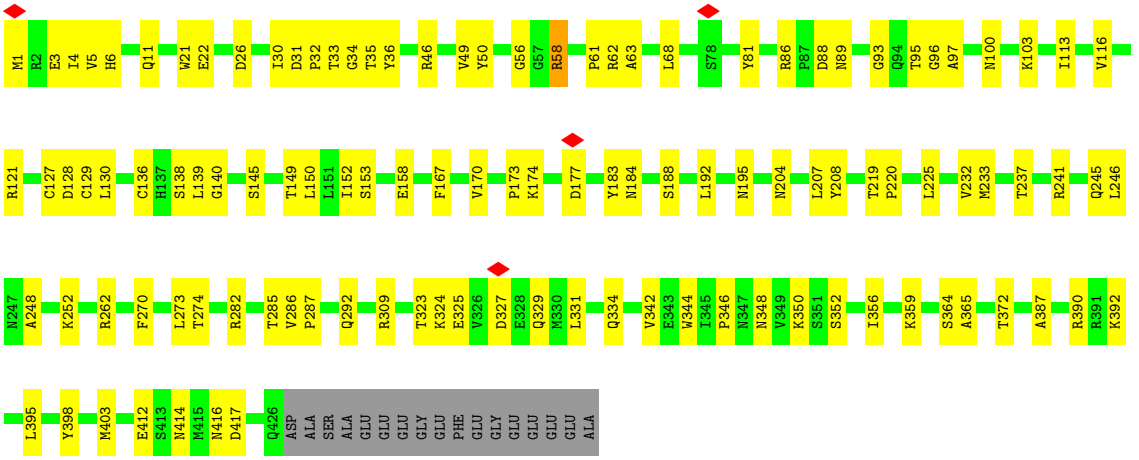

- Molecule 1: Tubulin beta

Chain W6:



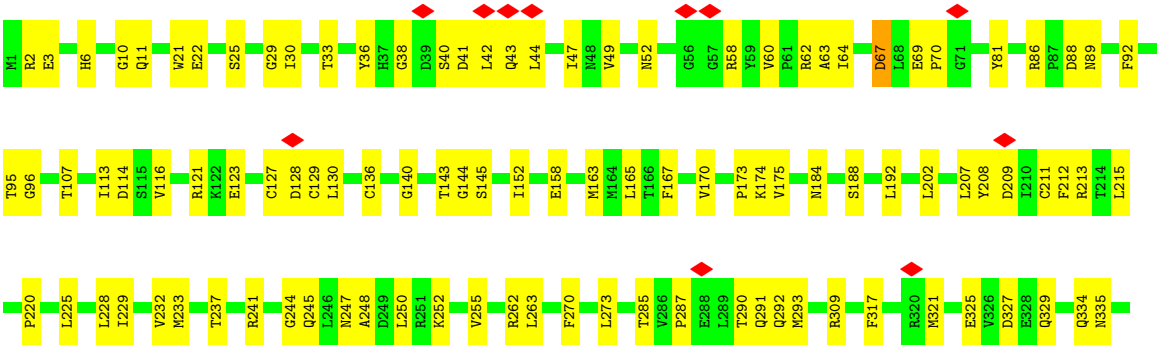

- Molecule 1: Tubulin beta

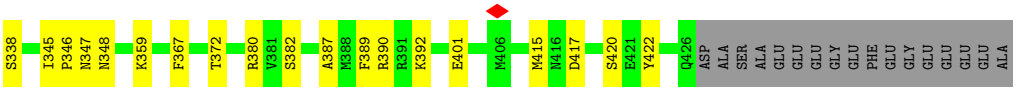
Chain W8:




- Molecule 1: Tubulin beta

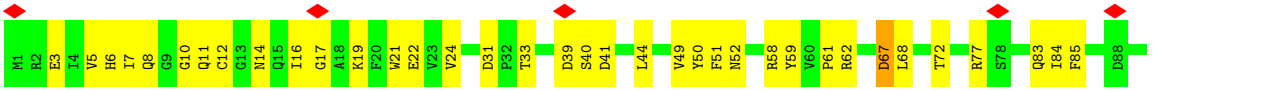
Chain X0:

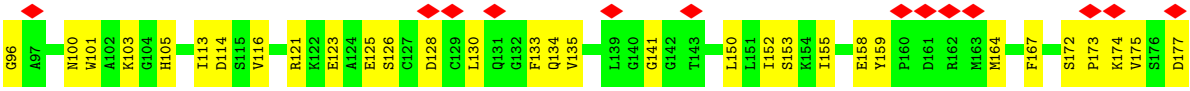


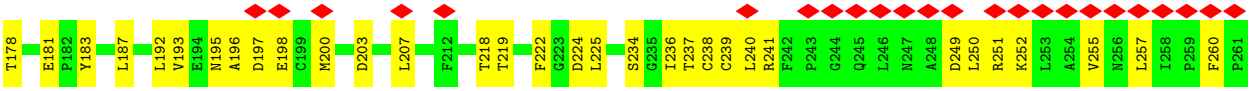


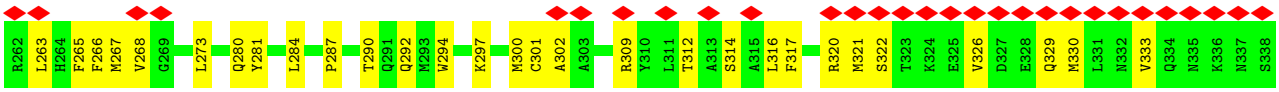

• Molecule 1: Tubulin beta

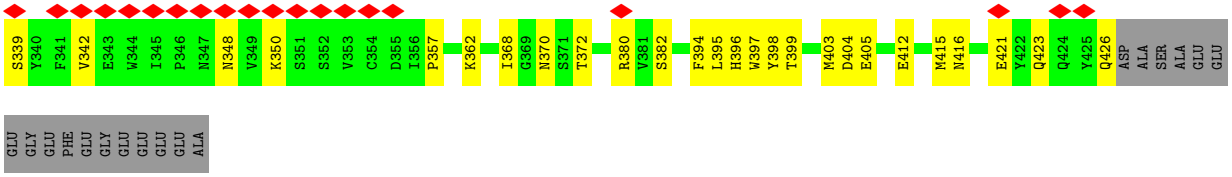
Chain X2:



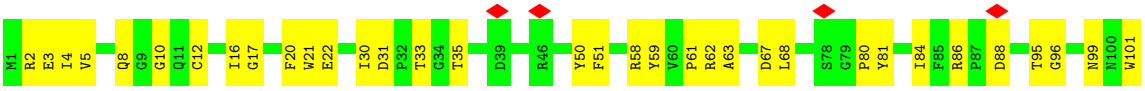



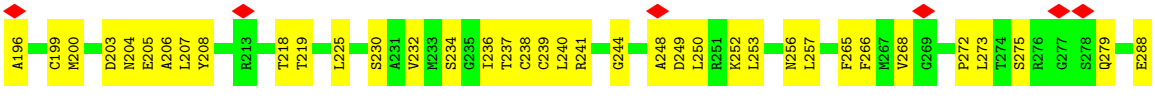



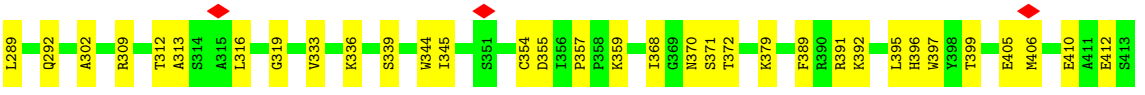



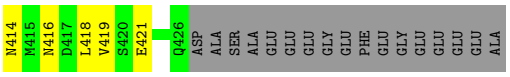

• Molecule 1: Tubulin beta

Chain X4:



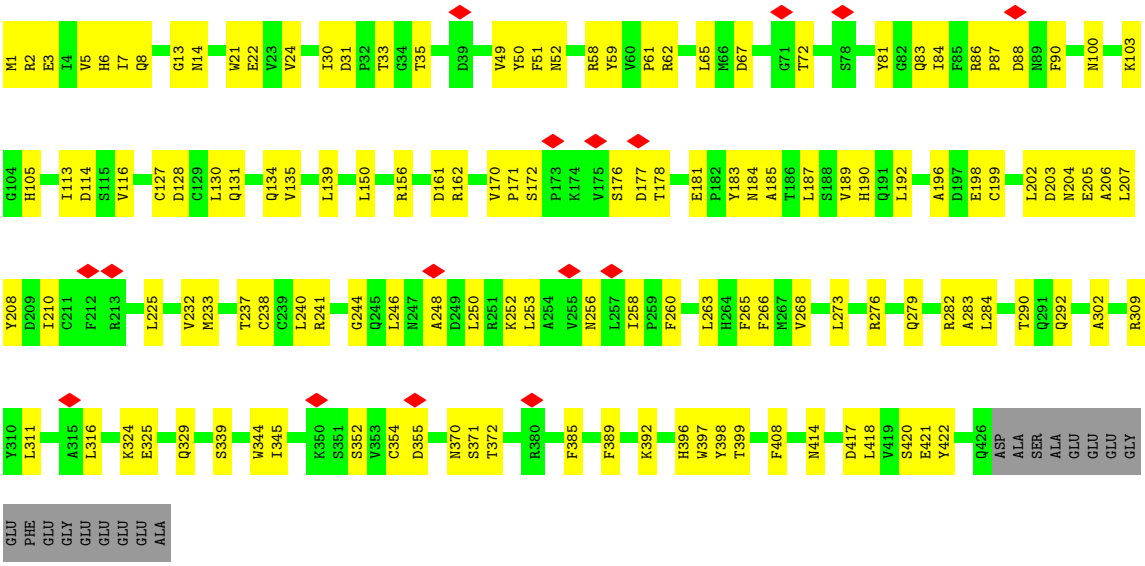


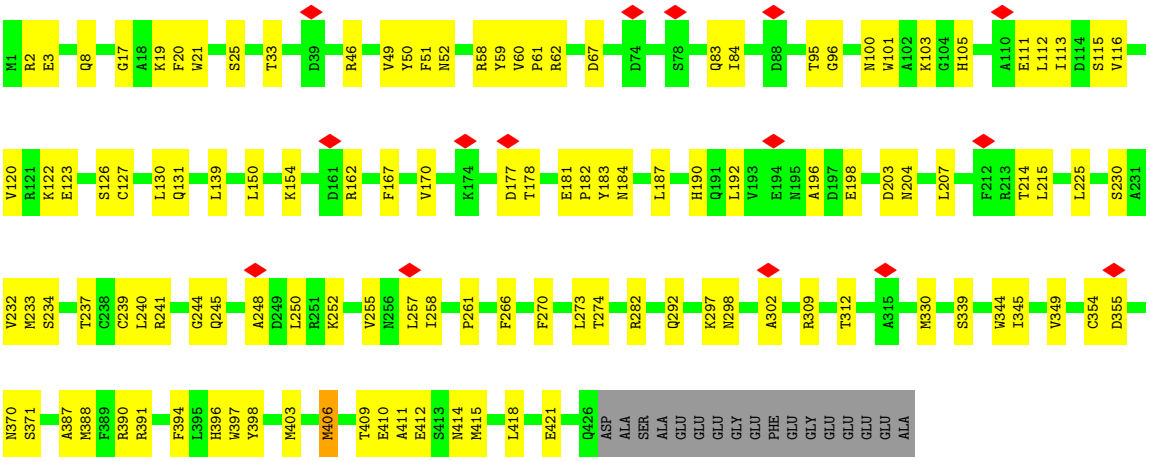

• Molecule 1: Tubulin beta

Chain X6:



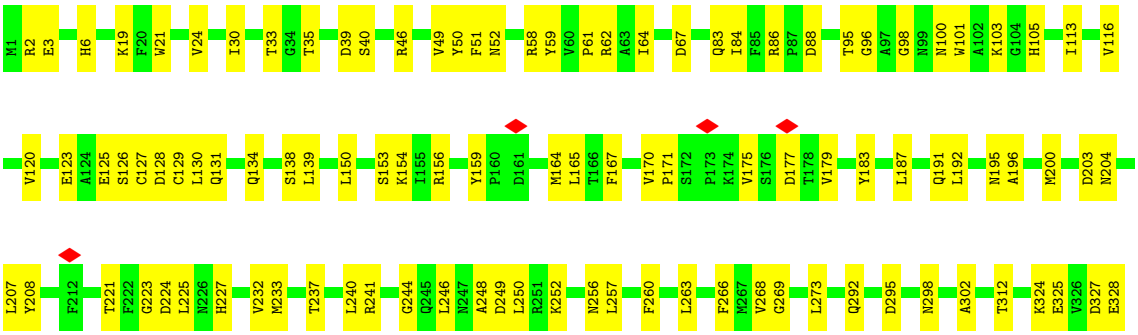

• Molecule 1: Tubulin beta

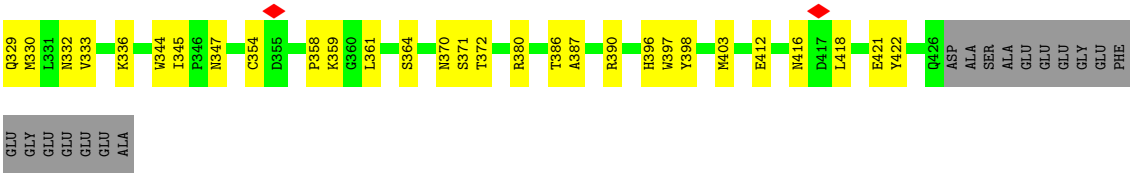
Chain X8:




• Molecule 1: Tubulin beta

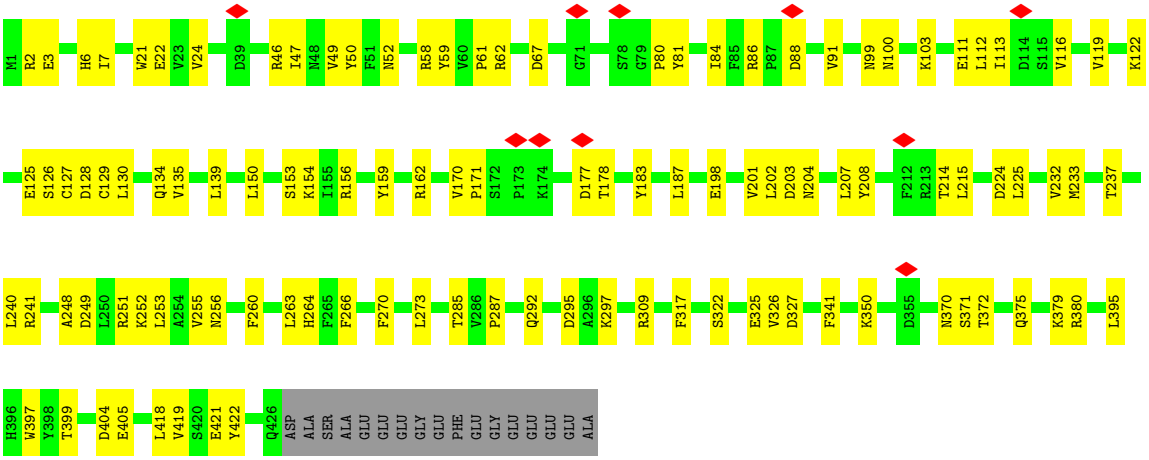
Chain Y0:





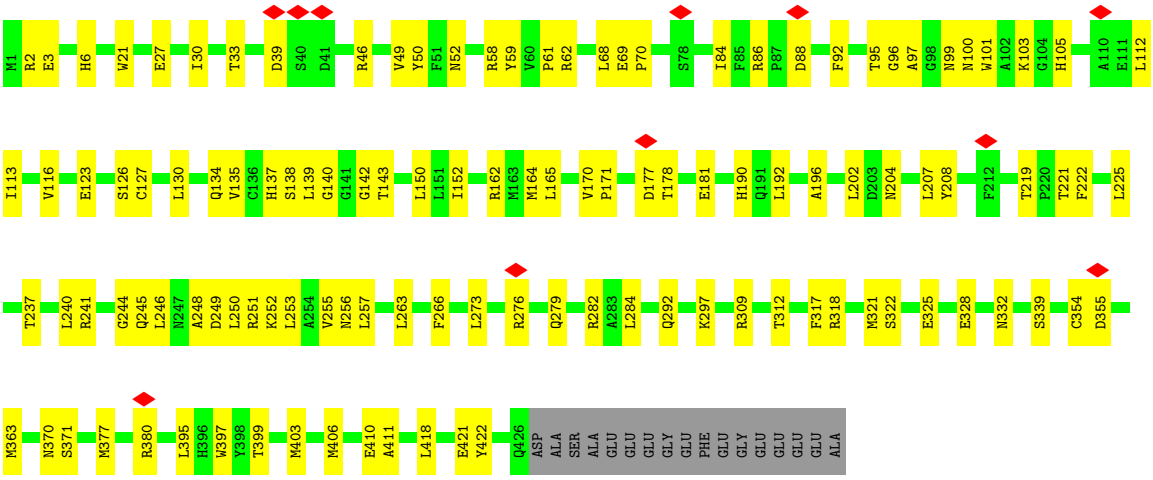

- Molecule 1: Tubulin beta

Chain Y2:



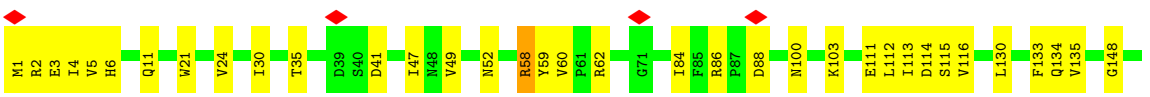

- Molecule 1: Tubulin beta

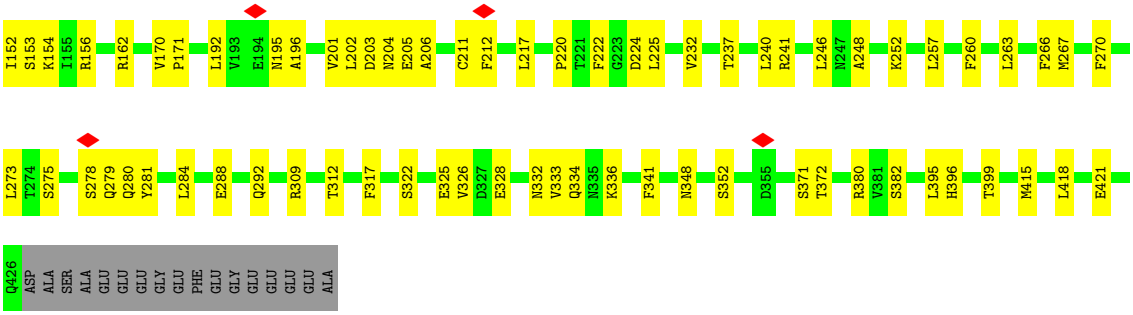
Chain Y4:




- Molecule 1: Tubulin beta

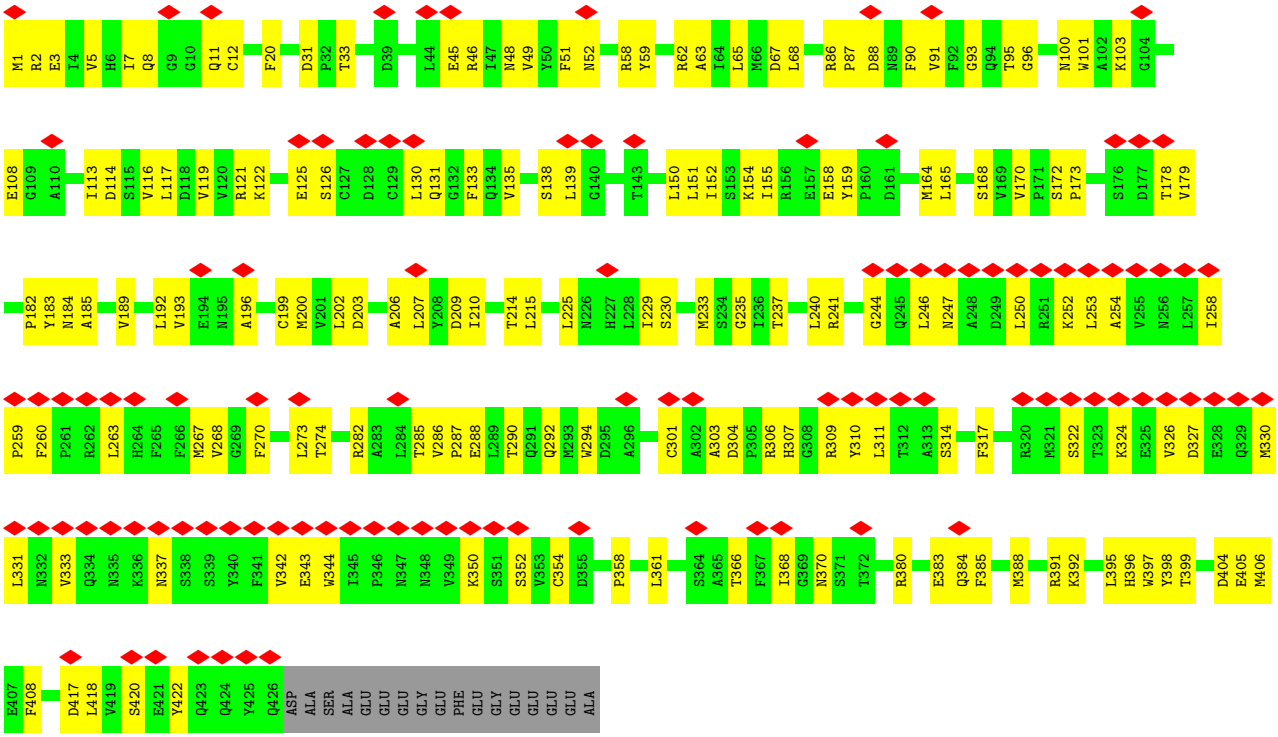
Chain Y6:





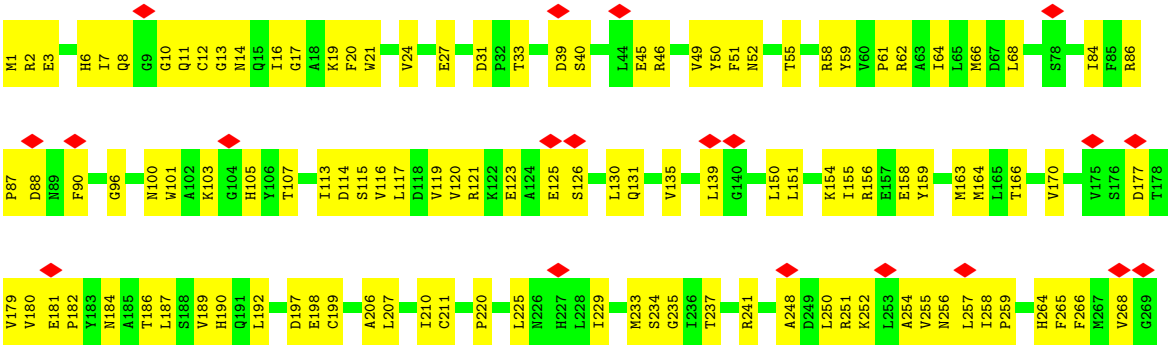

- Molecule 1: Tubulin beta

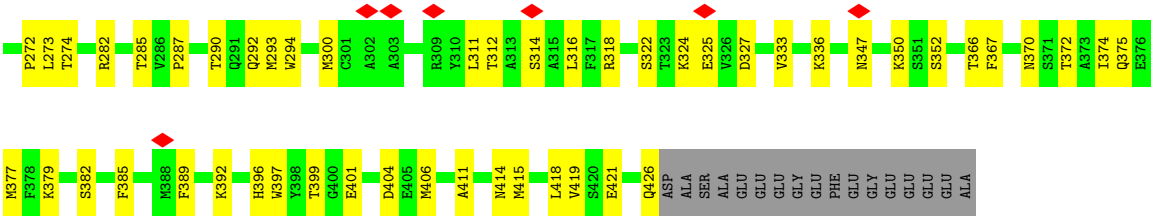
Chain Y8:




- Molecule 1: Tubulin beta

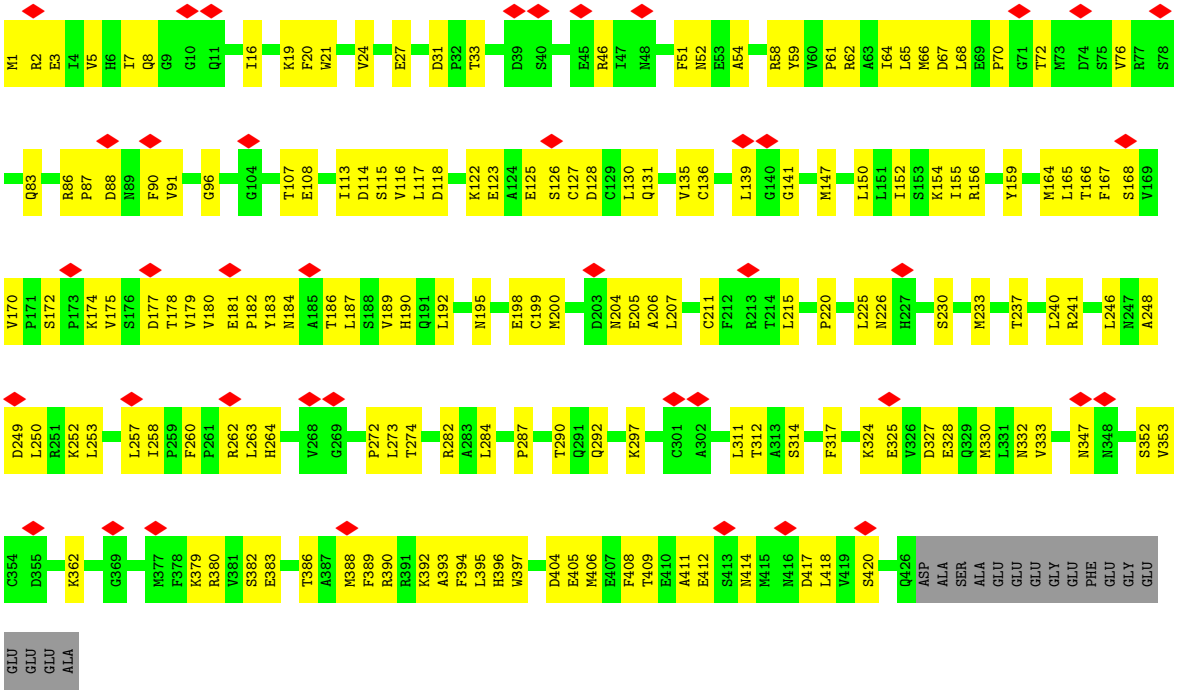
Chain Z0:





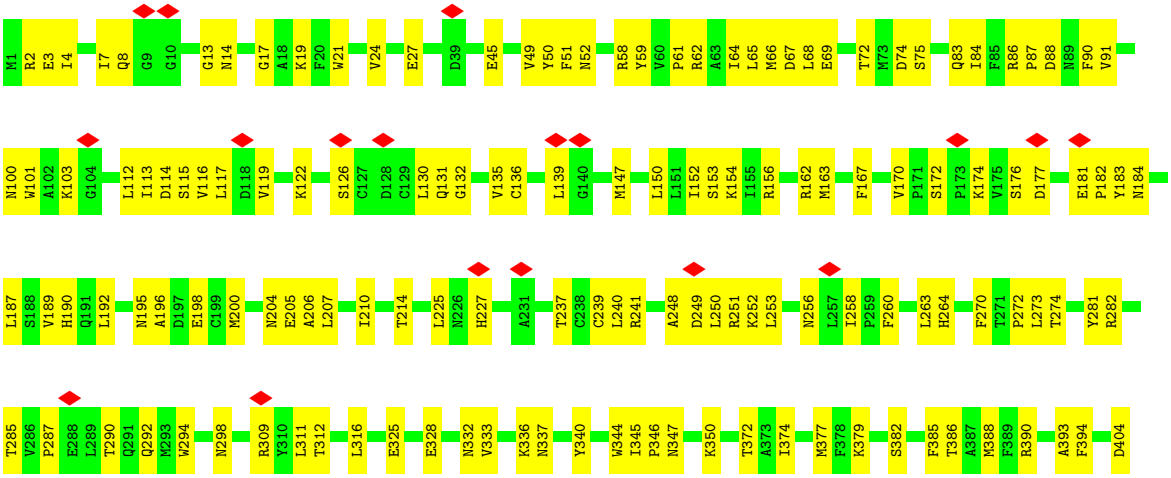

• Molecule 1: Tubulin beta

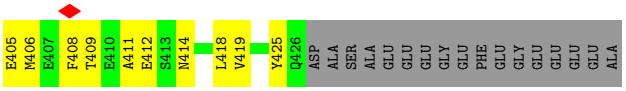
Chain Z2:




• Molecule 1: Tubulin beta

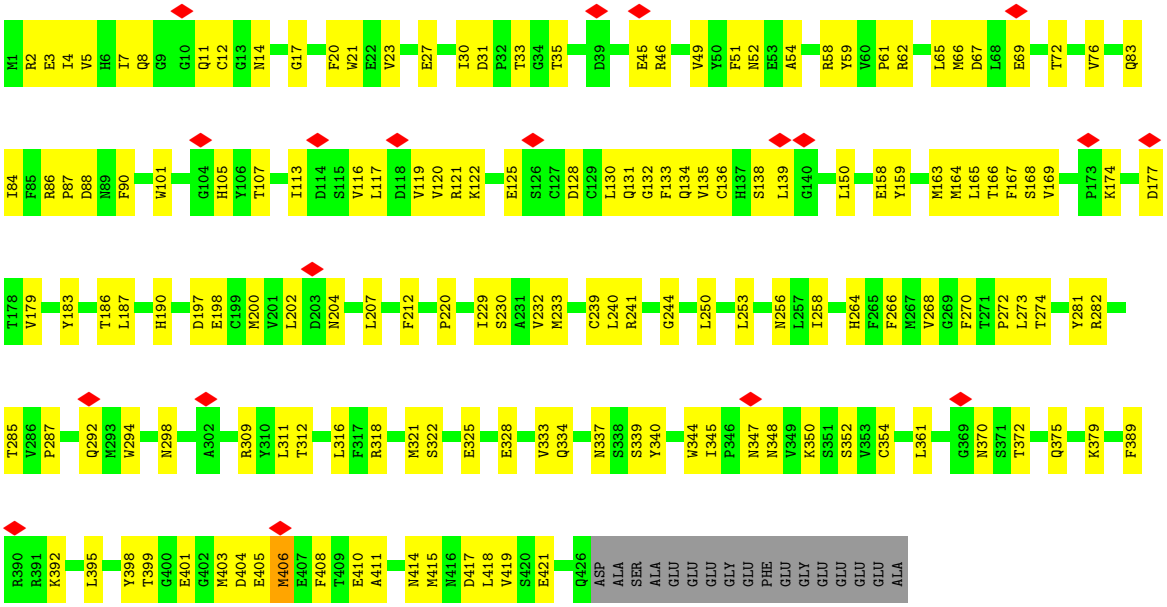
Chain Z4:





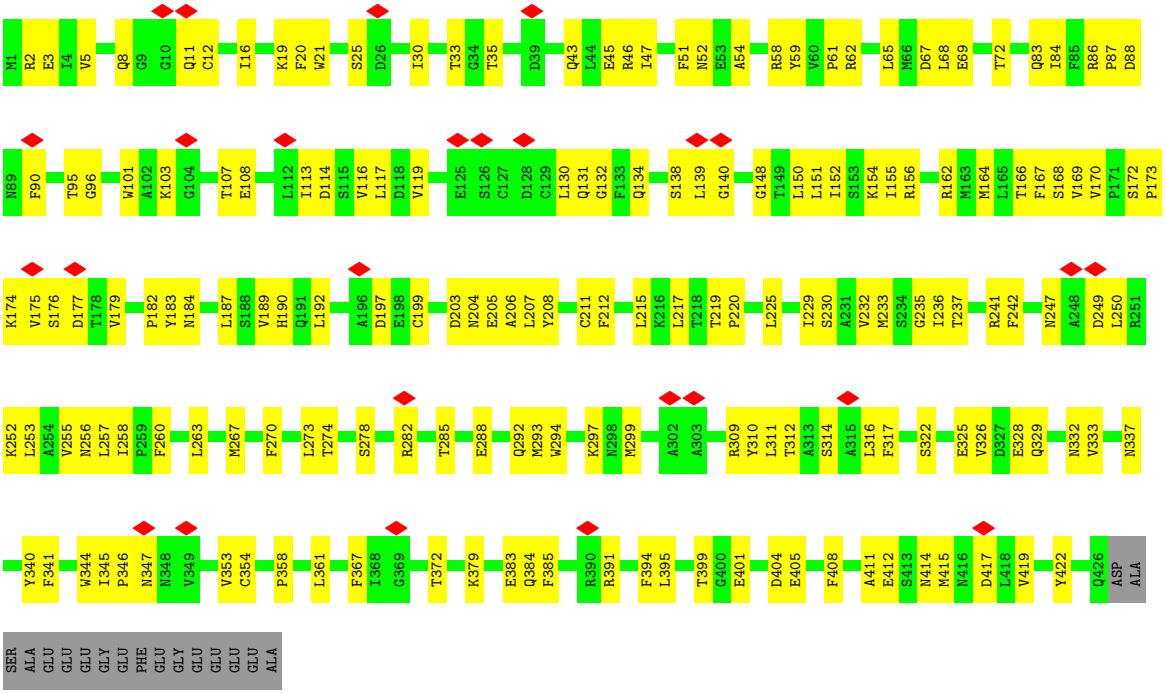

• Molecule 1: Tubulin beta

Chain Z6:



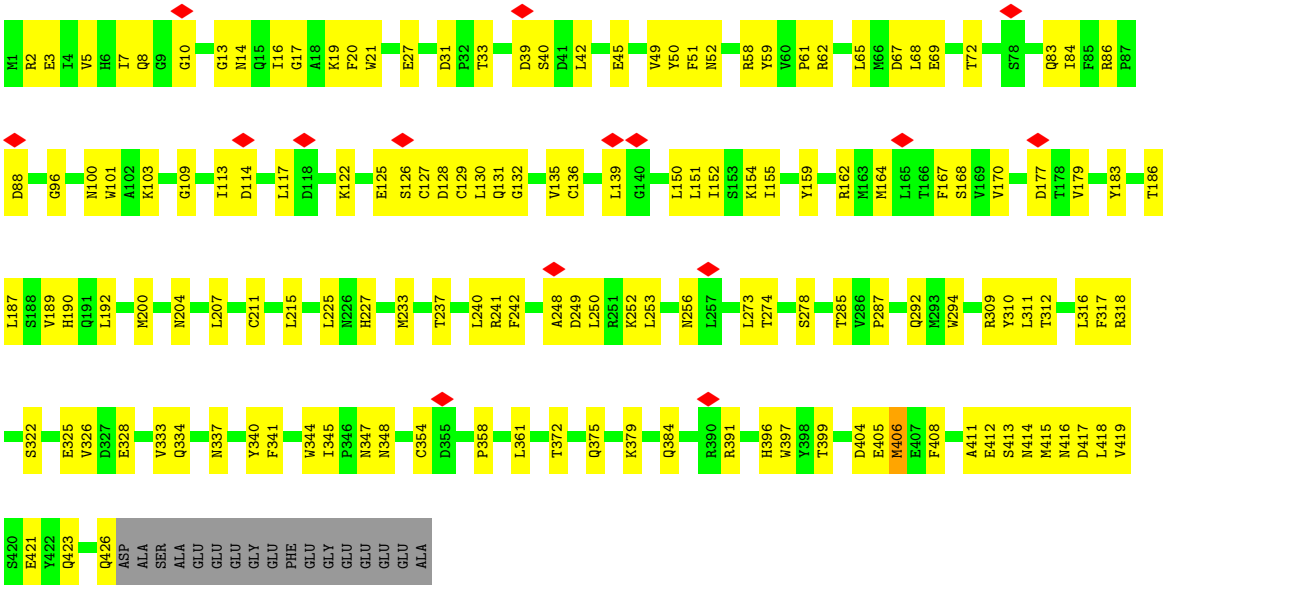

• Molecule 1: Tubulin beta

Chain Z8:



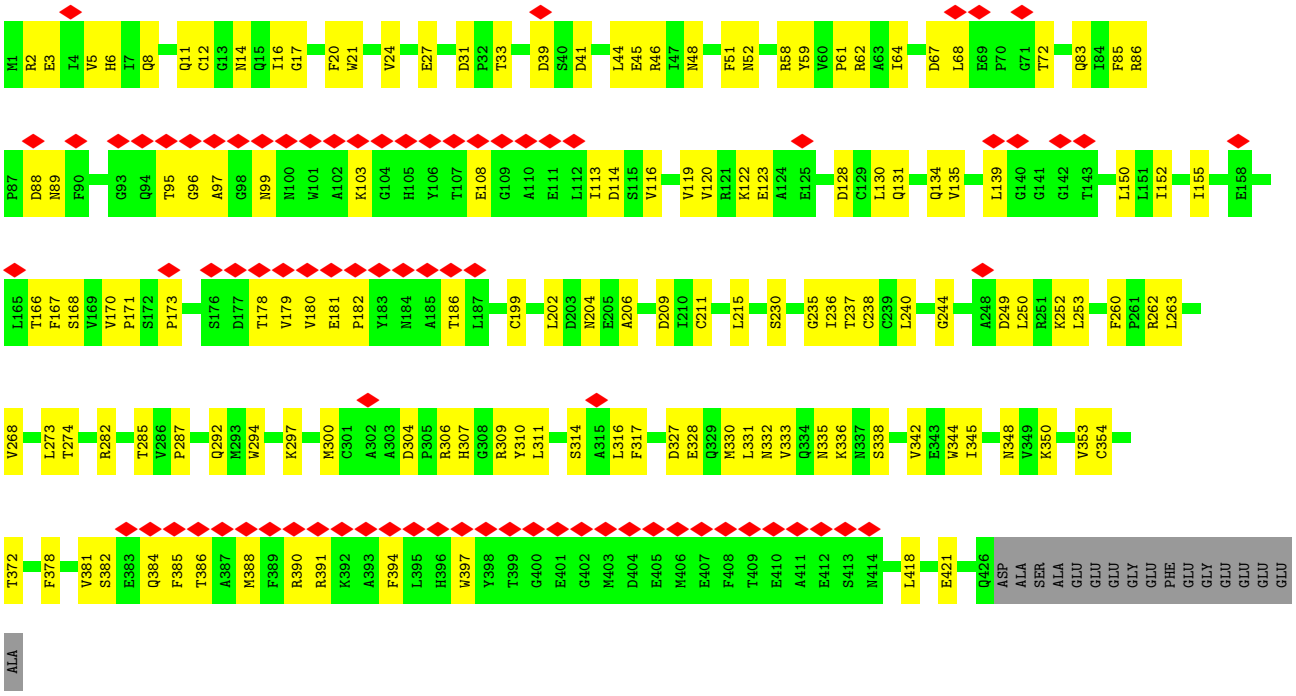
- Molecule 1: Tubulin beta

Chain 0A:



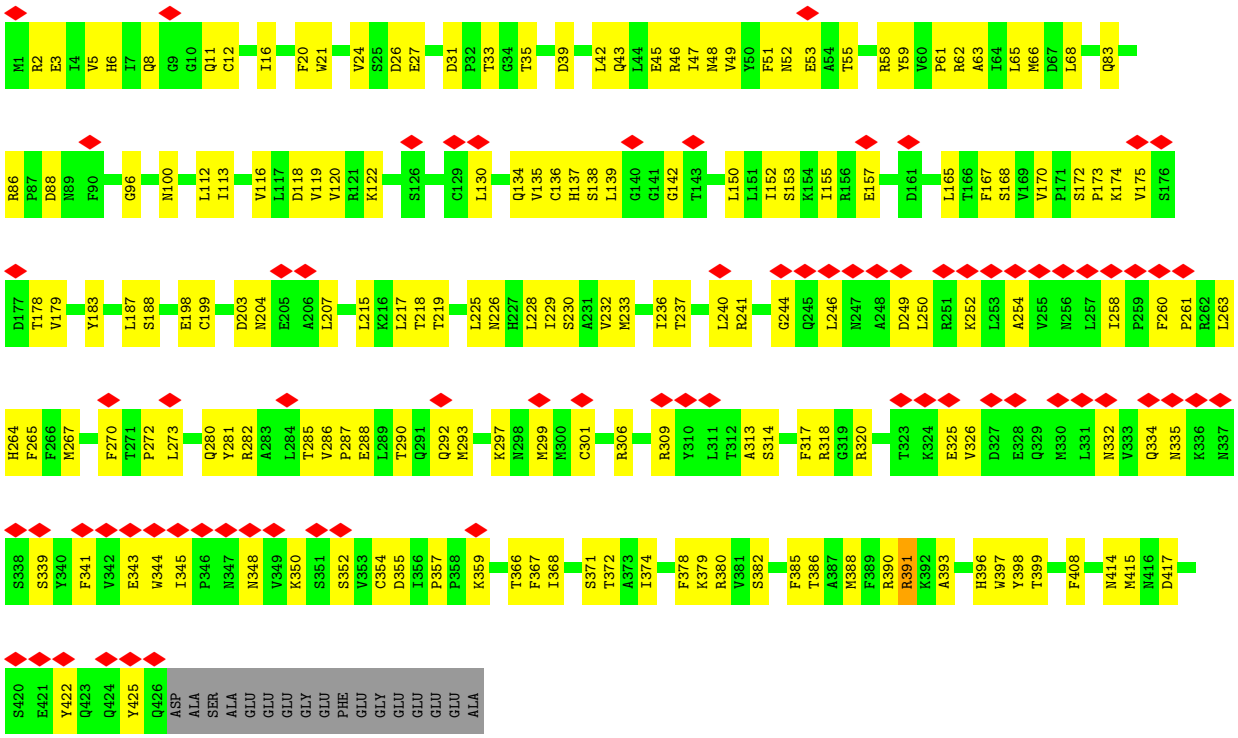

- Molecule 1: Tubulin beta

Chain 0C:



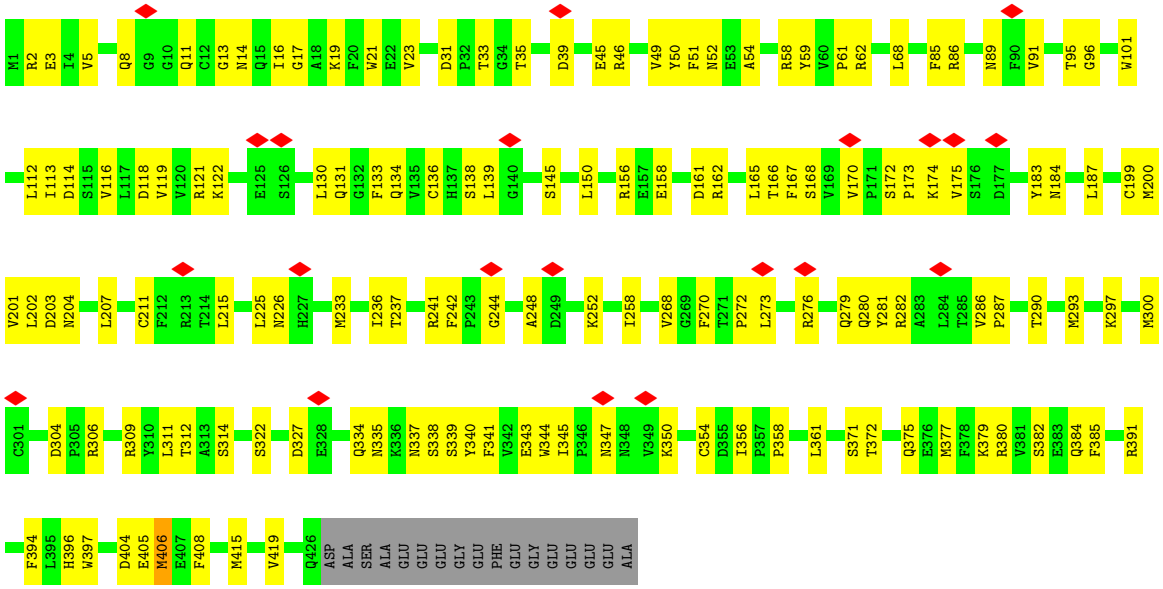

- Molecule 1: Tubulin beta

Chain 0E:



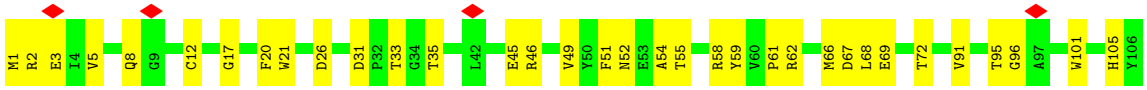

- Molecule 1: Tubulin beta

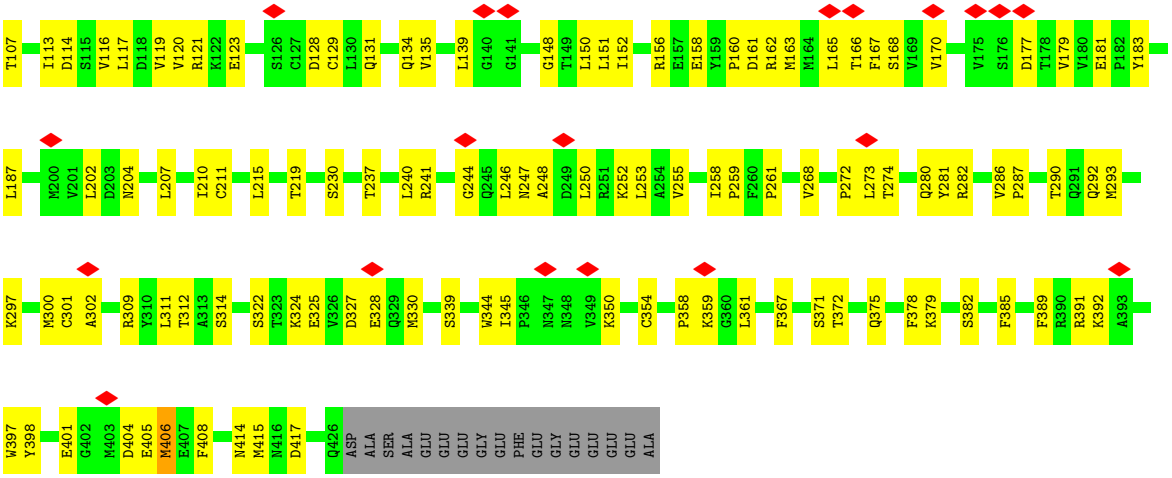
Chain 0G:




- Molecule 1: Tubulin beta

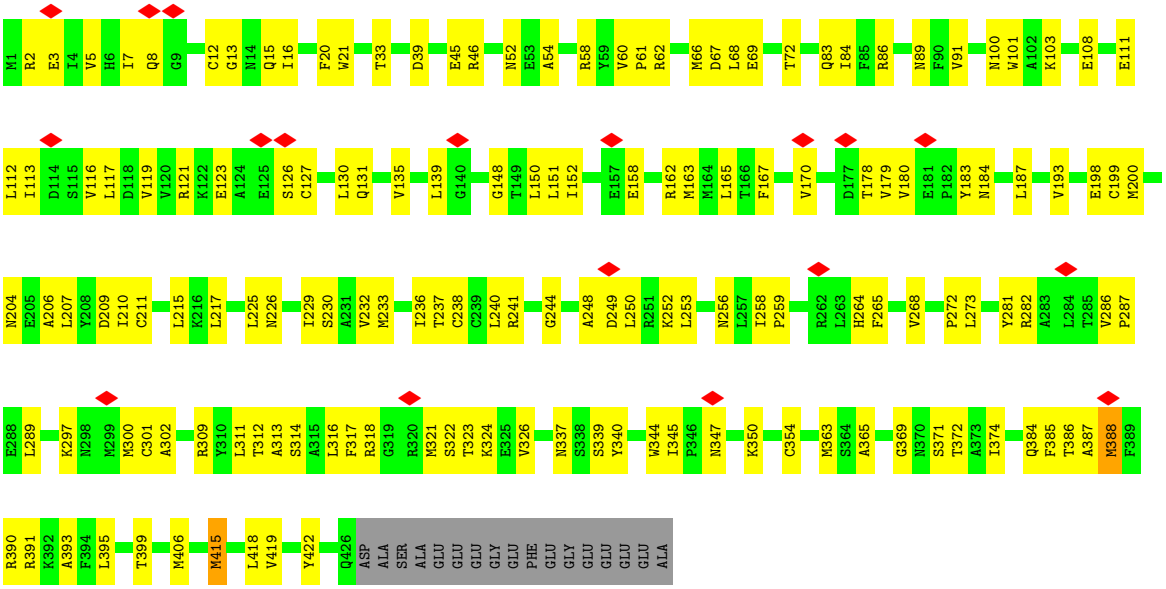
Chain 0I:





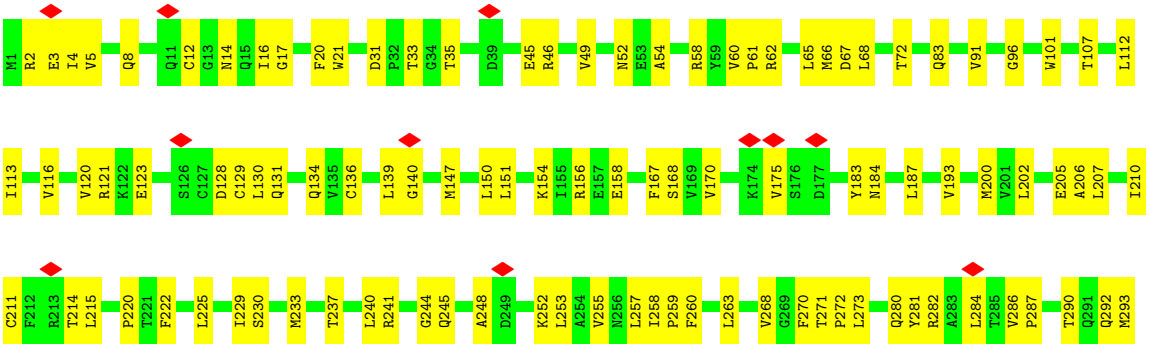

- Molecule 1: Tubulin beta

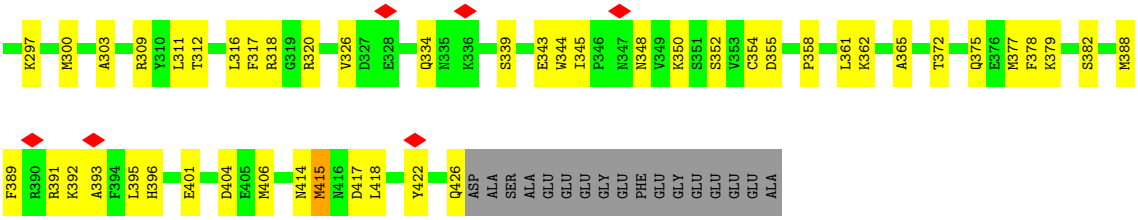
Chain 0K:




- Molecule 1: Tubulin beta

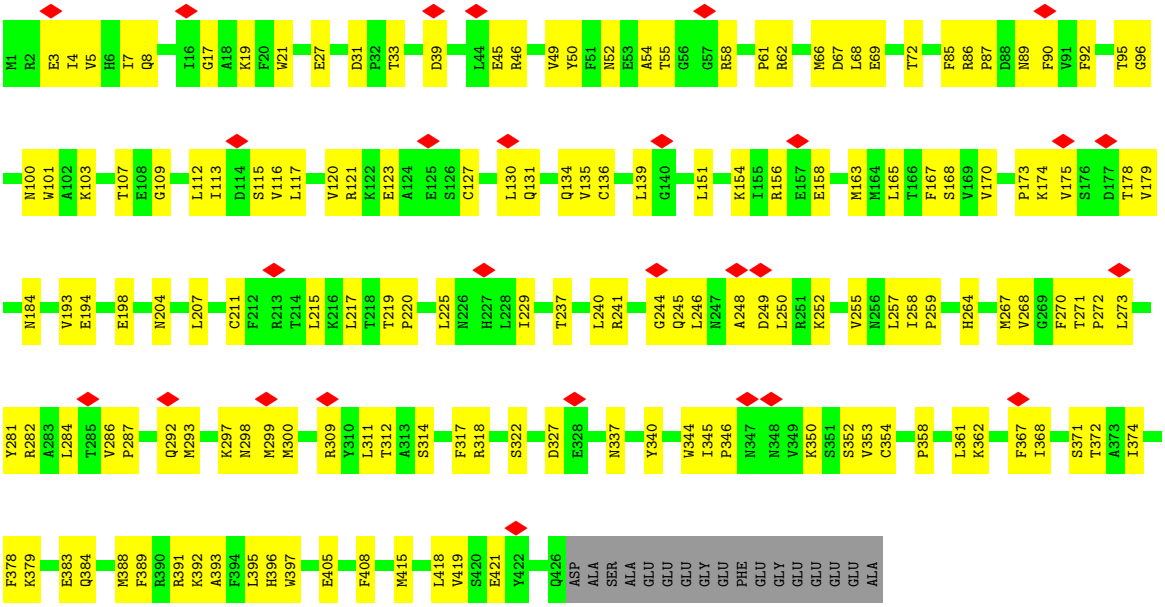
Chain 0M:





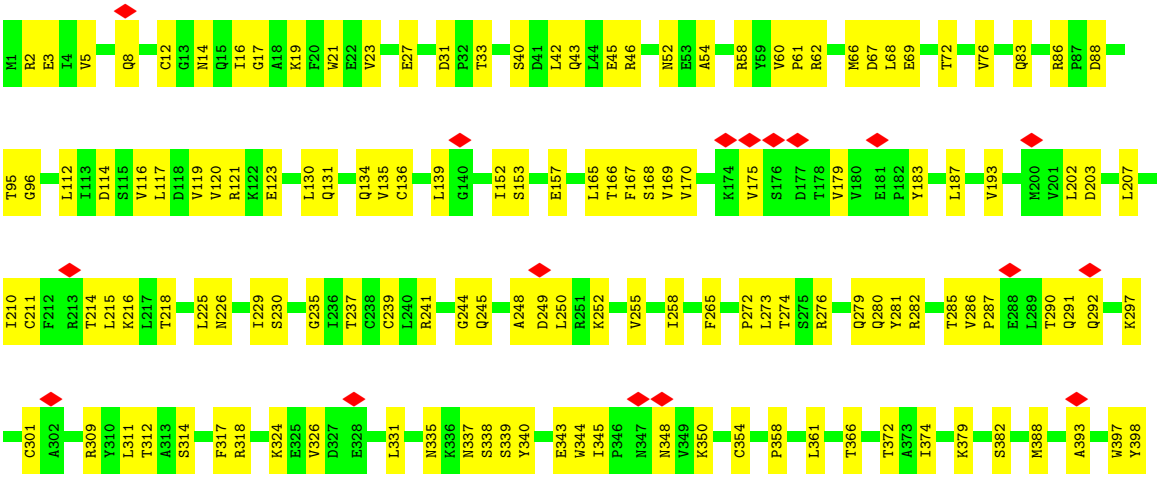

• Molecule 1: Tubulin beta

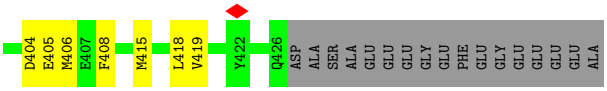
Chain 0O:




• Molecule 1: Tubulin beta

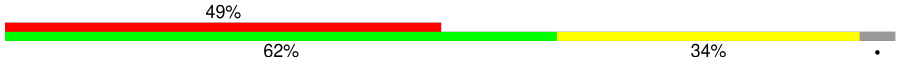
Chain 0Q:

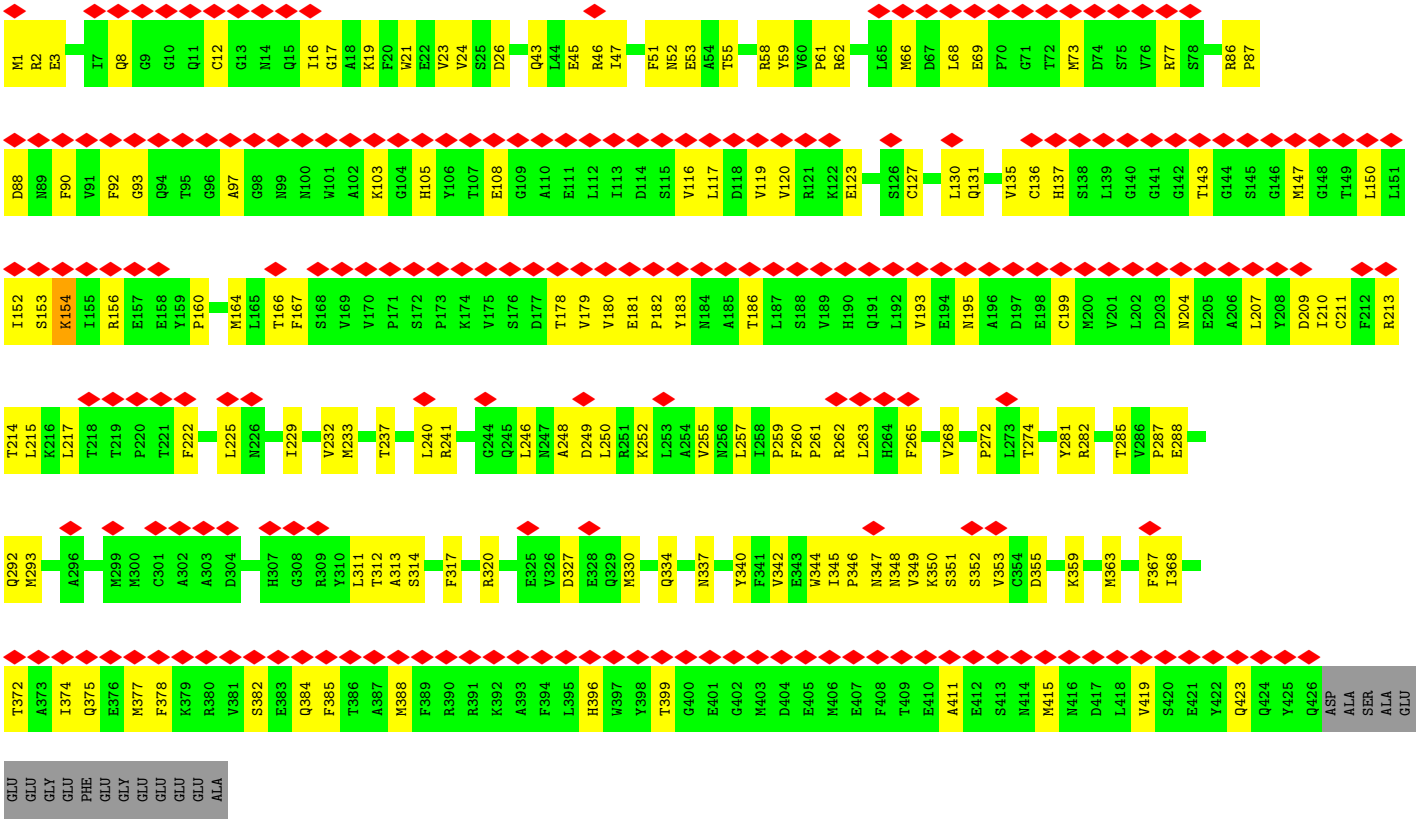





• Molecule 1: Tubulin beta

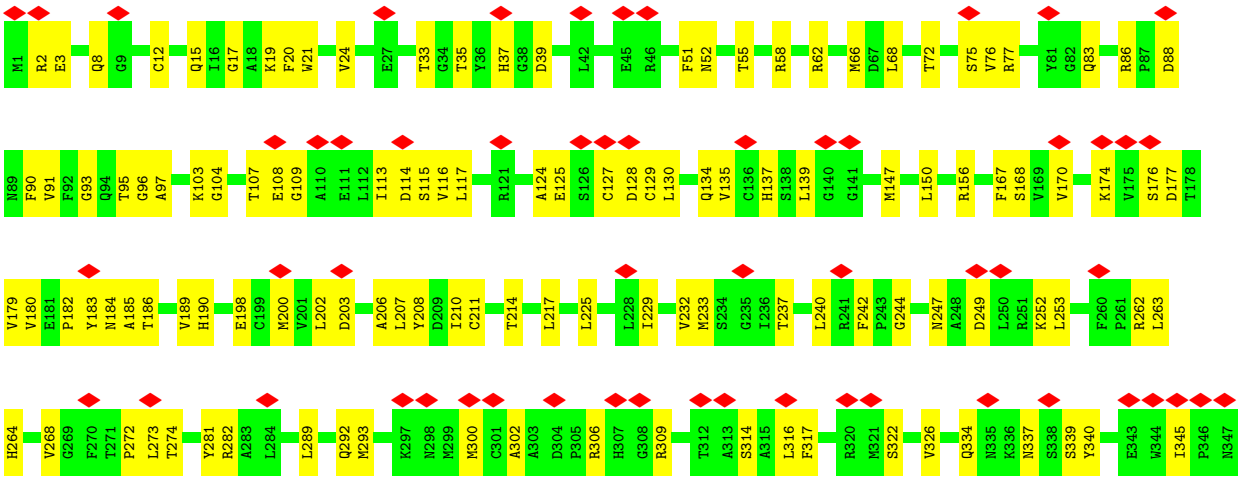
Chain 0S:

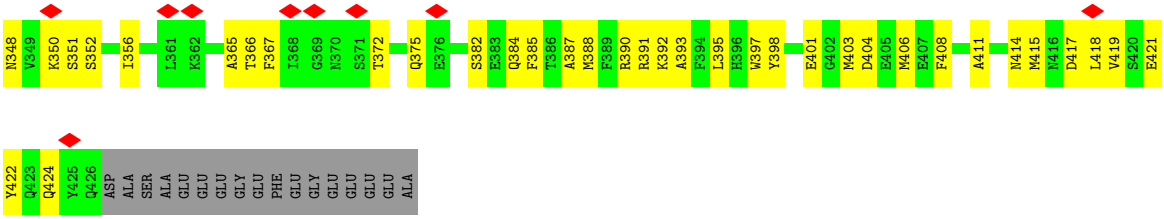



• Molecule 1: Tubulin beta

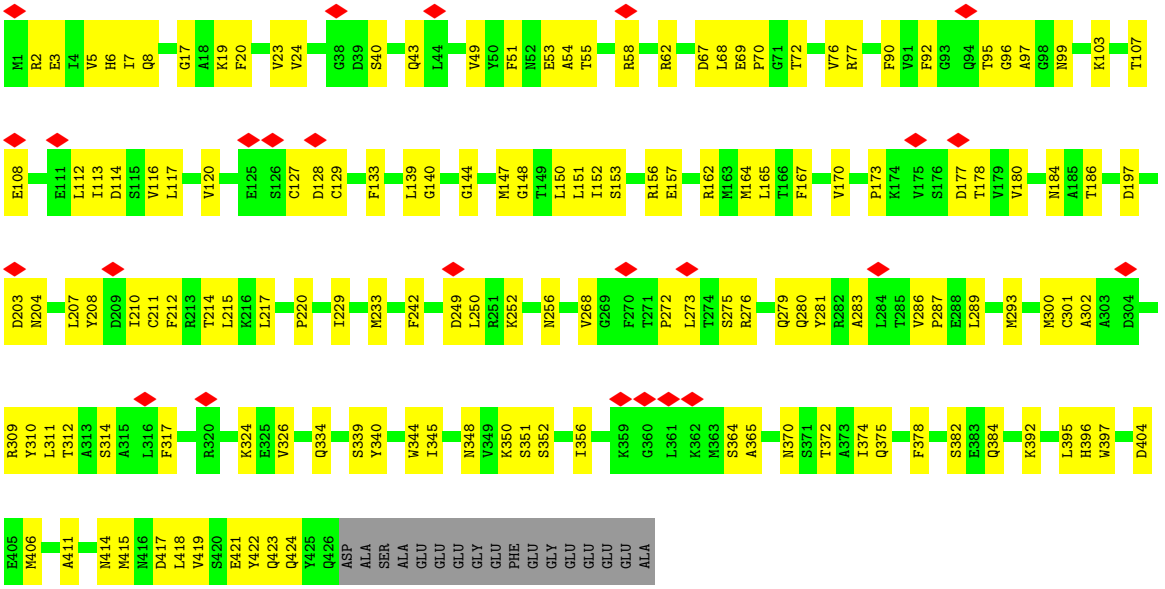
Chain 0U:





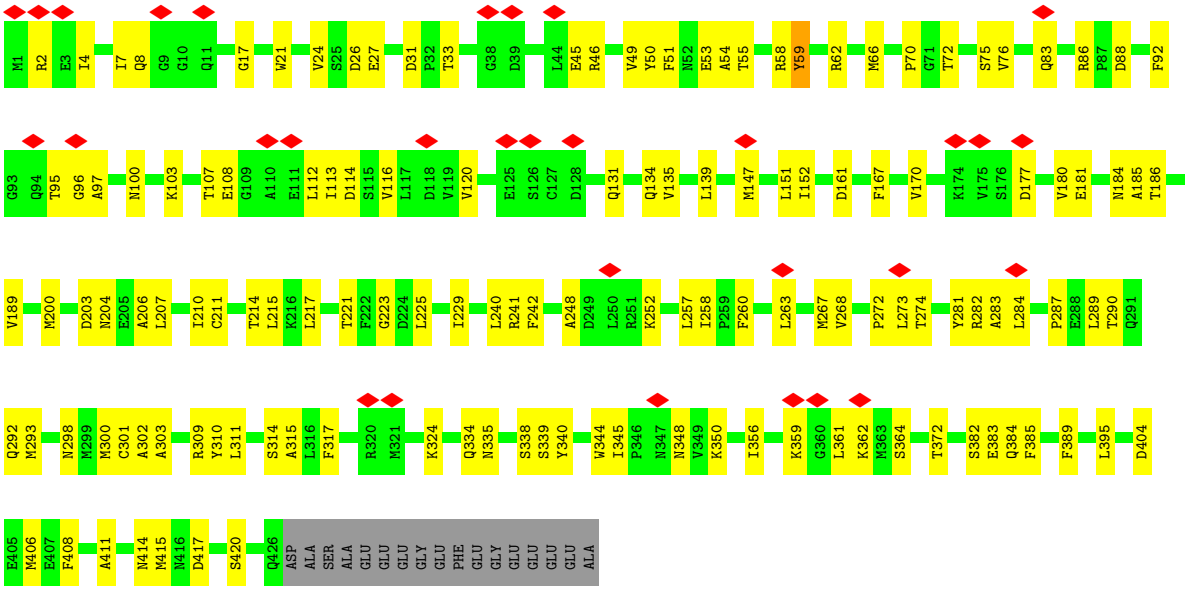

• Molecule 1: Tubulin beta

Chain 0W:



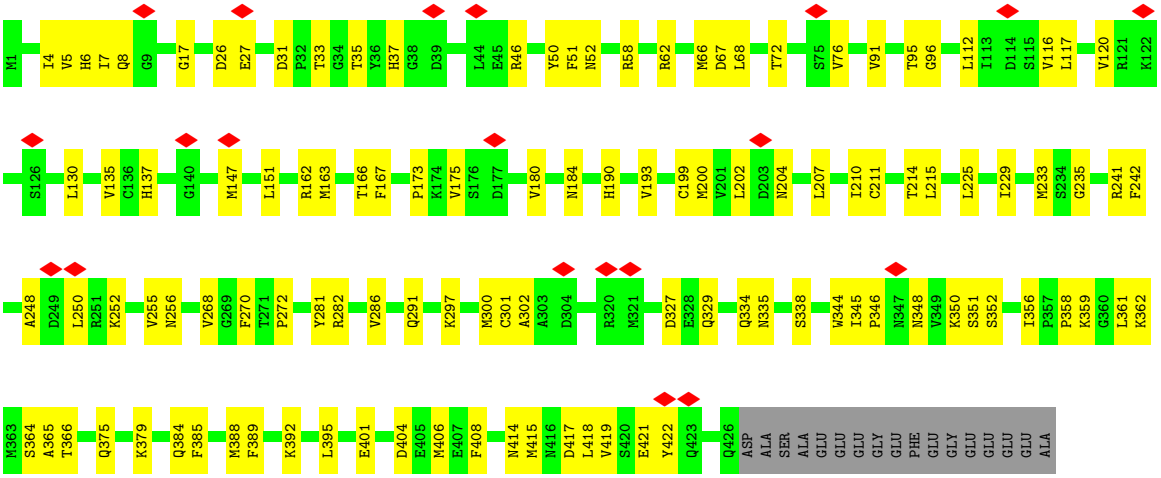

• Molecule 1: Tubulin beta

Chain 0Y:



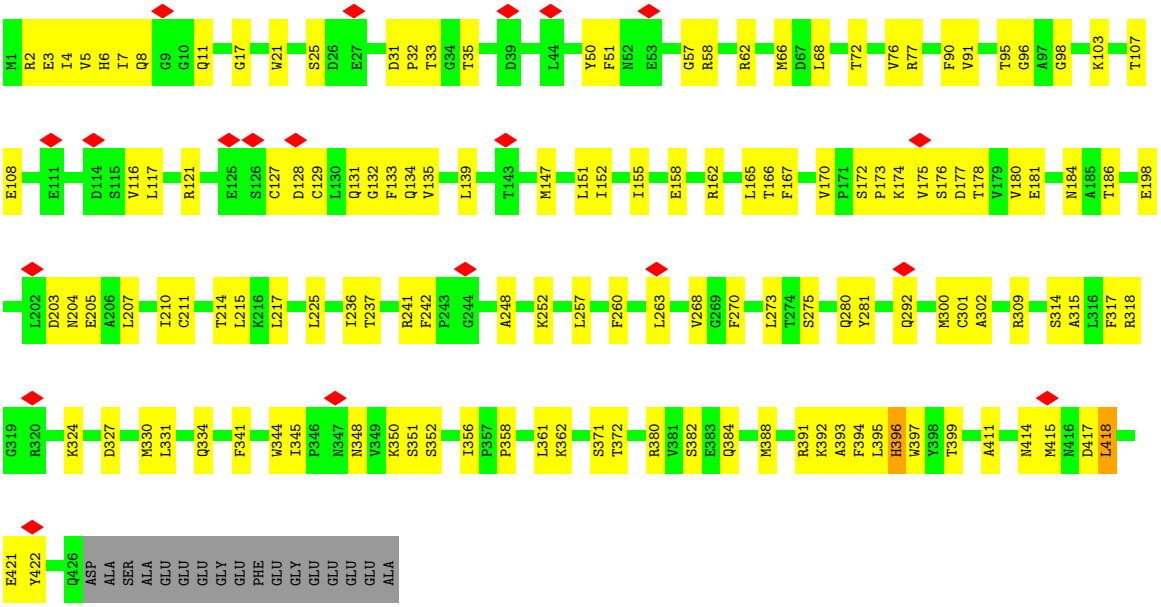
• Molecule 1: Tubulin beta

Chain 1A:



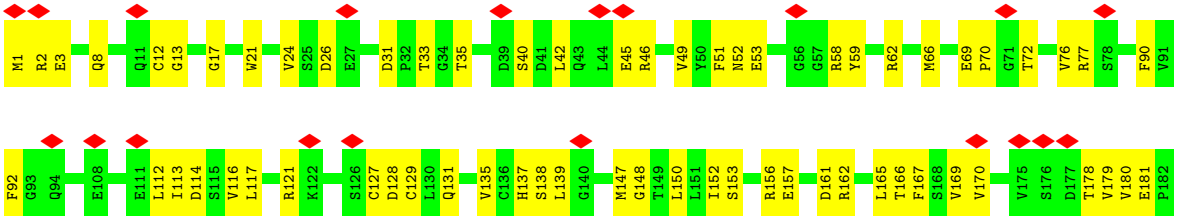

• Molecule 1: Tubulin beta

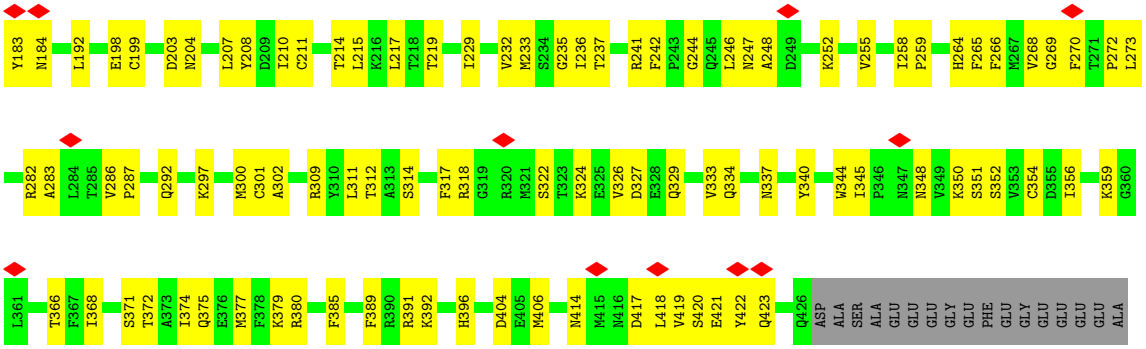
Chain 1C:




• Molecule 1: Tubulin beta

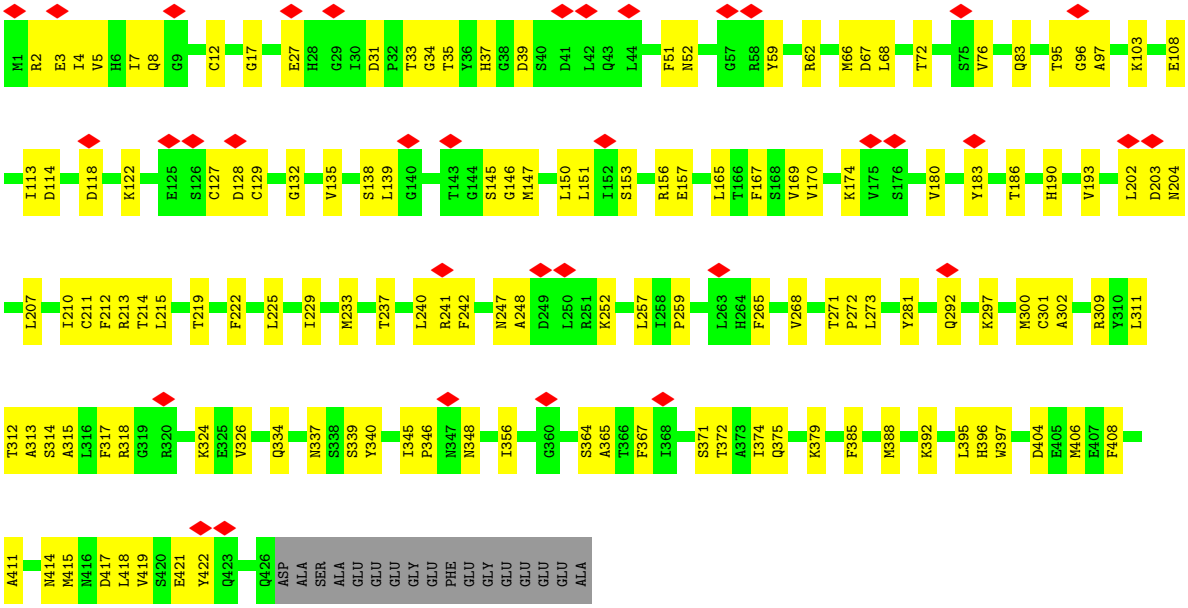
Chain 1E:





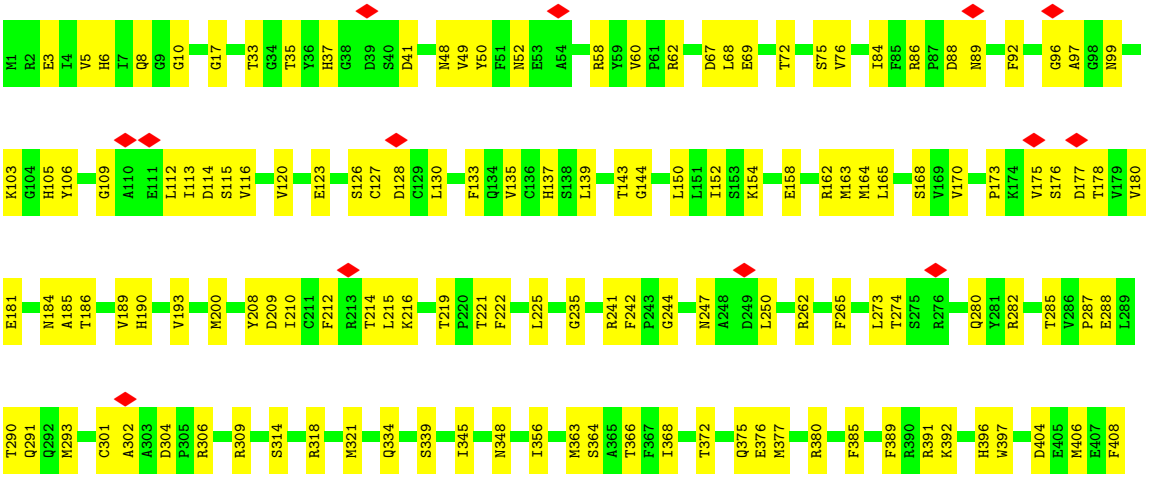

• Molecule 1: Tubulin beta

Chain 1G: 8% 65% 31%



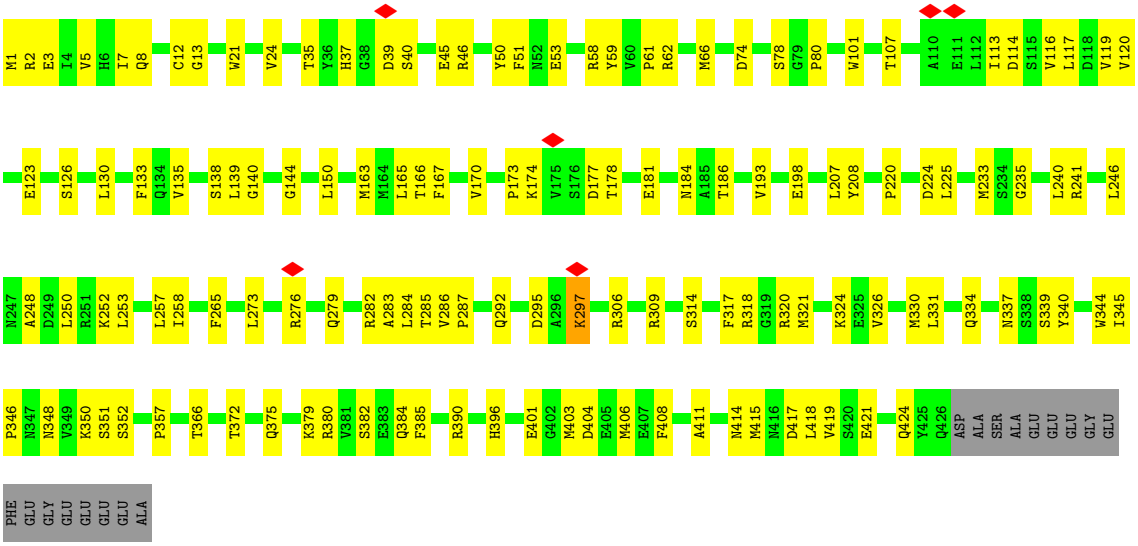

• Molecule 1: Tubulin beta

Chain 1K: 64% 32%



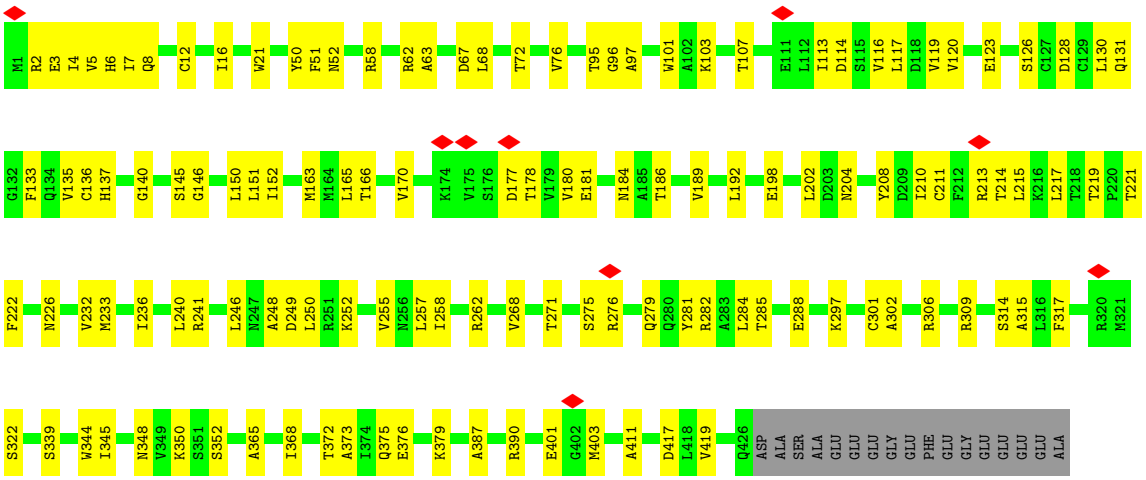
• Molecule 1: Tubulin beta

Chain 1M:



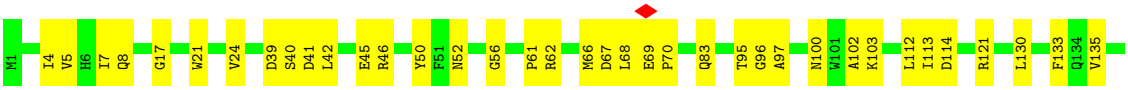

• Molecule 1: Tubulin beta

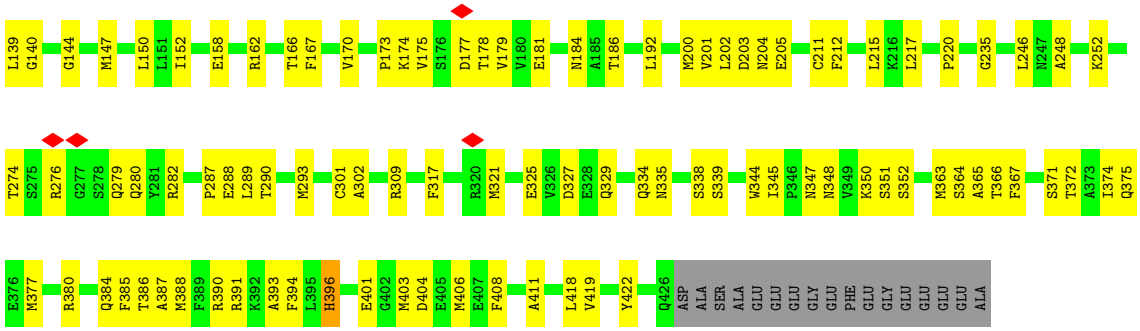
Chain 1O:




• Molecule 1: Tubulin beta

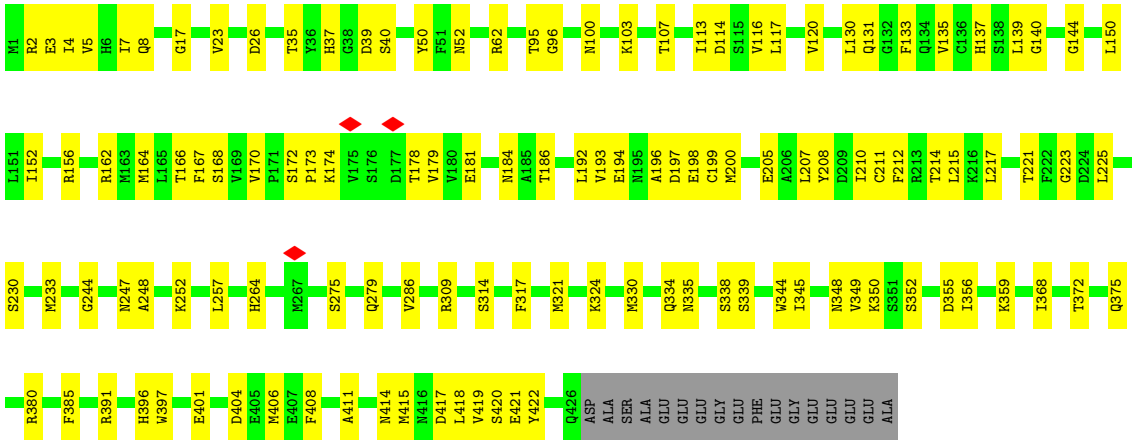
Chain 1Q:





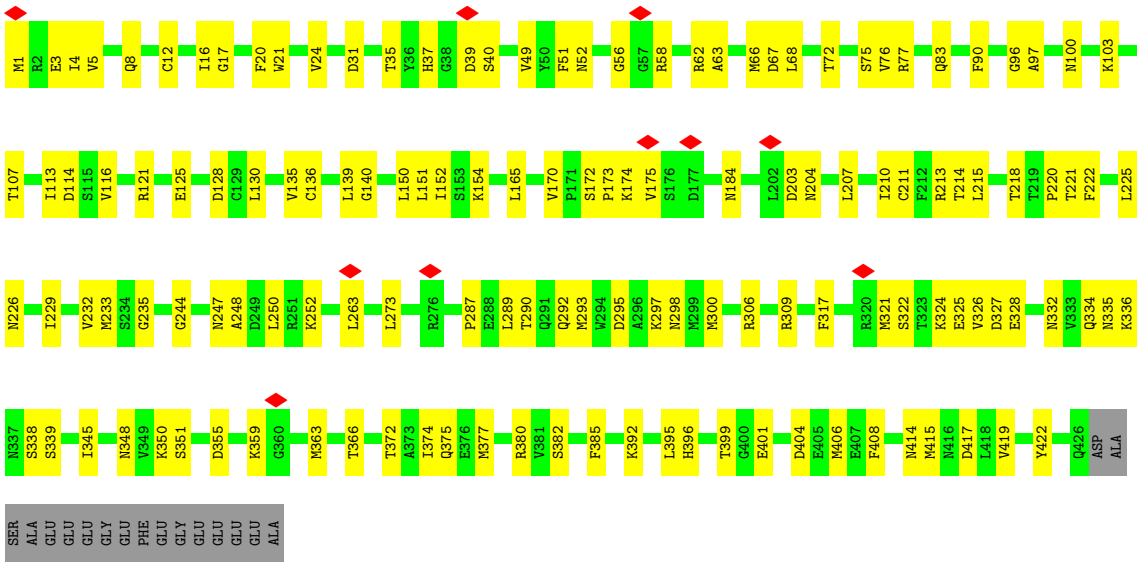

• Molecule 1: Tubulin beta

Chain 1S:



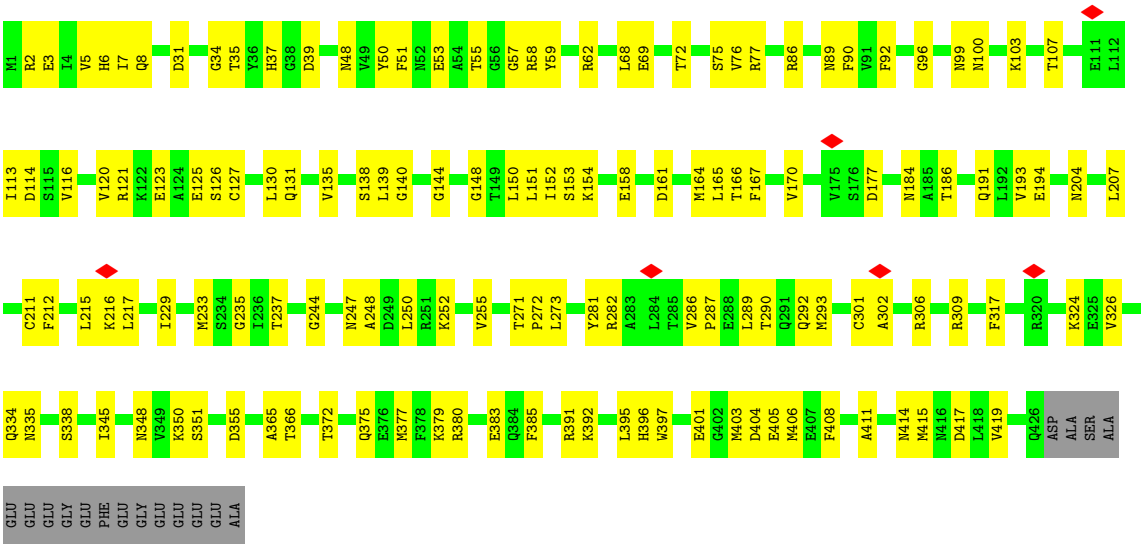

• Molecule 1: Tubulin beta

Chain 1U:



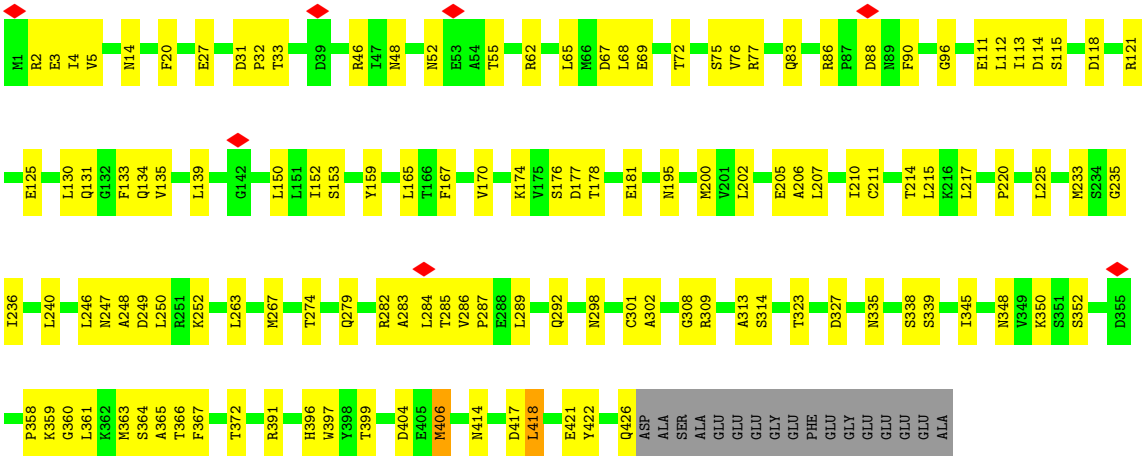

• Molecule 1: Tubulin beta

Chain 1W:



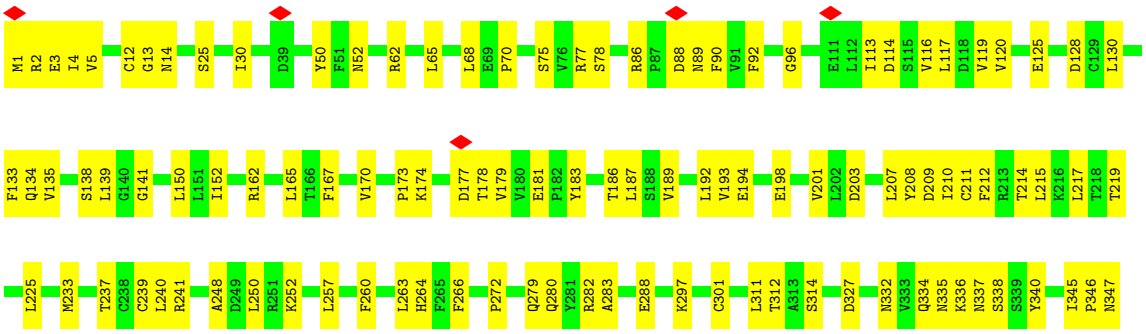

- Molecule 1: Tubulin beta

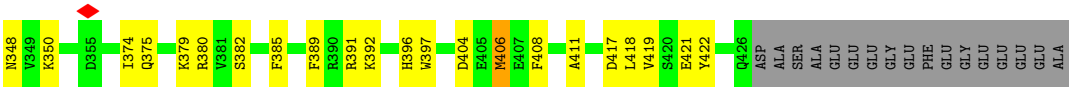
Chain 2A:




- Molecule 1: Tubulin beta

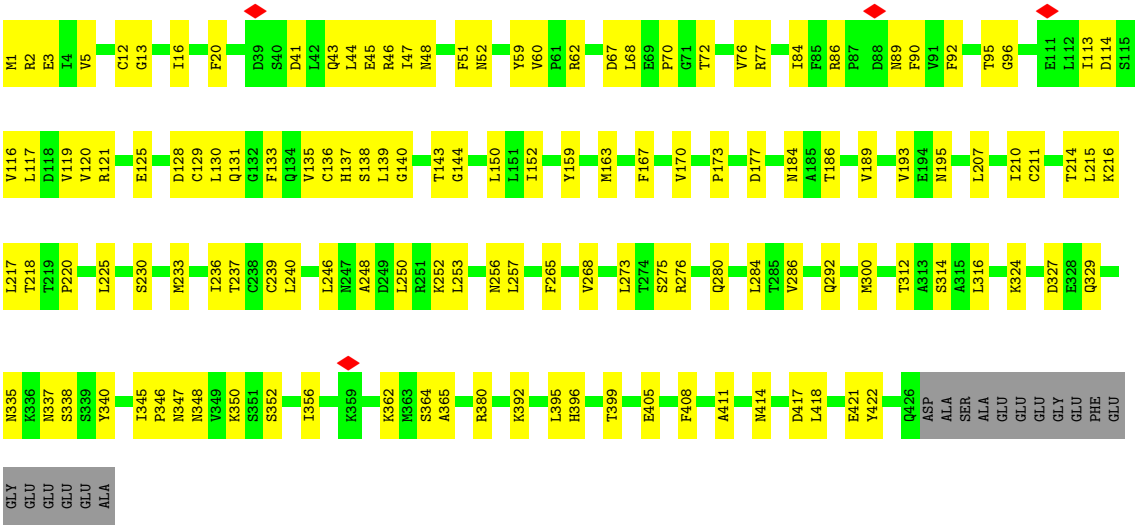
Chain 2C:





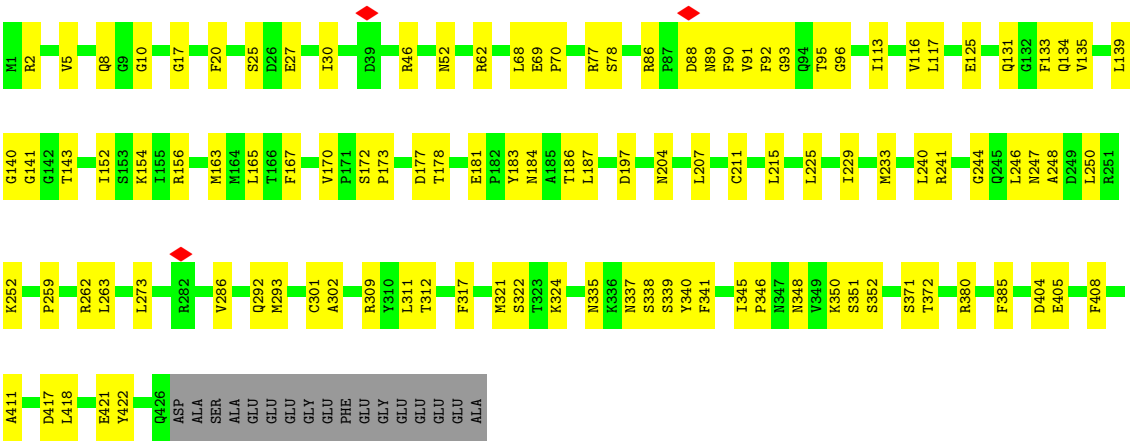

• Molecule 1: Tubulin beta

Chain 2E:



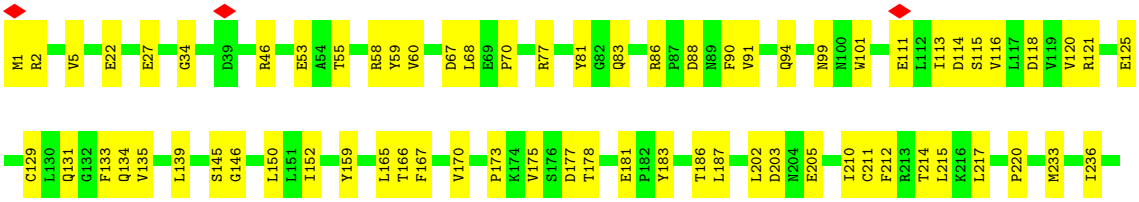

• Molecule 1: Tubulin beta

Chain 2G:




• Molecule 1: Tubulin beta

Chain 2I:



C239 L240 R241 G244 N247 A248 K252 P259 F270 L273 T274 S275 Q279 T285 V286 P287 E288 Q292 M300 C301 A302 R309 Y310 L311 T312 A313 S314 K324 D327 N335 K336 N337 S338 S339 Y340 F341 P346 K350 S351 D355 K359

F367 Q375 R380 F385 F389 R390 R391 L395 H396 W397 Y398 T399 M403 D404 E405 M406 E407 F408 A411 L418 V419 Y422 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 2K:

M1 R2 E3 I4 V5 G10 W21 G38 D39 N48 V49 Y50 F51 N52 G56 G57 P61 R62 L68 T72 S75 V76 R77 S78 R86 P87 D88 T95 G96 E111 L112 I113 D114 S115 V116 R121 E125 D128 C129 L130 F133 Q134 L139

G140 G141 G142 T143 G144 L151 I152 R156 E157 E158 R162 M163 M164 F167 V170 P173 K174 V175 S176 D177 T178 V179 N184 D197 E198 C199 M200 V201 L202 L207 Y208 C211 L215 K216 L217 L225 M233 S234 G235 L240 R241 A248 K252

F265 F266 L273 T274 S275 R276 Q280 Y281 R282 V286 P287 Q292 R309 S314 F317 M321 E325 Q334 S339 I345 P346 N347 N348 V349 K350 S351 S352 V353 P358 L361 T366 T372 R380 H396 T399 D404 E405 M406 Q426

ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 2M:

M1 R2 V5 H6 I7 Q8 C12 G17 F20 D31 P32 T33 G34 T35 Y36 H37 G38 D39 Q43 L44 E45 R46 I47 N48 V49 N52 R62 M66 D67 L68 D74 R77 S78 Q83 D88 N89 F90 Q94 T95 G96 A110 I113 D114 S115

V116 L117 D118 V119 V120 R121 K122 E123 A124 E125 S126 C129 Q134 V135 S138 L139 G140 G144 G148 I152 M164 L165 T166 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 E181 P182 Y183 N184 A185 T186 V189 E194 M200 V201 L202 D203 N204 L207

I210 C211 T214 L215 P220 D224 L225 M233 I236 R241 G244 N247 A248 D249 L250 R251 K252 L253 N256 R262 V268 T274 R282 A283 L284 T285 V286 P287 C301 A302 R309 T312 A313 S314 A315 L316 F317 T323 K324 E325 V326 D327

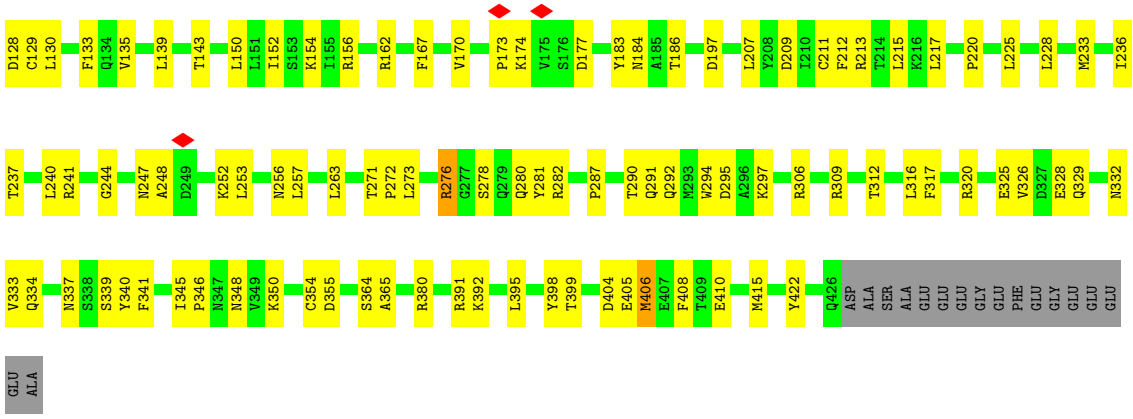
E328 N335 K336 N337 S338 S339 Y340 F341 I345 P346 N347 N348 V349 K350 D355 F367 I368 S371 T372 R380 V381 S382 F385 R391 L395 H396 W397 Y398 T399 D404 E405 M406 E407 F408 A411 N414 M415 E421 Q424 Y425 Q426 ASP ALA SER ALA GLU

GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

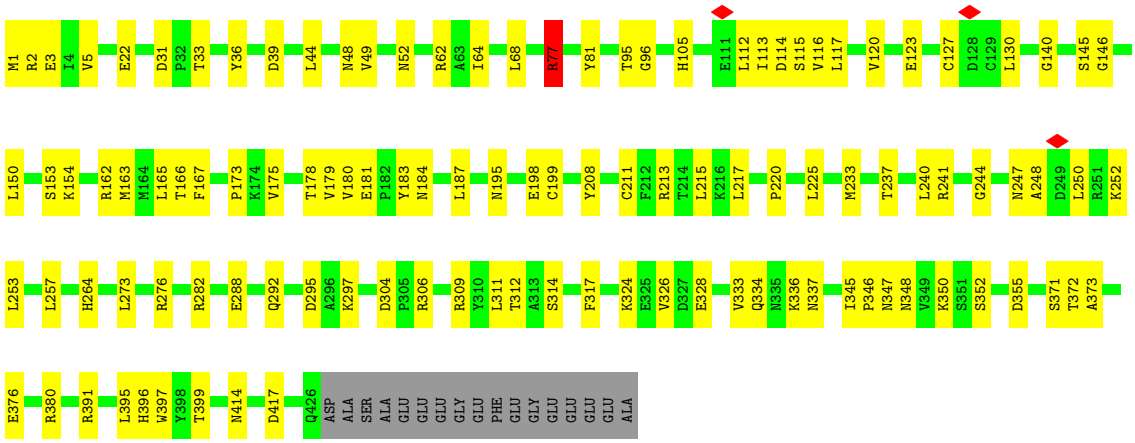
Chain 2Q:

M1 R2 E3 I4 V5 H6 I7 G10 D31 T35 D39 S40 E45 R46 V49 N52 T55 R58 R62 E69 R77 R86 N89 F90 V91 T95 G96 W101 T107 E108 E111 L112 I113 D114 S115 V116 R121 E125 S126 C127



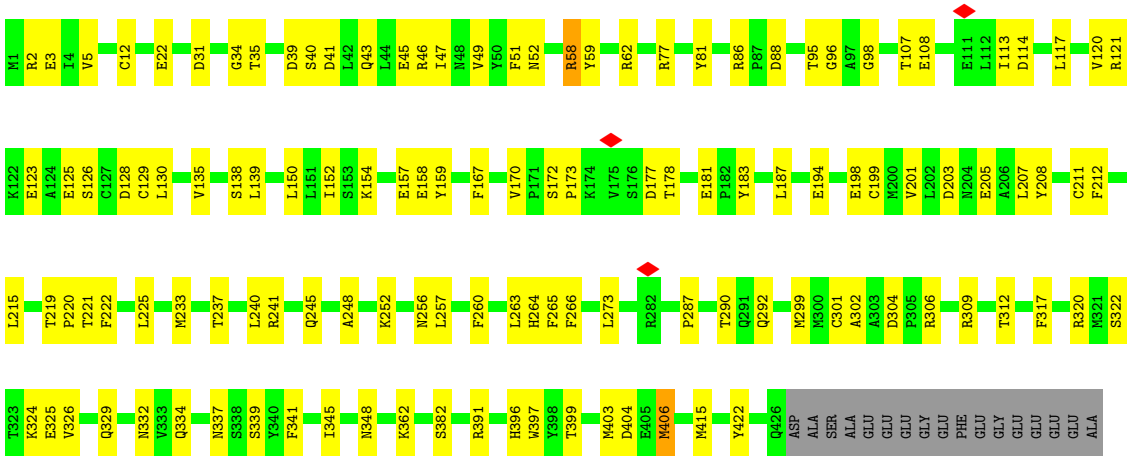

• Molecule 1: Tubulin beta

Chain 2S:



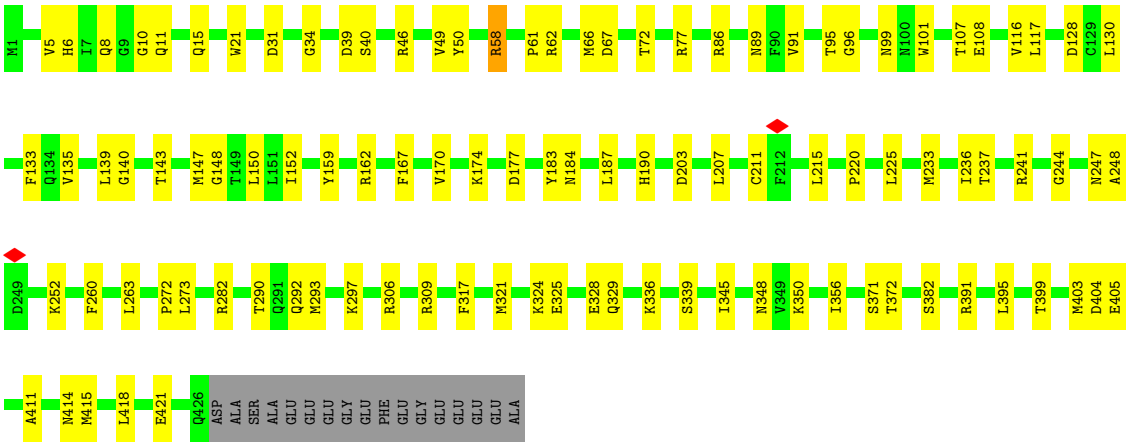

• Molecule 1: Tubulin beta

Chain 2U:



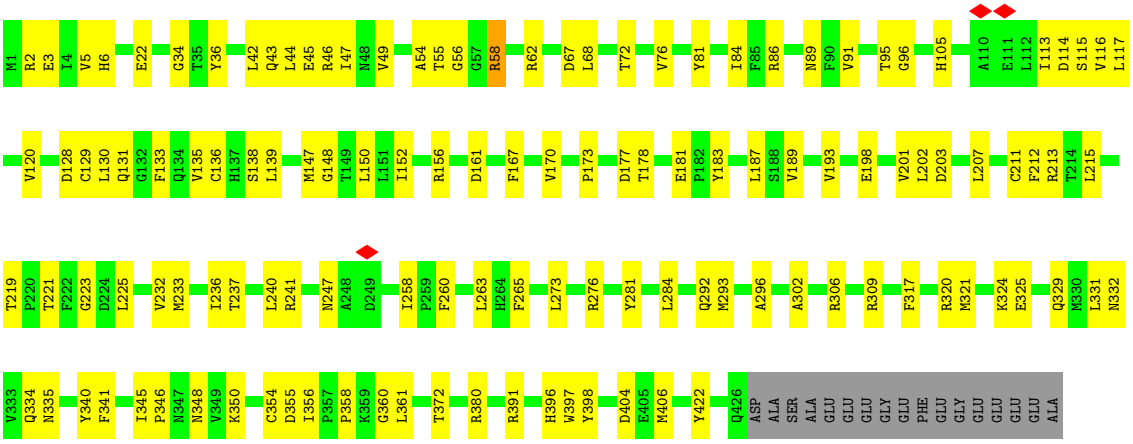

• Molecule 1: Tubulin beta

Chain 2W:



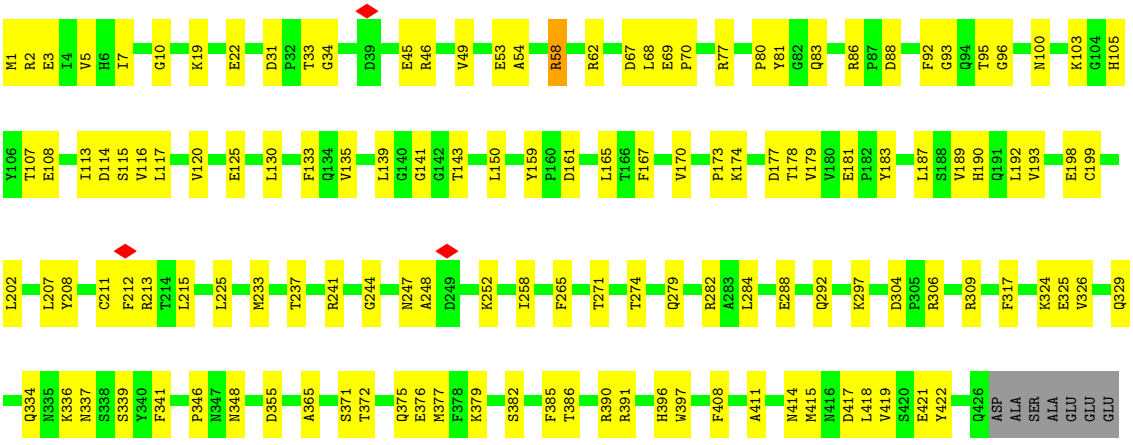

- Molecule 1: Tubulin beta

Chain 2Y:




- Molecule 1: Tubulin beta

Chain 3A:



GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3C:

M1 R2 E3 I4 V5 H6 I7 C12 G13 E22 G34 T35 L42 Q43 L44 E45 R46 I47 N48 V49 Y50 F51 N52 E53 A54 T55 R58 Y59 R62 R77 Y81 R86 P87 D88 N89 T95 G96 A97 G98 N99 N100 K103 G104 H105 A110 E111 L112 I113

V116 L117 D118 V119 V120 R121 D128 C129 L130 V135 C136 H137 S138 L139 G140 G141 S145 G146 M147 G148 T149 L150 L151 I152 S153 D161 R162 L165 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 V201

L202 D203 N204 E205 A206 L207 Y208 C211 F212 R213 T214 L215 K216 L217 M233 I236 T237 C238 C239 L240 R241 G244 Q245 L246 N247 A248 D249 L250 R251 K252 V255 N256 L257 F266 T274 S275 Q279 T285 V286 P287 Q291 M299 M300 C301 A302 R306 R309

T312 L316 F317 R320 T323 K324 E325 V326 Q329 N332 V333 Q334 N337 S338 S339 I345 P346 N347 N348 V349 K350 S351 S352 D355 K359 G360 L361 K362 M363 S371 T372 Q375 E376 K379 R380 V381 S382 T386 A387 M388 F389 R390 R391 K392 A393 F394

L395 H396 W397 Y398 T399 M406 E410 M415 Q426 ASP ALA SER ALA GLU GLU GLU GLY GLU PHE GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3G:

M1 R2 E3 H6 I7 Q8 I30 G34 D39 S40 R46 V49 Y50 F51 N52 E53 G57 R58 Y59 V60 P61 R62 L65 M66 T72 V76 R77 Q83 R86 P87 D88 N89 F90 Q94 T95 N99 N100 K103 E111 L112 I113 D114 S115 V116

L117 V120 R121 K122 D128 C129 L130 Q134 V135 S138 L139 G140 M147 L150 L151 I152 R156 P160 D161 M164 F167 V170 P171 S172 P173 K174 V175 S176 D177 T178 E181 N184 L192 N195 A196 D197 E198 L202 D203 N204 E205 D209 I210

C211 L215 T218 T219 I229 M233 T237 L240 R241 G244 N247 A248 K252 L253 H264 T271 P272 L273 T274 S275 R276 Q280 Y281 R282 V286 P287 M293 A302 R309 L316 F317 K324 E325 V326 Q334 I345 P346 N347 N348 V349

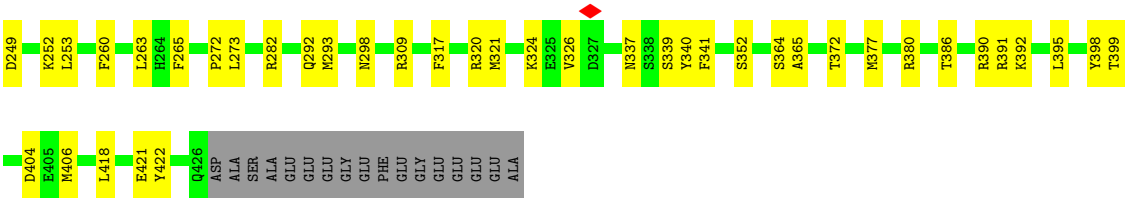
K350 S351 T372 R380 V381 S382 R391 M406 E410 M415 Q426 ASP ALA SER ALA GLU GLU GLU GLU GLY GLU PHE GLU GLU GLY GLU GLU GLU GLU ALA

- Molecule 1: Tubulin beta

Chain 3I:

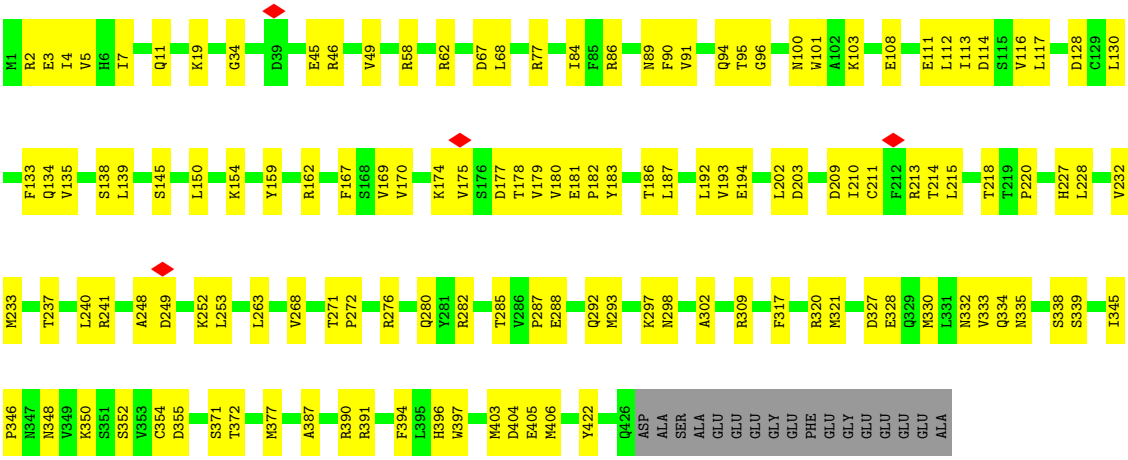
M1 R2 E3 I4 V5 H6 I7 Q8 Q11 W21 I30 D31 P32 T33 G34 D39 Y50 F51 N52 R58 Y59 V60 P61 R62 D67 L68 E69 P70 R77 Y81 F90 Q94 T95 L112 I113 D114 S115 V116 L117 D118 V119 V120 R121 D128 C129 Q134

V135 C136 H137 S138 L139 G140 S145 D161 R162 T166 F167 V170 P173 D177 P182 Y183 N184 A185 T186 L187 L192 C199 L202 D203 N204 E205 Y208 D209 I210 C211 L215 K216 L217 T218 T219 P220 L225 M233 T237 G244 Q245 L246 N247 A248



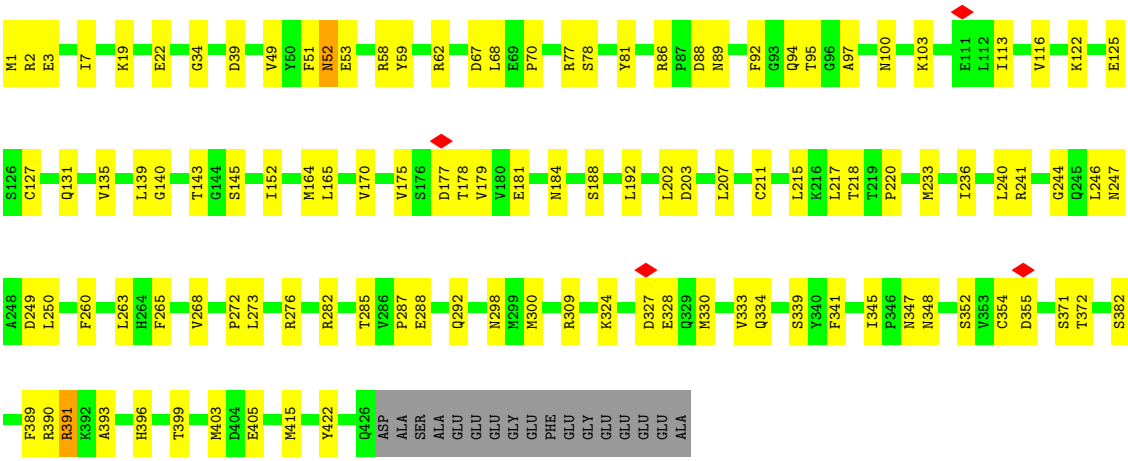

• Molecule 1: Tubulin beta

Chain 3K:



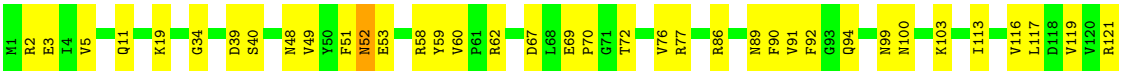

• Molecule 1: Tubulin beta

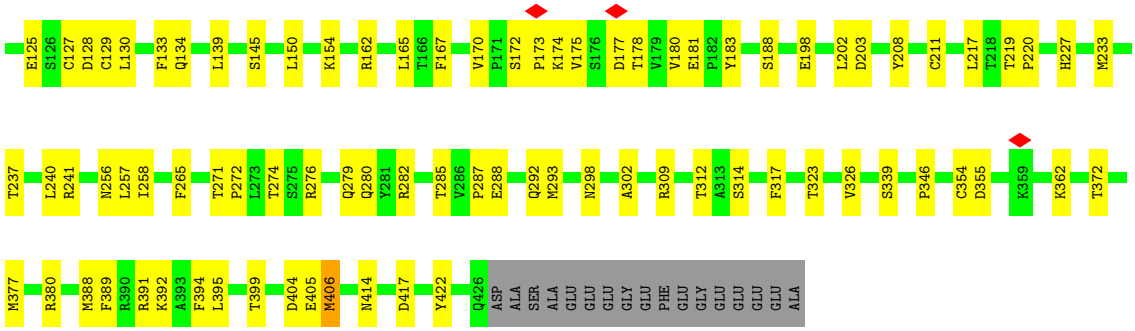
Chain 3M:




• Molecule 1: Tubulin beta

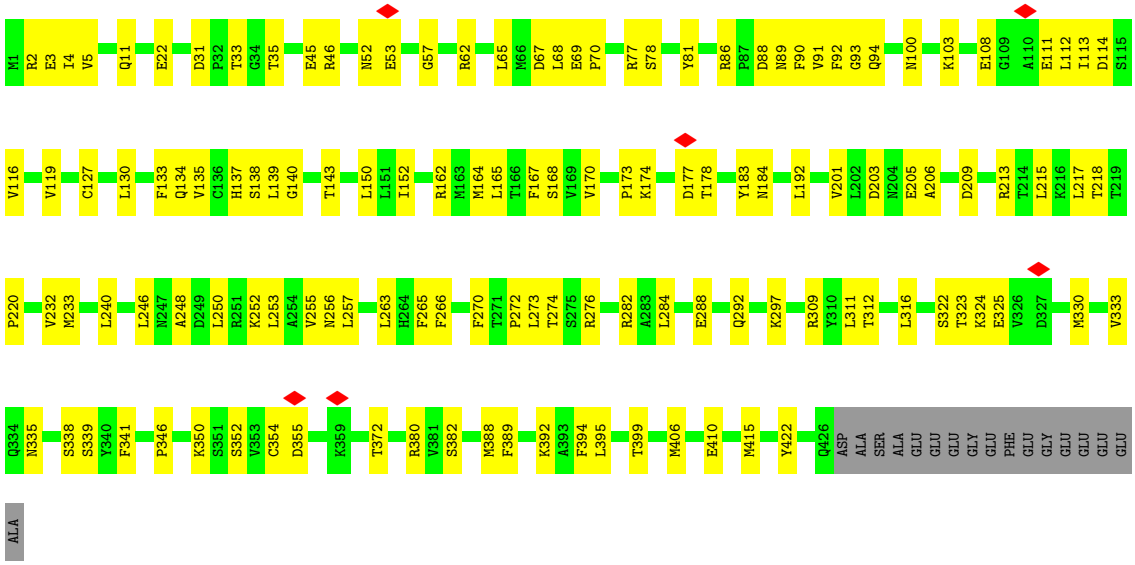
Chain 3O:





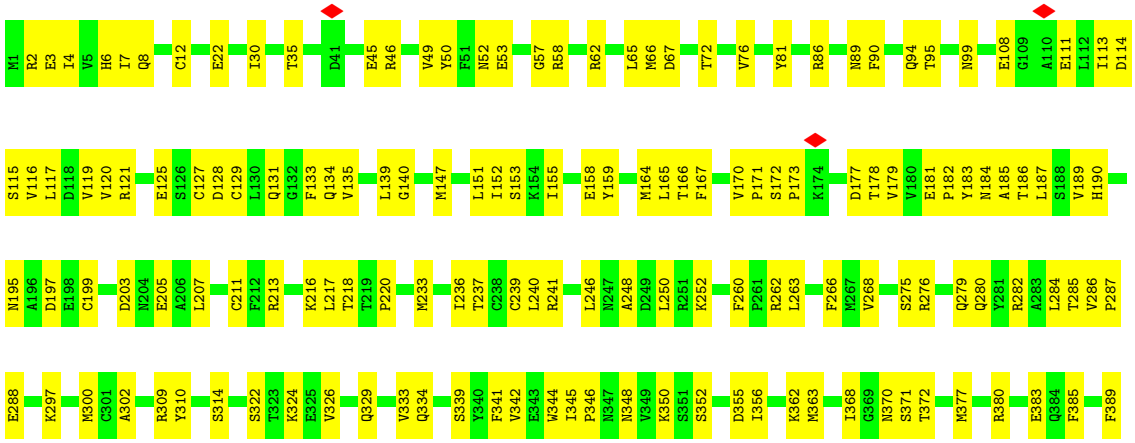

• Molecule 1: Tubulin beta

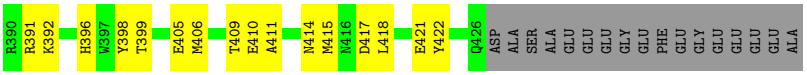
Chain 3Q:




• Molecule 1: Tubulin beta

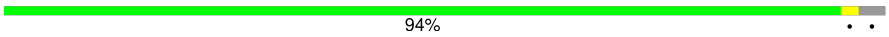
Chain 3S:

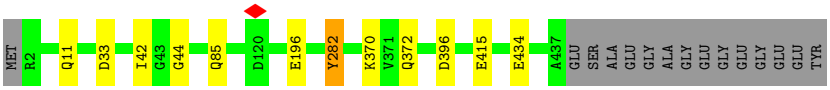





- Molecule 2: Tubulin alpha

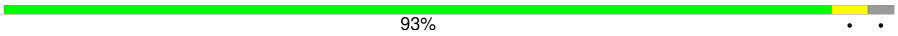
Chain 2:

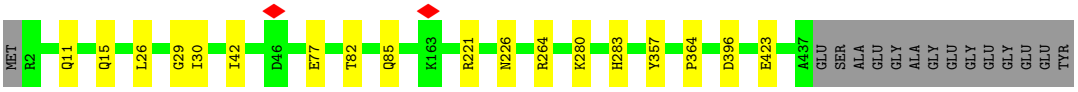



- Molecule 2: Tubulin alpha

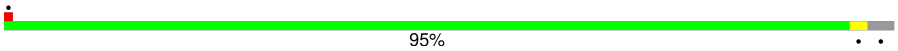
Chain 4:

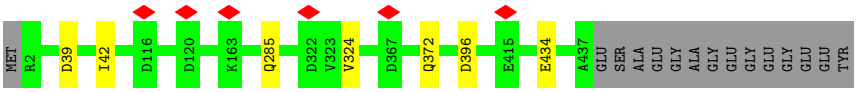



- Molecule 2: Tubulin alpha

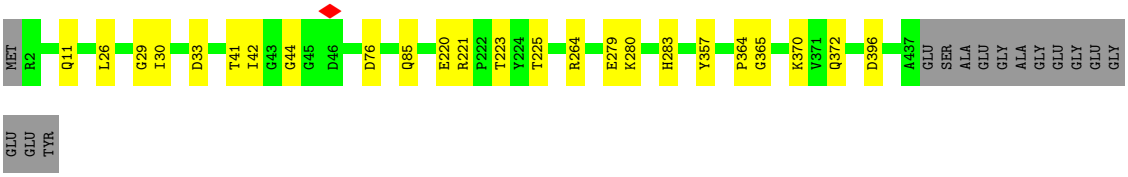
Chain 6:



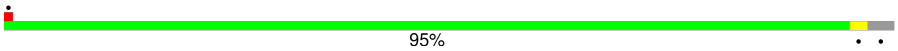

- Molecule 2: Tubulin alpha

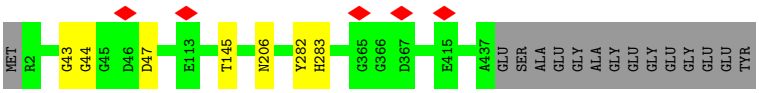
Chain 8:




- Molecule 2: Tubulin alpha

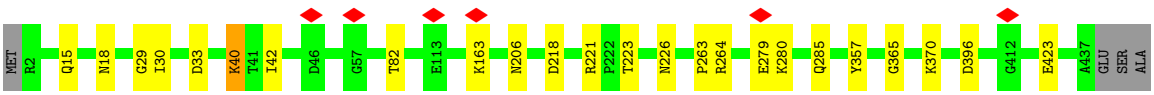
Chain A0:

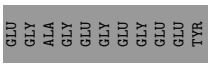



- Molecule 2: Tubulin alpha

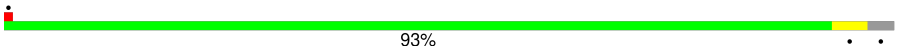
Chain A2:

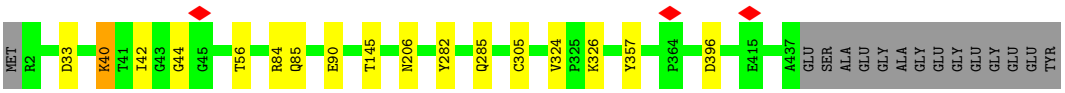





• Molecule 2: Tubulin alpha

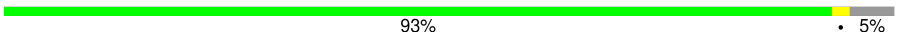
Chain A4:

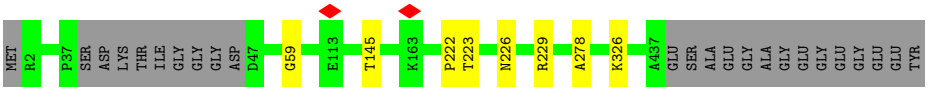



• Molecule 2: Tubulin alpha

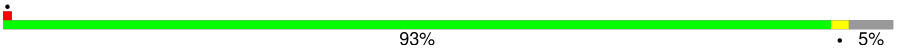
Chain A8:



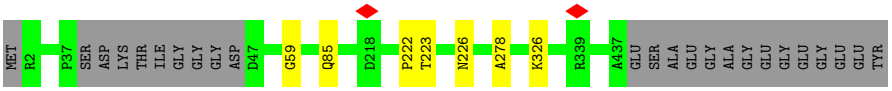

• Molecule 2: Tubulin alpha

Chain B0:



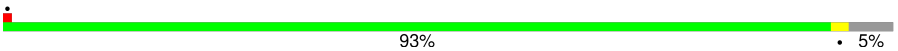
• Molecule 2: Tubulin alpha

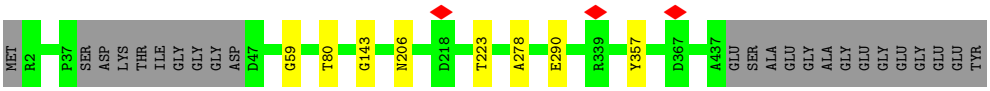
Chain B2:




• Molecule 2: Tubulin alpha

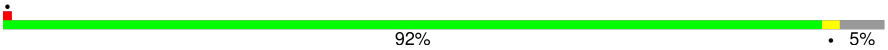
Chain B4:

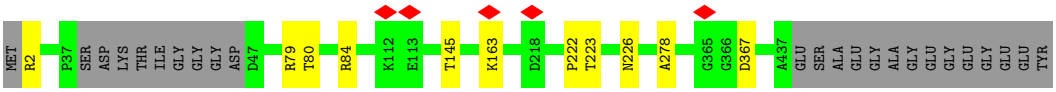



• Molecule 2: Tubulin alpha

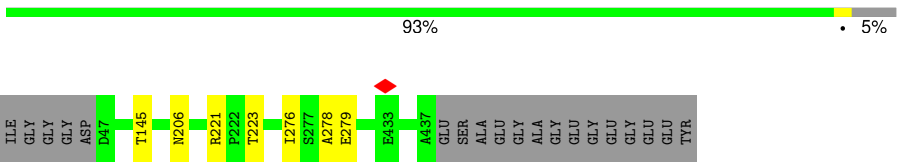
Chain B7:



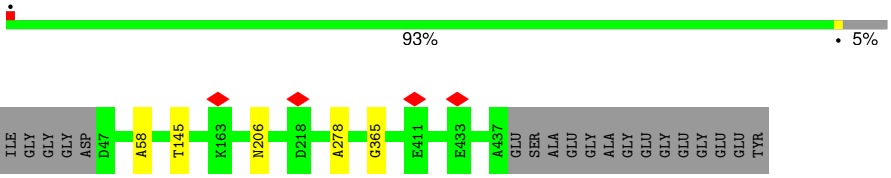

• Molecule 2: Tubulin alpha

Chain B9:



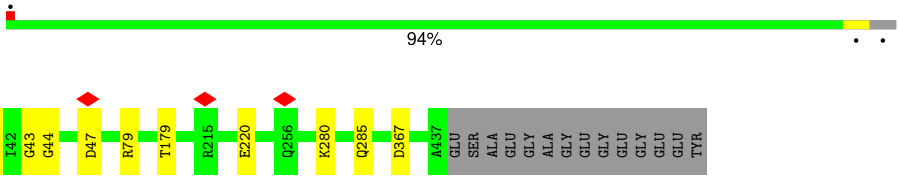

• Molecule 2: Tubulin alpha

Chain C1:



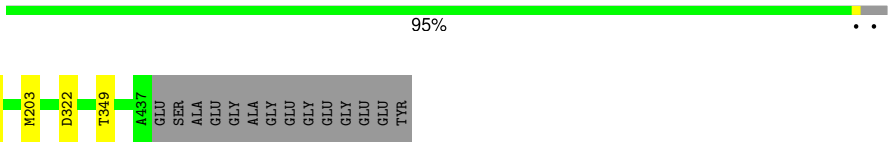

• Molecule 2: Tubulin alpha

Chain C5:



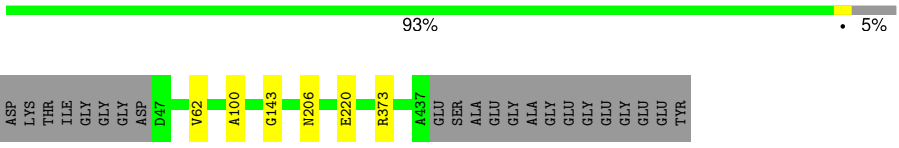

• Molecule 2: Tubulin alpha

Chain C7:



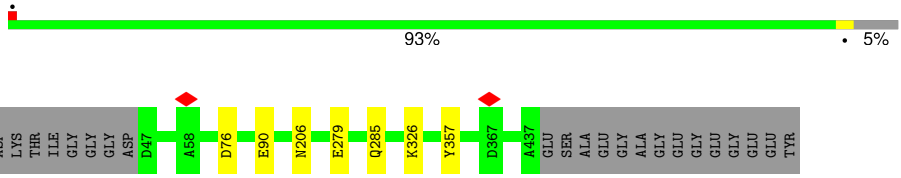

• Molecule 2: Tubulin alpha

Chain C9:



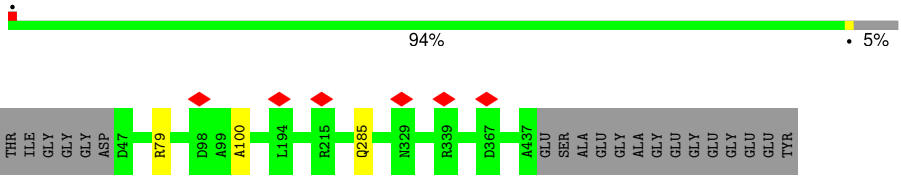

• Molecule 2: Tubulin alpha

Chain D1:



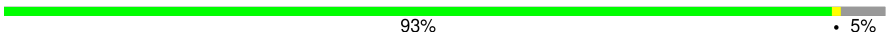

• Molecule 2: Tubulin alpha

Chain D3:



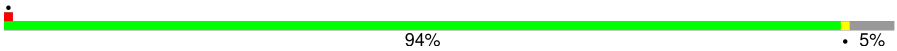
- Molecule 2: Tubulin alpha

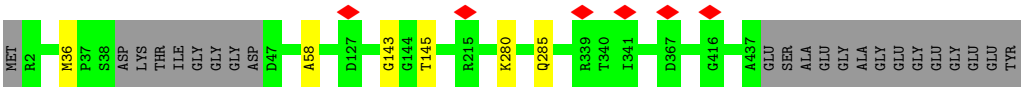
Chain D5:



- Molecule 2: Tubulin alpha

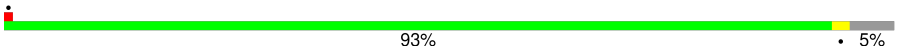
Chain D7:

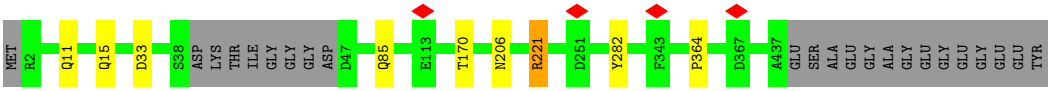



- Molecule 2: Tubulin alpha

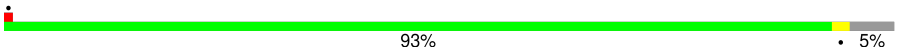
Chain E1:

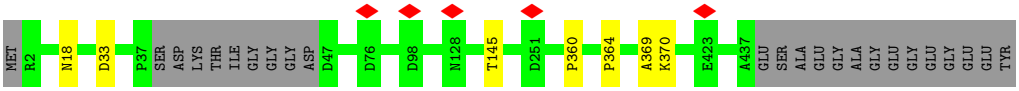



- Molecule 2: Tubulin alpha

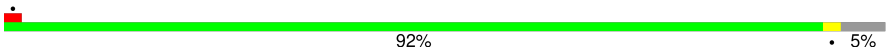
Chain E3:

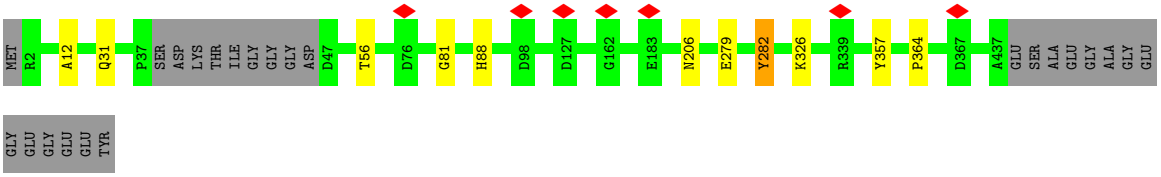



- Molecule 2: Tubulin alpha

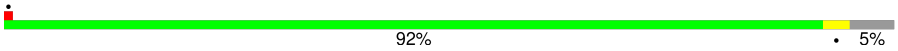
Chain E5:

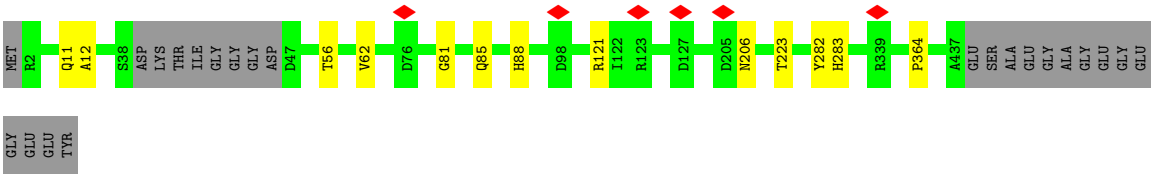



- Molecule 2: Tubulin alpha

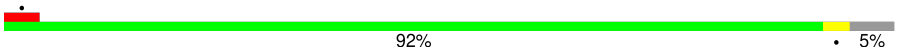
Chain E7:

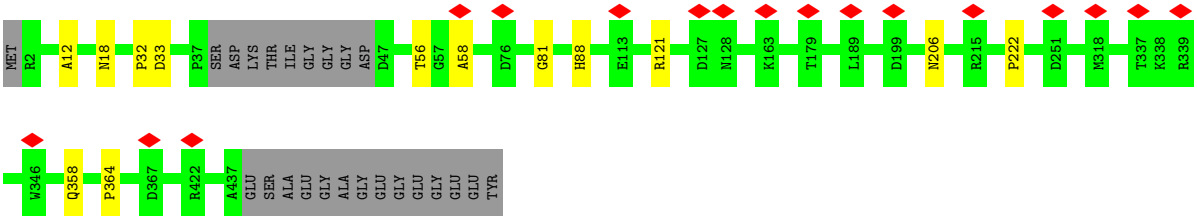


- Molecule 2: Tubulin alpha

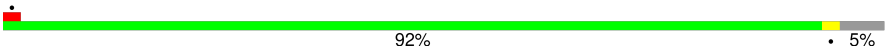
Chain E9:

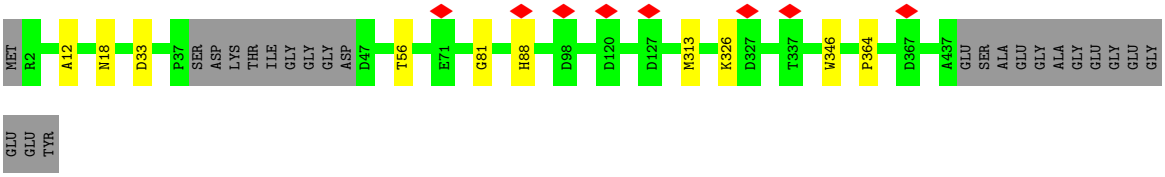



- Molecule 2: Tubulin alpha

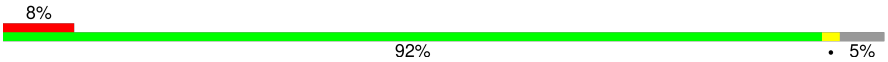
Chain F1:

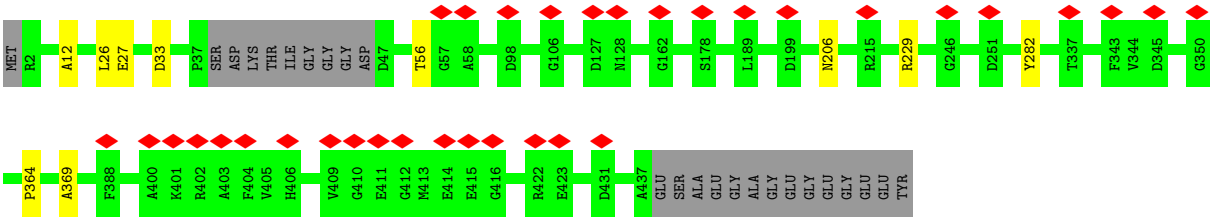



- Molecule 2: Tubulin alpha

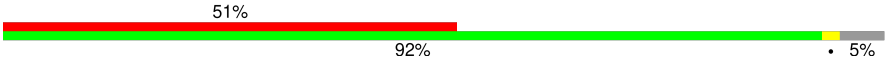
Chain F3:

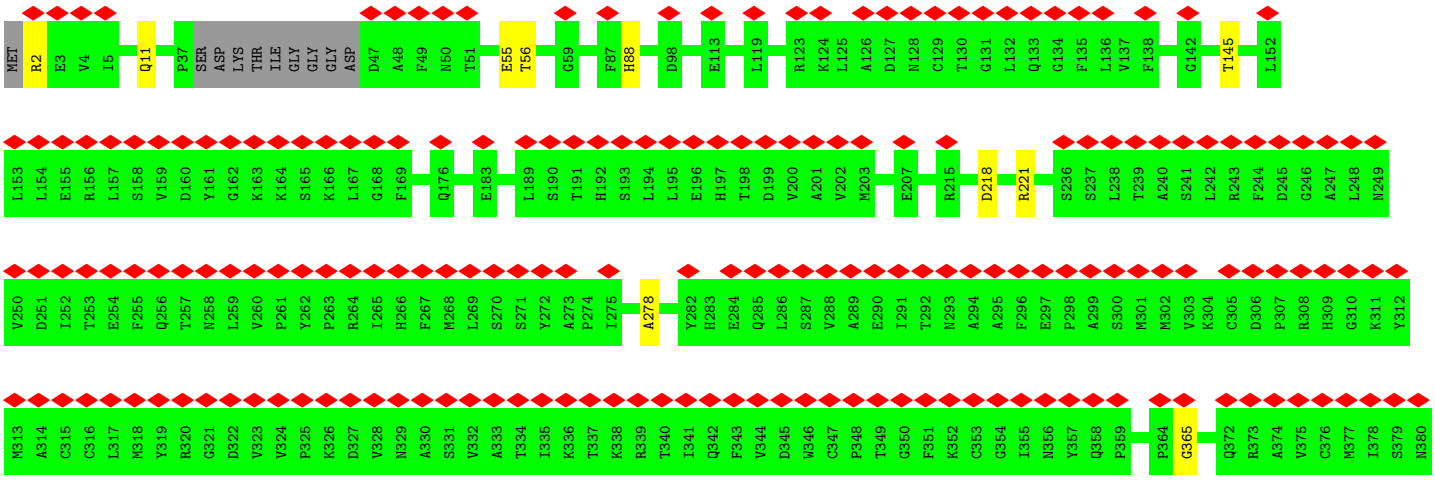


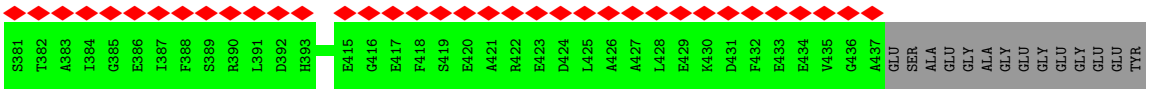




- Molecule 2: Tubulin alpha

Chain F5:

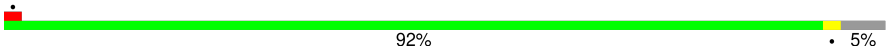


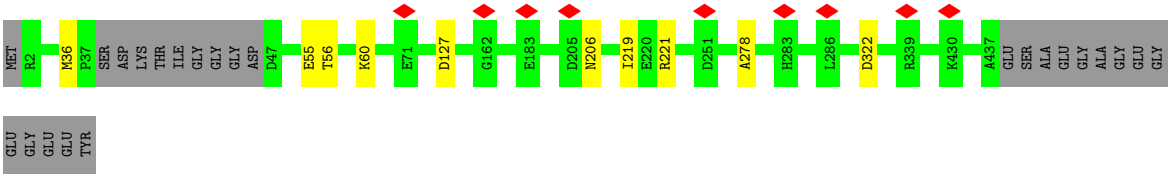






• Molecule 2: Tubulin alpha

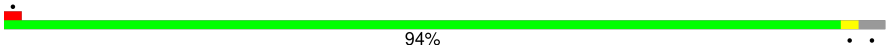
Chain F7:

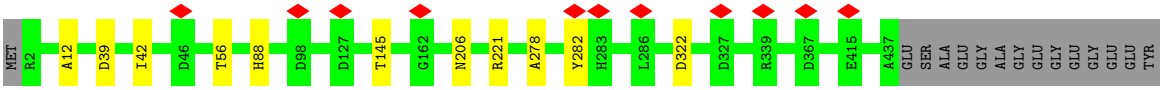



• Molecule 2: Tubulin alpha

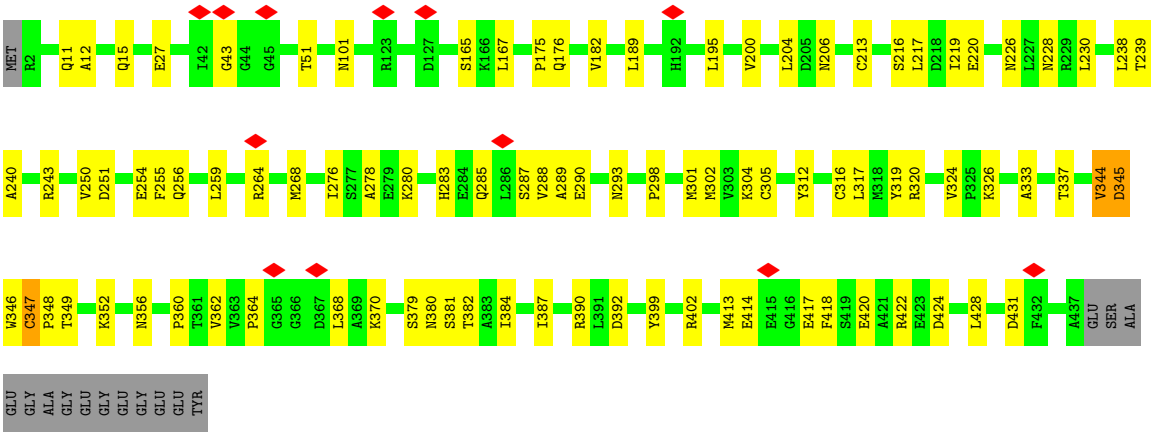
Chain F9:



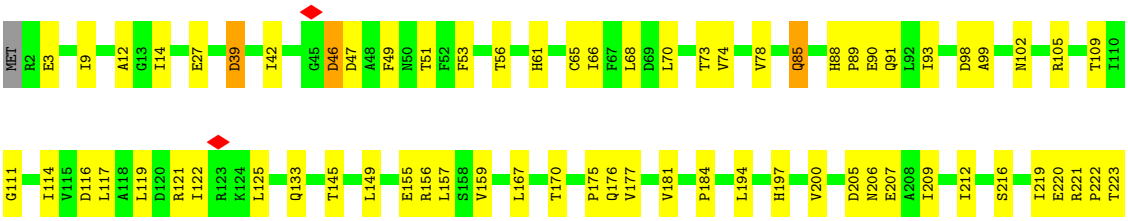

• Molecule 2: Tubulin alpha

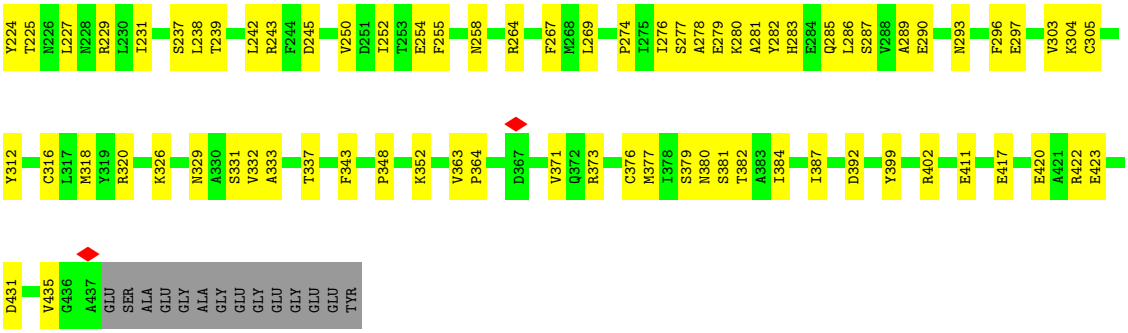
Chain G1:




• Molecule 2: Tubulin alpha

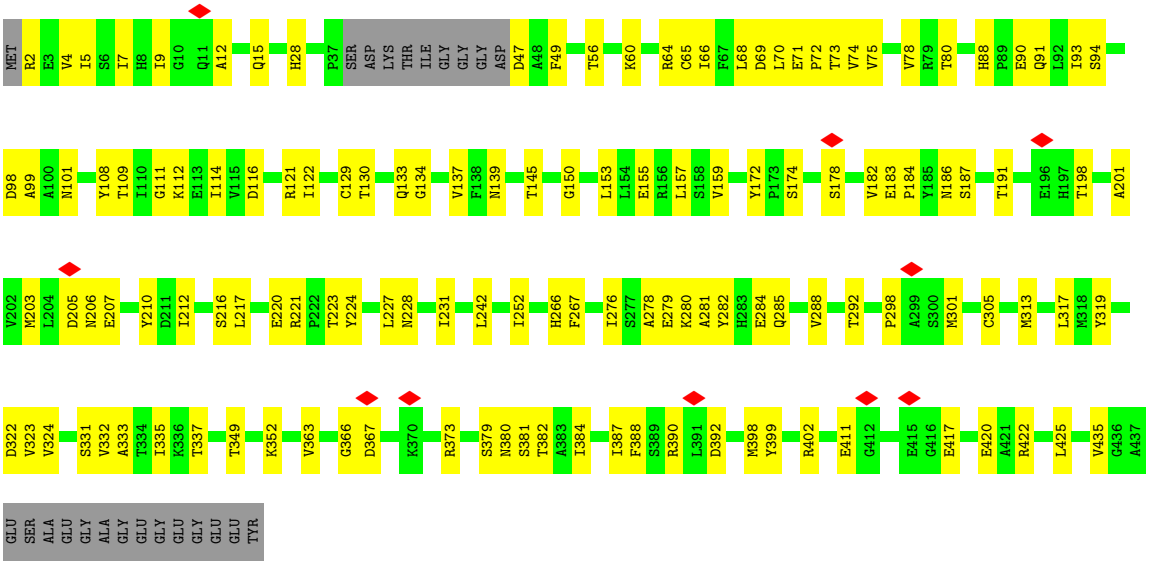
Chain G3:





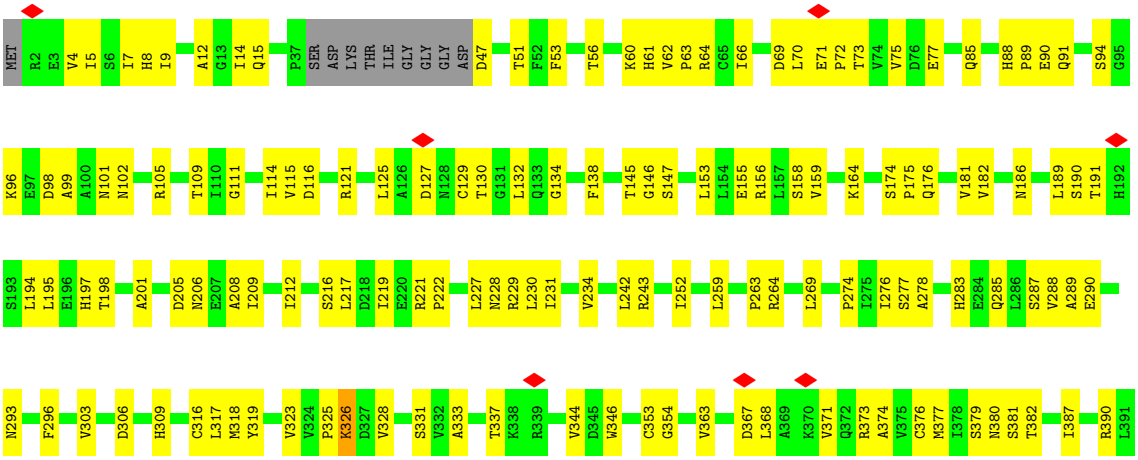

• Molecule 2: Tubulin alpha

Chain G5:



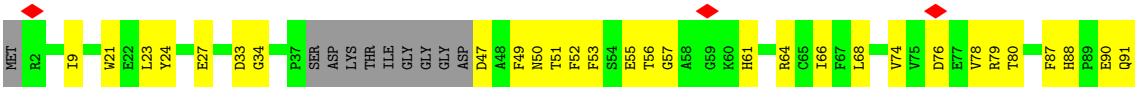

• Molecule 2: Tubulin alpha

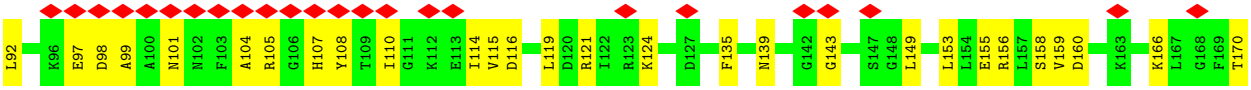
Chain G7:

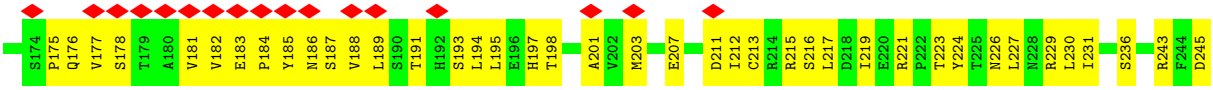


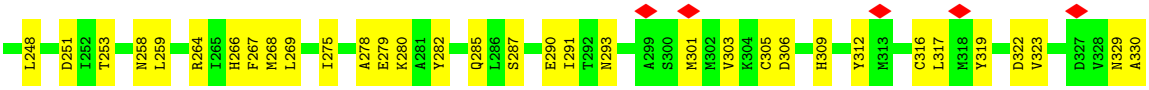
• Molecule 2: Tubulin alpha

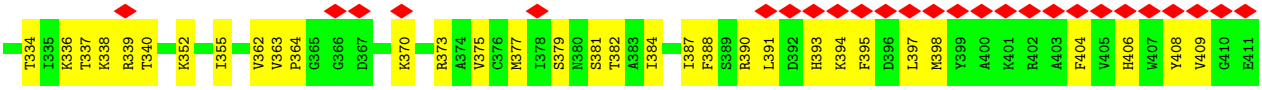
Chain G9:

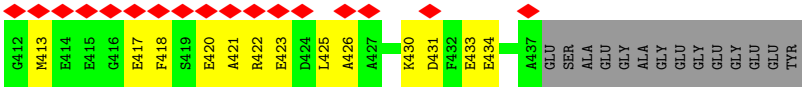


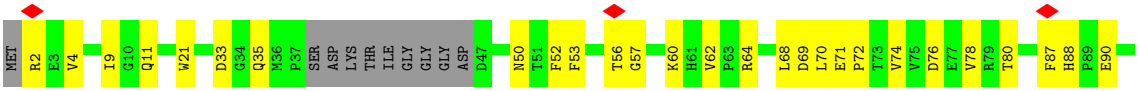



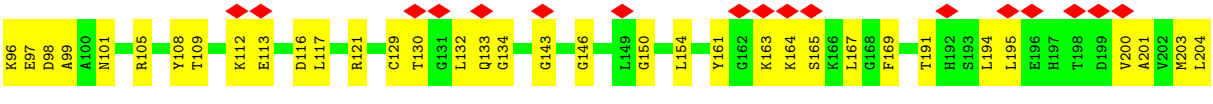



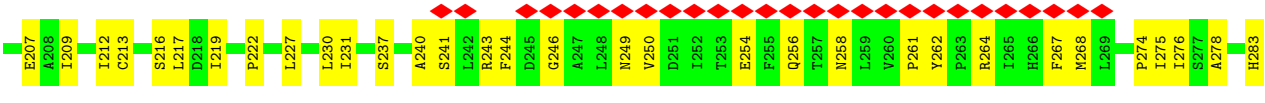



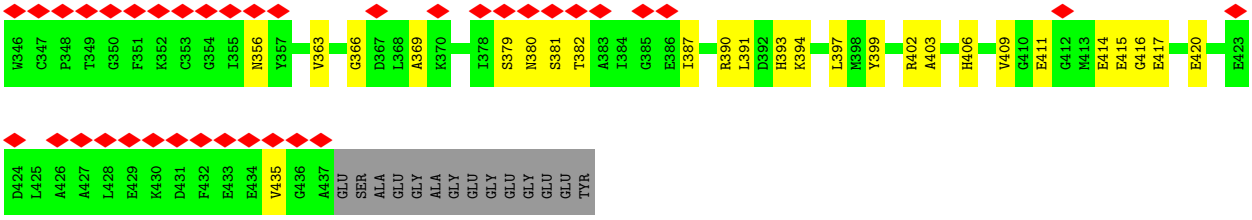

• Molecule 2: Tubulin alpha

Chain H1:



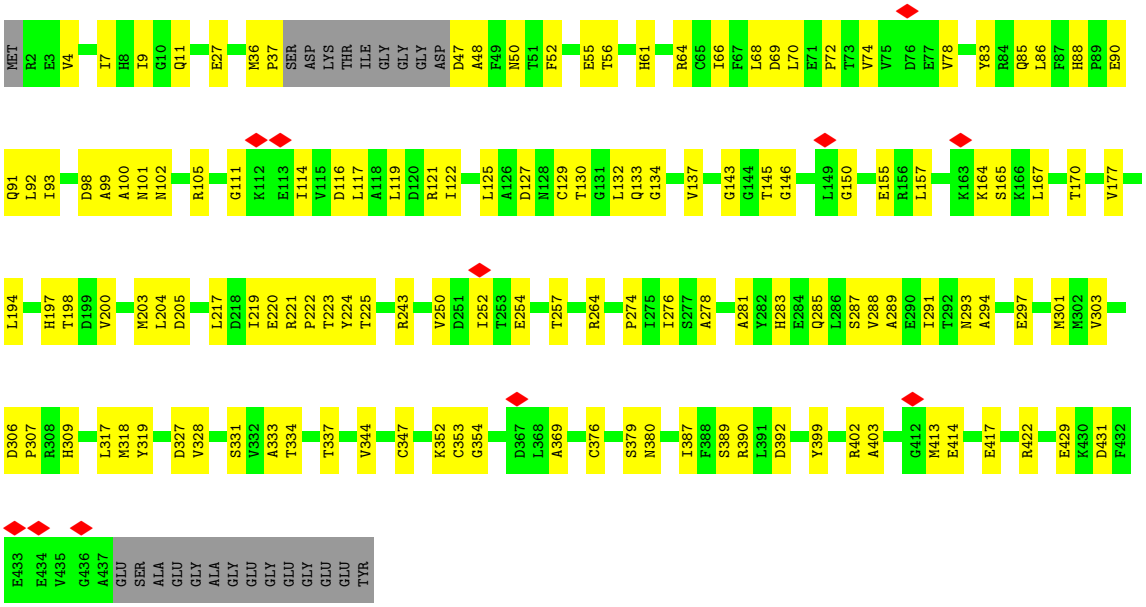





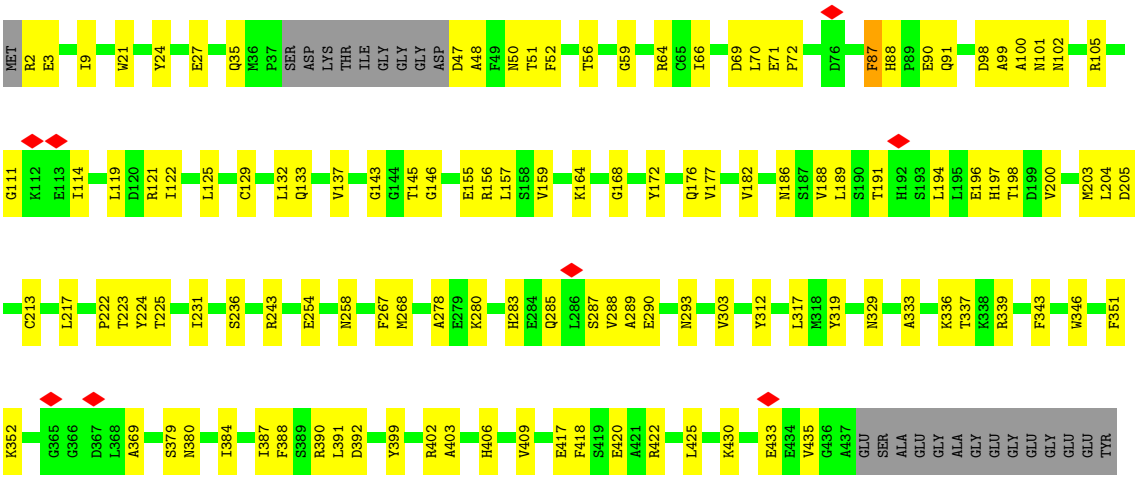

• Molecule 2: Tubulin alpha

Chain H3:



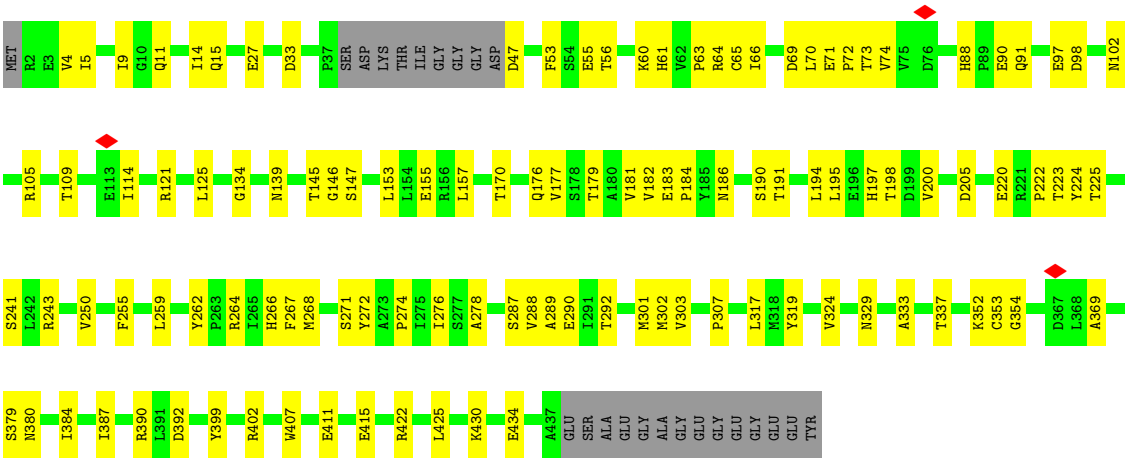

• Molecule 2: Tubulin alpha

Chain H5:



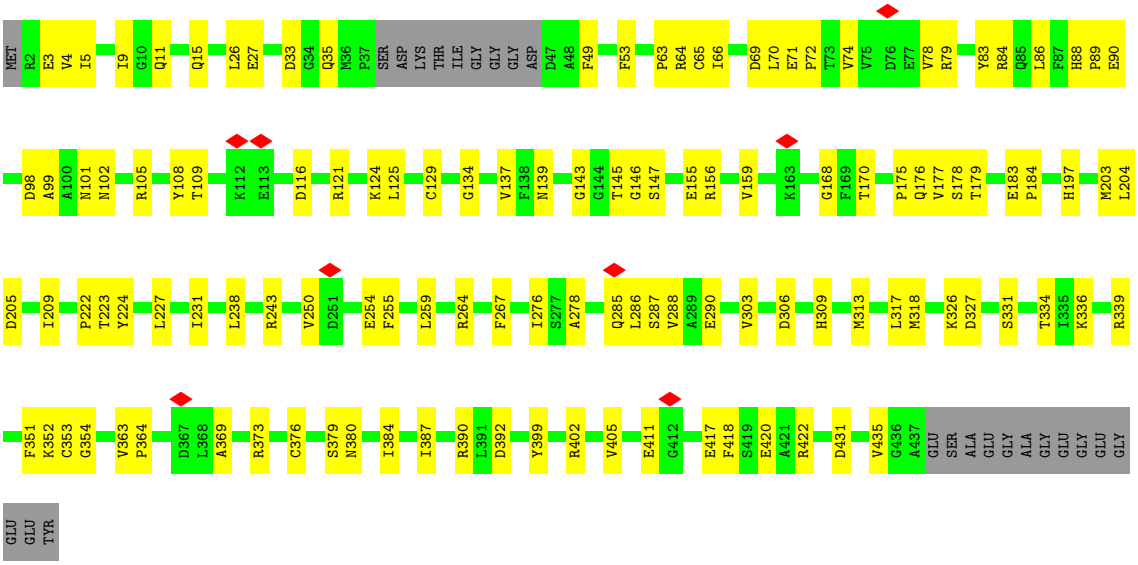

• Molecule 2: Tubulin alpha

Chain H7:



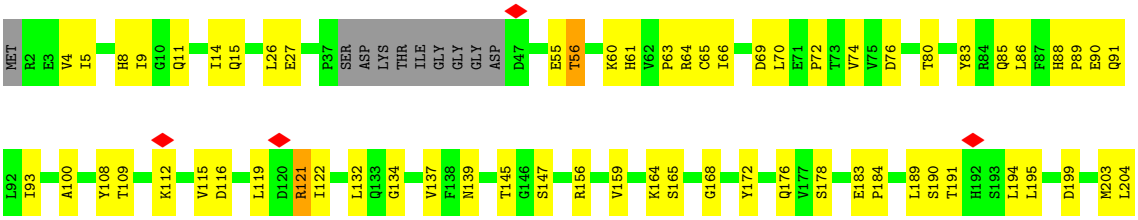

• Molecule 2: Tubulin alpha

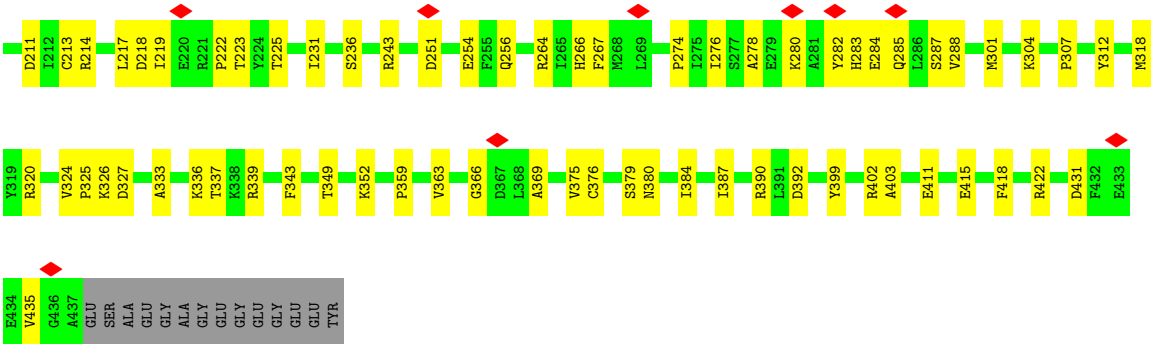
Chain H9:




• Molecule 2: Tubulin alpha

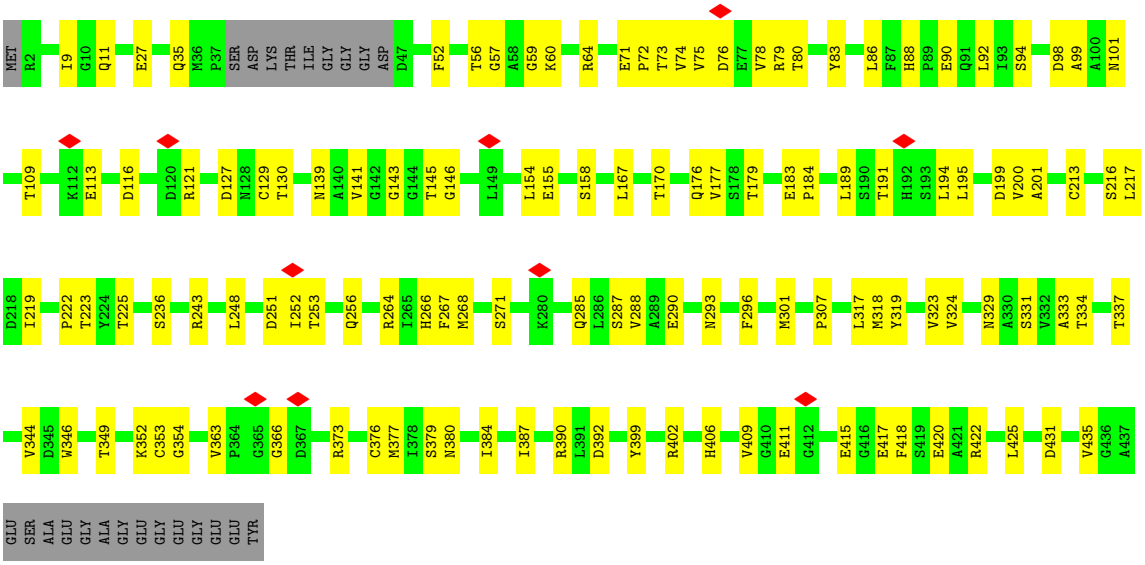
Chain I1:





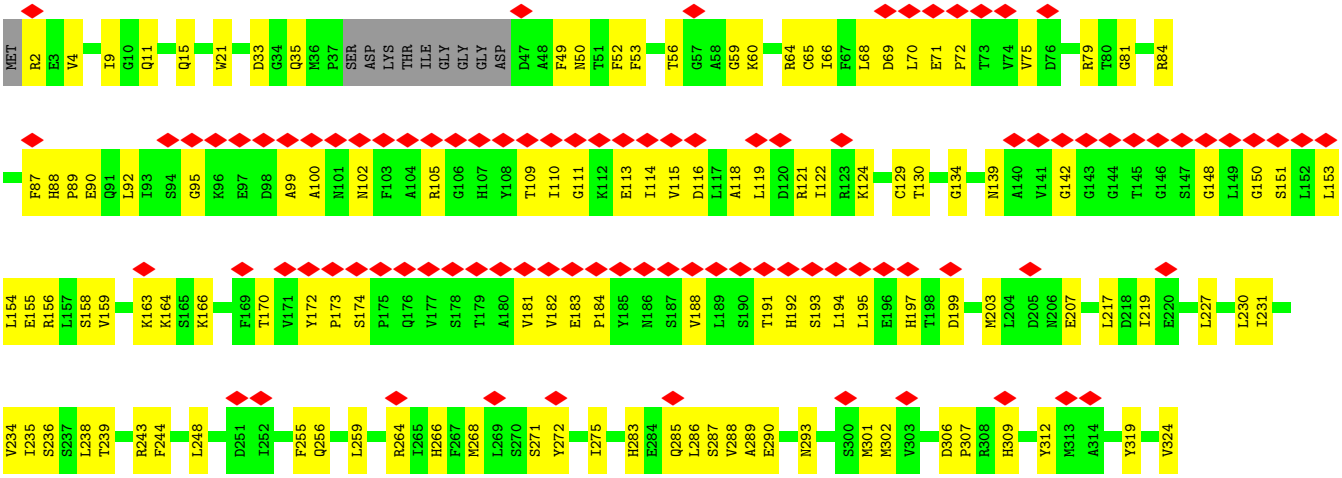

• Molecule 2: Tubulin alpha

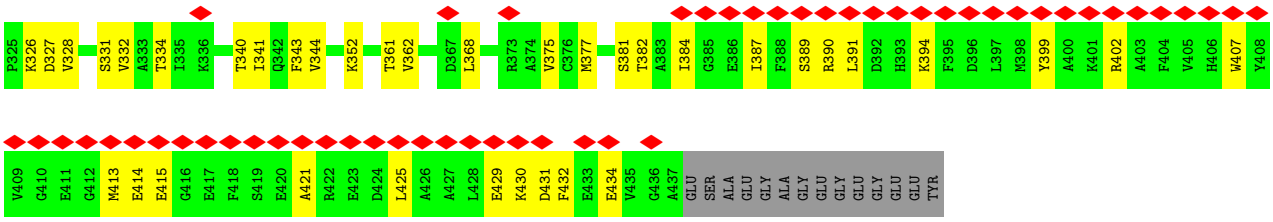
Chain I3:




• Molecule 2: Tubulin alpha

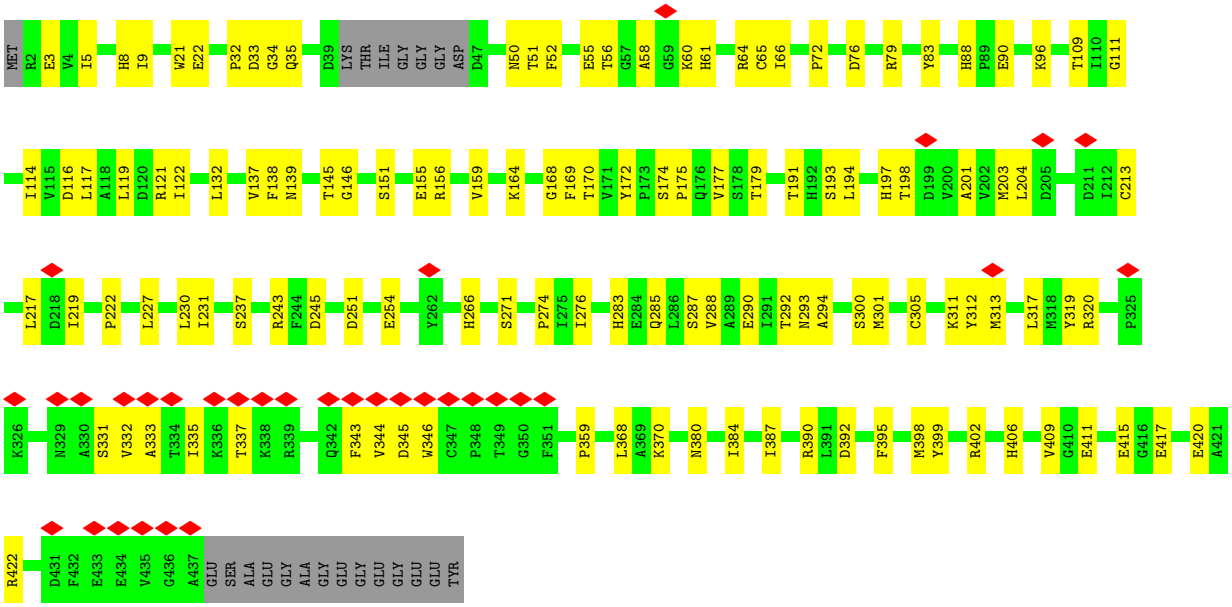
Chain I5:





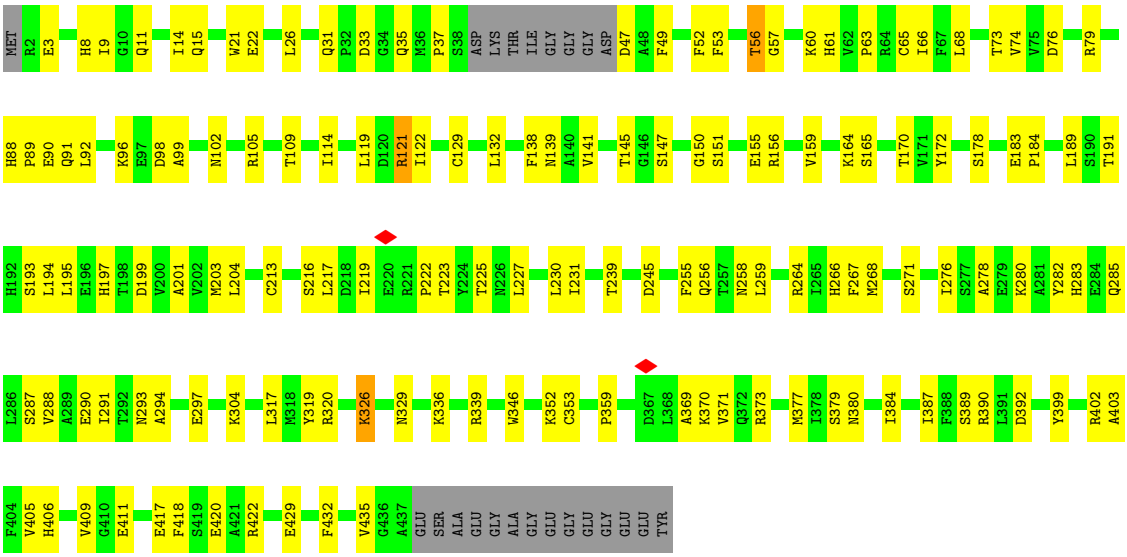

• Molecule 2: Tubulin alpha

Chain I7:



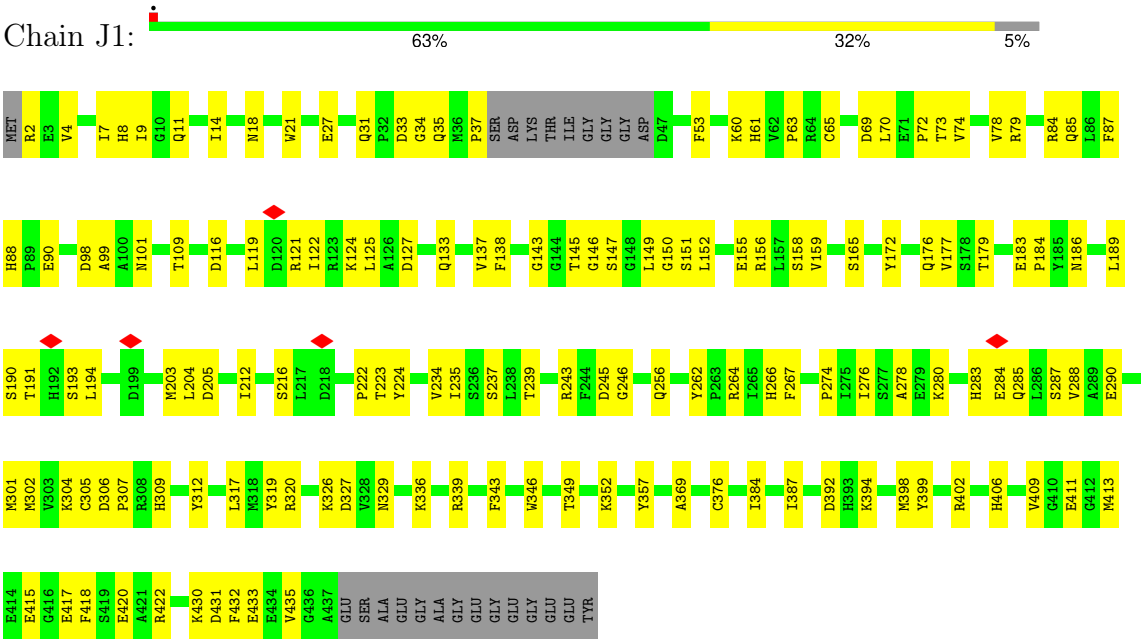

• Molecule 2: Tubulin alpha

Chain I9:



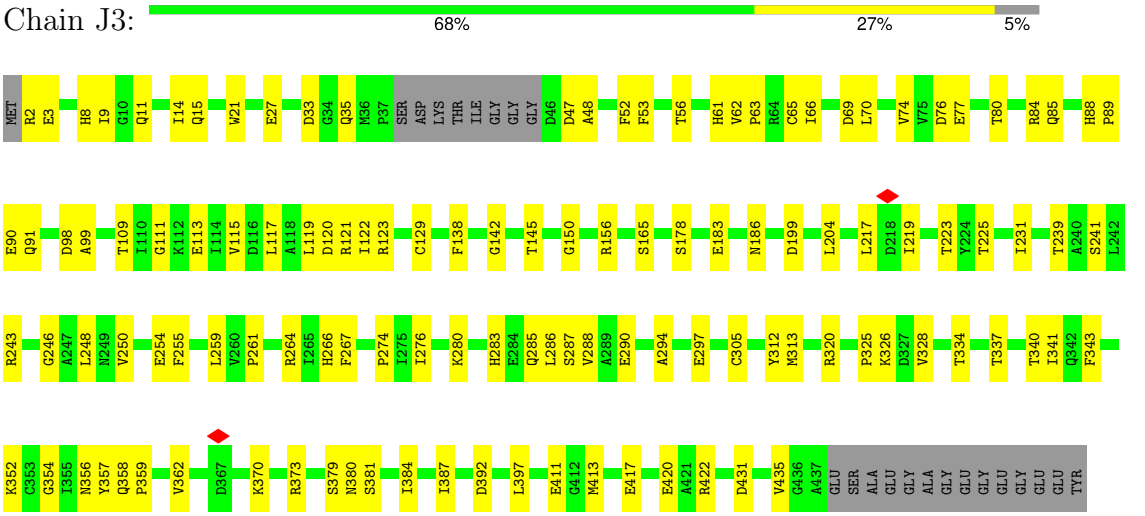
- Molecule 2: Tubulin alpha

Chain J1:



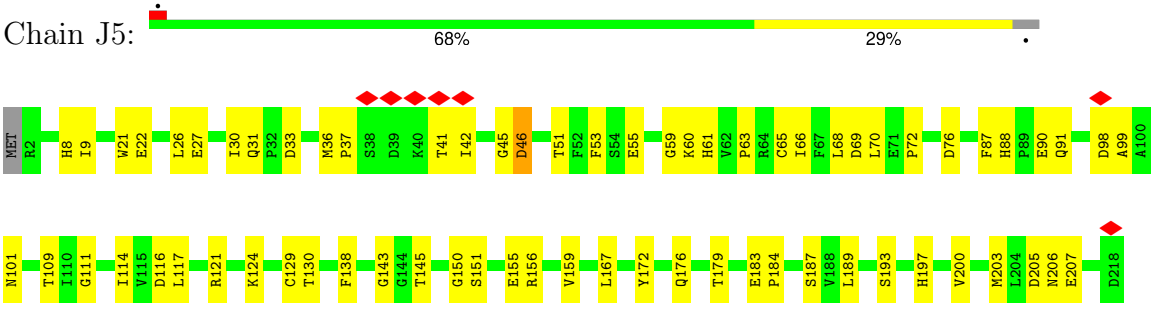

- Molecule 2: Tubulin alpha

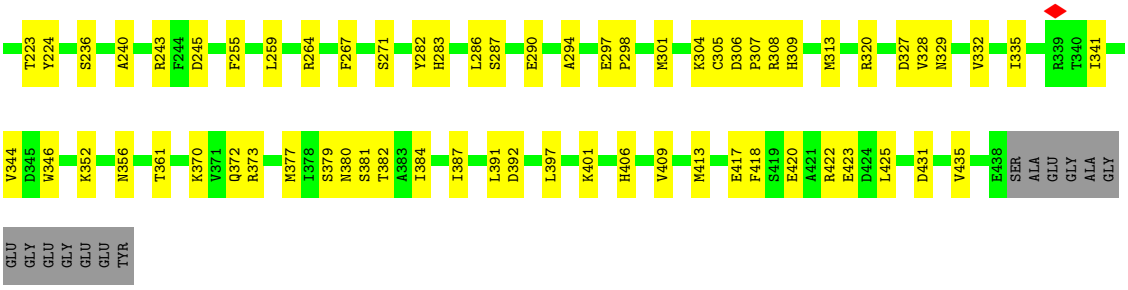
Chain J3:




- Molecule 2: Tubulin alpha

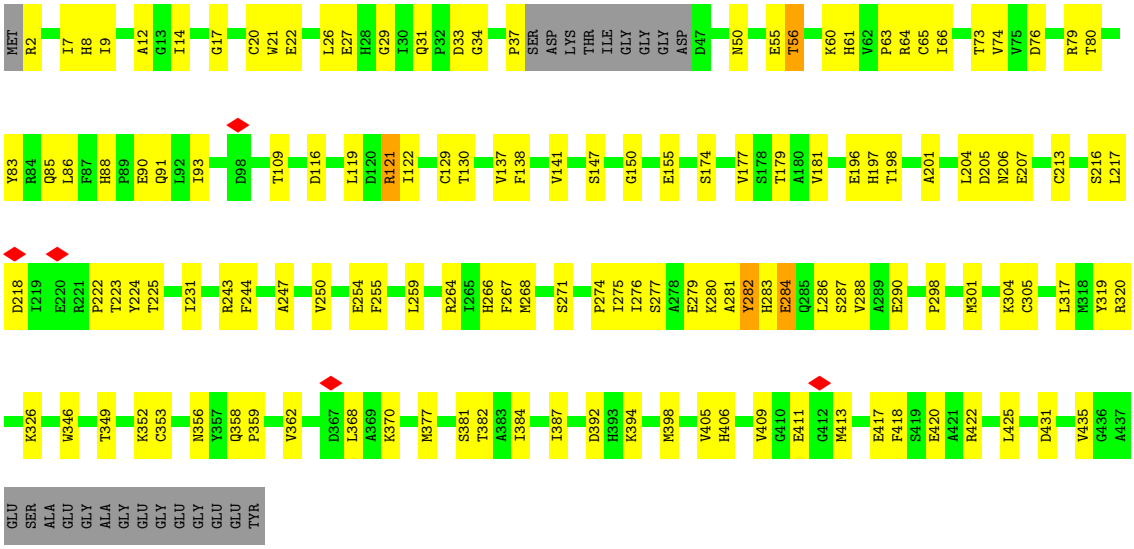
Chain J5:





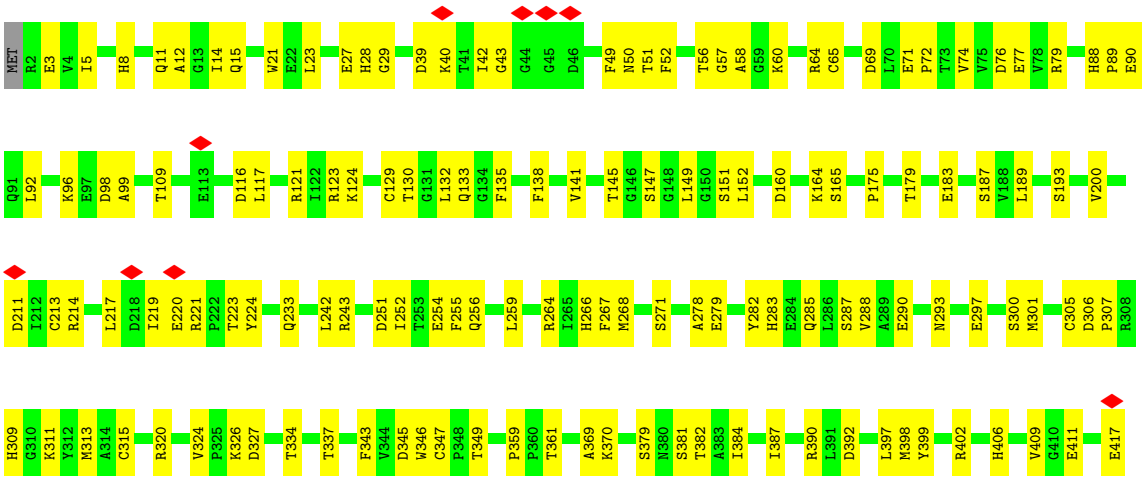

- Molecule 2: Tubulin alpha

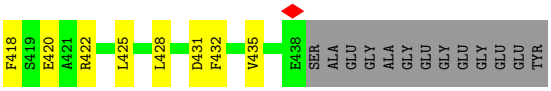
Chain J7:




- Molecule 2: Tubulin alpha

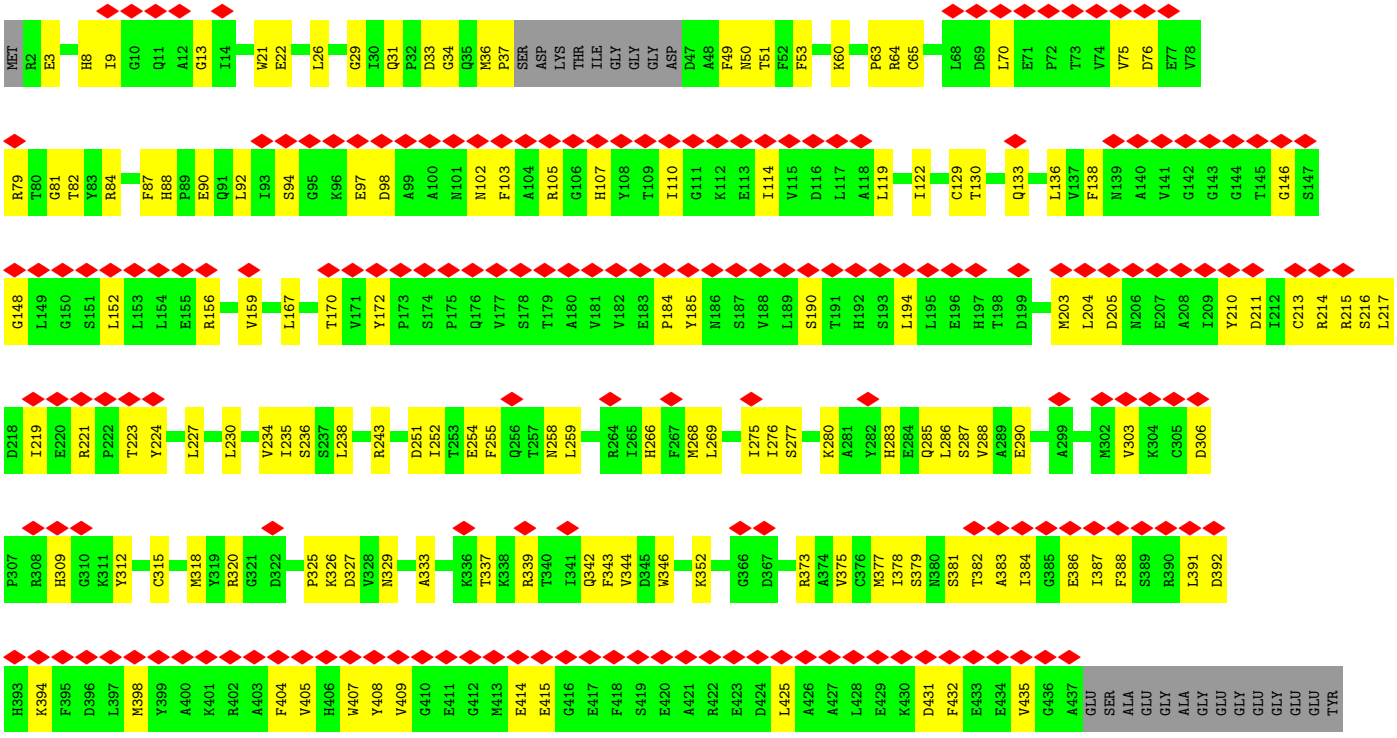
Chain J9:





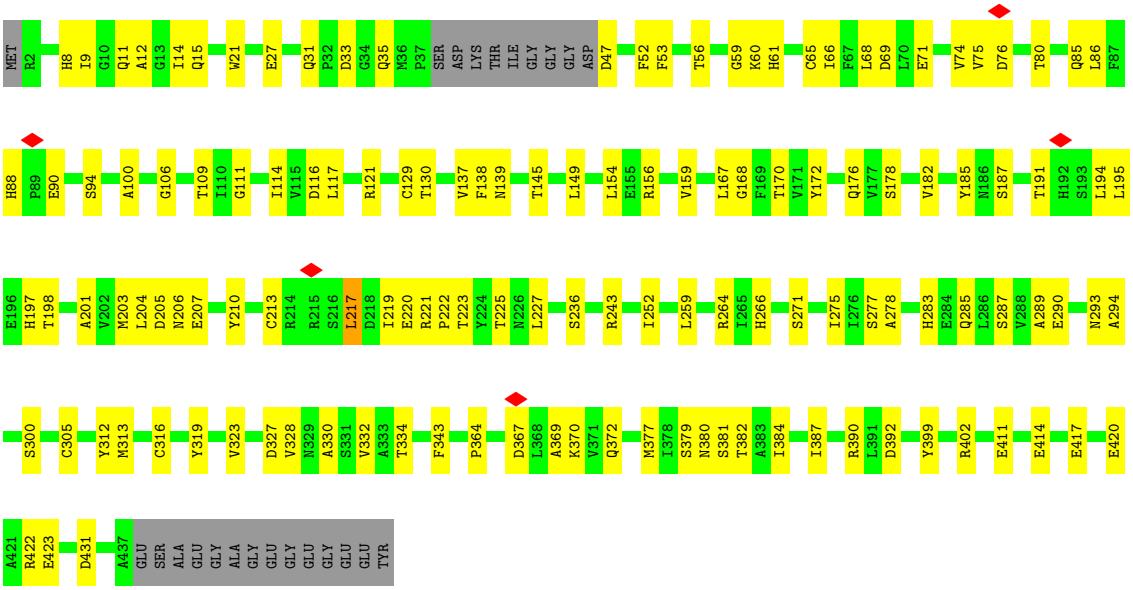

• Molecule 2: Tubulin alpha

Chain K1:




• Molecule 2: Tubulin alpha

Chain K3:



- Molecule 2: Tubulin alpha

Chain K5: 70% 24% 5%

MET R2 I7 H8 I9 G10 Q11 A12 G13 I14 Q15 N18 W21 E27 D33 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 F53 K60 H61 V62 P63 R64 C65 I66 D69 L70 V74 V75 D76 E77 T80 H88 P89 E90 D98 A99

T109 L119 D120 R121 I122 L125 C129 T130 V137 G146 G150 E155 L167 T170 Q176 V177 S178 E183 P184 S187 V188 L189 S190 T191 L194 L195 E196 H197 T198 D199 V200 N206 E207 C213 L217 D218 I219 T223 Y224 T225 T239

L242 R243 F244 D245 G246 I252 T253 E254 P261 R264 I265 H266 F267 E279 K280 H283 E284 Q285 L286 S287 V288 A289 E290 K304 M313 V324 D327 I335 R339 V344 D345 W346 K352 C353 N356 Y357 D367 R373 I384 I387 R390

L391 D392 L397 M398 Y399 A400 K401 R402 V405 E411 G412 M413 E414 E417 F418 S419 E420 A421 R422 K430 D431 E434 V435 G436 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain K7: 70% 25% 5%

MET R2 E3 I7 H8 I9 A12 W21 E27 D33 G34 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 N50 T51 F52 F53 K60 H61 R64 C65 D69 L70 E71 P72 R79 R84 H88 P89 E90 Q91 D98 A99 A100 N101 Y108

T109 K112 R121 L125 C129 T130 V137 F138 T145 G146 S151 R156 V159 L167 P175 Q176 A180 E183 S187 T191 H192 S193 L194 T198 D199 V200 A201 D205 N206 C213 R214 R215 I219 T223 Y224 L227 I231

R243 V250 D251 I252 T253 E254 F255 L259 R264 F267 M268 P274 A278 Y282 H283 L286 S287 V288 A289 E290 I291 T292 H309 C316 L317 M318 Y319 V324 P325 K326 N329 A330 S331 T334 I335 K336 R339 Q342 F343 V344 D345 W346 D367 L368

A369 C376 M377 I378 S379 N380 S381 T382 A383 I384 I387 Y399 R402 V405 E411 G412 M413 E417 F418 S419 E420 D431 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

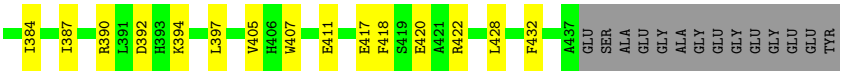
- Molecule 2: Tubulin alpha

Chain K9: 71% 24% 5%

MET R2 E3 V4 I7 H8 I9 G10 Q11 I14 W21 E27 Q31 P32 D33 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 F52 F53 H61 V62 P63 I66 F67 L68 P72 T73 V74 V75 D76 Q85 H88 P89 E90 K96 E97 D98

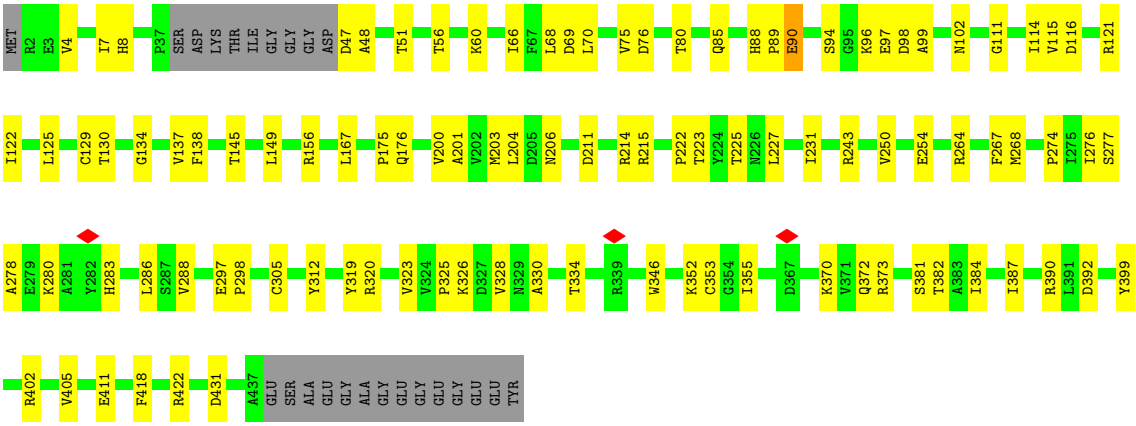
A99 A100 N101 N102 R105 D116 L117 A118 L119 D120 R121 I122 L125 C129 T130 G134 F135 L136 V137 G146 G150 L157 K163 T170 S174 P175 Q176 V177 S178 E183 S187 V188 L189 S190 T191 L194 A201 D205 N206 I209 R215 S216

L217 P222 L230 T239 A240 S241 L242 R243 V250 E254 F255 N258 L259 M268 S271 P274 I275 I276 S277 A278 A281 Y282 H283 S287 V288 A289 E290 K304 K311 K326 N329 T334 T337 Q342 W346 K352 A369 M377



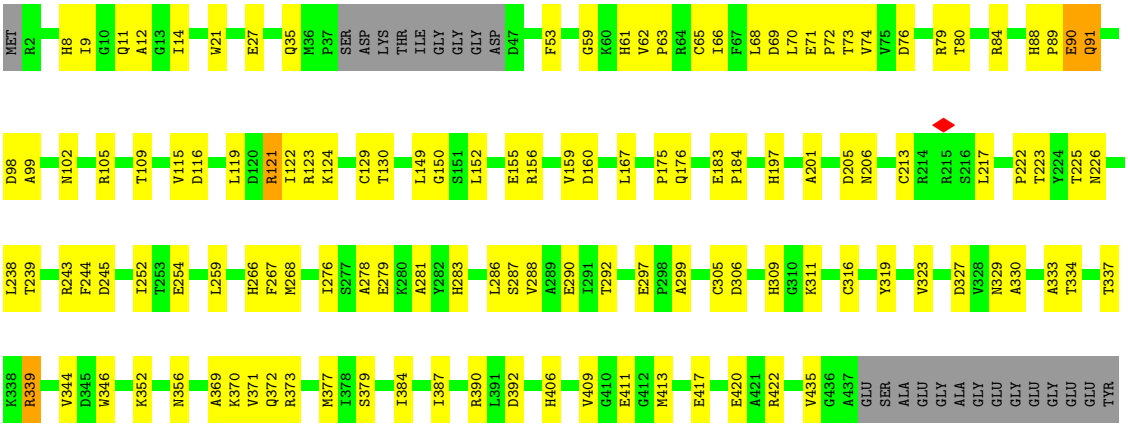

• Molecule 2: Tubulin alpha

Chain L1:



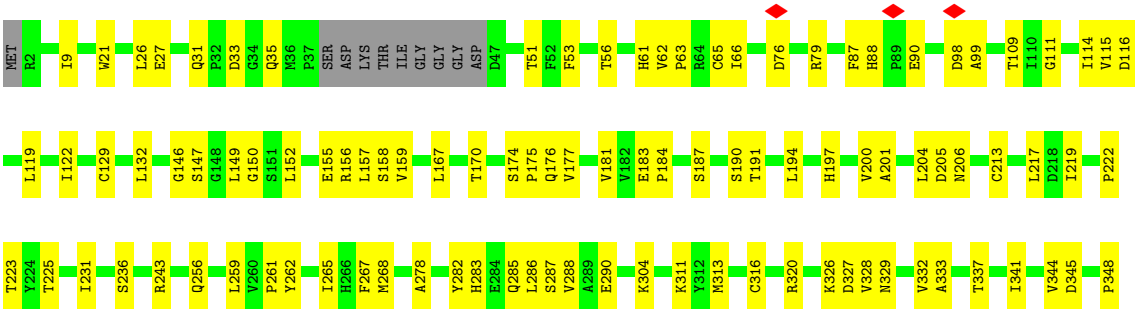

• Molecule 2: Tubulin alpha

Chain L3:



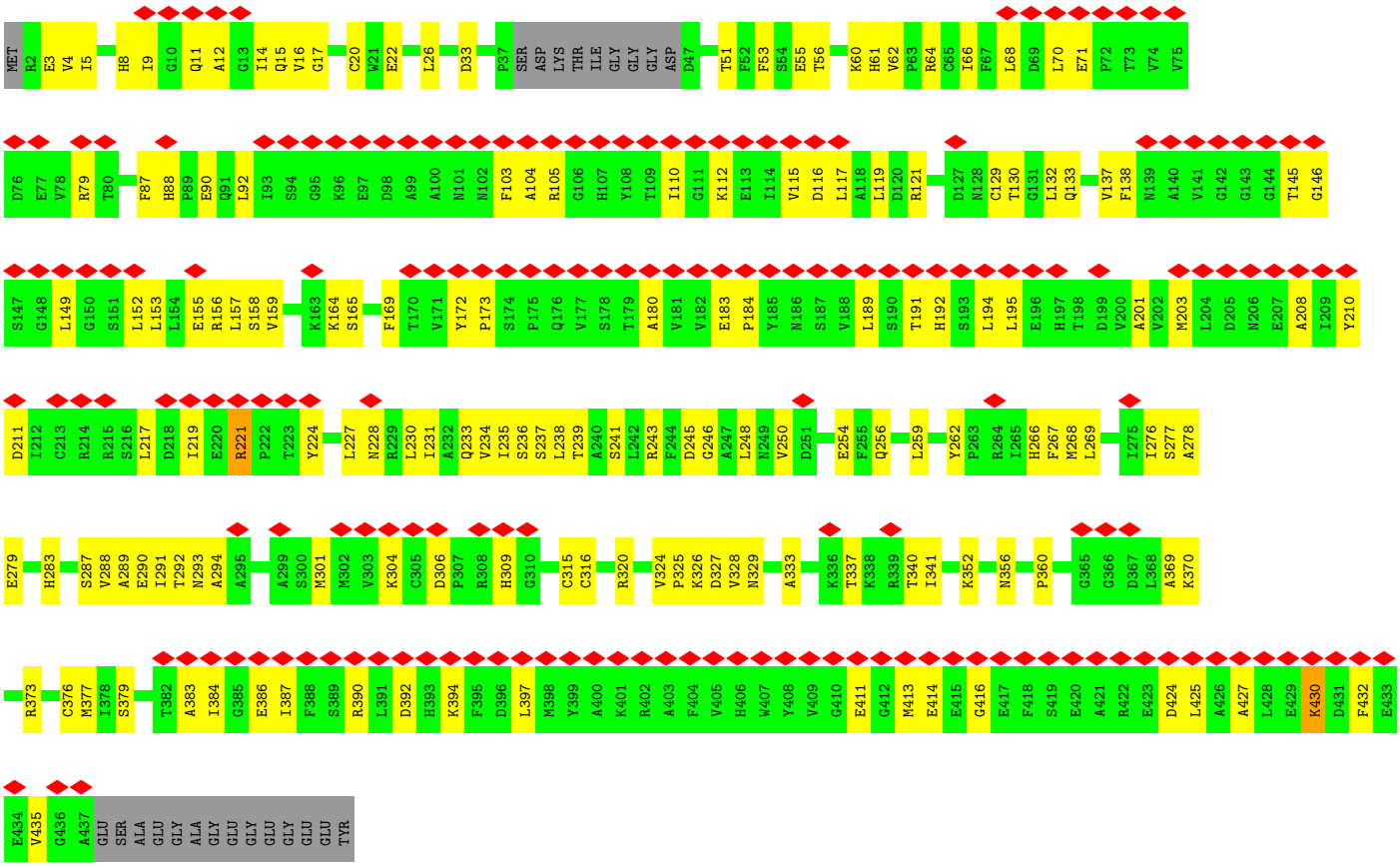

• Molecule 2: Tubulin alpha

Chain L5:



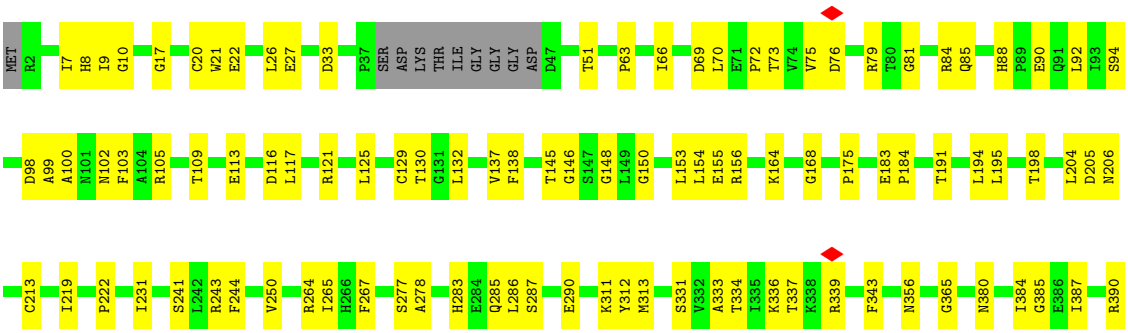
• Molecule 2: Tubulin alpha

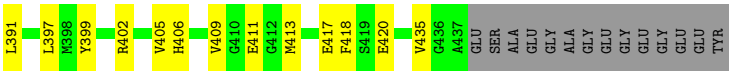
Chain L7:




• Molecule 2: Tubulin alpha

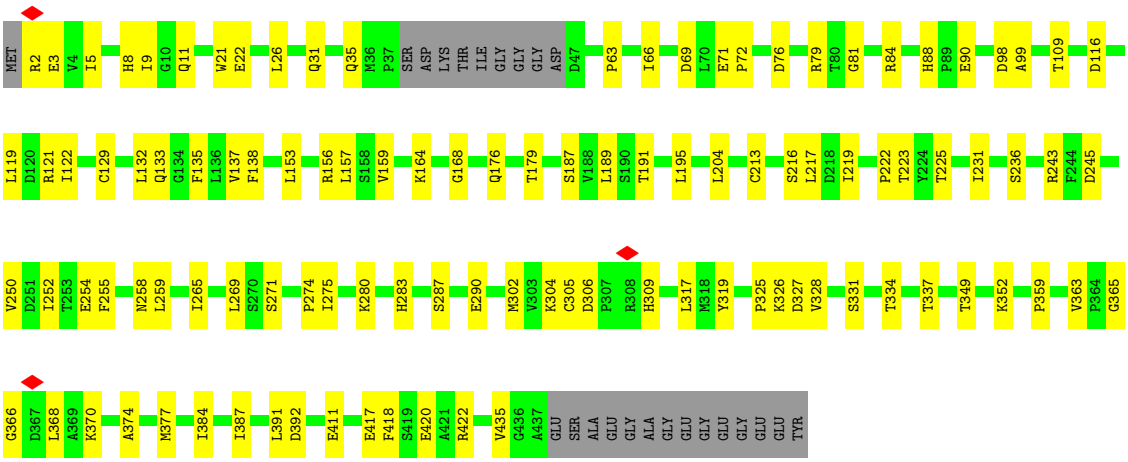
Chain L9:





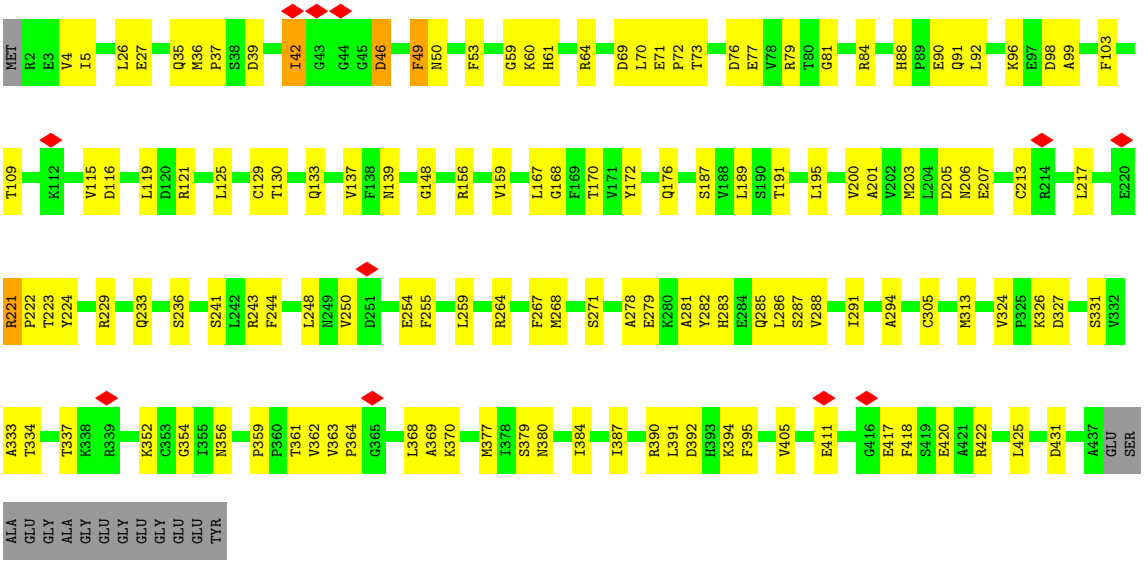

• Molecule 2: Tubulin alpha

Chain M1:



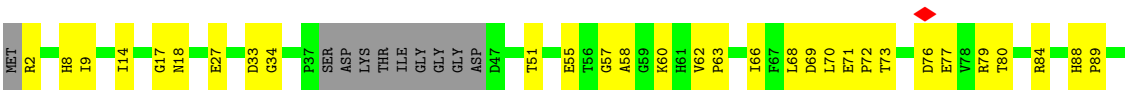

• Molecule 2: Tubulin alpha

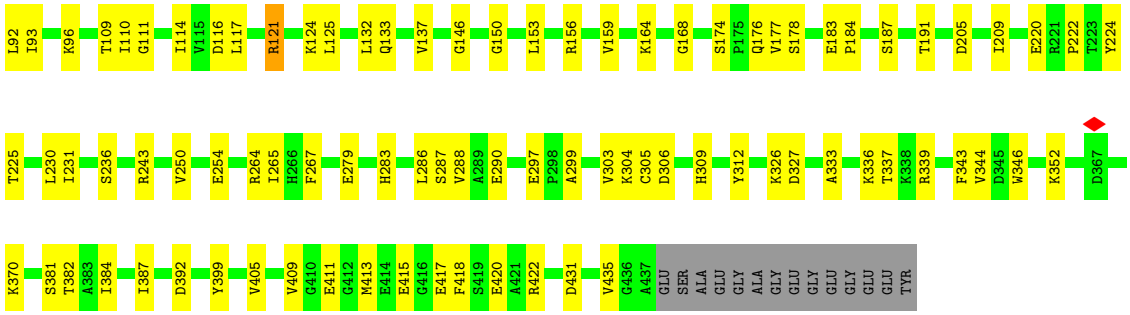
Chain M3:




• Molecule 2: Tubulin alpha

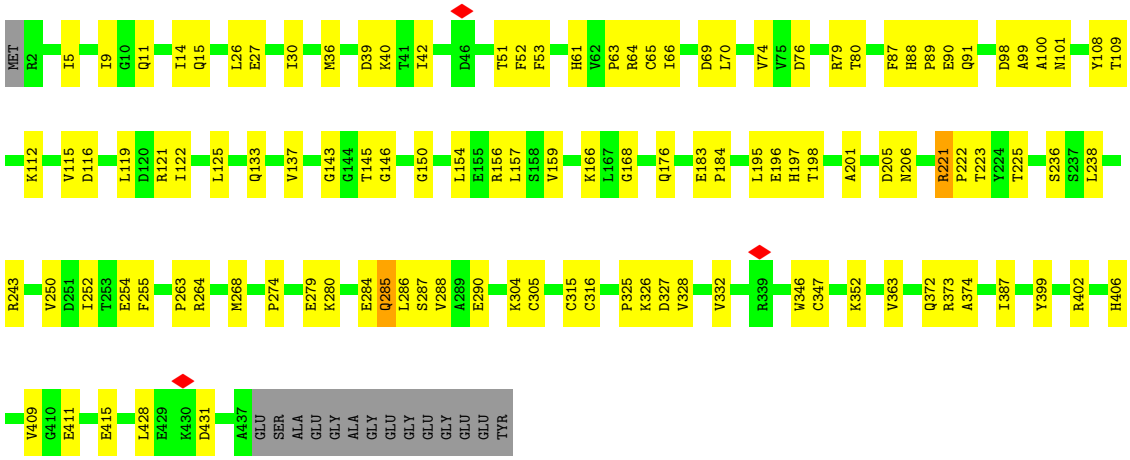
Chain M5:





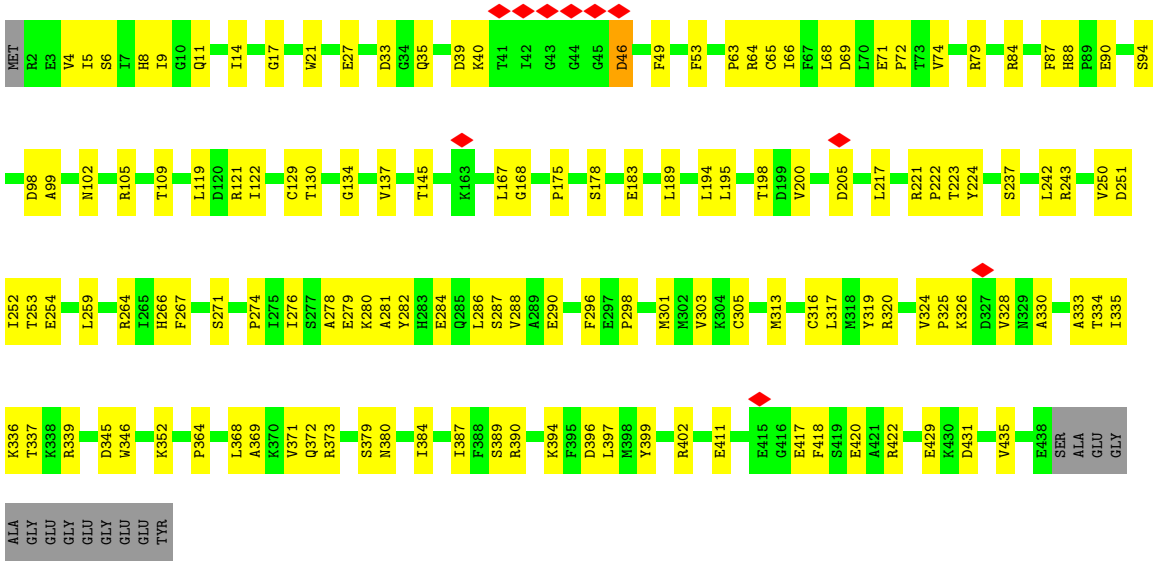

- Molecule 2: Tubulin alpha

Chain M7:



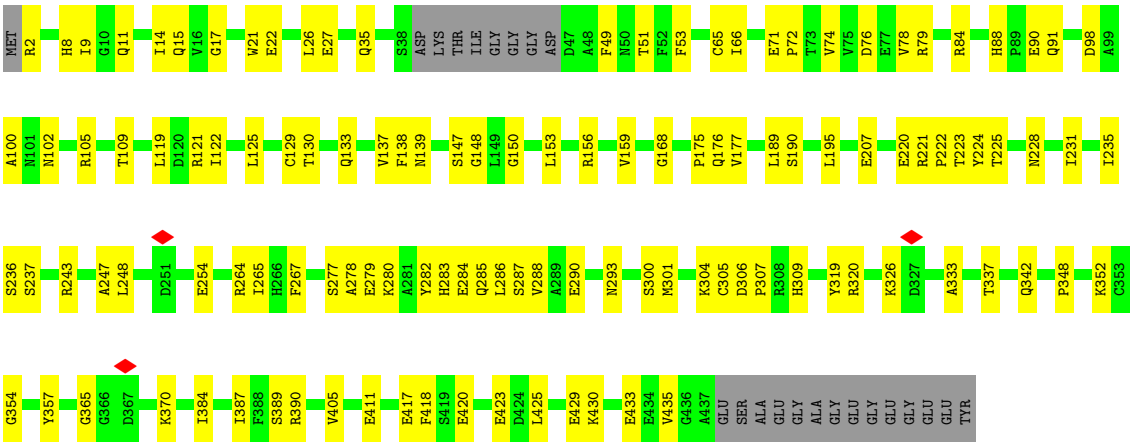

- Molecule 2: Tubulin alpha

Chain M9:



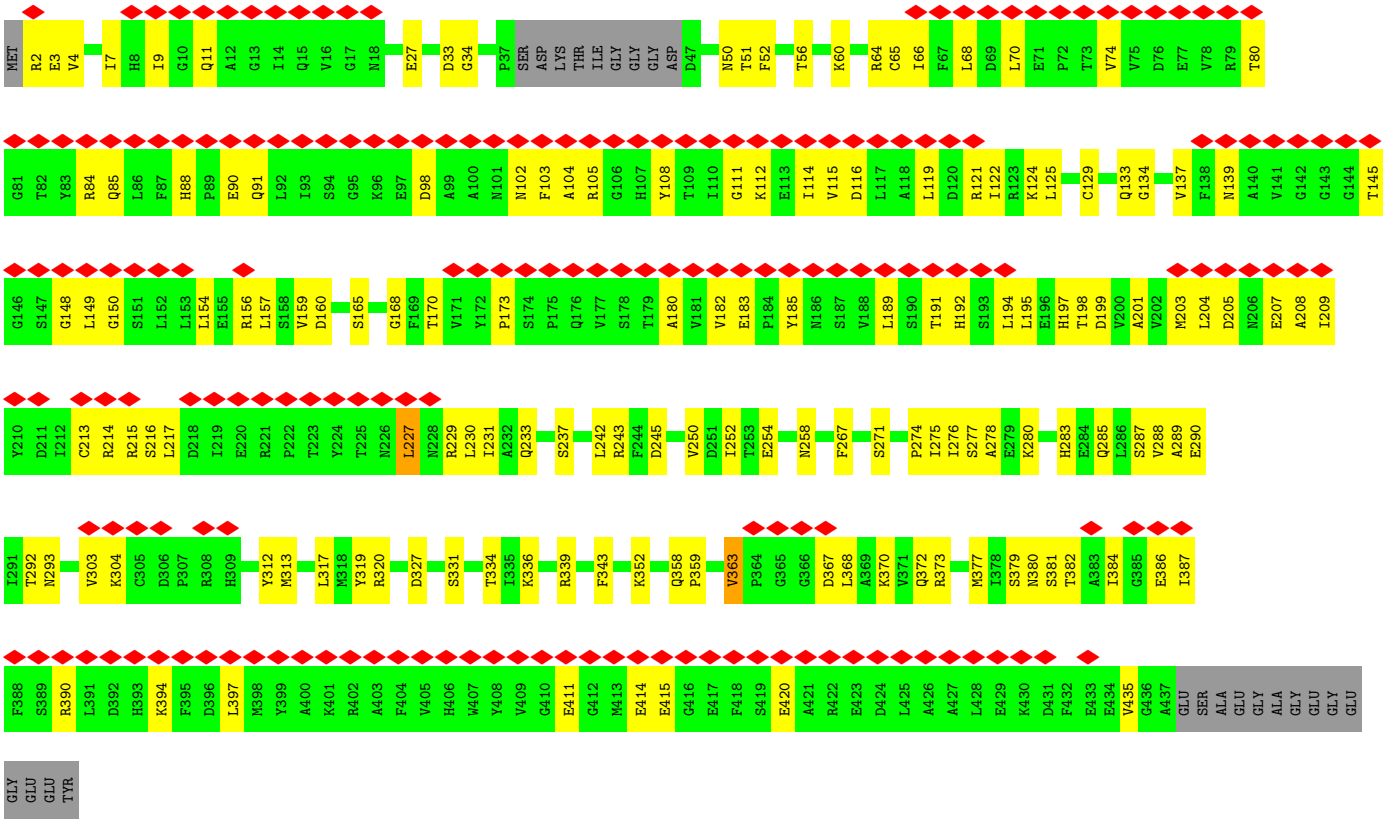

- Molecule 2: Tubulin alpha

Chain N1:




- Molecule 2: Tubulin alpha

Chain N3:

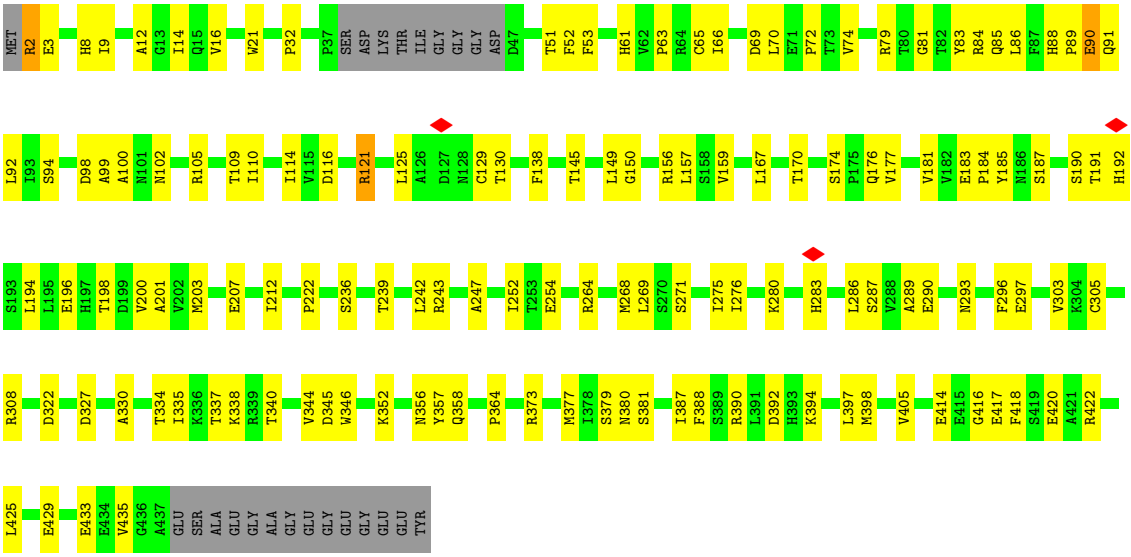



- Molecule 2: Tubulin alpha

Chain N5:

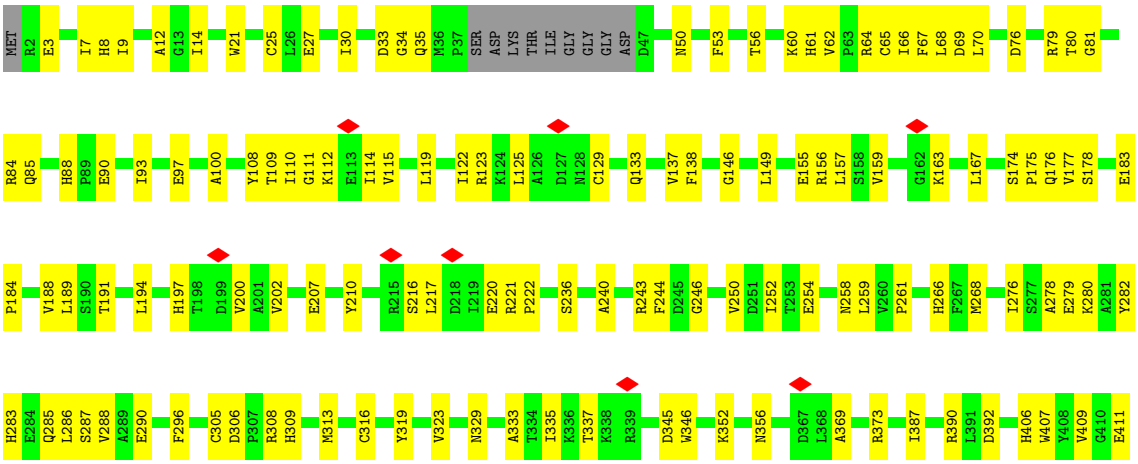
- Molecule 2: Tubulin alpha

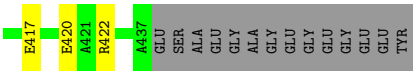
Chain N7:




- Molecule 2: Tubulin alpha

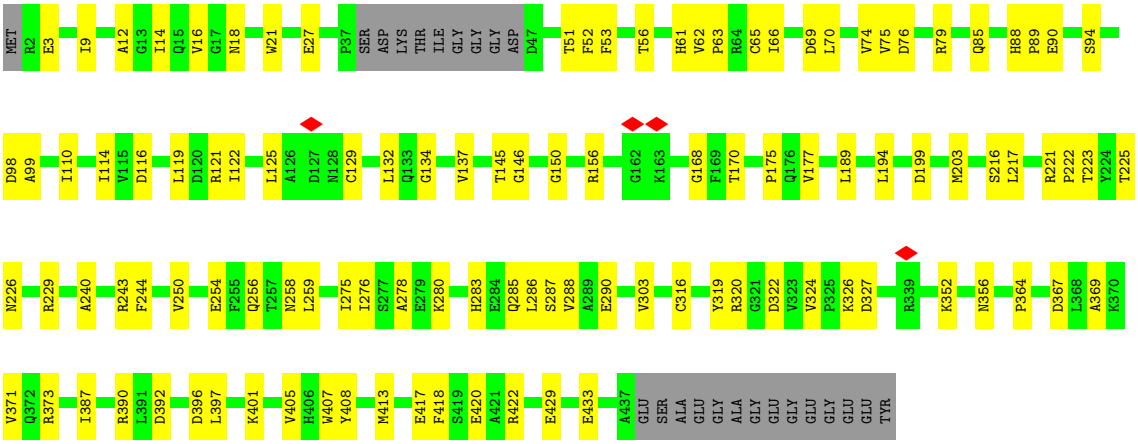
Chain N9:





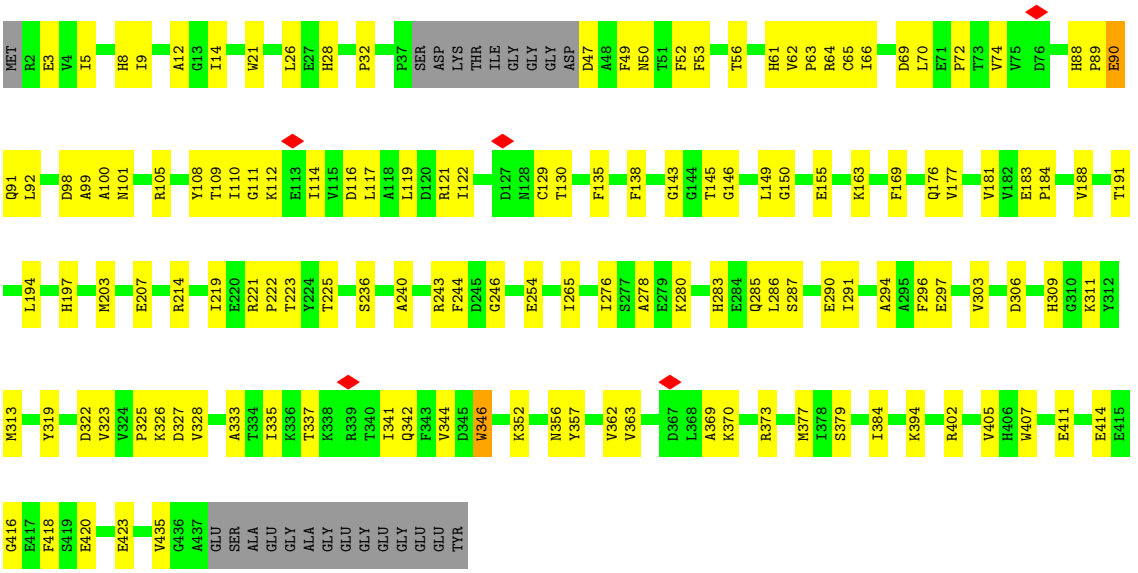

• Molecule 2: Tubulin alpha

Chain O1:



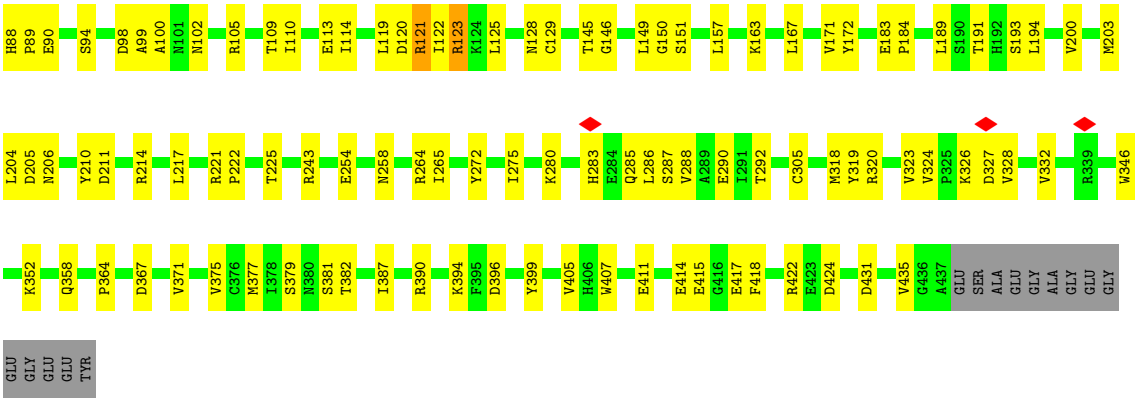

• Molecule 2: Tubulin alpha

Chain O3:



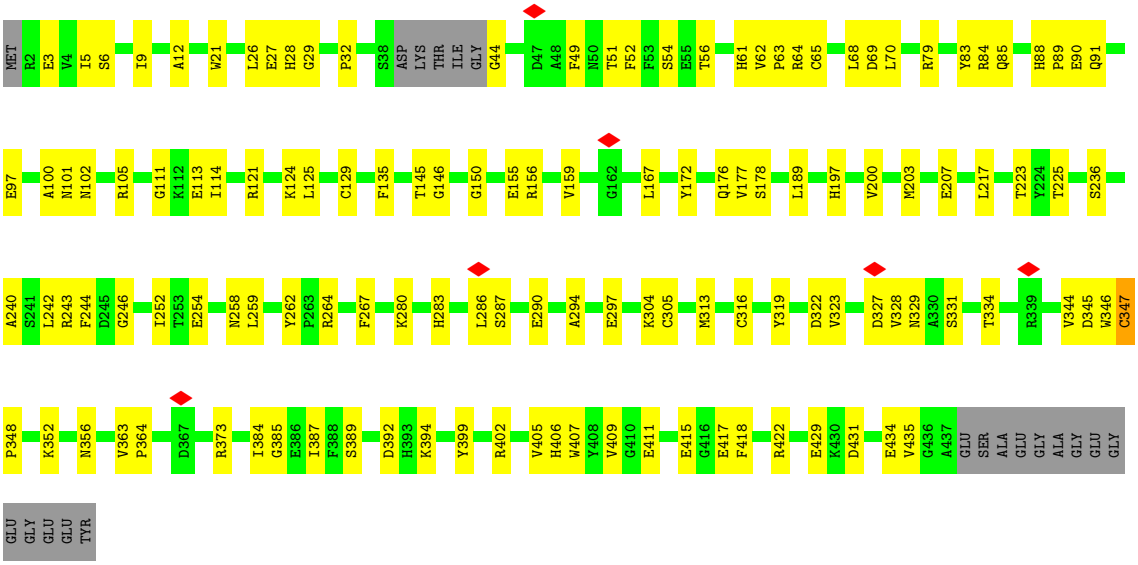

• Molecule 2: Tubulin alpha

Chain O5:



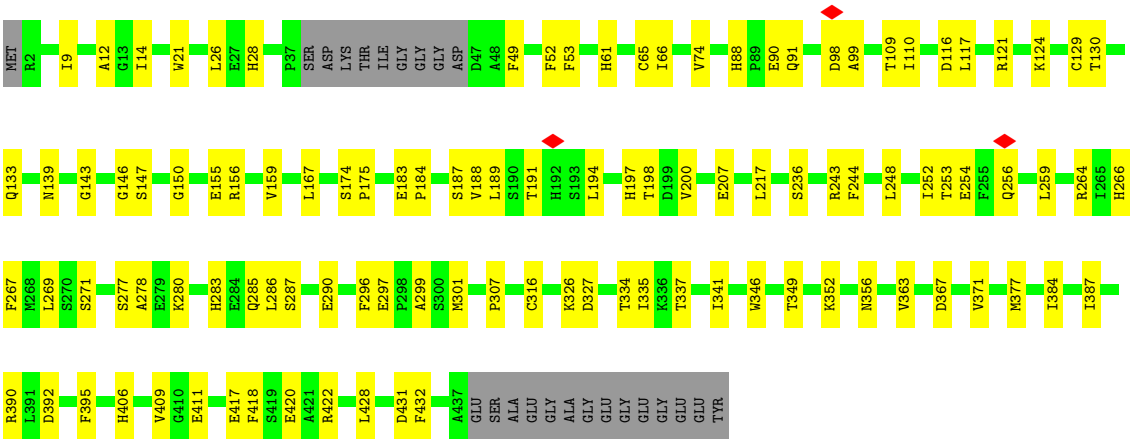

• Molecule 2: Tubulin alpha

Chain O7:



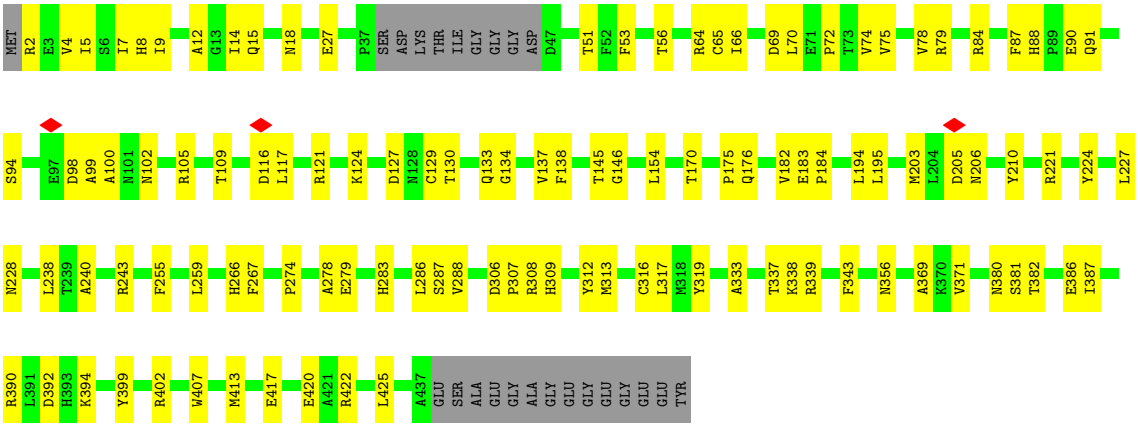

• Molecule 2: Tubulin alpha

Chain O9:



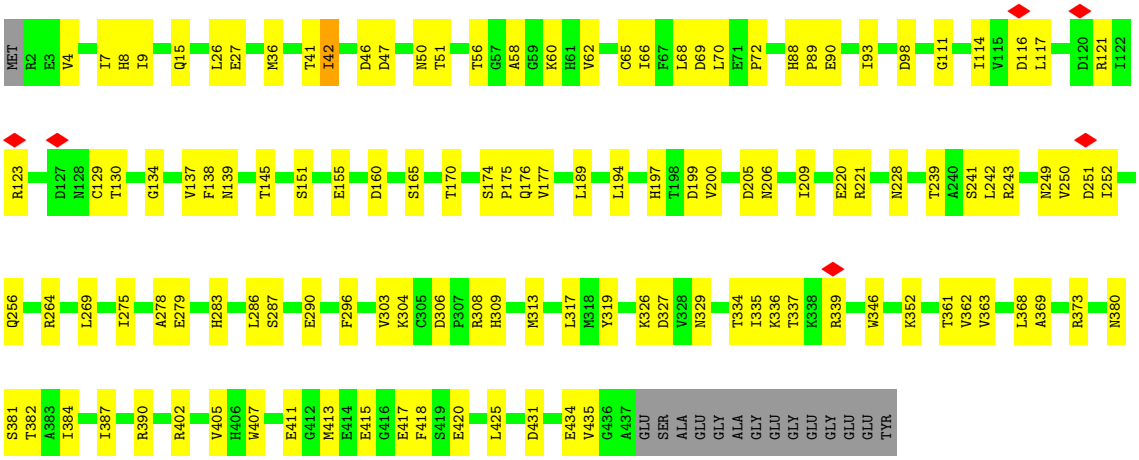
- Molecule 2: Tubulin alpha

Chain P3:



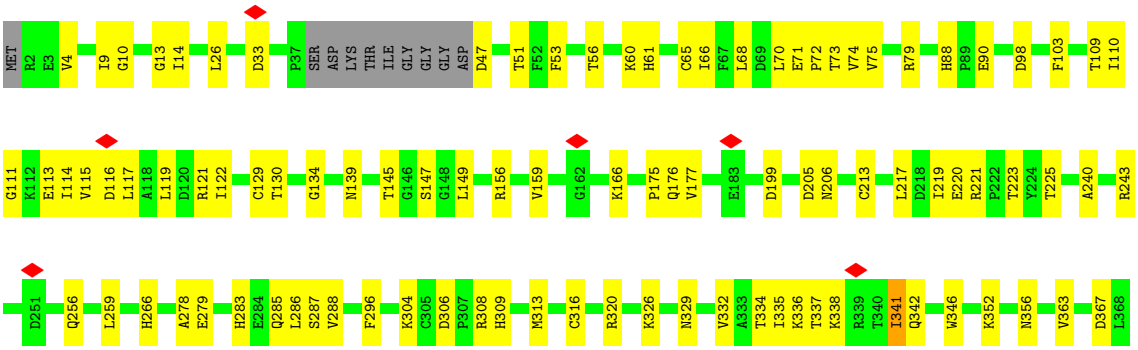

- Molecule 2: Tubulin alpha

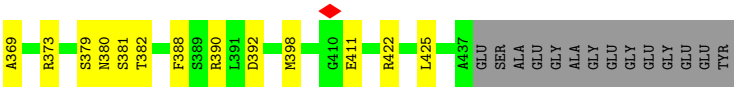
Chain P5:




- Molecule 2: Tubulin alpha

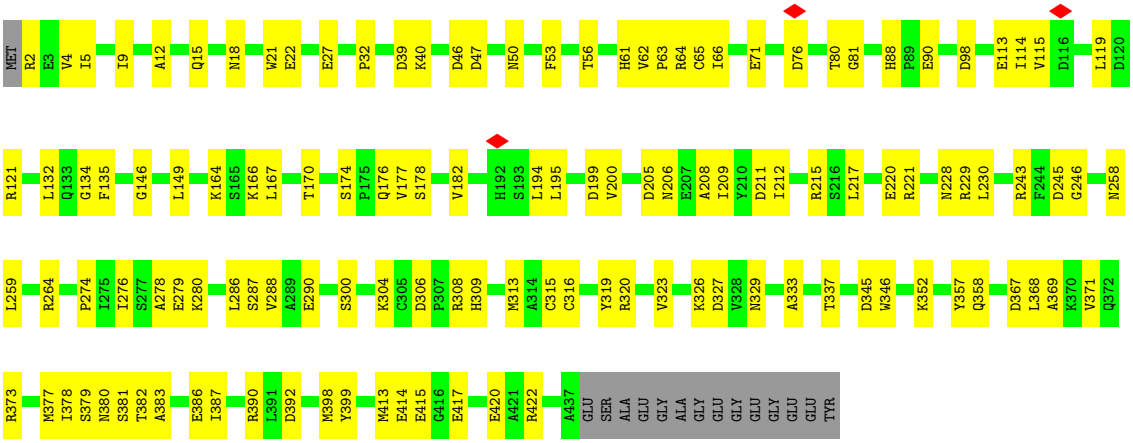
Chain P7:





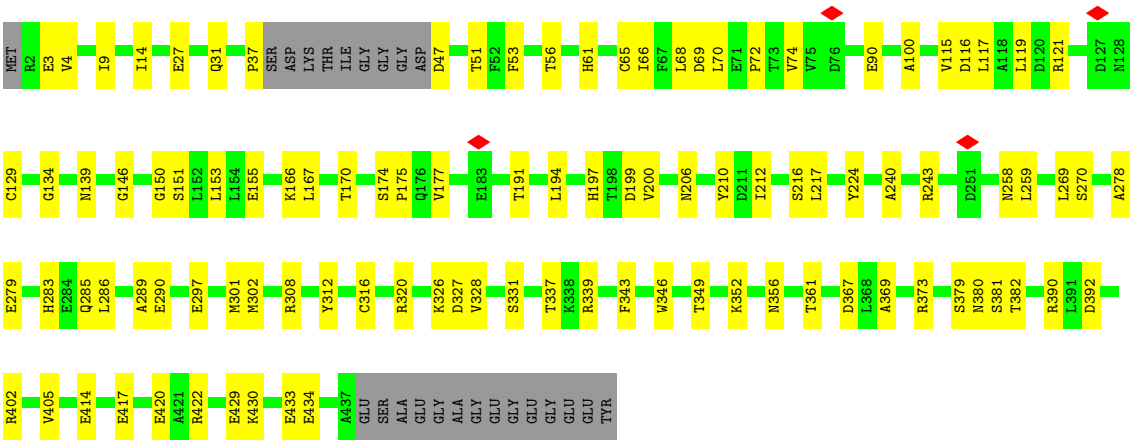

• Molecule 2: Tubulin alpha

Chain P9:



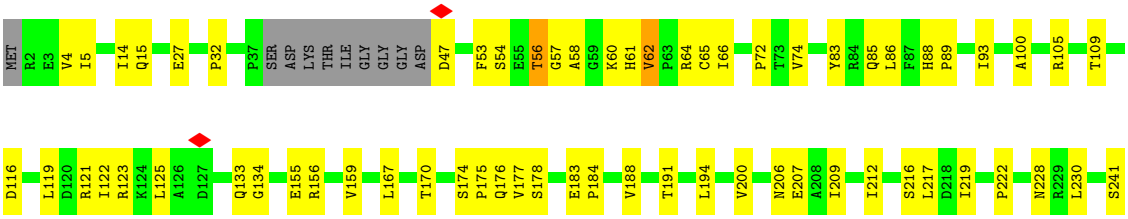

• Molecule 2: Tubulin alpha

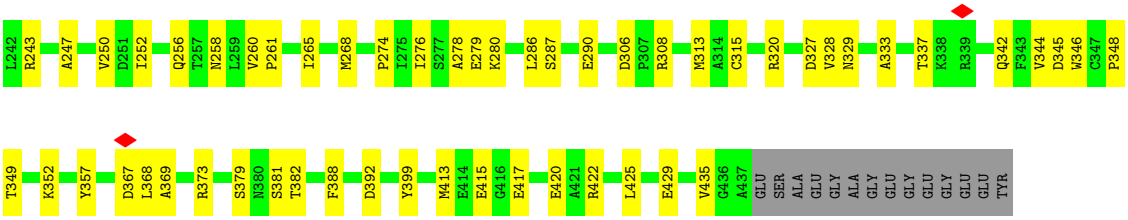
Chain Q1:




• Molecule 2: Tubulin alpha

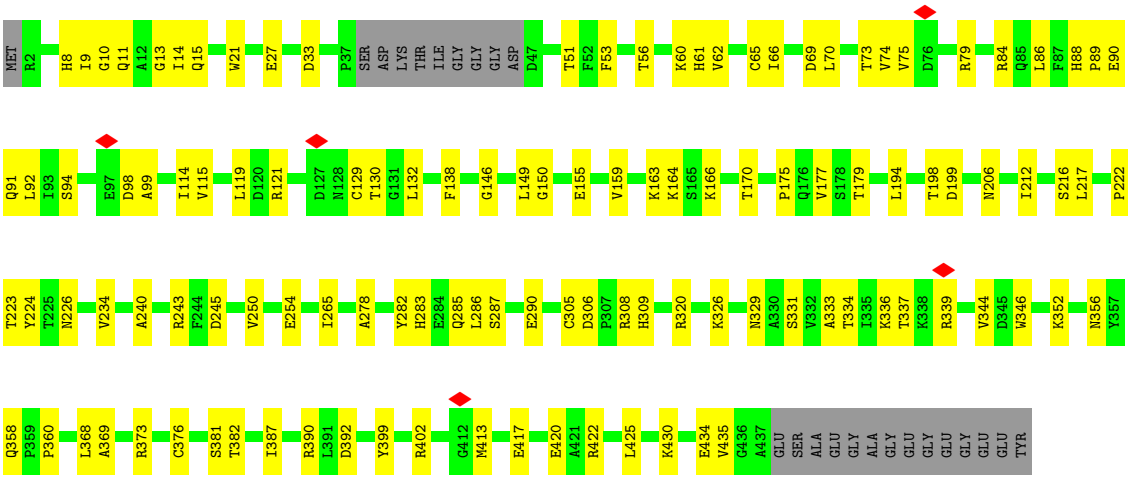
Chain Q3:





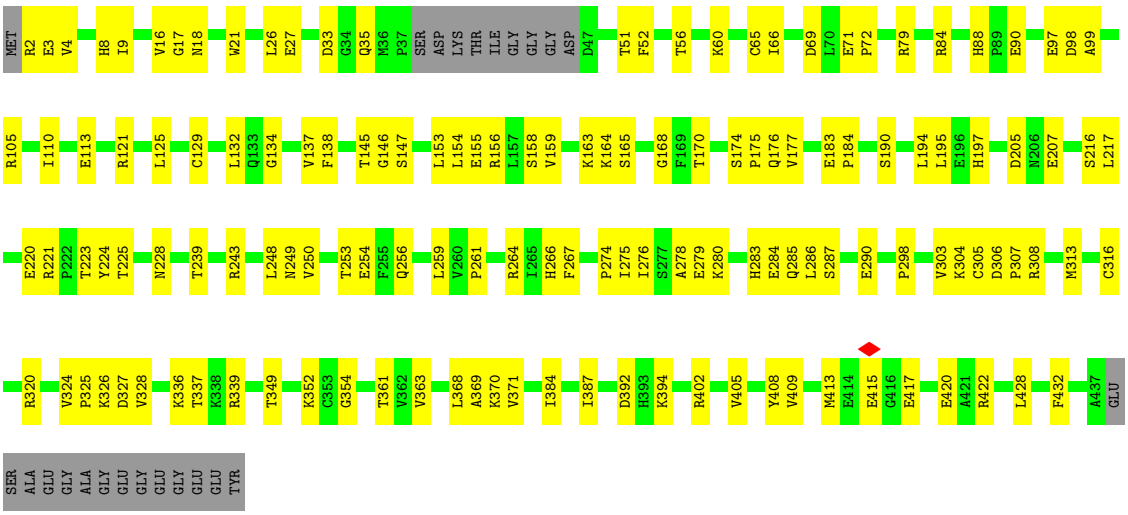

• Molecule 2: Tubulin alpha

Chain Q5:



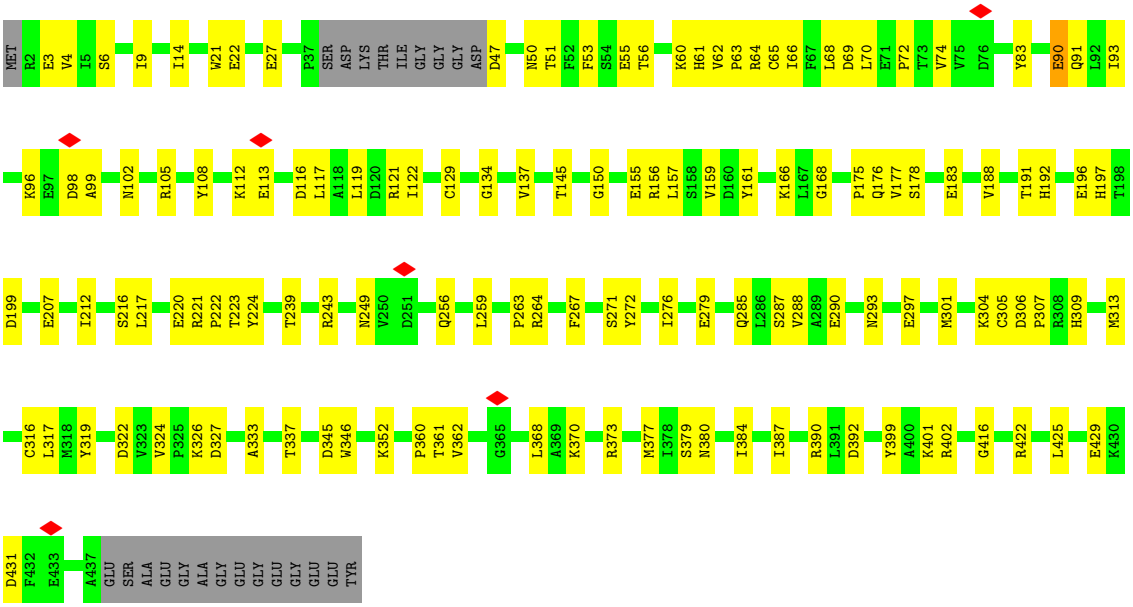

• Molecule 2: Tubulin alpha

Chain Q9:



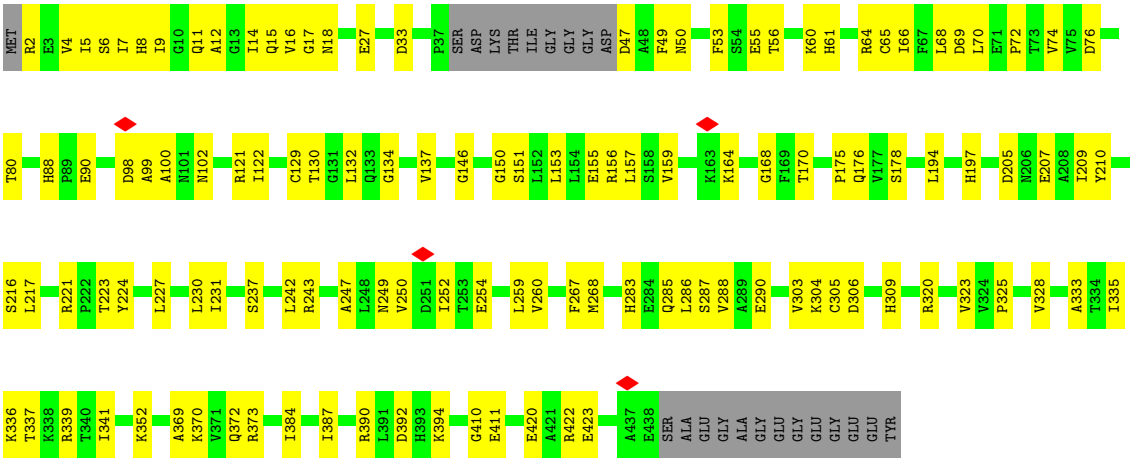

• Molecule 2: Tubulin alpha

Chain R1:



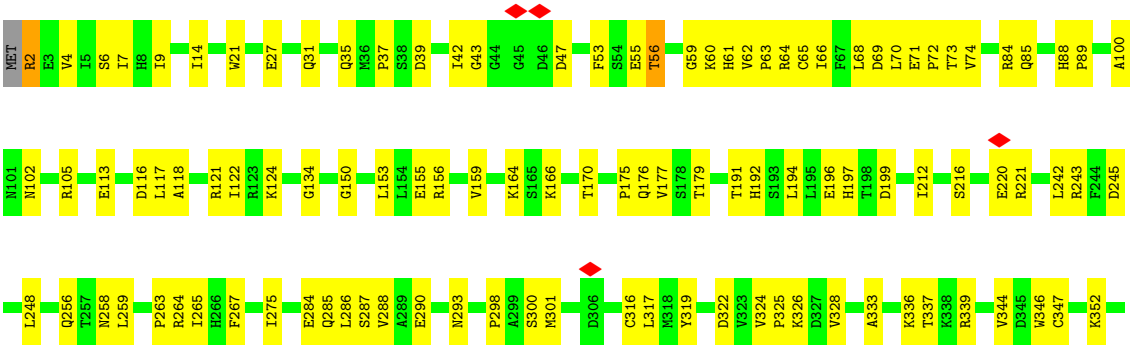

- Molecule 2: Tubulin alpha

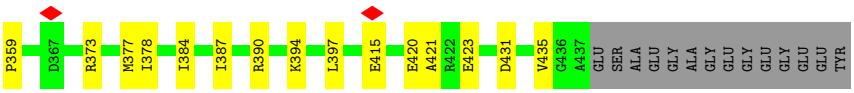
Chain R3:




- Molecule 2: Tubulin alpha

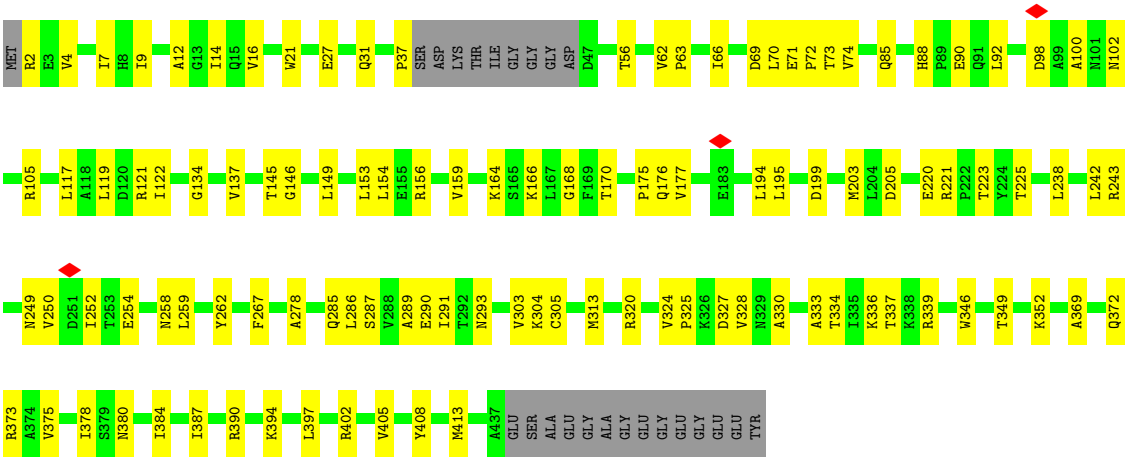
Chain R5:





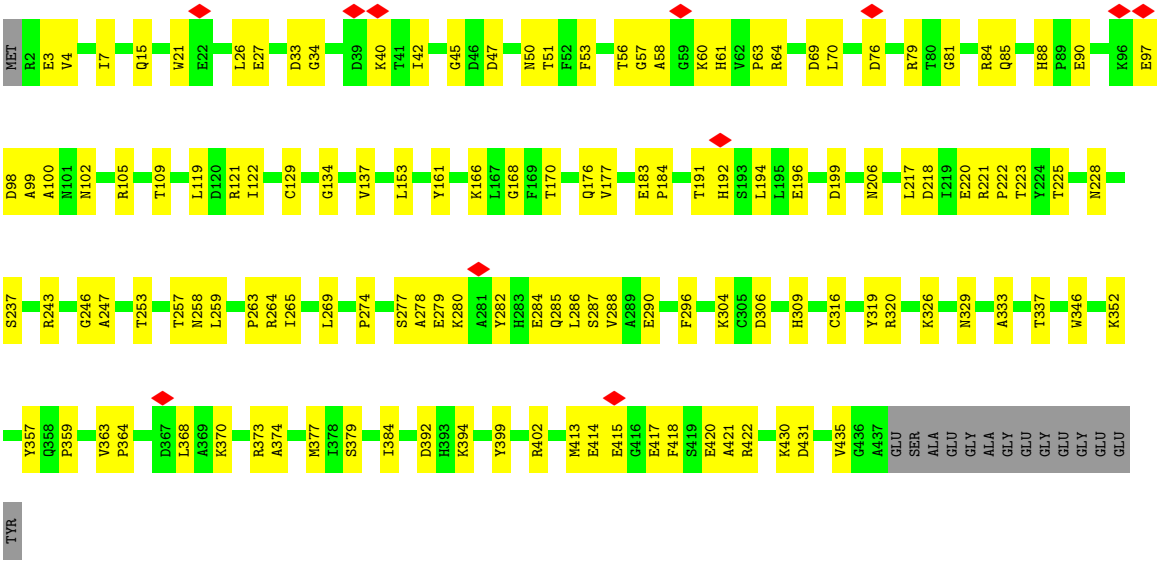

• Molecule 2: Tubulin alpha

Chain R7:



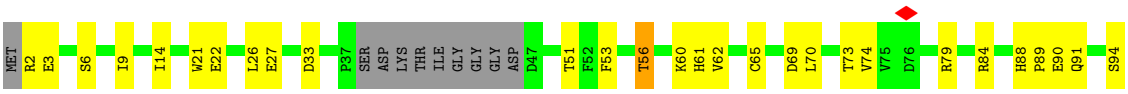

• Molecule 2: Tubulin alpha

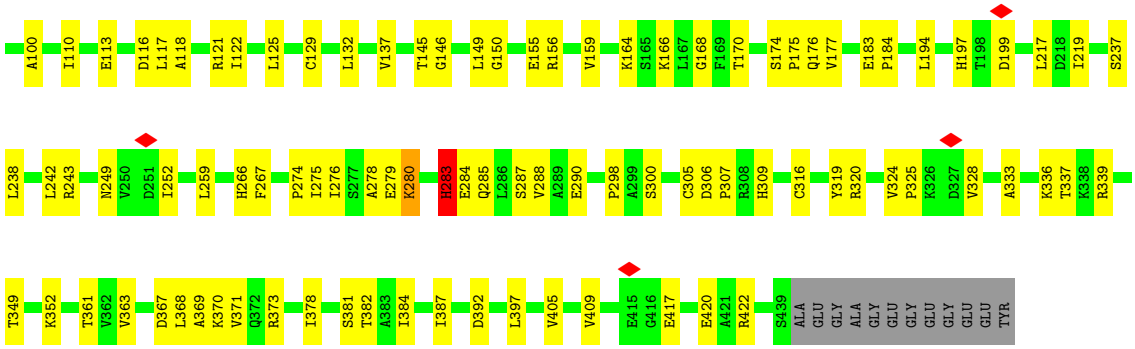
Chain R9:




• Molecule 2: Tubulin alpha

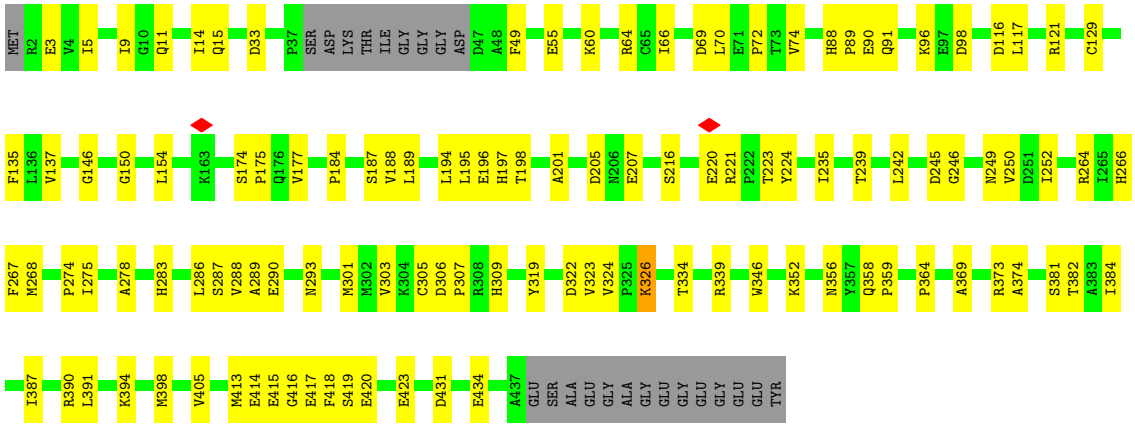
Chain S1:





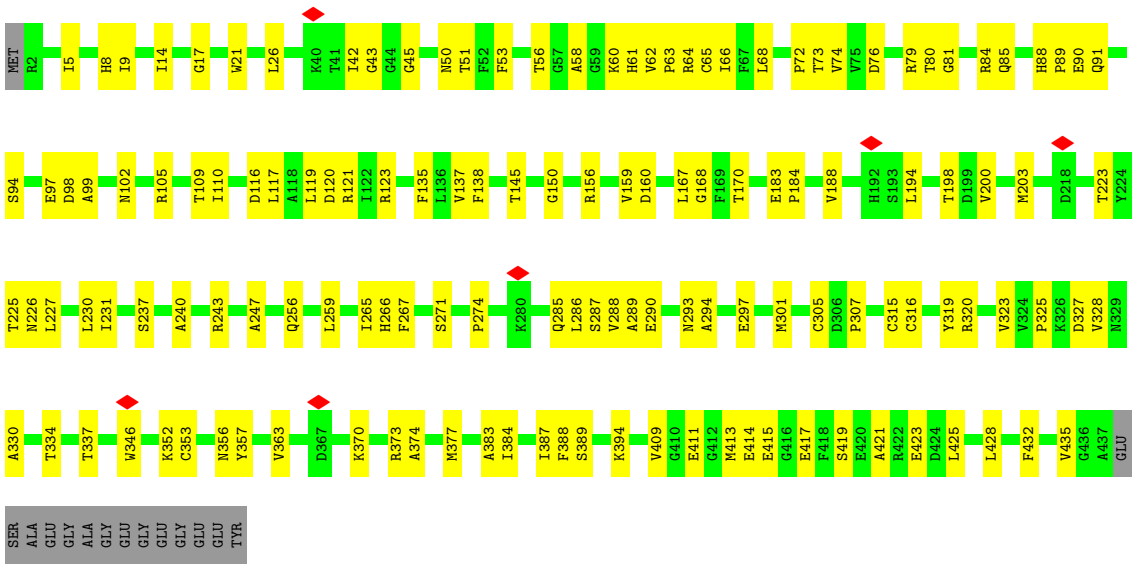

- Molecule 2: Tubulin alpha

Chain S5:



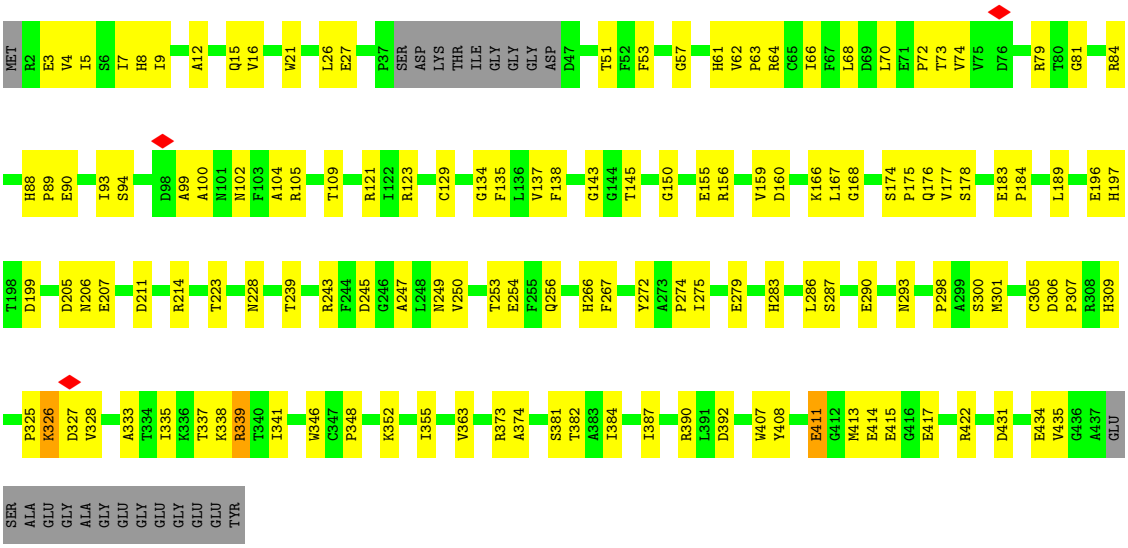

- Molecule 2: Tubulin alpha

Chain S7:



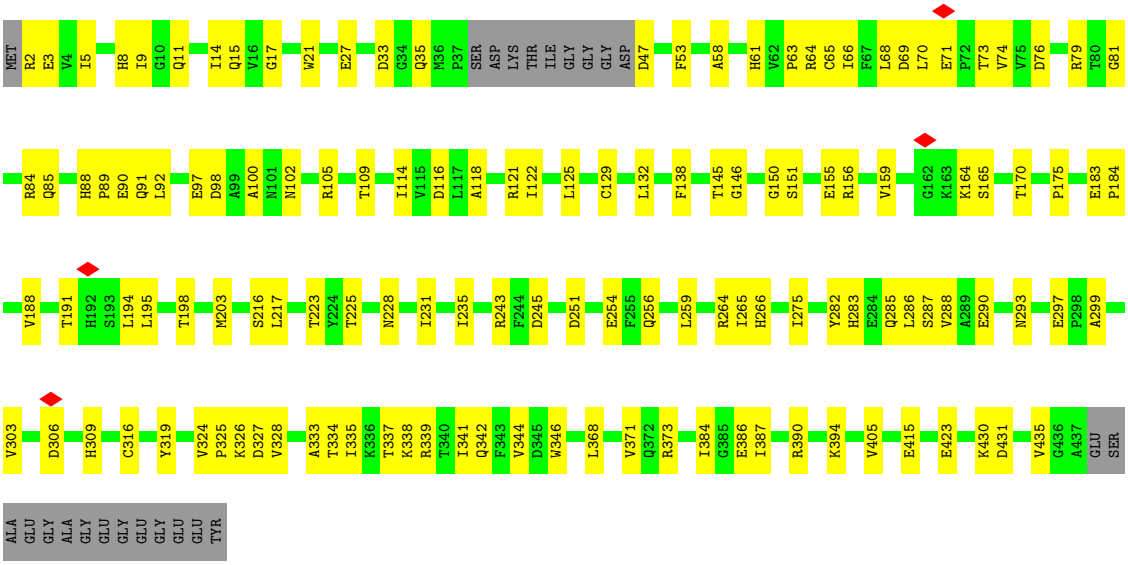

- Molecule 2: Tubulin alpha

Chain S9:



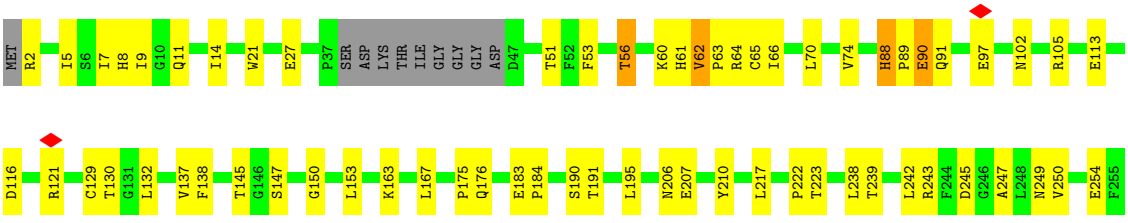

- Molecule 2: Tubulin alpha

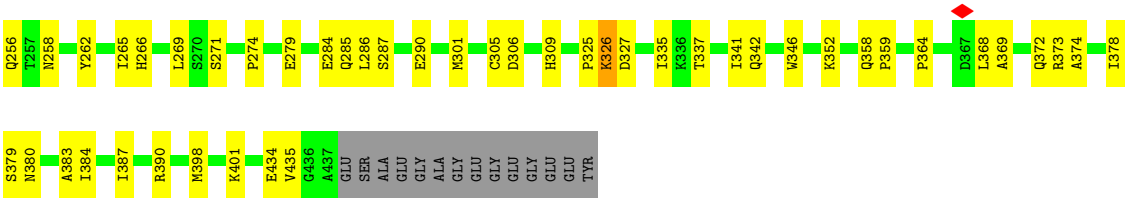
Chain T1:




- Molecule 2: Tubulin alpha

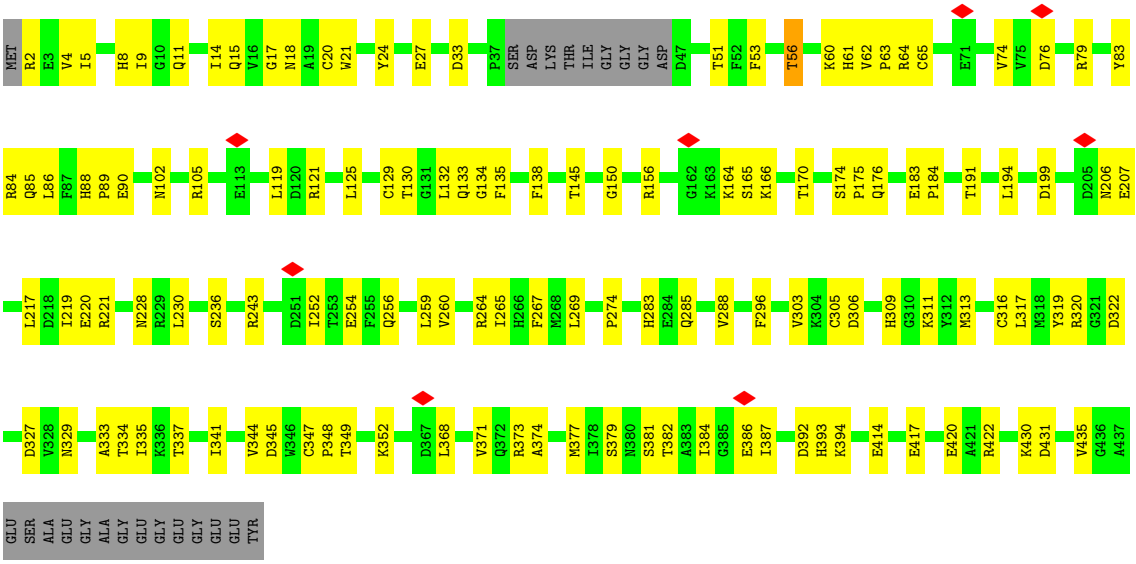
Chain T3:





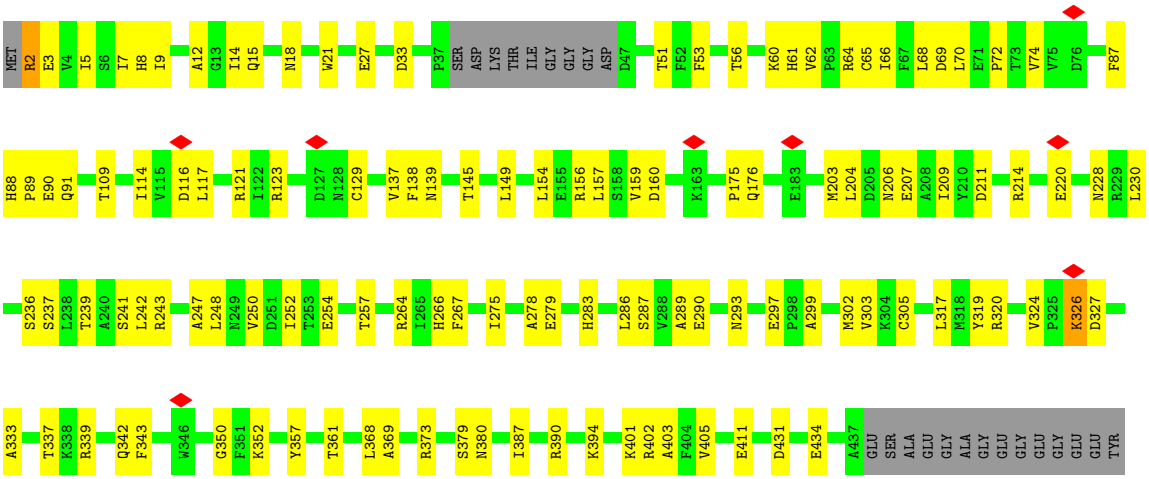

• Molecule 2: Tubulin alpha

Chain T5:



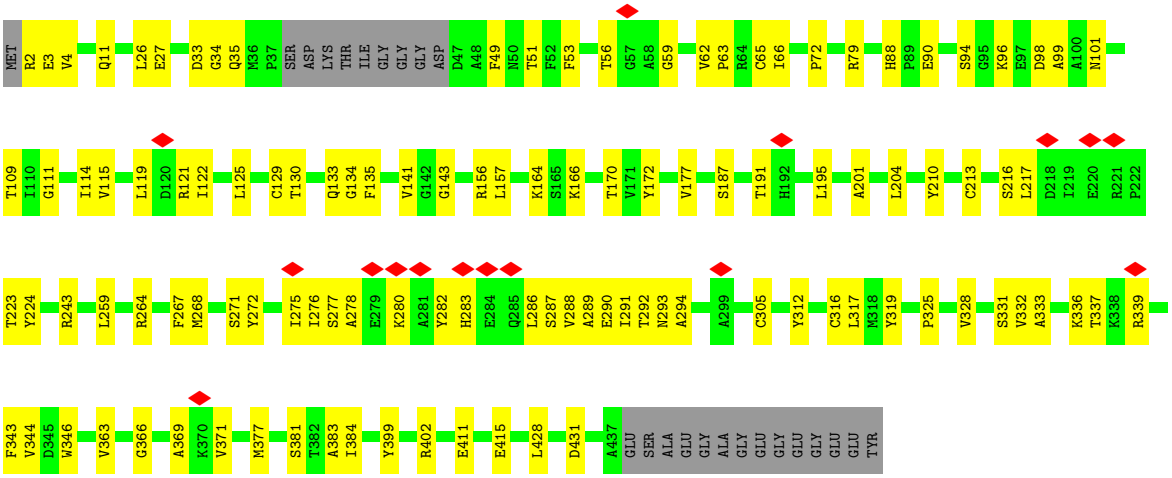

• Molecule 2: Tubulin alpha

Chain T7:



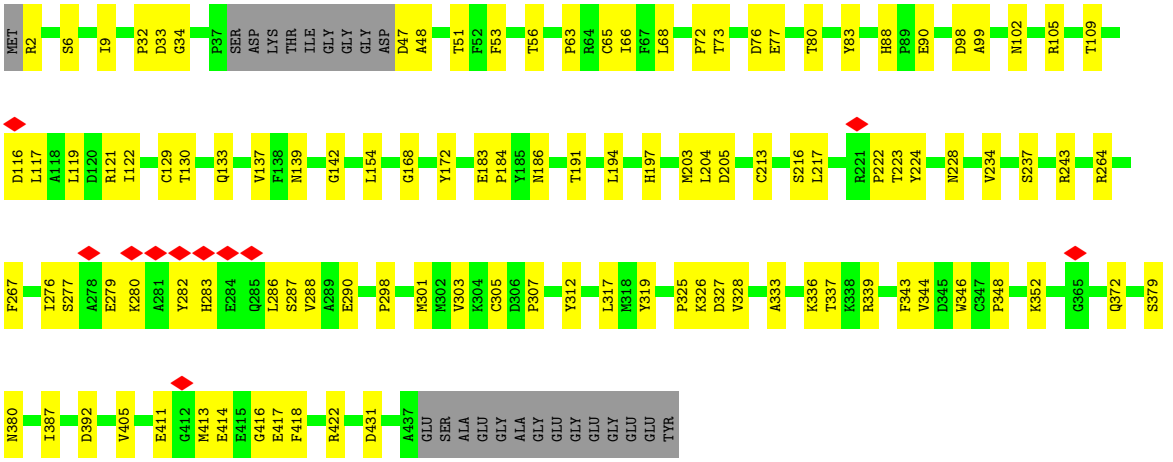

• Molecule 2: Tubulin alpha

Chain U1:



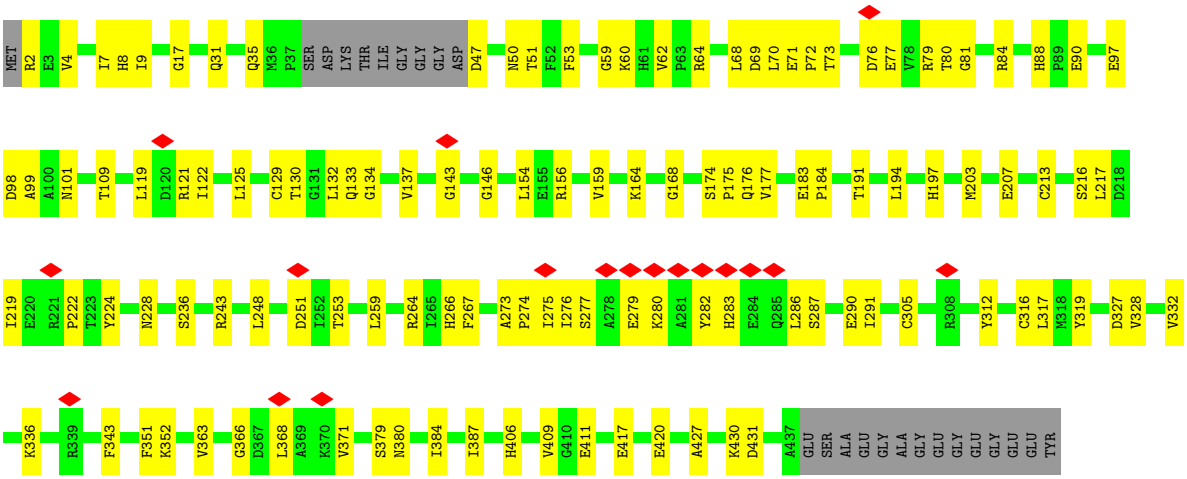

- Molecule 2: Tubulin alpha

Chain U3:




- Molecule 2: Tubulin alpha

Chain U5:



• Molecule 2: Tubulin alpha

Chain U7: 69% 25% 5%

MET R2 I5 I9 G10 Q11 Q15 W21 L26 E27 P32 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 T56 G59 K60 P63 R64 C65 I66 F67 L68 P72 T73 V74 V75 D76 E77 V78 R79 Y83 R84 Q85 H88

P89 E90 I93 S94 A100 N101 T109 L119 D120 R121 I122 L125 C129 T130 Q133 G143 G146 L154 P175 Q176 V177 T191 H192 S193 L194 L195 E196 H197 V200 M203 L204 C213 L217 R221 P222 T223 Y224 T225 L242 R243 A247

L248 N249 V250 D251 E254 F255 Q256 R264 F267 M268 L269 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 E290 A299 S300 M301 M302 V303 K304 C305 D306 P307 L317 M318 Y319 R320 P325 K326 D327 V328 N329 A333 T334 I335 K336 T337 T340 I341 G350 F351 K352

I355 N356 Y357 Q358 P359 V363 P364 G365 G366 D367 K370 I384 I387 R390 D396 Y399 R402 V405 H406 V409 G410 E411 E415 F418 R422 L425 D431 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

• Molecule 2: Tubulin alpha

Chain U9: 65% 29% 5%

MET R2 E3 V4 I5 I9 G10 Q11 I14 Q15 E27 P32 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 F52 F53 T56 G57 H61 R64 C65 I66 F67 L68 D69 L70 E71 P72 T73 V74 V75 D76 E77 V78 R79 T80 G81 T82 Y83 R84 Q85 L86

F87 H88 P89 E90 Q91 L92 I93 E97 D98 A99 A100 N101 N102 R105 Y108 T109 K112 D116 L117 A118 L119 D120 R121 I122 L125 A126 D127 N128 C129 T130 G131 L132 Q133 G134 V137 F138 N139 G150 L154 K163 K164 L167 G168 E183 P184 S187

T191 H192 S193 L194 L195 E196 H197 V200 D211 I212 C213 L217 D218 I219 E220 R221 P222 T223 Y224 N228 T239 R243 G246 A247 L248 N249 I252 T253 E254 F255 Q256 R264 S270 S271 E279 K280 A281 Y282 H283 E284 Q285 L286 S287 E290 I291 K304 C305

K311 Y312 M313 L317 M318 Y319 P325 K326 D327 V328 T334 I335 K336 T337 K338 R339 Q342 F343 V344 T349 G350 F351 K352 C353 G354 D367 I384 I387 L397 M398 Y399 R402 E411 R422 A426 A427 L428 D431 F432 A437 GLU SER ALA GLU

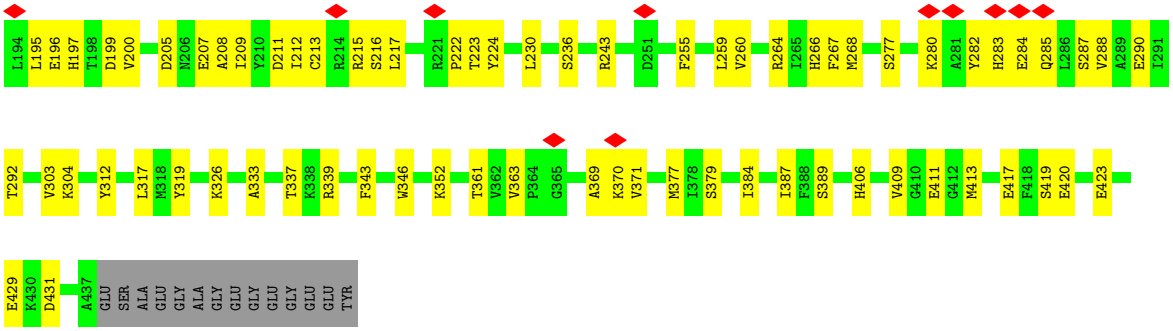
GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

• Molecule 2: Tubulin alpha

Chain V1: 65% 29% 5%

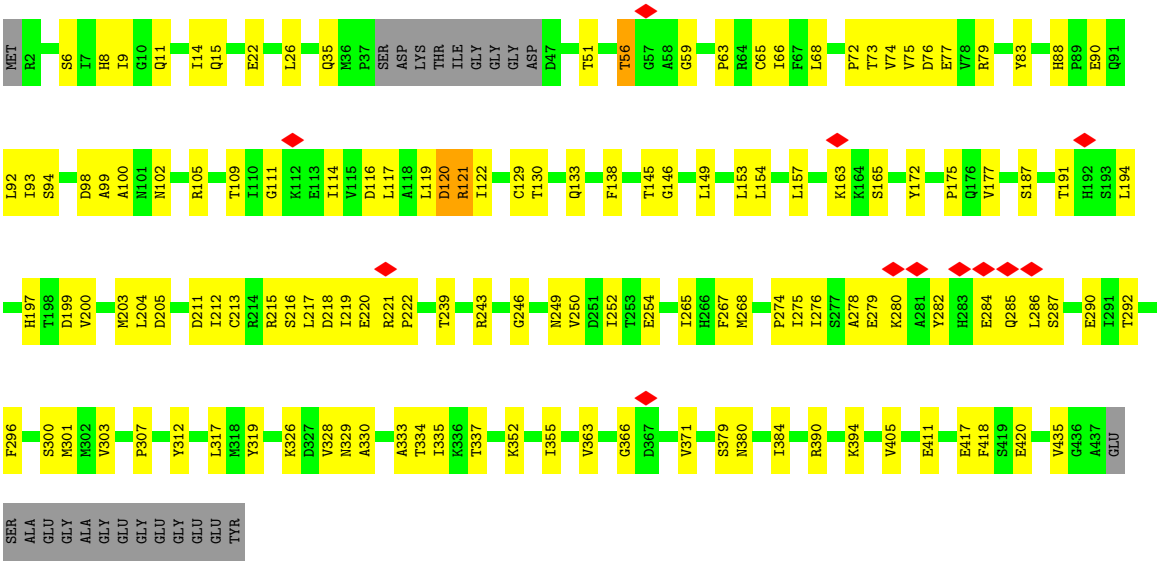
MET R2 E3 V4 I5 S6 I7 H8 I9 G10 I14 E22 L26 E27 P32 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 E55 T56 G59 K60 I66 F67 L68 D69 L70 E71 P72 V75 D76 R79 Y83 L86 F87 H88 P89 E90

Q91 S94 D98 A99 N102 R105 T109 K112 D116 L117 A118 L119 D120 R121 L125 C129 T130 G131 L132 Q133 G134 N139 G146 S147 G150 L153 L154 K163 K164 S165 K166 T170 P175 Q176 V177 E183 P184 S187 S190 T191



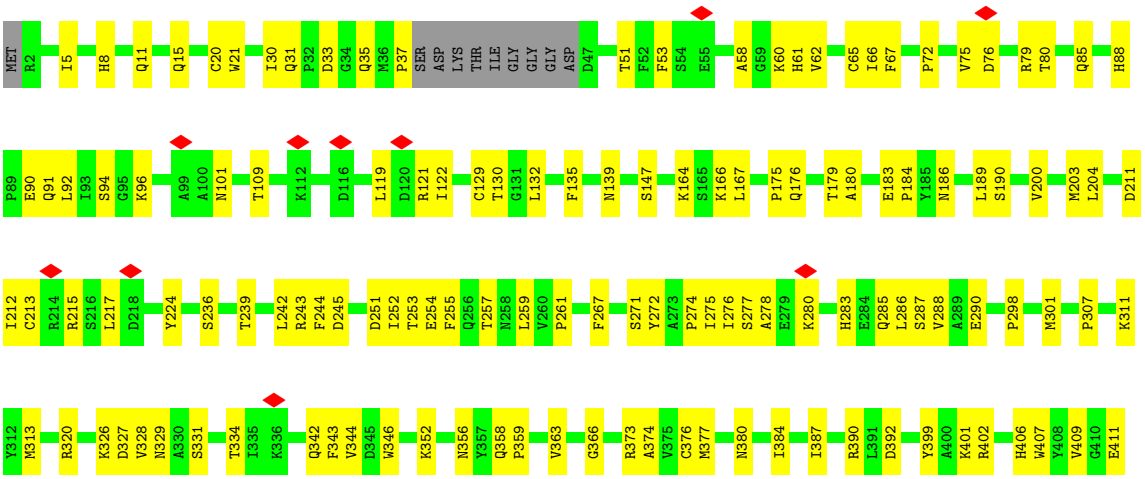

• Molecule 2: Tubulin alpha

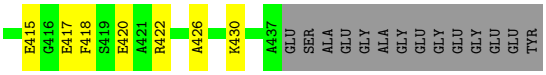
Chain V3:




• Molecule 2: Tubulin alpha

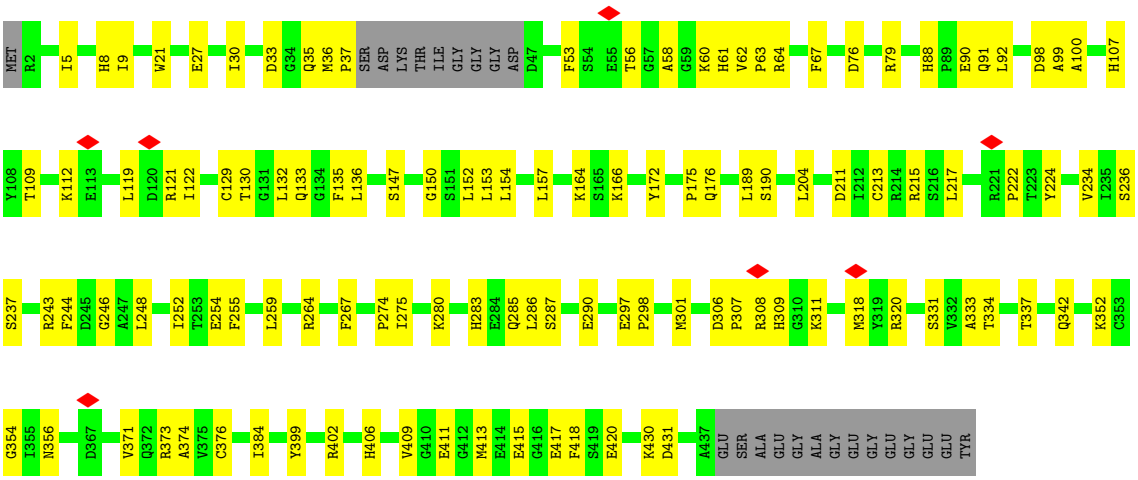
Chain V7:





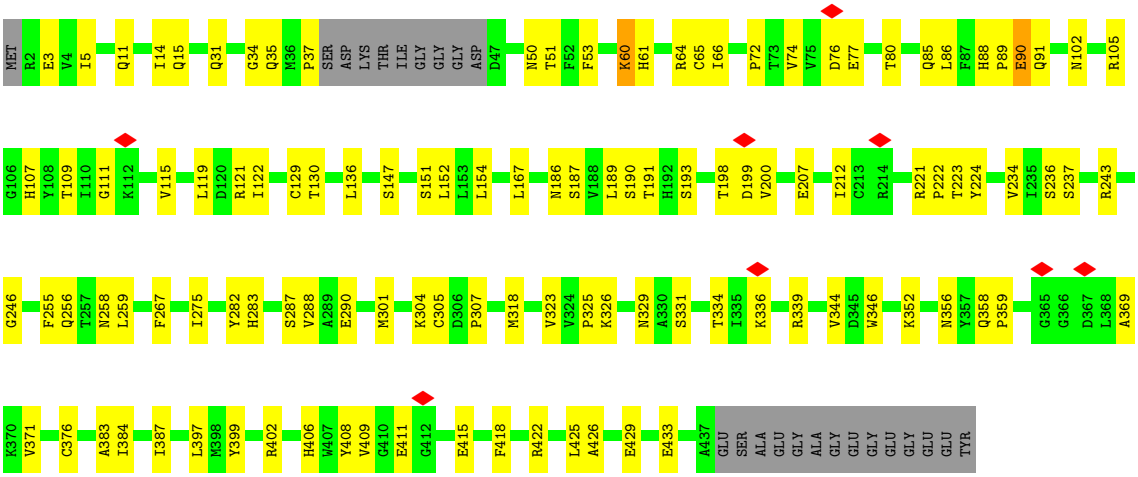

• Molecule 2: Tubulin alpha

Chain V9:



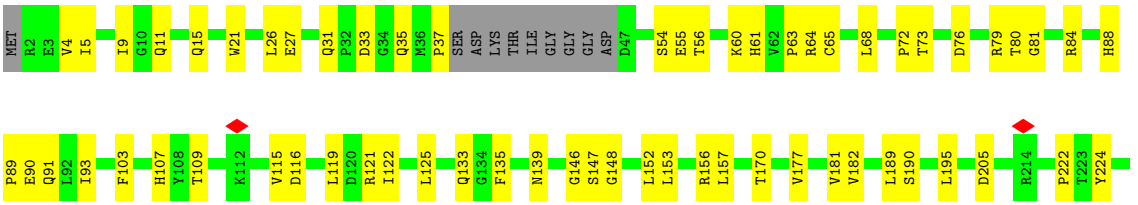

• Molecule 2: Tubulin alpha

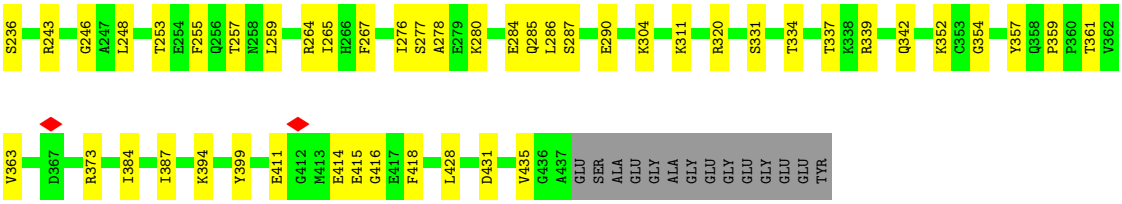
Chain W1:




• Molecule 2: Tubulin alpha

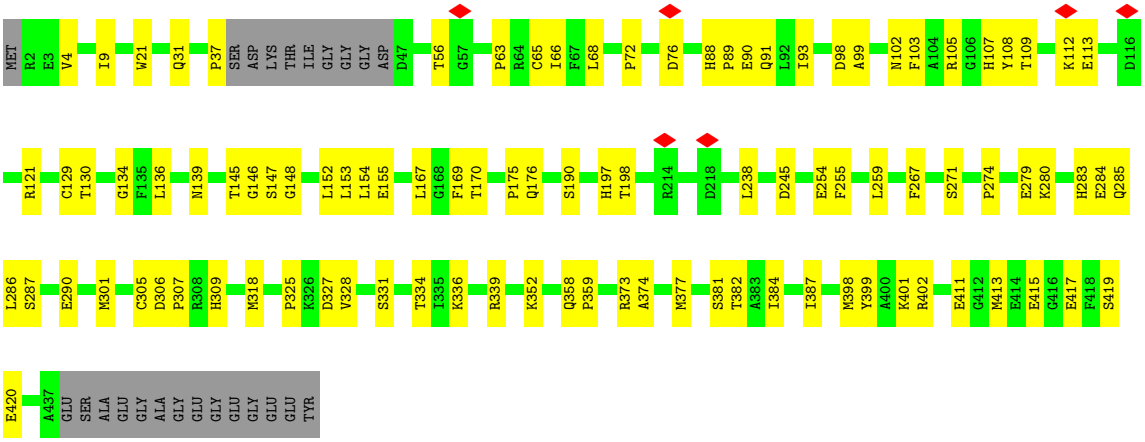
Chain W3:





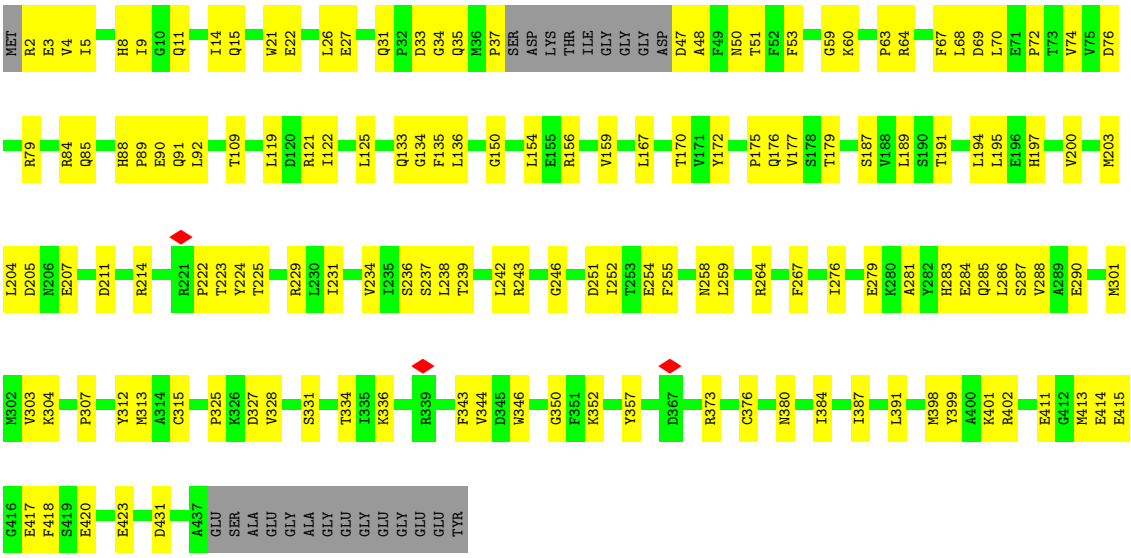

- Molecule 2: Tubulin alpha

Chain W5:



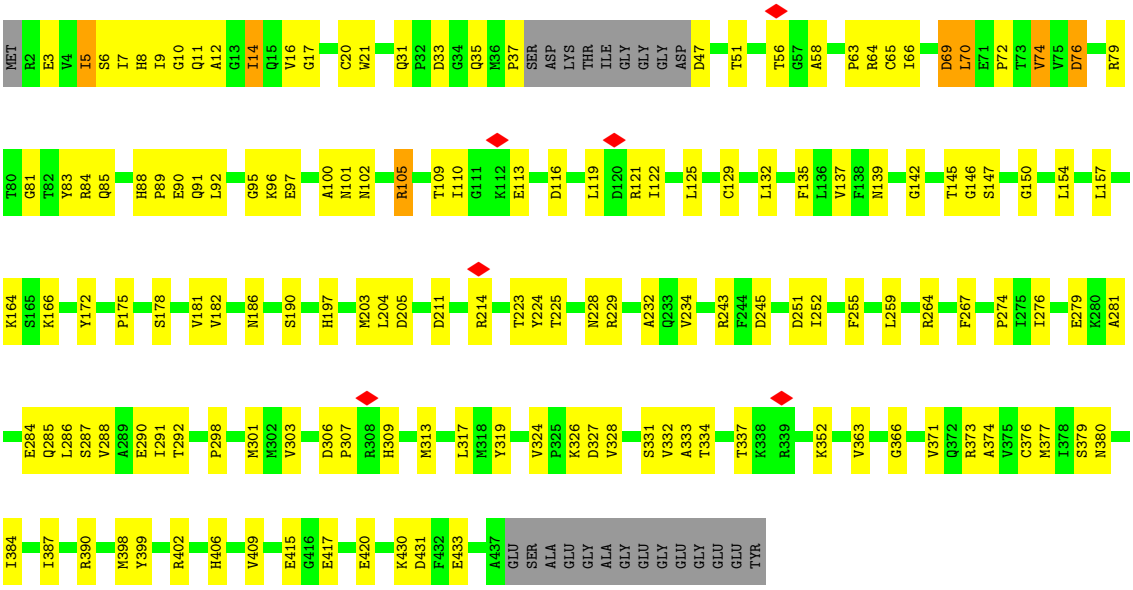

- Molecule 2: Tubulin alpha

Chain W7:



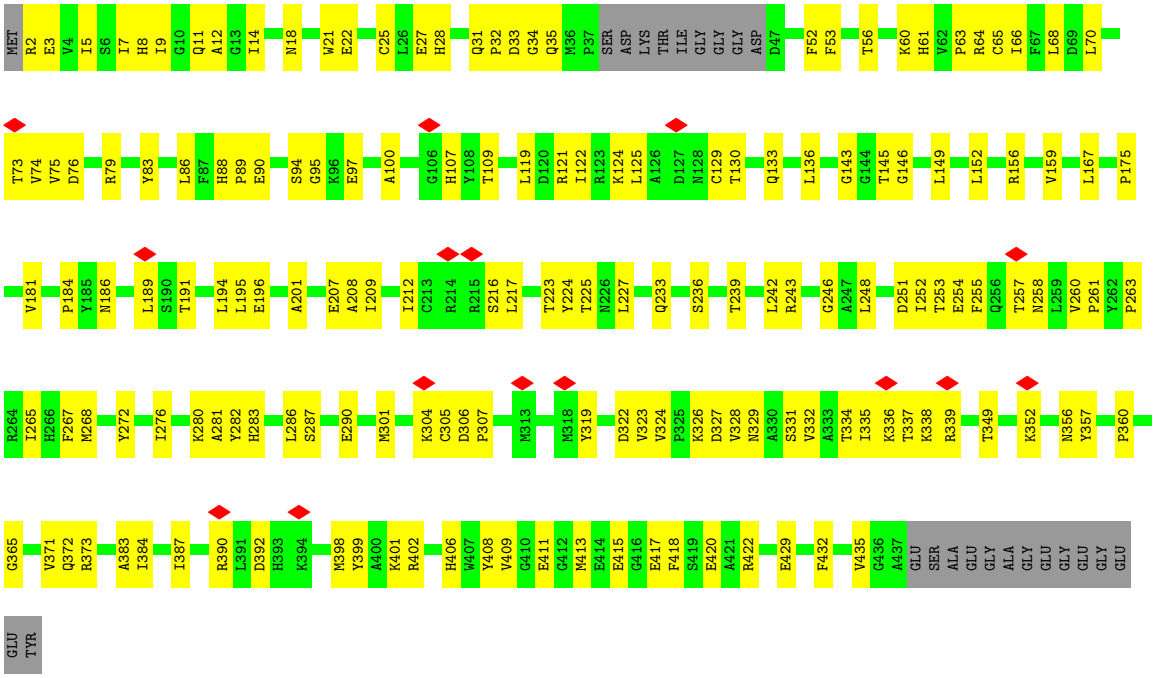

- Molecule 2: Tubulin alpha

Chain W9:



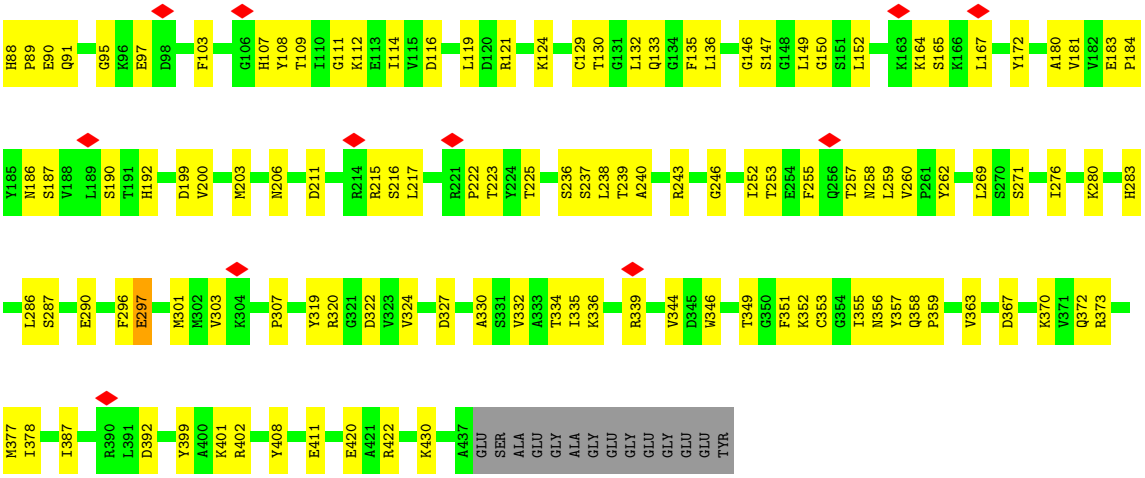

- Molecule 2: Tubulin alpha

Chain X3:



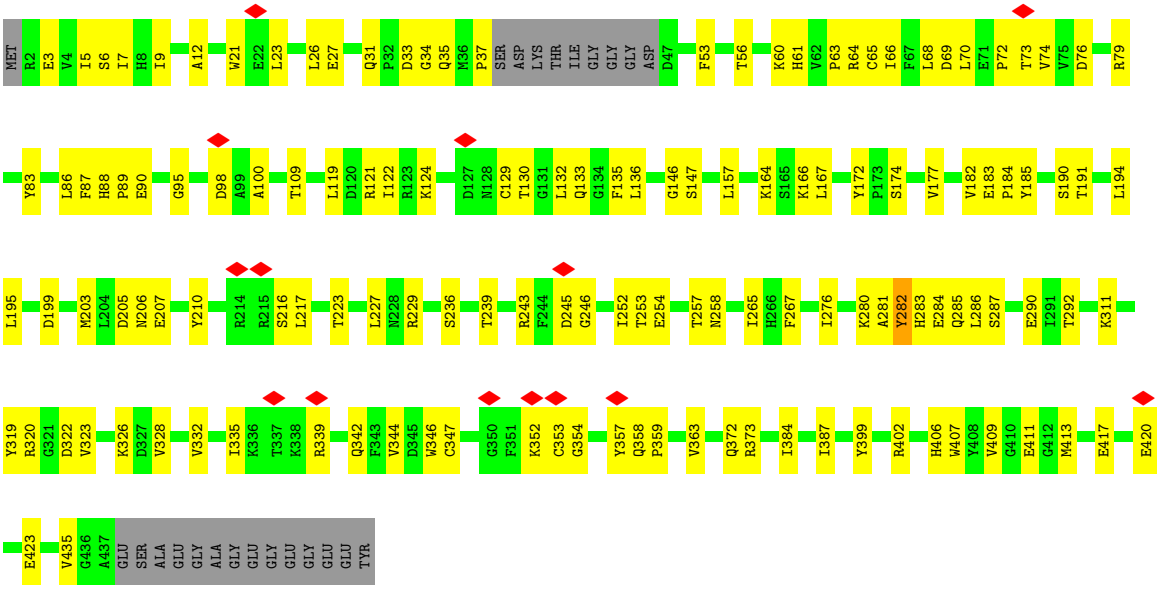

- Molecule 2: Tubulin alpha

Chain X5:



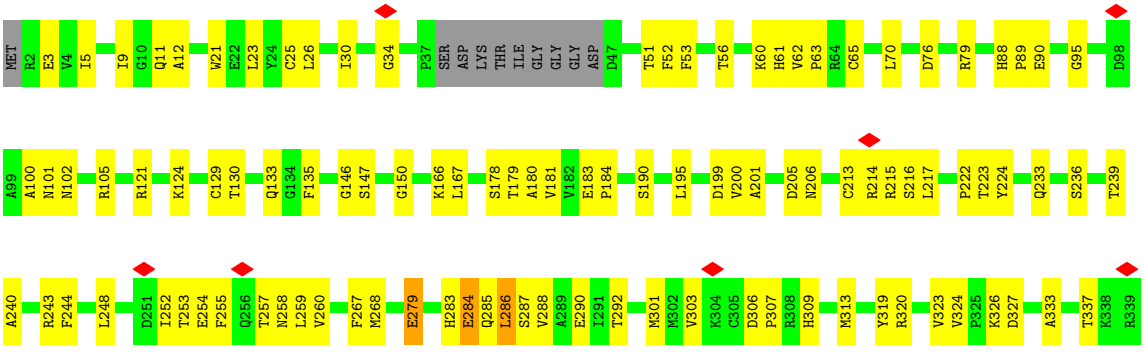

- Molecule 2: Tubulin alpha

Chain X7:



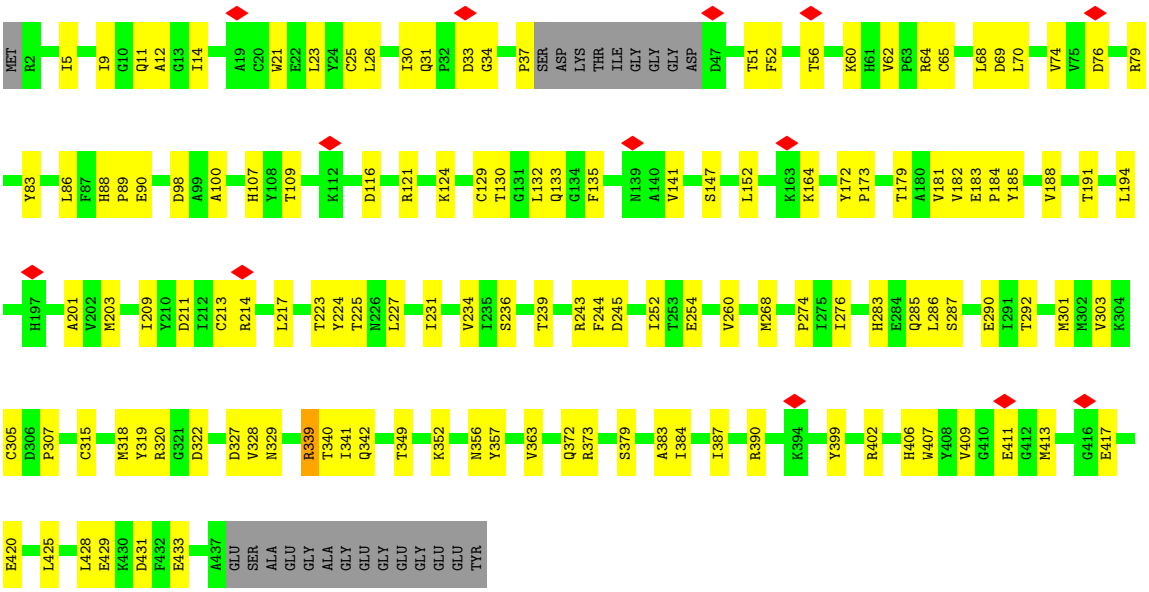

- Molecule 2: Tubulin alpha

Chain X9:



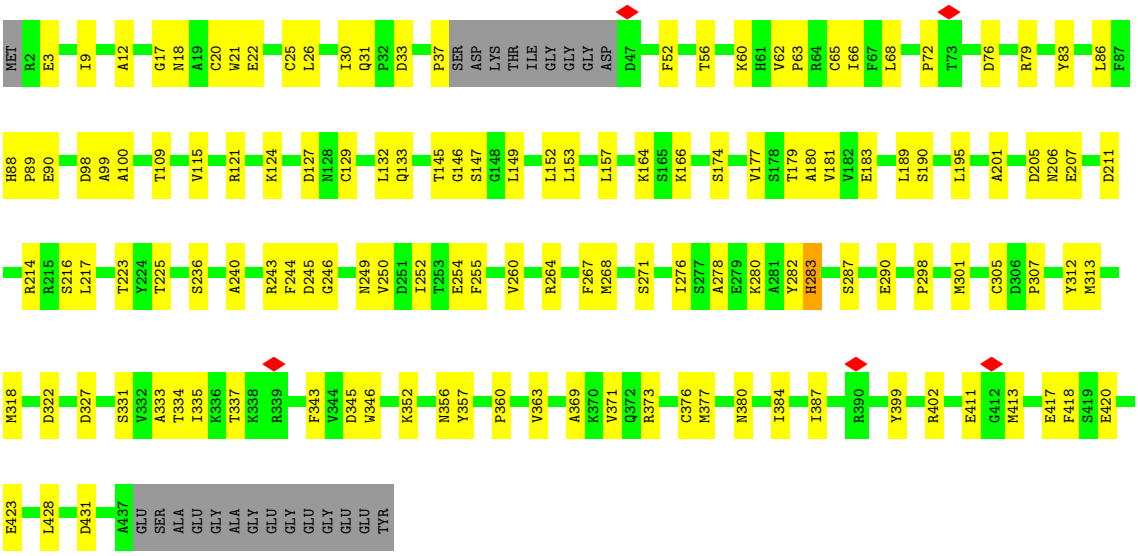
• Molecule 2: Tubulin alpha

Chain Y1:



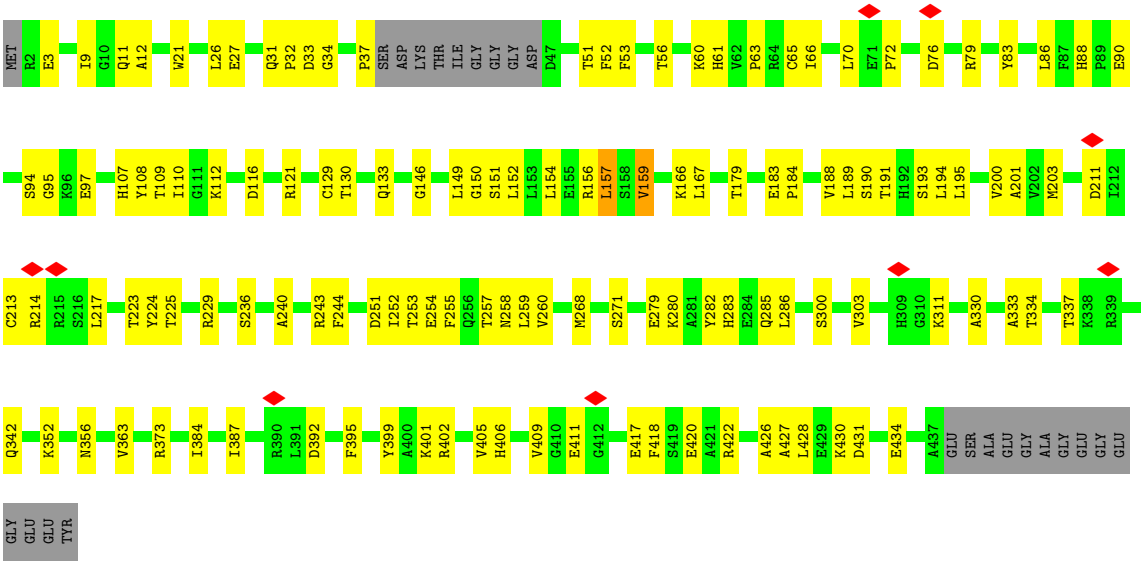

• Molecule 2: Tubulin alpha

Chain Y3:



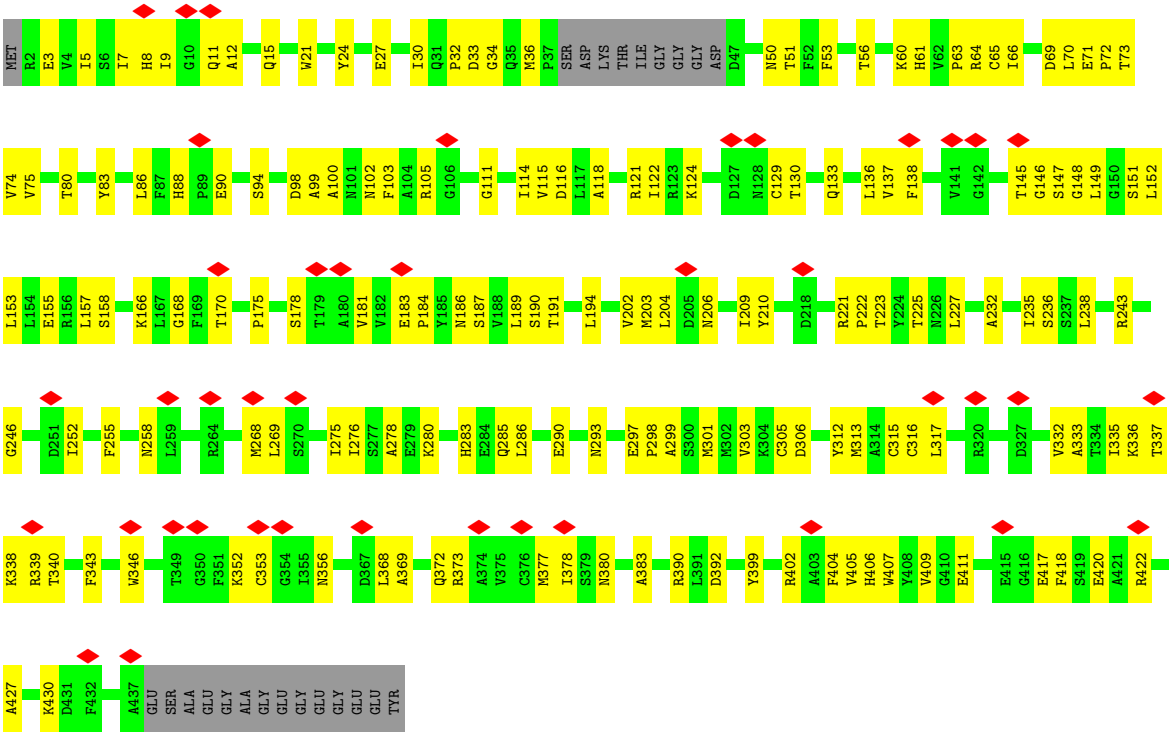

• Molecule 2: Tubulin alpha

Chain Y5:



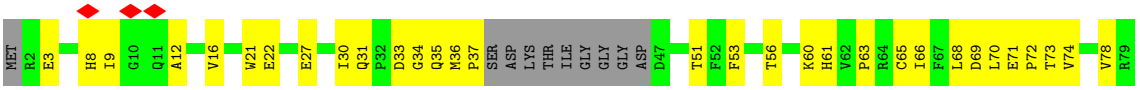

- Molecule 2: Tubulin alpha

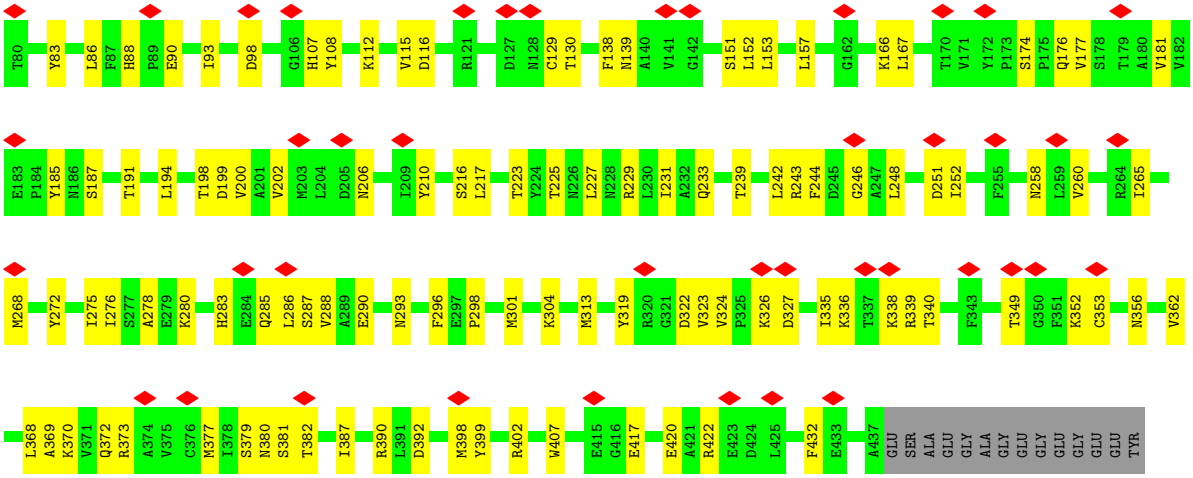
Chain Y9:




- Molecule 2: Tubulin alpha

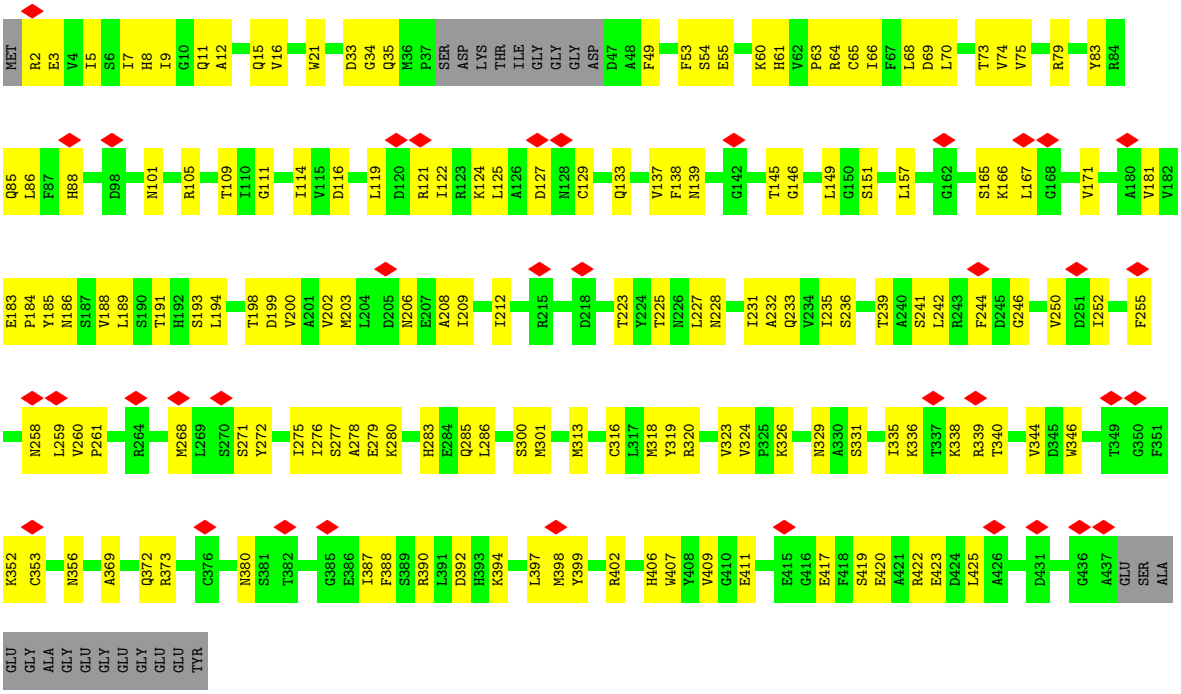
Chain Z1:





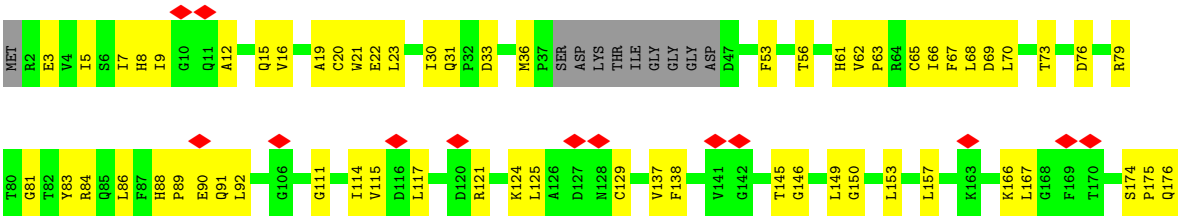

- Molecule 2: Tubulin alpha

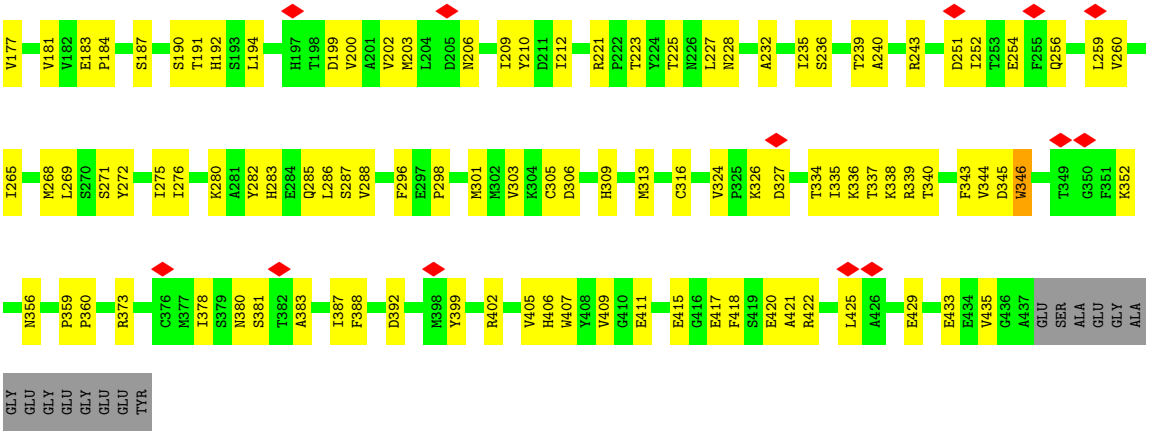
Chain Z3:




- Molecule 2: Tubulin alpha

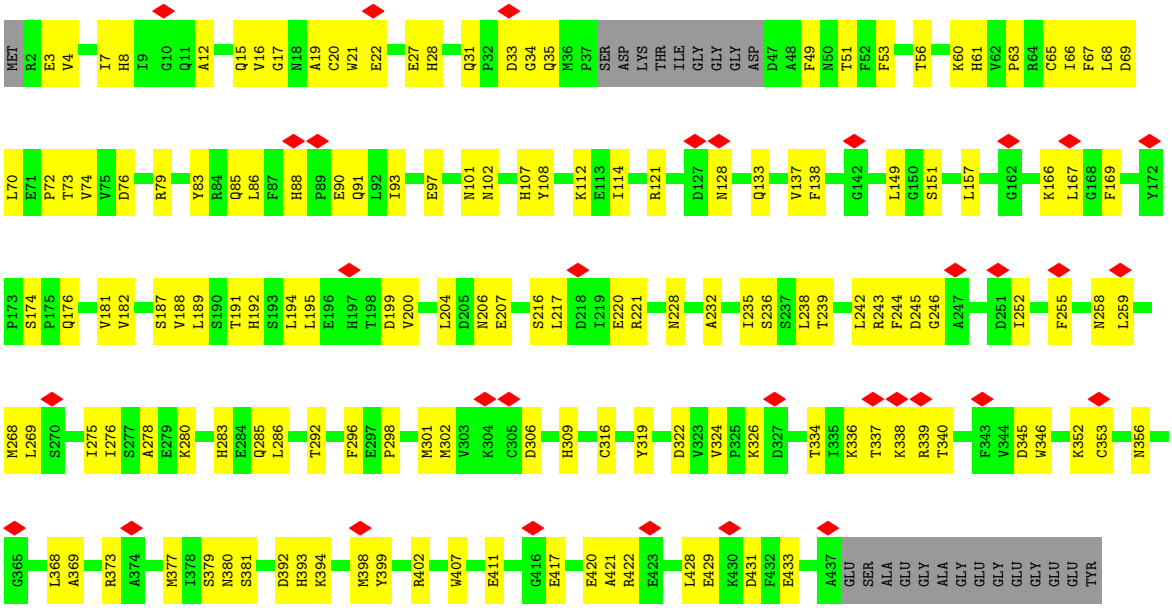
Chain Z5:





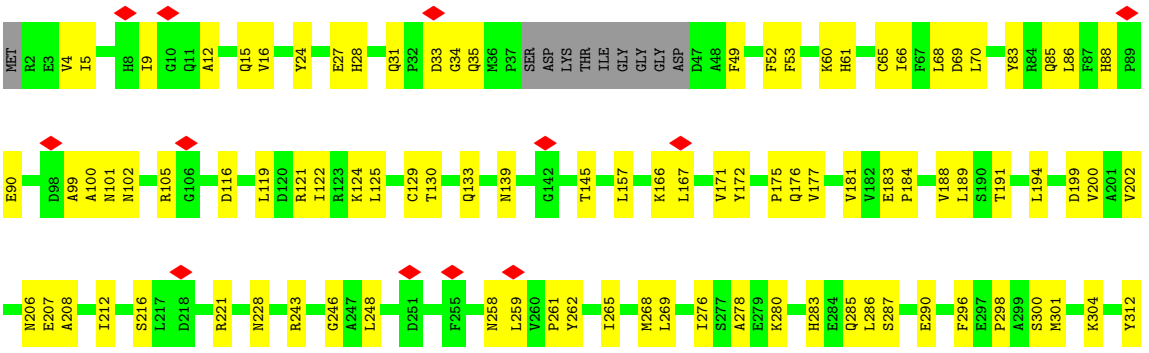

- Molecule 2: Tubulin alpha

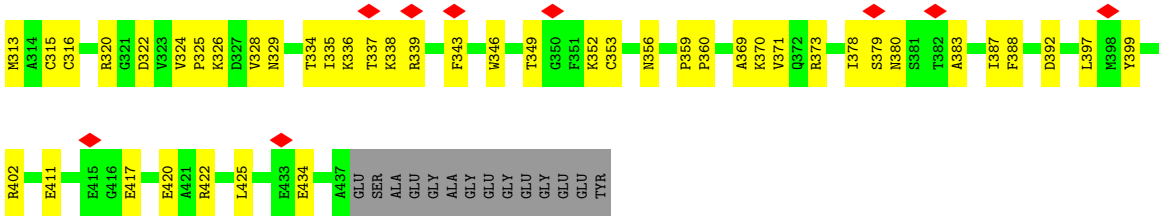
Chain Z7:




- Molecule 2: Tubulin alpha

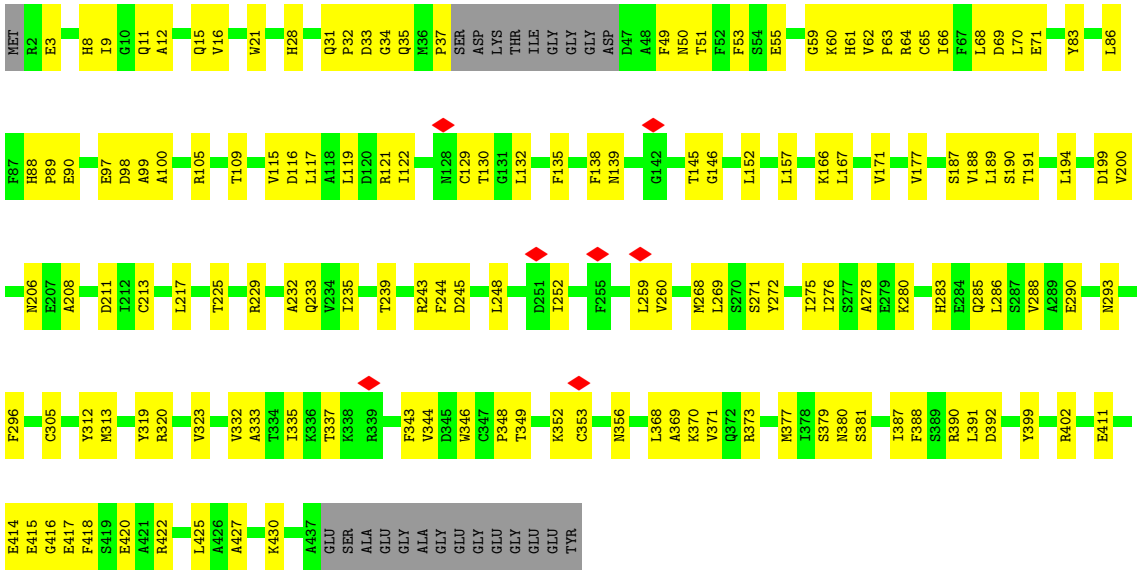
Chain Z9:





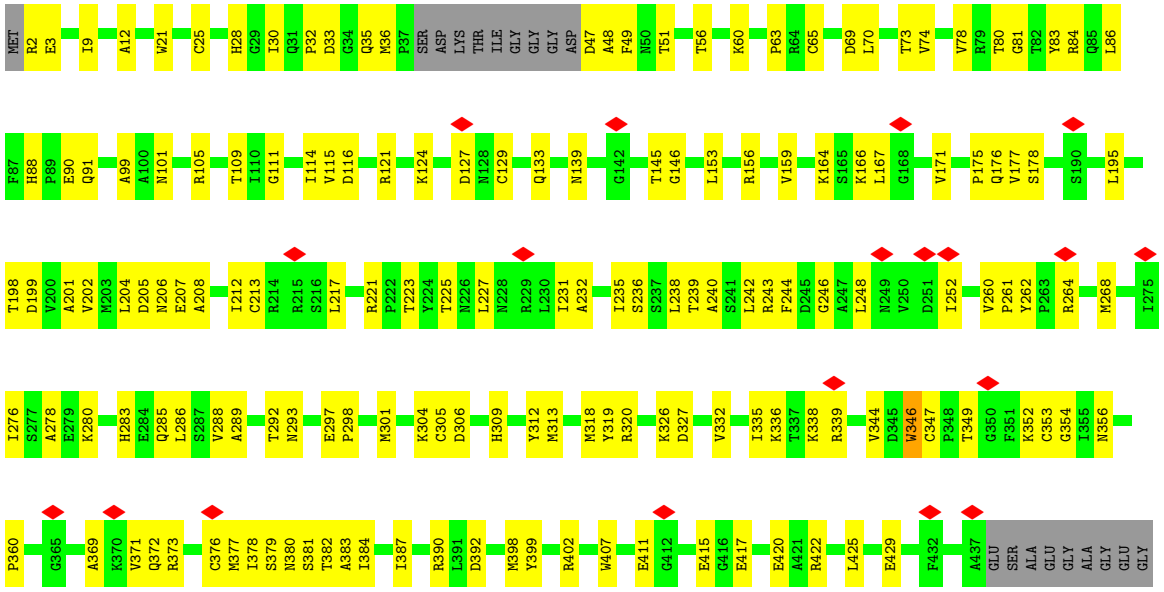

• Molecule 2: Tubulin alpha

Chain 0B:




• Molecule 2: Tubulin alpha

Chain 0F:



GLU GLY GLU GLU TYR

• Molecule 2: Tubulin alpha

Chain 0H:

MET R2 E3 I7 H8 I9 A12 Q15 C20 W21 E27 H28 G29 I30 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 E55 T56 K60 P63 R64 C65 I66 F67 L68 D69 L70 E71 P72 T73 V74 V78 G81 T82 Y83

R84 Q85 L86 F87 H88 P89 E90 A100 N101 N102 R105 T109 I110 V115 R121 I122 R123 K124 L132 Q133 V137 G142 T145 G146 S147 G148 L149 G150 L153 R156 V159 K166 L167 V171 P175 Q176 E183 P184 S190 T191 L194

T198 A201 V202 M203 L204 D205 N206 E207 A208 I209 Y210 D211 I212 C213 R214 L217 R221 P222 L227 N228 R229 V234 T239 L242 R243 F244 D245 G246 D251 I252 T257 N258 L259 V260 R264 F267 S271 Y272 A273 P274 A278 E279 K280 H283 E284 Q285

L286 S287 V288 A289 E290 I291 T292 N293 E297 P298 A299 S300 M301 K304 C305 D306 H309 C316 R320 G321 D322 D327 A330 S331 V332 A333 T334 I335 K336 T337 K338 R339 W346 C347 G350 C353 G354 I355 N356 D367 L368 A369 K370 R373 C376 M377 I378

S381 T382 A383 I384 I387 R390 L391 D392 L397 M398 Y399 A400 K401 R402 A403 H406 W407 E411 G412 E417 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

• Molecule 2: Tubulin alpha

Chain 0J:

MET R2 E3 V4 I5 I9 A12 Q15 V16 W21 C25 H28 G29 I30 Q31 P32 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 S54 E55 T56 G57 K60 H61 R64 C65 I66 F67 L68 D69 L70 T73 V74

V75 R79 T82 Y83 R84 Q85 L86 F87 H88 P89 E90 I93 S94 D98 A99 A100 T109 I110 G111 I114 V115 D116 L117 A118 L119 D120 R121 I122 R123 K124 L125 A126 D127 F135 L136 V137 G142 G146 S147 L153 R156 V159 G162 L167 G168 F169

S174 P175 Q176 V177 S178 V181 S187 S190 T198 A201 V202 M203 L204 D205 N206 E207 A208 I209 Y210 D211 I212 R215 S216 L217 R221 P222 N228 R229 A232 I235 L242 R243 F244 D245 G246 A247 D251 I252 F255 Q256 T257 N258 L259 V260 R264

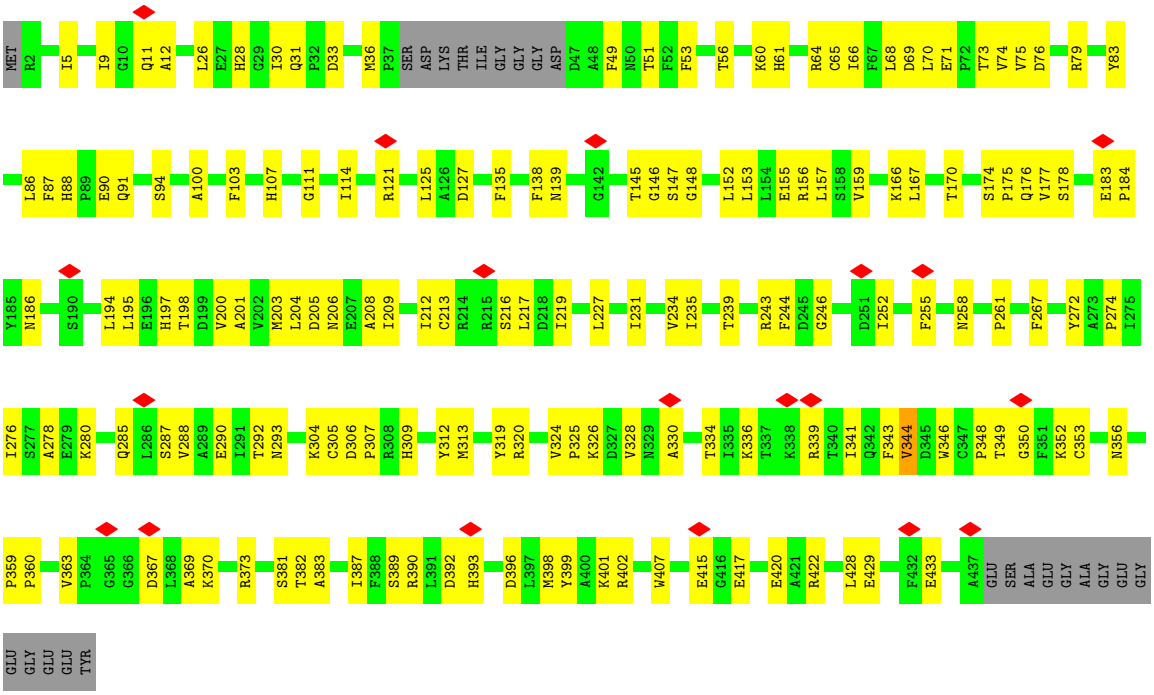
F267 M268 L269 S270 S271 P274 I275 I276 S277 A278 H283 L286 S287 V288 T292 N293 E297 P298 A299 S300 M301 K304 M313 M318 Y319 R320 G321 D322 P325 V328 N329 A330 S331 V332 A333 T334 I335 K336 T337 K338 R339 T340 F343 W346 T349 G350

N356 P360 T361 V362 G365 G366 D367 L368 A369 K370 R373 C376 N380 S381 T382 A383 I384 I387 R390 L391 D392 H393 M398 Y399 R402 W407 E411 R422 E429 F432 E433 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU

GLU TYR

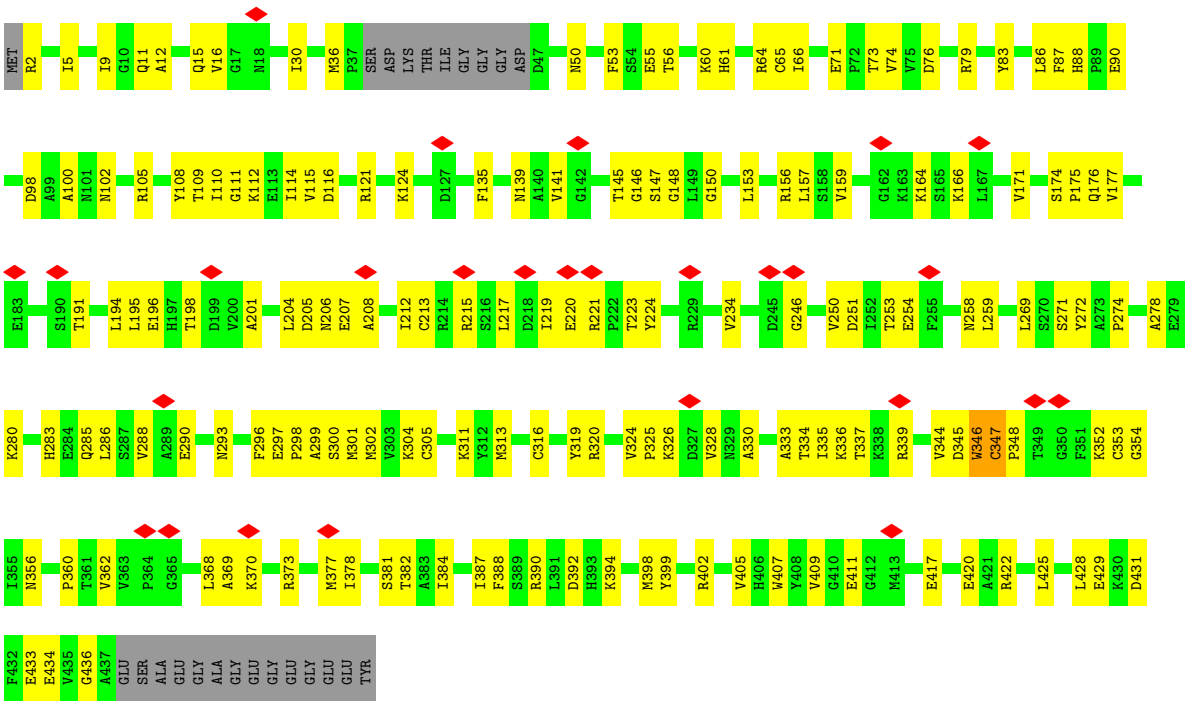
• Molecule 2: Tubulin alpha

Chain 0L: 59% 36% 5%




- Molecule 2: Tubulin alpha

Chain 0N: 6% 57% 37% 5%




- Molecule 2: Tubulin alpha

Chain 0P: 65% 30% 5%

MET R2 I5 H8 I9 A12 Q15 N18 C25 H28 Q31 P32 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 E55 T56 K60 R64 C65 I66 D69 L70 D76 R79 Y83 L86 F87 H88 F89

E90 N102 R105 T109 I110 G111 I114 V115 D116 R121 C129 L132 F138 N139 A140 V141 G142 T145 G146 L152 L153 R156 V159 G162 K163 K164 S165 K166 L167 S174 P175 Q176 V177 E183 T191 L194 T198 D199 V200 A201 D205

N206 I212 C213 S216 L217 D218 I219 E220 R221 P222 T223 Y224 N228 V234 T239 R243 F244 D245 G246 D251 I252 F255 Q256 T257 N258 L259 Y262 I265 M268 Y272 A273 P274 I275 I276 S277 A278 E279 K280 H283 L286 S287 V288 A289 E290 I291 T292

F296 E297 P298 M301 Y312 C316 Y319 R320 P325 K326 D327 V328 N329 A330 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 K352 C353 N356 A369 Q372 R373 S381 T382 I387 R390 L391 D392 L397

M398 Y399 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E417 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 0R: 5% 59% 36% 5%

MET R2 I5 S6 I7 H8 I9 A12 G17 N18 A19 C20 Y24 C25 L26 E27 H28 D33 G34 Q35 M36 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 A48 F49 N50 T51 F52 F53 S54 E55 T56 G57 K60 R64 C65 I66 E71 P72 T73 V74 V75 D76

E77 V78 R79 Y83 R84 Q85 L86 F87 H88 P89 E90 D98 A99 A100 H107 Y108 T109 I110 G111 K112 E113 I114 V115 D116 R121 I122 R123 K124 Q133 F138 N139 G142 T145 G146 S147 G148 L149 L152 L153 L154 E155 R156 L157 S158 V159 G162 K163 K164 S165 K166

L167 S174 P175 Q176 V177 E183 P184 Y185 V188 L189 S190 T191 H192 S193 L194 L195 E196 H197 T198 D199 V200 A201 V202 M203 E207 C213 R214 R215 S216 L217 Q233 S237 L238 T239 A240 R243 F244 D245 G246 N249 F255 N258 L259 V260 H266 S271

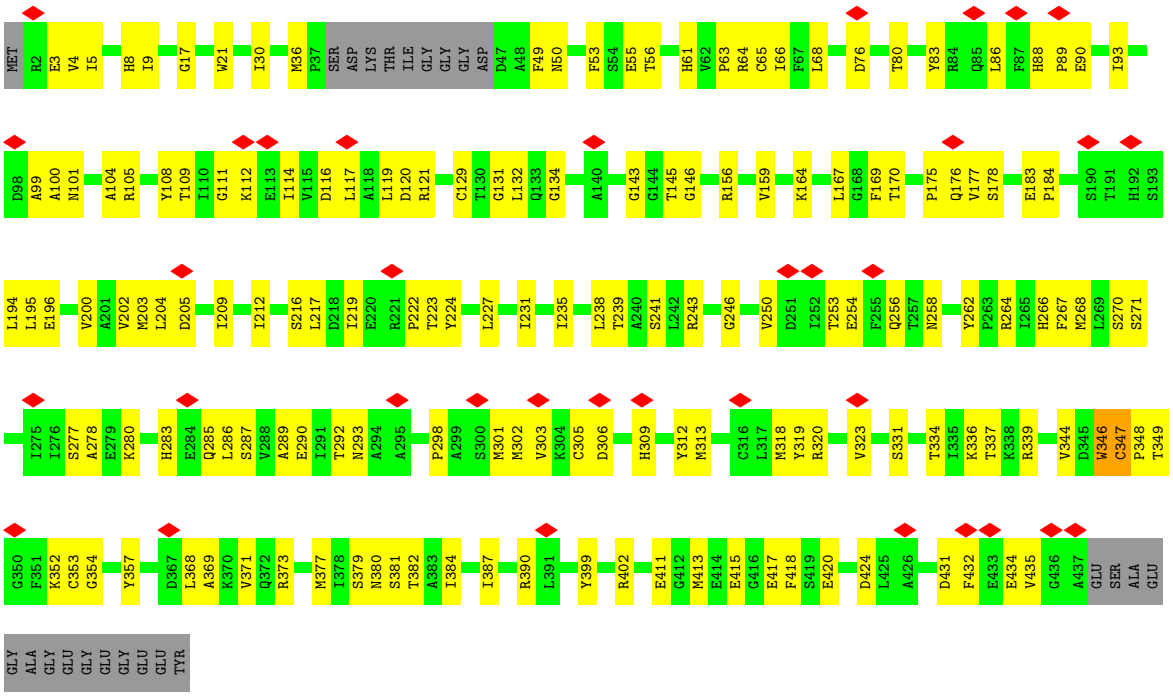
P274 I275 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 F296 E297 P298 M301 K304 C305 D306 H309 Y312 M318 Y319 R320 V323 V324 P325 K326 D327 V328 N329 A330 T334 I335 K336 T337 K338 R339 T340 I341 G350 F351 K352 C353

G354 I355 N356 V363 P364 G365 G366 D367 L368 A369 K370 V371 Q372 R373 G376 M377 I378 S379 N380 S381 T382 I387 R390 L391 D392 H393 K394 F395 D396 L397 M398 Y399 R402 A403 H406 W407 E411 E417 F418 S419 E420 A421 R422 A437 GLU SER ALA GLU GLY ALA GLY

GLU GLY GLU GLY GLU GLU TYR

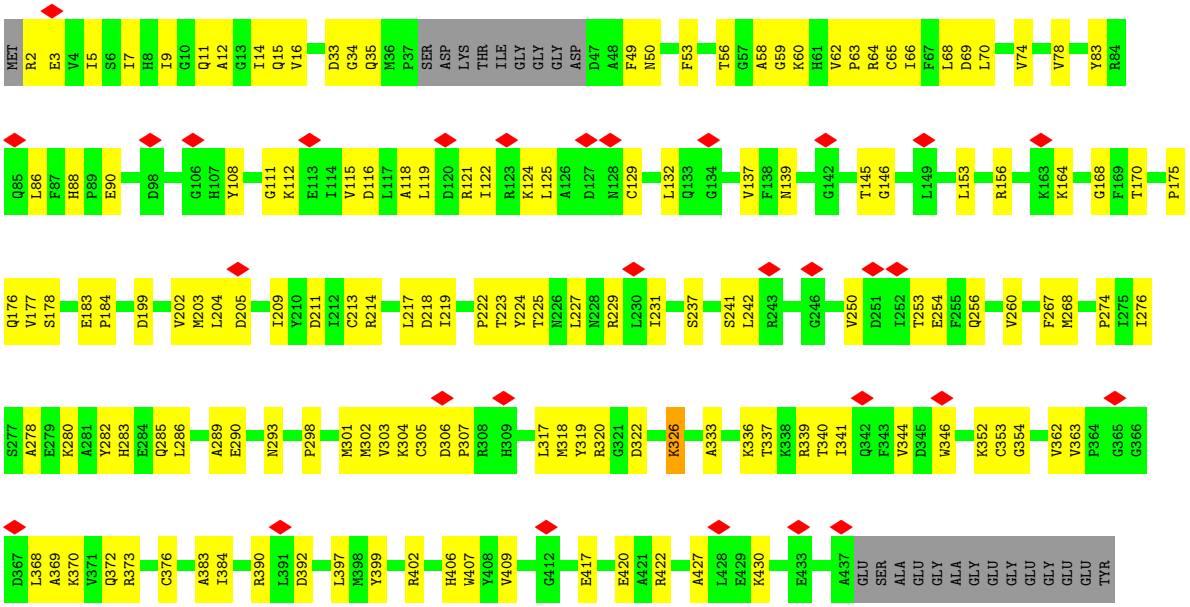
- Molecule 2: Tubulin alpha

Chain 0V: 8% 59% 35% 5%



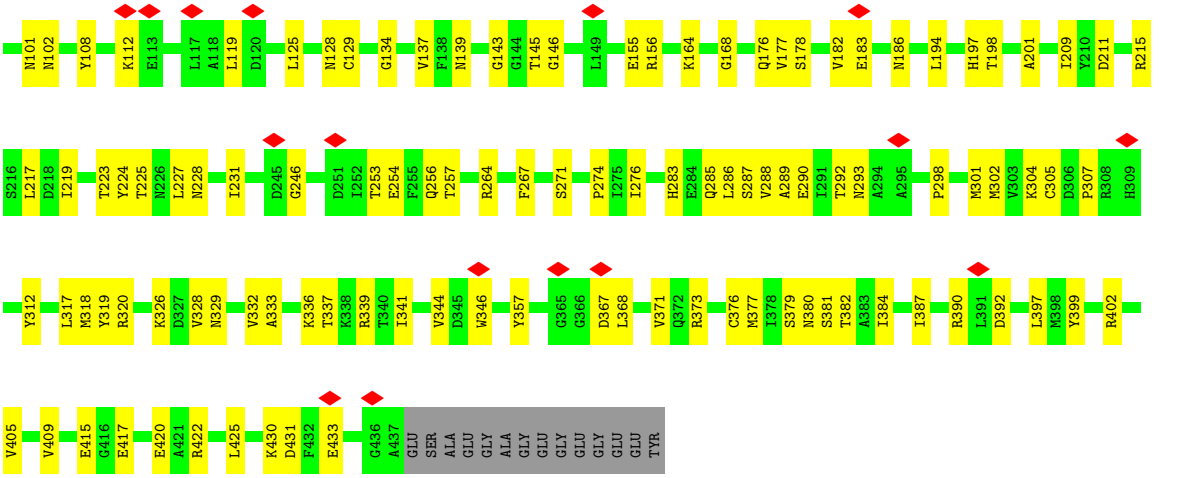

- Molecule 2: Tubulin alpha

Chain 0X:



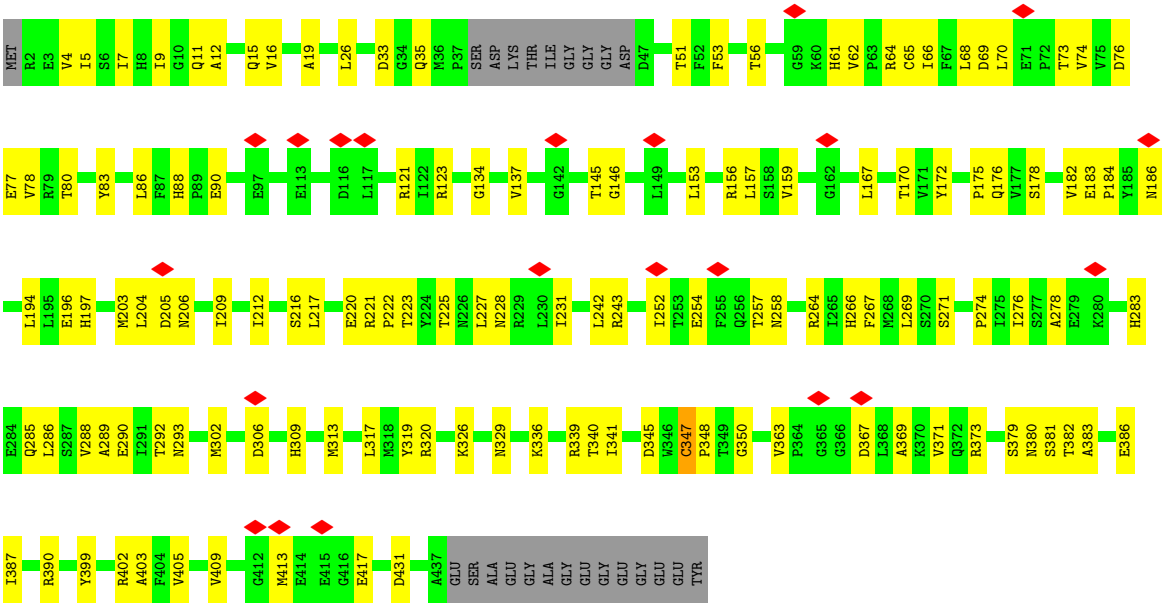

- Molecule 2: Tubulin alpha

Chain 0Z:



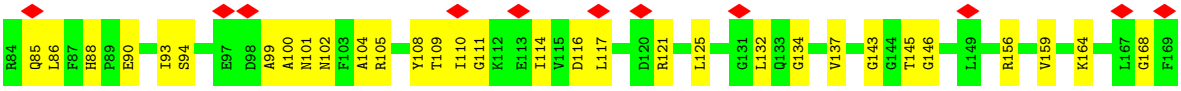

- Molecule 2: Tubulin alpha

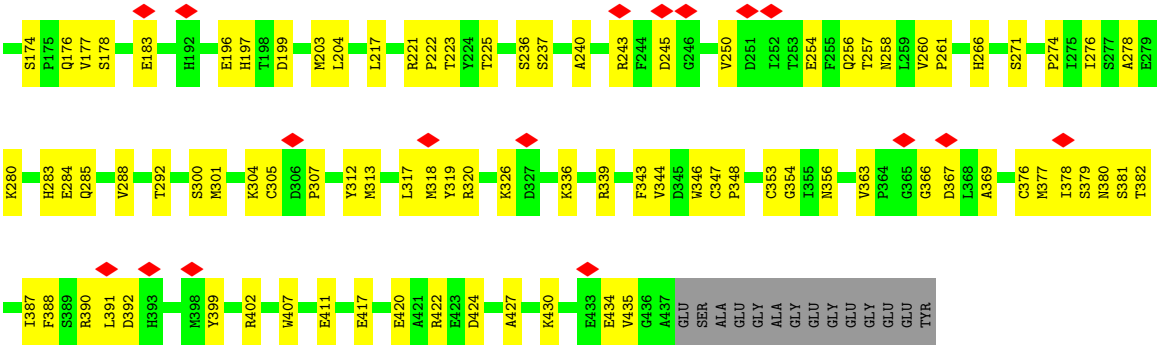
Chain 1B:




- Molecule 2: Tubulin alpha

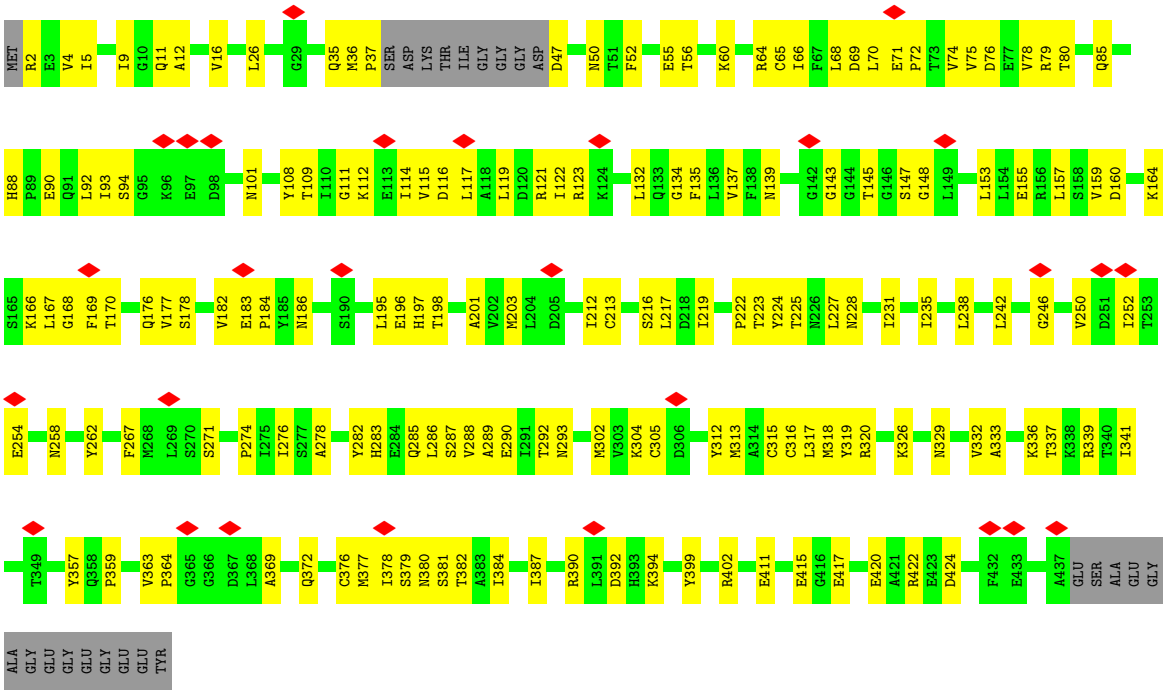
Chain 1D:





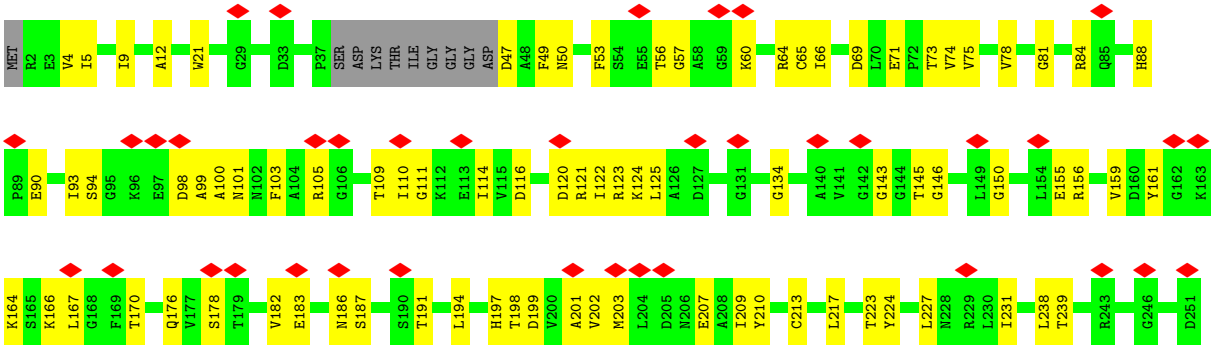

- Molecule 2: Tubulin alpha

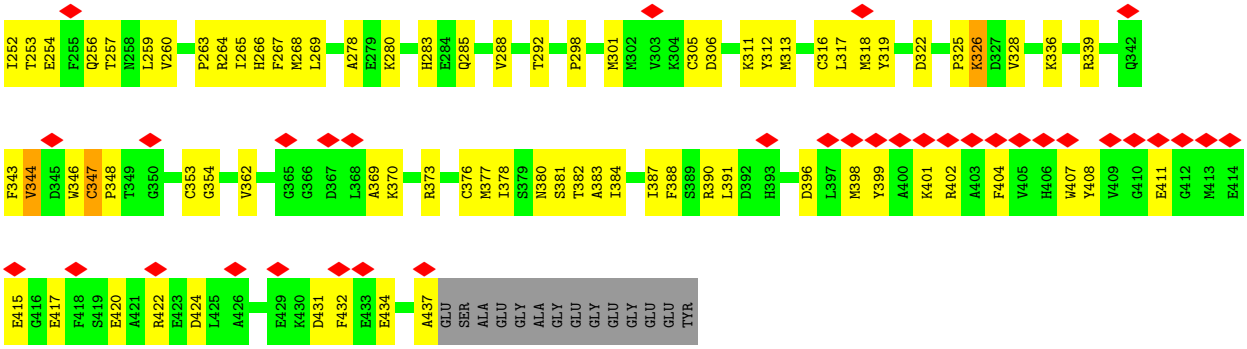
Chain 1F:




- Molecule 2: Tubulin alpha

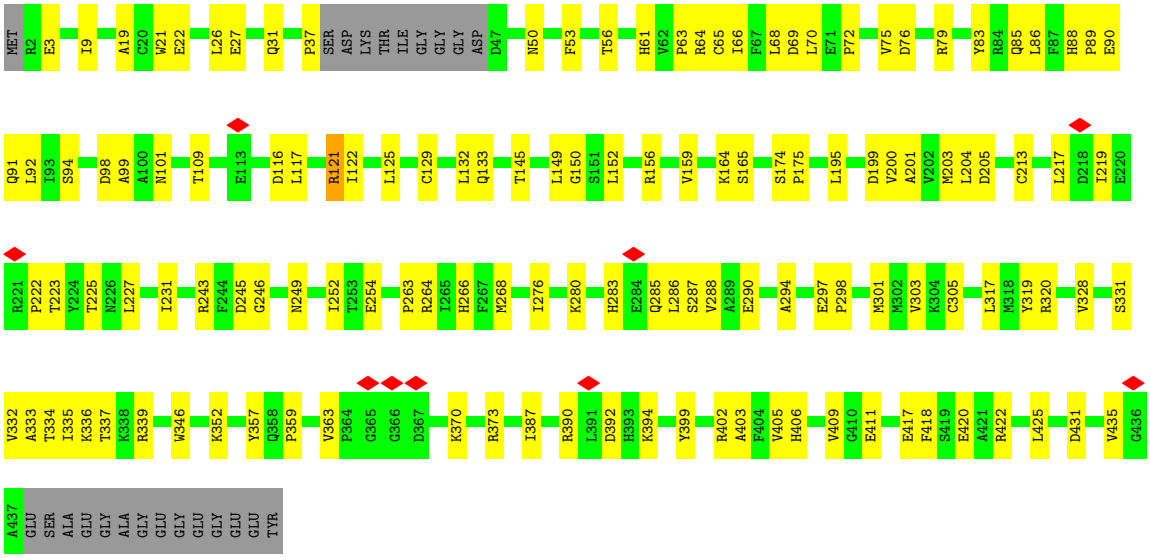
Chain 1H:





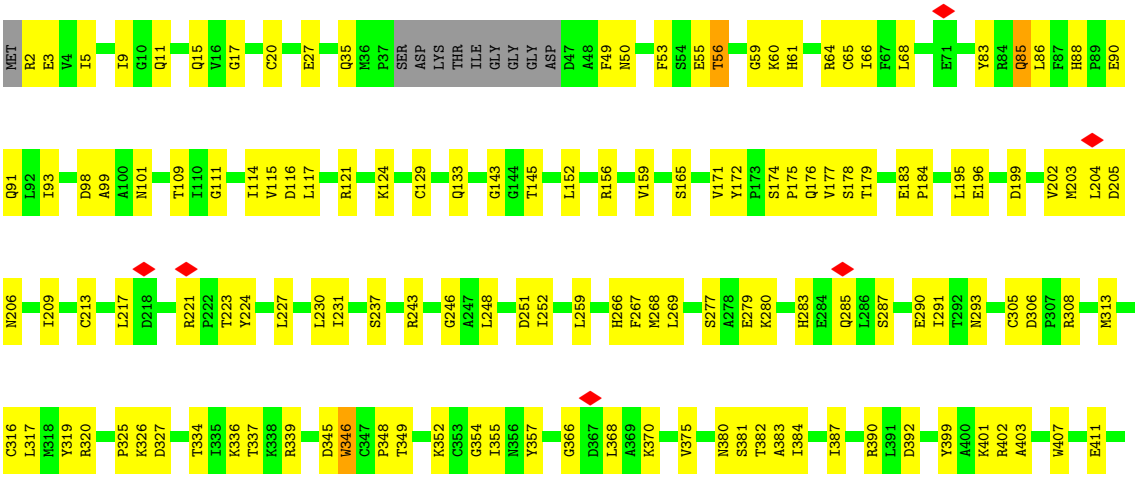

- Molecule 2: Tubulin alpha

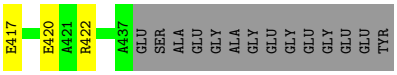
Chain 1L:




- Molecule 2: Tubulin alpha

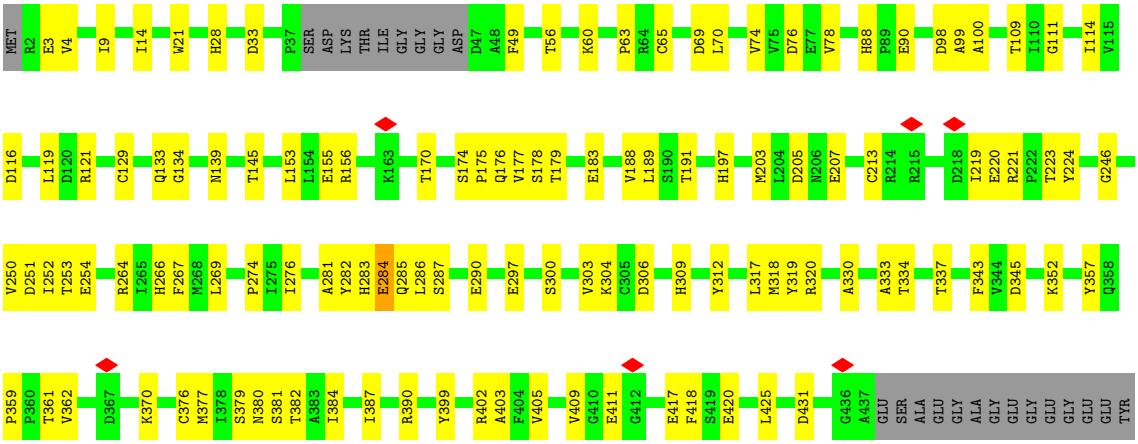
Chain 1N:





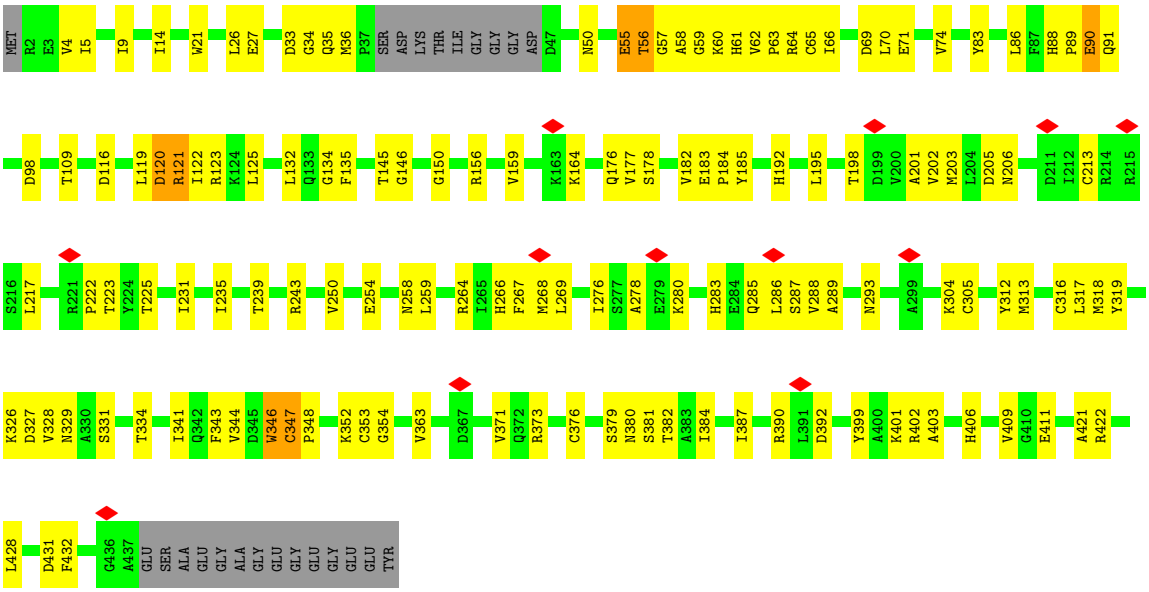

• Molecule 2: Tubulin alpha

Chain 1P:



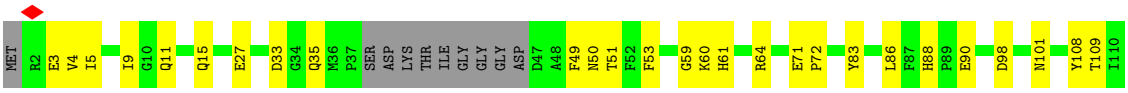

• Molecule 2: Tubulin alpha

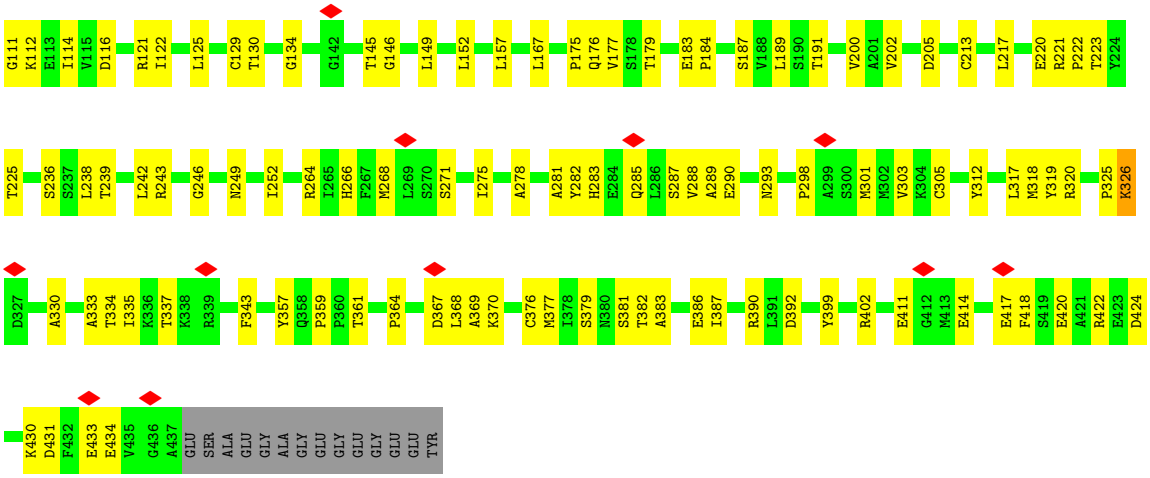
Chain 1R:




• Molecule 2: Tubulin alpha

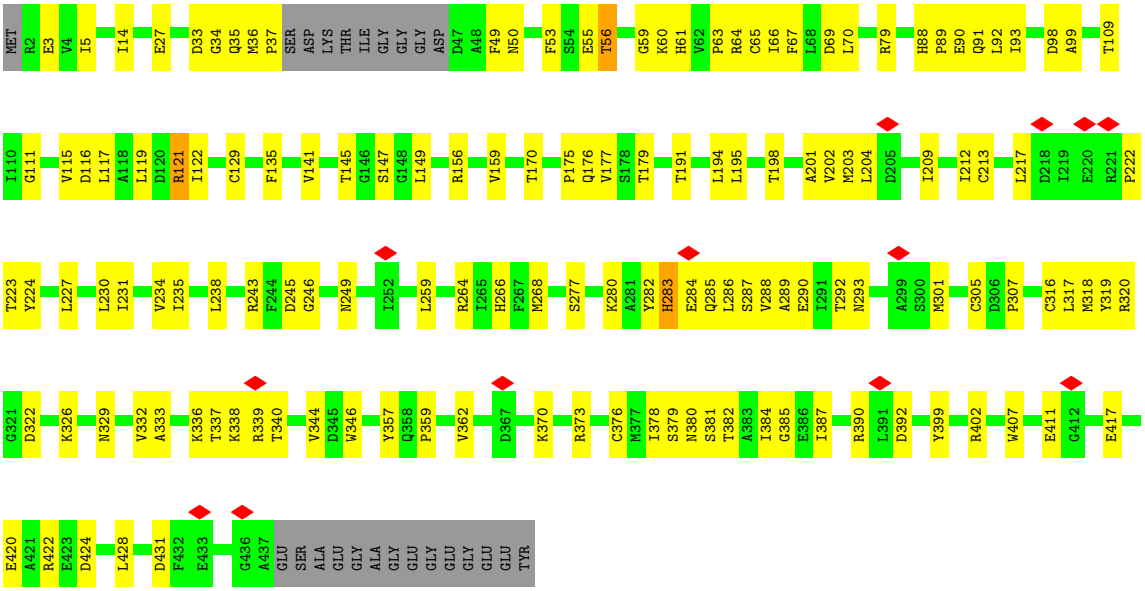
Chain 1T:





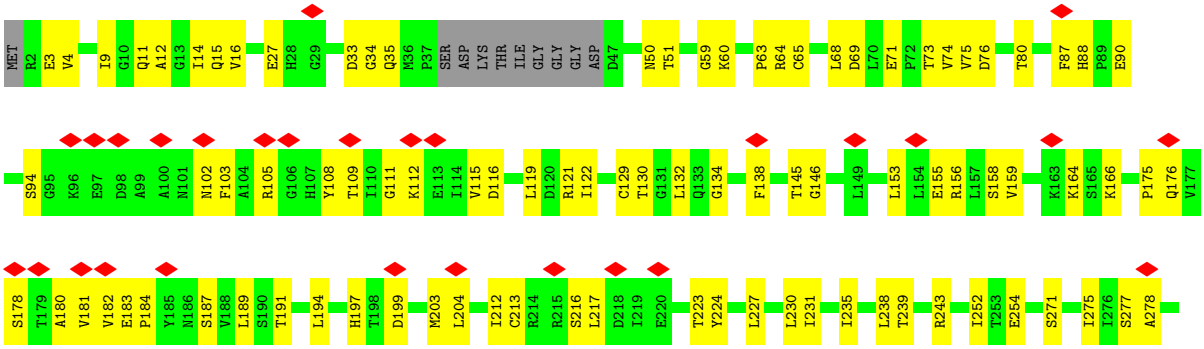

- Molecule 2: Tubulin alpha

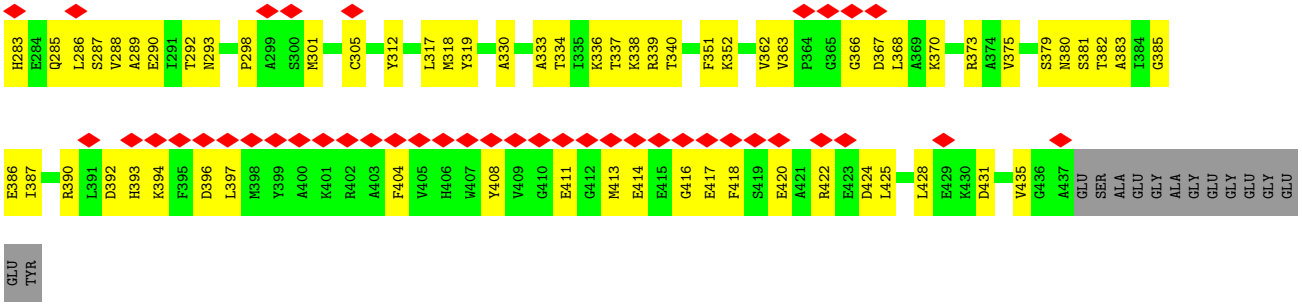
Chain 1V:




- Molecule 2: Tubulin alpha

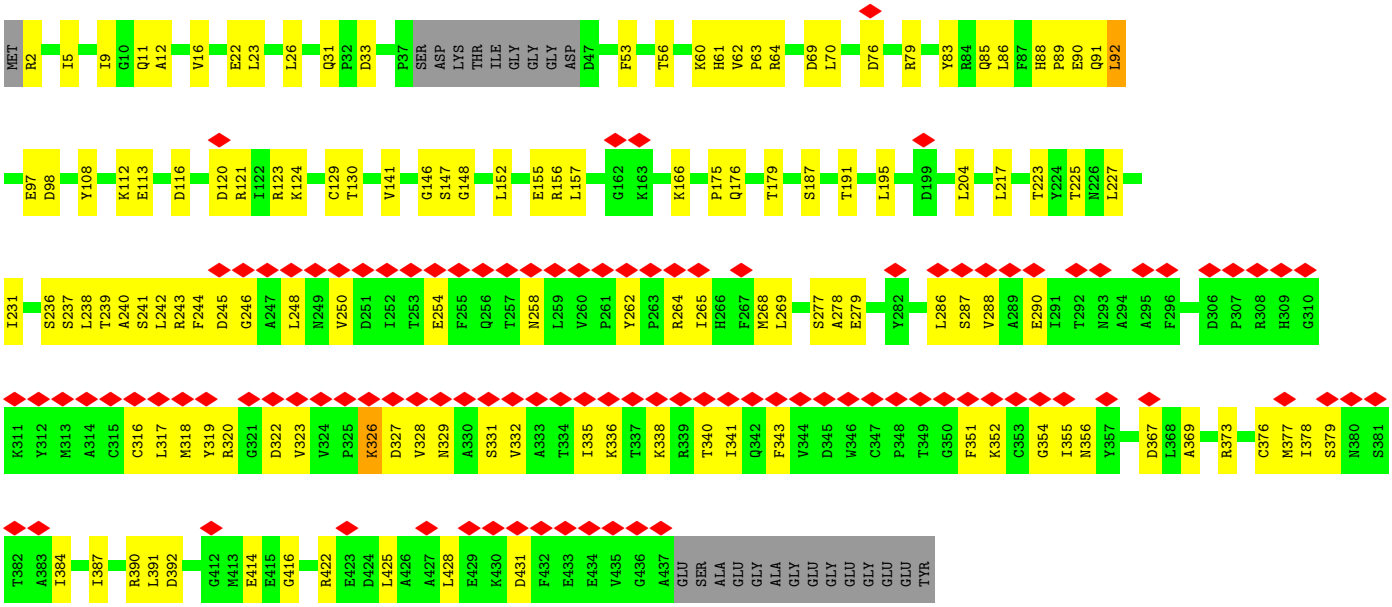
Chain 1X:





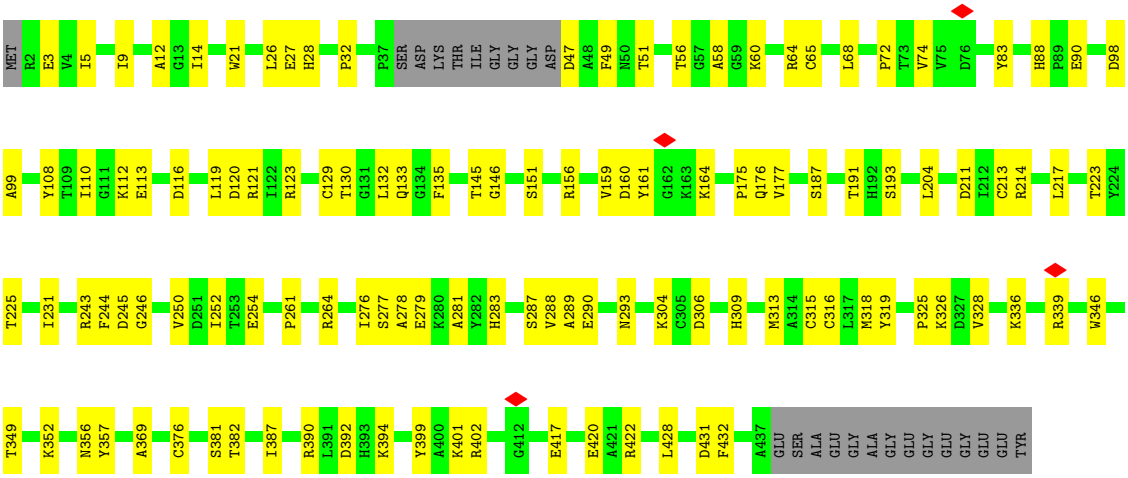

- Molecule 2: Tubulin alpha

Chain 1Z:



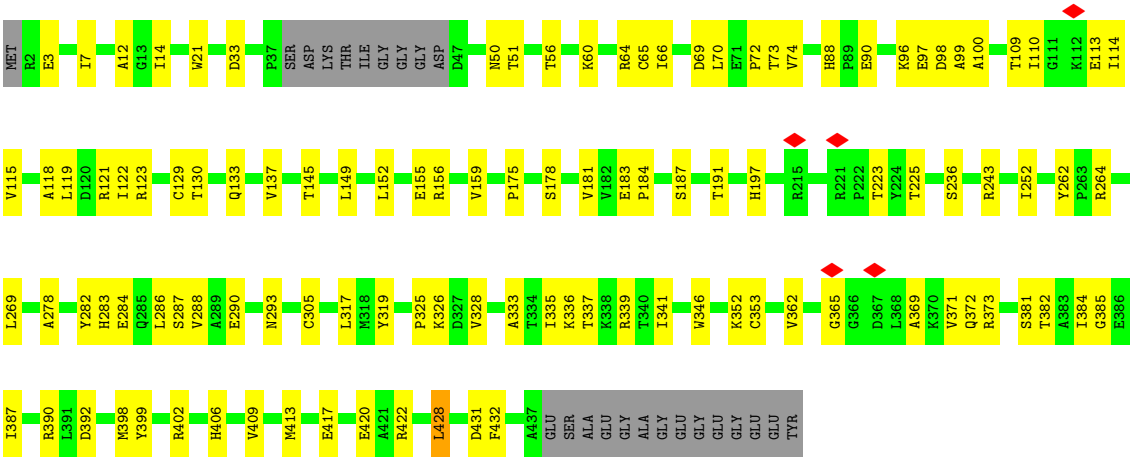

- Molecule 2: Tubulin alpha

Chain 2B:



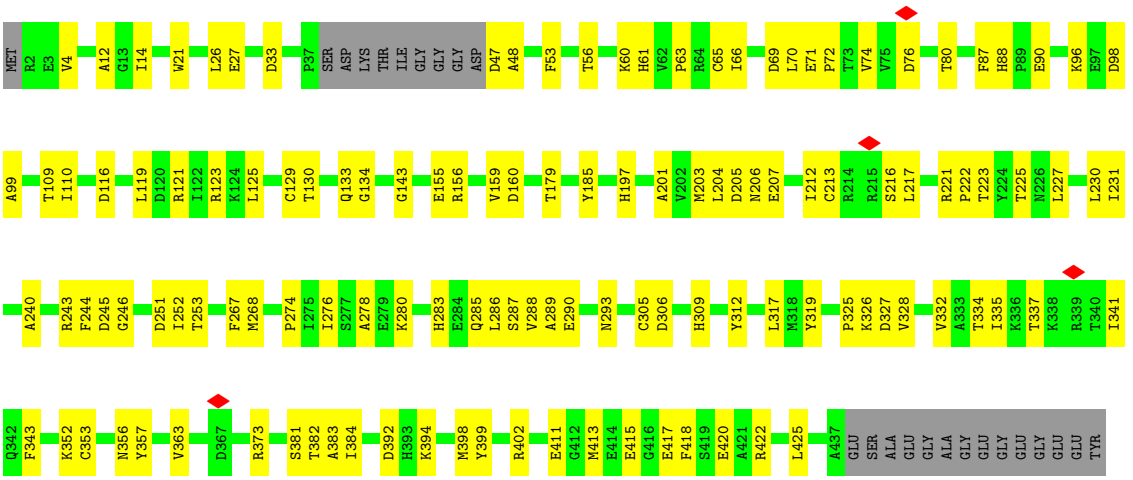
- Molecule 2: Tubulin alpha

Chain 2D:



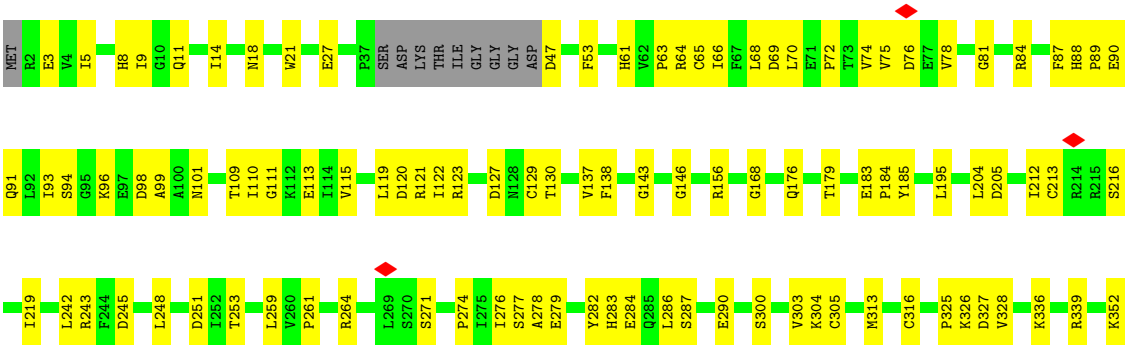

- Molecule 2: Tubulin alpha

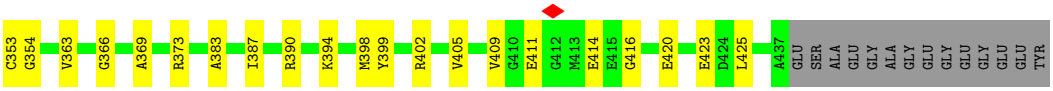
Chain 2F:




- Molecule 2: Tubulin alpha

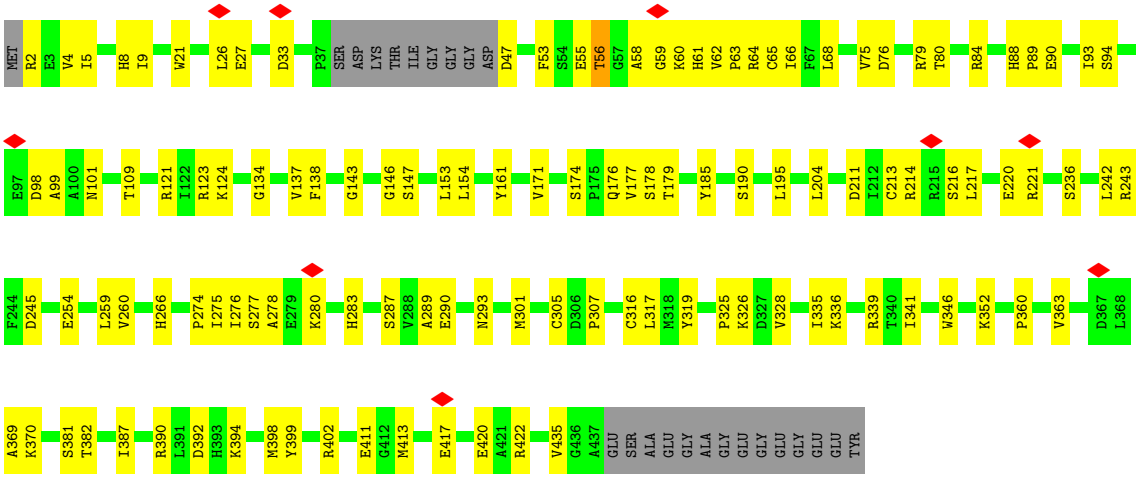
Chain 2H:





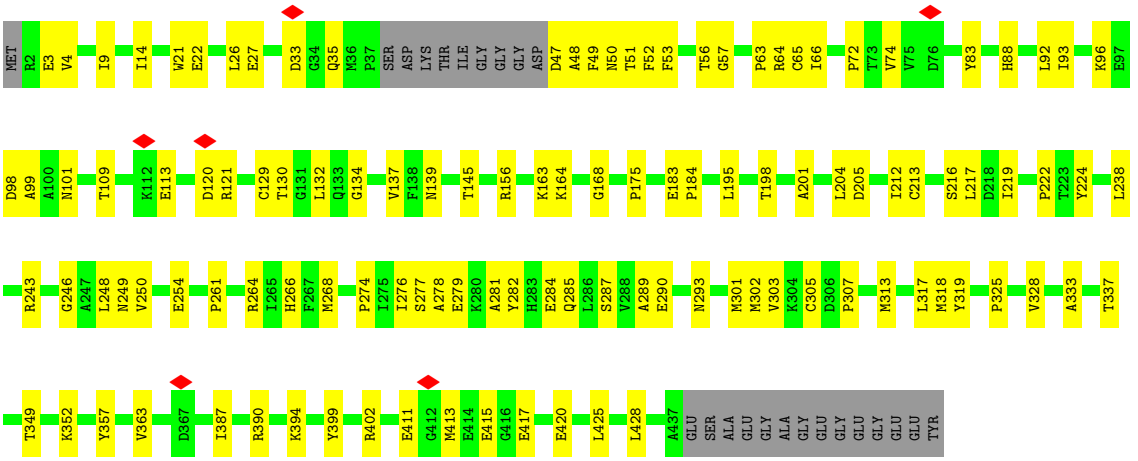

- Molecule 2: Tubulin alpha

Chain 2J:



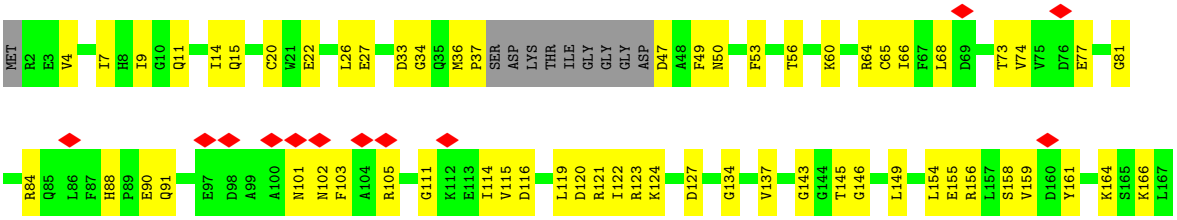

- Molecule 2: Tubulin alpha

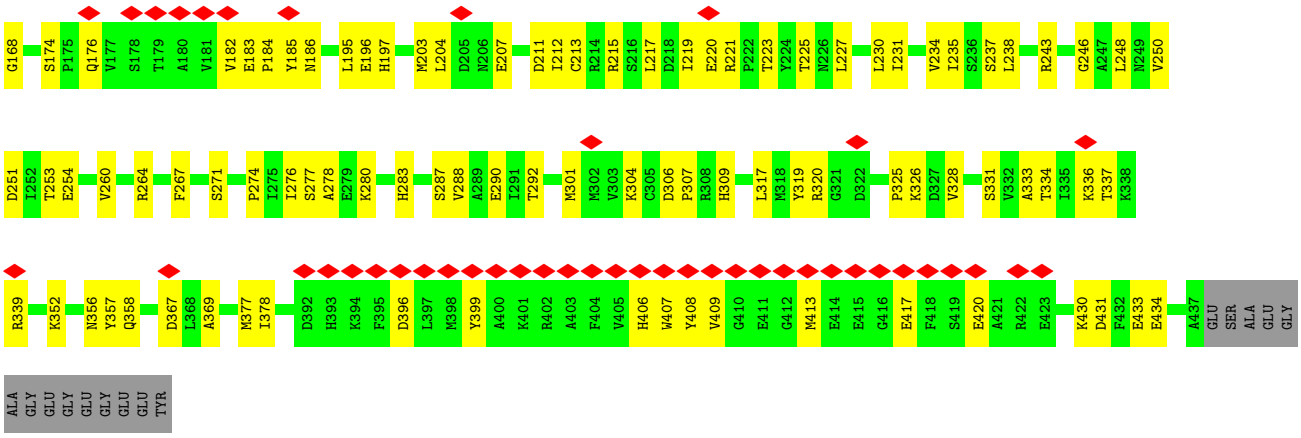
Chain 2L:




- Molecule 2: Tubulin alpha

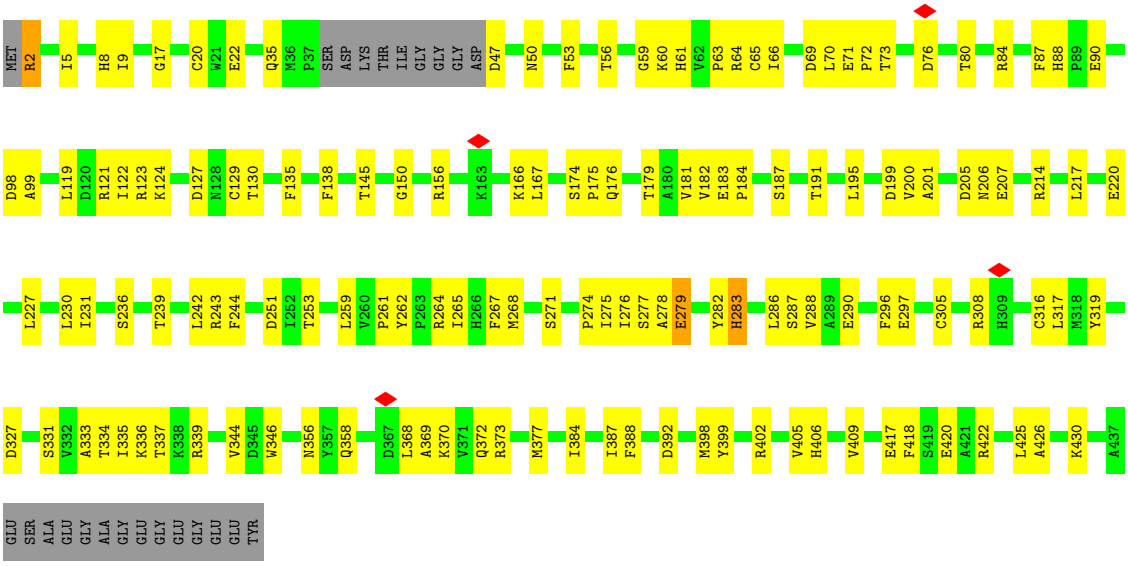
Chain 2N:





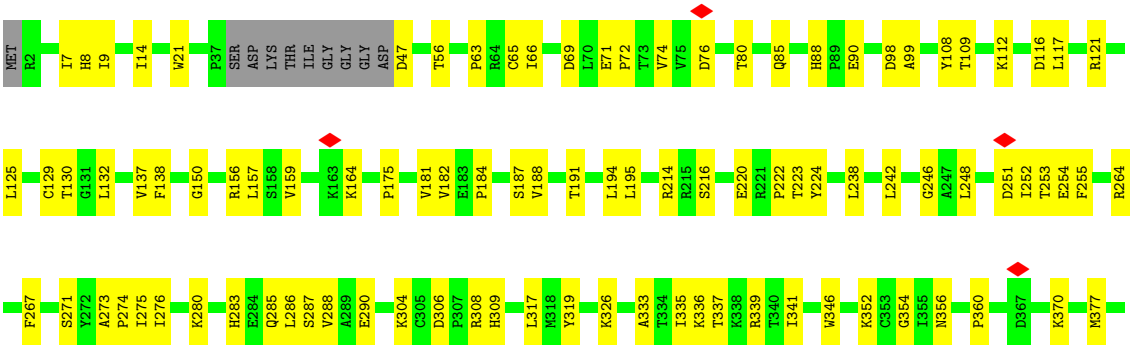

- Molecule 2: Tubulin alpha

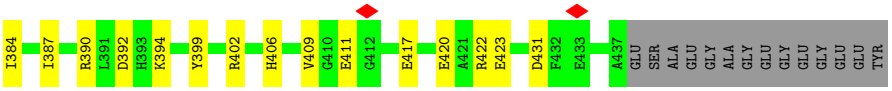
Chain 2P:




- Molecule 2: Tubulin alpha

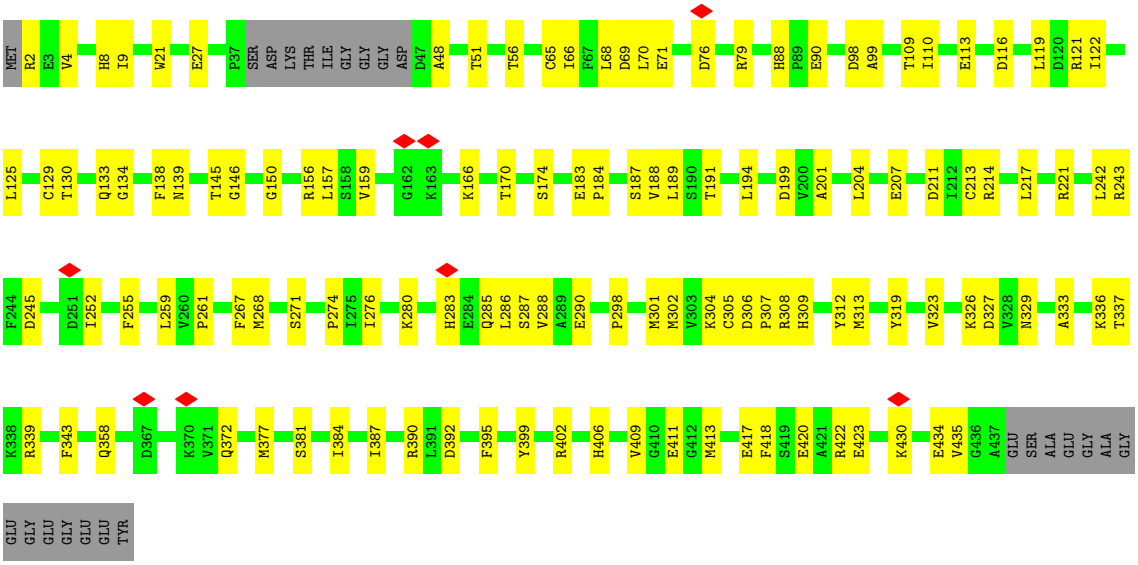
Chain 2R:





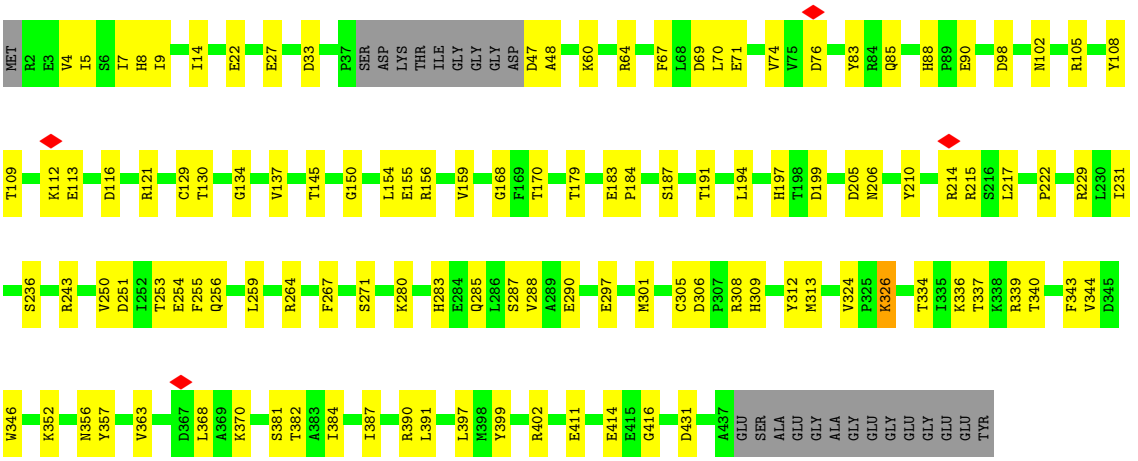

• Molecule 2: Tubulin alpha

Chain 2T:



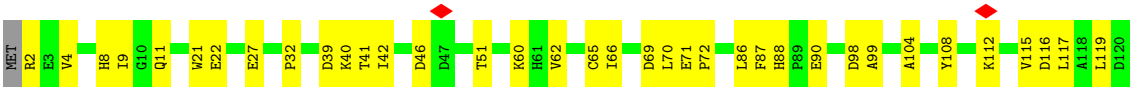

• Molecule 2: Tubulin alpha

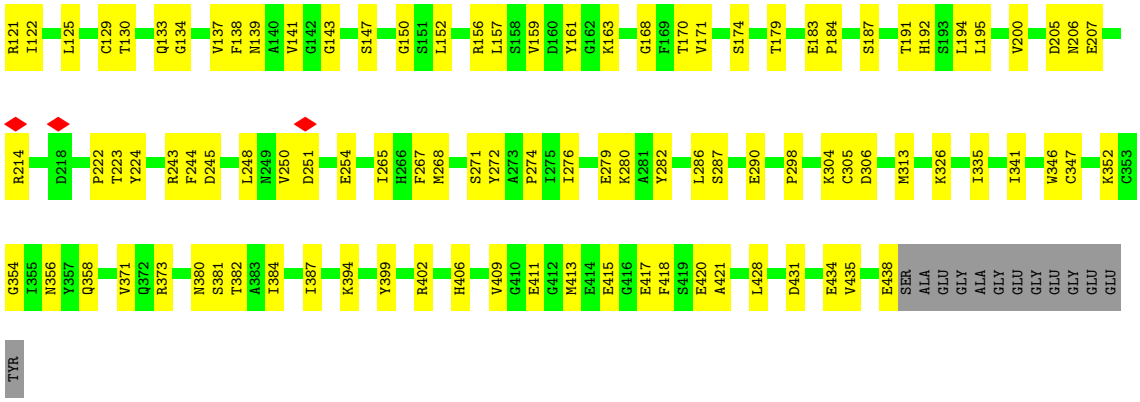
Chain 2V:




• Molecule 2: Tubulin alpha

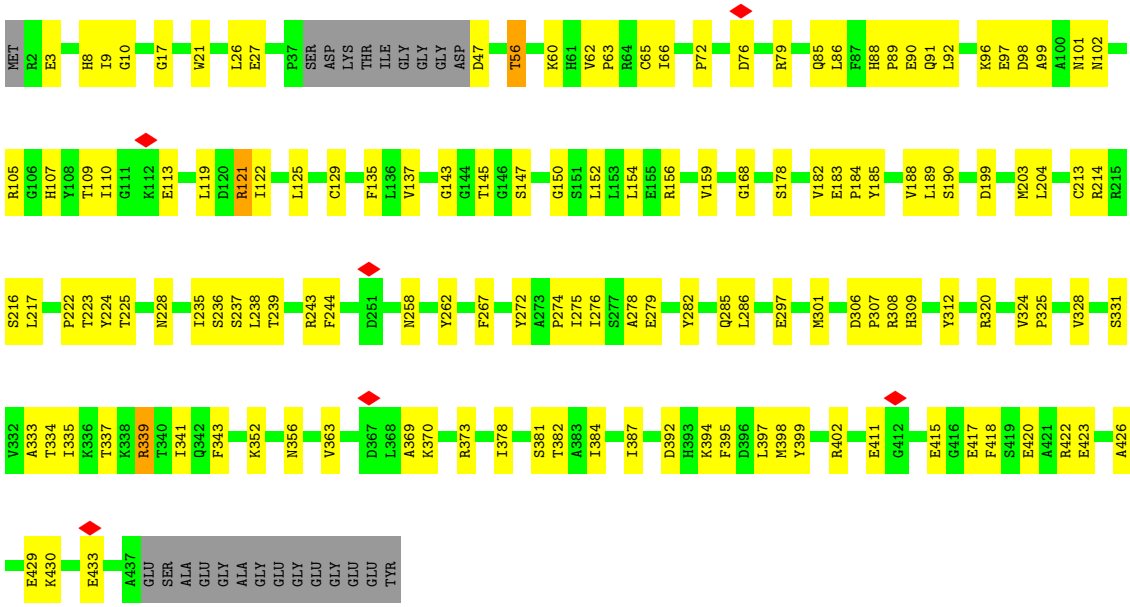
Chain 2X:





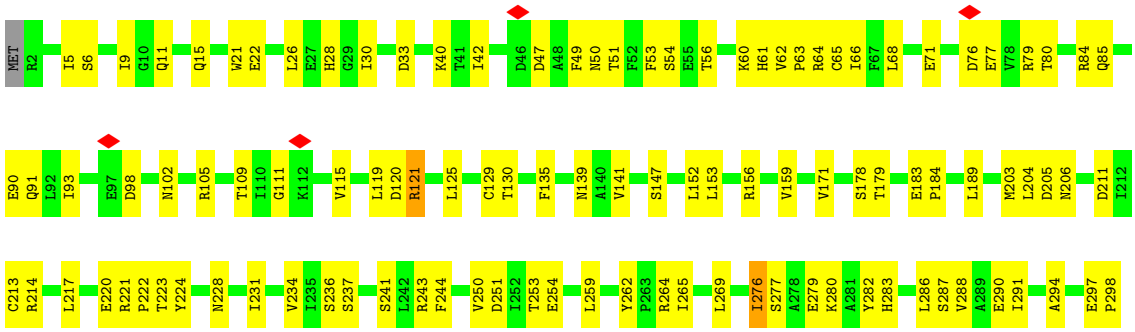

• Molecule 2: Tubulin alpha

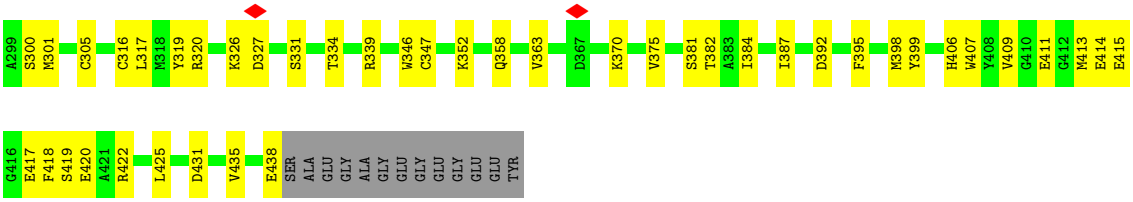
Chain 2Z:




• Molecule 2: Tubulin alpha

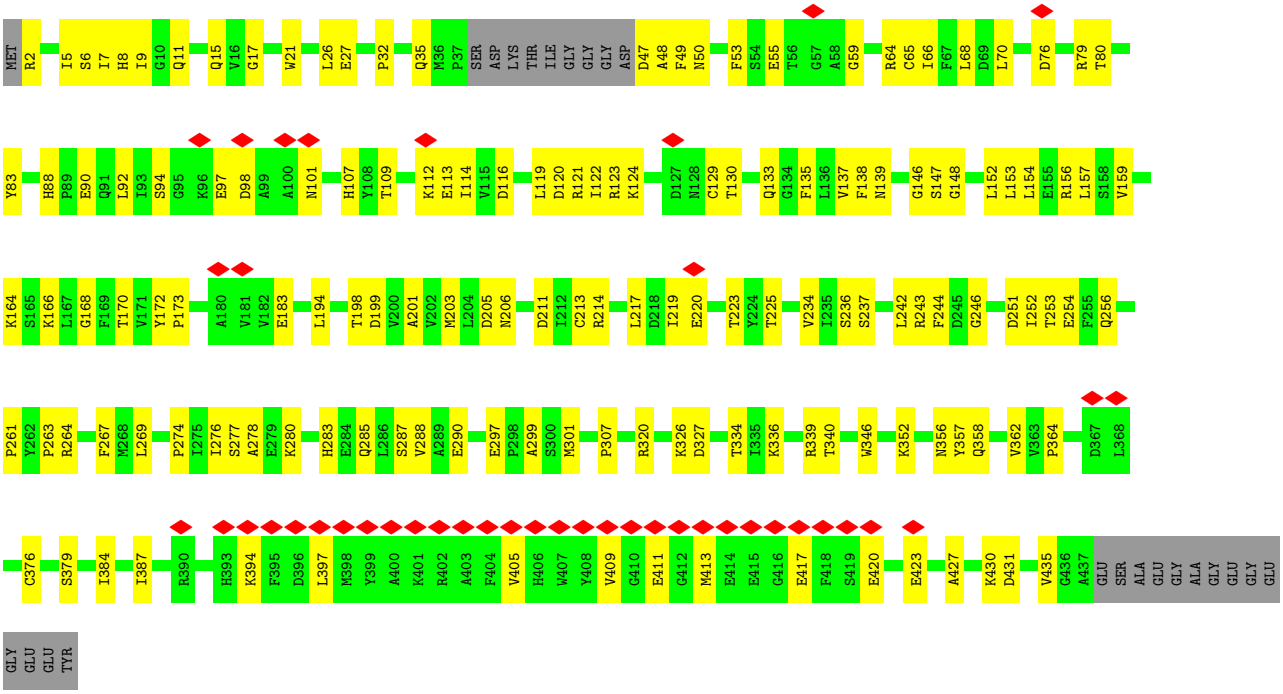
Chain 3B:





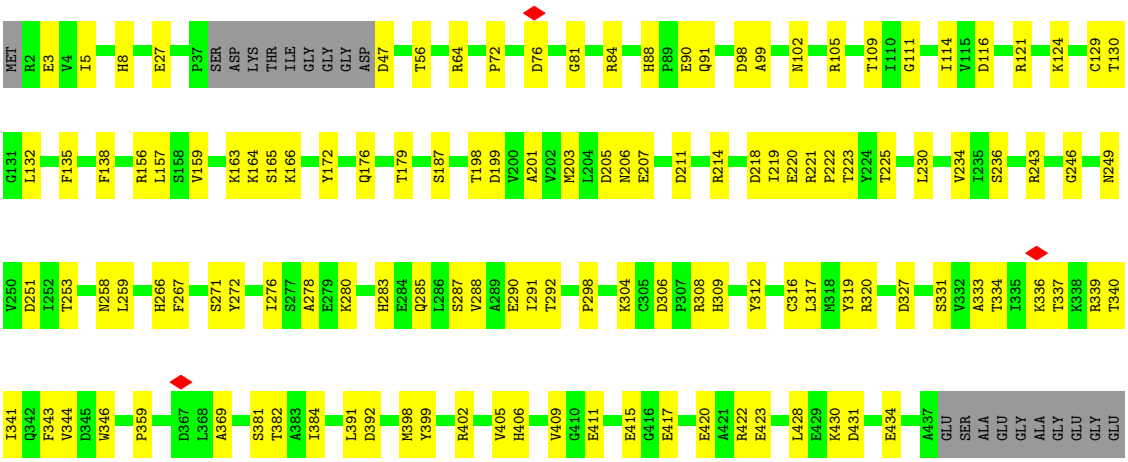

• Molecule 2: Tubulin alpha

Chain 3D:




• Molecule 2: Tubulin alpha

Chain 3F:



GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3H: 67% 27% 5%

MET R2 E3 V4 I5 I9 I14 W21 L26 E27 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 T56 P63 R64 C65 I66 P72 T73 V74 V75 D76 T80 R84 E90 Q91 D98 A99 V115 D116 L117 R121 K124

D127 N128 C129 F135 G146 S147 L152 L153 R156 V159 K163 K164 L167 S174 P175 Q176 V177 V182 E183 P184 Y185 S190 D199 V200 A201 V202 M203 L204 D205 N206 I219 E220 R221 P222 I231 S236 A240 R243 F244 D245 G246 V250 D251

E254 F255 Q256 P261 R264 F267 M268 L269 P274 I275 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 E290 I291 T292 N293 M301 C305 D306 P307 R308 H309 Y312 M313 R320 V324 D327 R339 T340 I341 Q342 F343 V344 D345 W346 T349

K352 N356 Y357 Q358 P359 V363 P364 G365 G366 D367 L368 A369 R373 A374 I384 R390 L391 D392 L397 M398 Y399 R402 E417 E420 A421 R422 D431 E434 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3J: 70% 25% 5%

MET R2 E3 H8 I9 I14 W21 E27 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 N50 T51 T56 R64 C65 L70 E71 P72 T73 V74 V75 D76 R79 H88 P89 E90 Q91 S94 D98 D116 L117 R121 I122 R123 K124 L125

A126 D127 N128 C129 Q133 F138 G146 R156 V159 S165 V177 S178 T179 E183 P184 H192 S193 L194 T198 D199 V200 C213 L217 E220 R221 P222 T223 Y224 S236 R243 G246 N249 I252 T253 E254 F255 Q256 T257 N258 L259 R264

F267 S271 Y272 I276 S277 A278 E279 K280 H283 E284 Q285 L286 S287 V288 A289 N293 M301 C305 D306 P307 L317 M318 Y319 K326 A333 T334 I335 K336 T337 K338 R339 T340 I341 Q342 F343 V344 D345 W346 T349 K352 N356 Y357 A369 R373

I384 I387 D392 H393 K394 L397 M398 Y399 R402 V405 E415 G416 E417 F418 S419 E420 A421 R422 D431 A437 GLU SER ALA GLU GLY ALA GLY GLU GLY GLU GLY GLU GLU TYR

- Molecule 2: Tubulin alpha

Chain 3L: 71% 24% 5%

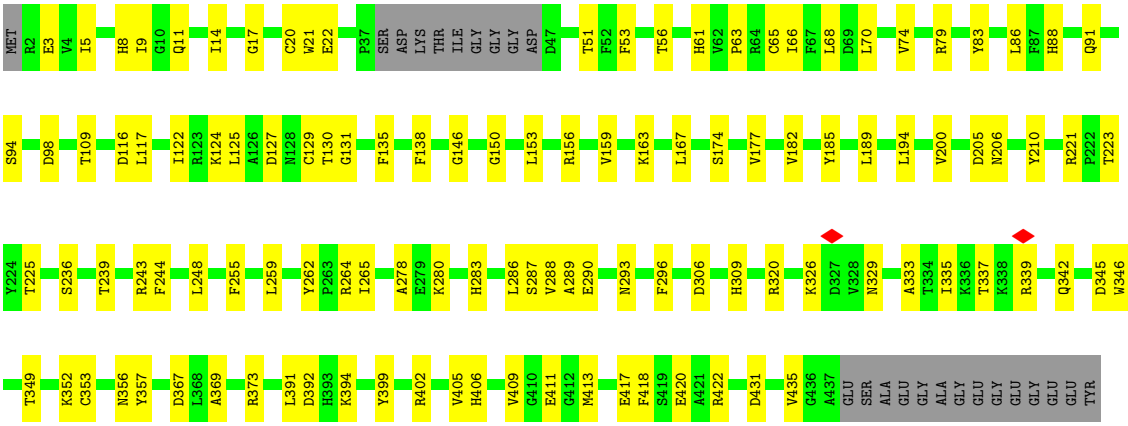
MET R2 E3 V4 I5 H8 I9 G10 Q11 I14 W21 E27 D33 P37 SER ASP LYS THR ILE GLY GLY GLY ASP D47 T51 T56 P63 R64 C65 E71 P72 D76 R79 R84 H88 Q91 D98 T109 L119 I122 R123

K124 L125 N128 C129 T130 G131 L132 Q133 G134 F135 F138 R156 V159 K163 K164 V177 S178 V182 E183 P184 Y185 V188 L189 L195 V200 C213 L217 D218 I219 E220 R221 P222 T223 Y224 S236 S237 L238 T239 R243 D251 I252 T253 E254 F255

L259 F267 M268 L269 S270 S271 K280 H283 L286 S287 V288 A289 E290 N293 F296 M301 C305 D306 P307 K326 A333 T334 I335 K336 T337 K338 R339 Q342 W346 T349 K352 N356 Y357 D367 R373 M377 I378 A383 I384 L391

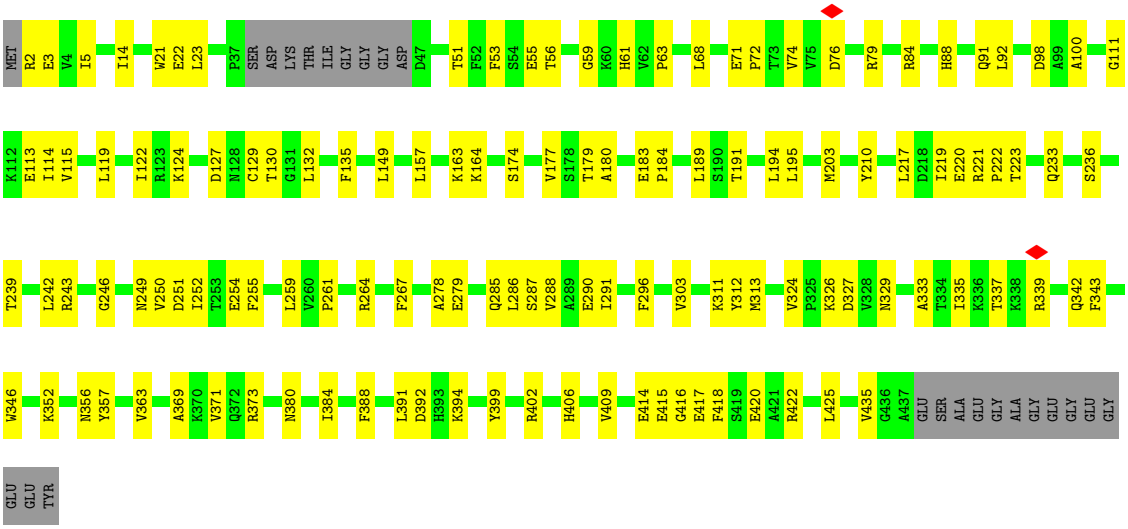
• Molecule 2: Tubulin alpha

Chain 3N:



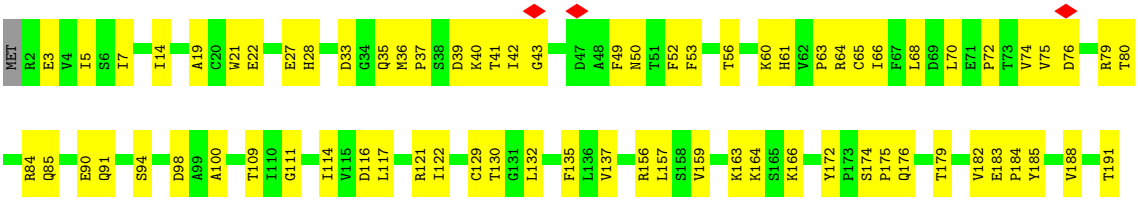

• Molecule 2: Tubulin alpha

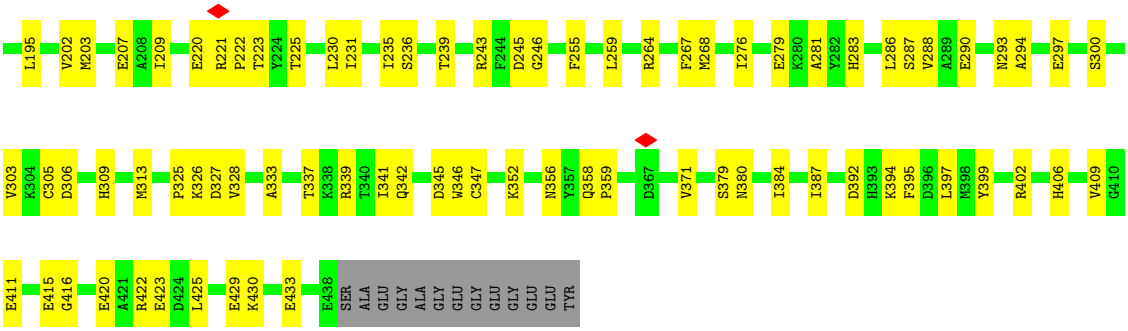
Chain 3P:




• Molecule 2: Tubulin alpha

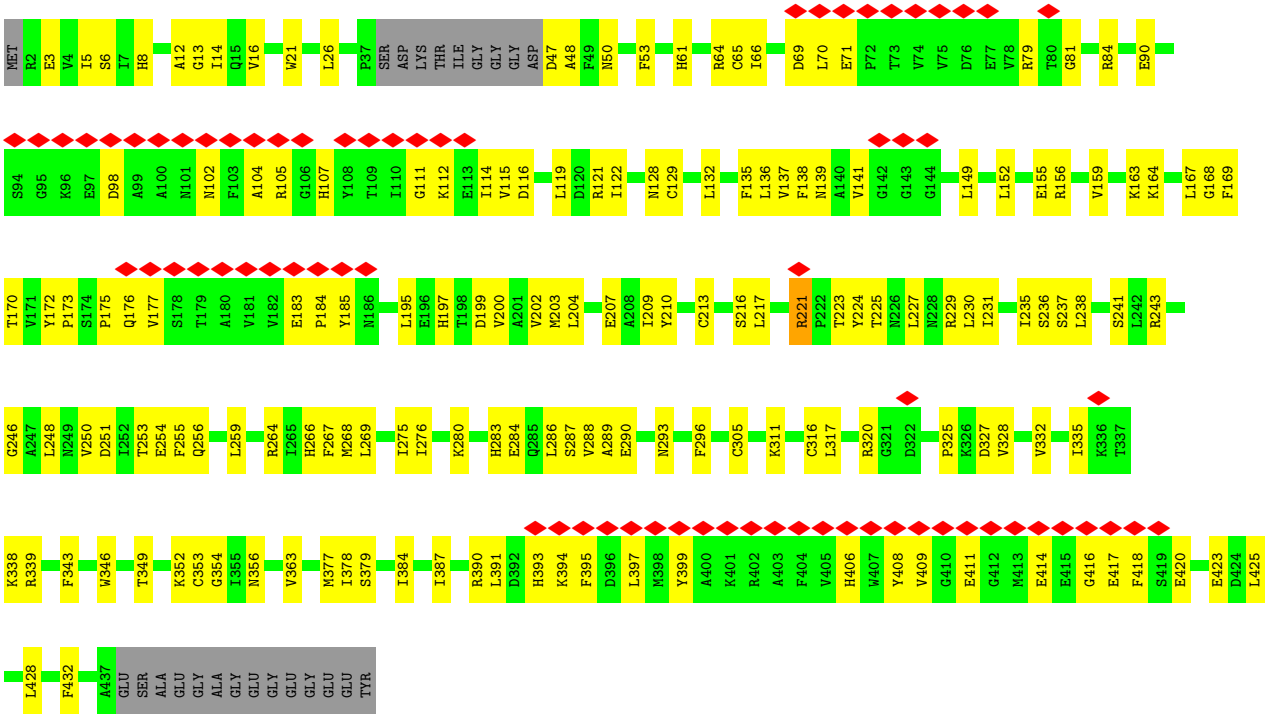
Chain 3R:





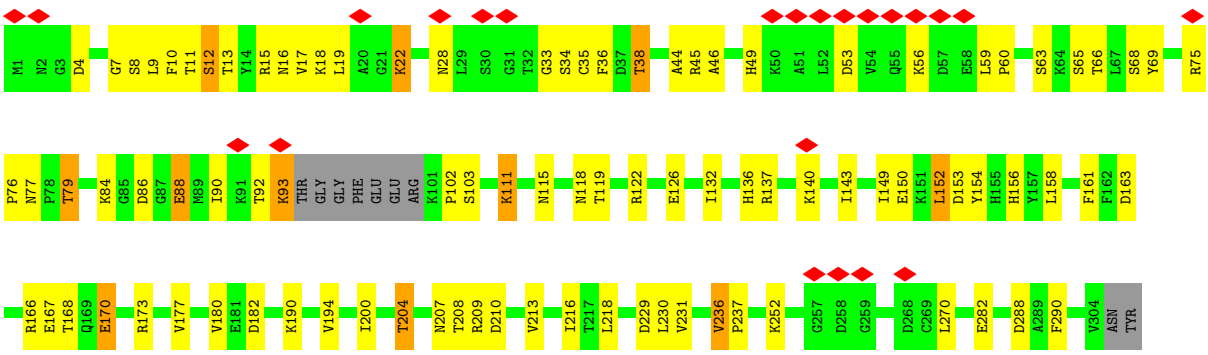

- Molecule 2: Tubulin alpha

Chain 3T:




- Molecule 3: PACRG

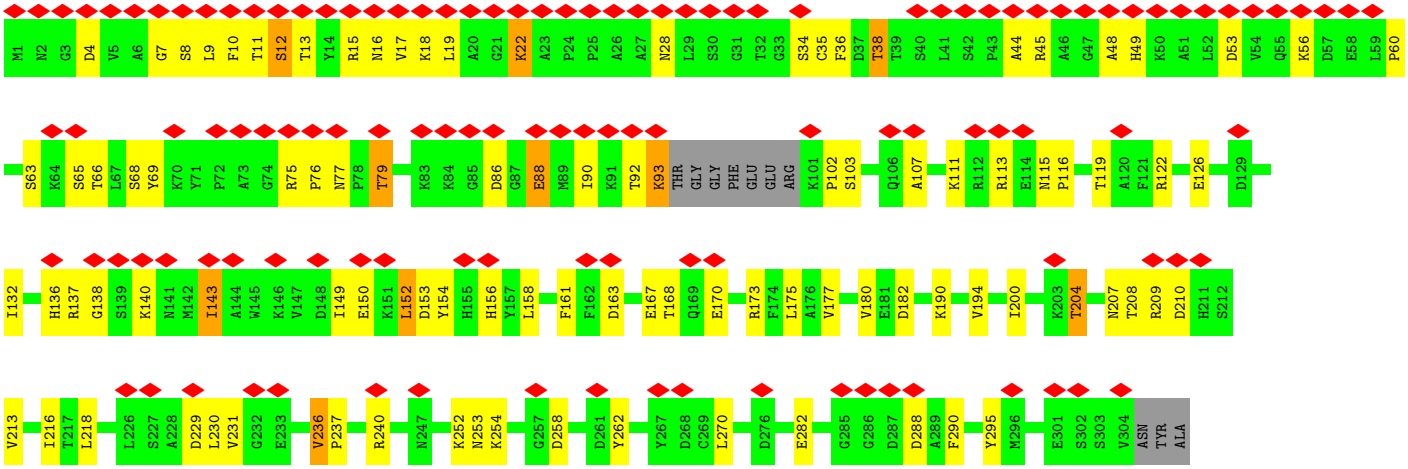
Chain 3V:



ALA

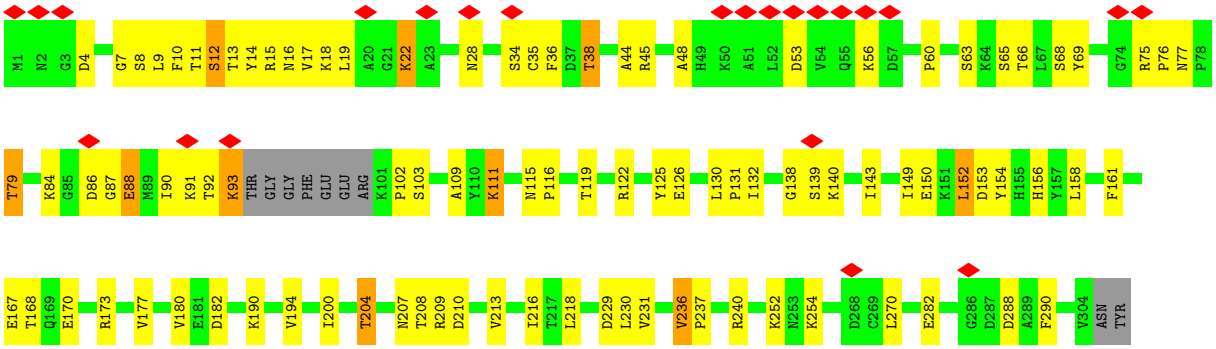
• Molecule 3: PACRG

Chain 3X:




• Molecule 3: PACRG

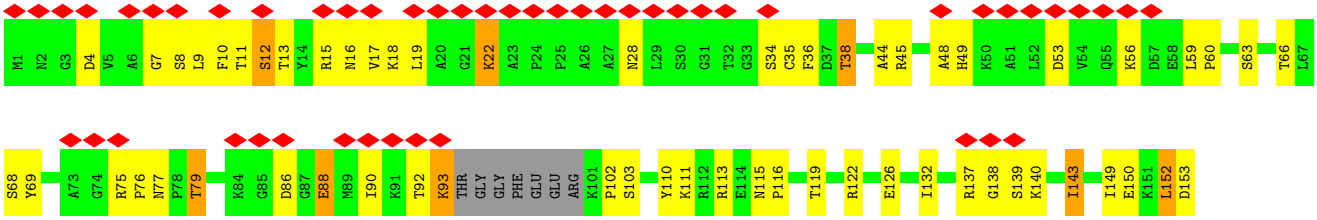
Chain 3Z:

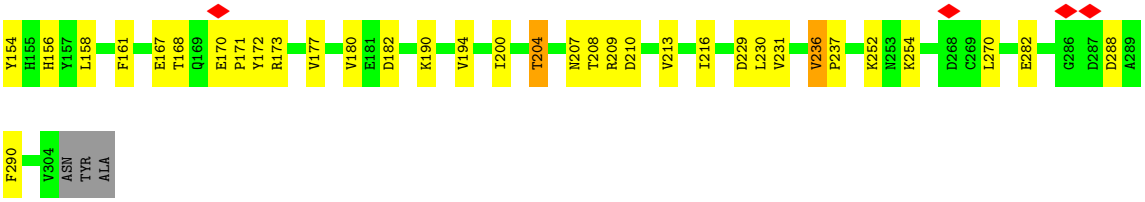



ALA

• Molecule 3: PACRG

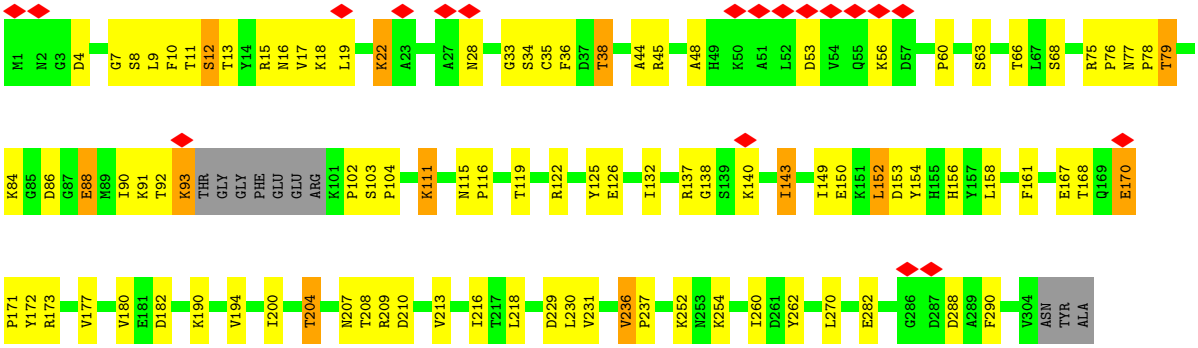
Chain 4B:





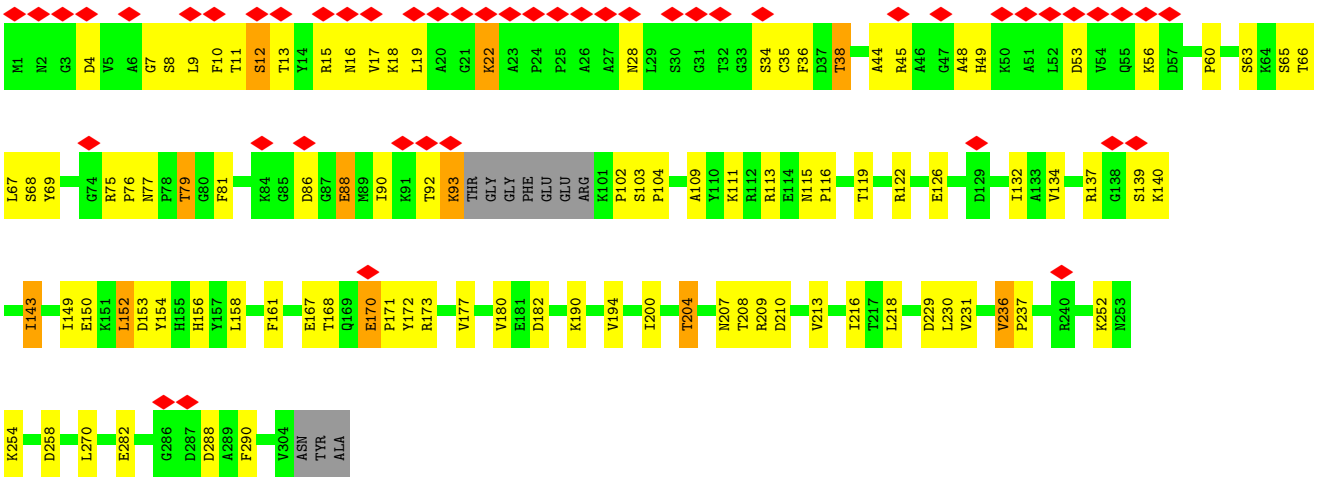

• Molecule 3: PACRG

Chain 4D:



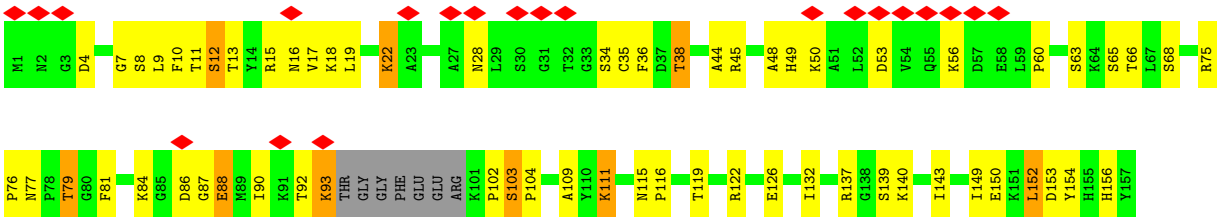

• Molecule 3: PACRG

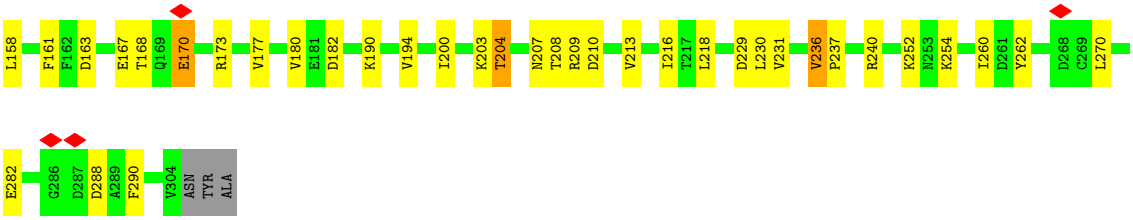
Chain 4F:




• Molecule 3: PACRG

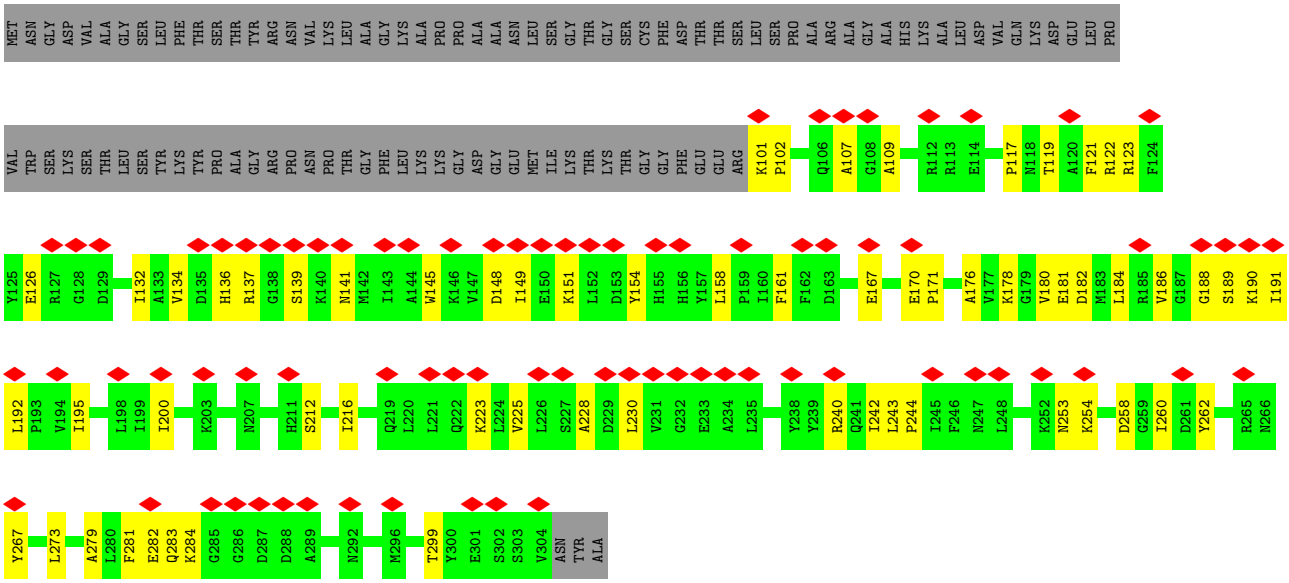
Chain 4H:





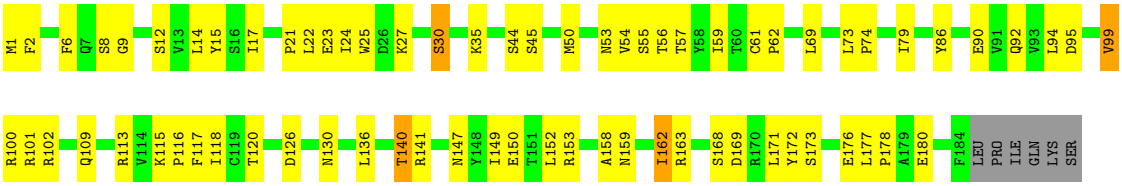

• Molecule 3: PACRG

Chain 4J:



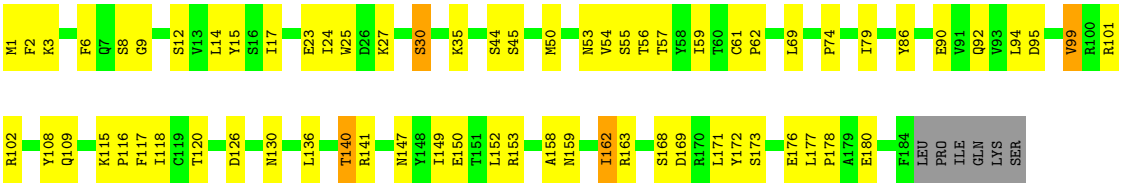

• Molecule 4: FAP20

Chain 3W:



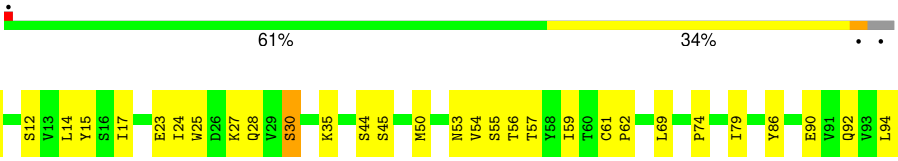

• Molecule 4: FAP20

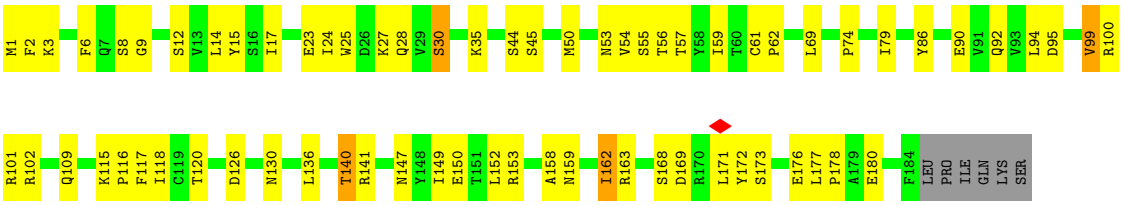
Chain 3Y:




• Molecule 4: FAP20

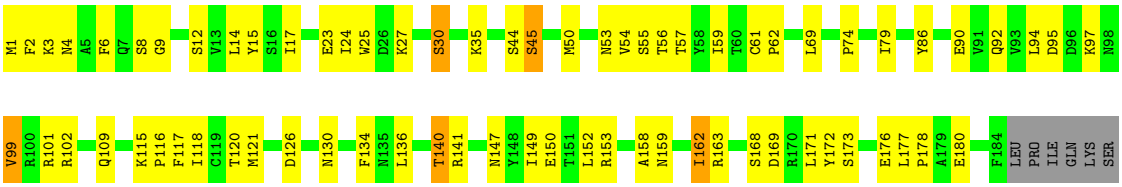
Chain 4A:



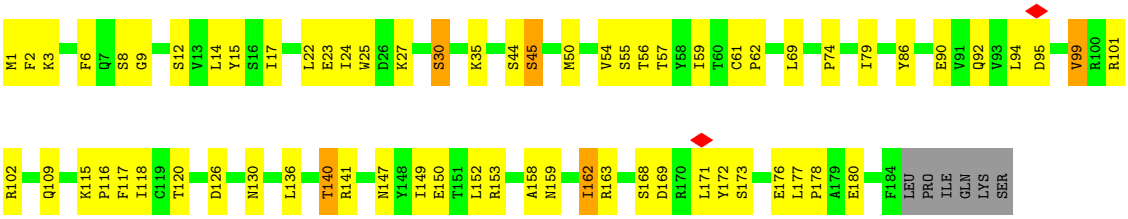

• Molecule 4: FAP20

Chain 4C:



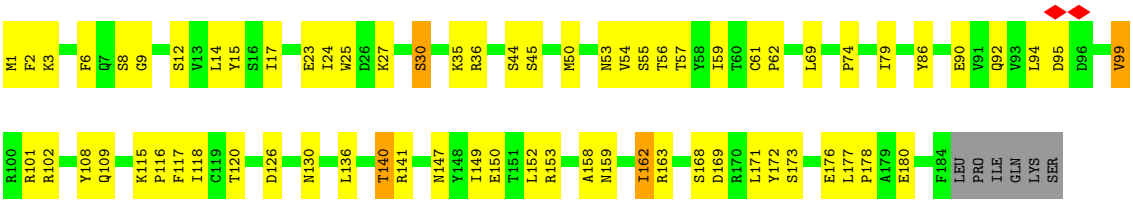

• Molecule 4: FAP20

Chain 4E:



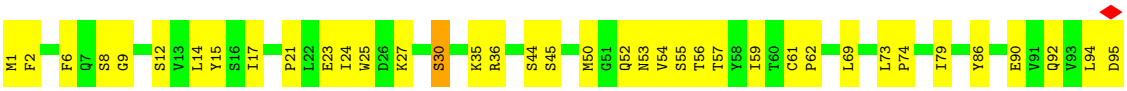

• Molecule 4: FAP20

Chain 4G:



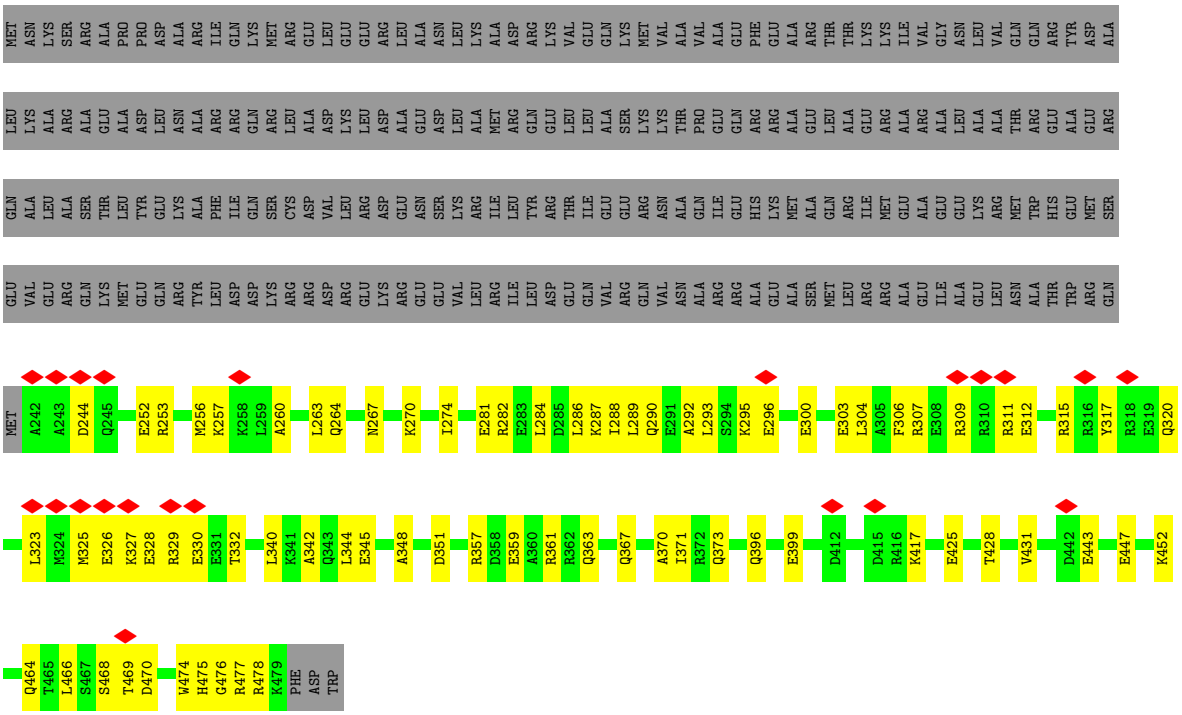

• Molecule 4: FAP20

Chain 4I:



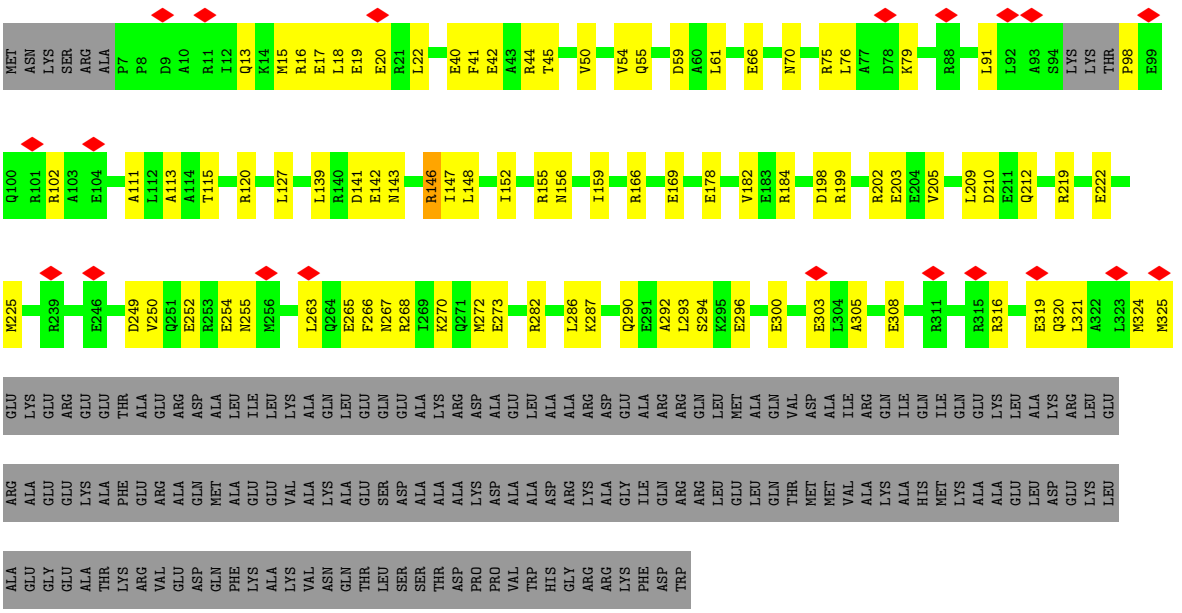
• Molecule 5: FAP53

Chain 4L:




• Molecule 5: FAP53

Chain 4M:



- Molecule 6: FAP127

Chain 4N:

MET SER ALA CYS ASP CYS THR CYS HIS ASP GLY GLY THR ARG ALA PRO LYS ARG GLY HIS LEU ALA ARG ALA VAL GLU GLN ARG GLU ALA ALA ARG ARG ILE ALA ALA ALA LYS SER GLU ILE ASN ARG TYR PHE ASN ASP GLN LYS VAL TYR ASP THR VAL ALA ALA ASN ALA VAL

LYS ASP ASP PHE LYS ARG LYS GLY ARG GLU PHE LYS GLU ARG ALA SER GLU ALA GLN MET LEU GLU SER LEU TYR GLN SER GLU ARG GLN LYS THR LEU ASN ALA ILE ARG ALA GLU GLU GLU GLU ARG ILE ALA VAL ALA MET ALA ARG LYS GLN GLN GLU LYS ASP ARG SER GLU ARG

GLU VAL GLN ARG LEU ARG GLU GLN SER ASP GLU LEU ARG SER LEU ALA GLU LYS ILE ARG VAL ALA ARG VAL ASN LYS GLU ARG SER ASP GLN LEU VAL GLU LYS LYS ILE ILE ILE GLY GLU GLN GLN GLU TYR ASP ARG ALA PHE ASN GLN PHE VAL ALA GLY ALA ALA ALA ALA GLU ALA

GLU ALA GLN GLU GLN GLU ASN GLN ALA LYS ARG ARG GLU ALA ASN VAL ARG ALA ARG MET VAL LEU GLU GLU GLN MET GLN GLU LYS ALA GLU ALA ARG LEU ALA GLU LEU GLU ALA VAL ARG GLU ARG ALA MET ILE ASP GLU VAL VAL ARG ARG ILE MET GLU GLU ASP ALA ALA

GLU MET ALA THR LYS ARG GLN ARG GLN GLU GLU THR LYS ASP PHE ILE SER HIS PHE LEU GLU GLN GLN ASP GLU LEU ARG ARG LYS GLU ARG GLU ALA ALA ALA GLU ASP LYS LYS ILE GLN GLU TYR TRP GLN SER VAL ARG GLU ARG GLU GLU ARG GLU ARG GLU GLU ALA LYS ARG

MET ARG LYS GLU ILE ALA ASP ARG MET TYR GLU LYS VAL LYS ARG GLU MET GLU ALA GLU MET ALA ARG ARG GLU GLU GLU GLU LEU ILE ASN MET LEU ARG ARG GLN GLU GLU GLU LEU GLU ALA LYS ARG ARG GLN GLU ASP ARG GLU LYS ALA GLU GLU GLU SER LYS GLU GLU

MET ARG ARG ALA ASN GLU TYR GLN MET LYS LEU LYS GLU GLU ARG GLU ALA ALA PHE ARG ALA GLU GLU GLU ALA PHE ARG GLN MET LEU ALA LYS PHE ALA GLU ASP GLU LYS LEU GLU GLU GLN MET ASN ALA GLN LYS ARG ARG MET ARG MET ALA GLU HIS ALA ARG GLU VAL GLN

ARG LEU ILE ASP GLU LYS ARG GLN ALA PHE GLU ALA ALA LYS ALA ARG GLU GLU ALA GLU ASP ALA ALA LYS ARG S446 E447 D448 V451 R452 V455 E456 E457 E458 K461 L462 L463 R464 E465 A466 A467 E468 L469 K470 D471 P474 R475 G476 V477 L478 I487 S488 L491

N497 ARG ALA LYS ALA THR GLN GLY ARG

- Molecule 6: FAP127

Chain 4O:

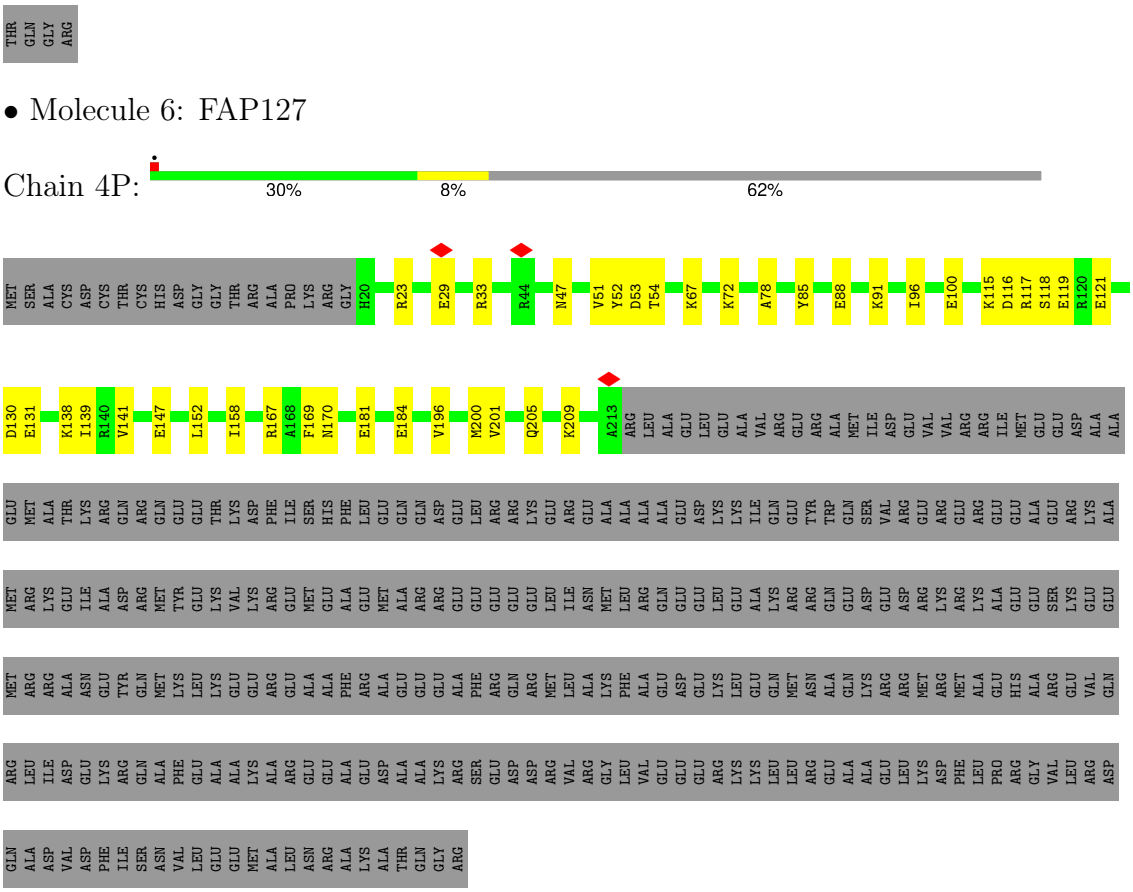
MET SER ALA CYS ASP CYS THR CYS HIS ASP GLY GLY THR ARG ALA PRO LYS ARG GLY H20 L21 A22 E26 Q27 R28 I34 A35 E36 N43 N47 V51 D62 D63 F64 K65 R66 R69 E70 F71 K72 E73 R74 A75 S76 E77 A78 Q79 M80 L81 E82 S83 L84 Y85

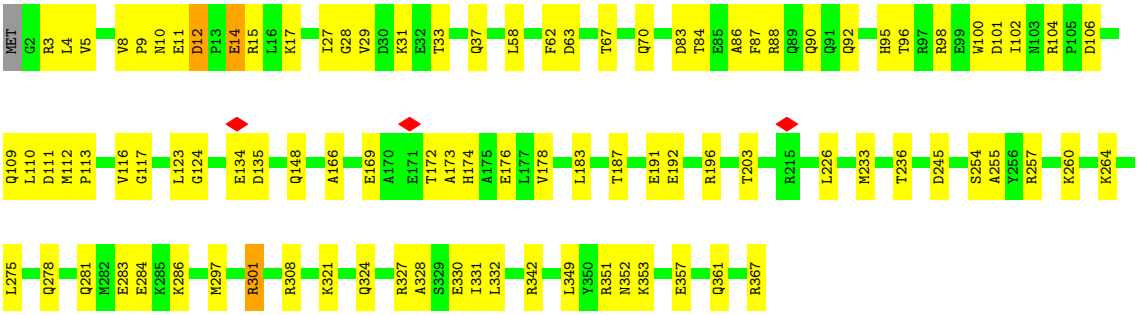
Q86 S87 E88 R89 Q90 K91 T92 L93 N94 A95 I96 R97 A98 E99 E100 E101 E102 R103 A107 E114 K115 S118 V122 R126 D130 E131 L135 A136 E137 K138 I139 R140 V141 K146 E147 R148 S149 D150 Y165 F169 E181 A182 Q183 E184 Q185 E186 K190

R199 E203 E208 E211 A212 A213 R214 L215 E219 R222 E223 R224 Q247 R248 E251 T252 K253 D254 H258 E261 Q262 Q263 D264 E265 R268 R271 A275 A276 E277 D278 K279 K280 Y284 W285 Q286 S287 V288 R289 E290 R291 E292 R293 E294 E295 A296 E297 R298

K299 A300 M301 R302 K303 E304 I305 A306 D307 R308 M309 Y310 E311 K312 V313 K314 R315 E316 M317 E318 A319 E320 M321 A322 R323 R324 E325 E326 E327 E328 E329 N332 M333 Q336 E337 D349 R350 K351 R352 K353 A354 E355 E356 S357 K358 E359 E360 M361 R362 R363 Q368 L371 R375 E376

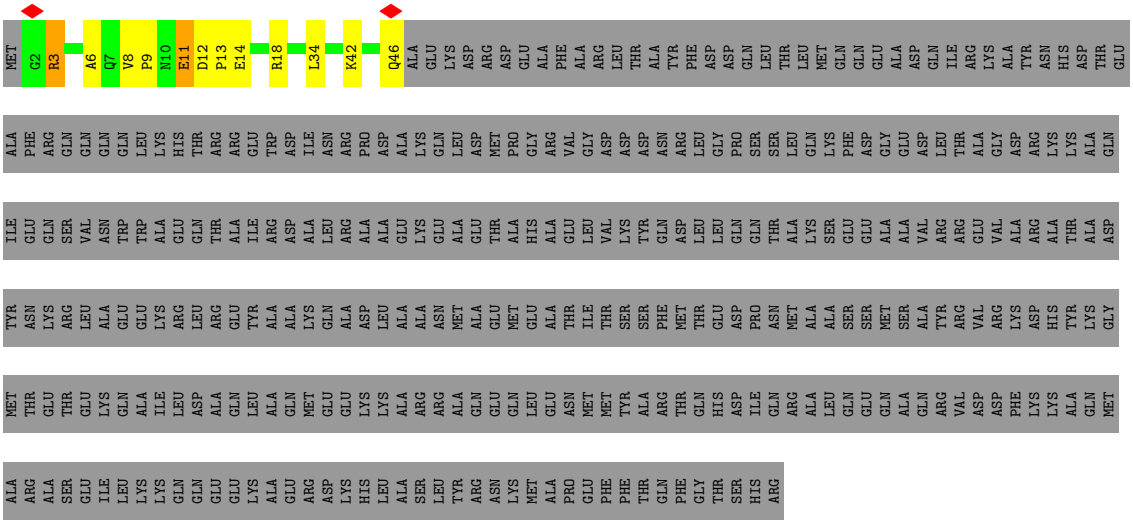
A377 R380 F386 R387 Q388 R389 M390 L391 F394 Q406 K407 R408 R409 M410 R411 H415 E418 R421 E425 D449 R452 G453 L454 V455 E456 E457 E458 R459 K460 K461 E465 L469 P474 R475 D483 V484 I487 V490 N497 ARG ALA LYS ALA


THR GLN GLY ARG
• Molecule 6: FAP127
Chain 4P:
30%
8%
62%
MET SER ALA CYS ASP CYS THR CYS HIS ASP GLY GLY THR ARG ALA PRO LYS ARG GLY H20 R23 E29 R33 R44 N47 V51 Y52 D53 T54 K67 K72 A78 Y85 E88 K91 I96 E100 K115 D116 R117 S118 E119 R120 E121
D130 E131 K138 I139 R140 V141 E147 L152 I158 R167 A168 F169 N170 E181 E184 V196 M200 V201 Q205 K209 A213 ARG LEU ALA GLU LEU GLU ALA VAL ARG GLU ARG ALA MET ILE ASP GLU VAL VAL ARG ILE MET GLU GLU ASP ALA ALA
GLU MET ALA THR LYS ARG GLN ARG GLN GLU GLU GLU THR LYS ASP PHE ILE SER HIS PHE LEU GLU GLN GLN GLN ASP GLU GLU LEU ARG ARG LYS GLU ARG GLU ALA ALA ALA ALA GLU ASP LYS LYS ILE GLN GLU TYR TRP GLN SER VAL ARG GLU ARG GLU GLU ARG LYS ALA
MET ARG LYS GLU ILE ALA ASP ARG MET TYR GLU LYS VAL LYS ARG GLU MET GLU ALA GLU MET ALA ARG ARG GLU GLU GLU GLU GLU LEU ILE ASN MET LEU ARG GLN GLU GLU LEU GLU ALA LYS ARG ARG GLN GLU ASP GLU ASP ARG LYS ARG LYS ALA GLU GLU SER LYS GLU GLU
MET ARG ARG ALA ASN GLU TYR GLN MET LYS LEU LYS GLU GLU ARG GLU ALA ALA PHE ARG ALA GLU GLU GLU ALA PHE ARG GLN ARG MET LEU ALA LYS PHE ALA GLU ASP GLU LYS LEU GLU GLN MET ASN ALA GLN GLN LYS ARG ARG MET ARG MET ALA GLU HIS ALA ARG GLU VAL GLN
ARG LEU ILE ASP GLU LYS ARG GLN ALA PHE GLU ALA ALA LYS ALA ARG GLU GLU GLU ALA GLU ASP ALA ALA LYS ARG SER GLU ASP ASP ARG VAL ARG GLY LEU VAL GLU GLU GLU ARG LYS LYS LEU LEU ARG GLU ALA ALA GLU LEU LYS ASP PHE LEU PRO ARG GLY VAL LEU ARG ASP
GLN ALA ASP VAL ASP PHE ILE SER ASN VAL LEU GLU GLU MET ALA LEU ASN ARG ALA LYS ALA THR GLN GLY ARG
• Molecule 7: RIB43a
Chain 4Q:
15%
83%
MET GLY ARG LEU VAL ALA GLN VAL PRO ASN GLU ASP PRO GLU ARG LEU LYS ARG VAL LEU ASP ALA LYS TRP ARG THR ILE GLY VAL ASP LYS GLU THR LEU GLU LEU GLN ALA GLN GLU LYS LYS ASP ARG GLU GLN ALA GLU LYS ASP ARG ASP GLU ALA PHE ALA ARG LEU ASP THR ASP
TYR PHE ASP ASP GLN LEU THR LEU MET GLN GLN GLU ALA ASP GLN ILE ARG LYS ALA TYR ASN HIS ASP THR GLU ALA PHE ARG GLN GLN GLN GLN LEU LYS HIS THR ARG ARG GLU TRP ASP ILE ASN ARG PRO ASP ALA LYS GLN LEU ASP MET PRO GLY ARG VAL GLY ASP ASP
ASN ARG LEU GLY PRO SER SER LEU GLN LYS PHE ASP GLY GLU ASP LEU THR ALA GLY ASP ARG LYS LYS ALA GLN ILE GLU GLN SER VAL ASN TRP TRP ALA GLU GLN THR ALA ILE ARG ASP ALA LEU ARG ALA ALA GLU LYS GLU ALA GLU THR ALA HIS ALA GLU LEU VAL LYS TYR
GLN ASP LEU LEU GLN GLN THR ALA LYS SER GLU GLU ALA VAL ARG ARG GLU VAL ALA ARG ALA THR ALA ASP TYR ASN LYS ARG LEU ALA GLU GLU LYS ARG LEU ARG GLU TYR ALA ALA LYS GLN ALA ASP LEU ALA ALA ALA ASN MET ALA GLU MET GLU ALA THR ILE THR SER SER
PHE MET THR GLU ASP PRO ASN MET ALA ALA SER SER MET SER ALA TYR ARG VAL ARG LYS ASP HIS TYR LYS GLY MET THR GLU THR GLU LYS GLN ALA ILE LEU ASP ALA GLN LEU ALA GLN MET GLU GLU LYS LYS ALA ARG ARG ALA GLN GLU GLN LEU GLU ASN MET MET TYR ALA
ARG THR GLN HIS D305 I306 F320 K321 K322 A323 Q324 Q336 N352 S365 H366 R367
• Molecule 7: RIB43a
Chain 4R:
74%
25%



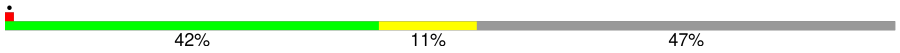

- Molecule 7: RIB43a

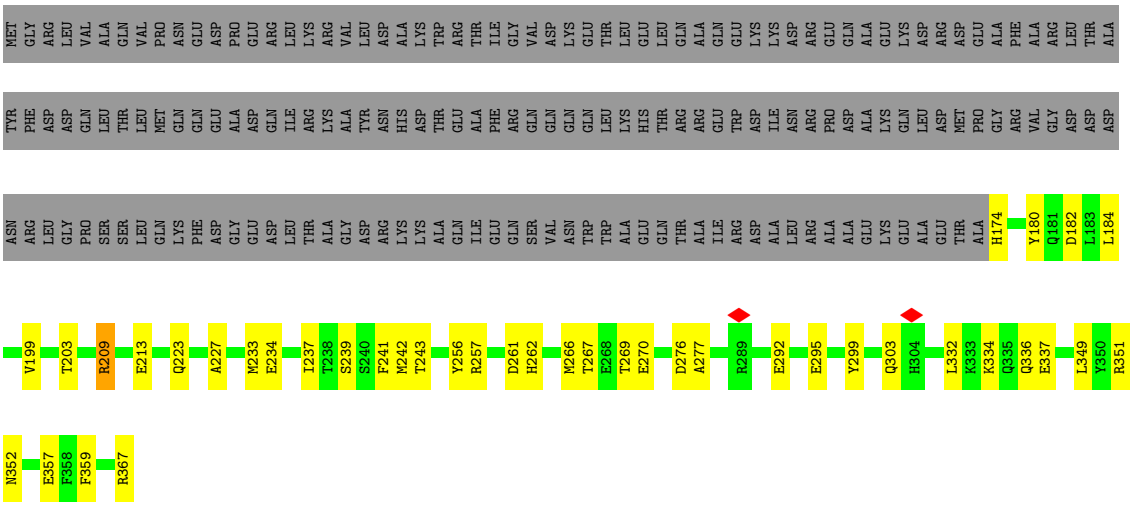
Chain 4S:




- Molecule 7: RIB43a

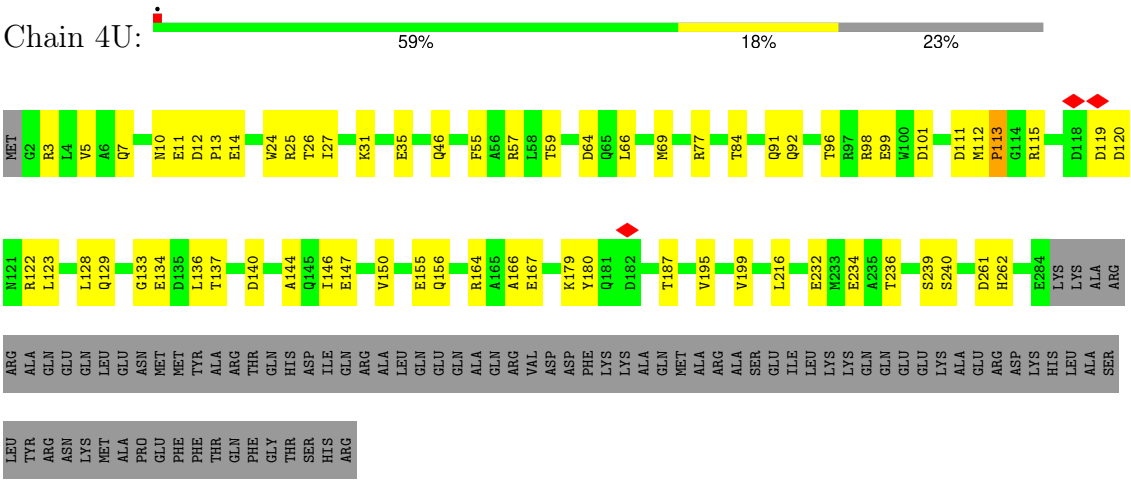
Chain 4T:



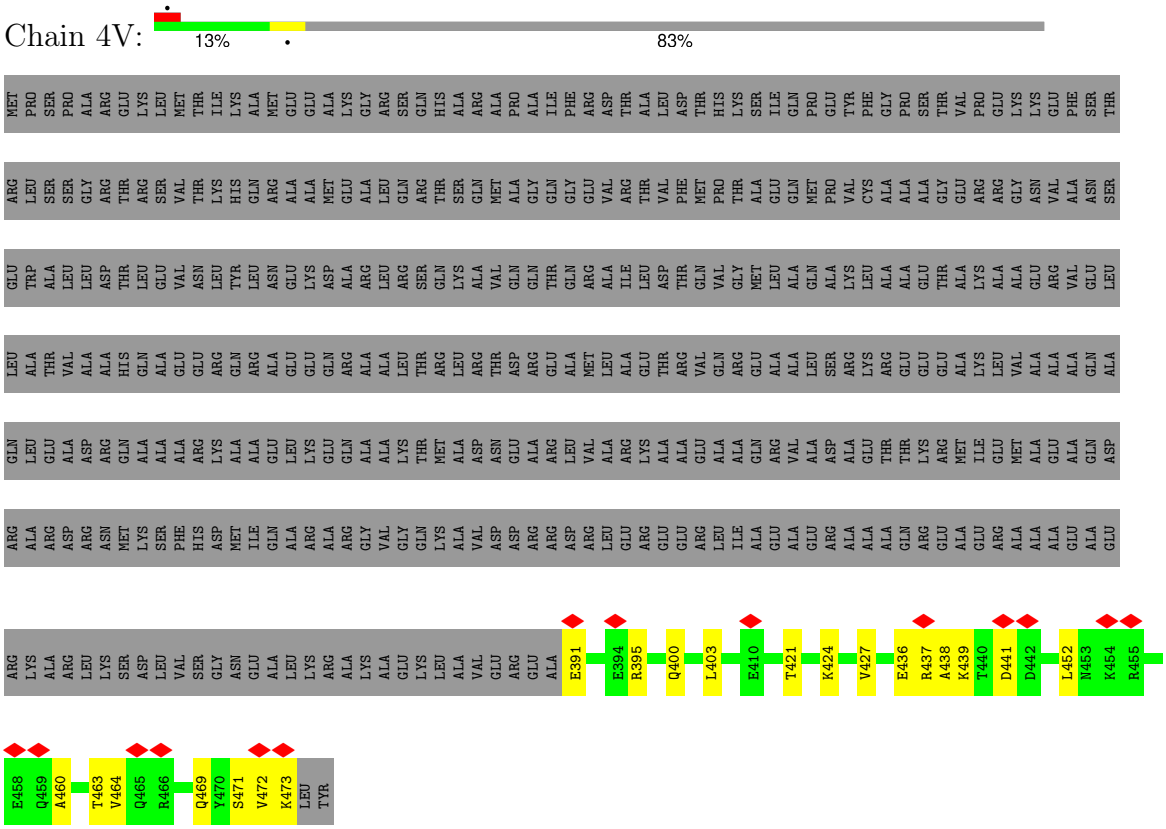

- Molecule 7: RIB43a

Chain 4U:



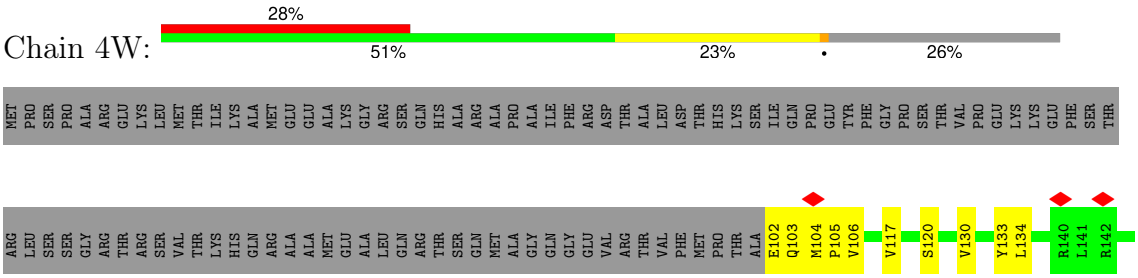

- Molecule 8: FAP112

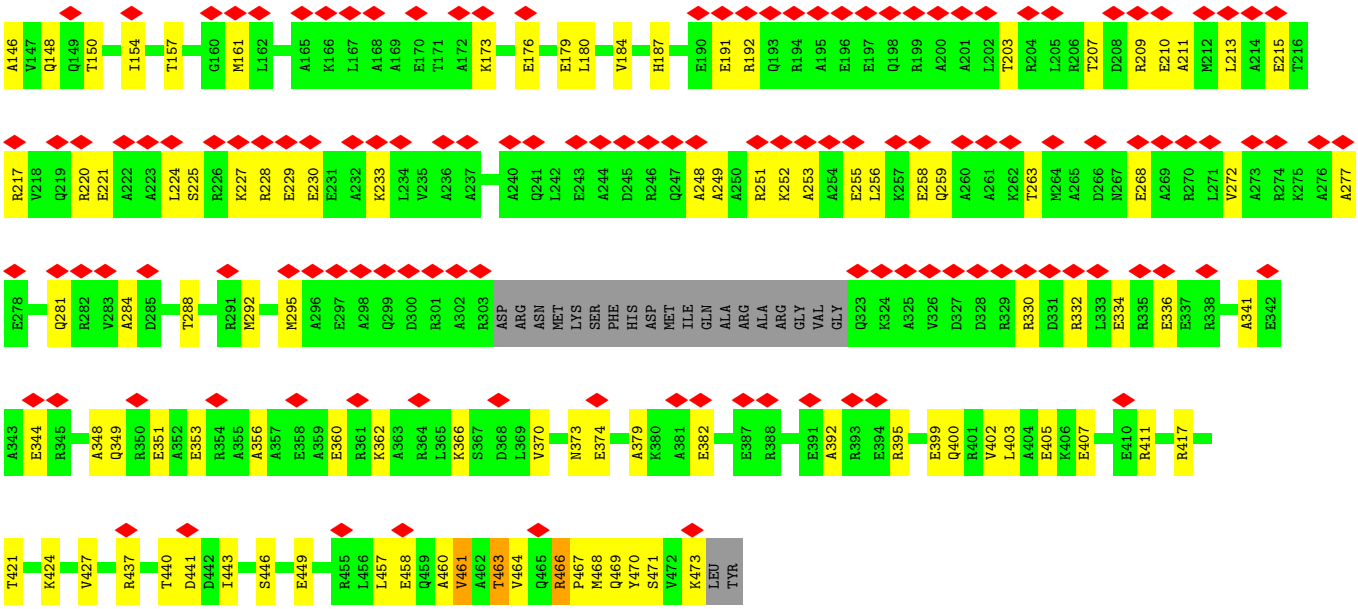
Chain 4V:




- Molecule 8: FAP112

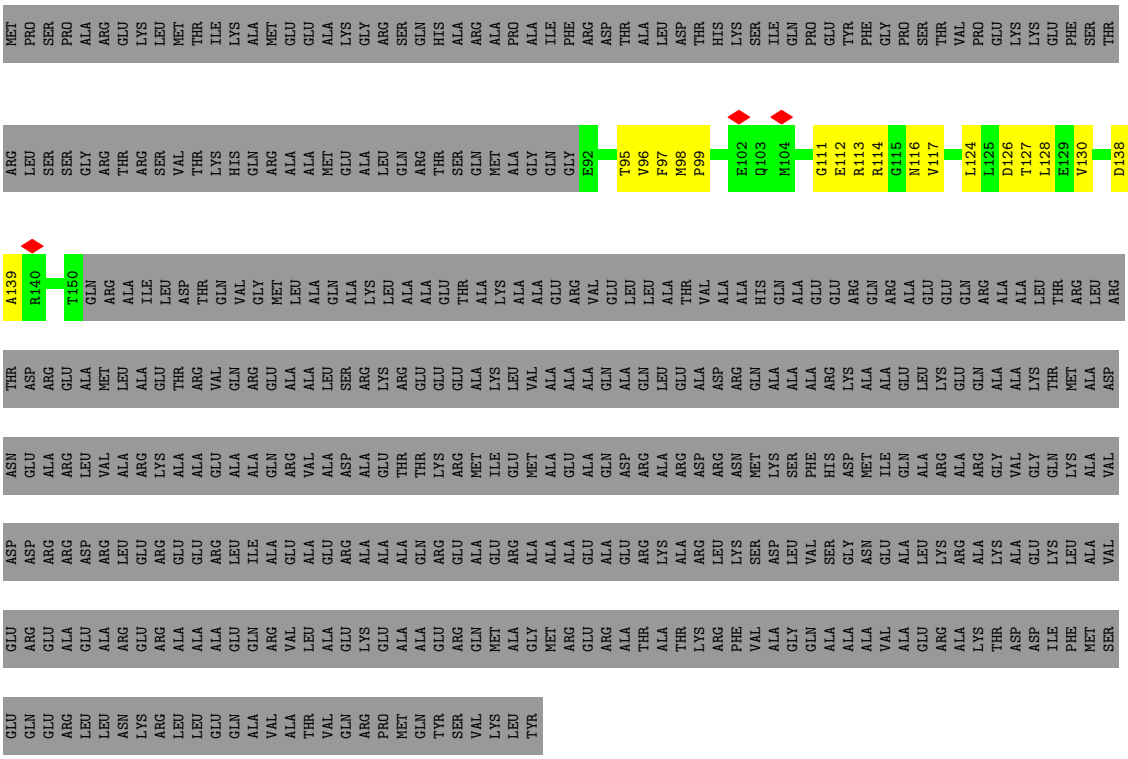
Chain 4W:





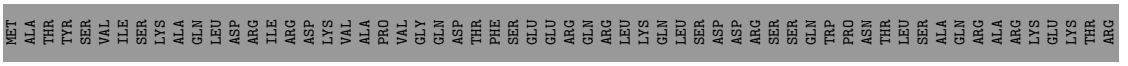

- Molecule 8: FAP112

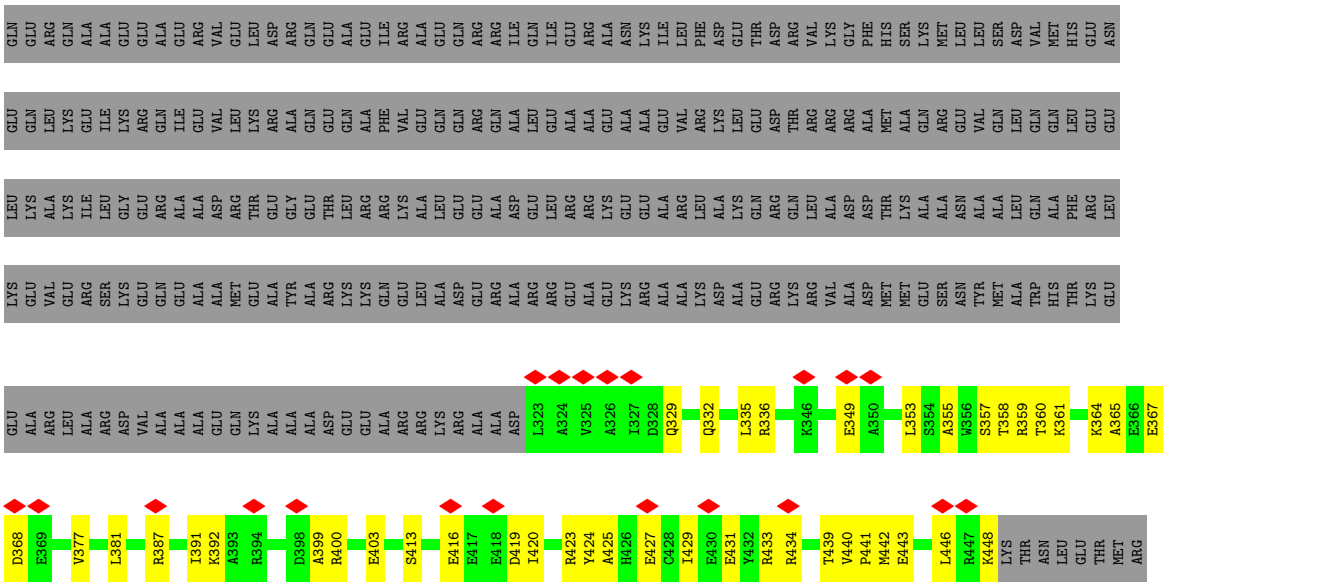
Chain 4X:




- Molecule 9: FAP210

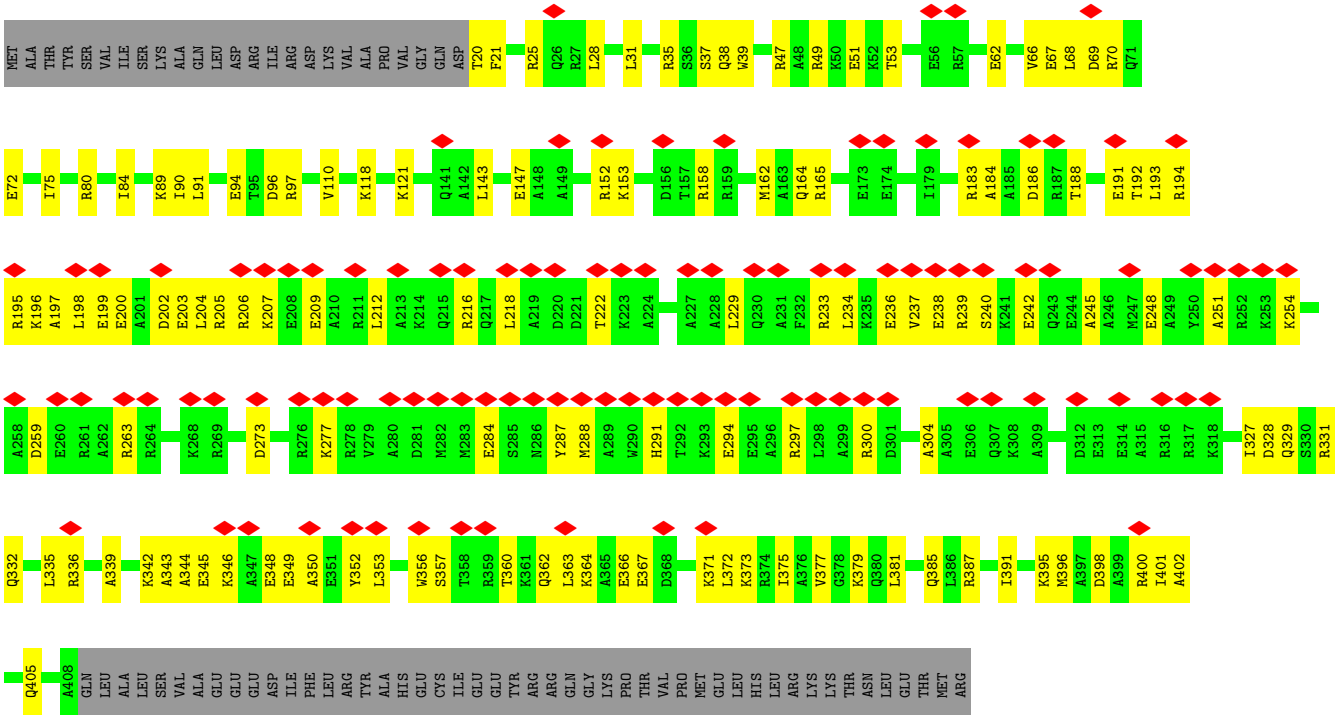
Chain 4Y:





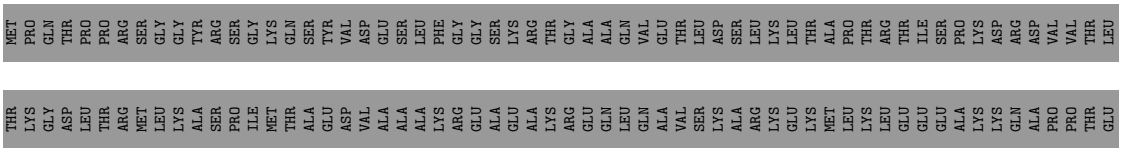
- Molecule 9: FAP210

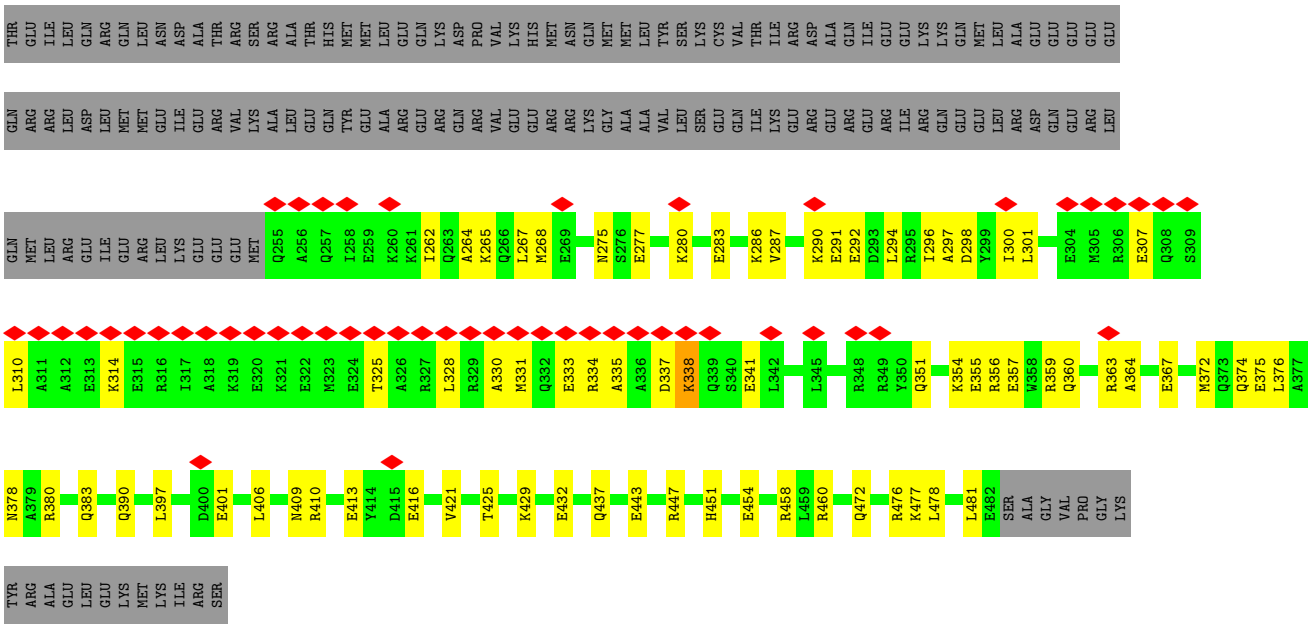
Chain 4Z:



- Molecule 10: FAP45

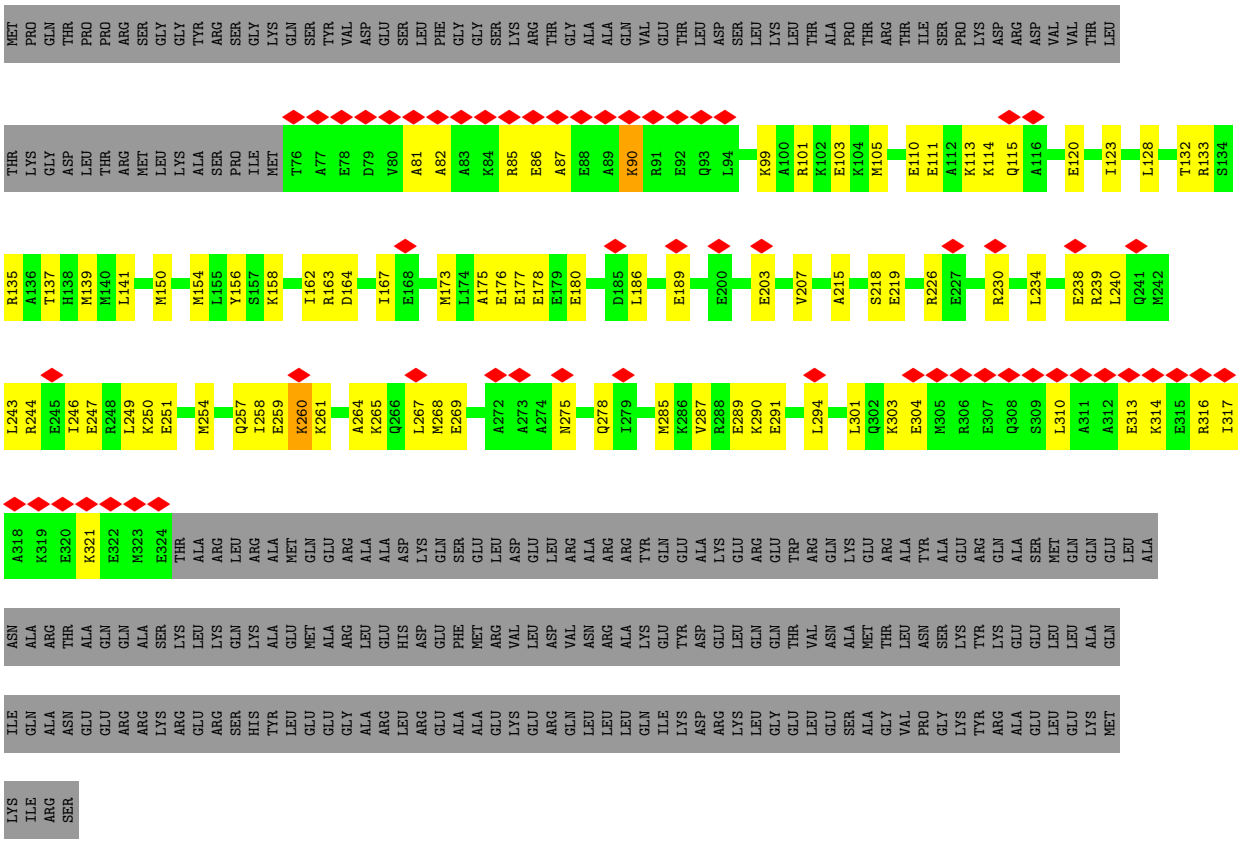
Chain 5A:





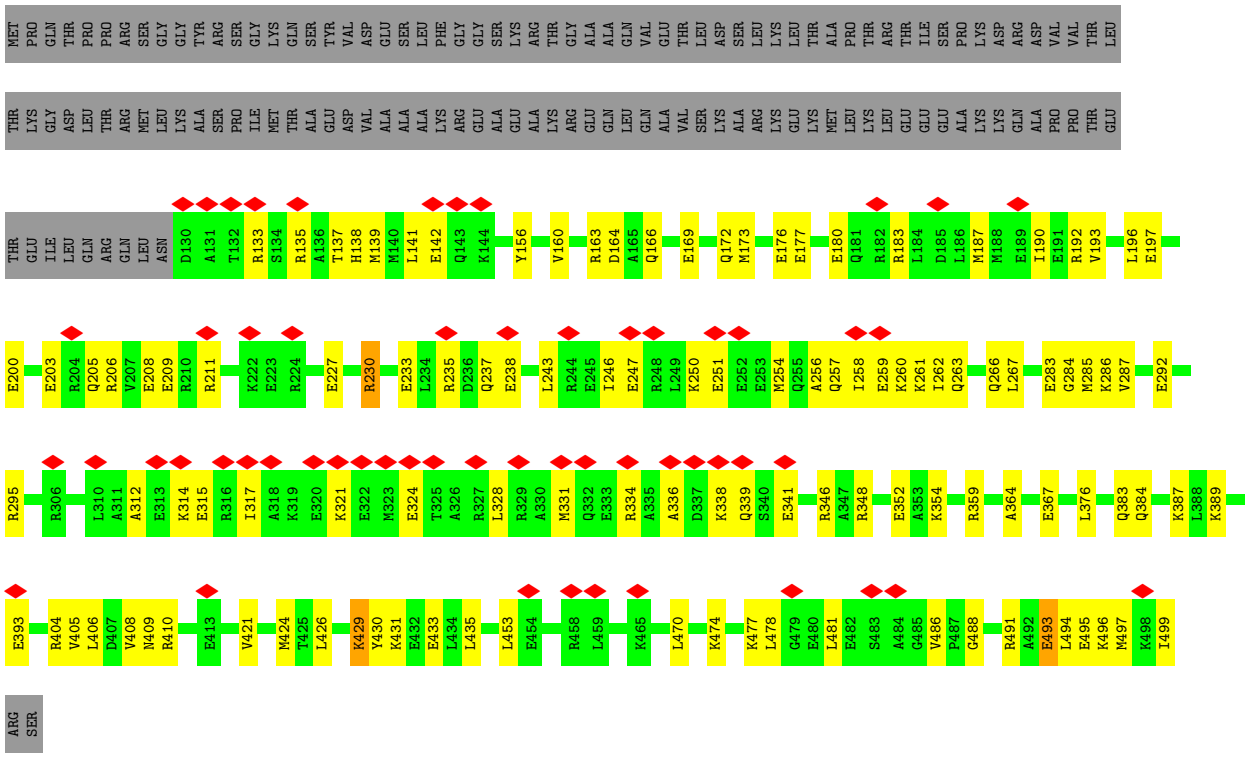

- Molecule 10: FAP45

Chain 5B:



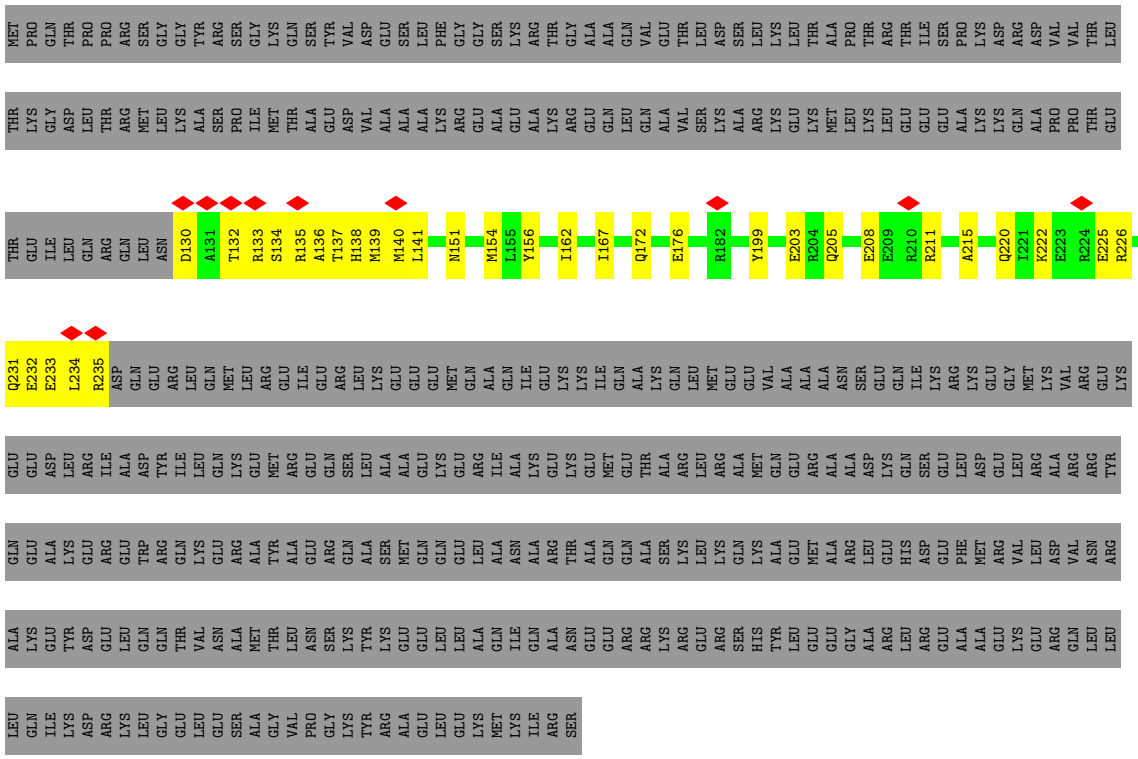

- Molecule 10: FAP45

Chain 5C:



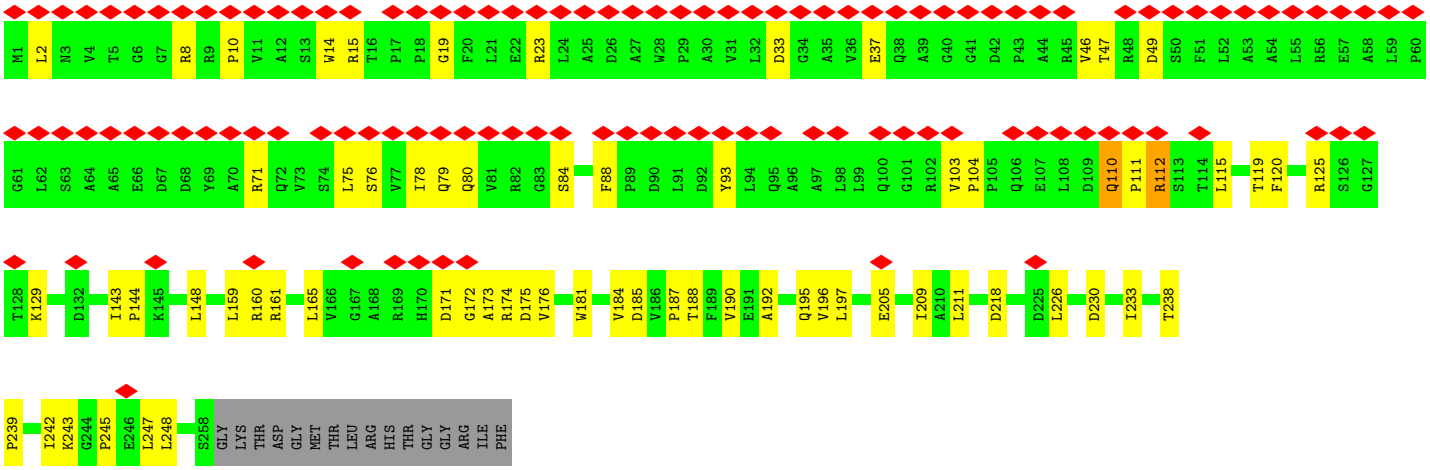
• Molecule 10: FAP45

Chain 5D: 14% 7% 79%



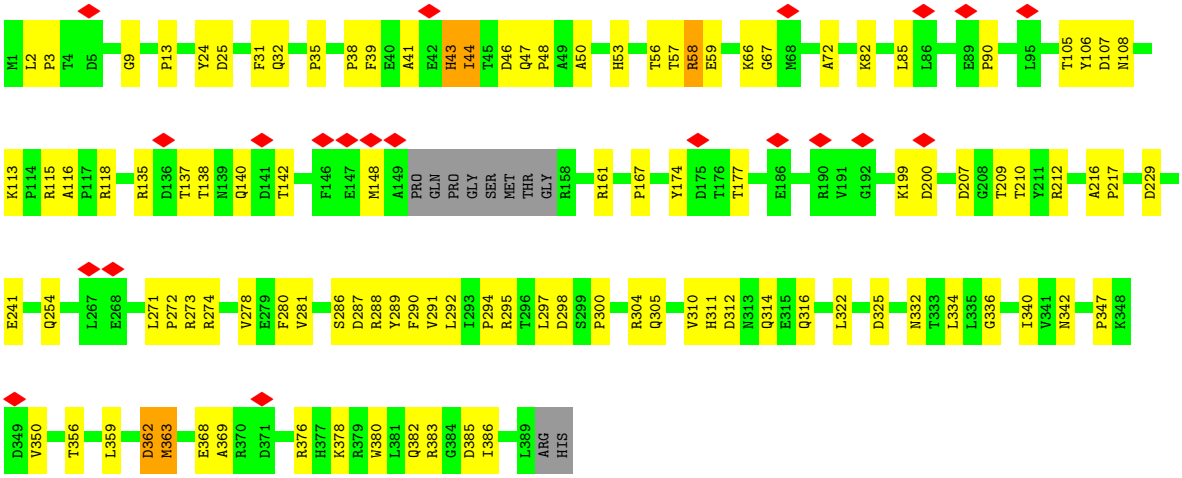
• Molecule 11: RIB30

Chain 5E:



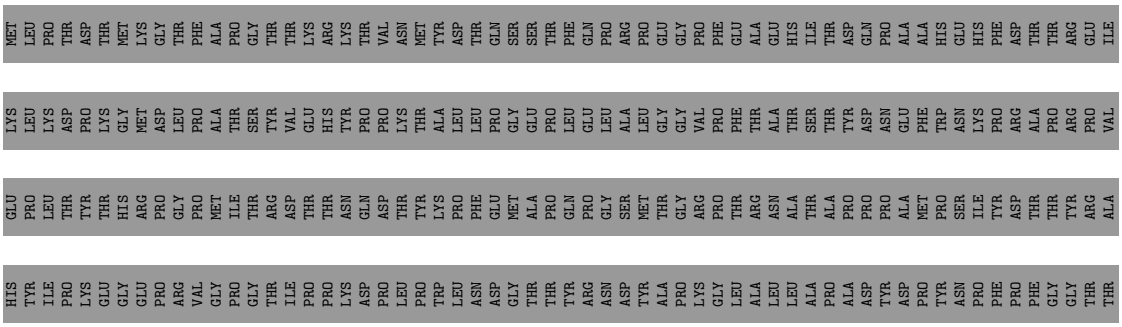

- Molecule 12: FAP363

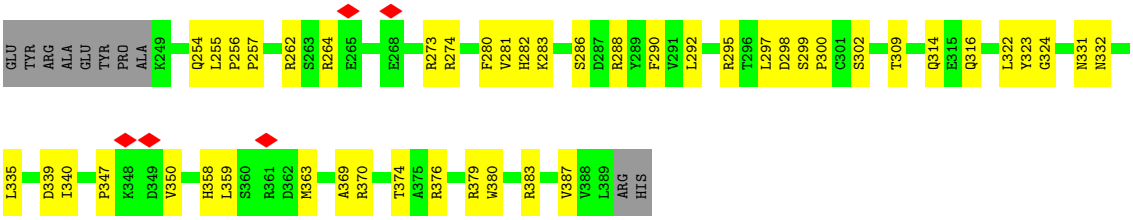
Chain 5F:




- Molecule 12: FAP363

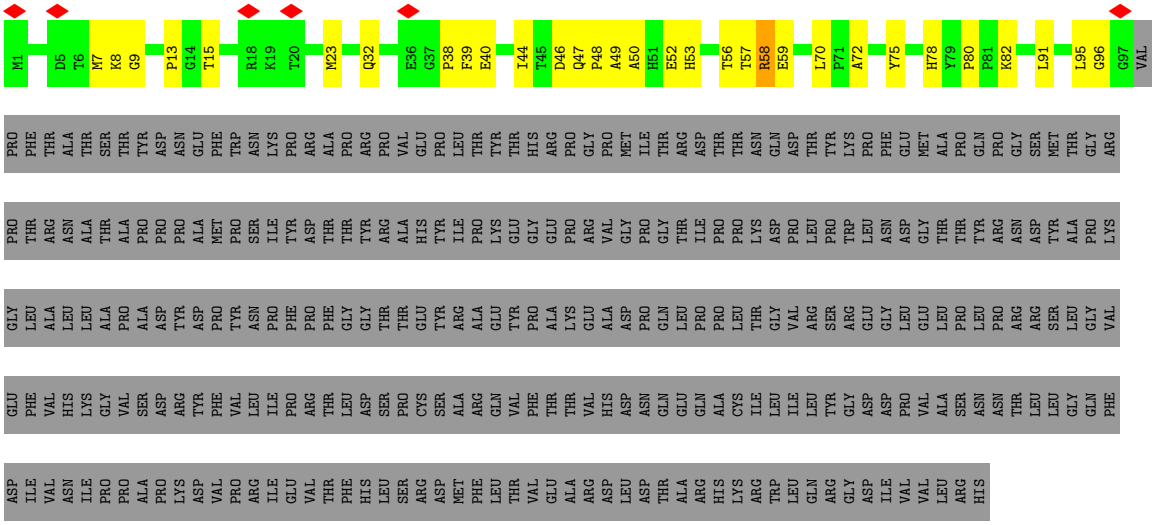
Chain 5G:





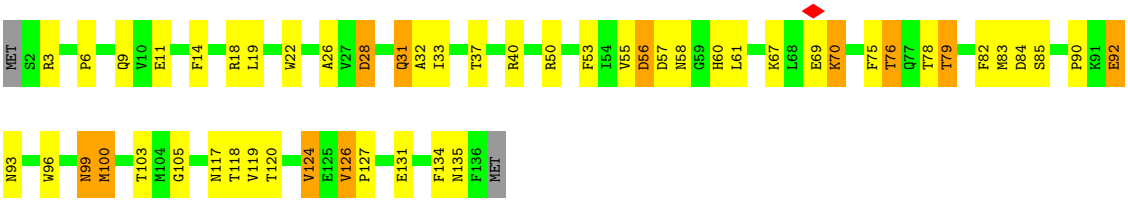

- Molecule 12: FAP363

Chain 7B:



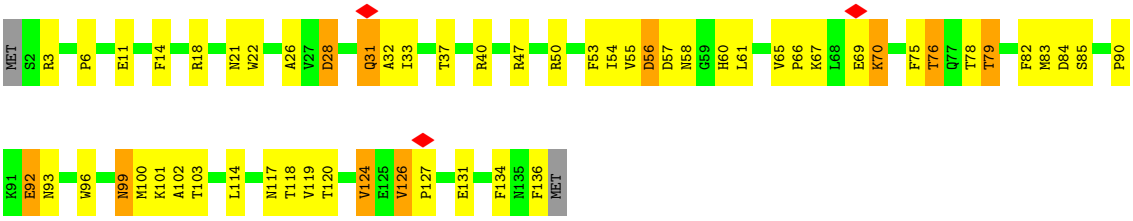

- Molecule 13: FAP126

Chain 5H:



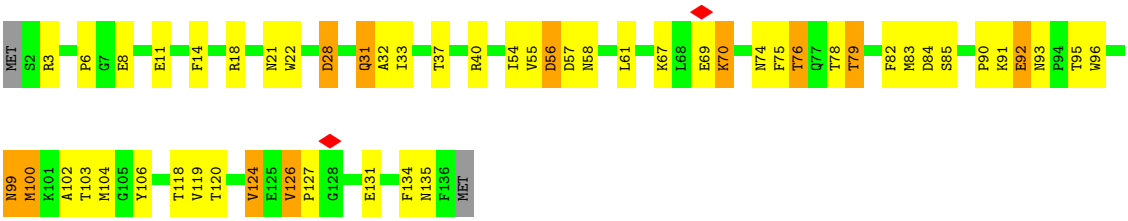

- Molecule 13: FAP126

Chain 5I:



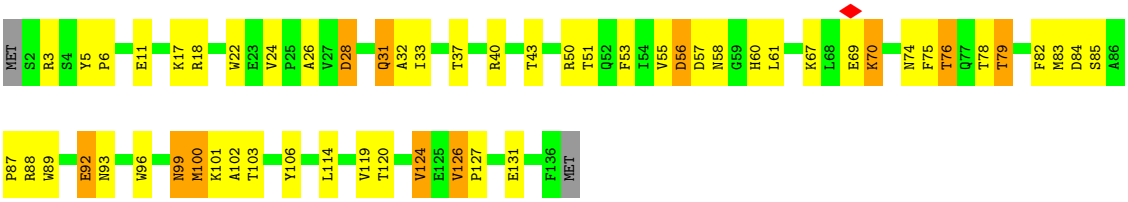

- Molecule 13: FAP126

Chain 5J:



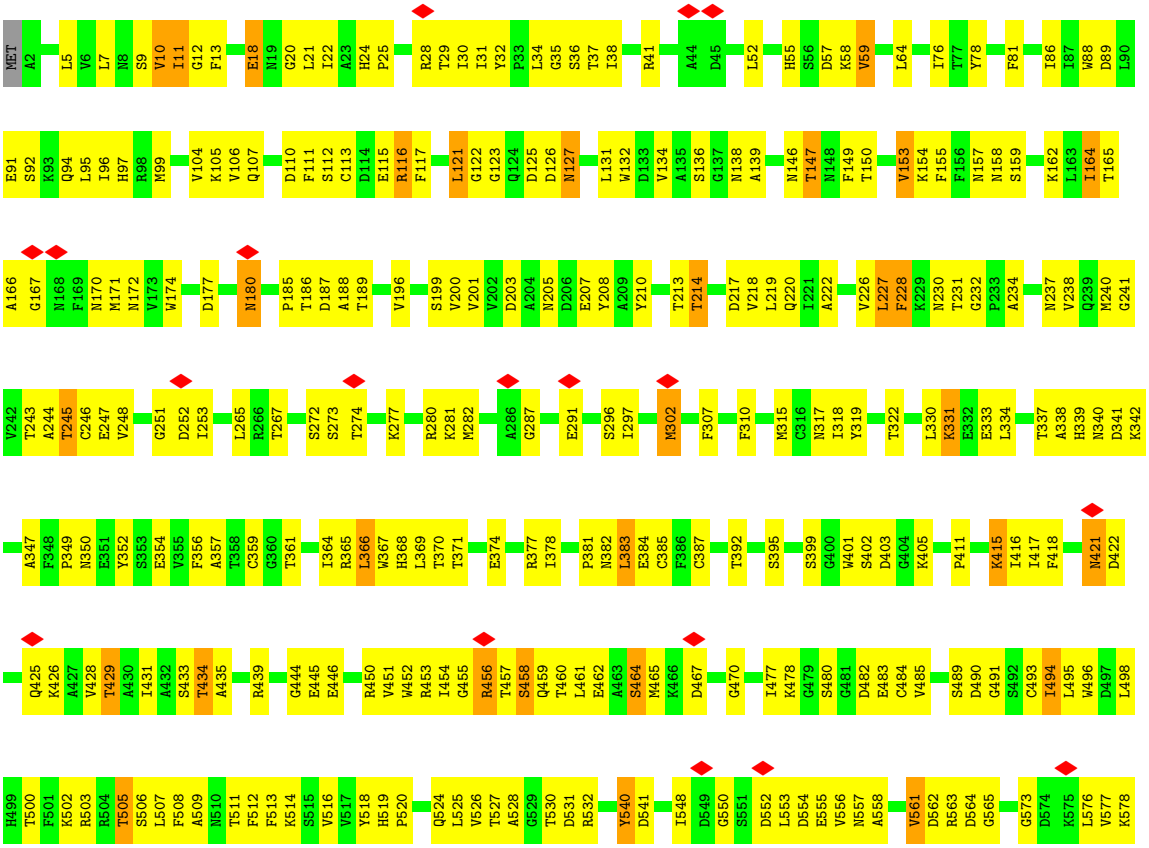

- Molecule 13: FAP126

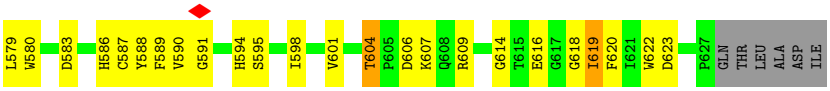
Chain 5K:




- Molecule 14: FAP52

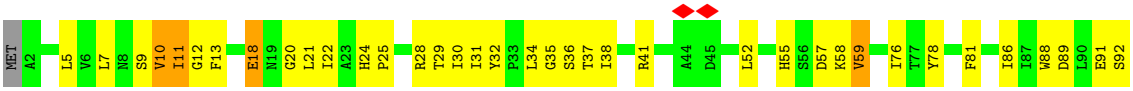
Chain 5L:

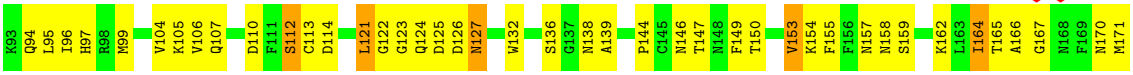


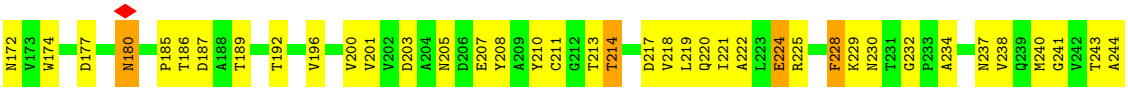


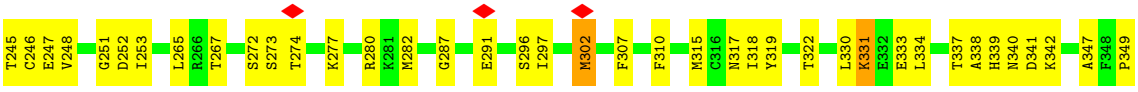

- Molecule 14: FAP52

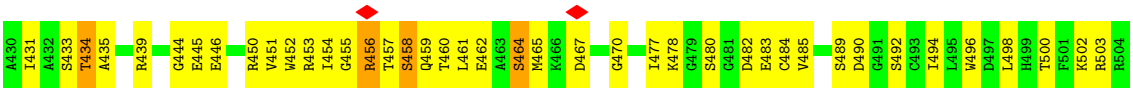
Chain 5M:

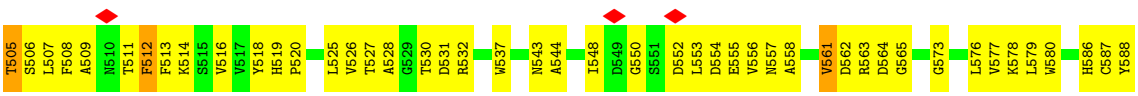


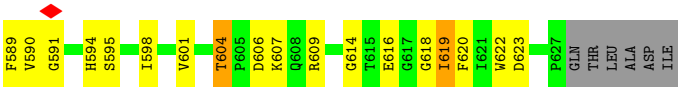



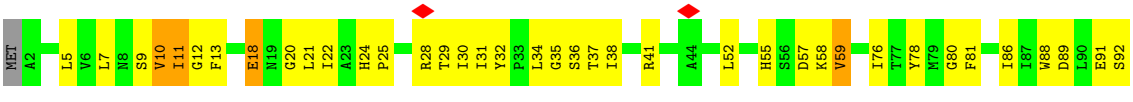


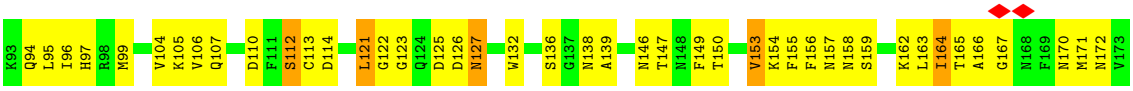



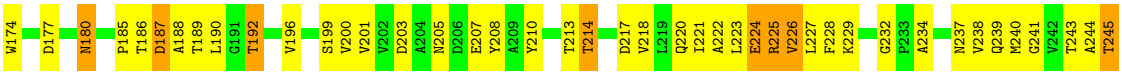



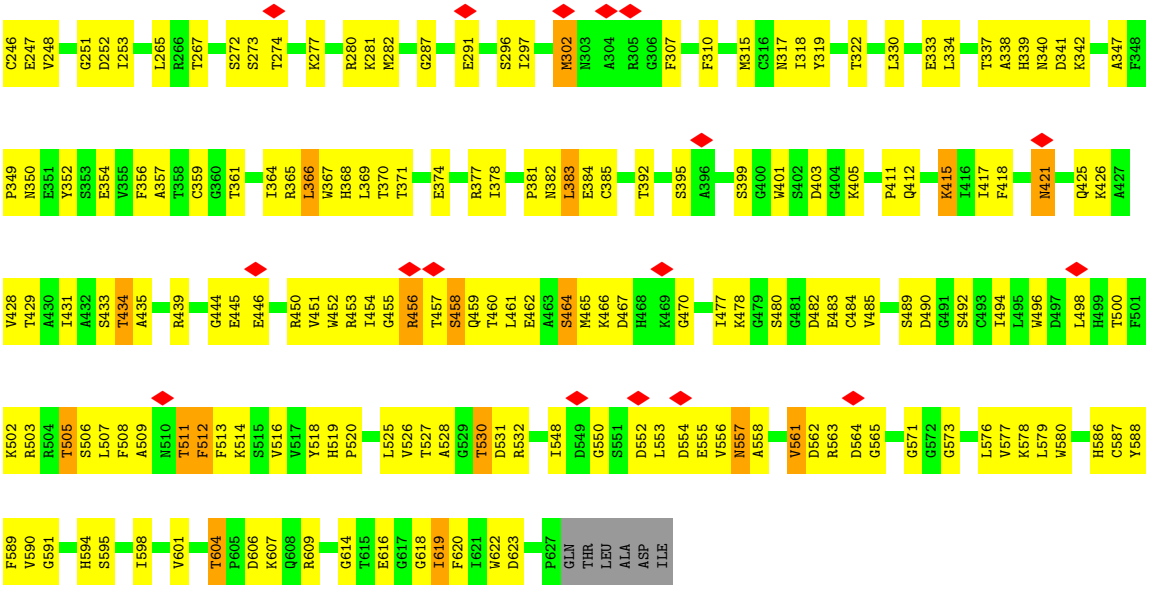

- Molecule 14: FAP52

Chain 5N:



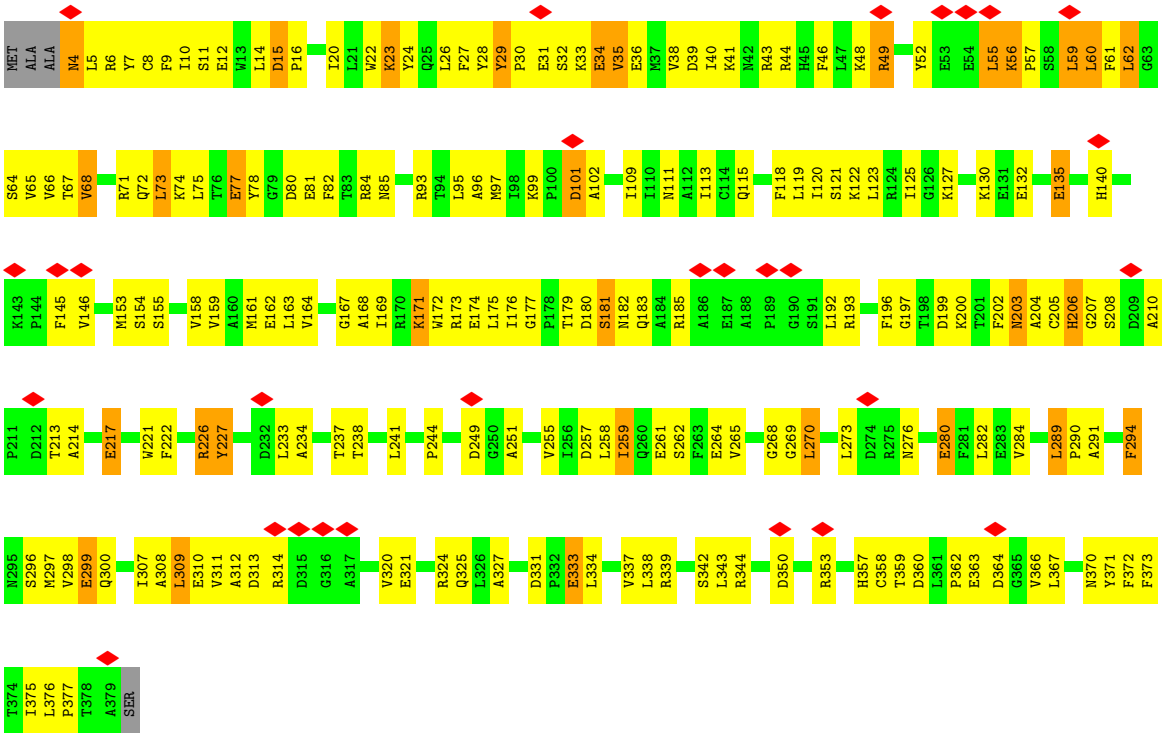





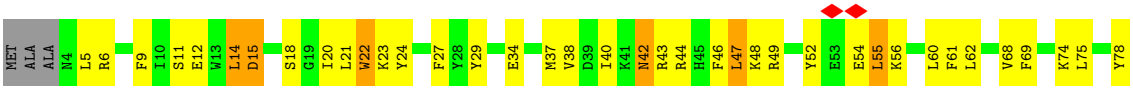

• Molecule 15: FAP67

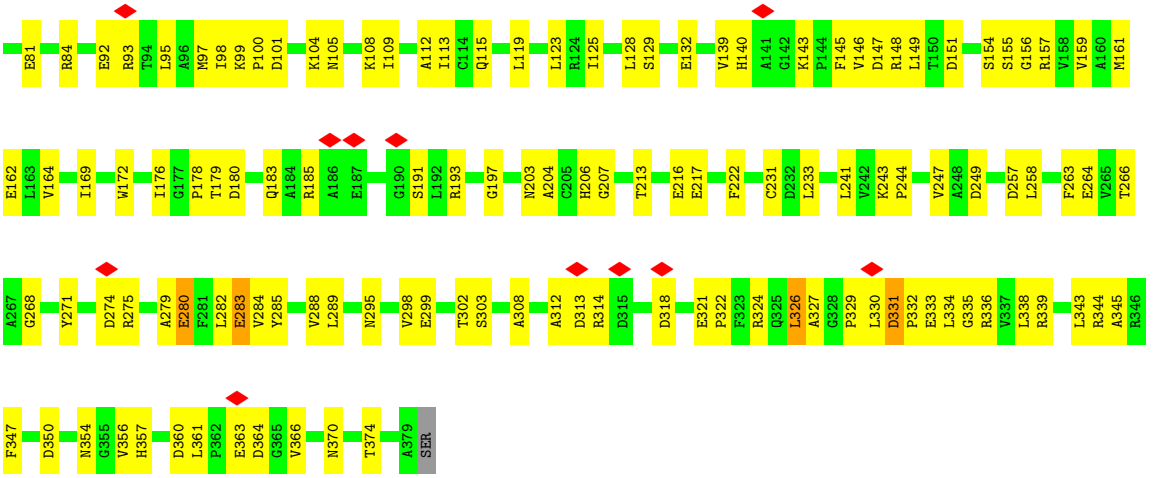
Chain 5O:




• Molecule 15: FAP67

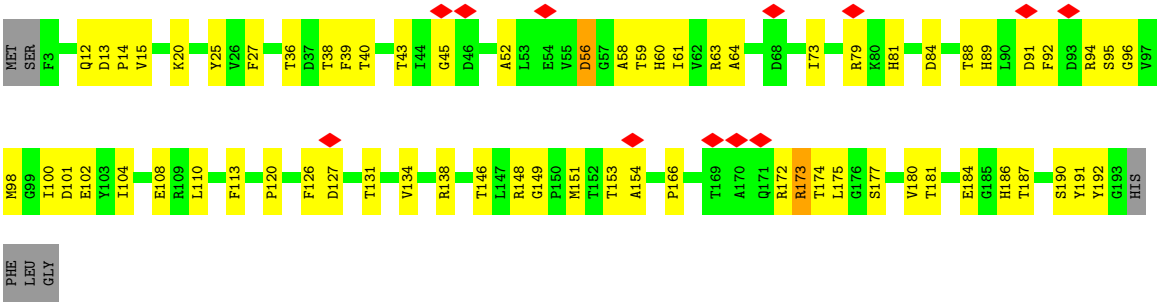
Chain 5P:





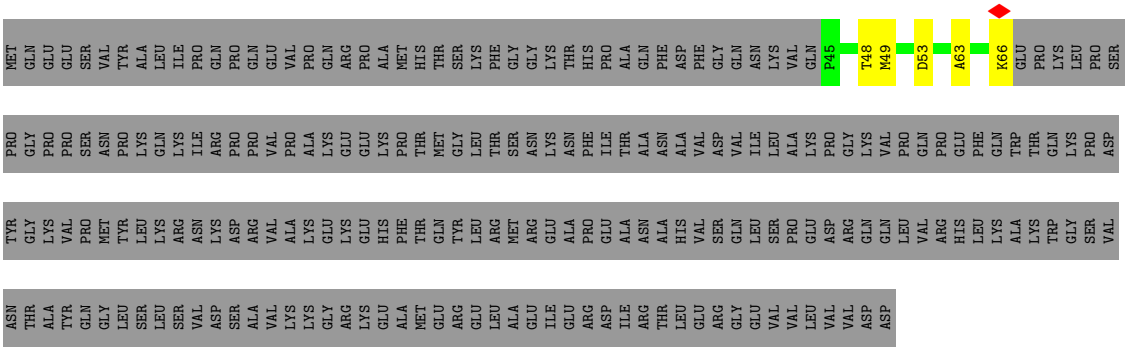

- Molecule 16: FAP85

Chain 5Q:



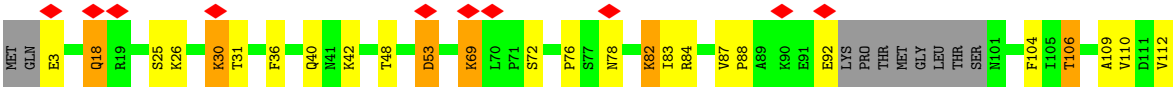

- Molecule 17: FAP106

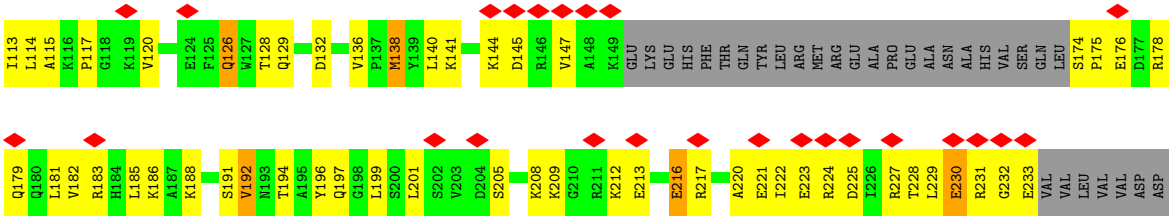
Chain 5R:




- Molecule 17: FAP106

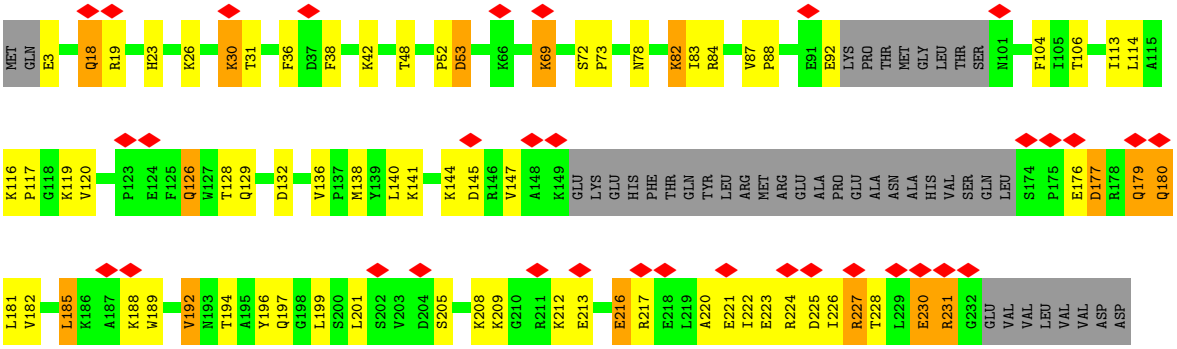
Chain 5S:





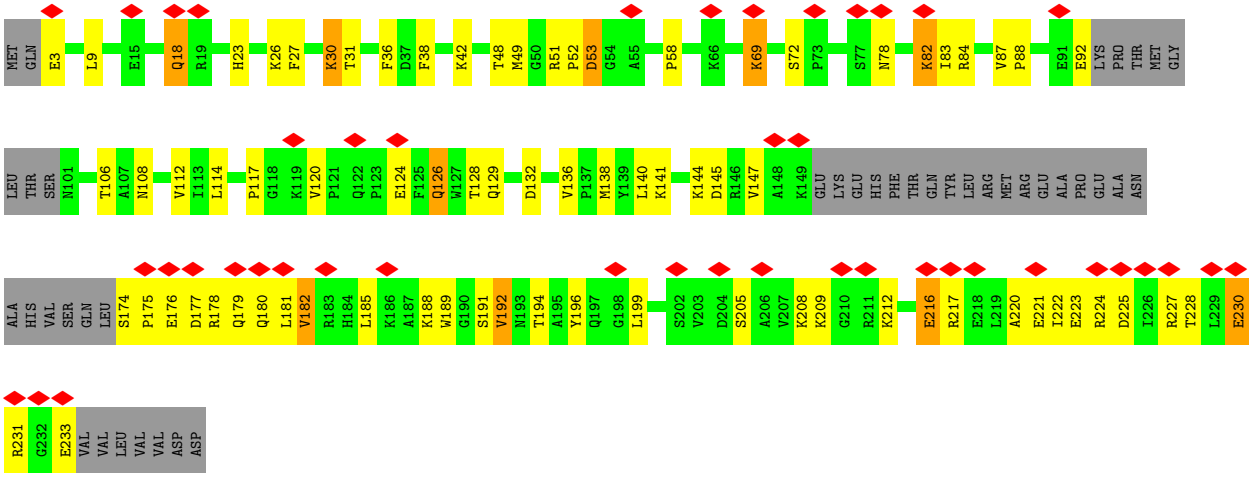

• Molecule 17: FAP106

Chain 5T:



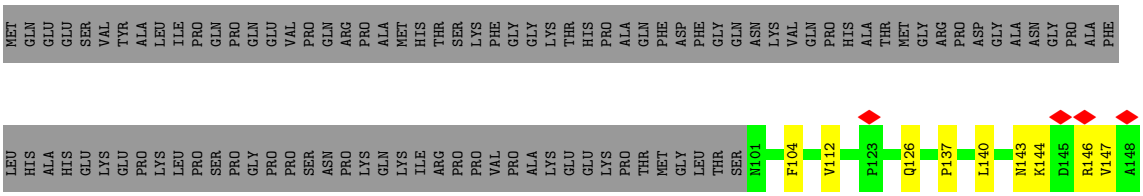

• Molecule 17: FAP106

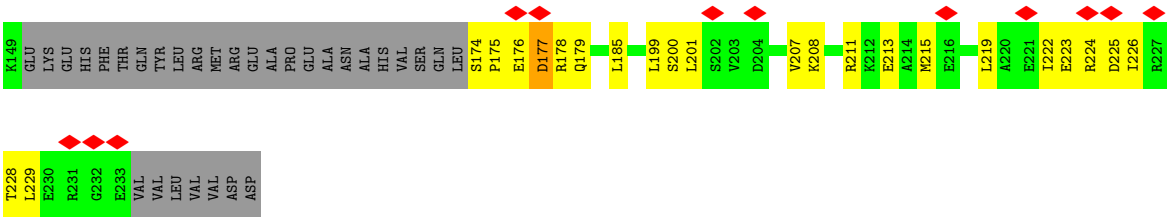
Chain 5U:




• Molecule 17: FAP106

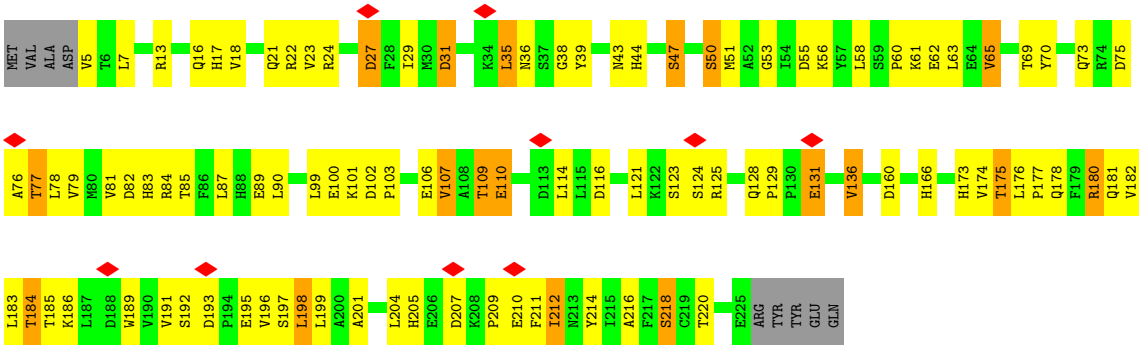
Chain 5V:





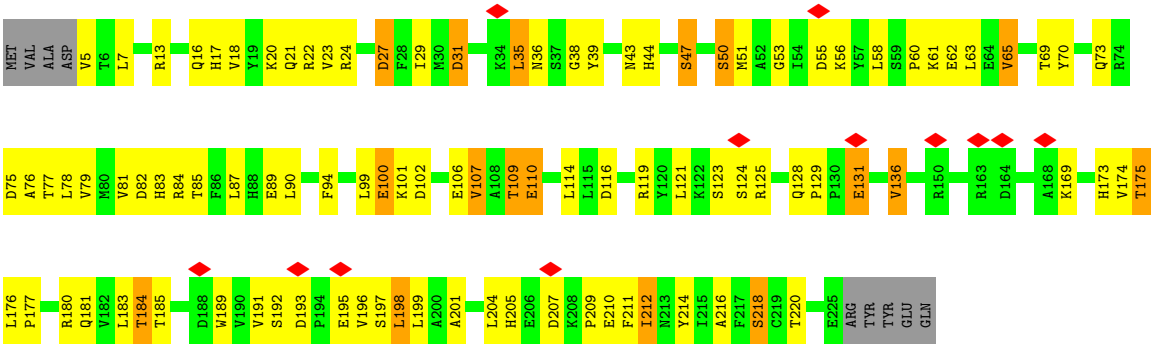

• Molecule 18: FAP115

Chain 5X:



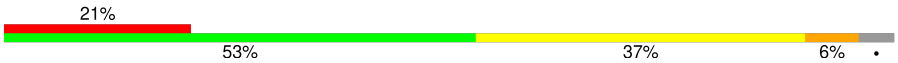

• Molecule 18: FAP115

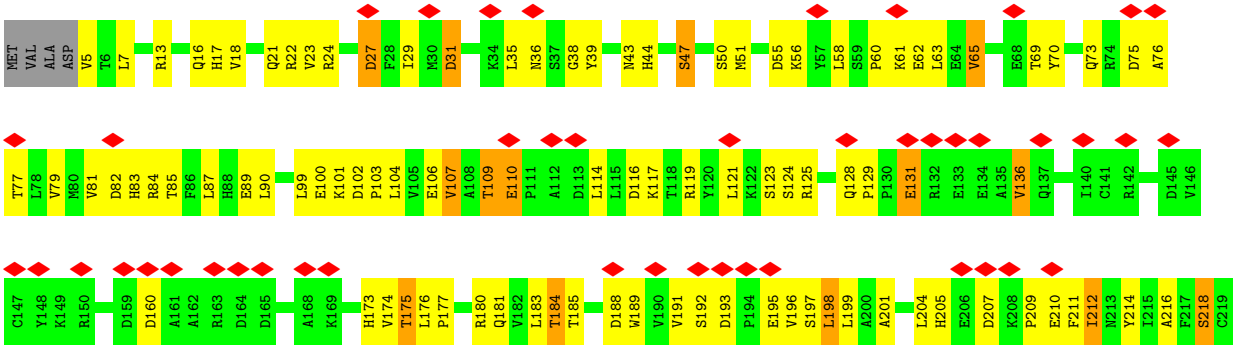
Chain 5Y:

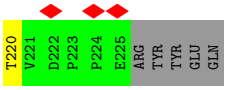



• Molecule 18: FAP115

Chain 5Z:

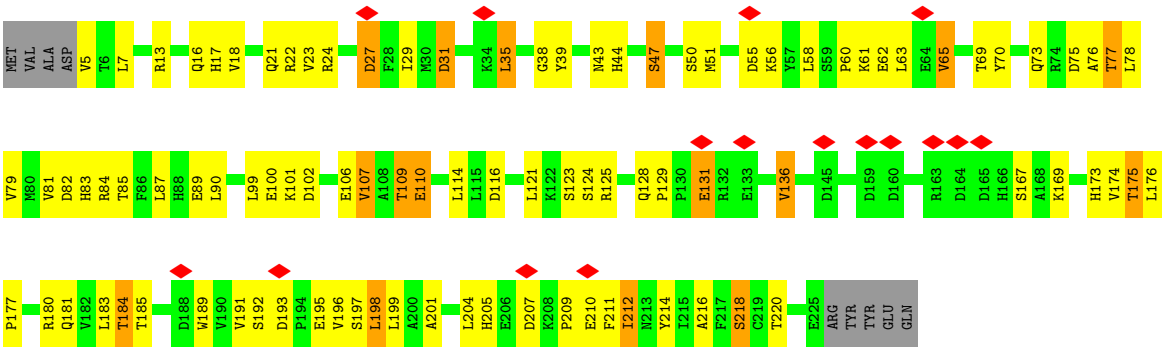




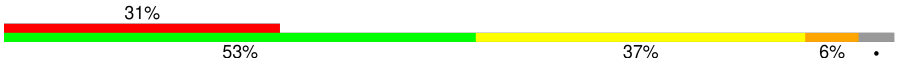

• Molecule 18: FAP115

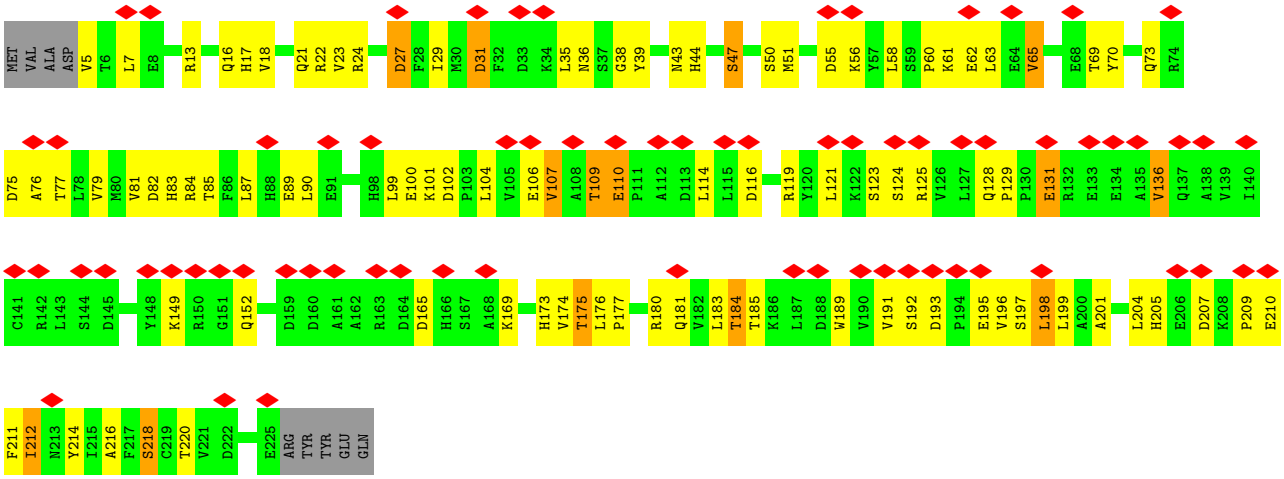
Chain 6A:




• Molecule 18: FAP115

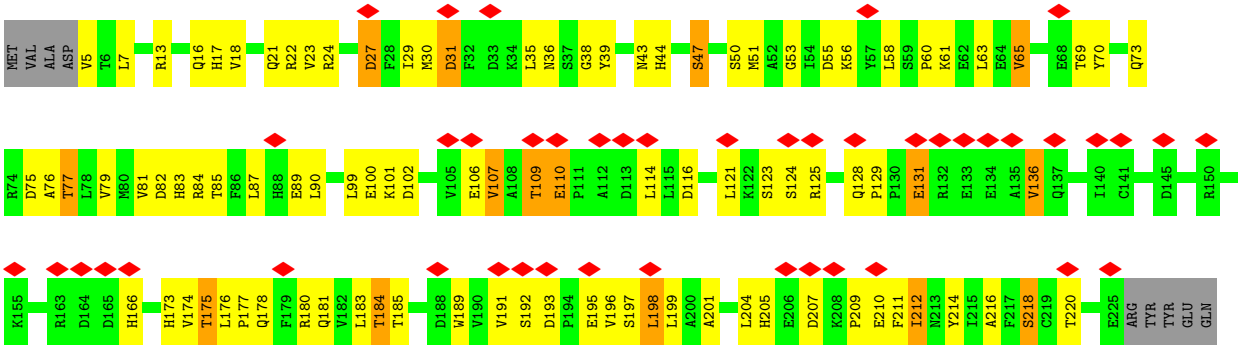
Chain 6B:



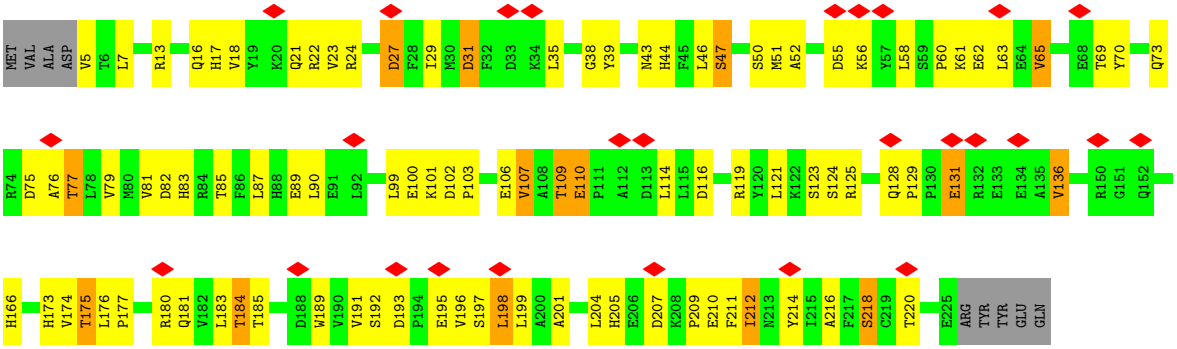

• Molecule 18: FAP115

Chain 6C:



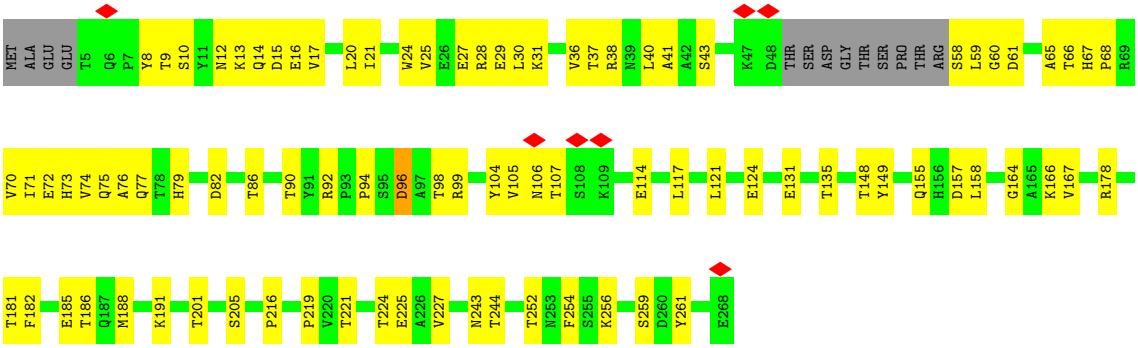
- Molecule 18: FAP115

Chain 6D:



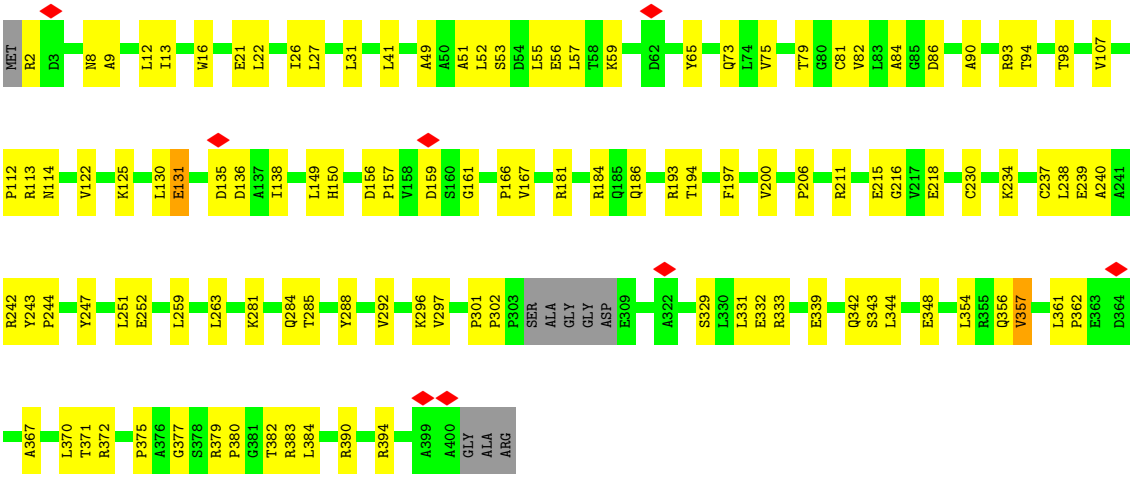

- Molecule 19: FAP143

Chain 6E:



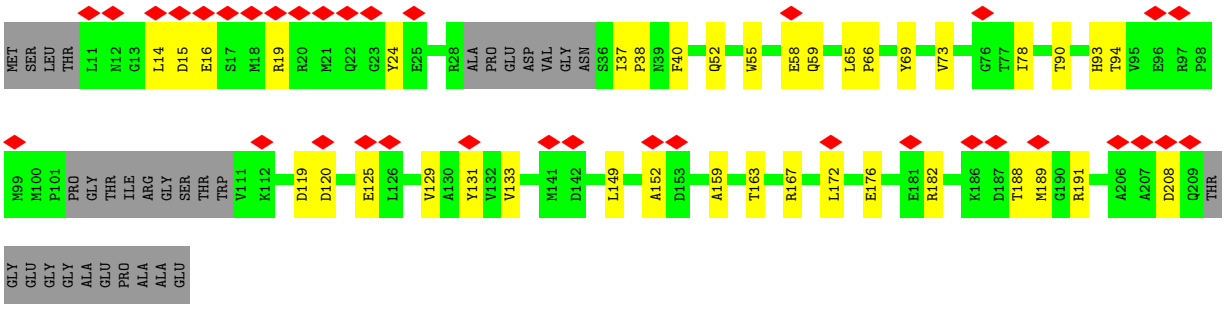

- Molecule 20: FAP161

Chain 6F:



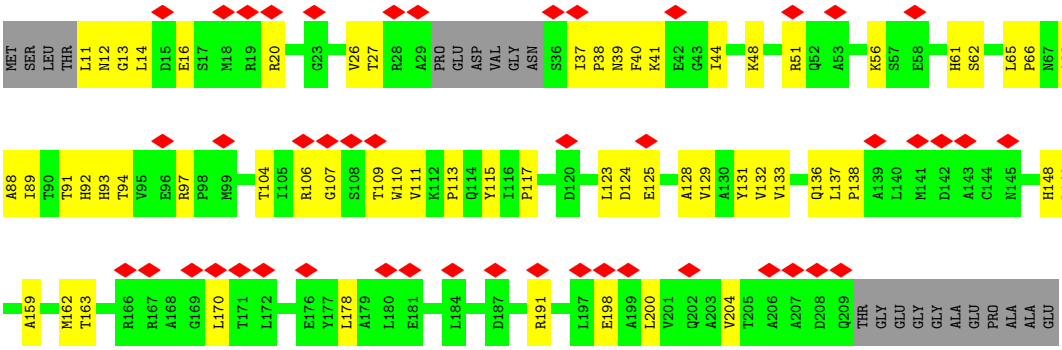

- Molecule 21: FAP166

Chain 6G:



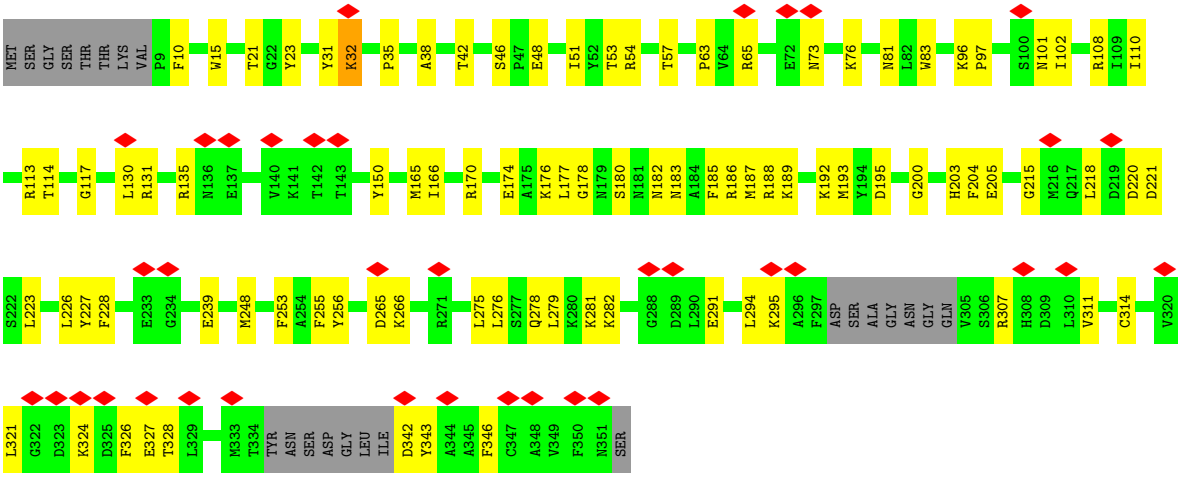

- Molecule 21: FAP166

Chain 6H:



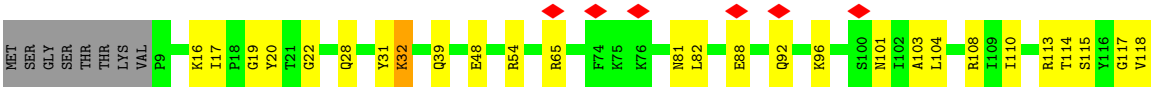

- Molecule 22: FAP252

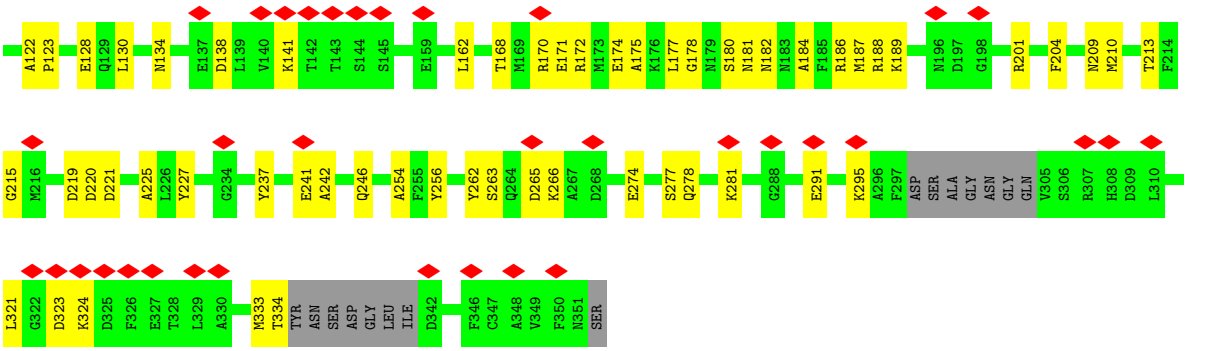
Chain 6I:




- Molecule 22: FAP252

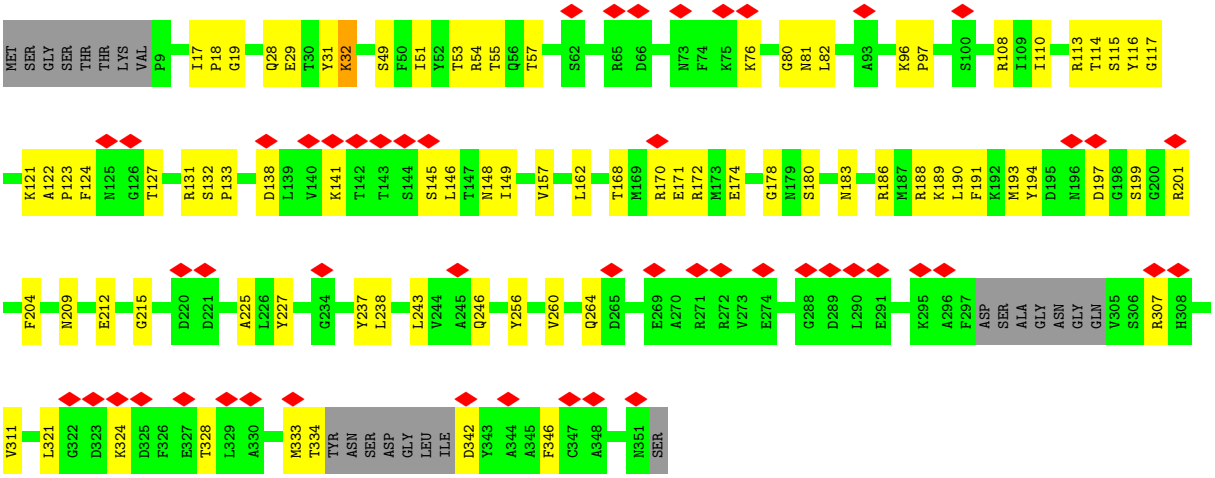
Chain 6J:





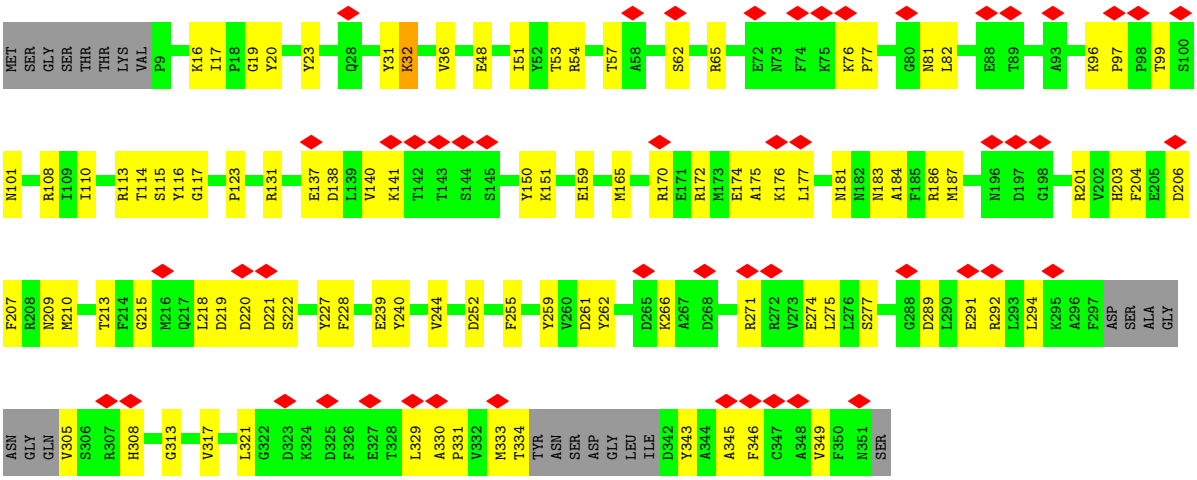

- Molecule 22: FAP252

Chain 6K:



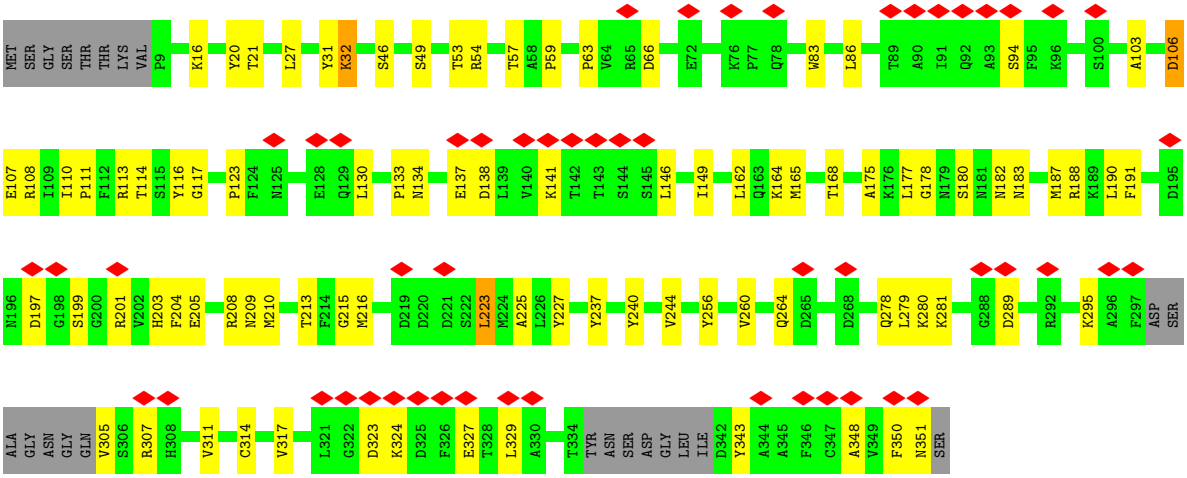

- Molecule 22: FAP252

Chain 6L:



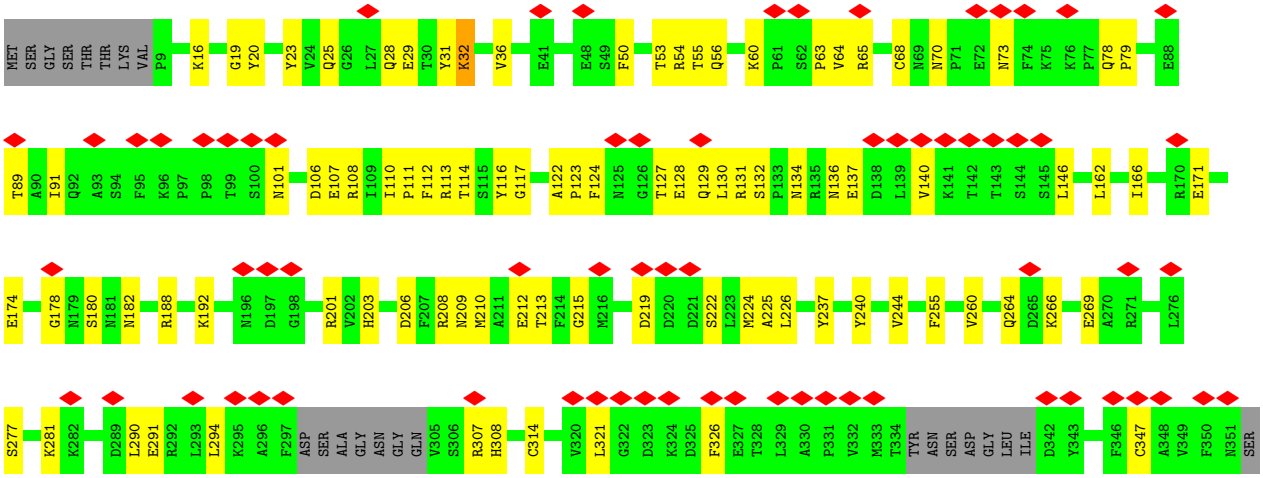

- Molecule 22: FAP252

Chain 6M:



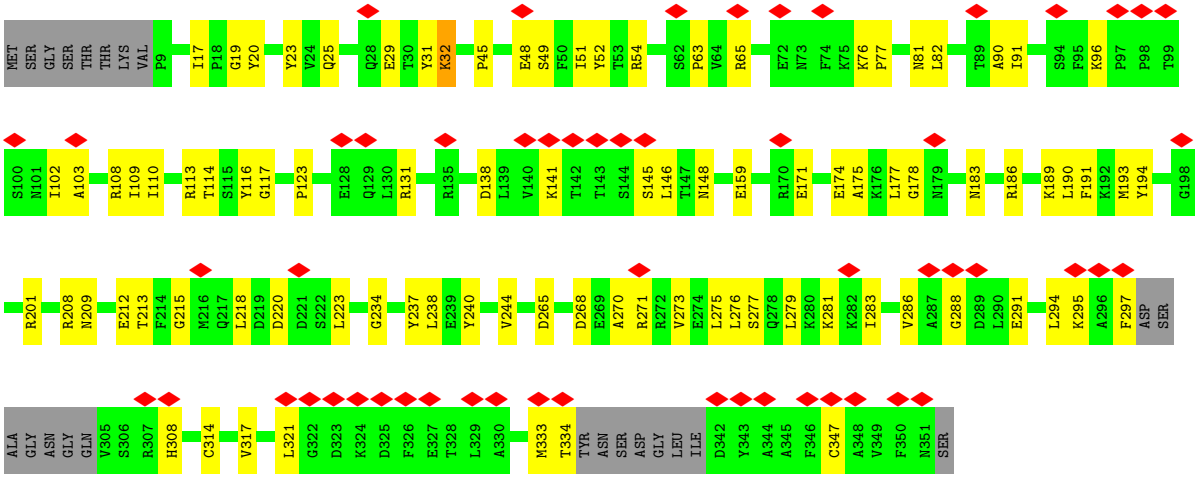

- Molecule 22: FAP252

Chain 6N:



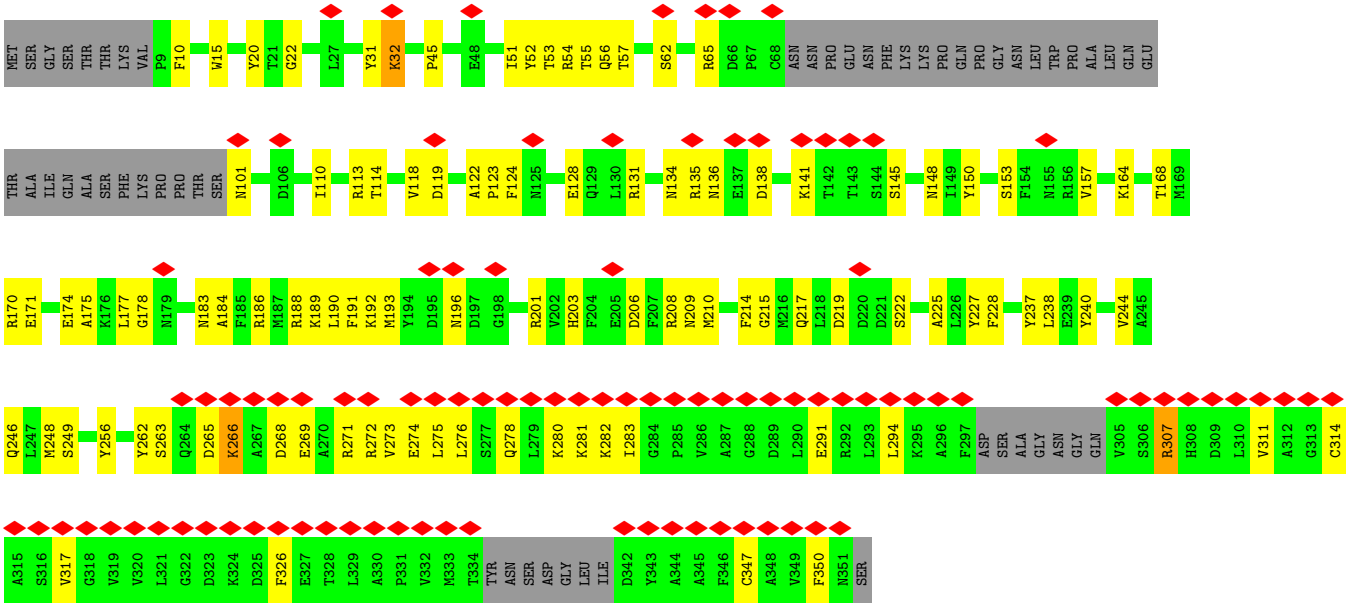

- Molecule 22: FAP252

Chain 6O:



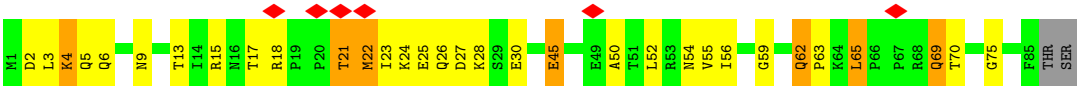
- Molecule 22: FAP252

Chain 6P:



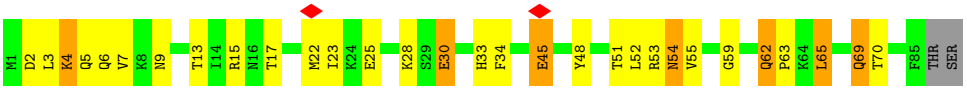

- Molecule 23: FAP276

Chain 6Q:



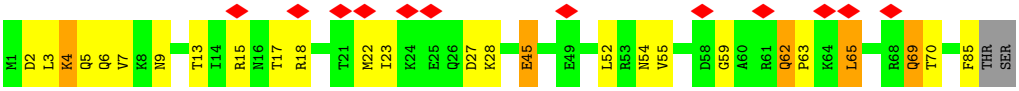

- Molecule 23: FAP276

Chain 6R:



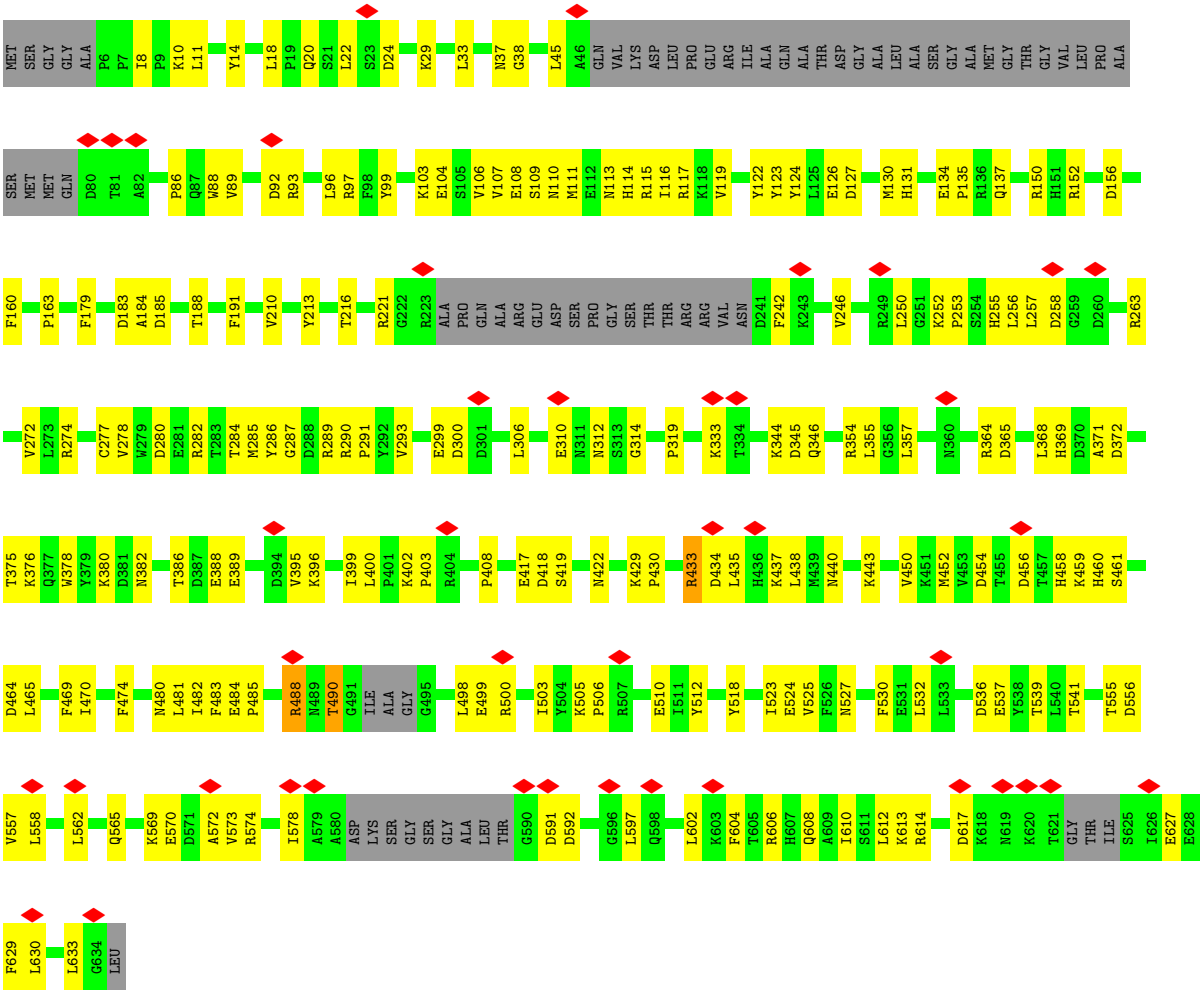

- Molecule 23: FAP276

Chain 6S:



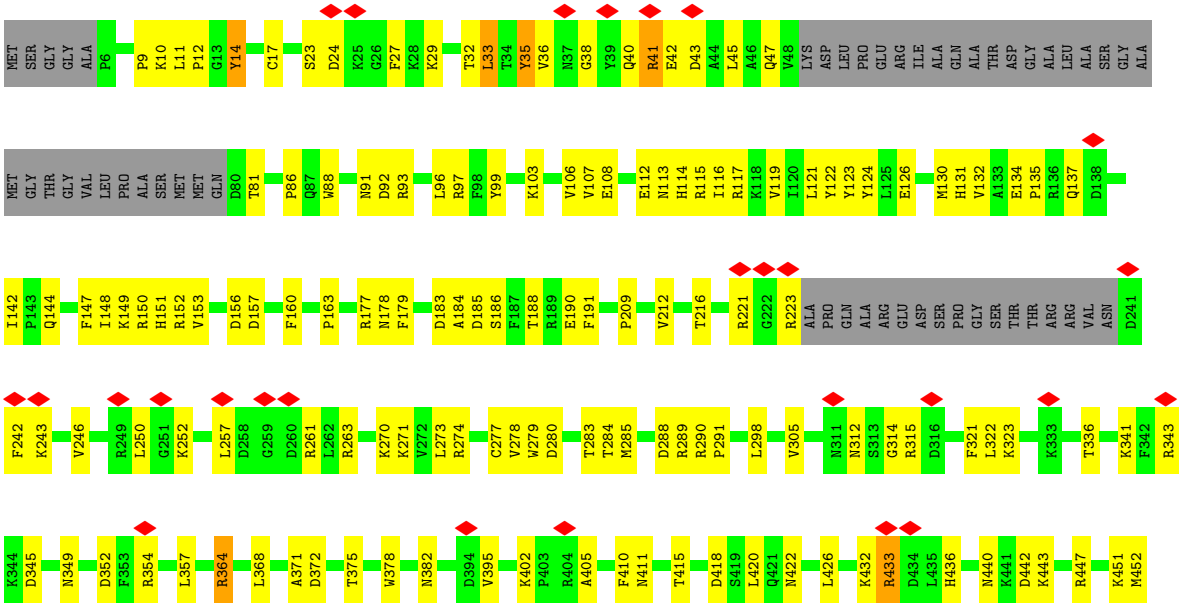

- Molecule 24: RIB72

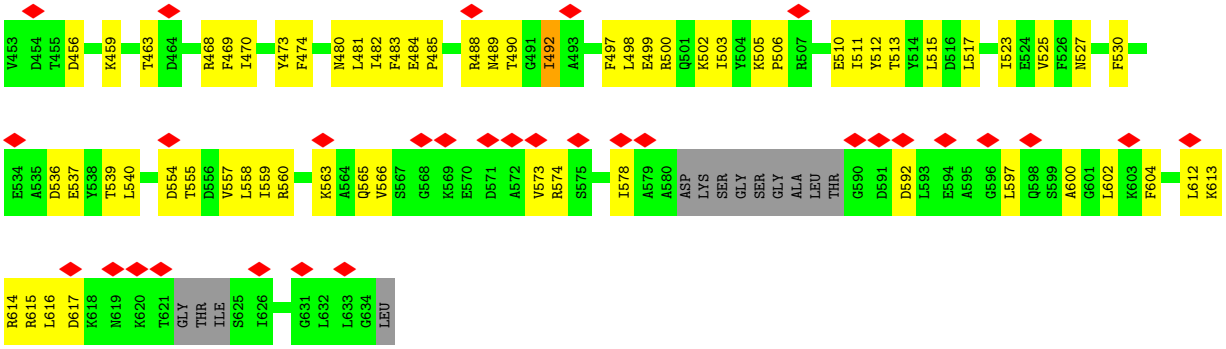
Chain 6T:



- Molecule 24: RIB72

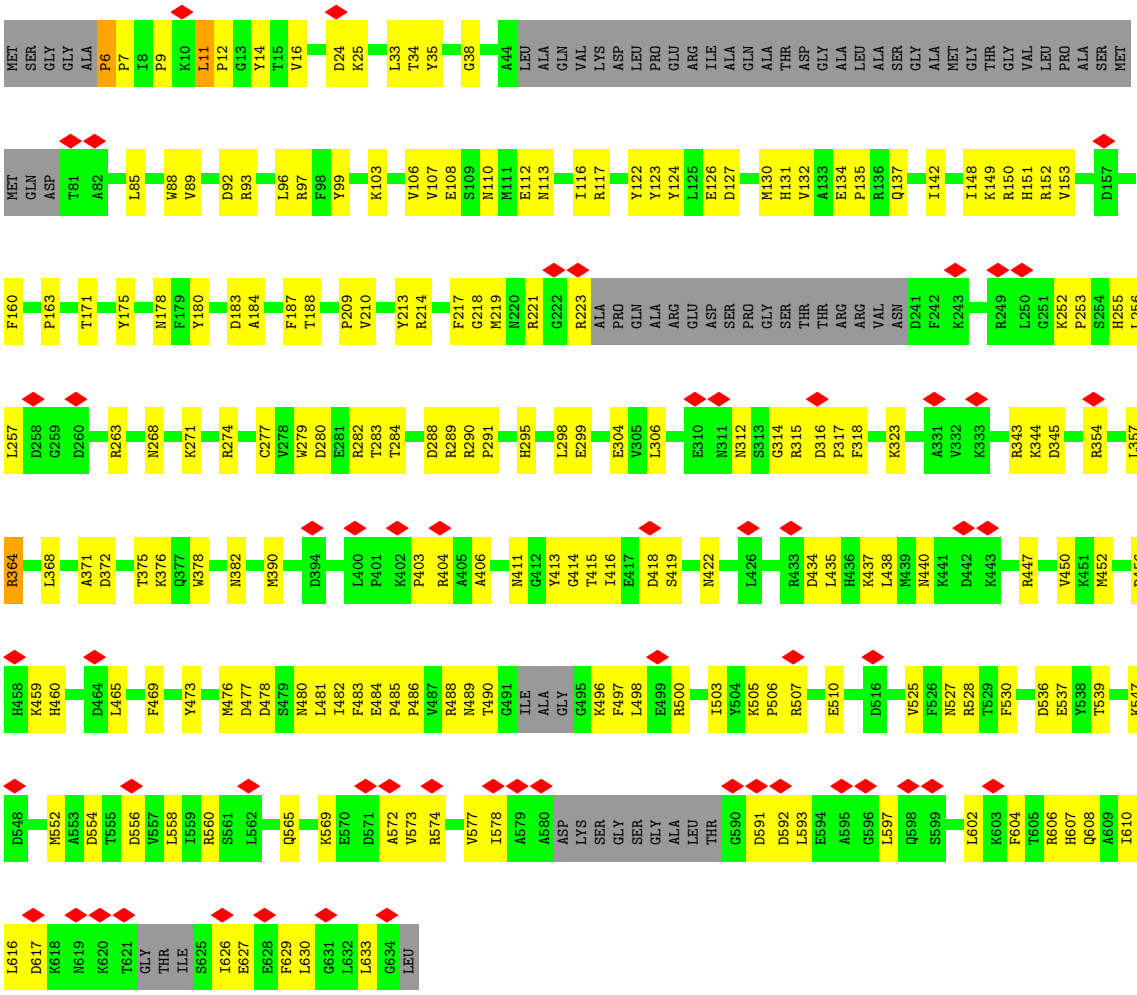
Chain 6U:





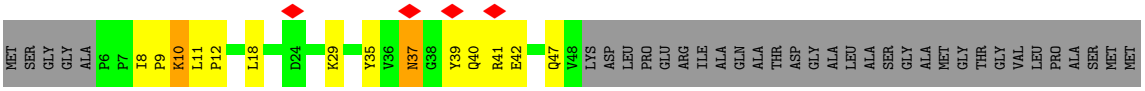

- Molecule 24: RIB72

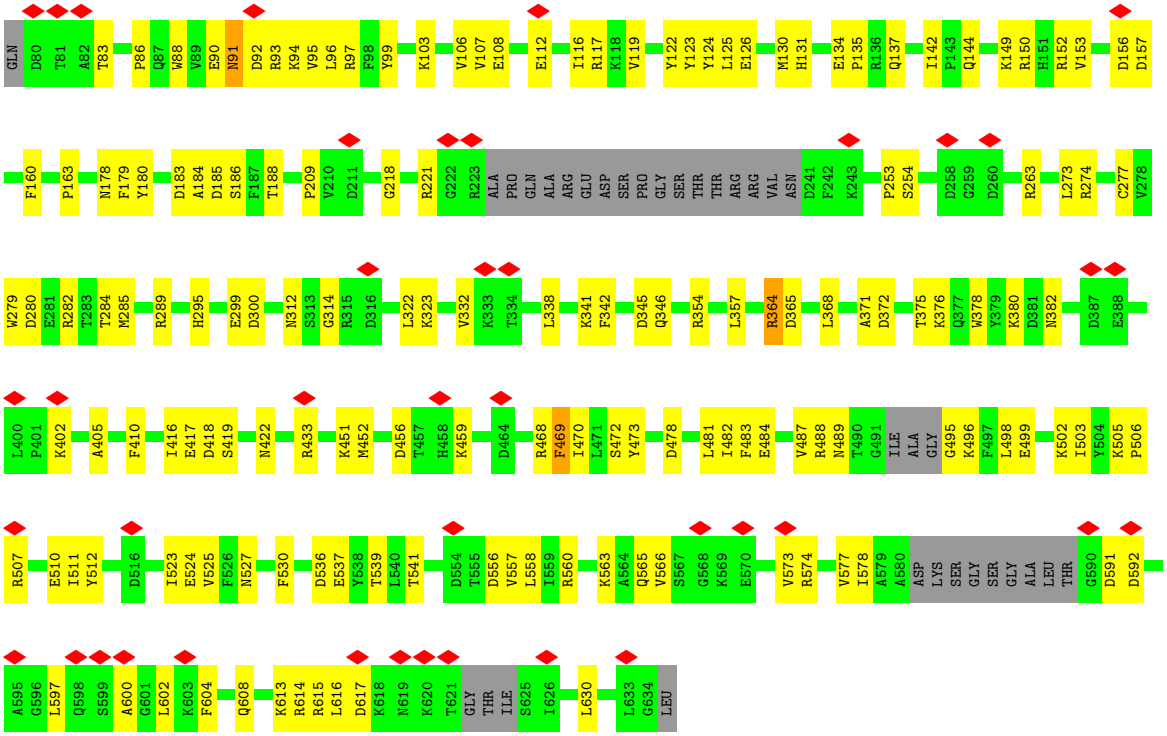
Chain 6V:




- Molecule 24: RIB72

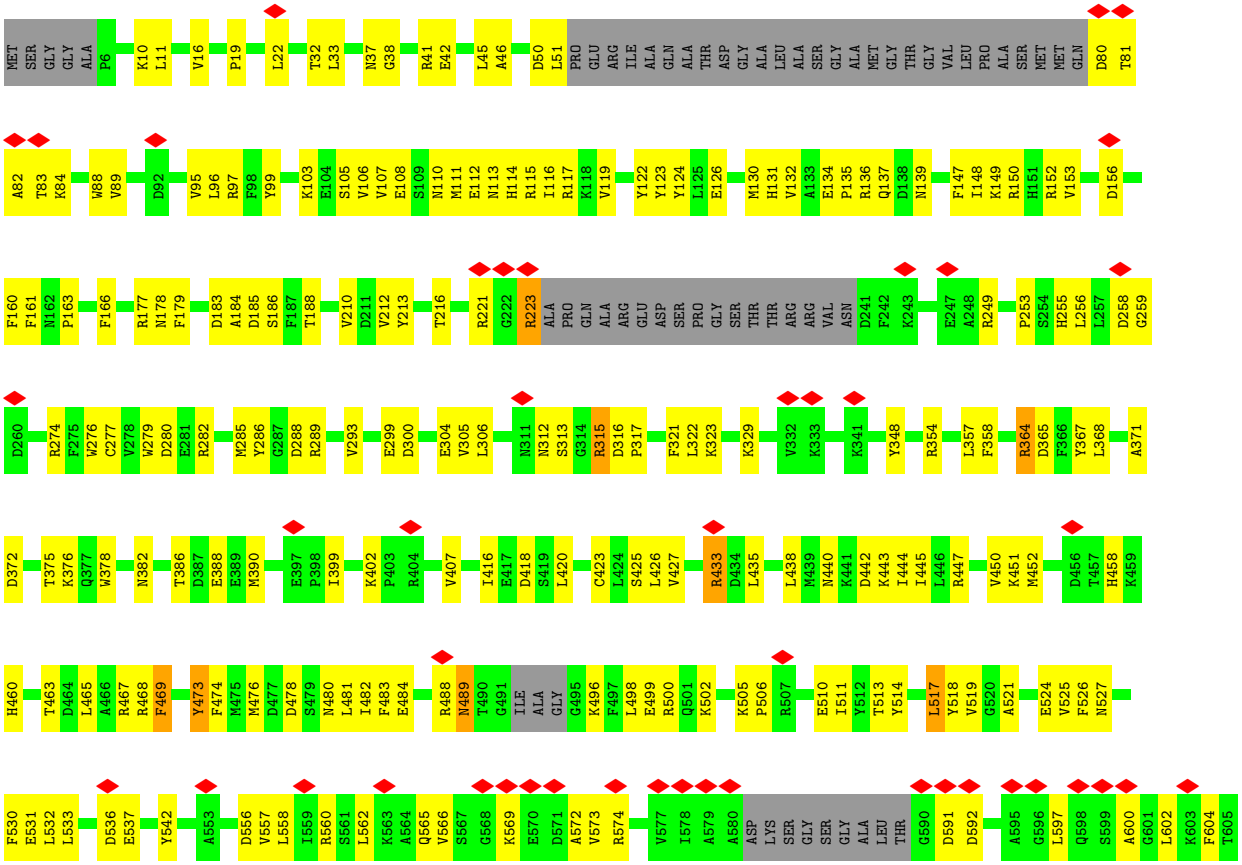
Chain 6W:

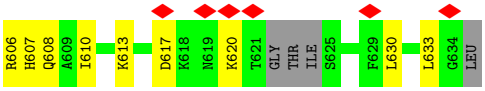




• Molecule 24: RIB72

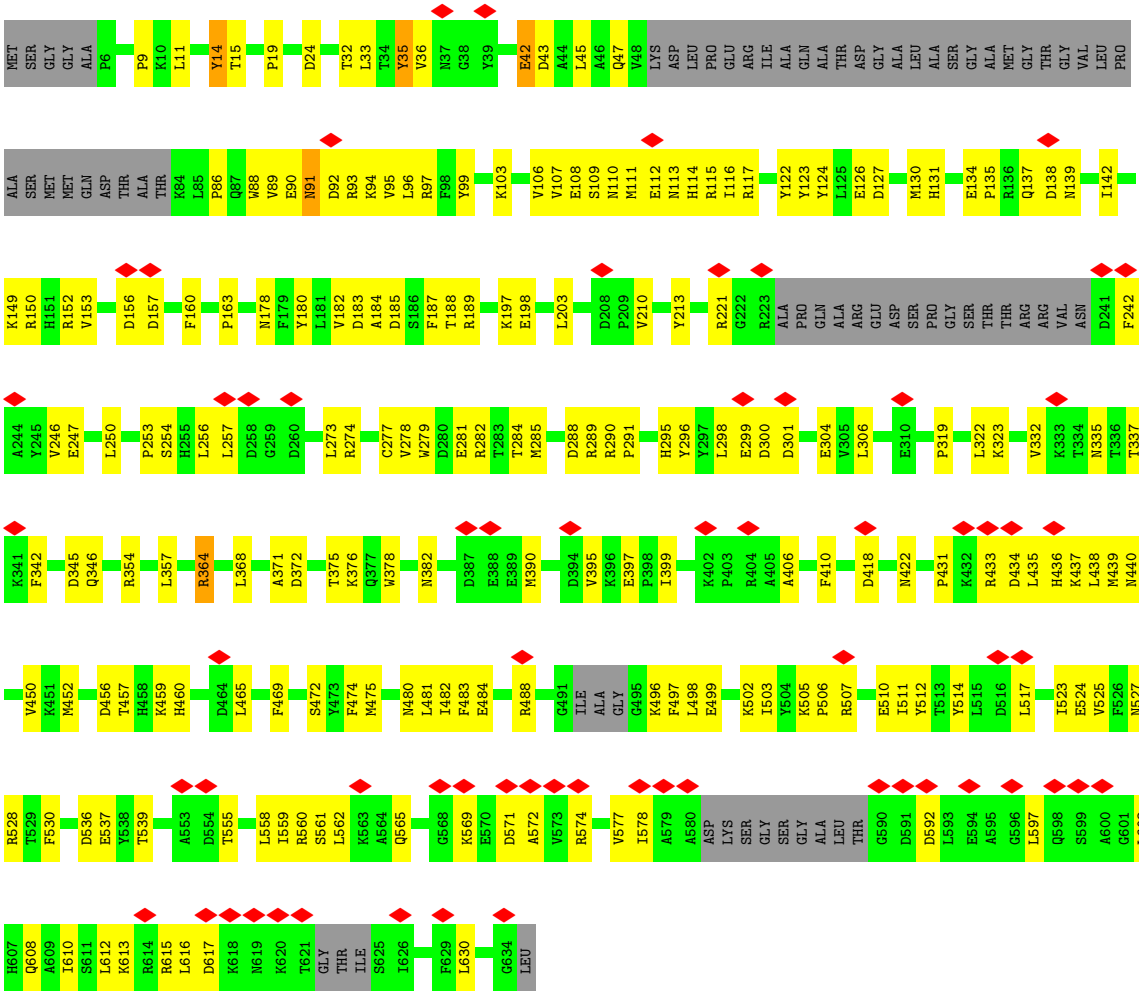
Chain 6X:





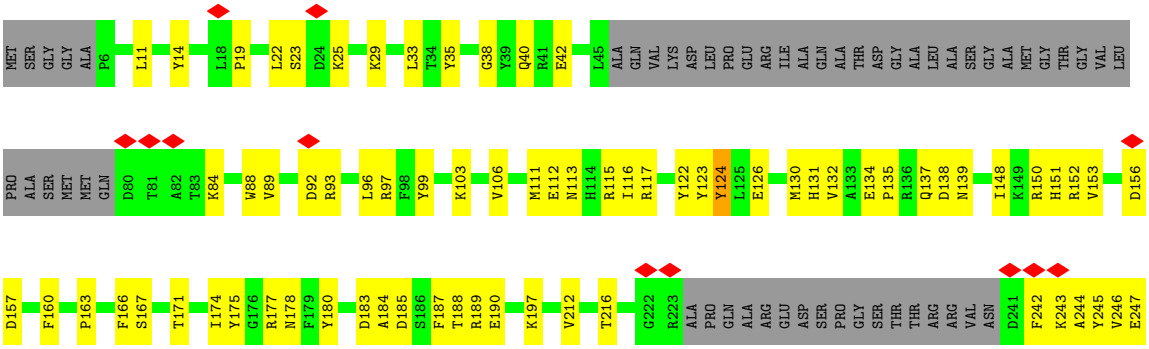

• Molecule 24: RIB72

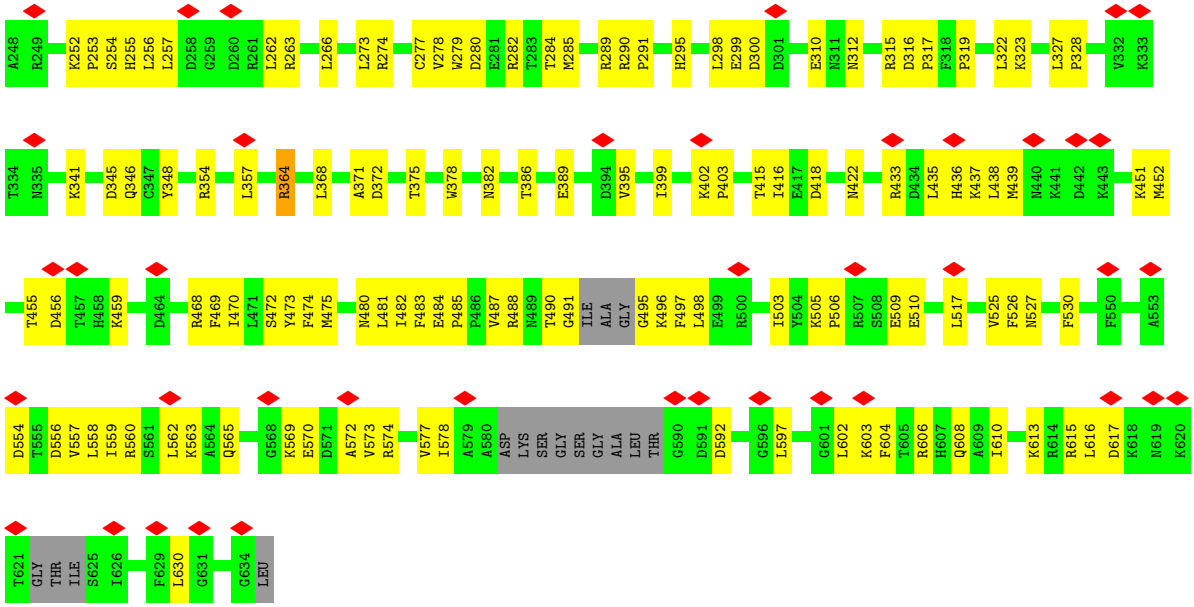
Chain 6Y:




• Molecule 24: RIB72

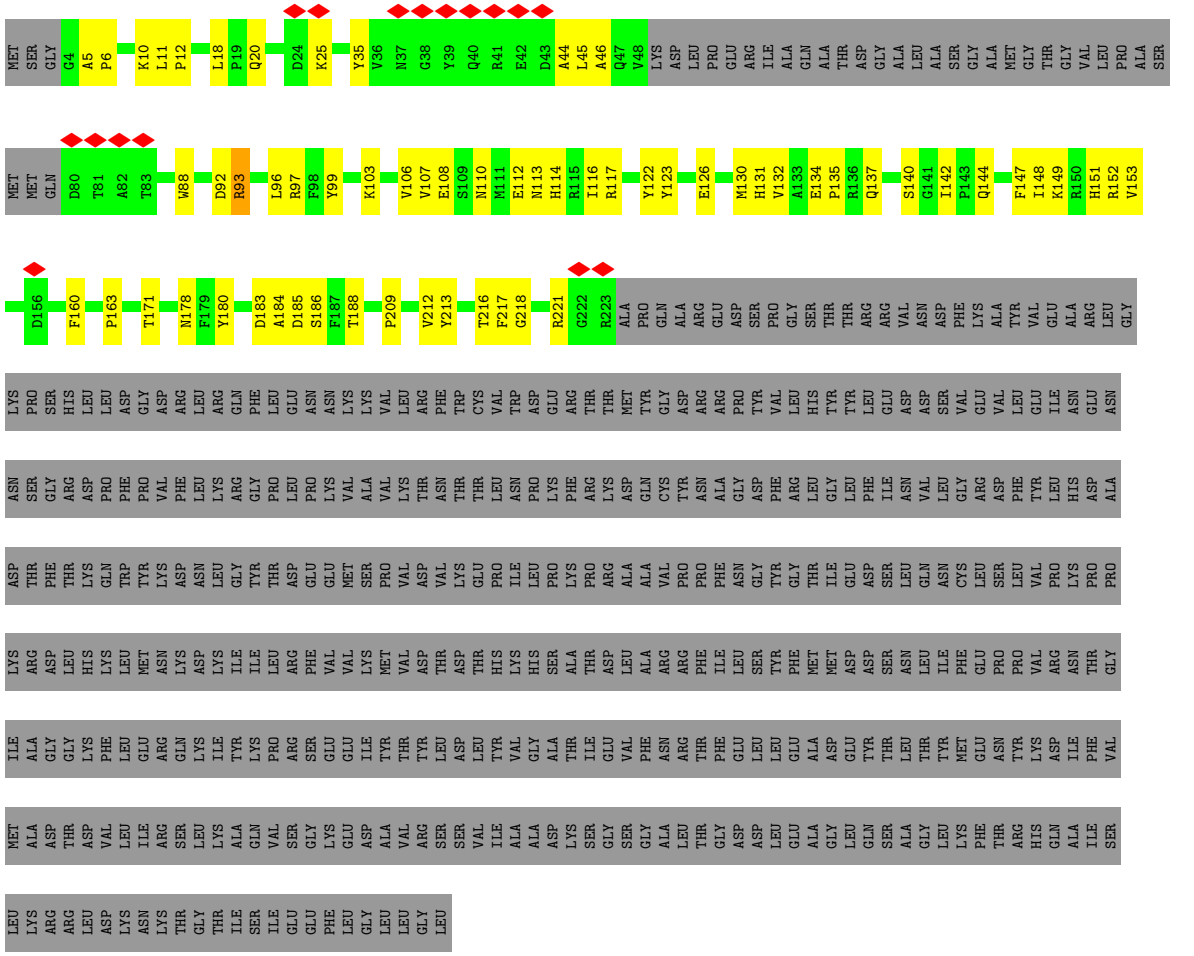
Chain 6Z:





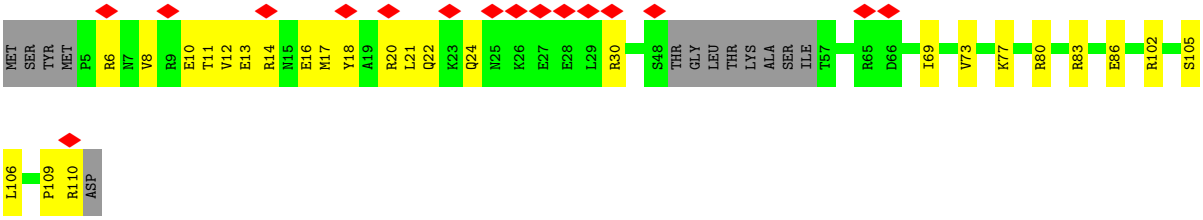

- Molecule 24: RIB72

Chain 7A:



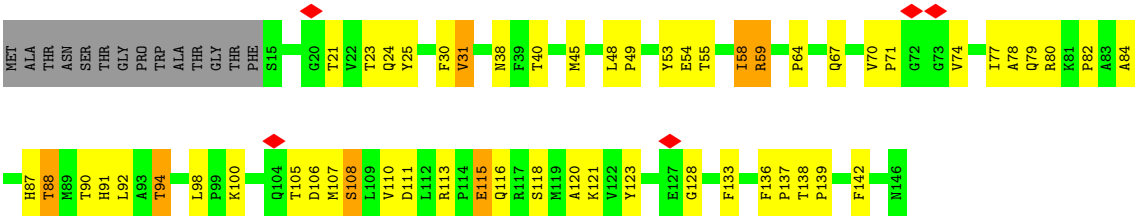
- Molecule 25: FAP141

Chain 7C:



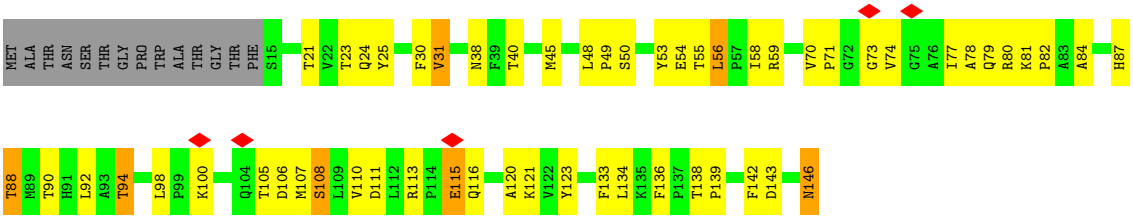

- Molecule 26: FAP222

Chain 7D:



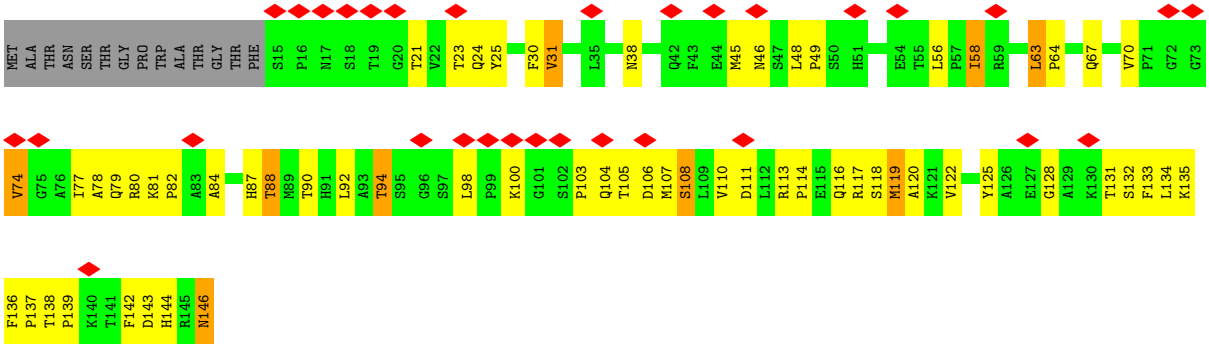

- Molecule 26: FAP222

Chain 7E:



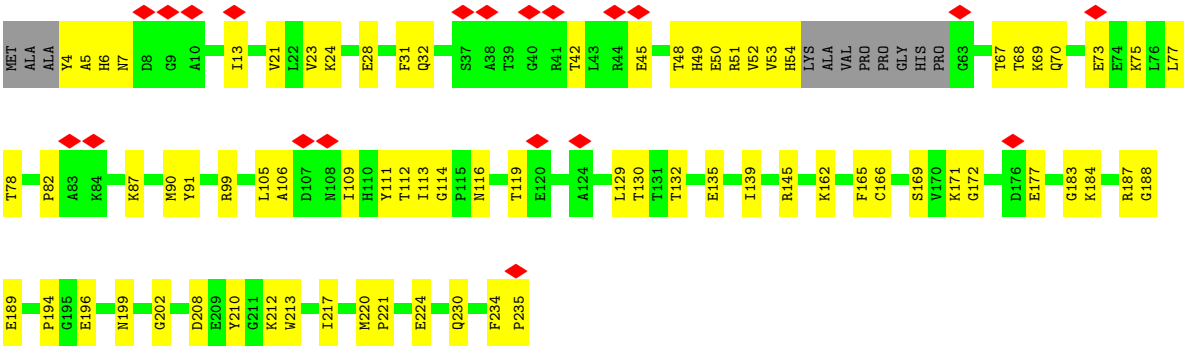

- Molecule 26: FAP222

Chain 7F:



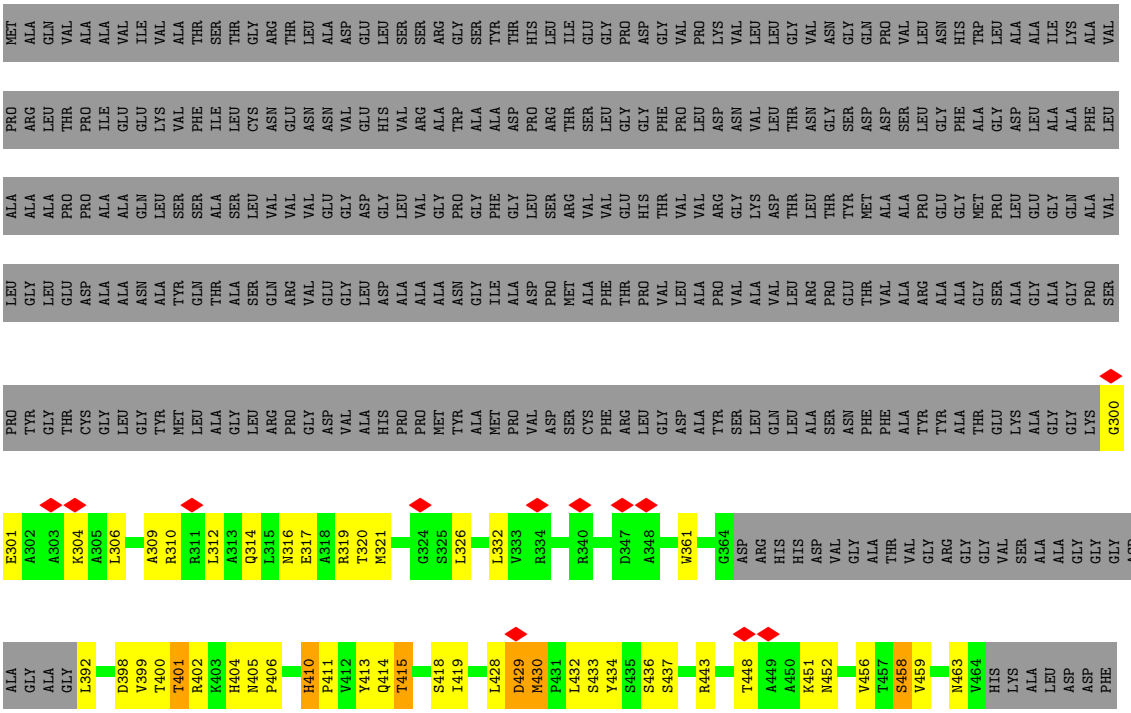

- Molecule 27: FAP95

Chain 7G:



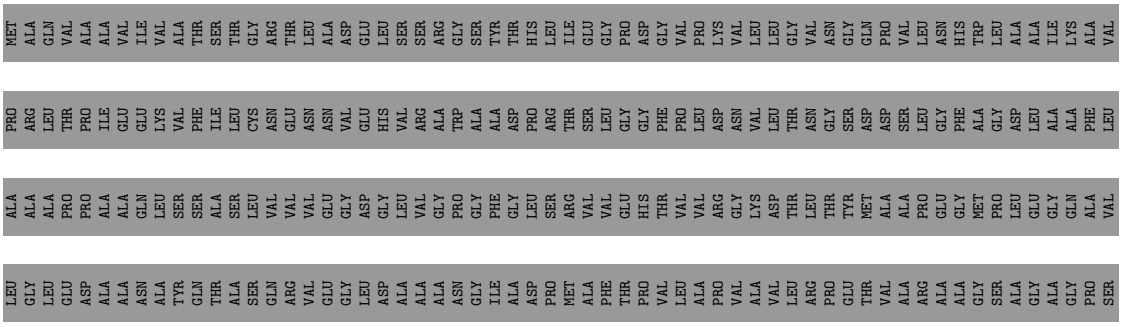

- Molecule 28: FAP182

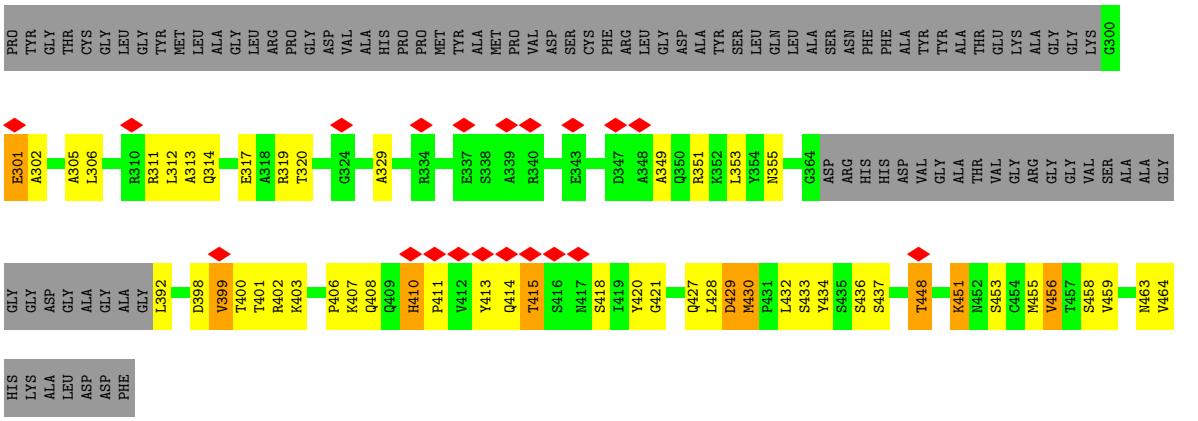
Chain 7H:




- Molecule 28: FAP182

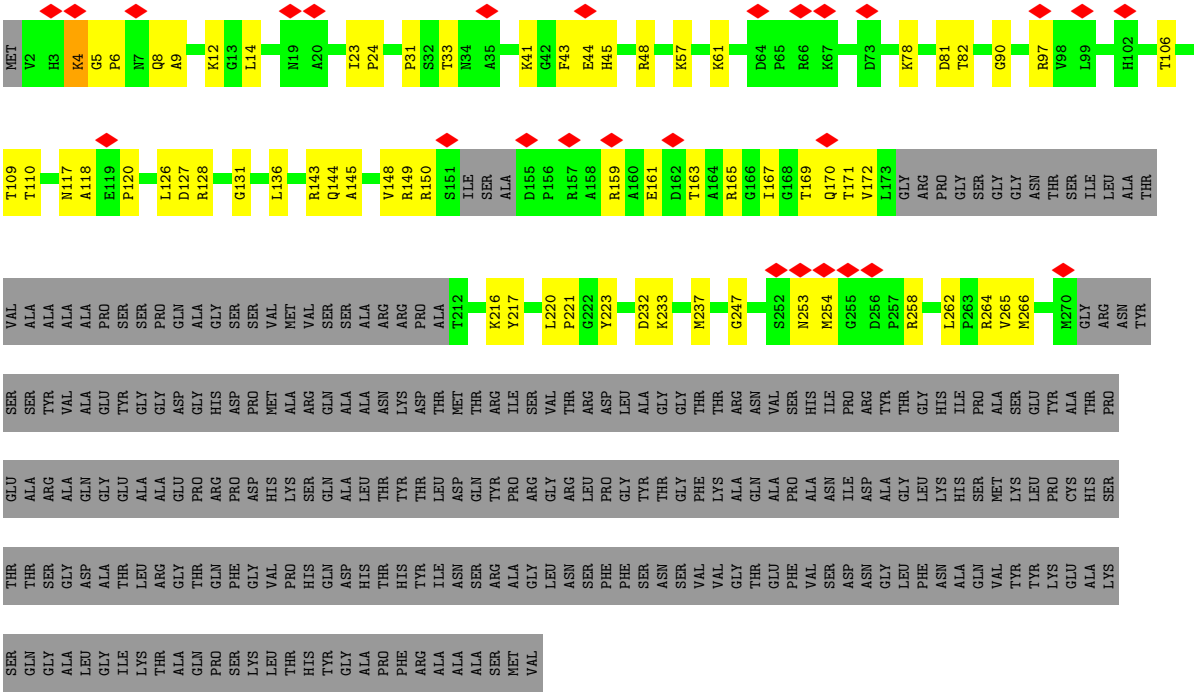
Chain 7X:





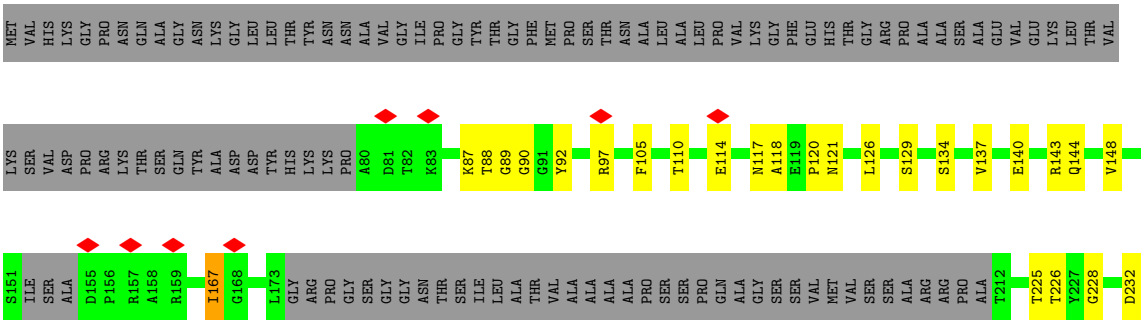

- Molecule 29: FAP129

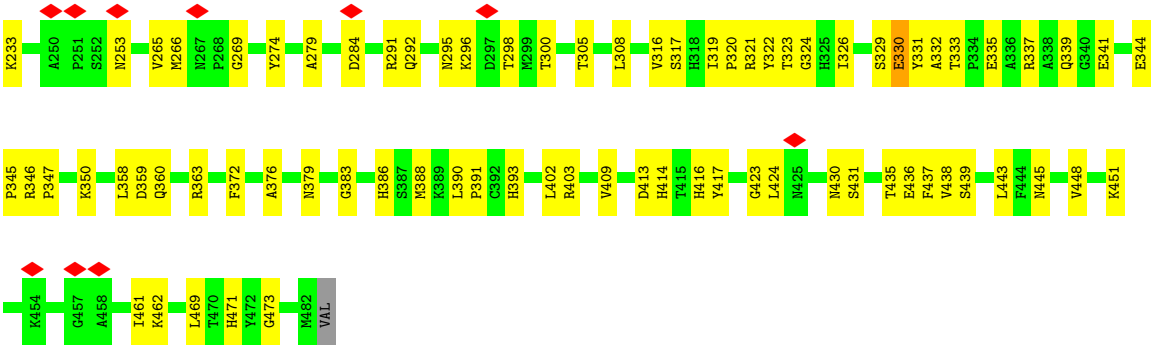
Chain 7I:




- Molecule 29: FAP129

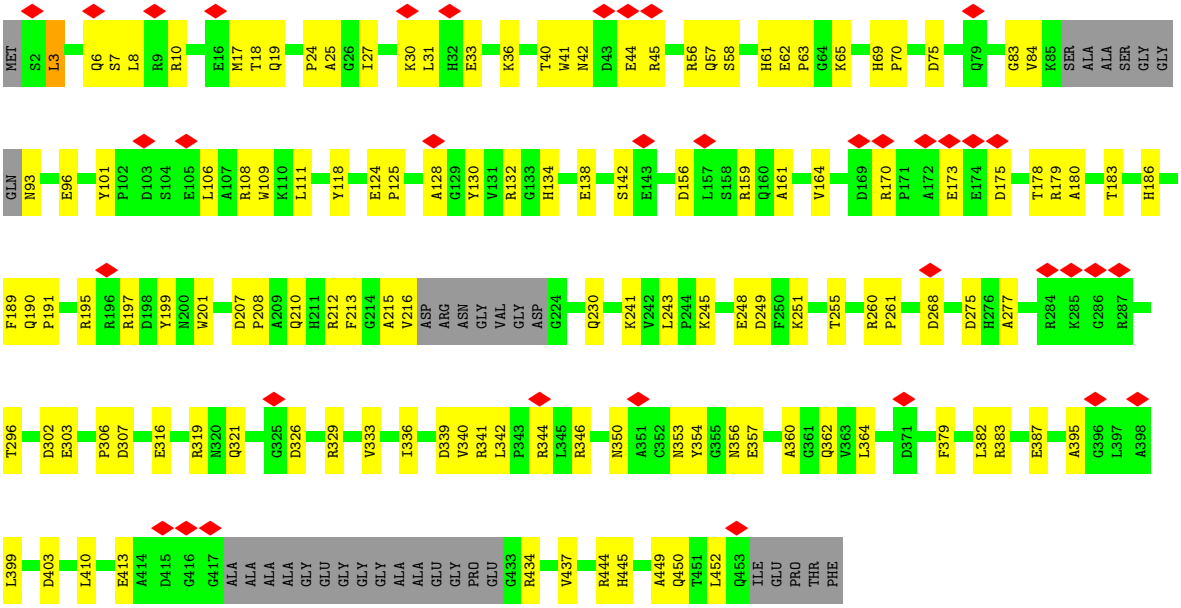
Chain 7J:





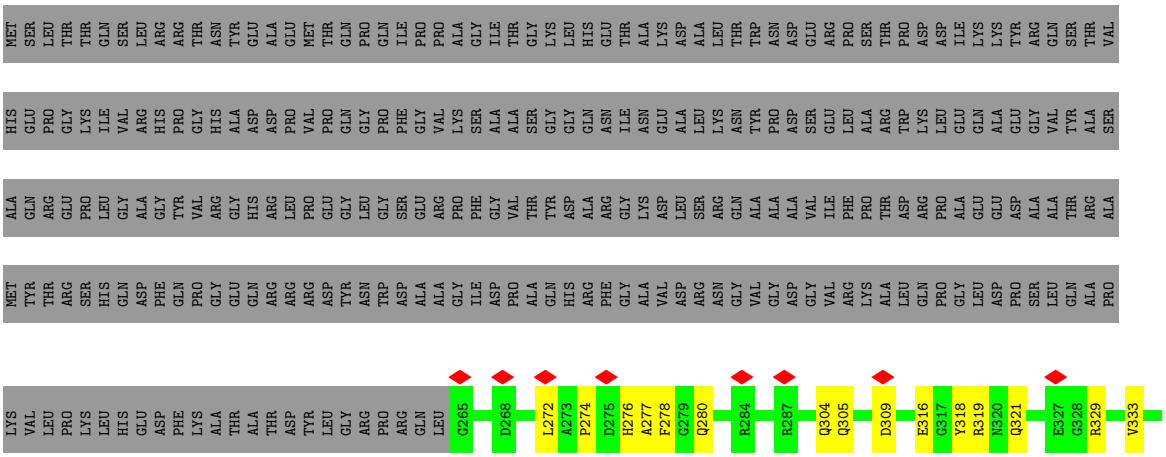

• Molecule 30: FAP21

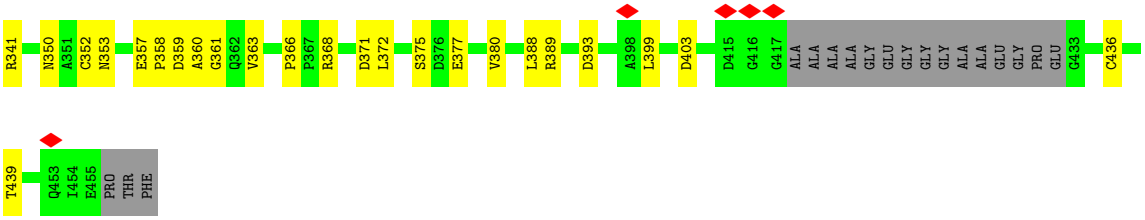
Chain 7K:




• Molecule 30: FAP21

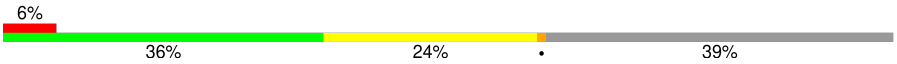
Chain 7L:

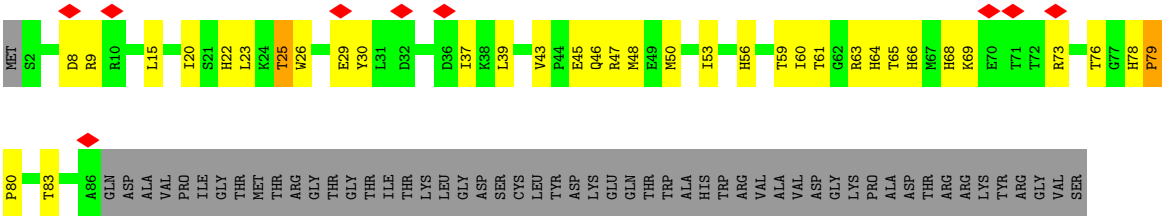





• Molecule 31: FAP273

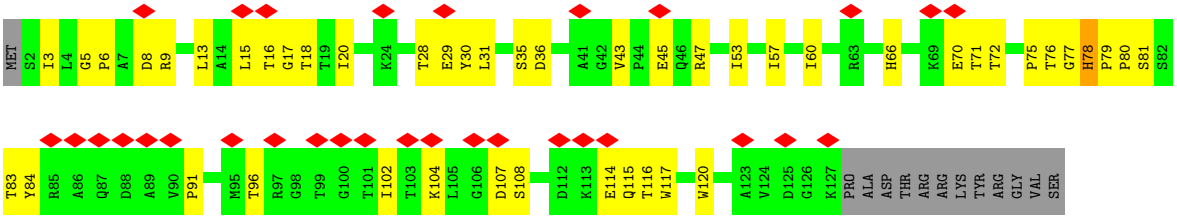
Chain 7M:



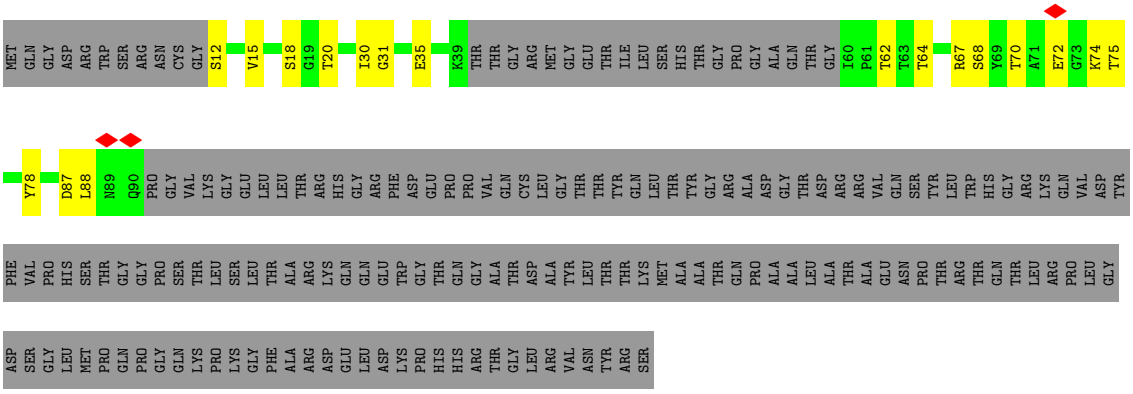

• Molecule 31: FAP273

Chain 7N:



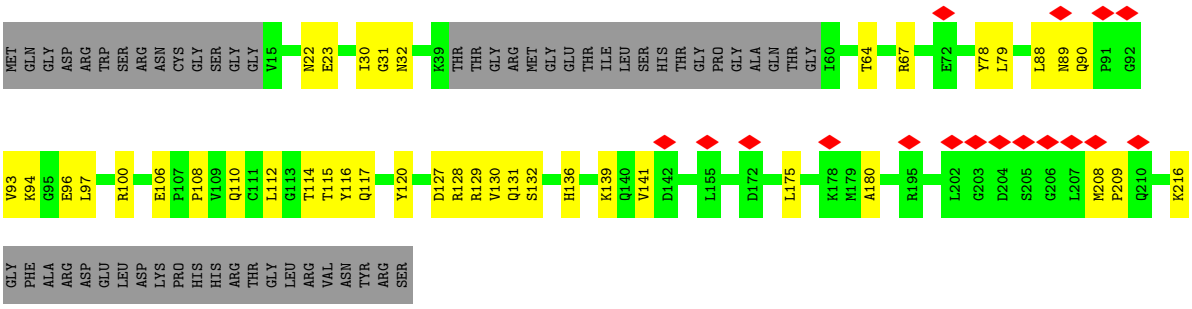

• Molecule 32: FAP107

Chain 7O:



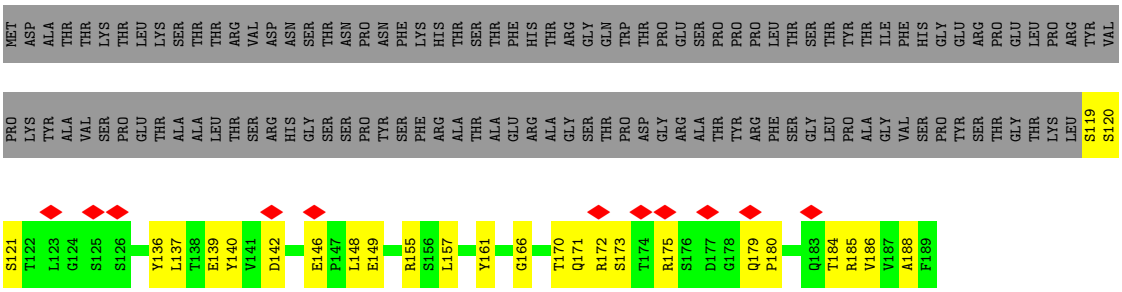

• Molecule 32: FAP107

Chain 7P:



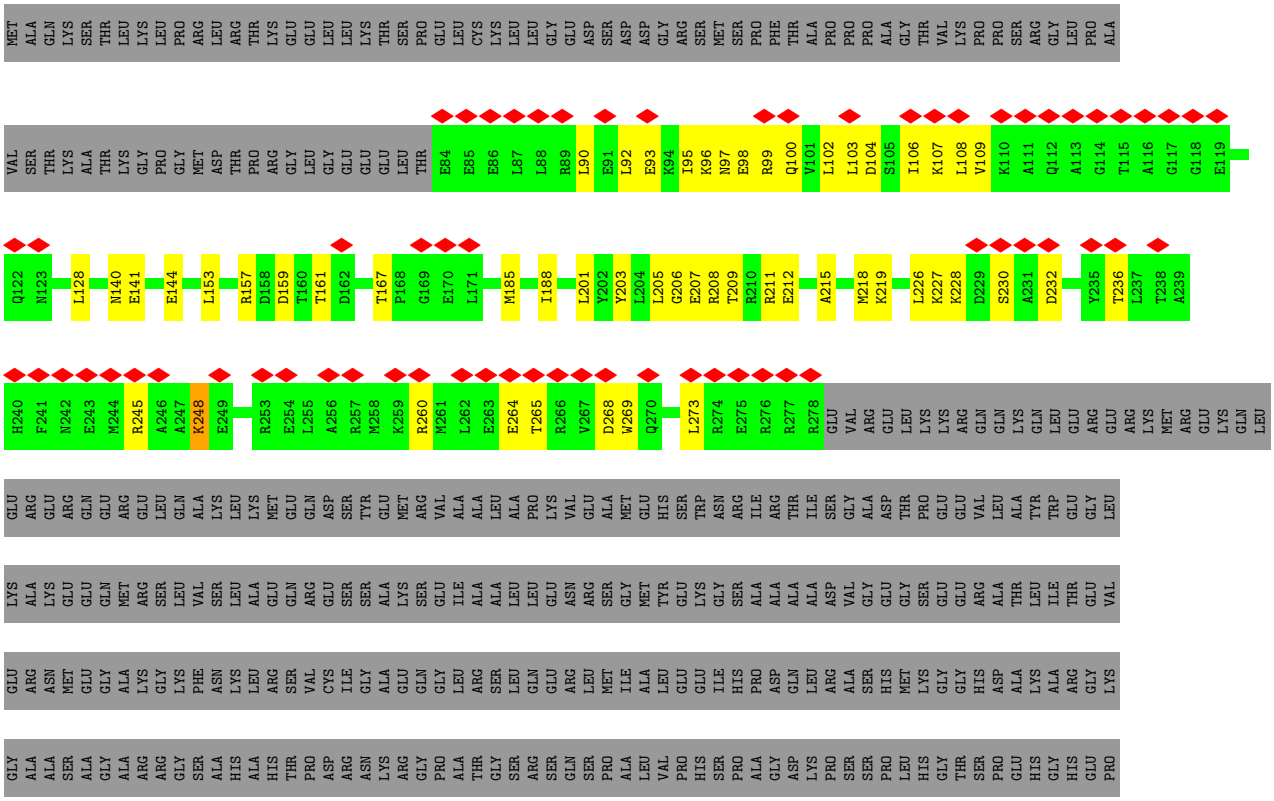

- Molecule 33: RIB21

Chain 7Q:




- Molecule 34: DC1

Chain 7R:



ILE PRO GLU GLY ALA GLU GLU LEU ALA GLY GLU ALA GLU MET VAL SER PRO LEU GLY ALA ASP GLY ASN THR ILE ASP ASP GLU HIS PHE PHE PRO GLU LEU LEU LEU THR SER VAL THR ASP ARG LEU ASN ARG VAL LEU VAL LEU ALA ALA GLU LEU ASP ALA GLN GLU PRO

ALA GLY ALA GLY GLU ASP GLY LEU PRO LEU SER GLY GLU PRO GLY ALA ASP GLY ALA GLU GLY ALA PRO ALA SER PRO SER ARG GLY ALA PRO GLU GLY LEU SER GLU SER GLU ARG THR LEU VAL LYS GLY MET ASN ARG ARG THR TRP THR GLY ALA PRO LEU LEU GLU THR ILE

ASN ALA SER PRO SER GLU ALA ALA LEU THR LEU ASN ILE LYS ARG LYS LYS GLY LYS LYS LYS GLU GLN GLN VAL GLN GLN PRO ASP LEU ASN ARG ILE LEU GLY TYR THR GLY SER ASP VAL GLU GLU GLU GLU PRO GLU SER GLU GLU GLU THR GLU GLU GLU ALA ASN LYS ASP ASP GLY

VAL VAL ASP ARG ASP TYR ILE LYS LEU ARG ALA LEU LYS MET SER GLN ARG LEU ALA ASN GLN GLN ARG ALA ILE LYS VAL

- Molecule 34: DC1

Chain 7S: 5% 16% 5% 79%

MET ALA GLN LYS SER THR LEU LYS LEU PRO ARG LEU ARG THR LYS GLU GLU LEU LEU LYS THR SER PRO GLU LEU CYS LYS LEU LEU GLY GLU ASP SER ASP ASP GLY ARG SER MET SER PRO PHE THR ALA PRO PRO PRO ALA GLY THR VAL LYS PRO PRO SER ARG GLY LEU PRO ALA

VAL SER THR LYS ALA THR LYS GLY PRO GLY MET ASP THR PRO ARG GLY LEU GLY GLU GLU GLU LEU THR GLU GLU GLU LEU LEU ARG LEU GLU LEU GLU LYS ILE LYS ASN GLU ARG GLN VAL LEU LEU ASP SER ILE LYS LEU VAL LYS ALA GLN ALA GLY THR ALA GLY GLY E119

N123 K126 R129 R130 L134 N140 K149 V152 Q156 T160 G169 E170 L171 I188 L201 L205 R210 R211 E212 H213 L214 A215 M216 D217 V220 L226 K227 K228 D229 D232 Y235 T238 A239 H240 F241 N242 E243 M244 R245 A246 A247 K248

E249 Q250 A251 E252 R253 E254 L255 A256 R257 M258 K259 R260 M261 L262 E263 E264 T265 R266 V267 D268 W269 Q270 K271 K272 L273 R274 E275 R276 R277 R278 GLU VAL ARG GLU LEU LYS LYS ARG GLN GLN LYS GLN LEU GLU ARG GLU ARG LYS MET ARG GLU LYS GLN LEU GLU ARG GLU ARG GLN GLU

ARG GLU LEU GLN ALA LYS LEU LYS MET GLU GLN ASP SER TYR GLU MET ARG VAL ALA ALA LEU ALA PRO LYS VAL GLU ALA MET GLU HIS SER TRP ASN ARG ILE ARG THR ILE SER GLY ALA ASP THR PRO GLU GLU VAL LEU ALA TYR TRP GLU GLY LEU LYS ALA LYS GLU GLN

MET ARG SER LEU VAL SER LEU ALA GLU GLN ARG GLU SER SER SER ALA LYS SER GLU ILE ALA ALA LEU LEU GLU ASN ARG SER GLY MET TYR GLU LYS GLY SER ALA ALA ALA ALA ASP VAL GLY GLU GLY SER GLU GLU ARG ALA THR LEU ILE THR GLU VAL GLU ARG ASN MET GLU GLY

ALA LYS GLY LYS PHE ASN LYS LEU ARG SER VAL CYS ILE GLY ALA GLU GLN GLY LEU ARG SER LEU GLU GLU ARG LEU MET ILE ALA LEU GLU GLU GLU ILE HIS PRO ASP GLN LEU ARG ALA SER HIS MET LYS GLY GLY HIS ASP ALA LYS ALA ARG GLY LYS GLY ALA ALA SER ALA GLY

ALA ARG ARG GLY SER ALA HIS ALA HIS THR PRO ASP ARG ASN LYS ARG GLY PRO ALA THR GLY SER ARG SER GLN SER PRO ALA LEU VAL PRO HIS SER PRO ALA GLY ASP LYS PRO SER SER PRO LEU HIS GLY THR SER PRO GLU HIS GLY HIS GLU PRO ILE PRO GLU GLY ALA GLU

GLU LEU ALA GLY GLU ALA GLU MET VAL SER PRO LEU GLY ALA ASP GLY ASN THR ILE ASP ASP GLU HIS PHE PHE PRO GLU LEU PRO GLU LEU LEU THR SER GLU ARG THR ASP ARG LEU ASN ARG VAL LEU VAL LEU ALA ALA GLU LEU ASP ALA GLN GLU PRO ALA GLY ALA GLU GLU

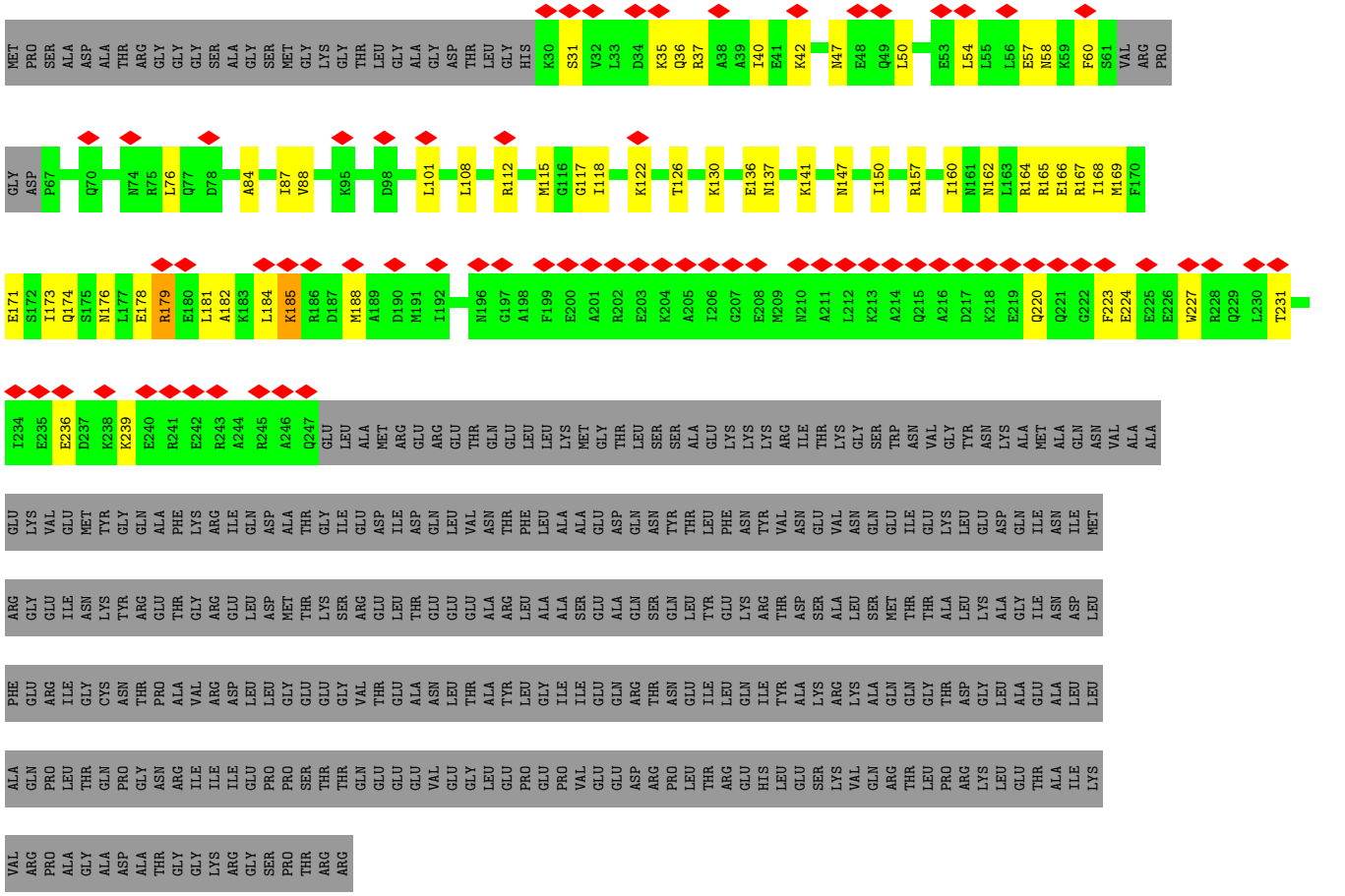
GLY LEU PRO LEU SER GLY GLU PRO GLY ALA ASP GLY ALA GLU GLY ALA ALA PRO ALA SER PRO SER ARG GLY ALA PRO GLU GLY LEU SER GLU SER GLU ARG THR LEU VAL LYS GLY MET ASN ARG ARG THR TRP THR GLY ALA PRO LEU LEU GLU THR ILE ASN ALA SER PRO GLU GLU

ALA ALA LEU THR LEU ASN ILE LYS ARG LYS LYS GLY LYS LYS LYS GLU GLN GLN VAL GLN PRO ASP LEU ASN ARG ILE LEU GLY TYR THR GLY SER ASP VAL GLU GLU GLU GLU PRO GLU SER GLU GLU GLU THR GLU GLU GLU ALA ASN LYS ASP ASP GLY VAL VAL ASP ARG ASP TYR

ILE LYS LEU ARG ALA LEU LYS MET SER GLN ARG LEU ALA ASN GLN GLN ARG ALA ILE LYS VAL

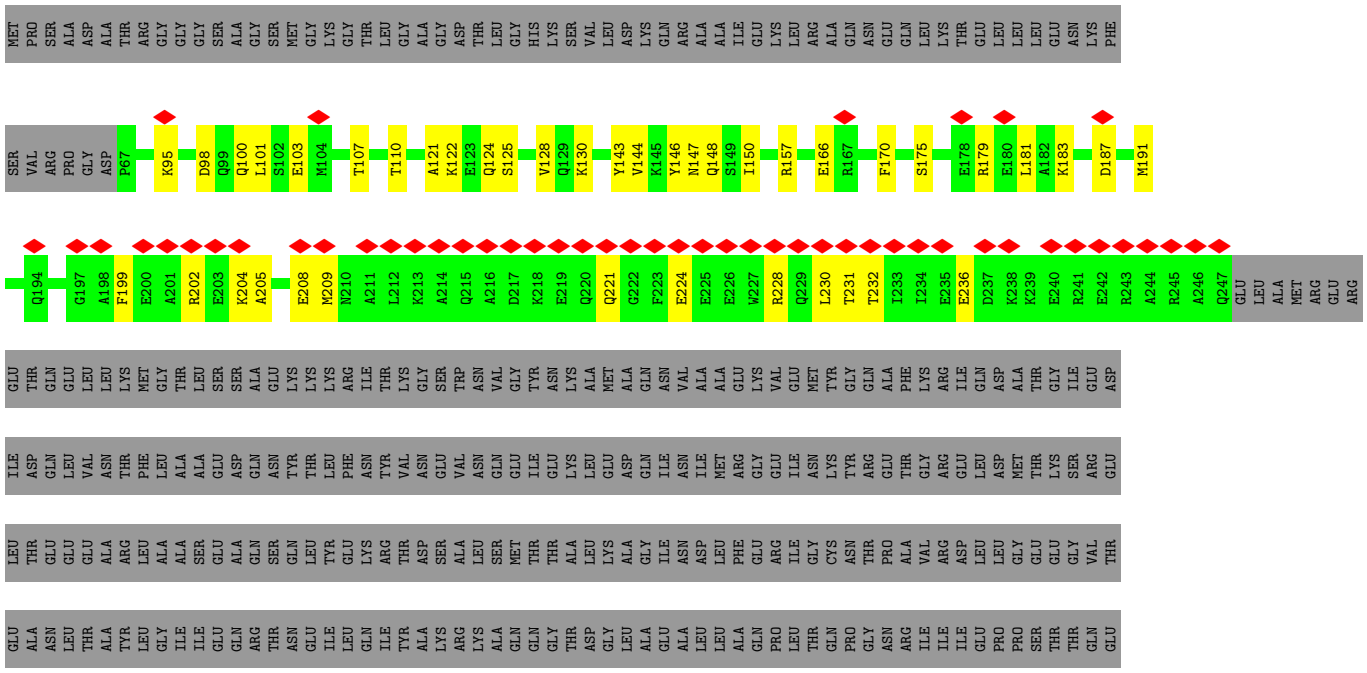
- Molecule 35: DC2

Chain 7T: 13% 28% 10% 61%



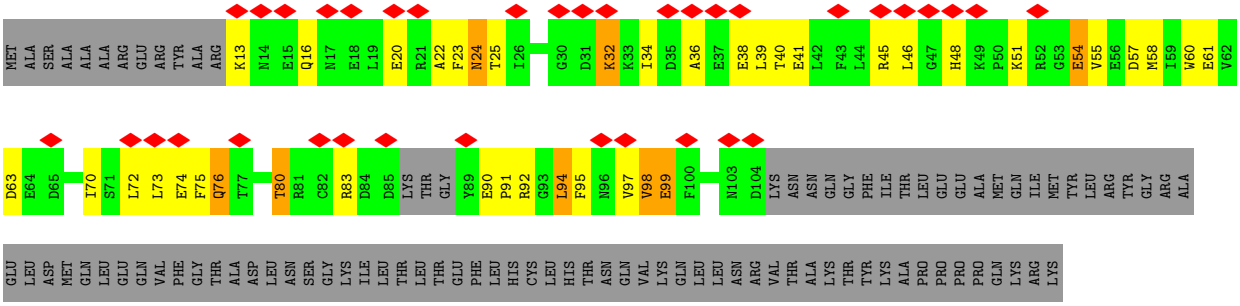

• Molecule 35: DC2

Chain 7U:



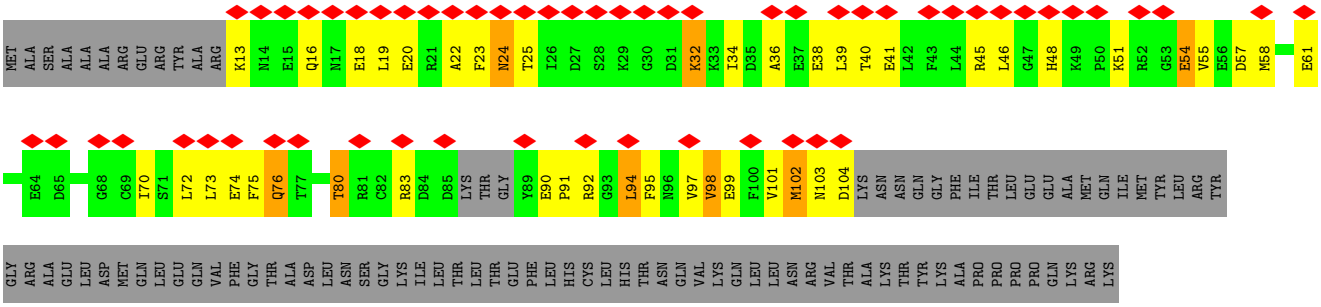
• Molecule 36: DC3

Chain 7V:



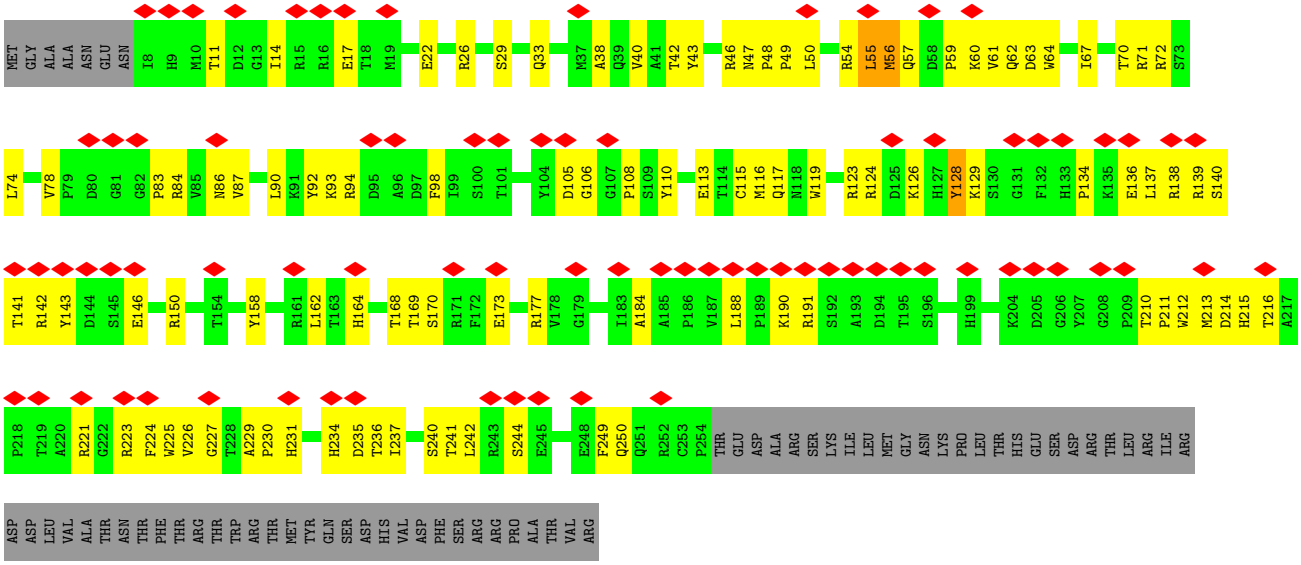

• Molecule 36: DC3

Chain 7W:



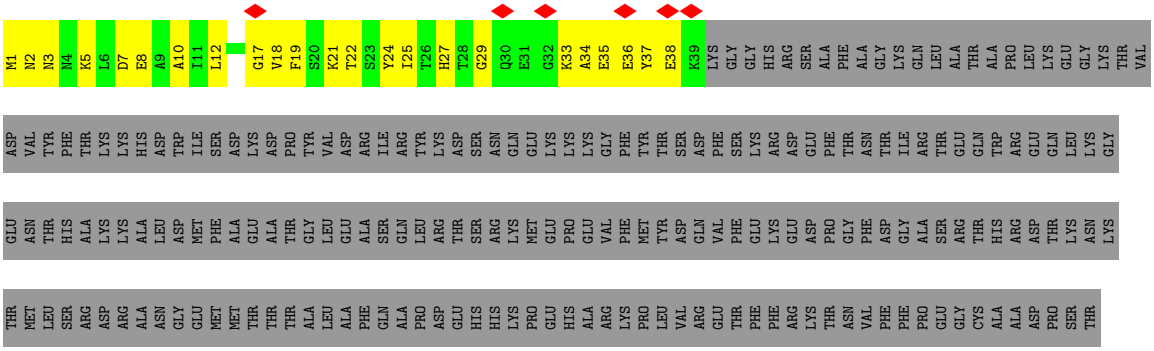

• Molecule 37: FAP68

Chain 7Y:



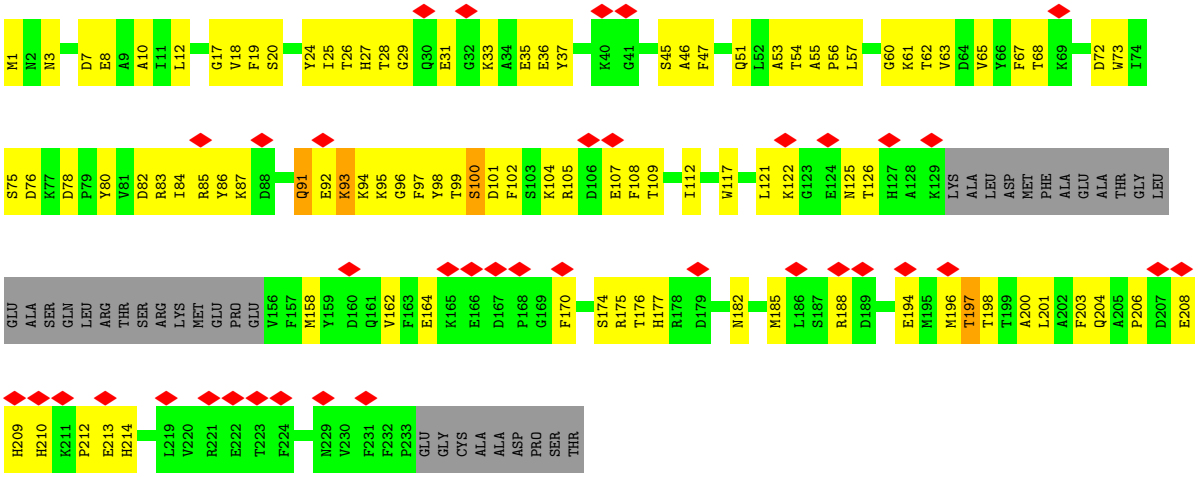
- Molecule 38: FAP90

Chain 7Z:



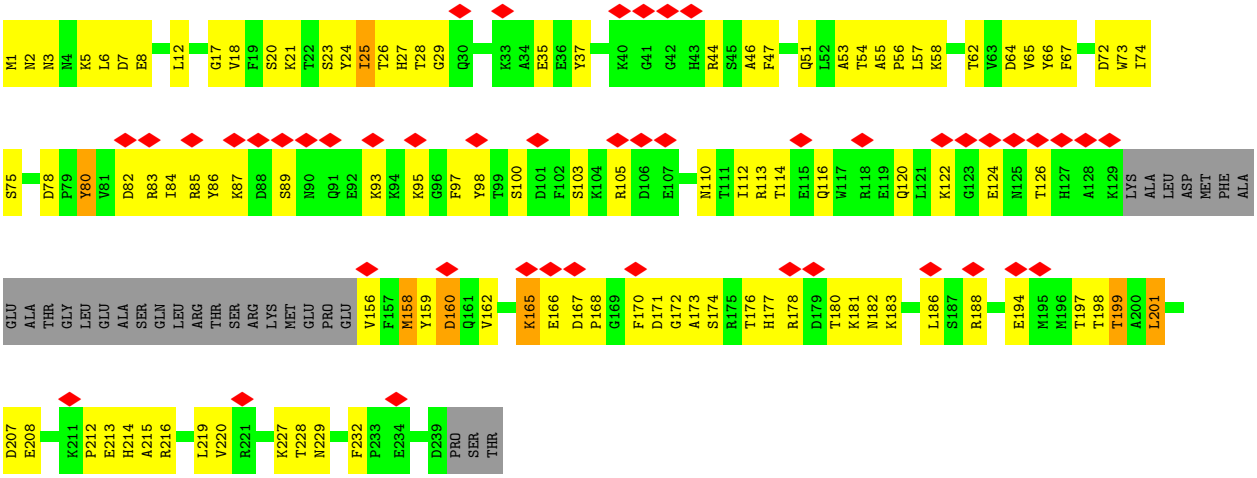

- Molecule 38: FAP90

Chain 8A:



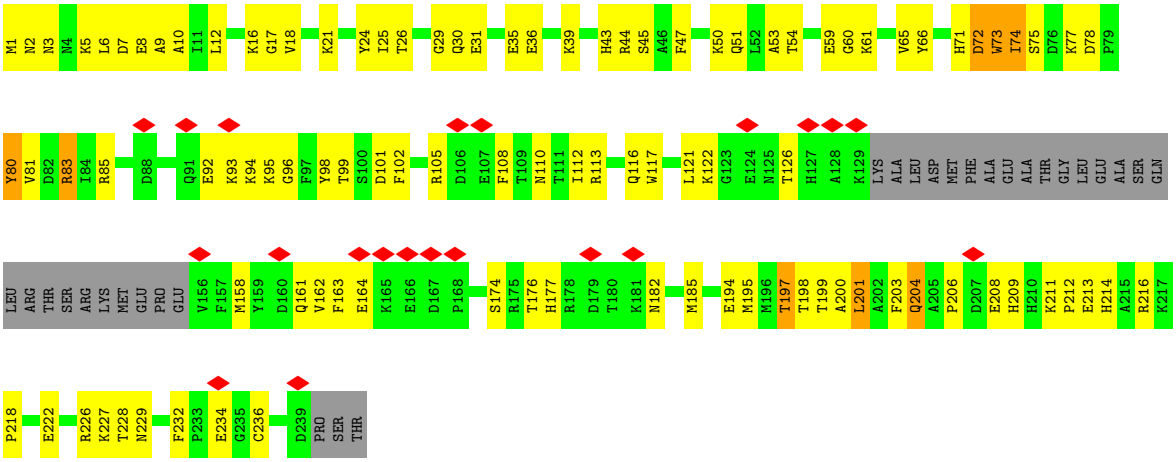

- Molecule 38: FAP90

Chain 8B:



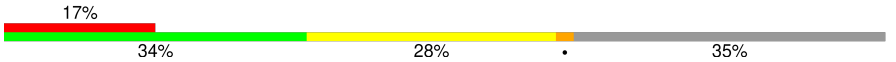
• Molecule 38: FAP90

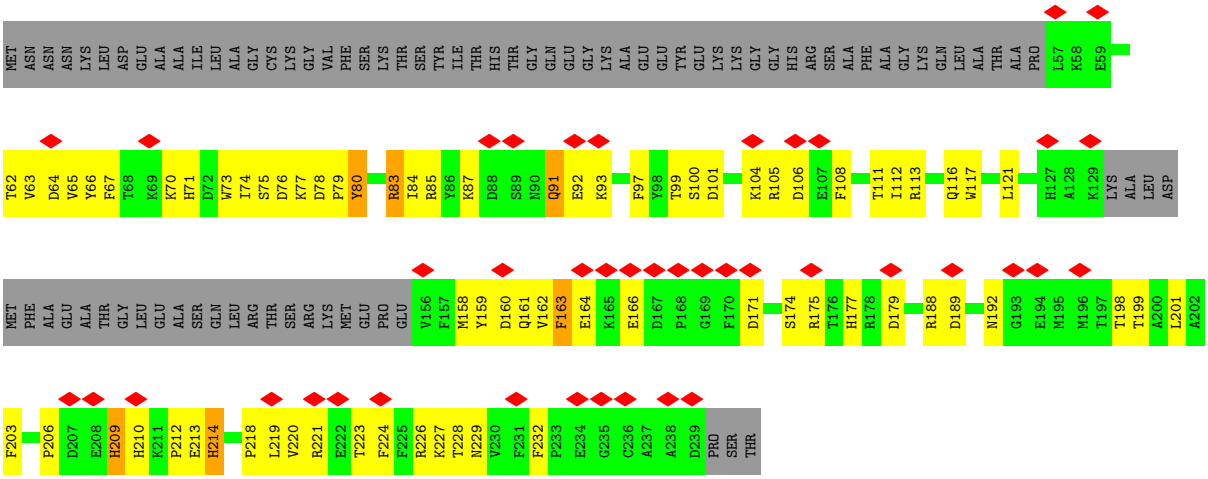
Chain 8C:




• Molecule 38: FAP90

Chain 8D:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 143765 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 38.9 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3100 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.122 | Depositor |
| Minimum map value | -0.042 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (Å) | 718.336, 718.336, 718.336 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.403, 1.403, 1.403 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | 0A | 0.33 | 0/3420 | 0.46 | 0/4628 |
| 1 | 0C | 0.30 | 0/3420 | 0.45 | 0/4628 |
| 1 | 0E | 0.31 | 0/3420 | 0.45 | 0/4628 |
| 1 | 0G | 0.32 | 0/3420 | 0.45 | 0/4628 |
| 1 | 0I | 0.32 | 0/3420 | 0.45 | 0/4628 |
| 1 | 0K | 0.35 | 0/3420 | 0.47 | 0/4628 |
| 1 | 0M | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | 0O | 0.33 | 0/3420 | 0.46 | 0/4628 |
| 1 | 0Q | 0.32 | 0/3420 | 0.44 | 0/4628 |
| 1 | 0S | 0.30 | 0/3420 | 0.47 | 0/4628 |
| 1 | 0U | 0.31 | 0/3420 | 0.46 | 0/4628 |
| 1 | 0W | 0.33 | 0/3420 | 0.47 | 0/4628 |
| 1 | 0Y | 0.33 | 0/3420 | 0.47 | 0/4628 |
| 1 | 1 | 0.43 | 0/1144 | 0.50 | 0/1538 |
| 1 | 1A | 0.35 | 0/3420 | 0.47 | 0/4628 |
| 1 | 1C | 0.35 | 0/3420 | 0.47 | 1/4628 (0.0%) |
| 1 | 1E | 0.33 | 0/3420 | 0.47 | 0/4628 |
| 1 | 1G | 0.33 | 0/3420 | 0.46 | 0/4628 |
| 1 | 1K | 0.32 | 0/3420 | 0.44 | 0/4628 |
| 1 | 1M | 0.34 | 0/3420 | 0.45 | 0/4628 |
| 1 | 1O | 0.34 | 0/3420 | 0.45 | 0/4628 |
| 1 | 1Q | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | 1S | 0.35 | 0/3420 | 0.45 | 0/4628 |
| 1 | 1U | 0.34 | 0/3420 | 0.47 | 0/4628 |
| 1 | 1W | 0.33 | 0/3420 | 0.44 | 0/4628 |
| 1 | 2A | 0.35 | 0/3420 | 0.47 | 1/4628 (0.0%) |
| 1 | 2C | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | 2E | 0.35 | 0/3420 | 0.45 | 0/4628 |
| 1 | 2G | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | 2I | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | 2K | 0.37 | 0/3420 | 0.45 | 0/4628 |
| 1 | 2M | 0.36 | 0/3420 | 0.46 | 0/4628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | 2Q | 0.39 | 0/3420 | 0.48 | 0/4628 |
| 1 | 2S | 0.39 | 0/3420 | 0.48 | 1/4628 (0.0%) |
| 1 | 2U | 0.39 | 0/3420 | 0.47 | 0/4628 |
| 1 | 2W | 0.41 | 0/3420 | 0.47 | 0/4628 |
| 1 | 2Y | 0.40 | 0/3420 | 0.48 | 0/4628 |
| 1 | 3 | 0.42 | 0/3471 | 0.48 | 0/4697 |
| 1 | 3A | 0.41 | 0/3420 | 0.48 | 0/4628 |
| 1 | 3C | 0.40 | 0/3420 | 0.47 | 0/4628 |
| 1 | 3G | 0.38 | 0/3420 | 0.47 | 0/4628 |
| 1 | 3I | 0.39 | 0/3420 | 0.47 | 0/4628 |
| 1 | 3K | 0.40 | 0/3420 | 0.48 | 0/4628 |
| 1 | 3M | 0.42 | 0/3420 | 0.50 | 1/4628 (0.0%) |
| 1 | 3O | 0.39 | 0/3420 | 0.50 | 0/4628 |
| 1 | 3Q | 0.40 | 0/3420 | 0.50 | 0/4628 |
| 1 | 3S | 0.43 | 0/3420 | 0.55 | 0/4628 |
| 1 | 5 | 0.41 | 0/3496 | 0.48 | 0/4730 |
| 1 | 7 | 0.43 | 0/3505 | 0.49 | 0/4742 |
| 1 | 9 | 0.44 | 0/3496 | 0.52 | 1/4730 (0.0%) |
| 1 | A1 | 0.40 | 0/3462 | 0.48 | 0/4685 |
| 1 | A3 | 0.32 | 0/3484 | 0.44 | 0/4714 |
| 1 | A5 | 0.38 | 0/3444 | 0.45 | 0/4661 |
| 1 | A7 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | A9 | 0.40 | 0/3420 | 0.47 | 0/4628 |
| 1 | B1 | 0.38 | 0/3420 | 0.45 | 0/4628 |
| 1 | B3 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | B5 | 0.41 | 0/3420 | 0.47 | 0/4628 |
| 1 | B8 | 0.37 | 0/3420 | 0.47 | 0/4628 |
| 1 | C0 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | C2 | 0.35 | 0/3420 | 0.44 | 0/4628 |
| 1 | C4 | 0.35 | 0/3420 | 0.45 | 0/4628 |
| 1 | C6 | 0.40 | 0/3420 | 0.48 | 0/4628 |
| 1 | C8 | 0.38 | 0/3420 | 0.48 | 0/4628 |
| 1 | D0 | 0.41 | 0/3420 | 0.47 | 0/4628 |
| 1 | D2 | 0.41 | 0/3420 | 0.49 | 1/4628 (0.0%) |
| 1 | D4 | 0.38 | 0/3420 | 0.48 | 0/4628 |
| 1 | D6 | 0.38 | 0/3420 | 0.47 | 0/4628 |
| 1 | D8 | 0.32 | 0/3420 | 0.46 | 0/4628 |
| 1 | E0 | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | E2 | 0.39 | 0/3420 | 0.48 | 0/4628 |
| 1 | E4 | 0.35 | 0/3420 | 0.47 | 0/4628 |
| 1 | E6 | 0.37 | 0/3420 | 0.47 | 0/4628 |
| 1 | E8 | 0.38 | 0/3420 | 0.48 | 0/4628 |
| 1 | F0 | 0.35 | 0/3420 | 0.47 | 0/4628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | F2 | 0.36 | 0/3420 | 0.47 | 0/4628 |
| 1 | F6 | 0.32 | 0/3420 | 0.47 | 1/4628 (0.0%) |
| 1 | F8 | 0.36 | 0/3420 | 0.46 | 0/4628 |
| 1 | G0 | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | G2 | 0.38 | 0/3420 | 0.47 | 0/4628 |
| 1 | G4 | 0.35 | 0/3420 | 0.45 | 0/4628 |
| 1 | G6 | 0.37 | 0/3420 | 0.48 | 0/4628 |
| 1 | G8 | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | H2 | 0.33 | 0/3420 | 0.46 | 0/4628 |
| 1 | H4 | 0.36 | 0/3420 | 0.48 | 0/4628 |
| 1 | H6 | 0.34 | 0/3420 | 0.45 | 0/4628 |
| 1 | H8 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | I0 | 0.36 | 0/3420 | 0.46 | 0/4628 |
| 1 | I2 | 0.36 | 0/3420 | 0.46 | 0/4628 |
| 1 | I4 | 0.36 | 0/3420 | 0.47 | 0/4628 |
| 1 | I8 | 0.37 | 0/3420 | 0.45 | 0/4628 |
| 1 | J0 | 0.39 | 0/3420 | 0.46 | 0/4628 |
| 1 | J2 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | J4 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | J6 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | J8 | 0.38 | 0/3420 | 0.45 | 0/4628 |
| 1 | K0 | 0.35 | 0/3420 | 0.45 | 0/4628 |
| 1 | K4 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | K6 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | K8 | 0.38 | 0/3420 | 0.45 | 0/4628 |
| 1 | L0 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | L2 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | L4 | 0.39 | 0/3420 | 0.46 | 0/4628 |
| 1 | L6 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | M0 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | M2 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | M4 | 0.36 | 0/3420 | 0.46 | 0/4628 |
| 1 | M6 | 0.39 | 0/3420 | 0.47 | 0/4628 |
| 1 | M8 | 0.36 | 0/3420 | 0.48 | 0/4628 |
| 1 | N0 | 0.39 | 0/3420 | 0.47 | 0/4628 |
| 1 | N2 | 0.36 | 0/3420 | 0.48 | 1/4628 (0.0%) |
| 1 | N6 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | N8 | 0.41 | 0/3420 | 0.47 | 0/4628 |
| 1 | O0 | 0.37 | 0/3420 | 0.47 | 0/4628 |
| 1 | O2 | 0.42 | 0/3420 | 0.49 | 0/4628 |
| 1 | O4 | 0.42 | 0/3420 | 0.48 | 0/4628 |
| 1 | O6 | 0.43 | 0/3420 | 0.47 | 0/4628 |
| 1 | O8 | 0.41 | 1/3420 (0.0%) | 0.46 | 0/4628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | P4 | 0.42 | 0/3420 | 0.47 | 0/4628 |
| 1 | P6 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | P8 | 0.41 | 0/3420 | 0.46 | 0/4628 |
| 1 | Q0 | 0.42 | 0/3420 | 0.48 | 1/4628 (0.0%) |
| 1 | Q2 | 0.41 | 0/3420 | 0.46 | 0/4628 |
| 1 | Q4 | 0.42 | 0/3420 | 0.47 | 0/4628 |
| 1 | Q6 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | Q8 | 0.33 | 0/3366 | 0.49 | 0/4556 |
| 1 | R0 | 0.42 | 0/3475 | 0.48 | 0/4702 |
| 1 | R2 | 0.40 | 0/3420 | 0.50 | 1/4628 (0.0%) |
| 1 | R4 | 0.43 | 0/3444 | 0.48 | 0/4661 |
| 1 | R6 | 0.42 | 0/3420 | 0.47 | 0/4628 |
| 1 | R8 | 0.41 | 0/3453 | 0.47 | 0/4673 |
| 1 | S0 | 0.41 | 0/3420 | 0.48 | 0/4628 |
| 1 | S2 | 0.41 | 0/3453 | 0.49 | 0/4673 |
| 1 | S4 | 0.37 | 0/3428 | 0.49 | 0/4639 |
| 1 | S6 | 0.41 | 0/3420 | 0.48 | 1/4628 (0.0%) |
| 1 | S8 | 0.41 | 0/3420 | 0.48 | 0/4628 |
| 1 | T0 | 0.42 | 0/3420 | 0.49 | 0/4628 |
| 1 | T2 | 0.44 | 0/3420 | 0.49 | 0/4628 |
| 1 | T4 | 0.40 | 0/3420 | 0.46 | 0/4628 |
| 1 | T6 | 0.44 | 1/3420 (0.0%) | 0.54 | 0/4628 |
| 1 | T8 | 0.38 | 0/3420 | 0.46 | 0/4628 |
| 1 | U2 | 0.36 | 0/3420 | 0.47 | 0/4628 |
| 1 | U4 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | U6 | 0.37 | 0/3420 | 0.47 | 0/4628 |
| 1 | U8 | 0.39 | 0/3444 | 0.49 | 0/4661 |
| 1 | V0 | 0.37 | 0/3420 | 0.45 | 0/4628 |
| 1 | V2 | 0.37 | 0/3420 | 0.47 | 0/4628 |
| 1 | V4 | 0.36 | 0/3420 | 0.45 | 0/4628 |
| 1 | V6 | 0.33 | 0/3420 | 0.46 | 0/4628 |
| 1 | V8 | 0.36 | 0/3420 | 0.47 | 0/4628 |
| 1 | W0 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | W2 | 0.37 | 0/3420 | 0.46 | 0/4628 |
| 1 | W4 | 0.40 | 0/3420 | 0.48 | 0/4628 |
| 1 | W6 | 0.36 | 0/3420 | 0.45 | 0/4628 |
| 1 | W8 | 0.38 | 0/3420 | 0.48 | 0/4628 |
| 1 | X0 | 0.36 | 0/3420 | 0.46 | 0/4628 |
| 1 | X2 | 0.31 | 0/3420 | 0.45 | 0/4628 |
| 1 | X4 | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | X6 | 0.35 | 0/3420 | 0.46 | 0/4628 |
| 1 | X8 | 0.36 | 0/3420 | 0.47 | 0/4628 |
| 1 | Y0 | 0.37 | 0/3420 | 0.47 | 0/4628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 1 | Y2 | 0.34 | 0/3420 | 0.46 | 0/4628 |
| 1 | Y4 | 0.39 | 0/3420 | 0.47 | 0/4628 |
| 1 | Y6 | 0.33 | 0/3420 | 0.45 | 0/4628 |
| 1 | Y8 | 0.29 | 0/3420 | 0.46 | 0/4628 |
| 1 | Z0 | 0.32 | 0/3420 | 0.46 | 0/4628 |
| 1 | Z2 | 0.32 | 0/3420 | 0.46 | 0/4628 |
| 1 | Z4 | 0.34 | 0/3420 | 0.48 | 0/4628 |
| 1 | Z6 | 0.34 | 0/3420 | 0.47 | 0/4628 |
| 1 | Z8 | 0.32 | 0/3420 | 0.46 | 0/4628 |
| 2 | 0B | 0.32 | 0/3389 | 0.46 | 0/4595 |
| 2 | 0F | 0.32 | 0/3389 | 0.47 | 0/4595 |
| 2 | 0H | 0.32 | 0/3389 | 0.46 | 0/4595 |
| 2 | 0J | 0.34 | 0/3389 | 0.48 | 0/4595 |
| 2 | 0L | 0.35 | 0/3389 | 0.49 | 1/4595 (0.0%) |
| 2 | 0N | 0.33 | 0/3389 | 0.47 | 0/4595 |
| 2 | 0P | 0.34 | 0/3389 | 0.48 | 0/4595 |
| 2 | 0R | 0.32 | 0/3389 | 0.47 | 0/4595 |
| 2 | 0V | 0.35 | 0/3389 | 0.47 | 0/4595 |
| 2 | 0X | 0.33 | 0/3389 | 0.47 | 0/4595 |
| 2 | 0Z | 0.36 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1B | 0.35 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1D | 0.34 | 0/3389 | 0.48 | 0/4595 |
| 2 | 1F | 0.34 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1H | 0.32 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1L | 0.34 | 0/3389 | 0.48 | 0/4595 |
| 2 | 1N | 0.36 | 0/3389 | 0.48 | 0/4595 |
| 2 | 1P | 0.37 | 0/3389 | 0.48 | 0/4595 |
| 2 | 1R | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | 1T | 0.34 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1V | 0.35 | 0/3389 | 0.48 | 0/4595 |
| 2 | 1X | 0.32 | 0/3389 | 0.47 | 0/4595 |
| 2 | 1Z | 0.33 | 0/3389 | 0.47 | 0/4595 |
| 2 | 2 | 0.41 | 0/3448 | 0.49 | 1/4675 (0.0%) |
| 2 | 2B | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | 2D | 0.35 | 0/3389 | 0.47 | 1/4595 (0.0%) |
| 2 | 2F | 0.37 | 0/3389 | 0.48 | 1/4595 (0.0%) |
| 2 | 2H | 0.38 | 0/3389 | 0.50 | 0/4595 |
| 2 | 2J | 0.38 | 0/3389 | 0.50 | 0/4595 |
| 2 | 2L | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | 2N | 0.33 | 0/3389 | 0.49 | 0/4595 |
| 2 | 2P | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | 2R | 0.40 | 0/3389 | 0.48 | 0/4595 |
| 2 | 2T | 0.39 | 0/3389 | 0.48 | 0/4595 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | 2V | 0.41 | 0/3389 | 0.49 | 0/4595 |
| 2 | 2X | 0.41 | 0/3457 | 0.49 | 1/4687 (0.0%) |
| 2 | 2Z | 0.41 | 0/3389 | 0.49 | 0/4595 |
| 2 | 3B | 0.43 | 0/3455 | 0.52 | 0/4684 |
| 2 | 3D | 0.36 | 0/3389 | 0.48 | 0/4595 |
| 2 | 3F | 0.37 | 0/3389 | 0.49 | 0/4595 |
| 2 | 3H | 0.39 | 0/3389 | 0.49 | 0/4595 |
| 2 | 3J | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | 3L | 0.41 | 0/3389 | 0.49 | 0/4595 |
| 2 | 3N | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | 3P | 0.39 | 0/3389 | 0.50 | 0/4595 |
| 2 | 3R | 0.40 | 0/3457 | 0.53 | 0/4687 |
| 2 | 3T | 0.36 | 0/3389 | 0.55 | 0/4595 |
| 2 | 4 | 0.43 | 0/3448 | 0.52 | 0/4675 |
| 2 | 6 | 0.41 | 0/3448 | 0.49 | 0/4675 |
| 2 | 8 | 0.44 | 0/3448 | 0.51 | 0/4675 |
| 2 | A0 | 0.41 | 0/3448 | 0.49 | 0/4675 |
| 2 | A2 | 0.35 | 0/3448 | 0.50 | 0/4675 |
| 2 | A4 | 0.41 | 0/3448 | 0.49 | 0/4675 |
| 2 | A8 | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | B0 | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | B2 | 0.40 | 0/3389 | 0.47 | 0/4595 |
| 2 | B4 | 0.42 | 0/3389 | 0.48 | 0/4595 |
| 2 | B7 | 0.38 | 0/3389 | 0.50 | 0/4595 |
| 2 | B9 | 0.40 | 0/3389 | 0.48 | 1/4595 (0.0%) |
| 2 | C1 | 0.37 | 0/3389 | 0.47 | 0/4595 |
| 2 | C5 | 0.39 | 0/3448 | 0.48 | 0/4675 |
| 2 | C7 | 0.40 | 0/3448 | 0.48 | 0/4675 |
| 2 | C9 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | D1 | 0.42 | 0/3389 | 0.51 | 1/4595 (0.0%) |
| 2 | D3 | 0.37 | 0/3395 | 0.47 | 0/4603 |
| 2 | D5 | 0.40 | 0/3389 | 0.49 | 0/4595 |
| 2 | D7 | 0.37 | 0/3395 | 0.48 | 0/4603 |
| 2 | E1 | 0.37 | 0/3395 | 0.48 | 0/4603 |
| 2 | E3 | 0.37 | 0/3389 | 0.47 | 0/4595 |
| 2 | E5 | 0.39 | 0/3389 | 0.49 | 0/4595 |
| 2 | E7 | 0.38 | 0/3395 | 0.50 | 0/4603 |
| 2 | E9 | 0.35 | 0/3389 | 0.49 | 0/4595 |
| 2 | F1 | 0.37 | 0/3389 | 0.49 | 0/4595 |
| 2 | F3 | 0.34 | 0/3389 | 0.49 | 0/4595 |
| 2 | F5 | 0.31 | 0/3389 | 0.46 | 0/4595 |
| 2 | F7 | 0.36 | 0/3389 | 0.47 | 0/4595 |
| 2 | F9 | 0.35 | 0/3448 | 0.46 | 0/4675 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | G1 | 0.38 | 0/3448 | 0.50 | 0/4675 |
| 2 | G3 | 0.39 | 0/3448 | 0.51 | 0/4675 |
| 2 | G5 | 0.34 | 0/3389 | 0.47 | 0/4595 |
| 2 | G7 | 0.35 | 0/3389 | 0.47 | 0/4595 |
| 2 | G9 | 0.33 | 0/3389 | 0.47 | 0/4595 |
| 2 | H1 | 0.31 | 0/3389 | 0.47 | 0/4595 |
| 2 | H3 | 0.38 | 0/3389 | 0.48 | 0/4595 |
| 2 | H5 | 0.35 | 0/3389 | 0.47 | 1/4595 (0.0%) |
| 2 | H7 | 0.38 | 0/3389 | 0.48 | 0/4595 |
| 2 | H9 | 0.38 | 0/3389 | 0.48 | 0/4595 |
| 2 | I1 | 0.35 | 0/3389 | 0.49 | 0/4595 |
| 2 | I3 | 0.36 | 0/3389 | 0.47 | 0/4595 |
| 2 | I5 | 0.31 | 0/3389 | 0.46 | 0/4595 |
| 2 | I7 | 0.35 | 0/3403 | 0.47 | 0/4614 |
| 2 | I9 | 0.40 | 0/3395 | 0.49 | 0/4603 |
| 2 | J1 | 0.37 | 0/3389 | 0.47 | 0/4595 |
| 2 | J3 | 0.43 | 0/3397 | 0.52 | 0/4606 |
| 2 | J5 | 0.42 | 0/3457 | 0.52 | 2/4687 (0.0%) |
| 2 | J7 | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | J9 | 0.37 | 0/3457 | 0.48 | 0/4687 |
| 2 | K1 | 0.32 | 0/3389 | 0.46 | 0/4595 |
| 2 | K3 | 0.35 | 0/3389 | 0.48 | 0/4595 |
| 2 | K5 | 0.39 | 0/3389 | 0.48 | 0/4595 |
| 2 | K7 | 0.36 | 0/3389 | 0.47 | 0/4595 |
| 2 | K9 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | L1 | 0.38 | 0/3389 | 0.47 | 0/4595 |
| 2 | L3 | 0.39 | 0/3389 | 0.49 | 0/4595 |
| 2 | L5 | 0.39 | 0/3389 | 0.49 | 0/4595 |
| 2 | L7 | 0.31 | 0/3389 | 0.47 | 0/4595 |
| 2 | L9 | 0.35 | 0/3389 | 0.47 | 0/4595 |
| 2 | M1 | 0.37 | 0/3389 | 0.49 | 0/4595 |
| 2 | M3 | 0.37 | 0/3448 | 0.48 | 0/4675 |
| 2 | M5 | 0.40 | 0/3389 | 0.49 | 0/4595 |
| 2 | M7 | 0.38 | 0/3448 | 0.49 | 0/4675 |
| 2 | M9 | 0.41 | 0/3457 | 0.50 | 0/4687 |
| 2 | N1 | 0.40 | 0/3395 | 0.53 | 0/4603 |
| 2 | N3 | 0.30 | 0/3389 | 0.47 | 0/4595 |
| 2 | N5 | 0.38 | 0/3389 | 0.50 | 0/4595 |
| 2 | N7 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | N9 | 0.39 | 0/3389 | 0.50 | 0/4595 |
| 2 | O1 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | O3 | 0.42 | 0/3389 | 0.51 | 0/4595 |
| 2 | O5 | 0.41 | 0/3389 | 0.50 | 0/4595 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | O7 | 0.42 | 0/3411 | 0.52 | 0/4624 |
| 2 | O9 | 0.38 | 0/3389 | 0.47 | 0/4595 |
| 2 | P3 | 0.41 | 0/3389 | 0.49 | 1/4595 (0.0%) |
| 2 | P5 | 0.42 | 0/3448 | 0.51 | 0/4675 |
| 2 | P7 | 0.41 | 0/3389 | 0.48 | 0/4595 |
| 2 | P9 | 0.42 | 0/3448 | 0.49 | 0/4675 |
| 2 | Q1 | 0.42 | 0/3389 | 0.50 | 0/4595 |
| 2 | Q3 | 0.42 | 0/3389 | 0.51 | 0/4595 |
| 2 | Q5 | 0.43 | 0/3389 | 0.50 | 0/4595 |
| 2 | Q9 | 0.40 | 0/3389 | 0.48 | 0/4595 |
| 2 | R1 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | R3 | 0.41 | 0/3398 | 0.51 | 0/4607 |
| 2 | R5 | 0.42 | 0/3448 | 0.51 | 0/4675 |
| 2 | R7 | 0.42 | 0/3389 | 0.49 | 0/4595 |
| 2 | R9 | 0.42 | 0/3448 | 0.49 | 0/4675 |
| 2 | S1 | 0.43 | 0/3404 | 0.55 | 2/4615 (0.0%) |
| 2 | S5 | 0.40 | 0/3389 | 0.48 | 0/4595 |
| 2 | S7 | 0.42 | 0/3448 | 0.55 | 1/4675 (0.0%) |
| 2 | S9 | 0.41 | 0/3389 | 0.49 | 0/4595 |
| 2 | T1 | 0.43 | 0/3389 | 0.50 | 0/4595 |
| 2 | T3 | 0.44 | 0/3389 | 0.50 | 0/4595 |
| 2 | T5 | 0.41 | 0/3389 | 0.49 | 0/4595 |
| 2 | T7 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | U1 | 0.35 | 0/3389 | 0.47 | 0/4595 |
| 2 | U3 | 0.37 | 0/3389 | 0.48 | 0/4595 |
| 2 | U5 | 0.36 | 0/3389 | 0.48 | 0/4595 |
| 2 | U7 | 0.39 | 0/3389 | 0.50 | 0/4595 |
| 2 | U9 | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | V1 | 0.38 | 0/3389 | 0.50 | 0/4595 |
| 2 | V3 | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | V7 | 0.36 | 0/3389 | 0.47 | 0/4595 |
| 2 | V9 | 0.37 | 0/3389 | 0.48 | 0/4595 |
| 2 | W1 | 0.38 | 0/3389 | 0.49 | 0/4595 |
| 2 | W3 | 0.41 | 0/3389 | 0.50 | 0/4595 |
| 2 | W5 | 0.39 | 0/3389 | 0.49 | 0/4595 |
| 2 | W7 | 0.39 | 0/3389 | 0.50 | 0/4595 |
| 2 | W9 | 0.43 | 0/3389 | 0.55 | 0/4595 |
| 2 | X3 | 0.33 | 0/3389 | 0.49 | 0/4595 |
| 2 | X5 | 0.36 | 0/3389 | 0.49 | 0/4595 |
| 2 | X7 | 0.34 | 0/3389 | 0.50 | 1/4595 (0.0%) |
| 2 | X9 | 0.37 | 0/3389 | 0.49 | 0/4595 |
| 2 | Y1 | 0.35 | 0/3389 | 0.49 | 1/4595 (0.0%) |
| 2 | Y3 | 0.35 | 0/3389 | 0.48 | 0/4595 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | Y5 | 0.35 | 0/3389 | 0.48 | 0/4595 |
| 2 | Y9 | 0.32 | 0/3389 | 0.47 | 0/4595 |
| 2 | Z1 | 0.31 | 0/3389 | 0.47 | 0/4595 |
| 2 | Z3 | 0.34 | 0/3389 | 0.48 | 0/4595 |
| 2 | Z5 | 0.36 | 0/3389 | 0.49 | 0/4595 |
| 2 | Z7 | 0.33 | 0/3389 | 0.47 | 0/4595 |
| 2 | Z9 | 0.32 | 0/3389 | 0.46 | 0/4595 |
| 3 | 3V | 0.39 | 0/2383 | 0.50 | 0/3226 |
| 3 | 3X | 0.38 | 0/2383 | 0.49 | 0/3226 |
| 3 | 3Z | 0.38 | 0/2383 | 0.49 | 0/3226 |
| 3 | 4B | 0.38 | 0/2383 | 0.49 | 0/3226 |
| 3 | 4D | 0.38 | 0/2383 | 0.49 | 0/3226 |
| 3 | 4F | 0.39 | 0/2383 | 0.49 | 0/3226 |
| 3 | 4H | 0.38 | 0/2383 | 0.49 | 0/3226 |
| 3 | 4J | 0.30 | 0/1682 | 0.47 | 0/2279 |
| 4 | 3W | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 3Y | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 4A | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 4C | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 4E | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 4G | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 4 | 4I | 0.41 | 0/1548 | 0.48 | 0/2090 |
| 5 | 4L | 0.34 | 0/1931 | 0.46 | 0/2570 |
| 5 | 4M | 0.35 | 0/2638 | 0.45 | 0/3512 |
| 6 | 4N | 0.30 | 0/424 | 0.46 | 0/567 |
| 6 | 4O | 0.32 | 0/4020 | 0.43 | 0/5336 |
| 6 | 4P | 0.35 | 0/1597 | 0.40 | 0/2126 |
| 7 | 4Q | 0.35 | 0/532 | 0.39 | 0/706 |
| 7 | 4R | 0.39 | 0/3021 | 0.47 | 0/4049 |
| 7 | 4S | 0.41 | 0/374 | 0.50 | 0/501 |
| 7 | 4T | 0.36 | 0/1592 | 0.43 | 0/2125 |
| 7 | 4U | 0.38 | 1/2314 (0.0%) | 0.47 | 1/3110 (0.0%) |
| 8 | 4V | 0.29 | 0/656 | 0.43 | 0/875 |
| 8 | 4W | 0.30 | 0/2757 | 0.43 | 0/3687 |
| 8 | 4X | 0.32 | 0/467 | 0.51 | 0/632 |
| 9 | 4Y | 0.31 | 0/1014 | 0.42 | 0/1357 |
| 9 | 4Z | 0.31 | 0/3176 | 0.47 | 0/4229 |
| 10 | 5A | 0.33 | 0/1912 | 0.46 | 0/2536 |
| 10 | 5B | 0.31 | 0/2081 | 0.44 | 0/2756 |
| 10 | 5C | 0.33 | 0/3120 | 0.43 | 0/4136 |
| 10 | 5D | 0.32 | 0/905 | 0.42 | 0/1198 |
| 11 | 5E | 0.34 | 0/2021 | 0.51 | 0/2754 |
| 12 | 5F | 0.38 | 0/3116 | 0.54 | 3/4267 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 12 | 5G | 0.35 | 0/1148 | 0.54 | 0/1564 |
| 12 | 7B | 0.37 | 0/775 | 0.55 | 0/1055 |
| 13 | 5H | 0.39 | 0/1098 | 0.54 | 0/1490 |
| 13 | 5I | 0.39 | 0/1098 | 0.54 | 0/1490 |
| 13 | 5J | 0.39 | 0/1098 | 0.54 | 0/1490 |
| 13 | 5K | 0.39 | 0/1098 | 0.54 | 0/1490 |
| 14 | 5L | 0.40 | 0/4851 | 0.57 | 0/6582 |
| 14 | 5M | 0.40 | 0/4851 | 0.57 | 1/6582 (0.0%) |
| 14 | 5N | 0.40 | 0/4851 | 0.59 | 1/6582 (0.0%) |
| 15 | 5O | 0.43 | 0/2991 | 0.62 | 0/4048 |
| 15 | 5P | 0.38 | 0/2991 | 0.53 | 0/4048 |
| 16 | 5Q | 0.38 | 0/1564 | 0.49 | 0/2126 |
| 17 | 5R | 0.30 | 0/168 | 0.44 | 0/226 |
| 17 | 5S | 0.38 | 0/1612 | 0.58 | 0/2177 |
| 17 | 5T | 0.40 | 0/1603 | 0.56 | 0/2165 |
| 17 | 5U | 0.37 | 0/1612 | 0.57 | 0/2177 |
| 17 | 5V | 0.38 | 0/893 | 0.49 | 0/1198 |
| 18 | 5X | 0.40 | 0/1835 | 0.51 | 0/2488 |
| 18 | 5Y | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 18 | 5Z | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 18 | 6A | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 18 | 6B | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 18 | 6C | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 18 | 6D | 0.40 | 0/1835 | 0.50 | 0/2488 |
| 19 | 6E | 0.42 | 0/1991 | 0.57 | 1/2713 (0.0%) |
| 20 | 6F | 0.44 | 0/3010 | 0.54 | 0/4102 |
| 21 | 6G | 0.34 | 0/1450 | 0.51 | 0/1970 |
| 21 | 6H | 0.31 | 0/1527 | 0.49 | 0/2078 |
| 22 | 6I | 0.31 | 0/2678 | 0.46 | 0/3618 |
| 22 | 6J | 0.34 | 0/2678 | 0.45 | 0/3618 |
| 22 | 6K | 0.34 | 0/2678 | 0.46 | 0/3618 |
| 22 | 6L | 0.37 | 0/2678 | 0.45 | 0/3618 |
| 22 | 6M | 0.34 | 0/2678 | 0.45 | 0/3618 |
| 22 | 6N | 0.33 | 0/2678 | 0.45 | 0/3618 |
| 22 | 6O | 0.35 | 0/2678 | 0.46 | 0/3618 |
| 22 | 6P | 0.31 | 0/2416 | 0.47 | 0/3256 |
| 23 | 6Q | 0.42 | 0/710 | 0.55 | 0/957 |
| 23 | 6R | 0.46 | 0/710 | 0.58 | 0/957 |
| 23 | 6S | 0.44 | 0/710 | 0.55 | 0/957 |
| 24 | 6T | 0.36 | 0/4696 | 0.49 | 0/6341 |
| 24 | 6U | 0.39 | 0/4730 | 0.49 | 0/6389 |
| 24 | 6V | 0.38 | 0/4675 | 0.51 | 0/6312 |
| 24 | 6W | 0.40 | 0/4712 | 0.48 | 0/6363 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 24 | 6X | 0.42 | 0/4737 | 0.53 | 0/6396 |
| 24 | 6Y | 0.38 | 0/4685 | 0.50 | 0/6325 |
| 24 | 6Z | 0.38 | 0/4691 | 0.49 | 0/6334 |
| 24 | 7A | 0.37 | 0/1557 | 0.47 | 0/2105 |
| 25 | 7C | 0.37 | 0/802 | 0.50 | 0/1074 |
| 26 | 7D | 0.40 | 0/1045 | 0.60 | 1/1416 (0.1%) |
| 26 | 7E | 0.39 | 0/1045 | 0.58 | 0/1416 |
| 26 | 7F | 0.45 | 0/1045 | 0.55 | 0/1416 |
| 27 | 7G | 0.37 | 0/1771 | 0.48 | 0/2406 |
| 28 | 7H | 0.37 | 0/1066 | 0.53 | 0/1444 |
| 28 | 7X | 0.36 | 0/1066 | 0.53 | 0/1444 |
| 29 | 7I | 0.35 | 0/1752 | 0.48 | 0/2377 |
| 29 | 7J | 0.38 | 0/2803 | 0.49 | 0/3802 |
| 30 | 7K | 0.34 | 0/3351 | 0.48 | 0/4541 |
| 30 | 7L | 0.32 | 0/1358 | 0.46 | 0/1836 |
| 31 | 7M | 0.34 | 0/678 | 0.56 | 1/921 (0.1%) |
| 31 | 7N | 0.35 | 0/1000 | 0.59 | 1/1359 (0.1%) |
| 32 | 7O | 0.33 | 0/448 | 0.53 | 0/603 |
| 32 | 7P | 0.36 | 0/1428 | 0.49 | 0/1939 |
| 33 | 7Q | 0.37 | 0/578 | 0.50 | 0/783 |
| 34 | 7R | 0.28 | 0/1629 | 0.42 | 0/2171 |
| 34 | 7S | 0.27 | 0/1357 | 0.41 | 0/1808 |
| 35 | 7T | 0.29 | 0/1748 | 0.41 | 0/2324 |
| 35 | 7U | 0.29 | 0/1486 | 0.40 | 0/1977 |
| 36 | 7V | 0.33 | 0/745 | 0.54 | 0/999 |
| 36 | 7W | 0.32 | 0/745 | 0.54 | 0/999 |
| 37 | 7Y | 0.39 | 0/2025 | 0.56 | 0/2749 |
| 38 | 7Z | 0.38 | 0/301 | 0.55 | 0/401 |
| 38 | 8A | 0.40 | 0/1729 | 0.55 | 0/2316 |
| 38 | 8B | 0.39 | 0/1766 | 0.51 | 0/2366 |
| 38 | 8C | 0.40 | 0/1766 | 0.54 | 0/2366 |
| 38 | 8D | 0.42 | 0/1342 | 0.57 | 0/1799 |
| All | All | 0.38 | 3/1377068 (0.0%) | 0.48 | 37/1864119 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | T6 | 60 | VAL | CB-CG1 | 5.93 | 1.65 | 1.52 |
| 7 | 4U | 113 | PRO | N-CD | 5.70 | 1.55 | 1.47 |
| 1 | O8 | 281 | TYR | CD2-CE2 | -5.05 | 1.31 | 1.39 |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D1 | 357 | TYR | C-N-CA | -5.94 | 106.85 | 121.70 |
| 31 | 7N | 78 | HIS | CB-CA-C | 5.91 | 122.21 | 110.40 |
| 2 | B9 | 276 | ILE | CG1-CB-CG2 | -5.89 | 98.43 | 111.40 |
| 26 | 7D | 128 | GLY | N-CA-C | 5.88 | 127.80 | 113.10 |
| 2 | S1 | 283 | HIS | CB-CA-C | 5.79 | 121.98 | 110.40 |
| 2 | H5 | 87 | PHE | C-N-CA | -5.79 | 107.23 | 121.70 |
| 2 | P3 | 87 | PHE | C-N-CA | -5.78 | 107.25 | 121.70 |
| 2 | X7 | 87 | PHE | C-N-CA | -5.72 | 107.40 | 121.70 |
| 31 | 7M | 79 | PRO | N-CA-C | -5.66 | 97.39 | 112.10 |
| 1 | D2 | 263 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 2 | 0L | 87 | PHE | C-N-CA | -5.55 | 107.83 | 121.70 |
| 19 | 6E | 27 | GLU | N-CA-CB | 5.54 | 120.58 | 110.60 |
| 1 | 2S | 77 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 1 | 2A | 418 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 1 | 9 | 41 | ASP | CB-CG-OD1 | -5.49 | 113.36 | 118.30 |
| 1 | 1C | 418 | LEU | CA-CB-CG | 5.47 | 127.87 | 115.30 |
| 12 | 5F | 363 | MET | N-CA-CB | -5.45 | 100.80 | 110.60 |
| 1 | 3M | 391 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 1 | S6 | 263 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 2 | J5 | 87 | PHE | C-N-CA | -5.39 | 108.22 | 121.70 |
| 1 | N2 | 253 | LEU | N-CA-CB | 5.31 | 121.02 | 110.40 |
| 2 | S7 | 428 | LEU | CA-CB-CG | 5.27 | 127.42 | 115.30 |
| 1 | R2 | 27 | GLU | N-CA-CB | 5.26 | 120.07 | 110.60 |
| 2 | 2F | 87 | PHE | C-N-CA | -5.26 | 108.56 | 121.70 |
| 1 | Q0 | 253 | LEU | N-CA-CB | 5.24 | 120.88 | 110.40 |
| 7 | 4U | 12 | ASP | CB-CG-OD2 | 5.24 | 123.01 | 118.30 |
| 14 | 5N | 224 | GLU | C-N-CA | 5.20 | 134.70 | 121.70 |
| 12 | 5F | 229 | ASP | CB-CG-OD2 | 5.18 | 122.97 | 118.30 |
| 2 | J5 | 46 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 12 | 5F | 362 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 2 | Y1 | 357 | TYR | C-N-CA | -5.15 | 108.83 | 121.70 |
| 2 | 2D | 428 | LEU | CA-CB-CG | 5.14 | 127.13 | 115.30 |
| 2 | 2X | 87 | PHE | C-N-CA | -5.12 | 108.91 | 121.70 |
| 14 | 5M | 224 | GLU | CB-CA-C | 5.10 | 120.60 | 110.40 |
| 2 | S1 | 280 | LYS | N-CA-CB | 5.07 | 119.73 | 110.60 |
| 2 | 2 | 282 | TYR | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 1 | F6 | 253 | LEU | N-CA-CB | 5.01 | 120.42 | 110.40 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 0A | 3346 | 0 | 3238 | 108 | 0 |
| 1 | 0C | 3346 | 0 | 3238 | 102 | 0 |
| 1 | 0E | 3346 | 0 | 3240 | 136 | 0 |
| 1 | 0G | 3346 | 0 | 3240 | 126 | 0 |
| 1 | 0I | 3346 | 0 | 3238 | 117 | 0 |
| 1 | 0K | 3346 | 0 | 3238 | 128 | 0 |
| 1 | 0M | 3346 | 0 | 3238 | 120 | 0 |
| 1 | 0O | 3346 | 0 | 3238 | 138 | 0 |
| 1 | 0Q | 3346 | 0 | 3238 | 110 | 0 |
| 1 | 0S | 3346 | 0 | 3238 | 125 | 0 |
| 1 | 0U | 3346 | 0 | 3240 | 113 | 0 |
| 1 | 0W | 3346 | 0 | 3240 | 113 | 0 |
| 1 | 0Y | 3346 | 0 | 3238 | 97 | 0 |
| 1 | 1 | 1120 | 0 | 1071 | 15 | 0 |
| 1 | 1A | 3346 | 0 | 3238 | 90 | 0 |
| 1 | 1C | 3346 | 0 | 3238 | 106 | 0 |
| 1 | 1E | 3346 | 0 | 3240 | 112 | 0 |
| 1 | 1G | 3346 | 0 | 3238 | 106 | 0 |
| 1 | 1K | 3346 | 0 | 3240 | 99 | 0 |
| 1 | 1M | 3346 | 0 | 3240 | 97 | 0 |
| 1 | 1O | 3346 | 0 | 3240 | 94 | 0 |
| 1 | 1Q | 3346 | 0 | 3239 | 100 | 0 |
| 1 | 1S | 3346 | 0 | 3238 | 83 | 0 |
| 1 | 1U | 3346 | 0 | 3240 | 103 | 0 |
| 1 | 1W | 3346 | 0 | 3238 | 92 | 0 |
| 1 | 2A | 3346 | 0 | 3238 | 108 | 0 |
| 1 | 2C | 3346 | 0 | 3238 | 97 | 0 |
| 1 | 2E | 3346 | 0 | 3238 | 103 | 0 |
| 1 | 2G | 3346 | 0 | 3238 | 77 | 0 |
| 1 | 2I | 3346 | 0 | 3238 | 108 | 0 |
| 1 | 2K | 3346 | 0 | 3238 | 76 | 0 |
| 1 | 2M | 3346 | 0 | 3240 | 109 | 0 |
| 1 | 2Q | 3346 | 0 | 3236 | 157 | 0 |
| 1 | 2S | 3346 | 0 | 3238 | 86 | 0 |
| 1 | 2U | 3346 | 0 | 3238 | 99 | 0 |
| 1 | 2W | 3346 | 0 | 3239 | 76 | 0 |
| 1 | 2Y | 3346 | 0 | 3238 | 121 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 3 | 3397 | 0 | 3275 | 22 | 0 |
| 1 | 3A | 3346 | 0 | 3238 | 113 | 0 |
| 1 | 3C | 3346 | 0 | 3238 | 143 | 0 |
| 1 | 3G | 3346 | 0 | 3238 | 92 | 0 |
| 1 | 3I | 3346 | 0 | 3239 | 95 | 0 |
| 1 | 3K | 3346 | 0 | 3239 | 114 | 0 |
| 1 | 3M | 3346 | 0 | 3239 | 106 | 0 |
| 1 | 3O | 3346 | 0 | 3239 | 103 | 0 |
| 1 | 3Q | 3346 | 0 | 3240 | 106 | 0 |
| 1 | 3S | 3346 | 0 | 3239 | 148 | 0 |
| 1 | 5 | 3421 | 0 | 3295 | 32 | 0 |
| 1 | 7 | 3430 | 0 | 3299 | 17 | 0 |
| 1 | 9 | 3421 | 0 | 3295 | 32 | 0 |
| 1 | A1 | 3388 | 0 | 3268 | 14 | 0 |
| 1 | A3 | 3410 | 0 | 3286 | 65 | 0 |
| 1 | A5 | 3370 | 0 | 3259 | 11 | 0 |
| 1 | A7 | 3346 | 0 | 3240 | 14 | 0 |
| 1 | A9 | 3346 | 0 | 3238 | 9 | 0 |
| 1 | B1 | 3346 | 0 | 3240 | 12 | 0 |
| 1 | B3 | 3346 | 0 | 3240 | 9 | 0 |
| 1 | B5 | 3346 | 0 | 3238 | 12 | 0 |
| 1 | B8 | 3346 | 0 | 3240 | 19 | 0 |
| 1 | C0 | 3346 | 0 | 3238 | 4 | 0 |
| 1 | C2 | 3346 | 0 | 3240 | 9 | 0 |
| 1 | C4 | 3346 | 0 | 3240 | 6 | 0 |
| 1 | C6 | 3346 | 0 | 3240 | 7 | 0 |
| 1 | C8 | 3346 | 0 | 3239 | 6 | 0 |
| 1 | D0 | 3346 | 0 | 3240 | 8 | 0 |
| 1 | D2 | 3346 | 0 | 3240 | 6 | 0 |
| 1 | D4 | 3346 | 0 | 3240 | 12 | 0 |
| 1 | D6 | 3346 | 0 | 3240 | 10 | 0 |
| 1 | D8 | 3346 | 0 | 3240 | 3 | 0 |
| 1 | E0 | 3346 | 0 | 3240 | 11 | 0 |
| 1 | E2 | 3346 | 0 | 3240 | 16 | 0 |
| 1 | E4 | 3346 | 0 | 3238 | 9 | 0 |
| 1 | E6 | 3346 | 0 | 3238 | 22 | 0 |
| 1 | E8 | 3346 | 0 | 3239 | 12 | 0 |
| 1 | F0 | 3346 | 0 | 3238 | 6 | 0 |
| 1 | F2 | 3346 | 0 | 3240 | 10 | 0 |
| 1 | F6 | 3346 | 0 | 3240 | 12 | 0 |
| 1 | F8 | 3346 | 0 | 3238 | 11 | 0 |
| 1 | G0 | 3346 | 0 | 3238 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | G2 | 3346 | 0 | 3240 | 123 | 0 |
| 1 | G4 | 3346 | 0 | 3238 | 96 | 0 |
| 1 | G6 | 3346 | 0 | 3240 | 127 | 0 |
| 1 | G8 | 3346 | 0 | 3240 | 118 | 0 |
| 1 | H2 | 3346 | 0 | 3238 | 98 | 0 |
| 1 | H4 | 3346 | 0 | 3240 | 98 | 0 |
| 1 | H6 | 3346 | 0 | 3238 | 99 | 0 |
| 1 | H8 | 3346 | 0 | 3238 | 73 | 0 |
| 1 | I0 | 3346 | 0 | 3238 | 98 | 0 |
| 1 | I2 | 3346 | 0 | 3240 | 106 | 0 |
| 1 | I4 | 3346 | 0 | 3237 | 126 | 0 |
| 1 | I8 | 3346 | 0 | 3238 | 97 | 0 |
| 1 | J0 | 3346 | 0 | 3238 | 89 | 0 |
| 1 | J2 | 3346 | 0 | 3238 | 82 | 0 |
| 1 | J4 | 3346 | 0 | 3238 | 79 | 0 |
| 1 | J6 | 3346 | 0 | 3239 | 82 | 0 |
| 1 | J8 | 3346 | 0 | 3239 | 70 | 0 |
| 1 | K0 | 3346 | 0 | 3238 | 76 | 0 |
| 1 | K4 | 3346 | 0 | 3239 | 83 | 0 |
| 1 | K6 | 3346 | 0 | 3239 | 71 | 0 |
| 1 | K8 | 3346 | 0 | 3240 | 83 | 0 |
| 1 | L0 | 3346 | 0 | 3240 | 76 | 0 |
| 1 | L2 | 3346 | 0 | 3238 | 82 | 0 |
| 1 | L4 | 3346 | 0 | 3239 | 100 | 0 |
| 1 | L6 | 3346 | 0 | 3238 | 110 | 0 |
| 1 | M0 | 3346 | 0 | 3239 | 86 | 0 |
| 1 | M2 | 3346 | 0 | 3238 | 84 | 0 |
| 1 | M4 | 3346 | 0 | 3238 | 85 | 0 |
| 1 | M6 | 3346 | 0 | 3238 | 119 | 0 |
| 1 | M8 | 3346 | 0 | 3240 | 81 | 0 |
| 1 | N0 | 3346 | 0 | 3238 | 85 | 0 |
| 1 | N2 | 3346 | 0 | 3240 | 104 | 0 |
| 1 | N6 | 3346 | 0 | 3239 | 85 | 0 |
| 1 | N8 | 3346 | 0 | 3239 | 86 | 0 |
| 1 | O0 | 3346 | 0 | 3238 | 73 | 0 |
| 1 | O2 | 3346 | 0 | 3239 | 97 | 0 |
| 1 | O4 | 3346 | 0 | 3237 | 101 | 0 |
| 1 | O6 | 3346 | 0 | 3239 | 76 | 0 |
| 1 | O8 | 3346 | 0 | 3239 | 75 | 0 |
| 1 | P4 | 3346 | 0 | 3238 | 103 | 0 |
| 1 | P6 | 3346 | 0 | 3238 | 69 | 0 |
| 1 | P8 | 3346 | 0 | 3239 | 80 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | Q0 | 3346 | 0 | 3240 | 73 | 0 |
| 1 | Q2 | 3346 | 0 | 3238 | 86 | 0 |
| 1 | Q4 | 3346 | 0 | 3238 | 85 | 0 |
| 1 | Q6 | 3346 | 0 | 3239 | 77 | 0 |
| 1 | Q8 | 3293 | 0 | 3182 | 122 | 0 |
| 1 | R0 | 3401 | 0 | 3278 | 89 | 0 |
| 1 | R2 | 3346 | 0 | 3238 | 97 | 0 |
| 1 | R4 | 3370 | 0 | 3257 | 102 | 0 |
| 1 | R6 | 3346 | 0 | 3238 | 91 | 0 |
| 1 | R8 | 3379 | 0 | 3264 | 89 | 0 |
| 1 | S0 | 3346 | 0 | 3239 | 100 | 0 |
| 1 | S2 | 3379 | 0 | 3263 | 96 | 0 |
| 1 | S4 | 3354 | 0 | 3244 | 144 | 0 |
| 1 | S6 | 3346 | 0 | 3240 | 101 | 0 |
| 1 | S8 | 3346 | 0 | 3239 | 116 | 0 |
| 1 | T0 | 3346 | 0 | 3240 | 107 | 0 |
| 1 | T2 | 3346 | 0 | 3239 | 122 | 0 |
| 1 | T4 | 3346 | 0 | 3238 | 109 | 0 |
| 1 | T6 | 3346 | 0 | 3239 | 157 | 0 |
| 1 | T8 | 3346 | 0 | 3239 | 99 | 0 |
| 1 | U2 | 3346 | 0 | 3239 | 87 | 0 |
| 1 | U4 | 3346 | 0 | 3238 | 83 | 0 |
| 1 | U6 | 3346 | 0 | 3238 | 99 | 0 |
| 1 | U8 | 3370 | 0 | 3259 | 89 | 0 |
| 1 | V0 | 3346 | 0 | 3240 | 80 | 0 |
| 1 | V2 | 3346 | 0 | 3238 | 92 | 0 |
| 1 | V4 | 3346 | 0 | 3240 | 79 | 0 |
| 1 | V6 | 3346 | 0 | 3240 | 135 | 0 |
| 1 | V8 | 3346 | 0 | 3238 | 93 | 0 |
| 1 | W0 | 3346 | 0 | 3238 | 85 | 0 |
| 1 | W2 | 3346 | 0 | 3238 | 83 | 0 |
| 1 | W4 | 3346 | 0 | 3238 | 93 | 0 |
| 1 | W6 | 3346 | 0 | 3240 | 82 | 0 |
| 1 | W8 | 3346 | 0 | 3238 | 86 | 0 |
| 1 | X0 | 3346 | 0 | 3238 | 120 | 0 |
| 1 | X2 | 3346 | 0 | 3240 | 124 | 0 |
| 1 | X4 | 3346 | 0 | 3238 | 110 | 0 |
| 1 | X6 | 3346 | 0 | 3238 | 105 | 0 |
| 1 | X8 | 3346 | 0 | 3240 | 90 | 0 |
| 1 | Y0 | 3346 | 0 | 3239 | 101 | 0 |
| 1 | Y2 | 3346 | 0 | 3240 | 79 | 0 |
| 1 | Y4 | 3346 | 0 | 3239 | 92 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | Y6 | 3346 | 0 | 3239 | 74 | 0 |
| 1 | Y8 | 3346 | 0 | 3240 | 130 | 0 |
| 1 | Z0 | 3346 | 0 | 3238 | 135 | 0 |
| 1 | Z2 | 3346 | 0 | 3239 | 131 | 0 |
| 1 | Z4 | 3346 | 0 | 3240 | 110 | 0 |
| 1 | Z6 | 3346 | 0 | 3238 | 116 | 0 |
| 1 | Z8 | 3346 | 0 | 3240 | 142 | 0 |
| 2 | 0B | 3318 | 0 | 3259 | 112 | 0 |
| 2 | 0F | 3318 | 0 | 3259 | 123 | 0 |
| 2 | 0H | 3318 | 0 | 3259 | 118 | 0 |
| 2 | 0J | 3318 | 0 | 3259 | 122 | 0 |
| 2 | 0L | 3318 | 0 | 3259 | 129 | 0 |
| 2 | 0N | 3318 | 0 | 3259 | 138 | 0 |
| 2 | 0P | 3318 | 0 | 3259 | 101 | 0 |
| 2 | 0R | 3318 | 0 | 3259 | 125 | 0 |
| 2 | 0V | 3318 | 0 | 3259 | 122 | 0 |
| 2 | 0X | 3318 | 0 | 3259 | 116 | 0 |
| 2 | 0Z | 3318 | 0 | 3259 | 124 | 0 |
| 2 | 1B | 3318 | 0 | 3259 | 96 | 0 |
| 2 | 1D | 3318 | 0 | 3259 | 123 | 0 |
| 2 | 1F | 3318 | 0 | 3259 | 125 | 0 |
| 2 | 1H | 3318 | 0 | 3259 | 123 | 0 |
| 2 | 1L | 3318 | 0 | 3259 | 101 | 0 |
| 2 | 1N | 3318 | 0 | 3259 | 116 | 0 |
| 2 | 1P | 3318 | 0 | 3259 | 93 | 0 |
| 2 | 1R | 3318 | 0 | 3259 | 111 | 0 |
| 2 | 1T | 3318 | 0 | 3259 | 95 | 0 |
| 2 | 1V | 3318 | 0 | 3259 | 114 | 0 |
| 2 | 1X | 3318 | 0 | 3259 | 110 | 0 |
| 2 | 1Z | 3318 | 0 | 3259 | 118 | 0 |
| 2 | 2 | 3376 | 0 | 3313 | 19 | 0 |
| 2 | 2B | 3318 | 0 | 3259 | 95 | 0 |
| 2 | 2D | 3318 | 0 | 3259 | 85 | 0 |
| 2 | 2F | 3318 | 0 | 3259 | 106 | 0 |
| 2 | 2H | 3318 | 0 | 3259 | 124 | 0 |
| 2 | 2J | 3318 | 0 | 3259 | 95 | 0 |
| 2 | 2L | 3318 | 0 | 3259 | 96 | 0 |
| 2 | 2N | 3318 | 0 | 3259 | 123 | 0 |
| 2 | 2P | 3318 | 0 | 3259 | 118 | 0 |
| 2 | 2R | 3318 | 0 | 3259 | 85 | 0 |
| 2 | 2T | 3318 | 0 | 3259 | 107 | 0 |
| 2 | 2V | 3318 | 0 | 3259 | 95 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | 2X | 3385 | 0 | 3319 | 112 | 0 |
| 2 | 2Z | 3318 | 0 | 3259 | 130 | 0 |
| 2 | 3B | 3383 | 0 | 3314 | 142 | 0 |
| 2 | 3D | 3318 | 0 | 3259 | 124 | 0 |
| 2 | 3F | 3318 | 0 | 3259 | 95 | 0 |
| 2 | 3H | 3318 | 0 | 3259 | 96 | 0 |
| 2 | 3J | 3318 | 0 | 3259 | 90 | 0 |
| 2 | 3L | 3318 | 0 | 3259 | 82 | 0 |
| 2 | 3N | 3318 | 0 | 3259 | 99 | 0 |
| 2 | 3P | 3318 | 0 | 3259 | 102 | 0 |
| 2 | 3R | 3385 | 0 | 3319 | 110 | 0 |
| 2 | 3T | 3318 | 0 | 3259 | 139 | 0 |
| 2 | 4 | 3376 | 0 | 3313 | 32 | 0 |
| 2 | 6 | 3376 | 0 | 3313 | 10 | 0 |
| 2 | 8 | 3376 | 0 | 3312 | 56 | 0 |
| 2 | A0 | 3376 | 0 | 3313 | 13 | 0 |
| 2 | A2 | 3376 | 0 | 3312 | 69 | 0 |
| 2 | A4 | 3376 | 0 | 3313 | 12 | 0 |
| 2 | A8 | 3318 | 0 | 3259 | 8 | 0 |
| 2 | B0 | 3318 | 0 | 3259 | 8 | 0 |
| 2 | B2 | 3318 | 0 | 3259 | 8 | 0 |
| 2 | B4 | 3318 | 0 | 3259 | 9 | 0 |
| 2 | B7 | 3318 | 0 | 3259 | 10 | 0 |
| 2 | B9 | 3318 | 0 | 3259 | 9 | 0 |
| 2 | C1 | 3318 | 0 | 3259 | 7 | 0 |
| 2 | C5 | 3376 | 0 | 3313 | 14 | 0 |
| 2 | C7 | 3376 | 0 | 3313 | 4 | 0 |
| 2 | C9 | 3318 | 0 | 3259 | 8 | 0 |
| 2 | D1 | 3318 | 0 | 3259 | 6 | 0 |
| 2 | D3 | 3324 | 0 | 3264 | 4 | 0 |
| 2 | D5 | 3318 | 0 | 3259 | 9 | 0 |
| 2 | D7 | 3324 | 0 | 3264 | 10 | 0 |
| 2 | E1 | 3324 | 0 | 3264 | 9 | 0 |
| 2 | E3 | 3318 | 0 | 3259 | 7 | 0 |
| 2 | E5 | 3318 | 0 | 3259 | 31 | 0 |
| 2 | E7 | 3324 | 0 | 3264 | 26 | 0 |
| 2 | E9 | 3318 | 0 | 3259 | 17 | 0 |
| 2 | F1 | 3318 | 0 | 3259 | 11 | 0 |
| 2 | F3 | 3318 | 0 | 3259 | 11 | 0 |
| 2 | F5 | 3318 | 0 | 3259 | 11 | 0 |
| 2 | F7 | 3318 | 0 | 3259 | 12 | 0 |
| 2 | F9 | 3376 | 0 | 3313 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | G1 | 3376 | 0 | 3313 | 71 | 0 |
| 2 | G3 | 3376 | 0 | 3313 | 133 | 0 |
| 2 | G5 | 3318 | 0 | 3259 | 107 | 0 |
| 2 | G7 | 3318 | 0 | 3259 | 116 | 0 |
| 2 | G9 | 3318 | 0 | 3259 | 149 | 0 |
| 2 | H1 | 3318 | 0 | 3259 | 117 | 0 |
| 2 | H3 | 3318 | 0 | 3259 | 107 | 0 |
| 2 | H5 | 3318 | 0 | 3259 | 86 | 0 |
| 2 | H7 | 3318 | 0 | 3259 | 85 | 0 |
| 2 | H9 | 3318 | 0 | 3259 | 83 | 0 |
| 2 | I1 | 3318 | 0 | 3259 | 104 | 0 |
| 2 | I3 | 3318 | 0 | 3259 | 96 | 0 |
| 2 | I5 | 3318 | 0 | 3259 | 135 | 0 |
| 2 | I7 | 3332 | 0 | 3268 | 106 | 0 |
| 2 | I9 | 3324 | 0 | 3264 | 110 | 0 |
| 2 | J1 | 3318 | 0 | 3259 | 108 | 0 |
| 2 | J3 | 3326 | 0 | 3263 | 103 | 0 |
| 2 | J5 | 3385 | 0 | 3319 | 101 | 0 |
| 2 | J7 | 3318 | 0 | 3259 | 128 | 0 |
| 2 | J9 | 3385 | 0 | 3319 | 127 | 0 |
| 2 | K1 | 3318 | 0 | 3259 | 135 | 0 |
| 2 | K3 | 3318 | 0 | 3259 | 106 | 0 |
| 2 | K5 | 3318 | 0 | 3259 | 85 | 0 |
| 2 | K7 | 3318 | 0 | 3259 | 86 | 0 |
| 2 | K9 | 3318 | 0 | 3259 | 89 | 0 |
| 2 | L1 | 3318 | 0 | 3259 | 72 | 0 |
| 2 | L3 | 3318 | 0 | 3259 | 115 | 0 |
| 2 | L5 | 3318 | 0 | 3259 | 99 | 0 |
| 2 | L7 | 3318 | 0 | 3259 | 124 | 0 |
| 2 | L9 | 3318 | 0 | 3259 | 82 | 0 |
| 2 | M1 | 3318 | 0 | 3259 | 86 | 0 |
| 2 | M3 | 3376 | 0 | 3313 | 129 | 0 |
| 2 | M5 | 3318 | 0 | 3259 | 110 | 0 |
| 2 | M7 | 3376 | 0 | 3313 | 106 | 0 |
| 2 | M9 | 3385 | 0 | 3319 | 115 | 0 |
| 2 | N1 | 3324 | 0 | 3264 | 106 | 0 |
| 2 | N3 | 3318 | 0 | 3259 | 128 | 0 |
| 2 | N5 | 3318 | 0 | 3259 | 96 | 0 |
| 2 | N7 | 3318 | 0 | 3259 | 105 | 0 |
| 2 | N9 | 3318 | 0 | 3259 | 105 | 0 |
| 2 | O1 | 3318 | 0 | 3259 | 92 | 0 |
| 2 | O3 | 3318 | 0 | 3259 | 125 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | O5 | 3318 | 0 | 3259 | 108 | 0 |
| 2 | O7 | 3340 | 0 | 3274 | 122 | 0 |
| 2 | O9 | 3318 | 0 | 3259 | 78 | 0 |
| 2 | P3 | 3318 | 0 | 3259 | 95 | 0 |
| 2 | P5 | 3376 | 0 | 3313 | 112 | 0 |
| 2 | P7 | 3318 | 0 | 3259 | 82 | 0 |
| 2 | P9 | 3376 | 0 | 3313 | 92 | 0 |
| 2 | Q1 | 3318 | 0 | 3259 | 70 | 0 |
| 2 | Q3 | 3318 | 0 | 3259 | 96 | 0 |
| 2 | Q5 | 3318 | 0 | 3259 | 94 | 0 |
| 2 | Q9 | 3318 | 0 | 3259 | 111 | 0 |
| 2 | R1 | 3318 | 0 | 3259 | 95 | 0 |
| 2 | R3 | 3327 | 0 | 3265 | 83 | 0 |
| 2 | R5 | 3376 | 0 | 3313 | 100 | 0 |
| 2 | R7 | 3318 | 0 | 3259 | 81 | 0 |
| 2 | R9 | 3376 | 0 | 3313 | 102 | 0 |
| 2 | S1 | 3333 | 0 | 3270 | 98 | 0 |
| 2 | S5 | 3318 | 0 | 3259 | 86 | 0 |
| 2 | S7 | 3376 | 0 | 3313 | 105 | 0 |
| 2 | S9 | 3318 | 0 | 3259 | 110 | 0 |
| 2 | T1 | 3318 | 0 | 3259 | 107 | 0 |
| 2 | T3 | 3318 | 0 | 3259 | 94 | 0 |
| 2 | T5 | 3318 | 0 | 3259 | 100 | 0 |
| 2 | T7 | 3318 | 0 | 3259 | 98 | 0 |
| 2 | U1 | 3318 | 0 | 3259 | 83 | 0 |
| 2 | U3 | 3318 | 0 | 3259 | 72 | 0 |
| 2 | U5 | 3318 | 0 | 3259 | 89 | 0 |
| 2 | U7 | 3318 | 0 | 3259 | 83 | 0 |
| 2 | U9 | 3318 | 0 | 3259 | 113 | 0 |
| 2 | V1 | 3318 | 0 | 3259 | 101 | 0 |
| 2 | V3 | 3318 | 0 | 3259 | 94 | 0 |
| 2 | V7 | 3318 | 0 | 3259 | 102 | 0 |
| 2 | V9 | 3318 | 0 | 3259 | 85 | 0 |
| 2 | W1 | 3318 | 0 | 3259 | 98 | 0 |
| 2 | W3 | 3318 | 0 | 3259 | 80 | 0 |
| 2 | W5 | 3318 | 0 | 3259 | 76 | 0 |
| 2 | W7 | 3318 | 0 | 3259 | 118 | 0 |
| 2 | W9 | 3318 | 0 | 3259 | 150 | 0 |
| 2 | X3 | 3318 | 0 | 3259 | 124 | 0 |
| 2 | X5 | 3318 | 0 | 3259 | 115 | 0 |
| 2 | X7 | 3318 | 0 | 3259 | 121 | 0 |
| 2 | X9 | 3318 | 0 | 3259 | 98 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | Y1 | 3318 | 0 | 3259 | 95 | 0 |
| 2 | Y3 | 3318 | 0 | 3259 | 116 | 0 |
| 2 | Y5 | 3318 | 0 | 3259 | 102 | 0 |
| 2 | Y9 | 3318 | 0 | 3259 | 118 | 0 |
| 2 | Z1 | 3318 | 0 | 3259 | 105 | 0 |
| 2 | Z3 | 3318 | 0 | 3259 | 119 | 0 |
| 2 | Z5 | 3318 | 0 | 3259 | 128 | 0 |
| 2 | Z7 | 3318 | 0 | 3259 | 116 | 0 |
| 2 | Z9 | 3318 | 0 | 3259 | 108 | 0 |
| 3 | 3V | 2329 | 0 | 2356 | 83 | 0 |
| 3 | 3X | 2329 | 0 | 2356 | 90 | 0 |
| 3 | 3Z | 2329 | 0 | 2356 | 79 | 0 |
| 3 | 4B | 2329 | 0 | 2356 | 76 | 0 |
| 3 | 4D | 2329 | 0 | 2356 | 84 | 0 |
| 3 | 4F | 2329 | 0 | 2356 | 86 | 0 |
| 3 | 4H | 2329 | 0 | 2356 | 84 | 0 |
| 3 | 4J | 1643 | 0 | 1662 | 50 | 0 |
| 4 | 3W | 1515 | 0 | 1526 | 49 | 0 |
| 4 | 3Y | 1515 | 0 | 1526 | 46 | 0 |
| 4 | 4A | 1515 | 0 | 1526 | 43 | 0 |
| 4 | 4C | 1515 | 0 | 1526 | 47 | 0 |
| 4 | 4E | 1515 | 0 | 1526 | 42 | 0 |
| 4 | 4G | 1515 | 0 | 1526 | 51 | 0 |
| 4 | 4I | 1515 | 0 | 1526 | 43 | 0 |
| 5 | 4L | 1921 | 0 | 1936 | 75 | 0 |
| 5 | 4M | 2622 | 0 | 2653 | 110 | 0 |
| 6 | 4N | 422 | 0 | 422 | 13 | 0 |
| 6 | 4O | 3995 | 0 | 3956 | 111 | 0 |
| 6 | 4P | 1588 | 0 | 1574 | 37 | 0 |
| 7 | 4Q | 525 | 0 | 521 | 15 | 0 |
| 7 | 4R | 2982 | 0 | 2914 | 102 | 0 |
| 7 | 4S | 371 | 0 | 380 | 20 | 0 |
| 7 | 4T | 1574 | 0 | 1556 | 42 | 0 |
| 7 | 4U | 2285 | 0 | 2221 | 66 | 0 |
| 8 | 4V | 653 | 0 | 667 | 19 | 0 |
| 8 | 4W | 2750 | 0 | 2805 | 116 | 0 |
| 8 | 4X | 462 | 0 | 459 | 48 | 0 |
| 9 | 4Y | 1004 | 0 | 1032 | 28 | 0 |
| 9 | 4Z | 3158 | 0 | 3201 | 130 | 0 |
| 10 | 5A | 1902 | 0 | 1930 | 65 | 0 |
| 10 | 5B | 2074 | 0 | 2132 | 82 | 0 |
| 10 | 5C | 3103 | 0 | 3156 | 110 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 10 | 5D | 901 | 0 | 914 | 26 | 0 |
| 11 | 5E | 1981 | 0 | 1969 | 58 | 0 |
| 12 | 5F | 3020 | 0 | 2948 | 105 | 0 |
| 12 | 5G | 1123 | 0 | 1132 | 34 | 0 |
| 12 | 7B | 753 | 0 | 735 | 41 | 0 |
| 13 | 5H | 1069 | 0 | 1048 | 45 | 0 |
| 13 | 5I | 1069 | 0 | 1048 | 49 | 0 |
| 13 | 5J | 1069 | 0 | 1048 | 44 | 0 |
| 13 | 5K | 1069 | 0 | 1048 | 50 | 0 |
| 14 | 5L | 4757 | 0 | 4692 | 251 | 0 |
| 14 | 5M | 4757 | 0 | 4691 | 242 | 0 |
| 14 | 5N | 4757 | 0 | 4692 | 244 | 0 |
| 15 | 5O | 2927 | 0 | 2895 | 247 | 0 |
| 15 | 5P | 2927 | 0 | 2895 | 188 | 0 |
| 16 | 5Q | 1523 | 0 | 1453 | 78 | 0 |
| 17 | 5R | 162 | 0 | 149 | 8 | 0 |
| 17 | 5S | 1572 | 0 | 1577 | 63 | 0 |
| 17 | 5T | 1563 | 0 | 1571 | 66 | 0 |
| 17 | 5U | 1572 | 0 | 1577 | 62 | 0 |
| 17 | 5V | 879 | 0 | 901 | 39 | 0 |
| 18 | 5X | 1793 | 0 | 1800 | 78 | 0 |
| 18 | 5Y | 1793 | 0 | 1800 | 72 | 0 |
| 18 | 5Z | 1793 | 0 | 1800 | 66 | 0 |
| 18 | 6A | 1793 | 0 | 1800 | 74 | 0 |
| 18 | 6B | 1793 | 0 | 1800 | 72 | 0 |
| 18 | 6C | 1793 | 0 | 1800 | 75 | 0 |
| 18 | 6D | 1793 | 0 | 1800 | 66 | 0 |
| 19 | 6E | 1952 | 0 | 1910 | 117 | 0 |
| 20 | 6F | 2950 | 0 | 2946 | 111 | 0 |
| 21 | 6G | 1420 | 0 | 1394 | 35 | 0 |
| 21 | 6H | 1493 | 0 | 1466 | 64 | 0 |
| 22 | 6I | 2617 | 0 | 2556 | 66 | 0 |
| 22 | 6J | 2617 | 0 | 2556 | 70 | 0 |
| 22 | 6K | 2617 | 0 | 2556 | 80 | 0 |
| 22 | 6L | 2617 | 0 | 2556 | 98 | 0 |
| 22 | 6M | 2617 | 0 | 2556 | 81 | 0 |
| 22 | 6N | 2617 | 0 | 2556 | 79 | 0 |
| 22 | 6O | 2617 | 0 | 2556 | 78 | 0 |
| 22 | 6P | 2366 | 0 | 2311 | 84 | 0 |
| 23 | 6Q | 694 | 0 | 690 | 30 | 0 |
| 23 | 6R | 694 | 0 | 690 | 41 | 0 |
| 23 | 6S | 694 | 0 | 690 | 27 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 24 | 6T | 4590 | 0 | 4521 | 203 | 0 |
| 24 | 6U | 4623 | 0 | 4558 | 209 | 0 |
| 24 | 6V | 4569 | 0 | 4501 | 195 | 0 |
| 24 | 6W | 4606 | 0 | 4538 | 187 | 0 |
| 24 | 6X | 4631 | 0 | 4566 | 291 | 0 |
| 24 | 6Y | 4579 | 0 | 4515 | 206 | 0 |
| 24 | 6Z | 4585 | 0 | 4516 | 200 | 0 |
| 24 | 7A | 1518 | 0 | 1462 | 61 | 0 |
| 25 | 7C | 794 | 0 | 816 | 30 | 0 |
| 26 | 7D | 1016 | 0 | 993 | 80 | 0 |
| 26 | 7E | 1016 | 0 | 993 | 82 | 0 |
| 26 | 7F | 1016 | 0 | 994 | 133 | 0 |
| 27 | 7G | 1728 | 0 | 1670 | 91 | 0 |
| 28 | 7H | 1046 | 0 | 1046 | 53 | 0 |
| 28 | 7X | 1046 | 0 | 1046 | 64 | 0 |
| 29 | 7I | 1716 | 0 | 1685 | 72 | 0 |
| 29 | 7J | 2741 | 0 | 2638 | 165 | 0 |
| 30 | 7K | 3276 | 0 | 3173 | 165 | 0 |
| 30 | 7L | 1333 | 0 | 1289 | 36 | 0 |
| 31 | 7M | 662 | 0 | 657 | 40 | 0 |
| 31 | 7N | 977 | 0 | 965 | 54 | 0 |
| 32 | 7O | 443 | 0 | 425 | 22 | 0 |
| 32 | 7P | 1398 | 0 | 1368 | 40 | 0 |
| 33 | 7Q | 567 | 0 | 551 | 27 | 0 |
| 34 | 7R | 1619 | 0 | 1650 | 45 | 0 |
| 34 | 7S | 1347 | 0 | 1357 | 33 | 0 |
| 35 | 7T | 1738 | 0 | 1787 | 53 | 0 |
| 35 | 7U | 1476 | 0 | 1506 | 34 | 0 |
| 36 | 7V | 735 | 0 | 696 | 33 | 0 |
| 36 | 7W | 735 | 0 | 696 | 42 | 0 |
| 37 | 7Y | 1971 | 0 | 1898 | 143 | 0 |
| 38 | 7Z | 298 | 0 | 291 | 35 | 0 |
| 38 | 8A | 1691 | 0 | 1638 | 195 | 0 |
| 38 | 8B | 1728 | 0 | 1666 | 168 | 0 |
| 38 | 8C | 1728 | 0 | 1666 | 193 | 0 |
| 38 | 8D | 1311 | 0 | 1252 | 139 | 0 |
| 39 | 0A | 28 | 0 | 12 | 1 | 0 |
| 39 | 0C | 28 | 0 | 12 | 2 | 0 |
| 39 | 0E | 28 | 0 | 12 | 3 | 0 |
| 39 | 0G | 28 | 0 | 12 | 2 | 0 |
| 39 | 0I | 28 | 0 | 12 | 1 | 0 |
| 39 | 0K | 28 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | 0M | 28 | 0 | 12 | 1 | 0 |
| 39 | 0O | 28 | 0 | 12 | 1 | 0 |
| 39 | 0Q | 28 | 0 | 12 | 1 | 0 |
| 39 | 0S | 28 | 0 | 12 | 2 | 0 |
| 39 | 0U | 28 | 0 | 12 | 1 | 0 |
| 39 | 0W | 28 | 0 | 12 | 2 | 0 |
| 39 | 0Y | 28 | 0 | 12 | 1 | 0 |
| 39 | 1A | 28 | 0 | 12 | 2 | 0 |
| 39 | 1C | 28 | 0 | 12 | 1 | 0 |
| 39 | 1E | 28 | 0 | 12 | 0 | 0 |
| 39 | 1G | 28 | 0 | 12 | 0 | 0 |
| 39 | 1K | 28 | 0 | 12 | 1 | 0 |
| 39 | 1M | 28 | 0 | 12 | 1 | 0 |
| 39 | 1O | 28 | 0 | 12 | 1 | 0 |
| 39 | 1Q | 28 | 0 | 12 | 1 | 0 |
| 39 | 1S | 28 | 0 | 12 | 1 | 0 |
| 39 | 1U | 28 | 0 | 12 | 0 | 0 |
| 39 | 1W | 28 | 0 | 12 | 2 | 0 |
| 39 | 2 | 28 | 0 | 12 | 0 | 0 |
| 39 | 2A | 28 | 0 | 12 | 0 | 0 |
| 39 | 2C | 28 | 0 | 12 | 1 | 0 |
| 39 | 2E | 28 | 0 | 12 | 1 | 0 |
| 39 | 2G | 28 | 0 | 12 | 3 | 0 |
| 39 | 2I | 28 | 0 | 12 | 0 | 0 |
| 39 | 2K | 28 | 0 | 12 | 2 | 0 |
| 39 | 2M | 28 | 0 | 12 | 2 | 0 |
| 39 | 2Q | 28 | 0 | 12 | 0 | 0 |
| 39 | 2S | 28 | 0 | 12 | 0 | 0 |
| 39 | 2U | 28 | 0 | 12 | 0 | 0 |
| 39 | 2W | 28 | 0 | 12 | 0 | 0 |
| 39 | 2Y | 28 | 0 | 12 | 0 | 0 |
| 39 | 3 | 28 | 0 | 12 | 2 | 0 |
| 39 | 3A | 28 | 0 | 12 | 1 | 0 |
| 39 | 3C | 28 | 0 | 12 | 1 | 0 |
| 39 | 3G | 28 | 0 | 12 | 0 | 0 |
| 39 | 3I | 28 | 0 | 12 | 1 | 0 |
| 39 | 3K | 28 | 0 | 12 | 1 | 0 |
| 39 | 3M | 28 | 0 | 12 | 0 | 0 |
| 39 | 3O | 28 | 0 | 12 | 1 | 0 |
| 39 | 3Q | 28 | 0 | 12 | 1 | 0 |
| 39 | 3S | 28 | 0 | 12 | 1 | 0 |
| 39 | 5 | 28 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | 7 | 28 | 0 | 12 | 3 | 0 |
| 39 | 9 | 28 | 0 | 12 | 1 | 0 |
| 39 | A1 | 28 | 0 | 12 | 0 | 0 |
| 39 | A3 | 28 | 0 | 12 | 0 | 0 |
| 39 | A5 | 28 | 0 | 12 | 1 | 0 |
| 39 | A7 | 28 | 0 | 12 | 2 | 0 |
| 39 | A9 | 28 | 0 | 12 | 0 | 0 |
| 39 | B1 | 28 | 0 | 12 | 1 | 0 |
| 39 | B3 | 28 | 0 | 12 | 1 | 0 |
| 39 | B5 | 28 | 0 | 12 | 0 | 0 |
| 39 | B8 | 28 | 0 | 12 | 2 | 0 |
| 39 | C0 | 28 | 0 | 12 | 0 | 0 |
| 39 | C2 | 28 | 0 | 12 | 0 | 0 |
| 39 | C4 | 28 | 0 | 12 | 3 | 0 |
| 39 | C6 | 28 | 0 | 12 | 3 | 0 |
| 39 | C8 | 28 | 0 | 12 | 3 | 0 |
| 39 | D0 | 28 | 0 | 12 | 5 | 0 |
| 39 | D2 | 28 | 0 | 12 | 2 | 0 |
| 39 | D4 | 28 | 0 | 12 | 3 | 0 |
| 39 | D6 | 28 | 0 | 12 | 3 | 0 |
| 39 | D8 | 28 | 0 | 12 | 1 | 0 |
| 39 | E0 | 28 | 0 | 12 | 4 | 0 |
| 39 | E2 | 28 | 0 | 12 | 2 | 0 |
| 39 | E4 | 28 | 0 | 12 | 0 | 0 |
| 39 | E6 | 28 | 0 | 12 | 1 | 0 |
| 39 | E8 | 28 | 0 | 12 | 1 | 0 |
| 39 | F0 | 28 | 0 | 12 | 2 | 0 |
| 39 | F2 | 28 | 0 | 12 | 3 | 0 |
| 39 | F6 | 28 | 0 | 12 | 0 | 0 |
| 39 | F8 | 28 | 0 | 12 | 0 | 0 |
| 39 | G0 | 28 | 0 | 12 | 0 | 0 |
| 39 | G2 | 28 | 0 | 12 | 0 | 0 |
| 39 | G4 | 28 | 0 | 12 | 1 | 0 |
| 39 | G6 | 28 | 0 | 12 | 0 | 0 |
| 39 | G8 | 28 | 0 | 12 | 1 | 0 |
| 39 | H2 | 28 | 0 | 12 | 1 | 0 |
| 39 | H4 | 28 | 0 | 12 | 1 | 0 |
| 39 | H6 | 28 | 0 | 12 | 1 | 0 |
| 39 | H8 | 28 | 0 | 12 | 0 | 0 |
| 39 | I0 | 28 | 0 | 12 | 0 | 0 |
| 39 | I2 | 28 | 0 | 12 | 0 | 0 |
| 39 | I4 | 28 | 0 | 12 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | I8 | 28 | 0 | 12 | 0 | 0 |
| 39 | J0 | 28 | 0 | 12 | 0 | 0 |
| 39 | J2 | 28 | 0 | 12 | 1 | 0 |
| 39 | J4 | 28 | 0 | 12 | 0 | 0 |
| 39 | J6 | 28 | 0 | 12 | 1 | 0 |
| 39 | J8 | 28 | 0 | 12 | 1 | 0 |
| 39 | K0 | 28 | 0 | 12 | 0 | 0 |
| 39 | K4 | 28 | 0 | 12 | 1 | 0 |
| 39 | K6 | 28 | 0 | 12 | 0 | 0 |
| 39 | K8 | 28 | 0 | 12 | 0 | 0 |
| 39 | L0 | 28 | 0 | 12 | 0 | 0 |
| 39 | L2 | 28 | 0 | 12 | 1 | 0 |
| 39 | L4 | 28 | 0 | 12 | 2 | 0 |
| 39 | L6 | 28 | 0 | 12 | 1 | 0 |
| 39 | M0 | 28 | 0 | 12 | 0 | 0 |
| 39 | M2 | 28 | 0 | 12 | 0 | 0 |
| 39 | M4 | 28 | 0 | 12 | 0 | 0 |
| 39 | M6 | 28 | 0 | 12 | 0 | 0 |
| 39 | M8 | 28 | 0 | 12 | 0 | 0 |
| 39 | N0 | 28 | 0 | 12 | 0 | 0 |
| 39 | N2 | 28 | 0 | 12 | 1 | 0 |
| 39 | N6 | 28 | 0 | 12 | 2 | 0 |
| 39 | N8 | 28 | 0 | 12 | 3 | 0 |
| 39 | O0 | 28 | 0 | 12 | 0 | 0 |
| 39 | O2 | 28 | 0 | 12 | 2 | 0 |
| 39 | O4 | 28 | 0 | 12 | 0 | 0 |
| 39 | O6 | 28 | 0 | 12 | 1 | 0 |
| 39 | O8 | 28 | 0 | 12 | 1 | 0 |
| 39 | P4 | 28 | 0 | 12 | 1 | 0 |
| 39 | P6 | 28 | 0 | 12 | 0 | 0 |
| 39 | P8 | 28 | 0 | 12 | 2 | 0 |
| 39 | Q0 | 28 | 0 | 12 | 0 | 0 |
| 39 | Q2 | 28 | 0 | 12 | 1 | 0 |
| 39 | Q4 | 28 | 0 | 12 | 1 | 0 |
| 39 | Q6 | 28 | 0 | 12 | 2 | 0 |
| 39 | Q8 | 28 | 0 | 12 | 0 | 0 |
| 39 | R0 | 28 | 0 | 12 | 0 | 0 |
| 39 | R2 | 28 | 0 | 12 | 0 | 0 |
| 39 | R4 | 28 | 0 | 12 | 1 | 0 |
| 39 | R6 | 28 | 0 | 12 | 1 | 0 |
| 39 | R8 | 28 | 0 | 12 | 0 | 0 |
| 39 | S0 | 28 | 0 | 12 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | S2 | 28 | 0 | 12 | 1 | 0 |
| 39 | S4 | 28 | 0 | 12 | 1 | 0 |
| 39 | S6 | 28 | 0 | 12 | 0 | 0 |
| 39 | S8 | 28 | 0 | 12 | 1 | 0 |
| 39 | T0 | 28 | 0 | 12 | 2 | 0 |
| 39 | T2 | 28 | 0 | 12 | 0 | 0 |
| 39 | T4 | 28 | 0 | 12 | 0 | 0 |
| 39 | T6 | 28 | 0 | 12 | 3 | 0 |
| 39 | T8 | 28 | 0 | 12 | 0 | 0 |
| 39 | U2 | 28 | 0 | 12 | 1 | 0 |
| 39 | U4 | 28 | 0 | 12 | 0 | 0 |
| 39 | U6 | 28 | 0 | 12 | 0 | 0 |
| 39 | U8 | 28 | 0 | 12 | 0 | 0 |
| 39 | V0 | 28 | 0 | 12 | 0 | 0 |
| 39 | V2 | 28 | 0 | 12 | 0 | 0 |
| 39 | V4 | 28 | 0 | 12 | 1 | 0 |
| 39 | V6 | 28 | 0 | 12 | 1 | 0 |
| 39 | V8 | 28 | 0 | 12 | 1 | 0 |
| 39 | W0 | 28 | 0 | 12 | 2 | 0 |
| 39 | W2 | 28 | 0 | 12 | 1 | 0 |
| 39 | W4 | 28 | 0 | 12 | 0 | 0 |
| 39 | W6 | 28 | 0 | 12 | 0 | 0 |
| 39 | W8 | 28 | 0 | 12 | 2 | 0 |
| 39 | X0 | 28 | 0 | 12 | 2 | 0 |
| 39 | X2 | 28 | 0 | 12 | 3 | 0 |
| 39 | X4 | 28 | 0 | 12 | 2 | 0 |
| 39 | X6 | 28 | 0 | 12 | 3 | 0 |
| 39 | X8 | 28 | 0 | 12 | 1 | 0 |
| 39 | Y0 | 28 | 0 | 12 | 2 | 0 |
| 39 | Y2 | 28 | 0 | 12 | 2 | 0 |
| 39 | Y4 | 28 | 0 | 12 | 3 | 0 |
| 39 | Y6 | 28 | 0 | 12 | 2 | 0 |
| 39 | Y8 | 28 | 0 | 12 | 2 | 0 |
| 39 | Z0 | 28 | 0 | 12 | 2 | 0 |
| 39 | Z2 | 28 | 0 | 12 | 3 | 0 |
| 39 | Z4 | 28 | 0 | 12 | 1 | 0 |
| 39 | Z6 | 28 | 0 | 12 | 2 | 0 |
| 39 | Z8 | 28 | 0 | 12 | 3 | 0 |
| 40 | 0A | 1 | 0 | 0 | 0 | 0 |
| 40 | 0B | 1 | 0 | 0 | 0 | 0 |
| 40 | 0F | 1 | 0 | 0 | 0 | 0 |
| 40 | 0H | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | 0J | 1 | 0 | 0 | 0 | 0 |
| 40 | 0L | 1 | 0 | 0 | 0 | 0 |
| 40 | 0N | 1 | 0 | 0 | 0 | 0 |
| 40 | 0P | 1 | 0 | 0 | 0 | 0 |
| 40 | 0R | 1 | 0 | 0 | 0 | 0 |
| 40 | 0W | 1 | 0 | 0 | 0 | 0 |
| 40 | 0X | 1 | 0 | 0 | 0 | 0 |
| 40 | 1A | 1 | 0 | 0 | 0 | 0 |
| 40 | 1B | 1 | 0 | 0 | 0 | 0 |
| 40 | 1D | 1 | 0 | 0 | 0 | 0 |
| 40 | 1F | 1 | 0 | 0 | 0 | 0 |
| 40 | 1H | 1 | 0 | 0 | 0 | 0 |
| 40 | 1L | 1 | 0 | 0 | 0 | 0 |
| 40 | 1N | 1 | 0 | 0 | 0 | 0 |
| 40 | 1P | 1 | 0 | 0 | 0 | 0 |
| 40 | 1R | 1 | 0 | 0 | 0 | 0 |
| 40 | 1T | 1 | 0 | 0 | 0 | 0 |
| 40 | 1V | 1 | 0 | 0 | 0 | 0 |
| 40 | 1X | 1 | 0 | 0 | 0 | 0 |
| 40 | 1Z | 1 | 0 | 0 | 0 | 0 |
| 40 | 2 | 1 | 0 | 0 | 0 | 0 |
| 40 | 2B | 1 | 0 | 0 | 0 | 0 |
| 40 | 2D | 1 | 0 | 0 | 0 | 0 |
| 40 | 2F | 1 | 0 | 0 | 0 | 0 |
| 40 | 2H | 1 | 0 | 0 | 0 | 0 |
| 40 | 2J | 1 | 0 | 0 | 0 | 0 |
| 40 | 2L | 1 | 0 | 0 | 0 | 0 |
| 40 | 2N | 1 | 0 | 0 | 0 | 0 |
| 40 | 2P | 1 | 0 | 0 | 0 | 0 |
| 40 | 2R | 1 | 0 | 0 | 0 | 0 |
| 40 | 2T | 1 | 0 | 0 | 0 | 0 |
| 40 | 2V | 1 | 0 | 0 | 0 | 0 |
| 40 | 2X | 1 | 0 | 0 | 0 | 0 |
| 40 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 40 | 3B | 1 | 0 | 0 | 0 | 0 |
| 40 | 3D | 1 | 0 | 0 | 0 | 0 |
| 40 | 3F | 1 | 0 | 0 | 0 | 0 |
| 40 | 3H | 1 | 0 | 0 | 0 | 0 |
| 40 | 3K | 1 | 0 | 0 | 0 | 0 |
| 40 | 3L | 1 | 0 | 0 | 0 | 0 |
| 40 | 3N | 1 | 0 | 0 | 0 | 0 |
| 40 | 3P | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | 3R | 1 | 0 | 0 | 0 | 0 |
| 40 | 3T | 1 | 0 | 0 | 0 | 0 |
| 40 | 4 | 1 | 0 | 0 | 0 | 0 |
| 40 | 6 | 1 | 0 | 0 | 0 | 0 |
| 40 | 8 | 1 | 0 | 0 | 0 | 0 |
| 40 | A0 | 1 | 0 | 0 | 0 | 0 |
| 40 | A2 | 1 | 0 | 0 | 0 | 0 |
| 40 | A4 | 1 | 0 | 0 | 0 | 0 |
| 40 | A8 | 1 | 0 | 0 | 0 | 0 |
| 40 | B0 | 1 | 0 | 0 | 0 | 0 |
| 40 | B2 | 1 | 0 | 0 | 0 | 0 |
| 40 | B4 | 1 | 0 | 0 | 0 | 0 |
| 40 | B7 | 1 | 0 | 0 | 0 | 0 |
| 40 | B9 | 1 | 0 | 0 | 0 | 0 |
| 40 | C1 | 1 | 0 | 0 | 0 | 0 |
| 40 | C5 | 1 | 0 | 0 | 0 | 0 |
| 40 | C7 | 1 | 0 | 0 | 0 | 0 |
| 40 | C9 | 1 | 0 | 0 | 0 | 0 |
| 40 | D1 | 1 | 0 | 0 | 0 | 0 |
| 40 | D3 | 1 | 0 | 0 | 0 | 0 |
| 40 | D5 | 1 | 0 | 0 | 0 | 0 |
| 40 | D7 | 1 | 0 | 0 | 0 | 0 |
| 40 | E1 | 1 | 0 | 0 | 0 | 0 |
| 40 | E3 | 1 | 0 | 0 | 0 | 0 |
| 40 | E5 | 1 | 0 | 0 | 0 | 0 |
| 40 | E7 | 1 | 0 | 0 | 0 | 0 |
| 40 | E9 | 1 | 0 | 0 | 0 | 0 |
| 40 | F1 | 1 | 0 | 0 | 0 | 0 |
| 40 | F3 | 1 | 0 | 0 | 0 | 0 |
| 40 | F5 | 1 | 0 | 0 | 0 | 0 |
| 40 | F7 | 1 | 0 | 0 | 0 | 0 |
| 40 | F9 | 1 | 0 | 0 | 0 | 0 |
| 40 | G1 | 1 | 0 | 0 | 0 | 0 |
| 40 | G3 | 1 | 0 | 0 | 0 | 0 |
| 40 | G5 | 1 | 0 | 0 | 0 | 0 |
| 40 | G7 | 1 | 0 | 0 | 0 | 0 |
| 40 | G9 | 1 | 0 | 0 | 0 | 0 |
| 40 | H2 | 1 | 0 | 0 | 0 | 0 |
| 40 | H3 | 1 | 0 | 0 | 0 | 0 |
| 40 | H5 | 1 | 0 | 0 | 0 | 0 |
| 40 | H8 | 1 | 0 | 0 | 0 | 0 |
| 40 | H9 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | I1 | 1 | 0 | 0 | 0 | 0 |
| 40 | I3 | 1 | 0 | 0 | 0 | 0 |
| 40 | I5 | 1 | 0 | 0 | 0 | 0 |
| 40 | I7 | 1 | 0 | 0 | 0 | 0 |
| 40 | I9 | 1 | 0 | 0 | 0 | 0 |
| 40 | J1 | 1 | 0 | 0 | 0 | 0 |
| 40 | J4 | 1 | 0 | 0 | 0 | 0 |
| 40 | J5 | 1 | 0 | 0 | 0 | 0 |
| 40 | J7 | 1 | 0 | 0 | 0 | 0 |
| 40 | J9 | 1 | 0 | 0 | 0 | 0 |
| 40 | K1 | 1 | 0 | 0 | 0 | 0 |
| 40 | K3 | 1 | 0 | 0 | 0 | 0 |
| 40 | K5 | 1 | 0 | 0 | 0 | 0 |
| 40 | K7 | 1 | 0 | 0 | 0 | 0 |
| 40 | K9 | 1 | 0 | 0 | 0 | 0 |
| 40 | L1 | 1 | 0 | 0 | 0 | 0 |
| 40 | L3 | 1 | 0 | 0 | 0 | 0 |
| 40 | L5 | 1 | 0 | 0 | 0 | 0 |
| 40 | L7 | 1 | 0 | 0 | 0 | 0 |
| 40 | L9 | 1 | 0 | 0 | 0 | 0 |
| 40 | M1 | 1 | 0 | 0 | 0 | 0 |
| 40 | M3 | 1 | 0 | 0 | 0 | 0 |
| 40 | M5 | 1 | 0 | 0 | 0 | 0 |
| 40 | M7 | 1 | 0 | 0 | 0 | 0 |
| 40 | M9 | 1 | 0 | 0 | 0 | 0 |
| 40 | N1 | 1 | 0 | 0 | 0 | 0 |
| 40 | N3 | 1 | 0 | 0 | 0 | 0 |
| 40 | N6 | 1 | 0 | 0 | 0 | 0 |
| 40 | N7 | 1 | 0 | 0 | 0 | 0 |
| 40 | O0 | 1 | 0 | 0 | 0 | 0 |
| 40 | O1 | 1 | 0 | 0 | 0 | 0 |
| 40 | O3 | 1 | 0 | 0 | 0 | 0 |
| 40 | O5 | 1 | 0 | 0 | 0 | 0 |
| 40 | O8 | 1 | 0 | 0 | 0 | 0 |
| 40 | O9 | 1 | 0 | 0 | 0 | 0 |
| 40 | P4 | 1 | 0 | 0 | 0 | 0 |
| 40 | P6 | 1 | 0 | 0 | 0 | 0 |
| 40 | P7 | 1 | 0 | 0 | 0 | 0 |
| 40 | P9 | 1 | 0 | 0 | 0 | 0 |
| 40 | Q1 | 1 | 0 | 0 | 0 | 0 |
| 40 | Q3 | 1 | 0 | 0 | 0 | 0 |
| 40 | Q5 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | Q9 | 1 | 0 | 0 | 0 | 0 |
| 40 | R1 | 1 | 0 | 0 | 0 | 0 |
| 40 | R3 | 1 | 0 | 0 | 0 | 0 |
| 40 | R6 | 1 | 0 | 0 | 0 | 0 |
| 40 | R7 | 1 | 0 | 0 | 0 | 0 |
| 40 | R9 | 1 | 0 | 0 | 0 | 0 |
| 40 | S1 | 1 | 0 | 0 | 0 | 0 |
| 40 | S5 | 1 | 0 | 0 | 0 | 0 |
| 40 | S7 | 1 | 0 | 0 | 0 | 0 |
| 40 | S9 | 1 | 0 | 0 | 0 | 0 |
| 40 | T1 | 1 | 0 | 0 | 0 | 0 |
| 40 | T3 | 1 | 0 | 0 | 0 | 0 |
| 40 | T5 | 1 | 0 | 0 | 0 | 0 |
| 40 | T7 | 1 | 0 | 0 | 0 | 0 |
| 40 | U1 | 1 | 0 | 0 | 0 | 0 |
| 40 | U3 | 1 | 0 | 0 | 0 | 0 |
| 40 | U5 | 1 | 0 | 0 | 0 | 0 |
| 40 | U7 | 1 | 0 | 0 | 0 | 0 |
| 40 | U9 | 1 | 0 | 0 | 0 | 0 |
| 40 | V2 | 1 | 0 | 0 | 0 | 0 |
| 40 | V3 | 1 | 0 | 0 | 0 | 0 |
| 40 | V7 | 1 | 0 | 0 | 0 | 0 |
| 40 | V9 | 1 | 0 | 0 | 0 | 0 |
| 40 | W2 | 1 | 0 | 0 | 0 | 0 |
| 40 | W3 | 1 | 0 | 0 | 0 | 0 |
| 40 | W5 | 1 | 0 | 0 | 0 | 0 |
| 40 | W8 | 1 | 0 | 0 | 0 | 0 |
| 40 | W9 | 1 | 0 | 0 | 0 | 0 |
| 40 | X3 | 1 | 0 | 0 | 0 | 0 |
| 40 | X5 | 1 | 0 | 0 | 0 | 0 |
| 40 | X7 | 1 | 0 | 0 | 0 | 0 |
| 40 | X9 | 1 | 0 | 0 | 0 | 0 |
| 40 | Y1 | 1 | 0 | 0 | 0 | 0 |
| 40 | Y3 | 1 | 0 | 0 | 0 | 0 |
| 40 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 40 | Y9 | 1 | 0 | 0 | 0 | 0 |
| 40 | Z2 | 1 | 0 | 0 | 0 | 0 |
| 40 | Z3 | 1 | 0 | 0 | 0 | 0 |
| 40 | Z5 | 1 | 0 | 0 | 0 | 0 |
| 40 | Z7 | 1 | 0 | 0 | 0 | 0 |
| 41 | 0A | 32 | 0 | 12 | 2 | 0 |
| 41 | 0C | 32 | 0 | 12 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | 0F | 32 | 0 | 12 | 3 | 0 |
| 41 | 0I | 32 | 0 | 12 | 3 | 0 |
| 41 | 0K | 32 | 0 | 12 | 2 | 0 |
| 41 | 0M | 32 | 0 | 12 | 3 | 0 |
| 41 | 0O | 32 | 0 | 12 | 2 | 0 |
| 41 | 0Q | 32 | 0 | 12 | 3 | 0 |
| 41 | 0S | 32 | 0 | 12 | 2 | 0 |
| 41 | 0V | 32 | 0 | 12 | 1 | 0 |
| 41 | 0Y | 32 | 0 | 12 | 1 | 0 |
| 41 | 1A | 32 | 0 | 12 | 1 | 0 |
| 41 | 1C | 32 | 0 | 12 | 1 | 0 |
| 41 | 1D | 32 | 0 | 12 | 1 | 0 |
| 41 | 1G | 32 | 0 | 12 | 1 | 0 |
| 41 | 1H | 32 | 0 | 12 | 2 | 0 |
| 41 | 1L | 32 | 0 | 12 | 1 | 0 |
| 41 | 1N | 32 | 0 | 12 | 1 | 0 |
| 41 | 1Q | 32 | 0 | 12 | 1 | 0 |
| 41 | 1S | 32 | 0 | 12 | 1 | 0 |
| 41 | 1T | 32 | 0 | 12 | 1 | 0 |
| 41 | 1W | 32 | 0 | 12 | 1 | 0 |
| 41 | 1X | 32 | 0 | 12 | 1 | 0 |
| 41 | 2A | 32 | 0 | 12 | 0 | 0 |
| 41 | 2C | 32 | 0 | 12 | 2 | 0 |
| 41 | 2E | 32 | 0 | 12 | 2 | 0 |
| 41 | 2G | 32 | 0 | 12 | 2 | 0 |
| 41 | 2I | 32 | 0 | 12 | 1 | 0 |
| 41 | 2K | 32 | 0 | 12 | 0 | 0 |
| 41 | 2L | 32 | 0 | 12 | 1 | 0 |
| 41 | 2N | 32 | 0 | 12 | 1 | 0 |
| 41 | 2Q | 32 | 0 | 12 | 1 | 0 |
| 41 | 2S | 32 | 0 | 12 | 0 | 0 |
| 41 | 2U | 32 | 0 | 12 | 1 | 0 |
| 41 | 2W | 32 | 0 | 12 | 1 | 0 |
| 41 | 2Y | 32 | 0 | 12 | 0 | 0 |
| 41 | 3 | 32 | 0 | 12 | 1 | 0 |
| 41 | 3A | 32 | 0 | 12 | 0 | 0 |
| 41 | 3C | 32 | 0 | 12 | 0 | 0 |
| 41 | 3D | 32 | 0 | 12 | 2 | 0 |
| 41 | 3G | 32 | 0 | 12 | 0 | 0 |
| 41 | 3I | 32 | 0 | 12 | 0 | 0 |
| 41 | 3K | 32 | 0 | 12 | 0 | 0 |
| 41 | 3M | 32 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | 3O | 32 | 0 | 12 | 1 | 0 |
| 41 | 3P | 32 | 0 | 12 | 0 | 0 |
| 41 | 3S | 32 | 0 | 12 | 0 | 0 |
| 41 | 3T | 32 | 0 | 12 | 0 | 0 |
| 41 | 4 | 32 | 0 | 12 | 1 | 0 |
| 41 | 7 | 32 | 0 | 12 | 0 | 0 |
| 41 | 8 | 32 | 0 | 12 | 1 | 0 |
| 41 | A1 | 32 | 0 | 12 | 2 | 0 |
| 41 | A2 | 32 | 0 | 12 | 1 | 0 |
| 41 | A4 | 32 | 0 | 12 | 2 | 0 |
| 41 | A9 | 32 | 0 | 12 | 1 | 0 |
| 41 | B0 | 32 | 0 | 12 | 2 | 0 |
| 41 | B2 | 32 | 0 | 12 | 0 | 0 |
| 41 | B5 | 32 | 0 | 12 | 2 | 0 |
| 41 | B7 | 32 | 0 | 12 | 1 | 0 |
| 41 | C0 | 32 | 0 | 12 | 2 | 0 |
| 41 | C1 | 32 | 0 | 12 | 2 | 0 |
| 41 | C5 | 32 | 0 | 12 | 2 | 0 |
| 41 | C8 | 32 | 0 | 12 | 1 | 0 |
| 41 | C9 | 32 | 0 | 12 | 5 | 0 |
| 41 | D1 | 32 | 0 | 12 | 1 | 0 |
| 41 | D3 | 32 | 0 | 12 | 2 | 0 |
| 41 | D5 | 32 | 0 | 12 | 1 | 0 |
| 41 | D7 | 32 | 0 | 12 | 2 | 0 |
| 41 | E1 | 32 | 0 | 12 | 3 | 0 |
| 41 | E4 | 32 | 0 | 12 | 1 | 0 |
| 41 | E6 | 32 | 0 | 12 | 2 | 0 |
| 41 | E8 | 32 | 0 | 12 | 3 | 0 |
| 41 | F0 | 32 | 0 | 12 | 2 | 0 |
| 41 | F1 | 32 | 0 | 12 | 1 | 0 |
| 41 | F3 | 32 | 0 | 12 | 2 | 0 |
| 41 | F5 | 32 | 0 | 12 | 2 | 0 |
| 41 | F8 | 32 | 0 | 12 | 1 | 0 |
| 41 | G0 | 32 | 0 | 12 | 3 | 0 |
| 41 | G1 | 32 | 0 | 12 | 2 | 0 |
| 41 | G4 | 32 | 0 | 12 | 2 | 0 |
| 41 | G5 | 32 | 0 | 12 | 3 | 0 |
| 41 | G7 | 32 | 0 | 12 | 2 | 0 |
| 41 | G9 | 32 | 0 | 12 | 1 | 0 |
| 41 | H2 | 32 | 0 | 12 | 1 | 0 |
| 41 | H3 | 32 | 0 | 12 | 1 | 0 |
| 41 | H6 | 32 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | H8 | 32 | 0 | 12 | 1 | 0 |
| 41 | I0 | 32 | 0 | 12 | 1 | 0 |
| 41 | I1 | 32 | 0 | 12 | 1 | 0 |
| 41 | I4 | 32 | 0 | 12 | 2 | 0 |
| 41 | I5 | 32 | 0 | 12 | 0 | 0 |
| 41 | I8 | 32 | 0 | 12 | 1 | 0 |
| 41 | J0 | 32 | 0 | 12 | 1 | 0 |
| 41 | J2 | 32 | 0 | 12 | 1 | 0 |
| 41 | J4 | 32 | 0 | 12 | 1 | 0 |
| 41 | J6 | 32 | 0 | 12 | 1 | 0 |
| 41 | J8 | 32 | 0 | 12 | 1 | 0 |
| 41 | K0 | 32 | 0 | 12 | 2 | 0 |
| 41 | K1 | 32 | 0 | 12 | 0 | 0 |
| 41 | K4 | 32 | 0 | 12 | 2 | 0 |
| 41 | K6 | 32 | 0 | 12 | 3 | 0 |
| 41 | K7 | 32 | 0 | 12 | 2 | 0 |
| 41 | K9 | 32 | 0 | 12 | 2 | 0 |
| 41 | L2 | 32 | 0 | 12 | 2 | 0 |
| 41 | L4 | 32 | 0 | 12 | 3 | 0 |
| 41 | L6 | 32 | 0 | 12 | 1 | 0 |
| 41 | L7 | 32 | 0 | 12 | 0 | 0 |
| 41 | M0 | 32 | 0 | 12 | 0 | 0 |
| 41 | M2 | 32 | 0 | 12 | 0 | 0 |
| 41 | M4 | 32 | 0 | 12 | 0 | 0 |
| 41 | M6 | 32 | 0 | 12 | 0 | 0 |
| 41 | M7 | 32 | 0 | 12 | 1 | 0 |
| 41 | N0 | 32 | 0 | 12 | 1 | 0 |
| 41 | N1 | 32 | 0 | 12 | 0 | 0 |
| 41 | N3 | 32 | 0 | 12 | 0 | 0 |
| 41 | N6 | 32 | 0 | 12 | 3 | 0 |
| 41 | N8 | 32 | 0 | 12 | 2 | 0 |
| 41 | O0 | 32 | 0 | 12 | 1 | 0 |
| 41 | O2 | 32 | 0 | 12 | 0 | 0 |
| 41 | O4 | 32 | 0 | 12 | 2 | 0 |
| 41 | O6 | 32 | 0 | 12 | 1 | 0 |
| 41 | O8 | 32 | 0 | 12 | 1 | 0 |
| 41 | O9 | 32 | 0 | 12 | 1 | 0 |
| 41 | P4 | 32 | 0 | 12 | 3 | 0 |
| 41 | P6 | 32 | 0 | 12 | 2 | 0 |
| 41 | P8 | 32 | 0 | 12 | 2 | 0 |
| 41 | P9 | 32 | 0 | 12 | 2 | 0 |
| 41 | Q2 | 32 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | Q4 | 32 | 0 | 12 | 1 | 0 |
| 41 | Q6 | 32 | 0 | 12 | 1 | 0 |
| 41 | R0 | 32 | 0 | 12 | 1 | 0 |
| 41 | R2 | 32 | 0 | 12 | 1 | 0 |
| 41 | R4 | 32 | 0 | 12 | 0 | 0 |
| 41 | R6 | 32 | 0 | 12 | 1 | 0 |
| 41 | R8 | 32 | 0 | 12 | 0 | 0 |
| 41 | S0 | 32 | 0 | 12 | 1 | 0 |
| 41 | S2 | 32 | 0 | 12 | 1 | 0 |
| 41 | S5 | 32 | 0 | 12 | 0 | 0 |
| 41 | S8 | 32 | 0 | 12 | 1 | 0 |
| 41 | S9 | 32 | 0 | 12 | 2 | 0 |
| 41 | T2 | 32 | 0 | 12 | 2 | 0 |
| 41 | T4 | 32 | 0 | 12 | 3 | 0 |
| 41 | T6 | 32 | 0 | 12 | 3 | 0 |
| 41 | T8 | 32 | 0 | 12 | 2 | 0 |
| 41 | U2 | 32 | 0 | 12 | 0 | 0 |
| 41 | U4 | 32 | 0 | 12 | 1 | 0 |
| 41 | U6 | 32 | 0 | 12 | 1 | 0 |
| 41 | U7 | 32 | 0 | 12 | 0 | 0 |
| 41 | U9 | 32 | 0 | 12 | 0 | 0 |
| 41 | V2 | 32 | 0 | 12 | 0 | 0 |
| 41 | V3 | 32 | 0 | 12 | 0 | 0 |
| 41 | V8 | 32 | 0 | 12 | 0 | 0 |
| 41 | W0 | 32 | 0 | 12 | 0 | 0 |
| 41 | W2 | 32 | 0 | 12 | 0 | 0 |
| 41 | W4 | 32 | 0 | 12 | 0 | 0 |
| 41 | W5 | 32 | 0 | 12 | 1 | 0 |
| 41 | W8 | 32 | 0 | 12 | 0 | 0 |
| 41 | X0 | 32 | 0 | 12 | 1 | 0 |
| 41 | X4 | 32 | 0 | 12 | 3 | 0 |
| 41 | X6 | 32 | 0 | 12 | 3 | 0 |
| 41 | X7 | 32 | 0 | 12 | 2 | 0 |
| 41 | Y0 | 32 | 0 | 12 | 3 | 0 |
| 41 | Y1 | 32 | 0 | 12 | 2 | 0 |
| 41 | Y4 | 32 | 0 | 12 | 2 | 0 |
| 41 | Y6 | 32 | 0 | 12 | 2 | 0 |
| 41 | Z0 | 32 | 0 | 12 | 1 | 0 |
| 41 | Z2 | 32 | 0 | 12 | 2 | 0 |
| 41 | Z3 | 32 | 0 | 12 | 2 | 0 |
| 41 | Z6 | 32 | 0 | 12 | 2 | 0 |
| 41 | Z7 | 32 | 0 | 12 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 1358547 | 0 | 1321887 | 33426 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (33426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3S:362:LYS:CE | 38:8D:166:GLU:HG3 | 1.25 | 1.64 |
| 2:E5:282:TYR:CZ | 22:6K:82:LEU:HD23 | 1.38 | 1.57 |
| 24:6X:451:LYS:CD | 24:6X:468:ARG:HH12 | 1.02 | 1.56 |
| 2:S1:88:HIS:CD2 | 2:S1:89:PRO:HD2 | 1.42 | 1.51 |
| 2:E5:282:TYR:CE1 | 22:6K:82:LEU:CD2 | 1.93 | 1.49 |
| 2:T7:88:HIS:CD2 | 2:T7:89:PRO:HD2 | 1.45 | 1.48 |
| 2:2Z:297:GLU:CD | 38:8C:74:ILE:HG22 | 1.21 | 1.48 |
| 2:E5:282:TYR:CE1 | 22:6K:82:LEU:HD22 | 1.47 | 1.47 |
| 38:8B:85:ARG:NH1 | 38:8B:87:LYS:HD3 | 1.26 | 1.45 |
| 2:3B:339:ARG:HE | 38:8C:39:LYS:NZ | 0.97 | 1.44 |
| 2:G3:42:ILE:HD11 | 24:6W:470:ILE:CD1 | 1.47 | 1.43 |
| 2:0Z:58:ALA:N | 9:4Z:165:ARG:HH22 | 1.08 | 1.43 |
| 2:K5:219:ILE:HG23 | 29:7I:14:LEU:CD1 | 1.48 | 1.43 |
| 1:A3:227:HIS:CE1 | 26:7F:133:PHE:O | 1.71 | 1.42 |
| 2:3B:339:ARG:NE | 38:8C:39:LYS:HZ1 | 1.14 | 1.41 |
| 1:5:227:HIS:CE1 | 26:7D:133:PHE:O | 1.70 | 1.41 |
| 2:1N:313:MET:CE | 2:1N:346:TRP:CZ2 | 2.01 | 1.41 |
| 2:8:370:LYS:CE | 24:6W:92:ASP:OD1 | 1.65 | 1.41 |
| 2:0Z:58:ALA:HB3 | 9:4Z:165:ARG:NH1 | 1.20 | 1.40 |
| 2:0Z:58:ALA:H | 9:4Z:165:ARG:NH2 | 1.17 | 1.40 |
| 2:0Z:58:ALA:CB | 9:4Z:165:ARG:NH1 | 1.85 | 1.40 |
| 2:Z5:88:HIS:CD2 | 2:Z5:89:PRO:HD2 | 1.56 | 1.39 |
| 1:2I:118:ASP:HB3 | 38:8C:99:THR:CG2 | 1.50 | 1.39 |
| 1:R2:92:PHE:CE2 | 24:6V:35:TYR:CE1 | 2.11 | 1.38 |
| 2:A2:370:LYS:CE | 24:6Y:92:ASP:OD1 | 1.71 | 1.38 |
| 2:E7:282:TYR:CZ | 22:6L:82:LEU:HD23 | 1.58 | 1.38 |
| 1:2Q:320:ARG:CZ | 38:8A:198:THR:HG22 | 1.55 | 1.37 |
| 2:0L:313:MET:CE | 2:0L:346:TRP:HZ2 | 1.38 | 1.36 |
| 15:5O:6:ARG:HD3 | 15:5O:27:PHE:CD2 | 1.60 | 1.36 |
| 2:M3:359:PRO:CB | 30:7K:212:ARG:HH21 | 1.35 | 1.35 |
| 1:2Q:320:ARG:NH2 | 38:8A:198:THR:HG22 | 1.36 | 1.35 |
| 2:J3:357:TYR:CB | 16:5Q:173:ARG:HE | 1.21 | 1.35 |
| 1:S2:80:PRO:CD | 7:4S:11:GLU:OE1 | 1.73 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1R:313:MET:CE | 2:1R:346:TRP:CZ2 | 2.09 | 1.34 |
| 14:5M:291:GLU:OE2 | 14:5M:317:ASN:ND2 | 1.59 | 1.33 |
| 1:E6:52:ASN:CA | 22:6L:181:ASN:ND2 | 1.92 | 1.33 |
| 2:G3:42:ILE:CD1 | 24:6W:470:ILE:HD11 | 1.56 | 1.33 |
| 24:6X:451:LYS:HD2 | 24:6X:468:ARG:NH1 | 1.03 | 1.32 |
| 2:E5:282:TYR:CZ | 22:6K:82:LEU:CD2 | 2.02 | 1.32 |
| 14:5N:210:TYR:CE1 | 14:5N:220:GLN:HG3 | 1.64 | 1.32 |
| 1:2Q:306:ARG:NH2 | 38:8A:99:THR:O | 1.58 | 1.32 |
| 1:3S:362:LYS:CE | 38:8D:166:GLU:CG | 2.08 | 1.32 |
| 1:3S:362:LYS:HE3 | 38:8D:166:GLU:CG | 1.58 | 1.31 |
| 1:9:227:HIS:CE1 | 26:7E:133:PHE:O | 1.82 | 1.31 |
| 2:K5:279:GLU:OE2 | 29:7I:24:PRO:CD | 1.65 | 1.31 |
| 2:J7:282:TYR:CD1 | 5:4M:209:LEU:HD21 | 1.66 | 1.31 |
| 1:2Q:306:ARG:NH2 | 38:8A:96:GLY:O | 1.60 | 1.30 |
| 14:5M:219:LEU:HD11 | 14:5M:228:PHE:CD2 | 1.65 | 1.30 |
| 1:3C:58:ARG:NH2 | 38:8D:158:MET:SD | 2.05 | 1.29 |
| 2:M9:282:TYR:CD1 | 30:7K:25:ALA:HB2 | 1.65 | 1.29 |
| 1:5:219:THR:OG1 | 26:7D:142:PHE:CE1 | 1.73 | 1.29 |
| 1:L6:41:ASP:OD1 | 29:7J:167:ILE:CD1 | 1.77 | 1.29 |
| 1:2E:95:THR:CG2 | 38:8B:83:ARG:HH12 | 1.44 | 1.29 |
| 1:H4:276:ARG:NH2 | 24:6U:489:ASN:O | 1.67 | 1.28 |
| 2:0Z:58:ALA:H | 9:4Z:165:ARG:CZ | 1.43 | 1.28 |
| 2:Q5:60:LYS:HE3 | 2:S1:283:HIS:NE2 | 1.45 | 1.28 |
| 38:8A:91:GLN:HB3 | 38:8A:102:PHE:CD1 | 1.69 | 1.28 |
| 2:Q5:60:LYS:CE | 2:S1:283:HIS:NE2 | 1.96 | 1.27 |
| 1:S0:92:PHE:CE2 | 24:6Z:40:GLN:NE2 | 1.98 | 1.27 |
| 2:Y3:282:TYR:CD2 | 8:4W:373:ASN:ND2 | 2.00 | 1.27 |
| 15:5O:52:TYR:CD2 | 15:5O:55:LEU:HD21 | 1.68 | 1.27 |
| 2:W9:88:HIS:CD2 | 2:W9:121:ARG:HH22 | 1.51 | 1.27 |
| 1:I4:218:THR:CG2 | 24:6Z:488:ARG:O | 1.81 | 1.27 |
| 1:E6:52:ASN:CA | 22:6L:181:ASN:HD22 | 1.46 | 1.26 |
| 2:1R:313:MET:HE1 | 2:1R:346:TRP:CZ2 | 1.68 | 1.26 |
| 1:R2:92:PHE:CE2 | 24:6V:35:TYR:HE1 | 1.46 | 1.26 |
| 1:I4:276:ARG:HD2 | 24:6Z:490:THR:O | 1.36 | 1.26 |
| 24:6X:316:ASP:OD2 | 24:6X:317:PRO:HD2 | 1.24 | 1.26 |
| 2:A0:44:GLY:N | 24:6X:124:TYR:OH | 1.69 | 1.25 |
| 2:A2:29:GLY:C | 26:7F:45:MET:CE | 2.05 | 1.25 |
| 2:E5:282:TYR:CE2 | 22:6K:82:LEU:HD23 | 1.70 | 1.25 |
| 2:P5:42:ILE:HD11 | 27:7G:213:TRP:CZ3 | 1.72 | 1.25 |
| 2:P5:88:HIS:ND1 | 2:P5:89:PRO:HD2 | 1.52 | 1.25 |
| 2:8:220:GLU:OE2 | 26:7E:81:LYS:HD2 | 1.33 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2E:95:THR:HG21 | 38:8B:83:ARG:NH1 | 1.50 | 1.24 |
| 2:E5:282:TYR:CG | 22:6K:82:LEU:HD21 | 1.72 | 1.24 |
| 2:1N:313:MET:HE1 | 2:1N:346:TRP:CH2 | 1.73 | 1.23 |
| 2:M3:359:PRO:HB2 | 30:7K:212:ARG:NH2 | 1.50 | 1.23 |
| 2:E5:282:TYR:CD1 | 22:6K:82:LEU:CD2 | 2.21 | 1.23 |
| 2:G3:88:HIS:CD2 | 2:G3:89:PRO:HD2 | 1.73 | 1.23 |
| 2:J7:80:THR:CB | 29:7J:390:LEU:HD21 | 1.69 | 1.23 |
| 1:I4:276:ARG:NH1 | 24:6Z:490:THR:O | 1.69 | 1.23 |
| 2:K5:219:ILE:CG2 | 29:7I:14:LEU:HD11 | 1.67 | 1.22 |
| 1:0M:393:ALA:HB2 | 2:0N:346:TRP:NE1 | 1.53 | 1.22 |
| 1:2Q:306:ARG:CZ | 38:8A:96:GLY:N | 2.03 | 1.22 |
| 2:8:42:ILE:CD1 | 24:6W:93:ARG:HH22 | 1.52 | 1.22 |
| 1:A3:227:HIS:NE2 | 26:7F:133:PHE:O | 1.73 | 1.22 |
| 1:E6:52:ASN:CB | 22:6L:181:ASN:HD21 | 1.52 | 1.22 |
| 2:J5:41:THR:CG2 | 2:J5:46:ASP:OD2 | 1.88 | 1.22 |
| 2:A2:29:GLY:C | 26:7F:45:MET:HE3 | 1.59 | 1.21 |
| 2:M3:279:GLU:OE1 | 30:7K:197:ARG:HG3 | 1.39 | 1.21 |
| 1:X0:42:LEU:HB2 | 8:4X:97:PHE:CZ | 1.74 | 1.21 |
| 2:3B:339:ARG:NE | 38:8C:39:LYS:NZ | 1.71 | 1.21 |
| 1:S2:80:PRO:HD2 | 7:4S:11:GLU:OE1 | 1.07 | 1.21 |
| 1:0M:393:ALA:CB | 2:0N:346:TRP:HE1 | 1.52 | 1.21 |
| 1:2Q:306:ARG:NH1 | 38:8A:96:GLY:N | 1.86 | 1.21 |
| 2:J7:282:TYR:CD1 | 5:4M:209:LEU:CD2 | 2.22 | 1.21 |
| 2:1Z:88:HIS:CD2 | 2:1Z:89:PRO:HD2 | 1.76 | 1.21 |
| 1:H6:276:ARG:NH2 | 24:6V:489:ASN:O | 1.74 | 1.20 |
| 2:S1:88:HIS:CD2 | 2:S1:89:PRO:CD | 2.23 | 1.20 |
| 1:T6:92:PHE:CZ | 24:7A:44:ALA:HB1 | 1.77 | 1.20 |
| 1:L4:37:HIS:HA | 29:7J:335:GLU:OE2 | 1.41 | 1.19 |
| 29:7J:319:ILE:CG2 | 29:7J:320:PRO:HD2 | 1.69 | 1.19 |
| 2:1N:313:MET:HE1 | 2:1N:346:TRP:CZ2 | 1.69 | 1.19 |
| 2:2P:22:GLU:OE1 | 38:8A:203:PHE:HD1 | 1.23 | 1.19 |
| 2:0Z:58:ALA:N | 9:4Z:165:ARG:NH2 | 1.72 | 1.18 |
| 14:5M:511:THR:OG1 | 14:5M:531:ASP:HB3 | 1.43 | 1.18 |
| 2:B9:279:GLU:OE1 | 18:6C:43:ASN:ND2 | 1.76 | 1.18 |
| 1:2Y:55:THR:O | 38:8C:161:GLN:NE2 | 1.77 | 1.18 |
| 15:5O:296:SER:O | 15:5O:299:GLU:HG3 | 1.40 | 1.18 |
| 2:M9:282:TYR:CE1 | 30:7K:25:ALA:HB2 | 1.80 | 1.17 |
| 1:M6:75:SER:HA | 15:5P:48:LYS:CE | 1.72 | 1.17 |
| 1:R2:94:GLN:HE22 | 13:5I:18:ARG:HA | 1.10 | 1.17 |
| 2:0Z:58:ALA:CB | 9:4Z:165:ARG:HH12 | 1.47 | 1.17 |
| 5:4M:76:LEU:HD23 | 15:5P:288:VAL:HG21 | 1.20 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8A:91:GLN:HB3 | 38:8A:102:PHE:CE1 | 1.79 | 1.16 |
| 2:A2:42:ILE:CD1 | 24:6Y:93:ARG:NH2 | 2.08 | 1.16 |
| 2:M9:279:GLU:OE2 | 29:7J:300:THR:HG21 | 1.43 | 1.16 |
| 24:6X:519:VAL:O | 24:6X:532:LEU:O | 1.60 | 1.16 |
| 1:3Q:248:ALA:HA | 1:3Q:252:LYS:HD2 | 1.25 | 1.16 |
| 1:B5:362:LYS:HD3 | 18:6A:24:ARG:HB2 | 1.23 | 1.16 |
| 1:E6:52:ASN:CB | 22:6L:181:ASN:ND2 | 2.07 | 1.15 |
| 2:T7:88:HIS:CD2 | 2:T7:89:PRO:CD | 2.28 | 1.15 |
| 2:A2:29:GLY:O | 26:7F:45:MET:HE3 | 0.98 | 1.15 |
| 2:E7:282:TYR:CE2 | 22:6L:82:LEU:CD2 | 2.29 | 1.15 |
| 1:I4:218:THR:OG1 | 24:6Z:488:ARG:O | 1.62 | 1.15 |
| 1:T0:248:ALA:HA | 1:T0:252:LYS:HD2 | 1.28 | 1.15 |
| 2:U9:88:HIS:ND1 | 2:U9:89:PRO:HD2 | 1.61 | 1.15 |
| 38:8C:36:GLU:OE1 | 38:8C:39:LYS:HE2 | 1.45 | 1.15 |
| 1:O2:79:GLY:CA | 37:7Y:191:ARG:HH22 | 1.59 | 1.15 |
| 2:1N:313:MET:HE3 | 2:1N:346:TRP:CZ2 | 1.72 | 1.15 |
| 1:2Y:56:GLY:HA3 | 38:8C:161:GLN:HG2 | 1.15 | 1.15 |
| 15:5O:99:LYS:HE3 | 15:5O:203:ASN:ND2 | 1.59 | 1.15 |
| 2:0L:313:MET:CE | 2:0L:346:TRP:CZ2 | 2.29 | 1.15 |
| 2:3P:279:GLU:OE2 | 14:5N:466:LYS:NZ | 1.80 | 1.15 |
| 2:J7:277:SER:HB2 | 2:J7:280:LYS:NZ | 1.62 | 1.14 |
| 7:4R:301:ARG:HG2 | 7:4R:301:ARG:HH21 | 1.06 | 1.14 |
| 1:A3:219:THR:OG1 | 26:7F:142:PHE:CD2 | 1.99 | 1.14 |
| 1:2Q:306:ARG:CZ | 38:8A:96:GLY:O | 1.95 | 1.14 |
| 1:2Q:320:ARG:CZ | 38:8A:198:THR:CG2 | 2.24 | 1.14 |
| 1:M8:248:ALA:HA | 1:M8:252:LYS:HD2 | 1.28 | 1.14 |
| 20:6F:361:LEU:HD12 | 20:6F:362:PRO:HD2 | 1.23 | 1.14 |
| 2:8:42:ILE:CD1 | 24:6W:93:ARG:NH2 | 2.07 | 1.14 |
| 14:5N:208:TYR:CG | 14:5N:220:GLN:NE2 | 2.15 | 1.14 |
| 15:5O:99:LYS:CE | 15:5O:203:ASN:HD21 | 1.60 | 1.14 |
| 2:8:370:LYS:HE2 | 24:6W:92:ASP:OD1 | 1.39 | 1.13 |
| 2:A2:42:ILE:HD12 | 24:6Y:93:ARG:NH2 | 1.52 | 1.13 |
| 15:5O:34:GLU:OE2 | 15:5O:49:ARG:HD3 | 1.47 | 1.13 |
| 2:N9:85:GLN:O | 2:P7:283:HIS:NE2 | 1.80 | 1.13 |
| 2:2X:282:TYR:OH | 10:5C:384:GLN:NE2 | 1.81 | 1.13 |
| 14:5L:110:ASP:OD1 | 14:5L:154:LYS:HA | 1.44 | 1.13 |
| 15:5P:329:PRO:HG3 | 15:5P:335:GLY:HA2 | 1.28 | 1.13 |
| 2:N7:121:ARG:HH21 | 2:N7:121:ARG:HG3 | 1.09 | 1.13 |
| 1:2Q:306:ARG:CD | 38:8A:96:GLY:HA3 | 1.78 | 1.13 |
| 2:H3:88:HIS:HD2 | 2:H3:121:ARG:NH2 | 1.46 | 1.13 |
| 2:K7:88:HIS:ND1 | 2:K7:89:PRO:HD2 | 1.65 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:467:ARG:NH1 | 24:6X:484:GLU:OE2 | 1.82 | 1.12 |
| 1:M6:75:SER:CA | 15:5P:48:LYS:HE3 | 1.78 | 1.12 |
| 2:N7:85:GLN:O | 2:P5:283:HIS:HE1 | 1.32 | 1.12 |
| 2:1R:313:MET:HE3 | 2:1R:346:TRP:CZ2 | 1.77 | 1.12 |
| 2:8:220:GLU:HG2 | 26:7E:81:LYS:HZ2 | 0.98 | 1.12 |
| 2:A2:370:LYS:HE3 | 24:6Y:92:ASP:OD1 | 1.33 | 1.12 |
| 2:E5:282:TYR:CD1 | 22:6K:82:LEU:HD21 | 1.81 | 1.12 |
| 1:R2:92:PHE:HE2 | 24:6V:35:TYR:CE1 | 1.59 | 1.12 |
| 2:Y3:282:TYR:HE2 | 8:4W:373:ASN:CB | 1.62 | 1.12 |
| 2:2Z:282:TYR:HE1 | 10:5C:435:LEU:HD21 | 0.96 | 1.12 |
| 2:J3:357:TYR:HB3 | 16:5Q:173:ARG:NE | 1.24 | 1.12 |
| 1:2Q:306:ARG:HD3 | 38:8A:96:GLY:HA3 | 1.28 | 1.12 |
| 2:2Z:297:GLU:CD | 38:8C:74:ILE:CG2 | 2.17 | 1.12 |
| 2:L3:89:PRO:HB3 | 29:7J:320:PRO:CG | 1.80 | 1.12 |
| 1:J8:40:SER:HA | 29:7J:388:MET:HG2 | 1.15 | 1.11 |
| 1:O2:79:GLY:HA2 | 37:7Y:191:ARG:HH22 | 1.03 | 1.11 |
| 2:1L:121:ARG:HH11 | 2:1L:121:ARG:HG2 | 1.15 | 1.11 |
| 1:B8:362:LYS:HD3 | 18:6B:24:ARG:HB2 | 1.26 | 1.11 |
| 2:G3:42:ILE:CD1 | 24:6W:470:ILE:CD1 | 2.21 | 1.11 |
| 2:G3:85:GLN:HE21 | 2:G3:85:GLN:HA | 1.11 | 1.11 |
| 1:L6:41:ASP:OD1 | 29:7J:167:ILE:HD13 | 1.47 | 1.11 |
| 15:5O:99:LYS:HE3 | 15:5O:203:ASN:HD21 | 1.03 | 1.11 |
| 15:5O:62:LEU:HD21 | 15:5O:77:GLU:HA | 1.32 | 1.11 |
| 2:8:221:ARG:O | 26:7E:77:ILE:O | 1.66 | 1.11 |
| 1:M6:46:ARG:CZ | 37:7Y:115:CYS:SG | 2.39 | 1.11 |
| 8:4W:457:LEU:O | 8:4W:461:VAL:HG12 | 1.48 | 1.11 |
| 29:7J:390:LEU:HB3 | 29:7J:391:PRO:HD2 | 1.15 | 1.11 |
| 1:I0:218:THR:OG1 | 24:6X:489:ASN:HB3 | 1.50 | 1.10 |
| 2:L3:84:ARG:HH12 | 29:7J:345:PRO:HA | 1.12 | 1.10 |
| 2:L3:89:PRO:HB3 | 29:7J:320:PRO:HG2 | 1.29 | 1.10 |
| 1:2I:118:ASP:CG | 38:8C:99:THR:HB | 1.70 | 1.10 |
| 1:H4:248:ALA:HA | 1:H4:252:LYS:HD2 | 1.31 | 1.10 |
| 1:I0:218:THR:HG23 | 24:6X:489:ASN:HA | 1.32 | 1.10 |
| 2:M3:359:PRO:CG | 30:7K:212:ARG:NH2 | 2.15 | 1.10 |
| 1:R4:391:ARG:HG3 | 1:R4:391:ARG:HH11 | 0.94 | 1.10 |
| 2:W9:7:ILE:HG13 | 2:W9:66:ILE:HB | 1.33 | 1.10 |
| 2:2P:22:GLU:OE1 | 38:8A:203:PHE:CD1 | 2.04 | 1.10 |
| 2:3B:22:GLU:OE1 | 38:8D:203:PHE:CD1 | 2.05 | 1.10 |
| 1:N2:248:ALA:HA | 1:N2:252:LYS:HD2 | 1.20 | 1.09 |
| 2:0L:313:MET:HE1 | 2:0L:346:TRP:HZ2 | 1.12 | 1.09 |
| 14:5L:115:GLU:O | 14:5L:134:VAL:HG11 | 1.52 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:291:ALA:HB1 | 15:5O:297:MET:HE1 | 1.31 | 1.09 |
| 26:7E:138:THR:HG22 | 26:7E:139:PRO:HD2 | 1.24 | 1.09 |
| 2:8:26:LEU:O | 24:6W:93:ARG:NH1 | 1.82 | 1.09 |
| 2:E5:282:TYR:OH | 22:6K:81:ASN:HA | 1.48 | 1.09 |
| 2:A2:221:ARG:O | 26:7F:77:ILE:O | 1.69 | 1.09 |
| 2:I1:121:ARG:HG2 | 2:I1:121:ARG:HH11 | 1.12 | 1.09 |
| 24:6X:316:ASP:OD2 | 24:6X:317:PRO:CD | 1.99 | 1.09 |
| 1:W8:56:GLY:HA2 | 8:4W:395:ARG:HD3 | 1.35 | 1.08 |
| 2:K9:85:GLN:OE1 | 30:7K:134:HIS:ND1 | 1.86 | 1.08 |
| 2:2N:123:ARG:HH12 | 38:8D:78:ASP:HB3 | 1.01 | 1.08 |
| 1:3C:355:ASP:OD1 | 38:8D:198:THR:HG22 | 1.54 | 1.08 |
| 24:6X:451:LYS:HD2 | 24:6X:468:ARG:CZ | 1.83 | 1.08 |
| 29:7J:390:LEU:HB3 | 29:7J:391:PRO:CD | 1.83 | 1.08 |
| 1:H2:218:THR:OG1 | 24:6T:488:ARG:O | 1.69 | 1.08 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:NH2 | 1.69 | 1.08 |
| 2:M3:42:ILE:HD12 | 2:M3:42:ILE:H | 1.19 | 1.07 |
| 2:P3:274:PRO:HG3 | 2:P3:286:LEU:HD21 | 1.27 | 1.07 |
| 1:2I:118:ASP:OD2 | 38:8C:99:THR:HB | 1.51 | 1.07 |
| 14:5M:219:LEU:HD11 | 14:5M:228:PHE:CE2 | 1.90 | 1.07 |
| 26:7D:138:THR:HG22 | 26:7D:139:PRO:HD2 | 1.11 | 1.07 |
| 2:1V:88:HIS:CD2 | 2:1V:89:PRO:HD2 | 1.89 | 1.07 |
| 2:2Z:282:TYR:CE1 | 10:5C:435:LEU:HD21 | 1.89 | 1.07 |
| 38:8D:206:PRO:HG2 | 38:8D:209:HIS:CE1 | 1.90 | 1.07 |
| 1:X0:42:LEU:HB2 | 8:4X:97:PHE:CE2 | 1.89 | 1.07 |
| 2:2Z:282:TYR:HE1 | 10:5C:435:LEU:CD2 | 1.67 | 1.07 |
| 38:8B:165:LYS:HD2 | 38:8B:165:LYS:H | 1.19 | 1.07 |
| 2:B9:279:GLU:CD | 18:6C:43:ASN:HD21 | 1.55 | 1.07 |
| 2:G7:90:GLU:HB3 | 2:G7:121:ARG:HH12 | 0.96 | 1.07 |
| 1:I2:218:THR:CG2 | 24:6Y:488:ARG:O | 2.01 | 1.07 |
| 2:1V:121:ARG:HH11 | 2:1V:121:ARG:HG2 | 1.11 | 1.07 |
| 2:A2:423:GLU:OE2 | 4:4G:108:TYR:CE1 | 2.07 | 1.07 |
| 2:2P:282:TYR:OH | 10:5C:164:ASP:OD2 | 1.73 | 1.07 |
| 1:K8:248:ALA:HA | 1:K8:252:LYS:HD3 | 1.30 | 1.06 |
| 2:1N:313:MET:CE | 2:1N:346:TRP:CH2 | 2.33 | 1.06 |
| 2:2T:308:ARG:NH2 | 38:8A:28:THR:HG22 | 1.70 | 1.06 |
| 2:J7:277:SER:HB2 | 2:J7:280:LYS:HZ2 | 0.96 | 1.06 |
| 2:M3:36:MET:HG3 | 2:M3:37:PRO:HD2 | 1.15 | 1.06 |
| 1:S0:91:VAL:HG11 | 1:S0:116:VAL:HG12 | 1.36 | 1.06 |
| 1:2Q:340:TYR:OH | 38:8A:95:LYS:O | 1.73 | 1.06 |
| 2:8:42:ILE:HD12 | 24:6W:93:ARG:NH2 | 1.49 | 1.06 |
| 38:8A:82:ASP:HB3 | 38:8A:112:ILE:HD13 | 1.38 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:8:220:GLU:CG | 26:7E:81:LYS:NZ | 2.19 | 1.06 |
| 1:S6:248:ALA:HA | 1:S6:252:LYS:HD3 | 1.36 | 1.06 |
| 17:5V:174:SER:OG | 17:5V:175:PRO:HD2 | 1.55 | 1.06 |
| 29:7J:319:ILE:HG22 | 29:7J:320:PRO:HD2 | 1.07 | 1.06 |
| 2:8:370:LYS:HE3 | 24:6W:92:ASP:OD1 | 1.45 | 1.05 |
| 1:A3:44:LEU:HD11 | 18:6C:36:ASN:O | 1.56 | 1.05 |
| 2:J7:80:THR:HB | 29:7J:390:LEU:CD2 | 1.85 | 1.05 |
| 2:W9:10:GLY:HA2 | 2:W9:69:ASP:OD2 | 1.55 | 1.05 |
| 2:1R:313:MET:CE | 2:1R:346:TRP:CH2 | 2.38 | 1.05 |
| 1:H6:276:ARG:NE | 24:6V:490:THR:O | 1.90 | 1.05 |
| 7:4S:12:ASP:OD1 | 7:4S:13:PRO:HD2 | 1.56 | 1.05 |
| 14:5L:116:ARG:HH11 | 14:5L:116:ARG:HB3 | 1.22 | 1.05 |
| 31:7M:80:PRO:HD2 | 31:7M:83:THR:OG1 | 1.57 | 1.05 |
| 1:2Q:306:ARG:CZ | 38:8A:96:GLY:CA | 2.34 | 1.05 |
| 1:2Q:306:ARG:CZ | 38:8A:99:THR:O | 2.04 | 1.05 |
| 1:E8:276:ARG:NH2 | 24:6X:313:SER:O | 1.89 | 1.05 |
| 26:7D:138:THR:HG22 | 26:7D:139:PRO:CD | 1.86 | 1.05 |
| 1:I4:218:THR:CB | 24:6Z:488:ARG:O | 2.05 | 1.04 |
| 26:7F:138:THR:HG22 | 26:7F:139:PRO:HD2 | 1.35 | 1.04 |
| 1:G6:78:SER:HB2 | 24:6Y:499:GLU:OE1 | 1.57 | 1.04 |
| 2:V1:88:HIS:HD2 | 2:V1:89:PRO:HD2 | 1.20 | 1.04 |
| 2:0Z:88:HIS:CD2 | 2:0Z:89:PRO:HD2 | 1.92 | 1.04 |
| 1:3M:391:ARG:HD2 | 2:3N:346:TRP:HB3 | 1.37 | 1.04 |
| 36:7W:32:LYS:HD3 | 36:7W:72:LEU:H | 1.20 | 1.04 |
| 1:2Y:355:ASP:OD2 | 38:8C:198:THR:HG23 | 1.55 | 1.04 |
| 1:3Q:252:LYS:HA | 1:3Q:255:VAL:HG12 | 1.34 | 1.04 |
| 2:G3:42:ILE:CG1 | 24:6W:470:ILE:HD13 | 1.88 | 1.04 |
| 2:G5:282:TYR:OH | 22:6N:134:ASN:ND2 | 1.90 | 1.04 |
| 1:U6:282:ARG:HH12 | 1:U6:288:GLU:HB3 | 1.19 | 1.04 |
| 1:W8:56:GLY:HA2 | 8:4W:395:ARG:CD | 1.86 | 1.04 |
| 2:G1:344:VAL:HG12 | 2:G1:347:CYS:HB3 | 1.39 | 1.04 |
| 1:I2:218:THR:HG23 | 24:6Y:488:ARG:O | 1.57 | 1.04 |
| 1:I2:248:ALA:HA | 1:I2:252:LYS:HD2 | 1.32 | 1.04 |
| 2:W9:7:ILE:HG22 | 2:W9:137:VAL:HG12 | 1.38 | 1.04 |
| 2:2T:308:ARG:HH21 | 38:8A:28:THR:HG22 | 1.21 | 1.04 |
| 36:7V:32:LYS:HD3 | 36:7V:72:LEU:H | 1.20 | 1.04 |
| 1:I0:218:THR:OG1 | 24:6X:489:ASN:N | 1.91 | 1.03 |
| 1:5:41:ASP:OD1 | 26:7D:25:TYR:CE2 | 2.11 | 1.03 |
| 2:J5:41:THR:HG23 | 2:J5:46:ASP:OD2 | 1.53 | 1.03 |
| 2:2Z:297:GLU:OE2 | 38:8C:74:ILE:HG22 | 1.58 | 1.03 |
| 15:5O:52:TYR:HD2 | 15:5O:55:LEU:HD21 | 1.04 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:514:TYR:HA | 24:6X:517:LEU:HD11 | 1.39 | 1.03 |
| 1:R2:92:PHE:CE1 | 24:6V:33:LEU:HD12 | 1.93 | 1.03 |
| 2:1N:313:MET:CE | 2:1N:346:TRP:HZ2 | 1.70 | 1.03 |
| 1:2I:118:ASP:HB3 | 38:8C:99:THR:CB | 1.87 | 1.03 |
| 2:3B:339:ARG:CD | 38:8C:39:LYS:HZ1 | 1.71 | 1.03 |
| 2:1F:85:GLN:O | 2:1V:283:HIS:CE1 | 2.12 | 1.03 |
| 2:2D:282:TYR:OH | 10:5A:380:ARG:HB3 | 1.59 | 1.03 |
| 2:2H:120:ASP:OD2 | 38:8B:27:HIS:CD2 | 2.11 | 1.03 |
| 1:2Q:306:ARG:CZ | 38:8A:96:GLY:H | 1.68 | 1.03 |
| 29:7I:4:LYS:HD2 | 29:7I:4:LYS:H | 1.20 | 1.03 |
| 2:J7:80:THR:HB | 29:7J:390:LEU:HD21 | 1.08 | 1.03 |
| 2:M7:285:GLN:HG3 | 30:7K:84:VAL:HG12 | 1.36 | 1.03 |
| 8:4W:468:MET:HE1 | 8:4W:470:TYR:OH | 1.57 | 1.03 |
| 1:I4:218:THR:OG1 | 24:6Z:488:ARG:C | 1.95 | 1.02 |
| 1:N2:252:LYS:HA | 1:N2:255:VAL:HG12 | 1.41 | 1.02 |
| 2:0L:313:MET:HE1 | 2:0L:346:TRP:CZ2 | 1.89 | 1.02 |
| 38:8B:85:ARG:NH1 | 38:8B:87:LYS:CD | 2.22 | 1.02 |
| 1:A3:282:ARG:O | 1:T6:54:ALA:HB1 | 1.58 | 1.02 |
| 2:0Z:58:ALA:N | 9:4Z:165:ARG:HH12 | 1.57 | 1.02 |
| 2:0Z:58:ALA:N | 9:4Z:165:ARG:NH1 | 2.07 | 1.02 |
| 1:2Y:56:GLY:CA | 38:8C:161:GLN:HG2 | 1.89 | 1.02 |
| 24:6X:514:TYR:HA | 24:6X:517:LEU:CD1 | 1.88 | 1.02 |
| 26:7F:58:ILE:HD12 | 26:7F:58:ILE:H | 1.22 | 1.02 |
| 38:8B:85:ARG:HH11 | 38:8B:87:LYS:CD | 1.71 | 1.02 |
| 2:M3:36:MET:HG3 | 2:M3:37:PRO:CD | 1.89 | 1.02 |
| 1:G6:78:SER:CB | 24:6Y:499:GLU:OE1 | 2.08 | 1.02 |
| 2:P5:88:HIS:CE1 | 2:P5:89:PRO:HD2 | 1.93 | 1.02 |
| 29:7J:344:GLU:OE2 | 29:7J:345:PRO:HD2 | 1.58 | 1.02 |
| 1:2I:118:ASP:CB | 38:8C:99:THR:HB | 1.90 | 1.01 |
| 2:E7:282:TYR:OH | 22:6L:81:ASN:HA | 1.56 | 1.01 |
| 2:2H:123:ARG:HH22 | 38:8B:37:TYR:HA | 1.22 | 1.01 |
| 1:2M:248:ALA:HA | 1:2M:252:LYS:HD3 | 1.40 | 1.01 |
| 14:5M:415:LYS:CE | 23:6R:22:MET:HB2 | 1.91 | 1.01 |
| 2:A2:40:LYS:NZ | 26:7F:45:MET:HB2 | 1.75 | 1.01 |
| 1:2Q:306:ARG:NE | 38:8A:96:GLY:CA | 2.23 | 1.01 |
| 14:5L:115:GLU:O | 14:5L:134:VAL:CG1 | 2.08 | 1.01 |
| 1:2I:118:ASP:HB3 | 38:8C:99:THR:HG21 | 1.36 | 1.01 |
| 7:4R:112:MET:HG3 | 7:4R:113:PRO:HD2 | 1.40 | 1.01 |
| 1:E6:52:ASN:HB3 | 22:6L:181:ASN:HD21 | 1.22 | 1.00 |
| 2:0X:56:THR:HB | 2:0X:60:LYS:HB3 | 1.43 | 1.00 |
| 2:0Z:58:ALA:H | 9:4Z:165:ARG:NH1 | 1.59 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2Q:320:ARG:NH2 | 38:8A:198:THR:CG2 | 2.22 | 1.00 |
| 2:0L:313:MET:HE3 | 2:0L:346:TRP:HZ2 | 1.26 | 1.00 |
| 1:2Y:306:ARG:HD3 | 38:8C:96:GLY:HA2 | 1.38 | 1.00 |
| 15:5O:99:LYS:CE | 15:5O:203:ASN:ND2 | 2.22 | 1.00 |
| 2:8:42:ILE:HD12 | 24:6W:93:ARG:HH22 | 1.04 | 1.00 |
| 2:E5:282:TYR:CD2 | 22:6K:82:LEU:HD21 | 1.96 | 1.00 |
| 2:W9:88:HIS:CD2 | 2:W9:121:ARG:NH2 | 2.28 | 1.00 |
| 15:5O:34:GLU:OE2 | 15:5O:49:ARG:CD | 2.10 | 1.00 |
| 2:E5:282:TYR:CE2 | 22:6K:82:LEU:CD2 | 2.36 | 1.00 |
| 2:Q5:60:LYS:HE2 | 2:S1:283:HIS:NE2 | 1.75 | 1.00 |
| 2:K5:279:GLU:OE2 | 29:7I:24:PRO:HD3 | 1.21 | 1.00 |
| 15:5O:6:ARG:HD3 | 15:5O:27:PHE:HD2 | 0.86 | 1.00 |
| 16:5Q:173:ARG:HH11 | 16:5Q:173:ARG:HG2 | 1.27 | 1.00 |
| 1:2Q:320:ARG:HH12 | 38:8A:198:THR:CA | 1.75 | 1.00 |
| 2:M1:90:GLU:HB3 | 1:N8:281:TYR:HE2 | 1.27 | 0.99 |
| 2:1R:313:MET:HE1 | 2:1R:346:TRP:CH2 | 1.95 | 0.99 |
| 1:3S:362:LYS:HE2 | 38:8D:166:GLU:CG | 1.88 | 0.99 |
| 1:L4:56:GLY:HA2 | 29:7J:331:TYR:HB2 | 1.42 | 0.99 |
| 2:0Z:58:ALA:CA | 9:4Z:165:ARG:NH1 | 2.24 | 0.99 |
| 15:5O:99:LYS:HG3 | 15:5O:203:ASN:O | 1.61 | 0.99 |
| 15:5P:12:GLU:HB2 | 15:5P:21:LEU:HD21 | 1.42 | 0.99 |
| 2:W7:85:GLN:O | 2:Y3:283:HIS:HE1 | 1.46 | 0.99 |
| 1:X0:42:LEU:CB | 8:4X:97:PHE:CZ | 2.43 | 0.99 |
| 1:1G:388:MET:HA | 1:1G:388:MET:HE2 | 1.44 | 0.99 |
| 1:2E:95:THR:CG2 | 38:8B:83:ARG:NH1 | 2.15 | 0.99 |
| 1:I4:218:THR:HG1 | 24:6Z:488:ARG:C | 1.65 | 0.99 |
| 14:5M:511:THR:OG1 | 14:5M:531:ASP:CB | 2.10 | 0.99 |
| 2:0Z:58:ALA:N | 9:4Z:165:ARG:CZ | 2.17 | 0.99 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:CZ | 1.92 | 0.99 |
| 2:Q5:60:LYS:HE2 | 2:S1:283:HIS:CD2 | 1.98 | 0.99 |
| 2:Y3:282:TYR:HE2 | 8:4W:373:ASN:HB2 | 1.23 | 0.99 |
| 2:M3:359:PRO:CB | 30:7K:212:ARG:NH2 | 2.10 | 0.98 |
| 1:2Q:306:ARG:NE | 38:8A:96:GLY:HA3 | 1.77 | 0.98 |
| 2:2Z:308:ARG:HH22 | 38:8C:72:ASP:HB2 | 1.27 | 0.98 |
| 15:5O:52:TYR:HD2 | 15:5O:55:LEU:CD2 | 1.74 | 0.98 |
| 38:8A:86:TYR:CE2 | 38:8A:104:LYS:HG2 | 1.98 | 0.98 |
| 2:2H:120:ASP:CG | 38:8B:27:HIS:NE2 | 2.16 | 0.98 |
| 29:7J:319:ILE:HG22 | 29:7J:320:PRO:CD | 1.93 | 0.98 |
| 2:H3:88:HIS:CD2 | 2:H3:121:ARG:NH2 | 2.31 | 0.98 |
| 2:L9:90:GLU:HB3 | 1:N6:281:TYR:HE2 | 1.24 | 0.98 |
| 2:1R:313:MET:HE1 | 2:1R:346:TRP:HZ2 | 1.27 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2Y:56:GLY:HA3 | 38:8C:161:GLN:CG | 1.91 | 0.98 |
| 1:M4:86:ARG:HG3 | 2:O1:283:HIS:HE1 | 1.29 | 0.98 |
| 15:5O:6:ARG:CD | 15:5O:27:PHE:HD2 | 1.76 | 0.98 |
| 2:G3:42:ILE:CG1 | 24:6W:470:ILE:CD1 | 2.40 | 0.98 |
| 1:H6:276:ARG:CZ | 24:6V:489:ASN:O | 2.12 | 0.98 |
| 1:I4:276:ARG:CD | 24:6Z:490:THR:O | 2.11 | 0.98 |
| 2:M9:282:TYR:CD1 | 30:7K:25:ALA:CB | 2.47 | 0.98 |
| 2:U9:100:ALA:HA | 1:V0:252:LYS:HG2 | 1.46 | 0.98 |
| 2:1D:85:GLN:O | 2:1T:283:HIS:HE1 | 1.44 | 0.98 |
| 1:M6:113:ILE:HD13 | 1:M6:150:LEU:HD22 | 1.46 | 0.98 |
| 2:Q3:88:HIS:CD2 | 2:Q3:89:PRO:HD2 | 1.99 | 0.98 |
| 2:Y3:282:TYR:HD2 | 8:4W:373:ASN:ND2 | 1.43 | 0.98 |
| 2:Z5:88:HIS:HD2 | 2:Z5:89:PRO:HD2 | 0.86 | 0.98 |
| 2:E7:282:TYR:CZ | 22:6L:82:LEU:CD2 | 2.30 | 0.98 |
| 1:2Y:306:ARG:CD | 38:8C:96:GLY:HA2 | 1.93 | 0.97 |
| 15:5O:56:LYS:H | 15:5O:56:LYS:HE2 | 1.28 | 0.97 |
| 2:O3:313:MET:HG2 | 2:O3:346:TRP:CZ3 | 1.99 | 0.97 |
| 38:8A:206:PRO:HG2 | 38:8A:209:HIS:NE2 | 1.79 | 0.97 |
| 14:5M:415:LYS:HE2 | 23:6R:22:MET:HB2 | 1.46 | 0.97 |
| 1:L0:113:ILE:HD13 | 1:L0:150:LEU:HD22 | 1.45 | 0.97 |
| 2:Y3:282:TYR:CE2 | 8:4W:373:ASN:CB | 2.47 | 0.97 |
| 2:1H:344:VAL:HG23 | 2:1H:347:CYS:HB3 | 1.44 | 0.97 |
| 38:8C:83:ARG:NH2 | 38:8C:85:ARG:HD2 | 1.78 | 0.97 |
| 1:Z2:113:ILE:HD13 | 1:Z2:150:LEU:HD22 | 1.43 | 0.97 |
| 2:P5:88:HIS:ND1 | 2:P5:89:PRO:CD | 2.27 | 0.97 |
| 2:S1:88:HIS:HD2 | 2:S1:89:PRO:HD2 | 1.29 | 0.97 |
| 5:4L:290:GLN:HE21 | 28:7H:309:ALA:HB1 | 1.28 | 0.97 |
| 7:4T:184:LEU:HD23 | 31:7M:78:HIS:ND1 | 1.79 | 0.97 |
| 20:6F:27:LEU:HD12 | 30:7K:3:LEU:HD12 | 1.47 | 0.97 |
| 2:2Z:297:GLU:OE1 | 38:8C:74:ILE:HG22 | 1.64 | 0.97 |
| 12:5F:271:LEU:HD23 | 12:7B:23:MET:HG2 | 1.47 | 0.97 |
| 1:A3:219:THR:OG1 | 26:7F:142:PHE:CE2 | 2.13 | 0.96 |
| 1:H6:276:ARG:NH1 | 24:6V:490:THR:HA | 1.80 | 0.96 |
| 2:1V:91:GLN:HA | 2:1V:121:ARG:HH12 | 1.27 | 0.96 |
| 2:E5:282:TYR:CD1 | 22:6K:82:LEU:HD22 | 1.95 | 0.96 |
| 1:M2:113:ILE:HD13 | 1:M2:150:LEU:HD22 | 1.47 | 0.96 |
| 2:N7:85:GLN:O | 2:P5:283:HIS:CE1 | 2.17 | 0.96 |
| 2:V1:88:HIS:CD2 | 2:V1:89:PRO:HD2 | 2.01 | 0.96 |
| 2:0L:313:MET:HE3 | 2:0L:346:TRP:CZ2 | 1.97 | 0.96 |
| 1:3S:362:LYS:HE2 | 38:8D:166:GLU:HG3 | 1.46 | 0.96 |
| 1:I0:218:THR:OG1 | 24:6X:489:ASN:CB | 2.13 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P4:71:GLY:HA3 | 27:7G:184:LYS:HA | 1.46 | 0.96 |
| 15:5O:12:GLU:OE1 | 15:5O:74:LYS:HE2 | 1.65 | 0.96 |
| 2:G7:90:GLU:HB3 | 2:G7:121:ARG:NH1 | 1.79 | 0.96 |
| 15:5P:329:PRO:CG | 15:5P:335:GLY:CA | 2.43 | 0.96 |
| 1:K8:113:ILE:HD13 | 1:K8:150:LEU:HD22 | 1.45 | 0.96 |
| 15:5O:145:PHE:CZ | 15:5O:200:LYS:NZ | 2.34 | 0.96 |
| 1:M4:86:ARG:HG3 | 2:O1:283:HIS:CE1 | 2.01 | 0.96 |
| 1:M6:75:SER:HA | 15:5P:48:LYS:HE3 | 0.97 | 0.96 |
| 2:Z5:88:HIS:CD2 | 2:Z5:89:PRO:CD | 2.49 | 0.96 |
| 2:J5:41:THR:HG21 | 2:J5:46:ASP:OD2 | 1.64 | 0.96 |
| 2:2J:88:HIS:ND1 | 2:2J:89:PRO:HD2 | 1.80 | 0.96 |
| 2:M3:359:PRO:HB2 | 30:7K:212:ARG:HH21 | 0.80 | 0.96 |
| 2:J7:218:ASP:OD2 | 2:J7:280:LYS:NZ | 1.97 | 0.95 |
| 1:M6:46:ARG:NH1 | 37:7Y:115:CYS:SG | 2.39 | 0.95 |
| 2:W9:9:ILE:HG22 | 2:W9:146:GLY:HA2 | 1.45 | 0.95 |
| 2:W9:88:HIS:HA | 2:Y5:283:HIS:CE1 | 2.01 | 0.95 |
| 1:2U:59:TYR:OH | 38:8B:182:ASN:OD1 | 1.84 | 0.95 |
| 2:2N:161:TYR:HE1 | 38:8D:80:TYR:HB2 | 1.31 | 0.95 |
| 1:2Q:306:ARG:NE | 38:8A:96:GLY:O | 1.99 | 0.95 |
| 1:2U:77:ARG:NH2 | 17:5T:197:GLN:O | 1.99 | 0.95 |
| 2:3B:339:ARG:HE | 38:8C:39:LYS:HZ3 | 0.98 | 0.95 |
| 2:M9:282:TYR:HD1 | 30:7K:25:ALA:HB2 | 1.28 | 0.95 |
| 1:2Q:113:ILE:HD13 | 1:2Q:150:LEU:HD22 | 1.45 | 0.95 |
| 2:A2:370:LYS:CD | 24:6Y:92:ASP:OD1 | 2.14 | 0.95 |
| 15:5O:34:GLU:CD | 15:5O:49:ARG:HD3 | 1.86 | 0.95 |
| 24:6X:315:ARG:HG2 | 24:6X:315:ARG:HH11 | 1.27 | 0.95 |
| 26:7D:59:ARG:NH2 | 26:7D:59:ARG:HB2 | 1.82 | 0.95 |
| 2:M3:279:GLU:OE1 | 30:7K:197:ARG:CG | 2.15 | 0.95 |
| 2:0Z:58:ALA:CA | 9:4Z:165:ARG:HH12 | 1.77 | 0.95 |
| 1:2I:121:ARG:HD2 | 38:8C:98:TYR:O | 1.66 | 0.95 |
| 38:8C:30:GLN:HE21 | 38:8C:31:GLU:HG2 | 1.29 | 0.95 |
| 2:2H:90:GLU:HB3 | 2:2H:121:ARG:HH22 | 1.30 | 0.95 |
| 15:5O:284:VAL:HG11 | 25:7C:80:ARG:HE | 1.31 | 0.95 |
| 1:R8:111:GLU:HG3 | 13:5J:119:VAL:HG11 | 1.48 | 0.94 |
| 15:5P:329:PRO:HG2 | 15:5P:335:GLY:HA3 | 1.47 | 0.94 |
| 2:A2:29:GLY:C | 26:7F:45:MET:HE1 | 1.79 | 0.94 |
| 2:W9:88:HIS:HB3 | 2:W9:91:GLN:HB2 | 1.48 | 0.94 |
| 1:1E:248:ALA:HA | 1:1E:252:LYS:HD3 | 1.47 | 0.94 |
| 26:7D:58:ILE:HD12 | 26:7D:58:ILE:H | 1.32 | 0.94 |
| 2:E7:282:TYR:CE1 | 22:6L:82:LEU:HD23 | 2.03 | 0.94 |
| 14:5M:363:PHE:CE1 | 14:5M:377:ARG:HD2 | 2.02 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M3:359:PRO:HG2 | 30:7K:212:ARG:NH2 | 1.81 | 0.94 |
| 2:2H:96:LYS:NZ | 38:8B:5:LYS:O | 2.00 | 0.94 |
| 1:5:337:ASN:HD21 | 3:3Z:69:TYR:H | 1.13 | 0.94 |
| 1:A3:227:HIS:HE1 | 26:7F:133:PHE:O | 1.46 | 0.94 |
| 2:M9:35:GLN:OE1 | 2:M9:40:LYS:NZ | 1.99 | 0.94 |
| 2:O3:313:MET:SD | 2:O3:346:TRP:HH2 | 1.91 | 0.94 |
| 2:P5:42:ILE:HD11 | 27:7G:213:TRP:CE3 | 2.03 | 0.94 |
| 2:W9:10:GLY:CA | 2:W9:69:ASP:OD2 | 2.14 | 0.94 |
| 2:3B:121:ARG:HD2 | 2:3B:125:LEU:HG | 1.49 | 0.93 |
| 26:7D:138:THR:CG2 | 26:7D:139:PRO:HD2 | 1.96 | 0.93 |
| 1:X0:42:LEU:CG | 8:4X:97:PHE:CZ | 2.51 | 0.93 |
| 1:0Y:207:LEU:HD11 | 1:0Y:229:ILE:HD11 | 1.48 | 0.93 |
| 15:5O:62:LEU:CD2 | 15:5O:77:GLU:HA | 1.96 | 0.93 |
| 15:5P:329:PRO:CG | 15:5P:335:GLY:HA2 | 1.98 | 0.93 |
| 1:E2:77:ARG:HH22 | 24:6U:426:LEU:HB2 | 1.26 | 0.93 |
| 2:2Z:88:HIS:ND1 | 2:2Z:89:PRO:HD2 | 1.84 | 0.93 |
| 2:A2:40:LYS:HZ1 | 26:7F:45:MET:HB2 | 1.25 | 0.93 |
| 2:2Z:297:GLU:OE2 | 38:8C:74:ILE:N | 2.02 | 0.93 |
| 15:5O:52:TYR:CD2 | 15:5O:55:LEU:CD2 | 2.50 | 0.93 |
| 22:6L:170:ARG:O | 22:6L:174:GLU:HG3 | 1.69 | 0.93 |
| 2:M7:285:GLN:HG3 | 30:7K:84:VAL:CG1 | 1.99 | 0.93 |
| 2:2H:120:ASP:CG | 38:8B:27:HIS:HE2 | 1.72 | 0.93 |
| 2:2P:358:GLN:HE22 | 38:8A:212:PRO:HB2 | 1.30 | 0.93 |
| 20:6F:361:LEU:CD1 | 20:6F:362:PRO:HD2 | 1.97 | 0.93 |
| 14:5L:188:ALA:HA | 14:5L:226:VAL:HG12 | 1.48 | 0.93 |
| 38:8B:85:ARG:HH12 | 38:8B:87:LYS:HD3 | 1.30 | 0.93 |
| 2:B2:85:GLN:NE2 | 18:5Z:210:GLU:OE2 | 2.01 | 0.93 |
| 2:M1:90:GLU:HB3 | 1:N8:281:TYR:CE2 | 2.03 | 0.93 |
| 2:0Z:58:ALA:HB3 | 9:4Z:165:ARG:HH11 | 1.10 | 0.93 |
| 14:5M:363:PHE:CD1 | 14:5M:377:ARG:HD2 | 2.04 | 0.93 |
| 26:7E:138:THR:CG2 | 26:7E:139:PRO:HD2 | 1.98 | 0.93 |
| 2:M9:35:GLN:CD | 2:M9:40:LYS:NZ | 2.21 | 0.93 |
| 2:0Z:56:THR:HG23 | 2:0Z:60:LYS:HB3 | 1.48 | 0.93 |
| 2:2Z:282:TYR:CE1 | 10:5C:435:LEU:CD2 | 2.48 | 0.93 |
| 15:5O:226:ARG:HG2 | 15:5O:226:ARG:HH11 | 1.34 | 0.93 |
| 2:O3:313:MET:SD | 2:O3:346:TRP:CH2 | 2.62 | 0.93 |
| 26:7E:138:THR:HG22 | 26:7E:139:PRO:CD | 1.97 | 0.93 |
| 2:G3:88:HIS:HD2 | 2:G3:89:PRO:HD2 | 1.21 | 0.92 |
| 2:J7:277:SER:CB | 2:J7:280:LYS:NZ | 2.31 | 0.92 |
| 2:L9:90:GLU:HB3 | 1:N6:281:TYR:CE2 | 2.03 | 0.92 |
| 1:3O:77:ARG:HH21 | 3:4F:19:LEU:HD23 | 1.31 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:337:ASN:HD21 | 3:3X:68:SER:HA | 1.33 | 0.92 |
| 1:M6:37:HIS:CE1 | 15:5P:295:ASN:ND2 | 2.37 | 0.92 |
| 1:1M:248:ALA:HA | 1:1M:252:LYS:HD3 | 1.49 | 0.92 |
| 1:2I:118:ASP:CB | 38:8C:99:THR:CG2 | 2.45 | 0.92 |
| 28:7H:410:HIS:HB3 | 28:7H:413:TYR:HB2 | 1.51 | 0.92 |
| 1:T6:92:PHE:O | 24:7A:35:TYR:OH | 1.86 | 0.92 |
| 26:7F:58:ILE:HD12 | 26:7F:58:ILE:N | 1.84 | 0.92 |
| 28:7X:410:HIS:HB3 | 28:7X:413:TYR:HB2 | 1.51 | 0.92 |
| 2:3B:22:GLU:OE1 | 38:8D:203:PHE:HD1 | 1.45 | 0.92 |
| 2:A2:223:THR:HG21 | 26:7F:111:ASP:OD1 | 1.67 | 0.92 |
| 2:J3:357:TYR:CB | 16:5Q:173:ARG:NE | 1.95 | 0.92 |
| 1:3K:77:ARG:HH21 | 3:4B:19:LEU:HD23 | 1.33 | 0.92 |
| 2:G5:282:TYR:CZ | 22:6N:134:ASN:ND2 | 2.37 | 0.92 |
| 2:3P:130:THR:OG1 | 3:4F:170:GLU:OE2 | 1.88 | 0.92 |
| 2:8:85:GLN:HE22 | 18:6A:78:LEU:HD13 | 1.25 | 0.92 |
| 2:I9:37:PRO:HB2 | 28:7H:401:THR:OG1 | 1.69 | 0.92 |
| 2:2H:88:HIS:CE1 | 2:2H:90:GLU:HB2 | 2.05 | 0.92 |
| 1:K4:113:ILE:HD13 | 1:K4:150:LEU:HD22 | 1.50 | 0.92 |
| 17:5V:174:SER:OG | 17:5V:175:PRO:CD | 2.17 | 0.92 |
| 1:A3:337:ASN:HD21 | 3:4H:68:SER:HA | 1.31 | 0.92 |
| 2:M7:221:ARG:HH21 | 30:7K:62:GLU:HB2 | 1.33 | 0.92 |
| 1:W0:202:LEU:HD23 | 1:W0:229:ILE:HD13 | 1.52 | 0.92 |
| 1:2A:111:GLU:OE2 | 38:8A:83:ARG:NH2 | 2.02 | 0.92 |
| 1:I4:276:ARG:NH1 | 24:6Z:490:THR:C | 2.24 | 0.91 |
| 1:2U:58:ARG:HB3 | 1:2U:58:ARG:NH1 | 1.85 | 0.91 |
| 17:5V:178:ARG:NH2 | 17:5V:229:LEU:O | 2.03 | 0.91 |
| 1:Y6:58:ARG:HG3 | 1:Y6:58:ARG:HH21 | 1.35 | 0.91 |
| 2:0Z:57:GLY:C | 9:4Z:165:ARG:HH22 | 1.73 | 0.91 |
| 1:3K:280:GLN:HG2 | 38:8B:162:VAL:HG22 | 1.52 | 0.91 |
| 1:H4:218:THR:OG1 | 24:6U:488:ARG:HB2 | 1.69 | 0.91 |
| 1:2Y:306:ARG:HD3 | 38:8C:96:GLY:CA | 1.98 | 0.91 |
| 1:I0:218:THR:CG2 | 24:6X:489:ASN:H | 1.83 | 0.91 |
| 2:0Z:58:ALA:O | 9:4Z:165:ARG:CZ | 2.18 | 0.91 |
| 1:1U:248:ALA:HA | 1:1U:252:LYS:HD3 | 1.49 | 0.91 |
| 2:Y3:157:LEU:HD11 | 2:Y3:166:LYS:HD3 | 1.53 | 0.91 |
| 2:2N:123:ARG:NH1 | 38:8D:78:ASP:HB3 | 1.85 | 0.91 |
| 2:J7:282:TYR:HD1 | 5:4M:209:LEU:HD21 | 1.11 | 0.91 |
| 2:T3:56:THR:HG23 | 2:T3:60:LYS:HB3 | 1.52 | 0.91 |
| 26:7F:138:THR:CG2 | 26:7F:139:PRO:HD2 | 2.01 | 0.91 |
| 2:G3:42:ILE:HG13 | 24:6W:470:ILE:HD13 | 1.47 | 0.91 |
| 2:M3:36:MET:CG | 2:M3:37:PRO:HD2 | 2.01 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6M:108:ARG:HD2 | 24:6X:285:MET:SD | 2.10 | 0.91 |
| 1:O2:79:GLY:CA | 37:7Y:191:ARG:NH2 | 2.34 | 0.91 |
| 1:I0:218:THR:HG21 | 24:6X:489:ASN:H | 1.36 | 0.91 |
| 2:J9:96:LYS:NZ | 28:7X:464:VAL:O | 2.03 | 0.91 |
| 2:2H:282:TYR:OH | 10:5B:164:ASP:OD1 | 1.87 | 0.91 |
| 2:J7:282:TYR:CE1 | 5:4M:209:LEU:CD2 | 2.52 | 0.91 |
| 2:N9:119:LEU:HD23 | 2:N9:122:ILE:HD11 | 1.53 | 0.91 |
| 2:2T:358:GLN:HE22 | 38:8B:212:PRO:HB2 | 1.34 | 0.90 |
| 1:I4:218:THR:HG23 | 24:6Z:488:ARG:O | 1.68 | 0.90 |
| 1:S4:46:ARG:HH21 | 1:S4:49:VAL:HB | 1.35 | 0.90 |
| 1:2I:118:ASP:HB3 | 38:8C:99:THR:HG22 | 1.53 | 0.90 |
| 1:2Y:320:ARG:NH2 | 38:8C:198:THR:HA | 1.86 | 0.90 |
| 15:5P:332:PRO:HG3 | 15:5P:350:ASP:C | 1.91 | 0.90 |
| 2:0Z:88:HIS:HD2 | 2:0Z:89:PRO:HD2 | 1.31 | 0.90 |
| 2:K1:224:TYR:HA | 2:K1:227:LEU:HD12 | 1.50 | 0.90 |
| 2:N3:386:GLU:HB2 | 2:N3:390:ARG:HH21 | 1.34 | 0.90 |
| 2:M3:362:VAL:HG11 | 2:M3:368:LEU:HB2 | 1.52 | 0.90 |
| 2:Z5:83:TYR:HB3 | 2:Z5:86:LEU:HB3 | 1.53 | 0.90 |
| 15:5O:208:SER:HB3 | 15:5O:217:GLU:OE1 | 1.70 | 0.90 |
| 2:A2:40:LYS:HZ3 | 26:7F:46:ASN:H | 1.18 | 0.90 |
| 1:I0:218:THR:OG1 | 24:6X:489:ASN:CA | 2.20 | 0.90 |
| 1:0C:113:ILE:HD13 | 1:0C:150:LEU:HD22 | 1.53 | 0.90 |
| 1:0M:393:ALA:HB2 | 2:0N:346:TRP:HE1 | 0.75 | 0.90 |
| 26:7F:132:SER:HA | 26:7F:135:LYS:HE2 | 1.54 | 0.90 |
| 38:8A:91:GLN:HB3 | 38:8A:102:PHE:HD1 | 1.30 | 0.90 |
| 2:A2:279:GLU:OE2 | 26:7F:82:PRO:HG2 | 1.70 | 0.90 |
| 2:Y5:157:LEU:HD21 | 2:Y5:166:LYS:HD3 | 1.53 | 0.90 |
| 1:3M:77:ARG:HH21 | 3:4D:19:LEU:HD23 | 1.37 | 0.90 |
| 14:5M:219:LEU:HD11 | 14:5M:228:PHE:HD2 | 1.34 | 0.90 |
| 38:8D:78:ASP:OD2 | 38:8D:79:PRO:HD2 | 1.70 | 0.90 |
| 2:O1:221:ARG:NH2 | 37:7Y:249:PHE:O | 2.04 | 0.90 |
| 1:R2:92:PHE:CD1 | 24:6V:33:LEU:HD12 | 2.05 | 0.90 |
| 2:1D:85:GLN:O | 2:1T:283:HIS:CE1 | 2.23 | 0.90 |
| 1:2I:118:ASP:HB3 | 38:8C:99:THR:HB | 1.52 | 0.90 |
| 2:2V:308:ARG:HH22 | 38:8B:72:ASP:HB2 | 1.34 | 0.90 |
| 15:5O:6:ARG:CD | 15:5O:27:PHE:CD2 | 2.51 | 0.90 |
| 22:6P:269:GLU:HA | 22:6P:272:ARG:HE | 1.35 | 0.90 |
| 2:M5:121:ARG:HH11 | 2:M5:121:ARG:HA | 1.35 | 0.90 |
| 2:Q9:18:ASN:HD21 | 12:7B:75:TYR:HE1 | 1.17 | 0.90 |
| 14:5M:415:LYS:HE2 | 23:6R:22:MET:CB | 2.00 | 0.90 |
| 2:J3:47:ASP:OD2 | 16:5Q:177:SER:OG | 1.90 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y8:8:GLN:HE22 | 1:Y8:63:ALA:HB1 | 1.36 | 0.89 |
| 15:5O:296:SER:HA | 15:5O:299:GLU:HG2 | 1.53 | 0.89 |
| 2:Y3:282:TYR:OH | 8:4W:370:VAL:HA | 1.72 | 0.89 |
| 2:K5:88:HIS:HB3 | 2:M1:283:HIS:ND1 | 1.88 | 0.89 |
| 10:5C:478:LEU:HD11 | 10:5C:495:GLU:HA | 1.54 | 0.89 |
| 1:W0:202:LEU:HD23 | 1:W0:229:ILE:CD1 | 2.02 | 0.89 |
| 8:4W:458:GLU:O | 8:4W:461:VAL:HG13 | 1.71 | 0.89 |
| 1:Q6:285:THR:HG22 | 1:Q6:287:PRO:HD2 | 1.52 | 0.89 |
| 1:T0:252:LYS:HA | 1:T0:255:VAL:HG12 | 1.54 | 0.89 |
| 2:Z7:66:ILE:HD12 | 2:Z7:68:LEU:HD11 | 1.55 | 0.89 |
| 17:5S:106:THR:O | 17:5S:110:VAL:HG23 | 1.71 | 0.89 |
| 1:Q4:285:THR:HG22 | 1:Q4:287:PRO:HD2 | 1.54 | 0.89 |
| 2:T5:264:ARG:NH1 | 2:T5:431:ASP:OD2 | 2.04 | 0.89 |
| 14:5N:208:TYR:CB | 14:5N:220:GLN:HE21 | 1.84 | 0.89 |
| 29:7J:253:ASN:HB3 | 30:7L:341:ARG:HH22 | 1.36 | 0.89 |
| 2:S5:264:ARG:NH1 | 2:S5:431:ASP:OD1 | 2.06 | 0.89 |
| 14:5N:210:TYR:HE1 | 14:5N:220:GLN:HG3 | 1.26 | 0.89 |
| 38:8A:91:GLN:CB | 38:8A:102:PHE:CD1 | 2.54 | 0.89 |
| 4:4I:35:LYS:NZ | 3:4J:254:LYS:O | 2.06 | 0.89 |
| 2:8:220:GLU:HG2 | 26:7E:81:LYS:NZ | 1.54 | 0.89 |
| 2:2D:282:TYR:OH | 10:5A:380:ARG:CB | 2.21 | 0.89 |
| 2:Z5:88:HIS:HD2 | 2:Z5:89:PRO:CD | 1.82 | 0.89 |
| 2:M7:285:GLN:HE21 | 30:7K:84:VAL:HG11 | 1.35 | 0.88 |
| 2:Q3:56:THR:HG22 | 2:Q3:60:LYS:HB3 | 1.53 | 0.88 |
| 29:7J:390:LEU:CB | 29:7J:391:PRO:CD | 2.51 | 0.88 |
| 2:G7:88:HIS:CD2 | 2:G7:89:PRO:HD2 | 2.08 | 0.88 |
| 1:W6:175:VAL:HG12 | 1:W6:205:GLU:HG2 | 1.56 | 0.88 |
| 2:I9:88:HIS:ND1 | 2:I9:89:PRO:HD2 | 1.88 | 0.88 |
| 2:L3:89:PRO:CB | 29:7J:320:PRO:CG | 2.52 | 0.88 |
| 1:R4:424:GLN:HE22 | 17:5T:104:PHE:H | 1.22 | 0.88 |
| 2:M3:359:PRO:CG | 30:7K:212:ARG:HH21 | 1.81 | 0.88 |
| 2:P5:42:ILE:CD1 | 27:7G:213:TRP:CZ3 | 2.56 | 0.88 |
| 2:2N:161:TYR:HE1 | 38:8D:80:TYR:CB | 1.86 | 0.88 |
| 14:5N:210:TYR:CE1 | 14:5N:220:GLN:CG | 2.54 | 0.88 |
| 1:1G:207:LEU:HD11 | 1:1G:229:ILE:HD11 | 1.56 | 0.88 |
| 1:2A:418:LEU:HG | 1:2A:422:TYR:HE2 | 1.39 | 0.88 |
| 24:6U:81:THR:O | 26:7D:59:ARG:NH1 | 2.06 | 0.88 |
| 2:I1:121:ARG:HG2 | 2:I1:121:ARG:NH1 | 1.80 | 0.88 |
| 1:I2:252:LYS:HA | 1:I2:255:VAL:HG12 | 1.54 | 0.88 |
| 2:M7:89:PRO:HG2 | 19:6E:25:VAL:CG1 | 2.04 | 0.88 |
| 2:2Z:121:ARG:HH11 | 2:2Z:121:ARG:CG | 1.87 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L3:84:ARG:NH1 | 29:7J:345:PRO:HA | 1.89 | 0.87 |
| 2:W9:5:ILE:HD12 | 2:W9:125:LEU:HD23 | 1.57 | 0.87 |
| 2:1V:121:ARG:HD2 | 2:1V:121:ARG:O | 1.74 | 0.87 |
| 2:2P:84:ARG:HB3 | 38:8A:188:ARG:HH12 | 1.39 | 0.87 |
| 7:4R:8:VAL:HG22 | 7:4R:9:PRO:HD2 | 1.56 | 0.87 |
| 7:4S:3:ARG:HG2 | 7:4S:3:ARG:HH11 | 1.38 | 0.87 |
| 2:M7:89:PRO:CB | 19:6E:25:VAL:HG11 | 2.03 | 0.87 |
| 1:R4:391:ARG:HG3 | 1:R4:391:ARG:NH1 | 1.74 | 0.87 |
| 1:X6:7:ILE:HB | 1:X6:135:VAL:HG12 | 1.55 | 0.87 |
| 1:0M:391:ARG:HD3 | 2:0N:346:TRP:HB2 | 1.56 | 0.87 |
| 15:5P:329:PRO:HG2 | 15:5P:335:GLY:CA | 2.03 | 0.87 |
| 1:N2:113:ILE:HD13 | 1:N2:150:LEU:HD22 | 1.56 | 0.87 |
| 24:6X:444:ILE:C | 24:6X:445:ILE:HD12 | 1.95 | 0.87 |
| 2:J9:72:PRO:HG3 | 1:K0:1:MET:HG2 | 1.54 | 0.87 |
| 2:S5:88:HIS:HB3 | 2:S5:91:GLN:HG3 | 1.57 | 0.87 |
| 2:1Z:88:HIS:HB3 | 2:1Z:91:GLN:HG3 | 1.56 | 0.87 |
| 1:G8:248:ALA:HA | 1:G8:252:LYS:HD3 | 1.53 | 0.87 |
| 15:5O:289:LEU:N | 15:5O:290:PRO:HD2 | 1.89 | 0.87 |
| 15:5P:329:PRO:HG3 | 15:5P:335:GLY:CA | 2.02 | 0.87 |
| 18:6D:5:VAL:HG11 | 18:6D:62:GLU:HG2 | 1.56 | 0.87 |
| 24:6X:463:THR:O | 24:6X:467:ARG:HG3 | 1.74 | 0.87 |
| 1:B3:362:LYS:HG2 | 24:6W:108:GLU:HG3 | 1.56 | 0.87 |
| 1:K8:248:ALA:CA | 1:K8:252:LYS:HD3 | 2.05 | 0.87 |
| 2:T1:88:HIS:HB2 | 2:T1:91:GLN:HB2 | 1.56 | 0.87 |
| 38:8A:73:TRP:CZ2 | 38:8A:76:ASP:HB3 | 2.09 | 0.87 |
| 2:8:220:GLU:CG | 26:7E:81:LYS:HZ3 | 1.82 | 0.87 |
| 2:8:370:LYS:HE3 | 24:6W:92:ASP:CG | 1.83 | 0.87 |
| 1:H4:175:VAL:HG22 | 2:H5:329:ASN:HD21 | 1.38 | 0.87 |
| 2:N7:121:ARG:HG3 | 2:N7:121:ARG:NH2 | 1.88 | 0.87 |
| 1:R4:391:ARG:HH11 | 1:R4:391:ARG:CG | 1.85 | 0.87 |
| 2:0V:347:CYS:SG | 2:0V:347:CYS:O | 2.32 | 0.87 |
| 5:4M:294:SER:HA | 28:7X:306:LEU:HD11 | 1.55 | 0.87 |
| 15:5P:34:GLU:OE2 | 15:5P:49:ARG:HG2 | 1.75 | 0.87 |
| 1:J6:212:PHE:HE1 | 2:J7:326:LYS:HE3 | 1.40 | 0.87 |
| 1:J8:40:SER:CA | 29:7J:388:MET:HG2 | 2.05 | 0.87 |
| 2:X5:301:MET:HE1 | 2:X5:307:PRO:HD3 | 1.55 | 0.87 |
| 2:A2:370:LYS:HE2 | 24:6Y:92:ASP:OD1 | 1.75 | 0.86 |
| 2:Y3:282:TYR:CE2 | 8:4W:373:ASN:HB2 | 2.10 | 0.86 |
| 37:7Y:115:CYS:SG | 37:7Y:115:CYS:O | 2.33 | 0.86 |
| 1:2Q:320:ARG:NH1 | 38:8A:198:THR:CG2 | 2.37 | 0.86 |
| 2:B9:221:ARG:NH2 | 18:6C:27:ASP:O | 2.06 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2U:58:ARG:HB3 | 1:2U:58:ARG:HH11 | 1.38 | 0.86 |
| 24:6Z:130:MET:HE1 | 24:6Z:174:ILE:HD11 | 1.57 | 0.86 |
| 26:7F:63:LEU:HD22 | 26:7F:63:LEU:H | 1.39 | 0.86 |
| 1:I0:218:THR:CG2 | 24:6X:489:ASN:HA | 2.05 | 0.86 |
| 2:1V:121:ARG:HH11 | 2:1V:121:ARG:CG | 1.87 | 0.86 |
| 2:A2:29:GLY:HA2 | 26:7F:45:MET:SD | 2.15 | 0.86 |
| 1:I4:218:THR:HG21 | 24:6Z:488:ARG:O | 1.74 | 0.86 |
| 1:X0:40:SER:HG | 8:4X:97:PHE:HD2 | 0.90 | 0.86 |
| 2:1B:347:CYS:SG | 2:1B:347:CYS:O | 2.33 | 0.86 |
| 1:2A:121:ARG:NH2 | 38:8A:100:SER:OG | 2.08 | 0.86 |
| 1:K8:248:ALA:HA | 1:K8:252:LYS:CD | 2.04 | 0.86 |
| 1:E6:52:ASN:OD1 | 22:6L:181:ASN:ND2 | 2.08 | 0.86 |
| 1:I4:276:ARG:CZ | 24:6Z:490:THR:O | 2.22 | 0.86 |
| 1:2M:173:PRO:HD2 | 1:2M:380:ARG:HE | 1.40 | 0.86 |
| 1:A3:219:THR:CB | 26:7F:142:PHE:CE2 | 2.59 | 0.86 |
| 5:4L:290:GLN:HE21 | 28:7H:309:ALA:CB | 1.89 | 0.86 |
| 26:7F:119:MET:HA | 26:7F:119:MET:CE | 2.05 | 0.86 |
| 1:O2:79:GLY:HA2 | 37:7Y:191:ARG:NH2 | 1.88 | 0.86 |
| 2:R5:56:THR:HG23 | 2:R5:60:LYS:HB3 | 1.57 | 0.86 |
| 2:G3:88:HIS:CD2 | 2:G3:89:PRO:CD | 2.58 | 0.86 |
| 2:0H:60:LYS:HD3 | 2:0H:88:HIS:CE1 | 2.10 | 0.86 |
| 1:2Q:77:ARG:NH2 | 17:5S:197:GLN:O | 2.08 | 0.86 |
| 8:4V:391:GLU:HG3 | 8:4V:395:ARG:HH11 | 1.40 | 0.86 |
| 10:5A:287:VAL:HA | 10:5A:290:LYS:HD2 | 1.58 | 0.86 |
| 1:Q8:233:MET:HA | 1:Q8:236:ILE:HD12 | 1.58 | 0.85 |
| 1:T2:375:GLN:HB3 | 1:T2:422:TYR:HD2 | 1.40 | 0.85 |
| 2:8:220:GLU:CG | 26:7E:81:LYS:HZ2 | 1.83 | 0.85 |
| 1:R8:175:VAL:HG22 | 2:R9:329:ASN:HD21 | 1.42 | 0.85 |
| 1:S2:80:PRO:HD3 | 7:4S:11:GLU:OE1 | 1.76 | 0.85 |
| 2:U7:88:HIS:ND1 | 2:U7:89:PRO:HD2 | 1.91 | 0.85 |
| 1:0U:207:LEU:HD11 | 1:0U:229:ILE:HD11 | 1.56 | 0.85 |
| 1:1M:375:GLN:HB2 | 1:1M:419:VAL:HG23 | 1.56 | 0.85 |
| 2:2N:161:TYR:CE1 | 38:8D:80:TYR:CB | 2.59 | 0.85 |
| 7:4R:112:MET:HG3 | 7:4R:113:PRO:CD | 2.06 | 0.85 |
| 24:6W:41:ARG:HE | 24:6W:41:ARG:HA | 1.40 | 0.85 |
| 38:8A:82:ASP:HB2 | 38:8A:112:ILE:HG21 | 1.56 | 0.85 |
| 38:8B:201:LEU:O | 38:8B:201:LEU:HD12 | 1.76 | 0.85 |
| 2:8:220:GLU:HG3 | 26:7E:81:LYS:HZ3 | 1.40 | 0.85 |
| 1:G2:391:ARG:HG3 | 1:G2:391:ARG:HH11 | 1.39 | 0.85 |
| 1:H2:276:ARG:HB2 | 24:6T:490:THR:HG21 | 1.57 | 0.85 |
| 1:I0:219:THR:HG21 | 24:6X:488:ARG:HD2 | 1.58 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I7:370:LYS:HD2 | 5:4L:263:LEU:HD22 | 1.59 | 0.85 |
| 2:M9:282:TYR:HD1 | 30:7K:25:ALA:CB | 1.84 | 0.85 |
| 1:T0:248:ALA:CA | 1:T0:252:LYS:HD2 | 2.05 | 0.85 |
| 14:5M:594:HIS:H | 14:5M:620:PHE:HE2 | 1.21 | 0.85 |
| 1:U2:220:PRO:HD2 | 2:U3:326:LYS:HD3 | 1.57 | 0.85 |
| 2:V3:154:LEU:HD22 | 2:V3:197:HIS:HB3 | 1.58 | 0.85 |
| 7:4R:301:ARG:HG2 | 7:4R:301:ARG:NH2 | 1.86 | 0.85 |
| 15:5O:203:ASN:H | 15:5O:203:ASN:HD22 | 1.24 | 0.85 |
| 24:6X:519:VAL:HG13 | 24:6X:533:LEU:O | 1.75 | 0.85 |
| 1:G6:78:SER:OG | 24:6Y:499:GLU:OE1 | 1.94 | 0.85 |
| 1:L4:44:LEU:CD2 | 29:7J:339:GLN:OE1 | 2.25 | 0.85 |
| 1:O2:280:GLN:NE2 | 37:7Y:211:PRO:O | 2.08 | 0.85 |
| 2:0N:102:ASN:HD21 | 2:0N:411:GLU:HG3 | 1.42 | 0.85 |
| 1:1U:16:ILE:HD11 | 1:1U:136:CYS:HB3 | 1.57 | 0.85 |
| 2:2Z:121:ARG:HH11 | 2:2Z:121:ARG:HG2 | 1.41 | 0.85 |
| 2:3F:220:GLU:HG2 | 38:8A:177:HIS:HB2 | 1.56 | 0.85 |
| 15:5P:326:LEU:O | 15:5P:326:LEU:HD12 | 1.76 | 0.85 |
| 22:6J:65:ARG:HE | 22:6J:101:ASN:HB3 | 1.41 | 0.85 |
| 1:Q8:46:ARG:HG2 | 1:Q8:241:ARG:HA | 1.58 | 0.85 |
| 14:5L:594:HIS:H | 14:5L:620:PHE:HE2 | 1.21 | 0.85 |
| 1:5:219:THR:OG1 | 26:7D:142:PHE:CD1 | 2.05 | 0.85 |
| 14:5N:594:HIS:H | 14:5N:620:PHE:HE2 | 1.21 | 0.85 |
| 1:L6:41:ASP:OD1 | 29:7J:167:ILE:HD11 | 1.74 | 0.85 |
| 1:N0:87:PRO:HD2 | 2:O7:283:HIS:HB2 | 1.58 | 0.85 |
| 2:3B:22:GLU:OE1 | 38:8D:203:PHE:CE1 | 2.29 | 0.85 |
| 17:5U:178:ARG:O | 17:5U:182:VAL:HG22 | 1.77 | 0.85 |
| 1:0E:390:ARG:HH21 | 1:0E:390:ARG:HB3 | 1.42 | 0.85 |
| 1:0Y:54:ALA:HB3 | 1:0Y:58:ARG:HB3 | 1.58 | 0.85 |
| 1:2Q:320:ARG:HH12 | 38:8A:198:THR:N | 1.73 | 0.85 |
| 14:5L:188:ALA:HA | 14:5L:226:VAL:CG1 | 2.07 | 0.85 |
| 1:1:337:ASN:HD21 | 3:3V:69:TYR:H | 1.20 | 0.85 |
| 2:B0:59:GLY:HA3 | 24:6U:263:ARG:HH11 | 1.42 | 0.85 |
| 2:L3:84:ARG:HH12 | 29:7J:345:PRO:CA | 1.88 | 0.85 |
| 2:M5:88:HIS:CD2 | 2:M5:89:PRO:HD2 | 2.11 | 0.85 |
| 2:P5:42:ILE:HD11 | 27:7G:213:TRP:HZ3 | 1.33 | 0.85 |
| 2:Y5:56:THR:HG22 | 2:0B:285:GLN:HB2 | 1.58 | 0.85 |
| 2:3B:85:GLN:O | 2:3R:283:HIS:CE1 | 2.30 | 0.85 |
| 15:5P:331:ASP:OD1 | 15:5P:331:ASP:N | 2.09 | 0.85 |
| 16:5Q:15:VAL:HG13 | 16:5Q:151:MET:HE1 | 1.56 | 0.85 |
| 2:W1:88:HIS:CD2 | 2:W1:90:GLU:HB3 | 2.12 | 0.84 |
| 1:1W:55:THR:HG21 | 1:2M:284:LEU:HD23 | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J7:282:TYR:HE1 | 5:4M:210:ASP:OD1 | 1.56 | 0.84 |
| 2:K9:76:ASP:OD2 | 1:L0:46:ARG:NH2 | 2.11 | 0.84 |
| 2:2H:120:ASP:OD1 | 38:8B:27:HIS:NE2 | 2.09 | 0.84 |
| 15:5O:176:ILE:HG22 | 15:5O:205:CYS:SG | 2.17 | 0.84 |
| 18:6B:27:ASP:OD1 | 18:6B:27:ASP:N | 2.05 | 0.84 |
| 1:S0:92:PHE:CD2 | 24:6Z:40:GLN:NE2 | 2.44 | 0.84 |
| 12:5F:271:LEU:CD2 | 12:7B:23:MET:HG2 | 2.06 | 0.84 |
| 14:5M:219:LEU:CD1 | 14:5M:228:PHE:CE2 | 2.60 | 0.84 |
| 18:6C:27:ASP:OD1 | 18:6C:27:ASP:N | 2.05 | 0.84 |
| 1:V6:2:ARG:HB2 | 1:V6:46:ARG:HH22 | 1.43 | 0.84 |
| 18:6A:27:ASP:OD1 | 18:6A:27:ASP:N | 2.05 | 0.84 |
| 2:N5:88:HIS:HE1 | 2:N5:90:GLU:HB2 | 1.41 | 0.84 |
| 2:W1:224:TYR:HB2 | 1:W2:245:GLN:HE21 | 1.43 | 0.84 |
| 1:1K:242:PHE:HB3 | 1:1K:356:ILE:HD13 | 1.56 | 0.84 |
| 1:2I:220:PRO:HD2 | 2:2J:326:LYS:HD2 | 1.59 | 0.84 |
| 8:4W:463:THR:HG21 | 8:4X:128:LEU:CD1 | 2.07 | 0.84 |
| 14:5N:208:TYR:CD1 | 14:5N:220:GLN:NE2 | 2.45 | 0.84 |
| 15:5O:6:ARG:HH11 | 15:5O:27:PHE:HE2 | 1.24 | 0.84 |
| 18:5Y:27:ASP:OD1 | 18:5Y:27:ASP:N | 2.05 | 0.84 |
| 2:E5:282:TYR:CD2 | 22:6K:82:LEU:CD2 | 2.59 | 0.84 |
| 1:S0:150:LEU:HD11 | 17:5U:58:PRO:HB3 | 1.59 | 0.84 |
| 2:3R:130:THR:OG1 | 3:4H:170:GLU:OE2 | 1.94 | 0.84 |
| 15:5O:213:THR:O | 15:5O:217:GLU:HG2 | 1.77 | 0.84 |
| 23:6R:28:LYS:HA | 23:6R:28:LYS:HE2 | 1.59 | 0.84 |
| 1:3I:77:ARG:HH21 | 3:3Z:19:LEU:HD23 | 1.42 | 0.84 |
| 2:K1:133:GLN:HE22 | 2:K1:251:ASP:HB2 | 1.42 | 0.84 |
| 1:M2:418:LEU:HG | 1:M2:422:TYR:HE2 | 1.43 | 0.84 |
| 2:M7:284:GLU:OE2 | 2:M7:285:GLN:O | 1.96 | 0.84 |
| 1:S2:125:GLU:OE2 | 1:S2:159:TYR:OH | 1.96 | 0.84 |
| 2:W5:56:THR:HG22 | 2:Y1:285:GLN:HB2 | 1.59 | 0.84 |
| 1:W8:113:ILE:HD13 | 1:W8:150:LEU:HD22 | 1.60 | 0.84 |
| 1:1C:388:MET:HE2 | 2:1D:348:PRO:HD2 | 1.58 | 0.84 |
| 14:5M:219:LEU:CD1 | 14:5M:228:PHE:CD2 | 2.56 | 0.84 |
| 14:5N:225:ARG:HB3 | 14:5N:227:LEU:HD13 | 1.59 | 0.84 |
| 18:6D:27:ASP:OD1 | 18:6D:27:ASP:N | 2.05 | 0.84 |
| 2:A2:226:ASN:OD1 | 26:7F:78:ALA:HB1 | 1.78 | 0.84 |
| 1:B5:362:LYS:NZ | 18:6A:24:ARG:HD3 | 1.91 | 0.84 |
| 1:K0:220:PRO:HD2 | 2:K1:326:LYS:HD2 | 1.59 | 0.84 |
| 2:N5:88:HIS:CE1 | 2:N5:90:GLU:HB2 | 2.11 | 0.84 |
| 2:1L:121:ARG:HG2 | 2:1L:121:ARG:NH1 | 1.87 | 0.84 |
| 1:2Q:320:ARG:HH12 | 38:8A:198:THR:HA | 1.42 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z0:207:LEU:HD11 | 1:Z0:229:ILE:HD11 | 1.60 | 0.84 |
| 1:Z4:113:ILE:HD13 | 1:Z4:150:LEU:HD22 | 1.58 | 0.84 |
| 2:1L:88:HIS:HD2 | 2:2B:283:HIS:HB3 | 1.41 | 0.84 |
| 3:4B:60:PRO:HG2 | 3:4B:102:PRO:HB3 | 1.60 | 0.84 |
| 3:4F:60:PRO:HG2 | 3:4F:102:PRO:HB3 | 1.60 | 0.84 |
| 18:5Z:27:ASP:OD1 | 18:5Z:27:ASP:N | 2.05 | 0.84 |
| 24:6X:483:PHE:HB2 | 24:6X:496:LYS:HA | 1.60 | 0.84 |
| 1:1:306:ARG:NH1 | 3:3V:60:PRO:O | 2.10 | 0.83 |
| 1:1G:375:GLN:HB2 | 1:1G:419:VAL:HG13 | 1.60 | 0.83 |
| 2:2D:156:ARG:NH2 | 38:8A:29:GLY:O | 2.11 | 0.83 |
| 18:5X:27:ASP:OD1 | 18:5X:27:ASP:N | 2.05 | 0.83 |
| 37:7Y:55:LEU:HD12 | 37:7Y:55:LEU:O | 1.77 | 0.83 |
| 2:O5:90:GLU:HA | 2:O5:90:GLU:OE2 | 1.78 | 0.83 |
| 1:R2:94:GLN:NE2 | 13:5I:18:ARG:HA | 1.92 | 0.83 |
| 1:1U:165:LEU:HD21 | 1:1U:250:LEU:HD21 | 1.59 | 0.83 |
| 3:3X:60:PRO:HG2 | 3:3X:102:PRO:HB3 | 1.61 | 0.83 |
| 2:W7:90:GLU:HB3 | 2:W7:121:ARG:HH12 | 1.42 | 0.83 |
| 1:2E:95:THR:HG21 | 38:8B:83:ARG:HH12 | 0.68 | 0.83 |
| 3:4H:60:PRO:HG2 | 3:4H:102:PRO:HB3 | 1.60 | 0.83 |
| 15:5O:59:LEU:HD12 | 15:5O:59:LEU:O | 1.78 | 0.83 |
| 26:7E:58:ILE:HD12 | 26:7E:58:ILE:H | 1.41 | 0.83 |
| 26:7F:138:THR:HG22 | 26:7F:139:PRO:CD | 2.07 | 0.83 |
| 2:G3:42:ILE:HD11 | 24:6W:470:ILE:HD11 | 0.85 | 0.83 |
| 2:M7:90:GLU:N | 1:O4:281:TYR:OH | 2.11 | 0.83 |
| 1:R2:94:GLN:HE22 | 13:5I:18:ARG:CA | 1.90 | 0.83 |
| 2:X7:157:LEU:HD11 | 2:X7:166:LYS:HD3 | 1.61 | 0.83 |
| 3:3V:60:PRO:HG2 | 3:3V:102:PRO:HB3 | 1.61 | 0.83 |
| 3:3Z:60:PRO:HG2 | 3:3Z:102:PRO:HB3 | 1.60 | 0.83 |
| 3:4D:60:PRO:HG2 | 3:4D:102:PRO:HB3 | 1.60 | 0.83 |
| 4:4G:35:LYS:NZ | 3:4H:254:LYS:O | 2.11 | 0.83 |
| 17:5U:174:SER:CB | 17:5U:175:PRO:HD2 | 2.08 | 0.83 |
| 38:8C:36:GLU:OE1 | 38:8C:39:LYS:CE | 2.26 | 0.83 |
| 1:M0:86:ARG:HB3 | 2:N7:283:HIS:CE1 | 2.14 | 0.83 |
| 1:M6:1:MET:HE1 | 37:7Y:116:MET:HB2 | 1.58 | 0.83 |
| 2:W9:88:HIS:HA | 2:Y5:283:HIS:NE2 | 1.92 | 0.83 |
| 15:5O:226:ARG:HH11 | 15:5O:226:ARG:CG | 1.91 | 0.83 |
| 20:6F:73:GLN:HB2 | 20:6F:292:VAL:HB | 1.61 | 0.83 |
| 24:6X:514:TYR:CA | 24:6X:517:LEU:CD1 | 2.56 | 0.83 |
| 24:6X:558:LEU:HD22 | 24:6X:608:GLN:HB3 | 1.58 | 0.83 |
| 2:G7:90:GLU:CB | 2:G7:121:ARG:HH12 | 1.86 | 0.83 |
| 1:1O:16:ILE:HD11 | 1:1O:136:CYS:HB3 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H3:56:THR:HA | 2:I9:285:GLN:HB2 | 1.60 | 0.83 |
| 2:M1:84:ARG:NH2 | 27:7G:111:TYR:O | 2.11 | 0.83 |
| 1:S0:92:PHE:CE2 | 24:6Z:33:LEU:HD23 | 2.11 | 0.83 |
| 2:M9:35:GLN:CD | 2:M9:40:LYS:HZ2 | 1.82 | 0.83 |
| 2:M9:279:GLU:OE1 | 2:M9:279:GLU:N | 2.12 | 0.83 |
| 2:P9:398:MET:HG2 | 1:Q0:345:ILE:HD13 | 1.61 | 0.83 |
| 22:6M:59:PRO:HB3 | 22:6M:108:ARG:NH2 | 1.94 | 0.83 |
| 2:K5:219:ILE:CG2 | 29:7I:14:LEU:CD1 | 2.42 | 0.83 |
| 1:Y2:248:ALA:HA | 1:Y2:252:LYS:HD3 | 1.61 | 0.83 |
| 2:1P:284:GLU:HA | 2:1P:284:GLU:OE1 | 1.77 | 0.83 |
| 1:2Q:320:ARG:NH1 | 38:8A:198:THR:HG23 | 1.94 | 0.83 |
| 1:3C:35:THR:HG21 | 38:8D:161:GLN:HE22 | 1.44 | 0.83 |
| 2:3F:130:THR:OG1 | 3:3V:170:GLU:OE2 | 1.95 | 0.83 |
| 2:S7:42:ILE:HG13 | 2:S7:43:GLY:H | 1.42 | 0.83 |
| 1:0K:388:MET:HE3 | 2:0L:348:PRO:HD3 | 1.60 | 0.83 |
| 24:6V:547:LYS:HG2 | 24:6V:554:ASP:HB3 | 1.60 | 0.83 |
| 1:F8:276:ARG:HD3 | 24:6U:410:PHE:HA | 1.58 | 0.82 |
| 29:7J:388:MET:HA | 29:7J:388:MET:CE | 2.09 | 0.82 |
| 2:Z9:9:ILE:HG13 | 2:Z9:139:ASN:HB3 | 1.60 | 0.82 |
| 1:1O:248:ALA:HA | 1:1O:252:LYS:HD3 | 1.60 | 0.82 |
| 1:2S:77:ARG:HH22 | 38:8B:220:VAL:HA | 1.44 | 0.82 |
| 7:4U:187:THR:HG21 | 31:7N:78:HIS:CE1 | 2.14 | 0.82 |
| 24:6Z:130:MET:SD | 24:6Z:166:PHE:CZ | 2.72 | 0.82 |
| 2:P5:269:LEU:HD22 | 2:P5:303:VAL:HG11 | 1.60 | 0.82 |
| 2:Y9:298:PRO:HA | 2:Y9:301:MET:HG3 | 1.60 | 0.82 |
| 26:7D:138:THR:CG2 | 26:7D:139:PRO:CD | 2.56 | 0.82 |
| 1:Q4:396:HIS:HA | 1:Q4:399:THR:HG22 | 1.60 | 0.82 |
| 1:U8:113:ILE:HD13 | 1:U8:150:LEU:HD22 | 1.61 | 0.82 |
| 2:0H:102:ASN:HD21 | 2:0H:411:GLU:HG3 | 1.44 | 0.82 |
| 2:1Z:123:ARG:NH1 | 38:7Z:35:GLU:OE2 | 2.12 | 0.82 |
| 2:4:280:LYS:HZ2 | 26:7D:64:PRO:HG2 | 1.39 | 0.82 |
| 2:A2:82:THR:HG23 | 26:7F:118:SER:HB2 | 1.62 | 0.82 |
| 1:2K:211:CYS:HA | 1:2K:215:LEU:HB2 | 1.60 | 0.82 |
| 14:5L:116:ARG:HB3 | 14:5L:116:ARG:NH1 | 1.93 | 0.82 |
| 17:5S:178:ARG:NH2 | 17:5S:229:LEU:O | 2.12 | 0.82 |
| 24:6X:451:LYS:CG | 24:6X:468:ARG:HH12 | 1.92 | 0.82 |
| 34:7R:230:SER:HB2 | 35:7T:184:LEU:HD22 | 1.60 | 0.82 |
| 1:Q8:235:GLY:HA3 | 1:Q8:366:THR:HG21 | 1.62 | 0.82 |
| 2:R5:85:GLN:O | 2:T1:283:HIS:HE1 | 1.62 | 0.82 |
| 1:V8:7:ILE:HB | 1:V8:135:VAL:HG12 | 1.60 | 0.82 |
| 2:1F:90:GLU:HB3 | 2:1F:121:ARG:HH12 | 1.44 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:5F:378:LYS:NZ | 12:7B:40:GLU:OE2 | 2.13 | 0.82 |
| 2:2:396:ASP:OD1 | 4:3W:53:ASN:ND2 | 2.12 | 0.82 |
| 2:M3:283:HIS:NE2 | 30:7K:199:TYR:OH | 2.07 | 0.82 |
| 1:X0:42:LEU:HD23 | 8:4X:97:PHE:CE2 | 2.14 | 0.82 |
| 1:Z0:379:LYS:HD3 | 1:Z0:419:VAL:HG21 | 1.60 | 0.82 |
| 2:1D:56:THR:HA | 2:1T:285:GLN:HB2 | 1.61 | 0.82 |
| 1:2E:95:THR:CB | 38:8B:83:ARG:NH1 | 2.43 | 0.82 |
| 1:2Q:306:ARG:CZ | 38:8A:96:GLY:C | 2.47 | 0.82 |
| 15:5P:333:GLU:HG3 | 30:7K:106:LEU:HD23 | 1.62 | 0.82 |
| 2:P9:176:GLN:HE22 | 2:P9:304:LYS:HE2 | 1.43 | 0.82 |
| 1:T8:418:LEU:HG | 1:T8:422:TYR:HE2 | 1.42 | 0.82 |
| 2:X3:56:THR:HG22 | 2:Y9:285:GLN:HB2 | 1.61 | 0.82 |
| 1:S0:92:PHE:CD2 | 24:6Z:33:LEU:HD23 | 2.14 | 0.82 |
| 2:U9:9:ILE:HG22 | 2:U9:68:LEU:HD11 | 1.62 | 0.82 |
| 2:V1:56:THR:HG23 | 2:V1:60:LYS:HB3 | 1.62 | 0.82 |
| 2:W1:85:GLN:O | 2:X7:283:HIS:NE2 | 2.12 | 0.82 |
| 2:1V:245:ASP:HA | 2:1V:249:ASN:HD21 | 1.43 | 0.82 |
| 1:O2:7:ILE:HB | 1:O2:135:VAL:HG12 | 1.61 | 0.81 |
| 2:X7:88:HIS:HB3 | 2:Z3:283:HIS:CE1 | 2.15 | 0.81 |
| 2:Z1:9:ILE:HG13 | 2:Z1:139:ASN:HB3 | 1.62 | 0.81 |
| 2:Z1:242:LEU:HD12 | 2:Z1:252:ILE:HD11 | 1.62 | 0.81 |
| 18:5X:5:VAL:HG11 | 18:5X:62:GLU:HG2 | 1.62 | 0.81 |
| 24:6Z:130:MET:SD | 24:6Z:166:PHE:HZ | 2.03 | 0.81 |
| 2:A0:43:GLY:HA2 | 24:6X:124:TYR:HE2 | 1.43 | 0.81 |
| 2:A2:40:LYS:NZ | 26:7F:46:ASN:H | 1.78 | 0.81 |
| 1:T4:173:PRO:HB3 | 1:T4:384:GLN:HE22 | 1.45 | 0.81 |
| 2:Z9:352:LYS:NZ | 2:Z9:353:CYS:O | 2.14 | 0.81 |
| 1:0I:33:THR:O | 1:0I:58:ARG:NH2 | 2.10 | 0.81 |
| 2:1Z:88:HIS:HD2 | 2:1Z:89:PRO:HD2 | 1.40 | 0.81 |
| 2:2N:161:TYR:CE1 | 38:8D:80:TYR:HB3 | 2.15 | 0.81 |
| 10:5C:477:LYS:HB3 | 10:5D:154:MET:HE1 | 1.62 | 0.81 |
| 15:5O:6:ARG:NH1 | 15:5O:27:PHE:CE2 | 2.48 | 0.81 |
| 15:5O:36:GLU:OE2 | 15:5O:49:ARG:HG2 | 1.79 | 0.81 |
| 1:5:337:ASN:ND2 | 3:3Z:69:TYR:H | 1.77 | 0.81 |
| 1:H6:276:ARG:NH1 | 24:6V:489:ASN:O | 2.14 | 0.81 |
| 1:I2:175:VAL:HG12 | 2:I3:329:ASN:HD21 | 1.45 | 0.81 |
| 2:P5:56:THR:HG23 | 2:P5:60:LYS:HB3 | 1.61 | 0.81 |
| 2:U9:154:LEU:HD22 | 2:U9:197:HIS:HB3 | 1.63 | 0.81 |
| 1:1W:375:GLN:HB2 | 1:1W:419:VAL:HG13 | 1.61 | 0.81 |
| 17:5T:227:ARG:O | 17:5T:230:GLU:HG3 | 1.79 | 0.81 |
| 24:6T:558:LEU:HD22 | 24:6T:608:GLN:HB3 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6V:6:PRO:N | 24:6V:7:PRO:CD | 2.42 | 0.81 |
| 1:O8:220:PRO:HD2 | 2:O9:326:LYS:HD3 | 1.61 | 0.81 |
| 1:0Y:53:GLU:OE2 | 1:0Y:53:GLU:HA | 1.79 | 0.81 |
| 2:G3:85:GLN:HA | 2:G3:85:GLN:NE2 | 1.90 | 0.81 |
| 1:I4:276:ARG:HH11 | 24:6Z:490:THR:C | 1.83 | 0.81 |
| 2:L3:276:ILE:HD11 | 2:L3:281:ALA:HA | 1.60 | 0.81 |
| 1:M2:220:PRO:HD2 | 2:M3:326:LYS:HD3 | 1.60 | 0.81 |
| 2:V9:255:PHE:HA | 2:V9:259:LEU:HD13 | 1.61 | 0.81 |
| 2:W7:154:LEU:HD22 | 2:W7:197:HIS:HB3 | 1.63 | 0.81 |
| 1:0G:11:GLN:NE2 | 39:0G:501:GDP:O1A | 2.14 | 0.81 |
| 2:2H:88:HIS:CE1 | 2:2H:90:GLU:CB | 2.63 | 0.81 |
| 14:5N:511:THR:HB | 14:5N:531:ASP:HB3 | 1.63 | 0.81 |
| 22:6P:138:ASP:HA | 22:6P:141:LYS:HD2 | 1.61 | 0.81 |
| 1:J4:113:ILE:HG13 | 1:J4:150:LEU:HD22 | 1.60 | 0.81 |
| 2:K7:88:HIS:HD1 | 2:K7:89:PRO:HD2 | 1.45 | 0.81 |
| 1:T4:173:PRO:HG2 | 1:T4:380:ARG:HH21 | 1.45 | 0.81 |
| 2:U3:154:LEU:HD22 | 2:U3:197:HIS:HB3 | 1.61 | 0.81 |
| 2:V1:264:ARG:NH2 | 2:V1:431:ASP:OD2 | 2.14 | 0.81 |
| 2:0N:234:VAL:HG21 | 2:0N:302:MET:HE1 | 1.62 | 0.81 |
| 1:0W:249:ASP:H | 1:0W:252:LYS:HD2 | 1.45 | 0.81 |
| 2:2L:101:ASN:OD1 | 1:2M:252:LYS:HE3 | 1.81 | 0.81 |
| 2:2P:262:TYR:HB2 | 2:2P:265:ILE:HG12 | 1.61 | 0.81 |
| 2:2Z:308:ARG:NH2 | 38:8C:72:ASP:HB2 | 1.96 | 0.81 |
| 1:5:227:HIS:NE2 | 26:7D:133:PHE:O | 2.12 | 0.81 |
| 2:8:29:GLY:C | 26:7E:45:MET:HE3 | 1.99 | 0.81 |
| 2:E7:282:TYR:CD2 | 22:6L:82:LEU:HD21 | 2.16 | 0.81 |
| 1:0S:237:THR:HG23 | 1:0S:241:ARG:HH21 | 1.45 | 0.81 |
| 1:I0:218:THR:HG1 | 24:6X:489:ASN:N | 1.78 | 0.81 |
| 1:I2:218:THR:HG21 | 24:6Y:488:ARG:O | 1.81 | 0.81 |
| 1:T2:245:GLN:HE21 | 12:5F:177:THR:HG21 | 1.44 | 0.81 |
| 2:U9:88:HIS:ND1 | 2:U9:89:PRO:CD | 2.41 | 0.81 |
| 1:E6:52:ASN:CG | 22:6L:181:ASN:ND2 | 2.32 | 0.81 |
| 1:G2:248:ALA:HA | 1:G2:252:LYS:HD3 | 1.62 | 0.81 |
| 1:G2:272:PRO:HB2 | 1:G2:282:ARG:HH12 | 1.43 | 0.81 |
| 1:L4:44:LEU:HD23 | 29:7J:339:GLN:OE1 | 1.78 | 0.81 |
| 2:L7:88:HIS:HB3 | 2:N3:283:HIS:ND1 | 1.96 | 0.81 |
| 2:O1:88:HIS:ND1 | 2:O1:89:PRO:HD2 | 1.94 | 0.81 |
| 1:S0:92:PHE:CZ | 24:6Z:40:GLN:HG3 | 2.16 | 0.81 |
| 1:1C:4:ILE:HB | 1:1C:50:TYR:HE1 | 1.45 | 0.81 |
| 2:2L:276:ILE:CG2 | 2:2L:281:ALA:HB2 | 2.09 | 0.81 |
| 1:3G:218:THR:OG1 | 17:5S:213:GLU:OE1 | 1.99 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:4M:76:LEU:HB2 | 15:5P:361:LEU:HD11 | 1.61 | 0.81 |
| 14:5L:112:SER:CA | 14:5L:155:PHE:HD2 | 1.94 | 0.81 |
| 1:3M:34:GLY:O | 1:3M:58:ARG:HA | 1.81 | 0.81 |
| 24:6U:469:PHE:HA | 24:6U:485:PRO:HD2 | 1.60 | 0.81 |
| 2:A2:40:LYS:NZ | 26:7F:46:ASN:N | 2.28 | 0.80 |
| 2:H3:90:GLU:HB3 | 2:H3:121:ARG:HH12 | 1.44 | 0.80 |
| 2:J3:90:GLU:HB3 | 2:J3:121:ARG:HH12 | 1.45 | 0.80 |
| 2:M5:121:ARG:HH11 | 2:M5:121:ARG:CB | 1.94 | 0.80 |
| 2:U7:154:LEU:HD22 | 2:U7:197:HIS:HB3 | 1.61 | 0.80 |
| 1:0W:55:THR:HG22 | 1:1M:284:LEU:CD1 | 2.12 | 0.80 |
| 2:2H:279:GLU:OE1 | 10:5B:167:ILE:HG12 | 1.81 | 0.80 |
| 2:L3:89:PRO:CB | 29:7J:320:PRO:HG2 | 2.10 | 0.80 |
| 2:S7:94:SER:OG | 26:7D:67:GLN:OE1 | 1.99 | 0.80 |
| 1:S8:375:GLN:HB2 | 1:S8:419:VAL:HG23 | 1.63 | 0.80 |
| 2:0H:60:LYS:HD3 | 2:0H:88:HIS:HE1 | 1.45 | 0.80 |
| 1:2Q:306:ARG:NH1 | 38:8A:95:LYS:C | 2.34 | 0.80 |
| 22:6M:63:PRO:HB2 | 24:6X:399:ILE:HG22 | 1.63 | 0.80 |
| 1:T4:390:ARG:NH1 | 1:T4:390:ARG:HB3 | 1.97 | 0.80 |
| 2:Z7:181:VAL:HG22 | 1:Z8:256:ASN:HD22 | 1.46 | 0.80 |
| 2:0V:100:ALA:HA | 1:0W:252:LYS:HG2 | 1.62 | 0.80 |
| 2:1F:85:GLN:O | 2:1V:283:HIS:HE1 | 1.58 | 0.80 |
| 2:1V:33:ASP:O | 2:1V:60:LYS:NZ | 2.15 | 0.80 |
| 2:1Z:121:ARG:HD3 | 2:1Z:121:ARG:O | 1.81 | 0.80 |
| 2:2N:250:VAL:HB | 2:2N:254:GLU:HG3 | 1.63 | 0.80 |
| 15:5O:34:GLU:CG | 15:5O:49:ARG:HD3 | 2.11 | 0.80 |
| 2:K1:277:SER:H | 2:K1:280:LYS:HZ3 | 1.29 | 0.80 |
| 2:M1:81:GLY:O | 2:M1:84:ARG:NH1 | 2.15 | 0.80 |
| 1:V6:7:ILE:HB | 1:V6:135:VAL:HG12 | 1.62 | 0.80 |
| 2:W9:274:PRO:HG3 | 2:W9:286:LEU:HD21 | 1.61 | 0.80 |
| 26:7F:146:ASN:H | 26:7F:146:ASN:HD22 | 1.29 | 0.80 |
| 2:8:29:GLY:C | 26:7E:45:MET:CE | 2.49 | 0.80 |
| 2:O3:90:GLU:HB3 | 2:O3:121:ARG:HH22 | 1.47 | 0.80 |
| 2:O5:89:PRO:HG2 | 2:Q3:279:GLU:OE1 | 1.81 | 0.80 |
| 24:6X:514:TYR:O | 24:6X:517:LEU:CD1 | 2.30 | 0.80 |
| 24:6Y:42:GLU:OE2 | 24:6Y:42:GLU:N | 2.13 | 0.80 |
| 1:B8:362:LYS:HZ3 | 18:6B:24:ARG:HD3 | 1.44 | 0.80 |
| 2:J5:282:TYR:HE1 | 5:4M:159:ILE:HD11 | 1.47 | 0.80 |
| 2:K3:154:LEU:HG | 2:K3:197:HIS:HB3 | 1.63 | 0.80 |
| 2:1F:90:GLU:CB | 2:1F:121:ARG:HH12 | 1.93 | 0.80 |
| 15:5O:99:LYS:CG | 15:5O:203:ASN:O | 2.29 | 0.80 |
| 2:A0:43:GLY:HA2 | 24:6X:124:TYR:CE2 | 2.16 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J3:48:ALA:HB2 | 16:5Q:174:THR:OG1 | 1.81 | 0.80 |
| 2:S1:22:GLU:OE2 | 12:5F:82:LYS:NZ | 2.14 | 0.80 |
| 2:X5:5:ILE:HG22 | 2:X5:64:ARG:HB3 | 1.63 | 0.80 |
| 2:1F:93:ILE:HD12 | 2:1F:117:LEU:HD21 | 1.64 | 0.80 |
| 2:1V:92:LEU:N | 2:1V:92:LEU:HD23 | 1.95 | 0.80 |
| 5:4M:293:LEU:HD12 | 28:7X:305:ALA:CB | 2.12 | 0.80 |
| 1:L4:36:TYR:O | 29:7J:335:GLU:OE2 | 1.99 | 0.80 |
| 2:P3:274:PRO:HG3 | 2:P3:286:LEU:CD2 | 2.12 | 0.80 |
| 2:3F:88:HIS:HB2 | 2:3F:91:GLN:HE22 | 1.46 | 0.80 |
| 1:I0:218:THR:HG1 | 24:6X:488:ARG:HG2 | 1.47 | 0.80 |
| 1:Y2:7:ILE:HB | 1:Y2:135:VAL:HG12 | 1.64 | 0.80 |
| 2:3B:339:ARG:CD | 38:8C:39:LYS:NZ | 2.36 | 0.80 |
| 14:5N:188:ALA:HA | 14:5N:226:VAL:HB | 1.62 | 0.80 |
| 15:5O:12:GLU:OE1 | 15:5O:74:LYS:CE | 2.30 | 0.80 |
| 26:7D:59:ARG:HB2 | 26:7D:59:ARG:HH21 | 1.43 | 0.80 |
| 1:W0:202:LEU:CD2 | 1:W0:229:ILE:HD13 | 2.12 | 0.80 |
| 1:1A:375:GLN:HB2 | 1:1A:419:VAL:HG13 | 1.63 | 0.80 |
| 1:2U:320:ARG:HH22 | 38:8B:198:THR:HA | 1.45 | 0.80 |
| 2:3H:163:LYS:HE3 | 3:3X:137:ARG:HG2 | 1.64 | 0.80 |
| 2:3P:239:THR:HG23 | 2:3P:243:ARG:HE | 1.46 | 0.80 |
| 2:3T:428:LEU:HG | 2:3T:432:PHE:CE2 | 2.16 | 0.80 |
| 2:I3:57:GLY:N | 2:J9:285:GLN:HG3 | 1.96 | 0.79 |
| 1:I8:175:VAL:HG12 | 2:I9:329:ASN:HD21 | 1.47 | 0.79 |
| 2:S7:334:THR:HG22 | 13:5H:134:PHE:H | 1.45 | 0.79 |
| 2:W1:255:PHE:HA | 2:W1:259:LEU:HD13 | 1.64 | 0.79 |
| 2:0X:399:TYR:O | 2:0X:402:ARG:NH1 | 2.15 | 0.79 |
| 1:1E:375:GLN:HB2 | 1:1E:419:VAL:HG13 | 1.64 | 0.79 |
| 2:3J:88:HIS:HB2 | 2:3J:91:GLN:HE22 | 1.47 | 0.79 |
| 29:7I:165:ARG:HH12 | 29:7I:232:ASP:HA | 1.46 | 0.79 |
| 2:M5:58:ALA:CB | 37:7Y:214:ASP:HB3 | 2.13 | 0.79 |
| 2:O1:199:ASP:HB3 | 2:O1:256:GLN:HE22 | 1.44 | 0.79 |
| 1:V6:215:LEU:HB3 | 1:V6:217:LEU:HD23 | 1.64 | 0.79 |
| 1:Z4:8:GLN:NE2 | 1:Z4:13:GLY:O | 2.15 | 0.79 |
| 1:2A:68:LEU:HB3 | 1:2A:96:GLY:HA2 | 1.63 | 0.79 |
| 2:3R:221:ARG:NH1 | 38:8D:179:ASP:OD1 | 2.14 | 0.79 |
| 24:6Y:254:SER:HA | 24:6Y:257:LEU:HD12 | 1.63 | 0.79 |
| 1:5:227:HIS:HE1 | 26:7D:133:PHE:O | 1.18 | 0.79 |
| 1:B8:362:LYS:NZ | 18:6B:24:ARG:HD3 | 1.96 | 0.79 |
| 1:R0:67:ASP:OD2 | 1:R0:72:THR:OG1 | 2.00 | 0.79 |
| 1:X4:250:LEU:HA | 1:X4:253:LEU:HD12 | 1.64 | 0.79 |
| 2:X9:56:THR:HG22 | 2:Z5:285:GLN:HB2 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1O:113:ILE:HD13 | 1:1O:150:LEU:HD22 | 1.63 | 0.79 |
| 1:2Q:306:ARG:NE | 38:8A:96:GLY:C | 2.35 | 0.79 |
| 24:6W:91:ASN:HB3 | 24:6W:94:LYS:HD2 | 1.64 | 0.79 |
| 24:6X:467:ARG:HH11 | 24:6X:484:GLU:CD | 1.84 | 0.79 |
| 1:E2:320:ARG:HH12 | 22:6J:115:SER:HA | 1.45 | 0.79 |
| 1:Q8:162:ARG:HA | 1:Q8:251:ARG:HH22 | 1.48 | 0.79 |
| 2:R5:85:GLN:O | 2:T1:283:HIS:CE1 | 2.35 | 0.79 |
| 2:S5:334:THR:HG22 | 13:5H:19:LEU:HB3 | 1.64 | 0.79 |
| 1:Z6:7:ILE:HB | 1:Z6:135:VAL:HG12 | 1.64 | 0.79 |
| 2:0H:176:GLN:HE22 | 2:0H:304:LYS:HE2 | 1.45 | 0.79 |
| 5:4M:293:LEU:HB3 | 28:7X:306:LEU:CD2 | 2.13 | 0.79 |
| 1:R8:125:GLU:OE2 | 1:R8:159:TYR:OH | 2.01 | 0.79 |
| 1:S4:396:HIS:HA | 1:S4:399:THR:HG22 | 1.64 | 0.79 |
| 1:3M:391:ARG:HH22 | 2:3N:435:VAL:HG13 | 1.46 | 0.79 |
| 2:3N:122:ILE:HA | 2:3N:125:LEU:HD12 | 1.64 | 0.79 |
| 1:3Q:252:LYS:HA | 1:3Q:255:VAL:CG1 | 2.10 | 0.79 |
| 17:5S:178:ARG:NH2 | 17:5S:232:GLY:O | 2.16 | 0.79 |
| 20:6F:31:LEU:HD11 | 30:7K:8:LEU:HD12 | 1.62 | 0.79 |
| 24:6Z:613:LYS:O | 24:6Z:617:ASP:HB2 | 1.83 | 0.79 |
| 2:G3:278:ALA:HB3 | 22:6M:215:GLY:HA2 | 1.65 | 0.79 |
| 2:H3:88:HIS:HD2 | 2:H3:121:ARG:HH22 | 1.25 | 0.79 |
| 2:J9:324:VAL:HG21 | 2:J9:326:LYS:HZ3 | 1.48 | 0.79 |
| 1:T4:282:ARG:HH21 | 1:T4:288:GLU:HG3 | 1.47 | 0.79 |
| 2:K5:279:GLU:OE2 | 29:7I:24:PRO:HD2 | 1.80 | 0.79 |
| 2:M7:89:PRO:CG | 19:6E:25:VAL:HG11 | 2.13 | 0.79 |
| 1:R4:67:ASP:OD2 | 1:R4:72:THR:OG1 | 2.01 | 0.79 |
| 2:R5:88:HIS:CD2 | 2:R5:89:PRO:HD2 | 2.17 | 0.79 |
| 2:S5:339:ARG:HB3 | 13:5H:26:ALA:HB2 | 1.65 | 0.79 |
| 2:U5:154:LEU:HD22 | 2:U5:197:HIS:HB3 | 1.63 | 0.79 |
| 2:2H:123:ARG:HH22 | 38:8B:37:TYR:CA | 1.94 | 0.79 |
| 2:2N:161:TYR:CD1 | 38:8D:80:TYR:HB3 | 2.16 | 0.79 |
| 1:3S:396:HIS:HA | 1:3S:399:THR:HG22 | 1.63 | 0.79 |
| 24:6T:470:ILE:CD1 | 24:6T:485:PRO:CG | 2.60 | 0.79 |
| 36:7W:98:VAL:O | 36:7W:102:MET:HB2 | 1.82 | 0.79 |
| 1:M6:220:PRO:HD2 | 2:M7:326:LYS:HD3 | 1.63 | 0.79 |
| 2:O1:226:ASN:HD21 | 37:7Y:250:GLN:HE22 | 1.27 | 0.79 |
| 2:P5:90:GLU:CB | 2:P5:121:ARG:HH12 | 1.94 | 0.79 |
| 1:Q4:391:ARG:HH11 | 2:Q5:346:TRP:HE1 | 1.28 | 0.79 |
| 1:Q6:113:ILE:HD13 | 1:Q6:150:LEU:HD22 | 1.63 | 0.79 |
| 1:1O:211:CYS:HA | 1:1O:215:LEU:HB2 | 1.64 | 0.79 |
| 22:6L:177:LEU:HD11 | 22:6L:252:ASP:CG | 2.03 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8A:87:LYS:O | 38:8A:87:LYS:HD2 | 1.82 | 0.79 |
| 2:E1:364:PRO:HG2 | 22:6J:123:PRO:HB2 | 1.65 | 0.79 |
| 2:H1:317:LEU:HB3 | 2:H1:319:TYR:HE1 | 1.48 | 0.79 |
| 2:Q9:280:LYS:HA | 2:Q9:283:HIS:CD2 | 2.18 | 0.79 |
| 2:T1:324:VAL:H | 7:4U:25:ARG:HH21 | 1.28 | 0.79 |
| 2:T5:56:THR:HG23 | 2:T5:60:LYS:HB3 | 1.63 | 0.79 |
| 2:Y3:9:ILE:HG12 | 2:Y3:68:LEU:HD21 | 1.64 | 0.79 |
| 1:Z4:7:ILE:HB | 1:Z4:135:VAL:HG12 | 1.64 | 0.79 |
| 2:Z5:324:VAL:HG22 | 2:Z5:326:LYS:H | 1.48 | 0.79 |
| 1:0E:390:ARG:HB3 | 1:0E:390:ARG:NH2 | 1.96 | 0.79 |
| 1:0M:5:VAL:HG23 | 1:0M:62:ARG:HG2 | 1.65 | 0.79 |
| 1:1U:4:ILE:HG22 | 1:1U:49:VAL:HG22 | 1.65 | 0.79 |
| 20:6F:125:LYS:HD2 | 20:6F:344:LEU:HD21 | 1.65 | 0.79 |
| 24:6X:451:LYS:CG | 24:6X:468:ARG:NH1 | 2.44 | 0.79 |
| 24:6X:482:ILE:HB | 24:6X:498:LEU:HB3 | 1.65 | 0.79 |
| 2:A2:29:GLY:CA | 26:7F:45:MET:CE | 2.61 | 0.79 |
| 1:R4:135:VAL:HG11 | 1:R4:152:ILE:HD11 | 1.65 | 0.79 |
| 1:X2:7:ILE:HB | 1:X2:135:VAL:HG12 | 1.64 | 0.79 |
| 1:0S:375:GLN:HB2 | 1:0S:419:VAL:HG23 | 1.65 | 0.79 |
| 1:2Q:320:ARG:HH22 | 38:8A:198:THR:HA | 1.46 | 0.79 |
| 2:J7:277:SER:CB | 2:J7:280:LYS:HZ2 | 1.84 | 0.78 |
| 2:J7:358:GLN:HE21 | 29:7J:416:HIS:HB2 | 1.46 | 0.78 |
| 2:W3:255:PHE:HA | 2:W3:259:LEU:HD13 | 1.65 | 0.78 |
| 1:X6:204:ASN:HD21 | 39:X6:502:GDP:HN22 | 1.29 | 0.78 |
| 2:Z5:265:ILE:HD11 | 2:Z5:435:VAL:HG21 | 1.64 | 0.78 |
| 19:6E:70:VAL:HG12 | 19:6E:71:ILE:HG23 | 1.64 | 0.78 |
| 24:6X:451:LYS:CD | 24:6X:468:ARG:NH1 | 1.87 | 0.78 |
| 38:8C:8:GLU:HG3 | 38:8C:21:LYS:HD3 | 1.65 | 0.78 |
| 38:8D:206:PRO:HG2 | 38:8D:209:HIS:HE1 | 1.41 | 0.78 |
| 2:4:15:GLN:NE2 | 26:7D:113:ARG:HH22 | 1.80 | 0.78 |
| 1:H2:211:CYS:HA | 1:H2:215:LEU:HB2 | 1.66 | 0.78 |
| 2:M5:121:ARG:HH11 | 2:M5:121:ARG:CA | 1.95 | 0.78 |
| 1:U2:276:ARG:HH11 | 1:U2:279:GLN:HB3 | 1.46 | 0.78 |
| 1:0W:54:ALA:HB3 | 1:0W:58:ARG:HB3 | 1.65 | 0.78 |
| 38:8A:91:GLN:CB | 38:8A:102:PHE:HD1 | 1.95 | 0.78 |
| 2:G3:90:GLU:HB3 | 2:G3:121:ARG:HH12 | 1.49 | 0.78 |
| 2:M1:275:ILE:HD12 | 2:M1:368:LEU:HD21 | 1.65 | 0.78 |
| 2:V1:132:LEU:HD22 | 2:V1:164:LYS:HD3 | 1.65 | 0.78 |
| 14:5L:116:ARG:HH11 | 14:5L:116:ARG:CB | 1.96 | 0.78 |
| 26:7F:138:THR:CG2 | 26:7F:139:PRO:CD | 2.62 | 0.78 |
| 2:I1:88:HIS:CD2 | 2:I1:89:PRO:HD2 | 2.18 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:274:PRO:HG3 | 2:W9:286:LEU:CD2 | 2.13 | 0.78 |
| 1:Y8:45:GLU:HG3 | 1:Y8:46:ARG:HG2 | 1.63 | 0.78 |
| 1:Z0:397:TRP:HE1 | 2:Z1:260:VAL:HB | 1.48 | 0.78 |
| 2:Z7:352:LYS:NZ | 2:Z7:353:CYS:O | 2.17 | 0.78 |
| 1:1C:51:PHE:O | 1:1C:62:ARG:NH2 | 2.16 | 0.78 |
| 2:1V:79:ARG:HE | 2:1V:92:LEU:HD12 | 1.48 | 0.78 |
| 14:5M:489:SER:HA | 14:5M:512:PHE:HB3 | 1.63 | 0.78 |
| 19:6E:92:ARG:HD3 | 19:6E:99:ARG:NE | 1.99 | 0.78 |
| 1:K6:113:ILE:HD13 | 1:K6:150:LEU:HD22 | 1.65 | 0.78 |
| 2:N9:56:THR:HG22 | 2:P7:285:GLN:HB2 | 1.65 | 0.78 |
| 2:V1:76:ASP:HA | 2:V1:79:ARG:HB2 | 1.65 | 0.78 |
| 1:X0:42:LEU:HD23 | 8:4X:97:PHE:CZ | 2.19 | 0.78 |
| 1:X0:42:LEU:HG | 8:4X:97:PHE:CZ | 2.17 | 0.78 |
| 2:Y1:56:THR:HG22 | 2:Z7:285:GLN:HB2 | 1.63 | 0.78 |
| 2:0H:88:HIS:HB3 | 2:0X:283:HIS:ND1 | 1.98 | 0.78 |
| 1:1C:418:LEU:HG | 1:1C:422:TYR:HE2 | 1.47 | 0.78 |
| 14:5N:107:GLN:H | 14:5N:122:GLY:HA2 | 1.47 | 0.78 |
| 37:7Y:221:ARG:HB3 | 37:7Y:231:HIS:CD2 | 2.19 | 0.78 |
| 1:1:379:LYS:HZ3 | 3:3V:49:HIS:CD2 | 1.99 | 0.78 |
| 2:8:221:ARG:NH1 | 26:7E:73:GLY:O | 2.14 | 0.78 |
| 1:1S:334:GLN:HE22 | 1:1S:348:ASN:H | 1.31 | 0.78 |
| 1:2Y:355:ASP:OD2 | 38:8C:198:THR:CG2 | 2.32 | 0.78 |
| 24:6Z:597:LEU:HB3 | 24:6Z:602:LEU:HD21 | 1.65 | 0.78 |
| 2:W9:11:GLN:OE1 | 2:W9:74:VAL:HB | 1.84 | 0.78 |
| 2:W9:154:LEU:HD22 | 2:W9:197:HIS:HB3 | 1.65 | 0.78 |
| 2:Z5:9:ILE:HG22 | 2:Z5:146:GLY:HA2 | 1.65 | 0.78 |
| 10:5C:334:ARG:NH2 | 14:5M:543:ASN:OD1 | 2.16 | 0.78 |
| 2:J7:181:VAL:HG12 | 1:J8:256:ASN:HD22 | 1.47 | 0.78 |
| 1:N2:249:ASP:OD2 | 1:N2:252:LYS:HE3 | 1.83 | 0.78 |
| 1:S0:92:PHE:HE2 | 24:6Z:40:GLN:HE21 | 0.80 | 0.78 |
| 1:S4:125:GLU:OE1 | 3:3V:66:THR:HG23 | 1.84 | 0.78 |
| 1:Y8:165:LEU:HD21 | 1:Y8:250:LEU:HD21 | 1.64 | 0.78 |
| 1:Z8:379:LYS:HD3 | 1:Z8:419:VAL:HG21 | 1.66 | 0.78 |
| 2:0H:399:TYR:O | 2:0H:402:ARG:NH1 | 2.15 | 0.78 |
| 2:0L:157:LEU:HD22 | 2:0L:166:LYS:HD3 | 1.66 | 0.78 |
| 2:0P:399:TYR:O | 2:0P:402:ARG:NH1 | 2.16 | 0.78 |
| 1:1Q:334:GLN:HE22 | 1:1Q:348:ASN:H | 1.29 | 0.78 |
| 1:3A:113:ILE:HD13 | 1:3A:150:LEU:HD22 | 1.64 | 0.78 |
| 1:3S:362:LYS:NZ | 38:8D:166:GLU:HG3 | 1.98 | 0.78 |
| 14:5L:107:GLN:H | 14:5L:122:GLY:HA2 | 1.47 | 0.78 |
| 22:6L:108:ARG:NH2 | 24:6W:284:THR:O | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:78:SER:HB2 | 24:6V:149:LYS:HG3 | 1.65 | 0.78 |
| 2:M3:359:PRO:HG2 | 30:7K:212:ARG:HH22 | 1.46 | 0.78 |
| 2:Q5:56:THR:HG23 | 2:Q5:60:LYS:HB3 | 1.65 | 0.78 |
| 2:Q5:132:LEU:HD22 | 2:Q5:164:LYS:HD3 | 1.65 | 0.78 |
| 1:S8:94:GLN:HB3 | 24:6W:35:TYR:CE1 | 2.18 | 0.78 |
| 1:X2:342:VAL:HG12 | 1:X2:348:ASN:HD21 | 1.48 | 0.78 |
| 2:1F:56:THR:HA | 2:1V:285:GLN:HB2 | 1.65 | 0.78 |
| 2:1N:313:MET:HE1 | 2:1N:346:TRP:HH2 | 1.48 | 0.78 |
| 14:5M:107:GLN:H | 14:5M:122:GLY:HA2 | 1.47 | 0.78 |
| 26:7F:21:THR:HG21 | 26:7F:120:ALA:HA | 1.65 | 0.78 |
| 31:7N:66:HIS:HD2 | 31:7N:76:THR:HA | 1.48 | 0.78 |
| 2:D7:280:LYS:NZ | 18:6D:166:HIS:HB3 | 1.98 | 0.78 |
| 2:F9:88:HIS:HB3 | 2:H5:283:HIS:ND1 | 1.99 | 0.78 |
| 1:J0:334:GLN:HE22 | 1:J0:348:ASN:H | 1.30 | 0.78 |
| 2:J7:218:ASP:OD2 | 2:J7:280:LYS:CE | 2.31 | 0.78 |
| 1:Y2:252:LYS:HE2 | 1:Y2:350:LYS:HE2 | 1.66 | 0.78 |
| 15:5O:99:LYS:NZ | 15:5O:203:ASN:HD21 | 1.81 | 0.78 |
| 22:6O:114:THR:HG23 | 22:6O:117:GLY:H | 1.46 | 0.78 |
| 2:H3:88:HIS:HD2 | 2:H3:121:ARG:HH21 | 1.30 | 0.77 |
| 1:I2:391:ARG:HD3 | 2:I3:346:TRP:HE1 | 1.48 | 0.77 |
| 2:X3:305:CYS:HB2 | 2:X3:387:ILE:HD11 | 1.66 | 0.77 |
| 2:2D:282:TYR:CZ | 10:5A:380:ARG:HD3 | 2.19 | 0.77 |
| 1:2S:334:GLN:HE22 | 1:2S:348:ASN:H | 1.30 | 0.77 |
| 2:3D:288:VAL:HG21 | 2:3D:327:ASP:HB2 | 1.64 | 0.77 |
| 6:4O:408:ARG:NH2 | 29:7J:435:THR:O | 2.17 | 0.77 |
| 24:6X:95:VAL:HG12 | 24:6X:124:TYR:HD2 | 1.49 | 0.77 |
| 24:6X:514:TYR:CA | 24:6X:517:LEU:HD11 | 2.13 | 0.77 |
| 1:R2:92:PHE:CZ | 24:6V:35:TYR:HE1 | 2.02 | 0.77 |
| 1:T2:263:LEU:HD22 | 1:T2:422:TYR:HE1 | 1.49 | 0.77 |
| 1:T6:125:GLU:OE2 | 1:T6:159:TYR:OH | 2.00 | 0.77 |
| 2:T7:88:HIS:CG | 2:T7:89:PRO:HD2 | 2.17 | 0.77 |
| 2:Z3:157:LEU:HD22 | 2:Z3:166:LYS:HD3 | 1.65 | 0.77 |
| 8:4W:468:MET:CE | 8:4W:470:TYR:OH | 2.31 | 0.77 |
| 26:7F:63:LEU:HD22 | 26:7F:63:LEU:N | 1.98 | 0.77 |
| 2:N1:90:GLU:HB3 | 1:O8:281:TYR:CE2 | 2.18 | 0.77 |
| 1:2C:418:LEU:HG | 1:2C:422:TYR:HE2 | 1.48 | 0.77 |
| 1:3I:220:PRO:HD2 | 2:3J:326:LYS:HD3 | 1.65 | 0.77 |
| 15:5O:65:VAL:HG22 | 15:5O:74:LYS:HB3 | 1.66 | 0.77 |
| 15:5P:34:GLU:CD | 15:5P:49:ARG:HE | 1.86 | 0.77 |
| 24:6V:11:LEU:HB3 | 24:6V:12:PRO:HD2 | 1.64 | 0.77 |
| 36:7W:99:GLU:O | 36:7W:103:ASN:CG | 2.22 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:219:THR:CB | 26:7D:142:PHE:CE1 | 2.67 | 0.77 |
| 1:M6:37:HIS:CE1 | 15:5P:295:ASN:HD21 | 1.98 | 0.77 |
| 1:N0:388:MET:HE2 | 2:N1:348:PRO:HD2 | 1.65 | 0.77 |
| 2:R9:364:PRO:HD3 | 33:7Q:188:ALA:HB2 | 1.65 | 0.77 |
| 2:W7:255:PHE:HA | 2:W7:259:LEU:HD13 | 1.65 | 0.77 |
| 1:0K:33:THR:O | 1:0K:58:ARG:NH2 | 2.18 | 0.77 |
| 1:3S:276:ARG:HH12 | 17:5V:219:LEU:HD13 | 1.50 | 0.77 |
| 7:4U:26:THR:HG21 | 19:6E:261:TYR:HB2 | 1.65 | 0.77 |
| 14:5L:381:PRO:HD2 | 23:6Q:59:GLY:HA3 | 1.65 | 0.77 |
| 14:5N:511:THR:HG21 | 14:5N:531:ASP:H | 1.48 | 0.77 |
| 16:5Q:88:THR:HG23 | 16:5Q:89:HIS:HD2 | 1.49 | 0.77 |
| 17:5T:189:TRP:HD1 | 17:5T:222:ILE:CG2 | 1.96 | 0.77 |
| 21:6G:65:LEU:HD12 | 21:6G:66:PRO:HD2 | 1.66 | 0.77 |
| 23:6R:13:THR:O | 23:6R:17:THR:HG23 | 1.85 | 0.77 |
| 1:E8:276:ARG:CZ | 24:6X:313:SER:O | 2.31 | 0.77 |
| 2:L3:276:ILE:CD1 | 2:L3:281:ALA:HA | 2.14 | 0.77 |
| 2:L7:119:LEU:HD11 | 2:L7:156:ARG:HD3 | 1.64 | 0.77 |
| 1:R0:45:GLU:HG3 | 1:R0:46:ARG:HG2 | 1.66 | 0.77 |
| 1:R4:217:LEU:HD22 | 7:4R:134:GLU:HB2 | 1.66 | 0.77 |
| 2:S5:33:ASP:O | 2:S5:60:LYS:NZ | 2.16 | 0.77 |
| 1:Z0:139:LEU:HD12 | 1:Z0:170:VAL:HG22 | 1.65 | 0.77 |
| 2:1R:313:MET:CE | 2:1R:346:TRP:HZ2 | 1.82 | 0.77 |
| 2:6:39:ASP:OD1 | 24:6V:187:PHE:N | 2.17 | 0.77 |
| 1:A3:219:THR:HB | 26:7F:142:PHE:CE2 | 2.17 | 0.77 |
| 1:H4:113:ILE:HA | 1:H4:116:VAL:HG22 | 1.67 | 0.77 |
| 1:H8:113:ILE:HG13 | 1:H8:150:LEU:HD22 | 1.66 | 0.77 |
| 1:L0:339:SER:H | 34:7R:140:ASN:HD21 | 1.32 | 0.77 |
| 2:O9:88:HIS:HB2 | 2:O9:91:GLN:HE22 | 1.48 | 0.77 |
| 1:P4:286:VAL:HG23 | 1:P4:287:PRO:HD3 | 1.65 | 0.77 |
| 2:Q5:308:ARG:NH1 | 2:V3:282:TYR:OH | 2.18 | 0.77 |
| 2:W3:267:PHE:HB2 | 2:W3:384:ILE:HD12 | 1.64 | 0.77 |
| 1:3S:362:LYS:HE3 | 38:8D:166:GLU:HG3 | 0.78 | 0.77 |
| 7:4T:184:LEU:CD2 | 31:7M:78:HIS:ND1 | 2.48 | 0.77 |
| 26:7D:136:PHE:HB3 | 26:7D:137:PRO:HD2 | 1.65 | 0.77 |
| 29:7I:254:MET:HE1 | 30:7K:341:ARG:HD3 | 1.66 | 0.77 |
| 1:M6:75:SER:CA | 15:5P:48:LYS:CE | 2.51 | 0.77 |
| 2:W9:88:HIS:NE2 | 2:W9:121:ARG:NH2 | 2.31 | 0.77 |
| 1:0O:134:GLN:HE21 | 1:0O:167:PHE:HE2 | 1.33 | 0.77 |
| 2:2R:195:LEU:HD11 | 2:2R:264:ARG:HH11 | 1.50 | 0.77 |
| 31:7N:80:PRO:HD2 | 31:7N:83:THR:CG2 | 2.14 | 0.77 |
| 2:G9:27:GLU:OE2 | 2:G9:243:ARG:NH1 | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J8:220:PRO:HD2 | 2:J9:326:LYS:HD3 | 1.67 | 0.77 |
| 1:M8:173:PRO:HD2 | 1:M8:380:ARG:HH21 | 1.50 | 0.77 |
| 2:Q9:176:GLN:HE22 | 2:Q9:304:LYS:HE2 | 1.49 | 0.77 |
| 1:T6:22:GLU:OE2 | 24:7A:10:LYS:NZ | 2.15 | 0.77 |
| 2:W3:88:HIS:CD2 | 2:W3:89:PRO:HD2 | 2.20 | 0.77 |
| 2:W7:276:ILE:HD11 | 2:W7:281:ALA:HA | 1.65 | 0.77 |
| 1:0G:33:THR:O | 1:0G:58:ARG:NH2 | 2.18 | 0.77 |
| 1:0G:248:ALA:HA | 1:0G:252:LYS:HD3 | 1.64 | 0.77 |
| 1:3M:272:PRO:HB2 | 1:3M:282:ARG:HH12 | 1.49 | 0.77 |
| 19:6E:92:ARG:HG3 | 19:6E:99:ARG:HE | 1.48 | 0.77 |
| 1:G4:285:THR:HG22 | 1:G4:287:PRO:HD2 | 1.65 | 0.77 |
| 1:G2:392:LYS:HE3 | 1:G2:395:LEU:HD23 | 1.64 | 0.77 |
| 2:Z3:34:GLY:HA3 | 2:Z3:60:LYS:HZ2 | 1.50 | 0.77 |
| 1:0C:97:ALA:HA | 1:0C:103:LYS:HD2 | 1.67 | 0.77 |
| 2:2Z:370:LYS:HD2 | 10:5C:433:GLU:HG3 | 1.66 | 0.77 |
| 14:5N:187:ASP:OD1 | 14:5N:187:ASP:N | 2.17 | 0.77 |
| 24:6X:514:TYR:C | 24:6X:517:LEU:CD1 | 2.54 | 0.77 |
| 2:K1:102:ASN:HB3 | 2:K1:105:ARG:HB2 | 1.67 | 0.76 |
| 2:P9:90:GLU:HB3 | 2:P9:121:ARG:HH12 | 1.50 | 0.76 |
| 1:W6:215:LEU:HB3 | 1:W6:217:LEU:HD23 | 1.67 | 0.76 |
| 2:Y5:255:PHE:HA | 2:Y5:259:LEU:HD13 | 1.67 | 0.76 |
| 1:Z2:125:GLU:OE2 | 1:Z2:159:TYR:OH | 2.03 | 0.76 |
| 1:0I:68:LEU:HB3 | 1:0I:96:GLY:HA2 | 1.67 | 0.76 |
| 2:A2:33:ASP:HB3 | 18:6C:77:THR:HG21 | 1.65 | 0.76 |
| 2:J3:287:SER:N | 2:J3:290:GLU:OE2 | 2.17 | 0.76 |
| 2:M9:279:GLU:OE2 | 29:7J:300:THR:CG2 | 2.30 | 0.76 |
| 2:R9:51:THR:HG21 | 2:R9:243:ARG:HG2 | 1.67 | 0.76 |
| 2:Z5:276:ILE:HG23 | 2:Z5:280:LYS:HB3 | 1.66 | 0.76 |
| 2:Z9:370:LYS:NZ | 2:Z9:371:VAL:O | 2.18 | 0.76 |
| 2:2Z:297:GLU:CD | 38:8C:74:ILE:H | 1.88 | 0.76 |
| 14:5L:110:ASP:OD1 | 14:5L:154:LYS:CA | 2.32 | 0.76 |
| 1:I4:215:LEU:HB3 | 1:I4:217:LEU:HD23 | 1.67 | 0.76 |
| 1:J0:43:GLN:NE2 | 28:7H:413:TYR:OH | 2.18 | 0.76 |
| 2:N3:370:LYS:HG3 | 30:7L:277:ALA:HA | 1.68 | 0.76 |
| 1:V0:67:ASP:OD2 | 1:V0:72:THR:OG1 | 2.04 | 0.76 |
| 2:Z3:206:ASN:OD1 | 41:Z3:501:GTP:N2 | 2.17 | 0.76 |
| 2:Z7:128:ASN:HD21 | 2:0N:290:GLU:HB3 | 1.48 | 0.76 |
| 1:1G:113:ILE:HG21 | 1:1G:150:LEU:HD22 | 1.67 | 0.76 |
| 2:2J:75:VAL:HG21 | 2:2J:94:SER:HB2 | 1.66 | 0.76 |
| 1:Q2:375:GLN:HB2 | 1:Q2:419:VAL:HG23 | 1.67 | 0.76 |
| 2:Q5:56:THR:HA | 2:S1:285:GLN:HB2 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:93:GLY:HA2 | 13:5I:118:THR:HG23 | 1.68 | 0.76 |
| 1:X0:40:SER:OG | 8:4X:97:PHE:HD2 | 1.67 | 0.76 |
| 1:3M:52:ASN:H | 1:3M:52:ASN:HD22 | 1.28 | 0.76 |
| 2:3T:288:VAL:HG21 | 2:3T:327:ASP:HB2 | 1.65 | 0.76 |
| 24:6Y:597:LEU:HB3 | 24:6Y:602:LEU:HD21 | 1.67 | 0.76 |
| 2:8:42:ILE:HD13 | 24:6W:93:ARG:NH2 | 1.98 | 0.76 |
| 1:A7:280:GLN:HE22 | 24:6T:106:VAL:HA | 1.47 | 0.76 |
| 2:E7:282:TYR:CD2 | 22:6L:82:LEU:CD2 | 2.68 | 0.76 |
| 2:O5:377:MET:SD | 2:O5:379:SER:OG | 2.42 | 0.76 |
| 1:W4:322:SER:O | 1:W4:325:GLU:HG2 | 1.86 | 0.76 |
| 1:Y0:248:ALA:HA | 1:Y0:252:LYS:HD2 | 1.67 | 0.76 |
| 14:5M:38:ILE:HD11 | 14:5M:52:LEU:HD12 | 1.68 | 0.76 |
| 15:5O:6:ARG:HD3 | 15:5O:27:PHE:CE2 | 2.19 | 0.76 |
| 22:6L:333:MET:HG2 | 22:6L:334:THR:HG23 | 1.65 | 0.76 |
| 26:7E:138:THR:CG2 | 26:7E:139:PRO:CD | 2.61 | 0.76 |
| 1:9:42:LEU:HD21 | 26:7E:121:LYS:HE3 | 1.66 | 0.76 |
| 2:E7:282:TYR:HH | 22:6L:81:ASN:HA | 1.50 | 0.76 |
| 1:E8:276:ARG:NE | 24:6X:313:SER:O | 2.18 | 0.76 |
| 2:M7:264:ARG:NH1 | 2:M7:431:ASP:OD2 | 2.18 | 0.76 |
| 1:O0:245:GLN:HE21 | 27:7G:68:THR:HG21 | 1.50 | 0.76 |
| 2:V7:255:PHE:HA | 2:V7:259:LEU:HD13 | 1.66 | 0.76 |
| 2:0J:9:ILE:HG22 | 2:0J:146:GLY:HA2 | 1.67 | 0.76 |
| 2:1L:85:GLN:O | 2:2B:283:HIS:NE2 | 2.18 | 0.76 |
| 14:5N:38:ILE:HD11 | 14:5N:52:LEU:HD12 | 1.67 | 0.76 |
| 24:6Z:122:TYR:HB2 | 24:6Z:131:HIS:HB3 | 1.65 | 0.76 |
| 2:4:396:ASP:OD1 | 4:3Y:53:ASN:ND2 | 2.15 | 0.76 |
| 1:K6:67:ASP:OD2 | 1:K6:72:THR:OG1 | 2.04 | 0.76 |
| 1:L4:37:HIS:CA | 29:7J:335:GLU:OE2 | 2.30 | 0.76 |
| 1:R0:125:GLU:OE2 | 1:R0:159:TYR:OH | 2.03 | 0.76 |
| 1:Z8:117:LEU:HD11 | 1:Z8:154:LYS:HD3 | 1.68 | 0.76 |
| 2:0N:56:THR:HA | 2:1D:285:GLN:HB2 | 1.68 | 0.76 |
| 1:0W:51:PHE:O | 1:0W:62:ARG:NH2 | 2.19 | 0.76 |
| 5:4L:286:LEU:O | 5:4L:290:GLN:HG3 | 1.85 | 0.76 |
| 14:5L:38:ILE:HD11 | 14:5L:52:LEU:HD12 | 1.68 | 0.76 |
| 15:5P:15:ASP:OD1 | 15:5P:15:ASP:N | 2.18 | 0.76 |
| 29:7I:131:GLY:O | 29:7I:170:GLN:NE2 | 2.17 | 0.76 |
| 36:7W:97:VAL:O | 36:7W:101:VAL:HG12 | 1.86 | 0.76 |
| 1:A5:423:GLN:NE2 | 3:4J:107:ALA:O | 2.18 | 0.76 |
| 1:G0:388:MET:HE3 | 2:G1:346:TRP:O | 1.86 | 0.76 |
| 1:G6:78:SER:OG | 24:6Y:499:GLU:CD | 2.24 | 0.76 |
| 1:L4:52:ASN:OD1 | 1:L4:62:ARG:NH2 | 2.19 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M8:248:ALA:CA | 1:M8:252:LYS:HD2 | 2.12 | 0.76 |
| 1:N0:276:ARG:NH1 | 1:N0:279:GLN:OE1 | 2.17 | 0.76 |
| 2:N7:121:ARG:HH21 | 2:N7:121:ARG:CG | 1.94 | 0.76 |
| 2:R9:218:ASP:OD2 | 2:R9:280:LYS:NZ | 2.18 | 0.76 |
| 2:Y9:427:ALA:HA | 2:Y9:430:LYS:HD2 | 1.67 | 0.76 |
| 2:0L:399:TYR:O | 2:0L:402:ARG:NH1 | 2.18 | 0.76 |
| 1:3C:172:SER:OG | 1:3C:380:ARG:NH2 | 2.19 | 0.76 |
| 2:3N:56:THR:OG1 | 3:4D:34:SER:HA | 1.86 | 0.76 |
| 24:6U:41:ARG:HA | 24:6U:41:ARG:HE | 1.50 | 0.76 |
| 24:6Y:480:ASN:HD21 | 24:6Y:503:ILE:HD12 | 1.51 | 0.76 |
| 1:O4:277:GLY:HA2 | 19:6E:29:GLU:HG2 | 1.68 | 0.76 |
| 2:P3:279:GLU:OE1 | 2:P3:279:GLU:N | 2.14 | 0.76 |
| 1:S4:74:ASP:OD1 | 24:6U:33:LEU:CD1 | 2.34 | 0.76 |
| 1:V6:342:VAL:HG12 | 1:V6:348:ASN:HD21 | 1.50 | 0.76 |
| 2:3B:42:ILE:HD11 | 14:5N:139:ALA:HB1 | 1.67 | 0.76 |
| 2:3B:85:GLN:O | 2:3R:283:HIS:HE1 | 1.69 | 0.76 |
| 2:3B:90:GLU:HB3 | 2:3B:121:ARG:HH22 | 1.49 | 0.76 |
| 14:5L:112:SER:HB2 | 14:5L:159:SER:HB2 | 1.67 | 0.76 |
| 24:6W:488:ARG:NH1 | 24:6W:488:ARG:HB3 | 2.00 | 0.76 |
| 24:6X:445:ILE:HG13 | 24:6X:474:PHE:CD1 | 2.21 | 0.76 |
| 24:7A:96:LEU:HB2 | 24:7A:123:TYR:HB3 | 1.66 | 0.76 |
| 1:G6:248:ALA:HA | 1:G6:252:LYS:HD3 | 1.67 | 0.76 |
| 2:H3:88:HIS:CD2 | 2:H3:121:ARG:HH22 | 1.96 | 0.76 |
| 1:H6:276:ARG:CZ | 24:6V:490:THR:O | 2.34 | 0.76 |
| 2:J3:358:GLN:NE2 | 16:5Q:172:ARG:HG2 | 2.00 | 0.76 |
| 2:Y9:88:HIS:HB3 | 2:0F:283:HIS:ND1 | 2.01 | 0.76 |
| 2:Z7:102:ASN:HD21 | 2:Z7:411:GLU:HG3 | 1.51 | 0.76 |
| 2:1Z:88:HIS:HD2 | 2:2P:283:HIS:HB3 | 1.49 | 0.76 |
| 7:4R:135:ASP:O | 19:6E:191:LYS:NZ | 2.18 | 0.76 |
| 2:8:85:GLN:NE2 | 18:6A:78:LEU:HD13 | 2.00 | 0.75 |
| 1:E6:58:ARG:HD3 | 1:G2:280:GLN:HE22 | 1.50 | 0.75 |
| 2:G3:85:GLN:HE21 | 2:G3:85:GLN:CA | 1.92 | 0.75 |
| 2:I5:88:HIS:HB3 | 2:K1:283:HIS:ND1 | 2.01 | 0.75 |
| 1:O4:7:ILE:HB | 1:O4:135:VAL:HG12 | 1.69 | 0.75 |
| 1:U2:211:CYS:HA | 1:U2:215:LEU:HB2 | 1.67 | 0.75 |
| 1:Z0:164:MET:HE3 | 1:Z0:197:ASP:H | 1.51 | 0.75 |
| 2:1R:347:CYS:O | 2:1R:347:CYS:SG | 2.44 | 0.75 |
| 1:1U:175:VAL:HG12 | 2:1V:329:ASN:HD21 | 1.51 | 0.75 |
| 2:2J:90:GLU:OE1 | 2:2J:90:GLU:HA | 1.85 | 0.75 |
| 2:2X:358:GLN:HE22 | 38:8C:212:PRO:HB2 | 1.49 | 0.75 |
| 18:6A:101:LYS:O | 24:6X:178:ASN:ND2 | 2.18 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:6H:51:ARG:HE | 21:6H:89:ILE:HD13 | 1.51 | 0.75 |
| 1:3:78:SER:HB2 | 24:6U:149:LYS:HG3 | 1.66 | 0.75 |
| 2:4:29:GLY:C | 26:7D:45:MET:HE3 | 2.06 | 0.75 |
| 2:J3:85:GLN:O | 2:K9:283:HIS:CE1 | 2.40 | 0.75 |
| 2:K1:31:GLN:HE21 | 2:K1:37:PRO:HG3 | 1.51 | 0.75 |
| 2:N1:265:ILE:HD11 | 2:N1:435:VAL:HG21 | 1.67 | 0.75 |
| 2:P9:132:LEU:HD22 | 2:P9:164:LYS:HD3 | 1.68 | 0.75 |
| 2:V3:119:LEU:HA | 2:V3:122:ILE:HG22 | 1.68 | 0.75 |
| 1:Y8:122:LYS:HD2 | 1:0E:292:GLN:HE22 | 1.49 | 0.75 |
| 1:0G:113:ILE:HD13 | 1:0G:150:LEU:HD22 | 1.67 | 0.75 |
| 2:2N:123:ARG:HH22 | 38:8D:78:ASP:CG | 1.88 | 0.75 |
| 2:3P:267:PHE:HB2 | 2:3P:384:ILE:HD12 | 1.68 | 0.75 |
| 14:5N:381:PRO:HD2 | 23:6S:59:GLY:HA3 | 1.68 | 0.75 |
| 26:7E:146:ASN:O | 26:7E:146:ASN:ND2 | 2.15 | 0.75 |
| 1:F8:279:GLN:NE2 | 24:6U:411:ASN:HB2 | 2.00 | 0.75 |
| 2:L3:377:MET:SD | 2:L3:379:SER:OG | 2.43 | 0.75 |
| 1:0K:388:MET:CE | 2:0L:348:PRO:HD3 | 2.16 | 0.75 |
| 1:0S:209:ASP:HA | 1:0S:213:ARG:HH11 | 1.51 | 0.75 |
| 24:6X:469:PHE:HB3 | 24:6X:484:GLU:HB3 | 1.68 | 0.75 |
| 1:M6:46:ARG:NH2 | 37:7Y:115:CYS:SG | 2.58 | 0.75 |
| 1:S6:67:ASP:OD2 | 1:S6:72:THR:OG1 | 2.03 | 0.75 |
| 1:T6:92:PHE:CE1 | 24:7A:35:TYR:HE1 | 2.04 | 0.75 |
| 1:W8:6:HIS:HE2 | 1:W8:136:CYS:HG | 1.33 | 0.75 |
| 2:0Z:387:ILE:HG12 | 2:0Z:390:ARG:HH22 | 1.50 | 0.75 |
| 1:3C:334:GLN:HE22 | 1:3C:348:ASN:H | 1.33 | 0.75 |
| 14:5M:415:LYS:NZ | 23:6R:22:MET:HG3 | 2.00 | 0.75 |
| 37:7Y:221:ARG:HB3 | 37:7Y:231:HIS:HD2 | 1.49 | 0.75 |
| 1:B3:39:ASP:OD1 | 18:5Z:117:LYS:HG2 | 1.87 | 0.75 |
| 1:G2:259:PRO:HG3 | 1:G2:311:LEU:HD21 | 1.67 | 0.75 |
| 2:G3:282:TYR:CD1 | 22:6M:133:PRO:HG3 | 2.22 | 0.75 |
| 2:R5:27:GLU:OE1 | 2:R5:243:ARG:NH1 | 2.20 | 0.75 |
| 2:U9:100:ALA:HA | 1:V0:252:LYS:CG | 2.17 | 0.75 |
| 1:V6:52:ASN:OD1 | 1:V6:62:ARG:NH2 | 2.18 | 0.75 |
| 2:X9:26:LEU:HD21 | 2:X9:363:VAL:HG12 | 1.68 | 0.75 |
| 1:0E:215:LEU:HD22 | 1:0E:217:LEU:HB2 | 1.66 | 0.75 |
| 1:2K:215:LEU:HB3 | 1:2K:217:LEU:HD23 | 1.67 | 0.75 |
| 1:3M:113:ILE:HA | 1:3M:116:VAL:HG12 | 1.68 | 0.75 |
| 10:5D:130:ASP:HA | 10:5D:133:ARG:HD2 | 1.67 | 0.75 |
| 38:8C:74:ILE:HD12 | 38:8C:74:ILE:O | 1.86 | 0.75 |
| 1:C2:277:GLY:HA2 | 24:7A:142:ILE:HG22 | 1.67 | 0.75 |
| 2:G7:132:LEU:HD22 | 2:G7:164:LYS:HD3 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L7:9:ILE:HG22 | 2:L7:146:GLY:HA2 | 1.67 | 0.75 |
| 2:R7:90:GLU:HB3 | 2:R7:121:ARG:HH12 | 1.50 | 0.75 |
| 2:T7:88:HIS:NE2 | 2:T7:89:PRO:HD2 | 1.99 | 0.75 |
| 2:U5:228:ASN:HD21 | 41:U6:501:GTP:HN1 | 1.34 | 0.75 |
| 2:X9:377:MET:SD | 2:X9:379:SER:OG | 2.43 | 0.75 |
| 1:Y2:260:PHE:HB2 | 1:Y2:263:LEU:HG | 1.69 | 0.75 |
| 2:Y9:56:THR:HA | 2:0F:285:GLN:HB2 | 1.68 | 0.75 |
| 2:0H:239:THR:HG23 | 2:0H:243:ARG:HE | 1.52 | 0.75 |
| 1:2Y:34:GLY:O | 1:2Y:58:ARG:HA | 1.86 | 0.75 |
| 2:3R:279:GLU:OE2 | 2:3R:279:GLU:N | 2.18 | 0.75 |
| 15:5O:16:PRO:O | 27:7G:87:LYS:HE2 | 1.87 | 0.75 |
| 24:6X:514:TYR:HA | 24:6X:517:LEU:HD13 | 1.69 | 0.75 |
| 31:7N:17:GLY:HA2 | 31:7N:20:ILE:HG22 | 1.66 | 0.75 |
| 1:Q0:52:ASN:OD1 | 1:Q0:62:ARG:NH2 | 2.20 | 0.75 |
| 2:R9:176:GLN:HE22 | 2:R9:304:LYS:HE2 | 1.50 | 0.75 |
| 1:S4:213:ARG:HE | 1:S4:297:LYS:HD2 | 1.52 | 0.75 |
| 1:X4:333:VAL:HA | 1:X4:336:LYS:HD3 | 1.69 | 0.75 |
| 1:3Q:113:ILE:HA | 1:3Q:116:VAL:HG12 | 1.68 | 0.75 |
| 8:4W:460:ALA:HB2 | 8:4X:128:LEU:HD22 | 1.68 | 0.75 |
| 22:6O:54:ARG:HG3 | 24:6Z:285:MET:HG2 | 1.66 | 0.75 |
| 29:7J:390:LEU:HG | 29:7J:391:PRO:HD3 | 1.67 | 0.75 |
| 2:G5:276:ILE:HD11 | 2:G5:281:ALA:HA | 1.68 | 0.75 |
| 1:Q8:227:HIS:NE2 | 24:6T:10:LYS:O | 2.20 | 0.75 |
| 2:W9:14:ILE:HG13 | 2:W9:74:VAL:HG21 | 1.67 | 0.75 |
| 2:0R:399:TYR:O | 2:0R:402:ARG:NH1 | 2.20 | 0.75 |
| 2:1N:399:TYR:O | 2:1N:402:ARG:NH1 | 2.20 | 0.75 |
| 1:3K:77:ARG:NH2 | 3:4B:19:LEU:HD23 | 2.00 | 0.75 |
| 31:7M:64:HIS:O | 31:7M:76:THR:HG23 | 1.87 | 0.75 |
| 1:E0:219:THR:N | 24:6T:312:ASN:OD1 | 2.14 | 0.75 |
| 2:H7:88:HIS:HB2 | 2:J3:283:HIS:ND1 | 2.02 | 0.75 |
| 1:Y4:50:TYR:CE2 | 1:Y4:241:ARG:HD3 | 2.21 | 0.75 |
| 2:Z1:352:LYS:NZ | 2:Z1:353:CYS:O | 2.20 | 0.75 |
| 2:0B:9:ILE:HG22 | 2:0B:68:LEU:HD21 | 1.67 | 0.75 |
| 1:0K:179:VAL:HG22 | 2:0L:258:ASN:HD22 | 1.50 | 0.75 |
| 1:0Y:55:THR:HG21 | 1:1O:284:LEU:HD23 | 1.69 | 0.75 |
| 1:1E:379:LYS:HG2 | 1:1E:419:VAL:HG11 | 1.69 | 0.75 |
| 2:1R:313:MET:HE3 | 2:1R:346:TRP:CH2 | 2.16 | 0.75 |
| 1:2Q:306:ARG:NH1 | 38:8A:96:GLY:H | 1.68 | 0.75 |
| 22:6M:134:ASN:O | 22:6M:208:ARG:NH1 | 2.20 | 0.75 |
| 1:1:379:LYS:NZ | 3:3V:49:HIS:CD2 | 2.54 | 0.74 |
| 1:U6:248:ALA:HA | 1:U6:252:LYS:HD2 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W3:88:HIS:CE1 | 2:W3:90:GLU:HB3 | 2.21 | 0.74 |
| 1:Y6:58:ARG:HH21 | 1:Y6:58:ARG:CG | 2.00 | 0.74 |
| 2:0N:399:TYR:O | 2:0N:402:ARG:NH1 | 2.20 | 0.74 |
| 1:1W:211:CYS:HA | 1:1W:215:LEU:HB2 | 1.67 | 0.74 |
| 2:3D:214:ARG:NH2 | 38:8D:66:TYR:HA | 2.02 | 0.74 |
| 26:7F:58:ILE:H | 26:7F:58:ILE:CD1 | 1.99 | 0.74 |
| 38:8A:82:ASP:CB | 38:8A:112:ILE:HD13 | 2.16 | 0.74 |
| 2:A2:423:GLU:OE2 | 4:4G:108:TYR:OH | 1.60 | 0.74 |
| 1:G8:80:PRO:HB3 | 24:6Z:526:PHE:HE2 | 1.51 | 0.74 |
| 2:O7:313:MET:HE1 | 2:O7:346:TRP:CH2 | 2.22 | 0.74 |
| 1:P4:175:VAL:HG12 | 2:P5:329:ASN:HD21 | 1.51 | 0.74 |
| 2:1F:11:GLN:HE22 | 1:1G:247:ASN:H | 1.34 | 0.74 |
| 2:1L:399:TYR:O | 2:1L:402:ARG:NH1 | 2.19 | 0.74 |
| 1:2Q:334:GLN:HE22 | 1:2Q:348:ASN:H | 1.33 | 0.74 |
| 8:4W:463:THR:HG21 | 8:4X:128:LEU:HD13 | 1.68 | 0.74 |
| 15:5P:332:PRO:HG3 | 15:5P:350:ASP:O | 1.87 | 0.74 |
| 26:7D:58:ILE:HD11 | 26:7D:82:PRO:CB | 2.16 | 0.74 |
| 29:7J:344:GLU:CD | 29:7J:345:PRO:HD2 | 2.06 | 0.74 |
| 2:H5:88:HIS:HB3 | 2:J1:283:HIS:ND1 | 2.02 | 0.74 |
| 1:K8:175:VAL:HG22 | 2:K9:329:ASN:HD21 | 1.53 | 0.74 |
| 2:Q5:75:VAL:HG21 | 2:Q5:94:SER:HB2 | 1.67 | 0.74 |
| 1:V0:345:ILE:O | 1:V0:348:ASN:ND2 | 2.21 | 0.74 |
| 2:Y3:282:TYR:HE2 | 8:4W:373:ASN:HB3 | 1.50 | 0.74 |
| 1:0Q:8:GLN:HE21 | 1:0Q:14:ASN:HA | 1.51 | 0.74 |
| 2:2X:286:LEU:O | 2:2X:373:ARG:NH1 | 2.20 | 0.74 |
| 1:3K:113:ILE:HA | 1:3K:116:VAL:HG12 | 1.67 | 0.74 |
| 2:3R:287:SER:N | 2:3R:290:GLU:OE2 | 2.16 | 0.74 |
| 3:4D:7:GLY:HA2 | 3:4D:140:LYS:HG2 | 1.67 | 0.74 |
| 15:5P:185:ARG:NH1 | 15:5P:197:GLY:O | 2.21 | 0.74 |
| 38:7Z:8:GLU:O | 38:7Z:12:LEU:HB2 | 1.87 | 0.74 |
| 1:A3:219:THR:HB | 26:7F:142:PHE:CZ | 2.22 | 0.74 |
| 1:F0:11:GLN:NE2 | 39:F0:502:GDP:O1A | 2.19 | 0.74 |
| 2:K7:88:HIS:ND1 | 2:K7:89:PRO:CD | 2.49 | 0.74 |
| 2:K9:90:GLU:HB3 | 2:K9:121:ARG:HH22 | 1.52 | 0.74 |
| 2:L9:90:GLU:N | 1:N6:281:TYR:OH | 2.19 | 0.74 |
| 2:Q1:308:ARG:NH1 | 2:U9:282:TYR:OH | 2.21 | 0.74 |
| 2:U5:213:CYS:HA | 2:U5:217:LEU:HB2 | 1.69 | 0.74 |
| 1:V2:218:THR:O | 2:V3:326:LYS:NZ | 2.20 | 0.74 |
| 1:V4:211:CYS:HA | 1:V4:215:LEU:HB2 | 1.69 | 0.74 |
| 1:V6:235:GLY:HA2 | 1:V6:318:ARG:HH11 | 1.52 | 0.74 |
| 2:X9:287:SER:N | 2:X9:290:GLU:OE2 | 2.19 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0U:68:LEU:HD23 | 1:0U:93:GLY:HA3 | 1.69 | 0.74 |
| 2:1T:27:GLU:OE1 | 2:1T:243:ARG:NH1 | 2.21 | 0.74 |
| 1:3O:77:ARG:NH2 | 3:4F:19:LEU:HD23 | 2.00 | 0.74 |
| 2:3T:241:SER:HA | 2:3T:356:ASN:HD21 | 1.51 | 0.74 |
| 14:5M:381:PRO:HD2 | 23:6R:59:GLY:HA3 | 1.68 | 0.74 |
| 1:I4:211:CYS:HA | 1:I4:215:LEU:HB2 | 1.67 | 0.74 |
| 1:N2:320:ARG:HH12 | 29:7J:110:THR:HA | 1.52 | 0.74 |
| 1:W6:190:HIS:CD2 | 1:W6:411:ALA:HA | 2.22 | 0.74 |
| 1:W8:207:LEU:HB3 | 1:W8:225:LEU:HD22 | 1.70 | 0.74 |
| 2:2H:90:GLU:HB3 | 2:2H:121:ARG:NH2 | 2.01 | 0.74 |
| 1:3K:213:ARG:HD3 | 1:3K:297:LYS:HE3 | 1.68 | 0.74 |
| 2:3L:392:ASP:OD2 | 2:3L:422:ARG:NH1 | 2.19 | 0.74 |
| 3:4H:7:GLY:HA2 | 3:4H:140:LYS:HG2 | 1.67 | 0.74 |
| 8:4W:466:ARG:HD3 | 8:4W:466:ARG:O | 1.86 | 0.74 |
| 1:5:40:SER:C | 26:7D:25:TYR:CE2 | 2.59 | 0.74 |
| 1:J8:40:SER:HA | 29:7J:388:MET:CG | 2.09 | 0.74 |
| 1:L4:320:ARG:HH22 | 29:7J:350:LYS:HA | 1.53 | 0.74 |
| 1:S8:94:GLN:OE1 | 24:6W:42:GLU:OE1 | 2.05 | 0.74 |
| 2:V3:239:THR:HG23 | 2:V3:243:ARG:HE | 1.52 | 0.74 |
| 2:Y9:72:PRO:HD2 | 1:Z0:2:ARG:HH12 | 1.51 | 0.74 |
| 3:3V:7:GLY:HA2 | 3:3V:140:LYS:HG2 | 1.67 | 0.74 |
| 3:3X:7:GLY:HA2 | 3:3X:140:LYS:HG2 | 1.67 | 0.74 |
| 3:3Z:7:GLY:HA2 | 3:3Z:140:LYS:HG2 | 1.67 | 0.74 |
| 3:4B:7:GLY:HA2 | 3:4B:140:LYS:HG2 | 1.67 | 0.74 |
| 15:5P:12:GLU:CB | 15:5P:21:LEU:HD21 | 2.18 | 0.74 |
| 17:5V:185:LEU:HB3 | 17:5V:226:ILE:HD11 | 1.68 | 0.74 |
| 22:6M:130:LEU:HD23 | 22:6M:209:ASN:HD21 | 1.52 | 0.74 |
| 22:6N:54:ARG:HG3 | 24:6Y:285:MET:HG2 | 1.66 | 0.74 |
| 27:7G:67:THR:HG23 | 27:7G:70:GLN:H | 1.52 | 0.74 |
| 1:0K:388:MET:SD | 2:0L:348:PRO:HD3 | 2.27 | 0.74 |
| 1:1G:388:MET:HE2 | 1:1G:388:MET:CA | 2.17 | 0.74 |
| 3:4F:7:GLY:HA2 | 3:4F:140:LYS:HG2 | 1.67 | 0.74 |
| 26:7E:58:ILE:HD12 | 26:7E:58:ILE:N | 2.01 | 0.74 |
| 2:D7:280:LYS:CE | 18:6D:166:HIS:HB3 | 2.18 | 0.74 |
| 1:I0:218:THR:CG2 | 24:6X:489:ASN:N | 2.50 | 0.74 |
| 1:O4:280:GLN:OE1 | 19:6E:75:GLN:HG3 | 1.87 | 0.74 |
| 2:R9:263:PRO:O | 17:5U:84:ARG:NH1 | 2.20 | 0.74 |
| 2:S1:53:PHE:HB3 | 2:S1:61:HIS:HB3 | 1.69 | 0.74 |
| 2:W1:237:SER:HB2 | 2:W1:318:MET:HE1 | 1.70 | 0.74 |
| 1:3G:95:THR:HG21 | 3:3X:138:GLY:HA2 | 1.70 | 0.74 |
| 14:5L:121:LEU:HD22 | 14:5L:153:VAL:HG13 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:121:LEU:HD22 | 14:5M:153:VAL:HG13 | 1.69 | 0.74 |
| 14:5N:121:LEU:HD22 | 14:5N:153:VAL:HG13 | 1.69 | 0.74 |
| 2:A2:423:GLU:OE2 | 4:4G:108:TYR:CZ | 2.07 | 0.74 |
| 2:E1:33:ASP:HB3 | 22:6J:130:LEU:HD12 | 1.69 | 0.74 |
| 2:M1:365:GLY:O | 30:7K:260:ARG:NH1 | 2.20 | 0.74 |
| 2:N1:287:SER:N | 2:N1:290:GLU:OE2 | 2.20 | 0.74 |
| 2:N3:384:ILE:HA | 2:N3:387:ILE:HD12 | 1.69 | 0.74 |
| 2:V3:100:ALA:HA | 1:V4:252:LYS:HG2 | 1.68 | 0.74 |
| 2:W7:88:HIS:HD2 | 2:W7:90:GLU:H | 1.34 | 0.74 |
| 1:Z0:3:GLU:HB2 | 1:Z0:130:LEU:HA | 1.68 | 0.74 |
| 1:Z6:379:LYS:HD3 | 1:Z6:419:VAL:HG21 | 1.68 | 0.74 |
| 2:0N:324:VAL:HG12 | 2:0N:326:LYS:H | 1.52 | 0.74 |
| 1:2U:113:ILE:HD13 | 1:2U:150:LEU:HD22 | 1.67 | 0.74 |
| 1:3O:5:VAL:HG12 | 1:3O:62:ARG:HD3 | 1.68 | 0.74 |
| 7:4S:11:GLU:OE2 | 7:4S:11:GLU:N | 2.21 | 0.74 |
| 15:5P:52:TYR:CE2 | 15:5P:54:GLU:HB3 | 2.23 | 0.74 |
| 2:I5:172:TYR:CZ | 2:I5:203:MET:HG2 | 2.23 | 0.74 |
| 2:K9:85:GLN:CD | 30:7K:134:HIS:HD1 | 1.90 | 0.74 |
| 1:S6:248:ALA:HA | 1:S6:252:LYS:CD | 2.18 | 0.74 |
| 2:T7:279:GLU:OE1 | 2:T7:279:GLU:HA | 1.88 | 0.74 |
| 1:U6:137:HIS:HE2 | 1:U6:168:SER:HG | 1.34 | 0.74 |
| 1:U8:249:ASP:H | 1:U8:252:LYS:HD2 | 1.53 | 0.74 |
| 1:V0:211:CYS:HA | 1:V0:215:LEU:HB2 | 1.70 | 0.74 |
| 1:Z8:68:LEU:HB3 | 1:Z8:96:GLY:HA2 | 1.70 | 0.74 |
| 2:0P:220:GLU:HG3 | 2:0P:221:ARG:HG3 | 1.69 | 0.74 |
| 1:1A:334:GLN:HE22 | 1:1A:348:ASN:H | 1.35 | 0.74 |
| 1:2A:215:LEU:HB3 | 1:2A:217:LEU:HD23 | 1.68 | 0.74 |
| 22:6N:108:ARG:NH2 | 24:6Y:284:THR:O | 2.21 | 0.74 |
| 24:6X:517:LEU:HD12 | 24:6X:517:LEU:N | 2.02 | 0.74 |
| 1:G4:139:LEU:HD12 | 1:G4:170:VAL:HG22 | 1.70 | 0.73 |
| 2:U3:228:ASN:HD21 | 41:U4:501:GTP:HN1 | 1.34 | 0.73 |
| 2:X9:88:HIS:HB3 | 2:Z5:283:HIS:ND1 | 2.03 | 0.73 |
| 2:Y3:56:THR:HG22 | 2:Z9:285:GLN:HB2 | 1.70 | 0.73 |
| 1:2U:126:SER:O | 38:8B:178:ARG:NH2 | 2.19 | 0.73 |
| 2:3T:223:THR:HG23 | 2:3T:225:THR:H | 1.52 | 0.73 |
| 4:3Y:74:PRO:HD2 | 4:3Y:169:ASP:HA | 1.69 | 0.73 |
| 24:6V:456:ASP:O | 24:6V:459:LYS:NZ | 2.20 | 0.73 |
| 37:7Y:177:ARG:HB2 | 37:7Y:177:ARG:HH11 | 1.53 | 0.73 |
| 38:8B:85:ARG:HH11 | 38:8B:87:LYS:HD3 | 0.93 | 0.73 |
| 1:L6:67:ASP:OD2 | 1:L6:72:THR:OG1 | 2.05 | 0.73 |
| 1:M6:1:MET:CE | 37:7Y:116:MET:HB2 | 2.16 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W1:89:PRO:HB2 | 2:X7:280:LYS:HZ1 | 1.53 | 0.73 |
| 2:X5:297:GLU:HA | 2:X5:297:GLU:OE2 | 1.88 | 0.73 |
| 2:0B:177:VAL:HA | 1:0C:331:LEU:HD11 | 1.70 | 0.73 |
| 1:0G:8:GLN:HE21 | 1:0G:14:ASN:HA | 1.53 | 0.73 |
| 1:0G:139:LEU:HD12 | 1:0G:170:VAL:HG12 | 1.69 | 0.73 |
| 1:0Y:180:VAL:HG23 | 1:0Y:184:ASN:HD21 | 1.53 | 0.73 |
| 2:2H:113:GLU:HG2 | 38:8B:7:ASP:HA | 1.68 | 0.73 |
| 1:2Q:320:ARG:NH1 | 38:8A:198:THR:HA | 2.02 | 0.73 |
| 1:2U:41:ASP:OD1 | 38:8B:183:LYS:NZ | 2.21 | 0.73 |
| 4:4C:74:PRO:HD2 | 4:4C:169:ASP:HA | 1.69 | 0.73 |
| 4:4G:74:PRO:HD2 | 4:4G:169:ASP:HA | 1.69 | 0.73 |
| 24:6X:569:LYS:HB3 | 24:6X:572:ALA:HB3 | 1.69 | 0.73 |
| 38:8A:86:TYR:HE2 | 38:8A:104:LYS:HG2 | 1.53 | 0.73 |
| 38:8C:35:GLU:OE1 | 38:8C:39:LYS:HE3 | 1.87 | 0.73 |
| 2:L3:66:ILE:HD12 | 2:L3:121:ARG:HG2 | 1.69 | 0.73 |
| 1:N8:390:ARG:HB3 | 2:N9:346:TRP:HZ3 | 1.53 | 0.73 |
| 1:V4:345:ILE:O | 1:V4:348:ASN:ND2 | 2.20 | 0.73 |
| 1:X2:50:TYR:HH | 1:X2:237:THR:HG1 | 1.26 | 0.73 |
| 1:Z4:139:LEU:HD12 | 1:Z4:170:VAL:HG12 | 1.69 | 0.73 |
| 1:1U:345:ILE:O | 1:1U:348:ASN:ND2 | 2.21 | 0.73 |
| 2:2L:246:GLY:H | 2:2L:249:ASN:HD21 | 1.35 | 0.73 |
| 9:4Z:35:ARG:NH1 | 14:5L:583:ASP:OD1 | 2.22 | 0.73 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:CD | 2.18 | 0.73 |
| 24:6T:613:LYS:O | 24:6T:617:ASP:HB2 | 1.88 | 0.73 |
| 1:A3:383:GLU:OE2 | 3:4H:50:LYS:NZ | 2.22 | 0.73 |
| 2:E7:282:TYR:CE2 | 22:6L:82:LEU:HD22 | 2.09 | 0.73 |
| 1:H6:272:PRO:HB2 | 1:H6:282:ARG:HH12 | 1.53 | 0.73 |
| 2:I5:105:ARG:HH12 | 2:I5:407:TRP:HZ3 | 1.35 | 0.73 |
| 2:J1:346:TRP:CH2 | 2:J1:435:VAL:HG23 | 2.23 | 0.73 |
| 1:J2:178:THR:HB | 1:J2:181:GLU:HG3 | 1.69 | 0.73 |
| 2:X5:52:PHE:HZ | 2:X5:239:THR:HG21 | 1.53 | 0.73 |
| 38:8A:83:ARG:HG3 | 38:8A:85:ARG:HG2 | 1.70 | 0.73 |
| 2:H3:278:ALA:HA | 2:H3:369:ALA:HB2 | 1.68 | 0.73 |
| 1:Y6:273:LEU:H | 1:Y6:292:GLN:HE22 | 1.34 | 0.73 |
| 2:Z9:100:ALA:HA | 1:0A:252:LYS:HE2 | 1.71 | 0.73 |
| 2:0F:206:ASN:OD1 | 41:0F:501:GTP:N2 | 2.22 | 0.73 |
| 1:1G:311:LEU:HD23 | 1:1G:312:THR:HG23 | 1.71 | 0.73 |
| 4:4I:74:PRO:HD2 | 4:4I:169:ASP:HA | 1.69 | 0.73 |
| 15:5O:56:LYS:H | 15:5O:56:LYS:CE | 2.01 | 0.73 |
| 15:5O:200:LYS:HD3 | 15:5O:200:LYS:C | 2.08 | 0.73 |
| 15:5P:12:GLU:HB2 | 15:5P:21:LEU:CD2 | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E6:52:ASN:HA | 22:6L:181:ASN:HD22 | 0.64 | 0.73 |
| 2:M3:221:ARG:HH22 | 30:7K:189:PHE:H | 1.36 | 0.73 |
| 2:R3:336:LYS:O | 2:R3:339:ARG:NH2 | 2.22 | 0.73 |
| 2:U7:100:ALA:HA | 1:U8:252:LYS:HG2 | 1.71 | 0.73 |
| 1:Y8:273:LEU:H | 1:Y8:292:GLN:HE22 | 1.36 | 0.73 |
| 2:Z1:108:TYR:O | 2:Z1:112:LYS:NZ | 2.19 | 0.73 |
| 2:Z7:91:GLN:HE22 | 2:0N:283:HIS:HE1 | 1.37 | 0.73 |
| 2:0F:286:LEU:HD11 | 2:0F:372:GLN:HB2 | 1.70 | 0.73 |
| 1:0U:139:LEU:HD12 | 1:0U:170:VAL:HG22 | 1.71 | 0.73 |
| 1:1E:51:PHE:O | 1:1E:62:ARG:NH2 | 2.22 | 0.73 |
| 2:1F:9:ILE:HG22 | 2:1F:68:LEU:HD11 | 1.69 | 0.73 |
| 2:1X:414:GLU:HG2 | 2:1X:416:GLY:H | 1.52 | 0.73 |
| 4:4A:74:PRO:HD2 | 4:4A:169:ASP:HA | 1.69 | 0.73 |
| 24:6T:488:ARG:HD2 | 24:6T:488:ARG:N | 2.03 | 0.73 |
| 26:7F:113:ARG:HB2 | 26:7F:116:GLN:HG3 | 1.71 | 0.73 |
| 1:E2:77:ARG:NH2 | 24:6U:426:LEU:HB2 | 2.03 | 0.73 |
| 2:G3:42:ILE:CG1 | 24:6W:470:ILE:HD11 | 2.16 | 0.73 |
| 2:G3:206:ASN:OD1 | 41:G4:501:GTP:N2 | 2.21 | 0.73 |
| 1:H4:218:THR:HG21 | 24:6U:488:ARG:HA | 1.71 | 0.73 |
| 1:I0:45:GLU:HG3 | 1:I0:46:ARG:HG2 | 1.70 | 0.73 |
| 1:I8:375:GLN:HB2 | 1:I8:419:VAL:HG23 | 1.71 | 0.73 |
| 2:J7:281:ALA:HA | 2:J7:284:GLU:HG3 | 1.71 | 0.73 |
| 1:X6:279:GLN:HE22 | 8:4W:184:VAL:HG22 | 1.53 | 0.73 |
| 1:1K:68:LEU:HB3 | 1:1K:96:GLY:HA2 | 1.71 | 0.73 |
| 2:1R:35:GLN:HB3 | 2:1R:59:GLY:O | 1.89 | 0.73 |
| 1:1S:375:GLN:HB2 | 1:1S:419:VAL:HG13 | 1.71 | 0.73 |
| 1:3S:285:THR:HG23 | 1:3S:288:GLU:H | 1.54 | 0.73 |
| 4:3W:74:PRO:HD2 | 4:3W:169:ASP:HA | 1.69 | 0.73 |
| 18:5X:136:VAL:HG23 | 18:5X:198:LEU:HB3 | 1.70 | 0.73 |
| 18:5Z:136:VAL:HG23 | 18:5Z:198:LEU:HB3 | 1.70 | 0.73 |
| 2:I5:324:VAL:HG21 | 2:I5:326:LYS:HZ3 | 1.54 | 0.73 |
| 2:J5:282:TYR:OH | 5:4M:156:ASN:OD1 | 2.05 | 0.73 |
| 2:V1:195:LEU:HD21 | 2:V1:264:ARG:HD2 | 1.71 | 0.73 |
| 2:Z5:206:ASN:OD1 | 41:Z6:501:GTP:N2 | 2.20 | 0.73 |
| 2:Z7:34:GLY:HA3 | 2:Z7:60:LYS:HZ2 | 1.54 | 0.73 |
| 2:0B:370:LYS:NZ | 2:0B:371:VAL:O | 2.22 | 0.73 |
| 2:0N:108:TYR:O | 2:0N:112:LYS:NZ | 2.21 | 0.73 |
| 2:0P:88:HIS:HB3 | 2:1F:283:HIS:ND1 | 2.04 | 0.73 |
| 1:3K:272:PRO:HB2 | 1:3K:282:ARG:HH12 | 1.53 | 0.73 |
| 1:3O:51:PHE:HB3 | 1:3O:59:TYR:HB3 | 1.69 | 0.73 |
| 4:4E:74:PRO:HD2 | 4:4E:169:ASP:HA | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:4R:284:GLU:OE2 | 33:7Q:184:THR:HA | 1.89 | 0.73 |
| 18:5Y:136:VAL:HG23 | 18:5Y:198:LEU:HB3 | 1.70 | 0.73 |
| 2:6:396:ASP:OD1 | 4:4A:53:ASN:ND2 | 2.21 | 0.73 |
| 1:I2:211:CYS:HA | 1:I2:215:LEU:HB2 | 1.71 | 0.73 |
| 1:K8:52:ASN:OD1 | 1:K8:62:ARG:NH2 | 2.21 | 0.73 |
| 2:M5:121:ARG:HB2 | 2:M5:121:ARG:NH1 | 2.03 | 0.73 |
| 2:P3:274:PRO:CG | 2:P3:286:LEU:HD21 | 2.13 | 0.73 |
| 2:0P:278:ALA:HA | 2:0P:369:ALA:HB2 | 1.70 | 0.73 |
| 2:1H:90:GLU:HG2 | 2:1H:121:ARG:HH22 | 1.54 | 0.73 |
| 1:2A:125:GLU:OE2 | 1:2A:159:TYR:OH | 2.05 | 0.73 |
| 2:2D:133:GLN:HB3 | 2:2D:252:ILE:HG21 | 1.70 | 0.73 |
| 14:5M:378:ILE:HG22 | 23:6R:55:VAL:HB | 1.71 | 0.73 |
| 24:6T:97:ARG:H | 24:6T:188:THR:HG21 | 1.53 | 0.73 |
| 2:A2:357:TYR:HB3 | 24:6Y:150:ARG:HH12 | 1.53 | 0.73 |
| 1:G8:33:THR:O | 1:G8:58:ARG:NH2 | 2.22 | 0.73 |
| 2:H7:317:LEU:HB3 | 2:H7:319:TYR:HE1 | 1.53 | 0.73 |
| 2:J5:413:MET:HB3 | 2:J5:417:GLU:OE2 | 1.88 | 0.73 |
| 2:J7:282:TYR:CE1 | 5:4M:210:ASP:OD1 | 2.40 | 0.73 |
| 2:P7:308:ARG:NH1 | 2:U5:282:TYR:OH | 2.21 | 0.73 |
| 1:S2:190:HIS:HD2 | 1:S2:414:ASN:HD22 | 1.36 | 0.73 |
| 2:Y9:114:ILE:HG21 | 2:Y9:149:LEU:HD22 | 1.70 | 0.73 |
| 2:Z1:206:ASN:OD1 | 41:Z2:501:GTP:N2 | 2.22 | 0.73 |
| 1:0Q:45:GLU:HG3 | 1:0Q:46:ARG:HG2 | 1.71 | 0.73 |
| 1:0Y:345:ILE:O | 1:0Y:348:ASN:ND2 | 2.20 | 0.73 |
| 1:1G:388:MET:HA | 1:1G:388:MET:CE | 2.19 | 0.73 |
| 5:4L:284:LEU:HA | 5:4L:287:LYS:HG3 | 1.69 | 0.73 |
| 10:5B:287:VAL:HA | 10:5B:290:LYS:HD2 | 1.71 | 0.73 |
| 13:5I:136:PHE:HD2 | 19:6E:259:SER:HB2 | 1.53 | 0.73 |
| 18:6A:136:VAL:HG23 | 18:6A:198:LEU:HB3 | 1.70 | 0.73 |
| 18:6B:136:VAL:HG23 | 18:6B:198:LEU:HB3 | 1.70 | 0.73 |
| 18:6D:136:VAL:HG23 | 18:6D:198:LEU:HB3 | 1.70 | 0.73 |
| 1:5:40:SER:C | 26:7D:25:TYR:HE2 | 1.93 | 0.72 |
| 2:Y3:282:TYR:CE2 | 8:4W:373:ASN:ND2 | 2.54 | 0.72 |
| 2:0F:83:TYR:HB3 | 2:0F:86:LEU:HB3 | 1.72 | 0.72 |
| 2:0H:83:TYR:HB3 | 2:0H:86:LEU:HB3 | 1.70 | 0.72 |
| 1:0O:215:LEU:HD21 | 1:0O:273:LEU:HD12 | 1.71 | 0.72 |
| 2:1B:290:GLU:HA | 2:1B:293:ASN:HD22 | 1.54 | 0.72 |
| 2:2L:276:ILE:HG21 | 2:2L:281:ALA:HB2 | 1.70 | 0.72 |
| 2:3D:122:ILE:HD11 | 2:3D:157:LEU:HD21 | 1.71 | 0.72 |
| 18:6C:136:VAL:HG23 | 18:6C:198:LEU:HB3 | 1.70 | 0.72 |
| 25:7C:73:VAL:HG22 | 25:7C:77:LYS:HE3 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:7D:58:ILE:HD11 | 26:7D:82:PRO:HB3 | 1.71 | 0.72 |
| 2:I1:264:ARG:NH1 | 2:I1:431:ASP:OD2 | 2.20 | 0.72 |
| 2:N5:88:HIS:HE1 | 2:N5:90:GLU:CB | 2.02 | 0.72 |
| 1:O0:268:VAL:HG23 | 1:O0:300:MET:HB2 | 1.70 | 0.72 |
| 2:Q5:392:ASP:OD2 | 2:Q5:422:ARG:NH1 | 2.22 | 0.72 |
| 1:R0:345:ILE:O | 1:R0:348:ASN:ND2 | 2.20 | 0.72 |
| 1:R4:200:MET:HE3 | 1:R4:268:VAL:HG21 | 1.72 | 0.72 |
| 1:U4:172:SER:OG | 1:U4:380:ARG:NH2 | 2.22 | 0.72 |
| 2:W9:81:GLY:O | 2:W9:84:ARG:HG3 | 1.89 | 0.72 |
| 1:0E:258:ILE:HD11 | 1:0E:261:PRO:HA | 1.70 | 0.72 |
| 2:0J:297:GLU:HG3 | 2:0J:299:ALA:H | 1.54 | 0.72 |
| 2:3F:344:VAL:HG12 | 2:3F:346:TRP:H | 1.53 | 0.72 |
| 2:3T:428:LEU:HG | 2:3T:432:PHE:HE2 | 1.54 | 0.72 |
| 8:4W:468:MET:HE1 | 8:4W:470:TYR:CZ | 2.24 | 0.72 |
| 15:5O:333:GLU:HB3 | 30:7K:241:LYS:NZ | 2.04 | 0.72 |
| 2:4:77:GLU:HG2 | 26:7D:115:GLU:HG2 | 1.71 | 0.72 |
| 2:8:396:ASP:OD1 | 4:4C:53:ASN:ND2 | 2.19 | 0.72 |
| 2:G1:101:ASN:OD1 | 1:G2:252:LYS:HE3 | 1.88 | 0.72 |
| 2:J5:91:GLN:HE21 | 2:J5:121:ARG:HH22 | 1.38 | 0.72 |
| 2:N9:33:ASP:O | 2:N9:60:LYS:NZ | 2.21 | 0.72 |
| 2:S7:223:THR:HG23 | 2:S7:225:THR:H | 1.54 | 0.72 |
| 1:V0:311:LEU:HD23 | 1:V0:342:VAL:HG21 | 1.70 | 0.72 |
| 2:V1:88:HIS:CE1 | 2:V1:90:GLU:HB3 | 2.24 | 0.72 |
| 1:0O:3:GLU:HB2 | 1:0O:130:LEU:HA | 1.71 | 0.72 |
| 1:1E:207:LEU:HD11 | 1:1E:229:ILE:HD11 | 1.71 | 0.72 |
| 1:1M:345:ILE:O | 1:1M:348:ASN:ND2 | 2.21 | 0.72 |
| 2:1N:280:LYS:HA | 2:1N:283:HIS:CD2 | 2.24 | 0.72 |
| 1:3I:34:GLY:O | 1:3I:58:ARG:HA | 1.89 | 0.72 |
| 1:3Q:248:ALA:CA | 1:3Q:252:LYS:HD2 | 2.14 | 0.72 |
| 24:6U:122:TYR:HB2 | 24:6U:131:HIS:HB3 | 1.71 | 0.72 |
| 1:1:306:ARG:HD3 | 3:3V:59:LEU:HD13 | 1.68 | 0.72 |
| 1:G2:139:LEU:HD12 | 1:G2:170:VAL:HG22 | 1.71 | 0.72 |
| 1:G4:2:ARG:HB3 | 1:G4:131:GLN:HB2 | 1.70 | 0.72 |
| 2:G9:279:GLU:OE1 | 2:G9:279:GLU:N | 2.20 | 0.72 |
| 2:J5:372:GLN:HE22 | 5:4M:148:LEU:HA | 1.54 | 0.72 |
| 2:Q9:336:LYS:O | 2:Q9:339:ARG:NH2 | 2.22 | 0.72 |
| 1:X8:113:ILE:HA | 1:X8:116:VAL:HG12 | 1.70 | 0.72 |
| 2:Z3:181:VAL:HG22 | 1:Z4:256:ASN:HD22 | 1.54 | 0.72 |
| 2:1D:399:TYR:O | 2:1D:402:ARG:NH1 | 2.23 | 0.72 |
| 2:1Z:377:MET:SD | 2:1Z:379:SER:OG | 2.44 | 0.72 |
| 16:5Q:45:GLY:HA2 | 16:5Q:58:ALA:HA | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6V:483:PHE:HB2 | 24:6V:496:LYS:HA | 1.71 | 0.72 |
| 38:8B:12:LEU:HB3 | 38:8B:18:VAL:HG21 | 1.72 | 0.72 |
| 38:8D:73:TRP:HD1 | 38:8D:75:SER:HB2 | 1.55 | 0.72 |
| 1:J2:71:GLY:HA2 | 16:5Q:175:LEU:HD21 | 1.71 | 0.72 |
| 1:J4:45:GLU:HG3 | 1:J4:46:ARG:HG2 | 1.72 | 0.72 |
| 2:J9:287:SER:N | 2:J9:290:GLU:OE2 | 2.20 | 0.72 |
| 1:N2:252:LYS:HA | 1:N2:255:VAL:CG1 | 2.19 | 0.72 |
| 1:O4:248:ALA:HA | 1:O4:252:LYS:HD2 | 1.71 | 0.72 |
| 2:O7:85:GLN:O | 2:Q5:283:HIS:NE2 | 2.21 | 0.72 |
| 1:Q2:311:LEU:HD23 | 1:Q2:312:THR:HG23 | 1.71 | 0.72 |
| 1:V0:5:VAL:HG23 | 1:V0:62:ARG:HG2 | 1.71 | 0.72 |
| 2:W9:255:PHE:HA | 2:W9:259:LEU:HD13 | 1.70 | 0.72 |
| 2:Z7:324:VAL:HG22 | 2:Z7:326:LYS:H | 1.55 | 0.72 |
| 1:1G:52:ASN:OD1 | 1:1G:62:ARG:NH2 | 2.20 | 0.72 |
| 1:2Y:54:ALA:HB3 | 1:2Y:58:ARG:HB3 | 1.70 | 0.72 |
| 18:5X:75:ASP:OD2 | 18:5X:76:ALA:N | 2.22 | 0.72 |
| 18:5Z:75:ASP:OD2 | 18:5Z:76:ALA:N | 2.22 | 0.72 |
| 18:6A:75:ASP:OD2 | 18:6A:76:ALA:N | 2.22 | 0.72 |
| 18:6B:75:ASP:OD2 | 18:6B:76:ALA:N | 2.22 | 0.72 |
| 18:6C:75:ASP:OD2 | 18:6C:76:ALA:N | 2.22 | 0.72 |
| 18:6D:75:ASP:OD2 | 18:6D:76:ALA:N | 2.22 | 0.72 |
| 24:6V:597:LEU:HB3 | 24:6V:602:LEU:HD21 | 1.69 | 0.72 |
| 1:H2:200:MET:HE3 | 1:H2:268:VAL:HG21 | 1.69 | 0.72 |
| 2:I1:90:GLU:OE2 | 2:I1:90:GLU:HA | 1.89 | 0.72 |
| 1:L6:339:SER:H | 34:7S:140:ASN:HD21 | 1.35 | 0.72 |
| 2:O3:313:MET:CG | 2:O3:346:TRP:CZ3 | 2.72 | 0.72 |
| 2:S9:88:HIS:HD2 | 2:S9:90:GLU:H | 1.35 | 0.72 |
| 1:Y8:202:LEU:CD2 | 1:Y8:229:ILE:HD13 | 2.18 | 0.72 |
| 2:Z5:15:GLN:HB3 | 2:Z5:228:ASN:HD21 | 1.53 | 0.72 |
| 2:0B:53:PHE:HB3 | 2:0B:61:HIS:HB3 | 1.72 | 0.72 |
| 2:0X:199:ASP:HB3 | 2:0X:256:GLN:HE22 | 1.52 | 0.72 |
| 2:1B:26:LEU:HD23 | 2:1B:363:VAL:HG12 | 1.70 | 0.72 |
| 5:4L:312:GLU:HA | 5:4L:315:ARG:HE | 1.53 | 0.72 |
| 14:5L:356:PHE:HB2 | 14:5L:367:TRP:HB2 | 1.70 | 0.72 |
| 14:5M:415:LYS:HE2 | 23:6R:22:MET:CG | 2.19 | 0.72 |
| 18:5Y:75:ASP:OD2 | 18:5Y:76:ALA:N | 2.22 | 0.72 |
| 2:H3:90:GLU:HB3 | 2:H3:121:ARG:NH1 | 2.05 | 0.72 |
| 1:H4:345:ILE:O | 1:H4:348:ASN:ND2 | 2.19 | 0.72 |
| 1:M8:175:VAL:HG22 | 1:M8:205:GLU:HG2 | 1.71 | 0.72 |
| 2:W5:287:SER:N | 2:W5:290:GLU:OE2 | 2.23 | 0.72 |
| 1:Y4:263:LEU:HG | 1:Y4:422:TYR:HE1 | 1.53 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0C:135:VAL:HG11 | 1:0C:152:ILE:HD11 | 1.72 | 0.72 |
| 2:0J:206:ASN:OD1 | 41:0K:501:GTP:N2 | 2.23 | 0.72 |
| 2:0X:88:HIS:CG | 2:1N:283:HIS:HB2 | 2.25 | 0.72 |
| 2:1B:399:TYR:O | 2:1B:402:ARG:NH1 | 2.23 | 0.72 |
| 2:1N:213:CYS:HA | 2:1N:217:LEU:HB2 | 1.72 | 0.72 |
| 1:3G:113:ILE:HA | 1:3G:116:VAL:HG12 | 1.69 | 0.72 |
| 2:3H:164:LYS:NZ | 3:3X:136:HIS:O | 2.21 | 0.72 |
| 2:3R:222:PRO:HD2 | 1:3S:324:LYS:HE3 | 1.72 | 0.72 |
| 15:5O:62:LEU:HD21 | 15:5O:77:GLU:CA | 2.16 | 0.72 |
| 15:5P:140:HIS:HB2 | 15:5P:146:VAL:HG11 | 1.71 | 0.72 |
| 16:5Q:173:ARG:HG2 | 16:5Q:173:ARG:NH1 | 1.99 | 0.72 |
| 24:6T:488:ARG:HD2 | 24:6T:488:ARG:H | 1.53 | 0.72 |
| 2:C1:278:ALA:HB3 | 18:6D:43:ASN:HD22 | 1.53 | 0.72 |
| 2:M1:176:GLN:HE22 | 2:M1:304:LYS:HE2 | 1.54 | 0.72 |
| 2:N5:154:LEU:HA | 2:N5:157:LEU:HD12 | 1.71 | 0.72 |
| 1:O0:2:ARG:HE | 1:O0:240:LEU:HD22 | 1.54 | 0.72 |
| 2:P5:308:ARG:NH1 | 2:U3:282:TYR:OH | 2.21 | 0.72 |
| 1:R2:334:GLN:HE22 | 1:R2:348:ASN:H | 1.37 | 0.72 |
| 1:T2:52:ASN:OD1 | 1:T2:62:ARG:NH2 | 2.22 | 0.72 |
| 1:V0:392:LYS:HD2 | 1:V0:395:LEU:HD22 | 1.71 | 0.72 |
| 1:V2:345:ILE:O | 1:V2:348:ASN:ND2 | 2.17 | 0.72 |
| 1:X0:42:LEU:HB2 | 8:4X:97:PHE:CE1 | 2.25 | 0.72 |
| 2:X9:279:GLU:H | 2:X9:279:GLU:CD | 1.93 | 0.72 |
| 1:Y4:207:LEU:HB3 | 1:Y4:225:LEU:HD22 | 1.72 | 0.72 |
| 2:Z3:114:ILE:HG21 | 2:Z3:149:LEU:HD22 | 1.72 | 0.72 |
| 2:0P:387:ILE:HG12 | 2:0P:390:ARG:HH22 | 1.52 | 0.72 |
| 2:1H:56:THR:HA | 2:1X:285:GLN:HB2 | 1.71 | 0.72 |
| 2:1P:88:HIS:HB3 | 2:2F:283:HIS:ND1 | 2.04 | 0.72 |
| 2:1T:399:TYR:O | 2:1T:402:ARG:NH1 | 2.23 | 0.72 |
| 2:2H:88:HIS:CE1 | 2:2H:121:ARG:HH22 | 2.07 | 0.72 |
| 2:2N:88:HIS:HB3 | 2:3D:283:HIS:ND1 | 2.05 | 0.72 |
| 1:3K:5:VAL:HG23 | 1:3K:62:ARG:HG2 | 1.71 | 0.72 |
| 1:3K:77:ARG:HH22 | 3:4B:18:LYS:HB3 | 1.53 | 0.72 |
| 2:3T:425:LEU:O | 2:3T:425:LEU:HD23 | 1.90 | 0.72 |
| 24:6U:566:VAL:HG23 | 24:6U:573:VAL:HG21 | 1.70 | 0.72 |
| 24:6W:41:ARG:HA | 24:6W:41:ARG:NE | 2.02 | 0.72 |
| 2:A0:145:THR:OG1 | 41:A1:501:GTP:O1B | 2.07 | 0.72 |
| 2:K1:33:ASP:O | 2:K1:60:LYS:NZ | 2.23 | 0.72 |
| 2:M3:36:MET:HG2 | 2:M3:42:ILE:HG13 | 1.70 | 0.72 |
| 2:M5:88:HIS:HD2 | 2:M5:89:PRO:HD2 | 1.52 | 0.72 |
| 2:O1:286:LEU:HD13 | 2:O1:371:VAL:HG23 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T0:218:THR:HG23 | 1:T0:219:THR:HG23 | 1.72 | 0.72 |
| 1:V2:165:LEU:HD21 | 1:V2:250:LEU:HD11 | 1.71 | 0.72 |
| 2:W9:145:THR:OG1 | 41:X0:501:GTP:O1B | 2.08 | 0.72 |
| 1:Z8:208:TYR:HE1 | 1:Z8:225:LEU:HD11 | 1.55 | 0.72 |
| 1:0M:68:LEU:HB3 | 1:0M:96:GLY:HA2 | 1.71 | 0.72 |
| 2:0V:202:VAL:HG12 | 2:0V:268:MET:HB2 | 1.71 | 0.72 |
| 2:1R:288:VAL:HG11 | 2:1R:328:VAL:HG12 | 1.71 | 0.72 |
| 2:3P:286:LEU:HD13 | 2:3P:371:VAL:HG23 | 1.70 | 0.72 |
| 10:5A:443:GLU:OE2 | 10:5A:447:ARG:NH1 | 2.23 | 0.72 |
| 14:5M:356:PHE:HB2 | 14:5M:367:TRP:HB2 | 1.71 | 0.72 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:HH21 | 1.53 | 0.72 |
| 15:5P:329:PRO:CG | 15:5P:335:GLY:HA3 | 2.14 | 0.72 |
| 19:6E:92:ARG:CD | 19:6E:99:ARG:HE | 2.02 | 0.72 |
| 24:6W:122:TYR:HB2 | 24:6W:131:HIS:HB3 | 1.72 | 0.72 |
| 36:7V:32:LYS:HD3 | 36:7V:72:LEU:N | 2.02 | 0.72 |
| 2:4:29:GLY:C | 26:7D:45:MET:CE | 2.59 | 0.72 |
| 2:H3:288:VAL:HG11 | 2:H3:328:VAL:HG12 | 1.71 | 0.72 |
| 1:J0:320:ARG:HH22 | 28:7H:419:ILE:HD11 | 1.54 | 0.72 |
| 2:M9:267:PHE:HB2 | 2:M9:384:ILE:HD12 | 1.71 | 0.72 |
| 1:U8:345:ILE:O | 1:U8:348:ASN:ND2 | 2.22 | 0.72 |
| 2:W7:88:HIS:CD2 | 2:W7:89:PRO:HD2 | 2.24 | 0.72 |
| 1:Z8:139:LEU:HD12 | 1:Z8:170:VAL:HG12 | 1.72 | 0.72 |
| 1:2W:67:ASP:OD2 | 1:2W:72:THR:OG1 | 2.06 | 0.72 |
| 1:2Y:45:GLU:HG3 | 1:2Y:46:ARG:HG2 | 1.71 | 0.72 |
| 1:2Y:340:TYR:OH | 38:8C:95:LYS:O | 2.08 | 0.72 |
| 1:3C:355:ASP:OD1 | 38:8D:198:THR:CG2 | 2.36 | 0.72 |
| 14:5N:356:PHE:HB2 | 14:5N:367:TRP:HB2 | 1.71 | 0.72 |
| 24:6T:597:LEU:HB3 | 24:6T:602:LEU:HD21 | 1.69 | 0.72 |
| 36:7W:98:VAL:O | 36:7W:102:MET:N | 2.20 | 0.72 |
| 38:8A:206:PRO:HG2 | 38:8A:209:HIS:CE1 | 2.25 | 0.72 |
| 1:F0:58:ARG:HD3 | 1:G6:280:GLN:HE22 | 1.54 | 0.71 |
| 2:G1:278:ALA:HB3 | 22:6L:215:GLY:HA2 | 1.71 | 0.71 |
| 1:H4:276:ARG:NH2 | 24:6U:490:THR:CA | 2.43 | 0.71 |
| 1:I8:271:THR:HG21 | 1:I8:293:MET:HG3 | 1.71 | 0.71 |
| 1:J4:273:LEU:H | 1:J4:292:GLN:HE22 | 1.38 | 0.71 |
| 2:M5:267:PHE:HB2 | 2:M5:384:ILE:HD12 | 1.72 | 0.71 |
| 1:T6:27:GLU:OE1 | 1:T6:241:ARG:NH1 | 2.22 | 0.71 |
| 2:V3:213:CYS:HA | 2:V3:217:LEU:HB2 | 1.72 | 0.71 |
| 1:X6:396:HIS:HA | 1:X6:399:THR:HG22 | 1.71 | 0.71 |
| 2:Z3:388:PHE:HB3 | 2:Z3:425:LEU:HD11 | 1.72 | 0.71 |
| 2:0B:88:HIS:HB3 | 2:0R:283:HIS:ND1 | 2.05 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0V:264:ARG:NH2 | 2:0V:431:ASP:OD2 | 2.22 | 0.71 |
| 1:1C:33:THR:O | 1:1C:58:ARG:NH2 | 2.19 | 0.71 |
| 2:2X:88:HIS:HB3 | 2:3N:283:HIS:ND1 | 2.05 | 0.71 |
| 1:3A:337:ASN:OD1 | 38:8C:53:ALA:N | 2.23 | 0.71 |
| 1:3S:140:GLY:O | 1:3S:184:ASN:ND2 | 2.23 | 0.71 |
| 17:5V:179:GLN:NE2 | 17:5V:179:GLN:HA | 2.05 | 0.71 |
| 2:A2:40:LYS:NZ | 26:7F:45:MET:N | 2.37 | 0.71 |
| 1:H6:276:ARG:CD | 24:6V:490:THR:O | 2.37 | 0.71 |
| 1:R2:92:PHE:CE1 | 24:6V:33:LEU:CD1 | 2.73 | 0.71 |
| 1:Z6:33:THR:O | 1:Z6:58:ARG:NH2 | 2.23 | 0.71 |
| 1:2M:68:LEU:HB3 | 1:2M:96:GLY:HA2 | 1.71 | 0.71 |
| 1:2Q:211:CYS:HA | 1:2Q:215:LEU:HB2 | 1.72 | 0.71 |
| 1:2W:5:VAL:HG12 | 1:2W:62:ARG:HD3 | 1.72 | 0.71 |
| 1:3A:34:GLY:O | 1:3A:58:ARG:HA | 1.91 | 0.71 |
| 21:6G:131:TYR:OH | 21:6G:208:ASP:OD1 | 2.07 | 0.71 |
| 29:7I:220:LEU:HD12 | 29:7I:221:PRO:HD2 | 1.72 | 0.71 |
| 1:N6:253:LEU:HD11 | 1:N6:316:LEU:HD11 | 1.72 | 0.71 |
| 2:O9:406:HIS:HA | 2:O9:409:VAL:HG12 | 1.72 | 0.71 |
| 2:P3:90:GLU:HB3 | 2:P3:121:ARG:HH12 | 1.56 | 0.71 |
| 1:Q4:175:VAL:HG22 | 2:Q5:329:ASN:HD21 | 1.54 | 0.71 |
| 2:S5:364:PRO:HB3 | 31:7M:47:ARG:HH12 | 1.53 | 0.71 |
| 1:S6:213:ARG:HH21 | 1:S6:297:LYS:HD3 | 1.55 | 0.71 |
| 1:T4:292:GLN:O | 1:T4:298:ASN:ND2 | 2.24 | 0.71 |
| 2:W5:284:GLU:OE1 | 2:W5:284:GLU:HA | 1.89 | 0.71 |
| 1:Z4:14:ASN:HD21 | 1:Z4:65:LEU:HB3 | 1.56 | 0.71 |
| 1:1O:215:LEU:HB3 | 1:1O:217:LEU:HD23 | 1.72 | 0.71 |
| 1:2I:118:ASP:OD2 | 38:8C:99:THR:CB | 2.35 | 0.71 |
| 2:3D:214:ARG:HH22 | 38:8D:66:TYR:HA | 1.55 | 0.71 |
| 2:3H:286:LEU:O | 2:3H:373:ARG:NH1 | 2.24 | 0.71 |
| 1:3Q:218:THR:HB | 38:8D:227:LYS:HA | 1.71 | 0.71 |
| 10:5C:334:ARG:HH11 | 10:5C:338:LYS:HD3 | 1.55 | 0.71 |
| 24:6X:451:LYS:CB | 24:6X:468:ARG:NH1 | 2.52 | 0.71 |
| 36:7W:32:LYS:HD3 | 36:7W:72:LEU:N | 2.02 | 0.71 |
| 38:8B:165:LYS:HD2 | 38:8B:165:LYS:N | 2.01 | 0.71 |
| 38:8C:72:ASP:N | 38:8C:72:ASP:OD2 | 2.19 | 0.71 |
| 1:1:337:ASN:ND2 | 3:3V:69:TYR:H | 1.88 | 0.71 |
| 1:3:262:ARG:HH12 | 3:3X:240:ARG:HH11 | 1.36 | 0.71 |
| 2:A4:357:TYR:HB3 | 26:7F:146:ASN:HA | 1.71 | 0.71 |
| 1:G0:32:PRO:HD2 | 24:6V:527:ASN:HD22 | 1.54 | 0.71 |
| 2:G1:344:VAL:CG1 | 2:G1:347:CYS:HB3 | 2.19 | 0.71 |
| 2:H5:132:LEU:HD22 | 2:H5:164:LYS:HD3 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J2:140:GLY:O | 1:J2:184:ASN:ND2 | 2.23 | 0.71 |
| 1:M2:145:SER:OG | 1:M2:188:SER:OG | 2.09 | 0.71 |
| 1:U8:113:ILE:HA | 1:U8:116:VAL:HG22 | 1.70 | 0.71 |
| 1:X2:67:ASP:OD2 | 1:X2:72:THR:OG1 | 2.07 | 0.71 |
| 1:X4:236:ILE:HD11 | 1:X4:368:ILE:HD11 | 1.71 | 0.71 |
| 1:Z2:67:ASP:OD2 | 1:Z2:72:THR:OG1 | 2.08 | 0.71 |
| 2:0L:198:THR:HG21 | 2:0L:201:ALA:HB2 | 1.71 | 0.71 |
| 1:0M:311:LEU:HD23 | 1:0M:312:THR:HG23 | 1.72 | 0.71 |
| 1:0O:45:GLU:HG3 | 1:0O:46:ARG:HG2 | 1.72 | 0.71 |
| 2:1H:202:VAL:HG12 | 2:1H:268:MET:HB2 | 1.72 | 0.71 |
| 1:1K:135:VAL:HG11 | 1:1K:152:ILE:HD11 | 1.72 | 0.71 |
| 1:1S:418:LEU:HG | 1:1S:422:TYR:HE2 | 1.55 | 0.71 |
| 1:3O:77:ARG:HH21 | 3:4F:19:LEU:CD2 | 2.02 | 0.71 |
| 2:3T:216:SER:OG | 2:3T:275:ILE:O | 2.06 | 0.71 |
| 3:3V:150:GLU:O | 3:3V:190:LYS:NZ | 2.22 | 0.71 |
| 3:3X:150:GLU:O | 3:3X:190:LYS:NZ | 2.22 | 0.71 |
| 3:3Z:150:GLU:O | 3:3Z:190:LYS:NZ | 2.22 | 0.71 |
| 3:4B:150:GLU:O | 3:4B:190:LYS:NZ | 2.22 | 0.71 |
| 3:4F:150:GLU:O | 3:4F:190:LYS:NZ | 2.22 | 0.71 |
| 14:5L:112:SER:HA | 14:5L:155:PHE:HD2 | 1.54 | 0.71 |
| 22:6J:108:ARG:NH2 | 24:6U:284:THR:O | 2.23 | 0.71 |
| 22:6L:177:LEU:HD23 | 22:6L:187:MET:CE | 2.19 | 0.71 |
| 29:7J:225:THR:HG23 | 29:7J:228:GLY:H | 1.55 | 0.71 |
| 35:7T:236:GLU:HA | 35:7T:239:LYS:HE3 | 1.71 | 0.71 |
| 1:G4:200:MET:HE3 | 1:G4:268:VAL:HG21 | 1.73 | 0.71 |
| 2:G7:9:ILE:HG22 | 2:G7:146:GLY:HA2 | 1.71 | 0.71 |
| 1:J2:113:ILE:HD13 | 1:J2:150:LEU:HD22 | 1.71 | 0.71 |
| 2:N5:88:HIS:CE1 | 2:N5:90:GLU:HG3 | 2.25 | 0.71 |
| 1:O8:58:ARG:HD3 | 1:Q6:280:GLN:HE22 | 1.54 | 0.71 |
| 1:O8:320:ARG:HH12 | 32:7P:64:THR:HA | 1.56 | 0.71 |
| 1:P4:345:ILE:O | 1:P4:348:ASN:ND2 | 2.23 | 0.71 |
| 1:S4:334:GLN:HE22 | 1:S4:348:ASN:H | 1.38 | 0.71 |
| 1:W8:139:LEU:HD12 | 1:W8:170:VAL:HG12 | 1.71 | 0.71 |
| 2:0J:9:ILE:HG13 | 2:0J:68:LEU:HD11 | 1.73 | 0.71 |
| 2:1H:9:ILE:HG22 | 2:1H:146:GLY:HA2 | 1.72 | 0.71 |
| 1:2S:306:ARG:HH22 | 38:8A:51:GLN:HA | 1.54 | 0.71 |
| 2:3D:88:HIS:HB3 | 2:3T:283:HIS:ND1 | 2.04 | 0.71 |
| 2:3L:339:ARG:HE | 2:3L:339:ARG:HA | 1.56 | 0.71 |
| 4:4A:35:LYS:NZ | 3:4B:254:LYS:O | 2.18 | 0.71 |
| 3:4D:150:GLU:O | 3:4D:190:LYS:NZ | 2.22 | 0.71 |
| 3:4H:150:GLU:O | 3:4H:190:LYS:NZ | 2.22 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5P:55:LEU:N | 15:5P:55:LEU:HD23 | 2.04 | 0.71 |
| 17:5U:174:SER:HB2 | 17:5U:175:PRO:HD2 | 1.72 | 0.71 |
| 24:6W:484:GLU:O | 24:6W:484:GLU:HG3 | 1.89 | 0.71 |
| 24:6X:95:VAL:CG1 | 24:6X:124:TYR:CD2 | 2.74 | 0.71 |
| 24:7A:97:ARG:H | 24:7A:188:THR:HG21 | 1.56 | 0.71 |
| 2:4:82:THR:HG22 | 26:7D:118:SER:H | 1.54 | 0.71 |
| 1:I2:345:ILE:O | 1:I2:348:ASN:ND2 | 2.24 | 0.71 |
| 2:M7:90:GLU:HB3 | 1:O4:281:TYR:CE2 | 2.25 | 0.71 |
| 1:T2:92:PHE:CE2 | 24:6Y:33:LEU:HB3 | 2.26 | 0.71 |
| 1:X4:218:THR:HG23 | 1:X4:219:THR:HG23 | 1.71 | 0.71 |
| 2:0X:340:THR:HG23 | 2:0X:341:ILE:HD12 | 1.72 | 0.71 |
| 1:2Y:320:ARG:CZ | 38:8C:198:THR:HA | 2.21 | 0.71 |
| 5:4M:293:LEU:CB | 28:7X:306:LEU:HD21 | 2.19 | 0.71 |
| 24:6T:10:LYS:HE3 | 12:7B:95:LEU:HD12 | 1.73 | 0.71 |
| 2:D5:279:GLU:OE2 | 18:6C:178:GLN:CD | 2.28 | 0.71 |
| 1:I2:180:VAL:HG23 | 1:I2:184:ASN:HD21 | 1.55 | 0.71 |
| 1:N2:248:ALA:CA | 1:N2:252:LYS:HD2 | 2.11 | 0.71 |
| 2:S9:415:GLU:OE2 | 2:S9:415:GLU:N | 2.23 | 0.71 |
| 2:U9:88:HIS:HE1 | 2:W5:280:LYS:HG2 | 1.55 | 0.71 |
| 2:W1:88:HIS:CD2 | 2:W1:121:ARG:HH22 | 2.08 | 0.71 |
| 2:Z1:53:PHE:HB3 | 2:Z1:61:HIS:HB3 | 1.71 | 0.71 |
| 1:Z2:7:ILE:HG22 | 1:Z2:64:ILE:HB | 1.72 | 0.71 |
| 2:Z5:202:VAL:HG22 | 2:Z5:268:MET:HB2 | 1.72 | 0.71 |
| 1:Z8:179:VAL:HG22 | 2:Z9:258:ASN:HD22 | 1.55 | 0.71 |
| 2:0R:352:LYS:NZ | 2:0R:353:CYS:O | 2.24 | 0.71 |
| 2:2H:120:ASP:OD2 | 38:8B:27:HIS:NE2 | 2.21 | 0.71 |
| 1:2I:118:ASP:CB | 38:8C:99:THR:CB | 2.57 | 0.71 |
| 1:2Q:276:ARG:HE | 10:5C:196:LEU:HG | 1.56 | 0.71 |
| 2:3P:84:ARG:HE | 23:6S:15:ARG:HH22 | 1.36 | 0.71 |
| 24:6X:130:MET:SD | 24:6X:166:PHE:CZ | 2.84 | 0.71 |
| 24:6X:481:LEU:HB3 | 24:6X:500:ARG:HB3 | 1.71 | 0.71 |
| 1:A9:320:ARG:HH12 | 18:5X:53:GLY:HA3 | 1.53 | 0.71 |
| 2:B0:206:ASN:ND2 | 41:B0:501:GTP:O2' | 2.24 | 0.71 |
| 2:D3:285:GLN:HE21 | 24:6X:253:PRO:HG2 | 1.56 | 0.71 |
| 2:E7:282:TYR:CG | 22:6L:82:LEU:HD21 | 2.25 | 0.71 |
| 2:G7:72:PRO:HG3 | 1:G8:1:MET:HG2 | 1.72 | 0.71 |
| 1:J6:131:GLN:HE21 | 1:J6:250:LEU:HB2 | 1.56 | 0.71 |
| 2:K1:133:GLN:NE2 | 2:K1:251:ASP:HB2 | 2.06 | 0.71 |
| 1:M2:190:HIS:HD2 | 1:M2:411:ALA:HA | 1.56 | 0.71 |
| 1:P6:52:ASN:OD1 | 1:P6:62:ARG:NH2 | 2.24 | 0.71 |
| 1:R0:10:GLY:O | 1:R0:14:ASN:ND2 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R5:263:PRO:O | 17:5T:84:ARG:NH1 | 2.23 | 0.71 |
| 2:S5:301:MET:HE1 | 2:S5:307:PRO:HD3 | 1.73 | 0.71 |
| 1:Y8:113:ILE:HD13 | 1:Y8:150:LEU:HD22 | 1.73 | 0.71 |
| 1:0I:49:VAL:HG21 | 1:0I:240:LEU:HD13 | 1.73 | 0.71 |
| 1:3C:306:ARG:HH22 | 38:8D:99:THR:H | 1.38 | 0.71 |
| 12:5F:359:LEU:HD21 | 12:5F:363:MET:SD | 2.31 | 0.71 |
| 15:5O:234:ALA:HB1 | 15:5O:366:VAL:HG23 | 1.72 | 0.71 |
| 15:5O:284:VAL:HG11 | 25:7C:80:ARG:NE | 2.04 | 0.71 |
| 18:5X:180:ARG:HD2 | 18:5X:196:VAL:HG11 | 1.72 | 0.71 |
| 19:6E:92:ARG:CG | 19:6E:99:ARG:HE | 2.03 | 0.71 |
| 20:6F:370:LEU:HD23 | 20:6F:384:LEU:HB2 | 1.73 | 0.71 |
| 24:6U:597:LEU:HB3 | 24:6U:602:LEU:HD21 | 1.70 | 0.71 |
| 29:7J:388:MET:HA | 29:7J:388:MET:HE3 | 1.72 | 0.71 |
| 1:E2:204:ASN:HD21 | 39:E2:501:GDP:HN22 | 1.38 | 0.71 |
| 2:F7:206:ASN:OD1 | 41:F8:501:GTP:N2 | 2.22 | 0.71 |
| 2:I3:195:LEU:HD21 | 2:I3:264:ARG:HD2 | 1.72 | 0.71 |
| 2:J3:88:HIS:CD2 | 2:J3:89:PRO:HD2 | 2.26 | 0.71 |
| 1:L0:334:GLN:HE22 | 1:L0:348:ASN:H | 1.38 | 0.71 |
| 1:M4:345:ILE:O | 1:M4:348:ASN:ND2 | 2.24 | 0.71 |
| 1:O2:396:HIS:HA | 1:O2:399:THR:HG22 | 1.73 | 0.71 |
| 1:O6:388:MET:CE | 2:O7:348:PRO:HD2 | 2.21 | 0.71 |
| 2:O7:29:GLY:HA2 | 32:7P:79:LEU:HD22 | 1.73 | 0.71 |
| 1:S8:263:LEU:HD22 | 1:S8:422:TYR:HE1 | 1.55 | 0.71 |
| 1:X8:50:TYR:OH | 1:X8:237:THR:OG1 | 2.07 | 0.71 |
| 2:Z3:83:TYR:HB3 | 2:Z3:86:LEU:HB3 | 1.73 | 0.71 |
| 1:0Y:107:THR:OG1 | 1:0Y:108:GLU:OE1 | 2.08 | 0.71 |
| 1:1U:67:ASP:OD2 | 1:1U:72:THR:OG1 | 2.07 | 0.71 |
| 2:3H:287:SER:N | 2:3H:290:GLU:OE2 | 2.22 | 0.71 |
| 24:6X:445:ILE:HG22 | 24:6X:447:ARG:HD2 | 1.72 | 0.71 |
| 2:A2:370:LYS:HD3 | 24:6Y:92:ASP:OD1 | 1.88 | 0.71 |
| 1:G2:391:ARG:HH11 | 1:G2:391:ARG:CG | 2.01 | 0.71 |
| 2:H3:274:PRO:HB2 | 2:H3:276:ILE:HG12 | 1.72 | 0.71 |
| 2:I7:33:ASP:O | 2:I7:60:LYS:NZ | 2.24 | 0.71 |
| 2:J3:85:GLN:O | 2:K9:283:HIS:HE1 | 1.73 | 0.71 |
| 2:L3:279:GLU:OE1 | 2:L3:279:GLU:N | 2.23 | 0.71 |
| 2:M7:108:TYR:O | 2:M7:112:LYS:NZ | 2.20 | 0.71 |
| 2:P3:307:PRO:HB2 | 2:P3:312:TYR:HE1 | 1.56 | 0.71 |
| 1:V6:175:VAL:HG13 | 2:V7:329:ASN:HD21 | 1.56 | 0.71 |
| 2:X5:88:HIS:HB3 | 2:Z1:283:HIS:ND1 | 2.06 | 0.71 |
| 1:Y8:117:LEU:HD11 | 1:Y8:154:LYS:HD3 | 1.71 | 0.71 |
| 2:0B:352:LYS:NZ | 2:0B:353:CYS:O | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0H:66:ILE:HG12 | 2:0H:122:ILE:HD11 | 1.71 | 0.71 |
| 1:0I:211:CYS:HA | 1:0I:215:LEU:HB2 | 1.73 | 0.71 |
| 1:0O:272:PRO:HB2 | 1:0O:282:ARG:HH12 | 1.52 | 0.71 |
| 1:0S:103:LYS:HE2 | 1:0S:108:GLU:HG2 | 1.73 | 0.71 |
| 1:2E:77:ARG:HH21 | 1:2E:90:PHE:HD2 | 1.38 | 0.71 |
| 2:2X:279:GLU:OE1 | 2:2X:279:GLU:N | 2.15 | 0.71 |
| 2:3J:246:GLY:H | 2:3J:249:ASN:HD21 | 1.39 | 0.71 |
| 3:3X:122:ARG:NH2 | 3:3X:167:GLU:OE1 | 2.23 | 0.71 |
| 5:4M:293:LEU:CB | 28:7X:306:LEU:CD2 | 2.69 | 0.71 |
| 8:4W:460:ALA:CB | 8:4X:128:LEU:HD22 | 2.20 | 0.71 |
| 22:6J:170:ARG:NH2 | 22:6J:246:GLN:O | 2.24 | 0.71 |
| 24:6V:97:ARG:H | 24:6V:188:THR:HG21 | 1.55 | 0.71 |
| 24:6V:268:ASN:HA | 24:6V:271:LYS:HD3 | 1.70 | 0.71 |
| 24:6V:577:VAL:HG21 | 24:6V:630:LEU:HD21 | 1.73 | 0.71 |
| 24:6X:514:TYR:O | 24:6X:517:LEU:HD13 | 1.89 | 0.71 |
| 38:8C:206:PRO:HG2 | 38:8C:209:HIS:NE2 | 2.05 | 0.71 |
| 1:G4:32:PRO:HD2 | 24:6X:527:ASN:HD22 | 1.56 | 0.70 |
| 1:G8:112:LEU:HB3 | 1:G8:147:MET:HE2 | 1.72 | 0.70 |
| 2:J7:90:GLU:HB3 | 2:J7:121:ARG:HH22 | 1.56 | 0.70 |
| 2:J7:277:SER:CB | 2:J7:280:LYS:HZ3 | 2.04 | 0.70 |
| 1:Q2:259:PRO:HG3 | 1:Q2:311:LEU:HD21 | 1.72 | 0.70 |
| 2:T1:286:LEU:O | 2:T1:373:ARG:NH1 | 2.24 | 0.70 |
| 1:T4:69:GLU:OE1 | 2:T5:2:ARG:NH1 | 2.24 | 0.70 |
| 1:X0:38:GLY:HA3 | 8:4X:95:THR:HG23 | 1.73 | 0.70 |
| 2:Z3:324:VAL:HG22 | 2:Z3:326:LYS:H | 1.55 | 0.70 |
| 2:Z5:298:PRO:HA | 2:Z5:301:MET:HG3 | 1.72 | 0.70 |
| 1:0E:207:LEU:HB3 | 1:0E:225:LEU:HD22 | 1.73 | 0.70 |
| 1:2M:110:ALA:HB3 | 38:8D:87:LYS:HD3 | 1.73 | 0.70 |
| 1:3C:34:GLY:O | 1:3C:58:ARG:HA | 1.90 | 0.70 |
| 1:3K:45:GLU:HG3 | 1:3K:46:ARG:HG2 | 1.73 | 0.70 |
| 3:4B:122:ARG:NH2 | 3:4B:167:GLU:OE1 | 2.23 | 0.70 |
| 3:4F:122:ARG:NH2 | 3:4F:167:GLU:OE1 | 2.23 | 0.70 |
| 14:5L:213:THR:OG1 | 14:5L:217:ASP:OD1 | 2.09 | 0.70 |
| 14:5M:213:THR:OG1 | 14:5M:217:ASP:OD1 | 2.09 | 0.70 |
| 14:5N:213:THR:OG1 | 14:5N:217:ASP:OD1 | 2.09 | 0.70 |
| 24:6T:96:LEU:HB2 | 24:6T:123:TYR:HB3 | 1.72 | 0.70 |
| 24:6X:597:LEU:HB3 | 24:6X:602:LEU:HD21 | 1.73 | 0.70 |
| 2:A2:33:ASP:CB | 18:6C:77:THR:HG21 | 2.21 | 0.70 |
| 1:H6:276:ARG:NH1 | 24:6V:490:THR:CA | 2.54 | 0.70 |
| 1:M0:86:ARG:HB3 | 2:N7:283:HIS:HE1 | 1.57 | 0.70 |
| 2:M3:369:ALA:HB1 | 30:7K:213:PHE:HD2 | 1.54 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R9:56:THR:HA | 2:T5:285:GLN:HB3 | 1.72 | 0.70 |
| 1:S2:345:ILE:O | 1:S2:348:ASN:ND2 | 2.24 | 0.70 |
| 2:U9:90:GLU:C | 2:U9:121:ARG:HH12 | 1.94 | 0.70 |
| 1:W8:220:PRO:HD2 | 2:W9:326:LYS:HD3 | 1.72 | 0.70 |
| 2:W9:286:LEU:O | 2:W9:373:ARG:NH1 | 2.24 | 0.70 |
| 2:X7:287:SER:N | 2:X7:290:GLU:OE2 | 2.24 | 0.70 |
| 2:X7:320:ARG:NH2 | 2:X7:358:GLN:OE1 | 2.25 | 0.70 |
| 2:Y9:352:LYS:NZ | 2:Y9:353:CYS:O | 2.24 | 0.70 |
| 1:0C:68:LEU:HB3 | 1:0C:96:GLY:HA2 | 1.71 | 0.70 |
| 2:0J:399:TYR:O | 2:0J:402:ARG:NH1 | 2.24 | 0.70 |
| 2:0Z:56:THR:HB | 2:1P:285:GLN:HB2 | 1.72 | 0.70 |
| 2:0Z:399:TYR:O | 2:0Z:402:ARG:NH1 | 2.23 | 0.70 |
| 7:4R:62:PHE:CZ | 24:6V:9:PRO:HD3 | 2.26 | 0.70 |
| 2:4:85:GLN:NE2 | 18:5Y:78:LEU:HB2 | 2.06 | 0.70 |
| 2:A8:278:ALA:HB3 | 18:5X:43:ASN:HD22 | 1.55 | 0.70 |
| 2:H1:88:HIS:HB3 | 2:I7:283:HIS:ND1 | 2.06 | 0.70 |
| 1:I4:113:ILE:HA | 1:I4:116:VAL:HG12 | 1.73 | 0.70 |
| 2:T7:297:GLU:HG3 | 2:T7:299:ALA:H | 1.54 | 0.70 |
| 1:X4:5:VAL:HG23 | 1:X4:62:ARG:HG2 | 1.73 | 0.70 |
| 1:0A:33:THR:O | 1:0A:58:ARG:NH2 | 2.24 | 0.70 |
| 1:1E:1:MET:HE1 | 1:1E:2:ARG:HG3 | 1.72 | 0.70 |
| 1:1Q:113:ILE:HD13 | 1:1Q:150:LEU:HD22 | 1.74 | 0.70 |
| 1:1Q:280:GLN:HG2 | 9:4Z:193:LEU:HG | 1.72 | 0.70 |
| 2:1R:399:TYR:O | 2:1R:402:ARG:NH1 | 2.24 | 0.70 |
| 2:1X:336:LYS:O | 2:1X:339:ARG:NH2 | 2.21 | 0.70 |
| 2:2B:399:TYR:O | 2:2B:402:ARG:NH1 | 2.23 | 0.70 |
| 1:2M:165:LEU:HD21 | 1:2M:250:LEU:HD11 | 1.73 | 0.70 |
| 1:2Q:320:ARG:NH2 | 38:8A:198:THR:HA | 2.04 | 0.70 |
| 1:3K:113:ILE:HD13 | 1:3K:150:LEU:HD22 | 1.73 | 0.70 |
| 3:4D:122:ARG:NH2 | 3:4D:167:GLU:OE1 | 2.23 | 0.70 |
| 7:4R:29:VAL:HG21 | 7:4R:31:LYS:HE2 | 1.73 | 0.70 |
| 15:5O:234:ALA:HB1 | 15:5O:366:VAL:CG2 | 2.21 | 0.70 |
| 15:5P:334:LEU:O | 15:5P:334:LEU:HD23 | 1.90 | 0.70 |
| 29:7J:332:ALA:HB3 | 29:7J:337:ARG:HE | 1.55 | 0.70 |
| 1:B1:320:ARG:HH12 | 18:5Y:53:GLY:HA3 | 1.55 | 0.70 |
| 1:H2:122:LYS:HE3 | 1:I8:291:GLN:HB3 | 1.73 | 0.70 |
| 1:L2:57:GLY:HA2 | 30:7K:56:ARG:HH22 | 1.54 | 0.70 |
| 2:L5:377:MET:SD | 2:L5:379:SER:OG | 2.45 | 0.70 |
| 1:M6:67:ASP:OD2 | 1:M6:72:THR:OG1 | 2.09 | 0.70 |
| 2:O5:128:ASN:ND2 | 2:O5:128:ASN:O | 2.24 | 0.70 |
| 2:P9:56:THR:HG21 | 2:P9:62:VAL:HG13 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q2:178:THR:HG22 | 2:Q3:352:LYS:HZ3 | 1.56 | 0.70 |
| 1:R6:135:VAL:HG21 | 1:R6:152:ILE:HD11 | 1.74 | 0.70 |
| 1:S0:125:GLU:OE2 | 1:S0:159:TYR:OH | 2.09 | 0.70 |
| 2:U7:56:THR:HG23 | 2:U7:60:LYS:HB3 | 1.72 | 0.70 |
| 1:V2:248:ALA:HA | 1:V2:252:LYS:HD2 | 1.73 | 0.70 |
| 1:W8:219:THR:HA | 2:W9:326:LYS:HE2 | 1.73 | 0.70 |
| 1:X6:192:LEU:HD22 | 1:X6:196:ALA:HB2 | 1.71 | 0.70 |
| 1:Z0:33:THR:O | 1:Z0:58:ARG:NH2 | 2.23 | 0.70 |
| 1:0K:45:GLU:HG3 | 1:0K:46:ARG:HG2 | 1.72 | 0.70 |
| 2:0Z:88:HIS:CD2 | 2:0Z:89:PRO:CD | 2.72 | 0.70 |
| 1:2G:309:ARG:NH1 | 1:2G:339:SER:O | 2.24 | 0.70 |
| 2:2N:217:LEU:HG | 2:2N:219:ILE:HG12 | 1.73 | 0.70 |
| 3:4H:122:ARG:NH2 | 3:4H:167:GLU:OE1 | 2.23 | 0.70 |
| 17:5T:189:TRP:HD1 | 17:5T:222:ILE:HG23 | 1.56 | 0.70 |
| 24:6W:597:LEU:HB3 | 24:6W:602:LEU:HD21 | 1.72 | 0.70 |
| 1:R6:52:ASN:OD1 | 1:R6:62:ARG:NH2 | 2.25 | 0.70 |
| 2:T1:287:SER:N | 2:T1:290:GLU:OE2 | 2.23 | 0.70 |
| 1:T4:391:ARG:O | 1:T4:391:ARG:HG3 | 1.91 | 0.70 |
| 2:Z5:56:THR:HA | 2:0L:285:GLN:HG2 | 1.74 | 0.70 |
| 2:0P:9:ILE:HG12 | 2:0P:153:LEU:HD21 | 1.74 | 0.70 |
| 1:0S:181:GLU:HG2 | 1:0S:182:PRO:HD3 | 1.71 | 0.70 |
| 2:2B:90:GLU:O | 2:2B:121:ARG:NH1 | 2.18 | 0.70 |
| 1:2C:272:PRO:HB2 | 1:2C:282:ARG:HH12 | 1.56 | 0.70 |
| 1:2Q:320:ARG:NH1 | 38:8A:198:THR:CA | 2.52 | 0.70 |
| 1:2Y:56:GLY:HA3 | 38:8C:161:GLN:HE21 | 1.56 | 0.70 |
| 2:2Z:88:HIS:HB3 | 2:2Z:91:GLN:HG2 | 1.74 | 0.70 |
| 2:3F:287:SER:N | 2:3F:290:GLU:OE2 | 2.25 | 0.70 |
| 3:3V:122:ARG:NH2 | 3:3V:167:GLU:OE1 | 2.23 | 0.70 |
| 3:3Z:122:ARG:NH2 | 3:3Z:167:GLU:OE1 | 2.23 | 0.70 |
| 9:4Z:328:ASP:HB3 | 9:4Z:331:ARG:HH21 | 1.55 | 0.70 |
| 14:5L:180:ASN:OD1 | 14:5L:180:ASN:N | 2.25 | 0.70 |
| 14:5M:180:ASN:OD1 | 14:5M:180:ASN:N | 2.25 | 0.70 |
| 15:5O:289:LEU:N | 15:5O:290:PRO:CD | 2.54 | 0.70 |
| 24:6T:107:VAL:HG12 | 24:6T:108:GLU:H | 1.57 | 0.70 |
| 24:6Z:244:ALA:HB1 | 24:6Z:257:LEU:HD11 | 1.71 | 0.70 |
| 29:7I:126:LEU:HD13 | 30:7K:321:GLN:HB2 | 1.72 | 0.70 |
| 2:G9:191:THR:HA | 2:G9:194:LEU:HB3 | 1.74 | 0.70 |
| 2:J3:357:TYR:HB3 | 16:5Q:173:ARG:CD | 2.20 | 0.70 |
| 2:L3:371:VAL:HG22 | 2:L3:373:ARG:H | 1.56 | 0.70 |
| 2:S1:336:LYS:O | 2:S1:339:ARG:NH2 | 2.24 | 0.70 |
| 1:S4:26:ASP:OD1 | 24:6U:10:LYS:CE | 2.40 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W1:267:PHE:HB2 | 2:W1:384:ILE:HD12 | 1.73 | 0.70 |
| 1:W2:30:ILE:HG22 | 1:W2:36:TYR:HA | 1.73 | 0.70 |
| 2:X7:406:HIS:HA | 2:X7:409:VAL:HG12 | 1.74 | 0.70 |
| 1:0I:45:GLU:HG3 | 1:0I:46:ARG:HG2 | 1.73 | 0.70 |
| 2:0V:56:THR:HA | 2:1L:285:GLN:HB2 | 1.73 | 0.70 |
| 2:0X:11:GLN:OE1 | 2:0X:15:GLN:NE2 | 2.25 | 0.70 |
| 2:1P:33:ASP:O | 2:1P:60:LYS:NZ | 2.24 | 0.70 |
| 1:1S:5:VAL:HG12 | 1:1S:62:ARG:HD3 | 1.73 | 0.70 |
| 2:1T:318:MET:HB2 | 2:1T:376:CYS:HB3 | 1.73 | 0.70 |
| 2:3B:279:GLU:OE2 | 2:3B:279:GLU:N | 2.12 | 0.70 |
| 21:6H:111:VAL:N | 24:6X:82:ALA:O | 2.23 | 0.70 |
| 22:6N:110:ILE:O | 22:6N:113:ARG:NH1 | 2.25 | 0.70 |
| 24:6W:525:VAL:HB | 24:6W:530:PHE:HE2 | 1.55 | 0.70 |
| 26:7F:119:MET:HA | 26:7F:119:MET:HE3 | 1.74 | 0.70 |
| 27:7G:91:TYR:HE1 | 27:7G:99:ARG:HG2 | 1.57 | 0.70 |
| 2:G5:9:ILE:HG13 | 2:G5:139:ASN:HB3 | 1.73 | 0.70 |
| 1:G8:52:ASN:OD1 | 1:G8:62:ARG:NH2 | 2.25 | 0.70 |
| 2:H3:91:GLN:HE22 | 2:H3:125:LEU:HD21 | 1.57 | 0.70 |
| 2:L3:89:PRO:CB | 29:7J:320:PRO:HG3 | 2.20 | 0.70 |
| 1:L6:219:THR:HB | 2:L7:324:VAL:HG11 | 1.73 | 0.70 |
| 1:N8:282:ARG:NH2 | 1:N8:288:GLU:OE2 | 2.24 | 0.70 |
| 2:R5:196:GLU:HG2 | 17:5T:82:LYS:NZ | 2.05 | 0.70 |
| 2:R9:81:GLY:O | 2:R9:84:ARG:NH1 | 2.25 | 0.70 |
| 1:S0:418:LEU:HG | 1:S0:422:TYR:HE2 | 1.57 | 0.70 |
| 2:S1:367:ASP:OD1 | 7:4R:342:ARG:NH1 | 2.24 | 0.70 |
| 1:S4:337:ASN:HD21 | 17:5R:48:THR:H | 1.40 | 0.70 |
| 1:S4:392:LYS:HD2 | 1:S4:392:LYS:N | 2.07 | 0.70 |
| 2:U1:344:VAL:HG22 | 2:U1:346:TRP:H | 1.55 | 0.70 |
| 2:V1:9:ILE:HG22 | 2:V1:146:GLY:HA2 | 1.74 | 0.70 |
| 2:W9:287:SER:N | 2:W9:290:GLU:OE2 | 2.23 | 0.70 |
| 2:Z9:88:HIS:HB3 | 2:0P:283:HIS:ND1 | 2.06 | 0.70 |
| 2:0J:115:VAL:HG23 | 2:0J:153:LEU:HD23 | 1.74 | 0.70 |
| 1:0S:211:CYS:HA | 1:0S:215:LEU:HB2 | 1.74 | 0.70 |
| 2:1D:9:ILE:HG22 | 2:1D:146:GLY:HA2 | 1.74 | 0.70 |
| 1:3K:276:ARG:HH12 | 17:5T:216:GLU:HB3 | 1.56 | 0.70 |
| 1:3M:77:ARG:NH2 | 3:4D:19:LEU:HD23 | 2.05 | 0.70 |
| 2:3N:51:THR:HG21 | 2:3N:243:ARG:HG2 | 1.73 | 0.70 |
| 1:3O:391:ARG:HH22 | 2:3P:435:VAL:HA | 1.56 | 0.70 |
| 9:4Z:152:ARG:HH22 | 9:4Z:153:LYS:HE2 | 1.55 | 0.70 |
| 12:5F:13:PRO:HG3 | 12:5G:298:ASP:HB2 | 1.74 | 0.70 |
| 15:5O:28:TYR:OH | 15:5O:57:PRO:HG3 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:6F:65:TYR:HB2 | 20:6F:138:ILE:HD11 | 1.73 | 0.70 |
| 22:6K:108:ARG:NH2 | 24:6V:284:THR:O | 2.25 | 0.70 |
| 22:6L:110:ILE:O | 22:6L:113:ARG:NH1 | 2.24 | 0.70 |
| 36:7V:95:PHE:O | 36:7V:99:GLU:HG2 | 1.92 | 0.70 |
| 2:E5:282:TYR:OH | 22:6K:80:GLY:O | 2.08 | 0.70 |
| 2:H5:317:LEU:HD11 | 2:H5:351:PHE:HD1 | 1.56 | 0.70 |
| 1:H6:2:ARG:HB3 | 1:H6:131:GLN:HB2 | 1.73 | 0.70 |
| 2:J1:11:GLN:NE2 | 1:J2:247:ASN:OD1 | 2.25 | 0.70 |
| 1:M2:58:ARG:HG2 | 2:N9:282:TYR:CE1 | 2.27 | 0.70 |
| 2:M5:72:PRO:HD2 | 1:M6:2:ARG:HH12 | 1.57 | 0.70 |
| 2:M5:121:ARG:HH11 | 2:M5:121:ARG:HB2 | 1.56 | 0.70 |
| 2:R9:286:LEU:O | 2:R9:373:ARG:NH1 | 2.25 | 0.70 |
| 2:W7:287:SER:N | 2:W7:290:GLU:OE2 | 2.23 | 0.70 |
| 1:Y8:189:VAL:HA | 1:Y8:192:LEU:HB3 | 1.74 | 0.70 |
| 1:0U:51:PHE:O | 1:0U:62:ARG:NH2 | 2.24 | 0.70 |
| 1:1S:211:CYS:HA | 1:1S:215:LEU:HB2 | 1.72 | 0.70 |
| 2:1X:33:ASP:O | 2:1X:60:LYS:NZ | 2.25 | 0.70 |
| 1:2A:77:ARG:HH21 | 1:2A:90:PHE:HD2 | 1.40 | 0.70 |
| 1:2A:211:CYS:HA | 1:2A:215:LEU:HB2 | 1.74 | 0.70 |
| 2:2X:306:ASP:OD2 | 38:8B:23:SER:OG | 2.03 | 0.70 |
| 1:3K:94:GLN:NE2 | 3:4B:139:SER:O | 2.25 | 0.70 |
| 22:6I:108:ARG:NH2 | 24:6T:284:THR:O | 2.25 | 0.70 |
| 24:6X:107:VAL:HG12 | 24:6X:108:GLU:H | 1.56 | 0.70 |
| 2:A2:370:LYS:HG2 | 24:6Y:89:VAL:HG23 | 1.74 | 0.70 |
| 2:F1:88:HIS:ND1 | 2:G7:283:HIS:HA | 2.06 | 0.70 |
| 1:M4:211:CYS:HA | 1:M4:215:LEU:HB2 | 1.74 | 0.70 |
| 1:P4:392:LYS:HD2 | 1:P4:395:LEU:HD22 | 1.73 | 0.70 |
| 1:P6:139:LEU:HD12 | 1:P6:170:VAL:HG22 | 1.72 | 0.70 |
| 1:R2:194:GLU:OE2 | 1:R2:414:ASN:ND2 | 2.24 | 0.70 |
| 2:S5:220:GLU:HG2 | 2:S5:221:ARG:HG3 | 1.72 | 0.70 |
| 2:V1:175:PRO:HB2 | 2:V1:176:GLN:HE21 | 1.57 | 0.70 |
| 1:W2:145:SER:HG | 1:W2:188:SER:HG | 1.38 | 0.70 |
| 1:X0:42:LEU:HG | 8:4X:97:PHE:HZ | 1.55 | 0.70 |
| 2:X3:287:SER:N | 2:X3:290:GLU:OE2 | 2.24 | 0.70 |
| 1:Z4:311:LEU:HD23 | 1:Z4:312:THR:HG23 | 1.73 | 0.70 |
| 1:0G:45:GLU:HG3 | 1:0G:46:ARG:HG2 | 1.72 | 0.70 |
| 1:1M:309:ARG:NH1 | 1:1M:339:SER:O | 2.25 | 0.70 |
| 2:2D:399:TYR:O | 2:2D:402:ARG:NH1 | 2.25 | 0.70 |
| 2:2H:88:HIS:CE1 | 2:2H:121:ARG:NH2 | 2.60 | 0.70 |
| 1:2Q:306:ARG:NH2 | 38:8A:99:THR:C | 2.43 | 0.70 |
| 2:3B:51:THR:HG21 | 2:3B:243:ARG:HG2 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3H:90:GLU:O | 2:3H:121:ARG:NH1 | 2.24 | 0.70 |
| 1:3O:2:ARG:HE | 1:3O:240:LEU:HD22 | 1.56 | 0.70 |
| 22:6I:63:PRO:HB2 | 24:6T:399:ILE:HG13 | 1.74 | 0.70 |
| 22:6I:108:ARG:NH2 | 24:6T:282:ARG:O | 2.24 | 0.70 |
| 24:6U:456:ASP:O | 24:6U:459:LYS:NZ | 2.23 | 0.70 |
| 24:6W:456:ASP:O | 24:6W:459:LYS:NZ | 2.23 | 0.70 |
| 1:A3:337:ASN:ND2 | 3:4H:68:SER:HA | 2.06 | 0.70 |
| 2:G9:221:ARG:NH1 | 22:6P:178:GLY:O | 2.24 | 0.70 |
| 2:H7:71:GLU:HG3 | 1:H8:2:ARG:HH12 | 1.57 | 0.70 |
| 1:I0:180:VAL:HG23 | 1:I0:184:ASN:HD21 | 1.57 | 0.70 |
| 2:I5:33:ASP:O | 2:I5:60:LYS:NZ | 2.25 | 0.70 |
| 1:J0:309:ARG:H | 1:J0:372:THR:HG22 | 1.56 | 0.70 |
| 2:J3:413:MET:HB3 | 2:J3:417:GLU:OE2 | 1.92 | 0.70 |
| 2:Q9:415:GLU:OE1 | 17:5S:113:ILE:HG23 | 1.91 | 0.70 |
| 2:S9:88:HIS:CD2 | 2:S9:89:PRO:HD2 | 2.27 | 0.70 |
| 1:V4:125:GLU:OE1 | 1:X0:291:GLN:NE2 | 2.25 | 0.70 |
| 2:Y1:88:HIS:HB3 | 2:Z7:283:HIS:ND1 | 2.07 | 0.70 |
| 1:Y8:52:ASN:OD1 | 1:Y8:62:ARG:NH2 | 2.25 | 0.70 |
| 2:0Z:108:TYR:O | 2:0Z:112:LYS:NZ | 2.21 | 0.70 |
| 2:0Z:224:TYR:O | 2:0Z:228:ASN:ND2 | 2.22 | 0.70 |
| 2:1D:132:LEU:HD22 | 2:1D:164:LYS:HD3 | 1.71 | 0.70 |
| 2:1F:317:LEU:HB3 | 2:1F:319:TYR:HE1 | 1.57 | 0.70 |
| 2:1L:88:HIS:CD2 | 2:1L:89:PRO:HD2 | 2.27 | 0.70 |
| 2:1X:317:LEU:HB3 | 2:1X:319:TYR:HE1 | 1.57 | 0.70 |
| 1:2I:311:LEU:HD23 | 1:2I:312:THR:HG23 | 1.72 | 0.70 |
| 2:3L:163:LYS:HE3 | 3:4B:137:ARG:HG2 | 1.72 | 0.70 |
| 1:3M:391:ARG:HD3 | 1:3M:393:ALA:HB2 | 1.72 | 0.70 |
| 7:4R:8:VAL:HG22 | 7:4R:9:PRO:CD | 2.21 | 0.70 |
| 8:4W:362:LYS:HG2 | 8:4W:366:LYS:HE3 | 1.73 | 0.70 |
| 19:6E:16:GLU:HA | 19:6E:16:GLU:OE1 | 1.92 | 0.70 |
| 22:6N:108:ARG:NH2 | 24:6Y:282:ARG:O | 2.25 | 0.70 |
| 24:6X:32:THR:HG23 | 24:6X:33:LEU:HD12 | 1.72 | 0.70 |
| 31:7N:80:PRO:HD2 | 31:7N:83:THR:HG21 | 1.72 | 0.70 |
| 1:A3:215:LEU:HD11 | 26:7F:136:PHE:CE2 | 2.26 | 0.69 |
| 2:C5:179:THR:HG1 | 41:C5:501:GTP:HO3' | 1.37 | 0.69 |
| 2:I9:287:SER:N | 2:I9:290:GLU:OE2 | 2.24 | 0.69 |
| 2:M3:221:ARG:HH22 | 30:7K:189:PHE:N | 1.91 | 0.69 |
| 2:S7:203:MET:N | 2:S7:203:MET:SD | 2.65 | 0.69 |
| 2:V7:31:GLN:HE21 | 2:V7:37:PRO:HG3 | 1.55 | 0.69 |
| 2:Z1:166:LYS:N | 2:Z1:199:ASP:OD2 | 2.23 | 0.69 |
| 1:Z2:33:THR:O | 1:Z2:58:ARG:NH2 | 2.23 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0W:334:GLN:HE22 | 1:0W:348:ASN:H | 1.38 | 0.69 |
| 2:1D:101:ASN:OD1 | 1:1E:252:LYS:HE3 | 1.92 | 0.69 |
| 2:1H:253:THR:HA | 2:1H:256:GLN:HE21 | 1.57 | 0.69 |
| 2:1Z:268:MET:HB3 | 2:1Z:378:ILE:HD11 | 1.72 | 0.69 |
| 2:2Z:297:GLU:CG | 38:8C:74:ILE:HG22 | 2.19 | 0.69 |
| 2:3P:124:LYS:NZ | 3:4F:36:PHE:HA | 2.07 | 0.69 |
| 15:5O:30:PRO:O | 15:5O:33:LYS:HD2 | 1.91 | 0.69 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:HD3 | 1.72 | 0.69 |
| 24:6T:456:ASP:O | 24:6T:459:LYS:NZ | 2.23 | 0.69 |
| 24:6U:92:ASP:OD1 | 24:6U:93:ARG:N | 2.24 | 0.69 |
| 24:6Z:96:LEU:HB2 | 24:6Z:123:TYR:HB3 | 1.73 | 0.69 |
| 35:7U:157:ARG:NH2 | 36:7W:57:ASP:OD1 | 2.24 | 0.69 |
| 38:8C:204:GLN:HA | 38:8C:204:GLN:HE21 | 1.56 | 0.69 |
| 2:A2:40:LYS:NZ | 26:7F:45:MET:CA | 2.55 | 0.69 |
| 1:G4:334:GLN:HE22 | 1:G4:348:ASN:H | 1.39 | 0.69 |
| 2:H5:90:GLU:HB3 | 2:H5:121:ARG:HH22 | 1.57 | 0.69 |
| 1:I8:140:GLY:O | 1:I8:184:ASN:ND2 | 2.25 | 0.69 |
| 2:J1:191:THR:HA | 2:J1:194:LEU:HB3 | 1.74 | 0.69 |
| 1:J8:272:PRO:HB2 | 1:J8:282:ARG:HH12 | 1.56 | 0.69 |
| 1:L4:53:GLU:OE2 | 29:7J:329:SER:HB3 | 1.92 | 0.69 |
| 2:M3:27:GLU:OE1 | 2:M3:243:ARG:NH1 | 2.24 | 0.69 |
| 2:Q9:18:ASN:ND2 | 12:7B:75:TYR:HE1 | 1.91 | 0.69 |
| 1:T0:222:PHE:HB2 | 7:4T:367:ARG:HG2 | 1.73 | 0.69 |
| 2:W7:175:PRO:HB2 | 2:W7:176:GLN:HE21 | 1.57 | 0.69 |
| 2:W9:72:PRO:HD2 | 1:X0:2:ARG:HH12 | 1.57 | 0.69 |
| 1:X8:273:LEU:H | 1:X8:292:GLN:HE22 | 1.40 | 0.69 |
| 1:Z6:20:PHE:CE1 | 1:Z6:233:MET:HG2 | 2.27 | 0.69 |
| 1:0W:113:ILE:HD11 | 1:0W:151:LEU:HA | 1.73 | 0.69 |
| 1:0W:214:THR:O | 1:0W:275:SER:OG | 2.10 | 0.69 |
| 1:1A:350:LYS:NZ | 1:1A:352:SER:OG | 2.25 | 0.69 |
| 2:1P:220:GLU:HG2 | 2:1P:221:ARG:HG3 | 1.74 | 0.69 |
| 2:2B:336:LYS:O | 2:2B:339:ARG:NH2 | 2.24 | 0.69 |
| 1:2E:125:GLU:O | 38:8A:3:ASN:ND2 | 2.23 | 0.69 |
| 2:2N:123:ARG:HD3 | 38:8D:75:SER:HB3 | 1.74 | 0.69 |
| 2:2R:308:ARG:HH22 | 38:8A:72:ASP:HB2 | 1.57 | 0.69 |
| 1:2Y:56:GLY:HA3 | 38:8C:161:GLN:NE2 | 2.08 | 0.69 |
| 2:3B:222:PRO:HD2 | 1:3C:324:LYS:HE3 | 1.72 | 0.69 |
| 2:3P:250:VAL:HB | 2:3P:254:GLU:HG3 | 1.74 | 0.69 |
| 6:4O:93:LEU:HD21 | 30:7K:449:ALA:HA | 1.73 | 0.69 |
| 14:5M:365:ARG:NH2 | 14:5M:377:ARG:NH1 | 2.40 | 0.69 |
| 15:5O:363:GLU:O | 27:7G:99:ARG:NH1 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Y:107:VAL:HG22 | 24:6Y:108:GLU:H | 1.58 | 0.69 |
| 1:A7:276:ARG:HH12 | 24:6T:210:VAL:HG11 | 1.55 | 0.69 |
| 2:H1:132:LEU:HD22 | 2:H1:164:LYS:HD3 | 1.74 | 0.69 |
| 1:H2:345:ILE:O | 1:H2:348:ASN:ND2 | 2.24 | 0.69 |
| 2:J9:324:VAL:HG21 | 2:J9:326:LYS:NZ | 2.06 | 0.69 |
| 2:L5:311:LYS:HE3 | 2:L5:344:VAL:HA | 1.75 | 0.69 |
| 2:O1:226:ASN:HD21 | 37:7Y:250:GLN:NE2 | 1.91 | 0.69 |
| 2:W5:72:PRO:HD2 | 1:W6:2:ARG:HH12 | 1.56 | 0.69 |
| 2:W7:85:GLN:O | 2:Y3:283:HIS:CE1 | 2.38 | 0.69 |
| 2:Y1:287:SER:N | 2:Y1:290:GLU:OE2 | 2.24 | 0.69 |
| 1:Y8:5:VAL:HG22 | 1:Y8:62:ARG:HD3 | 1.74 | 0.69 |
| 1:Z6:5:VAL:HG22 | 1:Z6:62:ARG:HD3 | 1.74 | 0.69 |
| 1:0K:183:TYR:CZ | 1:0K:388:MET:HB3 | 2.28 | 0.69 |
| 1:0W:350:LYS:NZ | 1:0W:351:SER:O | 2.24 | 0.69 |
| 2:1V:121:ARG:HG2 | 2:1V:121:ARG:NH1 | 1.93 | 0.69 |
| 2:1Z:156:ARG:HH22 | 38:7Z:29:GLY:HA2 | 1.56 | 0.69 |
| 2:2H:156:ARG:NH2 | 38:8B:29:GLY:HA2 | 2.07 | 0.69 |
| 2:2N:336:LYS:O | 2:2N:339:ARG:NH2 | 2.24 | 0.69 |
| 2:2P:88:HIS:HB3 | 2:3F:283:HIS:ND1 | 2.07 | 0.69 |
| 2:3J:267:PHE:HB2 | 2:3J:384:ILE:HD12 | 1.74 | 0.69 |
| 2:3N:286:LEU:O | 2:3N:373:ARG:NH1 | 2.24 | 0.69 |
| 2:3T:71:GLU:HG2 | 2:3T:98:ASP:HB3 | 1.74 | 0.69 |
| 10:5B:257:GLN:OE1 | 10:5B:260:LYS:HE3 | 1.93 | 0.69 |
| 15:5O:338:LEU:HD12 | 15:5O:339:ARG:HG2 | 1.74 | 0.69 |
| 23:6R:54:ASN:N | 23:6R:54:ASN:OD1 | 2.25 | 0.69 |
| 29:7J:316:VAL:CG1 | 29:7J:341:GLU:HA | 2.21 | 0.69 |
| 2:D1:285:GLN:HE21 | 24:6W:253:PRO:HG2 | 1.58 | 0.69 |
| 1:I2:113:ILE:HG13 | 1:I2:150:LEU:HD22 | 1.74 | 0.69 |
| 2:I9:88:HIS:HA | 2:K5:283:HIS:ND1 | 2.07 | 0.69 |
| 2:J1:33:ASP:O | 2:J1:60:LYS:NZ | 2.24 | 0.69 |
| 1:K4:362:LYS:HA | 6:4O:169:PHE:HZ | 1.57 | 0.69 |
| 1:Q8:28:HIS:HE1 | 1:Q8:241:ARG:HE | 1.40 | 0.69 |
| 2:Q9:51:THR:HG21 | 2:Q9:243:ARG:HG2 | 1.73 | 0.69 |
| 1:T4:217:LEU:HD22 | 7:4U:134:GLU:HB3 | 1.73 | 0.69 |
| 1:U8:372:THR:HG21 | 1:U8:426:GLN:HB2 | 1.72 | 0.69 |
| 2:V7:239:THR:HG23 | 2:V7:243:ARG:HE | 1.58 | 0.69 |
| 2:X5:206:ASN:OD1 | 41:X6:501:GTP:N2 | 2.25 | 0.69 |
| 1:Z0:52:ASN:OD1 | 1:Z0:62:ARG:NH2 | 2.25 | 0.69 |
| 2:Z1:233:GLN:NE2 | 2:Z1:272:TYR:OH | 2.24 | 0.69 |
| 2:0R:336:LYS:O | 2:0R:339:ARG:NH2 | 2.26 | 0.69 |
| 2:1F:115:VAL:HG23 | 2:1F:153:LEU:HD23 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1Q:5:VAL:HG12 | 1:1Q:62:ARG:HD3 | 1.74 | 0.69 |
| 1:2C:375:GLN:HB2 | 1:2C:419:VAL:HG23 | 1.74 | 0.69 |
| 2:2P:214:ARG:NH1 | 38:7Z:17:GLY:O | 2.26 | 0.69 |
| 1:2S:306:ARG:NH2 | 38:8A:51:GLN:OE1 | 2.25 | 0.69 |
| 2:3P:124:LYS:HZ3 | 3:4F:36:PHE:HA | 1.56 | 0.69 |
| 1:3S:190:HIS:CD2 | 1:3S:411:ALA:HA | 2.27 | 0.69 |
| 14:5M:365:ARG:NH2 | 14:5M:377:ARG:HH11 | 1.90 | 0.69 |
| 28:7H:399:VAL:HG22 | 28:7H:430:MET:SD | 2.32 | 0.69 |
| 1:3:262:ARG:NH1 | 3:3X:295:TYR:OH | 2.25 | 0.69 |
| 1:G8:175:VAL:HG12 | 2:G9:329:ASN:HD21 | 1.57 | 0.69 |
| 2:I1:121:ARG:HH11 | 2:I1:121:ARG:CG | 1.96 | 0.69 |
| 2:M7:285:GLN:HE21 | 30:7K:84:VAL:CG1 | 2.04 | 0.69 |
| 2:N3:192:HIS:NE2 | 2:N3:420:GLU:OE1 | 2.21 | 0.69 |
| 2:N5:88:HIS:CE1 | 2:N5:90:GLU:CB | 2.75 | 0.69 |
| 2:R5:166:LYS:N | 2:R5:199:ASP:OD2 | 2.24 | 0.69 |
| 2:S1:100:ALA:HA | 1:S2:252:LYS:HE2 | 1.75 | 0.69 |
| 1:S4:337:ASN:OD1 | 17:5R:48:THR:OG1 | 2.09 | 0.69 |
| 2:S5:245:ASP:HB3 | 24:6U:29:LYS:HD3 | 1.74 | 0.69 |
| 2:U9:220:GLU:HG2 | 2:U9:221:ARG:HG3 | 1.74 | 0.69 |
| 1:X0:42:LEU:CD2 | 8:4X:97:PHE:CZ | 2.76 | 0.69 |
| 1:Z8:3:GLU:HB2 | 1:Z8:130:LEU:HA | 1.73 | 0.69 |
| 1:1G:334:GLN:HE22 | 1:1G:348:ASN:H | 1.38 | 0.69 |
| 2:1P:399:TYR:O | 2:1P:402:ARG:NH1 | 2.25 | 0.69 |
| 2:1R:88:HIS:HB3 | 2:1R:91:GLN:HG3 | 1.73 | 0.69 |
| 2:1T:387:ILE:HG12 | 2:1T:390:ARG:HH22 | 1.57 | 0.69 |
| 1:3C:362:LYS:HD2 | 1:3C:363:MET:HG3 | 1.72 | 0.69 |
| 2:3R:50:ASN:O | 2:3R:64:ARG:NH2 | 2.24 | 0.69 |
| 14:5N:512:PHE:HD1 | 14:5N:512:PHE:N | 1.89 | 0.69 |
| 15:5P:162:GLU:HB2 | 15:5P:222:PHE:HE1 | 1.58 | 0.69 |
| 24:6V:354:ARG:HB2 | 24:6V:357:LEU:HG | 1.75 | 0.69 |
| 24:6Z:456:ASP:O | 24:6Z:459:LYS:NZ | 2.25 | 0.69 |
| 2:H1:9:ILE:HG22 | 2:H1:146:GLY:HA2 | 1.73 | 0.69 |
| 2:J9:88:HIS:HB3 | 2:L5:283:HIS:ND1 | 2.07 | 0.69 |
| 1:L2:219:THR:OG1 | 29:7J:430:ASN:OD1 | 2.10 | 0.69 |
| 2:L5:88:HIS:CG | 2:N1:283:HIS:HB2 | 2.27 | 0.69 |
| 1:N0:285:THR:HG23 | 1:N0:288:GLU:H | 1.58 | 0.69 |
| 2:O9:287:SER:N | 2:O9:290:GLU:OE2 | 2.16 | 0.69 |
| 2:P9:287:SER:N | 2:P9:290:GLU:OE2 | 2.25 | 0.69 |
| 1:R8:248:ALA:HA | 1:R8:252:LYS:HD2 | 1.74 | 0.69 |
| 1:S8:45:GLU:HG3 | 1:S8:46:ARG:HG2 | 1.73 | 0.69 |
| 2:S9:155:GLU:OE2 | 2:S9:197:HIS:NE2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S9:267:PHE:HB2 | 2:S9:384:ILE:HD12 | 1.73 | 0.69 |
| 1:V6:257:LEU:HA | 1:V6:312:THR:HG21 | 1.74 | 0.69 |
| 2:W9:14:ILE:HD11 | 2:W9:74:VAL:HG11 | 1.74 | 0.69 |
| 2:Z3:279:GLU:HG2 | 2:Z3:280:LYS:HD2 | 1.74 | 0.69 |
| 2:Z5:388:PHE:HB3 | 2:Z5:425:LEU:HD11 | 1.75 | 0.69 |
| 1:0S:259:PRO:HG3 | 1:0S:311:LEU:HD21 | 1.75 | 0.69 |
| 2:1L:121:ARG:O | 2:1L:121:ARG:HD2 | 1.92 | 0.69 |
| 1:1O:248:ALA:CA | 1:1O:252:LYS:HD3 | 2.22 | 0.69 |
| 2:2D:56:THR:HA | 2:2T:285:GLN:HB2 | 1.74 | 0.69 |
| 1:2I:53:GLU:CD | 1:2I:53:GLU:H | 1.94 | 0.69 |
| 1:2K:199:CYS:HG | 1:2K:265:PHE:HE1 | 1.40 | 0.69 |
| 1:2Q:52:ASN:OD1 | 1:2Q:62:ARG:NH2 | 2.26 | 0.69 |
| 2:2T:358:GLN:NE2 | 38:8B:212:PRO:HB2 | 2.06 | 0.69 |
| 15:5O:34:GLU:OE2 | 15:5O:49:ARG:CG | 2.40 | 0.69 |
| 22:6I:294:LEU:HD22 | 22:6I:343:TYR:HB2 | 1.75 | 0.69 |
| 22:6P:262:TYR:HA | 22:6P:266:LYS:HE2 | 1.74 | 0.69 |
| 24:6X:139:ASN:HD22 | 24:6X:223:ARG:HH21 | 1.38 | 0.69 |
| 38:8B:166:GLU:N | 38:8B:166:GLU:OE2 | 2.23 | 0.69 |
| 1:D4:204:ASN:HD21 | 39:D4:501:GDP:HN22 | 1.39 | 0.69 |
| 1:I0:218:THR:CG2 | 24:6X:489:ASN:CA | 2.70 | 0.69 |
| 1:L6:172:SER:OG | 1:L6:380:ARG:NH2 | 2.26 | 0.69 |
| 2:N9:220:GLU:HG2 | 2:N9:221:ARG:HG3 | 1.75 | 0.69 |
| 1:T4:45:GLU:OE2 | 21:6H:97:ARG:NH1 | 2.25 | 0.69 |
| 1:T6:92:PHE:HZ | 24:7A:44:ALA:HB1 | 1.54 | 0.69 |
| 2:U5:203:MET:HE1 | 2:U5:267:PHE:HB3 | 1.74 | 0.69 |
| 1:0M:3:GLU:HB2 | 1:0M:130:LEU:HD13 | 1.73 | 0.69 |
| 2:0N:9:ILE:HG22 | 2:0N:146:GLY:HA2 | 1.75 | 0.69 |
| 2:0P:9:ILE:HG22 | 2:0P:146:GLY:HA2 | 1.74 | 0.69 |
| 2:0P:55:GLU:O | 2:1F:285:GLN:NE2 | 2.25 | 0.69 |
| 1:3Q:252:LYS:CA | 1:3Q:255:VAL:HG12 | 2.19 | 0.69 |
| 4:4C:35:LYS:NZ | 3:4D:254:LYS:O | 2.20 | 0.69 |
| 5:4L:260:ALA:O | 5:4L:264:GLN:HG2 | 1.93 | 0.69 |
| 5:4M:293:LEU:CD1 | 28:7X:305:ALA:HB1 | 2.22 | 0.69 |
| 7:4U:112:MET:SD | 7:4U:113:PRO:HD2 | 2.33 | 0.69 |
| 12:5F:271:LEU:HD23 | 12:7B:23:MET:CG | 2.22 | 0.69 |
| 22:6L:183:ASN:O | 22:6L:186:ARG:N | 2.26 | 0.69 |
| 24:6T:470:ILE:HD13 | 24:6T:485:PRO:HG3 | 1.73 | 0.69 |
| 24:6X:122:TYR:HB2 | 24:6X:131:HIS:HB3 | 1.75 | 0.69 |
| 24:6X:354:ARG:HB2 | 24:6X:357:LEU:HD12 | 1.74 | 0.69 |
| 38:8A:206:PRO:CG | 38:8A:209:HIS:CE1 | 2.75 | 0.69 |
| 38:8B:86:TYR:O | 38:8B:89:SER:N | 2.19 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:40:SER:O | 26:7D:25:TYR:CE2 | 2.45 | 0.69 |
| 1:B3:277:GLY:HA2 | 24:6W:142:ILE:HG22 | 1.75 | 0.69 |
| 2:D3:79:ARG:NH2 | 22:6N:19:GLY:O | 2.25 | 0.69 |
| 1:F8:276:ARG:HH21 | 24:6U:420:LEU:HA | 1.58 | 0.69 |
| 1:G2:45:GLU:HG3 | 1:G2:46:ARG:HG2 | 1.73 | 0.69 |
| 2:G5:221:ARG:HG3 | 22:6N:178:GLY:HA2 | 1.75 | 0.69 |
| 2:H7:392:ASP:OD2 | 2:H7:422:ARG:NH1 | 2.25 | 0.69 |
| 1:H8:345:ILE:O | 1:H8:348:ASN:ND2 | 2.24 | 0.69 |
| 1:I2:334:GLN:HE22 | 1:I2:348:ASN:H | 1.38 | 0.69 |
| 2:J5:42:ILE:HG21 | 5:4L:478:ARG:CZ | 2.23 | 0.69 |
| 2:J7:279:GLU:HA | 2:J7:279:GLU:OE2 | 1.92 | 0.69 |
| 1:J8:178:THR:HG23 | 1:J8:181:GLU:HG3 | 1.74 | 0.69 |
| 2:M3:90:GLU:HG3 | 2:M3:121:ARG:NH1 | 2.08 | 0.69 |
| 2:M7:89:PRO:CG | 19:6E:25:VAL:CG1 | 2.71 | 0.69 |
| 2:N1:71:GLU:HB3 | 2:N1:98:ASP:HB2 | 1.74 | 0.69 |
| 1:N6:65:LEU:HD12 | 1:N6:90:PHE:HE1 | 1.57 | 0.69 |
| 2:R3:286:LEU:O | 2:R3:373:ARG:NH1 | 2.26 | 0.69 |
| 2:S7:88:HIS:HB3 | 2:S7:91:GLN:HG3 | 1.75 | 0.69 |
| 2:S7:287:SER:N | 2:S7:290:GLU:OE2 | 2.22 | 0.69 |
| 2:T5:368:LEU:O | 7:4U:156:GLN:NE2 | 2.26 | 0.69 |
| 1:W0:135:VAL:HG11 | 1:W0:152:ILE:HD11 | 1.74 | 0.69 |
| 2:W7:264:ARG:NH2 | 2:W7:431:ASP:OD2 | 2.25 | 0.69 |
| 2:W9:276:ILE:HD11 | 2:W9:281:ALA:HA | 1.74 | 0.69 |
| 2:X3:399:TYR:OH | 2:X3:415:GLU:OE2 | 2.08 | 0.69 |
| 2:Y5:72:PRO:HG3 | 1:Y6:1:MET:HG2 | 1.74 | 0.69 |
| 2:Z1:336:LYS:O | 2:Z1:339:ARG:NH2 | 2.26 | 0.69 |
| 2:Z3:392:ASP:OD2 | 2:Z3:422:ARG:NH1 | 2.25 | 0.69 |
| 1:0A:396:HIS:HA | 1:0A:399:THR:HG22 | 1.73 | 0.69 |
| 1:0G:68:LEU:HB3 | 1:0G:96:GLY:HA2 | 1.75 | 0.69 |
| 2:1V:399:TYR:O | 2:1V:402:ARG:NH1 | 2.25 | 0.69 |
| 2:1X:213:CYS:HA | 2:1X:217:LEU:HB2 | 1.74 | 0.69 |
| 1:2C:113:ILE:HA | 1:2C:116:VAL:HG22 | 1.73 | 0.69 |
| 2:2F:123:ARG:HD2 | 38:8B:75:SER:HB3 | 1.73 | 0.69 |
| 1:3C:211:CYS:HA | 1:3C:215:LEU:HB2 | 1.75 | 0.69 |
| 1:3I:77:ARG:NH2 | 3:3Z:19:LEU:HD23 | 2.07 | 0.69 |
| 1:3M:220:PRO:HD2 | 2:3N:326:LYS:HD3 | 1.74 | 0.69 |
| 15:5O:41:LYS:HZ2 | 15:5O:41:LYS:HB3 | 1.57 | 0.69 |
| 18:6A:5:VAL:CG1 | 18:6A:62:GLU:HG2 | 2.22 | 0.69 |
| 22:6M:180:SER:OG | 22:6M:182:ASN:ND2 | 2.26 | 0.69 |
| 22:6O:108:ARG:NH2 | 24:6Z:284:THR:O | 2.26 | 0.69 |
| 24:6T:606:ARG:O | 24:6T:610:ILE:HG12 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:7D:78:ALA:HB3 | 26:7D:111:ASP:HB3 | 1.74 | 0.69 |
| 26:7E:78:ALA:HB3 | 26:7E:111:ASP:HB3 | 1.74 | 0.69 |
| 38:8A:91:GLN:HB3 | 38:8A:102:PHE:HE1 | 1.52 | 0.69 |
| 38:8D:166:GLU:OE1 | 38:8D:166:GLU:N | 2.21 | 0.69 |
| 2:K1:79:ARG:NH1 | 2:K1:92:LEU:O | 2.25 | 0.69 |
| 2:K1:255:PHE:HA | 2:K1:259:LEU:HD13 | 1.74 | 0.69 |
| 2:M1:219:ILE:HG13 | 30:7K:261:PRO:HA | 1.75 | 0.69 |
| 2:M9:27:GLU:OE1 | 2:M9:243:ARG:NH1 | 2.24 | 0.69 |
| 1:O2:248:ALA:HA | 1:O2:252:LYS:HD2 | 1.75 | 0.69 |
| 1:T2:177:ASP:O | 2:T3:352:LYS:HA | 1.93 | 0.69 |
| 2:U1:213:CYS:HA | 2:U1:217:LEU:HB2 | 1.73 | 0.69 |
| 1:U8:211:CYS:HA | 1:U8:215:LEU:HB2 | 1.75 | 0.69 |
| 2:Z7:236:SER:OG | 2:Z7:243:ARG:NH2 | 2.26 | 0.69 |
| 2:0B:233:GLN:NE2 | 2:0B:272:TYR:OH | 2.26 | 0.69 |
| 2:1N:90:GLU:HB3 | 2:1N:121:ARG:HH22 | 1.58 | 0.69 |
| 2:1R:213:CYS:HA | 2:1R:217:LEU:HB2 | 1.75 | 0.69 |
| 2:1T:108:TYR:O | 2:1T:112:LYS:NZ | 2.25 | 0.69 |
| 2:2L:14:ILE:HD11 | 2:2L:74:VAL:HG22 | 1.75 | 0.69 |
| 1:3A:282:ARG:HH21 | 1:3A:288:GLU:HG3 | 1.58 | 0.69 |
| 2:3N:56:THR:OG1 | 3:4D:33:GLY:O | 2.10 | 0.69 |
| 1:3Q:77:ARG:HH12 | 3:4H:18:LYS:HB3 | 1.58 | 0.69 |
| 12:5F:271:LEU:HB3 | 12:5F:272:PRO:HD3 | 1.75 | 0.69 |
| 14:5N:28:ARG:HG2 | 14:5N:28:ARG:HH11 | 1.57 | 0.69 |
| 14:5N:208:TYR:CD2 | 14:5N:220:GLN:NE2 | 2.60 | 0.69 |
| 17:5S:181:LEU:HD23 | 17:5S:181:LEU:C | 2.13 | 0.69 |
| 2:B7:278:ALA:HB3 | 18:6B:43:ASN:HD22 | 1.56 | 0.69 |
| 2:G7:195:LEU:HD21 | 2:G7:428:LEU:HD12 | 1.75 | 0.69 |
| 2:K1:172:TYR:CE2 | 2:K1:203:MET:HG3 | 2.28 | 0.69 |
| 1:O2:391:ARG:HB3 | 1:O2:391:ARG:NH2 | 2.08 | 0.69 |
| 2:T7:88:HIS:CG | 2:T7:89:PRO:CD | 2.75 | 0.69 |
| 1:W2:145:SER:OG | 1:W2:188:SER:OG | 2.10 | 0.69 |
| 1:W6:309:ARG:H | 1:W6:372:THR:HG22 | 1.58 | 0.69 |
| 1:X0:29:GLY:HA3 | 8:4X:95:THR:HG22 | 1.74 | 0.69 |
| 2:X3:276:ILE:HG23 | 2:X3:280:LYS:HB2 | 1.75 | 0.69 |
| 2:0J:90:GLU:O | 2:0J:121:ARG:NH1 | 2.26 | 0.69 |
| 2:1Z:9:ILE:HG22 | 2:1Z:146:GLY:HA2 | 1.74 | 0.69 |
| 1:2I:77:ARG:HH21 | 1:2I:90:PHE:HD2 | 1.39 | 0.69 |
| 2:2P:358:GLN:HE21 | 38:8A:214:HIS:H | 1.41 | 0.69 |
| 2:3D:223:THR:HG23 | 2:3D:225:THR:H | 1.58 | 0.69 |
| 2:3J:27:GLU:OE1 | 2:3J:243:ARG:NH1 | 2.26 | 0.69 |
| 5:4M:113:ALA:HB2 | 6:4O:336:GLN:HE22 | 1.58 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:365:ARG:NH1 | 14:5M:377:ARG:NH1 | 2.40 | 0.69 |
| 15:5P:125:ILE:HG12 | 15:5P:159:VAL:HG22 | 1.75 | 0.69 |
| 18:6D:101:LYS:O | 24:7A:178:ASN:ND2 | 2.25 | 0.69 |
| 22:6I:177:LEU:HB2 | 22:6I:183:ASN:HB2 | 1.75 | 0.69 |
| 24:6T:470:ILE:CD1 | 24:6T:485:PRO:HG2 | 2.22 | 0.69 |
| 24:6W:97:ARG:NH2 | 24:6W:99:TYR:OH | 2.26 | 0.69 |
| 24:6X:130:MET:SD | 24:6X:166:PHE:HZ | 2.16 | 0.69 |
| 29:7J:126:LEU:HD13 | 30:7L:321:GLN:HB2 | 1.75 | 0.69 |
| 38:8A:91:GLN:CB | 38:8A:102:PHE:CE1 | 2.70 | 0.69 |
| 1:1:379:LYS:NZ | 3:3V:49:HIS:HD2 | 1.90 | 0.68 |
| 1:H2:276:ARG:HB2 | 24:6T:490:THR:CG2 | 2.22 | 0.68 |
| 2:K1:81:GLY:O | 2:K1:84:ARG:NH1 | 2.25 | 0.68 |
| 1:K6:350:LYS:NZ | 1:K6:351:SER:O | 2.26 | 0.68 |
| 2:Q5:60:LYS:HE3 | 2:S1:283:HIS:CE1 | 2.25 | 0.68 |
| 1:U6:345:ILE:O | 1:U6:348:ASN:ND2 | 2.26 | 0.68 |
| 1:Y0:260:PHE:HB2 | 1:Y0:263:LEU:HG | 1.75 | 0.68 |
| 1:Y2:125:GLU:OE2 | 1:Y2:159:TYR:OH | 2.11 | 0.68 |
| 1:0E:8:GLN:HE22 | 1:0E:63:ALA:HB1 | 1.58 | 0.68 |
| 1:0E:345:ILE:O | 1:0E:348:ASN:ND2 | 2.25 | 0.68 |
| 2:0F:387:ILE:HD12 | 2:0F:390:ARG:HH22 | 1.56 | 0.68 |
| 2:0N:157:LEU:HD22 | 2:0N:166:LYS:HD3 | 1.75 | 0.68 |
| 2:0N:313:MET:HG3 | 2:0N:346:TRP:CZ3 | 2.27 | 0.68 |
| 1:0W:139:LEU:HD12 | 1:0W:170:VAL:HG22 | 1.75 | 0.68 |
| 1:1E:272:PRO:HB2 | 1:1E:282:ARG:HH12 | 1.56 | 0.68 |
| 2:1F:55:GLU:O | 2:1V:285:GLN:NE2 | 2.25 | 0.68 |
| 2:1F:399:TYR:O | 2:1F:402:ARG:NH1 | 2.26 | 0.68 |
| 2:1T:220:GLU:HG2 | 2:1T:221:ARG:HG3 | 1.73 | 0.68 |
| 1:2I:53:GLU:N | 1:2I:53:GLU:OE1 | 2.26 | 0.68 |
| 1:2M:125:GLU:O | 38:8C:3:ASN:ND2 | 2.23 | 0.68 |
| 14:5M:28:ARG:HG2 | 14:5M:28:ARG:HH11 | 1.57 | 0.68 |
| 14:5N:512:PHE:N | 14:5N:512:PHE:CD1 | 2.59 | 0.68 |
| 15:5O:34:GLU:OE1 | 15:5O:35:VAL:N | 2.26 | 0.68 |
| 15:5P:330:LEU:HD23 | 15:5P:330:LEU:C | 2.14 | 0.68 |
| 24:6X:613:LYS:O | 24:6X:617:ASP:HB2 | 1.93 | 0.68 |
| 24:6Z:378:TRP:O | 24:6Z:382:ASN:ND2 | 2.26 | 0.68 |
| 26:7F:78:ALA:HB3 | 26:7F:111:ASP:HB3 | 1.75 | 0.68 |
| 1:5:245:GLN:HG2 | 26:7D:113:ARG:NH1 | 2.07 | 0.68 |
| 2:G1:345:ASP:N | 2:G1:345:ASP:OD1 | 2.27 | 0.68 |
| 2:G5:90:GLU:HB3 | 2:G5:121:ARG:HH12 | 1.58 | 0.68 |
| 2:H7:97:GLU:OE2 | 1:H8:251:ARG:NH2 | 2.26 | 0.68 |
| 2:K9:90:GLU:HB3 | 2:K9:121:ARG:NH2 | 2.07 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M3:42:ILE:H | 2:M3:42:ILE:CD1 | 1.92 | 0.68 |
| 2:M3:90:GLU:O | 2:M3:121:ARG:NH1 | 2.27 | 0.68 |
| 2:N3:115:VAL:HB | 2:N3:149:LEU:HD11 | 1.75 | 0.68 |
| 1:N8:178:THR:HG22 | 2:N9:352:LYS:HZ3 | 1.58 | 0.68 |
| 2:R5:264:ARG:NH1 | 2:R5:431:ASP:OD2 | 2.26 | 0.68 |
| 2:R7:62:VAL:HG21 | 2:R7:88:HIS:HB2 | 1.73 | 0.68 |
| 2:U1:336:LYS:O | 2:U1:339:ARG:NH2 | 2.25 | 0.68 |
| 1:U2:345:ILE:O | 1:U2:348:ASN:ND2 | 2.26 | 0.68 |
| 1:W8:56:GLY:HA2 | 8:4W:395:ARG:HD2 | 1.74 | 0.68 |
| 1:Y6:135:VAL:HG11 | 1:Y6:152:ILE:HD11 | 1.75 | 0.68 |
| 1:0E:45:GLU:HG3 | 1:0E:46:ARG:HG2 | 1.75 | 0.68 |
| 2:2H:286:LEU:O | 2:2H:373:ARG:NH1 | 2.26 | 0.68 |
| 1:2I:121:ARG:NH1 | 38:8C:99:THR:HA | 2.08 | 0.68 |
| 1:2S:304:ASP:OD2 | 38:8A:45:SER:OG | 2.06 | 0.68 |
| 2:3B:287:SER:N | 2:3B:290:GLU:OE2 | 2.25 | 0.68 |
| 1:3S:276:ARG:NH2 | 17:5V:223:GLU:OE2 | 2.24 | 0.68 |
| 8:4W:463:THR:HG21 | 8:4X:128:LEU:HD12 | 1.74 | 0.68 |
| 14:5L:28:ARG:HH11 | 14:5L:28:ARG:HG2 | 1.57 | 0.68 |
| 15:5O:296:SER:O | 15:5O:299:GLU:CG | 2.31 | 0.68 |
| 24:6V:107:VAL:HG22 | 24:6V:108:GLU:H | 1.57 | 0.68 |
| 1:B8:358:PRO:O | 18:6B:22:ARG:NH2 | 2.25 | 0.68 |
| 2:G7:85:GLN:OE1 | 2:G7:85:GLN:HA | 1.92 | 0.68 |
| 2:J7:282:TYR:CD1 | 5:4M:209:LEU:HD22 | 2.25 | 0.68 |
| 2:N1:88:HIS:O | 1:O8:281:TYR:OH | 2.11 | 0.68 |
| 2:N3:207:GLU:HB3 | 2:N3:304:LYS:HG3 | 1.74 | 0.68 |
| 2:O1:69:ASP:OD1 | 2:O1:70:LEU:N | 2.26 | 0.68 |
| 1:P4:320:ARG:HG2 | 1:P4:355:ASP:HB2 | 1.75 | 0.68 |
| 2:T1:327:ASP:OD2 | 7:4U:25:ARG:NH1 | 2.20 | 0.68 |
| 1:U4:375:GLN:HB3 | 1:U4:422:TYR:HD2 | 1.59 | 0.68 |
| 2:U9:287:SER:OG | 2:U9:290:GLU:OE1 | 2.11 | 0.68 |
| 1:X2:68:LEU:HB3 | 1:X2:96:GLY:HA2 | 1.75 | 0.68 |
| 2:0V:9:ILE:HG22 | 2:0V:146:GLY:HA2 | 1.75 | 0.68 |
| 2:0V:399:TYR:O | 2:0V:402:ARG:NH1 | 2.26 | 0.68 |
| 2:1X:275:ILE:HD12 | 2:1X:368:LEU:HD11 | 1.76 | 0.68 |
| 1:2I:125:GLU:O | 38:8B:3:ASN:ND2 | 2.24 | 0.68 |
| 1:2U:212:PHE:CZ | 2:2V:326:LYS:HD3 | 2.28 | 0.68 |
| 1:3Q:183:TYR:HE2 | 1:3Q:394:PHE:HB2 | 1.59 | 0.68 |
| 24:6X:95:VAL:HG12 | 24:6X:124:TYR:CD2 | 2.28 | 0.68 |
| 24:6X:566:VAL:HG21 | 24:6X:633:LEU:HD21 | 1.74 | 0.68 |
| 38:8A:12:LEU:HB3 | 38:8A:18:VAL:HG21 | 1.74 | 0.68 |
| 2:8:33:ASP:HB3 | 18:6A:77:THR:HG21 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E2:219:THR:N | 24:6U:312:ASN:OD1 | 2.15 | 0.68 |
| 1:H2:330:MET:HB3 | 1:H2:349:VAL:HG11 | 1.76 | 0.68 |
| 1:J8:41:ASP:H | 29:7J:388:MET:HB2 | 1.59 | 0.68 |
| 1:Q0:334:GLN:HE22 | 1:Q0:348:ASN:H | 1.40 | 0.68 |
| 2:T5:334:THR:HG22 | 13:5J:134:PHE:H | 1.57 | 0.68 |
| 2:X5:56:THR:HG22 | 2:Z1:285:GLN:HB2 | 1.74 | 0.68 |
| 2:Y3:282:TYR:CE2 | 8:4W:373:ASN:HB3 | 2.25 | 0.68 |
| 1:Z0:389:PHE:O | 1:Z0:392:LYS:NZ | 2.22 | 0.68 |
| 1:Z4:248:ALA:HA | 1:Z4:252:LYS:HD3 | 1.75 | 0.68 |
| 2:0X:132:LEU:HD22 | 2:0X:164:LYS:HD3 | 1.74 | 0.68 |
| 2:1D:278:ALA:HA | 2:1D:369:ALA:HB2 | 1.76 | 0.68 |
| 1:1Q:350:LYS:NZ | 1:1Q:351:SER:O | 2.27 | 0.68 |
| 2:2R:88:HIS:HB3 | 2:3H:283:HIS:ND1 | 2.09 | 0.68 |
| 1:2S:52:ASN:OD1 | 1:2S:62:ARG:NH2 | 2.27 | 0.68 |
| 2:C5:79:ARG:NH2 | 22:6J:19:GLY:O | 2.24 | 0.68 |
| 2:I7:88:HIS:HB3 | 2:K3:283:HIS:ND1 | 2.09 | 0.68 |
| 2:M5:76:ASP:OD2 | 1:M6:46:ARG:NH2 | 2.27 | 0.68 |
| 1:P6:257:LEU:HD21 | 1:P6:314:SER:HB3 | 1.75 | 0.68 |
| 2:Q3:88:HIS:CD2 | 2:Q3:89:PRO:CD | 2.76 | 0.68 |
| 1:Q6:45:GLU:HG2 | 1:Q6:46:ARG:HG2 | 1.74 | 0.68 |
| 1:Q6:375:GLN:HB2 | 1:Q6:419:VAL:HG13 | 1.76 | 0.68 |
| 1:R4:345:ILE:O | 1:R4:348:ASN:ND2 | 2.27 | 0.68 |
| 2:S9:414:GLU:N | 2:S9:414:GLU:OE1 | 2.25 | 0.68 |
| 1:W2:140:GLY:O | 1:W2:184:ASN:ND2 | 2.24 | 0.68 |
| 1:Y0:113:ILE:HA | 1:Y0:116:VAL:HG12 | 1.75 | 0.68 |
| 2:Z3:191:THR:HA | 2:Z3:194:LEU:HB3 | 1.74 | 0.68 |
| 1:2C:173:PRO:HD2 | 1:2C:380:ARG:HE | 1.58 | 0.68 |
| 2:3B:392:ASP:OD2 | 2:3B:422:ARG:NH1 | 2.27 | 0.68 |
| 1:3G:34:GLY:O | 1:3G:58:ARG:HA | 1.94 | 0.68 |
| 12:5F:281:VAL:HG23 | 12:5F:286:SER:HA | 1.76 | 0.68 |
| 15:5O:324:ARG:NH1 | 15:5O:360:ASP:O | 2.25 | 0.68 |
| 17:5T:181:LEU:HD23 | 17:5T:181:LEU:C | 2.14 | 0.68 |
| 29:7J:265:VAL:HG12 | 29:7J:266:MET:H | 1.58 | 0.68 |
| 2:D5:279:GLU:OE2 | 18:6C:178:GLN:NE2 | 2.27 | 0.68 |
| 1:D6:45:GLU:OE1 | 22:6O:20:TYR:OH | 2.09 | 0.68 |
| 1:G2:32:PRO:HD2 | 24:6W:527:ASN:HD22 | 1.58 | 0.68 |
| 2:I5:79:ARG:NH1 | 2:I5:92:LEU:O | 2.26 | 0.68 |
| 2:J9:381:SER:OG | 2:J9:382:THR:N | 2.26 | 0.68 |
| 2:K1:172:TYR:N | 2:K1:204:LEU:O | 2.25 | 0.68 |
| 2:L9:336:LYS:O | 2:L9:339:ARG:NH2 | 2.25 | 0.68 |
| 2:M5:287:SER:N | 2:M5:290:GLU:OE2 | 2.19 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O6:276:ARG:NH1 | 32:7P:97:LEU:O | 2.27 | 0.68 |
| 1:P4:19:LYS:NZ | 27:7G:177:GLU:OE2 | 2.27 | 0.68 |
| 2:P5:42:ILE:CD1 | 27:7G:213:TRP:HZ3 | 2.02 | 0.68 |
| 1:Q0:216:LYS:NZ | 5:4M:42:GLU:OE2 | 2.23 | 0.68 |
| 1:R8:5:VAL:HG23 | 1:R8:62:ARG:HG2 | 1.74 | 0.68 |
| 1:T4:248:ALA:HA | 1:T4:252:LYS:HD2 | 1.74 | 0.68 |
| 1:U8:67:ASP:OD2 | 1:U8:72:THR:OG1 | 2.09 | 0.68 |
| 1:W8:149:THR:HA | 1:W8:152:ILE:HD12 | 1.75 | 0.68 |
| 2:Y9:136:LEU:HD11 | 2:Y9:235:ILE:HD11 | 1.75 | 0.68 |
| 1:Z0:207:LEU:HB3 | 1:Z0:225:LEU:HD22 | 1.76 | 0.68 |
| 2:Z9:268:MET:SD | 2:Z9:380:ASN:HB2 | 2.33 | 0.68 |
| 1:0G:58:ARG:HH11 | 1:0W:281:TYR:HE1 | 1.42 | 0.68 |
| 2:1L:387:ILE:HG12 | 2:1L:390:ARG:HH22 | 1.58 | 0.68 |
| 2:2V:33:ASP:O | 2:2V:60:LYS:NZ | 2.27 | 0.68 |
| 2:3D:297:GLU:HG3 | 2:3D:299:ALA:H | 1.58 | 0.68 |
| 2:3L:189:LEU:HD11 | 2:3L:418:PHE:HE1 | 1.58 | 0.68 |
| 2:3P:339:ARG:NH2 | 2:3P:342:GLN:HB3 | 2.08 | 0.68 |
| 15:5O:34:GLU:CG | 15:5O:49:ARG:NH2 | 2.52 | 0.68 |
| 19:6E:72:GLU:HG2 | 19:6E:77:GLN:HE21 | 1.59 | 0.68 |
| 2:G3:90:GLU:CB | 2:G3:121:ARG:HH12 | 2.06 | 0.68 |
| 2:H3:317:LEU:HB3 | 2:H3:319:TYR:HE1 | 1.57 | 0.68 |
| 2:H5:27:GLU:OE1 | 2:H5:243:ARG:NH1 | 2.27 | 0.68 |
| 2:I5:88:HIS:HB3 | 2:K1:283:HIS:CE1 | 2.29 | 0.68 |
| 2:J7:255:PHE:HA | 2:J7:259:LEU:HD13 | 1.76 | 0.68 |
| 2:L3:297:GLU:HG2 | 2:L3:299:ALA:H | 1.58 | 0.68 |
| 1:M2:324:LYS:HD2 | 1:M2:328:GLU:OE1 | 1.94 | 0.68 |
| 2:M3:36:MET:CG | 2:M3:37:PRO:CD | 2.66 | 0.68 |
| 1:M6:86:ARG:HB3 | 2:O3:283:HIS:CE1 | 2.29 | 0.68 |
| 1:N0:276:ARG:HH12 | 30:7L:366:PRO:HB3 | 1.58 | 0.68 |
| 2:O1:90:GLU:HB2 | 2:O1:121:ARG:HH12 | 1.58 | 0.68 |
| 2:O3:90:GLU:HB3 | 2:O3:121:ARG:NH2 | 2.08 | 0.68 |
| 2:R5:117:LEU:O | 2:R5:121:ARG:HG2 | 1.94 | 0.68 |
| 2:R5:287:SER:N | 2:R5:290:GLU:OE2 | 2.27 | 0.68 |
| 2:S1:274:PRO:HB2 | 2:S1:276:ILE:HG12 | 1.76 | 0.68 |
| 1:U4:412:GLU:OE2 | 1:U4:416:ASN:ND2 | 2.27 | 0.68 |
| 2:V9:91:GLN:HE22 | 2:X5:283:HIS:CE1 | 2.12 | 0.68 |
| 1:W6:211:CYS:HA | 1:W6:215:LEU:HB2 | 1.76 | 0.68 |
| 2:W9:224:TYR:H | 1:X0:245:GLN:NE2 | 1.92 | 0.68 |
| 2:X7:136:LEU:HD22 | 2:X7:167:LEU:HB2 | 1.76 | 0.68 |
| 1:Z6:273:LEU:H | 1:Z6:292:GLN:HE22 | 1.42 | 0.68 |
| 1:0G:211:CYS:HA | 1:0G:215:LEU:HB2 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0M:139:LEU:HD12 | 1:0M:170:VAL:HG12 | 1.74 | 0.68 |
| 1:2A:220:PRO:HD2 | 2:2B:326:LYS:HD2 | 1.74 | 0.68 |
| 1:2M:309:ARG:NH1 | 1:2M:341:PHE:O | 2.26 | 0.68 |
| 1:2Q:320:ARG:HH22 | 38:8A:198:THR:CA | 2.05 | 0.68 |
| 7:4R:5:VAL:HG23 | 12:7B:15:THR:HG21 | 1.76 | 0.68 |
| 7:4R:301:ARG:HH21 | 7:4R:301:ARG:CG | 1.93 | 0.68 |
| 11:5E:211:LEU:HD23 | 11:5E:233:ILE:HG12 | 1.75 | 0.68 |
| 14:5N:456:ARG:NE | 14:5N:456:ARG:HA | 2.08 | 0.68 |
| 15:5O:289:LEU:H | 15:5O:290:PRO:HD2 | 1.58 | 0.68 |
| 24:6W:107:VAL:HG22 | 24:6W:108:GLU:H | 1.58 | 0.68 |
| 24:6Z:469:PHE:HA | 24:6Z:485:PRO:HD2 | 1.75 | 0.68 |
| 26:7F:106:ASP:OD1 | 26:7F:107:MET:N | 2.26 | 0.68 |
| 34:7R:269:TRP:HB3 | 35:7T:223:PHE:CE2 | 2.28 | 0.68 |
| 2:A8:229:ARG:NH2 | 18:5X:50:SER:OG | 2.26 | 0.68 |
| 2:G9:264:ARG:NH2 | 2:G9:431:ASP:OD2 | 2.27 | 0.68 |
| 1:J8:375:GLN:HB2 | 1:J8:419:VAL:HG23 | 1.76 | 0.68 |
| 2:K3:377:MET:SD | 2:K3:379:SER:OG | 2.45 | 0.68 |
| 2:R9:85:GLN:NE2 | 33:7Q:171:GLN:O | 2.27 | 0.68 |
| 2:X7:344:VAL:HG22 | 2:X7:346:TRP:H | 1.58 | 0.68 |
| 2:Y1:88:HIS:HB3 | 2:Z7:283:HIS:CE1 | 2.29 | 0.68 |
| 2:Y5:9:ILE:HG22 | 2:Y5:146:GLY:HA2 | 1.74 | 0.68 |
| 1:0A:5:VAL:HG22 | 1:0A:62:ARG:HD3 | 1.74 | 0.68 |
| 1:1E:248:ALA:CA | 1:1E:252:LYS:HD3 | 2.22 | 0.68 |
| 14:5L:456:ARG:NE | 14:5L:456:ARG:HA | 2.08 | 0.68 |
| 14:5L:491:GLY:HA2 | 14:5L:511:THR:O | 1.94 | 0.68 |
| 14:5N:146:ASN:HD21 | 14:5N:172:ASN:HD21 | 1.38 | 0.68 |
| 15:5P:52:TYR:CD2 | 15:5P:54:GLU:HB3 | 2.29 | 0.68 |
| 17:5U:174:SER:OG | 17:5U:175:PRO:HD2 | 1.94 | 0.68 |
| 22:6O:333:MET:HG3 | 22:6O:334:THR:HG23 | 1.76 | 0.68 |
| 24:7A:122:TYR:HB2 | 24:7A:131:HIS:HB3 | 1.74 | 0.68 |
| 26:7D:21:THR:HG21 | 26:7D:120:ALA:HA | 1.76 | 0.68 |
| 26:7E:21:THR:HG21 | 26:7E:120:ALA:HA | 1.76 | 0.68 |
| 31:7N:5:GLY:O | 31:7N:9:ARG:NH1 | 2.27 | 0.68 |
| 1:I4:31:ASP:OD1 | 28:7X:311:ARG:NH2 | 2.26 | 0.68 |
| 2:M3:42:ILE:HD12 | 2:M3:42:ILE:N | 2.01 | 0.68 |
| 1:N2:113:ILE:HA | 1:N2:116:VAL:HG22 | 1.76 | 0.68 |
| 2:O7:313:MET:CE | 2:O7:346:TRP:CH2 | 2.77 | 0.68 |
| 2:P7:9:ILE:HG13 | 2:P7:139:ASN:HB3 | 1.75 | 0.68 |
| 1:V8:334:GLN:HE22 | 1:V8:348:ASN:H | 1.41 | 0.68 |
| 1:Z4:117:LEU:HD11 | 1:Z4:154:LYS:HD3 | 1.75 | 0.68 |
| 1:2E:125:GLU:OE2 | 1:2E:159:TYR:OH | 2.11 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2H:98:ASP:OD1 | 2:2H:99:ALA:N | 2.27 | 0.68 |
| 2:2N:27:GLU:OE1 | 2:2N:243:ARG:NH1 | 2.26 | 0.68 |
| 1:2Q:3:GLU:HB2 | 1:2Q:130:LEU:HA | 1.76 | 0.68 |
| 2:2X:214:ARG:NH1 | 38:8B:17:GLY:O | 2.27 | 0.68 |
| 2:3B:42:ILE:HD11 | 14:5N:139:ALA:CB | 2.23 | 0.68 |
| 1:3C:139:LEU:HD12 | 1:3C:170:VAL:HG12 | 1.74 | 0.68 |
| 2:3H:221:ARG:NH1 | 23:6Q:70:THR:O | 2.24 | 0.68 |
| 1:3Q:220:PRO:HD2 | 2:3R:326:LYS:HD3 | 1.76 | 0.68 |
| 1:3S:2:ARG:HE | 1:3S:240:LEU:HD22 | 1.58 | 0.68 |
| 14:5M:456:ARG:NE | 14:5M:456:ARG:HA | 2.08 | 0.68 |
| 15:5O:173:ARG:NH1 | 15:5O:207:GLY:O | 2.27 | 0.68 |
| 15:5P:338:LEU:HD12 | 15:5P:338:LEU:C | 2.15 | 0.68 |
| 24:6U:469:PHE:CB | 24:6U:484:GLU:HA | 2.24 | 0.68 |
| 2:A8:59:GLY:HA3 | 24:6T:263:ARG:HH11 | 1.58 | 0.68 |
| 2:G7:182:VAL:HG23 | 2:G7:186:ASN:HD21 | 1.59 | 0.68 |
| 2:I1:9:ILE:HG13 | 2:I1:139:ASN:HB3 | 1.76 | 0.68 |
| 1:K4:113:ILE:HA | 1:K4:116:VAL:HG22 | 1.76 | 0.68 |
| 2:K5:219:ILE:HG23 | 29:7I:14:LEU:HD11 | 0.72 | 0.68 |
| 1:M4:113:ILE:HG12 | 1:M4:117:LEU:HD23 | 1.76 | 0.68 |
| 2:N3:370:LYS:NZ | 30:7L:274:PRO:O | 2.23 | 0.68 |
| 2:O1:286:LEU:O | 2:O1:373:ARG:NH1 | 2.27 | 0.68 |
| 2:O7:91:GLN:HA | 2:O7:121:ARG:HH12 | 1.59 | 0.68 |
| 1:T8:333:VAL:HG12 | 13:5K:102:ALA:HB3 | 1.75 | 0.68 |
| 1:V8:183:TYR:HB3 | 1:V8:398:TYR:HE2 | 1.59 | 0.68 |
| 1:X6:250:LEU:HD12 | 1:X6:250:LEU:H | 1.59 | 0.68 |
| 2:Y3:90:GLU:HB3 | 2:Y3:121:ARG:HH22 | 1.58 | 0.68 |
| 1:Z8:45:GLU:HG3 | 1:Z8:46:ARG:HG2 | 1.76 | 0.68 |
| 1:0O:175:VAL:HG22 | 2:0P:329:ASN:HD21 | 1.58 | 0.68 |
| 2:0P:239:THR:HG23 | 2:0P:243:ARG:HE | 1.59 | 0.68 |
| 1:0Y:309:ARG:NH1 | 1:0Y:339:SER:O | 2.27 | 0.68 |
| 2:1F:336:LYS:O | 2:1F:339:ARG:NH2 | 2.26 | 0.68 |
| 1:1K:309:ARG:H | 1:1K:372:THR:HG22 | 1.58 | 0.68 |
| 1:1O:345:ILE:O | 1:1O:348:ASN:ND2 | 2.26 | 0.68 |
| 2:2F:88:HIS:HB3 | 2:2V:283:HIS:ND1 | 2.09 | 0.68 |
| 2:2N:120:ASP:HB3 | 38:8D:73:TRP:CG | 2.29 | 0.68 |
| 2:2Z:121:ARG:CG | 2:2Z:121:ARG:NH1 | 2.55 | 0.68 |
| 1:3Q:2:ARG:HE | 1:3Q:240:LEU:HD22 | 1.59 | 0.68 |
| 14:5L:115:GLU:O | 14:5L:134:VAL:HG12 | 1.91 | 0.68 |
| 14:5M:146:ASN:HD21 | 14:5M:172:ASN:HD21 | 1.38 | 0.68 |
| 14:5N:415:LYS:HG2 | 23:6S:23:ILE:HD11 | 1.75 | 0.68 |
| 15:5O:376:LEU:N | 15:5O:377:PRO:HD2 | 2.09 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:444:ILE:O | 24:6X:445:ILE:HD12 | 1.94 | 0.68 |
| 24:6X:451:LYS:CE | 24:6X:468:ARG:HH12 | 1.98 | 0.68 |
| 31:7M:20:ILE:HD11 | 31:7M:23:LEU:HD12 | 1.76 | 0.68 |
| 1:I0:218:THR:CB | 24:6X:489:ASN:H | 2.07 | 0.67 |
| 2:L7:55:GLU:O | 2:N3:285:GLN:NE2 | 2.26 | 0.67 |
| 2:M7:51:THR:HG21 | 2:M7:243:ARG:HG2 | 1.76 | 0.67 |
| 2:Q3:56:THR:CG2 | 2:Q3:60:LYS:HB3 | 2.22 | 0.67 |
| 1:R6:293:MET:HE1 | 1:R6:317:PHE:HE1 | 1.58 | 0.67 |
| 2:X7:276:ILE:HG23 | 2:X7:280:LYS:HB2 | 1.75 | 0.67 |
| 1:0A:190:HIS:CD2 | 1:0A:411:ALA:HA | 2.29 | 0.67 |
| 1:0U:77:ARG:O | 1:0U:83:GLN:NE2 | 2.26 | 0.67 |
| 1:1E:273:LEU:H | 1:1E:292:GLN:HE22 | 1.42 | 0.67 |
| 2:1T:88:HIS:HB3 | 2:2J:283:HIS:ND1 | 2.09 | 0.67 |
| 2:1X:224:TYR:HA | 2:1X:227:LEU:HD12 | 1.75 | 0.67 |
| 2:2D:88:HIS:CE1 | 2:2T:283:HIS:HA | 2.29 | 0.67 |
| 1:2S:337:ASN:OD1 | 38:8A:53:ALA:N | 2.23 | 0.67 |
| 1:3C:245:GLN:HE21 | 38:8D:198:THR:HG21 | 1.59 | 0.67 |
| 2:3F:336:LYS:O | 2:3F:339:ARG:NH2 | 2.26 | 0.67 |
| 2:3T:289:ALA:O | 2:3T:293:ASN:ND2 | 2.27 | 0.67 |
| 3:3X:38:THR:HG21 | 4:3Y:3:LYS:HB2 | 1.75 | 0.67 |
| 14:5L:146:ASN:HD21 | 14:5L:172:ASN:HD21 | 1.38 | 0.67 |
| 20:6F:27:LEU:CD1 | 30:7K:3:LEU:HD12 | 2.23 | 0.67 |
| 24:6X:130:MET:HE1 | 24:6X:161:PHE:CG | 2.30 | 0.67 |
| 26:7D:106:ASP:OD1 | 26:7D:107:MET:N | 2.26 | 0.67 |
| 2:J7:80:THR:HB | 29:7J:390:LEU:CG | 2.24 | 0.67 |
| 1:L6:99:ASN:ND2 | 2:L7:254:GLU:OE1 | 2.27 | 0.67 |
| 2:N5:88:HIS:CD2 | 2:N5:89:PRO:HD2 | 2.30 | 0.67 |
| 2:P3:308:ARG:NH1 | 2:U1:282:TYR:OH | 2.23 | 0.67 |
| 2:P5:264:ARG:NH2 | 2:P5:431:ASP:OD2 | 2.27 | 0.67 |
| 2:S7:42:ILE:HG13 | 2:S7:43:GLY:N | 2.09 | 0.67 |
| 2:S7:286:LEU:O | 2:S7:373:ARG:NH1 | 2.27 | 0.67 |
| 2:T3:90:GLU:OE2 | 2:T3:90:GLU:HA | 1.93 | 0.67 |
| 1:T4:190:HIS:HD2 | 1:T4:414:ASN:HD22 | 1.41 | 0.67 |
| 1:V0:52:ASN:OD1 | 1:V0:62:ARG:NH2 | 2.27 | 0.67 |
| 1:V4:5:VAL:HG23 | 1:V4:62:ARG:HG2 | 1.75 | 0.67 |
| 2:V7:75:VAL:HG21 | 2:V7:94:SER:HB3 | 1.75 | 0.67 |
| 2:X3:88:HIS:HB3 | 2:Y9:283:HIS:ND1 | 2.08 | 0.67 |
| 1:Y8:327:ASP:HA | 1:Y8:330:MET:HE1 | 1.76 | 0.67 |
| 2:Z9:53:PHE:HB3 | 2:Z9:61:HIS:HB3 | 1.75 | 0.67 |
| 1:0A:16:ILE:HD11 | 1:0A:136:CYS:HB2 | 1.76 | 0.67 |
| 2:0B:191:THR:HA | 2:0B:194:LEU:HB3 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0C:52:ASN:OD1 | 1:0C:62:ARG:NH2 | 2.28 | 0.67 |
| 2:0H:203:MET:HE1 | 2:0H:267:PHE:HB3 | 1.76 | 0.67 |
| 2:0R:100:ALA:HA | 1:0S:252:LYS:HE2 | 1.76 | 0.67 |
| 2:0R:183:GLU:HG3 | 2:0R:184:PRO:HD3 | 1.75 | 0.67 |
| 1:0U:289:LEU:HD21 | 1:0U:365:ALA:HB3 | 1.75 | 0.67 |
| 1:0Y:4:ILE:HB | 1:0Y:50:TYR:HE1 | 1.57 | 0.67 |
| 2:2H:279:GLU:OE1 | 10:5B:167:ILE:CG1 | 2.42 | 0.67 |
| 2:2Z:214:ARG:HH22 | 38:8C:61:LYS:HA | 1.58 | 0.67 |
| 2:2Z:339:ARG:NH2 | 38:8C:77:LYS:O | 2.26 | 0.67 |
| 2:3D:164:LYS:O | 2:3D:166:LYS:NZ | 2.28 | 0.67 |
| 2:3F:399:TYR:OH | 2:3F:415:GLU:OE2 | 2.06 | 0.67 |
| 7:4R:8:VAL:CG2 | 7:4R:9:PRO:HD2 | 2.24 | 0.67 |
| 14:5L:598:ILE:HA | 14:5L:614:GLY:HA2 | 1.75 | 0.67 |
| 14:5N:5:LEU:HB3 | 14:5N:590:VAL:HB | 1.77 | 0.67 |
| 26:7E:106:ASP:OD1 | 26:7E:107:MET:N | 2.26 | 0.67 |
| 32:7P:93:VAL:HG13 | 32:7P:94:LYS:H | 1.59 | 0.67 |
| 2:F9:206:ASN:OD1 | 41:G0:501:GTP:N2 | 2.26 | 0.67 |
| 2:M7:36:MET:HG3 | 2:M7:42:ILE:HG12 | 1.76 | 0.67 |
| 2:M9:279:GLU:H | 2:M9:279:GLU:CD | 1.97 | 0.67 |
| 1:N0:128:ASP:O | 20:6F:2:ARG:NH2 | 2.27 | 0.67 |
| 2:N5:244:PHE:HB2 | 2:N5:356:ASN:HD21 | 1.59 | 0.67 |
| 1:S4:274:THR:HG21 | 1:S4:282:ARG:HD2 | 1.75 | 0.67 |
| 1:U2:418:LEU:HG | 1:U2:422:TYR:HE2 | 1.59 | 0.67 |
| 1:U4:52:ASN:OD1 | 1:U4:62:ARG:NH2 | 2.25 | 0.67 |
| 2:U5:275:ILE:HG13 | 2:U5:368:LEU:HD11 | 1.77 | 0.67 |
| 2:V7:267:PHE:HB2 | 2:V7:384:ILE:HD12 | 1.73 | 0.67 |
| 1:W2:139:LEU:HD12 | 1:W2:170:VAL:HG12 | 1.76 | 0.67 |
| 2:X5:223:THR:HG23 | 2:X5:225:THR:H | 1.59 | 0.67 |
| 1:0M:45:GLU:HG3 | 1:0M:46:ARG:HG2 | 1.76 | 0.67 |
| 1:1C:139:LEU:HD12 | 1:1C:170:VAL:HG22 | 1.75 | 0.67 |
| 1:1C:180:VAL:HG23 | 1:1C:184:ASN:HD21 | 1.59 | 0.67 |
| 2:1V:121:ARG:HD2 | 2:1V:121:ARG:C | 2.14 | 0.67 |
| 1:2A:121:ARG:NH1 | 38:8A:100:SER:OG | 2.27 | 0.67 |
| 2:2N:116:ASP:HB2 | 38:8D:73:TRP:CZ3 | 2.29 | 0.67 |
| 2:2N:213:CYS:HA | 2:2N:217:LEU:HB3 | 1.75 | 0.67 |
| 1:3Q:69:GLU:C | 1:3Q:92:PHE:HZ | 1.98 | 0.67 |
| 2:3T:425:LEU:HD23 | 2:3T:425:LEU:C | 2.14 | 0.67 |
| 14:5L:514:LYS:HD3 | 14:5L:557:ASN:HB3 | 1.76 | 0.67 |
| 14:5M:598:ILE:HA | 14:5M:614:GLY:HA2 | 1.76 | 0.67 |
| 14:5N:208:TYR:HB3 | 14:5N:220:GLN:HE21 | 1.56 | 0.67 |
| 15:5O:60:LEU:C | 15:5O:60:LEU:HD12 | 2.15 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:296:SER:HA | 15:5O:299:GLU:CG | 2.24 | 0.67 |
| 22:6I:110:ILE:O | 22:6I:113:ARG:NH1 | 2.27 | 0.67 |
| 22:6P:266:LYS:HA | 22:6P:269:GLU:HG3 | 1.76 | 0.67 |
| 29:7J:435:THR:HG22 | 29:7J:437:PHE:H | 1.59 | 0.67 |
| 38:8B:25:ILE:HD13 | 38:8B:25:ILE:C | 2.14 | 0.67 |
| 2:H7:90:GLU:O | 2:H7:121:ARG:NH1 | 2.26 | 0.67 |
| 1:H8:156:ARG:NH1 | 1:H8:197:ASP:OD1 | 2.27 | 0.67 |
| 2:J3:264:ARG:NH2 | 2:J3:431:ASP:OD2 | 2.27 | 0.67 |
| 2:K7:336:LYS:O | 2:K7:339:ARG:NH2 | 2.27 | 0.67 |
| 1:M2:67:ASP:OD2 | 1:M2:72:THR:OG1 | 2.13 | 0.67 |
| 2:N9:122:ILE:HD12 | 2:N9:157:LEU:HD21 | 1.76 | 0.67 |
| 1:O0:358:PRO:HG2 | 1:O0:361:LEU:HD12 | 1.76 | 0.67 |
| 1:Q2:68:LEU:HB3 | 1:Q2:96:GLY:HA2 | 1.75 | 0.67 |
| 1:Q6:1:MET:N | 1:Q6:3:GLU:OE2 | 2.27 | 0.67 |
| 2:S1:90:GLU:HB3 | 2:S1:121:ARG:HH22 | 1.58 | 0.67 |
| 1:W4:334:GLN:HE22 | 1:W4:348:ASN:H | 1.41 | 0.67 |
| 2:0F:288:VAL:HG13 | 2:0F:319:TYR:HE2 | 1.59 | 0.67 |
| 1:0O:273:LEU:H | 1:0O:292:GLN:HE22 | 1.40 | 0.67 |
| 1:1A:200:MET:HE3 | 1:1A:268:VAL:HG21 | 1.77 | 0.67 |
| 2:1B:340:THR:HG23 | 2:1B:341:ILE:HD12 | 1.76 | 0.67 |
| 1:1C:334:GLN:HE22 | 1:1C:348:ASN:H | 1.41 | 0.67 |
| 1:1S:335:ASN:O | 1:1S:338:SER:OG | 2.12 | 0.67 |
| 2:2L:113:GLU:HG2 | 38:8C:7:ASP:HA | 1.75 | 0.67 |
| 2:2P:417:GLU:HA | 2:2P:420:GLU:HG2 | 1.76 | 0.67 |
| 1:2U:51:PHE:HB3 | 1:2U:59:TYR:HB3 | 1.77 | 0.67 |
| 1:3Q:232:VAL:HG22 | 1:3Q:270:PHE:HB2 | 1.76 | 0.67 |
| 2:3T:225:THR:HG22 | 2:3T:229:ARG:HE | 1.59 | 0.67 |
| 5:4M:76:LEU:HD22 | 15:5P:284:VAL:HG12 | 1.76 | 0.67 |
| 14:5L:5:LEU:HB3 | 14:5L:590:VAL:HB | 1.77 | 0.67 |
| 14:5M:5:LEU:HB3 | 14:5M:590:VAL:HB | 1.77 | 0.67 |
| 14:5N:598:ILE:HA | 14:5N:614:GLY:HA2 | 1.76 | 0.67 |
| 15:5P:331:ASP:OD2 | 15:5P:334:LEU:CD1 | 2.41 | 0.67 |
| 18:5Y:109:THR:OG1 | 18:5Y:110:GLU:OE2 | 2.10 | 0.67 |
| 20:6F:31:LEU:CD1 | 30:7K:8:LEU:HD12 | 2.23 | 0.67 |
| 22:6P:268:ASP:HA | 22:6P:271:ARG:HG2 | 1.77 | 0.67 |
| 24:6Y:130:MET:HG3 | 24:6Y:153:VAL:HG12 | 1.77 | 0.67 |
| 2:I5:56:THR:HA | 2:K1:285:GLN:HB2 | 1.76 | 0.67 |
| 2:N3:359:PRO:HD3 | 29:7J:90:GLY:HA3 | 1.75 | 0.67 |
| 2:O3:265:ILE:CD1 | 2:O3:435:VAL:HG21 | 2.24 | 0.67 |
| 1:P4:52:ASN:OD1 | 1:P4:62:ARG:NH2 | 2.27 | 0.67 |
| 2:P5:90:GLU:HB2 | 2:P5:121:ARG:HH12 | 1.57 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P5:90:GLU:HB3 | 2:P5:121:ARG:HH12 | 1.57 | 0.67 |
| 2:Q5:245:ASP:HB3 | 20:6F:263:LEU:HD21 | 1.76 | 0.67 |
| 2:T1:35:GLN:NE2 | 24:6W:83:THR:OG1 | 2.25 | 0.67 |
| 1:U8:3:GLU:HB3 | 1:U8:130:LEU:HA | 1.75 | 0.67 |
| 2:Y3:88:HIS:HB3 | 2:Z9:283:HIS:CE1 | 2.30 | 0.67 |
| 2:Z9:392:ASP:OD2 | 2:Z9:422:ARG:NH1 | 2.28 | 0.67 |
| 1:0K:268:VAL:O | 1:0K:300:MET:N | 2.24 | 0.67 |
| 1:0Q:135:VAL:HG21 | 1:0Q:152:ILE:HD11 | 1.77 | 0.67 |
| 2:0V:387:ILE:HG12 | 2:0V:390:ARG:HH22 | 1.58 | 0.67 |
| 1:1C:350:LYS:NZ | 1:1C:352:SER:OG | 2.26 | 0.67 |
| 2:1F:250:VAL:HG23 | 2:1F:254:GLU:HG3 | 1.77 | 0.67 |
| 1:1G:379:LYS:HD3 | 1:1G:419:VAL:HG11 | 1.74 | 0.67 |
| 1:1O:67:ASP:OD2 | 1:1O:72:THR:OG1 | 2.11 | 0.67 |
| 1:1O:140:GLY:O | 1:1O:184:ASN:ND2 | 2.27 | 0.67 |
| 2:1T:264:ARG:NH2 | 2:1T:431:ASP:OD2 | 2.26 | 0.67 |
| 1:2I:134:GLN:HE21 | 1:2I:167:PHE:HE2 | 1.41 | 0.67 |
| 2:2R:222:PRO:HD2 | 1:2S:324:LYS:HE3 | 1.77 | 0.67 |
| 7:4U:234:GLU:HG3 | 31:7N:15:LEU:HD21 | 1.75 | 0.67 |
| 11:5E:161:ARG:NH1 | 11:5E:195:GLN:OE1 | 2.28 | 0.67 |
| 14:5L:199:SER:HG | 14:5L:245:THR:HG1 | 1.40 | 0.67 |
| 15:5P:243:LYS:NZ | 15:5P:354:ASN:OD1 | 2.25 | 0.67 |
| 17:5V:224:ARG:HB3 | 17:5V:224:ARG:NH2 | 2.09 | 0.67 |
| 18:6A:109:THR:OG1 | 18:6A:110:GLU:OE2 | 2.10 | 0.67 |
| 18:6B:109:THR:OG1 | 18:6B:110:GLU:OE2 | 2.10 | 0.67 |
| 18:6C:109:THR:OG1 | 18:6C:110:GLU:OE2 | 2.10 | 0.67 |
| 22:6I:180:SER:OG | 22:6I:182:ASN:ND2 | 2.27 | 0.67 |
| 24:6Z:354:ARG:HB2 | 24:6Z:357:LEU:HG | 1.76 | 0.67 |
| 24:6Z:470:ILE:HD12 | 24:6Z:485:PRO:HD3 | 1.76 | 0.67 |
| 38:8A:182:ASN:HB3 | 38:8A:185:MET:HB2 | 1.76 | 0.67 |
| 2:B7:226:ASN:ND2 | 18:6B:51:MET:SD | 2.67 | 0.67 |
| 1:D4:45:GLU:OE1 | 22:6N:20:TYR:OH | 2.06 | 0.67 |
| 1:F6:32:PRO:HD2 | 24:6T:527:ASN:HD22 | 1.60 | 0.67 |
| 2:G5:288:VAL:HG11 | 2:G5:323:VAL:HG13 | 1.77 | 0.67 |
| 1:H8:309:ARG:H | 1:H8:372:THR:HG22 | 1.58 | 0.67 |
| 2:L3:84:ARG:HD2 | 29:7J:319:ILE:HD11 | 1.75 | 0.67 |
| 2:N7:293:ASN:HD22 | 32:7O:18:SER:HB2 | 1.59 | 0.67 |
| 2:O3:236:SER:OG | 2:O3:243:ARG:NH2 | 2.27 | 0.67 |
| 1:O6:177:ASP:O | 2:O7:352:LYS:HA | 1.94 | 0.67 |
| 2:R1:176:GLN:HE22 | 2:R1:304:LYS:HE2 | 1.58 | 0.67 |
| 1:R8:345:ILE:O | 1:R8:348:ASN:ND2 | 2.28 | 0.67 |
| 2:S1:88:HIS:HD2 | 2:S1:89:PRO:CD | 1.84 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:391:ARG:HD2 | 13:5H:55:VAL:HB | 1.77 | 0.67 |
| 1:S6:135:VAL:HG11 | 1:S6:152:ILE:HD11 | 1.76 | 0.67 |
| 1:U8:45:GLU:HG3 | 1:U8:46:ARG:HG2 | 1.77 | 0.67 |
| 2:W3:287:SER:N | 2:W3:290:GLU:OE2 | 2.23 | 0.67 |
| 1:X0:42:LEU:CG | 8:4X:97:PHE:HZ | 2.04 | 0.67 |
| 1:X8:207:LEU:HB3 | 1:X8:225:LEU:HD22 | 1.76 | 0.67 |
| 1:Z4:309:ARG:H | 1:Z4:372:THR:HG22 | 1.60 | 0.67 |
| 1:0E:165:LEU:HD21 | 1:0E:250:LEU:HD11 | 1.76 | 0.67 |
| 2:0J:259:LEU:HB3 | 2:0J:268:MET:HE2 | 1.77 | 0.67 |
| 1:1C:270:PHE:HD2 | 1:1C:273:LEU:HD21 | 1.59 | 0.67 |
| 2:1V:88:HIS:CD2 | 2:1V:89:PRO:CD | 2.73 | 0.67 |
| 1:2Y:56:GLY:CA | 38:8C:161:GLN:HE21 | 2.07 | 0.67 |
| 2:3R:392:ASP:OD2 | 2:3R:422:ARG:NH1 | 2.27 | 0.67 |
| 15:5O:208:SER:CB | 15:5O:217:GLU:OE1 | 2.43 | 0.67 |
| 18:5Z:109:THR:OG1 | 18:5Z:110:GLU:OE2 | 2.10 | 0.67 |
| 22:6K:170:ARG:NH2 | 22:6K:246:GLN:O | 2.26 | 0.67 |
| 24:6X:517:LEU:HD12 | 24:6X:517:LEU:H | 1.60 | 0.67 |
| 1:1:306:ARG:NH2 | 3:3V:60:PRO:O | 2.26 | 0.67 |
| 1:3:337:ASN:ND2 | 3:3X:68:SER:HA | 2.08 | 0.67 |
| 1:G2:134:GLN:HE21 | 1:G2:167:PHE:HE2 | 1.42 | 0.67 |
| 2:G3:282:TYR:OH | 22:6M:134:ASN:ND2 | 2.27 | 0.67 |
| 1:I0:113:ILE:HA | 1:I0:116:VAL:HG22 | 1.77 | 0.67 |
| 2:K1:287:SER:N | 2:K1:290:GLU:OE2 | 2.28 | 0.67 |
| 1:K8:113:ILE:HA | 1:K8:116:VAL:HG22 | 1.76 | 0.67 |
| 1:L4:178:THR:HG22 | 2:L5:352:LYS:HE2 | 1.76 | 0.67 |
| 1:M0:113:ILE:HA | 1:M0:116:VAL:HG12 | 1.77 | 0.67 |
| 1:S4:139:LEU:HD12 | 1:S4:170:VAL:HG12 | 1.76 | 0.67 |
| 1:T0:333:VAL:HG22 | 13:5I:102:ALA:HB3 | 1.76 | 0.67 |
| 1:T2:92:PHE:CZ | 24:6Y:33:LEU:HB3 | 2.29 | 0.67 |
| 1:T6:16:ILE:HD13 | 1:T6:229:ILE:HD13 | 1.77 | 0.67 |
| 1:X2:8:GLN:HG2 | 1:X2:17:GLY:HA3 | 1.77 | 0.67 |
| 2:X3:387:ILE:HD12 | 2:X3:390:ARG:HH22 | 1.59 | 0.67 |
| 1:Y8:202:LEU:HD23 | 1:Y8:229:ILE:CD1 | 2.25 | 0.67 |
| 2:Z7:338:LYS:NZ | 2:Z7:340:THR:OG1 | 2.26 | 0.67 |
| 1:0U:392:LYS:HG3 | 1:0U:395:LEU:HD22 | 1.76 | 0.67 |
| 1:1U:211:CYS:HA | 1:1U:215:LEU:HB2 | 1.76 | 0.67 |
| 2:2D:282:TYR:CE2 | 10:5A:380:ARG:HD3 | 2.28 | 0.67 |
| 2:2N:264:ARG:NH2 | 2:2N:431:ASP:OD2 | 2.28 | 0.67 |
| 1:3G:345:ILE:O | 1:3G:348:ASN:ND2 | 2.25 | 0.67 |
| 6:4O:65:LYS:HB3 | 6:4O:66:ARG:HH21 | 1.60 | 0.67 |
| 18:6D:109:THR:OG1 | 18:6D:110:GLU:OE2 | 2.10 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:6H:37:ILE:HG13 | 21:6H:38:PRO:HD2 | 1.76 | 0.67 |
| 30:7K:6:GLN:OE1 | 30:7K:6:GLN:HA | 1.95 | 0.67 |
| 2:F5:278:ALA:HB3 | 22:6I:215:GLY:HA2 | 1.77 | 0.67 |
| 2:F7:221:ARG:HG3 | 22:6J:178:GLY:HA2 | 1.76 | 0.67 |
| 2:H3:88:HIS:HB3 | 2:H3:91:GLN:HG2 | 1.76 | 0.67 |
| 2:H5:56:THR:HA | 2:J1:285:GLN:HB2 | 1.77 | 0.67 |
| 1:J6:334:GLN:HE22 | 1:J6:348:ASN:H | 1.43 | 0.67 |
| 2:M7:285:GLN:CG | 30:7K:84:VAL:CG1 | 2.70 | 0.67 |
| 1:O0:52:ASN:OD1 | 1:O0:62:ARG:NH2 | 2.27 | 0.67 |
| 1:O6:67:ASP:OD2 | 1:O6:72:THR:OG1 | 2.13 | 0.67 |
| 1:S2:222:PHE:HB2 | 7:4R:367:ARG:HG2 | 1.76 | 0.67 |
| 2:T3:176:GLN:HE21 | 13:5J:90:PRO:HG3 | 1.60 | 0.67 |
| 1:T4:253:LEU:HD11 | 1:T4:316:LEU:HD21 | 1.76 | 0.67 |
| 1:T4:345:ILE:O | 1:T4:348:ASN:ND2 | 2.28 | 0.67 |
| 1:U8:3:GLU:OE2 | 1:U8:62:ARG:NH1 | 2.28 | 0.67 |
| 1:V8:177:ASP:O | 2:V9:352:LYS:HA | 1.93 | 0.67 |
| 2:Z1:298:PRO:HA | 2:Z1:301:MET:HG3 | 1.77 | 0.67 |
| 2:Z3:70:LEU:HG | 2:Z3:145:THR:HG23 | 1.75 | 0.67 |
| 1:0A:122:LYS:O | 1:0A:126:SER:OG | 2.11 | 0.67 |
| 1:1S:178:THR:HG23 | 1:1S:181:GLU:HG3 | 1.76 | 0.67 |
| 2:1Z:195:LEU:HD21 | 2:1Z:264:ARG:HD2 | 1.76 | 0.67 |
| 2:2D:90:GLU:HB2 | 2:2D:121:ARG:HH22 | 1.59 | 0.67 |
| 2:2D:336:LYS:O | 2:2D:339:ARG:NH2 | 2.27 | 0.67 |
| 2:2V:264:ARG:NH2 | 2:2V:431:ASP:OD2 | 2.28 | 0.67 |
| 2:3D:320:ARG:NH2 | 2:3D:358:GLN:OE1 | 2.27 | 0.67 |
| 2:3L:413:MET:HB3 | 2:3L:417:GLU:OE2 | 1.94 | 0.67 |
| 6:4P:29:GLU:OE1 | 6:4P:33:ARG:NE | 2.28 | 0.67 |
| 18:5X:31:ASP:N | 18:5X:31:ASP:OD2 | 2.27 | 0.67 |
| 24:6V:6:PRO:N | 24:6V:7:PRO:HD3 | 2.10 | 0.67 |
| 24:6Z:130:MET:CE | 24:6Z:174:ILE:HD11 | 2.25 | 0.67 |
| 29:7I:258:ARG:NE | 30:7K:342:LEU:HD11 | 2.09 | 0.67 |
| 1:C4:1:MET:HG2 | 22:6I:21:THR:HG21 | 1.77 | 0.67 |
| 2:E5:282:TYR:HH | 22:6K:81:ASN:CA | 2.05 | 0.67 |
| 1:G2:112:LEU:HB3 | 1:G2:147:MET:HE3 | 1.77 | 0.67 |
| 1:H2:51:PHE:O | 1:H2:62:ARG:NH2 | 2.27 | 0.67 |
| 2:H5:90:GLU:HG2 | 2:H5:121:ARG:HH12 | 1.59 | 0.67 |
| 2:I1:399:TYR:O | 2:I1:402:ARG:NH1 | 2.26 | 0.67 |
| 1:J0:140:GLY:O | 1:J0:184:ASN:ND2 | 2.27 | 0.67 |
| 1:J6:139:LEU:HD12 | 1:J6:170:VAL:HG12 | 1.75 | 0.67 |
| 1:J6:175:VAL:HG22 | 1:J6:205:GLU:HG3 | 1.76 | 0.67 |
| 2:J7:80:THR:CG2 | 29:7J:390:LEU:HD21 | 2.25 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J9:50:ASN:O | 2:J9:64:ARG:NH2 | 2.18 | 0.67 |
| 2:L7:87:PHE:HB3 | 2:L7:92:LEU:HD11 | 1.77 | 0.67 |
| 2:M3:53:PHE:HB3 | 2:M3:61:HIS:HB3 | 1.77 | 0.67 |
| 2:N1:27:GLU:OE1 | 2:N1:243:ARG:NH1 | 2.28 | 0.67 |
| 2:O3:287:SER:N | 2:O3:290:GLU:OE2 | 2.26 | 0.67 |
| 1:O4:274:THR:HG21 | 1:O4:282:ARG:HD2 | 1.75 | 0.67 |
| 2:Q5:417:GLU:HA | 2:Q5:420:GLU:HG2 | 1.77 | 0.67 |
| 1:S4:220:PRO:HD2 | 2:S5:326:LYS:HG2 | 1.77 | 0.67 |
| 1:S6:227:HIS:CG | 7:4T:241:PHE:HZ | 2.12 | 0.67 |
| 1:S6:248:ALA:CA | 1:S6:252:LYS:HD3 | 2.21 | 0.67 |
| 1:U8:52:ASN:OD1 | 1:U8:62:ARG:NH2 | 2.27 | 0.67 |
| 2:U9:353:CYS:SG | 2:U9:354:GLY:N | 2.68 | 0.67 |
| 2:W7:76:ASP:OD2 | 1:W8:46:ARG:NH2 | 2.27 | 0.67 |
| 1:X4:153:SER:HB3 | 1:X4:195:ASN:HD21 | 1.60 | 0.67 |
| 1:Y0:50:TYR:OH | 1:Y0:237:THR:OG1 | 2.13 | 0.67 |
| 2:0V:176:GLN:HG2 | 2:0V:177:VAL:HG23 | 1.76 | 0.67 |
| 1:1A:350:LYS:NZ | 1:1A:351:SER:O | 2.27 | 0.67 |
| 1:1E:2:ARG:HB3 | 1:1E:131:GLN:HB2 | 1.77 | 0.67 |
| 1:1G:211:CYS:HA | 1:1G:215:LEU:HB2 | 1.76 | 0.67 |
| 1:1K:377:MET:SD | 1:1K:380:ARG:NH2 | 2.68 | 0.67 |
| 2:1P:90:GLU:HG2 | 2:1P:121:ARG:HH12 | 1.59 | 0.67 |
| 1:1Q:139:LEU:HD12 | 1:1Q:170:VAL:HG12 | 1.77 | 0.67 |
| 1:1U:175:VAL:HG12 | 2:1V:329:ASN:ND2 | 2.09 | 0.67 |
| 2:1X:34:GLY:HA3 | 2:1X:60:LYS:HZ2 | 1.59 | 0.67 |
| 2:2T:358:GLN:HE21 | 38:8B:214:HIS:H | 1.42 | 0.67 |
| 1:2Y:306:ARG:CD | 38:8C:96:GLY:CA | 2.68 | 0.67 |
| 5:4M:294:SER:CA | 28:7X:306:LEU:HD11 | 2.25 | 0.67 |
| 18:5X:109:THR:OG1 | 18:5X:110:GLU:OE2 | 2.10 | 0.67 |
| 21:6H:109:THR:HA | 24:6X:82:ALA:HB3 | 1.77 | 0.67 |
| 22:6J:180:SER:OG | 22:6J:182:ASN:ND2 | 2.28 | 0.67 |
| 24:6Y:613:LYS:O | 24:6Y:617:ASP:HB2 | 1.95 | 0.67 |
| 1:E8:279:GLN:NE2 | 22:6M:103:ALA:O | 2.27 | 0.67 |
| 2:H1:9:ILE:HG12 | 2:H1:68:LEU:HD11 | 1.77 | 0.67 |
| 1:K6:52:ASN:OD1 | 1:K6:62:ARG:NH2 | 2.28 | 0.67 |
| 1:M0:86:ARG:HB2 | 1:M0:89:ASN:HB2 | 1.75 | 0.67 |
| 2:O5:424:ASP:OD1 | 2:V1:339:ARG:NH2 | 2.28 | 0.67 |
| 1:P4:311:LEU:HD23 | 1:P4:312:THR:HG23 | 1.77 | 0.67 |
| 2:P9:417:GLU:HA | 2:P9:420:GLU:HG3 | 1.77 | 0.67 |
| 1:Q4:375:GLN:HB2 | 1:Q4:419:VAL:HG13 | 1.77 | 0.67 |
| 2:R5:72:PRO:HG3 | 1:R6:1:MET:HG2 | 1.75 | 0.67 |
| 1:R6:244:GLY:H | 1:R6:247:ASN:HD21 | 1.43 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R7:85:GLN:OE1 | 2:R7:85:GLN:HA | 1.95 | 0.67 |
| 2:U5:287:SER:OG | 2:U5:290:GLU:OE1 | 2.12 | 0.67 |
| 2:V3:217:LEU:HB3 | 2:V3:219:ILE:HD12 | 1.77 | 0.67 |
| 1:X2:257:LEU:HD12 | 1:X2:312:THR:HG23 | 1.76 | 0.67 |
| 1:X8:131:GLN:HE21 | 1:X8:250:LEU:HD13 | 1.59 | 0.67 |
| 1:Y8:2:ARG:HB3 | 1:Y8:131:GLN:HB2 | 1.75 | 0.67 |
| 1:Z6:122:LYS:HD2 | 1:0M:292:GLN:HE22 | 1.59 | 0.67 |
| 1:0Q:210:ILE:HD11 | 1:0Q:273:LEU:HD12 | 1.77 | 0.67 |
| 2:0R:387:ILE:HG12 | 2:0R:390:ARG:HH22 | 1.59 | 0.67 |
| 1:1M:45:GLU:HG2 | 1:1M:46:ARG:HG2 | 1.76 | 0.67 |
| 1:1M:309:ARG:H | 1:1M:372:THR:HG22 | 1.60 | 0.67 |
| 1:1Q:387:ALA:HA | 1:1Q:390:ARG:HH21 | 1.59 | 0.67 |
| 2:1Z:319:TYR:HB3 | 2:1Z:323:VAL:HG21 | 1.74 | 0.67 |
| 1:2U:219:THR:HB | 2:2V:324:VAL:HG11 | 1.77 | 0.67 |
| 1:2Y:276:ARG:NH2 | 10:5C:409:ASN:OD1 | 2.27 | 0.67 |
| 2:3B:53:PHE:CD2 | 2:3B:61:HIS:HB3 | 2.30 | 0.67 |
| 5:4L:306:PHE:HA | 5:4L:309:ARG:HD3 | 1.77 | 0.67 |
| 9:4Z:25:ARG:HB3 | 14:5L:540:TYR:HD1 | 1.59 | 0.67 |
| 9:4Z:245:ALA:O | 9:4Z:248:GLU:HG3 | 1.95 | 0.67 |
| 14:5M:365:ARG:CZ | 14:5M:377:ARG:NH1 | 2.58 | 0.67 |
| 18:5X:128:GLN:OE1 | 18:5X:128:GLN:N | 2.19 | 0.67 |
| 24:6X:606:ARG:O | 24:6X:610:ILE:HG13 | 1.95 | 0.67 |
| 24:6Y:95:VAL:H | 24:6Y:187:PHE:HE2 | 1.43 | 0.67 |
| 2:G3:282:TYR:CE1 | 22:6M:133:PRO:HG2 | 2.29 | 0.66 |
| 2:G3:371:VAL:HG12 | 2:G3:373:ARG:H | 1.59 | 0.66 |
| 2:J1:88:HIS:CG | 2:K7:283:HIS:HA | 2.30 | 0.66 |
| 2:K3:210:TYR:HE1 | 2:K3:227:LEU:HD11 | 1.61 | 0.66 |
| 2:K5:33:ASP:O | 2:K5:60:LYS:NZ | 2.27 | 0.66 |
| 1:K6:211:CYS:HA | 1:K6:215:LEU:HB2 | 1.77 | 0.66 |
| 2:M5:58:ALA:HB1 | 37:7Y:214:ASP:HB3 | 1.76 | 0.66 |
| 1:O4:391:ARG:HD3 | 2:O5:346:TRP:CE2 | 2.30 | 0.66 |
| 2:O7:27:GLU:OE1 | 2:O7:243:ARG:NH1 | 2.28 | 0.66 |
| 2:S5:287:SER:N | 2:S5:290:GLU:OE2 | 2.25 | 0.66 |
| 1:V8:282:ARG:NH2 | 1:V8:288:GLU:OE2 | 2.25 | 0.66 |
| 2:V9:267:PHE:HB2 | 2:V9:384:ILE:HD12 | 1.75 | 0.66 |
| 1:W0:334:GLN:HE22 | 1:W0:348:ASN:H | 1.41 | 0.66 |
| 2:W5:255:PHE:HA | 2:W5:259:LEU:HD13 | 1.76 | 0.66 |
| 2:W7:223:THR:OG1 | 1:W8:245:GLN:NE2 | 2.25 | 0.66 |
| 1:X2:273:LEU:H | 1:X2:292:GLN:HE22 | 1.43 | 0.66 |
| 2:X7:203:MET:HE1 | 2:X7:387:ILE:HD13 | 1.76 | 0.66 |
| 2:Z5:114:ILE:HG21 | 2:Z5:149:LEU:HD22 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:56:THR:HA | 2:0N:285:GLN:HG2 | 1.76 | 0.66 |
| 2:0V:217:LEU:HB3 | 2:0V:219:ILE:HG12 | 1.77 | 0.66 |
| 2:0X:108:TYR:O | 2:0X:112:LYS:NZ | 2.21 | 0.66 |
| 1:1A:204:ASN:HD21 | 39:1A:503:GDP:HN22 | 1.42 | 0.66 |
| 2:1L:121:ARG:HD2 | 2:1L:121:ARG:C | 2.15 | 0.66 |
| 2:1T:33:ASP:O | 2:1T:60:LYS:NZ | 2.27 | 0.66 |
| 1:3C:45:GLU:HG3 | 1:3C:46:ARG:HG2 | 1.76 | 0.66 |
| 4:3W:35:LYS:NZ | 3:3X:254:LYS:O | 2.24 | 0.66 |
| 18:5Y:31:ASP:N | 18:5Y:31:ASP:OD2 | 2.27 | 0.66 |
| 18:6A:31:ASP:N | 18:6A:31:ASP:OD2 | 2.27 | 0.66 |
| 18:6D:31:ASP:N | 18:6D:31:ASP:OD2 | 2.27 | 0.66 |
| 24:6T:525:VAL:HB | 24:6T:530:PHE:HE2 | 1.60 | 0.66 |
| 30:7K:56:ARG:HG3 | 30:7K:58:SER:H | 1.60 | 0.66 |
| 1:A3:44:LEU:HD21 | 18:6C:84:ARG:HH22 | 1.60 | 0.66 |
| 2:B7:145:THR:OG1 | 41:B7:501:GTP:O1B | 2.12 | 0.66 |
| 2:D7:285:GLN:HE21 | 24:6Z:253:PRO:HG2 | 1.58 | 0.66 |
| 2:F5:55:GLU:O | 2:H1:285:GLN:NE2 | 2.28 | 0.66 |
| 2:G3:176:GLN:HE22 | 2:G3:304:LYS:HE2 | 1.60 | 0.66 |
| 2:G5:9:ILE:HG21 | 2:G5:153:LEU:HD21 | 1.76 | 0.66 |
| 2:L9:413:MET:HB3 | 2:L9:417:GLU:OE2 | 1.95 | 0.66 |
| 1:M6:7:ILE:HB | 1:M6:135:VAL:HG12 | 1.77 | 0.66 |
| 2:O3:32:PRO:HG3 | 19:6E:94:PRO:HD2 | 1.76 | 0.66 |
| 2:O9:26:LEU:HD21 | 2:O9:363:VAL:HG12 | 1.75 | 0.66 |
| 1:R2:173:PRO:HD2 | 1:R2:380:ARG:CZ | 2.24 | 0.66 |
| 1:S2:173:PRO:HB3 | 1:S2:384:GLN:HE22 | 1.60 | 0.66 |
| 1:S2:190:HIS:CD2 | 1:S2:414:ASN:HD22 | 2.12 | 0.66 |
| 2:S9:176:GLN:HE21 | 13:5I:90:PRO:HG3 | 1.59 | 0.66 |
| 1:T4:390:ARG:HB3 | 1:T4:390:ARG:CZ | 2.23 | 0.66 |
| 1:U4:190:HIS:CD2 | 1:U4:411:ALA:HA | 2.30 | 0.66 |
| 2:U9:100:ALA:CA | 1:V0:252:LYS:HG2 | 2.24 | 0.66 |
| 1:W6:207:LEU:HB3 | 1:W6:225:LEU:HD22 | 1.76 | 0.66 |
| 1:Z2:139:LEU:HD12 | 1:Z2:170:VAL:HG22 | 1.76 | 0.66 |
| 1:Z2:190:HIS:HD2 | 1:Z2:414:ASN:HB2 | 1.60 | 0.66 |
| 1:Z6:125:GLU:OE2 | 1:Z6:159:TYR:OH | 2.12 | 0.66 |
| 2:0B:278:ALA:HA | 2:0B:369:ALA:HB2 | 1.77 | 0.66 |
| 2:0Z:58:ALA:CA | 9:4Z:165:ARG:CZ | 2.69 | 0.66 |
| 1:1G:95:THR:OG1 | 1:1G:108:GLU:OE2 | 2.13 | 0.66 |
| 2:1Z:248:LEU:HD22 | 2:1Z:354:GLY:HA2 | 1.78 | 0.66 |
| 1:2G:311:LEU:HD23 | 1:2G:312:THR:HG23 | 1.77 | 0.66 |
| 1:3S:211:CYS:SG | 1:3S:220:PRO:HB3 | 2.35 | 0.66 |
| 18:5Z:31:ASP:N | 18:5Z:31:ASP:OD2 | 2.27 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:6B:31:ASP:N | 18:6B:31:ASP:OD2 | 2.27 | 0.66 |
| 18:6C:31:ASP:N | 18:6C:31:ASP:OD2 | 2.27 | 0.66 |
| 24:6W:97:ARG:H | 24:6W:188:THR:HG21 | 1.59 | 0.66 |
| 24:6Z:525:VAL:HB | 24:6Z:530:PHE:HE2 | 1.60 | 0.66 |
| 1:9:320:ARG:NH2 | 26:7E:111:ASP:OD2 | 2.28 | 0.66 |
| 1:B5:362:LYS:HE3 | 24:6X:108:GLU:HG3 | 1.77 | 0.66 |
| 2:E5:282:TYR:HH | 22:6K:81:ASN:HA | 1.60 | 0.66 |
| 2:I7:317:LEU:HB3 | 2:I7:319:TYR:HE1 | 1.60 | 0.66 |
| 1:L0:207:LEU:HB3 | 1:L0:225:LEU:HD22 | 1.76 | 0.66 |
| 2:N5:88:HIS:CE1 | 2:N5:90:GLU:CG | 2.78 | 0.66 |
| 2:P3:88:HIS:CG | 2:Q9:283:HIS:HB2 | 2.30 | 0.66 |
| 2:Q1:278:ALA:HA | 2:Q1:369:ALA:HB2 | 1.77 | 0.66 |
| 1:Q6:224:ASP:OD1 | 1:Q6:225:LEU:N | 2.28 | 0.66 |
| 1:S0:52:ASN:OD1 | 1:S0:62:ARG:NH2 | 2.28 | 0.66 |
| 1:S6:213:ARG:HH22 | 13:5H:117:ASN:ND2 | 1.92 | 0.66 |
| 2:S9:104:ALA:HB2 | 2:S9:413:MET:HG3 | 1.78 | 0.66 |
| 1:U2:248:ALA:HA | 1:U2:252:LYS:HD2 | 1.75 | 0.66 |
| 2:W7:224:TYR:HB2 | 1:W8:245:GLN:HE21 | 1.59 | 0.66 |
| 1:X6:250:LEU:HA | 1:X6:253:LEU:HD12 | 1.76 | 0.66 |
| 2:Y1:339:ARG:O | 2:Y1:342:GLN:NE2 | 2.23 | 0.66 |
| 1:Y8:33:THR:O | 1:Y8:58:ARG:NH2 | 2.29 | 0.66 |
| 2:Z1:202:VAL:HG22 | 2:Z1:268:MET:HB2 | 1.77 | 0.66 |
| 2:Z3:338:LYS:HG3 | 2:Z3:340:THR:HG22 | 1.77 | 0.66 |
| 1:Z4:2:ARG:HB3 | 1:Z4:131:GLN:HB2 | 1.77 | 0.66 |
| 2:Z7:7:ILE:HB | 2:Z7:137:VAL:HG12 | 1.77 | 0.66 |
| 1:0A:139:LEU:HD12 | 1:0A:170:VAL:HG12 | 1.78 | 0.66 |
| 2:0N:88:HIS:HB3 | 2:1D:283:HIS:ND1 | 2.10 | 0.66 |
| 2:0R:108:TYR:O | 2:0R:112:LYS:NZ | 2.28 | 0.66 |
| 1:0W:55:THR:HG23 | 1:1M:282:ARG:O | 1.94 | 0.66 |
| 2:1F:169:PHE:CE1 | 2:1F:235:ILE:HD11 | 2.30 | 0.66 |
| 1:2A:125:GLU:O | 38:7Z:3:ASN:ND2 | 2.26 | 0.66 |
| 2:2B:26:LEU:HD21 | 10:5A:325:THR:HG23 | 1.78 | 0.66 |
| 2:2B:27:GLU:OE2 | 2:2B:243:ARG:NH1 | 2.28 | 0.66 |
| 1:2E:95:THR:HB | 38:8B:83:ARG:NH1 | 2.10 | 0.66 |
| 2:2J:360:PRO:O | 2:2J:370:LYS:NZ | 2.27 | 0.66 |
| 1:3S:282:ARG:HH21 | 1:3S:288:GLU:HG2 | 1.60 | 0.66 |
| 3:3Z:38:THR:HA | 3:3Z:126:GLU:OE2 | 1.95 | 0.66 |
| 3:4D:38:THR:HA | 3:4D:126:GLU:OE2 | 1.95 | 0.66 |
| 5:4M:293:LEU:HD12 | 28:7X:305:ALA:HB3 | 1.75 | 0.66 |
| 7:4T:234:GLU:HG3 | 31:7M:15:LEU:HD21 | 1.78 | 0.66 |
| 14:5M:365:ARG:CZ | 14:5M:377:ARG:HH11 | 2.08 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:11:LEU:HB3 | 24:6U:12:PRO:HD2 | 1.76 | 0.66 |
| 24:6X:97:ARG:H | 24:6X:188:THR:HG21 | 1.58 | 0.66 |
| 31:7N:75:PRO:HB2 | 31:7N:78:HIS:CD2 | 2.30 | 0.66 |
| 2:8:30:ILE:N | 26:7E:45:MET:HE1 | 2.10 | 0.66 |
| 2:C5:285:GLN:HE21 | 24:6T:253:PRO:HG2 | 1.58 | 0.66 |
| 2:J9:392:ASP:OD2 | 2:J9:422:ARG:NH1 | 2.28 | 0.66 |
| 1:M8:48:ASN:HD22 | 19:6E:21:ILE:HB | 1.59 | 0.66 |
| 1:O4:263:LEU:HD13 | 1:O4:422:TYR:HE1 | 1.60 | 0.66 |
| 2:P7:9:ILE:HG22 | 2:P7:68:LEU:HD11 | 1.78 | 0.66 |
| 1:Q0:273:LEU:H | 1:Q0:292:GLN:HE22 | 1.42 | 0.66 |
| 2:S1:287:SER:N | 2:S1:290:GLU:OE2 | 2.28 | 0.66 |
| 1:U4:334:GLN:HE22 | 1:U4:348:ASN:H | 1.44 | 0.66 |
| 1:X0:52:ASN:OD1 | 1:X0:62:ARG:NH2 | 2.29 | 0.66 |
| 1:Y0:358:PRO:HG2 | 1:Y0:361:LEU:HB2 | 1.77 | 0.66 |
| 2:Y1:211:ASP:OD1 | 2:Y1:214:ARG:NH2 | 2.28 | 0.66 |
| 2:Y5:406:HIS:HA | 2:Y5:409:VAL:HG12 | 1.78 | 0.66 |
| 1:Z2:165:LEU:HD11 | 1:Z2:200:MET:HE3 | 1.78 | 0.66 |
| 1:Z6:311:LEU:HD23 | 1:Z6:312:THR:HG23 | 1.78 | 0.66 |
| 1:0U:180:VAL:HG23 | 1:0U:184:ASN:HD21 | 1.60 | 0.66 |
| 1:1A:33:THR:O | 1:1A:58:ARG:NH2 | 2.28 | 0.66 |
| 1:1E:211:CYS:HA | 1:1E:215:LEU:HB2 | 1.78 | 0.66 |
| 1:1O:373:ALA:O | 1:1O:376:GLU:HG2 | 1.95 | 0.66 |
| 1:1W:140:GLY:O | 1:1W:184:ASN:ND2 | 2.28 | 0.66 |
| 2:2F:27:GLU:OE1 | 2:2F:243:ARG:NH1 | 2.28 | 0.66 |
| 1:3I:309:ARG:NH1 | 1:3I:339:SER:O | 2.29 | 0.66 |
| 3:3V:38:THR:HA | 3:3V:126:GLU:OE2 | 1.95 | 0.66 |
| 3:3X:28:ASN:ND2 | 3:3X:115:ASN:OD1 | 2.28 | 0.66 |
| 3:3Z:28:ASN:ND2 | 3:3Z:115:ASN:OD1 | 2.28 | 0.66 |
| 3:4B:28:ASN:ND2 | 3:4B:115:ASN:OD1 | 2.28 | 0.66 |
| 3:4D:28:ASN:ND2 | 3:4D:115:ASN:OD1 | 2.28 | 0.66 |
| 3:4D:200:ILE:O | 3:4D:204:THR:OG1 | 2.14 | 0.66 |
| 3:4F:28:ASN:ND2 | 3:4F:115:ASN:OD1 | 2.28 | 0.66 |
| 3:4H:200:ILE:O | 3:4H:204:THR:OG1 | 2.14 | 0.66 |
| 5:4M:293:LEU:HD12 | 28:7X:305:ALA:HB1 | 1.77 | 0.66 |
| 15:5O:169:ILE:HD11 | 15:5O:208:SER:O | 1.95 | 0.66 |
| 15:5O:364:ASP:OD1 | 25:7C:80:ARG:NH1 | 2.28 | 0.66 |
| 15:5O:371:TYR:HD1 | 15:5O:375:ILE:HD12 | 1.59 | 0.66 |
| 38:8A:87:LYS:HD2 | 38:8A:87:LYS:C | 2.16 | 0.66 |
| 1:A9:358:PRO:O | 18:5X:22:ARG:NH2 | 2.29 | 0.66 |
| 2:E7:81:GLY:HA3 | 22:6M:116:TYR:HE2 | 1.61 | 0.66 |
| 2:H3:90:GLU:CB | 2:H3:121:ARG:HH12 | 2.09 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H9:5:ILE:HG22 | 2:H9:64:ARG:HB3 | 1.77 | 0.66 |
| 2:J5:286:LEU:O | 2:J5:373:ARG:NH1 | 2.27 | 0.66 |
| 1:K0:58:ARG:HG2 | 1:L6:280:GLN:HE22 | 1.61 | 0.66 |
| 2:L1:90:GLU:HB3 | 2:L1:121:ARG:HH12 | 1.60 | 0.66 |
| 1:M2:78:SER:HA | 15:5O:48:LYS:HG3 | 1.78 | 0.66 |
| 1:M6:125:GLU:HG2 | 37:7Y:93:LYS:HG3 | 1.78 | 0.66 |
| 2:N9:69:ASP:OD1 | 2:N9:70:LEU:N | 2.29 | 0.66 |
| 1:P6:301:CYS:SG | 1:P6:302:ALA:N | 2.68 | 0.66 |
| 1:Q8:172:SER:OG | 1:Q8:380:ARG:NH2 | 2.29 | 0.66 |
| 1:R6:2:ARG:HB3 | 1:R6:131:GLN:HB2 | 1.76 | 0.66 |
| 1:S4:311:LEU:HD13 | 1:S4:342:VAL:HG21 | 1.77 | 0.66 |
| 1:T2:190:HIS:CD2 | 1:T2:411:ALA:HA | 2.31 | 0.66 |
| 1:T6:92:PHE:CE1 | 24:7A:35:TYR:CE1 | 2.84 | 0.66 |
| 1:U4:248:ALA:HA | 1:U4:252:LYS:HD2 | 1.76 | 0.66 |
| 2:U5:132:LEU:HD22 | 2:U5:164:LYS:HD3 | 1.75 | 0.66 |
| 2:W1:336:LYS:O | 2:W1:339:ARG:NH2 | 2.28 | 0.66 |
| 1:Y4:244:GLY:HA2 | 1:Y4:355:ASP:HB2 | 1.78 | 0.66 |
| 2:Y9:100:ALA:HA | 1:Z0:252:LYS:HE2 | 1.78 | 0.66 |
| 1:Z0:207:LEU:HD13 | 1:Z0:225:LEU:HB3 | 1.76 | 0.66 |
| 1:Z8:215:LEU:HD21 | 1:Z8:273:LEU:HD12 | 1.76 | 0.66 |
| 2:0N:344:VAL:HG13 | 2:0N:347:CYS:HB3 | 1.76 | 0.66 |
| 1:0W:207:LEU:HD11 | 1:0W:229:ILE:HD11 | 1.78 | 0.66 |
| 1:2E:68:LEU:HB3 | 1:2E:96:GLY:HA2 | 1.76 | 0.66 |
| 1:2E:113:ILE:HG12 | 1:2E:150:LEU:HD22 | 1.77 | 0.66 |
| 1:3M:7:ILE:HB | 1:3M:135:VAL:HG12 | 1.77 | 0.66 |
| 1:3S:205:GLU:HA | 1:3S:205:GLU:OE1 | 1.96 | 0.66 |
| 1:3S:377:MET:HA | 1:3S:380:ARG:HD2 | 1.78 | 0.66 |
| 3:3V:28:ASN:ND2 | 3:3V:115:ASN:OD1 | 2.28 | 0.66 |
| 3:3V:46:ALA:HB1 | 3:3V:115:ASN:HB3 | 1.76 | 0.66 |
| 3:3V:200:ILE:O | 3:3V:204:THR:OG1 | 2.14 | 0.66 |
| 3:3X:38:THR:HA | 3:3X:126:GLU:OE2 | 1.95 | 0.66 |
| 3:3Z:200:ILE:O | 3:3Z:204:THR:OG1 | 2.14 | 0.66 |
| 3:4B:38:THR:HA | 3:4B:126:GLU:OE2 | 1.95 | 0.66 |
| 3:4F:38:THR:HA | 3:4F:126:GLU:OE2 | 1.95 | 0.66 |
| 3:4H:28:ASN:ND2 | 3:4H:115:ASN:OD1 | 2.28 | 0.66 |
| 3:4H:38:THR:HA | 3:4H:126:GLU:OE2 | 1.96 | 0.66 |
| 10:5B:257:GLN:HG3 | 10:5B:261:LYS:NZ | 2.10 | 0.66 |
| 14:5N:127:ASN:HB2 | 38:8D:227:LYS:NZ | 2.10 | 0.66 |
| 17:5V:224:ARG:HB3 | 17:5V:224:ARG:HH21 | 1.59 | 0.66 |
| 18:6A:5:VAL:O | 18:6A:5:VAL:HG12 | 1.96 | 0.66 |
| 18:6D:128:GLN:OE1 | 18:6D:128:GLN:N | 2.19 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6P:135:ARG:O | 24:6Z:436:HIS:NE2 | 2.28 | 0.66 |
| 24:6V:606:ARG:O | 24:6V:610:ILE:HG13 | 1.95 | 0.66 |
| 27:7G:221:PRO:HG2 | 27:7G:224:GLU:HG3 | 1.77 | 0.66 |
| 34:7S:245:ARG:HA | 34:7S:248:LYS:HE3 | 1.78 | 0.66 |
| 2:4:357:TYR:HB3 | 24:6U:150:ARG:HH12 | 1.60 | 0.66 |
| 1:7:337:ASN:HD21 | 3:4B:69:TYR:H | 1.44 | 0.66 |
| 1:A3:285:THR:HG22 | 26:7F:74:VAL:HG11 | 1.75 | 0.66 |
| 1:D8:45:GLU:OE1 | 22:6P:20:TYR:OH | 2.11 | 0.66 |
| 1:G2:67:ASP:OD2 | 1:G2:72:THR:OG1 | 2.08 | 0.66 |
| 1:G6:220:PRO:HD2 | 2:G7:326:LYS:HG2 | 1.77 | 0.66 |
| 2:H1:399:TYR:O | 2:H1:402:ARG:NH1 | 2.29 | 0.66 |
| 2:H9:317:LEU:HD11 | 2:H9:351:PHE:HD2 | 1.60 | 0.66 |
| 2:I7:56:THR:HA | 2:K3:285:GLN:HB2 | 1.78 | 0.66 |
| 2:I9:90:GLU:HB3 | 2:I9:121:ARG:HH22 | 1.61 | 0.66 |
| 1:L4:44:LEU:HD21 | 29:7J:339:GLN:OE1 | 1.95 | 0.66 |
| 1:L6:139:LEU:HD12 | 1:L6:170:VAL:HG12 | 1.77 | 0.66 |
| 2:L9:287:SER:N | 2:L9:290:GLU:OE2 | 2.23 | 0.66 |
| 2:M3:233:GLN:NE2 | 2:M3:361:THR:O | 2.29 | 0.66 |
| 2:N5:388:PHE:HB3 | 2:N5:425:LEU:HD11 | 1.76 | 0.66 |
| 2:O3:313:MET:SD | 2:O3:346:TRP:CZ3 | 2.89 | 0.66 |
| 1:T2:174:LYS:HD3 | 13:5J:14:PHE:CD2 | 2.31 | 0.66 |
| 2:T3:222:PRO:HD2 | 1:T4:324:LYS:HD3 | 1.77 | 0.66 |
| 1:T6:77:ARG:NH2 | 24:7A:46:ALA:HB1 | 2.09 | 0.66 |
| 1:U6:273:LEU:H | 1:U6:292:GLN:HE22 | 1.43 | 0.66 |
| 2:U7:213:CYS:HA | 2:U7:217:LEU:HB2 | 1.78 | 0.66 |
| 2:U9:132:LEU:HD22 | 2:U9:164:LYS:HD3 | 1.76 | 0.66 |
| 2:V1:90:GLU:HG3 | 2:V1:121:ARG:HH11 | 1.60 | 0.66 |
| 1:X4:113:ILE:HA | 1:X4:116:VAL:HG12 | 1.75 | 0.66 |
| 2:X9:88:HIS:HB3 | 2:Z5:283:HIS:CE1 | 2.31 | 0.66 |
| 2:Z5:336:LYS:O | 2:Z5:339:ARG:NH2 | 2.29 | 0.66 |
| 1:0K:183:TYR:OH | 1:0K:388:MET:HB3 | 1.95 | 0.66 |
| 2:0L:206:ASN:OD1 | 41:0M:501:GTP:N2 | 2.28 | 0.66 |
| 1:0W:397:TRP:HE1 | 2:0X:260:VAL:HG23 | 1.60 | 0.66 |
| 2:1B:278:ALA:HA | 2:1B:369:ALA:HB2 | 1.78 | 0.66 |
| 1:1O:213:ARG:HE | 1:1O:297:LYS:HZ2 | 1.43 | 0.66 |
| 2:1Z:223:THR:HG23 | 2:1Z:225:THR:HG22 | 1.76 | 0.66 |
| 2:3B:33:ASP:O | 2:3B:60:LYS:NZ | 2.29 | 0.66 |
| 1:3C:113:ILE:HA | 1:3C:116:VAL:HG12 | 1.77 | 0.66 |
| 2:3F:221:ARG:NH1 | 38:8A:176:THR:OG1 | 2.28 | 0.66 |
| 2:3J:88:HIS:HB2 | 2:3J:91:GLN:NE2 | 2.09 | 0.66 |
| 3:3X:200:ILE:O | 3:3X:204:THR:OG1 | 2.14 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4B:200:ILE:O | 3:4B:204:THR:OG1 | 2.14 | 0.66 |
| 3:4F:200:ILE:O | 3:4F:204:THR:OG1 | 2.14 | 0.66 |
| 7:4Q:306:ILE:HD11 | 24:6T:8:ILE:HA | 1.78 | 0.66 |
| 14:5L:210:TYR:CE1 | 14:5L:220:GLN:HB2 | 2.31 | 0.66 |
| 14:5L:341:ASP:OD1 | 14:5L:342:LYS:N | 2.27 | 0.66 |
| 14:5N:341:ASP:OD1 | 14:5N:342:LYS:N | 2.27 | 0.66 |
| 15:5O:99:LYS:NZ | 15:5O:203:ASN:ND2 | 2.40 | 0.66 |
| 24:6Z:416:ILE:HD12 | 24:6Z:416:ILE:H | 1.60 | 0.66 |
| 25:7C:83:ARG:NH2 | 25:7C:86:GLU:OE2 | 2.28 | 0.66 |
| 29:7J:319:ILE:HG23 | 29:7J:320:PRO:HD2 | 1.72 | 0.66 |
| 1:E6:33:THR:HG23 | 24:6W:405:ALA:HB2 | 1.77 | 0.66 |
| 2:F3:282:TYR:OH | 22:6O:81:ASN:HA | 1.95 | 0.66 |
| 2:G1:206:ASN:OD1 | 41:G1:501:GTP:N2 | 2.28 | 0.66 |
| 1:H8:139:LEU:HD12 | 1:H8:170:VAL:HG12 | 1.76 | 0.66 |
| 1:M4:12:CYS:SG | 1:M4:138:SER:HB3 | 2.35 | 0.66 |
| 1:M6:362:LYS:HB2 | 30:7K:101:TYR:CE2 | 2.30 | 0.66 |
| 2:O3:377:MET:SD | 2:O3:379:SER:HB2 | 2.36 | 0.66 |
| 1:O6:135:VAL:HG11 | 1:O6:152:ILE:HD11 | 1.77 | 0.66 |
| 2:T3:88:HIS:ND1 | 2:T3:89:PRO:HD2 | 2.10 | 0.66 |
| 2:U9:88:HIS:CE1 | 2:U9:89:PRO:HD2 | 2.31 | 0.66 |
| 2:U9:264:ARG:NH2 | 2:U9:431:ASP:OD2 | 2.29 | 0.66 |
| 2:Y5:157:LEU:C | 2:Y5:157:LEU:HD12 | 2.16 | 0.66 |
| 1:2M:52:ASN:OD1 | 1:2M:62:ARG:NH2 | 2.28 | 0.66 |
| 1:2Q:306:ARG:NH1 | 38:8A:94:LYS:O | 2.29 | 0.66 |
| 2:2T:287:SER:N | 2:2T:290:GLU:OE2 | 2.28 | 0.66 |
| 1:2Y:296:ALA:O | 38:8C:105:ARG:NH2 | 2.21 | 0.66 |
| 2:3L:280:LYS:HA | 2:3L:283:HIS:HB3 | 1.78 | 0.66 |
| 9:4Z:398:ASP:HA | 9:4Z:401:ILE:HD12 | 1.75 | 0.66 |
| 14:5M:341:ASP:OD1 | 14:5M:342:LYS:N | 2.27 | 0.66 |
| 14:5M:392:THR:HG21 | 14:5M:435:ALA:HA | 1.77 | 0.66 |
| 14:5N:392:THR:HG21 | 14:5N:435:ALA:HA | 1.77 | 0.66 |
| 14:5N:558:ALA:HB1 | 14:5N:601:VAL:HG12 | 1.77 | 0.66 |
| 24:6T:469:PHE:CE2 | 24:6T:482:ILE:HG23 | 2.31 | 0.66 |
| 2:A2:396:ASP:OD2 | 4:4G:53:ASN:ND2 | 2.28 | 0.66 |
| 2:I9:222:PRO:HD2 | 1:J0:324:LYS:HE3 | 1.78 | 0.66 |
| 1:L4:125:GLU:OE2 | 1:L4:159:TYR:OH | 2.14 | 0.66 |
| 2:N9:240:ALA:HB1 | 2:N9:356:ASN:HD22 | 1.58 | 0.66 |
| 2:O1:287:SER:N | 2:O1:290:GLU:OE2 | 2.26 | 0.66 |
| 1:T4:387:ALA:HA | 1:T4:390:ARG:HH12 | 1.61 | 0.66 |
| 1:W8:26:ASP:O | 1:W8:359:LYS:NZ | 2.27 | 0.66 |
| 2:X3:406:HIS:HA | 2:X3:409:VAL:HG22 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y3:287:SER:N | 2:Y3:290:GLU:OE2 | 2.29 | 0.66 |
| 1:Z2:179:VAL:HG22 | 2:Z3:258:ASN:HD22 | 1.61 | 0.66 |
| 1:Z2:311:LEU:HD23 | 1:Z2:312:THR:HG23 | 1.76 | 0.66 |
| 2:0B:392:ASP:OD2 | 2:0B:422:ARG:NH1 | 2.28 | 0.66 |
| 1:0G:3:GLU:HB2 | 1:0G:130:LEU:HA | 1.78 | 0.66 |
| 1:0K:3:GLU:HB2 | 1:0K:130:LEU:HA | 1.78 | 0.66 |
| 1:0S:45:GLU:HG3 | 1:0S:46:ARG:HG2 | 1.76 | 0.66 |
| 2:1V:145:THR:OG1 | 41:1W:501:GTP:O1B | 2.14 | 0.66 |
| 2:3J:289:ALA:O | 2:3J:293:ASN:ND2 | 2.28 | 0.66 |
| 2:3R:70:LEU:HB2 | 2:3R:98:ASP:HA | 1.77 | 0.66 |
| 2:3T:406:HIS:HA | 2:3T:409:VAL:HG12 | 1.78 | 0.66 |
| 14:5L:392:THR:HG21 | 14:5L:435:ALA:HA | 1.77 | 0.66 |
| 15:5O:140:HIS:HB3 | 15:5O:146:VAL:HG21 | 1.77 | 0.66 |
| 15:5O:193:ARG:NH2 | 15:5O:205:CYS:O | 2.28 | 0.66 |
| 20:6F:166:PRO:HG2 | 20:6F:194:THR:HG21 | 1.78 | 0.66 |
| 30:7L:360:ALA:HA | 30:7L:363:VAL:HG22 | 1.78 | 0.66 |
| 2:D5:285:GLN:HE21 | 24:6Y:253:PRO:HG2 | 1.59 | 0.66 |
| 2:I5:264:ARG:NH2 | 2:I5:431:ASP:OD2 | 2.28 | 0.66 |
| 2:I9:47:ASP:OD1 | 28:7H:443:ARG:NH2 | 2.29 | 0.66 |
| 2:K7:309:HIS:HB3 | 35:7T:165:ARG:HH21 | 1.59 | 0.66 |
| 2:L5:236:SER:OG | 2:L5:243:ARG:NH2 | 2.29 | 0.66 |
| 1:N8:320:ARG:NH1 | 27:7G:130:THR:O | 2.29 | 0.66 |
| 2:O1:244:PHE:HB2 | 2:O1:356:ASN:HD21 | 1.59 | 0.66 |
| 1:S0:177:ASP:O | 2:S1:352:LYS:HA | 1.96 | 0.66 |
| 2:S1:56:THR:HG23 | 2:S1:60:LYS:HB3 | 1.77 | 0.66 |
| 1:S2:45:GLU:HG3 | 1:S2:46:ARG:HG2 | 1.77 | 0.66 |
| 1:T2:53:GLU:OE2 | 26:7E:71:PRO:O | 2.13 | 0.66 |
| 1:T6:94:GLN:HB3 | 24:7A:35:TYR:CE2 | 2.31 | 0.66 |
| 1:W0:220:PRO:HD2 | 2:W1:326:LYS:HD2 | 1.78 | 0.66 |
| 2:W9:9:ILE:HD13 | 2:W9:150:GLY:HA2 | 1.78 | 0.66 |
| 2:X9:301:MET:HE1 | 2:X9:307:PRO:HD3 | 1.78 | 0.66 |
| 1:Y2:375:GLN:HB2 | 1:Y2:419:VAL:HG23 | 1.78 | 0.66 |
| 1:Z2:135:VAL:HG21 | 1:Z2:152:ILE:HD11 | 1.77 | 0.66 |
| 1:Z2:392:LYS:HB3 | 1:Z2:395:LEU:HD12 | 1.77 | 0.66 |
| 1:0A:58:ARG:HD3 | 1:0Q:280:GLN:HE22 | 1.61 | 0.66 |
| 1:0A:413:SER:HA | 1:0A:416:ASN:HD22 | 1.61 | 0.66 |
| 2:0H:322:ASP:HB2 | 2:0H:373:ARG:HH21 | 1.60 | 0.66 |
| 2:0Z:336:LYS:O | 2:0Z:339:ARG:NH2 | 2.28 | 0.66 |
| 2:1H:49:PHE:HB2 | 2:1H:53:PHE:HD2 | 1.61 | 0.66 |
| 1:1O:248:ALA:CB | 1:1O:252:LYS:HD3 | 2.24 | 0.66 |
| 1:1U:113:ILE:HA | 1:1U:116:VAL:HG22 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1X:392:ASP:OD2 | 2:1X:422:ARG:NH1 | 2.29 | 0.66 |
| 2:2F:244:PHE:HB2 | 2:2F:356:ASN:HD21 | 1.59 | 0.66 |
| 2:2T:417:GLU:HA | 2:2T:420:GLU:HG2 | 1.78 | 0.66 |
| 1:2U:45:GLU:HG3 | 1:2U:46:ARG:HG2 | 1.75 | 0.66 |
| 2:3L:51:THR:HG21 | 2:3L:243:ARG:HG2 | 1.77 | 0.66 |
| 5:4M:75:ARG:NH1 | 15:5P:363:GLU:OE2 | 2.29 | 0.66 |
| 15:5P:14:LEU:H | 15:5P:14:LEU:CD2 | 2.08 | 0.66 |
| 15:5P:34:GLU:OE2 | 15:5P:49:ARG:NE | 2.29 | 0.66 |
| 18:5Y:128:GLN:OE1 | 18:5Y:128:GLN:N | 2.19 | 0.66 |
| 22:6J:265:ASP:OD1 | 22:6J:266:LYS:N | 2.29 | 0.66 |
| 22:6O:271:ARG:HH12 | 22:6O:275:LEU:HG | 1.60 | 0.66 |
| 24:6T:470:ILE:CD1 | 24:6T:485:PRO:HG3 | 2.25 | 0.66 |
| 24:6X:315:ARG:HH11 | 24:6X:315:ARG:CG | 2.06 | 0.66 |
| 2:A2:29:GLY:HA2 | 26:7F:45:MET:CE | 2.24 | 0.66 |
| 2:F7:56:THR:HA | 2:H3:285:GLN:HB2 | 1.76 | 0.66 |
| 1:F8:279:GLN:HE21 | 24:6U:411:ASN:HB2 | 1.59 | 0.66 |
| 1:G6:211:CYS:HA | 1:G6:215:LEU:HB2 | 1.76 | 0.66 |
| 2:I3:88:HIS:CG | 2:J9:283:HIS:HB3 | 2.30 | 0.66 |
| 1:I4:26:ASP:O | 1:I4:359:LYS:NZ | 2.23 | 0.66 |
| 2:J1:88:HIS:HB3 | 2:K7:283:HIS:ND1 | 2.11 | 0.66 |
| 2:L1:250:VAL:HG23 | 2:L1:254:GLU:HG3 | 1.77 | 0.66 |
| 2:M9:46:ASP:OD1 | 2:M9:46:ASP:N | 2.29 | 0.66 |
| 1:O8:113:ILE:HA | 1:O8:116:VAL:HG12 | 1.78 | 0.66 |
| 1:Q0:67:ASP:OD2 | 1:Q0:72:THR:OG1 | 2.12 | 0.66 |
| 2:Q5:287:SER:N | 2:Q5:290:GLU:OE2 | 2.29 | 0.66 |
| 2:T1:264:ARG:NH1 | 2:T1:431:ASP:OD2 | 2.29 | 0.66 |
| 1:T6:45:GLU:HG3 | 1:T6:46:ARG:HG2 | 1.78 | 0.66 |
| 2:V7:286:LEU:O | 2:V7:373:ARG:NH1 | 2.29 | 0.66 |
| 2:W7:413:MET:HB3 | 2:W7:417:GLU:OE2 | 1.96 | 0.66 |
| 2:Y5:211:ASP:OD1 | 2:Y5:214:ARG:NH2 | 2.28 | 0.66 |
| 1:Z8:131:GLN:HG2 | 1:Z8:250:LEU:HD13 | 1.77 | 0.66 |
| 1:0I:311:LEU:HD23 | 1:0I:312:THR:HG23 | 1.77 | 0.66 |
| 1:1E:139:LEU:HD12 | 1:1E:170:VAL:HG22 | 1.77 | 0.66 |
| 1:2A:165:LEU:HD11 | 1:2A:250:LEU:HD13 | 1.78 | 0.66 |
| 1:2U:320:ARG:NH2 | 38:8B:198:THR:HA | 2.10 | 0.66 |
| 1:3K:178:THR:HB | 1:3K:181:GLU:HG3 | 1.76 | 0.66 |
| 2:3L:84:ARG:HE | 23:6R:15:ARG:HH22 | 1.43 | 0.66 |
| 2:3R:313:MET:HB2 | 2:3R:380:ASN:HB3 | 1.78 | 0.66 |
| 15:5O:9:PHE:HA | 15:5O:78:TYR:HA | 1.77 | 0.66 |
| 15:5O:289:LEU:C | 15:5O:289:LEU:HD23 | 2.16 | 0.66 |
| 18:6A:128:GLN:OE1 | 18:6A:128:GLN:N | 2.19 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6P:307:ARG:HH21 | 22:6P:326:PHE:HB2 | 1.60 | 0.66 |
| 26:7F:63:LEU:H | 26:7F:63:LEU:CD2 | 2.09 | 0.66 |
| 36:7V:94:LEU:O | 36:7V:98:VAL:HG12 | 1.95 | 0.66 |
| 1:F8:32:PRO:HD2 | 24:6U:527:ASN:HD22 | 1.60 | 0.65 |
| 2:G1:264:ARG:NH2 | 2:G1:431:ASP:OD2 | 2.28 | 0.65 |
| 1:I0:219:THR:CG2 | 24:6X:488:ARG:HD2 | 2.26 | 0.65 |
| 1:I0:220:PRO:HD2 | 2:I1:326:LYS:HD3 | 1.77 | 0.65 |
| 1:I8:45:GLU:HG3 | 1:I8:46:ARG:HG2 | 1.78 | 0.65 |
| 2:K1:288:VAL:HG11 | 2:K1:327:ASP:HB2 | 1.77 | 0.65 |
| 2:K5:90:GLU:HB3 | 2:K5:121:ARG:HH22 | 1.61 | 0.65 |
| 2:M3:370:LYS:HB2 | 30:7K:212:ARG:HD2 | 1.78 | 0.65 |
| 2:M7:76:ASP:OD2 | 1:M8:46:ARG:NH2 | 2.29 | 0.65 |
| 2:O5:88:HIS:ND1 | 2:O5:89:PRO:HD2 | 2.11 | 0.65 |
| 2:R7:223:THR:OG1 | 1:R8:245:GLN:NE2 | 2.29 | 0.65 |
| 2:R7:286:LEU:O | 2:R7:373:ARG:NH1 | 2.29 | 0.65 |
| 1:T8:287:PRO:HB3 | 13:5K:100:MET:SD | 2.36 | 0.65 |
| 2:X3:335:ILE:HA | 2:X3:338:LYS:HG2 | 1.78 | 0.65 |
| 2:Z9:399:TYR:O | 2:Z9:402:ARG:NH1 | 2.29 | 0.65 |
| 2:0B:399:TYR:O | 2:0B:402:ARG:NH1 | 2.30 | 0.65 |
| 1:0G:272:PRO:HB2 | 1:0G:282:ARG:HH12 | 1.60 | 0.65 |
| 2:0R:324:VAL:HG12 | 2:0R:326:LYS:H | 1.61 | 0.65 |
| 1:0U:232:VAL:HG11 | 1:0U:268:VAL:HG21 | 1.78 | 0.65 |
| 1:1Q:377:MET:SD | 1:1Q:380:ARG:NH2 | 2.69 | 0.65 |
| 2:2H:399:TYR:O | 2:2H:402:ARG:NH1 | 2.28 | 0.65 |
| 2:3N:296:PHE:HE2 | 2:3N:335:ILE:HD13 | 1.60 | 0.65 |
| 1:3S:6:HIS:HD2 | 1:3S:134:GLN:HG3 | 1.61 | 0.65 |
| 4:4I:52:GLN:NE2 | 3:4J:299:THR:OG1 | 2.28 | 0.65 |
| 14:5L:112:SER:N | 14:5L:155:PHE:HD2 | 1.93 | 0.65 |
| 18:5Z:128:GLN:OE1 | 18:5Z:128:GLN:N | 2.19 | 0.65 |
| 18:6B:128:GLN:OE1 | 18:6B:128:GLN:N | 2.19 | 0.65 |
| 18:6C:128:GLN:OE1 | 18:6C:128:GLN:N | 2.19 | 0.65 |
| 20:6F:285:THR:HA | 20:6F:288:TYR:CE2 | 2.31 | 0.65 |
| 24:6T:569:LYS:HB2 | 24:6T:572:ALA:HB3 | 1.78 | 0.65 |
| 1:3:194:GLU:OE2 | 3:3X:240:ARG:NH1 | 2.29 | 0.65 |
| 2:G7:387:ILE:HG12 | 2:G7:390:ARG:HH22 | 1.60 | 0.65 |
| 1:P8:165:LEU:HD11 | 1:P8:250:LEU:HD11 | 1.79 | 0.65 |
| 1:Q4:272:PRO:HB2 | 1:Q4:282:ARG:HH12 | 1.61 | 0.65 |
| 1:T6:73:MET:HA | 1:T6:76:VAL:HG12 | 1.79 | 0.65 |
| 1:V6:4:ILE:HG22 | 1:V6:49:VAL:HG22 | 1.78 | 0.65 |
| 1:W4:177:ASP:O | 2:W5:352:LYS:HA | 1.95 | 0.65 |
| 2:W5:76:ASP:OD2 | 1:W6:46:ARG:NH2 | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X0:6:HIS:HE2 | 1:X0:136:CYS:HG | 1.37 | 0.65 |
| 2:Y5:244:PHE:HB2 | 2:Y5:356:ASN:HD21 | 1.61 | 0.65 |
| 1:0E:287:PRO:HA | 1:0E:290:THR:HG22 | 1.77 | 0.65 |
| 2:0L:90:GLU:O | 2:0L:121:ARG:NH1 | 2.28 | 0.65 |
| 2:0R:157:LEU:HD22 | 2:0R:166:LYS:HD3 | 1.78 | 0.65 |
| 1:0S:52:ASN:OD1 | 1:0S:62:ARG:NH2 | 2.29 | 0.65 |
| 1:1A:248:ALA:HA | 1:1A:252:LYS:HD2 | 1.79 | 0.65 |
| 2:1T:101:ASN:OD1 | 1:1U:252:LYS:HE3 | 1.96 | 0.65 |
| 2:2Z:88:HIS:CE1 | 2:2Z:89:PRO:HD2 | 2.30 | 0.65 |
| 15:5O:121:SER:O | 15:5O:270:LEU:HD22 | 1.95 | 0.65 |
| 30:7K:108:ARG:CZ | 37:7Y:142:ARG:HD3 | 2.26 | 0.65 |
| 1:5:423:GLN:HB3 | 3:3Z:109:ALA:HB2 | 1.77 | 0.65 |
| 2:B2:223:THR:HG22 | 18:5Z:51:MET:HE3 | 1.77 | 0.65 |
| 1:F6:78:SER:HB3 | 24:6T:499:GLU:HB3 | 1.77 | 0.65 |
| 1:G8:190:HIS:CD2 | 1:G8:411:ALA:HA | 2.32 | 0.65 |
| 1:H2:11:GLN:N | 39:H2:503:GDP:O2B | 2.28 | 0.65 |
| 1:H8:211:CYS:HA | 1:H8:215:LEU:HB2 | 1.77 | 0.65 |
| 2:K5:287:SER:N | 2:K5:290:GLU:OE2 | 2.29 | 0.65 |
| 2:M1:31:GLN:HG2 | 29:7I:82:THR:HG21 | 1.78 | 0.65 |
| 1:Q4:91:VAL:HG11 | 1:Q4:116:VAL:HG12 | 1.78 | 0.65 |
| 1:S8:409:THR:HB | 13:5I:50:ARG:HD3 | 1.77 | 0.65 |
| 2:V1:413:MET:HB3 | 2:V1:417:GLU:OE2 | 1.96 | 0.65 |
| 1:V4:68:LEU:HB3 | 1:V4:96:GLY:HA2 | 1.78 | 0.65 |
| 1:V6:205:GLU:HG3 | 1:V6:302:ALA:HB2 | 1.78 | 0.65 |
| 2:W9:274:PRO:HB3 | 2:W9:286:LEU:HD11 | 1.77 | 0.65 |
| 2:X3:319:TYR:HB3 | 2:X3:323:VAL:HG21 | 1.78 | 0.65 |
| 1:Y2:252:LYS:HE2 | 1:Y2:350:LYS:CE | 2.26 | 0.65 |
| 1:Z2:7:ILE:HD11 | 1:Z2:135:VAL:HG22 | 1.79 | 0.65 |
| 1:0E:334:GLN:HE22 | 1:0E:348:ASN:H | 1.43 | 0.65 |
| 2:0H:56:THR:HA | 2:0X:285:GLN:HB2 | 1.78 | 0.65 |
| 1:1E:286:VAL:HG23 | 1:1E:287:PRO:HD3 | 1.77 | 0.65 |
| 2:1H:317:LEU:HB3 | 2:1H:319:TYR:HE1 | 1.60 | 0.65 |
| 2:1T:222:PRO:HD2 | 1:1U:324:LYS:HE3 | 1.78 | 0.65 |
| 2:1T:392:ASP:OD2 | 2:1T:422:ARG:NH1 | 2.28 | 0.65 |
| 1:2Y:360:GLY:HA2 | 10:5C:408:VAL:HG21 | 1.77 | 0.65 |
| 1:3S:276:ARG:HH22 | 17:5V:219:LEU:HD22 | 1.60 | 0.65 |
| 5:4L:359:GLU:OE1 | 5:4L:363:GLN:NE2 | 2.28 | 0.65 |
| 8:4W:230:GLU:HA | 8:4W:233:LYS:HD2 | 1.77 | 0.65 |
| 15:5O:56:LYS:HB2 | 15:5O:59:LEU:HB3 | 1.78 | 0.65 |
| 15:5P:14:LEU:H | 15:5P:14:LEU:HD23 | 1.61 | 0.65 |
| 15:5P:279:ALA:HA | 15:5P:298:VAL:HG21 | 1.76 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:7E:50:SER:N | 26:7E:56:LEU:CD2 | 2.59 | 0.65 |
| 2:A4:145:THR:OG1 | 41:A4:501:GTP:O1B | 2.14 | 0.65 |
| 1:E6:33:THR:HG21 | 22:6L:262:TYR:HB2 | 1.76 | 0.65 |
| 1:G2:345:ILE:O | 1:G2:348:ASN:ND2 | 2.30 | 0.65 |
| 2:I3:27:GLU:OE1 | 2:I3:243:ARG:NH1 | 2.29 | 0.65 |
| 1:K4:20:PHE:HA | 1:K4:230:SER:OG | 1.97 | 0.65 |
| 2:K5:413:MET:HB3 | 2:K5:417:GLU:OE2 | 1.97 | 0.65 |
| 1:L6:20:PHE:HA | 1:L6:230:SER:OG | 1.97 | 0.65 |
| 1:M8:57:GLY:H | 19:6E:14:GLN:NE2 | 1.95 | 0.65 |
| 1:P6:345:ILE:O | 1:P6:348:ASN:ND2 | 2.29 | 0.65 |
| 1:Q0:156:ARG:NH1 | 1:Q0:197:ASP:OD1 | 2.29 | 0.65 |
| 2:Q1:155:GLU:HG2 | 2:Q1:197:HIS:CE1 | 2.32 | 0.65 |
| 2:Q3:105:ARG:O | 2:Q3:109:THR:OG1 | 2.13 | 0.65 |
| 2:R1:263:PRO:O | 17:5S:84:ARG:NH1 | 2.29 | 0.65 |
| 1:S0:135:VAL:HG21 | 1:S0:152:ILE:HD11 | 1.79 | 0.65 |
| 1:T4:309:ARG:NH1 | 1:T4:339:SER:O | 2.28 | 0.65 |
| 2:T7:9:ILE:HG13 | 2:T7:139:ASN:HB3 | 1.79 | 0.65 |
| 2:V7:406:HIS:HA | 2:V7:409:VAL:HG22 | 1.78 | 0.65 |
| 1:X2:6:HIS:HB2 | 1:X2:134:GLN:HE21 | 1.62 | 0.65 |
| 2:X3:223:THR:HG23 | 2:X3:225:THR:H | 1.60 | 0.65 |
| 1:X6:389:PHE:O | 1:X6:392:LYS:NZ | 2.26 | 0.65 |
| 1:Y8:202:LEU:HD23 | 1:Y8:229:ILE:HD13 | 1.76 | 0.65 |
| 2:0F:344:VAL:HB | 2:0F:346:TRP:NE1 | 2.11 | 0.65 |
| 2:0P:206:ASN:OD1 | 41:0Q:501:GTP:N2 | 2.27 | 0.65 |
| 1:1O:249:ASP:OD1 | 1:1O:250:LEU:N | 2.27 | 0.65 |
| 2:1P:264:ARG:NH2 | 2:1P:431:ASP:OD2 | 2.28 | 0.65 |
| 2:1Z:258:ASN:HB2 | 2:1Z:352:LYS:HZ3 | 1.60 | 0.65 |
| 1:2G:248:ALA:HA | 1:2G:252:LYS:HD2 | 1.79 | 0.65 |
| 1:2K:68:LEU:HB3 | 1:2K:96:GLY:HA2 | 1.76 | 0.65 |
| 2:2L:276:ILE:HG22 | 2:2L:281:ALA:HB2 | 1.77 | 0.65 |
| 1:2W:207:LEU:HB3 | 1:2W:225:LEU:HD22 | 1.78 | 0.65 |
| 1:2Y:113:ILE:HA | 1:2Y:116:VAL:HG22 | 1.77 | 0.65 |
| 2:3J:255:PHE:HA | 2:3J:259:LEU:HD13 | 1.79 | 0.65 |
| 2:3P:255:PHE:HA | 2:3P:259:LEU:HD13 | 1.78 | 0.65 |
| 14:5N:199:SER:HG | 14:5N:245:THR:HG1 | 1.38 | 0.65 |
| 22:6O:138:ASP:HA | 22:6O:141:LYS:HE2 | 1.79 | 0.65 |
| 36:7W:94:LEU:O | 36:7W:98:VAL:HG12 | 1.95 | 0.65 |
| 1:E0:276:ARG:HH12 | 24:6T:287:GLY:H | 1.44 | 0.65 |
| 2:G1:250:VAL:HG23 | 2:G1:254:GLU:HG3 | 1.78 | 0.65 |
| 2:H1:289:ALA:O | 2:H1:293:ASN:ND2 | 2.30 | 0.65 |
| 2:I1:100:ALA:HB1 | 1:I2:252:LYS:HB3 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I1:336:LYS:O | 2:I1:339:ARG:NH2 | 2.29 | 0.65 |
| 1:I8:236:ILE:HG23 | 1:I8:237:THR:HG23 | 1.78 | 0.65 |
| 1:L0:113:ILE:HA | 1:L0:116:VAL:HG22 | 1.78 | 0.65 |
| 2:M7:221:ARG:NH2 | 30:7K:62:GLU:HB2 | 2.08 | 0.65 |
| 2:N3:139:ASN:HD21 | 2:N3:170:THR:HG22 | 1.61 | 0.65 |
| 2:N5:5:ILE:HG22 | 2:N5:64:ARG:HB3 | 1.78 | 0.65 |
| 2:O5:254:GLU:OE1 | 2:O5:352:LYS:NZ | 2.27 | 0.65 |
| 2:P7:335:ILE:HG22 | 2:P7:341:ILE:HD13 | 1.77 | 0.65 |
| 2:R3:7:ILE:HD11 | 2:R3:137:VAL:HG12 | 1.79 | 0.65 |
| 1:T6:211:CYS:SG | 1:T6:220:PRO:HB3 | 2.36 | 0.65 |
| 1:V2:121:ARG:NH2 | 1:V2:158:GLU:OE2 | 2.29 | 0.65 |
| 2:V3:109:THR:OG1 | 2:V3:411:GLU:OE2 | 2.14 | 0.65 |
| 2:V7:88:HIS:HB2 | 2:X3:283:HIS:ND1 | 2.12 | 0.65 |
| 1:W2:113:ILE:HD13 | 1:W2:150:LEU:HD22 | 1.77 | 0.65 |
| 2:Y5:236:SER:O | 2:Y5:243:ARG:NH2 | 2.29 | 0.65 |
| 2:0F:305:CYS:HB2 | 2:0F:387:ILE:HD11 | 1.77 | 0.65 |
| 1:1A:51:PHE:O | 1:1A:62:ARG:NH2 | 2.28 | 0.65 |
| 1:1M:12:CYS:SG | 1:1M:13:GLY:N | 2.68 | 0.65 |
| 2:1R:392:ASP:OD2 | 2:1R:422:ARG:NH1 | 2.29 | 0.65 |
| 2:1T:183:GLU:HG3 | 2:1T:184:PRO:HD3 | 1.77 | 0.65 |
| 2:2Z:297:GLU:OE2 | 38:8C:74:ILE:CG2 | 2.37 | 0.65 |
| 2:3D:133:GLN:HB3 | 2:3D:252:ILE:HG21 | 1.79 | 0.65 |
| 2:3L:183:GLU:HG3 | 2:3L:184:PRO:HD3 | 1.78 | 0.65 |
| 1:3O:94:GLN:NE2 | 3:4F:139:SER:O | 2.30 | 0.65 |
| 15:5O:255:VAL:O | 15:5O:259:ILE:HG22 | 1.95 | 0.65 |
| 22:6P:45:PRO:HB2 | 22:6P:52:TYR:HB2 | 1.78 | 0.65 |
| 26:7F:119:MET:HA | 26:7F:119:MET:HE2 | 1.76 | 0.65 |
| 1:A5:11:GLN:N | 39:A5:501:GDP:O2B | 2.28 | 0.65 |
| 1:B1:204:ASN:OD1 | 39:B1:501:GDP:O2' | 2.13 | 0.65 |
| 1:C2:359:LYS:NZ | 24:7A:110:ASN:OD1 | 2.18 | 0.65 |
| 2:G1:348:PRO:HG2 | 2:G1:349:THR:HG23 | 1.79 | 0.65 |
| 2:K5:399:TYR:O | 2:K5:402:ARG:NH1 | 2.30 | 0.65 |
| 2:L9:132:LEU:HD22 | 2:L9:164:LYS:HD3 | 1.77 | 0.65 |
| 2:Q1:381:SER:OG | 2:Q1:382:THR:N | 2.27 | 0.65 |
| 1:Q6:58:ARG:HD3 | 1:S2:280:GLN:HE22 | 1.61 | 0.65 |
| 1:R8:52:ASN:OD1 | 1:R8:62:ARG:NH2 | 2.30 | 0.65 |
| 1:T4:52:ASN:OD1 | 1:T4:62:ARG:NH2 | 2.30 | 0.65 |
| 1:T6:392:LYS:HD2 | 1:T6:395:LEU:HD22 | 1.79 | 0.65 |
| 2:V1:213:CYS:HA | 2:V1:217:LEU:HB2 | 1.77 | 0.65 |
| 1:X4:190:HIS:HD2 | 1:X4:414:ASN:HD22 | 1.44 | 0.65 |
| 2:Z9:206:ASN:OD1 | 41:0A:501:GTP:N2 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0N:198:THR:HG21 | 2:0N:201:ALA:HB2 | 1.79 | 0.65 |
| 1:0Y:215:LEU:HB3 | 1:0Y:217:LEU:HG | 1.78 | 0.65 |
| 2:1H:66:ILE:HD11 | 2:1H:93:ILE:HG12 | 1.78 | 0.65 |
| 1:1U:290:THR:HA | 1:1U:293:MET:HB2 | 1.78 | 0.65 |
| 2:1V:381:SER:OG | 2:1V:382:THR:N | 2.30 | 0.65 |
| 2:2B:161:TYR:CD1 | 38:8A:80:TYR:HB3 | 2.32 | 0.65 |
| 1:2M:286:VAL:HG21 | 1:2M:325:GLU:HB3 | 1.78 | 0.65 |
| 2:2V:214:ARG:HD3 | 38:8B:65:VAL:HG22 | 1.79 | 0.65 |
| 2:3F:27:GLU:OE1 | 2:3F:243:ARG:NH1 | 2.30 | 0.65 |
| 2:3L:124:LYS:NZ | 3:4B:35:CYS:SG | 2.69 | 0.65 |
| 2:3P:287:SER:N | 2:3P:290:GLU:OE2 | 2.29 | 0.65 |
| 8:4W:461:VAL:O | 8:4W:464:VAL:O | 2.14 | 0.65 |
| 14:5M:150:THR:HA | 14:5M:166:ALA:HA | 1.77 | 0.65 |
| 15:5O:132:GLU:HA | 15:5O:135:GLU:OE1 | 1.97 | 0.65 |
| 38:8D:78:ASP:OD2 | 38:8D:79:PRO:CD | 2.42 | 0.65 |
| 2:K1:414:GLU:HG2 | 2:K1:415:GLU:H | 1.61 | 0.65 |
| 1:K6:113:ILE:HA | 1:K6:116:VAL:HG22 | 1.79 | 0.65 |
| 2:L3:286:LEU:HD13 | 2:L3:371:VAL:HG23 | 1.78 | 0.65 |
| 2:M1:370:LYS:HE2 | 30:7K:277:ALA:HB2 | 1.78 | 0.65 |
| 2:N1:254:GLU:HB3 | 2:N1:352:LYS:HE2 | 1.77 | 0.65 |
| 2:R9:287:SER:N | 2:R9:290:GLU:OE2 | 2.23 | 0.65 |
| 1:S2:377:MET:HA | 1:S2:380:ARG:HE | 1.62 | 0.65 |
| 1:T0:345:ILE:O | 1:T0:348:ASN:ND2 | 2.30 | 0.65 |
| 1:U2:5:VAL:HG23 | 1:U2:62:ARG:HG2 | 1.77 | 0.65 |
| 1:U4:140:GLY:O | 1:U4:184:ASN:ND2 | 2.28 | 0.65 |
| 1:U6:67:ASP:OD2 | 1:U6:72:THR:OG1 | 2.14 | 0.65 |
| 1:W2:113:ILE:HA | 1:W2:116:VAL:HG12 | 1.79 | 0.65 |
| 1:W2:177:ASP:O | 2:W3:352:LYS:HA | 1.97 | 0.65 |
| 2:Y3:250:VAL:HB | 2:Y3:254:GLU:HG3 | 1.79 | 0.65 |
| 2:Y5:70:LEU:HD13 | 2:Y5:95:GLY:HA3 | 1.77 | 0.65 |
| 2:0F:88:HIS:HB3 | 2:0V:283:HIS:ND1 | 2.12 | 0.65 |
| 2:0J:90:GLU:HB3 | 2:0J:121:ARG:HH22 | 1.62 | 0.65 |
| 1:0K:388:MET:CE | 1:0K:388:MET:N | 2.60 | 0.65 |
| 1:0U:387:ALA:HA | 1:0U:390:ARG:HH21 | 1.62 | 0.65 |
| 2:1D:145:THR:OG1 | 41:1D:501:GTP:O1B | 2.12 | 0.65 |
| 1:1E:301:CYS:SG | 1:1E:302:ALA:N | 2.70 | 0.65 |
| 1:1U:113:ILE:HD13 | 1:1U:150:LEU:HD22 | 1.77 | 0.65 |
| 2:1V:90:GLU:HG2 | 2:1V:90:GLU:O | 1.97 | 0.65 |
| 1:2E:211:CYS:HA | 1:2E:215:LEU:HB2 | 1.78 | 0.65 |
| 1:2Y:340:TYR:CE2 | 38:8C:95:LYS:O | 2.49 | 0.65 |
| 2:2Z:96:LYS:HA | 1:3A:1:MET:HE1 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2Z:182:VAL:HG12 | 2:2Z:185:TYR:HB2 | 1.78 | 0.65 |
| 2:2Z:279:GLU:OE2 | 2:2Z:279:GLU:N | 2.24 | 0.65 |
| 1:3C:306:ARG:HE | 38:8D:97:PHE:HD2 | 1.44 | 0.65 |
| 1:3G:276:ARG:HH12 | 17:5S:216:GLU:HB3 | 1.62 | 0.65 |
| 8:4W:102:GLU:HG3 | 8:4W:103:GLN:HG2 | 1.78 | 0.65 |
| 10:5C:477:LYS:HB3 | 10:5D:154:MET:CE | 2.26 | 0.65 |
| 14:5L:150:THR:HA | 14:5L:166:ALA:HA | 1.77 | 0.65 |
| 14:5N:150:THR:HA | 14:5N:166:ALA:HA | 1.77 | 0.65 |
| 24:6X:573:VAL:HG12 | 24:6X:600:ALA:HB1 | 1.79 | 0.65 |
| 2:A2:40:LYS:HZ2 | 26:7F:46:ASN:N | 1.93 | 0.65 |
| 2:A2:221:ARG:CB | 26:7F:77:ILE:O | 2.44 | 0.65 |
| 2:G3:88:HIS:HD2 | 2:G3:89:PRO:CD | 1.99 | 0.65 |
| 1:G4:52:ASN:OD1 | 1:G4:62:ARG:NH2 | 2.29 | 0.65 |
| 2:G7:227:LEU:O | 2:G7:231:ILE:HG12 | 1.97 | 0.65 |
| 1:H4:276:ARG:NH2 | 24:6U:490:THR:HA | 2.11 | 0.65 |
| 1:H6:345:ILE:O | 1:H6:348:ASN:ND2 | 2.23 | 0.65 |
| 2:I7:5:ILE:HG22 | 2:I7:64:ARG:HB3 | 1.77 | 0.65 |
| 2:I9:183:GLU:HG3 | 2:I9:184:PRO:HD3 | 1.77 | 0.65 |
| 2:J7:33:ASP:O | 2:J7:60:LYS:NZ | 2.29 | 0.65 |
| 2:L5:352:LYS:NZ | 2:L5:353:CYS:O | 2.30 | 0.65 |
| 1:M6:357:PRO:HG2 | 37:7Y:142:ARG:HH12 | 1.61 | 0.65 |
| 2:M7:89:PRO:HG2 | 19:6E:25:VAL:HG11 | 1.73 | 0.65 |
| 2:O3:265:ILE:HD11 | 2:O3:435:VAL:HG21 | 1.78 | 0.65 |
| 2:P9:46:ASP:OD1 | 2:P9:47:ASP:N | 2.27 | 0.65 |
| 1:Q0:5:VAL:HG12 | 1:Q0:62:ARG:HD3 | 1.79 | 0.65 |
| 1:Q2:27:GLU:OE1 | 1:Q2:241:ARG:NH1 | 2.27 | 0.65 |
| 2:R9:57:GLY:H | 2:T5:285:GLN:HB3 | 1.61 | 0.65 |
| 2:T3:129:CYS:SG | 2:T3:132:LEU:HB2 | 2.36 | 0.65 |
| 1:T6:52:ASN:N | 1:T6:60:VAL:O | 2.29 | 0.65 |
| 1:V0:3:GLU:HB3 | 1:V0:130:LEU:HA | 1.77 | 0.65 |
| 2:W1:34:GLY:HA3 | 2:W1:60:LYS:HZ1 | 1.61 | 0.65 |
| 2:W9:33:ASP:HA | 2:W9:85:GLN:HB2 | 1.79 | 0.65 |
| 1:X4:204:ASN:HD21 | 39:X4:502:GDP:HN22 | 1.43 | 0.65 |
| 1:Y4:2:ARG:HE | 1:Y4:240:LEU:HD22 | 1.61 | 0.65 |
| 1:Y4:52:ASN:OD1 | 1:Y4:62:ARG:NH2 | 2.30 | 0.65 |
| 1:Z0:181:GLU:HG3 | 1:Z0:182:PRO:HD3 | 1.79 | 0.65 |
| 2:Z1:191:THR:HA | 2:Z1:194:LEU:HB3 | 1.79 | 0.65 |
| 2:0N:398:MET:HG2 | 1:0O:345:ILE:HG12 | 1.78 | 0.65 |
| 1:1A:4:ILE:HB | 1:1A:50:TYR:HE1 | 1.62 | 0.65 |
| 2:1N:392:ASP:OD2 | 2:1N:422:ARG:NH1 | 2.30 | 0.65 |
| 1:3C:174:LYS:HE3 | 38:8D:106:ASP:OD2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3K:233:MET:O | 1:3K:237:THR:HG22 | 1.96 | 0.65 |
| 1:3O:125:GLU:OE1 | 4:4E:45:SER:OG | 2.15 | 0.65 |
| 2:3P:254:GLU:HB3 | 2:3P:352:LYS:HE2 | 1.77 | 0.65 |
| 2:3R:56:THR:OG1 | 3:4H:34:SER:HA | 1.97 | 0.65 |
| 10:5A:310:LEU:O | 10:5A:314:LYS:HG2 | 1.96 | 0.65 |
| 10:5B:81:ALA:HB1 | 10:5B:85:ARG:HH21 | 1.62 | 0.65 |
| 14:5L:89:ASP:HB2 | 14:5L:96:ILE:HD11 | 1.77 | 0.65 |
| 14:5L:558:ALA:HB1 | 14:5L:601:VAL:HG12 | 1.79 | 0.65 |
| 14:5M:89:ASP:HB2 | 14:5M:96:ILE:HD11 | 1.77 | 0.65 |
| 14:5M:558:ALA:HB1 | 14:5M:601:VAL:HG12 | 1.79 | 0.65 |
| 24:6Z:327:LEU:HD12 | 24:6Z:328:PRO:HD2 | 1.77 | 0.65 |
| 36:7V:16:GLN:O | 36:7V:20:GLU:HG2 | 1.97 | 0.65 |
| 1:5:41:ASP:OD1 | 26:7D:25:TYR:CD2 | 2.44 | 0.65 |
| 2:8:283:HIS:HB3 | 2:T1:88:HIS:HD2 | 1.59 | 0.65 |
| 2:C7:41:THR:HG21 | 24:6U:274:ARG:CZ | 2.27 | 0.65 |
| 2:H1:57:GLY:H | 2:I7:285:GLN:HB2 | 1.62 | 0.65 |
| 2:H1:288:VAL:O | 2:H1:292:THR:OG1 | 2.13 | 0.65 |
| 2:H9:336:LYS:O | 2:H9:339:ARG:NH2 | 2.30 | 0.65 |
| 2:I1:11:GLN:OE1 | 2:I1:15:GLN:NE2 | 2.30 | 0.65 |
| 2:I5:154:LEU:HG | 2:I5:197:HIS:HB3 | 1.77 | 0.65 |
| 2:J7:29:GLY:HA2 | 29:7J:409:VAL:HG11 | 1.77 | 0.65 |
| 1:L4:45:GLU:HG3 | 1:L4:46:ARG:HG2 | 1.78 | 0.65 |
| 2:M9:399:TYR:O | 2:M9:402:ARG:NH1 | 2.30 | 0.65 |
| 2:N5:203:MET:HB2 | 2:N5:303:VAL:HG21 | 1.78 | 0.65 |
| 2:O3:90:GLU:HG3 | 2:O3:121:ARG:NH1 | 2.12 | 0.65 |
| 2:P9:32:PRO:HG3 | 19:6E:155:GLN:HB3 | 1.77 | 0.65 |
| 2:R7:31:GLN:HE21 | 2:R7:37:PRO:HG3 | 1.61 | 0.65 |
| 2:R9:296:PHE:HE1 | 2:R9:377:MET:HG3 | 1.62 | 0.65 |
| 1:W4:34:GLY:O | 1:W4:58:ARG:HA | 1.97 | 0.65 |
| 1:W6:140:GLY:O | 1:W6:184:ASN:ND2 | 2.23 | 0.65 |
| 1:X4:177:ASP:O | 2:X5:352:LYS:HA | 1.96 | 0.65 |
| 2:X7:9:ILE:HG22 | 2:X7:146:GLY:HA2 | 1.77 | 0.65 |
| 2:Z7:114:ILE:HD11 | 2:Z7:149:LEU:HD22 | 1.79 | 0.65 |
| 1:0M:33:THR:O | 1:0M:58:ARG:NH2 | 2.30 | 0.65 |
| 1:0M:54:ALA:HB3 | 1:0M:58:ARG:HB3 | 1.79 | 0.65 |
| 1:0S:90:PHE:HB3 | 1:0S:92:PHE:CE1 | 2.32 | 0.65 |
| 1:0Y:334:GLN:HE22 | 1:0Y:348:ASN:H | 1.45 | 0.65 |
| 2:1H:399:TYR:O | 2:1H:402:ARG:NH1 | 2.28 | 0.65 |
| 2:1N:88:HIS:HB3 | 2:1N:91:GLN:HG3 | 1.78 | 0.65 |
| 1:2C:248:ALA:HA | 1:2C:252:LYS:HD2 | 1.79 | 0.65 |
| 1:2G:52:ASN:OD1 | 1:2G:62:ARG:NH2 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2Q:287:PRO:HA | 1:2Q:290:THR:HG22 | 1.78 | 0.65 |
| 1:2Q:306:ARG:NH2 | 38:8A:96:GLY:H | 1.94 | 0.65 |
| 2:2R:85:GLN:HG3 | 14:5L:503:ARG:HH22 | 1.61 | 0.65 |
| 1:3Q:140:GLY:O | 1:3Q:184:ASN:ND2 | 2.25 | 0.65 |
| 14:5N:89:ASP:HB2 | 14:5N:96:ILE:HD11 | 1.77 | 0.65 |
| 16:5Q:120:PRO:HB3 | 16:5Q:146:THR:HG21 | 1.78 | 0.65 |
| 20:6F:239:GLU:HB3 | 20:6F:252:GLU:HB3 | 1.78 | 0.65 |
| 22:6J:48:GLU:HG2 | 22:6J:113:ARG:HD3 | 1.77 | 0.65 |
| 24:6U:96:LEU:HB2 | 24:6U:123:TYR:HB3 | 1.77 | 0.65 |
| 24:6V:122:TYR:HB2 | 24:6V:131:HIS:HB3 | 1.79 | 0.65 |
| 36:7W:16:GLN:O | 36:7W:20:GLU:HG2 | 1.97 | 0.65 |
| 36:7W:74:GLU:N | 36:7W:74:GLU:OE1 | 2.30 | 0.65 |
| 37:7Y:55:LEU:HD12 | 37:7Y:55:LEU:C | 2.16 | 0.65 |
| 1:G4:190:HIS:CD2 | 1:G4:411:ALA:HA | 2.32 | 0.65 |
| 2:G5:206:ASN:OD1 | 41:G5:501:GTP:N2 | 2.30 | 0.65 |
| 2:H1:244:PHE:O | 2:H1:249:ASN:ND2 | 2.29 | 0.65 |
| 2:I7:90:GLU:HB3 | 2:I7:121:ARG:HH22 | 1.61 | 0.65 |
| 2:M5:58:ALA:HB3 | 37:7Y:215:HIS:H | 1.61 | 0.65 |
| 2:M7:11:GLN:OE1 | 2:M7:15:GLN:NE2 | 2.29 | 0.65 |
| 1:O4:2:ARG:HE | 1:O4:240:LEU:HD22 | 1.62 | 0.65 |
| 1:P8:392:LYS:HD2 | 1:P8:395:LEU:HD22 | 1.78 | 0.65 |
| 2:R3:392:ASP:OD2 | 2:R3:422:ARG:NH1 | 2.30 | 0.65 |
| 1:T2:263:LEU:HD22 | 1:T2:422:TYR:CE1 | 2.31 | 0.65 |
| 1:T4:67:ASP:OD2 | 1:T4:72:THR:OG1 | 2.14 | 0.65 |
| 1:T6:309:ARG:H | 1:T6:372:THR:HG22 | 1.62 | 0.65 |
| 2:U7:109:THR:OG1 | 2:U7:411:GLU:OE2 | 2.12 | 0.65 |
| 1:W6:345:ILE:O | 1:W6:348:ASN:ND2 | 2.30 | 0.65 |
| 1:W8:334:GLN:HE22 | 1:W8:348:ASN:H | 1.44 | 0.65 |
| 1:X4:33:THR:O | 1:X4:58:ARG:NH2 | 2.30 | 0.65 |
| 2:Y1:5:ILE:HG22 | 2:Y1:64:ARG:HB3 | 1.77 | 0.65 |
| 2:0J:298:PRO:HA | 2:0J:301:MET:HG2 | 1.79 | 0.65 |
| 1:0Y:211:CYS:HA | 1:0Y:215:LEU:HB2 | 1.78 | 0.65 |
| 2:1F:56:THR:O | 2:1F:60:LYS:HB2 | 1.96 | 0.65 |
| 2:1N:313:MET:HE3 | 2:1N:346:TRP:CH2 | 2.19 | 0.65 |
| 2:1R:90:GLU:HB3 | 2:1R:121:ARG:HH12 | 1.62 | 0.65 |
| 2:1V:91:GLN:HG2 | 2:1V:121:ARG:HH22 | 1.61 | 0.65 |
| 1:2W:135:VAL:HG21 | 1:2W:152:ILE:HD11 | 1.77 | 0.65 |
| 1:3I:52:ASN:HD22 | 1:3I:52:ASN:H | 1.45 | 0.65 |
| 2:3L:267:PHE:HB2 | 2:3L:384:ILE:HD12 | 1.77 | 0.65 |
| 1:3S:309:ARG:O | 1:3S:371:SER:OG | 2.13 | 0.65 |
| 4:4I:92:GLN:HG2 | 4:4I:102:ARG:HG2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:4O:74:ARG:HH22 | 6:4O:75:ALA:HB2 | 1.61 | 0.65 |
| 18:6A:5:VAL:HG11 | 18:6A:62:GLU:HG2 | 1.78 | 0.65 |
| 24:6T:354:ARG:HB2 | 24:6T:357:LEU:HG | 1.79 | 0.65 |
| 24:6X:96:LEU:HB2 | 24:6X:123:TYR:HB3 | 1.78 | 0.65 |
| 24:6X:467:ARG:NH1 | 24:6X:484:GLU:CD | 2.48 | 0.65 |
| 26:7D:58:ILE:HD12 | 26:7D:58:ILE:N | 2.04 | 0.65 |
| 36:7V:74:GLU:N | 36:7V:74:GLU:OE1 | 2.30 | 0.65 |
| 1:G8:392:LYS:HD2 | 1:G8:395:LEU:HD22 | 1.79 | 0.64 |
| 1:H4:309:ARG:H | 1:H4:372:THR:HG22 | 1.62 | 0.64 |
| 2:I9:223:THR:HG23 | 2:I9:225:THR:H | 1.61 | 0.64 |
| 2:J7:80:THR:HB | 29:7J:390:LEU:HD11 | 1.79 | 0.64 |
| 2:K7:88:HIS:CE1 | 2:K7:89:PRO:HD2 | 2.30 | 0.64 |
| 1:L0:12:CYS:SG | 1:L0:138:SER:HB2 | 2.37 | 0.64 |
| 2:M3:264:ARG:NH2 | 2:M3:431:ASP:OD2 | 2.30 | 0.64 |
| 2:M5:381:SER:OG | 2:M5:382:THR:N | 2.30 | 0.64 |
| 2:N3:271:SER:HB3 | 2:N3:377:MET:HB3 | 1.80 | 0.64 |
| 2:N5:85:GLN:O | 2:P3:283:HIS:NE2 | 2.26 | 0.64 |
| 1:N6:309:ARG:H | 1:N6:372:THR:HG22 | 1.62 | 0.64 |
| 1:P4:107:THR:OG1 | 1:P4:108:GLU:OE1 | 2.08 | 0.64 |
| 2:P7:206:ASN:OD1 | 41:P8:501:GTP:N2 | 2.29 | 0.64 |
| 2:P7:392:ASP:OD2 | 2:P7:422:ARG:NH1 | 2.30 | 0.64 |
| 1:S8:375:GLN:HB3 | 1:S8:422:TYR:HD2 | 1.59 | 0.64 |
| 1:T6:213:ARG:HE | 1:T6:297:LYS:HD2 | 1.61 | 0.64 |
| 1:X6:139:LEU:HD12 | 1:X6:170:VAL:HG12 | 1.79 | 0.64 |
| 2:Y3:282:TYR:OH | 8:4W:370:VAL:CA | 2.44 | 0.64 |
| 2:Z1:56:THR:HA | 2:0H:285:GLN:HG2 | 1.77 | 0.64 |
| 1:Z8:207:LEU:HB3 | 1:Z8:225:LEU:HD22 | 1.79 | 0.64 |
| 1:0I:54:ALA:HB3 | 1:0I:58:ARG:HB2 | 1.79 | 0.64 |
| 1:1Q:279:GLN:OE1 | 9:4Z:196:LYS:NZ | 2.31 | 0.64 |
| 2:1R:56:THR:HG23 | 2:1R:60:LYS:HB3 | 1.78 | 0.64 |
| 1:1W:345:ILE:O | 1:1W:348:ASN:ND2 | 2.28 | 0.64 |
| 2:1Z:62:VAL:HG21 | 2:1Z:88:HIS:HB2 | 1.80 | 0.64 |
| 1:2A:135:VAL:HG21 | 1:2A:152:ILE:HD11 | 1.78 | 0.64 |
| 2:2N:220:GLU:HG2 | 2:2N:221:ARG:HG3 | 1.78 | 0.64 |
| 2:2P:167:LEU:HD23 | 2:2P:200:VAL:HB | 1.78 | 0.64 |
| 2:2V:267:PHE:HB2 | 2:2V:384:ILE:HD12 | 1.79 | 0.64 |
| 22:6K:333:MET:HG3 | 22:6K:334:THR:HG23 | 1.79 | 0.64 |
| 22:6M:280:LYS:HE3 | 22:6M:350:PHE:HA | 1.79 | 0.64 |
| 22:6P:65:ARG:HE | 22:6P:101:ASN:HB2 | 1.61 | 0.64 |
| 23:6S:45:GLU:OE1 | 23:6S:45:GLU:HA | 1.96 | 0.64 |
| 24:6U:278:VAL:HG11 | 24:6U:395:VAL:HG11 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:444:ILE:HD13 | 24:6X:542:TYR:CE1 | 2.32 | 0.64 |
| 24:7A:6:PRO:HD3 | 31:7N:84:TYR:HD1 | 1.62 | 0.64 |
| 2:A2:40:LYS:HZ2 | 26:7F:45:MET:HB2 | 1.62 | 0.64 |
| 2:A2:223:THR:HG22 | 26:7F:78:ALA:CB | 2.27 | 0.64 |
| 2:F5:56:THR:HA | 2:H1:285:GLN:HB2 | 1.77 | 0.64 |
| 1:H6:309:ARG:H | 1:H6:372:THR:HG22 | 1.62 | 0.64 |
| 1:I8:220:PRO:HD2 | 2:I9:326:LYS:HG2 | 1.79 | 0.64 |
| 2:J7:80:THR:CA | 29:7J:390:LEU:HD21 | 2.26 | 0.64 |
| 2:J7:381:SER:OG | 2:J7:382:THR:N | 2.30 | 0.64 |
| 2:L5:176:GLN:HE22 | 2:L5:304:LYS:HE2 | 1.62 | 0.64 |
| 1:M2:33:THR:O | 1:M2:58:ARG:NH1 | 2.31 | 0.64 |
| 1:M6:1:MET:CE | 37:7Y:116:MET:CB | 2.75 | 0.64 |
| 1:M8:86:ARG:HB3 | 2:O5:283:HIS:CE1 | 2.32 | 0.64 |
| 2:N5:35:GLN:HB3 | 2:N5:59:GLY:O | 1.97 | 0.64 |
| 2:O5:191:THR:HA | 2:O5:194:LEU:HB3 | 1.77 | 0.64 |
| 1:P6:3:GLU:HG3 | 1:P6:127:CYS:HB2 | 1.80 | 0.64 |
| 2:Q5:250:VAL:HB | 2:Q5:254:GLU:HG3 | 1.79 | 0.64 |
| 2:U1:216:SER:O | 2:U1:280:LYS:NZ | 2.30 | 0.64 |
| 1:U2:140:GLY:O | 1:U2:184:ASN:ND2 | 2.31 | 0.64 |
| 1:X4:238:CYS:SG | 1:X4:316:LEU:HD21 | 2.37 | 0.64 |
| 1:0O:5:VAL:HG23 | 1:0O:62:ARG:HG2 | 1.78 | 0.64 |
| 2:1D:346:TRP:HE3 | 2:1D:346:TRP:O | 1.80 | 0.64 |
| 2:1X:394:LYS:HD2 | 2:1X:397:LEU:HD12 | 1.78 | 0.64 |
| 2:2T:109:THR:OG1 | 2:2T:411:GLU:OE2 | 2.14 | 0.64 |
| 1:2U:3:GLU:HB2 | 1:2U:130:LEU:HA | 1.78 | 0.64 |
| 2:3D:287:SER:N | 2:3D:290:GLU:OE2 | 2.29 | 0.64 |
| 1:3M:391:ARG:CD | 2:3N:346:TRP:HB3 | 2.21 | 0.64 |
| 2:3R:19:ALA:O | 2:3R:22:GLU:HG3 | 1.97 | 0.64 |
| 10:5D:232:GLU:HA | 10:5D:235:ARG:HE | 1.62 | 0.64 |
| 14:5L:112:SER:HA | 14:5L:155:PHE:CD2 | 2.31 | 0.64 |
| 21:6H:137:LEU:HD11 | 21:6H:198:GLU:HG2 | 1.77 | 0.64 |
| 22:6M:177:LEU:HB2 | 22:6M:183:ASN:HB2 | 1.79 | 0.64 |
| 23:6Q:45:GLU:OE1 | 23:6Q:45:GLU:HA | 1.96 | 0.64 |
| 23:6R:45:GLU:OE1 | 23:6R:45:GLU:HA | 1.96 | 0.64 |
| 24:6X:315:ARG:HG2 | 24:6X:315:ARG:NH1 | 2.07 | 0.64 |
| 24:6X:489:ASN:C | 24:6X:489:ASN:HD22 | 1.99 | 0.64 |
| 28:7H:451:LYS:HG3 | 28:7H:452:ASN:N | 2.12 | 0.64 |
| 1:G2:388:MET:CE | 2:G3:348:PRO:HD2 | 2.26 | 0.64 |
| 2:I7:399:TYR:O | 2:I7:402:ARG:NH1 | 2.31 | 0.64 |
| 2:J9:213:CYS:HA | 2:J9:217:LEU:HB2 | 1.78 | 0.64 |
| 2:M5:336:LYS:O | 2:M5:339:ARG:NH2 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N2:60:VAL:HG11 | 1:N2:86:ARG:HE | 1.61 | 0.64 |
| 2:Q9:223:THR:HG22 | 2:Q9:224:TYR:H | 1.62 | 0.64 |
| 2:R1:161:TYR:HD1 | 13:5H:124:VAL:HG13 | 1.61 | 0.64 |
| 1:R6:237:THR:HG23 | 1:R6:240:LEU:HD13 | 1.79 | 0.64 |
| 2:R9:98:ASP:OD1 | 2:R9:99:ALA:N | 2.29 | 0.64 |
| 1:S4:309:ARG:NH1 | 1:S4:339:SER:O | 2.31 | 0.64 |
| 1:T6:73:MET:HA | 1:T6:76:VAL:CG1 | 2.28 | 0.64 |
| 1:T8:180:VAL:HG23 | 1:T8:184:ASN:HD21 | 1.61 | 0.64 |
| 2:U1:264:ARG:NH2 | 2:U1:431:ASP:OD2 | 2.30 | 0.64 |
| 2:U5:7:ILE:HD11 | 2:U5:68:LEU:HD21 | 1.78 | 0.64 |
| 1:V8:91:VAL:HG11 | 1:V8:119:VAL:HG21 | 1.79 | 0.64 |
| 2:W7:236:SER:O | 2:W7:243:ARG:NH2 | 2.30 | 0.64 |
| 2:Z3:105:ARG:O | 2:Z3:109:THR:OG1 | 2.14 | 0.64 |
| 1:0G:304:ASP:OD1 | 1:0G:306:ARG:NH1 | 2.29 | 0.64 |
| 1:2A:121:ARG:CZ | 38:8A:100:SER:OG | 2.46 | 0.64 |
| 2:2N:223:THR:HG23 | 2:2N:225:THR:HG22 | 1.80 | 0.64 |
| 2:3L:221:ARG:NH1 | 23:6R:70:THR:O | 2.30 | 0.64 |
| 2:3L:255:PHE:HA | 2:3L:259:LEU:HD13 | 1.79 | 0.64 |
| 2:3P:56:THR:OG1 | 3:4F:34:SER:HA | 1.96 | 0.64 |
| 1:3S:275:SER:O | 1:3S:279:GLN:HG2 | 1.97 | 0.64 |
| 4:3W:92:GLN:HG2 | 4:3W:102:ARG:HG2 | 1.78 | 0.64 |
| 4:4G:92:GLN:HG2 | 4:4G:102:ARG:HG2 | 1.78 | 0.64 |
| 6:4O:47:ASN:O | 6:4O:51:VAL:HG23 | 1.98 | 0.64 |
| 9:4Z:91:LEU:HA | 9:4Z:94:GLU:HG3 | 1.78 | 0.64 |
| 10:5D:134:SER:O | 10:5D:138:HIS:ND1 | 2.26 | 0.64 |
| 15:5O:34:GLU:HG3 | 15:5O:49:ARG:NE | 2.10 | 0.64 |
| 21:6G:172:LEU:HD22 | 21:6G:176:GLU:HG2 | 1.79 | 0.64 |
| 24:6Y:483:PHE:HB2 | 24:6Y:496:LYS:HA | 1.79 | 0.64 |
| 24:6Z:97:ARG:NH2 | 24:6Z:99:TYR:OH | 2.29 | 0.64 |
| 26:7E:50:SER:CA | 26:7E:56:LEU:HD23 | 2.27 | 0.64 |
| 36:7W:19:LEU:N | 36:7W:102:MET:HE2 | 2.13 | 0.64 |
| 38:8B:82:ASP:HA | 38:8B:112:ILE:HD13 | 1.78 | 0.64 |
| 2:B0:278:ALA:HB3 | 18:5Y:43:ASN:HD22 | 1.62 | 0.64 |
| 2:F1:56:THR:HG23 | 2:G7:285:GLN:HA | 1.79 | 0.64 |
| 1:K4:172:SER:HB3 | 1:K4:175:VAL:HG22 | 1.79 | 0.64 |
| 2:K5:77:GLU:HG3 | 29:7I:43:PHE:HZ | 1.62 | 0.64 |
| 1:K6:12:CYS:SG | 1:K6:138:SER:HB2 | 2.36 | 0.64 |
| 2:L3:66:ILE:HG21 | 2:L3:122:ILE:HD11 | 1.77 | 0.64 |
| 1:M0:272:PRO:HB2 | 1:M0:282:ARG:HH12 | 1.61 | 0.64 |
| 2:M1:392:ASP:OD2 | 2:M1:422:ARG:NH1 | 2.30 | 0.64 |
| 2:P7:337:THR:HG22 | 25:7C:21:LEU:HD13 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:177:ASP:O | 2:Q1:352:LYS:HA | 1.97 | 0.64 |
| 1:T6:320:ARG:HH12 | 33:7Q:139:GLU:HA | 1.63 | 0.64 |
| 1:T8:190:HIS:NE2 | 1:T8:410:GLU:HG3 | 2.13 | 0.64 |
| 1:V4:45:GLU:N | 1:V4:45:GLU:OE1 | 2.31 | 0.64 |
| 2:W3:109:THR:OG1 | 2:W3:411:GLU:OE2 | 2.16 | 0.64 |
| 2:W7:224:TYR:H | 1:W8:245:GLN:NE2 | 1.94 | 0.64 |
| 2:X5:167:LEU:HA | 2:X5:200:VAL:HG13 | 1.78 | 0.64 |
| 1:Y8:58:ARG:HD3 | 1:0E:280:GLN:HE22 | 1.62 | 0.64 |
| 2:Z7:53:PHE:HB3 | 2:Z7:61:HIS:HB3 | 1.79 | 0.64 |
| 2:0N:388:PHE:HB3 | 2:0N:425:LEU:HD11 | 1.79 | 0.64 |
| 1:0Q:139:LEU:HD12 | 1:0Q:170:VAL:HG12 | 1.79 | 0.64 |
| 2:1B:11:GLN:OE1 | 2:1B:15:GLN:NE2 | 2.31 | 0.64 |
| 2:2F:399:TYR:O | 2:2F:402:ARG:NH1 | 2.31 | 0.64 |
| 2:2J:161:TYR:CE1 | 38:8C:80:TYR:HB3 | 2.33 | 0.64 |
| 1:3C:138:SER:OG | 1:3C:139:LEU:N | 2.29 | 0.64 |
| 1:3C:173:PRO:HD2 | 1:3C:380:ARG:HE | 1.62 | 0.64 |
| 1:3I:211:CYS:HA | 1:3I:215:LEU:HB2 | 1.79 | 0.64 |
| 4:3Y:92:GLN:HG2 | 4:3Y:102:ARG:HG2 | 1.78 | 0.64 |
| 4:4E:92:GLN:HG2 | 4:4E:102:ARG:HG2 | 1.78 | 0.64 |
| 7:4R:96:THR:HG21 | 21:6G:73:VAL:HG13 | 1.78 | 0.64 |
| 14:5N:112:SER:HA | 14:5N:155:PHE:HD2 | 1.62 | 0.64 |
| 15:5O:72:GLN:O | 15:5O:72:GLN:HG3 | 1.95 | 0.64 |
| 20:6F:361:LEU:HD12 | 20:6F:362:PRO:CD | 2.16 | 0.64 |
| 24:6T:278:VAL:HG21 | 24:6T:395:VAL:HG11 | 1.80 | 0.64 |
| 24:6Y:36:VAL:HB | 24:6Y:45:LEU:HD11 | 1.79 | 0.64 |
| 24:6Y:96:LEU:HB2 | 24:6Y:123:TYR:HB3 | 1.78 | 0.64 |
| 34:7R:201:LEU:HD21 | 36:7V:91:PRO:HB3 | 1.80 | 0.64 |
| 37:7Y:223:ARG:HD3 | 37:7Y:225:TRP:CH2 | 2.32 | 0.64 |
| 2:4:423:GLU:HG3 | 4:3Y:108:TYR:OH | 1.98 | 0.64 |
| 1:5:78:SER:CB | 24:6V:149:LYS:HG3 | 2.27 | 0.64 |
| 1:9:83:GLN:NE2 | 24:6X:177:ARG:HH12 | 1.94 | 0.64 |
| 2:G7:96:LYS:HB3 | 1:G8:1:MET:HE2 | 1.79 | 0.64 |
| 1:H2:35:THR:HG22 | 28:7H:312:LEU:HD21 | 1.80 | 0.64 |
| 1:H2:140:GLY:O | 1:H2:184:ASN:ND2 | 2.30 | 0.64 |
| 2:H3:27:GLU:OE1 | 2:H3:243:ARG:NH1 | 2.31 | 0.64 |
| 2:I3:392:ASP:OD2 | 2:I3:422:ARG:NH1 | 2.31 | 0.64 |
| 1:I8:2:ARG:HB3 | 1:I8:131:GLN:HB2 | 1.80 | 0.64 |
| 2:J1:432:PHE:HA | 2:J1:435:VAL:HG12 | 1.77 | 0.64 |
| 1:K8:177:ASP:O | 2:K9:352:LYS:HA | 1.97 | 0.64 |
| 2:M5:109:THR:OG1 | 2:M5:411:GLU:OE2 | 2.14 | 0.64 |
| 1:M6:73:MET:HA | 1:M6:76:VAL:HG22 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N3:317:LEU:HB3 | 2:N3:319:TYR:HE1 | 1.61 | 0.64 |
| 2:N5:88:HIS:HE1 | 2:N5:90:GLU:CG | 2.10 | 0.64 |
| 1:O4:178:THR:OG1 | 2:O5:258:ASN:ND2 | 2.26 | 0.64 |
| 2:O7:207:GLU:HG2 | 2:O7:304:LYS:HD2 | 1.78 | 0.64 |
| 2:O9:155:GLU:HG2 | 2:O9:197:HIS:CE1 | 2.32 | 0.64 |
| 2:R3:100:ALA:HA | 1:R4:252:LYS:HE2 | 1.79 | 0.64 |
| 1:S4:177:ASP:O | 2:S5:352:LYS:HA | 1.96 | 0.64 |
| 1:T2:220:PRO:HD2 | 2:T3:326:LYS:HG2 | 1.80 | 0.64 |
| 1:U2:52:ASN:OD1 | 1:U2:62:ARG:NH2 | 2.31 | 0.64 |
| 1:V2:273:LEU:H | 1:V2:292:GLN:HE22 | 1.44 | 0.64 |
| 2:W5:399:TYR:OH | 2:W5:415:GLU:OE2 | 2.16 | 0.64 |
| 1:X2:320:ARG:HH22 | 1:X2:357:PRO:HG3 | 1.62 | 0.64 |
| 2:Z5:157:LEU:HD22 | 2:Z5:166:LYS:HD3 | 1.80 | 0.64 |
| 1:Z8:250:LEU:HA | 1:Z8:253:LEU:HD12 | 1.79 | 0.64 |
| 2:0H:305:CYS:HB3 | 2:0H:387:ILE:HD11 | 1.77 | 0.64 |
| 1:0M:286:VAL:HG23 | 1:0M:287:PRO:HD3 | 1.78 | 0.64 |
| 2:0P:129:CYS:SG | 2:0P:132:LEU:HB2 | 2.38 | 0.64 |
| 1:0Y:51:PHE:O | 1:0Y:62:ARG:NH2 | 2.31 | 0.64 |
| 2:1L:264:ARG:NH2 | 2:1L:431:ASP:OD2 | 2.31 | 0.64 |
| 2:2H:120:ASP:CG | 38:8B:27:HIS:CD2 | 2.66 | 0.64 |
| 2:2V:414:GLU:HG2 | 2:2V:416:GLY:H | 1.62 | 0.64 |
| 1:3A:418:LEU:HG | 1:3A:422:TYR:HE2 | 1.61 | 0.64 |
| 1:3C:245:GLN:CG | 38:8D:198:THR:HG21 | 2.28 | 0.64 |
| 1:3C:248:ALA:HA | 1:3C:252:LYS:HD2 | 1.80 | 0.64 |
| 2:3F:163:LYS:HE3 | 3:3V:137:ARG:HG2 | 1.78 | 0.64 |
| 2:3T:213:CYS:HA | 2:3T:217:LEU:HD12 | 1.80 | 0.64 |
| 4:4A:92:GLN:HG2 | 4:4A:102:ARG:HG2 | 1.78 | 0.64 |
| 12:5F:209:THR:HG23 | 12:5F:212:ARG:H | 1.62 | 0.64 |
| 14:5M:112:SER:HA | 14:5M:155:PHE:HD2 | 1.62 | 0.64 |
| 15:5P:52:TYR:CD2 | 15:5P:55:LEU:HD21 | 2.33 | 0.64 |
| 22:6M:114:THR:HG23 | 22:6M:117:GLY:H | 1.61 | 0.64 |
| 24:6X:482:ILE:HD12 | 24:6X:498:LEU:HD23 | 1.79 | 0.64 |
| 31:7N:102:ILE:HG13 | 31:7N:107:ASP:HB3 | 1.80 | 0.64 |
| 2:H3:413:MET:HB3 | 2:H3:417:GLU:OE2 | 1.96 | 0.64 |
| 1:I0:218:THR:HG23 | 24:6X:489:ASN:CA | 2.16 | 0.64 |
| 2:I7:406:HIS:HA | 2:I7:409:VAL:HG22 | 1.78 | 0.64 |
| 1:I8:211:CYS:HA | 1:I8:215:LEU:HB2 | 1.79 | 0.64 |
| 2:I9:392:ASP:OD2 | 2:I9:422:ARG:NH1 | 2.31 | 0.64 |
| 1:K4:211:CYS:HA | 1:K4:215:LEU:HB2 | 1.79 | 0.64 |
| 1:K6:220:PRO:HD2 | 2:K7:326:LYS:HD2 | 1.78 | 0.64 |
| 2:L5:129:CYS:SG | 2:L5:132:LEU:HB2 | 2.38 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N5:387:ILE:HG12 | 2:N5:390:ARG:HH22 | 1.61 | 0.64 |
| 2:N9:236:SER:OG | 2:N9:243:ARG:NH2 | 2.31 | 0.64 |
| 2:R9:264:ARG:HD3 | 17:5U:87:VAL:HG23 | 1.79 | 0.64 |
| 1:S4:2:ARG:HD2 | 1:S4:131:GLN:HB2 | 1.79 | 0.64 |
| 1:S4:186:THR:HG23 | 1:S4:187:LEU:HD12 | 1.80 | 0.64 |
| 2:U9:336:LYS:O | 2:U9:339:ARG:NH2 | 2.29 | 0.64 |
| 1:V8:2:ARG:HE | 1:V8:240:LEU:HD22 | 1.61 | 0.64 |
| 2:X5:344:VAL:HG13 | 2:X5:346:TRP:H | 1.63 | 0.64 |
| 1:X6:2:ARG:HE | 1:X6:240:LEU:HD22 | 1.62 | 0.64 |
| 1:Z4:252:LYS:HE2 | 1:Z4:350:LYS:HE2 | 1.79 | 0.64 |
| 2:0F:336:LYS:O | 2:0F:339:ARG:NH2 | 2.30 | 0.64 |
| 1:0I:259:PRO:HG3 | 1:0I:311:LEU:HD21 | 1.80 | 0.64 |
| 1:0K:178:THR:HG22 | 1:0K:180:VAL:H | 1.63 | 0.64 |
| 2:0L:387:ILE:HD12 | 2:0L:390:ARG:HH22 | 1.62 | 0.64 |
| 2:0N:392:ASP:OD2 | 2:0N:422:ARG:NH1 | 2.31 | 0.64 |
| 1:0W:350:LYS:NZ | 1:0W:352:SER:OG | 2.31 | 0.64 |
| 1:0Y:7:ILE:HD13 | 1:0Y:151:LEU:HD21 | 1.80 | 0.64 |
| 2:1L:245:ASP:HA | 2:1L:249:ASN:HD21 | 1.61 | 0.64 |
| 2:1L:336:LYS:O | 2:1L:339:ARG:NH2 | 2.29 | 0.64 |
| 1:1Q:309:ARG:H | 1:1Q:372:THR:HG22 | 1.63 | 0.64 |
| 2:1R:27:GLU:OE1 | 2:1R:243:ARG:NH1 | 2.30 | 0.64 |
| 1:2K:51:PHE:O | 1:2K:62:ARG:NH2 | 2.31 | 0.64 |
| 2:3N:255:PHE:HA | 2:3N:259:LEU:HD13 | 1.80 | 0.64 |
| 12:5F:41:ALA:HB3 | 12:5F:44:ILE:HG22 | 1.80 | 0.64 |
| 20:6F:342:GLN:HB2 | 20:6F:344:LEU:HD23 | 1.80 | 0.64 |
| 24:6Y:86:PRO:HD2 | 24:6Y:89:VAL:CG1 | 2.28 | 0.64 |
| 2:G3:221:ARG:HG3 | 22:6M:178:GLY:HA2 | 1.80 | 0.64 |
| 1:G4:350:LYS:NZ | 1:G4:351:SER:O | 2.30 | 0.64 |
| 2:I3:57:GLY:H | 2:J9:285:GLN:HG3 | 1.61 | 0.64 |
| 2:J3:27:GLU:OE1 | 2:J3:243:ARG:NH1 | 2.30 | 0.64 |
| 2:L5:155:GLU:HG2 | 2:L5:197:HIS:CE1 | 2.32 | 0.64 |
| 1:M4:6:HIS:HE2 | 1:M4:136:CYS:HG | 1.44 | 0.64 |
| 1:O6:388:MET:HE3 | 2:O7:348:PRO:HD2 | 1.80 | 0.64 |
| 2:R9:206:ASN:OD1 | 41:S0:501:GTP:N2 | 2.31 | 0.64 |
| 2:T3:287:SER:N | 2:T3:290:GLU:OE2 | 2.31 | 0.64 |
| 2:T5:220:GLU:HG2 | 2:T5:221:ARG:HG3 | 1.79 | 0.64 |
| 2:Z3:286:LEU:O | 2:Z3:373:ARG:NH1 | 2.30 | 0.64 |
| 2:Z5:346:TRP:CD1 | 2:Z5:346:TRP:C | 2.71 | 0.64 |
| 2:Z9:298:PRO:HA | 2:Z9:301:MET:HG3 | 1.78 | 0.64 |
| 1:0C:139:LEU:HD21 | 1:0C:168:SER:HB2 | 1.79 | 0.64 |
| 1:0C:394:PHE:HE2 | 1:0C:397:TRP:HE3 | 1.45 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0H:56:THR:N | 2:0H:60:LYS:O | 2.30 | 0.64 |
| 1:0K:54:ALA:HB3 | 1:0K:58:ARG:HB3 | 1.79 | 0.64 |
| 1:0M:320:ARG:HG2 | 1:0M:355:ASP:HB2 | 1.79 | 0.64 |
| 1:0Q:272:PRO:HB2 | 1:0Q:282:ARG:HH12 | 1.61 | 0.64 |
| 1:0W:215:LEU:HB3 | 1:0W:217:LEU:HG | 1.79 | 0.64 |
| 2:1L:286:LEU:O | 2:1L:373:ARG:NH1 | 2.31 | 0.64 |
| 2:1N:204:LEU:HD11 | 2:1N:209:ILE:HD11 | 1.80 | 0.64 |
| 1:2K:134:GLN:HE21 | 1:2K:167:PHE:HE2 | 1.45 | 0.64 |
| 1:2M:211:CYS:HA | 1:2M:215:LEU:HB2 | 1.79 | 0.64 |
| 1:2M:391:ARG:NH2 | 2:2N:434:GLU:O | 2.31 | 0.64 |
| 1:3Q:45:GLU:HG3 | 1:3Q:46:ARG:HG2 | 1.78 | 0.64 |
| 5:4M:143:ASN:O | 5:4M:147:ILE:HG13 | 1.98 | 0.64 |
| 6:4O:288:VAL:HA | 6:4O:291:ARG:HD2 | 1.80 | 0.64 |
| 7:4R:324:GLN:NE2 | 24:6Z:22:LEU:O | 2.30 | 0.64 |
| 14:5L:428:VAL:HA | 14:5L:444:GLY:HA2 | 1.80 | 0.64 |
| 14:5M:428:VAL:HA | 14:5M:444:GLY:HA2 | 1.80 | 0.64 |
| 34:7S:188:ILE:HG13 | 35:7U:143:TYR:HE1 | 1.62 | 0.64 |
| 2:A8:223:THR:HG23 | 18:5X:51:MET:HE3 | 1.80 | 0.64 |
| 1:G6:32:PRO:HD2 | 24:6Y:527:ASN:HD22 | 1.61 | 0.64 |
| 2:I7:287:SER:N | 2:I7:290:GLU:OE2 | 2.29 | 0.64 |
| 1:J4:359:LYS:NZ | 16:5Q:13:ASP:OD1 | 2.31 | 0.64 |
| 2:J5:88:HIS:ND1 | 2:L1:283:HIS:HA | 2.13 | 0.64 |
| 2:J7:282:TYR:CE1 | 5:4M:209:LEU:HD22 | 2.33 | 0.64 |
| 1:L6:339:SER:H | 34:7S:140:ASN:ND2 | 1.96 | 0.64 |
| 2:L9:88:HIS:O | 1:N6:281:TYR:OH | 2.15 | 0.64 |
| 2:O1:53:PHE:HB3 | 2:O1:61:HIS:HB3 | 1.80 | 0.64 |
| 2:O1:240:ALA:HB1 | 2:O1:356:ASN:HD22 | 1.63 | 0.64 |
| 1:O2:65:LEU:HD13 | 1:O2:90:PHE:HE1 | 1.63 | 0.64 |
| 1:O2:393:ALA:CB | 2:O3:346:TRP:HE1 | 2.10 | 0.64 |
| 1:O6:52:ASN:OD1 | 1:O6:62:ARG:NH2 | 2.31 | 0.64 |
| 1:R4:11:GLN:N | 39:R4:502:GDP:O1B | 2.29 | 0.64 |
| 2:R7:56:THR:HA | 2:T3:285:GLN:HB2 | 1.79 | 0.64 |
| 2:S7:305:CYS:HB2 | 2:S7:383:ALA:HB1 | 1.79 | 0.64 |
| 2:S9:408:TYR:HB3 | 2:S9:413:MET:HE2 | 1.79 | 0.64 |
| 1:T2:106:TYR:HE2 | 3:4D:78:PRO:HA | 1.62 | 0.64 |
| 2:U5:274:PRO:HG3 | 2:U5:286:LEU:HD11 | 1.79 | 0.64 |
| 1:U6:211:CYS:HA | 1:U6:215:LEU:HB2 | 1.79 | 0.64 |
| 1:W2:190:HIS:CD2 | 1:W2:411:ALA:HA | 2.33 | 0.64 |
| 1:Z0:207:LEU:HD11 | 1:Z0:229:ILE:CD1 | 2.28 | 0.64 |
| 2:0L:9:ILE:HG12 | 2:0L:153:LEU:HD21 | 1.78 | 0.64 |
| 2:0V:336:LYS:O | 2:0V:339:ARG:NH2 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1D:199:ASP:HB3 | 2:1D:256:GLN:NE2 | 2.12 | 0.64 |
| 2:1X:102:ASN:HD22 | 2:1X:105:ARG:HB2 | 1.62 | 0.64 |
| 2:2P:399:TYR:O | 2:2P:402:ARG:NH1 | 2.31 | 0.64 |
| 2:2Z:267:PHE:HB2 | 2:2Z:384:ILE:HD12 | 1.79 | 0.64 |
| 2:3B:298:PRO:HA | 2:3B:301:MET:HG3 | 1.79 | 0.64 |
| 1:3C:299:MET:O | 38:8D:105:ARG:NH2 | 2.31 | 0.64 |
| 1:3C:306:ARG:HH12 | 38:8D:100:SER:HA | 1.63 | 0.64 |
| 2:3L:236:SER:OG | 2:3L:243:ARG:NH2 | 2.30 | 0.64 |
| 4:4C:92:GLN:HG2 | 4:4C:102:ARG:HG2 | 1.78 | 0.64 |
| 10:5C:481:LEU:HD11 | 10:5C:494:LEU:HD23 | 1.78 | 0.64 |
| 14:5L:450:ARG:HG2 | 14:5L:464:SER:HB2 | 1.79 | 0.64 |
| 14:5L:509:ALA:HB3 | 14:5L:513:PHE:CZ | 2.33 | 0.64 |
| 14:5N:428:VAL:HA | 14:5N:444:GLY:HA2 | 1.80 | 0.64 |
| 24:6U:469:PHE:CE2 | 24:6U:482:ILE:HG23 | 2.32 | 0.64 |
| 24:6X:451:LYS:CB | 24:6X:468:ARG:HH11 | 2.11 | 0.64 |
| 31:7N:78:HIS:O | 31:7N:80:PRO:HD3 | 1.98 | 0.64 |
| 38:8B:82:ASP:N | 38:8B:82:ASP:OD1 | 2.31 | 0.64 |
| 2:G5:278:ALA:HB3 | 22:6N:215:GLY:HA2 | 1.78 | 0.64 |
| 2:G7:289:ALA:O | 2:G7:293:ASN:ND2 | 2.30 | 0.64 |
| 1:I0:51:PHE:O | 1:I0:62:ARG:NH2 | 2.31 | 0.64 |
| 2:J7:222:PRO:HD2 | 1:J8:324:LYS:HE3 | 1.80 | 0.64 |
| 2:L5:259:LEU:HD11 | 2:L5:316:CYS:HB2 | 1.80 | 0.64 |
| 1:M0:177:ASP:O | 2:M1:352:LYS:HA | 1.97 | 0.64 |
| 2:M3:195:LEU:HD21 | 2:M3:264:ARG:HH11 | 1.62 | 0.64 |
| 1:M4:53:GLU:OE2 | 1:M4:57:GLY:N | 2.26 | 0.64 |
| 2:N9:90:GLU:OE1 | 2:N9:90:GLU:HA | 1.98 | 0.64 |
| 1:O2:253:LEU:HD11 | 1:O2:316:LEU:HD11 | 1.78 | 0.64 |
| 2:P3:381:SER:OG | 2:P3:382:THR:N | 2.31 | 0.64 |
| 2:P5:90:GLU:HB2 | 2:P5:121:ARG:HH22 | 1.62 | 0.64 |
| 1:P8:2:ARG:HB3 | 1:P8:131:GLN:HB2 | 1.80 | 0.64 |
| 2:P9:392:ASP:OD2 | 2:P9:422:ARG:NH1 | 2.31 | 0.64 |
| 2:R1:223:THR:HG22 | 2:R1:224:TYR:H | 1.63 | 0.64 |
| 2:U1:88:HIS:HB3 | 2:V7:283:HIS:ND1 | 2.12 | 0.64 |
| 1:V8:33:THR:HA | 8:4V:471:SER:OG | 1.98 | 0.64 |
| 1:V8:113:ILE:HD13 | 1:V8:150:LEU:HD22 | 1.79 | 0.64 |
| 1:X4:192:LEU:HD22 | 1:X4:196:ALA:HB2 | 1.79 | 0.64 |
| 1:Z6:3:GLU:HB2 | 1:Z6:130:LEU:HA | 1.79 | 0.64 |
| 2:0P:276:ILE:HG23 | 2:0P:280:LYS:HB3 | 1.80 | 0.64 |
| 2:0X:145:THR:OG1 | 41:0Y:501:GTP:O1B | 2.16 | 0.64 |
| 2:1R:222:PRO:HD2 | 1:1S:324:LYS:HE3 | 1.80 | 0.64 |
| 1:2E:95:THR:CB | 38:8B:83:ARG:HH12 | 2.06 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2F:123:ARG:NH1 | 38:8B:75:SER:O | 2.31 | 0.64 |
| 1:2Q:113:ILE:HA | 1:2Q:116:VAL:HG22 | 1.80 | 0.64 |
| 2:2T:88:HIS:HB3 | 2:3J:283:HIS:ND1 | 2.13 | 0.64 |
| 4:3Y:141:ARG:HH11 | 4:3Y:147:ASN:HB3 | 1.63 | 0.64 |
| 14:5M:382:ASN:ND2 | 23:6R:62:GLN:O | 2.31 | 0.64 |
| 14:5N:450:ARG:HG2 | 14:5N:464:SER:HB2 | 1.79 | 0.64 |
| 15:5P:299:GLU:HA | 15:5P:302:THR:HG22 | 1.78 | 0.64 |
| 15:5P:326:LEU:HD12 | 15:5P:326:LEU:C | 2.17 | 0.64 |
| 22:6I:65:ARG:HE | 22:6I:101:ASN:HB2 | 1.61 | 0.64 |
| 22:6M:188:ARG:NH2 | 22:6M:256:TYR:O | 2.31 | 0.64 |
| 24:6W:416:ILE:HD12 | 24:6W:416:ILE:H | 1.63 | 0.64 |
| 37:7Y:59:PRO:O | 37:7Y:62:GLN:N | 2.30 | 0.64 |
| 38:8B:201:LEU:HD12 | 38:8B:201:LEU:C | 2.16 | 0.64 |
| 2:A0:283:HIS:CD2 | 2:T3:62:VAL:HB | 2.33 | 0.64 |
| 1:A3:41:ASP:HA | 26:7F:25:TYR:CE2 | 2.33 | 0.64 |
| 1:A3:44:LEU:CD1 | 18:6C:36:ASN:O | 2.42 | 0.64 |
| 1:C2:358:PRO:O | 18:6D:22:ARG:NH2 | 2.31 | 0.64 |
| 1:H6:276:ARG:HH11 | 24:6V:490:THR:HA | 1.59 | 0.64 |
| 1:J0:309:ARG:NH1 | 1:J0:339:SER:O | 2.31 | 0.64 |
| 1:J8:309:ARG:H | 1:J8:372:THR:HG22 | 1.62 | 0.64 |
| 1:K4:31:ASP:OD2 | 1:K4:33:THR:OG1 | 2.14 | 0.64 |
| 2:L7:172:TYR:CE2 | 2:L7:203:MET:HG2 | 2.33 | 0.64 |
| 2:M5:76:ASP:HB2 | 37:7Y:119:TRP:CH2 | 2.33 | 0.64 |
| 2:M7:27:GLU:OE1 | 2:M7:243:ARG:NH1 | 2.30 | 0.64 |
| 2:N9:50:ASN:O | 2:N9:64:ARG:NH2 | 2.30 | 0.64 |
| 1:O4:263:LEU:HD13 | 1:O4:422:TYR:CE1 | 2.33 | 0.64 |
| 2:R9:287:SER:OG | 2:R9:290:GLU:OE1 | 2.15 | 0.64 |
| 1:S2:263:LEU:HD21 | 1:S2:425:TYR:HD2 | 1.63 | 0.64 |
| 1:S4:26:ASP:OD1 | 24:6U:10:LYS:HE2 | 1.97 | 0.64 |
| 1:T2:139:LEU:HD12 | 1:T2:170:VAL:HG12 | 1.78 | 0.64 |
| 1:T2:309:ARG:H | 1:T2:372:THR:HG22 | 1.63 | 0.64 |
| 1:T4:306:ARG:HH12 | 13:5J:106:TYR:HB2 | 1.63 | 0.64 |
| 2:Z7:169:PHE:HB3 | 2:Z7:204:LEU:HD11 | 1.78 | 0.64 |
| 1:0A:130:LEU:HD23 | 1:0A:162:ARG:HG3 | 1.78 | 0.64 |
| 2:0B:244:PHE:HB2 | 2:0B:356:ASN:HD21 | 1.62 | 0.64 |
| 2:0J:88:HIS:CE1 | 2:0Z:283:HIS:HA | 2.33 | 0.64 |
| 1:0M:211:CYS:HA | 1:0M:215:LEU:HB2 | 1.80 | 0.64 |
| 1:0S:26:ASP:O | 1:0S:359:LYS:NZ | 2.28 | 0.64 |
| 1:1A:361:LEU:HD12 | 1:1A:362:LYS:H | 1.63 | 0.64 |
| 1:1Q:177:ASP:O | 2:1R:352:LYS:HA | 1.97 | 0.64 |
| 2:2J:88:HIS:ND1 | 2:2J:89:PRO:CD | 2.59 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2P:398:MET:HG2 | 1:2Q:345:ILE:HD13 | 1.78 | 0.64 |
| 1:2Q:306:ARG:HH12 | 38:8A:95:LYS:HA | 1.62 | 0.64 |
| 1:2S:5:VAL:HG23 | 1:2S:62:ARG:HG2 | 1.79 | 0.64 |
| 2:2V:255:PHE:HA | 2:2V:259:LEU:HD13 | 1.80 | 0.64 |
| 2:3F:76:ASP:OD2 | 1:3G:46:ARG:NH2 | 2.31 | 0.64 |
| 1:3O:285:THR:HG23 | 1:3O:288:GLU:H | 1.62 | 0.64 |
| 1:3Q:205:GLU:HG2 | 1:3Q:206:ALA:N | 2.13 | 0.64 |
| 2:3R:236:SER:OG | 2:3R:243:ARG:NH2 | 2.31 | 0.64 |
| 2:3T:199:ASP:OD2 | 2:3T:256:GLN:HG2 | 1.98 | 0.64 |
| 2:3T:267:PHE:HB3 | 2:3T:384:ILE:HG21 | 1.79 | 0.64 |
| 14:5M:450:ARG:HG2 | 14:5M:464:SER:HB2 | 1.79 | 0.64 |
| 35:7T:157:ARG:NH2 | 36:7V:57:ASP:OD1 | 2.31 | 0.64 |
| 1:F2:58:ARG:HD3 | 1:G8:280:GLN:HE22 | 1.63 | 0.63 |
| 1:F8:78:SER:HB3 | 24:6U:499:GLU:HB3 | 1.78 | 0.63 |
| 2:G5:72:PRO:HD2 | 1:G6:2:ARG:NH1 | 2.12 | 0.63 |
| 1:G6:190:HIS:CD2 | 1:G6:411:ALA:HA | 2.33 | 0.63 |
| 2:J9:5:ILE:HG22 | 2:J9:64:ARG:HB3 | 1.79 | 0.63 |
| 2:M3:39:ASP:O | 15:5O:80:ASP:OD1 | 2.16 | 0.63 |
| 2:M3:267:PHE:HB2 | 2:M3:384:ILE:HD12 | 1.78 | 0.63 |
| 1:R2:45:GLU:HG2 | 1:R2:46:ARG:HG2 | 1.79 | 0.63 |
| 2:S5:286:LEU:O | 2:S5:373:ARG:NH1 | 2.30 | 0.63 |
| 1:U8:178:THR:HG23 | 1:U8:181:GLU:HG3 | 1.79 | 0.63 |
| 2:V1:88:HIS:HD2 | 2:V1:89:PRO:CD | 2.04 | 0.63 |
| 1:V4:52:ASN:OD1 | 1:V4:62:ARG:NH2 | 2.32 | 0.63 |
| 2:X5:320:ARG:NH2 | 2:X5:358:GLN:OE1 | 2.31 | 0.63 |
| 1:0A:3:GLU:HB2 | 1:0A:130:LEU:HA | 1.80 | 0.63 |
| 1:0C:31:ASP:OD2 | 1:0C:33:THR:OG1 | 2.15 | 0.63 |
| 1:0E:388:MET:HE1 | 2:0F:347:CYS:HA | 1.79 | 0.63 |
| 2:1B:56:THR:HA | 2:1R:285:GLN:HB2 | 1.79 | 0.63 |
| 2:1V:27:GLU:OE1 | 2:1V:243:ARG:NH1 | 2.30 | 0.63 |
| 2:1V:213:CYS:HA | 2:1V:217:LEU:HB2 | 1.79 | 0.63 |
| 2:2J:123:ARG:NH1 | 38:8C:78:ASP:O | 2.25 | 0.63 |
| 2:2T:56:THR:HA | 2:3J:285:GLN:HB2 | 1.78 | 0.63 |
| 2:3P:279:GLU:OE1 | 2:3P:279:GLU:N | 2.26 | 0.63 |
| 4:4G:141:ARG:HH11 | 4:4G:147:ASN:HB3 | 1.63 | 0.63 |
| 14:5N:165:THR:HG22 | 14:5N:171:MET:SD | 2.37 | 0.63 |
| 19:6E:167:VAL:HB | 19:6E:178:ARG:HH12 | 1.63 | 0.63 |
| 24:6X:460:HIS:HB2 | 24:6X:465:LEU:HD22 | 1.80 | 0.63 |
| 2:2:85:GLN:NE2 | 18:5X:78:LEU:HD22 | 2.13 | 0.63 |
| 1:7:337:ASN:HD21 | 3:4B:68:SER:HA | 1.62 | 0.63 |
| 1:C2:362:LYS:HD3 | 18:6D:24:ARG:HA | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:80:PRO:HB3 | 24:6X:526:PHE:HE2 | 1.63 | 0.63 |
| 1:G8:32:PRO:HD2 | 24:6Z:527:ASN:HD22 | 1.62 | 0.63 |
| 1:L2:134:GLN:HE21 | 1:L2:167:PHE:HE2 | 1.46 | 0.63 |
| 2:M1:88:HIS:O | 1:N8:281:TYR:OH | 2.16 | 0.63 |
| 1:M4:54:ALA:HA | 2:O1:285:GLN:HB2 | 1.79 | 0.63 |
| 2:M5:225:THR:OG1 | 37:7Y:150:ARG:HD3 | 1.98 | 0.63 |
| 1:M8:361:LEU:HD13 | 1:M8:364:SER:HB2 | 1.81 | 0.63 |
| 1:R2:11:GLN:NE2 | 2:R3:249:ASN:OD1 | 2.31 | 0.63 |
| 2:R5:298:PRO:HA | 2:R5:301:MET:HG3 | 1.80 | 0.63 |
| 1:R6:165:LEU:HD11 | 1:R6:250:LEU:HD11 | 1.79 | 0.63 |
| 2:S7:42:ILE:HA | 7:4T:256:TYR:HB3 | 1.78 | 0.63 |
| 2:T1:339:ARG:NH2 | 2:T1:342:GLN:HB3 | 2.14 | 0.63 |
| 2:T5:5:ILE:HG22 | 2:T5:64:ARG:HB3 | 1.80 | 0.63 |
| 2:T7:206:ASN:OD1 | 41:T8:501:GTP:N2 | 2.31 | 0.63 |
| 1:U8:124:ALA:HB1 | 1:U8:130:LEU:HD11 | 1.78 | 0.63 |
| 1:V2:31:ASP:OD2 | 1:V2:33:THR:OG1 | 2.17 | 0.63 |
| 1:V8:273:LEU:H | 1:V8:292:GLN:HE22 | 1.45 | 0.63 |
| 2:W1:236:SER:O | 2:W1:243:ARG:NH2 | 2.29 | 0.63 |
| 2:W9:88:HIS:HB3 | 2:W9:91:GLN:CB | 2.25 | 0.63 |
| 2:X7:339:ARG:HH21 | 2:X7:342:GLN:HA | 1.61 | 0.63 |
| 1:Y0:221:THR:HG23 | 1:Y0:223:GLY:H | 1.61 | 0.63 |
| 1:Z6:14:ASN:ND2 | 1:Z6:65:LEU:HG | 2.14 | 0.63 |
| 1:0G:286:VAL:HG23 | 1:0G:287:PRO:HD3 | 1.79 | 0.63 |
| 1:0I:134:GLN:HE21 | 1:0I:167:PHE:HE2 | 1.46 | 0.63 |
| 2:0L:91:GLN:HE22 | 2:0L:125:LEU:HD11 | 1.64 | 0.63 |
| 2:0X:392:ASP:OD2 | 2:0X:422:ARG:NH1 | 2.31 | 0.63 |
| 2:2F:399:TYR:OH | 2:2F:415:GLU:OE2 | 2.09 | 0.63 |
| 1:2G:350:LYS:NZ | 1:2G:351:SER:O | 2.27 | 0.63 |
| 2:2T:305:CYS:HB3 | 2:2T:387:ILE:HD11 | 1.80 | 0.63 |
| 1:3K:34:GLY:HA3 | 1:3K:58:ARG:HD3 | 1.80 | 0.63 |
| 4:4I:141:ARG:HH11 | 4:4I:147:ASN:HB3 | 1.63 | 0.63 |
| 14:5L:347:ALA:HB3 | 14:5L:357:ALA:HB3 | 1.80 | 0.63 |
| 17:5S:109:ALA:O | 17:5S:113:ILE:HG13 | 1.99 | 0.63 |
| 24:6U:469:PHE:HB2 | 24:6U:484:GLU:HA | 1.80 | 0.63 |
| 24:6U:470:ILE:HD12 | 24:6U:485:PRO:HD3 | 1.80 | 0.63 |
| 38:8A:91:GLN:O | 38:8A:102:PHE:HE1 | 1.80 | 0.63 |
| 38:8B:73:TRP:HD1 | 38:8B:75:SER:HB2 | 1.63 | 0.63 |
| 1:D2:78:SER:HB2 | 24:6X:323:LYS:HG3 | 1.80 | 0.63 |
| 1:G2:388:MET:HE2 | 2:G3:348:PRO:HD2 | 1.78 | 0.63 |
| 1:I2:51:PHE:O | 1:I2:62:ARG:NH2 | 2.31 | 0.63 |
| 1:I2:175:VAL:HG12 | 2:I3:329:ASN:ND2 | 2.14 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J1:176:GLN:HE22 | 2:J1:304:LYS:HE2 | 1.63 | 0.63 |
| 1:L0:52:ASN:OD1 | 1:L0:62:ARG:NH2 | 2.31 | 0.63 |
| 2:M3:369:ALA:HB1 | 30:7K:213:PHE:CD2 | 2.34 | 0.63 |
| 2:N5:287:SER:N | 2:N5:290:GLU:OE2 | 2.30 | 0.63 |
| 2:O9:417:GLU:HA | 2:O9:420:GLU:HG2 | 1.80 | 0.63 |
| 2:P3:51:THR:HG21 | 2:P3:243:ARG:HG2 | 1.81 | 0.63 |
| 2:Q5:88:HIS:ND1 | 2:Q5:89:PRO:HD2 | 2.14 | 0.63 |
| 1:Q8:418:LEU:HG | 1:Q8:422:TYR:HE2 | 1.64 | 0.63 |
| 2:R1:317:LEU:HB3 | 2:R1:319:TYR:HE1 | 1.64 | 0.63 |
| 1:T2:334:GLN:HE22 | 1:T2:348:ASN:H | 1.46 | 0.63 |
| 2:U3:276:ILE:HB | 2:U3:280:LYS:HG3 | 1.79 | 0.63 |
| 1:V2:3:GLU:HB2 | 1:V2:130:LEU:HD13 | 1.80 | 0.63 |
| 2:X5:286:LEU:O | 2:X5:373:ARG:NH1 | 2.32 | 0.63 |
| 1:X6:172:SER:O | 1:X6:176:SER:OG | 2.14 | 0.63 |
| 1:Y4:137:HIS:ND1 | 1:Y4:138:SER:O | 2.29 | 0.63 |
| 2:Y9:278:ALA:HA | 2:Y9:369:ALA:HB2 | 1.80 | 0.63 |
| 1:Z0:58:ARG:HD3 | 1:0G:280:GLN:HE22 | 1.63 | 0.63 |
| 2:Z7:70:LEU:HD21 | 2:Z7:114:ILE:HD13 | 1.80 | 0.63 |
| 1:0I:139:LEU:HD12 | 1:0I:170:VAL:HG22 | 1.79 | 0.63 |
| 1:0M:112:LEU:HB3 | 1:0M:147:MET:HE1 | 1.79 | 0.63 |
| 1:0M:388:MET:SD | 2:0N:348:PRO:HD3 | 2.39 | 0.63 |
| 2:0P:198:THR:HG21 | 2:0P:201:ALA:HB2 | 1.79 | 0.63 |
| 1:1E:350:LYS:NZ | 1:1E:351:SER:O | 2.30 | 0.63 |
| 1:1M:113:ILE:HA | 1:1M:116:VAL:HG12 | 1.79 | 0.63 |
| 2:1P:223:THR:HG22 | 2:1P:224:TYR:H | 1.63 | 0.63 |
| 1:1S:199:CYS:SG | 1:1S:200:MET:N | 2.71 | 0.63 |
| 2:1T:175:PRO:HB3 | 2:1T:390:ARG:HE | 1.63 | 0.63 |
| 2:1T:246:GLY:H | 2:1T:249:ASN:HD21 | 1.47 | 0.63 |
| 2:2L:222:PRO:HD2 | 1:2M:324:LYS:HE3 | 1.79 | 0.63 |
| 2:2P:119:LEU:HA | 2:2P:122:ILE:HG12 | 1.79 | 0.63 |
| 2:2T:133:GLN:HB3 | 2:2T:252:ILE:HG21 | 1.79 | 0.63 |
| 1:2Y:58:ARG:HH12 | 1:2Y:84:ILE:HG22 | 1.62 | 0.63 |
| 1:3A:31:ASP:OD2 | 1:3A:33:THR:OG1 | 2.16 | 0.63 |
| 2:3J:165:SER:HA | 2:3J:199:ASP:OD2 | 1.97 | 0.63 |
| 1:3O:177:ASP:O | 2:3P:352:LYS:HA | 1.98 | 0.63 |
| 1:3S:172:SER:CB | 1:3S:205:GLU:HB2 | 2.29 | 0.63 |
| 1:3S:216:LYS:HB2 | 1:3S:275:SER:OG | 1.97 | 0.63 |
| 4:3W:141:ARG:HH11 | 4:3W:147:ASN:HB3 | 1.63 | 0.63 |
| 8:4W:253:ALA:HA | 8:4W:256:LEU:HD12 | 1.79 | 0.63 |
| 14:5N:347:ALA:HB3 | 14:5N:357:ALA:HB3 | 1.80 | 0.63 |
| 14:5N:557:ASN:OD1 | 14:5N:557:ASN:N | 2.30 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:213:THR:O | 15:5O:217:GLU:CG | 2.46 | 0.63 |
| 22:6I:110:ILE:HB | 22:6I:113:ARG:HH22 | 1.63 | 0.63 |
| 24:6U:354:ARG:HB2 | 24:6U:357:LEU:HG | 1.81 | 0.63 |
| 24:6X:130:MET:HE1 | 24:6X:161:PHE:CB | 2.28 | 0.63 |
| 24:6Y:514:TYR:HA | 24:6Y:517:LEU:HD13 | 1.80 | 0.63 |
| 24:6Z:197:LYS:HD3 | 24:6Z:197:LYS:O | 1.98 | 0.63 |
| 2:A2:42:ILE:HD13 | 24:6Y:93:ARG:CZ | 2.28 | 0.63 |
| 2:E7:282:TYR:CE1 | 22:6L:82:LEU:CD2 | 2.70 | 0.63 |
| 1:F2:12:CYS:HB3 | 39:F2:501:GDP:C8 | 2.32 | 0.63 |
| 2:G7:269:LEU:HD22 | 2:G7:303:VAL:HG21 | 1.80 | 0.63 |
| 2:G9:176:GLN:HG2 | 2:G9:177:VAL:HG23 | 1.81 | 0.63 |
| 2:H5:387:ILE:HG12 | 2:H5:390:ARG:HH22 | 1.64 | 0.63 |
| 2:M3:90:GLU:HG3 | 2:M3:121:ARG:HH12 | 1.61 | 0.63 |
| 1:R8:156:ARG:NH1 | 1:R8:197:ASP:OD1 | 2.31 | 0.63 |
| 1:T8:52:ASN:OD1 | 1:T8:62:ARG:NH2 | 2.30 | 0.63 |
| 2:U7:26:LEU:HD23 | 2:U7:363:VAL:HG12 | 1.81 | 0.63 |
| 2:V7:287:SER:N | 2:V7:290:GLU:OE2 | 2.25 | 0.63 |
| 2:Y9:9:ILE:HG22 | 2:Y9:146:GLY:HA2 | 1.79 | 0.63 |
| 1:Z0:190:HIS:CD2 | 1:Z0:411:ALA:HA | 2.33 | 0.63 |
| 1:0C:211:CYS:HA | 1:0C:215:LEU:HB2 | 1.80 | 0.63 |
| 2:0F:90:GLU:O | 2:0F:121:ARG:NH1 | 2.31 | 0.63 |
| 1:0I:272:PRO:HB2 | 1:0I:282:ARG:HH12 | 1.63 | 0.63 |
| 2:0J:398:MET:HG2 | 1:0K:345:ILE:HG12 | 1.81 | 0.63 |
| 1:0K:309:ARG:H | 1:0K:372:THR:HG22 | 1.63 | 0.63 |
| 1:1M:235:GLY:HA3 | 1:1M:366:THR:HG21 | 1.79 | 0.63 |
| 2:1R:55:GLU:O | 2:1R:55:GLU:HG3 | 1.97 | 0.63 |
| 2:1V:91:GLN:HA | 2:1V:121:ARG:NH1 | 2.07 | 0.63 |
| 2:2P:195:LEU:HD21 | 2:2P:264:ARG:HD2 | 1.79 | 0.63 |
| 1:2Y:332:ASN:OD1 | 38:8B:1:MET:HA | 1.98 | 0.63 |
| 1:3A:248:ALA:HA | 1:3A:252:LYS:HD2 | 1.80 | 0.63 |
| 1:3G:286:VAL:HG23 | 1:3G:287:PRO:HD3 | 1.79 | 0.63 |
| 1:3M:396:HIS:HA | 1:3M:399:THR:HG22 | 1.79 | 0.63 |
| 1:3Q:3:GLU:HG3 | 1:3Q:127:CYS:HB2 | 1.80 | 0.63 |
| 4:3W:35:LYS:NZ | 3:3X:253:ASN:OD1 | 2.18 | 0.63 |
| 4:4A:141:ARG:HH11 | 4:4A:147:ASN:HB3 | 1.63 | 0.63 |
| 4:4C:141:ARG:HH11 | 4:4C:147:ASN:HB3 | 1.63 | 0.63 |
| 4:4E:141:ARG:HH11 | 4:4E:147:ASN:HB3 | 1.63 | 0.63 |
| 5:4M:300:GLU:CD | 28:7X:301:GLU:OE2 | 2.36 | 0.63 |
| 5:4M:300:GLU:OE2 | 28:7X:301:GLU:OE2 | 2.15 | 0.63 |
| 6:4O:137:GLU:HA | 6:4O:140:ARG:HD2 | 1.78 | 0.63 |
| 7:4T:223:GLN:HB3 | 31:7M:22:HIS:NE2 | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:347:ALA:HB3 | 14:5M:357:ALA:HB3 | 1.80 | 0.63 |
| 17:5U:174:SER:CB | 17:5U:175:PRO:CD | 2.76 | 0.63 |
| 19:6E:20:LEU:HD21 | 19:6E:28:ARG:HH21 | 1.61 | 0.63 |
| 21:6G:14:LEU:HD13 | 21:6G:131:TYR:HE2 | 1.64 | 0.63 |
| 23:6R:5:GLN:NE2 | 23:6R:9:ASN:OD1 | 2.30 | 0.63 |
| 24:6Z:277:CYS:HA | 24:6Z:368:LEU:HA | 1.80 | 0.63 |
| 24:7A:6:PRO:CG | 31:7N:83:THR:HG23 | 2.29 | 0.63 |
| 38:8D:158:MET:O | 38:8D:162:VAL:HG23 | 1.99 | 0.63 |
| 1:G2:311:LEU:HD23 | 1:G2:312:THR:HG23 | 1.81 | 0.63 |
| 2:G9:213:CYS:HA | 2:G9:217:LEU:HB2 | 1.80 | 0.63 |
| 2:G9:306:ASP:OD1 | 2:G9:309:HIS:N | 2.32 | 0.63 |
| 2:I9:79:ARG:NH1 | 2:I9:92:LEU:O | 2.32 | 0.63 |
| 1:J0:107:THR:OG1 | 1:J0:401:GLU:OE2 | 2.16 | 0.63 |
| 2:J3:255:PHE:HA | 2:J3:259:LEU:HD13 | 1.80 | 0.63 |
| 2:J5:301:MET:HE1 | 2:J5:307:PRO:HD3 | 1.81 | 0.63 |
| 1:J6:73:MET:HB3 | 1:J6:77:ARG:HH12 | 1.61 | 0.63 |
| 1:K0:107:THR:OG1 | 1:K0:401:GLU:OE2 | 2.15 | 0.63 |
| 2:K7:267:PHE:HB2 | 2:K7:384:ILE:HD12 | 1.80 | 0.63 |
| 1:K8:375:GLN:HB2 | 1:K8:419:VAL:HG23 | 1.79 | 0.63 |
| 1:L0:339:SER:H | 34:7R:140:ASN:ND2 | 1.96 | 0.63 |
| 1:N8:153:SER:HA | 1:N8:195:ASN:HD22 | 1.63 | 0.63 |
| 1:N8:334:GLN:HE22 | 1:N8:348:ASN:H | 1.45 | 0.63 |
| 1:O2:178:THR:HG22 | 2:O3:352:LYS:HZ3 | 1.62 | 0.63 |
| 2:O7:90:GLU:HG3 | 2:O7:121:ARG:NH1 | 2.13 | 0.63 |
| 1:P6:248:ALA:HA | 1:P6:252:LYS:HD2 | 1.81 | 0.63 |
| 2:Q3:381:SER:OG | 2:Q3:382:THR:N | 2.29 | 0.63 |
| 2:R3:410:GLY:O | 17:5T:119:LYS:HE2 | 1.98 | 0.63 |
| 2:S1:9:ILE:HD13 | 2:S1:150:GLY:HA2 | 1.80 | 0.63 |
| 2:T7:286:LEU:O | 2:T7:373:ARG:NH1 | 2.31 | 0.63 |
| 2:U9:5:ILE:HG22 | 2:U9:64:ARG:HB3 | 1.80 | 0.63 |
| 2:W7:88:HIS:HB3 | 2:W7:91:GLN:HB2 | 1.80 | 0.63 |
| 1:X0:42:LEU:CB | 8:4X:97:PHE:CE2 | 2.74 | 0.63 |
| 1:X2:249:ASP:H | 1:X2:252:LYS:HD3 | 1.64 | 0.63 |
| 1:X8:397:TRP:HE1 | 2:X9:260:VAL:HB | 1.64 | 0.63 |
| 2:Y9:33:ASP:O | 2:Y9:60:LYS:NZ | 2.32 | 0.63 |
| 1:0A:20:PHE:CE1 | 1:0A:233:MET:HG2 | 2.34 | 0.63 |
| 1:0E:66:MET:HE1 | 1:0E:112:LEU:HD21 | 1.81 | 0.63 |
| 1:0Q:3:GLU:HB2 | 1:0Q:130:LEU:HA | 1.80 | 0.63 |
| 1:0S:2:ARG:HE | 1:0S:240:LEU:HD22 | 1.62 | 0.63 |
| 2:1D:344:VAL:HG21 | 2:1D:346:TRP:CD1 | 2.33 | 0.63 |
| 2:1N:85:GLN:O | 2:2D:283:HIS:NE2 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:234:VAL:O | 2:2N:237:SER:OG | 2.14 | 0.63 |
| 1:2U:34:GLY:O | 1:2U:58:ARG:HA | 1.98 | 0.63 |
| 2:2V:71:GLU:HB3 | 2:2V:98:ASP:OD1 | 1.99 | 0.63 |
| 2:3B:223:THR:HA | 1:3C:323:THR:HG22 | 1.81 | 0.63 |
| 1:3I:77:ARG:HH22 | 3:3Z:18:LYS:HB3 | 1.64 | 0.63 |
| 1:3K:2:ARG:HE | 1:3K:240:LEU:HD22 | 1.64 | 0.63 |
| 8:4W:463:THR:HG22 | 8:4W:464:VAL:HG22 | 1.78 | 0.63 |
| 18:5Z:101:LYS:O | 24:6W:178:ASN:ND2 | 2.31 | 0.63 |
| 20:6F:125:LYS:CD | 20:6F:344:LEU:HD21 | 2.29 | 0.63 |
| 24:6V:574:ARG:O | 24:6V:578:ILE:HG12 | 1.99 | 0.63 |
| 24:6W:378:TRP:O | 24:6W:382:ASN:ND2 | 2.32 | 0.63 |
| 24:6Y:456:ASP:O | 24:6Y:459:LYS:NZ | 2.31 | 0.63 |
| 34:7S:123:ASN:HA | 34:7S:126:LYS:HG2 | 1.80 | 0.63 |
| 38:8A:73:TRP:CE2 | 38:8A:76:ASP:HB3 | 2.33 | 0.63 |
| 2:C1:206:ASN:ND2 | 41:C1:501:GTP:O2' | 2.31 | 0.63 |
| 1:C2:320:ARG:NE | 18:6D:52:ALA:O | 2.31 | 0.63 |
| 1:G2:52:ASN:OD1 | 1:G2:62:ARG:NH2 | 2.32 | 0.63 |
| 2:I3:222:PRO:HD2 | 1:I4:324:LYS:HE3 | 1.81 | 0.63 |
| 1:I8:58:ARG:HG2 | 1:K4:280:GLN:HE22 | 1.63 | 0.63 |
| 1:I8:113:ILE:HD13 | 1:I8:150:LEU:HD22 | 1.81 | 0.63 |
| 1:J4:274:THR:HG21 | 1:J4:282:ARG:HD3 | 1.79 | 0.63 |
| 2:K7:121:ARG:HD2 | 2:K7:121:ARG:O | 1.97 | 0.63 |
| 2:L3:222:PRO:HD2 | 1:L4:324:LYS:HE3 | 1.80 | 0.63 |
| 2:L9:109:THR:OG1 | 2:L9:411:GLU:OE2 | 2.14 | 0.63 |
| 1:N8:2:ARG:HE | 1:N8:240:LEU:HD22 | 1.64 | 0.63 |
| 1:P4:45:GLU:HG3 | 1:P4:46:ARG:HG2 | 1.79 | 0.63 |
| 2:R7:287:SER:N | 2:R7:290:GLU:OE2 | 2.32 | 0.63 |
| 2:R9:196:GLU:HA | 17:5U:84:ARG:HD2 | 1.79 | 0.63 |
| 1:S4:287:PRO:HA | 1:S4:329:GLN:HE22 | 1.64 | 0.63 |
| 1:S6:209:ASP:OD1 | 1:S6:213:ARG:HD3 | 1.99 | 0.63 |
| 2:T7:53:PHE:HB3 | 2:T7:61:HIS:HB3 | 1.80 | 0.63 |
| 1:U8:140:GLY:O | 1:U8:184:ASN:ND2 | 2.29 | 0.63 |
| 2:W9:406:HIS:HA | 2:W9:409:VAL:HG22 | 1.81 | 0.63 |
| 1:X2:252:LYS:HD2 | 1:X2:252:LYS:H | 1.63 | 0.63 |
| 1:X6:5:VAL:HG23 | 1:X6:62:ARG:HG2 | 1.80 | 0.63 |
| 1:X8:184:ASN:OD1 | 1:X8:398:TYR:OH | 2.15 | 0.63 |
| 2:Y1:417:GLU:HA | 2:Y1:420:GLU:HG2 | 1.81 | 0.63 |
| 2:Y9:72:PRO:HD2 | 1:Z0:2:ARG:NH1 | 2.13 | 0.63 |
| 1:0A:2:ARG:HB3 | 1:0A:131:GLN:HB2 | 1.79 | 0.63 |
| 1:0K:388:MET:N | 1:0K:388:MET:HE1 | 2.14 | 0.63 |
| 1:0M:207:LEU:HD11 | 1:0M:229:ILE:HD11 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2I:125:GLU:OE2 | 1:2I:159:TYR:OH | 2.16 | 0.63 |
| 2:2P:230:LEU:HD11 | 2:2P:275:ILE:HD13 | 1.81 | 0.63 |
| 2:3F:124:LYS:HZ2 | 3:3V:36:PHE:HD1 | 1.45 | 0.63 |
| 2:3N:189:LEU:HD11 | 2:3N:418:PHE:HE1 | 1.63 | 0.63 |
| 1:3O:211:CYS:SG | 1:3O:220:PRO:HB3 | 2.39 | 0.63 |
| 6:4O:89:ARG:NH1 | 30:7K:450:GLN:O | 2.31 | 0.63 |
| 6:4P:47:ASN:O | 6:4P:51:VAL:HG23 | 1.98 | 0.63 |
| 11:5E:14:TRP:CZ3 | 11:5E:103:VAL:HG23 | 2.33 | 0.63 |
| 14:5L:112:SER:CA | 14:5L:155:PHE:CD2 | 2.80 | 0.63 |
| 14:5L:587:CYS:HB3 | 14:5L:589:PHE:HD1 | 1.63 | 0.63 |
| 15:5O:5:LEU:HD11 | 15:5O:82:PHE:HZ | 1.64 | 0.63 |
| 15:5O:73:LEU:H | 15:5O:73:LEU:HD23 | 1.62 | 0.63 |
| 15:5O:93:ARG:HG2 | 15:5O:164:VAL:HG22 | 1.81 | 0.63 |
| 15:5O:97:MET:SD | 15:5O:206:HIS:HB3 | 2.39 | 0.63 |
| 23:6Q:5:GLN:NE2 | 23:6Q:9:ASN:OD1 | 2.30 | 0.63 |
| 24:6T:482:ILE:HD13 | 24:6T:498:LEU:HD23 | 1.80 | 0.63 |
| 24:6V:613:LYS:O | 24:6V:617:ASP:HB2 | 1.98 | 0.63 |
| 24:6W:96:LEU:HB2 | 24:6W:123:TYR:HB3 | 1.80 | 0.63 |
| 31:7N:114:GLU:O | 31:7N:114:GLU:HG2 | 1.99 | 0.63 |
| 1:A7:11:GLN:N | 39:A7:501:GDP:O2B | 2.26 | 0.63 |
| 2:B0:226:ASN:ND2 | 18:5Y:51:MET:SD | 2.71 | 0.63 |
| 1:G2:135:VAL:HG21 | 1:G2:152:ILE:HD11 | 1.80 | 0.63 |
| 1:H4:113:ILE:HD13 | 1:H4:150:LEU:HD22 | 1.80 | 0.63 |
| 1:I0:219:THR:H | 24:6X:489:ASN:HB3 | 1.64 | 0.63 |
| 2:I3:90:GLU:HB3 | 2:I3:121:ARG:HH22 | 1.63 | 0.63 |
| 2:J1:392:ASP:OD2 | 2:J1:422:ARG:NH1 | 2.32 | 0.63 |
| 2:K9:189:LEU:HD11 | 2:K9:418:PHE:HE1 | 1.63 | 0.63 |
| 2:L5:9:ILE:HD13 | 2:L5:150:GLY:HA2 | 1.79 | 0.63 |
| 2:M7:406:HIS:HA | 2:M7:409:VAL:HG22 | 1.80 | 0.63 |
| 2:M9:222:PRO:HD2 | 1:N0:324:LYS:HE3 | 1.80 | 0.63 |
| 1:N2:391:ARG:HH22 | 2:N3:435:VAL:HA | 1.64 | 0.63 |
| 1:O6:2:ARG:HE | 1:O6:240:LEU:HD22 | 1.63 | 0.63 |
| 1:P8:53:GLU:OE1 | 7:4R:109:GLN:HG2 | 1.98 | 0.63 |
| 2:Q1:51:THR:HG21 | 2:Q1:243:ARG:HG2 | 1.80 | 0.63 |
| 2:Q1:392:ASP:OD2 | 2:Q1:422:ARG:NH1 | 2.32 | 0.63 |
| 2:Q9:409:VAL:HG11 | 17:5S:115:ALA:HB3 | 1.79 | 0.63 |
| 1:R8:101:TRP:HD1 | 1:R8:145:SER:HG | 1.45 | 0.63 |
| 2:S7:414:GLU:N | 2:S7:414:GLU:OE1 | 2.31 | 0.63 |
| 1:T6:139:LEU:HD12 | 1:T6:170:VAL:HG12 | 1.80 | 0.63 |
| 1:U2:226:ASN:HD21 | 39:U2:502:GDP:HN1 | 1.45 | 0.63 |
| 1:X0:107:THR:OG1 | 1:X0:401:GLU:OE2 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z6:52:ASN:OD1 | 1:Z6:62:ARG:NH2 | 2.32 | 0.63 |
| 2:0N:336:LYS:O | 2:0N:339:ARG:NH2 | 2.30 | 0.63 |
| 2:1F:392:ASP:OD2 | 2:1F:422:ARG:NH1 | 2.32 | 0.63 |
| 1:2A:114:ASP:HB2 | 38:8A:101:ASP:HB3 | 1.81 | 0.63 |
| 1:2E:12:CYS:SG | 1:2E:138:SER:HB3 | 2.39 | 0.63 |
| 2:2J:161:TYR:CD1 | 38:8C:80:TYR:HB3 | 2.33 | 0.63 |
| 2:2Z:88:HIS:ND1 | 2:2Z:89:PRO:CD | 2.60 | 0.63 |
| 2:3L:286:LEU:O | 2:3L:373:ARG:NH1 | 2.31 | 0.63 |
| 10:5C:477:LYS:NZ | 10:5D:151:ASN:OD1 | 2.31 | 0.63 |
| 14:5M:587:CYS:HB3 | 14:5M:589:PHE:HD1 | 1.63 | 0.63 |
| 23:6S:5:GLN:NE2 | 23:6S:9:ASN:OD1 | 2.30 | 0.63 |
| 24:6X:130:MET:HE1 | 24:6X:161:PHE:HB2 | 1.81 | 0.63 |
| 29:7J:319:ILE:CG2 | 29:7J:320:PRO:CD | 2.60 | 0.63 |
| 32:7P:129:ARG:HD2 | 32:7P:131:GLN:HE21 | 1.62 | 0.63 |
| 2:F9:56:THR:HA | 2:H5:285:GLN:HB2 | 1.81 | 0.63 |
| 1:G6:77:ARG:HG3 | 1:G6:90:PHE:HE2 | 1.63 | 0.63 |
| 1:G8:334:GLN:HE22 | 1:G8:348:ASN:H | 1.47 | 0.63 |
| 2:H1:11:GLN:NE2 | 1:H2:247:ASN:OD1 | 2.32 | 0.63 |
| 2:H3:85:GLN:OE1 | 2:H3:85:GLN:HA | 1.99 | 0.63 |
| 1:H6:218:THR:HB | 24:6V:488:ARG:HB3 | 1.81 | 0.63 |
| 2:H9:90:GLU:HG2 | 2:H9:121:ARG:HH12 | 1.63 | 0.63 |
| 2:I3:406:HIS:HA | 2:I3:409:VAL:HG22 | 1.81 | 0.63 |
| 1:I8:248:ALA:HA | 1:I8:252:LYS:HD2 | 1.80 | 0.63 |
| 2:J1:264:ARG:NH2 | 2:J1:431:ASP:OD2 | 2.32 | 0.63 |
| 2:K5:109:THR:OG1 | 2:K5:411:GLU:OE2 | 2.15 | 0.63 |
| 1:K8:207:LEU:HB3 | 1:K8:225:LEU:HD22 | 1.79 | 0.63 |
| 1:L0:134:GLN:HE21 | 1:L0:167:PHE:HE2 | 1.45 | 0.63 |
| 2:L3:287:SER:N | 2:L3:290:GLU:OE2 | 2.32 | 0.63 |
| 2:L7:370:LYS:HD2 | 6:4P:201:VAL:HG11 | 1.80 | 0.63 |
| 2:M3:50:ASN:O | 2:M3:64:ARG:NH2 | 2.32 | 0.63 |
| 1:M6:113:ILE:HA | 1:M6:116:VAL:HG12 | 1.79 | 0.63 |
| 2:N1:285:GLN:HG3 | 30:7L:333:VAL:HG21 | 1.80 | 0.63 |
| 2:O5:405:VAL:HG13 | 2:O5:418:PHE:HE2 | 1.63 | 0.63 |
| 1:P6:2:ARG:HB3 | 1:P6:131:GLN:HB2 | 1.79 | 0.63 |
| 1:P8:135:VAL:HG21 | 1:P8:152:ILE:HD11 | 1.80 | 0.63 |
| 2:R5:42:ILE:HD11 | 11:5E:129:LYS:HD2 | 1.81 | 0.63 |
| 2:S5:413:MET:HB3 | 2:S5:417:GLU:OE2 | 1.99 | 0.63 |
| 1:W0:140:GLY:O | 1:W0:184:ASN:ND2 | 2.32 | 0.63 |
| 2:W3:72:PRO:HD2 | 1:W4:2:ARG:HH12 | 1.64 | 0.63 |
| 1:W6:377:MET:SD | 1:W6:380:ARG:NH2 | 2.72 | 0.63 |
| 1:X4:2:ARG:HE | 1:X4:240:LEU:HD22 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0E:5:VAL:HG23 | 1:0E:62:ARG:HG2 | 1.80 | 0.63 |
| 2:1H:253:THR:HA | 2:1H:256:GLN:NE2 | 2.13 | 0.63 |
| 1:1M:2:ARG:HH21 | 1:1M:240:LEU:HA | 1.64 | 0.63 |
| 2:1R:269:LEU:HD11 | 2:1R:384:ILE:HG23 | 1.81 | 0.63 |
| 1:2C:207:LEU:HB3 | 1:2C:225:LEU:HD22 | 1.81 | 0.63 |
| 2:2D:428:LEU:HG | 2:2D:432:PHE:HE2 | 1.64 | 0.63 |
| 1:2I:135:VAL:HG21 | 1:2I:152:ILE:HD11 | 1.78 | 0.63 |
| 2:2L:156:ARG:NH2 | 38:8C:29:GLY:HA2 | 2.14 | 0.63 |
| 2:2V:109:THR:OG1 | 2:2V:411:GLU:OE2 | 2.13 | 0.63 |
| 1:2W:345:ILE:O | 1:2W:348:ASN:ND2 | 2.32 | 0.63 |
| 2:2Z:335:ILE:HG23 | 2:2Z:341:ILE:HD11 | 1.80 | 0.63 |
| 1:3S:117:LEU:HA | 1:3S:120:VAL:HG12 | 1.81 | 0.63 |
| 14:5N:587:CYS:HB3 | 14:5N:589:PHE:HD1 | 1.63 | 0.63 |
| 15:5P:280:GLU:HG3 | 19:6E:114:GLU:HG3 | 1.81 | 0.63 |
| 18:5X:180:ARG:HH21 | 18:5X:180:ARG:CG | 2.10 | 0.63 |
| 18:5Y:5:VAL:HG12 | 18:5Y:5:VAL:O | 1.99 | 0.63 |
| 19:6E:92:ARG:HG3 | 19:6E:99:ARG:NE | 2.14 | 0.63 |
| 24:6T:469:PHE:CD2 | 24:6T:482:ILE:HG23 | 2.34 | 0.63 |
| 31:7N:80:PRO:O | 31:7N:83:THR:HG22 | 1.98 | 0.63 |
| 1:9:78:SER:OG | 24:6X:149:LYS:HG3 | 1.99 | 0.63 |
| 1:A3:340:TYR:CD1 | 3:4H:104:PRO:HD3 | 2.33 | 0.63 |
| 2:F3:364:PRO:HG2 | 22:6P:123:PRO:HB2 | 1.79 | 0.63 |
| 2:G5:66:ILE:HG21 | 2:G5:122:ILE:HD11 | 1.81 | 0.63 |
| 1:J0:220:PRO:HD2 | 2:J1:326:LYS:HD3 | 1.80 | 0.63 |
| 1:J4:309:ARG:NH1 | 1:J4:339:SER:O | 2.32 | 0.63 |
| 1:J8:113:ILE:HA | 1:J8:116:VAL:HG12 | 1.81 | 0.63 |
| 2:L3:267:PHE:HB2 | 2:L3:384:ILE:HD12 | 1.81 | 0.63 |
| 1:M4:177:ASP:O | 2:M5:352:LYS:HA | 1.99 | 0.63 |
| 1:O2:130:LEU:HB2 | 1:O2:162:ARG:HE | 1.63 | 0.63 |
| 2:O7:286:LEU:O | 2:O7:373:ARG:NH1 | 2.32 | 0.63 |
| 1:O8:273:LEU:H | 1:O8:292:GLN:HE22 | 1.46 | 0.63 |
| 2:P9:15:GLN:HB3 | 2:P9:228:ASN:HD21 | 1.63 | 0.63 |
| 2:R1:290:GLU:HA | 2:R1:293:ASN:HD22 | 1.64 | 0.63 |
| 1:V6:113:ILE:HA | 1:V6:116:VAL:HG12 | 1.81 | 0.63 |
| 1:W0:207:LEU:HD11 | 1:W0:229:ILE:HD11 | 1.80 | 0.63 |
| 1:W2:309:ARG:NH1 | 1:W2:339:SER:O | 2.32 | 0.63 |
| 1:W8:128:ASP:OD1 | 1:W8:129:CYS:N | 2.32 | 0.63 |
| 2:X3:258:ASN:HB3 | 2:X3:352:LYS:HG3 | 1.80 | 0.63 |
| 1:Y0:192:LEU:HD22 | 1:Y0:196:ALA:HB2 | 1.81 | 0.63 |
| 1:Z2:52:ASN:OD1 | 1:Z2:62:ARG:NH2 | 2.32 | 0.63 |
| 2:Z3:15:GLN:HB3 | 2:Z3:228:ASN:HD21 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z5:286:LEU:O | 2:Z5:373:ARG:NH1 | 2.32 | 0.63 |
| 1:0E:52:ASN:OD1 | 1:0E:62:ARG:NH2 | 2.32 | 0.63 |
| 2:0F:313:MET:HG3 | 2:0F:346:TRP:CH2 | 2.34 | 0.63 |
| 2:0L:176:GLN:HE22 | 2:0L:304:LYS:HE2 | 1.63 | 0.63 |
| 1:0O:33:THR:O | 1:0O:58:ARG:NH2 | 2.32 | 0.63 |
| 2:0P:392:ASP:OD2 | 2:0P:422:ARG:NH1 | 2.31 | 0.63 |
| 2:0Z:317:LEU:HB3 | 2:0Z:319:TYR:HE1 | 1.64 | 0.63 |
| 2:1H:387:ILE:HG12 | 2:1H:390:ARG:HH22 | 1.64 | 0.63 |
| 1:1M:173:PRO:HB3 | 1:1M:384:GLN:HE22 | 1.64 | 0.63 |
| 2:1N:223:THR:HG22 | 2:1N:224:TYR:H | 1.63 | 0.63 |
| 1:1U:289:LEU:HD21 | 1:1U:363:MET:HG2 | 1.79 | 0.63 |
| 2:1V:277:SER:OG | 2:1V:280:LYS:HG2 | 1.99 | 0.63 |
| 1:3C:375:GLN:NE2 | 1:3C:376:GLU:OE1 | 2.32 | 0.63 |
| 2:3D:79:ARG:NH1 | 2:3D:94:SER:OG | 2.32 | 0.63 |
| 1:3S:172:SER:HB2 | 1:3S:205:GLU:HB2 | 1.81 | 0.63 |
| 14:5M:229:LYS:O | 14:5M:230:ASN:O | 2.16 | 0.63 |
| 22:6J:184:ALA:HA | 22:6J:187:MET:HE2 | 1.81 | 0.63 |
| 22:6P:227:TYR:HD1 | 22:6P:238:LEU:HD21 | 1.64 | 0.63 |
| 24:6T:470:ILE:HD12 | 24:6T:485:PRO:CG | 2.28 | 0.63 |
| 24:6T:482:ILE:HD12 | 24:6T:482:ILE:N | 2.13 | 0.63 |
| 36:7V:57:ASP:O | 36:7V:61:GLU:HG2 | 1.99 | 0.63 |
| 36:7W:57:ASP:O | 36:7W:61:GLU:HG2 | 1.99 | 0.63 |
| 1:B5:362:LYS:CE | 18:6A:24:ARG:HD3 | 2.28 | 0.62 |
| 2:H7:287:SER:N | 2:H7:290:GLU:OE2 | 2.32 | 0.62 |
| 2:I1:195:LEU:HD21 | 2:I1:264:ARG:HH21 | 1.64 | 0.62 |
| 2:I3:264:ARG:NH2 | 2:I3:431:ASP:OD2 | 2.32 | 0.62 |
| 1:I8:74:ASP:OD1 | 1:I8:77:ARG:NH1 | 2.31 | 0.62 |
| 1:J6:248:ALA:HA | 1:J6:252:LYS:HD2 | 1.81 | 0.62 |
| 1:K0:69:GLU:C | 1:K0:92:PHE:HZ | 2.01 | 0.62 |
| 2:K7:167:LEU:HD13 | 2:K7:200:VAL:HB | 1.81 | 0.62 |
| 2:M9:317:LEU:HB3 | 2:M9:319:TYR:HE1 | 1.63 | 0.62 |
| 1:Q8:361:LEU:HG | 24:6T:11:LEU:HD22 | 1.80 | 0.62 |
| 2:R7:90:GLU:HB2 | 2:R7:121:ARG:HH22 | 1.63 | 0.62 |
| 1:S2:52:ASN:OD1 | 1:S2:62:ARG:NH2 | 2.32 | 0.62 |
| 1:U6:3:GLU:HB3 | 1:U6:130:LEU:HA | 1.81 | 0.62 |
| 1:U6:282:ARG:NH1 | 1:U6:288:GLU:HB3 | 2.04 | 0.62 |
| 2:V3:56:THR:HA | 2:W9:285:GLN:HB2 | 1.80 | 0.62 |
| 1:V6:159:TYR:HB3 | 1:V6:162:ARG:HD3 | 1.81 | 0.62 |
| 1:W6:107:THR:OG1 | 1:W6:401:GLU:OE2 | 2.12 | 0.62 |
| 2:X5:83:TYR:HB3 | 2:X5:86:LEU:HB3 | 1.80 | 0.62 |
| 1:X6:244:GLY:HA2 | 1:X6:355:ASP:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y0:177:ASP:O | 2:Y1:352:LYS:HA | 1.98 | 0.62 |
| 2:Y9:90:GLU:O | 2:Y9:121:ARG:NH1 | 2.30 | 0.62 |
| 2:0L:407:TRP:HZ2 | 1:0M:258:ILE:HB | 1.64 | 0.62 |
| 1:0O:309:ARG:H | 1:0O:372:THR:HG22 | 1.64 | 0.62 |
| 2:0P:90:GLU:O | 2:0P:121:ARG:NH1 | 2.32 | 0.62 |
| 1:0Q:211:CYS:HA | 1:0Q:215:LEU:HB2 | 1.81 | 0.62 |
| 1:0W:309:ARG:NH1 | 1:0W:339:SER:O | 2.32 | 0.62 |
| 2:1L:72:PRO:HG3 | 1:1M:1:MET:HG2 | 1.81 | 0.62 |
| 1:1S:156:ARG:NH1 | 1:1S:197:ASP:OD1 | 2.32 | 0.62 |
| 1:2M:207:LEU:HB3 | 1:2M:225:LEU:HD22 | 1.81 | 0.62 |
| 2:2T:308:ARG:HH21 | 38:8A:28:THR:CG2 | 2.05 | 0.62 |
| 1:3A:139:LEU:HD12 | 1:3A:170:VAL:HG12 | 1.79 | 0.62 |
| 5:4L:292:ALA:HA | 5:4L:295:LYS:HD3 | 1.81 | 0.62 |
| 8:4W:467:PRO:HD3 | 8:4X:124:LEU:HD21 | 1.80 | 0.62 |
| 11:5E:184:VAL:HG21 | 11:5E:226:LEU:HD11 | 1.80 | 0.62 |
| 13:5J:92:GLU:H | 13:5J:92:GLU:CD | 2.02 | 0.62 |
| 13:5K:92:GLU:H | 13:5K:92:GLU:CD | 2.02 | 0.62 |
| 15:5O:101:ASP:OD2 | 15:5O:101:ASP:N | 2.19 | 0.62 |
| 22:6K:311:VAL:HA | 22:6K:321:LEU:HD23 | 1.80 | 0.62 |
| 22:6N:136:ASN:HD22 | 22:6N:208:ARG:HH22 | 1.44 | 0.62 |
| 24:6V:484:GLU:O | 24:6V:484:GLU:HG3 | 1.98 | 0.62 |
| 1:A3:383:GLU:OE2 | 3:4H:50:LYS:CE | 2.48 | 0.62 |
| 1:E6:52:ASN:HA | 22:6L:181:ASN:ND2 | 1.28 | 0.62 |
| 2:F5:221:ARG:NH1 | 22:6I:177:LEU:O | 2.31 | 0.62 |
| 2:H1:76:ASP:OD2 | 1:H2:46:ARG:NH2 | 2.32 | 0.62 |
| 1:I4:219:THR:HA | 2:I5:326:LYS:HZ1 | 1.63 | 0.62 |
| 2:J1:222:PRO:HD2 | 1:J2:324:LYS:HE3 | 1.80 | 0.62 |
| 2:J3:14:ILE:HD11 | 2:J3:74:VAL:HG13 | 1.80 | 0.62 |
| 2:J7:282:TYR:CE1 | 5:4M:209:LEU:HD23 | 2.34 | 0.62 |
| 1:K0:113:ILE:HA | 1:K0:116:VAL:HG12 | 1.80 | 0.62 |
| 1:M2:113:ILE:HA | 1:M2:116:VAL:HG22 | 1.81 | 0.62 |
| 2:M9:195:LEU:HD21 | 2:M9:264:ARG:HH11 | 1.62 | 0.62 |
| 2:P5:15:GLN:HB3 | 2:P5:228:ASN:HD21 | 1.63 | 0.62 |
| 2:Q3:83:TYR:HB3 | 2:Q3:86:LEU:HB3 | 1.81 | 0.62 |
| 2:Q3:308:ARG:NH1 | 2:V1:282:TYR:OH | 2.28 | 0.62 |
| 1:R4:156:ARG:NH1 | 1:R4:197:ASP:OD1 | 2.32 | 0.62 |
| 2:T5:267:PHE:HB2 | 2:T5:384:ILE:HD12 | 1.80 | 0.62 |
| 2:V1:88:HIS:CD2 | 2:V1:89:PRO:CD | 2.79 | 0.62 |
| 1:X0:335:ASN:O | 1:X0:338:SER:OG | 2.18 | 0.62 |
| 1:X2:3:GLU:HB2 | 1:X2:130:LEU:HA | 1.81 | 0.62 |
| 2:X7:9:ILE:HG13 | 2:X7:68:LEU:HD21 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z6:116:VAL:HA | 1:Z6:119:VAL:HG12 | 1.81 | 0.62 |
| 1:0A:113:ILE:HD11 | 1:0A:151:LEU:HA | 1.82 | 0.62 |
| 1:0C:273:LEU:H | 1:0C:292:GLN:HE22 | 1.45 | 0.62 |
| 2:0N:100:ALA:HA | 1:0O:252:LYS:HE2 | 1.80 | 0.62 |
| 2:0N:344:VAL:HG21 | 2:0N:346:TRP:HE3 | 1.64 | 0.62 |
| 2:0R:88:HIS:HB3 | 2:1H:283:HIS:ND1 | 2.13 | 0.62 |
| 2:0V:3:GLU:HG3 | 2:0V:129:CYS:HB2 | 1.81 | 0.62 |
| 1:1K:35:THR:HG1 | 1:1K:37:HIS:HE2 | 1.47 | 0.62 |
| 2:2F:204:LEU:HD23 | 2:2F:231:ILE:HD12 | 1.79 | 0.62 |
| 2:2H:279:GLU:OE1 | 10:5B:167:ILE:CD1 | 2.47 | 0.62 |
| 2:2Z:399:TYR:O | 2:2Z:402:ARG:NH1 | 2.32 | 0.62 |
| 1:3I:52:ASN:H | 1:3I:52:ASN:ND2 | 1.96 | 0.62 |
| 1:3M:249:ASP:OD1 | 1:3M:250:LEU:N | 2.30 | 0.62 |
| 13:5H:92:GLU:CD | 13:5H:92:GLU:H | 2.02 | 0.62 |
| 14:5L:511:THR:HB | 14:5L:531:ASP:HB3 | 1.81 | 0.62 |
| 19:6E:29:GLU:OE2 | 19:6E:29:GLU:HA | 1.99 | 0.62 |
| 24:6X:442:ASP:OD1 | 24:6X:443:LYS:HG3 | 1.99 | 0.62 |
| 1:G8:211:CYS:HA | 1:G8:215:LEU:HB2 | 1.81 | 0.62 |
| 2:H9:286:LEU:O | 2:H9:373:ARG:NH1 | 2.32 | 0.62 |
| 2:J1:283:HIS:HD2 | 2:J1:284:GLU:HB2 | 1.64 | 0.62 |
| 2:J7:267:PHE:HB2 | 2:J7:384:ILE:HD12 | 1.81 | 0.62 |
| 2:K1:213:CYS:HA | 2:K1:217:LEU:HB2 | 1.81 | 0.62 |
| 2:L5:98:ASP:OD1 | 2:L5:99:ALA:N | 2.32 | 0.62 |
| 2:M9:396:ASP:HB2 | 2:M9:422:ARG:HH12 | 1.64 | 0.62 |
| 1:N6:320:ARG:CZ | 32:7O:64:THR:HG22 | 2.29 | 0.62 |
| 2:O3:89:PRO:HG2 | 2:Q1:279:GLU:OE1 | 1.99 | 0.62 |
| 1:O6:253:LEU:HD11 | 1:O6:316:LEU:HD11 | 1.82 | 0.62 |
| 2:P5:69:ASP:OD1 | 2:P5:70:LEU:N | 2.32 | 0.62 |
| 1:R6:238:CYS:SG | 1:R6:318:ARG:NE | 2.73 | 0.62 |
| 2:R7:27:GLU:OE1 | 2:R7:243:ARG:NH1 | 2.32 | 0.62 |
| 1:S6:173:PRO:HB3 | 1:S6:384:GLN:HE22 | 1.62 | 0.62 |
| 2:U5:88:HIS:HB3 | 2:W1:283:HIS:ND1 | 2.14 | 0.62 |
| 2:U9:73:THR:O | 2:U9:77:GLU:HG2 | 1.98 | 0.62 |
| 2:W1:305:CYS:HB3 | 2:W1:387:ILE:HD11 | 1.80 | 0.62 |
| 1:W8:286:VAL:HG21 | 1:W8:325:GLU:HB3 | 1.81 | 0.62 |
| 1:X2:309:ARG:NH1 | 1:X2:339:SER:O | 2.32 | 0.62 |
| 1:X2:320:ARG:HH12 | 1:X2:357:PRO:HD3 | 1.63 | 0.62 |
| 2:0B:268:MET:HE2 | 2:0B:380:ASN:HB2 | 1.81 | 0.62 |
| 2:1N:85:GLN:CA | 2:1N:85:GLN:HE21 | 2.12 | 0.62 |
| 2:1P:387:ILE:HG12 | 2:1P:390:ARG:HH22 | 1.63 | 0.62 |
| 2:1V:170:THR:OG1 | 2:1V:203:MET:SD | 2.57 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:154:LEU:HG | 2:2N:197:HIS:HB3 | 1.81 | 0.62 |
| 2:2R:132:LEU:HD22 | 2:2R:164:LYS:HD3 | 1.80 | 0.62 |
| 1:3C:345:ILE:O | 1:3C:348:ASN:ND2 | 2.32 | 0.62 |
| 2:3N:417:GLU:HA | 2:3N:420:GLU:HG2 | 1.81 | 0.62 |
| 1:3S:362:LYS:HE2 | 38:8D:166:GLU:CB | 2.30 | 0.62 |
| 3:3Z:17:VAL:HG23 | 3:3Z:18:LYS:HG3 | 1.81 | 0.62 |
| 3:3Z:63:SER:OG | 3:3Z:68:SER:O | 2.16 | 0.62 |
| 3:4D:63:SER:OG | 3:4D:68:SER:O | 2.16 | 0.62 |
| 6:4O:421:ARG:O | 6:4O:425:GLU:HG2 | 1.99 | 0.62 |
| 11:5E:14:TRP:CH2 | 11:5E:103:VAL:CG2 | 2.83 | 0.62 |
| 13:5I:92:GLU:CD | 13:5I:92:GLU:H | 2.02 | 0.62 |
| 22:6K:180:SER:O | 22:6K:183:ASN:ND2 | 2.31 | 0.62 |
| 23:6R:48:TYR:CE2 | 23:6R:52:LEU:HD12 | 2.34 | 0.62 |
| 24:6X:95:VAL:CG1 | 24:6X:124:TYR:HD2 | 2.09 | 0.62 |
| 38:8B:160:ASP:N | 38:8B:160:ASP:OD2 | 2.32 | 0.62 |
| 38:8D:73:TRP:CD1 | 38:8D:75:SER:HB2 | 2.34 | 0.62 |
| 2:E5:364:PRO:HG2 | 22:6L:123:PRO:HB2 | 1.80 | 0.62 |
| 1:H8:177:ASP:O | 2:H9:352:LYS:HA | 1.99 | 0.62 |
| 2:I5:142:GLY:HA2 | 2:I5:183:GLU:HG3 | 1.81 | 0.62 |
| 1:I8:391:ARG:HD2 | 2:I9:346:TRP:CZ2 | 2.34 | 0.62 |
| 2:I9:132:LEU:HD22 | 2:I9:164:LYS:HD3 | 1.82 | 0.62 |
| 2:J5:33:ASP:O | 2:J5:60:LYS:NZ | 2.33 | 0.62 |
| 1:K0:345:ILE:O | 1:K0:348:ASN:ND2 | 2.29 | 0.62 |
| 2:M9:90:GLU:O | 2:M9:121:ARG:NH1 | 2.31 | 0.62 |
| 2:M9:396:ASP:HB2 | 2:M9:422:ARG:NH1 | 2.15 | 0.62 |
| 2:N9:244:PHE:HB2 | 2:N9:356:ASN:HD21 | 1.63 | 0.62 |
| 1:P8:55:THR:HG22 | 7:4R:111:ASP:OD1 | 1.98 | 0.62 |
| 2:Q3:14:ILE:HD11 | 2:Q3:74:VAL:HG22 | 1.81 | 0.62 |
| 1:R2:276:ARG:HH22 | 7:4R:70:GLN:HE21 | 1.47 | 0.62 |
| 2:S7:98:ASP:OD1 | 2:S7:99:ALA:N | 2.33 | 0.62 |
| 2:T3:337:THR:HG23 | 13:5J:21:ASN:HD22 | 1.63 | 0.62 |
| 1:T4:285:THR:HG23 | 1:T4:288:GLU:H | 1.63 | 0.62 |
| 2:T5:175:PRO:O | 2:T5:394:LYS:NZ | 2.32 | 0.62 |
| 1:T6:409:THR:HB | 13:5K:50:ARG:HD3 | 1.80 | 0.62 |
| 2:U3:90:GLU:HB3 | 2:V9:283:HIS:HE1 | 1.65 | 0.62 |
| 2:U9:195:LEU:HD21 | 2:U9:264:ARG:HH11 | 1.63 | 0.62 |
| 2:V9:399:TYR:OH | 2:V9:415:GLU:OE2 | 2.17 | 0.62 |
| 2:W1:287:SER:N | 2:W1:290:GLU:OE2 | 2.23 | 0.62 |
| 1:W2:52:ASN:OD1 | 1:W2:62:ARG:NH2 | 2.32 | 0.62 |
| 1:X8:198:GLU:HB3 | 1:X8:258:ILE:HD11 | 1.81 | 0.62 |
| 2:Z3:9:ILE:HG23 | 2:Z3:68:LEU:HD11 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z4:190:HIS:CD2 | 1:Z4:411:ALA:HA | 2.35 | 0.62 |
| 2:0F:399:TYR:O | 2:0F:402:ARG:NH1 | 2.32 | 0.62 |
| 2:1L:392:ASP:OD2 | 2:1L:422:ARG:NH1 | 2.33 | 0.62 |
| 1:1M:140:GLY:O | 1:1M:184:ASN:ND2 | 2.33 | 0.62 |
| 2:1N:5:ILE:HG22 | 2:1N:64:ARG:HB3 | 1.79 | 0.62 |
| 2:1N:35:GLN:HB3 | 2:1N:59:GLY:O | 1.99 | 0.62 |
| 2:1N:313:MET:HE1 | 2:1N:346:TRP:HZ2 | 1.42 | 0.62 |
| 1:1Q:375:GLN:HB2 | 1:1Q:419:VAL:HG23 | 1.82 | 0.62 |
| 1:1Q:418:LEU:HG | 1:1Q:422:TYR:HE2 | 1.64 | 0.62 |
| 2:1T:381:SER:OG | 2:1T:382:THR:N | 2.33 | 0.62 |
| 1:1W:139:LEU:HD12 | 1:1W:170:VAL:HG12 | 1.81 | 0.62 |
| 1:1W:334:GLN:HE22 | 1:1W:348:ASN:H | 1.44 | 0.62 |
| 1:2Q:211:CYS:SG | 1:2Q:220:PRO:HB3 | 2.38 | 0.62 |
| 2:2T:214:ARG:NH1 | 38:8A:17:GLY:O | 2.33 | 0.62 |
| 1:3A:334:GLN:HE22 | 1:3A:348:ASN:H | 1.46 | 0.62 |
| 1:3G:172:SER:HB3 | 1:3G:175:VAL:HG22 | 1.79 | 0.62 |
| 2:3J:122:ILE:HA | 2:3J:125:LEU:HD12 | 1.79 | 0.62 |
| 3:3V:17:VAL:HG23 | 3:3V:18:LYS:HG3 | 1.81 | 0.62 |
| 3:3X:17:VAL:HG23 | 3:3X:18:LYS:HG3 | 1.81 | 0.62 |
| 3:4B:17:VAL:HG23 | 3:4B:18:LYS:HG3 | 1.81 | 0.62 |
| 3:4D:17:VAL:HG23 | 3:4D:18:LYS:HG3 | 1.81 | 0.62 |
| 3:4H:17:VAL:HG23 | 3:4H:18:LYS:HG3 | 1.81 | 0.62 |
| 3:4H:63:SER:OG | 3:4H:68:SER:O | 2.16 | 0.62 |
| 7:4R:124:GLY:HA2 | 11:5E:174:ARG:HB3 | 1.80 | 0.62 |
| 1:D8:56:GLY:HA2 | 22:6P:54:ARG:HH21 | 1.63 | 0.62 |
| 2:H1:241:SER:O | 2:H1:249:ASN:ND2 | 2.33 | 0.62 |
| 2:H1:244:PHE:HB2 | 2:H1:356:ASN:HD21 | 1.65 | 0.62 |
| 1:H2:113:ILE:HG13 | 1:H2:117:LEU:HD23 | 1.82 | 0.62 |
| 1:H4:276:ARG:NH2 | 24:6U:489:ASN:C | 2.52 | 0.62 |
| 1:I0:218:THR:HG21 | 24:6X:489:ASN:N | 2.12 | 0.62 |
| 1:I2:33:THR:O | 1:I2:58:ARG:NH2 | 2.33 | 0.62 |
| 1:I4:220:PRO:HD2 | 2:I5:326:LYS:HD3 | 1.81 | 0.62 |
| 1:J6:218:THR:HG23 | 1:J6:219:THR:HG22 | 1.81 | 0.62 |
| 1:K0:119:VAL:O | 1:K0:123:GLU:HG2 | 1.99 | 0.62 |
| 2:K3:182:VAL:HG12 | 2:K3:185:TYR:HB2 | 1.82 | 0.62 |
| 1:K4:52:ASN:OD1 | 1:K4:62:ARG:NH2 | 2.32 | 0.62 |
| 2:L1:372:GLN:NE2 | 6:4O:360:GLU:OE2 | 2.33 | 0.62 |
| 2:M5:58:ALA:O | 37:7Y:215:HIS:HB2 | 1.99 | 0.62 |
| 2:N3:90:GLU:OE1 | 2:N3:91:GLN:NE2 | 2.32 | 0.62 |
| 1:N8:86:ARG:NH2 | 1:P6:281:TYR:O | 2.32 | 0.62 |
| 1:N8:272:PRO:HB2 | 1:N8:282:ARG:HH12 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O5:123:ARG:HG3 | 2:O5:123:ARG:HH11 | 1.64 | 0.62 |
| 2:P9:9:ILE:HG22 | 2:P9:146:GLY:HA2 | 1.82 | 0.62 |
| 1:Q0:392:LYS:HD2 | 1:Q0:395:LEU:HD22 | 1.81 | 0.62 |
| 2:Q3:388:PHE:HB3 | 2:Q3:425:LEU:HD11 | 1.81 | 0.62 |
| 2:R3:156:ARG:HA | 2:R3:159:VAL:HG12 | 1.82 | 0.62 |
| 1:S8:2:ARG:HB3 | 1:S8:131:GLN:HB2 | 1.80 | 0.62 |
| 2:S9:287:SER:N | 2:S9:290:GLU:OE2 | 2.27 | 0.62 |
| 2:T1:344:VAL:HG22 | 2:T1:346:TRP:H | 1.64 | 0.62 |
| 1:T2:68:LEU:HD12 | 1:T2:97:ALA:HB2 | 1.81 | 0.62 |
| 2:T3:372:GLN:HE22 | 7:4U:84:THR:HG21 | 1.63 | 0.62 |
| 1:V6:211:CYS:HA | 1:V6:215:LEU:HB2 | 1.80 | 0.62 |
| 1:X0:212:PHE:HE1 | 1:X0:220:PRO:HG3 | 1.64 | 0.62 |
| 1:Y6:224:ASP:OD1 | 1:Y6:225:LEU:N | 2.33 | 0.62 |
| 1:0E:270:PHE:CD2 | 1:0E:273:LEU:HD11 | 2.34 | 0.62 |
| 2:0L:9:ILE:HG22 | 2:0L:146:GLY:HA2 | 1.81 | 0.62 |
| 2:0P:56:THR:HA | 2:1F:285:GLN:HB2 | 1.81 | 0.62 |
| 2:1B:90:GLU:O | 2:1B:121:ARG:NH1 | 2.32 | 0.62 |
| 2:1P:287:SER:N | 2:1P:290:GLU:OE2 | 2.32 | 0.62 |
| 1:1W:350:LYS:NZ | 1:1W:351:SER:O | 2.32 | 0.62 |
| 2:2J:278:ALA:HA | 2:2J:369:ALA:HB2 | 1.79 | 0.62 |
| 2:2N:120:ASP:HB3 | 38:8D:73:TRP:CD1 | 2.34 | 0.62 |
| 2:2N:287:SER:N | 2:2N:290:GLU:OE2 | 2.31 | 0.62 |
| 1:2Y:211:CYS:HA | 1:2Y:215:LEU:HB2 | 1.80 | 0.62 |
| 2:3F:90:GLU:O | 2:3F:121:ARG:NH1 | 2.32 | 0.62 |
| 2:3J:405:VAL:HG13 | 2:3J:418:PHE:HE2 | 1.64 | 0.62 |
| 1:3K:218:THR:OG1 | 17:5T:213:GLU:OE1 | 2.16 | 0.62 |
| 1:3M:125:GLU:OE1 | 4:4C:45:SER:OG | 2.16 | 0.62 |
| 3:3V:63:SER:OG | 3:3V:68:SER:O | 2.16 | 0.62 |
| 3:3X:63:SER:OG | 3:3X:68:SER:O | 2.16 | 0.62 |
| 3:4B:63:SER:OG | 3:4B:68:SER:O | 2.16 | 0.62 |
| 3:4F:17:VAL:HG23 | 3:4F:18:LYS:HG3 | 1.81 | 0.62 |
| 3:4F:63:SER:OG | 3:4F:68:SER:O | 2.16 | 0.62 |
| 10:5C:478:LEU:HD23 | 10:5C:481:LEU:HD12 | 1.80 | 0.62 |
| 14:5L:516:VAL:HG22 | 14:5L:527:THR:HG22 | 1.81 | 0.62 |
| 14:5M:516:VAL:HG22 | 14:5M:527:THR:HG22 | 1.81 | 0.62 |
| 24:6W:354:ARG:HB2 | 24:6W:357:LEU:HG | 1.82 | 0.62 |
| 24:6Z:483:PHE:HB2 | 24:6Z:496:LYS:HA | 1.81 | 0.62 |
| 36:7W:51:LYS:HB2 | 36:7W:54:GLU:HB3 | 1.81 | 0.62 |
| 1:A7:94:GLN:HG2 | 24:6T:250:LEU:HD11 | 1.81 | 0.62 |
| 2:E9:364:PRO:HG2 | 22:6N:123:PRO:HB2 | 1.80 | 0.62 |
| 2:G3:109:THR:OG1 | 2:G3:411:GLU:OE2 | 2.17 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G5:282:TYR:CE1 | 22:6N:134:ASN:ND2 | 2.68 | 0.62 |
| 2:G9:195:LEU:HD11 | 2:G9:264:ARG:HH11 | 1.65 | 0.62 |
| 1:M0:221:THR:OG1 | 29:7I:97:ARG:NH1 | 2.33 | 0.62 |
| 1:M2:207:LEU:HB3 | 1:M2:225:LEU:HD22 | 1.80 | 0.62 |
| 2:O1:98:ASP:OD1 | 2:O1:99:ALA:N | 2.33 | 0.62 |
| 2:O7:156:ARG:HA | 2:O7:159:VAL:HG12 | 1.82 | 0.62 |
| 2:O9:259:LEU:HD21 | 2:O9:316:CYS:HB2 | 1.80 | 0.62 |
| 1:S2:139:LEU:HD12 | 1:S2:170:VAL:HG12 | 1.80 | 0.62 |
| 1:T2:292:GLN:HG2 | 1:T2:298:ASN:HD22 | 1.64 | 0.62 |
| 1:U6:177:ASP:O | 2:U7:352:LYS:HA | 1.99 | 0.62 |
| 2:U9:90:GLU:HB3 | 2:U9:121:ARG:NH2 | 2.15 | 0.62 |
| 2:V3:287:SER:OG | 2:V3:290:GLU:OE1 | 2.12 | 0.62 |
| 2:W5:90:GLU:HB3 | 2:W5:121:ARG:NH1 | 2.15 | 0.62 |
| 1:Y8:86:ARG:HH21 | 1:0E:282:ARG:HA | 1.64 | 0.62 |
| 2:0H:90:GLU:O | 2:0H:121:ARG:NH1 | 2.33 | 0.62 |
| 1:0S:131:GLN:HE21 | 1:0S:250:LEU:HB2 | 1.62 | 0.62 |
| 1:1G:271:THR:OG1 | 1:1G:292:GLN:OE1 | 2.16 | 0.62 |
| 1:1S:113:ILE:HA | 1:1S:116:VAL:HG22 | 1.82 | 0.62 |
| 2:1V:91:GLN:CA | 2:1V:121:ARG:HH12 | 2.08 | 0.62 |
| 2:1Z:121:ARG:HE | 2:1Z:124:LYS:HE3 | 1.64 | 0.62 |
| 2:1Z:262:TYR:HE1 | 2:1Z:264:ARG:HB2 | 1.65 | 0.62 |
| 2:2F:223:THR:HG23 | 2:2F:225:THR:H | 1.65 | 0.62 |
| 2:2L:195:LEU:HD21 | 2:2L:264:ARG:HD2 | 1.81 | 0.62 |
| 2:2R:287:SER:N | 2:2R:290:GLU:OE2 | 2.33 | 0.62 |
| 2:2T:255:PHE:HA | 2:2T:259:LEU:HD13 | 1.81 | 0.62 |
| 2:3B:282:TYR:OH | 10:5D:167:ILE:HD12 | 1.99 | 0.62 |
| 9:4Z:335:LEU:HB3 | 9:4Z:336:ARG:HH21 | 1.64 | 0.62 |
| 15:5O:73:LEU:H | 15:5O:73:LEU:CD2 | 2.12 | 0.62 |
| 15:5P:344:ARG:NH1 | 15:5P:356:VAL:O | 2.32 | 0.62 |
| 19:6E:96:ASP:N | 19:6E:96:ASP:OD2 | 2.31 | 0.62 |
| 2:8:370:LYS:NZ | 24:6W:92:ASP:OD1 | 2.31 | 0.62 |
| 2:A4:206:ASN:OD1 | 41:A4:501:GTP:N2 | 2.31 | 0.62 |
| 2:I9:336:LYS:O | 2:I9:339:ARG:NH2 | 2.33 | 0.62 |
| 1:J4:77:ARG:HH21 | 1:J4:90:PHE:HD2 | 1.47 | 0.62 |
| 2:J9:326:LYS:HG3 | 2:J9:327:ASP:N | 2.14 | 0.62 |
| 1:L2:391:ARG:HD2 | 2:L3:346:TRP:NE1 | 2.14 | 0.62 |
| 2:M5:132:LEU:HD22 | 2:M5:164:LYS:HD3 | 1.81 | 0.62 |
| 1:N6:178:THR:HG22 | 2:N7:352:LYS:HZ3 | 1.64 | 0.62 |
| 2:P3:69:ASP:OD1 | 2:P3:70:LEU:N | 2.32 | 0.62 |
| 2:R7:92:LEU:N | 2:R7:92:LEU:HD23 | 2.15 | 0.62 |
| 1:R8:93:GLY:HA2 | 13:5J:118:THR:HG23 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T2:309:ARG:NH1 | 1:T2:339:SER:O | 2.33 | 0.62 |
| 2:T7:402:ARG:HD2 | 2:T7:405:VAL:HG21 | 1.81 | 0.62 |
| 1:U4:135:VAL:HG21 | 1:U4:152:ILE:HD11 | 1.80 | 0.62 |
| 1:U6:190:HIS:CD2 | 1:U6:411:ALA:HA | 2.34 | 0.62 |
| 2:U9:90:GLU:HA | 2:U9:90:GLU:OE2 | 2.00 | 0.62 |
| 1:V2:207:LEU:HB3 | 1:V2:225:LEU:HD22 | 1.82 | 0.62 |
| 2:Z1:83:TYR:HB3 | 2:Z1:86:LEU:HB3 | 1.80 | 0.62 |
| 1:0G:248:ALA:CB | 1:0G:252:LYS:HD3 | 2.30 | 0.62 |
| 2:0J:100:ALA:HA | 1:0K:252:LYS:HE2 | 1.82 | 0.62 |
| 1:1Q:345:ILE:O | 1:1Q:348:ASN:ND2 | 2.32 | 0.62 |
| 1:3O:34:GLY:O | 1:3O:58:ARG:HA | 2.00 | 0.62 |
| 2:3T:176:GLN:NE2 | 2:3T:207:GLU:HG2 | 2.14 | 0.62 |
| 7:4U:179:LYS:HD3 | 33:7Q:121:SER:HA | 1.82 | 0.62 |
| 14:5M:489:SER:CA | 14:5M:512:PHE:HB3 | 2.30 | 0.62 |
| 14:5N:516:VAL:HG22 | 14:5N:527:THR:HG22 | 1.81 | 0.62 |
| 18:6B:101:LYS:O | 24:6Y:178:ASN:ND2 | 2.25 | 0.62 |
| 34:7R:99:ARG:HH12 | 34:7R:103:LEU:HD22 | 1.64 | 0.62 |
| 36:7V:51:LYS:HB2 | 36:7V:54:GLU:HB3 | 1.81 | 0.62 |
| 1:7:337:ASN:ND2 | 3:4B:69:TYR:H | 1.97 | 0.62 |
| 1:B3:358:PRO:O | 18:5Z:22:ARG:NH2 | 2.31 | 0.62 |
| 2:F9:42:ILE:HD11 | 24:6U:447:ARG:HB3 | 1.81 | 0.62 |
| 2:G5:392:ASP:OD2 | 2:G5:422:ARG:NH1 | 2.32 | 0.62 |
| 2:H5:336:LYS:O | 2:H5:339:ARG:NH2 | 2.32 | 0.62 |
| 2:H9:405:VAL:HG13 | 2:H9:418:PHE:HE2 | 1.63 | 0.62 |
| 2:J5:392:ASP:OD2 | 2:J5:422:ARG:NH1 | 2.33 | 0.62 |
| 1:L2:2:ARG:HE | 1:L2:240:LEU:HD22 | 1.64 | 0.62 |
| 2:L3:84:ARG:HH22 | 29:7J:345:PRO:HD3 | 1.63 | 0.62 |
| 1:N2:392:LYS:HD2 | 1:N2:395:LEU:HD22 | 1.81 | 0.62 |
| 2:O3:98:ASP:OD1 | 2:O3:99:ALA:N | 2.33 | 0.62 |
| 2:O3:313:MET:HG2 | 2:O3:346:TRP:CH2 | 2.35 | 0.62 |
| 1:R0:220:PRO:HD2 | 2:R1:326:LYS:HD3 | 1.82 | 0.62 |
| 2:R7:223:THR:HG23 | 2:R7:225:THR:H | 1.65 | 0.62 |
| 1:S6:190:HIS:HD2 | 1:S6:414:ASN:HB2 | 1.64 | 0.62 |
| 2:T7:90:GLU:O | 2:T7:90:GLU:HG2 | 1.97 | 0.62 |
| 1:U4:113:ILE:HA | 1:U4:116:VAL:HG22 | 1.81 | 0.62 |
| 1:V2:49:VAL:HG11 | 1:V2:241:ARG:HG2 | 1.82 | 0.62 |
| 1:V2:52:ASN:OD1 | 1:V2:62:ARG:NH2 | 2.30 | 0.62 |
| 1:W0:52:ASN:OD1 | 1:W0:62:ARG:NH2 | 2.32 | 0.62 |
| 2:W7:286:LEU:O | 2:W7:373:ARG:NH1 | 2.32 | 0.62 |
| 2:W9:100:ALA:O | 1:X0:255:VAL:HG11 | 1.99 | 0.62 |
| 1:Y0:207:LEU:HB3 | 1:Y0:225:LEU:HD22 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y4:263:LEU:HG | 1:Y4:422:TYR:CE1 | 2.34 | 0.62 |
| 2:Y5:88:HIS:HB3 | 2:0B:283:HIS:ND1 | 2.15 | 0.62 |
| 1:Z8:190:HIS:CD2 | 1:Z8:411:ALA:HA | 2.34 | 0.62 |
| 1:0A:39:ASP:OD1 | 1:0A:40:SER:N | 2.32 | 0.62 |
| 2:0F:56:THR:HA | 2:0V:285:GLN:HB2 | 1.82 | 0.62 |
| 1:0I:113:ILE:HA | 1:0I:116:VAL:HG22 | 1.82 | 0.62 |
| 1:0M:345:ILE:O | 1:0M:348:ASN:ND2 | 2.31 | 0.62 |
| 1:1G:7:ILE:HD13 | 1:1G:151:LEU:HD21 | 1.81 | 0.62 |
| 1:1K:345:ILE:O | 1:1K:348:ASN:ND2 | 2.30 | 0.62 |
| 2:1R:26:LEU:HD23 | 2:1R:363:VAL:HG12 | 1.81 | 0.62 |
| 2:1Z:5:ILE:HG22 | 2:1Z:64:ARG:HB3 | 1.81 | 0.62 |
| 2:2J:33:ASP:O | 2:2J:60:LYS:NZ | 2.32 | 0.62 |
| 1:2K:286:VAL:HG23 | 1:2K:287:PRO:HD3 | 1.82 | 0.62 |
| 1:2K:309:ARG:NH1 | 1:2K:339:SER:O | 2.33 | 0.62 |
| 1:3C:387:ALA:HA | 1:3C:390:ARG:HE | 1.65 | 0.62 |
| 2:3H:365:GLY:HA3 | 14:5L:422:ASP:OD1 | 1.98 | 0.62 |
| 1:3K:391:ARG:HH22 | 2:3L:435:VAL:HA | 1.65 | 0.62 |
| 14:5L:439:ARG:HH12 | 14:5L:453:ARG:HB2 | 1.63 | 0.62 |
| 14:5N:439:ARG:HH12 | 14:5N:453:ARG:HB2 | 1.63 | 0.62 |
| 14:5N:604:THR:OG1 | 14:5N:606:ASP:OD1 | 2.14 | 0.62 |
| 15:5O:11:SER:HB3 | 15:5O:75:LEU:HD23 | 1.82 | 0.62 |
| 15:5P:52:TYR:CE2 | 15:5P:54:GLU:CB | 2.82 | 0.62 |
| 15:5P:233:LEU:HG | 15:5P:266:THR:HG21 | 1.82 | 0.62 |
| 19:6E:205:SER:O | 21:6G:38:PRO:HB3 | 1.99 | 0.62 |
| 22:6M:208:ARG:HG2 | 22:6M:223:LEU:HD13 | 1.81 | 0.62 |
| 1:A1:337:ASN:ND2 | 3:4F:69:TYR:H | 1.98 | 0.62 |
| 2:G9:50:ASN:O | 2:G9:64:ARG:NH2 | 2.33 | 0.62 |
| 2:G9:115:VAL:HG23 | 2:G9:153:LEU:HD12 | 1.79 | 0.62 |
| 1:H2:135:VAL:HG21 | 1:H2:152:ILE:HD11 | 1.82 | 0.62 |
| 1:I0:52:ASN:OD1 | 1:I0:62:ARG:NH2 | 2.33 | 0.62 |
| 1:I0:392:LYS:HD2 | 1:I0:395:LEU:HD22 | 1.81 | 0.62 |
| 2:J1:394:LYS:HB2 | 1:J2:346:PRO:HG3 | 1.82 | 0.62 |
| 1:L4:211:CYS:HA | 1:L4:215:LEU:HB2 | 1.81 | 0.62 |
| 2:L7:384:ILE:HA | 2:L7:387:ILE:HG12 | 1.82 | 0.62 |
| 1:M6:125:GLU:OE2 | 1:M6:159:TYR:OH | 2.17 | 0.62 |
| 2:N1:90:GLU:CB | 1:O8:281:TYR:HE2 | 2.12 | 0.62 |
| 2:N1:176:GLN:HG2 | 2:N1:177:VAL:HG23 | 1.82 | 0.62 |
| 2:N5:289:ALA:O | 2:N5:293:ASN:ND2 | 2.33 | 0.62 |
| 1:O4:32:PRO:HB2 | 37:7Y:33:GLN:HE21 | 1.65 | 0.62 |
| 2:O7:88:HIS:HB3 | 2:O7:91:GLN:HG3 | 1.82 | 0.62 |
| 2:Q1:286:LEU:O | 2:Q1:373:ARG:NH1 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R1:27:GLU:OE1 | 2:R1:243:ARG:NH1 | 2.29 | 0.62 |
| 2:U7:287:SER:OG | 2:U7:290:GLU:OE1 | 2.13 | 0.62 |
| 2:V9:264:ARG:NH2 | 2:V9:431:ASP:OD2 | 2.33 | 0.62 |
| 2:W5:267:PHE:HB2 | 2:W5:384:ILE:HD12 | 1.81 | 0.62 |
| 1:Y6:113:ILE:HA | 1:Y6:116:VAL:HG12 | 1.82 | 0.62 |
| 1:Z2:190:HIS:CD2 | 1:Z2:411:ALA:HA | 2.35 | 0.62 |
| 1:Z2:380:ARG:NH1 | 1:Z2:383:GLU:OE2 | 2.28 | 0.62 |
| 2:Z5:67:PHE:HB2 | 2:Z5:92:LEU:HD22 | 1.82 | 0.62 |
| 1:0I:244:GLY:HA3 | 1:0I:354:CYS:HA | 1.82 | 0.62 |
| 1:0S:97:ALA:HA | 1:0S:103:LYS:HD2 | 1.80 | 0.62 |
| 1:1M:12:CYS:SG | 1:1M:138:SER:HB2 | 2.40 | 0.62 |
| 2:1N:11:GLN:OE1 | 2:1N:15:GLN:NE2 | 2.33 | 0.62 |
| 2:1N:313:MET:SD | 2:1N:346:TRP:HZ2 | 2.23 | 0.62 |
| 2:1V:318:MET:HB2 | 2:1V:376:CYS:HB3 | 1.81 | 0.62 |
| 2:1V:344:VAL:HG22 | 2:1V:346:TRP:H | 1.63 | 0.62 |
| 2:1Z:335:ILE:HG23 | 2:1Z:338:LYS:HE3 | 1.81 | 0.62 |
| 1:2A:2:ARG:HE | 1:2A:240:LEU:HD22 | 1.65 | 0.62 |
| 2:2L:109:THR:OG1 | 2:2L:411:GLU:OE2 | 2.16 | 0.62 |
| 1:2Q:45:GLU:HG3 | 1:2Q:46:ARG:HG2 | 1.80 | 0.62 |
| 1:3M:77:ARG:HH22 | 3:4D:18:LYS:HB3 | 1.64 | 0.62 |
| 7:4S:3:ARG:HG2 | 7:4S:3:ARG:NH1 | 2.13 | 0.62 |
| 14:5M:604:THR:OG1 | 14:5M:606:ASP:OD1 | 2.14 | 0.62 |
| 14:5N:166:ALA:HB2 | 14:5N:170:ASN:OD1 | 1.99 | 0.62 |
| 15:5P:105:ASN:HD21 | 15:5P:108:LYS:HD2 | 1.64 | 0.62 |
| 12:7B:44:ILE:HD11 | 12:7B:50:ALA:HA | 1.80 | 0.62 |
| 26:7E:50:SER:CA | 26:7E:56:LEU:CD2 | 2.77 | 0.62 |
| 38:8D:206:PRO:CG | 38:8D:209:HIS:CE1 | 2.76 | 0.62 |
| 1:B8:143:THR:OG1 | 39:B8:501:GDP:O1B | 2.18 | 0.62 |
| 2:G7:109:THR:OG1 | 2:G7:411:GLU:OE2 | 2.16 | 0.62 |
| 1:G8:2:ARG:HB3 | 1:G8:131:GLN:HB2 | 1.81 | 0.62 |
| 2:H1:240:ALA:O | 2:H1:356:ASN:ND2 | 2.33 | 0.62 |
| 2:H1:387:ILE:HG12 | 2:H1:390:ARG:HH22 | 1.64 | 0.62 |
| 2:I9:405:VAL:HG13 | 2:I9:418:PHE:HE2 | 1.65 | 0.62 |
| 2:K1:3:GLU:HG3 | 2:K1:51:THR:HA | 1.80 | 0.62 |
| 1:L0:12:CYS:SG | 1:L0:13:GLY:N | 2.73 | 0.62 |
| 2:L9:285:GLN:HG3 | 30:7K:333:VAL:HG21 | 1.81 | 0.62 |
| 1:M0:122:LYS:HD3 | 32:7O:12:SER:HB3 | 1.81 | 0.62 |
| 2:O3:90:GLU:HG3 | 2:O3:121:ARG:HH12 | 1.65 | 0.62 |
| 1:O4:309:ARG:H | 1:O4:372:THR:HG22 | 1.65 | 0.62 |
| 2:Q5:90:GLU:HB3 | 2:Q5:121:ARG:HH12 | 1.65 | 0.62 |
| 1:Q8:238:CYS:SG | 1:Q8:318:ARG:HD3 | 2.39 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S2:15:GLN:OE1 | 7:4R:367:ARG:NH1 | 2.33 | 0.62 |
| 2:U7:269:LEU:HD22 | 2:U7:303:VAL:HG11 | 1.82 | 0.62 |
| 2:U9:11:GLN:OE1 | 2:U9:15:GLN:NE2 | 2.32 | 0.62 |
| 1:V2:5:VAL:HG23 | 1:V2:62:ARG:HG2 | 1.81 | 0.62 |
| 1:V8:309:ARG:H | 1:V8:372:THR:HG22 | 1.63 | 0.62 |
| 2:V9:406:HIS:HA | 2:V9:409:VAL:HG22 | 1.81 | 0.62 |
| 2:W1:88:HIS:CD2 | 2:W1:90:GLU:CB | 2.83 | 0.62 |
| 2:Y3:9:ILE:HG22 | 2:Y3:146:GLY:HA2 | 1.82 | 0.62 |
| 2:Z9:157:LEU:HD22 | 2:Z9:166:LYS:HD3 | 1.82 | 0.62 |
| 1:0I:135:VAL:HB | 1:0I:166:THR:HG22 | 1.82 | 0.62 |
| 1:0M:113:ILE:HA | 1:0M:116:VAL:HG22 | 1.82 | 0.62 |
| 1:0W:276:ARG:NH1 | 1:0W:279:GLN:OE1 | 2.33 | 0.62 |
| 2:1H:164:LYS:O | 2:1H:166:LYS:NZ | 2.33 | 0.62 |
| 1:1K:304:ASP:OD1 | 1:1K:306:ARG:NH1 | 2.33 | 0.62 |
| 2:1X:11:GLN:OE1 | 2:1X:15:GLN:NE2 | 2.33 | 0.62 |
| 2:1Z:85:GLN:O | 2:2P:283:HIS:CE1 | 2.53 | 0.62 |
| 2:2P:358:GLN:HE21 | 38:8A:214:HIS:N | 1.97 | 0.62 |
| 1:2Q:320:ARG:HH22 | 38:8A:198:THR:CB | 2.13 | 0.62 |
| 1:2Y:345:ILE:O | 1:2Y:348:ASN:ND2 | 2.33 | 0.62 |
| 1:3G:276:ARG:NH1 | 17:5S:216:GLU:HB3 | 2.15 | 0.62 |
| 5:4L:263:LEU:O | 5:4L:267:ASN:ND2 | 2.32 | 0.62 |
| 9:4Y:358:THR:HA | 9:4Y:361:LYS:HD2 | 1.82 | 0.62 |
| 14:5L:166:ALA:HB2 | 14:5L:170:ASN:OD1 | 1.99 | 0.62 |
| 14:5L:205:ASN:ND2 | 14:5L:207:GLU:OE1 | 2.33 | 0.62 |
| 14:5L:604:THR:OG1 | 14:5L:606:ASP:OD1 | 2.14 | 0.62 |
| 14:5M:205:ASN:ND2 | 14:5M:207:GLU:OE1 | 2.33 | 0.62 |
| 14:5M:439:ARG:HH12 | 14:5M:453:ARG:HB2 | 1.63 | 0.62 |
| 14:5N:205:ASN:ND2 | 14:5N:207:GLU:OE1 | 2.33 | 0.62 |
| 15:5O:102:ALA:CB | 15:5O:204:ALA:HB1 | 2.30 | 0.62 |
| 22:6I:200:GLY:O | 22:6I:239:GLU:HA | 2.00 | 0.62 |
| 22:6P:170:ARG:NH2 | 22:6P:246:GLN:O | 2.33 | 0.62 |
| 24:6U:97:ARG:H | 24:6U:188:THR:HG21 | 1.65 | 0.62 |
| 24:6X:95:VAL:HG11 | 24:6X:124:TYR:CE2 | 2.35 | 0.62 |
| 24:6X:253:PRO:HB3 | 24:6X:255:HIS:CE1 | 2.35 | 0.62 |
| 38:8A:196:MET:HE2 | 38:8A:201:LEU:HD21 | 1.80 | 0.62 |
| 2:B7:367:ASP:OD1 | 18:6B:47:SER:OG | 1.91 | 0.61 |
| 2:G3:91:GLN:HG3 | 2:G3:121:ARG:NH2 | 2.15 | 0.61 |
| 1:G8:178:THR:OG1 | 2:G9:258:ASN:ND2 | 2.33 | 0.61 |
| 2:H1:195:LEU:HD21 | 2:H1:264:ARG:HD2 | 1.81 | 0.61 |
| 1:I0:309:ARG:H | 1:I0:372:THR:HG22 | 1.63 | 0.61 |
| 1:I4:345:ILE:O | 1:I4:348:ASN:ND2 | 2.26 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I7:55:GLU:O | 2:K3:285:GLN:NE2 | 2.33 | 0.61 |
| 2:J7:223:THR:OG1 | 1:J8:245:GLN:NE2 | 2.33 | 0.61 |
| 2:L1:90:GLU:HB3 | 2:L1:121:ARG:NH1 | 2.13 | 0.61 |
| 1:M2:334:GLN:HE22 | 1:M2:348:ASN:H | 1.47 | 0.61 |
| 2:M9:364:PRO:HB2 | 29:7J:291:ARG:HG3 | 1.82 | 0.61 |
| 2:N1:365:GLY:HA3 | 29:7J:118:ALA:HB1 | 1.81 | 0.61 |
| 2:O3:286:LEU:O | 2:O3:373:ARG:NH1 | 2.33 | 0.61 |
| 1:O8:2:ARG:HE | 1:O8:240:LEU:HD22 | 1.65 | 0.61 |
| 1:Q4:301:CYS:HB2 | 1:Q4:377:MET:HE1 | 1.82 | 0.61 |
| 1:Q8:200:MET:HE3 | 1:Q8:268:VAL:HG21 | 1.81 | 0.61 |
| 1:R2:11:GLN:HE22 | 2:R3:249:ASN:H | 1.47 | 0.61 |
| 1:S8:227:HIS:NE2 | 24:6W:10:LYS:O | 2.32 | 0.61 |
| 2:T3:398:MET:HG2 | 1:T4:345:ILE:HD13 | 1.82 | 0.61 |
| 2:U1:286:LEU:HD11 | 2:U1:291:ILE:HG23 | 1.82 | 0.61 |
| 1:V6:309:ARG:H | 1:V6:372:THR:HG22 | 1.65 | 0.61 |
| 2:Z7:298:PRO:HA | 2:Z7:301:MET:HG3 | 1.81 | 0.61 |
| 2:0N:195:LEU:HD23 | 2:0N:196:GLU:HG2 | 1.80 | 0.61 |
| 1:0Y:272:PRO:HB3 | 1:0Y:282:ARG:HH22 | 1.65 | 0.61 |
| 2:1R:223:THR:HG23 | 2:1R:225:THR:H | 1.66 | 0.61 |
| 1:1U:334:GLN:HE22 | 1:1U:348:ASN:H | 1.45 | 0.61 |
| 2:2B:123:ARG:NH1 | 38:8A:78:ASP:O | 2.31 | 0.61 |
| 2:2N:164:LYS:O | 2:2N:166:LYS:NZ | 2.33 | 0.61 |
| 2:2P:296:PHE:HE2 | 2:2P:335:ILE:HD13 | 1.65 | 0.61 |
| 2:2V:155:GLU:HG2 | 2:2V:197:HIS:CE1 | 2.35 | 0.61 |
| 1:2W:290:THR:HG21 | 1:2W:329:GLN:HE21 | 1.65 | 0.61 |
| 3:4J:117:PRO:HB2 | 3:4J:122:ARG:HH12 | 1.65 | 0.61 |
| 14:5M:166:ALA:HB2 | 14:5M:170:ASN:OD1 | 1.99 | 0.61 |
| 14:5N:11:ILE:HD12 | 14:5N:619:ILE:HD13 | 1.81 | 0.61 |
| 14:5N:112:SER:OG | 14:5N:114:ASP:OD1 | 2.17 | 0.61 |
| 17:5T:113:ILE:HG22 | 17:5T:114:LEU:HD22 | 1.82 | 0.61 |
| 24:6W:37:ASN:H | 24:6W:37:ASN:HD22 | 1.47 | 0.61 |
| 24:6Z:97:ARG:H | 24:6Z:188:THR:HG21 | 1.65 | 0.61 |
| 2:4:15:GLN:HE21 | 26:7D:113:ARG:NH2 | 1.96 | 0.61 |
| 2:8:76:ASP:OD2 | 18:6A:35:LEU:HD11 | 2.01 | 0.61 |
| 1:A9:79:GLY:HA3 | 24:6U:221:ARG:HH22 | 1.63 | 0.61 |
| 2:E7:85:GLN:O | 2:G3:283:HIS:NE2 | 2.11 | 0.61 |
| 2:G9:301:MET:HG2 | 2:G9:303:VAL:H | 1.65 | 0.61 |
| 2:I7:174:SER:OG | 2:I7:177:VAL:O | 2.18 | 0.61 |
| 2:K9:287:SER:N | 2:K9:290:GLU:OE2 | 2.33 | 0.61 |
| 1:L2:139:LEU:HD12 | 1:L2:170:VAL:HG12 | 1.82 | 0.61 |
| 1:L4:56:GLY:CA | 29:7J:331:TYR:HB2 | 2.25 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L9:154:LEU:HD21 | 2:L9:198:THR:HG23 | 1.82 | 0.61 |
| 2:N3:209:ILE:HG21 | 2:N3:227:LEU:HD13 | 1.81 | 0.61 |
| 2:N3:287:SER:N | 2:N3:290:GLU:OE2 | 2.32 | 0.61 |
| 2:S9:176:GLN:NE2 | 2:S9:207:GLU:OE2 | 2.34 | 0.61 |
| 1:T8:3:GLU:HG3 | 1:T8:127:CYS:HB2 | 1.82 | 0.61 |
| 1:T8:67:ASP:OD2 | 1:T8:72:THR:OG1 | 2.16 | 0.61 |
| 2:U3:172:TYR:N | 2:U3:204:LEU:O | 2.33 | 0.61 |
| 1:V2:107:THR:OG1 | 1:V2:401:GLU:OE2 | 2.14 | 0.61 |
| 1:W4:207:LEU:HB3 | 1:W4:225:LEU:HD22 | 1.82 | 0.61 |
| 1:X8:309:ARG:O | 1:X8:371:SER:OG | 2.16 | 0.61 |
| 2:Y1:236:SER:OG | 2:Y1:243:ARG:NH2 | 2.33 | 0.61 |
| 2:Z1:399:TYR:O | 2:Z1:402:ARG:NH1 | 2.33 | 0.61 |
| 1:0E:391:ARG:HG3 | 2:0F:346:TRP:HB3 | 1.80 | 0.61 |
| 1:0G:202:LEU:HD22 | 1:0G:300:MET:HB3 | 1.82 | 0.61 |
| 1:0G:252:LYS:HE2 | 1:0G:350:LYS:HE2 | 1.82 | 0.61 |
| 2:0L:336:LYS:O | 2:0L:339:ARG:NH2 | 2.29 | 0.61 |
| 1:0M:272:PRO:HB2 | 1:0M:282:ARG:HH12 | 1.64 | 0.61 |
| 2:0N:316:CYS:HB3 | 2:0N:378:ILE:HG23 | 1.81 | 0.61 |
| 1:0U:244:GLY:H | 1:0U:247:ASN:HD21 | 1.47 | 0.61 |
| 1:2Q:306:ARG:NH2 | 38:8A:96:GLY:C | 2.48 | 0.61 |
| 2:2X:22:GLU:OE1 | 38:8C:203:PHE:CE1 | 2.53 | 0.61 |
| 2:3J:339:ARG:HH22 | 2:3J:342:GLN:HB3 | 1.65 | 0.61 |
| 1:3K:345:ILE:O | 1:3K:348:ASN:ND2 | 2.32 | 0.61 |
| 2:3P:195:LEU:HD21 | 2:3P:264:ARG:HH11 | 1.66 | 0.61 |
| 1:3Q:309:ARG:NH1 | 1:3Q:339:SER:O | 2.32 | 0.61 |
| 24:6U:525:VAL:HB | 24:6U:530:PHE:HE2 | 1.65 | 0.61 |
| 2:8:29:GLY:HA2 | 26:7E:45:MET:CE | 2.28 | 0.61 |
| 1:A3:383:GLU:OE2 | 3:4H:50:LYS:HE2 | 2.00 | 0.61 |
| 2:F7:60:LYS:NZ | 2:H3:283:HIS:NE2 | 2.44 | 0.61 |
| 1:G4:173:PRO:HD2 | 1:G4:380:ARG:HE | 1.65 | 0.61 |
| 2:G5:72:PRO:HD2 | 1:G6:2:ARG:HH12 | 1.65 | 0.61 |
| 1:J0:320:ARG:NH2 | 28:7H:419:ILE:HD11 | 2.16 | 0.61 |
| 2:J3:48:ALA:HB2 | 16:5Q:174:THR:HG1 | 1.65 | 0.61 |
| 2:J5:76:ASP:OD2 | 1:J6:46:ARG:NH2 | 2.34 | 0.61 |
| 2:J9:42:ILE:HG22 | 2:J9:43:GLY:H | 1.65 | 0.61 |
| 2:L1:51:THR:HG21 | 2:L1:243:ARG:HG2 | 1.82 | 0.61 |
| 2:M9:287:SER:N | 2:M9:290:GLU:OE2 | 2.33 | 0.61 |
| 1:N0:156:ARG:NH1 | 1:N0:197:ASP:OD1 | 2.34 | 0.61 |
| 2:N3:50:ASN:O | 2:N3:64:ARG:NH2 | 2.33 | 0.61 |
| 2:Q9:183:GLU:HG3 | 2:Q9:184:PRO:HD3 | 1.80 | 0.61 |
| 1:S4:172:SER:HB3 | 1:S4:175:VAL:HG12 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:301:CYS:SG | 1:S4:302:ALA:N | 2.74 | 0.61 |
| 2:S7:66:ILE:HD12 | 2:S7:68:LEU:HD23 | 1.82 | 0.61 |
| 1:S8:177:ASP:O | 2:S9:352:LYS:HA | 2.00 | 0.61 |
| 1:T4:207:LEU:HB3 | 1:T4:225:LEU:HD22 | 1.82 | 0.61 |
| 1:T6:150:LEU:HD11 | 3:4H:76:PRO:HG3 | 1.80 | 0.61 |
| 1:T8:336:LYS:HD3 | 13:5K:101:LYS:HD3 | 1.80 | 0.61 |
| 1:U2:309:ARG:H | 1:U2:372:THR:HG22 | 1.64 | 0.61 |
| 2:U9:109:THR:OG1 | 2:U9:411:GLU:OE2 | 2.13 | 0.61 |
| 2:V7:213:CYS:HA | 2:V7:217:LEU:HB2 | 1.81 | 0.61 |
| 1:W2:207:LEU:HD11 | 1:W2:229:ILE:HD11 | 1.81 | 0.61 |
| 2:W7:225:THR:O | 2:W7:229:ARG:HG3 | 2.01 | 0.61 |
| 1:X0:237:THR:HG23 | 1:X0:241:ARG:HE | 1.65 | 0.61 |
| 2:X9:9:ILE:HG22 | 2:X9:146:GLY:HA2 | 1.82 | 0.61 |
| 1:0G:309:ARG:NH1 | 1:0G:339:SER:O | 2.33 | 0.61 |
| 2:0R:392:ASP:OD2 | 2:0R:422:ARG:NH1 | 2.33 | 0.61 |
| 1:1C:358:PRO:HG2 | 1:1C:361:LEU:HD23 | 1.81 | 0.61 |
| 1:1W:207:LEU:HD11 | 1:1W:229:ILE:HD11 | 1.82 | 0.61 |
| 1:2C:134:GLN:HE21 | 1:2C:167:PHE:HE2 | 1.47 | 0.61 |
| 1:2G:259:PRO:HG3 | 1:2G:311:LEU:HD21 | 1.83 | 0.61 |
| 2:2P:50:ASN:O | 2:2P:64:ARG:NH2 | 2.33 | 0.61 |
| 1:3A:193:VAL:HG22 | 1:3A:265:PHE:HZ | 1.64 | 0.61 |
| 2:3R:163:LYS:HE3 | 3:4H:137:ARG:HG2 | 1.81 | 0.61 |
| 14:5L:11:ILE:HD12 | 14:5L:619:ILE:HD13 | 1.82 | 0.61 |
| 14:5M:11:ILE:HD12 | 14:5M:619:ILE:HD13 | 1.82 | 0.61 |
| 14:5M:112:SER:OG | 14:5M:114:ASP:OD1 | 2.17 | 0.61 |
| 24:6W:482:ILE:HD12 | 24:6W:482:ILE:N | 2.15 | 0.61 |
| 24:6W:488:ARG:HB3 | 24:6W:488:ARG:HH11 | 1.66 | 0.61 |
| 2:G5:279:GLU:OE1 | 2:G5:279:GLU:N | 2.25 | 0.61 |
| 2:H1:56:THR:HA | 2:I7:285:GLN:HB2 | 1.81 | 0.61 |
| 2:H5:406:HIS:HA | 2:H5:409:VAL:HG22 | 1.82 | 0.61 |
| 1:H6:113:ILE:HA | 1:H6:116:VAL:HG22 | 1.82 | 0.61 |
| 2:K5:167:LEU:HA | 2:K5:200:VAL:HG13 | 1.82 | 0.61 |
| 1:Q0:135:VAL:HG21 | 1:Q0:152:ILE:HD11 | 1.82 | 0.61 |
| 1:Q4:391:ARG:NH1 | 2:Q5:346:TRP:HE1 | 1.99 | 0.61 |
| 1:T6:226:ASN:O | 1:T6:230:SER:N | 2.31 | 0.61 |
| 1:U6:128:ASP:OD1 | 1:U6:129:CYS:N | 2.33 | 0.61 |
| 1:V8:52:ASN:OD1 | 1:V8:62:ARG:NH2 | 2.34 | 0.61 |
| 1:W4:350:LYS:NZ | 1:W4:352:SER:OG | 2.32 | 0.61 |
| 1:W6:139:LEU:HD12 | 1:W6:170:VAL:HG12 | 1.82 | 0.61 |
| 1:0E:382:SER:HB3 | 1:0E:415:MET:HG2 | 1.83 | 0.61 |
| 1:0I:135:VAL:HG21 | 1:0I:152:ILE:HD11 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Q:309:ARG:H | 1:0Q:372:THR:HG22 | 1.64 | 0.61 |
| 2:0R:90:GLU:O | 2:0R:121:ARG:NH1 | 2.33 | 0.61 |
| 2:0Z:290:GLU:HA | 2:0Z:293:ASN:HD22 | 1.63 | 0.61 |
| 2:0Z:392:ASP:OD2 | 2:0Z:422:ARG:NH1 | 2.33 | 0.61 |
| 1:1A:379:LYS:HG3 | 1:1A:419:VAL:HG11 | 1.82 | 0.61 |
| 2:1R:176:GLN:HE22 | 2:1R:304:LYS:HE2 | 1.65 | 0.61 |
| 2:1V:392:ASP:OD2 | 2:1V:422:ARG:NH1 | 2.32 | 0.61 |
| 2:1Z:340:THR:HG23 | 2:1Z:341:ILE:HG12 | 1.81 | 0.61 |
| 1:2Q:272:PRO:HB2 | 1:2Q:282:ARG:HH12 | 1.63 | 0.61 |
| 7:4R:321:LYS:HD2 | 24:6Z:19:PRO:HG2 | 1.83 | 0.61 |
| 9:4Y:329:GLN:NE2 | 9:4Y:332:GLN:OE1 | 2.33 | 0.61 |
| 9:4Z:284:GLU:OE1 | 9:4Z:288:MET:HE3 | 1.99 | 0.61 |
| 14:5L:405:LYS:HE2 | 14:5L:421:ASN:HA | 1.80 | 0.61 |
| 14:5M:405:LYS:HE2 | 14:5M:421:ASN:HA | 1.80 | 0.61 |
| 14:5N:405:LYS:HE2 | 14:5N:421:ASN:HA | 1.80 | 0.61 |
| 15:5O:59:LEU:HD12 | 15:5O:59:LEU:C | 2.19 | 0.61 |
| 22:6K:53:THR:O | 22:6K:57:THR:OG1 | 2.18 | 0.61 |
| 29:7I:165:ARG:NH1 | 29:7I:232:ASP:HA | 2.14 | 0.61 |
| 36:7W:98:VAL:HA | 36:7W:101:VAL:CG1 | 2.30 | 0.61 |
| 37:7Y:173:GLU:HA | 37:7Y:173:GLU:OE1 | 2.00 | 0.61 |
| 1:B1:358:PRO:O | 18:5Y:22:ARG:NH2 | 2.33 | 0.61 |
| 1:G8:45:GLU:HG3 | 1:G8:46:ARG:HG2 | 1.82 | 0.61 |
| 2:I5:326:LYS:HG3 | 2:I5:327:ASP:N | 2.15 | 0.61 |
| 1:I8:107:THR:OG1 | 1:I8:401:GLU:OE2 | 2.14 | 0.61 |
| 1:J2:74:ASP:OD2 | 16:5Q:181:THR:HG21 | 2.00 | 0.61 |
| 2:J7:370:LYS:HD2 | 5:4M:205:VAL:HG23 | 1.83 | 0.61 |
| 2:K5:189:LEU:HD11 | 2:K5:418:PHE:HE1 | 1.65 | 0.61 |
| 1:K6:282:ARG:NH2 | 1:K6:288:GLU:OE2 | 2.30 | 0.61 |
| 2:K7:98:ASP:OD1 | 2:K7:99:ALA:N | 2.33 | 0.61 |
| 2:L9:222:PRO:HD2 | 1:M0:324:LYS:HE3 | 1.82 | 0.61 |
| 1:M4:12:CYS:SG | 1:M4:13:GLY:N | 2.74 | 0.61 |
| 2:M7:69:ASP:OD1 | 2:M7:70:LEU:N | 2.33 | 0.61 |
| 2:M7:90:GLU:HG3 | 2:M7:121:ARG:NH1 | 2.15 | 0.61 |
| 2:N1:265:ILE:CD1 | 2:N1:435:VAL:HG21 | 2.30 | 0.61 |
| 2:N7:98:ASP:OD1 | 2:N7:99:ALA:N | 2.33 | 0.61 |
| 2:N7:387:ILE:HG12 | 2:N7:390:ARG:HH22 | 1.66 | 0.61 |
| 1:O0:19:LYS:HZ3 | 27:7G:48:THR:HG1 | 1.48 | 0.61 |
| 1:O2:320:ARG:NH1 | 37:7Y:235:ASP:O | 2.33 | 0.61 |
| 2:O3:88:HIS:ND1 | 2:O3:89:PRO:HD2 | 2.16 | 0.61 |
| 1:P4:207:LEU:HB3 | 1:P4:225:LEU:HD22 | 1.82 | 0.61 |
| 1:P6:128:ASP:OD1 | 1:P6:129:CYS:N | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q4:178:THR:HG22 | 2:Q5:352:LYS:HZ3 | 1.65 | 0.61 |
| 1:Q6:33:THR:O | 1:Q6:58:ARG:NH2 | 2.33 | 0.61 |
| 1:S0:139:LEU:HD12 | 1:S0:170:VAL:HG22 | 1.82 | 0.61 |
| 1:S6:213:ARG:HH22 | 13:5H:117:ASN:HD21 | 1.47 | 0.61 |
| 1:S6:397:TRP:NE1 | 2:S7:256:GLN:O | 2.33 | 0.61 |
| 1:T2:2:ARG:HB3 | 1:T2:131:GLN:HB2 | 1.83 | 0.61 |
| 2:U9:98:ASP:OD1 | 2:U9:99:ALA:N | 2.33 | 0.61 |
| 1:V8:272:PRO:HB2 | 1:V8:282:ARG:HH12 | 1.65 | 0.61 |
| 1:W2:207:LEU:HB3 | 1:W2:225:LEU:HD22 | 1.81 | 0.61 |
| 1:X0:359:LYS:HG3 | 8:4X:96:VAL:HG22 | 1.81 | 0.61 |
| 2:X3:100:ALA:HA | 1:X4:252:LYS:HE2 | 1.82 | 0.61 |
| 2:X7:319:TYR:HB3 | 2:X7:323:VAL:HG21 | 1.80 | 0.61 |
| 1:X8:33:THR:O | 1:X8:58:ARG:NH2 | 2.34 | 0.61 |
| 2:X9:223:THR:HG22 | 2:X9:224:TYR:H | 1.65 | 0.61 |
| 1:Y8:8:GLN:NE2 | 1:Y8:63:ALA:HB1 | 2.12 | 0.61 |
| 1:Z0:68:LEU:HB3 | 1:Z0:96:GLY:HA2 | 1.82 | 0.61 |
| 1:0E:374:ILE:HD12 | 1:0E:378:PHE:HE2 | 1.65 | 0.61 |
| 1:0W:53:GLU:OE1 | 1:0W:53:GLU:HA | 1.99 | 0.61 |
| 2:1B:271:SER:HA | 2:1B:302:MET:HG2 | 1.81 | 0.61 |
| 1:1E:270:PHE:CD2 | 1:1E:273:LEU:HD21 | 2.36 | 0.61 |
| 2:1L:320:ARG:NH2 | 2:1L:359:PRO:O | 2.34 | 0.61 |
| 1:1Q:5:VAL:HG22 | 1:1Q:133:PHE:HD1 | 1.65 | 0.61 |
| 1:2M:309:ARG:NH1 | 1:2M:339:SER:O | 2.33 | 0.61 |
| 2:2P:35:GLN:HB3 | 2:2P:59:GLY:O | 2.00 | 0.61 |
| 2:2T:358:GLN:HE21 | 38:8B:214:HIS:N | 1.98 | 0.61 |
| 1:2Y:320:ARG:HH22 | 38:8C:198:THR:HA | 1.64 | 0.61 |
| 2:3B:413:MET:HB3 | 2:3B:417:GLU:OE2 | 2.01 | 0.61 |
| 2:3N:339:ARG:HH22 | 2:3N:342:GLN:HB3 | 1.66 | 0.61 |
| 3:4J:119:THR:HG22 | 3:4J:121:PHE:H | 1.63 | 0.61 |
| 18:6B:43:ASN:OD1 | 18:6B:44:HIS:N | 2.32 | 0.61 |
| 22:6M:137:GLU:HB3 | 22:6M:141:LYS:HE2 | 1.81 | 0.61 |
| 24:6X:277:CYS:HA | 24:6X:368:LEU:HA | 1.82 | 0.61 |
| 24:6Y:431:PRO:HB2 | 24:6Y:433:ARG:HH22 | 1.64 | 0.61 |
| 26:7E:50:SER:C | 26:7E:56:LEU:HD23 | 2.21 | 0.61 |
| 2:4:264:ARG:HD3 | 4:3Y:115:LYS:HD3 | 1.82 | 0.61 |
| 2:F3:56:THR:HG23 | 2:G9:285:GLN:HA | 1.80 | 0.61 |
| 1:G0:276:ARG:HD3 | 24:6V:419:SER:HB2 | 1.81 | 0.61 |
| 2:G3:287:SER:N | 2:G3:290:GLU:OE2 | 2.32 | 0.61 |
| 1:H2:272:PRO:HB2 | 1:H2:282:ARG:HH12 | 1.64 | 0.61 |
| 2:H5:392:ASP:OD2 | 2:H5:422:ARG:NH1 | 2.33 | 0.61 |
| 1:J0:40:SER:HB2 | 28:7H:413:TYR:HD1 | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J4:309:ARG:H | 1:J4:372:THR:HG22 | 1.66 | 0.61 |
| 1:J6:128:ASP:OD1 | 1:J6:129:CYS:N | 2.33 | 0.61 |
| 2:J7:76:ASP:HA | 2:J7:79:ARG:HB2 | 1.82 | 0.61 |
| 2:J7:405:VAL:HG13 | 2:J7:418:PHE:HE2 | 1.64 | 0.61 |
| 2:J9:399:TYR:O | 2:J9:402:ARG:NH1 | 2.34 | 0.61 |
| 1:K4:2:ARG:HE | 1:K4:240:LEU:HD22 | 1.66 | 0.61 |
| 1:L2:57:GLY:H | 30:7K:56:ARG:HH12 | 1.46 | 0.61 |
| 2:M7:195:LEU:HD11 | 2:M7:428:LEU:HD12 | 1.83 | 0.61 |
| 2:P5:206:ASN:OD1 | 41:P6:501:GTP:N2 | 2.33 | 0.61 |
| 1:R4:334:GLN:HE22 | 1:R4:347:ASN:HA | 1.66 | 0.61 |
| 1:S4:26:ASP:OD1 | 24:6U:10:LYS:HE3 | 1.99 | 0.61 |
| 1:S4:273:LEU:O | 1:S4:292:GLN:NE2 | 2.34 | 0.61 |
| 1:S6:52:ASN:OD1 | 1:S6:62:ARG:NH2 | 2.34 | 0.61 |
| 1:S8:213:ARG:HD3 | 1:S8:297:LYS:HD2 | 1.83 | 0.61 |
| 2:S9:298:PRO:HA | 2:S9:301:MET:HG3 | 1.81 | 0.61 |
| 2:T7:9:ILE:HG22 | 2:T7:68:LEU:HD11 | 1.83 | 0.61 |
| 1:U6:137:HIS:NE2 | 1:U6:168:SER:OG | 2.31 | 0.61 |
| 2:U9:384:ILE:HA | 2:U9:387:ILE:HD12 | 1.82 | 0.61 |
| 1:W0:49:VAL:HG11 | 1:W0:241:ARG:HG2 | 1.81 | 0.61 |
| 2:W1:109:THR:OG1 | 2:W1:411:GLU:OE2 | 2.15 | 0.61 |
| 2:Y3:223:THR:HG23 | 2:Y3:225:THR:H | 1.64 | 0.61 |
| 2:Y9:399:TYR:O | 2:Y9:402:ARG:NH1 | 2.33 | 0.61 |
| 1:Z2:16:ILE:HD11 | 1:Z2:136:CYS:HB2 | 1.82 | 0.61 |
| 2:0J:33:ASP:O | 2:0J:60:LYS:NZ | 2.34 | 0.61 |
| 2:0P:286:LEU:HD11 | 2:0P:372:GLN:HB2 | 1.83 | 0.61 |
| 1:0S:86:ARG:HG2 | 1:0S:88:ASP:H | 1.65 | 0.61 |
| 2:0X:83:TYR:HB3 | 2:0X:86:LEU:HB3 | 1.82 | 0.61 |
| 1:0Y:206:ALA:O | 1:0Y:210:ILE:HG12 | 2.01 | 0.61 |
| 2:1D:176:GLN:HE22 | 2:1D:304:LYS:HE2 | 1.65 | 0.61 |
| 2:1D:387:ILE:HG12 | 2:1D:390:ARG:HH22 | 1.64 | 0.61 |
| 2:1F:381:SER:OG | 2:1F:382:THR:N | 2.34 | 0.61 |
| 1:1K:113:ILE:HA | 1:1K:116:VAL:HG22 | 1.81 | 0.61 |
| 1:1M:107:THR:OG1 | 1:1M:401:GLU:OE2 | 2.17 | 0.61 |
| 2:1V:222:PRO:HD2 | 1:1W:324:LYS:HE3 | 1.83 | 0.61 |
| 2:2F:33:ASP:O | 2:2F:60:LYS:NZ | 2.33 | 0.61 |
| 1:2Y:135:VAL:HG21 | 1:2Y:152:ILE:HD11 | 1.83 | 0.61 |
| 1:3C:316:LEU:HD13 | 1:3C:352:SER:HB2 | 1.83 | 0.61 |
| 2:3H:399:TYR:O | 2:3H:402:ARG:NH1 | 2.34 | 0.61 |
| 1:3O:257:LEU:HD21 | 1:3O:314:SER:HB3 | 1.82 | 0.61 |
| 1:3O:362:LYS:NZ | 38:8C:164:GLU:OE1 | 2.32 | 0.61 |
| 2:3P:286:LEU:O | 2:3P:373:ARG:NH1 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:4W:468:MET:CE | 8:4W:470:TYR:CZ | 2.84 | 0.61 |
| 15:5O:99:LYS:N | 15:5O:204:ALA:O | 2.31 | 0.61 |
| 18:5X:43:ASN:OD1 | 18:5X:44:HIS:N | 2.32 | 0.61 |
| 18:5Z:43:ASN:OD1 | 18:5Z:44:HIS:N | 2.32 | 0.61 |
| 18:6A:43:ASN:OD1 | 18:6A:44:HIS:N | 2.32 | 0.61 |
| 18:6C:43:ASN:OD1 | 18:6C:44:HIS:N | 2.32 | 0.61 |
| 18:6D:43:ASN:OD1 | 18:6D:44:HIS:N | 2.32 | 0.61 |
| 19:6E:75:GLN:O | 37:7Y:60:LYS:NZ | 2.34 | 0.61 |
| 22:6P:219:ASP:OD1 | 22:6P:222:SER:OG | 2.10 | 0.61 |
| 24:6Y:91:ASN:HB3 | 24:6Y:94:LYS:HG3 | 1.81 | 0.61 |
| 24:6Y:525:VAL:HB | 24:6Y:530:PHE:HE2 | 1.65 | 0.61 |
| 26:7F:31:VAL:HG22 | 26:7F:107:MET:HB2 | 1.83 | 0.61 |
| 2:4:221:ARG:O | 26:7D:77:ILE:O | 2.18 | 0.61 |
| 1:G2:33:THR:O | 1:G2:58:ARG:NH2 | 2.34 | 0.61 |
| 2:G5:210:TYR:HB3 | 1:G6:324:LYS:HE2 | 1.81 | 0.61 |
| 2:G7:129:CYS:SG | 2:G7:130:THR:N | 2.73 | 0.61 |
| 1:G8:31:ASP:OD1 | 1:G8:35:THR:N | 2.27 | 0.61 |
| 1:J0:139:LEU:HD12 | 1:J0:170:VAL:HG12 | 1.83 | 0.61 |
| 1:J0:350:LYS:NZ | 1:J0:351:SER:O | 2.32 | 0.61 |
| 1:J2:309:ARG:H | 1:J2:372:THR:HG22 | 1.66 | 0.61 |
| 1:K4:362:LYS:HA | 6:4O:169:PHE:CZ | 2.35 | 0.61 |
| 1:L6:41:ASP:CG | 29:7J:167:ILE:HD13 | 2.21 | 0.61 |
| 1:L6:135:VAL:HG21 | 1:L6:152:ILE:HD11 | 1.80 | 0.61 |
| 2:L9:79:ARG:NH1 | 2:L9:92:LEU:O | 2.34 | 0.61 |
| 1:N6:2:ARG:HE | 1:N6:240:LEU:HD22 | 1.66 | 0.61 |
| 1:P6:177:ASP:O | 2:P7:352:LYS:HA | 2.01 | 0.61 |
| 2:Q5:98:ASP:OD1 | 2:Q5:99:ALA:N | 2.34 | 0.61 |
| 1:Q8:212:PHE:HE1 | 2:Q9:326:LYS:HE3 | 1.65 | 0.61 |
| 2:R9:364:PRO:HD2 | 12:5F:113:LYS:HD3 | 1.81 | 0.61 |
| 2:S5:14:ILE:HD11 | 2:S5:74:VAL:HG13 | 1.83 | 0.61 |
| 2:S7:419:SER:O | 2:S7:423:GLU:HG2 | 2.01 | 0.61 |
| 39:T0:501:GDP:O3B | 7:4U:3:ARG:NH1 | 2.34 | 0.61 |
| 2:T1:79:ARG:NH1 | 2:T1:92:LEU:O | 2.34 | 0.61 |
| 2:W5:31:GLN:HE21 | 2:W5:37:PRO:HG3 | 1.66 | 0.61 |
| 1:X0:64:ILE:HD11 | 1:X0:123:GLU:HG3 | 1.83 | 0.61 |
| 2:Z9:83:TYR:HB3 | 2:Z9:86:LEU:HB3 | 1.82 | 0.61 |
| 2:0F:318:MET:HB2 | 2:0F:376:CYS:HB3 | 1.81 | 0.61 |
| 1:0I:309:ARG:NH1 | 1:0I:339:SER:O | 2.34 | 0.61 |
| 1:0O:68:LEU:HB3 | 1:0O:96:GLY:HA2 | 1.83 | 0.61 |
| 2:0X:222:PRO:HD2 | 1:0Y:324:LYS:HE3 | 1.81 | 0.61 |
| 2:0Z:85:GLN:O | 2:1P:283:HIS:NE2 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1C:361:LEU:HD12 | 1:1C:362:LYS:H | 1.65 | 0.61 |
| 2:1X:287:SER:N | 2:1X:290:GLU:OE2 | 2.30 | 0.61 |
| 1:2E:248:ALA:HA | 1:2E:252:LYS:HD2 | 1.83 | 0.61 |
| 1:2E:396:HIS:HA | 1:2E:399:THR:HG22 | 1.83 | 0.61 |
| 2:2N:176:GLN:HE22 | 2:2N:304:LYS:HE2 | 1.65 | 0.61 |
| 2:2R:214:ARG:NH2 | 38:8A:60:GLY:O | 2.33 | 0.61 |
| 2:2T:267:PHE:HB2 | 2:2T:384:ILE:HD12 | 1.83 | 0.61 |
| 1:3C:55:THR:CG2 | 38:8D:164:GLU:HB2 | 2.31 | 0.61 |
| 2:3F:5:ILE:HG22 | 2:3F:64:ARG:HB3 | 1.81 | 0.61 |
| 5:4L:466:LEU:HD21 | 5:4M:139:LEU:HD23 | 1.82 | 0.61 |
| 10:5C:172:GLN:NE2 | 10:5C:176:GLU:HG3 | 2.15 | 0.61 |
| 14:5L:489:SER:HB3 | 14:5L:512:PHE:CD1 | 2.36 | 0.61 |
| 14:5L:548:ILE:HG22 | 14:5L:550:GLY:H | 1.65 | 0.61 |
| 14:5N:548:ILE:HG22 | 14:5N:550:GLY:H | 1.65 | 0.61 |
| 15:5O:203:ASN:HD22 | 15:5O:203:ASN:N | 1.93 | 0.61 |
| 15:5P:343:LEU:H | 15:5P:343:LEU:HD23 | 1.65 | 0.61 |
| 17:5S:181:LEU:HD23 | 17:5S:181:LEU:O | 2.00 | 0.61 |
| 18:5X:47:SER:O | 18:5X:51:MET:HG2 | 2.01 | 0.61 |
| 22:6N:114:THR:HG23 | 22:6N:117:GLY:H | 1.64 | 0.61 |
| 12:7B:49:ALA:O | 12:7B:52:GLU:HG3 | 2.00 | 0.61 |
| 37:7Y:113:GLU:HA | 37:7Y:113:GLU:OE2 | 2.01 | 0.61 |
| 2:F1:33:ASP:OD2 | 22:6O:131:ARG:NH1 | 2.33 | 0.61 |
| 1:H2:418:LEU:HG | 1:H2:422:TYR:HE2 | 1.65 | 0.61 |
| 2:H9:250:VAL:HB | 2:H9:254:GLU:HG3 | 1.83 | 0.61 |
| 2:H9:399:TYR:O | 2:H9:402:ARG:NH1 | 2.34 | 0.61 |
| 2:I3:57:GLY:O | 2:J9:285:GLN:NE2 | 2.20 | 0.61 |
| 2:K3:217:LEU:HD13 | 2:K3:275:ILE:HG22 | 1.82 | 0.61 |
| 1:K4:39:ASP:O | 29:7I:172:VAL:HG22 | 2.01 | 0.61 |
| 1:L6:248:ALA:HA | 1:L6:252:LYS:HD2 | 1.83 | 0.61 |
| 2:L7:90:GLU:H | 2:N3:283:HIS:CE1 | 2.18 | 0.61 |
| 1:N2:252:LYS:CA | 1:N2:255:VAL:HG12 | 2.25 | 0.61 |
| 1:N8:272:PRO:HB2 | 1:N8:282:ARG:NH1 | 2.15 | 0.61 |
| 2:P9:2:ARG:HH12 | 19:6E:166:LYS:HE3 | 1.64 | 0.61 |
| 1:Q2:166:THR:OG1 | 1:Q2:199:CYS:SG | 2.56 | 0.61 |
| 1:S4:26:ASP:O | 1:S4:359:LYS:NZ | 2.29 | 0.61 |
| 2:U3:413:MET:HB3 | 2:U3:417:GLU:OE2 | 2.01 | 0.61 |
| 2:V1:109:THR:OG1 | 2:V1:411:GLU:OE2 | 2.17 | 0.61 |
| 1:V6:343:GLU:HG2 | 1:V6:344:TRP:HD1 | 1.65 | 0.61 |
| 2:V9:189:LEU:HD11 | 2:V9:418:PHE:HE1 | 1.66 | 0.61 |
| 2:W1:406:HIS:HA | 2:W1:409:VAL:HG22 | 1.82 | 0.61 |
| 2:W3:337:THR:O | 2:W3:339:ARG:NH1 | 2.28 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W4:68:LEU:HD12 | 1:W4:143:THR:HG22 | 1.82 | 0.61 |
| 1:W8:138:SER:OG | 1:W8:139:LEU:N | 2.33 | 0.61 |
| 1:X6:177:ASP:O | 2:X7:352:LYS:HA | 2.01 | 0.61 |
| 1:X8:237:THR:O | 1:X8:241:ARG:NE | 2.33 | 0.61 |
| 1:Y0:263:LEU:HD22 | 1:Y0:422:TYR:HE1 | 1.66 | 0.61 |
| 2:Z3:12:ALA:HB2 | 41:Z3:501:GTP:C8 | 2.36 | 0.61 |
| 2:Z9:9:ILE:HG22 | 2:Z9:68:LEU:HD11 | 1.83 | 0.61 |
| 2:0F:2:ARG:HA | 2:0F:133:GLN:HE21 | 1.66 | 0.61 |
| 2:0H:167:LEU:HG | 2:0H:252:ILE:HD11 | 1.83 | 0.61 |
| 2:0H:206:ASN:OD1 | 41:0I:501:GTP:N2 | 2.31 | 0.61 |
| 1:0S:3:GLU:HB2 | 1:0S:130:LEU:HA | 1.81 | 0.61 |
| 2:0V:346:TRP:HD1 | 2:0V:346:TRP:H | 1.47 | 0.61 |
| 2:0X:289:ALA:O | 2:0X:293:ASN:ND2 | 2.34 | 0.61 |
| 2:1D:381:SER:OG | 2:1D:382:THR:N | 2.34 | 0.61 |
| 2:1F:85:GLN:O | 2:1V:283:HIS:NE2 | 2.34 | 0.61 |
| 1:1K:235:GLY:HA3 | 1:1K:366:THR:HG21 | 1.83 | 0.61 |
| 1:1O:52:ASN:OD1 | 1:1O:62:ARG:NH2 | 2.34 | 0.61 |
| 2:1Z:121:ARG:HD3 | 2:1Z:121:ARG:C | 2.20 | 0.61 |
| 2:2X:98:ASP:OD1 | 2:2X:99:ALA:N | 2.34 | 0.61 |
| 2:3N:221:ARG:NE | 38:8C:174:SER:OG | 2.34 | 0.61 |
| 1:3S:280:GLN:HG2 | 38:8D:162:VAL:HG13 | 1.81 | 0.61 |
| 8:4W:440:THR:HA | 8:4W:443:ILE:HD13 | 1.82 | 0.61 |
| 15:5P:157:ARG:NE | 15:5P:231:CYS:SG | 2.67 | 0.61 |
| 18:5Y:43:ASN:OD1 | 18:5Y:44:HIS:N | 2.32 | 0.61 |
| 18:6A:47:SER:O | 18:6A:51:MET:HG2 | 2.01 | 0.61 |
| 19:6E:82:ASP:O | 37:7Y:64:TRP:NE1 | 2.32 | 0.61 |
| 20:6F:122:VAL:HG13 | 20:6F:377:GLY:HA2 | 1.82 | 0.61 |
| 22:6N:136:ASN:OD1 | 24:6X:440:ASN:ND2 | 2.33 | 0.61 |
| 24:6W:484:GLU:HG2 | 24:6W:495:GLY:O | 2.00 | 0.61 |
| 37:7Y:72:ARG:HG2 | 37:7Y:72:ARG:NH2 | 2.16 | 0.61 |
| 38:8A:10:ALA:HA | 38:8A:17:GLY:HA2 | 1.82 | 0.61 |
| 1:9:245:GLN:HG2 | 26:7E:113:ARG:NH1 | 2.15 | 0.61 |
| 1:E8:58:ARG:HD3 | 1:G4:280:GLN:HE22 | 1.64 | 0.61 |
| 2:F3:206:ASN:OD1 | 41:F3:501:GTP:N2 | 2.26 | 0.61 |
| 1:G2:391:ARG:HH22 | 2:G3:435:VAL:HA | 1.65 | 0.61 |
| 2:G3:227:LEU:O | 2:G3:231:ILE:HG12 | 2.01 | 0.61 |
| 2:G3:282:TYR:CD1 | 22:6M:133:PRO:CG | 2.84 | 0.61 |
| 1:H2:156:ARG:NH1 | 1:H2:197:ASP:OD1 | 2.34 | 0.61 |
| 1:J2:211:CYS:HA | 1:J2:215:LEU:HB2 | 1.83 | 0.61 |
| 1:J2:274:THR:HG21 | 1:J2:282:ARG:HD2 | 1.83 | 0.61 |
| 2:K7:274:PRO:HG3 | 2:K7:286:LEU:HD11 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L0:139:LEU:HD12 | 1:L0:170:VAL:HG12 | 1.83 | 0.61 |
| 1:M0:52:ASN:OD1 | 1:M0:62:ARG:NH2 | 2.34 | 0.61 |
| 2:O3:191:THR:HA | 2:O3:194:LEU:HB3 | 1.83 | 0.61 |
| 1:O4:83:GLN:HE21 | 37:7Y:26:ARG:HG2 | 1.65 | 0.61 |
| 2:O5:125:LEU:O | 2:O5:125:LEU:HD12 | 2.00 | 0.61 |
| 1:P6:156:ARG:NH1 | 1:P6:197:ASP:OD1 | 2.33 | 0.61 |
| 1:Q4:166:THR:OG1 | 1:Q4:199:CYS:SG | 2.59 | 0.61 |
| 2:Q9:98:ASP:OD1 | 2:Q9:99:ALA:N | 2.34 | 0.61 |
| 1:S4:286:VAL:HG12 | 1:S4:329:GLN:HE21 | 1.66 | 0.61 |
| 2:S5:417:GLU:HA | 2:S5:420:GLU:HG2 | 1.83 | 0.61 |
| 2:U1:88:HIS:CG | 2:V7:283:HIS:HA | 2.35 | 0.61 |
| 2:U1:277:SER:OG | 2:U1:278:ALA:N | 2.28 | 0.61 |
| 1:V2:67:ASP:N | 1:V2:67:ASP:OD1 | 2.34 | 0.61 |
| 1:V6:256:ASN:HB2 | 1:V6:350:LYS:NZ | 2.15 | 0.61 |
| 2:W1:11:GLN:OE1 | 2:W1:15:GLN:NE2 | 2.34 | 0.61 |
| 1:X4:248:ALA:HA | 1:X4:252:LYS:HD2 | 1.83 | 0.61 |
| 1:Y4:279:GLN:HG2 | 1:Y4:282:ARG:HH21 | 1.66 | 0.61 |
| 2:Y9:12:ALA:HB2 | 41:Z0:501:GTP:C8 | 2.36 | 0.61 |
| 1:Z0:45:GLU:HG2 | 1:Z0:46:ARG:HG2 | 1.82 | 0.61 |
| 1:Z6:139:LEU:HD21 | 1:Z6:168:SER:HB2 | 1.83 | 0.61 |
| 2:0F:47:ASP:OD1 | 2:0F:48:ALA:N | 2.34 | 0.61 |
| 2:0R:50:ASN:O | 2:0R:64:ARG:NH2 | 2.34 | 0.61 |
| 1:1G:259:PRO:HG3 | 1:1G:311:LEU:HD21 | 1.83 | 0.61 |
| 1:1K:3:GLU:HB2 | 1:1K:130:LEU:HA | 1.83 | 0.61 |
| 2:1X:394:LYS:HA | 2:1X:397:LEU:HG | 1.83 | 0.61 |
| 1:2A:286:VAL:HG23 | 1:2A:287:PRO:HD3 | 1.83 | 0.61 |
| 1:2E:67:ASP:OD1 | 1:2E:72:THR:OG1 | 2.18 | 0.61 |
| 1:2K:248:ALA:HA | 1:2K:252:LYS:HD2 | 1.82 | 0.61 |
| 1:2Q:130:LEU:HB2 | 1:2Q:162:ARG:HE | 1.65 | 0.61 |
| 2:3F:56:THR:OG1 | 3:3V:34:SER:HA | 2.01 | 0.61 |
| 2:3F:317:LEU:HB3 | 2:3F:319:TYR:HE1 | 1.65 | 0.61 |
| 2:3H:320:ARG:NH2 | 2:3H:358:GLN:OE1 | 2.33 | 0.61 |
| 1:3K:280:GLN:HG2 | 38:8B:162:VAL:CG2 | 2.29 | 0.61 |
| 10:5C:137:THR:O | 10:5C:141:LEU:HG | 2.01 | 0.61 |
| 11:5E:47:THR:HG22 | 11:5E:49:ASP:H | 1.65 | 0.61 |
| 14:5M:548:ILE:HG22 | 14:5M:550:GLY:H | 1.65 | 0.61 |
| 15:5O:366:VAL:O | 15:5O:370:ASN:ND2 | 2.34 | 0.61 |
| 17:5T:185:LEU:HD12 | 17:5T:226:ILE:HG13 | 1.81 | 0.61 |
| 18:5Y:47:SER:O | 18:5Y:51:MET:HG2 | 2.01 | 0.61 |
| 18:5Z:47:SER:O | 18:5Z:51:MET:HG2 | 2.01 | 0.61 |
| 18:6B:47:SER:O | 18:6B:51:MET:HG2 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:6C:5:VAL:HG12 | 18:6C:5:VAL:O | 2.01 | 0.61 |
| 18:6C:47:SER:O | 18:6C:51:MET:HG2 | 2.01 | 0.61 |
| 18:6D:47:SER:O | 18:6D:51:MET:HG2 | 2.01 | 0.61 |
| 22:6K:124:PHE:HB2 | 22:6K:127:THR:HG23 | 1.83 | 0.61 |
| 23:6R:25:GLU:OE1 | 23:6R:25:GLU:HA | 2.01 | 0.61 |
| 24:6Y:97:ARG:H | 24:6Y:188:THR:CG2 | 2.13 | 0.61 |
| 26:7D:31:VAL:HG22 | 26:7D:107:MET:HB2 | 1.83 | 0.61 |
| 26:7E:31:VAL:HG22 | 26:7E:107:MET:HB2 | 1.83 | 0.61 |
| 26:7F:146:ASN:H | 26:7F:146:ASN:ND2 | 1.98 | 0.61 |
| 30:7L:389:ARG:NH2 | 30:7L:393:ASP:OD1 | 2.34 | 0.61 |
| 34:7R:205:LEU:HD12 | 36:7V:91:PRO:HG3 | 1.82 | 0.61 |
| 2:8:26:LEU:HD22 | 26:7E:48:LEU:HD11 | 1.83 | 0.61 |
| 2:8:370:LYS:HG3 | 24:6W:88:TRP:HZ3 | 1.65 | 0.61 |
| 1:G2:65:LEU:HD12 | 1:G2:90:PHE:CE1 | 2.36 | 0.61 |
| 2:J1:417:GLU:HA | 2:J1:420:GLU:HG2 | 1.83 | 0.61 |
| 2:J9:278:ALA:HA | 2:J9:369:ALA:HB2 | 1.82 | 0.61 |
| 2:M5:121:ARG:CB | 2:M5:121:ARG:NH1 | 2.63 | 0.61 |
| 2:O3:319:TYR:HB3 | 2:O3:323:VAL:HG21 | 1.82 | 0.61 |
| 2:O5:100:ALA:HA | 1:O6:252:LYS:HE3 | 1.83 | 0.61 |
| 1:Q0:396:HIS:HA | 1:Q0:399:THR:HG22 | 1.82 | 0.61 |
| 1:Q6:334:GLN:HE22 | 1:Q6:348:ASN:H | 1.49 | 0.61 |
| 2:S1:79:ARG:NH1 | 2:S1:94:SER:OG | 2.34 | 0.61 |
| 2:U5:73:THR:O | 2:U5:77:GLU:HG2 | 2.01 | 0.61 |
| 1:U8:68:LEU:HB3 | 1:U8:96:GLY:HA2 | 1.82 | 0.61 |
| 2:V3:51:THR:HG21 | 2:V3:243:ARG:HG2 | 1.82 | 0.61 |
| 2:W1:89:PRO:HB2 | 2:X7:280:LYS:NZ | 2.16 | 0.61 |
| 2:W7:2:ARG:HA | 2:W7:133:GLN:HE21 | 1.65 | 0.61 |
| 1:X2:67:ASP:N | 1:X2:67:ASP:OD1 | 2.33 | 0.61 |
| 1:X6:178:THR:OG1 | 2:X7:258:ASN:ND2 | 2.34 | 0.61 |
| 2:Y9:191:THR:HA | 2:Y9:194:LEU:HB3 | 1.82 | 0.61 |
| 2:Z1:210:TYR:CE1 | 2:Z1:227:LEU:HD21 | 2.36 | 0.61 |
| 2:Z7:417:GLU:HA | 2:Z7:420:GLU:HG2 | 1.83 | 0.61 |
| 1:0C:394:PHE:CE2 | 1:0C:397:TRP:HE3 | 2.19 | 0.61 |
| 1:0E:6:HIS:CE1 | 1:0E:8:GLN:HG3 | 2.36 | 0.61 |
| 2:0F:166:LYS:NZ | 2:0F:199:ASP:OD2 | 2.33 | 0.61 |
| 2:0J:278:ALA:HA | 2:0J:369:ALA:HB2 | 1.82 | 0.61 |
| 2:0P:56:THR:N | 2:0P:60:LYS:O | 2.33 | 0.61 |
| 1:0Q:5:VAL:HG23 | 1:0Q:62:ARG:HG2 | 1.82 | 0.61 |
| 1:0Y:389:PHE:CE1 | 1:0Y:395:LEU:HD11 | 2.36 | 0.61 |
| 2:1B:53:PHE:HB3 | 2:1B:61:HIS:HB3 | 1.83 | 0.61 |
| 2:1V:287:SER:N | 2:1V:290:GLU:OE2 | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2D:387:ILE:HG12 | 2:2D:390:ARG:HH22 | 1.66 | 0.61 |
| 1:2U:320:ARG:CZ | 38:8B:201:LEU:HD23 | 2.30 | 0.61 |
| 2:3D:50:ASN:O | 2:3D:64:ARG:NH2 | 2.33 | 0.61 |
| 2:3H:264:ARG:NH2 | 2:3H:431:ASP:OD2 | 2.34 | 0.61 |
| 2:3R:182:VAL:HG12 | 2:3R:185:TYR:HB2 | 1.82 | 0.61 |
| 6:4N:451:VAL:O | 6:4N:455:VAL:HG23 | 2.01 | 0.61 |
| 11:5E:115:LEU:HD12 | 11:5E:119:THR:O | 2.00 | 0.61 |
| 14:5L:21:LEU:HD21 | 14:5L:310:PHE:HB3 | 1.82 | 0.61 |
| 14:5M:21:LEU:HD21 | 14:5M:310:PHE:HB3 | 1.82 | 0.61 |
| 14:5M:415:LYS:HE3 | 23:6R:22:MET:HB2 | 1.79 | 0.61 |
| 1:9:281:TYR:HD2 | 1:T2:60:VAL:HG11 | 1.65 | 0.60 |
| 1:A9:277:GLY:HA2 | 24:6U:142:ILE:HG22 | 1.83 | 0.60 |
| 1:B1:39:ASP:O | 18:5Y:119:ARG:NH1 | 2.33 | 0.60 |
| 1:E0:32:PRO:HG3 | 24:6T:402:LYS:HE3 | 1.81 | 0.60 |
| 2:G3:42:ILE:CD1 | 24:6W:470:ILE:HD13 | 2.17 | 0.60 |
| 2:G5:282:TYR:CE2 | 22:6N:212:GLU:OE1 | 2.54 | 0.60 |
| 1:G8:180:VAL:HG23 | 1:G8:184:ASN:HD21 | 1.66 | 0.60 |
| 2:G9:90:GLU:OE1 | 2:I5:283:HIS:ND1 | 2.33 | 0.60 |
| 1:H2:309:ARG:H | 1:H2:372:THR:HG22 | 1.65 | 0.60 |
| 2:I1:222:PRO:HD2 | 1:I2:324:LYS:HE3 | 1.82 | 0.60 |
| 2:I1:267:PHE:HB2 | 2:I1:384:ILE:HD12 | 1.82 | 0.60 |
| 2:K1:315:CYS:HG | 2:K1:379:SER:HG | 1.46 | 0.60 |
| 2:K3:364:PRO:HB2 | 29:7I:233:LYS:HG2 | 1.82 | 0.60 |
| 1:K8:134:GLN:HE21 | 1:K8:167:PHE:HE2 | 1.48 | 0.60 |
| 1:L2:211:CYS:HA | 1:L2:215:LEU:HB2 | 1.83 | 0.60 |
| 1:Q4:279:GLN:OE1 | 20:6F:93:ARG:NH2 | 2.34 | 0.60 |
| 2:R1:379:SER:OG | 2:R1:380:ASN:N | 2.34 | 0.60 |
| 1:S0:92:PHE:CZ | 24:6Z:40:GLN:CG | 2.83 | 0.60 |
| 1:S2:33:THR:HG22 | 1:S2:58:ARG:HH22 | 1.64 | 0.60 |
| 2:T1:102:ASN:HB3 | 2:T1:105:ARG:HB3 | 1.83 | 0.60 |
| 2:W5:109:THR:OG1 | 2:W5:411:GLU:OE2 | 2.15 | 0.60 |
| 2:W7:267:PHE:HB2 | 2:W7:384:ILE:HD12 | 1.81 | 0.60 |
| 2:Z1:115:VAL:HG21 | 2:Z1:152:LEU:HD22 | 1.83 | 0.60 |
| 2:Z1:319:TYR:HB3 | 2:Z1:323:VAL:HG21 | 1.83 | 0.60 |
| 2:Z5:405:VAL:HG13 | 2:Z5:418:PHE:HE2 | 1.65 | 0.60 |
| 1:Z6:285:THR:HB | 1:Z6:287:PRO:HD2 | 1.83 | 0.60 |
| 1:0E:218:THR:HG23 | 1:0E:219:THR:HG23 | 1.83 | 0.60 |
| 1:0M:270:PHE:HD2 | 1:0M:273:LEU:HD11 | 1.66 | 0.60 |
| 1:1C:268:VAL:O | 1:1C:300:MET:N | 2.34 | 0.60 |
| 2:1H:65:CYS:SG | 2:1H:66:ILE:N | 2.74 | 0.60 |
| 2:1T:287:SER:N | 2:1T:290:GLU:OE2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1Z:113:GLU:HG2 | 38:7Z:7:ASP:HA | 1.82 | 0.60 |
| 1:2E:163:MET:HB3 | 1:2E:250:LEU:HD22 | 1.82 | 0.60 |
| 1:2M:286:VAL:HG23 | 1:2M:287:PRO:HD3 | 1.82 | 0.60 |
| 2:3B:339:ARG:CG | 38:8C:39:LYS:HZ2 | 2.14 | 0.60 |
| 2:3D:394:LYS:HA | 2:3D:397:LEU:HG | 1.82 | 0.60 |
| 2:3H:276:ILE:HG13 | 2:3H:280:LYS:HB2 | 1.83 | 0.60 |
| 2:3R:416:GLY:O | 2:3R:420:GLU:HG2 | 1.99 | 0.60 |
| 1:3S:211:CYS:SG | 1:3S:217:LEU:HB2 | 2.40 | 0.60 |
| 14:5N:21:LEU:HD21 | 14:5N:310:PHE:HB3 | 1.82 | 0.60 |
| 22:6N:180:SER:OG | 22:6N:182:ASN:ND2 | 2.33 | 0.60 |
| 26:7D:38:ASN:ND2 | 26:7D:54:GLU:OE1 | 2.30 | 0.60 |
| 38:8A:84:ILE:HG23 | 38:8A:84:ILE:O | 2.01 | 0.60 |
| 2:2:415:GLU:OE2 | 4:3W:86:TYR:CZ | 2.53 | 0.60 |
| 2:E5:282:TYR:OH | 22:6K:82:LEU:N | 2.34 | 0.60 |
| 2:E9:58:ALA:HB2 | 24:6X:435:LEU:HD13 | 1.81 | 0.60 |
| 2:G1:195:LEU:HD21 | 2:G1:264:ARG:HD2 | 1.83 | 0.60 |
| 2:H1:363:VAL:HG23 | 2:H1:366:GLY:HA3 | 1.83 | 0.60 |
| 2:J9:301:MET:HE1 | 2:J9:307:PRO:HD3 | 1.82 | 0.60 |
| 2:K3:223:THR:OG1 | 1:K4:245:GLN:NE2 | 2.34 | 0.60 |
| 1:L2:257:LEU:HA | 1:L2:312:THR:HG21 | 1.84 | 0.60 |
| 2:L3:417:GLU:HA | 2:L3:420:GLU:HG2 | 1.84 | 0.60 |
| 2:L5:174:SER:HB3 | 2:L5:177:VAL:O | 2.00 | 0.60 |
| 1:M6:73:MET:CE | 1:M6:90:PHE:HB3 | 2.32 | 0.60 |
| 2:M7:198:THR:HG21 | 2:M7:201:ALA:HB2 | 1.83 | 0.60 |
| 2:N1:119:LEU:HA | 2:N1:122:ILE:HG22 | 1.83 | 0.60 |
| 2:N9:88:HIS:CD2 | 2:P7:283:HIS:HB3 | 2.37 | 0.60 |
| 1:O2:134:GLN:HE21 | 1:O2:167:PHE:HE2 | 1.47 | 0.60 |
| 2:O3:69:ASP:OD1 | 2:O3:70:LEU:N | 2.34 | 0.60 |
| 2:O5:27:GLU:OE1 | 2:O5:243:ARG:NH1 | 2.27 | 0.60 |
| 2:P7:114:ILE:HG21 | 2:P7:149:LEU:HD22 | 1.83 | 0.60 |
| 2:Q3:417:GLU:HA | 2:Q3:420:GLU:HG2 | 1.84 | 0.60 |
| 1:R8:238:CYS:SG | 1:R8:318:ARG:NE | 2.74 | 0.60 |
| 2:R9:166:LYS:N | 2:R9:199:ASP:OD2 | 2.32 | 0.60 |
| 1:T4:287:PRO:HB3 | 13:5J:100:MET:SD | 2.41 | 0.60 |
| 2:U1:287:SER:N | 2:U1:290:GLU:OE2 | 2.33 | 0.60 |
| 1:V6:343:GLU:HG2 | 1:V6:344:TRP:CD1 | 2.36 | 0.60 |
| 1:Y0:139:LEU:HD12 | 1:Y0:170:VAL:HG12 | 1.82 | 0.60 |
| 2:Z1:12:ALA:HB2 | 41:Z2:501:GTP:C8 | 2.37 | 0.60 |
| 1:Z8:208:TYR:CE1 | 1:Z8:225:LEU:HD11 | 2.35 | 0.60 |
| 2:0B:239:THR:HG23 | 2:0B:243:ARG:HE | 1.66 | 0.60 |
| 2:0F:239:THR:HG23 | 2:0F:243:ARG:HE | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0G:165:LEU:HD13 | 1:0G:167:PHE:HZ | 1.65 | 0.60 |
| 1:0K:165:LEU:HD22 | 1:0K:167:PHE:HE1 | 1.66 | 0.60 |
| 2:0L:352:LYS:NZ | 2:0L:353:CYS:O | 2.34 | 0.60 |
| 1:0M:334:GLN:HE22 | 1:0M:348:ASN:H | 1.49 | 0.60 |
| 1:0U:177:ASP:O | 2:0V:352:LYS:HA | 2.00 | 0.60 |
| 2:1D:392:ASP:OD2 | 2:1D:422:ARG:NH1 | 2.34 | 0.60 |
| 1:1Q:276:ARG:NH2 | 9:4Z:203:GLU:OE2 | 2.31 | 0.60 |
| 2:2B:392:ASP:OD2 | 2:2B:422:ARG:NH1 | 2.34 | 0.60 |
| 1:2I:285:THR:HG23 | 1:2I:288:GLU:H | 1.65 | 0.60 |
| 2:2J:381:SER:OG | 2:2J:382:THR:N | 2.34 | 0.60 |
| 2:2N:102:ASN:HB2 | 2:2N:407:TRP:CH2 | 2.36 | 0.60 |
| 2:2P:214:ARG:CZ | 38:7Z:18:VAL:HA | 2.32 | 0.60 |
| 2:2P:308:ARG:HH12 | 38:7Z:24:TYR:N | 1.99 | 0.60 |
| 2:2Z:88:HIS:HB3 | 2:2Z:91:GLN:CG | 2.31 | 0.60 |
| 1:3I:139:LEU:HD12 | 1:3I:170:VAL:HG12 | 1.83 | 0.60 |
| 2:3P:71:GLU:HB3 | 2:3P:98:ASP:OD1 | 2.01 | 0.60 |
| 1:3S:380:ARG:O | 1:3S:383:GLU:HG3 | 2.00 | 0.60 |
| 7:4U:144:ALA:HB1 | 31:7N:115:GLN:HE22 | 1.65 | 0.60 |
| 7:4U:234:GLU:OE2 | 12:5G:295:ARG:NH1 | 2.34 | 0.60 |
| 15:5O:344:ARG:NH2 | 15:5O:358:CYS:SG | 2.74 | 0.60 |
| 16:5Q:187:THR:HG23 | 16:5Q:190:SER:H | 1.66 | 0.60 |
| 17:5S:174:SER:HB2 | 17:5S:175:PRO:HD2 | 1.83 | 0.60 |
| 22:6K:51:ILE:HA | 22:6K:54:ARG:HD3 | 1.81 | 0.60 |
| 25:7C:80:ARG:HD2 | 27:7G:91:TYR:OH | 2.01 | 0.60 |
| 38:8C:83:ARG:HD3 | 38:8C:83:ARG:O | 2.01 | 0.60 |
| 1:C2:79:GLY:HA3 | 24:7A:221:ARG:HH22 | 1.65 | 0.60 |
| 2:G3:381:SER:OG | 2:G3:382:THR:N | 2.32 | 0.60 |
| 2:J1:145:THR:OG1 | 41:J2:501:GTP:O1B | 2.19 | 0.60 |
| 2:J7:109:THR:OG1 | 2:J7:411:GLU:OE2 | 2.20 | 0.60 |
| 2:J7:207:GLU:OE1 | 2:J7:304:LYS:HE3 | 2.01 | 0.60 |
| 1:M6:5:VAL:HG23 | 1:M6:62:ARG:HG2 | 1.84 | 0.60 |
| 2:M9:282:TYR:HE1 | 30:7K:25:ALA:HB2 | 1.60 | 0.60 |
| 1:N2:140:GLY:O | 1:N2:184:ASN:ND2 | 2.34 | 0.60 |
| 2:N3:289:ALA:O | 2:N3:293:ASN:ND2 | 2.33 | 0.60 |
| 2:O3:313:MET:CG | 2:O3:346:TRP:CH2 | 2.85 | 0.60 |
| 2:O7:203:MET:HE1 | 2:O7:267:PHE:HB3 | 1.84 | 0.60 |
| 2:O9:269:LEU:HG | 2:O9:384:ILE:HD11 | 1.82 | 0.60 |
| 2:P7:56:THR:HA | 2:R3:285:GLN:HB2 | 1.82 | 0.60 |
| 1:Q2:176:SER:HB3 | 2:Q3:349:THR:CG2 | 2.32 | 0.60 |
| 1:Q4:33:THR:O | 1:Q4:58:ARG:NH2 | 2.34 | 0.60 |
| 1:T4:175:VAL:HG22 | 2:T5:329:ASN:HD21 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T4:190:HIS:CD2 | 1:T4:414:ASN:HD22 | 2.19 | 0.60 |
| 1:T6:92:PHE:CZ | 24:7A:44:ALA:CB | 2.71 | 0.60 |
| 2:V9:254:GLU:HB3 | 2:V9:352:LYS:HE2 | 1.83 | 0.60 |
| 1:W0:207:LEU:HB3 | 1:W0:225:LEU:HD22 | 1.82 | 0.60 |
| 1:W6:266:PHE:HE1 | 1:W6:370:ASN:HD22 | 1.47 | 0.60 |
| 2:W9:279:GLU:OE2 | 2:W9:279:GLU:HA | 2.01 | 0.60 |
| 1:X2:11:GLN:HG3 | 1:X2:72:THR:HG22 | 1.83 | 0.60 |
| 2:X3:336:LYS:O | 2:X3:339:ARG:NH2 | 2.34 | 0.60 |
| 1:X4:3:GLU:HB2 | 1:X4:130:LEU:HA | 1.81 | 0.60 |
| 1:X4:275:SER:O | 1:X4:279:GLN:HG3 | 2.01 | 0.60 |
| 2:X9:90:GLU:HG2 | 2:Z5:280:LYS:HE2 | 1.82 | 0.60 |
| 2:Z7:83:TYR:HB3 | 2:Z7:86:LEU:HB3 | 1.82 | 0.60 |
| 2:0H:392:ASP:OD2 | 2:0H:422:ARG:NH1 | 2.34 | 0.60 |
| 1:0S:103:LYS:CE | 1:0S:108:GLU:HG2 | 2.31 | 0.60 |
| 1:1C:397:TRP:CE3 | 1:1C:397:TRP:HA | 2.35 | 0.60 |
| 2:1H:145:THR:OG1 | 41:1H:501:GTP:O1B | 2.19 | 0.60 |
| 2:1L:88:HIS:CD2 | 2:2B:283:HIS:HB3 | 2.31 | 0.60 |
| 1:1O:113:ILE:HA | 1:1O:116:VAL:HG22 | 1.83 | 0.60 |
| 2:1X:27:GLU:OE1 | 2:1X:243:ARG:NH1 | 2.34 | 0.60 |
| 1:2K:50:TYR:CE2 | 1:2K:241:ARG:HD3 | 2.36 | 0.60 |
| 1:2Q:128:ASP:OD1 | 1:2Q:129:CYS:N | 2.34 | 0.60 |
| 1:2Q:248:ALA:HA | 1:2Q:252:LYS:HD2 | 1.82 | 0.60 |
| 2:2X:46:ASP:OD2 | 38:8C:211:LYS:HE2 | 2.00 | 0.60 |
| 1:3C:350:LYS:NZ | 1:3C:352:SER:OG | 2.34 | 0.60 |
| 1:3Q:113:ILE:HD13 | 1:3Q:150:LEU:HD22 | 1.83 | 0.60 |
| 2:3R:245:ASP:OD2 | 14:5N:192:THR:HG22 | 2.01 | 0.60 |
| 3:4F:38:THR:HG21 | 4:4G:3:LYS:HB2 | 1.82 | 0.60 |
| 5:4L:270:LYS:O | 5:4L:274:ILE:HG12 | 2.01 | 0.60 |
| 9:4Z:401:ILE:O | 9:4Z:405:GLN:HG3 | 2.01 | 0.60 |
| 15:5O:199:ASP:O | 15:5O:202:PHE:O | 2.20 | 0.60 |
| 17:5T:189:TRP:CD1 | 17:5T:222:ILE:CG2 | 2.82 | 0.60 |
| 24:6U:107:VAL:HG22 | 24:6U:108:GLU:H | 1.65 | 0.60 |
| 24:6X:514:TYR:O | 24:6X:517:LEU:HD12 | 2.00 | 0.60 |
| 24:7A:11:LEU:HD12 | 24:7A:12:PRO:HD2 | 1.84 | 0.60 |
| 35:7T:174:GLN:O | 35:7T:178:GLU:HG2 | 2.01 | 0.60 |
| 2:G7:317:LEU:HB3 | 2:G7:319:TYR:HE1 | 1.67 | 0.60 |
| 2:H3:387:ILE:HG12 | 2:H3:390:ARG:HH22 | 1.65 | 0.60 |
| 2:H3:392:ASP:OD2 | 2:H3:422:ARG:NH1 | 2.35 | 0.60 |
| 1:I0:218:THR:H | 24:6X:489:ASN:CB | 2.15 | 0.60 |
| 2:K7:381:SER:OG | 2:K7:382:THR:N | 2.32 | 0.60 |
| 1:K8:248:ALA:CB | 1:K8:252:LYS:HD3 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L4:2:ARG:HE | 1:L4:240:LEU:HD22 | 1.65 | 0.60 |
| 2:L7:79:ARG:NH1 | 2:L7:92:LEU:O | 2.35 | 0.60 |
| 1:M4:279:GLN:HB3 | 30:7K:170:ARG:HH22 | 1.66 | 0.60 |
| 1:N8:309:ARG:H | 1:N8:372:THR:HG22 | 1.67 | 0.60 |
| 2:P3:307:PRO:HB2 | 2:P3:312:TYR:CE1 | 2.36 | 0.60 |
| 2:Q9:33:ASP:OD2 | 2:Q9:35:GLN:NE2 | 2.33 | 0.60 |
| 1:R8:257:LEU:HD21 | 1:R8:314:SER:HB3 | 1.83 | 0.60 |
| 1:S0:334:GLN:HE22 | 1:S0:348:ASN:H | 1.48 | 0.60 |
| 1:T6:221:THR:HG23 | 1:T6:223:GLY:H | 1.65 | 0.60 |
| 1:T6:328:GLU:HB3 | 17:5U:38:PHE:CZ | 2.36 | 0.60 |
| 2:T7:211:ASP:OD2 | 13:5K:88:ARG:NE | 2.21 | 0.60 |
| 1:U8:334:GLN:HE22 | 1:U8:348:ASN:H | 1.49 | 0.60 |
| 1:V6:140:GLY:O | 1:V6:184:ASN:ND2 | 2.34 | 0.60 |
| 2:V7:399:TYR:OH | 2:V7:415:GLU:OE2 | 2.19 | 0.60 |
| 1:X2:33:THR:O | 1:X2:58:ARG:NH2 | 2.34 | 0.60 |
| 1:Y2:111:GLU:HG2 | 1:Y2:112:LEU:HD22 | 1.84 | 0.60 |
| 1:Z2:21:TRP:HA | 1:Z2:24:VAL:HG22 | 1.83 | 0.60 |
| 1:0A:113:ILE:HD13 | 1:0A:150:LEU:HD22 | 1.83 | 0.60 |
| 1:0U:334:GLN:HE22 | 1:0U:348:ASN:H | 1.49 | 0.60 |
| 2:0X:9:ILE:HG22 | 2:0X:146:GLY:HA2 | 1.82 | 0.60 |
| 2:0Z:58:ALA:HB2 | 9:4Z:165:ARG:HH12 | 1.59 | 0.60 |
| 1:1E:8:GLN:O | 1:1E:66:MET:HG2 | 2.01 | 0.60 |
| 2:1P:320:ARG:NH2 | 2:1P:359:PRO:O | 2.34 | 0.60 |
| 2:1Z:121:ARG:NE | 2:1Z:124:LYS:HE3 | 2.16 | 0.60 |
| 2:2B:132:LEU:HD22 | 2:2B:164:LYS:HD3 | 1.83 | 0.60 |
| 1:2Q:263:LEU:HD13 | 1:2Q:422:TYR:HE1 | 1.66 | 0.60 |
| 1:2Q:271:THR:HG23 | 1:2Q:365:ALA:HB3 | 1.83 | 0.60 |
| 2:2V:308:ARG:NH2 | 38:8B:72:ASP:HB2 | 2.11 | 0.60 |
| 1:3A:45:GLU:HG3 | 1:3A:46:ARG:HG2 | 1.82 | 0.60 |
| 2:3P:88:HIS:HB3 | 2:3P:91:GLN:NE2 | 2.17 | 0.60 |
| 2:3P:242:LEU:HD11 | 2:3P:252:ILE:HG12 | 1.83 | 0.60 |
| 2:3R:91:GLN:HE21 | 3:4H:36:PHE:HE2 | 1.50 | 0.60 |
| 14:5L:36:SER:N | 14:5L:595:SER:OG | 2.33 | 0.60 |
| 26:7E:38:ASN:ND2 | 26:7E:54:GLU:OE1 | 2.30 | 0.60 |
| 28:7H:399:VAL:O | 28:7H:402:ARG:HG2 | 2.01 | 0.60 |
| 34:7S:156:GLN:O | 34:7S:160:THR:HG23 | 2.01 | 0.60 |
| 2:8:29:GLY:C | 26:7E:45:MET:HE1 | 2.19 | 0.60 |
| 1:G6:77:ARG:HG3 | 1:G6:90:PHE:CE2 | 2.35 | 0.60 |
| 2:G7:174:SER:OG | 2:G7:205:ASP:OD1 | 2.19 | 0.60 |
| 2:H7:379:SER:OG | 2:H7:380:ASN:N | 2.33 | 0.60 |
| 1:J8:2:ARG:HE | 1:J8:240:LEU:HD22 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K3:387:ILE:HG12 | 2:K3:390:ARG:HH22 | 1.67 | 0.60 |
| 2:L5:181:VAL:HB | 1:L6:256:ASN:HD22 | 1.66 | 0.60 |
| 2:O5:11:GLN:OE1 | 2:O5:15:GLN:NE2 | 2.34 | 0.60 |
| 2:P9:18:ASN:ND2 | 19:6E:149:TYR:HE1 | 2.00 | 0.60 |
| 1:Q2:54:ALA:HA | 1:R8:283:ALA:HB2 | 1.84 | 0.60 |
| 1:R2:102:ALA:HB1 | 1:R2:401:GLU:HB3 | 1.82 | 0.60 |
| 2:R5:196:GLU:HG2 | 17:5T:82:LYS:HZ2 | 1.66 | 0.60 |
| 1:R6:37:HIS:O | 11:5E:71:ARG:NH1 | 2.29 | 0.60 |
| 1:S0:94:GLN:HE22 | 13:5K:17:LYS:C | 2.04 | 0.60 |
| 2:S1:267:PHE:HB2 | 2:S1:384:ILE:HD12 | 1.83 | 0.60 |
| 2:S9:176:GLN:NE2 | 13:5I:90:PRO:HG3 | 2.17 | 0.60 |
| 2:T5:86:LEU:O | 2:T5:86:LEU:HD12 | 2.01 | 0.60 |
| 2:V1:389:SER:N | 2:V1:429:GLU:OE1 | 2.35 | 0.60 |
| 1:V8:56:GLY:O | 8:4V:469:GLN:NE2 | 2.34 | 0.60 |
| 1:W0:161:ASP:O | 1:W0:162:ARG:NH1 | 2.32 | 0.60 |
| 1:W4:113:ILE:HA | 1:W4:116:VAL:HG12 | 1.82 | 0.60 |
| 2:W5:113:GLU:N | 2:W5:113:GLU:OE2 | 2.35 | 0.60 |
| 2:W5:413:MET:HB3 | 2:W5:417:GLU:OE2 | 2.01 | 0.60 |
| 1:X2:268:VAL:HG23 | 1:X2:300:MET:HB2 | 1.84 | 0.60 |
| 1:X8:181:GLU:HG3 | 1:X8:182:PRO:HD3 | 1.83 | 0.60 |
| 1:X8:391:ARG:HG3 | 2:X9:346:TRP:HB3 | 1.83 | 0.60 |
| 1:Y2:201:VAL:HG12 | 1:Y2:266:PHE:O | 2.01 | 0.60 |
| 1:Y2:397:TRP:HE1 | 2:Y3:260:VAL:HB | 1.65 | 0.60 |
| 1:Y8:193:VAL:HG11 | 1:Y8:418:LEU:HD11 | 1.83 | 0.60 |
| 1:Z2:114:ASP:OD1 | 1:Z2:115:SER:N | 2.34 | 0.60 |
| 1:0I:20:PHE:HA | 1:0I:230:SER:OG | 2.01 | 0.60 |
| 2:0R:298:PRO:HA | 2:0R:301:MET:HG3 | 1.82 | 0.60 |
| 2:0V:167:LEU:HB3 | 2:0V:169:PHE:HE1 | 1.65 | 0.60 |
| 2:1D:250:VAL:HG23 | 2:1D:254:GLU:HG3 | 1.84 | 0.60 |
| 1:1K:163:MET:HB3 | 1:1K:250:LEU:HD22 | 1.82 | 0.60 |
| 1:1M:186:THR:HG22 | 1:1M:411:ALA:HB1 | 1.82 | 0.60 |
| 2:1N:56:THR:HG23 | 2:1N:60:LYS:HB3 | 1.84 | 0.60 |
| 1:2C:52:ASN:OD1 | 1:2C:62:ARG:NH2 | 2.35 | 0.60 |
| 2:2D:123:ARG:NH2 | 38:8A:37:TYR:HA | 2.17 | 0.60 |
| 2:2F:222:PRO:HD2 | 1:2G:324:LYS:HE3 | 1.82 | 0.60 |
| 2:2T:280:LYS:HA | 2:2T:283:HIS:ND1 | 2.16 | 0.60 |
| 1:2W:211:CYS:HA | 1:2W:215:LEU:HB2 | 1.83 | 0.60 |
| 2:3B:223:THR:HG21 | 1:3C:245:GLN:HE22 | 1.67 | 0.60 |
| 2:3J:70:LEU:HB2 | 2:3J:98:ASP:HA | 1.84 | 0.60 |
| 1:3O:272:PRO:HB2 | 1:3O:282:ARG:HH12 | 1.66 | 0.60 |
| 2:3P:222:PRO:HD2 | 1:3Q:324:LYS:HE3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:3W:44:SER:OG | 4:3W:163:ARG:NH1 | 2.34 | 0.60 |
| 4:3Y:44:SER:OG | 4:3Y:163:ARG:NH1 | 2.34 | 0.60 |
| 4:4A:44:SER:OG | 4:4A:163:ARG:NH1 | 2.34 | 0.60 |
| 4:4I:44:SER:OG | 4:4I:163:ARG:NH1 | 2.34 | 0.60 |
| 14:5N:36:SER:N | 14:5N:595:SER:OG | 2.33 | 0.60 |
| 15:5O:210:ALA:HB3 | 15:5O:213:THR:HG23 | 1.82 | 0.60 |
| 22:6I:54:ARG:HG3 | 24:6T:285:MET:HG2 | 1.83 | 0.60 |
| 24:6V:569:LYS:HB2 | 24:6V:572:ALA:HB3 | 1.84 | 0.60 |
| 1:A3:283:ALA:HB2 | 1:T6:54:ALA:HA | 1.82 | 0.60 |
| 2:G3:221:ARG:NH1 | 22:6M:178:GLY:O | 2.34 | 0.60 |
| 2:H3:399:TYR:O | 2:H3:402:ARG:NH1 | 2.35 | 0.60 |
| 2:H7:222:PRO:HD2 | 1:H8:324:LYS:HE3 | 1.81 | 0.60 |
| 2:H7:399:TYR:O | 2:H7:402:ARG:NH1 | 2.35 | 0.60 |
| 2:J9:88:HIS:CG | 2:L5:283:HIS:HA | 2.36 | 0.60 |
| 2:J9:90:GLU:HG3 | 2:J9:121:ARG:NH1 | 2.17 | 0.60 |
| 1:L0:211:CYS:HA | 1:L0:215:LEU:HB2 | 1.83 | 0.60 |
| 2:L7:156:ARG:HA | 2:L7:159:VAL:HG22 | 1.83 | 0.60 |
| 2:M3:73:THR:O | 2:M3:77:GLU:HG2 | 2.02 | 0.60 |
| 1:N2:125:GLU:OE2 | 1:N2:159:TYR:OH | 2.20 | 0.60 |
| 1:N8:177:ASP:O | 2:N9:352:LYS:HA | 2.01 | 0.60 |
| 2:P9:166:LYS:N | 2:P9:199:ASP:OD2 | 2.27 | 0.60 |
| 1:Q8:77:ARG:HG2 | 24:6T:45:LEU:HD13 | 1.83 | 0.60 |
| 1:R2:178:THR:HB | 1:R2:181:GLU:HG3 | 1.82 | 0.60 |
| 1:R6:177:ASP:O | 2:R7:352:LYS:HA | 2.00 | 0.60 |
| 2:S9:250:VAL:HG23 | 2:S9:254:GLU:HG3 | 1.82 | 0.60 |
| 1:U2:113:ILE:HA | 1:U2:116:VAL:HG22 | 1.82 | 0.60 |
| 1:U4:224:ASP:OD2 | 1:U4:225:LEU:N | 2.35 | 0.60 |
| 2:U5:109:THR:OG1 | 2:U5:411:GLU:OE2 | 2.15 | 0.60 |
| 1:V0:207:LEU:HB3 | 1:V0:225:LEU:HD22 | 1.82 | 0.60 |
| 2:W1:119:LEU:HA | 2:W1:122:ILE:HG22 | 1.84 | 0.60 |
| 2:W5:98:ASP:OD1 | 2:W5:99:ALA:N | 2.35 | 0.60 |
| 2:W9:9:ILE:CG2 | 2:W9:146:GLY:HA2 | 2.28 | 0.60 |
| 1:Y6:248:ALA:HA | 1:Y6:252:LYS:HD2 | 1.84 | 0.60 |
| 2:Y9:202:VAL:HG22 | 2:Y9:268:MET:HB2 | 1.83 | 0.60 |
| 1:Z0:179:VAL:HG23 | 1:Z0:180:VAL:HG13 | 1.82 | 0.60 |
| 2:Z3:352:LYS:NZ | 2:Z3:353:CYS:O | 2.34 | 0.60 |
| 1:0G:248:ALA:CA | 1:0G:252:LYS:HD3 | 2.31 | 0.60 |
| 1:1O:262:ARG:NH2 | 1:1O:417:ASP:OD1 | 2.34 | 0.60 |
| 1:1Q:102:ALA:HB1 | 1:1Q:401:GLU:HG2 | 1.84 | 0.60 |
| 1:2A:211:CYS:SG | 1:2A:217:LEU:HB2 | 2.42 | 0.60 |
| 1:2W:248:ALA:HA | 1:2W:252:LYS:HD2 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2X:222:PRO:HD2 | 1:2Y:324:LYS:HD2 | 1.83 | 0.60 |
| 2:3L:71:GLU:HB3 | 2:3L:98:ASP:OD1 | 2.02 | 0.60 |
| 2:3L:289:ALA:O | 2:3L:293:ASN:ND2 | 2.35 | 0.60 |
| 2:3R:339:ARG:NH1 | 2:3R:341:ILE:O | 2.34 | 0.60 |
| 4:4E:44:SER:OG | 4:4E:163:ARG:NH1 | 2.34 | 0.60 |
| 4:4G:44:SER:OG | 4:4G:163:ARG:NH1 | 2.34 | 0.60 |
| 7:4R:297:MET:HG3 | 20:6F:130:LEU:HD21 | 1.83 | 0.60 |
| 14:5L:22:ILE:HG13 | 14:5L:31:ILE:HG23 | 1.84 | 0.60 |
| 14:5M:363:PHE:CD1 | 14:5M:377:ARG:CD | 2.81 | 0.60 |
| 14:5N:22:ILE:HG13 | 14:5N:31:ILE:HG23 | 1.84 | 0.60 |
| 14:5N:511:THR:HG21 | 14:5N:531:ASP:N | 2.15 | 0.60 |
| 15:5P:43:ARG:HD3 | 37:7Y:72:ARG:O | 2.02 | 0.60 |
| 21:6H:14:LEU:HG | 21:6H:131:TYR:HE2 | 1.65 | 0.60 |
| 24:6T:10:LYS:NZ | 12:7B:96:GLY:O | 2.33 | 0.60 |
| 37:7Y:141:THR:HG22 | 37:7Y:142:ARG:H | 1.65 | 0.60 |
| 2:2:282:TYR:OH | 24:6T:89:VAL:HG21 | 2.01 | 0.60 |
| 1:A9:320:ARG:NH1 | 18:5X:53:GLY:HA3 | 2.16 | 0.60 |
| 1:B3:80:PRO:HD2 | 24:6W:221:ARG:HH12 | 1.67 | 0.60 |
| 1:F2:279:GLN:NE2 | 22:6O:103:ALA:O | 2.35 | 0.60 |
| 2:H1:33:ASP:O | 2:H1:60:LYS:NZ | 2.32 | 0.60 |
| 1:K4:3:GLU:HB2 | 1:K4:130:LEU:HA | 1.83 | 0.60 |
| 2:K7:377:MET:SD | 2:K7:379:SER:OG | 2.56 | 0.60 |
| 1:L6:2:ARG:HE | 1:L6:240:LEU:HD22 | 1.65 | 0.60 |
| 1:M2:140:GLY:O | 1:M2:184:ASN:ND2 | 2.32 | 0.60 |
| 1:M6:107:THR:OG1 | 1:M6:108:GLU:OE1 | 2.17 | 0.60 |
| 1:M8:177:ASP:O | 2:M9:352:LYS:HA | 2.01 | 0.60 |
| 2:M9:336:LYS:O | 2:M9:339:ARG:NH2 | 2.35 | 0.60 |
| 1:N6:309:ARG:NH1 | 1:N6:339:SER:O | 2.35 | 0.60 |
| 2:N9:100:ALA:HA | 1:O0:252:LYS:HE2 | 1.83 | 0.60 |
| 2:O1:223:THR:HG23 | 2:O1:225:THR:H | 1.65 | 0.60 |
| 2:O3:145:THR:OG1 | 41:O4:501:GTP:O1B | 2.20 | 0.60 |
| 1:O4:131:GLN:HE21 | 1:O4:250:LEU:HB2 | 1.66 | 0.60 |
| 2:P5:176:GLN:HE22 | 2:P5:304:LYS:HE2 | 1.67 | 0.60 |
| 1:R6:227:HIS:NE2 | 24:6X:10:LYS:O | 2.35 | 0.60 |
| 1:S6:345:ILE:O | 1:S6:348:ASN:ND2 | 2.35 | 0.60 |
| 1:T6:53:GLU:N | 1:T6:53:GLU:OE2 | 2.33 | 0.60 |
| 1:V4:2:ARG:HB3 | 1:V4:131:GLN:HB2 | 1.83 | 0.60 |
| 2:W9:264:ARG:NH2 | 2:W9:431:ASP:OD2 | 2.34 | 0.60 |
| 1:Y6:334:GLN:NE2 | 1:Y6:348:ASN:OD1 | 2.35 | 0.60 |
| 2:Z1:417:GLU:HA | 2:Z1:420:GLU:HG2 | 1.84 | 0.60 |
| 2:Z5:212:ILE:HG23 | 2:Z5:275:ILE:HD12 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z9:90:GLU:HB2 | 2:0P:283:HIS:CE1 | 2.36 | 0.60 |
| 1:0C:3:GLU:HB2 | 1:0C:130:LEU:HA | 1.84 | 0.60 |
| 2:0N:220:GLU:HG2 | 2:0N:221:ARG:HG3 | 1.84 | 0.60 |
| 1:0Y:2:ARG:HB3 | 1:0Y:131:GLN:HB2 | 1.84 | 0.60 |
| 1:1A:272:PRO:HB2 | 1:1A:282:ARG:HH12 | 1.67 | 0.60 |
| 2:1N:287:SER:N | 2:1N:290:GLU:OE2 | 2.34 | 0.60 |
| 1:1S:330:MET:HB3 | 1:1S:349:VAL:HG11 | 1.83 | 0.60 |
| 1:2C:391:ARG:HG3 | 2:2D:346:TRP:CD2 | 2.35 | 0.60 |
| 2:2H:156:ARG:HH22 | 38:8B:29:GLY:HA2 | 1.67 | 0.60 |
| 1:3M:345:ILE:O | 1:3M:348:ASN:ND2 | 2.35 | 0.60 |
| 4:4C:44:SER:OG | 4:4C:163:ARG:NH1 | 2.34 | 0.60 |
| 11:5E:19:GLY:O | 11:5E:23:ARG:HD3 | 2.02 | 0.60 |
| 13:5J:31:GLN:OE1 | 13:5J:32:ALA:N | 2.34 | 0.60 |
| 14:5M:22:ILE:HG13 | 14:5M:31:ILE:HG23 | 1.84 | 0.60 |
| 14:5M:36:SER:N | 14:5M:595:SER:OG | 2.33 | 0.60 |
| 14:5M:434:THR:HG21 | 14:5M:439:ARG:HB2 | 1.83 | 0.60 |
| 15:5P:324:ARG:NH1 | 15:5P:360:ASP:O | 2.35 | 0.60 |
| 16:5Q:184:GLU:OE1 | 16:5Q:184:GLU:N | 2.33 | 0.60 |
| 20:6F:150:HIS:CE1 | 20:6F:157:PRO:HG3 | 2.36 | 0.60 |
| 37:7Y:72:ARG:HG2 | 37:7Y:72:ARG:HH21 | 1.66 | 0.60 |
| 1:G2:49:VAL:HG11 | 1:G2:241:ARG:HG2 | 1.83 | 0.60 |
| 2:G5:317:LEU:HB3 | 2:G5:319:TYR:HE1 | 1.66 | 0.60 |
| 2:I3:287:SER:N | 2:I3:290:GLU:OE2 | 2.34 | 0.60 |
| 2:J3:88:HIS:HD2 | 2:K9:283:HIS:HB3 | 1.66 | 0.60 |
| 1:J4:334:GLN:HE22 | 1:J4:348:ASN:H | 1.48 | 0.60 |
| 2:J5:145:THR:OG1 | 41:J6:501:GTP:O1B | 2.20 | 0.60 |
| 2:L1:98:ASP:OD1 | 2:L1:99:ALA:N | 2.35 | 0.60 |
| 2:L3:14:ILE:HD11 | 2:L3:74:VAL:HG13 | 1.84 | 0.60 |
| 2:L3:90:GLU:CD | 29:7J:321:ARG:HH21 | 2.05 | 0.60 |
| 2:N1:287:SER:OG | 2:N1:290:GLU:OE1 | 2.18 | 0.60 |
| 2:O3:240:ALA:HB1 | 2:O3:356:ASN:HD22 | 1.67 | 0.60 |
| 1:O4:391:ARG:HH22 | 2:O5:435:VAL:HA | 1.67 | 0.60 |
| 2:O5:189:LEU:HD11 | 2:O5:418:PHE:HE1 | 1.67 | 0.60 |
| 1:P4:2:ARG:HB3 | 1:P4:131:GLN:HB2 | 1.83 | 0.60 |
| 1:R0:93:GLY:HA2 | 13:5H:118:THR:HG23 | 1.83 | 0.60 |
| 1:R6:5:VAL:HG12 | 1:R6:62:ARG:HD3 | 1.83 | 0.60 |
| 1:S8:157:GLU:OE2 | 3:3Z:90:ILE:HD12 | 2.01 | 0.60 |
| 1:S8:263:LEU:HD22 | 1:S8:422:TYR:CE1 | 2.36 | 0.60 |
| 1:T4:224:ASP:OD1 | 7:4U:133:GLY:HA3 | 2.01 | 0.60 |
| 2:U7:267:PHE:HB2 | 2:U7:384:ILE:HD12 | 1.84 | 0.60 |
| 2:V1:377:MET:SD | 2:V1:379:SER:HB3 | 2.42 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V3:76:ASP:OD2 | 1:V4:46:ARG:NH2 | 2.35 | 0.60 |
| 1:X0:67:ASP:N | 1:X0:67:ASP:OD1 | 2.34 | 0.60 |
| 1:X6:265:PHE:HD2 | 1:X6:422:TYR:HH | 1.48 | 0.60 |
| 2:Z7:206:ASN:OD1 | 41:Z7:501:GTP:N2 | 2.24 | 0.60 |
| 2:1L:122:ILE:HA | 2:1L:125:LEU:HB2 | 1.84 | 0.60 |
| 1:1O:180:VAL:HG23 | 1:1O:184:ASN:HD21 | 1.67 | 0.60 |
| 1:1Q:179:VAL:HG22 | 2:1R:258:ASN:HD22 | 1.66 | 0.60 |
| 1:2E:52:ASN:OD1 | 1:2E:62:ARG:NH2 | 2.34 | 0.60 |
| 1:2G:2:ARG:HE | 1:2G:240:LEU:HD22 | 1.66 | 0.60 |
| 1:2U:139:LEU:HD12 | 1:2U:170:VAL:HG22 | 1.84 | 0.60 |
| 2:3J:133:GLN:HB3 | 2:3J:252:ILE:HG21 | 1.83 | 0.60 |
| 1:3K:213:ARG:HB2 | 1:3K:297:LYS:NZ | 2.17 | 0.60 |
| 2:3N:392:ASP:OD2 | 2:3N:422:ARG:NH1 | 2.34 | 0.60 |
| 8:4W:468:MET:O | 8:4X:127:THR:HG21 | 2.02 | 0.60 |
| 9:4Z:204:LEU:HA | 9:4Z:207:LYS:HE2 | 1.82 | 0.60 |
| 10:5D:137:THR:O | 10:5D:141:LEU:HG | 2.02 | 0.60 |
| 12:5F:380:TRP:NE1 | 12:7B:38:PRO:HG2 | 2.15 | 0.60 |
| 14:5L:434:THR:HG21 | 14:5L:439:ARG:HB2 | 1.83 | 0.60 |
| 14:5N:434:THR:HG21 | 14:5N:439:ARG:HB2 | 1.83 | 0.60 |
| 15:5O:41:LYS:HB3 | 15:5O:41:LYS:NZ | 2.15 | 0.60 |
| 24:6Z:132:VAL:HB | 24:6Z:148:ILE:HB | 1.82 | 0.60 |
| 2:C5:36:MET:HB2 | 22:6I:76:LYS:HE3 | 1.84 | 0.60 |
| 2:H1:340:THR:HG23 | 2:H1:341:ILE:HG12 | 1.83 | 0.60 |
| 2:H3:100:ALA:HB1 | 1:H4:252:LYS:HB3 | 1.82 | 0.60 |
| 1:H6:68:LEU:HB3 | 1:H6:96:GLY:HA2 | 1.84 | 0.60 |
| 1:I2:309:ARG:H | 1:I2:372:THR:HG22 | 1.67 | 0.60 |
| 2:I5:70:LEU:HD13 | 2:I5:95:GLY:HA3 | 1.83 | 0.60 |
| 1:K0:330:MET:HB3 | 1:K0:349:VAL:HG11 | 1.83 | 0.60 |
| 2:K5:176:GLN:HE22 | 2:K5:304:LYS:HE2 | 1.67 | 0.60 |
| 2:K9:222:PRO:HD2 | 1:L0:324:LYS:HE3 | 1.83 | 0.60 |
| 2:L3:183:GLU:HG3 | 2:L3:184:PRO:HD3 | 1.84 | 0.60 |
| 2:M1:132:LEU:HD22 | 2:M1:164:LYS:HD3 | 1.84 | 0.60 |
| 1:M2:177:ASP:O | 2:M3:352:LYS:HA | 2.02 | 0.60 |
| 2:M3:283:HIS:NE2 | 30:7K:199:TYR:CZ | 2.53 | 0.60 |
| 2:P3:238:LEU:HD11 | 2:P3:255:PHE:CZ | 2.37 | 0.60 |
| 2:P5:9:ILE:HG22 | 2:P5:68:LEU:HD11 | 1.82 | 0.60 |
| 2:P9:381:SER:OG | 2:P9:382:THR:N | 2.32 | 0.60 |
| 1:Q4:135:VAL:HG21 | 1:Q4:152:ILE:HD11 | 1.84 | 0.60 |
| 1:R6:77:ARG:HG2 | 24:6X:45:LEU:HD11 | 1.83 | 0.60 |
| 2:R9:53:PHE:HB3 | 2:R9:61:HIS:HB3 | 1.84 | 0.60 |
| 2:S7:50:ASN:O | 2:S7:64:ARG:NH2 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S8:1:MET:HE2 | 1:S8:1:MET:HA | 1.83 | 0.60 |
| 1:U6:328:GLU:O | 1:U6:332:ASN:ND2 | 2.34 | 0.60 |
| 2:W1:76:ASP:OD2 | 1:W2:46:ARG:NH2 | 2.35 | 0.60 |
| 1:W4:248:ALA:HA | 1:W4:252:LYS:HD2 | 1.84 | 0.60 |
| 2:W9:51:THR:HG21 | 2:W9:243:ARG:HG2 | 1.84 | 0.60 |
| 1:X0:207:LEU:HB3 | 1:X0:225:LEU:HD22 | 1.84 | 0.60 |
| 2:X5:26:LEU:HD21 | 2:X5:363:VAL:HG12 | 1.84 | 0.60 |
| 1:Y0:171:PRO:O | 1:Y0:380:ARG:NH2 | 2.35 | 0.60 |
| 2:Y1:76:ASP:HA | 2:Y1:79:ARG:HB2 | 1.84 | 0.60 |
| 1:0G:54:ALA:N | 1:0G:58:ARG:O | 2.32 | 0.60 |
| 1:0K:116:VAL:HA | 1:0K:119:VAL:HG12 | 1.83 | 0.60 |
| 2:0P:145:THR:OG1 | 41:0Q:501:GTP:O1B | 2.20 | 0.60 |
| 2:0R:56:THR:N | 2:0R:60:LYS:O | 2.35 | 0.60 |
| 1:0S:210:ILE:O | 1:0S:214:THR:OG1 | 2.16 | 0.60 |
| 2:1D:90:GLU:HB3 | 2:1D:121:ARG:NH2 | 2.17 | 0.60 |
| 1:1U:140:GLY:O | 1:1U:184:ASN:ND2 | 2.35 | 0.60 |
| 2:2B:211:ASP:OD2 | 2:2B:214:ARG:NH2 | 2.35 | 0.60 |
| 2:2L:96:LYS:NZ | 38:8C:5:LYS:O | 2.27 | 0.60 |
| 2:2V:250:VAL:HG23 | 2:2V:254:GLU:HG3 | 1.82 | 0.60 |
| 1:3I:208:TYR:HE1 | 1:3I:225:LEU:HD11 | 1.67 | 0.60 |
| 13:5I:31:GLN:OE1 | 13:5I:32:ALA:N | 2.34 | 0.60 |
| 14:5N:415:LYS:NZ | 23:6S:22:MET:HB2 | 2.17 | 0.60 |
| 15:5O:179:THR:HA | 15:5O:193:ARG:HH11 | 1.67 | 0.60 |
| 19:6E:79:HIS:CD2 | 37:7Y:49:PRO:HB3 | 2.37 | 0.60 |
| 24:6U:41:ARG:HE | 24:6U:41:ARG:CA | 2.14 | 0.60 |
| 24:6Y:32:THR:HG23 | 24:6Y:33:LEU:HG | 1.84 | 0.60 |
| 26:7D:94:THR:O | 26:7D:94:THR:OG1 | 2.20 | 0.60 |
| 26:7F:94:THR:O | 26:7F:94:THR:OG1 | 2.20 | 0.60 |
| 35:7U:187:ASP:O | 35:7U:191:MET:HG2 | 2.01 | 0.60 |
| 2:E7:206:ASN:OD1 | 41:E8:501:GTP:N2 | 2.25 | 0.60 |
| 2:F3:369:ALA:HB1 | 22:6O:82:LEU:HD13 | 1.83 | 0.60 |
| 2:G3:133:GLN:HG3 | 2:G3:242:LEU:HD11 | 1.83 | 0.60 |
| 1:G4:74:ASP:O | 1:G4:78:SER:OG | 2.20 | 0.60 |
| 2:H1:406:HIS:HA | 2:H1:409:VAL:HG22 | 1.83 | 0.60 |
| 1:H2:68:LEU:HB3 | 1:H2:96:GLY:HA2 | 1.83 | 0.60 |
| 2:H7:27:GLU:OE1 | 2:H7:243:ARG:NH1 | 2.35 | 0.60 |
| 1:I4:276:ARG:NE | 24:6Z:490:THR:O | 2.35 | 0.60 |
| 2:I7:320:ARG:NH2 | 2:I7:359:PRO:O | 2.34 | 0.60 |
| 2:K3:287:SER:N | 2:K3:290:GLU:OE2 | 2.35 | 0.60 |
| 1:K6:5:VAL:HG12 | 1:K6:62:ARG:HD3 | 1.84 | 0.60 |
| 2:K7:194:LEU:O | 2:K7:198:THR:HG22 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L5:9:ILE:HG22 | 2:L5:146:GLY:HA2 | 1.83 | 0.60 |
| 2:M1:287:SER:N | 2:M1:290:GLU:OE2 | 2.35 | 0.60 |
| 2:N7:236:SER:OG | 2:N7:243:ARG:NH2 | 2.34 | 0.60 |
| 2:Q1:69:ASP:OD1 | 2:Q1:70:LEU:N | 2.34 | 0.60 |
| 1:Q2:238:CYS:SG | 1:Q2:318:ARG:NE | 2.75 | 0.60 |
| 1:R0:94:GLN:HG2 | 13:5H:119:VAL:O | 2.02 | 0.60 |
| 2:T5:132:LEU:O | 2:T5:164:LYS:NZ | 2.35 | 0.60 |
| 1:T6:334:GLN:HE22 | 1:T6:348:ASN:H | 1.50 | 0.60 |
| 1:V6:253:LEU:HA | 1:V6:350:LYS:NZ | 2.17 | 0.60 |
| 1:V6:292:GLN:O | 1:V6:298:ASN:ND2 | 2.32 | 0.60 |
| 2:W3:33:ASP:O | 2:W3:60:LYS:NZ | 2.35 | 0.60 |
| 2:W5:415:GLU:OE2 | 2:W5:419:SER:OG | 2.20 | 0.60 |
| 2:X5:121:ARG:HE | 2:X5:124:LYS:NZ | 2.00 | 0.60 |
| 2:X7:100:ALA:HA | 1:X8:252:LYS:HG2 | 1.84 | 0.60 |
| 1:Y0:397:TRP:HE1 | 2:Y1:260:VAL:HB | 1.67 | 0.60 |
| 2:Y1:25:CYS:O | 2:Y1:30:ILE:N | 2.32 | 0.60 |
| 1:Z4:58:ARG:HH11 | 1:Z4:84:ILE:HA | 1.67 | 0.60 |
| 1:Z8:116:VAL:HA | 1:Z8:119:VAL:HG12 | 1.82 | 0.60 |
| 2:Z9:101:ASN:HD22 | 1:0A:256:ASN:HD21 | 1.49 | 0.60 |
| 1:0M:309:ARG:NH1 | 1:0M:339:SER:O | 2.35 | 0.60 |
| 2:0X:66:ILE:HD12 | 2:0X:68:LEU:HD23 | 1.84 | 0.60 |
| 1:1C:128:ASP:OD1 | 1:1C:129:CYS:N | 2.34 | 0.60 |
| 2:1F:267:PHE:HB2 | 2:1F:384:ILE:HD12 | 1.83 | 0.60 |
| 2:1H:66:ILE:HG21 | 2:1H:122:ILE:HD11 | 1.84 | 0.60 |
| 2:1T:145:THR:OG1 | 41:1T:501:GTP:O1B | 2.18 | 0.60 |
| 1:2A:4:ILE:HD11 | 1:2A:240:LEU:HD12 | 1.83 | 0.60 |
| 2:2F:130:THR:OG1 | 38:8B:116:GLN:NE2 | 2.35 | 0.60 |
| 2:2H:88:HIS:CE1 | 2:2H:90:GLU:HB3 | 2.36 | 0.60 |
| 1:2M:67:ASP:CG | 1:2M:68:LEU:H | 2.06 | 0.60 |
| 2:2P:98:ASP:OD1 | 2:2P:99:ALA:N | 2.35 | 0.60 |
| 2:2V:214:ARG:HH22 | 1:2W:324:LYS:HD3 | 1.65 | 0.60 |
| 1:3O:77:ARG:NH1 | 3:4F:18:LYS:HB3 | 2.17 | 0.60 |
| 5:4M:222:GLU:OE1 | 29:7J:403:ARG:NH2 | 2.35 | 0.60 |
| 13:5H:31:GLN:OE1 | 13:5H:32:ALA:N | 2.34 | 0.60 |
| 13:5K:31:GLN:OE1 | 13:5K:32:ALA:N | 2.34 | 0.60 |
| 15:5O:73:LEU:HD23 | 15:5O:73:LEU:O | 2.01 | 0.60 |
| 19:6E:92:ARG:HD3 | 19:6E:99:ARG:HE | 1.65 | 0.60 |
| 24:6X:574:ARG:HE | 24:6X:630:LEU:HD21 | 1.67 | 0.60 |
| 26:7E:94:THR:O | 26:7E:94:THR:OG1 | 2.20 | 0.60 |
| 35:7T:84:ALA:O | 35:7T:88:VAL:HG23 | 2.01 | 0.60 |
| 1:G0:224:ASP:OD1 | 24:6V:414:GLY:HA2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G2:207:LEU:HB3 | 1:G2:225:LEU:HD22 | 1.84 | 0.59 |
| 2:H3:301:MET:HE1 | 2:H3:307:PRO:HD3 | 1.84 | 0.59 |
| 1:I8:359:LYS:HD2 | 1:I8:360:GLY:H | 1.66 | 0.59 |
| 2:I9:53:PHE:HB3 | 2:I9:61:HIS:HB3 | 1.83 | 0.59 |
| 2:J3:69:ASP:OD1 | 2:J3:70:LEU:N | 2.35 | 0.59 |
| 2:J5:31:GLN:HG3 | 2:J5:37:PRO:HD3 | 1.82 | 0.59 |
| 2:L7:289:ALA:O | 2:L7:293:ASN:ND2 | 2.35 | 0.59 |
| 1:M2:190:HIS:CD2 | 1:M2:411:ALA:HA | 2.36 | 0.59 |
| 2:M3:76:ASP:OD2 | 1:M4:46:ARG:NH2 | 2.35 | 0.59 |
| 1:O0:177:ASP:O | 2:O1:352:LYS:HA | 2.02 | 0.59 |
| 2:O5:81:GLY:O | 2:O5:84:ARG:NH1 | 2.34 | 0.59 |
| 2:P5:189:LEU:HD11 | 2:P5:418:PHE:HE1 | 1.66 | 0.59 |
| 2:P7:90:GLU:O | 2:P7:121:ARG:NH1 | 2.32 | 0.59 |
| 2:R1:399:TYR:O | 2:R1:402:ARG:NH1 | 2.35 | 0.59 |
| 1:R2:52:ASN:OD1 | 1:R2:62:ARG:NH2 | 2.35 | 0.59 |
| 1:U4:211:CYS:HA | 1:U4:215:LEU:HB2 | 1.82 | 0.59 |
| 2:U9:284:GLU:O | 2:U9:285:GLN:NE2 | 2.35 | 0.59 |
| 1:V2:156:ARG:NH1 | 1:V2:197:ASP:OD1 | 2.34 | 0.59 |
| 1:V6:125:GLU:OE2 | 1:V6:159:TYR:OH | 2.17 | 0.59 |
| 1:V8:170:VAL:N | 1:V8:202:LEU:O | 2.32 | 0.59 |
| 2:V9:98:ASP:OD1 | 2:V9:99:ALA:N | 2.35 | 0.59 |
| 1:W0:107:THR:OG1 | 1:W0:401:GLU:OE2 | 2.13 | 0.59 |
| 2:W5:155:GLU:HG3 | 2:W5:197:HIS:NE2 | 2.16 | 0.59 |
| 1:W8:49:VAL:HG11 | 1:W8:241:ARG:HG2 | 1.84 | 0.59 |
| 1:X2:218:THR:HG23 | 1:X2:219:THR:HG23 | 1.84 | 0.59 |
| 2:Y1:406:HIS:HA | 2:Y1:409:VAL:HG22 | 1.84 | 0.59 |
| 2:0H:398:MET:HG2 | 1:0I:345:ILE:HG12 | 1.83 | 0.59 |
| 1:0O:392:LYS:HB3 | 1:0O:395:LEU:HD22 | 1.84 | 0.59 |
| 2:0R:278:ALA:HA | 2:0R:369:ALA:HB2 | 1.84 | 0.59 |
| 1:1C:211:CYS:HA | 1:1C:215:LEU:HB2 | 1.84 | 0.59 |
| 2:1N:85:GLN:HE21 | 2:1N:85:GLN:HA | 1.67 | 0.59 |
| 2:2J:88:HIS:CE1 | 2:2J:89:PRO:HD2 | 2.37 | 0.59 |
| 2:2L:27:GLU:OE1 | 2:2L:243:ARG:NH1 | 2.35 | 0.59 |
| 1:3C:391:ARG:HH22 | 2:3D:435:VAL:HA | 1.67 | 0.59 |
| 2:3F:278:ALA:HA | 2:3F:369:ALA:HB2 | 1.81 | 0.59 |
| 5:4M:252:GLU:HA | 5:4M:255:ASN:ND2 | 2.17 | 0.59 |
| 9:4Y:424:TYR:O | 9:4Y:427:GLU:HG3 | 2.01 | 0.59 |
| 14:5L:226:VAL:HG12 | 14:5L:226:VAL:O | 2.02 | 0.59 |
| 22:6I:150:TYR:HB3 | 22:6I:228:PHE:HD1 | 1.66 | 0.59 |
| 26:7E:59:ARG:HG2 | 26:7E:59:ARG:HH11 | 1.67 | 0.59 |
| 1:B8:94:GLN:HG2 | 24:6Y:250:LEU:HD11 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G3:49:PHE:HB2 | 2:G3:53:PHE:HD2 | 1.67 | 0.59 |
| 1:I8:175:VAL:HG12 | 2:I9:329:ASN:ND2 | 2.15 | 0.59 |
| 2:I9:33:ASP:O | 2:I9:60:LYS:NZ | 2.34 | 0.59 |
| 1:J4:67:ASP:OD2 | 1:J4:72:THR:OG1 | 2.20 | 0.59 |
| 2:L1:405:VAL:HG13 | 2:L1:418:PHE:HE2 | 1.68 | 0.59 |
| 2:N9:417:GLU:HA | 2:N9:420:GLU:HG2 | 1.82 | 0.59 |
| 1:P8:53:GLU:OE1 | 7:4R:109:GLN:CG | 2.50 | 0.59 |
| 1:Q8:113:ILE:HA | 1:Q8:116:VAL:HG12 | 1.84 | 0.59 |
| 2:R3:98:ASP:OD1 | 2:R3:99:ALA:N | 2.34 | 0.59 |
| 2:R7:413:MET:O | 17:5U:117:PRO:HG3 | 2.02 | 0.59 |
| 1:T0:65:LEU:HD12 | 1:T0:90:PHE:CE1 | 2.36 | 0.59 |
| 2:T1:334:THR:HG22 | 13:5I:134:PHE:H | 1.66 | 0.59 |
| 1:T4:238:CYS:SG | 1:T4:318:ARG:NE | 2.75 | 0.59 |
| 1:T6:414:ASN:ND2 | 3:4H:84:LYS:HD2 | 2.16 | 0.59 |
| 1:V4:3:GLU:HB2 | 1:V4:130:LEU:HD13 | 1.84 | 0.59 |
| 1:V4:67:ASP:OD2 | 1:V4:72:THR:OG1 | 2.15 | 0.59 |
| 1:X6:113:ILE:HA | 1:X6:116:VAL:HG22 | 1.84 | 0.59 |
| 2:Y1:109:THR:OG1 | 2:Y1:411:GLU:OE2 | 2.19 | 0.59 |
| 1:Y4:328:GLU:O | 1:Y4:332:ASN:ND2 | 2.35 | 0.59 |
| 1:Y8:125:GLU:OE2 | 1:Y8:159:TYR:OH | 2.19 | 0.59 |
| 2:Z7:91:GLN:HE22 | 2:0N:283:HIS:CE1 | 2.17 | 0.59 |
| 1:Z8:311:LEU:HD23 | 1:Z8:312:THR:HG23 | 1.83 | 0.59 |
| 2:Z9:166:LYS:N | 2:Z9:199:ASP:OD2 | 2.35 | 0.59 |
| 1:0A:2:ARG:HE | 1:0A:240:LEU:HD22 | 1.67 | 0.59 |
| 1:0K:393:ALA:C | 1:0K:395:LEU:H | 2.06 | 0.59 |
| 2:0L:320:ARG:HD3 | 2:0L:360:PRO:HG3 | 1.83 | 0.59 |
| 2:0N:221:ARG:HB3 | 1:0O:322:SER:OG | 2.02 | 0.59 |
| 1:0S:342:VAL:HG12 | 1:0S:348:ASN:HD21 | 1.67 | 0.59 |
| 2:0V:381:SER:OG | 2:0V:382:THR:N | 2.35 | 0.59 |
| 1:1E:72:THR:O | 1:1E:76:VAL:HG23 | 2.03 | 0.59 |
| 1:1S:113:ILE:HD13 | 1:1S:150:LEU:HD22 | 1.84 | 0.59 |
| 2:2B:279:GLU:HA | 2:2B:279:GLU:OE2 | 2.01 | 0.59 |
| 1:2I:91:VAL:HG11 | 1:2I:116:VAL:HG12 | 1.84 | 0.59 |
| 1:2I:215:LEU:HD21 | 1:2I:273:LEU:HD12 | 1.85 | 0.59 |
| 2:2N:9:ILE:HG22 | 2:2N:146:GLY:HA2 | 1.84 | 0.59 |
| 1:2Q:209:ASP:OD2 | 38:8A:105:ARG:O | 2.20 | 0.59 |
| 1:2Q:320:ARG:CZ | 38:8A:198:THR:HA | 2.32 | 0.59 |
| 1:2Q:391:ARG:HG3 | 2:2R:346:TRP:CD2 | 2.36 | 0.59 |
| 2:2V:340:THR:OG1 | 38:8B:78:ASP:OD2 | 2.10 | 0.59 |
| 2:2V:399:TYR:O | 2:2V:402:ARG:NH1 | 2.35 | 0.59 |
| 1:2Y:6:HIS:NE2 | 1:2Y:136:CYS:SG | 2.75 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2Z:258:ASN:OD1 | 2:2Z:352:LYS:NZ | 2.33 | 0.59 |
| 2:3L:124:LYS:HZ2 | 3:4B:36:PHE:HD1 | 1.50 | 0.59 |
| 1:3M:178:THR:HG23 | 1:3M:181:GLU:HG3 | 1.83 | 0.59 |
| 10:5A:397:LEU:O | 10:5A:401:GLU:HG2 | 2.01 | 0.59 |
| 12:5F:58:ARG:O | 12:5F:59:GLU:HG3 | 2.02 | 0.59 |
| 12:5F:298:ASP:HB2 | 12:7B:13:PRO:CG | 2.32 | 0.59 |
| 14:5L:31:ILE:HD11 | 14:5L:38:ILE:HD12 | 1.84 | 0.59 |
| 14:5M:31:ILE:HD11 | 14:5M:38:ILE:HD12 | 1.84 | 0.59 |
| 14:5N:31:ILE:HD11 | 14:5N:38:ILE:HD12 | 1.84 | 0.59 |
| 17:5S:53:ASP:N | 17:5S:53:ASP:OD1 | 2.32 | 0.59 |
| 17:5S:220:ALA:HA | 17:5S:223:GLU:HB2 | 1.83 | 0.59 |
| 17:5T:53:ASP:N | 17:5T:53:ASP:OD1 | 2.32 | 0.59 |
| 17:5T:220:ALA:HA | 17:5T:223:GLU:HB2 | 1.83 | 0.59 |
| 18:5Y:181:GLN:O | 18:5Y:185:THR:OG1 | 2.19 | 0.59 |
| 24:6T:135:PRO:HG2 | 24:6T:137:GLN:HE22 | 1.66 | 0.59 |
| 24:6V:525:VAL:HB | 24:6V:530:PHE:HE2 | 1.65 | 0.59 |
| 38:8A:93:LYS:HE3 | 38:8A:93:LYS:O | 2.02 | 0.59 |
| 2:A2:263:PRO:HG2 | 4:4G:116:PRO:HG3 | 1.82 | 0.59 |
| 1:G2:149:THR:HB | 1:G2:191:GLN:HG2 | 1.83 | 0.59 |
| 2:G5:15:GLN:HB3 | 2:G5:228:ASN:HD21 | 1.67 | 0.59 |
| 1:H6:257:LEU:HD21 | 1:H6:314:SER:HB3 | 1.84 | 0.59 |
| 2:I3:176:GLN:HG2 | 2:I3:177:VAL:HG23 | 1.84 | 0.59 |
| 2:J3:33:ASP:OD1 | 2:J3:35:GLN:NE2 | 2.35 | 0.59 |
| 2:L3:69:ASP:OD1 | 2:L3:70:LEU:N | 2.35 | 0.59 |
| 2:L7:183:GLU:HG3 | 2:L7:184:PRO:HD3 | 1.84 | 0.59 |
| 1:M2:52:ASN:OD1 | 1:M2:62:ARG:NH2 | 2.35 | 0.59 |
| 2:M5:27:GLU:OE1 | 2:M5:243:ARG:NH1 | 2.34 | 0.59 |
| 2:M7:399:TYR:OH | 2:M7:415:GLU:OE1 | 2.18 | 0.59 |
| 1:N8:135:VAL:HG21 | 1:N8:152:ILE:HD11 | 1.82 | 0.59 |
| 1:Q0:248:ALA:HA | 1:Q0:252:LYS:HD3 | 1.84 | 0.59 |
| 1:R0:49:VAL:HG11 | 1:R0:241:ARG:HG2 | 1.84 | 0.59 |
| 1:R8:190:HIS:NE2 | 1:R8:410:GLU:OE2 | 2.36 | 0.59 |
| 1:S6:292:GLN:HG2 | 1:S6:298:ASN:HD22 | 1.67 | 0.59 |
| 1:S8:309:ARG:NH1 | 1:S8:339:SER:O | 2.35 | 0.59 |
| 2:S9:253:THR:HA | 2:S9:256:GLN:OE1 | 2.02 | 0.59 |
| 2:T5:259:LEU:HD21 | 2:T5:316:CYS:HB2 | 1.83 | 0.59 |
| 1:T8:375:GLN:HB2 | 1:T8:419:VAL:HG13 | 1.83 | 0.59 |
| 1:T8:418:LEU:HG | 1:T8:422:TYR:CE2 | 2.32 | 0.59 |
| 2:U1:172:TYR:N | 2:U1:204:LEU:O | 2.34 | 0.59 |
| 2:U3:286:LEU:H | 2:U3:286:LEU:HD23 | 1.68 | 0.59 |
| 1:U8:177:ASP:O | 2:U9:352:LYS:HA | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V0:177:ASP:O | 2:V1:352:LYS:HA | 2.01 | 0.59 |
| 1:V8:58:ARG:NH1 | 1:V8:84:ILE:HA | 2.18 | 0.59 |
| 1:V8:211:CYS:HA | 1:V8:215:LEU:HB2 | 1.85 | 0.59 |
| 1:W0:183:TYR:HB3 | 1:W0:398:TYR:HE2 | 1.67 | 0.59 |
| 1:X4:309:ARG:NH1 | 1:X4:339:SER:O | 2.36 | 0.59 |
| 2:X7:90:GLU:OE1 | 2:X7:90:GLU:N | 2.34 | 0.59 |
| 2:Y1:52:PHE:CE2 | 2:Y1:243:ARG:HD3 | 2.37 | 0.59 |
| 1:Y4:177:ASP:O | 2:Y5:352:LYS:HA | 2.01 | 0.59 |
| 2:Y5:53:PHE:HB3 | 2:Y5:61:HIS:HB3 | 1.84 | 0.59 |
| 2:Y5:223:THR:HG22 | 2:Y5:224:TYR:H | 1.67 | 0.59 |
| 1:Y6:112:LEU:O | 1:Y6:115:SER:OG | 2.18 | 0.59 |
| 1:Y6:171:PRO:O | 1:Y6:380:ARG:NH2 | 2.35 | 0.59 |
| 1:Y8:86:ARG:NH2 | 1:0E:281:TYR:O | 2.34 | 0.59 |
| 1:0C:166:THR:HG23 | 1:0C:199:CYS:HB3 | 1.83 | 0.59 |
| 2:0J:167:LEU:HG | 2:0J:252:ILE:HD11 | 1.85 | 0.59 |
| 1:0S:207:LEU:HD11 | 1:0S:229:ILE:HD11 | 1.83 | 0.59 |
| 1:0W:7:ILE:HD13 | 1:0W:151:LEU:HD21 | 1.82 | 0.59 |
| 1:0W:55:THR:HG22 | 1:1M:284:LEU:HD12 | 1.84 | 0.59 |
| 2:0X:336:LYS:O | 2:0X:339:ARG:NH2 | 2.32 | 0.59 |
| 2:1D:336:LYS:O | 2:1D:339:ARG:NH2 | 2.35 | 0.59 |
| 1:1Q:396:HIS:H | 1:1Q:396:HIS:CD2 | 2.19 | 0.59 |
| 1:1W:244:GLY:H | 1:1W:247:ASN:HD21 | 1.49 | 0.59 |
| 2:2H:282:TYR:CZ | 10:5B:164:ASP:OD1 | 2.55 | 0.59 |
| 2:2Z:222:PRO:HD2 | 1:3A:324:LYS:HE3 | 1.83 | 0.59 |
| 1:3M:285:THR:HG23 | 1:3M:288:GLU:H | 1.67 | 0.59 |
| 12:5F:53:HIS:O | 12:5F:58:ARG:NH2 | 2.35 | 0.59 |
| 14:5N:127:ASN:HB2 | 38:8D:227:LYS:HZ3 | 1.67 | 0.59 |
| 18:6D:181:GLN:O | 18:6D:185:THR:OG1 | 2.19 | 0.59 |
| 22:6N:63:PRO:HB2 | 24:6Y:399:ILE:HG12 | 1.83 | 0.59 |
| 24:6W:566:VAL:HG23 | 24:6W:573:VAL:HG11 | 1.84 | 0.59 |
| 24:6Y:97:ARG:H | 24:6Y:188:THR:HG21 | 1.68 | 0.59 |
| 34:7R:260:ARG:O | 34:7R:264:GLU:HG2 | 2.01 | 0.59 |
| 35:7T:162:ASN:O | 35:7T:166:GLU:HG2 | 2.03 | 0.59 |
| 1:G0:388:MET:SD | 2:G1:348:PRO:HD3 | 2.42 | 0.59 |
| 1:G8:139:LEU:HD12 | 1:G8:170:VAL:HG22 | 1.84 | 0.59 |
| 2:H1:394:LYS:HA | 2:H1:397:LEU:HG | 1.84 | 0.59 |
| 1:H2:334:GLN:HE22 | 1:H2:348:ASN:H | 1.50 | 0.59 |
| 2:I7:417:GLU:HA | 2:I7:420:GLU:HG2 | 1.84 | 0.59 |
| 1:K0:186:THR:HG23 | 1:K0:187:LEU:HD12 | 1.84 | 0.59 |
| 1:K4:345:ILE:O | 1:K4:348:ASN:ND2 | 2.36 | 0.59 |
| 1:K6:5:VAL:HG22 | 1:K6:133:PHE:HD1 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K9:101:ASN:HB2 | 1:L0:252:LYS:HG3 | 1.85 | 0.59 |
| 2:M3:46:ASP:HB2 | 2:M3:49:PHE:CD2 | 2.38 | 0.59 |
| 2:M3:391:LEU:HD23 | 2:M3:394:LYS:HD2 | 1.84 | 0.59 |
| 1:M8:309:ARG:NH1 | 1:M8:339:SER:O | 2.35 | 0.59 |
| 1:N2:221:THR:OG1 | 29:7J:97:ARG:NH1 | 2.35 | 0.59 |
| 1:N8:65:LEU:HD12 | 1:N8:90:PHE:CE1 | 2.38 | 0.59 |
| 2:P5:286:LEU:O | 2:P5:373:ARG:NH1 | 2.35 | 0.59 |
| 2:P9:308:ARG:NH1 | 2:U7:282:TYR:OH | 2.35 | 0.59 |
| 2:P9:387:ILE:HD12 | 2:P9:390:ARG:HH22 | 1.66 | 0.59 |
| 2:Q1:339:ARG:HD3 | 5:4M:18:LEU:HD21 | 1.84 | 0.59 |
| 1:Q8:23:VAL:O | 1:Q8:27:GLU:HG2 | 2.01 | 0.59 |
| 1:R8:198:GLU:HA | 1:R8:264:HIS:HB2 | 1.84 | 0.59 |
| 1:S0:4:ILE:HD11 | 1:S0:240:LEU:HD12 | 1.84 | 0.59 |
| 1:S4:50:TYR:OH | 1:S4:237:THR:OG1 | 2.21 | 0.59 |
| 2:S5:195:LEU:HD21 | 2:S5:264:ARG:HH21 | 1.66 | 0.59 |
| 1:V6:172:SER:OG | 1:V6:380:ARG:NH1 | 2.36 | 0.59 |
| 1:W4:68:LEU:HD23 | 1:W4:93:GLY:HA3 | 1.84 | 0.59 |
| 1:X0:211:CYS:HA | 1:X0:215:LEU:HB2 | 1.82 | 0.59 |
| 1:X6:309:ARG:O | 1:X6:371:SER:OG | 2.18 | 0.59 |
| 2:X7:223:THR:OG1 | 1:X8:245:GLN:NE2 | 2.35 | 0.59 |
| 2:X7:292:THR:OG1 | 2:X7:319:TYR:OH | 2.18 | 0.59 |
| 1:Z4:287:PRO:HA | 1:Z4:290:THR:HG22 | 1.83 | 0.59 |
| 1:0C:250:LEU:HD12 | 1:0C:250:LEU:H | 1.66 | 0.59 |
| 1:0E:165:LEU:HD12 | 1:0E:167:PHE:HE1 | 1.66 | 0.59 |
| 1:0U:52:ASN:OD1 | 1:0U:62:ARG:NH2 | 2.34 | 0.59 |
| 2:0Z:85:GLN:OE1 | 2:1P:283:HIS:CE1 | 2.54 | 0.59 |
| 2:1F:132:LEU:O | 2:1F:164:LYS:NZ | 2.34 | 0.59 |
| 1:1G:68:LEU:HB3 | 1:1G:96:GLY:HA2 | 1.85 | 0.59 |
| 1:1M:139:LEU:HD12 | 1:1M:170:VAL:HG22 | 1.85 | 0.59 |
| 1:1O:252:LYS:HE2 | 1:1O:350:LYS:HE2 | 1.85 | 0.59 |
| 2:1Z:343:PHE:HZ | 2:1Z:351:PHE:HE1 | 1.51 | 0.59 |
| 2:2D:286:LEU:O | 2:2D:373:ARG:NH1 | 2.35 | 0.59 |
| 2:2H:18:ASN:HD21 | 2:2H:78:VAL:HG22 | 1.66 | 0.59 |
| 2:3D:79:ARG:NH1 | 2:3D:92:LEU:O | 2.35 | 0.59 |
| 1:3G:248:ALA:HA | 1:3G:252:LYS:HD2 | 1.84 | 0.59 |
| 1:3K:95:THR:HG21 | 3:4B:138:GLY:HA2 | 1.84 | 0.59 |
| 11:5E:159:LEU:HD11 | 11:5E:230:ASP:OD1 | 2.02 | 0.59 |
| 13:5H:28:ASP:HA | 13:5H:31:GLN:HE21 | 1.67 | 0.59 |
| 13:5K:28:ASP:HA | 13:5K:31:GLN:HE21 | 1.67 | 0.59 |
| 14:5L:564:ASP:OD1 | 14:5L:565:GLY:N | 2.35 | 0.59 |
| 14:5M:564:ASP:OD1 | 14:5M:565:GLY:N | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5N:564:ASP:OD1 | 14:5N:565:GLY:N | 2.36 | 0.59 |
| 17:5U:220:ALA:HA | 17:5U:223:GLU:HB2 | 1.84 | 0.59 |
| 18:5Z:181:GLN:O | 18:5Z:185:THR:OG1 | 2.19 | 0.59 |
| 18:6A:181:GLN:O | 18:6A:185:THR:OG1 | 2.19 | 0.59 |
| 18:6B:181:GLN:O | 18:6B:185:THR:OG1 | 2.19 | 0.59 |
| 24:6Y:97:ARG:NH2 | 24:6Y:99:TYR:OH | 2.35 | 0.59 |
| 24:6Y:354:ARG:HB2 | 24:6Y:357:LEU:HG | 1.85 | 0.59 |
| 24:7A:132:VAL:HB | 24:7A:148:ILE:HB | 1.85 | 0.59 |
| 32:7P:175:LEU:HG | 32:7P:180:ALA:HB2 | 1.85 | 0.59 |
| 1:5:194:GLU:OE2 | 3:3Z:240:ARG:NH1 | 2.34 | 0.59 |
| 1:F8:216:LYS:C | 24:6U:422:ASN:HD21 | 2.05 | 0.59 |
| 2:G9:322:ASP:HB3 | 2:G9:373:ARG:HH21 | 1.68 | 0.59 |
| 1:H4:211:CYS:HA | 1:H4:215:LEU:HB2 | 1.82 | 0.59 |
| 2:H5:222:PRO:HD2 | 1:H6:324:LYS:HE3 | 1.85 | 0.59 |
| 1:H6:139:LEU:HG | 1:H6:168:SER:HB3 | 1.84 | 0.59 |
| 2:H9:379:SER:OG | 2:H9:380:ASN:N | 2.32 | 0.59 |
| 2:H9:387:ILE:HG12 | 2:H9:390:ARG:HH22 | 1.66 | 0.59 |
| 2:I3:179:THR:O | 1:I4:350:LYS:HD2 | 2.03 | 0.59 |
| 1:J2:139:LEU:HD12 | 1:J2:170:VAL:HG12 | 1.85 | 0.59 |
| 2:K3:145:THR:OG1 | 41:K4:501:GTP:O1B | 2.20 | 0.59 |
| 1:M0:3:GLU:HB2 | 1:M0:130:LEU:HA | 1.84 | 0.59 |
| 1:M4:200:MET:HE3 | 1:M4:268:VAL:HG21 | 1.84 | 0.59 |
| 2:M9:280:LYS:HZ2 | 29:7J:320:PRO:CB | 2.15 | 0.59 |
| 1:N2:199:CYS:HG | 1:N2:265:PHE:HD1 | 1.50 | 0.59 |
| 2:O1:199:ASP:HB3 | 2:O1:256:GLN:NE2 | 2.16 | 0.59 |
| 1:O4:190:HIS:CD2 | 1:O4:411:ALA:HA | 2.38 | 0.59 |
| 2:P3:129:CYS:SG | 2:P3:130:THR:N | 2.74 | 0.59 |
| 2:P7:90:GLU:HG2 | 2:P7:121:ARG:NH1 | 2.17 | 0.59 |
| 2:P7:166:LYS:N | 2:P7:199:ASP:OD2 | 2.35 | 0.59 |
| 1:T4:173:PRO:HB3 | 1:T4:384:GLN:NE2 | 2.17 | 0.59 |
| 1:T4:273:LEU:O | 1:T4:292:GLN:NE2 | 2.32 | 0.59 |
| 1:T4:407:GLU:OE2 | 3:4F:81:PHE:HB3 | 2.02 | 0.59 |
| 1:T6:178:THR:HB | 1:T6:181:GLU:HG3 | 1.83 | 0.59 |
| 1:V2:2:ARG:HB3 | 1:V2:131:GLN:HB2 | 1.84 | 0.59 |
| 2:V3:220:GLU:HG2 | 2:V3:221:ARG:HG3 | 1.84 | 0.59 |
| 1:V8:67:ASP:N | 1:V8:67:ASP:OD1 | 2.34 | 0.59 |
| 2:W9:224:TYR:HB2 | 1:X0:245:GLN:HE21 | 1.67 | 0.59 |
| 2:X3:236:SER:O | 2:X3:243:ARG:NH2 | 2.33 | 0.59 |
| 2:X7:284:GLU:HG2 | 2:X7:285:GLN:N | 2.18 | 0.59 |
| 1:Y2:122:LYS:O | 1:Y2:126:SER:OG | 2.14 | 0.59 |
| 1:Y6:11:GLN:N | 39:Y6:502:GDP:O1B | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y8:3:GLU:HB2 | 1:Y8:130:LEU:HA | 1.84 | 0.59 |
| 2:Z3:399:TYR:O | 2:Z3:402:ARG:NH1 | 2.36 | 0.59 |
| 1:Z4:190:HIS:HD2 | 1:Z4:414:ASN:HB2 | 1.67 | 0.59 |
| 2:Z5:265:ILE:CD1 | 2:Z5:435:VAL:HG21 | 2.31 | 0.59 |
| 2:0F:178:SER:HB3 | 1:0G:347:ASN:HD22 | 1.67 | 0.59 |
| 2:0H:387:ILE:HD13 | 2:0H:390:ARG:HH12 | 1.67 | 0.59 |
| 2:0J:381:SER:OG | 2:0J:382:THR:N | 2.35 | 0.59 |
| 2:0X:286:LEU:HD11 | 2:0X:372:GLN:HB2 | 1.84 | 0.59 |
| 1:1A:26:ASP:O | 1:1A:359:LYS:NZ | 2.23 | 0.59 |
| 1:1C:2:ARG:HB3 | 1:1C:131:GLN:HB2 | 1.84 | 0.59 |
| 1:1G:371:SER:OG | 1:1G:372:THR:N | 2.35 | 0.59 |
| 2:1H:88:HIS:CD2 | 2:1X:283:HIS:HB3 | 2.37 | 0.59 |
| 1:1K:86:ARG:HB3 | 1:1K:89:ASN:ND2 | 2.18 | 0.59 |
| 2:1N:259:LEU:HD21 | 2:1N:316:CYS:HB2 | 1.85 | 0.59 |
| 1:1O:276:ARG:HD3 | 9:4Z:147:GLU:OE1 | 2.02 | 0.59 |
| 1:1S:140:GLY:O | 1:1S:184:ASN:ND2 | 2.35 | 0.59 |
| 1:1U:309:ARG:H | 1:1U:372:THR:HG22 | 1.68 | 0.59 |
| 2:1X:271:SER:HB3 | 2:1X:301:MET:HA | 1.83 | 0.59 |
| 2:1Z:92:LEU:N | 2:1Z:92:LEU:HD23 | 2.17 | 0.59 |
| 1:2G:113:ILE:HA | 1:2G:116:VAL:HG12 | 1.85 | 0.59 |
| 2:2Z:297:GLU:OE1 | 38:8C:74:ILE:CG2 | 2.42 | 0.59 |
| 2:3H:267:PHE:HB2 | 2:3H:384:ILE:HD12 | 1.83 | 0.59 |
| 1:3M:49:VAL:HG11 | 1:3M:241:ARG:HG2 | 1.84 | 0.59 |
| 1:3M:175:VAL:HG22 | 2:3N:329:ASN:HD21 | 1.68 | 0.59 |
| 1:3O:237:THR:HG23 | 1:3O:241:ARG:HE | 1.68 | 0.59 |
| 1:3S:128:ASP:OD1 | 1:3S:129:CYS:N | 2.35 | 0.59 |
| 7:4R:8:VAL:CG2 | 7:4R:9:PRO:CD | 2.79 | 0.59 |
| 10:5B:120:GLU:HG3 | 10:5C:359:ARG:HH12 | 1.67 | 0.59 |
| 14:5L:382:ASN:ND2 | 23:6Q:62:GLN:O | 2.35 | 0.59 |
| 17:5U:53:ASP:N | 17:5U:53:ASP:OD1 | 2.32 | 0.59 |
| 18:6C:181:GLN:O | 18:6C:185:THR:OG1 | 2.19 | 0.59 |
| 22:6K:138:ASP:HA | 22:6K:141:LYS:HG3 | 1.84 | 0.59 |
| 22:6P:265:ASP:OD1 | 22:6P:266:LYS:N | 2.35 | 0.59 |
| 24:6V:376:LYS:HA | 24:6V:390:MET:HE2 | 1.84 | 0.59 |
| 30:7K:195:ARG:HD2 | 30:7K:197:ARG:HH21 | 1.67 | 0.59 |
| 37:7Y:140:SER:OG | 37:7Y:141:THR:O | 2.21 | 0.59 |
| 2:G5:178:SER:HB3 | 1:G6:347:ASN:HD22 | 1.66 | 0.59 |
| 1:J6:77:ARG:HD3 | 1:J6:90:PHE:HE2 | 1.68 | 0.59 |
| 2:J7:27:GLU:OE1 | 2:J7:243:ARG:NH1 | 2.35 | 0.59 |
| 2:K7:88:HIS:HD2 | 2:K7:91:GLN:HG3 | 1.67 | 0.59 |
| 2:L5:261:PRO:HG3 | 2:L5:313:MET:HE3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M4:88:ASP:H | 2:O1:283:HIS:CE1 | 2.20 | 0.59 |
| 2:M5:58:ALA:HB2 | 37:7Y:214:ASP:HB3 | 1.83 | 0.59 |
| 2:N1:79:ARG:O | 2:N1:84:ARG:HG2 | 2.03 | 0.59 |
| 2:N5:417:GLU:HA | 2:N5:420:GLU:HG2 | 1.83 | 0.59 |
| 1:O4:117:LEU:HA | 1:O4:120:VAL:HG12 | 1.83 | 0.59 |
| 1:O6:36:TYR:CZ | 1:O6:44:LEU:HD21 | 2.37 | 0.59 |
| 1:O6:354:CYS:SG | 1:O6:355:ASP:N | 2.76 | 0.59 |
| 1:P4:67:ASP:OD1 | 1:P4:72:THR:OG1 | 2.21 | 0.59 |
| 1:P6:289:LEU:HD23 | 1:P6:365:ALA:HB2 | 1.83 | 0.59 |
| 2:Q5:121:ARG:HD2 | 2:Q5:121:ARG:O | 2.03 | 0.59 |
| 1:R8:190:HIS:CD2 | 1:R8:414:ASN:HB2 | 2.37 | 0.59 |
| 2:R9:392:ASP:OD2 | 2:R9:422:ARG:NH1 | 2.36 | 0.59 |
| 2:S1:305:CYS:HB3 | 2:S1:387:ILE:HD11 | 1.85 | 0.59 |
| 1:S4:74:ASP:OD1 | 24:6U:33:LEU:HD11 | 2.02 | 0.59 |
| 2:S9:27:GLU:OE2 | 2:S9:243:ARG:NH1 | 2.36 | 0.59 |
| 1:T0:350:LYS:NZ | 1:T0:352:SER:OG | 2.35 | 0.59 |
| 1:T4:373:ALA:O | 1:T4:376:GLU:HG3 | 2.03 | 0.59 |
| 1:U2:177:ASP:O | 2:U3:352:LYS:HA | 2.02 | 0.59 |
| 1:W0:5:VAL:HG23 | 1:W0:62:ARG:HG2 | 1.84 | 0.59 |
| 1:W6:334:GLN:HE22 | 1:W6:348:ASN:H | 1.51 | 0.59 |
| 2:W9:399:TYR:O | 2:W9:402:ARG:NH1 | 2.35 | 0.59 |
| 2:X7:90:GLU:HB3 | 2:X7:121:ARG:HH12 | 1.67 | 0.59 |
| 2:X7:417:GLU:HA | 2:X7:420:GLU:HG2 | 1.85 | 0.59 |
| 1:Y4:3:GLU:HB2 | 1:Y4:130:LEU:HA | 1.84 | 0.59 |
| 2:Y9:53:PHE:HB3 | 2:Y9:61:HIS:HB3 | 1.84 | 0.59 |
| 2:Z3:33:ASP:OD2 | 2:Z3:35:GLN:NE2 | 2.36 | 0.59 |
| 1:Z6:202:LEU:HD23 | 1:Z6:229:ILE:HD13 | 1.84 | 0.59 |
| 1:Z6:204:ASN:ND2 | 39:Z6:502:GDP:HN22 | 2.01 | 0.59 |
| 2:Z7:166:LYS:N | 2:Z7:199:ASP:OD2 | 2.35 | 0.59 |
| 2:Z7:181:VAL:HG23 | 2:Z7:182:VAL:HG13 | 1.85 | 0.59 |
| 1:0E:68:LEU:HB3 | 1:0E:96:GLY:HA2 | 1.84 | 0.59 |
| 2:0F:109:THR:OG1 | 2:0F:411:GLU:OE2 | 2.20 | 0.59 |
| 2:0H:156:ARG:HA | 2:0H:159:VAL:HG12 | 1.85 | 0.59 |
| 1:0I:183:TYR:HB3 | 1:0I:398:TYR:HE2 | 1.68 | 0.59 |
| 1:0S:372:THR:OG1 | 1:0S:375:GLN:OE1 | 2.21 | 0.59 |
| 1:0Y:139:LEU:HD12 | 1:0Y:170:VAL:HG12 | 1.83 | 0.59 |
| 1:1A:256:ASN:ND2 | 1:1A:350:LYS:HB2 | 2.18 | 0.59 |
| 2:1H:318:MET:HB2 | 2:1H:376:CYS:HB3 | 1.84 | 0.59 |
| 1:1K:50:TYR:CE2 | 1:1K:241:ARG:HD3 | 2.38 | 0.59 |
| 1:2S:77:ARG:HH12 | 38:8B:220:VAL:N | 2.00 | 0.59 |
| 2:2V:287:SER:N | 2:2V:290:GLU:OE2 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2X:191:THR:HA | 2:2X:194:LEU:HB3 | 1.85 | 0.59 |
| 2:3B:417:GLU:HA | 2:3B:420:GLU:HG2 | 1.85 | 0.59 |
| 2:3D:129:CYS:SG | 2:3D:130:THR:N | 2.75 | 0.59 |
| 2:3J:90:GLU:O | 2:3J:121:ARG:NH1 | 2.36 | 0.59 |
| 6:4N:452:ARG:O | 6:4N:456:GLU:HG2 | 2.01 | 0.59 |
| 13:5I:28:ASP:HA | 13:5I:31:GLN:HE21 | 1.67 | 0.59 |
| 13:5J:28:ASP:HA | 13:5J:31:GLN:HE21 | 1.67 | 0.59 |
| 15:5O:68:VAL:O | 15:5O:71:ARG:HG2 | 2.02 | 0.59 |
| 15:5O:226:ARG:NH1 | 15:5O:226:ARG:HB3 | 2.17 | 0.59 |
| 18:5Z:110:GLU:OE2 | 18:5Z:110:GLU:N | 2.35 | 0.59 |
| 22:6M:278:GLN:HA | 22:6M:281:LYS:HD3 | 1.84 | 0.59 |
| 27:7G:116:ASN:HB2 | 27:7G:119:THR:HG23 | 1.83 | 0.59 |
| 38:8A:91:GLN:CG | 38:8A:102:PHE:HD1 | 2.15 | 0.59 |
| 2:2:282:TYR:HE1 | 24:6T:88:TRP:CH2 | 2.20 | 0.59 |
| 2:4:280:LYS:HG2 | 2:S7:89:PRO:HG2 | 1.84 | 0.59 |
| 1:9:41:ASP:OD1 | 26:7E:25:TYR:CE2 | 2.55 | 0.59 |
| 2:E7:364:PRO:HG2 | 22:6M:123:PRO:HB2 | 1.85 | 0.59 |
| 1:G2:404:ASP:HB2 | 1:G2:406:MET:SD | 2.43 | 0.59 |
| 1:G6:252:LYS:HE2 | 1:G6:350:LYS:HE2 | 1.85 | 0.59 |
| 1:G8:166:THR:HG1 | 1:G8:199:CYS:HG | 1.50 | 0.59 |
| 1:G8:286:VAL:HG23 | 1:G8:287:PRO:HD3 | 1.83 | 0.59 |
| 1:H2:97:ALA:HB3 | 1:H2:143:THR:HG22 | 1.84 | 0.59 |
| 2:J3:248:LEU:HD22 | 2:J3:354:GLY:HA2 | 1.84 | 0.59 |
| 2:K1:9:ILE:HG22 | 2:K1:146:GLY:HA2 | 1.85 | 0.59 |
| 2:M3:49:PHE:CD1 | 2:M3:49:PHE:C | 2.76 | 0.59 |
| 1:M6:12:CYS:SG | 1:M6:13:GLY:N | 2.76 | 0.59 |
| 2:O1:392:ASP:OD2 | 2:O1:422:ARG:NH1 | 2.36 | 0.59 |
| 2:P7:26:LEU:HD23 | 2:P7:363:VAL:HG12 | 1.84 | 0.59 |
| 2:Q3:342:GLN:HG3 | 2:Q3:342:GLN:O | 2.02 | 0.59 |
| 1:R2:309:ARG:H | 1:R2:372:THR:HG22 | 1.68 | 0.59 |
| 2:R3:333:ALA:O | 2:R3:337:THR:HG23 | 2.03 | 0.59 |
| 1:S8:405:GLU:HG2 | 13:5I:53:PHE:HZ | 1.67 | 0.59 |
| 2:T7:51:THR:HG21 | 2:T7:243:ARG:HG2 | 1.84 | 0.59 |
| 1:U4:67:ASP:N | 1:U4:67:ASP:OD1 | 2.35 | 0.59 |
| 2:U5:88:HIS:ND1 | 2:W1:283:HIS:HA | 2.17 | 0.59 |
| 1:V6:68:LEU:HB3 | 1:V6:96:GLY:HA2 | 1.83 | 0.59 |
| 2:W3:4:VAL:HG12 | 2:W3:133:GLN:HB2 | 1.85 | 0.59 |
| 1:W4:49:VAL:HG11 | 1:W4:241:ARG:HG2 | 1.83 | 0.59 |
| 1:X4:8:GLN:HE22 | 1:X4:63:ALA:HB1 | 1.67 | 0.59 |
| 2:Y5:189:LEU:HD11 | 2:Y5:418:PHE:HE1 | 1.67 | 0.59 |
| 2:Z7:268:MET:HG3 | 2:Z7:380:ASN:HB2 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z9:12:ALA:HB2 | 41:0A:501:GTP:C8 | 2.38 | 0.59 |
| 2:0J:115:VAL:HG22 | 2:0J:119:LEU:HD23 | 1.85 | 0.59 |
| 2:0P:262:TYR:HB2 | 2:0P:265:ILE:HG22 | 1.84 | 0.59 |
| 1:0Q:337:ASN:HB2 | 1:0Q:340:TYR:HD2 | 1.67 | 0.59 |
| 1:1Q:220:PRO:HD2 | 2:1R:326:LYS:HD2 | 1.85 | 0.59 |
| 1:1W:334:GLN:NE2 | 1:1W:348:ASN:OD1 | 2.36 | 0.59 |
| 2:1X:387:ILE:HG12 | 2:1X:390:ARG:HH22 | 1.66 | 0.59 |
| 1:2M:345:ILE:O | 1:2M:348:ASN:ND2 | 2.34 | 0.59 |
| 2:2V:306:ASP:HB3 | 2:2V:309:HIS:HD2 | 1.67 | 0.59 |
| 2:2X:244:PHE:HB2 | 2:2X:356:ASN:HD21 | 1.68 | 0.59 |
| 2:3B:53:PHE:HB3 | 2:3B:63:PRO:HA | 1.84 | 0.59 |
| 1:3C:309:ARG:H | 1:3C:372:THR:HG22 | 1.67 | 0.59 |
| 5:4L:282:ARG:O | 5:4L:286:LEU:HG | 2.02 | 0.59 |
| 5:4L:466:LEU:HD21 | 5:4M:139:LEU:CD2 | 2.32 | 0.59 |
| 14:5M:225:ARG:HH11 | 14:5M:225:ARG:HG2 | 1.68 | 0.59 |
| 18:5X:110:GLU:OE2 | 18:5X:110:GLU:N | 2.35 | 0.59 |
| 21:6H:106:ARG:NH2 | 24:6X:81:THR:OG1 | 2.35 | 0.59 |
| 22:6P:136:ASN:HD22 | 22:6P:208:ARG:HH22 | 1.50 | 0.59 |
| 26:7D:58:ILE:CD1 | 26:7D:82:PRO:HB3 | 2.33 | 0.59 |
| 29:7J:390:LEU:CG | 29:7J:391:PRO:HD3 | 2.33 | 0.59 |
| 38:8D:70:LYS:HD3 | 38:8D:71:HIS:N | 2.18 | 0.59 |
| 2:4:364:PRO:HB2 | 26:7D:53:TYR:CD1 | 2.37 | 0.59 |
| 2:8:223:THR:HG21 | 26:7E:111:ASP:OD1 | 2.03 | 0.59 |
| 2:A2:280:LYS:HZ2 | 26:7F:64:PRO:HG2 | 1.68 | 0.59 |
| 1:B1:276:ARG:NH1 | 24:6V:210:VAL:HG21 | 2.18 | 0.59 |
| 2:E5:81:GLY:HA3 | 22:6L:116:TYR:HE2 | 1.67 | 0.59 |
| 1:H6:211:CYS:HA | 1:H6:215:LEU:HB2 | 1.84 | 0.59 |
| 2:I5:90:GLU:HB2 | 2:K1:283:HIS:CE1 | 2.38 | 0.59 |
| 2:J3:156:ARG:HE | 35:7T:112:ARG:NH2 | 2.01 | 0.59 |
| 2:L3:339:ARG:NH2 | 34:7S:217:ASP:OD1 | 2.36 | 0.59 |
| 1:M6:1:MET:HE2 | 37:7Y:116:MET:CB | 2.33 | 0.59 |
| 2:Q5:129:CYS:SG | 2:Q5:130:THR:N | 2.75 | 0.59 |
| 1:R8:67:ASP:N | 1:R8:67:ASP:OD1 | 2.35 | 0.59 |
| 1:S0:92:PHE:HE2 | 24:6Z:40:GLN:NE2 | 1.64 | 0.59 |
| 1:T6:14:ASN:HD22 | 1:T6:65:LEU:HD23 | 1.68 | 0.59 |
| 2:T7:175:PRO:O | 2:T7:394:LYS:NZ | 2.35 | 0.59 |
| 2:U3:287:SER:N | 2:U3:290:GLU:OE2 | 2.35 | 0.59 |
| 1:U6:268:VAL:HG23 | 1:U6:368:ILE:HG13 | 1.83 | 0.59 |
| 1:V4:113:ILE:HA | 1:V4:116:VAL:HG22 | 1.85 | 0.59 |
| 1:W6:113:ILE:HA | 1:W6:116:VAL:HG12 | 1.85 | 0.59 |
| 2:W9:79:ARG:O | 2:W9:84:ARG:HG2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y8:260:PHE:HB3 | 1:Y8:263:LEU:HB2 | 1.84 | 0.59 |
| 2:Y9:11:GLN:HE22 | 2:Y9:74:VAL:HG11 | 1.68 | 0.59 |
| 1:Z6:8:GLN:HG2 | 1:Z6:17:GLY:HA3 | 1.84 | 0.59 |
| 1:0G:58:ARG:HD3 | 1:0W:280:GLN:HE22 | 1.67 | 0.59 |
| 2:0L:399:TYR:OH | 2:0L:415:GLU:OE2 | 2.10 | 0.59 |
| 2:0N:381:SER:OG | 2:0N:382:THR:N | 2.35 | 0.59 |
| 1:0Q:68:LEU:HB3 | 1:0Q:96:GLY:HA2 | 1.85 | 0.59 |
| 1:1S:52:ASN:OD1 | 1:1S:62:ARG:NH2 | 2.35 | 0.59 |
| 1:2A:248:ALA:HA | 1:2A:252:LYS:HD2 | 1.85 | 0.59 |
| 2:2D:96:LYS:HD2 | 1:2E:129:CYS:SG | 2.42 | 0.59 |
| 1:2U:212:PHE:HZ | 2:2V:326:LYS:HD3 | 1.68 | 0.59 |
| 1:3A:336:LYS:NZ | 38:8C:54:THR:O | 2.33 | 0.59 |
| 2:3D:236:SER:O | 2:3D:243:ARG:NH2 | 2.35 | 0.59 |
| 2:3D:336:LYS:O | 2:3D:339:ARG:NH2 | 2.35 | 0.59 |
| 1:3G:177:ASP:O | 2:3H:352:LYS:HA | 2.02 | 0.59 |
| 1:3I:177:ASP:O | 2:3J:352:LYS:HA | 2.03 | 0.59 |
| 1:3K:276:ARG:NH1 | 17:5T:216:GLU:HB3 | 2.17 | 0.59 |
| 2:3L:239:THR:HG23 | 2:3L:243:ARG:HE | 1.68 | 0.59 |
| 1:3O:309:ARG:NH1 | 1:3O:339:SER:O | 2.36 | 0.59 |
| 1:3S:49:VAL:HG11 | 1:3S:241:ARG:HG2 | 1.85 | 0.59 |
| 1:3S:94:GLN:HG3 | 1:3S:95:THR:HG23 | 1.84 | 0.59 |
| 15:5P:333:GLU:HG3 | 30:7K:106:LEU:CD2 | 2.32 | 0.59 |
| 18:5Y:110:GLU:OE2 | 18:5Y:110:GLU:N | 2.35 | 0.59 |
| 18:6A:110:GLU:OE2 | 18:6A:110:GLU:N | 2.35 | 0.59 |
| 18:6C:110:GLU:OE2 | 18:6C:110:GLU:N | 2.35 | 0.59 |
| 18:6D:110:GLU:OE2 | 18:6D:110:GLU:N | 2.35 | 0.59 |
| 22:6P:263:SER:O | 22:6P:266:LYS:HG3 | 2.02 | 0.59 |
| 23:6R:69:GLN:OE1 | 23:6R:69:GLN:N | 2.28 | 0.59 |
| 23:6S:15:ARG:HA | 23:6S:18:ARG:HG3 | 1.85 | 0.59 |
| 24:6U:469:PHE:HB2 | 24:6U:483:PHE:O | 2.03 | 0.59 |
| 29:7I:253:ASN:HB3 | 30:7K:341:ARG:NH2 | 2.17 | 0.59 |
| 34:7R:98:GLU:OE2 | 35:7T:47:ASN:ND2 | 2.30 | 0.59 |
| 2:8:283:HIS:HB3 | 2:T1:88:HIS:CD2 | 2.33 | 0.59 |
| 2:A2:423:GLU:OE2 | 4:4G:108:TYR:HE1 | 1.63 | 0.59 |
| 1:A5:281:TYR:HB3 | 1:T8:86:ARG:HG2 | 1.83 | 0.59 |
| 2:B2:59:GLY:HA3 | 24:6V:263:ARG:HH12 | 1.67 | 0.59 |
| 2:C9:206:ASN:ND2 | 41:C9:501:GTP:O2' | 2.36 | 0.59 |
| 1:G2:391:ARG:CG | 1:G2:391:ARG:NH1 | 2.64 | 0.59 |
| 2:G3:42:ILE:HG12 | 24:6W:470:ILE:CD1 | 2.30 | 0.59 |
| 2:H3:291:ILE:HA | 2:H3:294:ALA:HB3 | 1.84 | 0.59 |
| 1:H4:392:LYS:HD2 | 1:H4:395:LEU:HD22 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H6:166:THR:OG1 | 1:H6:199:CYS:SG | 2.59 | 0.59 |
| 2:H9:27:GLU:OE1 | 2:H9:243:ARG:NH1 | 2.32 | 0.59 |
| 2:H9:287:SER:N | 2:H9:290:GLU:OE2 | 2.26 | 0.59 |
| 1:I4:2:ARG:HE | 1:I4:240:LEU:HD22 | 1.68 | 0.59 |
| 2:J3:267:PHE:HB2 | 2:J3:384:ILE:HD12 | 1.85 | 0.59 |
| 2:L7:427:ALA:O | 2:L7:430:LYS:HG3 | 2.02 | 0.59 |
| 1:M2:58:ARG:HG2 | 2:N9:282:TYR:HE1 | 1.67 | 0.59 |
| 1:O2:208:TYR:CE1 | 1:O2:225:LEU:HD11 | 2.37 | 0.59 |
| 1:O4:208:TYR:HB3 | 2:O5:326:LYS:HZ3 | 1.68 | 0.59 |
| 2:O7:399:TYR:O | 2:O7:402:ARG:NH1 | 2.35 | 0.59 |
| 1:Q8:162:ARG:HA | 1:Q8:251:ARG:NH2 | 2.15 | 0.59 |
| 2:Q9:287:SER:N | 2:Q9:290:GLU:OE2 | 2.35 | 0.59 |
| 1:R4:2:ARG:HE | 1:R4:240:LEU:HD22 | 1.68 | 0.59 |
| 1:S8:334:GLN:HE22 | 1:S8:348:ASN:H | 1.49 | 0.59 |
| 1:T6:384:GLN:HE21 | 13:5K:5:TYR:HE2 | 1.51 | 0.59 |
| 2:T7:203:MET:HB2 | 2:T7:303:VAL:HG21 | 1.85 | 0.59 |
| 1:U6:190:HIS:HD2 | 1:U6:414:ASN:HB2 | 1.68 | 0.59 |
| 1:V6:287:PRO:HA | 1:V6:290:THR:HG22 | 1.84 | 0.59 |
| 1:V8:140:GLY:O | 1:V8:184:ASN:ND2 | 2.36 | 0.59 |
| 2:X5:52:PHE:CE2 | 2:X5:243:ARG:HD3 | 2.38 | 0.59 |
| 2:X7:353:CYS:SG | 2:X7:354:GLY:N | 2.76 | 0.59 |
| 2:Y5:213:CYS:HA | 2:Y5:217:LEU:HD13 | 1.85 | 0.59 |
| 2:Y9:111:GLY:HA2 | 2:Y9:114:ILE:HG22 | 1.85 | 0.59 |
| 1:Z2:3:GLU:HB2 | 1:Z2:130:LEU:HA | 1.83 | 0.59 |
| 1:Z4:190:HIS:NE2 | 1:Z4:414:ASN:OD1 | 2.35 | 0.59 |
| 2:Z9:388:PHE:HB3 | 2:Z9:425:LEU:HD11 | 1.85 | 0.59 |
| 1:0A:86:ARG:HG2 | 1:0A:88:ASP:H | 1.67 | 0.59 |
| 1:0I:139:LEU:HG | 1:0I:168:SER:HB2 | 1.85 | 0.59 |
| 2:0L:244:PHE:HB2 | 2:0L:356:ASN:HD21 | 1.67 | 0.59 |
| 1:1U:139:LEU:HD12 | 1:1U:170:VAL:HG22 | 1.84 | 0.59 |
| 2:2B:88:HIS:HB3 | 2:2R:283:HIS:ND1 | 2.18 | 0.59 |
| 1:2I:270:PHE:HD2 | 1:2I:273:LEU:HD21 | 1.67 | 0.59 |
| 1:2M:121:ARG:HH12 | 38:8D:100:SER:H | 1.49 | 0.59 |
| 2:2P:278:ALA:HA | 2:2P:369:ALA:HB2 | 1.83 | 0.59 |
| 2:2R:88:HIS:ND1 | 2:3H:283:HIS:HA | 2.18 | 0.59 |
| 1:2Y:320:ARG:HH22 | 38:8C:201:LEU:HB3 | 1.67 | 0.59 |
| 2:2Z:98:ASP:OD1 | 2:2Z:99:ALA:N | 2.34 | 0.59 |
| 2:3F:98:ASP:OD1 | 2:3F:99:ALA:N | 2.36 | 0.59 |
| 6:4O:386:PHE:HB3 | 6:4O:387:ARG:HH21 | 1.68 | 0.59 |
| 8:4W:259:GLN:O | 8:4W:263:THR:HG23 | 2.03 | 0.59 |
| 9:4Z:37:SER:OG | 9:4Z:38:GLN:OE1 | 2.20 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:375:ILE:HG23 | 9:4Z:379:LYS:HE2 | 1.84 | 0.59 |
| 10:5B:128:LEU:O | 10:5B:132:THR:HG23 | 2.03 | 0.59 |
| 14:5M:221:ILE:HD13 | 14:5M:228:PHE:HA | 1.84 | 0.59 |
| 15:5O:333:GLU:HB3 | 30:7K:241:LYS:HZ1 | 1.67 | 0.59 |
| 18:6B:110:GLU:OE2 | 18:6B:110:GLU:N | 2.35 | 0.59 |
| 23:6R:33:HIS:CE1 | 23:6R:51:THR:O | 2.56 | 0.59 |
| 24:6W:338:LEU:HB3 | 24:6W:341:LYS:HZ1 | 1.68 | 0.59 |
| 24:6X:525:VAL:HB | 24:6X:530:PHE:HE2 | 1.68 | 0.59 |
| 25:7C:8:VAL:O | 25:7C:12:VAL:HG23 | 2.03 | 0.59 |
| 34:7S:260:ARG:O | 34:7S:264:GLU:HG2 | 2.03 | 0.59 |
| 38:8C:44:ARG:HB2 | 38:8C:47:PHE:CD2 | 2.38 | 0.59 |
| 38:8C:73:TRP:HD1 | 38:8C:73:TRP:H | 1.51 | 0.59 |
| 1:9:280:GLN:OE1 | 1:T2:58:ARG:NH2 | 2.36 | 0.59 |
| 1:A3:41:ASP:HA | 26:7F:25:TYR:HE2 | 1.67 | 0.59 |
| 2:C9:373:ARG:HH22 | 24:6V:255:HIS:CD2 | 2.18 | 0.59 |
| 1:H6:237:THR:HG23 | 1:H6:240:LEU:HD13 | 1.84 | 0.59 |
| 1:H8:309:ARG:NH1 | 1:H8:339:SER:O | 2.36 | 0.59 |
| 2:L1:66:ILE:HD12 | 2:L1:68:LEU:HD23 | 1.85 | 0.59 |
| 2:L5:183:GLU:HG3 | 2:L5:184:PRO:HD3 | 1.85 | 0.59 |
| 1:M4:67:ASP:OD2 | 1:M4:72:THR:OG1 | 2.21 | 0.59 |
| 1:M6:37:HIS:CE1 | 15:5P:295:ASN:HD22 | 2.19 | 0.59 |
| 1:M6:382:SER:HB3 | 1:M6:415:MET:HG2 | 1.84 | 0.59 |
| 2:N7:340:THR:HG21 | 32:7O:15:VAL:HG12 | 1.85 | 0.59 |
| 1:O2:204:ASN:HD21 | 39:O2:502:GDP:HN22 | 1.51 | 0.59 |
| 2:O3:183:GLU:HG3 | 2:O3:184:PRO:HD3 | 1.83 | 0.59 |
| 1:O6:391:ARG:HG3 | 2:O7:346:TRP:CG | 2.37 | 0.59 |
| 1:P4:172:SER:HB3 | 1:P4:175:VAL:HG22 | 1.85 | 0.59 |
| 2:Q5:240:ALA:HB1 | 2:Q5:356:ASN:HD22 | 1.68 | 0.59 |
| 1:R2:172:SER:OG | 1:R2:380:ARG:NH2 | 2.36 | 0.59 |
| 1:R6:219:THR:HB | 2:R7:324:VAL:HG11 | 1.85 | 0.59 |
| 2:S1:9:ILE:HG22 | 2:S1:146:GLY:HA2 | 1.85 | 0.59 |
| 2:T7:379:SER:OG | 2:T7:380:ASN:N | 2.36 | 0.59 |
| 2:U9:246:GLY:H | 2:U9:249:ASN:HD21 | 1.49 | 0.59 |
| 2:V7:90:GLU:O | 2:V7:121:ARG:NH1 | 2.33 | 0.59 |
| 1:X6:31:ASP:OD2 | 1:X6:33:THR:OG1 | 2.18 | 0.59 |
| 1:0C:99:ASN:HB3 | 1:0C:180:VAL:HG11 | 1.84 | 0.59 |
| 1:0I:5:VAL:HG23 | 1:0I:62:ARG:HG2 | 1.85 | 0.59 |
| 1:0K:393:ALA:O | 1:0K:395:LEU:N | 2.36 | 0.59 |
| 2:0L:274:PRO:HB2 | 2:0L:276:ILE:HG12 | 1.85 | 0.59 |
| 1:1U:58:ARG:HG2 | 1:2K:280:GLN:HE22 | 1.67 | 0.59 |
| 1:1U:273:LEU:H | 1:1U:292:GLN:HE22 | 1.48 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1U:335:ASN:O | 1:1U:338:SER:OG | 2.21 | 0.59 |
| 1:1W:272:PRO:HB2 | 1:1W:282:ARG:HH12 | 1.68 | 0.59 |
| 1:2G:172:SER:HB2 | 1:2G:380:ARG:HH21 | 1.67 | 0.59 |
| 2:2H:53:PHE:HB3 | 2:2H:61:HIS:HB3 | 1.84 | 0.59 |
| 2:3B:399:TYR:OH | 2:3B:415:GLU:OE2 | 2.19 | 0.59 |
| 2:3F:88:HIS:HB2 | 2:3F:91:GLN:NE2 | 2.17 | 0.59 |
| 2:3H:358:GLN:NE2 | 2:3H:359:PRO:O | 2.35 | 0.59 |
| 1:3I:317:PHE:HB3 | 1:3I:321:MET:HE1 | 1.84 | 0.59 |
| 12:5F:44:ILE:HD11 | 12:5F:50:ALA:HB2 | 1.85 | 0.59 |
| 12:5F:47:GLN:N | 12:5F:48:PRO:HD2 | 2.17 | 0.59 |
| 15:5P:54:GLU:OE1 | 15:5P:54:GLU:HA | 2.03 | 0.59 |
| 17:5V:222:ILE:O | 17:5V:226:ILE:HG12 | 2.03 | 0.59 |
| 22:6P:269:GLU:HB2 | 22:6P:272:ARG:HH21 | 1.68 | 0.59 |
| 23:6Q:15:ARG:HA | 23:6Q:18:ARG:HG3 | 1.85 | 0.59 |
| 24:6Y:112:GLU:OE1 | 24:6Y:210:VAL:HG22 | 2.03 | 0.59 |
| 24:7A:212:VAL:O | 24:7A:216:THR:HG23 | 2.02 | 0.59 |
| 26:7D:79:GLN:NE2 | 26:7D:108:SER:O | 2.35 | 0.59 |
| 26:7E:79:GLN:NE2 | 26:7E:108:SER:O | 2.35 | 0.59 |
| 38:8A:92:GLU:O | 38:8A:92:GLU:HG3 | 2.03 | 0.59 |
| 1:A3:228:LEU:HD21 | 26:7F:136:PHE:CZ | 2.37 | 0.58 |
| 2:G3:209:ILE:HD13 | 2:G3:231:ILE:HD11 | 1.85 | 0.58 |
| 2:G7:217:LEU:HD21 | 2:G7:368:LEU:HD23 | 1.84 | 0.58 |
| 2:H5:88:HIS:CE1 | 2:J1:283:HIS:HA | 2.38 | 0.58 |
| 1:H6:334:GLN:HE22 | 1:H6:348:ASN:H | 1.51 | 0.58 |
| 1:I2:391:ARG:HB2 | 2:I3:346:TRP:HE1 | 1.68 | 0.58 |
| 1:J2:190:HIS:CD2 | 1:J2:411:ALA:HA | 2.38 | 0.58 |
| 2:N7:156:ARG:HA | 2:N7:159:VAL:HG12 | 1.85 | 0.58 |
| 2:N7:287:SER:N | 2:N7:290:GLU:OE2 | 2.23 | 0.58 |
| 1:P8:238:CYS:SG | 1:P8:318:ARG:NE | 2.75 | 0.58 |
| 2:R1:51:THR:HG21 | 2:R1:243:ARG:HG2 | 1.84 | 0.58 |
| 1:R2:7:ILE:HB | 1:R2:135:VAL:HG12 | 1.85 | 0.58 |
| 1:S4:11:GLN:HE22 | 2:S5:249:ASN:H | 1.50 | 0.58 |
| 2:S5:189:LEU:HD11 | 2:S5:418:PHE:HE1 | 1.67 | 0.58 |
| 2:S9:88:HIS:CD2 | 2:S9:90:GLU:H | 2.17 | 0.58 |
| 1:U4:51:PHE:O | 1:U4:62:ARG:NH2 | 2.35 | 0.58 |
| 1:U6:166:THR:OG1 | 1:U6:199:CYS:SG | 2.61 | 0.58 |
| 1:V6:58:ARG:HG2 | 1:X2:280:GLN:HE22 | 1.67 | 0.58 |
| 2:V9:88:HIS:CD2 | 2:X5:283:HIS:HB2 | 2.38 | 0.58 |
| 1:W2:375:GLN:HB2 | 1:W2:419:VAL:HG13 | 1.84 | 0.58 |
| 1:W6:49:VAL:HG11 | 1:W6:241:ARG:HG2 | 1.84 | 0.58 |
| 2:W7:384:ILE:HA | 2:W7:387:ILE:HD12 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:76:ASP:HA | 2:W9:79:ARG:HB2 | 1.85 | 0.58 |
| 1:X4:273:LEU:H | 1:X4:292:GLN:HE22 | 1.51 | 0.58 |
| 1:Y0:412:GLU:O | 1:Y0:416:ASN:ND2 | 2.36 | 0.58 |
| 1:Y8:246:LEU:O | 1:Y8:352:SER:OG | 2.21 | 0.58 |
| 2:Z5:12:ALA:HB2 | 41:Z6:501:GTP:C8 | 2.37 | 0.58 |
| 2:0H:336:LYS:O | 2:0H:339:ARG:NH2 | 2.30 | 0.58 |
| 1:0M:31:ASP:OD2 | 1:0M:33:THR:OG1 | 2.21 | 0.58 |
| 1:0S:186:THR:HG22 | 1:0S:411:ALA:HB1 | 1.85 | 0.58 |
| 1:0Y:204:ASN:OD1 | 39:0Y:502:GDP:O2' | 2.21 | 0.58 |
| 1:1A:211:CYS:HA | 1:1A:215:LEU:HB2 | 1.84 | 0.58 |
| 2:1V:56:THR:HA | 2:2L:285:GLN:HB2 | 1.84 | 0.58 |
| 2:2H:284:GLU:OE1 | 2:2H:284:GLU:HA | 2.03 | 0.58 |
| 1:3M:211:CYS:SG | 1:3M:220:PRO:HB3 | 2.43 | 0.58 |
| 2:3P:236:SER:OG | 2:3P:243:ARG:NH2 | 2.35 | 0.58 |
| 1:3S:362:LYS:CE | 38:8D:166:GLU:HG2 | 2.25 | 0.58 |
| 12:5F:56:THR:HG23 | 12:5F:57:THR:H | 1.67 | 0.58 |
| 15:5P:60:LEU:H | 15:5P:60:LEU:HD23 | 1.67 | 0.58 |
| 16:5Q:88:THR:HG23 | 16:5Q:89:HIS:CD2 | 2.36 | 0.58 |
| 17:5V:207:VAL:HG22 | 17:5V:211:ARG:HH12 | 1.67 | 0.58 |
| 19:6E:17:VAL:HG11 | 19:6E:28:ARG:HG2 | 1.85 | 0.58 |
| 22:6I:166:ILE:HD11 | 22:6I:226:LEU:HD11 | 1.85 | 0.58 |
| 23:6Q:69:GLN:OE1 | 23:6Q:69:GLN:N | 2.28 | 0.58 |
| 24:6Y:35:TYR:CD1 | 24:6Y:42:GLU:HG2 | 2.38 | 0.58 |
| 1:E6:204:ASN:HD21 | 39:E6:502:GDP:HN22 | 1.51 | 0.58 |
| 1:H2:177:ASP:O | 2:H3:352:LYS:HA | 2.03 | 0.58 |
| 2:H5:287:SER:N | 2:H5:290:GLU:OE2 | 2.34 | 0.58 |
| 1:H6:51:PHE:O | 1:H6:62:ARG:NH2 | 2.36 | 0.58 |
| 2:J1:119:LEU:HD11 | 2:J1:156:ARG:HD3 | 1.85 | 0.58 |
| 1:J2:350:LYS:NZ | 1:J2:351:SER:O | 2.36 | 0.58 |
| 1:J4:248:ALA:HA | 1:J4:252:LYS:HD2 | 1.84 | 0.58 |
| 2:M1:90:GLU:HG3 | 2:M1:121:ARG:HH12 | 1.68 | 0.58 |
| 2:M5:370:LYS:NZ | 30:7K:142:SER:O | 2.28 | 0.58 |
| 2:M9:109:THR:OG1 | 2:M9:411:GLU:OE2 | 2.16 | 0.58 |
| 2:O3:405:VAL:HG13 | 2:O3:418:PHE:HE2 | 1.68 | 0.58 |
| 2:O5:18:ASN:HD21 | 32:7P:116:TYR:HE1 | 1.51 | 0.58 |
| 2:O5:399:TYR:OH | 2:O5:415:GLU:OE2 | 2.13 | 0.58 |
| 1:O8:52:ASN:OD1 | 1:O8:62:ARG:NH2 | 2.36 | 0.58 |
| 2:Q3:286:LEU:O | 2:Q3:373:ARG:NH1 | 2.36 | 0.58 |
| 1:R0:173:PRO:HB3 | 1:R0:384:GLN:HE22 | 1.67 | 0.58 |
| 2:R3:7:ILE:HD12 | 2:R3:153:LEU:HD21 | 1.86 | 0.58 |
| 2:S1:333:ALA:O | 2:S1:337:THR:HG23 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T2:273:LEU:H | 1:T2:292:GLN:HE22 | 1.52 | 0.58 |
| 1:V2:285:THR:HG23 | 1:V2:288:GLU:H | 1.68 | 0.58 |
| 1:W4:138:SER:OG | 1:W4:139:LEU:N | 2.37 | 0.58 |
| 1:X0:140:GLY:O | 1:X0:184:ASN:ND2 | 2.37 | 0.58 |
| 1:X4:397:TRP:HE1 | 2:X5:260:VAL:HB | 1.68 | 0.58 |
| 2:Y5:279:GLU:HG2 | 2:Y5:280:LYS:HD3 | 1.83 | 0.58 |
| 1:Y6:201:VAL:HG12 | 1:Y6:266:PHE:O | 2.03 | 0.58 |
| 1:Y8:207:LEU:HD23 | 1:Y8:225:LEU:HB3 | 1.85 | 0.58 |
| 2:Z5:90:GLU:HB2 | 2:Z5:121:ARG:NH1 | 2.19 | 0.58 |
| 2:Z7:181:VAL:HG12 | 1:Z8:347:ASN:O | 2.03 | 0.58 |
| 1:Z8:412:GLU:HG2 | 1:Z8:415:MET:HE2 | 1.85 | 0.58 |
| 2:0J:55:GLU:O | 2:0Z:285:GLN:NE2 | 2.36 | 0.58 |
| 1:0M:67:ASP:OD2 | 1:0M:72:THR:OG1 | 2.17 | 0.58 |
| 1:0O:113:ILE:HA | 1:0O:116:VAL:HG22 | 1.84 | 0.58 |
| 1:0Q:117:LEU:HD13 | 1:0Q:121:ARG:HH22 | 1.67 | 0.58 |
| 2:1H:278:ALA:HA | 2:1H:369:ALA:HB2 | 1.85 | 0.58 |
| 2:1H:298:PRO:HA | 2:1H:301:MET:HG3 | 1.84 | 0.58 |
| 2:1H:322:ASP:HB3 | 2:1H:373:ARG:HH21 | 1.68 | 0.58 |
| 2:1N:336:LYS:O | 2:1N:339:ARG:NH2 | 2.35 | 0.58 |
| 2:1R:57:GLY:HA3 | 10:5B:156:TYR:OH | 2.03 | 0.58 |
| 2:2D:109:THR:HG23 | 2:2D:110:ILE:HG12 | 1.84 | 0.58 |
| 1:2M:253:LEU:HD11 | 1:2M:316:LEU:HD21 | 1.85 | 0.58 |
| 1:2Y:177:ASP:O | 2:2Z:352:LYS:HA | 2.03 | 0.58 |
| 1:3I:77:ARG:NE | 3:3Z:19:LEU:HA | 2.18 | 0.58 |
| 2:3L:182:VAL:HG12 | 2:3L:185:TYR:HB2 | 1.83 | 0.58 |
| 1:3M:391:ARG:HH21 | 2:3N:262:TYR:HE2 | 1.50 | 0.58 |
| 8:4X:112:GLU:O | 8:4X:116:ASN:ND2 | 2.36 | 0.58 |
| 10:5B:150:MET:O | 10:5B:154:MET:HG2 | 2.03 | 0.58 |
| 15:5O:111:ASN:ND2 | 15:5O:115:GLN:OE1 | 2.35 | 0.58 |
| 15:5P:21:LEU:HD23 | 15:5P:21:LEU:C | 2.22 | 0.58 |
| 18:5X:101:LYS:O | 24:6U:178:ASN:ND2 | 2.32 | 0.58 |
| 24:6V:11:LEU:CB | 24:6V:12:PRO:HD2 | 2.31 | 0.58 |
| 38:8A:196:MET:CE | 38:8A:201:LEU:HD21 | 2.32 | 0.58 |
| 2:G1:43:GLY:O | 24:6V:447:ARG:NH1 | 2.36 | 0.58 |
| 1:G4:219:THR:N | 24:6X:418:ASP:OD1 | 2.35 | 0.58 |
| 1:G4:388:MET:HG3 | 1:G4:393:ALA:HB3 | 1.86 | 0.58 |
| 2:I7:392:ASP:OD2 | 2:I7:422:ARG:NH1 | 2.35 | 0.58 |
| 1:J4:139:LEU:HD12 | 1:J4:170:VAL:HG12 | 1.85 | 0.58 |
| 1:J6:2:ARG:HB3 | 1:J6:131:GLN:HB2 | 1.83 | 0.58 |
| 1:K0:211:CYS:HA | 1:K0:215:LEU:HB2 | 1.86 | 0.58 |
| 2:K1:84:ARG:HH12 | 28:7X:407:LYS:HG3 | 1.67 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L0:39:ASP:OD1 | 1:L0:40:SER:N | 2.34 | 0.58 |
| 2:M9:90:GLU:HB2 | 1:O6:281:TYR:CE2 | 2.38 | 0.58 |
| 1:N0:334:GLN:HE22 | 1:N0:348:ASN:H | 1.51 | 0.58 |
| 2:O3:56:THR:HG21 | 2:Q1:283:HIS:O | 2.03 | 0.58 |
| 2:O7:189:LEU:HD11 | 2:O7:418:PHE:HE1 | 1.68 | 0.58 |
| 1:P8:272:PRO:HB2 | 1:P8:282:ARG:HH12 | 1.66 | 0.58 |
| 1:Q0:193:VAL:HG23 | 1:Q0:194:GLU:HG2 | 1.84 | 0.58 |
| 1:Q8:177:ASP:O | 2:Q9:352:LYS:HA | 2.02 | 0.58 |
| 2:R1:102:ASN:HB3 | 2:R1:105:ARG:HB3 | 1.85 | 0.58 |
| 2:R1:196:GLU:HA | 17:5S:84:ARG:HD2 | 1.84 | 0.58 |
| 2:R3:151:SER:O | 2:R3:155:GLU:HG3 | 2.03 | 0.58 |
| 1:S8:280:GLN:OE1 | 1:S8:280:GLN:N | 2.36 | 0.58 |
| 1:T6:337:ASN:HD21 | 17:5U:48:THR:H | 1.50 | 0.58 |
| 2:U3:73:THR:O | 2:U3:77:GLU:HG2 | 2.02 | 0.58 |
| 1:W0:30:ILE:HG22 | 1:W0:36:TYR:HA | 1.84 | 0.58 |
| 2:W1:384:ILE:HA | 2:W1:387:ILE:HD12 | 1.84 | 0.58 |
| 1:X0:359:LYS:HG3 | 8:4X:96:VAL:CG2 | 2.33 | 0.58 |
| 1:X8:192:LEU:HD22 | 1:X8:196:ALA:HB2 | 1.85 | 0.58 |
| 2:Y5:282:TYR:O | 8:4W:424:LYS:NZ | 2.31 | 0.58 |
| 2:Z3:69:ASP:OD1 | 2:Z3:70:LEU:N | 2.36 | 0.58 |
| 1:Z6:274:THR:OG1 | 1:Z6:282:ARG:NH1 | 2.35 | 0.58 |
| 2:0B:109:THR:OG1 | 2:0B:411:GLU:OE2 | 2.17 | 0.58 |
| 2:0F:292:THR:HG1 | 2:0F:319:TYR:HH | 1.52 | 0.58 |
| 2:0J:5:ILE:HD11 | 2:0J:135:PHE:CE1 | 2.38 | 0.58 |
| 1:0Q:33:THR:O | 1:0Q:58:ARG:NH2 | 2.36 | 0.58 |
| 2:0V:63:PRO:HB2 | 2:0V:65:CYS:SG | 2.43 | 0.58 |
| 2:0V:238:LEU:HA | 2:0V:318:MET:SD | 2.43 | 0.58 |
| 2:0Z:73:THR:HA | 1:1A:46:ARG:HH21 | 1.68 | 0.58 |
| 2:1P:381:SER:OG | 2:1P:382:THR:N | 2.37 | 0.58 |
| 2:1X:9:ILE:HG22 | 2:1X:146:GLY:HA2 | 1.86 | 0.58 |
| 2:2J:109:THR:OG1 | 2:2J:411:GLU:OE2 | 2.20 | 0.58 |
| 2:2L:289:ALA:O | 2:2L:293:ASN:ND2 | 2.37 | 0.58 |
| 2:2R:392:ASP:OD2 | 2:2R:422:ARG:NH1 | 2.35 | 0.58 |
| 1:3C:140:GLY:O | 1:3C:184:ASN:ND2 | 2.35 | 0.58 |
| 2:3L:72:PRO:HD2 | 1:3M:2:ARG:HH12 | 1.67 | 0.58 |
| 2:3P:399:TYR:O | 2:3P:402:ARG:NH1 | 2.36 | 0.58 |
| 13:5H:18:ARG:HB3 | 24:6T:38:GLY:HA2 | 1.86 | 0.58 |
| 13:5H:28:ASP:HA | 13:5H:31:GLN:NE2 | 2.19 | 0.58 |
| 13:5J:28:ASP:HA | 13:5J:31:GLN:NE2 | 2.19 | 0.58 |
| 13:5K:28:ASP:HA | 13:5K:31:GLN:NE2 | 2.19 | 0.58 |
| 15:5O:34:GLU:OE2 | 15:5O:49:ARG:HG2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:270:LEU:HD12 | 15:5O:307:ILE:HD11 | 1.85 | 0.58 |
| 19:6E:98:THR:O | 19:6E:98:THR:HG23 | 2.02 | 0.58 |
| 22:6N:70:ASN:O | 22:6N:73:ASN:ND2 | 2.37 | 0.58 |
| 22:6O:45:PRO:HB3 | 22:6O:51:ILE:HG23 | 1.86 | 0.58 |
| 23:6S:69:GLN:OE1 | 23:6S:69:GLN:N | 2.28 | 0.58 |
| 24:6Y:242:PHE:O | 24:6Y:246:VAL:HG23 | 2.04 | 0.58 |
| 26:7F:79:GLN:NE2 | 26:7F:108:SER:O | 2.35 | 0.58 |
| 36:7V:32:LYS:CD | 36:7V:72:LEU:H | 2.07 | 0.58 |
| 38:8C:83:ARG:HD3 | 38:8C:83:ARG:N | 2.17 | 0.58 |
| 1:F2:11:GLN:N | 39:F2:501:GDP:O1B | 2.28 | 0.58 |
| 2:I5:164:LYS:O | 2:I5:166:LYS:NZ | 2.35 | 0.58 |
| 1:J2:71:GLY:CA | 16:5Q:175:LEU:HD21 | 2.33 | 0.58 |
| 2:J5:417:GLU:HA | 2:J5:420:GLU:HG2 | 1.85 | 0.58 |
| 2:K5:223:THR:HG23 | 2:K5:225:THR:H | 1.68 | 0.58 |
| 1:M0:211:CYS:HA | 1:M0:215:LEU:HB2 | 1.85 | 0.58 |
| 1:M2:86:ARG:HB3 | 2:N9:283:HIS:CE1 | 2.38 | 0.58 |
| 2:M3:109:THR:OG1 | 2:M3:411:GLU:OE2 | 2.19 | 0.58 |
| 2:N1:76:ASP:OD1 | 1:N2:46:ARG:NH2 | 2.35 | 0.58 |
| 2:N3:381:SER:OG | 2:N3:382:THR:N | 2.37 | 0.58 |
| 2:N9:259:LEU:HD11 | 2:N9:316:CYS:HB2 | 1.85 | 0.58 |
| 2:P9:27:GLU:OE1 | 2:P9:243:ARG:NH1 | 2.36 | 0.58 |
| 2:P9:278:ALA:HA | 2:P9:369:ALA:HB2 | 1.85 | 0.58 |
| 1:Q0:125:GLU:OE2 | 1:R6:291:GLN:NE2 | 2.36 | 0.58 |
| 2:Q1:53:PHE:HB3 | 2:Q1:61:HIS:HB3 | 1.84 | 0.58 |
| 1:Q6:52:ASN:OD1 | 1:Q6:62:ARG:NH2 | 2.37 | 0.58 |
| 1:S0:5:VAL:HG23 | 1:S0:62:ARG:HG2 | 1.84 | 0.58 |
| 1:S4:113:ILE:HG13 | 1:S4:150:LEU:HD22 | 1.85 | 0.58 |
| 2:V3:284:GLU:O | 2:V3:285:GLN:NE2 | 2.36 | 0.58 |
| 1:V6:192:LEU:HD22 | 1:V6:196:ALA:HB2 | 1.85 | 0.58 |
| 2:V7:392:ASP:OD2 | 2:V7:422:ARG:NH1 | 2.35 | 0.58 |
| 1:W2:138:SER:OG | 1:W2:139:LEU:N | 2.36 | 0.58 |
| 2:W7:398:MET:SD | 1:W8:346:PRO:HD2 | 2.43 | 0.58 |
| 1:X0:345:ILE:O | 1:X0:348:ASN:ND2 | 2.37 | 0.58 |
| 2:X3:9:ILE:HG12 | 2:X3:68:LEU:HD21 | 1.85 | 0.58 |
| 2:X5:236:SER:O | 2:X5:243:ARG:NH2 | 2.35 | 0.58 |
| 1:Y4:276:ARG:HD3 | 8:4W:405:GLU:OE2 | 2.03 | 0.58 |
| 2:Z5:88:HIS:ND1 | 2:Z5:90:GLU:HG2 | 2.19 | 0.58 |
| 1:Z6:4:ILE:HG22 | 1:Z6:49:VAL:HG22 | 1.84 | 0.58 |
| 2:0J:5:ILE:HD11 | 2:0J:135:PHE:HE1 | 1.69 | 0.58 |
| 2:0L:33:ASP:O | 2:0L:60:LYS:NZ | 2.36 | 0.58 |
| 1:0S:68:LEU:HD13 | 1:0S:93:GLY:HA3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0S:209:ASP:HA | 1:0S:213:ARG:NH1 | 2.17 | 0.58 |
| 1:0U:273:LEU:H | 1:0U:292:GLN:HE22 | 1.49 | 0.58 |
| 2:1H:305:CYS:HB2 | 2:1H:387:ILE:HD11 | 1.86 | 0.58 |
| 1:1K:180:VAL:HG23 | 1:1K:184:ASN:HD21 | 1.66 | 0.58 |
| 1:1Q:248:ALA:HA | 1:1Q:252:LYS:HD2 | 1.84 | 0.58 |
| 2:2H:205:ASP:OD1 | 2:2H:303:VAL:HA | 2.04 | 0.58 |
| 2:2H:352:LYS:NZ | 2:2H:353:CYS:O | 2.35 | 0.58 |
| 2:2N:203:MET:HE3 | 2:2N:267:PHE:HD1 | 1.67 | 0.58 |
| 1:2U:128:ASP:OD1 | 1:2U:129:CYS:N | 2.35 | 0.58 |
| 2:2V:215:ARG:HB2 | 38:8B:66:TYR:HE1 | 1.68 | 0.58 |
| 1:2W:391:ARG:NH1 | 2:2X:438:GLU:OE1 | 2.36 | 0.58 |
| 1:2Y:237:THR:O | 1:2Y:241:ARG:NE | 2.37 | 0.58 |
| 1:3I:248:ALA:HA | 1:3I:252:LYS:HD2 | 1.84 | 0.58 |
| 6:4O:62:ASP:O | 6:4O:66:ARG:HG2 | 2.04 | 0.58 |
| 10:5A:356:ARG:HA | 10:5A:359:ARG:HD2 | 1.85 | 0.58 |
| 13:5I:28:ASP:HA | 13:5I:31:GLN:NE2 | 2.19 | 0.58 |
| 13:5K:82:PHE:CD1 | 13:5K:83:MET:HG2 | 2.38 | 0.58 |
| 14:5N:224:GLU:O | 14:5N:224:GLU:HG2 | 2.02 | 0.58 |
| 22:6K:114:THR:HG23 | 22:6K:117:GLY:H | 1.68 | 0.58 |
| 24:6X:96:LEU:HD22 | 24:6X:188:THR:HG22 | 1.85 | 0.58 |
| 28:7H:451:LYS:HG3 | 28:7H:452:ASN:H | 1.68 | 0.58 |
| 35:7T:227:TRP:O | 35:7T:231:THR:HG23 | 2.03 | 0.58 |
| 38:8A:213:GLU:HG2 | 38:8A:214:HIS:N | 2.17 | 0.58 |
| 2:4:423:GLU:OE2 | 4:3Y:54:VAL:HG23 | 2.02 | 0.58 |
| 1:G2:276:ARG:HD3 | 24:6W:419:SER:HB2 | 1.84 | 0.58 |
| 1:G8:80:PRO:HB3 | 24:6Z:526:PHE:CE2 | 2.34 | 0.58 |
| 1:H2:97:ALA:HA | 1:H2:103:LYS:HE3 | 1.83 | 0.58 |
| 2:J1:63:PRO:HB2 | 2:J1:65:CYS:SG | 2.43 | 0.58 |
| 2:J1:287:SER:N | 2:J1:290:GLU:OE2 | 2.37 | 0.58 |
| 2:K3:167:LEU:HD21 | 2:K3:252:ILE:HD12 | 1.85 | 0.58 |
| 1:L2:257:LEU:HD21 | 1:L2:314:SER:HB3 | 1.85 | 0.58 |
| 1:L6:183:TYR:HE2 | 1:L6:394:PHE:HB2 | 1.68 | 0.58 |
| 2:L7:279:GLU:OE1 | 6:4P:209:LYS:NZ | 2.36 | 0.58 |
| 2:M9:286:LEU:O | 30:7K:27:ILE:HG22 | 2.04 | 0.58 |
| 2:N5:392:ASP:OD2 | 2:N5:422:ARG:NH1 | 2.37 | 0.58 |
| 2:N9:119:LEU:HD23 | 2:N9:122:ILE:CD1 | 2.31 | 0.58 |
| 1:O6:393:ALA:O | 1:O6:395:LEU:N | 2.37 | 0.58 |
| 1:P4:374:ILE:O | 1:P4:377:MET:HG3 | 2.03 | 0.58 |
| 1:Q2:107:THR:OG1 | 1:Q2:108:GLU:OE1 | 2.15 | 0.58 |
| 1:S0:91:VAL:CG1 | 1:S0:116:VAL:HG12 | 2.24 | 0.58 |
| 1:T0:201:VAL:HG21 | 1:T0:374:ILE:HD11 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T0:213:ARG:HH22 | 13:5I:117:ASN:ND2 | 2.01 | 0.58 |
| 2:T3:286:LEU:O | 2:T3:373:ARG:NH1 | 2.37 | 0.58 |
| 1:T6:177:ASP:O | 2:T7:352:LYS:HA | 2.03 | 0.58 |
| 1:T8:45:GLU:HG2 | 1:T8:46:ARG:HG2 | 1.84 | 0.58 |
| 2:U1:90:GLU:HB3 | 2:V7:283:HIS:CE1 | 2.37 | 0.58 |
| 1:V2:113:ILE:HA | 1:V2:116:VAL:HG22 | 1.84 | 0.58 |
| 1:V8:22:GLU:HG2 | 1:V8:81:TYR:HB2 | 1.85 | 0.58 |
| 1:X4:391:ARG:HD3 | 2:X5:346:TRP:CE2 | 2.38 | 0.58 |
| 2:X5:399:TYR:O | 2:X5:402:ARG:NH1 | 2.36 | 0.58 |
| 1:X6:172:SER:HB2 | 1:X6:205:GLU:OE1 | 2.02 | 0.58 |
| 2:X7:88:HIS:CE1 | 2:Z3:283:HIS:HA | 2.38 | 0.58 |
| 1:Y2:113:ILE:HA | 1:Y2:116:VAL:HG12 | 1.84 | 0.58 |
| 1:Y4:178:THR:OG1 | 2:Y5:258:ASN:ND2 | 2.36 | 0.58 |
| 2:Z1:210:TYR:HE1 | 2:Z1:227:LEU:HD21 | 1.68 | 0.58 |
| 2:0B:12:ALA:HB2 | 41:0C:501:GTP:C8 | 2.38 | 0.58 |
| 2:0B:157:LEU:HD13 | 2:0B:166:LYS:HD3 | 1.84 | 0.58 |
| 2:0B:427:ALA:HA | 2:0B:430:LYS:HD3 | 1.86 | 0.58 |
| 1:0M:3:GLU:O | 1:0M:131:GLN:N | 2.34 | 0.58 |
| 1:0O:391:ARG:O | 1:0O:391:ARG:HG3 | 2.03 | 0.58 |
| 1:1G:301:CYS:SG | 1:1G:302:ALA:N | 2.77 | 0.58 |
| 2:1L:88:HIS:HB3 | 2:1L:91:GLN:HG3 | 1.86 | 0.58 |
| 1:1O:3:GLU:HB2 | 1:1O:130:LEU:HA | 1.84 | 0.58 |
| 1:1U:107:THR:OG1 | 1:1U:401:GLU:OE2 | 2.21 | 0.58 |
| 2:1Z:113:GLU:OE1 | 2:1Z:113:GLU:N | 2.37 | 0.58 |
| 2:2D:264:ARG:NH2 | 2:2D:431:ASP:OD2 | 2.37 | 0.58 |
| 2:2D:284:GLU:HA | 2:2D:284:GLU:OE1 | 2.04 | 0.58 |
| 2:2L:66:ILE:HD11 | 2:2L:93:ILE:HD12 | 1.86 | 0.58 |
| 1:2U:334:GLN:HE22 | 1:2U:348:ASN:H | 1.49 | 0.58 |
| 1:3M:139:LEU:HD12 | 1:3M:170:VAL:HG12 | 1.84 | 0.58 |
| 1:3O:183:TYR:HE2 | 1:3O:394:PHE:HB2 | 1.67 | 0.58 |
| 1:3Q:138:SER:OG | 1:3Q:139:LEU:N | 2.37 | 0.58 |
| 9:4Z:251:ALA:HA | 9:4Z:254:LYS:HD2 | 1.86 | 0.58 |
| 10:5D:172:GLN:O | 10:5D:176:GLU:HG2 | 2.03 | 0.58 |
| 11:5E:46:VAL:HG23 | 11:5E:88:PHE:HD2 | 1.67 | 0.58 |
| 17:5V:177:ASP:N | 17:5V:177:ASP:OD2 | 2.36 | 0.58 |
| 20:6F:238:LEU:HD23 | 20:6F:240:ALA:H | 1.67 | 0.58 |
| 21:6H:88:ALA:O | 21:6H:92:HIS:HB2 | 2.03 | 0.58 |
| 24:6U:277:CYS:HA | 24:6U:368:LEU:HA | 1.84 | 0.58 |
| 24:6U:469:PHE:HA | 24:6U:485:PRO:CD | 2.32 | 0.58 |
| 24:6X:152:ARG:HD3 | 24:6X:160:PHE:CG | 2.39 | 0.58 |
| 2:4:280:LYS:HG2 | 2:S7:89:PRO:CG | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A3:340:TYR:HD1 | 3:4H:104:PRO:HD3 | 1.67 | 0.58 |
| 1:G8:31:ASP:OD2 | 1:G8:33:THR:OG1 | 2.20 | 0.58 |
| 1:G8:140:GLY:O | 1:G8:184:ASN:ND2 | 2.35 | 0.58 |
| 2:G9:219:ILE:HG23 | 22:6P:175:ALA:HB1 | 1.84 | 0.58 |
| 2:H7:72:PRO:HD2 | 1:H8:2:ARG:HH12 | 1.68 | 0.58 |
| 2:I5:195:LEU:HD11 | 2:I5:264:ARG:HH11 | 1.68 | 0.58 |
| 2:I9:22:GLU:O | 2:I9:26:LEU:HG | 2.03 | 0.58 |
| 2:J1:90:GLU:O | 2:J1:121:ARG:NH1 | 2.32 | 0.58 |
| 2:J5:305:CYS:HB3 | 2:J5:387:ILE:HD11 | 1.86 | 0.58 |
| 1:L2:113:ILE:HA | 1:L2:116:VAL:HG22 | 1.85 | 0.58 |
| 2:M7:89:PRO:HG2 | 19:6E:25:VAL:HG12 | 1.84 | 0.58 |
| 2:M7:109:THR:OG1 | 2:M7:411:GLU:OE2 | 2.18 | 0.58 |
| 2:N3:288:VAL:O | 2:N3:292:THR:HG23 | 2.04 | 0.58 |
| 2:P7:286:LEU:O | 2:P7:373:ARG:NH1 | 2.36 | 0.58 |
| 1:R0:52:ASN:OD1 | 1:R0:62:ARG:NH2 | 2.36 | 0.58 |
| 1:R4:3:GLU:HG3 | 1:R4:127:CYS:HB2 | 1.85 | 0.58 |
| 1:R4:335:ASN:O | 1:R4:338:SER:OG | 2.21 | 0.58 |
| 1:R8:391:ARG:HD3 | 2:R9:346:TRP:CE2 | 2.39 | 0.58 |
| 1:S4:5:VAL:HG12 | 1:S4:133:PHE:HD1 | 1.68 | 0.58 |
| 2:S7:414:GLU:CD | 2:S7:414:GLU:H | 2.06 | 0.58 |
| 2:T1:293:ASN:OD1 | 2:T1:338:LYS:NZ | 2.35 | 0.58 |
| 2:T5:311:LYS:HE3 | 2:T5:344:VAL:HA | 1.85 | 0.58 |
| 1:T8:190:HIS:HE2 | 1:T8:410:GLU:HG3 | 1.68 | 0.58 |
| 2:V9:286:LEU:O | 2:V9:373:ARG:NH1 | 2.37 | 0.58 |
| 2:W1:189:LEU:HD11 | 2:W1:418:PHE:HE1 | 1.67 | 0.58 |
| 2:Y1:133:GLN:HB3 | 2:Y1:252:ILE:HG21 | 1.86 | 0.58 |
| 2:Y9:178:SER:HB3 | 1:Z0:347:ASN:HD22 | 1.69 | 0.58 |
| 1:Z4:210:ILE:O | 1:Z4:214:THR:OG1 | 2.16 | 0.58 |
| 1:Z6:83:GLN:O | 1:0M:281:TYR:OH | 2.11 | 0.58 |
| 1:0C:342:VAL:HG12 | 1:0C:348:ASN:HD21 | 1.69 | 0.58 |
| 2:0F:244:PHE:HB2 | 2:0F:356:ASN:HD21 | 1.69 | 0.58 |
| 2:0N:83:TYR:HB3 | 2:0N:86:LEU:HB3 | 1.85 | 0.58 |
| 2:0N:191:THR:HA | 2:0N:194:LEU:HB3 | 1.84 | 0.58 |
| 1:0U:392:LYS:HG3 | 1:0U:395:LEU:CD2 | 2.34 | 0.58 |
| 2:1L:213:CYS:HA | 2:1L:217:LEU:HB2 | 1.86 | 0.58 |
| 2:1N:183:GLU:HG3 | 2:1N:184:PRO:HD3 | 1.84 | 0.58 |
| 1:1U:20:PHE:HB2 | 1:1U:233:MET:HE3 | 1.84 | 0.58 |
| 1:1U:248:ALA:CA | 1:1U:252:LYS:HD3 | 2.27 | 0.58 |
| 2:1V:209:ILE:HA | 2:1V:212:ILE:HD12 | 1.83 | 0.58 |
| 2:2B:72:PRO:HG3 | 1:2C:1:MET:HE2 | 1.85 | 0.58 |
| 2:2B:276:ILE:HG22 | 2:2B:281:ALA:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:406:HIS:HA | 2:2N:409:VAL:HG22 | 1.85 | 0.58 |
| 2:2P:336:LYS:O | 2:2P:339:ARG:NH2 | 2.35 | 0.58 |
| 2:2Z:56:THR:HG23 | 2:2Z:60:LYS:HB3 | 1.85 | 0.58 |
| 2:2Z:236:SER:O | 2:2Z:243:ARG:NH2 | 2.37 | 0.58 |
| 2:3B:265:ILE:HD13 | 2:3B:435:VAL:HG21 | 1.84 | 0.58 |
| 2:3D:90:GLU:O | 2:3D:121:ARG:NH1 | 2.34 | 0.58 |
| 2:3D:384:ILE:HA | 2:3D:387:ILE:HD12 | 1.84 | 0.58 |
| 1:3Q:272:PRO:HB2 | 1:3Q:282:ARG:HH12 | 1.68 | 0.58 |
| 2:3R:290:GLU:HA | 2:3R:293:ASN:HD22 | 1.69 | 0.58 |
| 5:4L:290:GLN:O | 28:7H:306:LEU:HD21 | 2.04 | 0.58 |
| 10:5C:336:ALA:O | 10:5C:339:GLN:HG3 | 2.03 | 0.58 |
| 14:5L:507:LEU:HD11 | 14:5L:525:LEU:HD12 | 1.83 | 0.58 |
| 22:6M:204:PHE:HB2 | 22:6M:223:LEU:HD21 | 1.86 | 0.58 |
| 24:6X:354:ARG:HB2 | 24:6X:357:LEU:CD1 | 2.33 | 0.58 |
| 24:6X:460:HIS:HB2 | 24:6X:465:LEU:CD2 | 2.34 | 0.58 |
| 36:7W:32:LYS:CD | 36:7W:72:LEU:H | 2.07 | 0.58 |
| 1:1:306:ARG:CZ | 3:3V:60:PRO:O | 2.51 | 0.58 |
| 2:E1:206:ASN:OD1 | 41:E1:501:GTP:N2 | 2.31 | 0.58 |
| 2:G1:195:LEU:CD1 | 2:G1:428:LEU:HD21 | 2.34 | 0.58 |
| 2:G7:115:VAL:HG23 | 2:G7:153:LEU:HD23 | 1.86 | 0.58 |
| 1:I2:166:THR:OG1 | 1:I2:199:CYS:SG | 2.58 | 0.58 |
| 2:I3:88:HIS:ND1 | 2:J9:283:HIS:O | 2.36 | 0.58 |
| 1:I8:309:ARG:H | 1:I8:372:THR:HG22 | 1.69 | 0.58 |
| 1:J2:71:GLY:HA2 | 16:5Q:175:LEU:HD11 | 1.85 | 0.58 |
| 1:J6:99:ASN:ND2 | 2:J7:254:GLU:OE1 | 2.36 | 0.58 |
| 1:K4:39:ASP:OD1 | 1:K4:40:SER:N | 2.33 | 0.58 |
| 2:K5:88:HIS:ND1 | 2:M1:283:HIS:HA | 2.18 | 0.58 |
| 2:M1:222:PRO:HD2 | 1:M2:324:LYS:HE3 | 1.86 | 0.58 |
| 2:M5:88:HIS:CD2 | 2:M5:89:PRO:CD | 2.86 | 0.58 |
| 1:M6:248:ALA:HA | 1:M6:252:LYS:HD2 | 1.86 | 0.58 |
| 1:N0:272:PRO:HB2 | 1:N0:282:ARG:HH22 | 1.69 | 0.58 |
| 1:N2:88:ASP:H | 2:O9:283:HIS:CE1 | 2.21 | 0.58 |
| 2:N3:209:ILE:HG23 | 2:N3:230:LEU:HD21 | 1.85 | 0.58 |
| 2:N9:33:ASP:OD1 | 2:N9:35:GLN:NE2 | 2.37 | 0.58 |
| 1:P8:3:GLU:HB2 | 1:P8:130:LEU:HD23 | 1.86 | 0.58 |
| 2:Q5:278:ALA:HA | 2:Q5:369:ALA:HB2 | 1.86 | 0.58 |
| 1:Q8:358:PRO:HG2 | 1:Q8:361:LEU:HB2 | 1.84 | 0.58 |
| 1:R0:274:THR:HG21 | 1:R0:282:ARG:HD2 | 1.85 | 0.58 |
| 2:R5:37:PRO:HA | 11:5E:8:ARG:HH11 | 1.69 | 0.58 |
| 2:S1:88:HIS:CD2 | 2:S1:89:PRO:HD3 | 2.36 | 0.58 |
| 2:T1:386:GLU:OE2 | 2:T1:390:ARG:NH1 | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T3:217:LEU:HD21 | 2:T3:368:LEU:HD23 | 1.86 | 0.58 |
| 1:T4:7:ILE:HB | 1:T4:135:VAL:HG12 | 1.85 | 0.58 |
| 1:T6:222:PHE:HD2 | 2:T7:247:ALA:HB1 | 1.69 | 0.58 |
| 1:V8:137:HIS:ND1 | 1:V8:138:SER:O | 2.35 | 0.58 |
| 1:Y0:123:GLU:O | 1:Y0:126:SER:OG | 2.18 | 0.58 |
| 1:Y2:309:ARG:NH1 | 1:Y2:341:PHE:O | 2.35 | 0.58 |
| 1:0K:309:ARG:NH1 | 1:0K:339:SER:O | 2.35 | 0.58 |
| 2:0L:5:ILE:HG22 | 2:0L:64:ARG:HB3 | 1.85 | 0.58 |
| 1:1C:77:ARG:HE | 1:1C:90:PHE:HE2 | 1.50 | 0.58 |
| 2:1F:50:ASN:O | 2:1F:64:ARG:NH2 | 2.36 | 0.58 |
| 2:1P:176:GLN:HE22 | 2:1P:304:LYS:HE2 | 1.69 | 0.58 |
| 1:1Q:404:ASP:HB3 | 1:1Q:406:MET:SD | 2.44 | 0.58 |
| 2:1V:5:ILE:HD11 | 2:1V:135:PHE:HE1 | 1.69 | 0.58 |
| 2:1V:338:LYS:HG3 | 2:1V:340:THR:HG22 | 1.85 | 0.58 |
| 2:1X:289:ALA:O | 2:1X:293:ASN:ND2 | 2.36 | 0.58 |
| 1:2A:67:ASP:OD2 | 1:2A:72:THR:OG1 | 2.09 | 0.58 |
| 2:2F:53:PHE:HB3 | 2:2F:61:HIS:HB3 | 1.86 | 0.58 |
| 2:2R:109:THR:OG1 | 2:2R:411:GLU:OE2 | 2.20 | 0.58 |
| 1:3A:77:ARG:NH1 | 38:8D:220:VAL:HA | 2.19 | 0.58 |
| 1:3O:256:ASN:O | 1:3O:312:THR:HG21 | 2.03 | 0.58 |
| 1:3O:285:THR:OG1 | 1:3O:287:PRO:HD2 | 2.04 | 0.58 |
| 6:4N:461:LYS:HD2 | 6:4N:465:GLU:OE2 | 2.03 | 0.58 |
| 8:4X:114:ARG:HA | 8:4X:117:VAL:HG12 | 1.85 | 0.58 |
| 10:5C:283:GLU:HA | 10:5C:286:LYS:HD2 | 1.85 | 0.58 |
| 13:5H:82:PHE:CD1 | 13:5H:83:MET:HG2 | 2.38 | 0.58 |
| 13:5I:82:PHE:CD1 | 13:5I:83:MET:HG2 | 2.38 | 0.58 |
| 13:5J:82:PHE:CD1 | 13:5J:83:MET:HG2 | 2.38 | 0.58 |
| 14:5N:385:CYS:HB2 | 14:5N:401:TRP:CZ3 | 2.39 | 0.58 |
| 15:5O:56:LYS:HE2 | 15:5O:56:LYS:N | 2.10 | 0.58 |
| 15:5P:101:ASP:O | 15:5P:104:LYS:NZ | 2.35 | 0.58 |
| 15:5P:123:LEU:HD13 | 15:5P:161:MET:HB3 | 1.85 | 0.58 |
| 21:6G:37:ILE:CG2 | 21:6G:40:PHE:HB3 | 2.34 | 0.58 |
| 1:9:41:ASP:OD2 | 26:7E:23:THR:HG21 | 2.02 | 0.58 |
| 1:A3:276:ARG:HH21 | 26:7F:138:THR:HG23 | 1.69 | 0.58 |
| 2:G7:278:ALA:HB3 | 22:6O:215:GLY:HA2 | 1.86 | 0.58 |
| 2:I5:9:ILE:HG13 | 2:I5:139:ASN:HB3 | 1.84 | 0.58 |
| 2:J7:88:HIS:CD2 | 2:L3:283:HIS:HB3 | 2.38 | 0.58 |
| 1:K0:309:ARG:H | 1:K0:372:THR:HG22 | 1.69 | 0.58 |
| 2:K5:27:GLU:OE1 | 2:K5:243:ARG:NH1 | 2.37 | 0.58 |
| 1:K8:379:LYS:HG3 | 1:K8:419:VAL:HG21 | 1.86 | 0.58 |
| 2:L7:340:THR:HG23 | 2:L7:341:ILE:HG12 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L9:417:GLU:HA | 2:L9:420:GLU:HG2 | 1.86 | 0.58 |
| 1:M2:77:ARG:NH1 | 15:5O:44:ARG:HD3 | 2.19 | 0.58 |
| 2:M7:90:GLU:HG3 | 2:M7:121:ARG:HH12 | 1.68 | 0.58 |
| 1:N0:128:ASP:OD1 | 1:N0:129:CYS:N | 2.37 | 0.58 |
| 2:N1:305:CYS:HB3 | 2:N1:387:ILE:HD11 | 1.84 | 0.58 |
| 2:N5:357:TYR:HB2 | 32:7O:87:ASP:OD2 | 2.04 | 0.58 |
| 1:O4:132:GLY:HA2 | 1:O4:162:ARG:HB3 | 1.85 | 0.58 |
| 2:O5:285:GLN:HG3 | 19:6E:13:LYS:HE3 | 1.86 | 0.58 |
| 1:P4:287:PRO:HA | 1:P4:290:THR:HG22 | 1.85 | 0.58 |
| 2:P9:413:MET:HB3 | 2:P9:417:GLU:OE2 | 2.04 | 0.58 |
| 2:Q3:88:HIS:NE2 | 2:R9:284:GLU:HG3 | 2.19 | 0.58 |
| 2:R1:3:GLU:HB2 | 2:R1:129:CYS:SG | 2.43 | 0.58 |
| 2:R3:369:ALA:HB1 | 7:4R:88:ARG:HD3 | 1.85 | 0.58 |
| 2:S7:137:VAL:HG22 | 2:S7:168:GLY:HA2 | 1.86 | 0.58 |
| 2:U5:98:ASP:OD1 | 2:U5:99:ALA:N | 2.36 | 0.58 |
| 1:V4:331:LEU:O | 1:V4:335:ASN:ND2 | 2.37 | 0.58 |
| 2:V9:132:LEU:HD22 | 2:V9:164:LYS:HD3 | 1.84 | 0.58 |
| 1:W0:11:GLN:N | 39:W0:502:GDP:O1B | 2.31 | 0.58 |
| 1:W4:140:GLY:O | 1:W4:184:ASN:ND2 | 2.36 | 0.58 |
| 2:X3:305:CYS:SG | 2:X3:383:ALA:HB1 | 2.44 | 0.58 |
| 1:Z2:68:LEU:HB3 | 1:Z2:96:GLY:HA2 | 1.85 | 0.58 |
| 1:Z4:49:VAL:HG21 | 1:Z4:241:ARG:HG2 | 1.86 | 0.58 |
| 1:Z8:207:LEU:HD23 | 1:Z8:225:LEU:HB3 | 1.86 | 0.58 |
| 1:0M:393:ALA:HB2 | 2:0N:346:TRP:CD1 | 2.37 | 0.58 |
| 2:0V:266:HIS:O | 2:0V:266:HIS:ND1 | 2.37 | 0.58 |
| 1:0W:309:ARG:H | 1:0W:372:THR:HG22 | 1.69 | 0.58 |
| 1:1A:72:THR:O | 1:1A:76:VAL:HG23 | 2.04 | 0.58 |
| 1:1C:7:ILE:HD13 | 1:1C:151:LEU:HD21 | 1.85 | 0.58 |
| 2:1D:69:ASP:OD1 | 2:1D:70:LEU:N | 2.36 | 0.58 |
| 1:1K:309:ARG:NH1 | 1:1K:339:SER:O | 2.37 | 0.58 |
| 1:1O:163:MET:HB3 | 1:1O:250:LEU:HD22 | 1.86 | 0.58 |
| 1:1O:177:ASP:O | 2:1P:352:LYS:HA | 2.04 | 0.58 |
| 2:1P:276:ILE:HG12 | 2:1P:281:ALA:HB2 | 1.86 | 0.58 |
| 1:1Q:96:GLY:O | 1:1Q:103:LYS:NZ | 2.27 | 0.58 |
| 2:1Z:70:LEU:HB2 | 2:1Z:98:ASP:HA | 1.86 | 0.58 |
| 1:2I:186:THR:HG22 | 1:2I:411:ALA:HB1 | 1.86 | 0.58 |
| 2:2T:336:LYS:O | 2:2T:339:ARG:NH2 | 2.36 | 0.58 |
| 2:3B:407:TRP:CD2 | 1:3C:255:VAL:HG12 | 2.39 | 0.58 |
| 2:3L:305:CYS:SG | 2:3L:383:ALA:HB1 | 2.44 | 0.58 |
| 2:3L:399:TYR:O | 2:3L:402:ARG:NH1 | 2.37 | 0.58 |
| 2:3N:130:THR:HB | 3:4D:170:GLU:OE2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3T:111:GLY:O | 2:3T:115:VAL:HG22 | 2.02 | 0.58 |
| 6:4P:78:ALA:HB2 | 20:6F:41:LEU:HD11 | 1.85 | 0.58 |
| 8:4W:443:ILE:HD11 | 8:4X:113:ARG:HE | 1.69 | 0.58 |
| 13:5K:70:LYS:HZ1 | 13:5K:75:PHE:HZ | 1.50 | 0.58 |
| 17:5S:188:LYS:O | 17:5S:192:VAL:HG23 | 2.04 | 0.58 |
| 18:6C:18:VAL:HG23 | 18:6C:23:VAL:HG13 | 1.84 | 0.58 |
| 21:6H:16:GLU:OE1 | 21:6H:20:ARG:NE | 2.35 | 0.58 |
| 22:6K:188:ARG:NH2 | 22:6K:256:TYR:O | 2.37 | 0.58 |
| 24:6W:123:TYR:CE2 | 24:6W:163:PRO:HG3 | 2.39 | 0.58 |
| 24:6X:212:VAL:O | 24:6X:216:THR:HG23 | 2.04 | 0.58 |
| 27:7G:23:VAL:HG23 | 27:7G:24:LYS:H | 1.68 | 0.58 |
| 31:7M:78:HIS:N | 31:7M:79:PRO:CD | 2.67 | 0.58 |
| 31:7N:80:PRO:HD2 | 31:7N:83:THR:HG22 | 1.85 | 0.58 |
| 34:7R:227:LYS:HA | 35:7T:181:LEU:HD21 | 1.85 | 0.58 |
| 36:7W:18:GLU:C | 36:7W:102:MET:HE2 | 2.24 | 0.58 |
| 2:B2:278:ALA:HB3 | 18:5Z:43:ASN:HD22 | 1.67 | 0.58 |
| 1:G4:78:SER:HB2 | 24:6X:499:GLU:N | 2.19 | 0.58 |
| 2:G9:99:ALA:HA | 2:G9:105:ARG:HD2 | 1.86 | 0.58 |
| 1:H4:277:GLY:CA | 24:6U:492:ILE:HG22 | 2.34 | 0.58 |
| 2:H7:301:MET:HE1 | 2:H7:307:PRO:HD3 | 1.85 | 0.58 |
| 2:I3:236:SER:O | 2:I3:243:ARG:NH2 | 2.37 | 0.58 |
| 2:I5:119:LEU:HD21 | 2:I5:156:ARG:HB3 | 1.84 | 0.58 |
| 2:I5:129:CYS:SG | 2:I5:130:THR:N | 2.77 | 0.58 |
| 2:I5:340:THR:HG23 | 2:I5:341:ILE:HG12 | 1.84 | 0.58 |
| 1:J2:88:ASP:O | 16:5Q:186:HIS:CD2 | 2.57 | 0.58 |
| 1:L4:37:HIS:HA | 29:7J:335:GLU:CD | 2.23 | 0.58 |
| 1:L6:173:PRO:HD2 | 1:L6:380:ARG:HE | 1.69 | 0.58 |
| 1:N0:113:ILE:HA | 1:N0:116:VAL:HG22 | 1.85 | 0.58 |
| 2:O3:176:GLN:NE2 | 2:O3:207:GLU:OE2 | 2.37 | 0.58 |
| 1:O6:277:GLY:HA2 | 20:6F:21:GLU:HG2 | 1.83 | 0.58 |
| 1:O8:27:GLU:OE2 | 1:O8:318:ARG:NH2 | 2.37 | 0.58 |
| 2:O9:129:CYS:SG | 2:O9:130:THR:N | 2.76 | 0.58 |
| 2:P7:278:ALA:HA | 2:P7:369:ALA:HB2 | 1.86 | 0.58 |
| 2:Q3:278:ALA:HA | 2:Q3:369:ALA:HB2 | 1.86 | 0.58 |
| 1:R0:117:LEU:HA | 1:R0:120:VAL:HG12 | 1.85 | 0.58 |
| 1:R2:4:ILE:HD11 | 1:R2:240:LEU:HD22 | 1.85 | 0.58 |
| 1:R8:128:ASP:OD1 | 1:R8:129:CYS:N | 2.35 | 0.58 |
| 2:R9:384:ILE:HD12 | 2:R9:384:ILE:H | 1.69 | 0.58 |
| 1:S0:2:ARG:HB3 | 1:S0:131:GLN:HB2 | 1.86 | 0.58 |
| 2:S1:166:LYS:N | 2:S1:199:ASP:OD2 | 2.36 | 0.58 |
| 1:S8:11:GLN:HA | 1:S8:72:THR:HG21 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T1:66:ILE:HD12 | 2:T1:68:LEU:HD23 | 1.86 | 0.58 |
| 1:T2:145:SER:HG | 1:T2:188:SER:HG | 1.43 | 0.58 |
| 1:U2:392:LYS:HD2 | 1:U2:395:LEU:HD22 | 1.86 | 0.58 |
| 2:U3:109:THR:OG1 | 2:U3:411:GLU:OE2 | 2.18 | 0.58 |
| 2:U7:405:VAL:HG13 | 2:U7:418:PHE:HE2 | 1.69 | 0.58 |
| 2:V3:218:ASP:OD2 | 2:V3:280:LYS:NZ | 2.37 | 0.58 |
| 1:V6:11:GLN:N | 39:V6:501:GDP:O2B | 2.34 | 0.58 |
| 1:W4:263:LEU:HD13 | 1:W4:422:TYR:CE1 | 2.39 | 0.58 |
| 1:X0:43:GLN:HE21 | 8:4X:97:PHE:CB | 2.17 | 0.58 |
| 1:X2:207:LEU:HD13 | 1:X2:225:LEU:HB3 | 1.85 | 0.58 |
| 2:Z3:276:ILE:HG23 | 2:Z3:280:LYS:HB2 | 1.86 | 0.58 |
| 1:0A:337:ASN:HB3 | 1:0A:340:TYR:HD2 | 1.68 | 0.58 |
| 1:0C:178:THR:HG22 | 1:0C:179:VAL:H | 1.68 | 0.58 |
| 1:0G:172:SER:HB3 | 1:0G:175:VAL:HG22 | 1.86 | 0.58 |
| 2:0J:313:MET:HB2 | 2:0J:380:ASN:HB3 | 1.85 | 0.58 |
| 1:0O:101:TRP:HB2 | 1:0O:184:ASN:OD1 | 2.02 | 0.58 |
| 1:0O:237:THR:HG23 | 1:0O:240:LEU:HD13 | 1.84 | 0.58 |
| 1:0Y:49:VAL:HG21 | 1:0Y:240:LEU:HD13 | 1.85 | 0.58 |
| 2:1B:387:ILE:HG12 | 2:1B:390:ARG:HH22 | 1.69 | 0.58 |
| 2:1F:119:LEU:HA | 2:1F:122:ILE:HG12 | 1.85 | 0.58 |
| 2:1F:288:VAL:O | 2:1F:292:THR:HG23 | 2.03 | 0.58 |
| 2:1R:119:LEU:HA | 2:1R:122:ILE:HG12 | 1.86 | 0.58 |
| 1:1U:67:ASP:OD1 | 1:1U:67:ASP:N | 2.37 | 0.58 |
| 2:2D:381:SER:OG | 2:2D:382:THR:N | 2.37 | 0.58 |
| 1:2I:273:LEU:O | 1:2I:292:GLN:NE2 | 2.37 | 0.58 |
| 2:2P:388:PHE:HB3 | 2:2P:425:LEU:HD11 | 1.86 | 0.58 |
| 1:3S:414:ASN:HA | 1:3S:417:ASP:OD2 | 2.04 | 0.58 |
| 4:3W:180:GLU:OE1 | 4:3W:180:GLU:N | 2.34 | 0.58 |
| 4:4I:180:GLU:OE1 | 4:4I:180:GLU:N | 2.34 | 0.58 |
| 7:4U:232:GLU:O | 7:4U:236:THR:HG22 | 2.04 | 0.58 |
| 8:4W:229:GLU:HG3 | 8:4W:233:LYS:HE2 | 1.86 | 0.58 |
| 8:4X:113:ARG:HA | 8:4X:116:ASN:HD21 | 1.68 | 0.58 |
| 10:5B:226:ARG:O | 10:5B:230:ARG:HG2 | 2.03 | 0.58 |
| 13:5K:57:ASP:OD1 | 13:5K:58:ASN:N | 2.36 | 0.58 |
| 14:5L:506:SER:HB2 | 14:5L:508:PHE:CZ | 2.39 | 0.58 |
| 18:6A:18:VAL:HG23 | 18:6A:23:VAL:HG13 | 1.84 | 0.58 |
| 18:6B:18:VAL:HG23 | 18:6B:23:VAL:HG13 | 1.84 | 0.58 |
| 18:6C:131:GLU:H | 18:6C:131:GLU:CD | 2.06 | 0.58 |
| 18:6D:18:VAL:HG23 | 18:6D:23:VAL:HG13 | 1.84 | 0.58 |
| 18:6D:131:GLU:H | 18:6D:131:GLU:CD | 2.06 | 0.58 |
| 38:8C:122:LYS:O | 38:8C:126:THR:HG23 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8D:201:LEU:HD23 | 38:8D:201:LEU:C | 2.24 | 0.58 |
| 2:8:29:GLY:CA | 26:7E:45:MET:CE | 2.82 | 0.58 |
| 1:9:44:LEU:HG | 18:6A:84:ARG:HH22 | 1.69 | 0.58 |
| 1:D6:56:GLY:H | 22:6O:54:ARG:HD2 | 1.68 | 0.58 |
| 2:G3:279:GLU:HG2 | 2:G3:280:LYS:H | 1.69 | 0.58 |
| 1:G4:135:VAL:HG21 | 1:G4:152:ILE:HD11 | 1.85 | 0.58 |
| 1:G6:80:PRO:O | 1:G6:81:TYR:HB2 | 2.04 | 0.58 |
| 2:H1:213:CYS:HA | 2:H1:217:LEU:HB2 | 1.85 | 0.58 |
| 2:I3:72:PRO:HG3 | 1:I4:1:MET:HG2 | 1.86 | 0.58 |
| 1:I4:334:GLN:HE22 | 1:I4:348:ASN:H | 1.52 | 0.58 |
| 1:J0:219:THR:HG21 | 5:4L:361:ARG:HH22 | 1.69 | 0.58 |
| 2:K3:264:ARG:NH2 | 2:K3:431:ASP:OD2 | 2.35 | 0.58 |
| 2:K5:80:THR:HG22 | 29:7I:48:ARG:HD2 | 1.86 | 0.58 |
| 2:K7:264:ARG:NH2 | 2:K7:431:ASP:OD2 | 2.37 | 0.58 |
| 1:K8:5:VAL:HG23 | 1:K8:62:ARG:HG2 | 1.85 | 0.58 |
| 1:L4:336:LYS:HG2 | 35:7U:148:GLN:OE1 | 2.04 | 0.58 |
| 2:L7:195:LEU:O | 2:L7:266:HIS:NE2 | 2.33 | 0.58 |
| 2:M5:220:GLU:HB3 | 30:7K:124:GLU:OE1 | 2.04 | 0.58 |
| 2:N5:4:VAL:HG12 | 2:N5:133:GLN:HB2 | 1.85 | 0.58 |
| 2:N5:246:GLY:HA3 | 2:N5:356:ASN:HA | 1.86 | 0.58 |
| 1:O0:309:ARG:H | 1:O0:372:THR:HG22 | 1.68 | 0.58 |
| 1:O2:181:GLU:HG2 | 1:O2:182:PRO:HD3 | 1.85 | 0.58 |
| 2:O5:98:ASP:OD1 | 2:O5:99:ALA:N | 2.36 | 0.58 |
| 2:P9:217:LEU:HD21 | 2:P9:368:LEU:HD23 | 1.86 | 0.58 |
| 1:Q8:122:LYS:NZ | 1:S4:291:GLN:OE1 | 2.28 | 0.58 |
| 2:Q9:113:GLU:HB3 | 13:5H:93:ASN:OD1 | 2.04 | 0.58 |
| 2:R1:222:PRO:HD2 | 1:R2:324:LYS:HE3 | 1.85 | 0.58 |
| 1:R6:113:ILE:HD11 | 1:R6:151:LEU:HD13 | 1.86 | 0.58 |
| 1:R8:273:LEU:H | 1:R8:292:GLN:HE22 | 1.51 | 0.58 |
| 1:S6:309:ARG:H | 1:S6:372:THR:HG22 | 1.69 | 0.58 |
| 2:S7:170:THR:HG21 | 2:S7:194:LEU:HD11 | 1.86 | 0.58 |
| 2:S7:305:CYS:HB3 | 2:S7:387:ILE:HD11 | 1.85 | 0.58 |
| 2:T3:266:HIS:ND1 | 2:T3:266:HIS:O | 2.37 | 0.58 |
| 2:U3:183:GLU:HG3 | 2:U3:184:PRO:HD3 | 1.86 | 0.58 |
| 2:V1:76:ASP:OD1 | 1:V2:46:ARG:NH2 | 2.36 | 0.58 |
| 2:V1:147:SER:OG | 2:V1:190:SER:OG | 2.15 | 0.58 |
| 2:V3:267:PHE:HB2 | 2:V3:384:ILE:HD12 | 1.85 | 0.58 |
| 1:W0:272:PRO:HB2 | 1:W0:282:ARG:HH12 | 1.68 | 0.58 |
| 2:W1:34:GLY:HA3 | 2:W1:60:LYS:NZ | 2.19 | 0.58 |
| 1:W2:190:HIS:HD2 | 1:W2:411:ALA:HA | 1.66 | 0.58 |
| 1:W8:113:ILE:HA | 1:W8:116:VAL:HG12 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X3:9:ILE:HG22 | 2:X3:146:GLY:HA2 | 1.86 | 0.58 |
| 2:X7:5:ILE:HG22 | 2:X7:64:ARG:HB3 | 1.86 | 0.58 |
| 2:Y3:223:THR:OG1 | 1:Y4:245:GLN:NE2 | 2.37 | 0.58 |
| 1:0G:116:VAL:HA | 1:0G:119:VAL:HG12 | 1.86 | 0.58 |
| 1:0K:113:ILE:HA | 1:0K:116:VAL:HG22 | 1.85 | 0.58 |
| 1:0K:248:ALA:HA | 1:0K:252:LYS:HD2 | 1.86 | 0.58 |
| 2:0Z:58:ALA:O | 9:4Z:165:ARG:NH2 | 2.36 | 0.58 |
| 2:1H:198:THR:HG21 | 2:1H:201:ALA:HB2 | 1.86 | 0.58 |
| 1:1S:23:VAL:HG11 | 1:1S:230:SER:HB2 | 1.86 | 0.58 |
| 1:2A:77:ARG:HE | 1:2A:90:PHE:HE2 | 1.52 | 0.58 |
| 2:2D:90:GLU:N | 2:2D:90:GLU:OE2 | 2.37 | 0.58 |
| 2:2D:398:MET:HG3 | 1:2E:346:PRO:HD2 | 1.86 | 0.58 |
| 2:2X:214:ARG:CZ | 38:8B:18:VAL:HA | 2.33 | 0.58 |
| 2:3J:51:THR:HG21 | 2:3J:243:ARG:HG2 | 1.85 | 0.58 |
| 1:3K:210:ILE:HA | 1:3K:297:LYS:NZ | 2.19 | 0.58 |
| 2:3L:223:THR:HG22 | 2:3L:224:TYR:H | 1.69 | 0.58 |
| 4:4A:180:GLU:OE1 | 4:4A:180:GLU:N | 2.34 | 0.58 |
| 4:4E:180:GLU:OE1 | 4:4E:180:GLU:N | 2.34 | 0.58 |
| 5:4L:417:LYS:NZ | 16:5Q:52:ALA:O | 2.37 | 0.58 |
| 5:4M:320:GLN:HB3 | 28:7X:428:LEU:HD11 | 1.85 | 0.58 |
| 6:4O:248:ARG:O | 6:4O:252:THR:HG23 | 2.04 | 0.58 |
| 7:4T:227:ALA:HB1 | 31:7M:20:ILE:HD12 | 1.84 | 0.58 |
| 10:5B:257:GLN:HG3 | 10:5B:261:LYS:HZ1 | 1.69 | 0.58 |
| 13:5H:57:ASP:OD1 | 13:5H:58:ASN:N | 2.36 | 0.58 |
| 13:5I:57:ASP:OD1 | 13:5I:58:ASN:N | 2.36 | 0.58 |
| 15:5O:226:ARG:HB3 | 15:5O:226:ARG:CZ | 2.34 | 0.58 |
| 16:5Q:191:TYR:OH | 35:7T:137:ASN:ND2 | 2.29 | 0.58 |
| 18:5X:131:GLU:H | 18:5X:131:GLU:CD | 2.06 | 0.58 |
| 18:5Y:18:VAL:HG23 | 18:5Y:23:VAL:HG13 | 1.84 | 0.58 |
| 18:5Z:131:GLU:H | 18:5Z:131:GLU:CD | 2.06 | 0.58 |
| 18:6B:131:GLU:H | 18:6B:131:GLU:CD | 2.06 | 0.58 |
| 24:6W:565:GLN:OE1 | 24:6W:602:LEU:HB2 | 2.04 | 0.58 |
| 30:7K:130:TYR:CE2 | 30:7K:132:ARG:HG2 | 2.38 | 0.58 |
| 35:7U:204:LYS:O | 35:7U:208:GLU:HG2 | 2.04 | 0.58 |
| 1:C4:142:GLY:N | 39:C4:501:GDP:O2B | 2.37 | 0.57 |
| 2:D1:279:GLU:OE1 | 18:6A:167:SER:HA | 2.04 | 0.57 |
| 2:G1:195:LEU:HD11 | 2:G1:428:LEU:HD21 | 1.84 | 0.57 |
| 1:G2:392:LYS:HG3 | 1:G2:395:LEU:HD22 | 1.86 | 0.57 |
| 2:I1:392:ASP:OD2 | 2:I1:422:ARG:NH1 | 2.37 | 0.57 |
| 2:J1:223:THR:HG22 | 2:J1:224:TYR:H | 1.68 | 0.57 |
| 1:J4:238:CYS:SG | 1:J4:318:ARG:NE | 2.77 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J6:175:VAL:CG2 | 1:J6:205:GLU:HG3 | 2.34 | 0.57 |
| 1:J6:177:ASP:O | 2:J7:352:LYS:HA | 2.04 | 0.57 |
| 1:J6:334:GLN:NE2 | 1:J6:348:ASN:OD1 | 2.37 | 0.57 |
| 2:L1:264:ARG:NH2 | 2:L1:431:ASP:OD2 | 2.37 | 0.57 |
| 2:M5:279:GLU:OE2 | 2:M5:279:GLU:N | 2.37 | 0.57 |
| 2:N1:248:LEU:HD22 | 2:N1:354:GLY:HA2 | 1.85 | 0.57 |
| 2:N1:267:PHE:HB2 | 2:N1:384:ILE:HD12 | 1.85 | 0.57 |
| 2:N1:417:GLU:HA | 2:N1:420:GLU:HG2 | 1.86 | 0.57 |
| 2:O1:88:HIS:CE1 | 2:O1:89:PRO:HD2 | 2.38 | 0.57 |
| 2:O5:211:ASP:OD1 | 2:O5:214:ARG:NH2 | 2.37 | 0.57 |
| 2:O7:91:GLN:HA | 2:O7:121:ARG:NH1 | 2.18 | 0.57 |
| 2:P3:75:VAL:HG12 | 2:P3:79:ARG:HE | 1.68 | 0.57 |
| 2:Q1:65:CYS:SG | 2:Q1:66:ILE:N | 2.76 | 0.57 |
| 1:Q8:198:GLU:HA | 1:Q8:264:HIS:HB2 | 1.86 | 0.57 |
| 2:Q9:9:ILE:HD11 | 2:Q9:153:LEU:HD23 | 1.85 | 0.57 |
| 2:R3:56:THR:HG23 | 2:R3:60:LYS:HB3 | 1.85 | 0.57 |
| 2:T1:9:ILE:HD13 | 2:T1:150:GLY:HA2 | 1.86 | 0.57 |
| 1:T2:164:MET:HB3 | 1:T2:197:ASP:OD2 | 2.04 | 0.57 |
| 1:T2:173:PRO:HB3 | 1:T2:384:GLN:HE22 | 1.69 | 0.57 |
| 1:T8:286:VAL:HG23 | 1:T8:287:PRO:HD3 | 1.86 | 0.57 |
| 1:T8:336:LYS:NZ | 1:T8:337:ASN:OD1 | 2.37 | 0.57 |
| 2:U1:109:THR:OG1 | 2:U1:411:GLU:OE2 | 2.18 | 0.57 |
| 2:V1:9:ILE:HG12 | 2:V1:68:LEU:HD11 | 1.85 | 0.57 |
| 1:V6:382:SER:HB3 | 1:V6:415:MET:HG2 | 1.86 | 0.57 |
| 1:W6:138:SER:OG | 1:W6:139:LEU:N | 2.37 | 0.57 |
| 1:X2:152:ILE:HD13 | 1:X2:155:ILE:HD11 | 1.86 | 0.57 |
| 1:X8:111:GLU:HG2 | 1:X8:112:LEU:HD22 | 1.84 | 0.57 |
| 1:X8:122:LYS:O | 1:X8:126:SER:OG | 2.17 | 0.57 |
| 2:Y9:102:ASN:HD21 | 2:Y9:411:GLU:HG3 | 1.68 | 0.57 |
| 1:Z0:190:HIS:NE2 | 1:Z0:414:ASN:OD1 | 2.36 | 0.57 |
| 2:Z5:53:PHE:HB3 | 2:Z5:61:HIS:HB3 | 1.86 | 0.57 |
| 1:Z8:211:CYS:SG | 1:Z8:220:PRO:HB3 | 2.43 | 0.57 |
| 1:0C:8:GLN:HE21 | 1:0C:14:ASN:HA | 1.67 | 0.57 |
| 1:0O:86:ARG:NH1 | 1:0O:89:ASN:OD1 | 2.37 | 0.57 |
| 2:0P:177:VAL:HB | 1:0Q:331:LEU:HD11 | 1.85 | 0.57 |
| 2:0V:132:LEU:HD22 | 2:0V:164:LYS:HD3 | 1.85 | 0.57 |
| 2:1B:73:THR:OG1 | 2:1B:77:GLU:OE1 | 2.19 | 0.57 |
| 2:1B:381:SER:OG | 2:1B:382:THR:N | 2.37 | 0.57 |
| 2:1H:178:SER:OG | 2:1H:183:GLU:OE2 | 2.19 | 0.57 |
| 2:1H:381:SER:OG | 2:1H:382:THR:N | 2.37 | 0.57 |
| 2:1P:175:PRO:HD2 | 2:1P:207:GLU:OE1 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1T:364:PRO:HG2 | 9:4Z:287:TYR:HE2 | 1.69 | 0.57 |
| 1:1U:252:LYS:HE2 | 1:1U:350:LYS:HE2 | 1.86 | 0.57 |
| 1:2A:3:GLU:HB2 | 1:2A:130:LEU:HD23 | 1.84 | 0.57 |
| 2:2D:183:GLU:HG3 | 2:2D:184:PRO:HD3 | 1.86 | 0.57 |
| 1:2M:139:LEU:HD12 | 1:2M:170:VAL:HG12 | 1.86 | 0.57 |
| 2:2T:399:TYR:O | 2:2T:402:ARG:NH1 | 2.34 | 0.57 |
| 1:2U:203:ASP:OD2 | 1:2U:302:ALA:N | 2.37 | 0.57 |
| 1:2W:130:LEU:HB2 | 1:2W:162:ARG:HE | 1.69 | 0.57 |
| 1:2W:272:PRO:HB2 | 1:2W:282:ARG:HH12 | 1.69 | 0.57 |
| 10:5B:264:ALA:O | 10:5B:267:LEU:HG | 2.03 | 0.57 |
| 12:5G:374:THR:HG23 | 12:5G:376:ARG:HG3 | 1.86 | 0.57 |
| 18:5X:18:VAL:HG23 | 18:5X:23:VAL:HG13 | 1.84 | 0.57 |
| 18:5Y:131:GLU:H | 18:5Y:131:GLU:CD | 2.06 | 0.57 |
| 31:7N:81:SER:HA | 31:7N:84:TYR:CD2 | 2.39 | 0.57 |
| 33:7Q:146:GLU:HB2 | 33:7Q:149:GLU:HG2 | 1.85 | 0.57 |
| 35:7T:176:ASN:OD1 | 35:7T:179:ARG:NH2 | 2.37 | 0.57 |
| 1:5:39:ASP:O | 26:7D:25:TYR:CD2 | 2.57 | 0.57 |
| 2:C1:365:GLY:HA2 | 18:6D:46:LEU:HB3 | 1.85 | 0.57 |
| 1:D6:204:ASN:HD21 | 39:D6:501:GDP:HN22 | 1.49 | 0.57 |
| 1:E2:33:THR:HG23 | 24:6U:405:ALA:HB2 | 1.87 | 0.57 |
| 1:G2:287:PRO:HA | 1:G2:290:THR:HG22 | 1.85 | 0.57 |
| 2:G3:56:THR:HA | 2:H9:285:GLN:HB2 | 1.86 | 0.57 |
| 2:G7:75:VAL:HG11 | 2:G7:94:SER:HB2 | 1.85 | 0.57 |
| 2:G9:88:HIS:CE1 | 2:I5:283:HIS:HA | 2.39 | 0.57 |
| 2:I5:90:GLU:H | 2:K1:283:HIS:CE1 | 2.22 | 0.57 |
| 2:I5:331:SER:O | 2:I5:334:THR:OG1 | 2.19 | 0.57 |
| 1:I8:273:LEU:H | 1:I8:292:GLN:HE22 | 1.52 | 0.57 |
| 2:I9:109:THR:OG1 | 2:I9:411:GLU:OE2 | 2.22 | 0.57 |
| 2:I9:213:CYS:HA | 2:I9:217:LEU:HB2 | 1.85 | 0.57 |
| 2:K3:195:LEU:HD21 | 2:K3:264:ARG:HD2 | 1.85 | 0.57 |
| 2:L1:129:CYS:SG | 2:L1:130:THR:N | 2.77 | 0.57 |
| 2:L1:392:ASP:OD2 | 2:L1:422:ARG:NH1 | 2.37 | 0.57 |
| 1:L4:121:ARG:NH2 | 1:L4:158:GLU:OE2 | 2.33 | 0.57 |
| 2:M1:109:THR:OG1 | 2:M1:411:GLU:OE2 | 2.22 | 0.57 |
| 1:M2:30:ILE:HG22 | 1:M2:36:TYR:HA | 1.87 | 0.57 |
| 1:M2:37:HIS:NE2 | 15:5O:276:ASN:OD1 | 2.35 | 0.57 |
| 2:M5:344:VAL:HG13 | 2:M5:346:TRP:H | 1.69 | 0.57 |
| 2:M7:286:LEU:O | 2:M7:373:ARG:NH1 | 2.36 | 0.57 |
| 1:N8:67:ASP:OD2 | 1:N8:68:LEU:N | 2.35 | 0.57 |
| 1:O8:276:ARG:HG2 | 1:O8:279:GLN:NE2 | 2.19 | 0.57 |
| 1:R0:223:GLY:HA3 | 7:4Q:365:SER:OG | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R1:287:SER:OG | 2:R1:288:VAL:N | 2.36 | 0.57 |
| 1:R2:177:ASP:O | 2:R3:352:LYS:HA | 2.04 | 0.57 |
| 2:R3:306:ASP:HB3 | 2:R3:309:HIS:HD2 | 1.68 | 0.57 |
| 1:R6:5:VAL:HG22 | 1:R6:133:PHE:HD1 | 1.69 | 0.57 |
| 1:S0:2:ARG:HE | 1:S0:240:LEU:HD22 | 1.68 | 0.57 |
| 1:S6:113:ILE:HD11 | 1:S6:151:LEU:HA | 1.86 | 0.57 |
| 1:S6:371:SER:OG | 1:S6:372:THR:N | 2.37 | 0.57 |
| 1:S8:22:GLU:HG2 | 1:S8:81:TYR:CD1 | 2.39 | 0.57 |
| 1:T6:207:LEU:HD13 | 1:T6:225:LEU:HB3 | 1.85 | 0.57 |
| 1:V2:257:LEU:HD21 | 1:V2:314:SER:HB3 | 1.86 | 0.57 |
| 1:V4:276:ARG:NH1 | 1:V4:279:GLN:OE1 | 2.36 | 0.57 |
| 1:V6:118:ASP:OD1 | 1:V6:121:ARG:NH1 | 2.37 | 0.57 |
| 2:V7:189:LEU:HD11 | 2:V7:418:PHE:HE1 | 1.69 | 0.57 |
| 1:V8:58:ARG:N | 8:4V:469:GLN:HE22 | 2.02 | 0.57 |
| 1:W0:418:LEU:O | 1:W0:421:GLU:HG2 | 2.05 | 0.57 |
| 2:W5:129:CYS:SG | 2:W5:130:THR:N | 2.76 | 0.57 |
| 2:W9:267:PHE:HB2 | 2:W9:384:ILE:HD12 | 1.85 | 0.57 |
| 1:X0:309:ARG:H | 1:X0:372:THR:HG22 | 1.68 | 0.57 |
| 1:Y4:135:VAL:HG11 | 1:Y4:152:ILE:HD11 | 1.86 | 0.57 |
| 1:Z2:287:PRO:HA | 1:Z2:290:THR:HG22 | 1.86 | 0.57 |
| 1:0E:397:TRP:NE1 | 2:0F:260:VAL:O | 2.33 | 0.57 |
| 2:0F:33:ASP:OD2 | 2:0F:35:GLN:NE2 | 2.37 | 0.57 |
| 2:0N:362:VAL:HG13 | 2:0N:370:LYS:HZ3 | 1.69 | 0.57 |
| 1:0S:204:ASN:OD1 | 39:0S:502:GDP:N2 | 2.35 | 0.57 |
| 2:0V:379:SER:OG | 2:0V:380:ASN:N | 2.35 | 0.57 |
| 1:1G:237:THR:HG23 | 1:1G:241:ARG:HE | 1.68 | 0.57 |
| 2:1L:287:SER:N | 2:1L:290:GLU:OE2 | 2.26 | 0.57 |
| 1:1M:248:ALA:CA | 1:1M:252:LYS:HD3 | 2.29 | 0.57 |
| 1:1U:210:ILE:O | 1:1U:214:THR:OG1 | 2.19 | 0.57 |
| 1:1W:248:ALA:HA | 1:1W:252:LYS:HD2 | 1.84 | 0.57 |
| 1:2C:2:ARG:HE | 1:2C:240:LEU:HD22 | 1.69 | 0.57 |
| 1:2I:350:LYS:NZ | 1:2I:351:SER:O | 2.35 | 0.57 |
| 2:2L:387:ILE:HG12 | 2:2L:390:ARG:HH22 | 1.70 | 0.57 |
| 1:2Y:128:ASP:OD1 | 1:2Y:129:CYS:N | 2.33 | 0.57 |
| 2:3H:116:ASP:OD1 | 2:3H:117:LEU:N | 2.37 | 0.57 |
| 1:3I:263:LEU:HD13 | 1:3I:422:TYR:CE1 | 2.39 | 0.57 |
| 4:3Y:180:GLU:OE1 | 4:3Y:180:GLU:N | 2.34 | 0.57 |
| 6:4P:115:LYS:O | 6:4P:119:GLU:HG2 | 2.04 | 0.57 |
| 8:4W:180:LEU:O | 8:4W:184:VAL:HG23 | 2.04 | 0.57 |
| 12:5G:331:ASN:HD22 | 31:7N:16:THR:HB | 1.69 | 0.57 |
| 13:5J:57:ASP:OD1 | 13:5J:58:ASN:N | 2.36 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:149:PHE:O | 14:5M:167:GLY:N | 2.36 | 0.57 |
| 18:5Z:18:VAL:HG23 | 18:5Z:23:VAL:HG13 | 1.84 | 0.57 |
| 18:6A:131:GLU:CD | 18:6A:131:GLU:H | 2.06 | 0.57 |
| 24:6T:122:TYR:HB2 | 24:6T:131:HIS:HB3 | 1.85 | 0.57 |
| 24:6U:378:TRP:O | 24:6U:382:ASN:ND2 | 2.37 | 0.57 |
| 24:6W:558:LEU:HD22 | 24:6W:608:GLN:HB3 | 1.86 | 0.57 |
| 24:6Z:212:VAL:O | 24:6Z:216:THR:HG23 | 2.04 | 0.57 |
| 2:8:29:GLY:HA2 | 26:7E:45:MET:SD | 2.43 | 0.57 |
| 2:F9:221:ARG:HG3 | 22:6K:178:GLY:HA2 | 1.85 | 0.57 |
| 2:I1:145:THR:OG1 | 41:I1:501:GTP:O1B | 2.23 | 0.57 |
| 1:I4:272:PRO:HB2 | 1:I4:282:ARG:HH12 | 1.68 | 0.57 |
| 2:I7:137:VAL:HG22 | 2:I7:168:GLY:HA2 | 1.87 | 0.57 |
| 2:I9:98:ASP:OD1 | 2:I9:99:ALA:N | 2.37 | 0.57 |
| 1:L2:5:VAL:HG23 | 1:L2:62:ARG:HG2 | 1.85 | 0.57 |
| 1:L6:382:SER:HB3 | 1:L6:415:MET:HG2 | 1.86 | 0.57 |
| 2:L7:287:SER:N | 2:L7:290:GLU:OE2 | 2.37 | 0.57 |
| 2:L7:414:GLU:HG3 | 2:L7:416:GLY:H | 1.68 | 0.57 |
| 2:M5:58:ALA:CB | 37:7Y:215:HIS:H | 2.16 | 0.57 |
| 1:M6:2:ARG:HB3 | 1:M6:131:GLN:HB2 | 1.87 | 0.57 |
| 2:M9:387:ILE:HG12 | 2:M9:390:ARG:HH22 | 1.69 | 0.57 |
| 1:N0:309:ARG:H | 1:N0:372:THR:HG22 | 1.68 | 0.57 |
| 1:N6:320:ARG:NH1 | 32:7O:62:THR:OG1 | 2.36 | 0.57 |
| 2:O9:392:ASP:OD2 | 2:O9:422:ARG:NH1 | 2.38 | 0.57 |
| 1:R0:20:PHE:HA | 1:R0:230:SER:HB2 | 1.87 | 0.57 |
| 2:R1:14:ILE:HD11 | 2:R1:74:VAL:HG13 | 1.86 | 0.57 |
| 2:R3:102:ASN:HD21 | 2:R3:411:GLU:HG3 | 1.69 | 0.57 |
| 2:R9:50:ASN:O | 2:R9:64:ARG:NH2 | 2.37 | 0.57 |
| 1:T2:2:ARG:HE | 1:T2:240:LEU:HD22 | 1.69 | 0.57 |
| 1:T2:49:VAL:HG11 | 1:T2:241:ARG:HG2 | 1.86 | 0.57 |
| 2:T7:339:ARG:HB3 | 13:5K:26:ALA:HB2 | 1.84 | 0.57 |
| 1:T8:209:ASP:OD1 | 13:5K:114:LEU:HB3 | 2.05 | 0.57 |
| 2:U1:195:LEU:HD11 | 2:U1:264:ARG:HH11 | 1.69 | 0.57 |
| 1:V0:51:PHE:O | 1:V0:62:ARG:NH2 | 2.37 | 0.57 |
| 2:W7:211:ASP:OD1 | 2:W7:214:ARG:NH2 | 2.37 | 0.57 |
| 2:X3:133:GLN:HB3 | 2:X3:252:ILE:HG21 | 1.86 | 0.57 |
| 1:X4:130:LEU:HB2 | 1:X4:162:ARG:HE | 1.69 | 0.57 |
| 2:Y3:399:TYR:O | 2:Y3:402:ARG:NH1 | 2.36 | 0.57 |
| 2:Y3:417:GLU:HA | 2:Y3:420:GLU:HG2 | 1.85 | 0.57 |
| 1:Y4:113:ILE:HA | 1:Y4:116:VAL:HG22 | 1.86 | 0.57 |
| 2:Z5:210:TYR:CE1 | 2:Z5:227:LEU:HD11 | 2.39 | 0.57 |
| 2:Z7:85:GLN:O | 2:Z7:88:HIS:NE2 | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:191:THR:HA | 2:Z7:194:LEU:HB3 | 1.84 | 0.57 |
| 1:Z8:328:GLU:O | 1:Z8:332:ASN:ND2 | 2.36 | 0.57 |
| 1:0A:122:LYS:HD2 | 1:0Q:292:GLN:HE22 | 1.69 | 0.57 |
| 1:0G:215:LEU:HD21 | 1:0G:273:LEU:HD12 | 1.85 | 0.57 |
| 2:0H:68:LEU:HD11 | 2:0H:153:LEU:HD21 | 1.86 | 0.57 |
| 1:0S:182:PRO:HG3 | 1:0S:384:GLN:HE21 | 1.68 | 0.57 |
| 1:0U:35:THR:OG1 | 1:0U:37:HIS:NE2 | 2.36 | 0.57 |
| 1:0U:309:ARG:H | 1:0U:372:THR:HG22 | 1.70 | 0.57 |
| 2:0X:278:ALA:HA | 2:0X:369:ALA:HB2 | 1.86 | 0.57 |
| 1:1E:31:ASP:OD1 | 1:1E:35:THR:N | 2.30 | 0.57 |
| 1:1G:4:ILE:HD11 | 1:1G:240:LEU:HD12 | 1.85 | 0.57 |
| 1:1M:282:ARG:NH2 | 1:1M:283:ALA:O | 2.34 | 0.57 |
| 2:1N:101:ASN:OD1 | 1:1O:252:LYS:HE3 | 2.04 | 0.57 |
| 2:1P:174:SER:HB3 | 2:1P:207:GLU:CD | 2.25 | 0.57 |
| 1:1S:107:THR:OG1 | 1:1S:401:GLU:OE2 | 2.22 | 0.57 |
| 1:2G:135:VAL:HG21 | 1:2G:152:ILE:HD11 | 1.87 | 0.57 |
| 1:2G:173:PRO:HD2 | 1:2G:380:ARG:HE | 1.69 | 0.57 |
| 2:2J:98:ASP:OD1 | 2:2J:99:ALA:N | 2.36 | 0.57 |
| 2:2R:191:THR:HA | 2:2R:194:LEU:HB2 | 1.86 | 0.57 |
| 2:2V:27:GLU:OE1 | 2:2V:243:ARG:NH1 | 2.33 | 0.57 |
| 1:2W:220:PRO:HD2 | 2:2X:326:LYS:HD3 | 1.85 | 0.57 |
| 1:3G:94:GLN:HG3 | 1:3G:95:THR:HG23 | 1.86 | 0.57 |
| 2:3J:221:ARG:NE | 38:8B:174:SER:OG | 2.38 | 0.57 |
| 1:3M:95:THR:HG21 | 3:4D:138:GLY:HA2 | 1.86 | 0.57 |
| 3:4B:38:THR:HG21 | 4:4C:3:LYS:HB2 | 1.86 | 0.57 |
| 4:4C:180:GLU:OE1 | 4:4C:180:GLU:N | 2.34 | 0.57 |
| 4:4G:180:GLU:OE1 | 4:4G:180:GLU:N | 2.34 | 0.57 |
| 6:4N:462:LEU:HA | 6:4N:465:GLU:OE2 | 2.05 | 0.57 |
| 7:4T:334:LYS:O | 7:4T:337:GLU:HG3 | 2.03 | 0.57 |
| 9:4Z:375:ILE:O | 9:4Z:379:LYS:HG2 | 2.04 | 0.57 |
| 10:5A:262:ILE:O | 10:5A:265:LYS:HG2 | 2.03 | 0.57 |
| 10:5D:199:TYR:O | 10:5D:203:GLU:HG3 | 2.03 | 0.57 |
| 14:5L:149:PHE:O | 14:5L:167:GLY:N | 2.36 | 0.57 |
| 14:5N:163:LEU:HD12 | 14:5N:171:MET:CE | 2.34 | 0.57 |
| 15:5P:366:VAL:O | 15:5P:370:ASN:ND2 | 2.37 | 0.57 |
| 22:6K:146:LEU:HA | 22:6K:149:ILE:HD12 | 1.86 | 0.57 |
| 22:6K:209:ASN:HA | 22:6K:212:GLU:OE1 | 2.04 | 0.57 |
| 22:6L:172:ARG:HH22 | 22:6L:176:LYS:CE | 2.17 | 0.57 |
| 27:7G:28:GLU:O | 27:7G:32:GLN:HG2 | 2.04 | 0.57 |
| 1:A3:83:GLN:HB2 | 24:6Z:177:ARG:HH22 | 1.68 | 0.57 |
| 2:B4:59:GLY:HA3 | 24:6W:263:ARG:HH11 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G3:70:LEU:HG | 2:G3:145:THR:HG23 | 1.86 | 0.57 |
| 2:G3:282:TYR:CE1 | 22:6M:133:PRO:CG | 2.86 | 0.57 |
| 1:I0:418:LEU:HG | 1:I0:422:TYR:HE2 | 1.69 | 0.57 |
| 2:J3:223:THR:HG23 | 2:J3:225:THR:H | 1.70 | 0.57 |
| 2:K3:222:PRO:HD2 | 1:K4:324:LYS:HE3 | 1.86 | 0.57 |
| 2:K7:88:HIS:HD1 | 2:M3:283:HIS:HB2 | 1.69 | 0.57 |
| 1:L6:334:GLN:HE22 | 1:L6:348:ASN:H | 1.52 | 0.57 |
| 1:M0:128:ASP:OD1 | 1:M0:129:CYS:N | 2.35 | 0.57 |
| 2:M5:264:ARG:NH2 | 2:M5:431:ASP:OD2 | 2.37 | 0.57 |
| 2:M7:90:GLU:O | 2:M7:121:ARG:NH1 | 2.33 | 0.57 |
| 2:N1:279:GLU:OE2 | 30:7L:319:ARG:N | 2.37 | 0.57 |
| 2:N9:125:LEU:HD23 | 2:N9:125:LEU:C | 2.24 | 0.57 |
| 2:O3:72:PRO:HD2 | 1:O4:2:ARG:HH12 | 1.68 | 0.57 |
| 2:O7:21:TRP:CZ2 | 2:O7:65:CYS:HB3 | 2.40 | 0.57 |
| 2:O7:392:ASP:OD2 | 2:O7:422:ARG:NH1 | 2.37 | 0.57 |
| 2:O7:405:VAL:HG13 | 2:O7:418:PHE:HE2 | 1.70 | 0.57 |
| 2:Q3:183:GLU:HG3 | 2:Q3:184:PRO:HD3 | 1.86 | 0.57 |
| 2:Q5:381:SER:OG | 2:Q5:382:THR:N | 2.35 | 0.57 |
| 1:R4:58:ARG:NH2 | 1:T0:280:GLN:OE1 | 2.38 | 0.57 |
| 2:S5:322:ASP:OD2 | 2:S5:373:ARG:NH2 | 2.36 | 0.57 |
| 2:S7:265:ILE:HD11 | 2:S7:435:VAL:HG21 | 1.85 | 0.57 |
| 2:T3:206:ASN:OD1 | 41:T4:501:GTP:N2 | 2.37 | 0.57 |
| 1:T4:392:LYS:HD2 | 1:T4:395:LEU:HD22 | 1.86 | 0.57 |
| 2:U9:77:GLU:OE1 | 1:V0:243:PRO:HB3 | 2.04 | 0.57 |
| 2:V3:120:ASP:OD1 | 2:V3:121:ARG:N | 2.37 | 0.57 |
| 1:V6:132:GLY:HA3 | 1:V6:163:MET:HB3 | 1.87 | 0.57 |
| 2:V9:236:SER:O | 2:V9:243:ARG:NH2 | 2.38 | 0.57 |
| 2:W7:31:GLN:HE21 | 2:W7:37:PRO:HG3 | 1.70 | 0.57 |
| 2:W9:70:LEU:HD13 | 2:W9:95:GLY:HA3 | 1.87 | 0.57 |
| 2:X3:189:LEU:HD11 | 2:X3:418:PHE:HE1 | 1.70 | 0.57 |
| 2:X5:186:ASN:OD1 | 2:X5:408:TYR:OH | 2.20 | 0.57 |
| 1:Z0:274:THR:OG1 | 1:Z0:282:ARG:NH1 | 2.37 | 0.57 |
| 2:0F:278:ALA:HA | 2:0F:369:ALA:HB2 | 1.86 | 0.57 |
| 1:0K:8:GLN:NE2 | 1:0K:13:GLY:O | 2.28 | 0.57 |
| 1:0K:15:GLN:HB3 | 1:0K:226:ASN:HD21 | 1.69 | 0.57 |
| 1:0S:334:GLN:HE22 | 1:0S:347:ASN:H | 1.51 | 0.57 |
| 2:0V:178:SER:OG | 2:0V:183:GLU:OE2 | 2.16 | 0.57 |
| 1:0W:128:ASP:OD1 | 1:0W:129:CYS:N | 2.35 | 0.57 |
| 2:1B:288:VAL:O | 2:1B:292:THR:HG23 | 2.04 | 0.57 |
| 2:1D:317:LEU:HB3 | 2:1D:319:TYR:HE1 | 1.68 | 0.57 |
| 2:1L:223:THR:HG23 | 2:1L:225:THR:H | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1M:177:ASP:N | 1:1M:181:GLU:OE2 | 2.38 | 0.57 |
| 2:1N:346:TRP:HD1 | 2:1N:346:TRP:H | 1.52 | 0.57 |
| 1:1O:252:LYS:HE2 | 1:1O:350:LYS:CE | 2.34 | 0.57 |
| 1:1Q:21:TRP:HA | 1:1Q:24:VAL:HG12 | 1.86 | 0.57 |
| 1:2C:12:CYS:SG | 1:2C:138:SER:HB2 | 2.44 | 0.57 |
| 2:2H:120:ASP:OD1 | 38:8B:24:TYR:CD2 | 2.56 | 0.57 |
| 2:2V:222:PRO:HD2 | 1:2W:324:LYS:HE3 | 1.86 | 0.57 |
| 2:2Z:384:ILE:HA | 2:2Z:387:ILE:HD12 | 1.87 | 0.57 |
| 2:3B:119:LEU:HD11 | 2:3B:156:ARG:HB3 | 1.85 | 0.57 |
| 1:3G:113:ILE:HD13 | 1:3G:150:LEU:HD22 | 1.87 | 0.57 |
| 2:3N:289:ALA:O | 2:3N:293:ASN:ND2 | 2.37 | 0.57 |
| 2:3P:392:ASP:OD2 | 2:3P:422:ARG:NH1 | 2.38 | 0.57 |
| 2:3T:248:LEU:HD22 | 2:3T:354:GLY:HA2 | 1.85 | 0.57 |
| 5:4M:252:GLU:HA | 5:4M:255:ASN:HD21 | 1.67 | 0.57 |
| 8:4W:417:ARG:O | 8:4W:421:THR:HG23 | 2.05 | 0.57 |
| 9:4Z:218:LEU:O | 9:4Z:222:THR:HG23 | 2.03 | 0.57 |
| 11:5E:14:TRP:CZ3 | 11:5E:103:VAL:CG2 | 2.87 | 0.57 |
| 14:5N:149:PHE:O | 14:5N:167:GLY:N | 2.36 | 0.57 |
| 12:7B:58:ARG:O | 12:7B:59:GLU:HG3 | 2.03 | 0.57 |
| 25:7C:110:ARG:HD2 | 25:7C:110:ARG:N | 2.20 | 0.57 |
| 30:7K:125:PRO:HB2 | 30:7K:128:ALA:HB3 | 1.85 | 0.57 |
| 38:8A:91:GLN:O | 38:8A:102:PHE:CE1 | 2.58 | 0.57 |
| 2:D5:79:ARG:NH2 | 22:6O:19:GLY:O | 2.37 | 0.57 |
| 2:E5:206:ASN:OD1 | 41:E6:501:GTP:N2 | 2.18 | 0.57 |
| 2:E9:33:ASP:HB3 | 22:6N:130:LEU:HD12 | 1.87 | 0.57 |
| 1:F8:218:THR:OG1 | 24:6U:418:ASP:OD1 | 2.21 | 0.57 |
| 2:G3:296:PHE:HE1 | 2:G3:377:MET:HG3 | 1.69 | 0.57 |
| 2:H1:116:ASP:OD1 | 2:H1:117:LEU:N | 2.36 | 0.57 |
| 2:H3:145:THR:OG1 | 41:H3:501:GTP:O1B | 2.22 | 0.57 |
| 1:I0:219:THR:HA | 2:I1:326:LYS:HZ2 | 1.68 | 0.57 |
| 2:I9:3:GLU:HB2 | 2:I9:129:CYS:SG | 2.44 | 0.57 |
| 1:J0:345:ILE:O | 1:J0:348:ASN:ND2 | 2.37 | 0.57 |
| 2:J9:98:ASP:OD1 | 2:J9:99:ALA:N | 2.38 | 0.57 |
| 2:K1:29:GLY:HA2 | 28:7X:402:ARG:NH2 | 2.19 | 0.57 |
| 1:L4:388:MET:HE2 | 2:L5:348:PRO:HD2 | 1.86 | 0.57 |
| 2:M3:313:MET:HB2 | 2:M3:380:ASN:HB3 | 1.87 | 0.57 |
| 1:M4:165:LEU:HD21 | 1:M4:250:LEU:HD21 | 1.87 | 0.57 |
| 1:N0:117:LEU:HA | 1:N0:120:VAL:HG12 | 1.86 | 0.57 |
| 2:N3:280:LYS:HA | 2:N3:283:HIS:HB3 | 1.86 | 0.57 |
| 2:N5:69:ASP:OD1 | 2:N5:70:LEU:N | 2.36 | 0.57 |
| 1:O8:248:ALA:HA | 1:O8:252:LYS:HD2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R0:67:ASP:N | 1:R0:67:ASP:OD1 | 2.37 | 0.57 |
| 1:R2:121:ARG:HD3 | 17:5S:48:THR:O | 2.05 | 0.57 |
| 1:R8:135:VAL:HG21 | 1:R8:152:ILE:HD11 | 1.85 | 0.57 |
| 2:S1:145:THR:OG1 | 41:S2:501:GTP:O1B | 2.22 | 0.57 |
| 2:S1:392:ASP:OD2 | 2:S1:422:ARG:NH1 | 2.37 | 0.57 |
| 2:S7:76:ASP:OD1 | 1:S8:46:ARG:NH2 | 2.38 | 0.57 |
| 1:T0:391:ARG:HD3 | 2:T1:346:TRP:CD1 | 2.39 | 0.57 |
| 2:T1:90:GLU:O | 2:T1:121:ARG:NH1 | 2.31 | 0.57 |
| 2:T3:176:GLN:NE2 | 13:5J:90:PRO:HG3 | 2.20 | 0.57 |
| 1:U4:121:ARG:NH2 | 1:U4:158:GLU:OE2 | 2.37 | 0.57 |
| 1:V6:273:LEU:H | 1:V6:292:GLN:HE22 | 1.51 | 0.57 |
| 1:W4:190:HIS:CD2 | 1:W4:411:ALA:HA | 2.39 | 0.57 |
| 1:X0:212:PHE:CE1 | 1:X0:220:PRO:HG3 | 2.39 | 0.57 |
| 2:X7:172:TYR:CE2 | 2:X7:203:MET:HG2 | 2.40 | 0.57 |
| 2:Y3:76:ASP:HA | 2:Y3:79:ARG:HB2 | 1.86 | 0.57 |
| 1:Z0:285:THR:HB | 1:Z0:287:PRO:HD2 | 1.87 | 0.57 |
| 2:Z7:336:LYS:O | 2:Z7:339:ARG:NH2 | 2.37 | 0.57 |
| 2:Z7:399:TYR:O | 2:Z7:402:ARG:NH1 | 2.37 | 0.57 |
| 1:0E:116:VAL:HA | 1:0E:119:VAL:HG12 | 1.86 | 0.57 |
| 2:0L:290:GLU:HA | 2:0L:293:ASN:HD22 | 1.70 | 0.57 |
| 1:0M:309:ARG:H | 1:0M:372:THR:HG22 | 1.70 | 0.57 |
| 1:0U:391:ARG:HH21 | 2:0V:435:VAL:HG22 | 1.69 | 0.57 |
| 2:0X:344:VAL:HG22 | 2:0X:346:TRP:H | 1.68 | 0.57 |
| 2:0Z:217:LEU:HB3 | 2:0Z:219:ILE:HD12 | 1.85 | 0.57 |
| 1:1E:148:GLY:O | 1:1E:152:ILE:HG13 | 2.03 | 0.57 |
| 2:1F:108:TYR:O | 2:1F:112:LYS:NZ | 2.26 | 0.57 |
| 2:1F:387:ILE:HG12 | 2:1F:390:ARG:HH22 | 1.69 | 0.57 |
| 1:1G:72:THR:O | 1:1G:76:VAL:HG23 | 2.04 | 0.57 |
| 2:1H:336:LYS:O | 2:1H:339:ARG:NH2 | 2.38 | 0.57 |
| 1:1O:350:LYS:NZ | 1:1O:352:SER:OG | 2.37 | 0.57 |
| 1:1U:97:ALA:HA | 1:1U:103:LYS:HE3 | 1.87 | 0.57 |
| 2:2J:123:ARG:NE | 38:8C:75:SER:HB3 | 2.20 | 0.57 |
| 1:2W:34:GLY:O | 1:2W:58:ARG:HA | 2.03 | 0.57 |
| 2:2Z:301:MET:HE1 | 2:2Z:307:PRO:HD3 | 1.85 | 0.57 |
| 2:3L:339:ARG:NH2 | 2:3L:342:GLN:HA | 2.18 | 0.57 |
| 1:3O:130:LEU:HB2 | 1:3O:162:ARG:HE | 1.70 | 0.57 |
| 4:3Y:27:LYS:HA | 4:3Y:59:ILE:HG22 | 1.87 | 0.57 |
| 3:4J:191:ILE:HD11 | 3:4J:228:ALA:HB2 | 1.86 | 0.57 |
| 7:4R:62:PHE:CE2 | 24:6V:9:PRO:HD3 | 2.39 | 0.57 |
| 8:4W:203:THR:O | 8:4W:207:THR:HG23 | 2.04 | 0.57 |
| 8:4W:458:GLU:O | 8:4W:461:VAL:CG1 | 2.49 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:5C:263:GLN:O | 10:5C:266:GLN:HG3 | 2.04 | 0.57 |
| 12:5F:298:ASP:CB | 12:7B:13:PRO:HG3 | 2.35 | 0.57 |
| 13:5I:70:LYS:HZ1 | 13:5I:75:PHE:HZ | 1.51 | 0.57 |
| 14:5M:219:LEU:CD1 | 14:5M:228:PHE:HD2 | 2.10 | 0.57 |
| 15:5O:52:TYR:CE2 | 15:5O:55:LEU:HD21 | 2.33 | 0.57 |
| 20:6F:84:ALA:HB1 | 20:6F:113:ARG:HG3 | 1.87 | 0.57 |
| 24:7A:107:VAL:HG22 | 24:7A:108:GLU:H | 1.70 | 0.57 |
| 2:A4:324:VAL:HG11 | 26:7F:142:PHE:HZ | 1.70 | 0.57 |
| 2:A8:222:PRO:HA | 18:5X:51:MET:HE1 | 1.86 | 0.57 |
| 2:E1:282:TYR:OH | 22:6I:81:ASN:HA | 2.05 | 0.57 |
| 1:G2:113:ILE:HG12 | 1:G2:117:LEU:HG | 1.87 | 0.57 |
| 1:G8:175:VAL:HG12 | 2:G9:329:ASN:ND2 | 2.19 | 0.57 |
| 2:H1:191:THR:HA | 2:H1:194:LEU:HG | 1.87 | 0.57 |
| 1:H6:262:ARG:HH21 | 1:H6:418:LEU:HD21 | 1.69 | 0.57 |
| 1:I2:391:ARG:HB2 | 2:I3:346:TRP:NE1 | 2.19 | 0.57 |
| 2:I9:121:ARG:O | 2:I9:121:ARG:HD2 | 2.05 | 0.57 |
| 2:K7:27:GLU:CD | 2:K7:243:ARG:HH12 | 2.08 | 0.57 |
| 2:K9:98:ASP:OD1 | 2:K9:99:ALA:N | 2.37 | 0.57 |
| 1:L0:272:PRO:HB2 | 1:L0:282:ARG:HH12 | 1.69 | 0.57 |
| 2:L3:259:LEU:HD11 | 2:L3:316:CYS:HB2 | 1.87 | 0.57 |
| 2:L7:269:LEU:N | 2:L7:379:SER:O | 2.34 | 0.57 |
| 1:M4:2:ARG:HB3 | 1:M4:131:GLN:HB2 | 1.85 | 0.57 |
| 2:M7:223:THR:HG23 | 2:M7:225:THR:H | 1.68 | 0.57 |
| 1:N0:388:MET:CE | 2:N1:348:PRO:HD2 | 2.33 | 0.57 |
| 2:N3:205:ASP:OD1 | 2:N3:303:VAL:HG13 | 2.04 | 0.57 |
| 2:N7:335:ILE:HD12 | 2:N7:338:LYS:HD2 | 1.86 | 0.57 |
| 2:N7:356:ASN:ND2 | 2:N7:358:GLN:H | 2.03 | 0.57 |
| 2:O1:51:THR:HG23 | 2:O1:52:PHE:CD2 | 2.39 | 0.57 |
| 2:O5:172:TYR:CE2 | 2:O5:203:MET:HG2 | 2.40 | 0.57 |
| 2:P5:381:SER:OG | 2:P5:382:THR:N | 2.37 | 0.57 |
| 1:P8:204:ASN:HD21 | 39:P8:502:GDP:HN22 | 1.52 | 0.57 |
| 1:Q8:211:CYS:HA | 1:Q8:215:LEU:HB2 | 1.87 | 0.57 |
| 1:Q8:262:ARG:NH2 | 1:Q8:417:ASP:OD1 | 2.37 | 0.57 |
| 1:R8:178:THR:HG22 | 2:R9:352:LYS:HZ3 | 1.70 | 0.57 |
| 1:S6:190:HIS:CD2 | 1:S6:414:ASN:HB2 | 2.39 | 0.57 |
| 1:T0:244:GLY:H | 1:T0:247:ASN:HD21 | 1.52 | 0.57 |
| 1:T8:135:VAL:HG21 | 1:T8:152:ILE:HD11 | 1.86 | 0.57 |
| 2:U3:9:ILE:HG22 | 2:U3:68:LEU:HD11 | 1.84 | 0.57 |
| 1:U8:335:ASN:O | 1:U8:338:SER:OG | 2.23 | 0.57 |
| 1:V0:97:ALA:HA | 1:V0:103:LYS:HE3 | 1.87 | 0.57 |
| 2:V1:98:ASP:OD1 | 2:V1:99:ALA:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V8:113:ILE:HA | 1:V8:116:VAL:HG22 | 1.86 | 0.57 |
| 1:V8:207:LEU:HB3 | 1:V8:225:LEU:HD22 | 1.86 | 0.57 |
| 2:W3:90:GLU:OE2 | 2:W3:90:GLU:HA | 2.04 | 0.57 |
| 2:W5:286:LEU:O | 2:W5:373:ARG:NH1 | 2.38 | 0.57 |
| 2:W9:16:VAL:HG22 | 2:W9:228:ASN:OD1 | 2.05 | 0.57 |
| 1:X8:250:LEU:HD12 | 1:X8:250:LEU:H | 1.68 | 0.57 |
| 1:Y6:333:VAL:HA | 1:Y6:336:LYS:HE2 | 1.87 | 0.57 |
| 1:0E:254:ALA:O | 1:0E:258:ILE:HG22 | 2.04 | 0.57 |
| 1:0G:309:ARG:H | 1:0G:372:THR:HG22 | 1.70 | 0.57 |
| 2:0P:259:LEU:HD21 | 2:0P:316:CYS:HB2 | 1.86 | 0.57 |
| 1:0S:136:CYS:HG | 1:0S:167:PHE:HD2 | 1.51 | 0.57 |
| 1:0U:182:PRO:HG3 | 1:0U:388:MET:HE3 | 1.86 | 0.57 |
| 2:0Z:289:ALA:O | 2:0Z:293:ASN:ND2 | 2.38 | 0.57 |
| 1:1A:207:LEU:HD11 | 1:1A:229:ILE:HD11 | 1.86 | 0.57 |
| 2:1D:83:TYR:HB3 | 2:1D:86:LEU:HB3 | 1.86 | 0.57 |
| 2:1F:274:PRO:HB2 | 2:1F:276:ILE:HG12 | 1.85 | 0.57 |
| 1:1K:177:ASP:O | 2:1L:352:LYS:HA | 2.05 | 0.57 |
| 2:1T:223:THR:HG23 | 2:1T:225:THR:HG22 | 1.86 | 0.57 |
| 1:1U:309:ARG:NH1 | 1:1U:339:SER:O | 2.37 | 0.57 |
| 2:1Z:317:LEU:HB3 | 2:1Z:319:TYR:HE1 | 1.70 | 0.57 |
| 1:2M:118:ASP:OD2 | 38:8D:99:THR:HB | 2.05 | 0.57 |
| 1:2S:3:GLU:HB2 | 1:2S:130:LEU:HA | 1.87 | 0.57 |
| 2:2V:229:ARG:HD3 | 2:2V:363:VAL:HG21 | 1.86 | 0.57 |
| 1:3C:105:HIS:CD2 | 1:3C:150:LEU:HB2 | 2.39 | 0.57 |
| 2:3H:306:ASP:HB3 | 2:3H:309:HIS:HD2 | 1.70 | 0.57 |
| 1:3O:309:ARG:H | 1:3O:372:THR:HG22 | 1.70 | 0.57 |
| 1:3S:285:THR:OG1 | 1:3S:287:PRO:HD2 | 2.04 | 0.57 |
| 4:4G:27:LYS:HA | 4:4G:59:ILE:HG22 | 1.87 | 0.57 |
| 13:5H:70:LYS:HZ1 | 13:5H:75:PHE:HZ | 1.51 | 0.57 |
| 13:5J:70:LYS:HZ1 | 13:5J:75:PHE:HZ | 1.51 | 0.57 |
| 14:5L:577:VAL:HG23 | 14:5L:594:HIS:HE1 | 1.67 | 0.57 |
| 14:5N:377:ARG:HH21 | 23:6S:52:LEU:HD11 | 1.68 | 0.57 |
| 24:6T:277:CYS:HA | 24:6T:368:LEU:HA | 1.86 | 0.57 |
| 24:6T:488:ARG:H | 24:6T:488:ARG:CD | 2.13 | 0.57 |
| 36:7V:58:MET:HG2 | 36:7V:94:LEU:HG | 1.87 | 0.57 |
| 36:7W:36:ALA:O | 36:7W:40:THR:HG23 | 2.05 | 0.57 |
| 38:8C:204:GLN:HE21 | 38:8C:204:GLN:CA | 2.17 | 0.57 |
| 1:3:280:GLN:HE22 | 1:S6:58:ARG:HG2 | 1.70 | 0.57 |
| 1:C2:362:LYS:HD3 | 18:6D:24:ARG:CA | 2.35 | 0.57 |
| 2:G7:206:ASN:OD1 | 41:G7:501:GTP:N2 | 2.37 | 0.57 |
| 2:G7:222:PRO:HD2 | 1:G8:324:LYS:HE3 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G8:172:SER:HB3 | 1:G8:175:VAL:HG22 | 1.86 | 0.57 |
| 2:G9:49:PHE:HB2 | 2:G9:53:PHE:HD2 | 1.69 | 0.57 |
| 1:H4:156:ARG:NH1 | 1:H4:197:ASP:OD1 | 2.38 | 0.57 |
| 1:H4:277:GLY:HA3 | 24:6U:492:ILE:HG22 | 1.86 | 0.57 |
| 2:I1:27:GLU:OE1 | 2:I1:243:ARG:NH1 | 2.37 | 0.57 |
| 2:I5:236:SER:O | 2:I5:243:ARG:NH2 | 2.38 | 0.57 |
| 1:I8:285:THR:HG23 | 1:I8:288:GLU:H | 1.69 | 0.57 |
| 2:J3:392:ASP:OD2 | 2:J3:422:ARG:NH1 | 2.38 | 0.57 |
| 2:L7:56:THR:HA | 2:N3:285:GLN:HB2 | 1.85 | 0.57 |
| 1:M0:107:THR:OG1 | 1:M0:401:GLU:OE2 | 2.15 | 0.57 |
| 1:M4:362:LYS:HD3 | 30:7K:173:GLU:HG3 | 1.87 | 0.57 |
| 1:M8:86:ARG:HB3 | 2:O5:283:HIS:HE1 | 1.68 | 0.57 |
| 1:M8:207:LEU:HB3 | 1:M8:225:LEU:HD22 | 1.86 | 0.57 |
| 2:N9:65:CYS:SG | 2:N9:66:ILE:N | 2.77 | 0.57 |
| 2:O5:222:PRO:HD2 | 1:O6:324:LYS:HE3 | 1.85 | 0.57 |
| 2:P5:50:ASN:HB3 | 27:7G:187:ARG:HH21 | 1.70 | 0.57 |
| 1:P8:45:GLU:HG3 | 1:P8:46:ARG:HG2 | 1.87 | 0.57 |
| 2:P9:286:LEU:O | 2:P9:373:ARG:NH1 | 2.37 | 0.57 |
| 1:Q0:248:ALA:HB2 | 1:Q0:252:LYS:HE2 | 1.86 | 0.57 |
| 2:Q9:225:THR:HG21 | 12:7B:78:HIS:CD2 | 2.40 | 0.57 |
| 2:R5:324:VAL:HG12 | 2:R5:326:LYS:H | 1.69 | 0.57 |
| 1:R6:130:LEU:HB2 | 1:R6:162:ARG:HE | 1.70 | 0.57 |
| 1:R8:117:LEU:HA | 1:R8:120:VAL:HG12 | 1.87 | 0.57 |
| 1:T0:252:LYS:CA | 1:T0:255:VAL:HG12 | 2.32 | 0.57 |
| 1:T4:350:LYS:NZ | 1:T4:351:SER:O | 2.38 | 0.57 |
| 1:T4:390:ARG:HG2 | 1:T4:390:ARG:O | 2.05 | 0.57 |
| 2:U9:399:TYR:O | 2:U9:402:ARG:NH1 | 2.37 | 0.57 |
| 1:W4:309:ARG:H | 1:W4:372:THR:HG22 | 1.69 | 0.57 |
| 2:W7:288:VAL:HG11 | 2:W7:327:ASP:HB2 | 1.86 | 0.57 |
| 2:X9:406:HIS:HA | 2:X9:409:VAL:HG22 | 1.86 | 0.57 |
| 2:X9:422:ARG:HH12 | 2:X9:426:ALA:HB2 | 1.70 | 0.57 |
| 1:Y0:100:ASN:HB3 | 1:Y0:103:LYS:HB2 | 1.84 | 0.57 |
| 1:Z2:139:LEU:HD21 | 1:Z2:168:SER:HB2 | 1.85 | 0.57 |
| 2:Z3:244:PHE:HB2 | 2:Z3:356:ASN:HD21 | 1.70 | 0.57 |
| 1:Z6:309:ARG:H | 1:Z6:372:THR:HG22 | 1.69 | 0.57 |
| 2:Z7:90:GLU:O | 2:Z7:121:ARG:NH1 | 2.37 | 0.57 |
| 1:0E:320:ARG:HG2 | 1:0E:355:ASP:HB3 | 1.87 | 0.57 |
| 2:0J:156:ARG:HA | 2:0J:159:VAL:HG22 | 1.87 | 0.57 |
| 1:0Q:72:THR:O | 1:0Q:76:VAL:HG23 | 2.04 | 0.57 |
| 1:0W:55:THR:HG22 | 1:1M:284:LEU:HD11 | 1.85 | 0.57 |
| 1:1A:301:CYS:SG | 1:1A:302:ALA:N | 2.77 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1F:213:CYS:HA | 2:1F:217:LEU:HB2 | 1.86 | 0.57 |
| 2:1H:265:ILE:HD12 | 2:1H:267:PHE:HD2 | 1.69 | 0.57 |
| 2:1N:305:CYS:SG | 2:1N:383:ALA:HB1 | 2.44 | 0.57 |
| 1:1S:350:LYS:NZ | 1:1S:352:SER:OG | 2.37 | 0.57 |
| 2:1V:34:GLY:HA3 | 2:1V:60:LYS:HZ2 | 1.69 | 0.57 |
| 2:1Z:338:LYS:HD2 | 2:1Z:340:THR:HG22 | 1.87 | 0.57 |
| 2:1Z:343:PHE:CZ | 2:1Z:351:PHE:HE1 | 2.22 | 0.57 |
| 1:2I:118:ASP:CB | 38:8C:99:THR:HG22 | 2.24 | 0.57 |
| 2:2R:336:LYS:O | 2:2R:339:ARG:NH2 | 2.38 | 0.57 |
| 2:2T:183:GLU:HG3 | 2:2T:184:PRO:HD3 | 1.85 | 0.57 |
| 2:3J:183:GLU:HG3 | 2:3J:184:PRO:HD3 | 1.86 | 0.57 |
| 1:3Q:217:LEU:HD22 | 38:8D:229:ASN:H | 1.70 | 0.57 |
| 2:3R:109:THR:OG1 | 2:3R:411:GLU:OE2 | 2.21 | 0.57 |
| 4:4C:27:LYS:HA | 4:4C:59:ILE:HG22 | 1.87 | 0.57 |
| 5:4L:466:LEU:O | 5:4M:146:ARG:NH2 | 2.38 | 0.57 |
| 6:4O:74:ARG:NH2 | 6:4O:75:ALA:HB2 | 2.19 | 0.57 |
| 9:4Z:239:ARG:O | 9:4Z:242:GLU:HG3 | 2.05 | 0.57 |
| 14:5M:24:HIS:HB2 | 14:5M:29:THR:HB | 1.85 | 0.57 |
| 15:5P:14:LEU:HD23 | 15:5P:14:LEU:O | 2.04 | 0.57 |
| 21:6G:37:ILE:HG23 | 21:6G:40:PHE:HB3 | 1.85 | 0.57 |
| 22:6K:110:ILE:O | 22:6K:113:ARG:NH1 | 2.38 | 0.57 |
| 24:6X:97:ARG:NH2 | 24:6X:99:TYR:OH | 2.37 | 0.57 |
| 25:7C:109:PRO:C | 25:7C:110:ARG:HD2 | 2.25 | 0.57 |
| 29:7J:388:MET:N | 29:7J:388:MET:SD | 2.77 | 0.57 |
| 30:7K:353:ASN:ND2 | 30:7K:357:GLU:OE1 | 2.37 | 0.57 |
| 37:7Y:11:THR:HA | 37:7Y:14:ILE:HD12 | 1.86 | 0.57 |
| 38:8C:73:TRP:N | 38:8C:73:TRP:CD1 | 2.73 | 0.57 |
| 1:7:337:ASN:ND2 | 3:4B:68:SER:HA | 2.18 | 0.57 |
| 2:G3:399:TYR:O | 2:G3:402:ARG:NH1 | 2.38 | 0.57 |
| 1:G6:73:MET:O | 1:G6:76:VAL:HG22 | 2.05 | 0.57 |
| 2:G9:406:HIS:HA | 2:G9:409:VAL:HG12 | 1.87 | 0.57 |
| 2:H3:222:PRO:HD2 | 1:H4:324:LYS:HE3 | 1.87 | 0.57 |
| 1:H6:113:ILE:HD13 | 1:H6:150:LEU:HD22 | 1.86 | 0.57 |
| 1:H6:128:ASP:OD1 | 1:H6:129:CYS:N | 2.38 | 0.57 |
| 2:H7:278:ALA:HA | 2:H7:369:ALA:HB2 | 1.87 | 0.57 |
| 1:H8:199:CYS:HB2 | 1:H8:265:PHE:HD1 | 1.68 | 0.57 |
| 1:H8:287:PRO:HA | 1:H8:290:THR:HG22 | 1.87 | 0.57 |
| 2:H9:392:ASP:OD2 | 2:H9:422:ARG:NH1 | 2.37 | 0.57 |
| 2:I7:313:MET:HB2 | 2:I7:380:ASN:HB3 | 1.86 | 0.57 |
| 2:J3:90:GLU:CB | 2:J3:121:ARG:HH12 | 2.16 | 0.57 |
| 2:K3:271:SER:OG | 2:K3:377:MET:HB3 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L4:39:ASP:O | 29:7J:339:GLN:NE2 | 2.38 | 0.57 |
| 1:N6:8:GLN:HG2 | 1:N6:17:GLY:HA3 | 1.87 | 0.57 |
| 2:O3:56:THR:HG22 | 2:Q1:285:GLN:HB2 | 1.86 | 0.57 |
| 2:O7:344:VAL:HG13 | 2:O7:347:CYS:H | 1.70 | 0.57 |
| 2:P3:14:ILE:HD11 | 2:P3:74:VAL:HG13 | 1.86 | 0.57 |
| 2:P5:296:PHE:HE2 | 2:P5:335:ILE:HG13 | 1.69 | 0.57 |
| 1:Q2:301:CYS:SG | 1:Q2:302:ALA:N | 2.78 | 0.57 |
| 2:Q9:137:VAL:HG11 | 2:Q9:154:LEU:HD21 | 1.85 | 0.57 |
| 1:R2:139:LEU:HD12 | 1:R2:170:VAL:HG12 | 1.86 | 0.57 |
| 1:T2:193:VAL:HG23 | 1:T2:194:GLU:HG2 | 1.86 | 0.57 |
| 2:T5:11:GLN:OE1 | 2:T5:15:GLN:NE2 | 2.37 | 0.57 |
| 1:T8:350:LYS:NZ | 1:T8:351:SER:O | 2.37 | 0.57 |
| 2:U7:85:GLN:OE1 | 2:U7:85:GLN:HA | 2.04 | 0.57 |
| 2:V1:287:SER:N | 2:V1:290:GLU:OE2 | 2.38 | 0.57 |
| 1:V4:135:VAL:HG21 | 1:V4:152:ILE:HD11 | 1.87 | 0.57 |
| 1:V6:49:VAL:HG21 | 1:V6:240:LEU:HD13 | 1.85 | 0.57 |
| 1:V6:256:ASN:HB2 | 1:V6:350:LYS:HZ3 | 1.70 | 0.57 |
| 1:W8:233:MET:O | 1:W8:237:THR:HG22 | 2.04 | 0.57 |
| 1:X0:43:GLN:HE21 | 8:4X:97:PHE:HB3 | 1.70 | 0.57 |
| 2:X5:327:ASP:N | 2:X5:327:ASP:OD2 | 2.37 | 0.57 |
| 2:X7:90:GLU:O | 2:X7:121:ARG:NH1 | 2.38 | 0.57 |
| 2:X7:284:GLU:HG2 | 2:X7:285:GLN:H | 1.70 | 0.57 |
| 1:X8:248:ALA:HA | 1:X8:252:LYS:HD2 | 1.86 | 0.57 |
| 2:X9:292:THR:OG1 | 2:X9:319:TYR:OH | 2.21 | 0.57 |
| 2:Y1:12:ALA:HB2 | 41:Y1:501:GTP:C8 | 2.40 | 0.57 |
| 2:Y9:313:MET:HE3 | 2:Y9:380:ASN:HB3 | 1.87 | 0.57 |
| 2:Y9:417:GLU:HA | 2:Y9:420:GLU:HG2 | 1.87 | 0.57 |
| 1:Z8:58:ARG:HH11 | 1:Z8:84:ILE:HA | 1.68 | 0.57 |
| 2:0H:115:VAL:HG23 | 2:0H:153:LEU:HD12 | 1.85 | 0.57 |
| 2:0J:88:HIS:HB3 | 2:0Z:283:HIS:ND1 | 2.19 | 0.57 |
| 2:0L:83:TYR:HB3 | 2:0L:86:LEU:HB3 | 1.85 | 0.57 |
| 2:0L:167:LEU:HD13 | 2:0L:200:VAL:HB | 1.87 | 0.57 |
| 2:1F:286:LEU:HD11 | 2:1F:372:GLN:HB2 | 1.86 | 0.57 |
| 2:1N:145:THR:OG1 | 41:1N:501:GTP:O1B | 2.21 | 0.57 |
| 1:2E:2:ARG:HB3 | 1:2E:131:GLN:HB2 | 1.87 | 0.57 |
| 1:2K:121:ARG:O | 1:2K:125:GLU:HG2 | 2.05 | 0.57 |
| 2:2P:217:LEU:HD11 | 2:2P:275:ILE:HD11 | 1.85 | 0.57 |
| 2:3B:11:GLN:OE1 | 2:3B:15:GLN:NE2 | 2.37 | 0.57 |
| 2:3B:77:GLU:OE2 | 38:8D:199:THR:OG1 | 2.10 | 0.57 |
| 1:3C:320:ARG:HH22 | 38:8D:198:THR:HA | 1.70 | 0.57 |
| 1:3G:2:ARG:HE | 1:3G:240:LEU:HD22 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3M:3:GLU:HG3 | 1:3M:127:CYS:HB2 | 1.85 | 0.57 |
| 2:3P:163:LYS:HE3 | 3:4F:137:ARG:HG2 | 1.87 | 0.57 |
| 2:3R:75:VAL:HG21 | 2:3R:94:SER:HB3 | 1.86 | 0.57 |
| 12:5G:322:LEU:HD13 | 12:5G:332:ASN:HB2 | 1.87 | 0.57 |
| 14:5M:577:VAL:HG23 | 14:5M:594:HIS:HE1 | 1.68 | 0.57 |
| 14:5N:577:VAL:HG23 | 14:5N:594:HIS:HE1 | 1.67 | 0.57 |
| 17:5V:208:LYS:HA | 17:5V:211:ARG:HH11 | 1.69 | 0.57 |
| 21:6H:37:ILE:HG21 | 21:6H:40:PHE:HD2 | 1.70 | 0.57 |
| 24:6T:378:TRP:O | 24:6T:382:ASN:ND2 | 2.38 | 0.57 |
| 24:6U:502:LYS:HB3 | 24:6U:511:ILE:HD12 | 1.87 | 0.57 |
| 26:7F:48:LEU:N | 26:7F:49:PRO:HD2 | 2.20 | 0.57 |
| 34:7S:171:LEU:HD11 | 35:7U:124:GLN:HE22 | 1.70 | 0.57 |
| 36:7V:36:ALA:O | 36:7V:40:THR:HG23 | 2.05 | 0.57 |
| 37:7Y:214:ASP:OD2 | 37:7Y:229:ALA:HB2 | 2.03 | 0.57 |
| 2:A2:40:LYS:HZ1 | 26:7F:45:MET:N | 2.03 | 0.57 |
| 1:B8:276:ARG:O | 24:6Y:115:ARG:NH2 | 2.35 | 0.57 |
| 2:C5:280:LYS:NZ | 18:5X:166:HIS:HB3 | 2.20 | 0.57 |
| 2:E9:206:ASN:OD1 | 41:F0:501:GTP:N2 | 2.28 | 0.57 |
| 1:F0:35:THR:HG21 | 22:6N:260:VAL:H | 1.68 | 0.57 |
| 2:F9:278:ALA:HB3 | 22:6K:215:GLY:HA2 | 1.86 | 0.57 |
| 2:G9:9:ILE:HG22 | 2:G9:68:LEU:HD22 | 1.87 | 0.57 |
| 1:H2:113:ILE:HA | 1:H2:116:VAL:HG22 | 1.87 | 0.57 |
| 1:I2:290:THR:HA | 1:I2:293:MET:HB2 | 1.87 | 0.57 |
| 2:I9:320:ARG:NH2 | 2:I9:359:PRO:O | 2.38 | 0.57 |
| 2:J1:189:LEU:HD11 | 2:J1:418:PHE:HE1 | 1.70 | 0.57 |
| 2:J7:216:SER:OG | 2:J7:275:ILE:O | 2.23 | 0.57 |
| 2:J9:320:ARG:NH2 | 2:J9:359:PRO:O | 2.38 | 0.57 |
| 2:K3:223:THR:HG23 | 2:K3:225:THR:H | 1.69 | 0.57 |
| 2:K5:417:GLU:HA | 2:K5:420:GLU:HG2 | 1.87 | 0.57 |
| 2:L1:206:ASN:OD1 | 41:L2:501:GTP:N2 | 2.36 | 0.57 |
| 1:L6:309:ARG:NH1 | 1:L6:339:SER:O | 2.38 | 0.57 |
| 2:L9:204:LEU:HD13 | 2:L9:231:ILE:HD12 | 1.85 | 0.57 |
| 1:N2:135:VAL:HG11 | 1:N2:152:ILE:HD11 | 1.87 | 0.57 |
| 1:N2:179:VAL:HG22 | 2:N3:258:ASN:HD22 | 1.69 | 0.57 |
| 1:N6:14:ASN:HD21 | 1:N6:67:ASP:HB3 | 1.69 | 0.57 |
| 2:N7:222:PRO:HD2 | 1:N8:324:LYS:HE3 | 1.87 | 0.57 |
| 1:Q0:318:ARG:HD3 | 1:Q0:358:PRO:HD3 | 1.87 | 0.57 |
| 2:Q5:286:LEU:O | 2:Q5:373:ARG:NH1 | 2.38 | 0.57 |
| 2:T3:88:HIS:CE1 | 2:T3:90:GLU:H | 2.23 | 0.57 |
| 1:T6:306:ARG:HH12 | 17:5U:51:ARG:C | 2.07 | 0.57 |
| 2:U1:399:TYR:OH | 2:U1:415:GLU:OE2 | 2.22 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U3:279:GLU:HB3 | 2:U3:283:HIS:CE1 | 2.40 | 0.57 |
| 2:W9:70:LEU:HB3 | 2:W9:97:GLU:O | 2.04 | 0.57 |
| 2:W9:132:LEU:HD22 | 2:W9:164:LYS:HD3 | 1.87 | 0.57 |
| 1:X2:173:PRO:HG2 | 1:X2:380:ARG:HH21 | 1.70 | 0.57 |
| 1:Y2:100:ASN:HB3 | 1:Y2:103:LYS:HB2 | 1.85 | 0.57 |
| 2:Y9:3:GLU:HG3 | 2:Y9:51:THR:HA | 1.87 | 0.57 |
| 2:Y9:392:ASP:OD2 | 2:Y9:422:ARG:NH1 | 2.38 | 0.57 |
| 1:Z0:182:PRO:HB2 | 1:Z0:385:PHE:HD2 | 1.70 | 0.57 |
| 1:Z4:135:VAL:HG21 | 1:Z4:152:ILE:HD11 | 1.86 | 0.57 |
| 1:0A:126:SER:HA | 1:0Q:291:GLN:HE22 | 1.69 | 0.57 |
| 1:0I:2:ARG:HB3 | 1:0I:131:GLN:HB2 | 1.87 | 0.57 |
| 1:0M:107:THR:OG1 | 1:0M:401:GLU:OE2 | 2.20 | 0.57 |
| 1:0O:388:MET:N | 1:0O:388:MET:HE2 | 2.20 | 0.57 |
| 2:0R:12:ALA:HB2 | 41:0S:501:GTP:C8 | 2.39 | 0.57 |
| 2:0R:24:TYR:O | 2:0R:27:GLU:HG2 | 2.05 | 0.57 |
| 1:1C:3:GLU:OE1 | 1:1C:62:ARG:HD2 | 2.05 | 0.57 |
| 2:1N:17:GLY:HA2 | 2:1N:20:CYS:HB3 | 1.87 | 0.57 |
| 1:1W:335:ASN:O | 1:1W:338:SER:OG | 2.22 | 0.57 |
| 1:2E:139:LEU:HD12 | 1:2E:170:VAL:HG22 | 1.87 | 0.57 |
| 1:2E:177:ASP:O | 2:2F:352:LYS:HA | 2.05 | 0.57 |
| 1:2U:125:GLU:OE2 | 1:2U:159:TYR:OH | 2.22 | 0.57 |
| 2:2X:2:ARG:HA | 2:2X:133:GLN:HE21 | 1.69 | 0.57 |
| 1:2Y:49:VAL:HG11 | 1:2Y:241:ARG:HG2 | 1.85 | 0.57 |
| 1:2Y:320:ARG:NH1 | 38:8C:197:THR:C | 2.58 | 0.57 |
| 2:3F:392:ASP:OD2 | 2:3F:422:ARG:NH1 | 2.38 | 0.57 |
| 1:3I:95:THR:HG21 | 3:3Z:138:GLY:HA2 | 1.87 | 0.57 |
| 1:3S:72:THR:O | 1:3S:76:VAL:HG23 | 2.05 | 0.57 |
| 9:4Z:202:ASP:OD1 | 9:4Z:206:ARG:NH1 | 2.36 | 0.57 |
| 14:5N:24:HIS:HB2 | 14:5N:29:THR:HB | 1.85 | 0.57 |
| 14:5N:28:ARG:HG2 | 14:5N:28:ARG:NH1 | 2.20 | 0.57 |
| 14:5N:157:ASN:ND2 | 14:5N:203:ASP:O | 2.38 | 0.57 |
| 15:5P:49:ARG:HG2 | 15:5P:49:ARG:O | 2.04 | 0.57 |
| 18:5X:7:LEU:HD13 | 18:5X:69:THR:HG21 | 1.86 | 0.57 |
| 18:5Y:39:TYR:CZ | 26:7D:24:GLN:OE1 | 2.58 | 0.57 |
| 18:6B:7:LEU:HD13 | 18:6B:69:THR:HG21 | 1.86 | 0.57 |
| 18:6C:7:LEU:HD13 | 18:6C:69:THR:HG21 | 1.86 | 0.57 |
| 22:6L:177:LEU:HD11 | 22:6L:252:ASP:OD2 | 2.04 | 0.57 |
| 22:6M:59:PRO:HB3 | 22:6M:108:ARG:HH22 | 1.68 | 0.57 |
| 22:6M:205:GLU:OE1 | 22:6M:205:GLU:N | 2.35 | 0.57 |
| 22:6O:271:ARG:HH22 | 22:6O:275:LEU:HD11 | 1.67 | 0.57 |
| 29:7J:359:ASP:OD1 | 29:7J:363:ARG:NH1 | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:7T:182:ALA:O | 35:7T:185:LYS:HG3 | 2.05 | 0.57 |
| 38:8A:73:TRP:HD1 | 38:8A:75:SER:HB2 | 1.69 | 0.57 |
| 1:E4:320:ARG:HH12 | 22:6K:115:SER:HA | 1.70 | 0.57 |
| 2:G3:290:GLU:HA | 2:G3:293:ASN:HD22 | 1.69 | 0.57 |
| 1:G6:33:THR:O | 1:G6:58:ARG:NH2 | 2.38 | 0.57 |
| 1:H2:114:ASP:N | 1:H2:114:ASP:OD1 | 2.38 | 0.57 |
| 2:H3:274:PRO:HB2 | 2:H3:276:ILE:CG1 | 2.35 | 0.57 |
| 1:I4:237:THR:CG2 | 1:I4:240:LEU:HD12 | 2.35 | 0.57 |
| 1:J4:43:GLN:HE21 | 16:5Q:15:VAL:HG21 | 1.69 | 0.57 |
| 2:J7:287:SER:N | 2:J7:290:GLU:OE2 | 2.38 | 0.57 |
| 2:L3:109:THR:OG1 | 2:L3:411:GLU:OE2 | 2.16 | 0.57 |
| 1:N2:86:ARG:HB3 | 2:O9:283:HIS:CE1 | 2.40 | 0.57 |
| 2:N5:121:ARG:HD2 | 2:N5:121:ARG:O | 2.04 | 0.57 |
| 1:P8:37:HIS:O | 21:6G:167:ARG:NH1 | 2.32 | 0.57 |
| 2:Q9:402:ARG:HB3 | 2:Q9:405:VAL:HG21 | 1.87 | 0.57 |
| 1:R8:190:HIS:CD2 | 1:R8:411:ALA:HA | 2.39 | 0.57 |
| 1:R8:334:GLN:HE22 | 1:R8:348:ASN:H | 1.53 | 0.57 |
| 2:S5:72:PRO:HD2 | 1:S6:2:ARG:HH12 | 1.69 | 0.57 |
| 2:S5:414:GLU:HG2 | 2:S5:416:GLY:H | 1.68 | 0.57 |
| 1:S6:67:ASP:N | 1:S6:67:ASP:OD1 | 2.36 | 0.57 |
| 2:S7:167:LEU:HD13 | 2:S7:200:VAL:HB | 1.87 | 0.57 |
| 2:S7:289:ALA:O | 2:S7:293:ASN:ND2 | 2.38 | 0.57 |
| 2:V1:177:VAL:HG13 | 1:V2:327:ASP:HB3 | 1.86 | 0.57 |
| 2:W1:88:HIS:NE2 | 2:W1:90:GLU:CB | 2.68 | 0.57 |
| 1:X0:42:LEU:HD23 | 8:4X:97:PHE:HE2 | 1.68 | 0.57 |
| 2:X3:22:GLU:HG3 | 2:X3:83:TYR:OH | 2.05 | 0.57 |
| 1:X6:263:LEU:HD22 | 1:X6:422:TYR:HE1 | 1.70 | 0.57 |
| 2:X9:236:SER:O | 2:X9:243:ARG:NH2 | 2.37 | 0.57 |
| 2:Y1:236:SER:O | 2:Y1:243:ARG:NH2 | 2.37 | 0.57 |
| 1:Y6:309:ARG:H | 1:Y6:372:THR:HG22 | 1.70 | 0.57 |
| 1:Y8:113:ILE:HA | 1:Y8:116:VAL:HG22 | 1.87 | 0.57 |
| 2:Z3:5:ILE:HG12 | 2:Z3:64:ARG:HB3 | 1.86 | 0.57 |
| 1:0A:167:PHE:HD1 | 1:0A:200:MET:HB2 | 1.70 | 0.57 |
| 1:0M:8:GLN:CD | 1:0M:17:GLY:HA3 | 2.25 | 0.57 |
| 1:0M:303:ALA:HB2 | 1:0M:377:MET:HG2 | 1.86 | 0.57 |
| 2:0P:177:VAL:HA | 1:0Q:331:LEU:HD21 | 1.85 | 0.57 |
| 1:0Q:31:ASP:OD2 | 1:0Q:33:THR:OG1 | 2.18 | 0.57 |
| 1:0S:233:MET:O | 1:0S:237:THR:HG22 | 2.04 | 0.57 |
| 1:0Y:8:GLN:O | 1:0Y:66:MET:HG3 | 2.05 | 0.57 |
| 2:1B:379:SER:OG | 2:1B:380:ASN:N | 2.36 | 0.57 |
| 1:1C:273:LEU:H | 1:1C:292:GLN:HE22 | 1.53 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1D:60:LYS:HE3 | 2:1T:282:TYR:O | 2.05 | 0.57 |
| 2:1D:88:HIS:HD2 | 2:1D:121:ARG:HH22 | 1.53 | 0.57 |
| 1:1O:178:THR:OG1 | 1:1O:181:GLU:HG3 | 2.05 | 0.57 |
| 2:1T:213:CYS:HA | 2:1T:217:LEU:HB2 | 1.85 | 0.57 |
| 2:2N:103:PHE:HB3 | 2:2N:408:TYR:HE2 | 1.69 | 0.57 |
| 2:2R:88:HIS:CE1 | 2:3H:283:HIS:HA | 2.40 | 0.57 |
| 2:2V:76:ASP:OD1 | 1:2W:46:ARG:NH2 | 2.38 | 0.57 |
| 2:3R:203:MET:HB2 | 2:3R:303:VAL:HG21 | 1.87 | 0.57 |
| 2:3R:223:THR:HG23 | 2:3R:225:THR:H | 1.69 | 0.57 |
| 4:3W:27:LYS:HA | 4:3W:59:ILE:HG22 | 1.87 | 0.57 |
| 4:4E:27:LYS:HA | 4:4E:59:ILE:HG22 | 1.87 | 0.57 |
| 5:4M:222:GLU:HA | 5:4M:225:MET:HG2 | 1.86 | 0.57 |
| 6:4O:301:MET:O | 6:4O:304:GLU:HG3 | 2.05 | 0.57 |
| 9:4Z:294:GLU:HA | 9:4Z:297:ARG:HD2 | 1.86 | 0.57 |
| 14:5L:24:HIS:HB2 | 14:5L:29:THR:HB | 1.86 | 0.57 |
| 14:5L:157:ASN:ND2 | 14:5L:203:ASP:O | 2.38 | 0.57 |
| 14:5M:28:ARG:HG2 | 14:5M:28:ARG:NH1 | 2.20 | 0.57 |
| 14:5M:157:ASN:ND2 | 14:5M:203:ASP:O | 2.38 | 0.57 |
| 14:5N:210:TYR:CZ | 14:5N:220:GLN:HG3 | 2.34 | 0.57 |
| 18:5Y:5:VAL:CG1 | 18:5Y:62:GLU:HG2 | 2.35 | 0.57 |
| 18:5Y:7:LEU:HD13 | 18:5Y:69:THR:HG21 | 1.86 | 0.57 |
| 18:5Z:7:LEU:HD13 | 18:5Z:69:THR:HG21 | 1.86 | 0.57 |
| 18:6A:7:LEU:HD13 | 18:6A:69:THR:HG21 | 1.86 | 0.57 |
| 18:6D:7:LEU:HD13 | 18:6D:69:THR:HG21 | 1.86 | 0.57 |
| 21:6G:125:GLU:OE2 | 21:6G:182:ARG:NH2 | 2.36 | 0.57 |
| 24:6Y:574:ARG:O | 24:6Y:578:ILE:HG12 | 2.05 | 0.57 |
| 28:7H:398:ASP:OD1 | 28:7H:400:THR:HG23 | 2.05 | 0.57 |
| 34:7R:102:LEU:HD13 | 35:7T:50:LEU:HD22 | 1.87 | 0.57 |
| 36:7W:58:MET:HG2 | 36:7W:94:LEU:HG | 1.87 | 0.57 |
| 37:7Y:237:ILE:O | 37:7Y:241:THR:HG23 | 2.04 | 0.57 |
| 38:8B:156:VAL:O | 38:8B:156:VAL:HG23 | 2.05 | 0.57 |
| 1:7:307:HIS:NE2 | 3:4B:59:LEU:HD11 | 2.19 | 0.56 |
| 2:E5:282:TYR:OH | 22:6K:81:ASN:CA | 2.23 | 0.56 |
| 1:F6:276:ARG:NH2 | 24:6T:408:PRO:O | 2.35 | 0.56 |
| 2:G3:245:ASP:N | 2:G3:245:ASP:OD1 | 2.38 | 0.56 |
| 1:G6:309:ARG:H | 1:G6:372:THR:HG22 | 1.70 | 0.56 |
| 2:H1:99:ALA:HA | 2:H1:105:ARG:HD3 | 1.85 | 0.56 |
| 2:H3:379:SER:OG | 2:H3:380:ASN:N | 2.36 | 0.56 |
| 1:H6:218:THR:CG2 | 24:6V:488:ARG:HB3 | 2.35 | 0.56 |
| 2:I1:318:MET:HB2 | 2:I1:376:CYS:HB3 | 1.86 | 0.56 |
| 2:I7:35:GLN:N | 2:I7:35:GLN:OE1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J0:248:ALA:HA | 1:J0:252:LYS:HD2 | 1.85 | 0.56 |
| 1:J0:404:ASP:HB3 | 1:J0:406:MET:SD | 2.45 | 0.56 |
| 1:J6:212:PHE:CE1 | 2:J7:326:LYS:HE3 | 2.31 | 0.56 |
| 1:J6:273:LEU:O | 1:J6:292:GLN:NE2 | 2.38 | 0.56 |
| 2:J9:251:ASP:H | 2:J9:254:GLU:HG2 | 1.70 | 0.56 |
| 2:J9:264:ARG:NH2 | 2:J9:431:ASP:OD2 | 2.38 | 0.56 |
| 2:K9:287:SER:OG | 2:K9:288:VAL:N | 2.38 | 0.56 |
| 2:L1:267:PHE:HB2 | 2:L1:384:ILE:HD12 | 1.86 | 0.56 |
| 1:L2:5:VAL:HG12 | 1:L2:133:PHE:HD1 | 1.70 | 0.56 |
| 1:L6:41:ASP:OD1 | 29:7J:167:ILE:HD12 | 1.95 | 0.56 |
| 2:N5:88:HIS:HD2 | 2:P3:283:HIS:HB3 | 1.70 | 0.56 |
| 1:O2:167:PHE:CZ | 1:O2:233:MET:HG2 | 2.39 | 0.56 |
| 1:O6:114:ASP:OD1 | 1:O6:115:SER:N | 2.38 | 0.56 |
| 2:Q3:62:VAL:HG21 | 2:Q3:88:HIS:HB2 | 1.86 | 0.56 |
| 2:R3:267:PHE:HB2 | 2:R3:384:ILE:HD12 | 1.87 | 0.56 |
| 1:S6:190:HIS:CD2 | 1:S6:411:ALA:HA | 2.40 | 0.56 |
| 2:S7:226:ASN:O | 2:S7:230:LEU:HG | 2.05 | 0.56 |
| 2:T5:217:LEU:HD11 | 2:T5:230:LEU:HD11 | 1.87 | 0.56 |
| 1:U8:51:PHE:O | 1:U8:62:ARG:NH2 | 2.38 | 0.56 |
| 1:V8:350:LYS:NZ | 1:V8:352:SER:OG | 2.29 | 0.56 |
| 2:W3:89:PRO:HD3 | 2:X9:283:HIS:CD2 | 2.39 | 0.56 |
| 1:W4:371:SER:OG | 1:W4:372:THR:N | 2.38 | 0.56 |
| 2:W7:72:PRO:HG3 | 1:W8:1:MET:HG3 | 1.87 | 0.56 |
| 2:X5:238:LEU:HD11 | 2:X5:255:PHE:CZ | 2.39 | 0.56 |
| 1:Y0:387:ALA:HA | 1:Y0:390:ARG:HE | 1.68 | 0.56 |
| 1:Y4:208:TYR:CE1 | 1:Y4:225:LEU:HD11 | 2.40 | 0.56 |
| 1:Z2:190:HIS:NE2 | 1:Z2:414:ASN:OD1 | 2.38 | 0.56 |
| 2:Z3:165:SER:HA | 2:Z3:199:ASP:OD2 | 2.05 | 0.56 |
| 1:Z4:204:ASN:ND2 | 39:Z4:501:GDP:HN22 | 2.03 | 0.56 |
| 1:Z8:220:PRO:HD2 | 2:Z9:326:LYS:HD2 | 1.87 | 0.56 |
| 1:0A:128:ASP:OD1 | 1:0A:129:CYS:N | 2.35 | 0.56 |
| 1:0G:8:GLN:CD | 1:0G:17:GLY:HA3 | 2.26 | 0.56 |
| 1:0K:113:ILE:HD12 | 1:0K:150:LEU:HB3 | 1.87 | 0.56 |
| 2:0L:51:THR:HG21 | 2:0L:243:ARG:HG2 | 1.87 | 0.56 |
| 2:0X:317:LEU:HB3 | 2:0X:319:TYR:HE1 | 1.70 | 0.56 |
| 2:0Z:58:ALA:CA | 9:4Z:165:ARG:NH2 | 2.66 | 0.56 |
| 2:1F:109:THR:OG1 | 2:1F:411:GLU:OE2 | 2.22 | 0.56 |
| 2:1L:27:GLU:OE1 | 2:1L:243:ARG:NH1 | 2.38 | 0.56 |
| 2:1P:109:THR:OG1 | 2:1P:411:GLU:OE2 | 2.23 | 0.56 |
| 2:2H:88:HIS:NE2 | 2:2X:280:LYS:HE3 | 2.20 | 0.56 |
| 2:2N:56:THR:HA | 2:3D:285:GLN:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:431:ASP:HA | 2:2N:434:GLU:HG2 | 1.86 | 0.56 |
| 1:3C:391:ARG:HD3 | 2:3D:346:TRP:CE2 | 2.39 | 0.56 |
| 2:3T:70:LEU:HD21 | 2:3T:149:LEU:HD21 | 1.86 | 0.56 |
| 4:3Y:149:ILE:HG22 | 4:3Y:150:GLU:HG2 | 1.87 | 0.56 |
| 4:4A:27:LYS:HA | 4:4A:59:ILE:HG22 | 1.87 | 0.56 |
| 4:4I:27:LYS:HA | 4:4I:59:ILE:HG22 | 1.87 | 0.56 |
| 5:4L:370:ALA:O | 5:4L:373:GLN:HG2 | 2.04 | 0.56 |
| 7:4T:266:MET:HG2 | 7:4T:270:GLU:HB2 | 1.87 | 0.56 |
| 14:5L:28:ARG:HG2 | 14:5L:28:ARG:NH1 | 2.20 | 0.56 |
| 14:5N:505:THR:OG1 | 14:5N:506:SER:N | 2.37 | 0.56 |
| 17:5T:188:LYS:O | 17:5T:192:VAL:HG23 | 2.05 | 0.56 |
| 22:6K:17:ILE:HG22 | 22:6K:19:GLY:H | 1.69 | 0.56 |
| 22:6P:283:ILE:HD12 | 22:6P:350:PHE:CD1 | 2.40 | 0.56 |
| 24:6U:274:ARG:NE | 24:6U:372:ASP:OD2 | 2.35 | 0.56 |
| 24:6Z:124:TYR:CD1 | 24:6Z:124:TYR:N | 2.73 | 0.56 |
| 24:7A:97:ARG:NH2 | 24:7A:99:TYR:OH | 2.38 | 0.56 |
| 27:7G:106:ALA:HB3 | 27:7G:109:ILE:HG22 | 1.87 | 0.56 |
| 1:9:228:LEU:HD21 | 26:7E:136:PHE:CZ | 2.39 | 0.56 |
| 1:A1:333:VAL:HG22 | 3:4F:67:LEU:HD13 | 1.87 | 0.56 |
| 1:A3:83:GLN:HB2 | 24:6Z:177:ARG:NH2 | 2.20 | 0.56 |
| 1:C2:359:LYS:HA | 18:6D:22:ARG:CZ | 2.35 | 0.56 |
| 1:G0:216:LYS:HD2 | 24:6V:422:ASN:HD21 | 1.68 | 0.56 |
| 1:G2:177:ASP:O | 2:G3:352:LYS:HA | 2.04 | 0.56 |
| 2:G5:2:ARG:NE | 2:G5:242:LEU:O | 2.37 | 0.56 |
| 2:J1:165:SER:HB3 | 2:J1:256:GLN:HE22 | 1.69 | 0.56 |
| 2:J3:113:GLU:N | 2:J3:113:GLU:OE1 | 2.38 | 0.56 |
| 1:K6:12:CYS:SG | 1:K6:13:GLY:N | 2.78 | 0.56 |
| 1:K6:309:ARG:NH1 | 1:K6:341:PHE:O | 2.38 | 0.56 |
| 2:K7:89:PRO:HD3 | 2:M3:283:HIS:CD2 | 2.40 | 0.56 |
| 1:L2:177:ASP:O | 2:L3:352:LYS:HA | 2.04 | 0.56 |
| 1:L6:336:LYS:HD3 | 28:7X:456:VAL:HG23 | 1.85 | 0.56 |
| 2:M7:98:ASP:OD1 | 2:M7:99:ALA:N | 2.38 | 0.56 |
| 1:O6:388:MET:HE2 | 2:O7:348:PRO:HD2 | 1.87 | 0.56 |
| 2:O9:191:THR:HA | 2:O9:194:LEU:HB3 | 1.86 | 0.56 |
| 2:P5:417:GLU:HA | 2:P5:420:GLU:HG2 | 1.87 | 0.56 |
| 1:Q8:317:PHE:HB2 | 1:Q8:353:VAL:HG22 | 1.87 | 0.56 |
| 2:Q9:250:VAL:HB | 2:Q9:254:GLU:HG3 | 1.87 | 0.56 |
| 2:R1:279:GLU:CD | 2:R1:279:GLU:H | 2.08 | 0.56 |
| 2:R5:259:LEU:HD11 | 2:R5:316:CYS:HB2 | 1.86 | 0.56 |
| 1:R6:49:VAL:HG11 | 1:R6:241:ARG:HG2 | 1.86 | 0.56 |
| 1:S4:113:ILE:HD11 | 1:S4:147:MET:HG3 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:272:PRO:HD3 | 1:S4:364:SER:HA | 1.87 | 0.56 |
| 1:S6:125:GLU:OE2 | 3:3X:66:THR:HG23 | 2.05 | 0.56 |
| 1:T2:43:GLN:NE2 | 12:5F:174:TYR:OH | 2.38 | 0.56 |
| 2:U3:392:ASP:OD2 | 2:U3:422:ARG:NH1 | 2.38 | 0.56 |
| 1:U8:117:LEU:HA | 1:U8:120:VAL:HG12 | 1.85 | 0.56 |
| 1:V0:113:ILE:HA | 1:V0:116:VAL:HG22 | 1.86 | 0.56 |
| 2:V7:399:TYR:O | 2:V7:402:ARG:NH1 | 2.37 | 0.56 |
| 1:V8:11:GLN:HG3 | 1:V8:72:THR:HG22 | 1.86 | 0.56 |
| 2:W3:76:ASP:OD2 | 1:W4:46:ARG:NH2 | 2.39 | 0.56 |
| 1:W6:52:ASN:OD1 | 1:W6:62:ARG:NH2 | 2.38 | 0.56 |
| 1:W8:34:GLY:O | 1:W8:58:ARG:HA | 2.05 | 0.56 |
| 1:X0:287:PRO:HD3 | 1:X0:325:GLU:OE1 | 2.05 | 0.56 |
| 1:X4:182:PRO:O | 1:X4:186:THR:OG1 | 2.15 | 0.56 |
| 1:X6:237:THR:HG23 | 1:X6:241:ARG:HH21 | 1.70 | 0.56 |
| 2:X7:346:TRP:CE3 | 2:X7:347:CYS:HB2 | 2.40 | 0.56 |
| 2:Z3:133:GLN:HG3 | 2:Z3:242:LEU:HD11 | 1.86 | 0.56 |
| 1:Z4:374:ILE:O | 1:Z4:377:MET:HG3 | 2.04 | 0.56 |
| 1:0C:2:ARG:HB3 | 1:0C:131:GLN:HB2 | 1.87 | 0.56 |
| 1:0C:21:TRP:HA | 1:0C:24:VAL:HG22 | 1.88 | 0.56 |
| 1:0E:286:VAL:HG23 | 1:0E:287:PRO:HD3 | 1.87 | 0.56 |
| 1:0K:163:MET:HB3 | 1:0K:250:LEU:HD22 | 1.86 | 0.56 |
| 1:0O:268:VAL:O | 1:0O:300:MET:N | 2.34 | 0.56 |
| 2:1H:109:THR:OG1 | 2:1H:411:GLU:OE2 | 2.22 | 0.56 |
| 1:1K:52:ASN:OD1 | 1:1K:62:ARG:NH2 | 2.38 | 0.56 |
| 2:1L:276:ILE:HG23 | 2:1L:280:LYS:HB2 | 1.87 | 0.56 |
| 1:1U:375:GLN:HB2 | 1:1U:419:VAL:HG23 | 1.86 | 0.56 |
| 1:1W:113:ILE:HD12 | 1:1W:150:LEU:HB3 | 1.86 | 0.56 |
| 2:1X:132:LEU:HD22 | 2:1X:164:LYS:HD3 | 1.87 | 0.56 |
| 1:2E:193:VAL:HG12 | 1:2E:265:PHE:HZ | 1.69 | 0.56 |
| 2:2H:282:TYR:CE1 | 10:5B:163:ARG:HD2 | 2.40 | 0.56 |
| 1:2I:404:ASP:HB3 | 1:2I:406:MET:SD | 2.45 | 0.56 |
| 2:2L:287:SER:N | 2:2L:290:GLU:OE2 | 2.38 | 0.56 |
| 2:2L:417:GLU:HA | 2:2L:420:GLU:HG2 | 1.85 | 0.56 |
| 1:2M:140:GLY:O | 1:2M:184:ASN:ND2 | 2.38 | 0.56 |
| 1:2U:301:CYS:O | 38:8B:105:ARG:NH1 | 2.37 | 0.56 |
| 2:2X:431:ASP:O | 2:2X:434:GLU:HG2 | 2.04 | 0.56 |
| 2:2Z:214:ARG:NH2 | 38:8C:60:GLY:O | 2.38 | 0.56 |
| 2:2Z:417:GLU:HA | 2:2Z:420:GLU:HG2 | 1.86 | 0.56 |
| 1:3O:173:PRO:HD2 | 1:3O:380:ARG:CZ | 2.35 | 0.56 |
| 2:3R:221:ARG:HB2 | 38:8D:174:SER:H | 1.70 | 0.56 |
| 8:4V:473:LYS:HE2 | 8:4W:134:LEU:HD22 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Y:413:SER:O | 9:4Y:416:GLU:HG3 | 2.04 | 0.56 |
| 14:5L:500:THR:OG1 | 14:5L:502:LYS:HG3 | 2.05 | 0.56 |
| 14:5M:500:THR:OG1 | 14:5M:502:LYS:HG3 | 2.05 | 0.56 |
| 14:5N:500:THR:OG1 | 14:5N:502:LYS:HG3 | 2.05 | 0.56 |
| 15:5O:20:ILE:HG23 | 27:7G:82:PRO:HB3 | 1.86 | 0.56 |
| 20:6F:55:LEU:HD22 | 20:6F:112:PRO:HA | 1.87 | 0.56 |
| 23:6R:48:TYR:HE2 | 23:6R:52:LEU:HD12 | 1.70 | 0.56 |
| 24:6Z:482:ILE:HG22 | 24:6Z:497:PHE:HB3 | 1.86 | 0.56 |
| 30:7K:57:GLN:HG3 | 30:7K:61:HIS:HD2 | 1.68 | 0.56 |
| 28:7X:406:PRO:HG2 | 28:7X:408:GLN:HE21 | 1.70 | 0.56 |
| 1:E6:52:ASN:CG | 22:6L:181:ASN:HD21 | 1.98 | 0.56 |
| 1:E8:77:ARG:HH11 | 24:6X:426:LEU:HG | 1.70 | 0.56 |
| 1:G2:325:GLU:HA | 1:G2:328:GLU:HG2 | 1.86 | 0.56 |
| 2:G3:98:ASP:OD1 | 2:G3:99:ALA:N | 2.37 | 0.56 |
| 1:G6:7:ILE:O | 1:G6:135:VAL:HA | 2.06 | 0.56 |
| 1:G6:78:SER:HA | 24:6Y:497:PHE:O | 2.05 | 0.56 |
| 1:H2:2:ARG:HB3 | 1:H2:131:GLN:HB2 | 1.86 | 0.56 |
| 1:H4:122:LYS:NZ | 1:J0:291:GLN:O | 2.37 | 0.56 |
| 1:I0:67:ASP:N | 1:I0:67:ASP:OD1 | 2.38 | 0.56 |
| 1:I0:345:ILE:O | 1:I0:348:ASN:ND2 | 2.38 | 0.56 |
| 1:I8:3:GLU:HB2 | 1:I8:130:LEU:HA | 1.87 | 0.56 |
| 1:J0:207:LEU:HB3 | 1:J0:225:LEU:HD22 | 1.88 | 0.56 |
| 2:J5:236:SER:OG | 2:J5:243:ARG:NH2 | 2.38 | 0.56 |
| 2:J5:406:HIS:HA | 2:J5:409:VAL:HG22 | 1.87 | 0.56 |
| 2:J7:80:THR:HB | 29:7J:390:LEU:CD1 | 2.35 | 0.56 |
| 2:K5:69:ASP:OD1 | 2:K5:70:LEU:N | 2.38 | 0.56 |
| 1:K6:285:THR:HG23 | 1:K6:288:GLU:H | 1.70 | 0.56 |
| 1:K8:307:HIS:NE2 | 35:7T:136:GLU:OE2 | 2.37 | 0.56 |
| 1:L4:350:LYS:NZ | 1:L4:351:SER:O | 2.37 | 0.56 |
| 1:M0:6:HIS:HE2 | 1:M0:136:CYS:HG | 1.53 | 0.56 |
| 2:M1:363:VAL:HG23 | 2:M1:366:GLY:HA3 | 1.86 | 0.56 |
| 2:M7:285:GLN:CG | 30:7K:84:VAL:HG12 | 2.22 | 0.56 |
| 1:N2:107:THR:OG1 | 1:N2:401:GLU:OE2 | 2.19 | 0.56 |
| 1:N2:139:LEU:HD12 | 1:N2:170:VAL:HG12 | 1.87 | 0.56 |
| 2:N3:275:ILE:HD12 | 2:N3:368:LEU:HD21 | 1.87 | 0.56 |
| 1:N6:191:GLN:HE21 | 1:N6:195:ASN:ND2 | 2.03 | 0.56 |
| 2:N7:69:ASP:OD1 | 2:N7:70:LEU:N | 2.37 | 0.56 |
| 2:N9:392:ASP:OD2 | 2:N9:422:ARG:NH1 | 2.38 | 0.56 |
| 1:O0:277:GLY:HA2 | 27:7G:31:PHE:HD2 | 1.70 | 0.56 |
| 2:O1:90:GLU:CB | 2:O1:121:ARG:HH12 | 2.17 | 0.56 |
| 1:O6:178:THR:HG22 | 2:O7:352:LYS:HZ3 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O7:44:GLY:HA3 | 20:6F:242:ARG:HH12 | 1.69 | 0.56 |
| 2:P5:220:GLU:HG2 | 2:P5:221:ARG:HG3 | 1.86 | 0.56 |
| 1:P6:70:PRO:N | 1:P6:92:PHE:HZ | 2.03 | 0.56 |
| 2:P7:220:GLU:HG2 | 2:P7:221:ARG:HG3 | 1.87 | 0.56 |
| 1:Q2:156:ARG:NH1 | 1:Q2:197:ASP:OD1 | 2.38 | 0.56 |
| 1:Q8:190:HIS:CD2 | 1:Q8:411:ALA:HA | 2.41 | 0.56 |
| 1:R8:220:PRO:HD2 | 2:R9:326:LYS:HD2 | 1.87 | 0.56 |
| 2:S1:381:SER:OG | 2:S1:382:THR:N | 2.37 | 0.56 |
| 1:S2:95:THR:HG21 | 1:S2:108:GLU:HG2 | 1.86 | 0.56 |
| 1:S4:50:TYR:CE2 | 1:S4:241:ARG:HD3 | 2.40 | 0.56 |
| 1:T0:336:LYS:HG3 | 13:5I:101:LYS:HD3 | 1.87 | 0.56 |
| 2:T3:305:CYS:SG | 2:T3:383:ALA:HB1 | 2.45 | 0.56 |
| 1:T4:334:GLN:HE22 | 1:T4:348:ASN:H | 1.52 | 0.56 |
| 1:T6:220:PRO:HD2 | 2:T7:326:LYS:HG2 | 1.87 | 0.56 |
| 1:U4:3:GLU:HB2 | 1:U4:130:LEU:HA | 1.87 | 0.56 |
| 1:W0:139:LEU:HD12 | 1:W0:170:VAL:HG12 | 1.88 | 0.56 |
| 2:W9:72:PRO:HD2 | 1:X0:2:ARG:NH1 | 2.20 | 0.56 |
| 1:X0:128:ASP:OD1 | 1:X0:129:CYS:N | 2.35 | 0.56 |
| 1:X2:178:THR:HA | 2:X3:352:LYS:CD | 2.34 | 0.56 |
| 1:X2:183:TYR:HB3 | 1:X2:398:TYR:HE2 | 1.69 | 0.56 |
| 2:X3:5:ILE:HG12 | 2:X3:64:ARG:HB3 | 1.88 | 0.56 |
| 2:X5:90:GLU:H | 2:Z1:283:HIS:CE1 | 2.23 | 0.56 |
| 1:X8:2:ARG:HE | 1:X8:240:LEU:HD22 | 1.69 | 0.56 |
| 1:X8:204:ASN:HD21 | 39:X8:501:GDP:HN22 | 1.53 | 0.56 |
| 2:X9:25:CYS:O | 2:X9:30:ILE:N | 2.24 | 0.56 |
| 2:X9:206:ASN:OD1 | 41:Y0:501:GTP:N2 | 2.37 | 0.56 |
| 2:Y1:305:CYS:SG | 2:Y1:383:ALA:HB1 | 2.45 | 0.56 |
| 2:Y3:179:THR:HG21 | 1:Y4:246:LEU:HD11 | 1.87 | 0.56 |
| 2:Y5:392:ASP:OD2 | 2:Y5:422:ARG:NH1 | 2.38 | 0.56 |
| 1:Y8:215:LEU:HD21 | 1:Y8:273:LEU:HD12 | 1.87 | 0.56 |
| 2:Y9:88:HIS:HB3 | 2:0F:283:HIS:CE1 | 2.40 | 0.56 |
| 1:Z0:107:THR:OG1 | 1:Z0:401:GLU:OE2 | 2.22 | 0.56 |
| 2:Z1:227:LEU:O | 2:Z1:231:ILE:HG12 | 2.05 | 0.56 |
| 2:Z5:223:THR:HG23 | 2:Z5:225:THR:H | 1.69 | 0.56 |
| 2:Z7:68:LEU:HG | 2:Z7:93:ILE:HB | 1.85 | 0.56 |
| 2:Z7:276:ILE:HG23 | 2:Z7:280:LYS:HB3 | 1.87 | 0.56 |
| 1:0G:31:ASP:OD1 | 1:0G:35:THR:N | 2.22 | 0.56 |
| 1:0I:248:ALA:HA | 1:0I:252:LYS:HD2 | 1.86 | 0.56 |
| 2:0J:83:TYR:HB3 | 2:0J:86:LEU:HB3 | 1.86 | 0.56 |
| 2:0L:276:ILE:HG23 | 2:0L:280:LYS:HB3 | 1.85 | 0.56 |
| 2:0P:381:SER:OG | 2:0P:382:THR:N | 2.37 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Q:54:ALA:HB3 | 1:0Q:58:ARG:HB3 | 1.88 | 0.56 |
| 2:0R:377:MET:SD | 2:0R:379:SER:HB2 | 2.45 | 0.56 |
| 1:0U:309:ARG:NH1 | 1:0U:339:SER:O | 2.38 | 0.56 |
| 1:0W:3:GLU:HG2 | 1:0W:127:CYS:SG | 2.44 | 0.56 |
| 1:0W:418:LEU:HG | 1:0W:422:TYR:HE2 | 1.70 | 0.56 |
| 2:0X:217:LEU:HB3 | 2:0X:219:ILE:HD12 | 1.88 | 0.56 |
| 2:1D:90:GLU:HB3 | 2:1D:121:ARG:HH22 | 1.71 | 0.56 |
| 1:1E:183:TYR:HA | 1:1E:385:PHE:HE1 | 1.70 | 0.56 |
| 1:1G:397:TRP:HE1 | 2:1H:260:VAL:HG13 | 1.71 | 0.56 |
| 2:1L:101:ASN:OD1 | 1:1M:252:LYS:HE3 | 2.05 | 0.56 |
| 1:1M:113:ILE:HD13 | 1:1M:150:LEU:HD22 | 1.86 | 0.56 |
| 2:1R:63:PRO:HB2 | 2:1R:65:CYS:SG | 2.45 | 0.56 |
| 2:1R:379:SER:OG | 2:1R:380:ASN:N | 2.39 | 0.56 |
| 2:1V:287:SER:OG | 2:1V:290:GLU:OE1 | 2.19 | 0.56 |
| 1:1W:72:THR:O | 1:1W:76:VAL:HG23 | 2.06 | 0.56 |
| 2:1Z:155:GLU:OE1 | 2:1Z:156:ARG:HD2 | 2.05 | 0.56 |
| 1:2E:218:THR:O | 2:2F:326:LYS:NZ | 2.31 | 0.56 |
| 1:2I:244:GLY:H | 1:2I:247:ASN:HD21 | 1.53 | 0.56 |
| 1:2K:396:HIS:HA | 1:2K:399:THR:HG22 | 1.88 | 0.56 |
| 1:2M:186:THR:HG22 | 1:2M:411:ALA:HB1 | 1.88 | 0.56 |
| 2:2X:274:PRO:HG2 | 2:2X:371:VAL:HG21 | 1.86 | 0.56 |
| 2:3B:251:ASP:H | 2:3B:254:GLU:HG2 | 1.71 | 0.56 |
| 2:3B:358:GLN:OE1 | 38:8D:214:HIS:CD2 | 2.59 | 0.56 |
| 2:3J:117:LEU:HD13 | 4:4A:6:PHE:HB2 | 1.85 | 0.56 |
| 2:3P:221:ARG:NH1 | 23:6S:70:THR:O | 2.31 | 0.56 |
| 1:3Q:203:ASP:HB2 | 1:3Q:205:GLU:OE2 | 2.06 | 0.56 |
| 1:3S:178:THR:HA | 2:3T:352:LYS:HD2 | 1.88 | 0.56 |
| 2:3T:236:SER:OG | 2:3T:243:ARG:NH2 | 2.39 | 0.56 |
| 3:3V:15:ARG:HA | 3:3V:19:LEU:HG | 1.88 | 0.56 |
| 4:3W:22:LEU:H | 3:3X:258:ASP:CG | 2.08 | 0.56 |
| 4:3W:149:ILE:HG22 | 4:3W:150:GLU:HG2 | 1.87 | 0.56 |
| 4:4A:149:ILE:HG22 | 4:4A:150:GLU:HG2 | 1.87 | 0.56 |
| 4:4C:149:ILE:HG22 | 4:4C:150:GLU:HG2 | 1.87 | 0.56 |
| 3:4D:15:ARG:HA | 3:4D:19:LEU:HG | 1.88 | 0.56 |
| 3:4F:15:ARG:HA | 3:4F:19:LEU:HG | 1.88 | 0.56 |
| 4:4G:149:ILE:HG22 | 4:4G:150:GLU:HG2 | 1.87 | 0.56 |
| 3:4J:148:ASP:OD1 | 3:4J:151:LYS:HG3 | 2.05 | 0.56 |
| 3:4J:242:ILE:HG13 | 3:4J:243:LEU:HD22 | 1.86 | 0.56 |
| 6:4P:167:ARG:HA | 6:4P:170:ASN:HD21 | 1.71 | 0.56 |
| 8:4X:96:VAL:HG12 | 8:4X:96:VAL:O | 2.05 | 0.56 |
| 9:4Y:399:ALA:O | 9:4Y:403:GLU:HG3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:202:ASP:O | 9:4Z:206:ARG:HG2 | 2.06 | 0.56 |
| 9:4Z:233:ARG:O | 9:4Z:236:GLU:HG3 | 2.04 | 0.56 |
| 9:4Z:273:ASP:O | 9:4Z:277:LYS:HG2 | 2.05 | 0.56 |
| 10:5A:374:GLN:O | 10:5A:378:ASN:ND2 | 2.37 | 0.56 |
| 10:5B:230:ARG:O | 10:5B:234:LEU:HG | 2.05 | 0.56 |
| 10:5D:211:ARG:HH12 | 10:5D:215:ALA:HB2 | 1.70 | 0.56 |
| 12:5F:107:ASP:OD2 | 33:7Q:175:ARG:HD3 | 2.05 | 0.56 |
| 12:5F:314:GLN:NE2 | 12:7B:57:THR:O | 2.38 | 0.56 |
| 15:5O:265:VAL:CG1 | 15:5O:309:LEU:HD12 | 2.36 | 0.56 |
| 15:5P:42:ASN:HD22 | 15:5P:44:ARG:HH12 | 1.53 | 0.56 |
| 18:5X:102:ASP:N | 18:5X:102:ASP:OD1 | 2.37 | 0.56 |
| 18:6B:5:VAL:O | 18:6B:5:VAL:HG12 | 2.06 | 0.56 |
| 22:6L:177:LEU:CD1 | 22:6L:252:ASP:OD2 | 2.53 | 0.56 |
| 22:6O:110:ILE:O | 22:6O:113:ARG:NH1 | 2.35 | 0.56 |
| 24:6T:556:ASP:OD1 | 24:6T:557:VAL:N | 2.39 | 0.56 |
| 24:6U:35:TYR:CE2 | 24:6U:42:GLU:HB2 | 2.40 | 0.56 |
| 24:6V:536:ASP:OD1 | 24:6V:537:GLU:N | 2.38 | 0.56 |
| 24:6Z:96:LEU:HD22 | 24:6Z:188:THR:HG22 | 1.88 | 0.56 |
| 24:6Z:416:ILE:HG12 | 24:6Z:509:GLU:OE2 | 2.06 | 0.56 |
| 12:7B:52:GLU:O | 12:7B:56:THR:HG23 | 2.06 | 0.56 |
| 26:7E:49:PRO:HA | 26:7E:55:THR:OG1 | 2.06 | 0.56 |
| 28:7H:434:TYR:CE2 | 28:7H:436:SER:HB3 | 2.39 | 0.56 |
| 29:7I:4:LYS:HD2 | 29:7I:4:LYS:N | 2.05 | 0.56 |
| 29:7J:376:ALA:HB3 | 29:7J:379:ASN:HD22 | 1.67 | 0.56 |
| 34:7R:273:LEU:HD12 | 35:7T:223:PHE:CZ | 2.39 | 0.56 |
| 28:7X:434:TYR:CE2 | 28:7X:436:SER:HB3 | 2.39 | 0.56 |
| 1:A7:80:PRO:HD2 | 24:6T:221:ARG:HH12 | 1.70 | 0.56 |
| 2:E3:33:ASP:OD2 | 22:6K:131:ARG:NH1 | 2.38 | 0.56 |
| 1:G2:156:ARG:NH1 | 1:G2:197:ASP:OD1 | 2.38 | 0.56 |
| 1:G8:219:THR:N | 24:6Z:418:ASP:OD1 | 2.37 | 0.56 |
| 2:H3:220:GLU:HG2 | 2:H3:221:ARG:HG3 | 1.88 | 0.56 |
| 2:H7:179:THR:O | 1:H8:350:LYS:HD2 | 2.05 | 0.56 |
| 1:I0:272:PRO:HB2 | 1:I0:282:ARG:HH12 | 1.71 | 0.56 |
| 1:I8:128:ASP:OD1 | 1:I8:129:CYS:N | 2.36 | 0.56 |
| 2:K1:82:THR:HG21 | 28:7X:421:GLY:HA3 | 1.87 | 0.56 |
| 1:L2:4:ILE:HB | 1:L2:50:TYR:HE1 | 1.69 | 0.56 |
| 2:L5:119:LEU:HA | 2:L5:122:ILE:HG22 | 1.88 | 0.56 |
| 1:N0:139:LEU:HD12 | 1:N0:170:VAL:HG12 | 1.88 | 0.56 |
| 1:N2:86:ARG:HB3 | 2:O9:283:HIS:HE1 | 1.71 | 0.56 |
| 2:N5:206:ASN:OD1 | 41:N6:501:GTP:N2 | 2.37 | 0.56 |
| 1:N6:20:PHE:HA | 1:N6:230:SER:OG | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O9:167:LEU:HG | 2:O9:252:ILE:HD11 | 1.88 | 0.56 |
| 1:P8:68:LEU:HB3 | 1:P8:96:GLY:HA2 | 1.86 | 0.56 |
| 2:S1:278:ALA:HA | 2:S1:369:ALA:HB2 | 1.86 | 0.56 |
| 1:S8:1:MET:HA | 1:S8:1:MET:CE | 2.36 | 0.56 |
| 2:S9:335:ILE:HG23 | 2:S9:341:ILE:HD11 | 1.87 | 0.56 |
| 2:T5:90:GLU:HB3 | 2:T5:121:ARG:NH1 | 2.20 | 0.56 |
| 2:U3:264:ARG:NH2 | 2:U3:431:ASP:OD2 | 2.39 | 0.56 |
| 1:W4:232:VAL:HG22 | 1:W4:270:PHE:HB2 | 1.88 | 0.56 |
| 1:X0:287:PRO:HA | 1:X0:290:THR:HG22 | 1.86 | 0.56 |
| 1:X2:113:ILE:HA | 1:X2:116:VAL:HG22 | 1.86 | 0.56 |
| 1:X2:238:CYS:SG | 1:X2:316:LEU:HD21 | 2.45 | 0.56 |
| 1:Z8:113:ILE:HA | 1:Z8:116:VAL:HG22 | 1.87 | 0.56 |
| 2:Z9:70:LEU:HG | 2:Z9:145:THR:HG23 | 1.87 | 0.56 |
| 1:0E:136:CYS:HG | 1:0E:167:PHE:HD2 | 1.54 | 0.56 |
| 2:0L:401:LYS:HD2 | 1:0M:344:TRP:CD2 | 2.40 | 0.56 |
| 2:0P:344:VAL:HG13 | 2:0P:346:TRP:CD1 | 2.41 | 0.56 |
| 1:1C:127:CYS:SG | 1:1C:128:ASP:N | 2.79 | 0.56 |
| 2:1D:222:PRO:HD2 | 1:1E:324:LYS:HE3 | 1.87 | 0.56 |
| 2:1F:183:GLU:HG3 | 2:1F:184:PRO:HD3 | 1.86 | 0.56 |
| 1:1G:35:THR:HG1 | 1:1G:37:HIS:HE2 | 1.49 | 0.56 |
| 2:1N:53:PHE:HB3 | 2:1N:61:HIS:HB3 | 1.87 | 0.56 |
| 1:1O:215:LEU:HB3 | 1:1O:217:LEU:CD2 | 2.35 | 0.56 |
| 2:1Z:387:ILE:HG12 | 2:1Z:390:ARG:HH22 | 1.69 | 0.56 |
| 2:1Z:392:ASP:OD2 | 2:1Z:422:ARG:NH1 | 2.38 | 0.56 |
| 2:1Z:414:GLU:HG2 | 2:1Z:416:GLY:H | 1.70 | 0.56 |
| 1:2W:306:ARG:NH1 | 38:8B:51:GLN:OE1 | 2.38 | 0.56 |
| 1:2Y:334:GLN:HE22 | 1:2Y:348:ASN:H | 1.53 | 0.56 |
| 1:3A:211:CYS:HA | 1:3A:215:LEU:HB2 | 1.86 | 0.56 |
| 1:3M:285:THR:OG1 | 1:3M:287:PRO:HD2 | 2.05 | 0.56 |
| 1:3Q:389:PHE:O | 1:3Q:392:LYS:NZ | 2.32 | 0.56 |
| 2:3R:406:HIS:HA | 2:3R:409:VAL:HG22 | 1.86 | 0.56 |
| 2:3T:104:ALA:H | 2:3T:408:TYR:HE2 | 1.51 | 0.56 |
| 3:3X:15:ARG:HA | 3:3X:19:LEU:HG | 1.88 | 0.56 |
| 3:4B:15:ARG:HA | 3:4B:19:LEU:HG | 1.88 | 0.56 |
| 4:4E:35:LYS:NZ | 3:4F:254:LYS:O | 2.30 | 0.56 |
| 4:4E:149:ILE:HG22 | 4:4E:150:GLU:HG2 | 1.87 | 0.56 |
| 3:4H:15:ARG:HA | 3:4H:19:LEU:HG | 1.88 | 0.56 |
| 4:4I:149:ILE:HG22 | 4:4I:150:GLU:HG2 | 1.87 | 0.56 |
| 5:4L:287:LYS:O | 5:4L:290:GLN:HB2 | 2.05 | 0.56 |
| 7:4R:166:ALA:HB1 | 11:5E:84:SER:N | 2.20 | 0.56 |
| 7:4U:101:ASP:N | 7:4U:101:ASP:OD1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:4X:111:GLY:HA2 | 8:4X:114:ARG:HH21 | 1.70 | 0.56 |
| 15:5O:102:ALA:HB2 | 15:5O:204:ALA:HB1 | 1.87 | 0.56 |
| 19:6E:41:ALA:HB2 | 19:6E:61:ASP:HB2 | 1.86 | 0.56 |
| 19:6E:92:ARG:CD | 19:6E:99:ARG:NE | 2.63 | 0.56 |
| 22:6L:204:PHE:HA | 22:6L:227:TYR:OH | 2.05 | 0.56 |
| 22:6O:291:GLU:HB3 | 22:6O:347:CYS:SG | 2.45 | 0.56 |
| 24:6X:117:ARG:NH1 | 24:6X:134:GLU:OE2 | 2.39 | 0.56 |
| 24:6X:514:TYR:CA | 24:6X:517:LEU:HD13 | 2.31 | 0.56 |
| 24:7A:96:LEU:HD22 | 24:7A:188:THR:HG22 | 1.87 | 0.56 |
| 27:7G:49:HIS:O | 27:7G:53:VAL:HG22 | 2.05 | 0.56 |
| 32:7P:128:ARG:HD2 | 32:7P:132:SER:OG | 2.05 | 0.56 |
| 34:7R:93:GLU:HA | 34:7R:96:LYS:HG2 | 1.87 | 0.56 |
| 2:B9:279:GLU:OE2 | 18:6C:44:HIS:CE1 | 2.59 | 0.56 |
| 1:F6:218:THR:HG21 | 24:6T:430:PRO:HA | 1.87 | 0.56 |
| 2:G1:381:SER:OG | 2:G1:382:THR:N | 2.38 | 0.56 |
| 2:G9:312:TYR:HD1 | 2:G9:381:SER:HB2 | 1.70 | 0.56 |
| 1:H2:285:THR:HG23 | 1:H2:287:PRO:HD2 | 1.86 | 0.56 |
| 1:I2:4:ILE:HB | 1:I2:50:TYR:HE1 | 1.70 | 0.56 |
| 1:I4:50:TYR:CE2 | 1:I4:241:ARG:HD3 | 2.40 | 0.56 |
| 2:I5:173:PRO:HB3 | 2:I5:183:GLU:CD | 2.26 | 0.56 |
| 2:J1:312:TYR:HB2 | 2:J1:343:PHE:HD1 | 1.70 | 0.56 |
| 1:J6:135:VAL:HG21 | 1:J6:152:ILE:HD11 | 1.88 | 0.56 |
| 1:J8:52:ASN:OD1 | 1:J8:62:ARG:NH2 | 2.39 | 0.56 |
| 1:L6:317:PHE:HE2 | 1:L6:326:VAL:HG13 | 1.69 | 0.56 |
| 2:L9:191:THR:HA | 2:L9:194:LEU:HB3 | 1.87 | 0.56 |
| 1:M8:3:GLU:HB2 | 1:M8:130:LEU:HA | 1.88 | 0.56 |
| 2:M9:274:PRO:HB2 | 2:M9:276:ILE:HG12 | 1.87 | 0.56 |
| 2:N5:276:ILE:HG23 | 2:N5:280:LYS:HB2 | 1.88 | 0.56 |
| 2:N5:405:VAL:HG13 | 2:N5:418:PHE:HE2 | 1.69 | 0.56 |
| 1:O4:2:ARG:HB3 | 1:O4:131:GLN:HB2 | 1.87 | 0.56 |
| 2:O5:9:ILE:HG22 | 2:O5:146:GLY:HA2 | 1.87 | 0.56 |
| 1:O8:190:HIS:CD2 | 1:O8:411:ALA:HA | 2.41 | 0.56 |
| 1:P4:213:ARG:HE | 1:P4:297:LYS:CE | 2.18 | 0.56 |
| 1:P4:391:ARG:HB2 | 2:P5:346:TRP:CZ3 | 2.41 | 0.56 |
| 2:P9:88:HIS:HB3 | 2:P9:90:GLU:H | 1.70 | 0.56 |
| 1:R0:424:GLN:HE22 | 17:5S:104:PHE:H | 1.53 | 0.56 |
| 2:R3:387:ILE:HG12 | 2:R3:390:ARG:HH22 | 1.71 | 0.56 |
| 1:R8:69:GLU:C | 1:R8:92:PHE:HZ | 2.08 | 0.56 |
| 2:R9:306:ASP:HB3 | 2:R9:309:HIS:HD2 | 1.69 | 0.56 |
| 1:S2:377:MET:HB3 | 1:S2:380:ARG:HH21 | 1.69 | 0.56 |
| 2:S7:240:ALA:HB1 | 2:S7:356:ASN:HD22 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S9:104:ALA:CB | 2:S9:413:MET:HG3 | 2.35 | 0.56 |
| 2:T7:275:ILE:HG13 | 2:T7:368:LEU:HD21 | 1.86 | 0.56 |
| 1:T8:139:LEU:HD12 | 1:T8:170:VAL:HG12 | 1.87 | 0.56 |
| 2:U7:75:VAL:HG12 | 2:U7:79:ARG:HE | 1.69 | 0.56 |
| 1:V0:68:LEU:HB3 | 1:V0:96:GLY:HA2 | 1.86 | 0.56 |
| 1:V6:3:GLU:HB3 | 1:V6:130:LEU:HA | 1.88 | 0.56 |
| 1:V6:22:GLU:HG2 | 1:V6:81:TYR:HB2 | 1.85 | 0.56 |
| 1:V6:199:CYS:HG | 1:V6:265:PHE:HD1 | 1.53 | 0.56 |
| 1:W0:33:THR:HG23 | 1:W0:35:THR:HG23 | 1.88 | 0.56 |
| 1:W0:177:ASP:O | 2:W1:352:LYS:HA | 2.06 | 0.56 |
| 2:X3:399:TYR:O | 2:X3:402:ARG:NH1 | 2.39 | 0.56 |
| 2:X5:109:THR:OG1 | 2:X5:411:GLU:OE2 | 2.15 | 0.56 |
| 2:Z1:31:GLN:HE21 | 2:Z1:37:PRO:HG3 | 1.71 | 0.56 |
| 2:Z3:278:ALA:HA | 2:Z3:369:ALA:HB2 | 1.88 | 0.56 |
| 1:0A:83:GLN:O | 1:0Q:281:TYR:OH | 2.16 | 0.56 |
| 2:0L:194:LEU:O | 2:0L:198:THR:HG22 | 2.04 | 0.56 |
| 2:0R:26:LEU:HD23 | 2:0R:363:VAL:HG12 | 1.88 | 0.56 |
| 1:0U:208:TYR:CE1 | 1:0U:225:LEU:HD21 | 2.40 | 0.56 |
| 2:0V:222:PRO:HD2 | 1:0W:324:LYS:HE3 | 1.86 | 0.56 |
| 2:1D:102:ASN:HD21 | 1:1E:255:VAL:HG21 | 1.70 | 0.56 |
| 1:1S:309:ARG:NH1 | 1:1S:339:SER:O | 2.39 | 0.56 |
| 2:1X:338:LYS:HG2 | 2:1X:340:THR:HG22 | 1.86 | 0.56 |
| 1:2E:418:LEU:HG | 1:2E:422:TYR:HE2 | 1.70 | 0.56 |
| 2:2L:274:PRO:HB2 | 2:2L:276:ILE:HG12 | 1.86 | 0.56 |
| 2:2Z:27:GLU:OE1 | 2:2Z:243:ARG:NH1 | 2.39 | 0.56 |
| 2:3H:278:ALA:HA | 2:3H:369:ALA:HB2 | 1.87 | 0.56 |
| 1:3I:391:ARG:HD3 | 2:3J:346:TRP:CZ2 | 2.40 | 0.56 |
| 1:3O:113:ILE:HA | 1:3O:116:VAL:HG12 | 1.88 | 0.56 |
| 1:3S:334:GLN:HE22 | 1:3S:348:ASN:H | 1.51 | 0.56 |
| 3:3Z:15:ARG:HA | 3:3Z:19:LEU:HG | 1.88 | 0.56 |
| 6:4N:463:LEU:HD12 | 6:4N:487:ILE:HD11 | 1.85 | 0.56 |
| 7:4R:95:HIS:HD1 | 7:4R:95:HIS:H | 1.54 | 0.56 |
| 12:5F:2:LEU:HD12 | 12:5F:3:PRO:HD2 | 1.87 | 0.56 |
| 12:5F:300:PRO:HG2 | 12:7B:13:PRO:HB3 | 1.88 | 0.56 |
| 14:5N:167:GLY:O | 14:5N:196:VAL:HG13 | 2.05 | 0.56 |
| 17:5U:188:LYS:O | 17:5U:192:VAL:HG23 | 2.05 | 0.56 |
| 18:5X:125:ARG:NH2 | 18:5X:204:LEU:O | 2.38 | 0.56 |
| 19:6E:20:LEU:CD2 | 19:6E:28:ARG:HH21 | 2.19 | 0.56 |
| 20:6F:329:SER:HA | 20:6F:332:GLU:OE2 | 2.05 | 0.56 |
| 22:6P:269:GLU:HA | 22:6P:272:ARG:NE | 2.13 | 0.56 |
| 24:6U:35:TYR:CD2 | 24:6U:42:GLU:HB2 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:7R:104:ASP:O | 34:7R:108:LEU:HG | 2.05 | 0.56 |
| 34:7S:263:GLU:O | 34:7S:267:VAL:HG23 | 2.05 | 0.56 |
| 36:7V:34:ILE:HB | 36:7V:70:ILE:HD11 | 1.86 | 0.56 |
| 36:7V:54:GLU:HG3 | 36:7V:55:VAL:N | 2.20 | 0.56 |
| 38:8C:201:LEU:O | 38:8C:201:LEU:HD13 | 2.05 | 0.56 |
| 2:C1:2:ARG:HH12 | 24:6Z:243:LYS:NZ | 2.03 | 0.56 |
| 2:F3:33:ASP:OD2 | 22:6P:131:ARG:NH1 | 2.37 | 0.56 |
| 2:G3:417:GLU:HA | 2:G3:420:GLU:HG2 | 1.88 | 0.56 |
| 1:G6:216:LYS:O | 24:6Y:422:ASN:ND2 | 2.32 | 0.56 |
| 2:G9:282:TYR:OH | 22:6P:134:ASN:ND2 | 2.39 | 0.56 |
| 2:I1:301:MET:HE1 | 2:I1:307:PRO:HD3 | 1.88 | 0.56 |
| 2:I1:326:LYS:HG3 | 2:I1:327:ASP:N | 2.21 | 0.56 |
| 2:I3:344:VAL:HG22 | 2:I3:346:TRP:HE3 | 1.70 | 0.56 |
| 2:J1:301:MET:HE1 | 2:J1:307:PRO:HD3 | 1.86 | 0.56 |
| 2:J5:189:LEU:HD11 | 2:J5:418:PHE:HE1 | 1.71 | 0.56 |
| 2:L7:115:VAL:HG23 | 2:L7:153:LEU:HD22 | 1.88 | 0.56 |
| 1:M2:309:ARG:NH1 | 1:M2:341:PHE:O | 2.39 | 0.56 |
| 2:M7:9:ILE:HG22 | 2:M7:146:GLY:HA2 | 1.86 | 0.56 |
| 2:M9:98:ASP:OD1 | 2:M9:99:ALA:N | 2.39 | 0.56 |
| 2:M9:250:VAL:HG11 | 2:M9:352:LYS:HE3 | 1.88 | 0.56 |
| 2:N5:137:VAL:HG22 | 2:N5:168:GLY:HA2 | 1.87 | 0.56 |
| 1:O0:101:TRP:CE3 | 1:O0:187:LEU:HD23 | 2.39 | 0.56 |
| 2:O1:280:LYS:HA | 2:O1:283:HIS:HB3 | 1.87 | 0.56 |
| 2:O5:14:ILE:HD11 | 2:O5:74:VAL:HG13 | 1.86 | 0.56 |
| 1:O6:245:GLN:HE21 | 32:7P:115:THR:HG21 | 1.71 | 0.56 |
| 1:P4:166:THR:OG1 | 1:P4:199:CYS:SG | 2.62 | 0.56 |
| 1:P4:177:ASP:O | 2:P5:352:LYS:HA | 2.06 | 0.56 |
| 2:R1:56:THR:HA | 2:S7:285:GLN:HB3 | 1.87 | 0.56 |
| 2:R1:267:PHE:HB2 | 2:R1:384:ILE:HD12 | 1.86 | 0.56 |
| 1:R6:208:TYR:CE1 | 1:R6:225:LEU:HD11 | 2.41 | 0.56 |
| 1:S0:248:ALA:HA | 1:S0:252:LYS:HD2 | 1.87 | 0.56 |
| 1:S4:173:PRO:HD3 | 1:S4:380:ARG:HD2 | 1.87 | 0.56 |
| 1:S6:391:ARG:HH22 | 2:S7:435:VAL:HA | 1.71 | 0.56 |
| 1:S8:94:GLN:HB3 | 24:6W:35:TYR:HE1 | 1.67 | 0.56 |
| 1:S8:107:THR:OG1 | 1:S8:108:GLU:OE1 | 2.22 | 0.56 |
| 2:T1:69:ASP:OD1 | 2:T1:70:LEU:N | 2.39 | 0.56 |
| 1:T2:320:ARG:HH12 | 12:5F:177:THR:HA | 1.70 | 0.56 |
| 1:T2:375:GLN:HB3 | 1:T2:422:TYR:CD2 | 2.31 | 0.56 |
| 1:T8:292:GLN:HG2 | 1:T8:298:ASN:ND2 | 2.21 | 0.56 |
| 2:U1:26:LEU:HD21 | 2:U1:363:VAL:HG12 | 1.87 | 0.56 |
| 1:U4:178:THR:HG23 | 1:U4:181:GLU:HG3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U6:113:ILE:HA | 1:U6:116:VAL:HG22 | 1.86 | 0.56 |
| 2:U7:11:GLN:OE1 | 2:U7:15:GLN:NE2 | 2.38 | 0.56 |
| 1:V6:5:VAL:HG12 | 1:V6:62:ARG:HD3 | 1.88 | 0.56 |
| 1:W0:178:THR:OG1 | 2:W1:258:ASN:ND2 | 2.38 | 0.56 |
| 1:W2:248:ALA:HA | 1:W2:252:LYS:HD2 | 1.88 | 0.56 |
| 2:W9:5:ILE:HD11 | 2:W9:122:ILE:HG13 | 1.88 | 0.56 |
| 2:W9:70:LEU:HD11 | 2:W9:110:ILE:HG21 | 1.88 | 0.56 |
| 1:X4:101:TRP:CE3 | 1:X4:187:LEU:HD23 | 2.40 | 0.56 |
| 1:Z0:372:THR:HG21 | 1:Z0:426:GLN:HB2 | 1.88 | 0.56 |
| 2:Z9:99:ALA:HA | 2:Z9:105:ARG:HD3 | 1.87 | 0.56 |
| 2:0B:11:GLN:OE1 | 2:0B:15:GLN:NE2 | 2.39 | 0.56 |
| 2:0L:76:ASP:OD1 | 2:0L:79:ARG:HD2 | 2.06 | 0.56 |
| 1:0U:404:ASP:HB3 | 1:0U:406:MET:SD | 2.45 | 0.56 |
| 1:1A:235:GLY:HA3 | 1:1A:366:THR:HG21 | 1.86 | 0.56 |
| 1:1E:3:GLU:HG2 | 1:1E:127:CYS:SG | 2.45 | 0.56 |
| 2:1F:116:ASP:N | 2:1F:116:ASP:OD1 | 2.38 | 0.56 |
| 2:1Z:239:THR:HG23 | 2:1Z:243:ARG:HE | 1.71 | 0.56 |
| 2:2H:27:GLU:OE1 | 2:2H:243:ARG:NH1 | 2.35 | 0.56 |
| 1:2I:248:ALA:HA | 1:2I:252:LYS:HD2 | 1.88 | 0.56 |
| 1:2Q:332:ASN:HD21 | 38:7Z:1:MET:HA | 1.70 | 0.56 |
| 2:2R:214:ARG:NE | 2:2R:220:GLU:OE2 | 2.39 | 0.56 |
| 1:2S:48:ASN:ND2 | 23:6Q:75:GLY:O | 2.38 | 0.56 |
| 2:2T:90:GLU:HG3 | 2:2T:121:ARG:NH1 | 2.20 | 0.56 |
| 2:3D:334:THR:HG21 | 38:8D:111:THR:HG22 | 1.88 | 0.56 |
| 2:3P:51:THR:HG21 | 2:3P:243:ARG:HG2 | 1.87 | 0.56 |
| 2:3P:100:ALA:HA | 1:3Q:252:LYS:HE2 | 1.87 | 0.56 |
| 2:3R:306:ASP:HB3 | 2:3R:309:HIS:HD2 | 1.70 | 0.56 |
| 2:3T:12:ALA:O | 2:3T:16:VAL:HG13 | 2.05 | 0.56 |
| 2:3T:230:LEU:HD12 | 2:3T:231:ILE:HD13 | 1.86 | 0.56 |
| 14:5N:378:ILE:HG22 | 23:6S:55:VAL:HB | 1.88 | 0.56 |
| 22:6O:186:ARG:O | 22:6O:189:LYS:HB2 | 2.05 | 0.56 |
| 31:7M:66:HIS:HD2 | 31:7M:76:THR:HA | 1.70 | 0.56 |
| 1:7:78:SER:OG | 24:6W:149:LYS:N | 2.39 | 0.56 |
| 1:G2:2:ARG:HE | 1:G2:240:LEU:HD22 | 1.71 | 0.56 |
| 2:G3:74:VAL:O | 2:G3:78:VAL:HG23 | 2.05 | 0.56 |
| 1:G4:54:ALA:HB3 | 1:G4:58:ARG:HB3 | 1.86 | 0.56 |
| 1:I0:139:LEU:HD12 | 1:I0:170:VAL:HG12 | 1.88 | 0.56 |
| 2:I9:217:LEU:HB3 | 2:I9:219:ILE:HD12 | 1.86 | 0.56 |
| 1:J2:88:ASP:O | 16:5Q:186:HIS:HD2 | 1.88 | 0.56 |
| 1:J4:259:PRO:HG2 | 1:J4:263:LEU:HD23 | 1.86 | 0.56 |
| 1:J6:309:ARG:H | 1:J6:372:THR:HG22 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J7:88:HIS:HD2 | 2:L3:283:HIS:HB3 | 1.71 | 0.56 |
| 2:J9:133:GLN:HE22 | 2:J9:242:LEU:HD21 | 1.70 | 0.56 |
| 2:J9:189:LEU:HD11 | 2:J9:418:PHE:HE1 | 1.70 | 0.56 |
| 2:K7:69:ASP:OD1 | 2:K7:71:GLU:N | 2.35 | 0.56 |
| 1:L0:58:ARG:N | 30:7K:118:TYR:OH | 2.38 | 0.56 |
| 2:L3:319:TYR:HB3 | 2:L3:323:VAL:HG21 | 1.87 | 0.56 |
| 2:M7:133:GLN:HB3 | 2:M7:252:ILE:HG21 | 1.88 | 0.56 |
| 2:M9:280:LYS:NZ | 29:7J:320:PRO:CB | 2.68 | 0.56 |
| 1:N6:248:ALA:HA | 1:N6:252:LYS:HD2 | 1.87 | 0.56 |
| 2:O5:221:ARG:HD2 | 32:7P:136:HIS:ND1 | 2.21 | 0.56 |
| 2:O5:305:CYS:HB3 | 2:O5:387:ILE:HD11 | 1.87 | 0.56 |
| 1:O6:131:GLN:HE21 | 1:O6:250:LEU:HB2 | 1.71 | 0.56 |
| 2:O7:223:THR:HG23 | 2:O7:225:THR:H | 1.71 | 0.56 |
| 2:P9:5:ILE:HD11 | 2:P9:135:PHE:CE1 | 2.41 | 0.56 |
| 2:Q3:5:ILE:HG22 | 2:Q3:64:ARG:HB3 | 1.87 | 0.56 |
| 1:R4:70:PRO:HA | 1:R4:92:PHE:CZ | 2.41 | 0.56 |
| 1:R4:180:VAL:HG22 | 2:R5:258:ASN:HD21 | 1.70 | 0.56 |
| 1:S2:49:VAL:HG11 | 1:S2:241:ARG:HG2 | 1.87 | 0.56 |
| 1:S6:50:TYR:CE2 | 1:S6:241:ARG:HD3 | 2.41 | 0.56 |
| 1:T0:207:LEU:HB3 | 1:T0:225:LEU:HD22 | 1.87 | 0.56 |
| 2:U3:56:THR:HA | 2:V9:285:GLN:HB2 | 1.87 | 0.56 |
| 1:V0:6:HIS:HE2 | 1:V0:136:CYS:HG | 1.54 | 0.56 |
| 2:V1:88:HIS:HB2 | 2:W7:283:HIS:HB3 | 1.88 | 0.56 |
| 1:V4:249:ASP:H | 1:V4:252:LYS:HD2 | 1.71 | 0.56 |
| 2:X9:254:GLU:HB3 | 2:X9:352:LYS:HE2 | 1.87 | 0.56 |
| 1:Y8:151:LEU:O | 1:Y8:155:ILE:HG12 | 2.05 | 0.56 |
| 1:Z4:3:GLU:HB2 | 1:Z4:130:LEU:HD12 | 1.88 | 0.56 |
| 2:Z7:12:ALA:HB2 | 41:Z7:501:GTP:C8 | 2.41 | 0.56 |
| 1:Z8:151:LEU:O | 1:Z8:155:ILE:HG12 | 2.06 | 0.56 |
| 2:Z9:5:ILE:HG21 | 2:Z9:122:ILE:HD11 | 1.88 | 0.56 |
| 1:0E:309:ARG:NH1 | 1:0E:343:GLU:OE1 | 2.38 | 0.56 |
| 1:0G:54:ALA:HB3 | 1:0G:58:ARG:HB3 | 1.87 | 0.56 |
| 2:0N:194:LEU:O | 2:0N:198:THR:HG22 | 2.04 | 0.56 |
| 1:0U:104:GLY:HA2 | 1:0U:147:MET:HE3 | 1.88 | 0.56 |
| 2:0X:353:CYS:SG | 2:0X:354:GLY:N | 2.78 | 0.56 |
| 2:1F:198:THR:HG21 | 2:1F:201:ALA:HB2 | 1.86 | 0.56 |
| 1:1M:165:LEU:HG | 1:1M:250:LEU:HD11 | 1.87 | 0.56 |
| 2:1R:195:LEU:HD21 | 2:1R:264:ARG:HD2 | 1.87 | 0.56 |
| 2:1T:287:SER:OG | 2:1T:288:VAL:N | 2.39 | 0.56 |
| 2:1V:224:TYR:HD1 | 2:1V:227:LEU:HD12 | 1.69 | 0.56 |
| 2:2B:176:GLN:HE22 | 2:2B:304:LYS:HE2 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2L:413:MET:HB3 | 2:2L:417:GLU:OE1 | 2.06 | 0.56 |
| 2:2N:101:ASN:HD22 | 2:2N:143:GLY:HA2 | 1.69 | 0.56 |
| 2:2P:358:GLN:NE2 | 38:8A:212:PRO:HB2 | 2.12 | 0.56 |
| 1:2Q:320:ARG:NH2 | 38:8A:198:THR:CB | 2.68 | 0.56 |
| 2:2T:98:ASP:OD1 | 2:2T:99:ALA:N | 2.39 | 0.56 |
| 1:2W:66:MET:SD | 1:2W:147:MET:HG2 | 2.46 | 0.56 |
| 2:2X:214:ARG:NH1 | 38:8B:18:VAL:HA | 2.21 | 0.56 |
| 2:3B:22:GLU:CD | 38:8D:203:PHE:HD1 | 2.08 | 0.56 |
| 2:3F:417:GLU:HA | 2:3F:420:GLU:HG2 | 1.86 | 0.56 |
| 1:3G:135:VAL:HG11 | 1:3G:152:ILE:HD11 | 1.88 | 0.56 |
| 2:3H:251:ASP:OD2 | 2:3H:254:GLU:HG2 | 2.05 | 0.56 |
| 1:3K:133:PHE:HZ | 1:3K:159:TYR:HD2 | 1.53 | 0.56 |
| 1:3M:276:ARG:HG2 | 38:8C:226:ARG:HH12 | 1.69 | 0.56 |
| 10:5C:321:LYS:O | 10:5C:324:GLU:HG3 | 2.05 | 0.56 |
| 14:5L:167:GLY:O | 14:5L:196:VAL:HG13 | 2.06 | 0.56 |
| 14:5M:167:GLY:O | 14:5M:196:VAL:HG13 | 2.06 | 0.56 |
| 14:5N:37:THR:HG22 | 14:5N:595:SER:HB3 | 1.88 | 0.56 |
| 18:5Y:102:ASP:OD1 | 18:5Y:102:ASP:N | 2.37 | 0.56 |
| 18:5Y:125:ARG:NH2 | 18:5Y:204:LEU:O | 2.38 | 0.56 |
| 18:6D:102:ASP:OD1 | 18:6D:102:ASP:N | 2.37 | 0.56 |
| 22:6J:54:ARG:HG3 | 24:6U:285:MET:HG2 | 1.87 | 0.56 |
| 24:6T:278:VAL:HG13 | 24:6T:369:HIS:CD2 | 2.41 | 0.56 |
| 24:6U:452:MET:HA | 24:6U:530:PHE:HA | 1.88 | 0.56 |
| 26:7D:84:ALA:O | 26:7D:88:THR:OG1 | 2.23 | 0.56 |
| 29:7J:292:GLN:HG2 | 30:7K:19:GLN:HE21 | 1.71 | 0.56 |
| 31:7N:104:LYS:HG3 | 31:7N:107:ASP:HB2 | 1.87 | 0.56 |
| 34:7S:211:ARG:O | 34:7S:214:LEU:HG | 2.06 | 0.56 |
| 1:B3:144:GLY:N | 39:B3:501:GDP:O2B | 2.38 | 0.56 |
| 1:B5:276:ARG:NH2 | 24:6X:210:VAL:HG21 | 2.21 | 0.56 |
| 2:B7:84:ARG:NH2 | 18:6B:210:GLU:OE2 | 2.18 | 0.56 |
| 2:C5:367:ASP:OD1 | 18:5X:181:GLN:NE2 | 2.39 | 0.56 |
| 1:G2:2:ARG:HB3 | 1:G2:131:GLN:HB2 | 1.88 | 0.56 |
| 2:G5:205:ASP:OD1 | 2:G5:206:ASN:N | 2.39 | 0.56 |
| 1:G8:334:GLN:NE2 | 1:G8:348:ASN:H | 2.02 | 0.56 |
| 2:H1:241:SER:OG | 2:H1:250:VAL:N | 2.38 | 0.56 |
| 2:H5:417:GLU:HA | 2:H5:420:GLU:HG2 | 1.88 | 0.56 |
| 2:H7:195:LEU:HD21 | 2:H7:264:ARG:HD2 | 1.88 | 0.56 |
| 2:I3:379:SER:OG | 2:I3:380:ASN:N | 2.37 | 0.56 |
| 1:I8:350:LYS:NZ | 1:I8:351:SER:O | 2.39 | 0.56 |
| 2:I9:145:THR:OG1 | 41:J0:501:GTP:O1B | 2.24 | 0.56 |
| 2:K1:259:LEU:HD23 | 2:K1:268:MET:HG2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K7:198:THR:HG21 | 2:K7:201:ALA:HB2 | 1.87 | 0.56 |
| 2:N1:333:ALA:O | 2:N1:337:THR:HG23 | 2.06 | 0.56 |
| 1:N6:193:VAL:HG13 | 1:N6:194:GLU:HG3 | 1.86 | 0.56 |
| 2:O9:53:PHE:HB3 | 2:O9:61:HIS:HB3 | 1.87 | 0.56 |
| 1:Q0:287:PRO:HA | 1:Q0:290:THR:HG22 | 1.87 | 0.56 |
| 2:Q5:413:MET:HB3 | 2:Q5:417:GLU:OE2 | 2.05 | 0.56 |
| 1:S0:71:GLY:HA2 | 24:6Z:29:LYS:HD3 | 1.87 | 0.56 |
| 2:S1:91:GLN:HG2 | 2:S1:121:ARG:HH21 | 1.70 | 0.56 |
| 1:S2:207:LEU:HB3 | 1:S2:225:LEU:HD22 | 1.86 | 0.56 |
| 2:S7:119:LEU:HD11 | 2:S7:156:ARG:HD3 | 1.86 | 0.56 |
| 1:T8:190:HIS:NE2 | 1:T8:414:ASN:OD1 | 2.39 | 0.56 |
| 1:U2:3:GLU:HB2 | 1:U2:130:LEU:HA | 1.87 | 0.56 |
| 2:U7:191:THR:HA | 2:U7:194:LEU:HB3 | 1.87 | 0.56 |
| 2:U9:286:LEU:HD11 | 2:U9:291:ILE:HG23 | 1.87 | 0.56 |
| 2:V3:274:PRO:HG3 | 2:V3:286:LEU:HD21 | 1.88 | 0.56 |
| 2:V7:109:THR:OG1 | 2:V7:411:GLU:OE2 | 2.21 | 0.56 |
| 2:V9:56:THR:HG21 | 2:V9:62:VAL:HG13 | 1.87 | 0.56 |
| 2:W1:88:HIS:HB3 | 2:W1:91:GLN:CG | 2.35 | 0.56 |
| 1:X2:240:LEU:HD11 | 1:X2:250:LEU:HD11 | 1.88 | 0.56 |
| 2:Y1:90:GLU:H | 2:Z7:283:HIS:HE1 | 1.52 | 0.56 |
| 1:Y2:3:GLU:HB2 | 1:Y2:130:LEU:HA | 1.86 | 0.56 |
| 2:Z7:3:GLU:HG3 | 2:Z7:51:THR:HA | 1.87 | 0.56 |
| 2:0F:145:THR:OG1 | 41:0F:501:GTP:O1B | 2.24 | 0.56 |
| 2:0H:69:ASP:OD1 | 2:0H:70:LEU:N | 2.37 | 0.56 |
| 1:0I:67:ASP:OD2 | 1:0I:72:THR:OG1 | 2.12 | 0.56 |
| 1:0M:389:PHE:O | 1:0M:392:LYS:NZ | 2.32 | 0.56 |
| 2:0N:50:ASN:O | 2:0N:64:ARG:NH2 | 2.37 | 0.56 |
| 2:0N:278:ALA:HA | 2:0N:369:ALA:HB2 | 1.88 | 0.56 |
| 2:0N:352:LYS:NZ | 2:0N:353:CYS:O | 2.39 | 0.56 |
| 1:1C:72:THR:O | 1:1C:76:VAL:HG23 | 2.06 | 0.56 |
| 1:1C:215:LEU:HB3 | 1:1C:217:LEU:HG | 1.88 | 0.56 |
| 2:1P:90:GLU:HG2 | 2:1P:121:ARG:NH1 | 2.20 | 0.56 |
| 1:1U:392:LYS:HD2 | 1:1U:395:LEU:HD22 | 1.87 | 0.56 |
| 1:2A:52:ASN:OD1 | 1:2A:62:ARG:NH2 | 2.38 | 0.56 |
| 1:2C:12:CYS:SG | 1:2C:13:GLY:N | 2.78 | 0.56 |
| 1:2I:34:GLY:O | 1:2I:58:ARG:HA | 2.05 | 0.56 |
| 2:2L:279:GLU:HA | 2:2L:279:GLU:OE2 | 2.04 | 0.56 |
| 1:2U:299:MET:O | 38:8B:105:ARG:NH2 | 2.39 | 0.56 |
| 1:3A:274:THR:CG2 | 1:3A:282:ARG:HH11 | 2.19 | 0.56 |
| 2:3F:220:GLU:HG2 | 38:8A:177:HIS:CB | 2.32 | 0.56 |
| 2:3H:392:ASP:OD2 | 2:3H:422:ARG:NH1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3S:22:GLU:HG2 | 1:3S:81:TYR:HB2 | 1.87 | 0.56 |
| 1:3S:329:GLN:O | 1:3S:333:VAL:HG23 | 2.06 | 0.56 |
| 2:3T:102:ASN:HB3 | 2:3T:105:ARG:HB3 | 1.88 | 0.56 |
| 2:3T:287:SER:N | 2:3T:290:GLU:OE2 | 2.38 | 0.56 |
| 3:3V:153:ASP:OD1 | 3:3V:156:HIS:N | 2.37 | 0.56 |
| 3:4H:153:ASP:OD1 | 3:4H:156:HIS:N | 2.37 | 0.56 |
| 5:4M:178:GLU:O | 5:4M:182:VAL:HG23 | 2.06 | 0.56 |
| 8:4V:472:VAL:HG22 | 8:4V:473:LYS:HG3 | 1.88 | 0.56 |
| 11:5E:171:ASP:OD1 | 11:5E:172:GLY:N | 2.37 | 0.56 |
| 14:5L:37:THR:HG22 | 14:5L:595:SER:HB3 | 1.88 | 0.56 |
| 18:5Z:102:ASP:N | 18:5Z:102:ASP:OD1 | 2.37 | 0.56 |
| 18:6B:102:ASP:N | 18:6B:102:ASP:OD1 | 2.37 | 0.56 |
| 18:6D:125:ARG:NH2 | 18:6D:204:LEU:O | 2.38 | 0.56 |
| 24:6T:469:PHE:HB2 | 24:6T:483:PHE:O | 2.06 | 0.56 |
| 24:6U:117:ARG:NH1 | 24:6U:134:GLU:OE2 | 2.39 | 0.56 |
| 26:7E:84:ALA:O | 26:7E:88:THR:OG1 | 2.23 | 0.56 |
| 29:7J:110:THR:O | 29:7J:114:GLU:HG3 | 2.05 | 0.56 |
| 31:7M:80:PRO:CD | 31:7M:83:THR:OG1 | 2.45 | 0.56 |
| 36:7W:54:GLU:HG3 | 36:7W:55:VAL:N | 2.20 | 0.56 |
| 2:A2:42:ILE:HD12 | 24:6Y:93:ARG:HH21 | 1.38 | 0.56 |
| 2:A2:221:ARG:HB2 | 26:7F:77:ILE:O | 2.06 | 0.56 |
| 1:D0:204:ASN:HD21 | 39:D0:501:GDP:HN22 | 1.52 | 0.56 |
| 1:G6:186:THR:HG22 | 1:G6:411:ALA:HB1 | 1.88 | 0.56 |
| 2:H5:278:ALA:HA | 2:H5:369:ALA:HB2 | 1.87 | 0.56 |
| 2:I5:195:LEU:HD21 | 2:I5:264:ARG:HD2 | 1.88 | 0.56 |
| 2:I5:413:MET:HG3 | 2:I5:414:GLU:H | 1.71 | 0.56 |
| 2:I9:417:GLU:HA | 2:I9:420:GLU:HG2 | 1.88 | 0.56 |
| 1:J8:211:CYS:HA | 1:J8:215:LEU:HB2 | 1.87 | 0.56 |
| 2:J9:88:HIS:CD2 | 2:L5:283:HIS:HA | 2.41 | 0.56 |
| 2:K9:119:LEU:HA | 2:K9:122:ILE:HG22 | 1.88 | 0.56 |
| 2:L1:102:ASN:HD21 | 2:L1:411:GLU:HG3 | 1.70 | 0.56 |
| 1:L4:31:ASP:OD1 | 1:L4:35:THR:N | 2.39 | 0.56 |
| 2:N3:9:ILE:HD12 | 2:N3:150:GLY:HA3 | 1.87 | 0.56 |
| 2:O1:324:VAL:HG12 | 2:O1:326:LYS:H | 1.70 | 0.56 |
| 1:O2:177:ASP:O | 2:O3:352:LYS:HA | 2.06 | 0.56 |
| 2:O3:346:TRP:CD1 | 2:O3:346:TRP:C | 2.78 | 0.56 |
| 1:O4:52:ASN:OD1 | 1:O4:62:ARG:NH2 | 2.39 | 0.56 |
| 2:O7:254:GLU:HB3 | 2:O7:352:LYS:HE2 | 1.87 | 0.56 |
| 1:P4:285:THR:HG22 | 1:P4:287:PRO:HD2 | 1.88 | 0.56 |
| 1:P6:49:VAL:HG11 | 1:P6:241:ARG:HG2 | 1.88 | 0.56 |
| 2:P7:88:HIS:CG | 2:R3:283:HIS:HB2 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P8:72:THR:O | 1:P8:76:VAL:HG23 | 2.05 | 0.56 |
| 1:Q0:252:LYS:HA | 1:Q0:255:VAL:HG12 | 1.88 | 0.56 |
| 1:Q4:177:ASP:O | 2:Q5:352:LYS:HA | 2.06 | 0.56 |
| 1:Q8:395:LEU:O | 1:Q8:399:THR:HG23 | 2.06 | 0.56 |
| 1:S2:113:ILE:HA | 1:S2:116:VAL:HG12 | 1.88 | 0.56 |
| 2:S7:81:GLY:O | 2:S7:84:ARG:NH1 | 2.39 | 0.56 |
| 2:S9:272:TYR:HB3 | 2:S9:275:ILE:HD11 | 1.88 | 0.56 |
| 1:T0:317:PHE:HB3 | 1:T0:321:MET:SD | 2.46 | 0.56 |
| 2:T3:14:ILE:HD11 | 2:T3:74:VAL:HG13 | 1.88 | 0.56 |
| 2:U1:135:PHE:HB2 | 2:U1:166:LYS:HG2 | 1.87 | 0.56 |
| 2:U1:164:LYS:O | 2:U1:166:LYS:NZ | 2.39 | 0.56 |
| 2:U7:79:ARG:NH1 | 2:U7:94:SER:OG | 2.39 | 0.56 |
| 2:V7:417:GLU:HA | 2:V7:420:GLU:HG2 | 1.88 | 0.56 |
| 1:V8:3:GLU:HB2 | 1:V8:130:LEU:HA | 1.88 | 0.56 |
| 1:W0:140:GLY:HA3 | 1:W0:181:GLU:OE1 | 2.06 | 0.56 |
| 2:W3:264:ARG:NH2 | 2:W3:431:ASP:OD2 | 2.39 | 0.56 |
| 2:W7:11:GLN:OE1 | 2:W7:15:GLN:NE2 | 2.39 | 0.56 |
| 1:X0:263:LEU:HG | 1:X0:422:TYR:CE1 | 2.41 | 0.56 |
| 1:X6:58:ARG:HH11 | 1:X6:84:ILE:HA | 1.69 | 0.56 |
| 2:X7:286:LEU:O | 2:X7:373:ARG:NH1 | 2.38 | 0.56 |
| 2:X9:167:LEU:HD13 | 2:X9:200:VAL:HB | 1.87 | 0.56 |
| 1:Y4:190:HIS:CD2 | 1:Y4:411:ALA:HA | 2.41 | 0.56 |
| 1:Y4:309:ARG:NH1 | 1:Y4:339:SER:O | 2.39 | 0.56 |
| 2:Z5:239:THR:HG23 | 2:Z5:243:ARG:HE | 1.71 | 0.56 |
| 2:0B:62:VAL:HG22 | 2:0B:88:HIS:CE1 | 2.41 | 0.56 |
| 2:0F:384:ILE:HD12 | 2:0F:384:ILE:H | 1.71 | 0.56 |
| 1:0M:121:ARG:NH2 | 1:0M:158:GLU:OE2 | 2.36 | 0.56 |
| 2:1F:290:GLU:HA | 2:1F:293:ASN:HD22 | 1.71 | 0.56 |
| 1:1Q:211:CYS:HA | 1:1Q:215:LEU:HB2 | 1.88 | 0.56 |
| 1:1S:186:THR:HG22 | 1:1S:411:ALA:HB1 | 1.88 | 0.56 |
| 1:1U:332:ASN:HD21 | 1:1U:336:LYS:HE3 | 1.71 | 0.56 |
| 2:2D:129:CYS:SG | 2:2D:130:THR:N | 2.79 | 0.56 |
| 1:2E:268:VAL:HG23 | 1:2E:300:MET:HB2 | 1.88 | 0.56 |
| 1:2M:165:LEU:HD23 | 1:2M:250:LEU:HD21 | 1.88 | 0.56 |
| 1:2M:337:ASN:HB3 | 1:2M:340:TYR:HD2 | 1.69 | 0.56 |
| 2:2P:63:PRO:HB2 | 2:2P:65:CYS:SG | 2.45 | 0.56 |
| 2:2R:406:HIS:HA | 2:2R:409:VAL:HG22 | 1.88 | 0.56 |
| 1:2S:213:ARG:HD2 | 38:8A:47:PHE:CE1 | 2.41 | 0.56 |
| 2:2T:122:ILE:HA | 2:2T:125:LEU:HD12 | 1.88 | 0.56 |
| 2:3D:121:ARG:HA | 2:3D:124:LYS:HZ2 | 1.70 | 0.56 |
| 1:3I:244:GLY:H | 1:3I:247:ASN:HD21 | 1.53 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4D:153:ASP:OD1 | 3:4D:156:HIS:N | 2.37 | 0.56 |
| 6:4O:219:GLU:OE2 | 6:4O:222:ARG:NH2 | 2.37 | 0.56 |
| 10:5B:244:ARG:O | 10:5B:247:GLU:HG3 | 2.05 | 0.56 |
| 10:5C:331:MET:HE1 | 10:5C:334:ARG:HH21 | 1.70 | 0.56 |
| 10:5D:232:GLU:HA | 10:5D:235:ARG:NE | 2.21 | 0.56 |
| 14:5L:555:GLU:O | 14:5L:573:GLY:N | 2.36 | 0.56 |
| 14:5M:37:THR:HG22 | 14:5M:595:SER:HB3 | 1.88 | 0.56 |
| 14:5M:124:GLN:HG3 | 38:8C:232:PHE:HD1 | 1.71 | 0.56 |
| 14:5M:555:GLU:O | 14:5M:573:GLY:N | 2.36 | 0.56 |
| 18:5Z:125:ARG:NH2 | 18:5Z:204:LEU:O | 2.38 | 0.56 |
| 18:6A:102:ASP:N | 18:6A:102:ASP:OD1 | 2.37 | 0.56 |
| 22:6N:137:GLU:HA | 22:6N:140:VAL:HG22 | 1.88 | 0.56 |
| 24:6Y:124:TYR:CE2 | 24:6Y:150:ARG:HG3 | 2.41 | 0.56 |
| 31:7N:43:VAL:O | 31:7N:47:ARG:HG2 | 2.06 | 0.56 |
| 36:7W:34:ILE:HB | 36:7W:70:ILE:HD11 | 1.86 | 0.56 |
| 38:7Z:36:GLU:OE1 | 38:7Z:37:TYR:N | 2.39 | 0.56 |
| 38:8B:158:MET:HA | 38:8B:158:MET:HE3 | 1.88 | 0.56 |
| 1:1:420:SER:OG | 3:3V:209:ARG:NH1 | 2.38 | 0.56 |
| 1:A5:281:TYR:OH | 1:T8:83:GLN:O | 2.07 | 0.56 |
| 2:E9:81:GLY:HA3 | 22:6N:116:TYR:HE2 | 1.70 | 0.56 |
| 1:G6:31:ASP:OD2 | 1:G6:33:THR:OG1 | 2.23 | 0.56 |
| 1:J8:249:ASP:O | 1:J8:253:LEU:HG | 2.06 | 0.56 |
| 2:K5:88:HIS:HB3 | 2:M1:283:HIS:CE1 | 2.41 | 0.56 |
| 2:L1:56:THR:HG23 | 2:L1:60:LYS:HB3 | 1.88 | 0.56 |
| 2:L1:274:PRO:HB2 | 2:L1:276:ILE:HG12 | 1.88 | 0.56 |
| 1:L2:135:VAL:HG21 | 1:L2:152:ILE:HD11 | 1.87 | 0.56 |
| 1:M0:404:ASP:OD1 | 1:M0:405:GLU:N | 2.39 | 0.56 |
| 2:N1:222:PRO:HD2 | 1:N2:324:LYS:HE3 | 1.87 | 0.56 |
| 1:N2:211:CYS:HA | 1:N2:215:LEU:HB2 | 1.88 | 0.56 |
| 1:N6:10:GLY:O | 1:N6:14:ASN:ND2 | 2.39 | 0.56 |
| 1:N6:396:HIS:HA | 1:N6:399:THR:HG22 | 1.87 | 0.56 |
| 2:O1:221:ARG:HD2 | 1:O2:325:GLU:OE2 | 2.05 | 0.56 |
| 2:O9:98:ASP:OD1 | 2:O9:99:ALA:N | 2.39 | 0.56 |
| 2:P7:296:PHE:CE2 | 2:P7:335:ILE:HG21 | 2.41 | 0.56 |
| 1:Q2:5:VAL:HG23 | 1:Q2:62:ARG:HG2 | 1.88 | 0.56 |
| 2:Q9:3:GLU:HB2 | 2:Q9:129:CYS:SG | 2.45 | 0.56 |
| 2:R3:305:CYS:HB3 | 2:R3:387:ILE:HD11 | 1.88 | 0.56 |
| 1:R4:121:ARG:NH2 | 1:R4:158:GLU:OE2 | 2.39 | 0.56 |
| 1:R6:69:GLU:HG3 | 1:R6:71:GLY:H | 1.71 | 0.56 |
| 1:S0:193:VAL:HG23 | 1:S0:194:GLU:HG2 | 1.88 | 0.56 |
| 1:S8:156:ARG:HH22 | 3:3Z:91:LYS:HE2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S8:194:GLU:HB3 | 3:3Z:87:GLY:HA3 | 1.88 | 0.56 |
| 1:T0:153:SER:O | 1:T0:157:GLU:HG2 | 2.05 | 0.56 |
| 2:T1:183:GLU:CD | 2:T1:184:PRO:HD3 | 2.25 | 0.56 |
| 2:T1:223:THR:HG23 | 2:T1:225:THR:H | 1.70 | 0.56 |
| 2:T7:123:ARG:NH2 | 2:T7:160:ASP:OD2 | 2.39 | 0.56 |
| 2:W9:3:GLU:HB2 | 2:W9:129:CYS:SG | 2.46 | 0.56 |
| 2:X3:191:THR:HA | 2:X3:194:LEU:HG | 1.88 | 0.56 |
| 2:Y5:83:TYR:HB3 | 2:Y5:86:LEU:HB3 | 1.87 | 0.56 |
| 1:Y6:246:LEU:HD22 | 1:Y6:352:SER:HA | 1.88 | 0.56 |
| 2:Y9:181:VAL:HB | 1:Z0:256:ASN:HD22 | 1.70 | 0.56 |
| 2:Z3:336:LYS:O | 2:Z3:339:ARG:NH2 | 2.38 | 0.56 |
| 1:Z8:252:LYS:HA | 1:Z8:255:VAL:HG22 | 1.88 | 0.56 |
| 1:0A:211:CYS:HA | 1:0A:215:LEU:HB2 | 1.88 | 0.56 |
| 1:0G:113:ILE:HA | 1:0G:116:VAL:HG22 | 1.88 | 0.56 |
| 1:0M:31:ASP:OD1 | 1:0M:35:THR:N | 2.27 | 0.56 |
| 2:0V:50:ASN:O | 2:0V:64:ARG:NH2 | 2.39 | 0.56 |
| 1:1K:33:THR:O | 1:1K:58:ARG:NH2 | 2.39 | 0.56 |
| 1:1K:285:THR:HG23 | 1:1K:288:GLU:H | 1.71 | 0.56 |
| 1:2I:177:ASP:O | 2:2J:352:LYS:HA | 2.06 | 0.56 |
| 1:2S:257:LEU:HD21 | 1:2S:314:SER:HB3 | 1.88 | 0.56 |
| 1:2Y:173:PRO:HD2 | 1:2Y:380:ARG:CZ | 2.36 | 0.56 |
| 2:3B:223:THR:HG22 | 2:3B:224:TYR:H | 1.71 | 0.56 |
| 1:3M:52:ASN:H | 1:3M:52:ASN:ND2 | 2.01 | 0.56 |
| 1:3Q:177:ASP:O | 2:3R:352:LYS:HA | 2.06 | 0.56 |
| 2:3R:37:PRO:O | 2:3R:41:THR:HG23 | 2.06 | 0.56 |
| 2:3T:246:GLY:HA3 | 2:3T:356:ASN:HA | 1.87 | 0.56 |
| 3:3Z:153:ASP:OD1 | 3:3Z:156:HIS:N | 2.37 | 0.56 |
| 5:4L:312:GLU:HB3 | 5:4L:315:ARG:HH21 | 1.70 | 0.56 |
| 14:5L:384:GLU:HB3 | 14:5L:402:SER:HB3 | 1.88 | 0.56 |
| 14:5N:382:ASN:ND2 | 23:6S:62:GLN:O | 2.39 | 0.56 |
| 15:5O:60:LEU:HD12 | 15:5O:60:LEU:O | 2.05 | 0.56 |
| 15:5O:296:SER:C | 15:5O:299:GLU:HG3 | 2.23 | 0.56 |
| 15:5P:52:TYR:CD2 | 15:5P:54:GLU:CB | 2.88 | 0.56 |
| 15:5P:331:ASP:OD2 | 15:5P:334:LEU:HD12 | 2.05 | 0.56 |
| 18:6C:102:ASP:N | 18:6C:102:ASP:OD1 | 2.37 | 0.56 |
| 19:6E:73:HIS:O | 19:6E:77:GLN:HG3 | 2.05 | 0.56 |
| 22:6I:294:LEU:HD13 | 22:6I:343:TYR:CD1 | 2.41 | 0.56 |
| 24:6Z:558:LEU:O | 24:6Z:562:LEU:HG | 2.06 | 0.56 |
| 24:7A:6:PRO:HG2 | 31:7N:83:THR:CG2 | 2.36 | 0.56 |
| 26:7F:84:ALA:O | 26:7F:88:THR:OG1 | 2.23 | 0.56 |
| 1:A3:215:LEU:CD1 | 26:7F:136:PHE:CD2 | 2.90 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B4:59:GLY:HA3 | 24:6W:263:ARG:NH1 | 2.21 | 0.55 |
| 1:I2:173:PRO:HB3 | 1:I2:384:GLN:HE22 | 1.70 | 0.55 |
| 2:I5:90:GLU:OE1 | 2:K1:283:HIS:ND1 | 2.38 | 0.55 |
| 1:I8:113:ILE:HA | 1:I8:116:VAL:HG12 | 1.87 | 0.55 |
| 1:I8:135:VAL:O | 1:I8:166:THR:HA | 2.06 | 0.55 |
| 1:J2:45:GLU:HG2 | 1:J2:46:ARG:HG2 | 1.88 | 0.55 |
| 2:J5:72:PRO:HG3 | 1:J6:1:MET:HG2 | 1.87 | 0.55 |
| 2:L1:223:THR:HG23 | 2:L1:225:THR:H | 1.71 | 0.55 |
| 1:M2:74:ASP:HB3 | 15:5O:48:LYS:HE2 | 1.88 | 0.55 |
| 1:M4:5:VAL:HG12 | 1:M4:133:PHE:HD1 | 1.70 | 0.55 |
| 2:M5:265:ILE:HD11 | 2:M5:435:VAL:HG21 | 1.88 | 0.55 |
| 1:O4:39:ASP:OD1 | 1:O4:40:SER:N | 2.39 | 0.55 |
| 2:P3:98:ASP:OD1 | 2:P3:99:ALA:N | 2.39 | 0.55 |
| 1:Q4:113:ILE:HA | 1:Q4:116:VAL:HG22 | 1.87 | 0.55 |
| 2:R3:137:VAL:HG22 | 2:R3:168:GLY:HA2 | 1.88 | 0.55 |
| 2:R3:306:ASP:HB3 | 2:R3:309:HIS:CD2 | 2.41 | 0.55 |
| 2:R9:222:PRO:HD2 | 1:S0:324:LYS:HE3 | 1.88 | 0.55 |
| 1:S2:329:GLN:HA | 1:S2:332:ASN:HD21 | 1.71 | 0.55 |
| 1:S6:125:GLU:CD | 3:3X:66:THR:HG23 | 2.26 | 0.55 |
| 2:S7:8:HIS:CD2 | 2:S7:17:GLY:HA3 | 2.40 | 0.55 |
| 1:T0:2:ARG:HE | 1:T0:240:LEU:HD22 | 1.71 | 0.55 |
| 2:T5:381:SER:OG | 2:T5:382:THR:N | 2.39 | 0.55 |
| 2:T7:3:GLU:HB2 | 2:T7:129:CYS:SG | 2.46 | 0.55 |
| 2:U9:11:GLN:NE2 | 1:V0:247:ASN:OD1 | 2.39 | 0.55 |
| 2:V3:301:MET:HE1 | 2:V3:307:PRO:HD3 | 1.87 | 0.55 |
| 1:W2:335:ASN:O | 1:W2:338:SER:OG | 2.25 | 0.55 |
| 2:W3:119:LEU:HA | 2:W3:122:ILE:HG22 | 1.88 | 0.55 |
| 2:W7:90:GLU:HB3 | 2:W7:121:ARG:NH1 | 2.19 | 0.55 |
| 2:W9:90:GLU:HB2 | 2:W9:121:ARG:HH12 | 1.70 | 0.55 |
| 2:X7:132:LEU:HD22 | 2:X7:164:LYS:HD3 | 1.87 | 0.55 |
| 2:Y3:236:SER:O | 2:Y3:243:ARG:NH2 | 2.38 | 0.55 |
| 1:Y4:171:PRO:O | 1:Y4:380:ARG:NH2 | 2.38 | 0.55 |
| 2:Z1:167:LEU:HD13 | 2:Z1:200:VAL:HB | 1.88 | 0.55 |
| 2:Z9:5:ILE:HD13 | 2:Z9:125:LEU:HD23 | 1.88 | 0.55 |
| 2:0J:274:PRO:HB2 | 2:0J:276:ILE:CG1 | 2.36 | 0.55 |
| 2:0N:9:ILE:HD13 | 2:0N:150:GLY:HA2 | 1.87 | 0.55 |
| 2:0R:244:PHE:HB2 | 2:0R:356:ASN:HD21 | 1.71 | 0.55 |
| 2:1R:286:LEU:O | 2:1R:373:ARG:NH1 | 2.38 | 0.55 |
| 2:2B:98:ASP:OD1 | 2:2B:99:ALA:N | 2.39 | 0.55 |
| 2:2B:278:ALA:HA | 2:2B:369:ALA:HB2 | 1.87 | 0.55 |
| 1:2C:335:ASN:O | 1:2C:338:SER:OG | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2F:109:THR:OG1 | 2:2F:411:GLU:OE2 | 2.22 | 0.55 |
| 2:2P:267:PHE:HB2 | 2:2P:384:ILE:HD12 | 1.89 | 0.55 |
| 2:2R:267:PHE:HB2 | 2:2R:384:ILE:HD12 | 1.88 | 0.55 |
| 2:2X:51:THR:HG21 | 2:2X:243:ARG:HG2 | 1.88 | 0.55 |
| 2:2X:381:SER:OG | 2:2X:382:THR:N | 2.38 | 0.55 |
| 2:2X:399:TYR:OH | 2:2X:415:GLU:OE2 | 2.21 | 0.55 |
| 2:3F:381:SER:OG | 2:3F:382:THR:N | 2.39 | 0.55 |
| 1:3M:282:ARG:HH21 | 1:3M:288:GLU:CD | 2.09 | 0.55 |
| 2:3R:255:PHE:HA | 2:3R:259:LEU:HD13 | 1.88 | 0.55 |
| 2:3R:399:TYR:O | 2:3R:402:ARG:NH1 | 2.39 | 0.55 |
| 1:3S:114:ASP:N | 1:3S:114:ASP:OD1 | 2.39 | 0.55 |
| 4:4I:90:GLU:OE2 | 4:4I:102:ARG:HD2 | 2.05 | 0.55 |
| 7:4R:297:MET:CG | 20:6F:130:LEU:HD21 | 2.36 | 0.55 |
| 14:5L:196:VAL:O | 14:5L:214:THR:N | 2.39 | 0.55 |
| 14:5L:359:CYS:HB2 | 14:5L:364:ILE:HD13 | 1.87 | 0.55 |
| 14:5M:359:CYS:HB2 | 14:5M:364:ILE:HD13 | 1.87 | 0.55 |
| 14:5M:384:GLU:HB3 | 14:5M:402:SER:HB3 | 1.88 | 0.55 |
| 14:5N:555:GLU:O | 14:5N:573:GLY:N | 2.36 | 0.55 |
| 18:6A:125:ARG:NH2 | 18:6A:204:LEU:O | 2.38 | 0.55 |
| 18:6B:125:ARG:NH2 | 18:6B:204:LEU:O | 2.38 | 0.55 |
| 18:6C:125:ARG:NH2 | 18:6C:204:LEU:O | 2.38 | 0.55 |
| 22:6O:49:SER:OG | 22:6O:51:ILE:HG22 | 2.06 | 0.55 |
| 24:6U:252:LYS:HG2 | 24:6U:257:LEU:HD21 | 1.87 | 0.55 |
| 24:6X:445:ILE:HG22 | 24:6X:447:ARG:CD | 2.37 | 0.55 |
| 24:6Y:14:TYR:CD2 | 24:6Y:14:TYR:N | 2.74 | 0.55 |
| 24:6Y:95:VAL:N | 24:6Y:187:PHE:HE2 | 2.04 | 0.55 |
| 35:7U:100:GLN:HA | 35:7U:103:GLU:HG3 | 1.87 | 0.55 |
| 2:8:33:ASP:CB | 18:6A:77:THR:HG21 | 2.36 | 0.55 |
| 2:A2:40:LYS:HZ3 | 26:7F:45:MET:N | 2.03 | 0.55 |
| 2:F3:282:TYR:CZ | 22:6O:82:LEU:HG | 2.41 | 0.55 |
| 1:H2:72:THR:O | 1:H2:76:VAL:HG23 | 2.06 | 0.55 |
| 1:H4:287:PRO:HA | 1:H4:290:THR:HG22 | 1.88 | 0.55 |
| 2:I1:72:PRO:HG3 | 1:I2:1:MET:HG2 | 1.88 | 0.55 |
| 1:I2:248:ALA:CA | 1:I2:252:LYS:HD2 | 2.22 | 0.55 |
| 1:I4:167:PHE:CZ | 1:I4:233:MET:HG2 | 2.41 | 0.55 |
| 2:I5:289:ALA:O | 2:I5:293:ASN:ND2 | 2.38 | 0.55 |
| 1:J4:177:ASP:O | 2:J5:352:LYS:HA | 2.06 | 0.55 |
| 1:J8:164:MET:HB3 | 1:J8:197:ASP:OD2 | 2.06 | 0.55 |
| 2:K3:88:HIS:CG | 2:L9:283:HIS:HB2 | 2.42 | 0.55 |
| 2:K3:399:TYR:O | 2:K3:402:ARG:NH1 | 2.39 | 0.55 |
| 1:K6:207:LEU:HB3 | 1:K6:225:LEU:HD22 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K6:257:LEU:HA | 1:K6:312:THR:HG21 | 1.89 | 0.55 |
| 1:K6:285:THR:OG1 | 1:K6:287:PRO:HD2 | 2.06 | 0.55 |
| 2:K9:281:ALA:C | 2:K9:283:HIS:H | 2.09 | 0.55 |
| 2:L1:222:PRO:HD2 | 1:L2:324:LYS:HE3 | 1.88 | 0.55 |
| 2:L9:76:ASP:HA | 2:L9:79:ARG:HB2 | 1.88 | 0.55 |
| 2:L9:195:LEU:HD21 | 2:L9:264:ARG:HH11 | 1.72 | 0.55 |
| 2:M5:58:ALA:CB | 37:7Y:214:ASP:CB | 2.84 | 0.55 |
| 1:M6:80:PRO:HB3 | 15:5P:69:PHE:CZ | 2.42 | 0.55 |
| 1:M6:86:ARG:HB3 | 2:O3:283:HIS:HE1 | 1.69 | 0.55 |
| 2:M7:399:TYR:O | 2:M7:402:ARG:NH1 | 2.40 | 0.55 |
| 1:O2:274:THR:CG2 | 1:O2:282:ARG:HD2 | 2.35 | 0.55 |
| 2:Q3:287:SER:N | 2:Q3:290:GLU:OE2 | 2.24 | 0.55 |
| 2:R5:71:GLU:OE1 | 2:R5:73:THR:OG1 | 2.24 | 0.55 |
| 2:R9:191:THR:HA | 2:R9:194:LEU:HB3 | 1.88 | 0.55 |
| 1:S4:77:ARG:HD2 | 24:6U:32:THR:HG21 | 1.87 | 0.55 |
| 1:T8:190:HIS:HD2 | 1:T8:414:ASN:HB2 | 1.71 | 0.55 |
| 2:U3:213:CYS:HA | 2:U3:217:LEU:HB2 | 1.87 | 0.55 |
| 1:V0:172:SER:OG | 1:V0:380:ARG:NH2 | 2.39 | 0.55 |
| 2:V3:129:CYS:SG | 2:V3:130:THR:N | 2.78 | 0.55 |
| 1:W0:167:PHE:CZ | 1:W0:233:MET:HG2 | 2.42 | 0.55 |
| 1:W8:3:GLU:OE2 | 1:W8:62:ARG:NH1 | 2.39 | 0.55 |
| 2:W9:88:HIS:CB | 2:W9:91:GLN:HB2 | 2.30 | 0.55 |
| 1:X6:51:PHE:HB3 | 1:X6:59:TYR:HB3 | 1.88 | 0.55 |
| 1:Y4:170:VAL:HG21 | 1:Y4:377:MET:SD | 2.46 | 0.55 |
| 2:Y5:88:HIS:HB3 | 2:0B:283:HIS:CE1 | 2.41 | 0.55 |
| 1:Y8:8:GLN:OE1 | 1:Y8:65:LEU:HD23 | 2.06 | 0.55 |
| 1:Y8:20:PHE:HA | 1:Y8:230:SER:OG | 2.06 | 0.55 |
| 2:Z1:129:CYS:SG | 2:Z1:130:THR:N | 2.79 | 0.55 |
| 1:0A:309:ARG:H | 1:0A:372:THR:HG22 | 1.71 | 0.55 |
| 2:0B:388:PHE:HB3 | 2:0B:425:LEU:HD11 | 1.87 | 0.55 |
| 1:0E:3:GLU:HB2 | 1:0E:130:LEU:HA | 1.88 | 0.55 |
| 1:0M:134:GLN:HE21 | 1:0M:167:PHE:HE2 | 1.54 | 0.55 |
| 2:0N:387:ILE:HD13 | 2:0N:390:ARG:HH12 | 1.72 | 0.55 |
| 2:0V:289:ALA:O | 2:0V:293:ASN:ND2 | 2.39 | 0.55 |
| 1:0Y:292:GLN:O | 1:0Y:298:ASN:ND2 | 2.27 | 0.55 |
| 2:0Z:318:MET:HB2 | 2:0Z:376:CYS:HB3 | 1.88 | 0.55 |
| 1:1A:180:VAL:HG23 | 1:1A:184:ASN:HD21 | 1.71 | 0.55 |
| 2:1R:88:HIS:CD2 | 2:1R:90:GLU:H | 2.25 | 0.55 |
| 2:2H:353:CYS:SG | 2:2H:354:GLY:N | 2.79 | 0.55 |
| 1:2M:74:ASP:O | 1:2M:78:SER:OG | 2.16 | 0.55 |
| 2:2P:405:VAL:HG13 | 2:2P:418:PHE:HE2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3I:233:MET:O | 1:3I:237:THR:HG22 | 2.06 | 0.55 |
| 1:3O:11:GLN:N | 39:3O:502:GDP:O1B | 2.32 | 0.55 |
| 2:3T:227:LEU:O | 2:3T:231:ILE:HG12 | 2.06 | 0.55 |
| 4:3Y:90:GLU:OE2 | 4:3Y:102:ARG:HD2 | 2.05 | 0.55 |
| 12:5G:282:HIS:HB2 | 12:5G:288:ARG:HG3 | 1.89 | 0.55 |
| 14:5L:117:PHE:HB3 | 14:5L:131:LEU:HD21 | 1.87 | 0.55 |
| 14:5M:196:VAL:O | 14:5M:214:THR:N | 2.39 | 0.55 |
| 14:5N:10:VAL:HG22 | 14:5N:620:PHE:CD1 | 2.41 | 0.55 |
| 14:5N:196:VAL:O | 14:5N:214:THR:N | 2.39 | 0.55 |
| 15:5O:78:TYR:OH | 15:5O:84:ARG:HG3 | 2.06 | 0.55 |
| 24:6V:110:ASN:ND2 | 24:6V:213:TYR:OH | 2.39 | 0.55 |
| 29:7J:322:TYR:CZ | 29:7J:324:GLY:HA3 | 2.41 | 0.55 |
| 1:5:204:ASN:HD21 | 39:5:501:GDP:HN22 | 1.54 | 0.55 |
| 1:A3:219:THR:CB | 26:7F:142:PHE:CZ | 2.88 | 0.55 |
| 2:A8:226:ASN:ND2 | 18:5X:51:MET:SD | 2.79 | 0.55 |
| 2:G9:221:ARG:HG3 | 22:6P:178:GLY:HA2 | 1.88 | 0.55 |
| 2:H9:222:PRO:HD2 | 1:I0:324:LYS:HE3 | 1.87 | 0.55 |
| 2:I1:165:SER:HB2 | 2:I1:256:GLN:HE21 | 1.71 | 0.55 |
| 1:I4:178:THR:HG22 | 2:I5:352:LYS:HE2 | 1.86 | 0.55 |
| 2:I9:406:HIS:HA | 2:I9:409:VAL:HG22 | 1.87 | 0.55 |
| 1:J4:140:GLY:O | 1:J4:184:ASN:ND2 | 2.40 | 0.55 |
| 2:K3:11:GLN:NE2 | 1:K4:247:ASN:OD1 | 2.40 | 0.55 |
| 1:K4:135:VAL:HG21 | 1:K4:152:ILE:HD11 | 1.89 | 0.55 |
| 2:K5:405:VAL:HG13 | 2:K5:418:PHE:HE2 | 1.71 | 0.55 |
| 2:K9:206:ASN:OD1 | 41:K9:501:GTP:N2 | 2.39 | 0.55 |
| 2:L3:115:VAL:HG22 | 2:L3:119:LEU:HD23 | 1.87 | 0.55 |
| 2:L3:406:HIS:HA | 2:L3:409:VAL:HG22 | 1.89 | 0.55 |
| 2:L5:27:GLU:CD | 2:L5:243:ARG:HH12 | 2.08 | 0.55 |
| 1:M6:317:PHE:HE2 | 1:M6:326:VAL:HG13 | 1.71 | 0.55 |
| 1:M8:285:THR:OG1 | 1:M8:287:PRO:HD2 | 2.07 | 0.55 |
| 2:N5:70:LEU:HD12 | 2:N5:99:ALA:HB2 | 1.88 | 0.55 |
| 1:N6:177:ASP:O | 2:N7:352:LYS:HA | 2.06 | 0.55 |
| 2:O3:244:PHE:HB2 | 2:O3:356:ASN:HD21 | 1.70 | 0.55 |
| 2:O7:91:GLN:CA | 2:O7:121:ARG:HH12 | 2.18 | 0.55 |
| 2:P5:46:ASP:O | 2:P5:47:ASP:HB3 | 2.06 | 0.55 |
| 2:Q3:58:ALA:HB3 | 7:4R:275:LEU:HD11 | 1.89 | 0.55 |
| 1:Q6:238:CYS:SG | 1:Q6:318:ARG:NE | 2.79 | 0.55 |
| 2:R1:98:ASP:OD1 | 2:R1:99:ALA:N | 2.39 | 0.55 |
| 2:R7:278:ALA:HA | 2:R7:369:ALA:HB2 | 1.89 | 0.55 |
| 1:S8:53:GLU:OE1 | 26:7D:71:PRO:O | 2.23 | 0.55 |
| 1:T0:363:MET:HB3 | 7:4T:352:ASN:ND2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U5:276:ILE:HB | 2:U5:280:LYS:HG3 | 1.87 | 0.55 |
| 2:U5:417:GLU:HA | 2:U5:420:GLU:HG2 | 1.89 | 0.55 |
| 2:U9:85:GLN:OE1 | 2:U9:85:GLN:HA | 2.07 | 0.55 |
| 1:V8:375:GLN:HB3 | 1:V8:422:TYR:HD2 | 1.70 | 0.55 |
| 2:V9:119:LEU:HA | 2:V9:122:ILE:HG22 | 1.88 | 0.55 |
| 1:W0:22:GLU:HG2 | 1:W0:81:TYR:HB2 | 1.89 | 0.55 |
| 1:W2:198:GLU:HB3 | 1:W2:258:ILE:HD11 | 1.87 | 0.55 |
| 2:W5:399:TYR:O | 2:W5:402:ARG:NH1 | 2.40 | 0.55 |
| 2:Y9:83:TYR:HB3 | 2:Y9:86:LEU:HB3 | 1.89 | 0.55 |
| 2:Z7:286:LEU:O | 2:Z7:373:ARG:NH1 | 2.40 | 0.55 |
| 2:Z9:90:GLU:O | 2:Z9:121:ARG:NH1 | 2.39 | 0.55 |
| 2:0F:12:ALA:HB2 | 41:0F:501:GTP:C8 | 2.41 | 0.55 |
| 2:0F:320:ARG:HD3 | 2:0F:360:PRO:HG3 | 1.88 | 0.55 |
| 1:0M:358:PRO:HG2 | 1:0M:361:LEU:HD13 | 1.88 | 0.55 |
| 1:0S:182:PRO:HG2 | 1:0S:388:MET:HE3 | 1.88 | 0.55 |
| 2:0X:58:ALA:HB2 | 9:4Y:441:PRO:HB3 | 1.87 | 0.55 |
| 1:1A:364:SER:OG | 1:1A:365:ALA:N | 2.39 | 0.55 |
| 2:1B:222:PRO:HD2 | 1:1C:324:LYS:HE3 | 1.88 | 0.55 |
| 1:1K:10:GLY:HA2 | 1:1K:143:THR:HG23 | 1.87 | 0.55 |
| 1:1O:72:THR:O | 1:1O:76:VAL:HG23 | 2.06 | 0.55 |
| 1:2A:5:VAL:HG12 | 1:2A:62:ARG:HD3 | 1.89 | 0.55 |
| 1:2G:211:CYS:HA | 1:2G:215:LEU:HB2 | 1.88 | 0.55 |
| 2:2H:123:ARG:HG2 | 38:8B:26:THR:HB | 1.87 | 0.55 |
| 1:2I:77:ARG:HE | 1:2I:90:PHE:HE2 | 1.53 | 0.55 |
| 2:2P:296:PHE:C | 38:7Z:25:ILE:HD11 | 2.27 | 0.55 |
| 1:2U:245:GLN:HE21 | 38:8B:198:THR:HG21 | 1.71 | 0.55 |
| 2:3B:189:LEU:HD11 | 2:3B:418:PHE:HE1 | 1.71 | 0.55 |
| 2:3B:406:HIS:HA | 2:3B:409:VAL:HG22 | 1.88 | 0.55 |
| 2:3D:70:LEU:HB2 | 2:3D:98:ASP:HA | 1.87 | 0.55 |
| 1:3K:309:ARG:NH1 | 1:3K:339:SER:O | 2.39 | 0.55 |
| 2:3P:189:LEU:HD11 | 2:3P:418:PHE:HE1 | 1.72 | 0.55 |
| 2:3R:116:ASP:OD1 | 2:3R:117:LEU:N | 2.39 | 0.55 |
| 2:3R:433:GLU:OE1 | 2:3R:433:GLU:N | 2.32 | 0.55 |
| 4:3W:90:GLU:OE2 | 4:3W:102:ARG:HD2 | 2.05 | 0.55 |
| 4:4A:90:GLU:OE2 | 4:4A:102:ARG:HD2 | 2.05 | 0.55 |
| 4:4E:90:GLU:OE2 | 4:4E:102:ARG:HD2 | 2.05 | 0.55 |
| 10:5D:133:ARG:O | 10:5D:137:THR:HG23 | 2.06 | 0.55 |
| 14:5L:10:VAL:HG22 | 14:5L:620:PHE:CD1 | 2.41 | 0.55 |
| 18:5X:181:GLN:O | 18:5X:185:THR:OG1 | 2.22 | 0.55 |
| 18:5Y:175:THR:OG1 | 18:5Y:177:PRO:HD2 | 2.06 | 0.55 |
| 18:5Z:175:THR:OG1 | 18:5Z:177:PRO:HD2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6J:277:SER:O | 22:6J:281:LYS:HG2 | 2.06 | 0.55 |
| 22:6N:219:ASP:OD1 | 22:6N:222:SER:OG | 2.20 | 0.55 |
| 23:6R:28:LYS:HA | 23:6R:28:LYS:CE | 2.33 | 0.55 |
| 24:6T:429:LYS:HD2 | 24:6T:430:PRO:HD2 | 1.89 | 0.55 |
| 24:6Y:431:PRO:HB2 | 24:6Y:433:ARG:NH2 | 2.22 | 0.55 |
| 24:7A:18:LEU:O | 24:7A:20:GLN:NE2 | 2.39 | 0.55 |
| 38:8B:158:MET:HE2 | 38:8B:158:MET:O | 2.07 | 0.55 |
| 2:A2:82:THR:CG2 | 26:7F:118:SER:HB2 | 2.35 | 0.55 |
| 1:G4:218:THR:OG1 | 24:6X:418:ASP:OD1 | 2.16 | 0.55 |
| 2:G9:278:ALA:HB3 | 22:6P:215:GLY:HA2 | 1.89 | 0.55 |
| 2:I1:203:MET:O | 2:I1:204:LEU:HD23 | 2.07 | 0.55 |
| 2:I5:119:LEU:HA | 2:I5:122:ILE:HG12 | 1.87 | 0.55 |
| 2:I5:227:LEU:O | 2:I5:231:ILE:HG12 | 2.06 | 0.55 |
| 1:J2:52:ASN:OD1 | 1:J2:62:ARG:NH2 | 2.39 | 0.55 |
| 2:J9:116:ASP:OD1 | 2:J9:117:LEU:N | 2.38 | 0.55 |
| 2:J9:220:GLU:HG2 | 2:J9:221:ARG:HG3 | 1.88 | 0.55 |
| 2:K1:37:PRO:HG2 | 28:7X:402:ARG:HB3 | 1.89 | 0.55 |
| 1:K4:177:ASP:O | 2:K5:352:LYS:HA | 2.06 | 0.55 |
| 2:K7:53:PHE:HB3 | 2:K7:61:HIS:HB3 | 1.89 | 0.55 |
| 2:L3:276:ILE:HD11 | 2:L3:281:ALA:CA | 2.33 | 0.55 |
| 2:M1:359:PRO:HD3 | 29:7I:90:GLY:HA3 | 1.87 | 0.55 |
| 2:N3:165:SER:HA | 2:N3:199:ASP:OD2 | 2.07 | 0.55 |
| 2:O3:90:GLU:CB | 2:O3:121:ARG:HH12 | 2.20 | 0.55 |
| 2:O3:100:ALA:HA | 1:O4:252:LYS:HE2 | 1.88 | 0.55 |
| 1:O8:139:LEU:HD12 | 1:O8:170:VAL:HG22 | 1.87 | 0.55 |
| 2:O9:21:TRP:CZ2 | 2:O9:65:CYS:HB2 | 2.42 | 0.55 |
| 1:P6:194:GLU:OE2 | 1:P6:262:ARG:NH1 | 2.38 | 0.55 |
| 1:P8:114:ASP:OD1 | 1:P8:115:SER:N | 2.40 | 0.55 |
| 2:P9:81:GLY:HA3 | 19:6E:149:TYR:HE2 | 1.72 | 0.55 |
| 2:Q1:14:ILE:HD11 | 2:Q1:74:VAL:HG13 | 1.87 | 0.55 |
| 1:Q2:388:MET:HE2 | 2:Q3:348:PRO:HD2 | 1.89 | 0.55 |
| 2:R5:170:THR:HG21 | 2:R5:194:LEU:HD11 | 1.88 | 0.55 |
| 1:S2:181:GLU:HG2 | 1:S2:182:PRO:HD3 | 1.88 | 0.55 |
| 2:T5:345:ASP:N | 2:T5:345:ASP:OD1 | 2.39 | 0.55 |
| 1:T6:253:LEU:HD11 | 1:T6:316:LEU:HD11 | 1.88 | 0.55 |
| 1:U4:190:HIS:HD2 | 1:U4:414:ASN:HB2 | 1.72 | 0.55 |
| 2:V1:384:ILE:HA | 2:V1:387:ILE:HD12 | 1.88 | 0.55 |
| 2:V3:417:GLU:HA | 2:V3:420:GLU:HG2 | 1.87 | 0.55 |
| 2:V9:172:TYR:N | 2:V9:204:LEU:O | 2.38 | 0.55 |
| 1:X2:135:VAL:HG21 | 1:X2:152:ILE:HD11 | 1.89 | 0.55 |
| 1:X2:172:SER:OG | 1:X2:380:ARG:NH2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X3:224:TYR:HD1 | 2:X3:227:LEU:HD12 | 1.70 | 0.55 |
| 2:X5:262:TYR:HH | 2:X5:346:TRP:HZ3 | 1.53 | 0.55 |
| 1:X6:309:ARG:NH1 | 1:X6:339:SER:O | 2.39 | 0.55 |
| 2:Y5:399:TYR:O | 2:Y5:402:ARG:NH1 | 2.39 | 0.55 |
| 1:Y8:244:GLY:HA3 | 1:Y8:354:CYS:HA | 1.88 | 0.55 |
| 1:Z4:101:TRP:HB2 | 1:Z4:184:ASN:OD1 | 2.07 | 0.55 |
| 2:Z9:183:GLU:CD | 2:Z9:184:PRO:HD3 | 2.26 | 0.55 |
| 2:Z9:315:CYS:SG | 2:Z9:316:CYS:N | 2.79 | 0.55 |
| 1:0E:267:MET:HG3 | 1:0E:301:CYS:HB3 | 1.88 | 0.55 |
| 2:0F:164:LYS:O | 2:0F:166:LYS:NZ | 2.39 | 0.55 |
| 2:0H:278:ALA:HA | 2:0H:369:ALA:HB2 | 1.88 | 0.55 |
| 1:0K:60:VAL:HG11 | 1:1A:281:TYR:HB3 | 1.87 | 0.55 |
| 1:0K:211:CYS:HA | 1:0K:215:LEU:HB2 | 1.87 | 0.55 |
| 1:0O:249:ASP:OD2 | 1:0O:250:LEU:N | 2.37 | 0.55 |
| 2:0V:145:THR:OG1 | 41:0V:501:GTP:O1B | 2.22 | 0.55 |
| 2:0V:336:LYS:NZ | 2:0V:349:THR:HA | 2.22 | 0.55 |
| 1:0W:211:CYS:HA | 1:0W:215:LEU:HB2 | 1.89 | 0.55 |
| 2:1B:264:ARG:NH1 | 2:1B:431:ASP:OD1 | 2.40 | 0.55 |
| 2:1D:33:ASP:OD2 | 2:1D:35:GLN:NE2 | 2.40 | 0.55 |
| 2:1D:72:PRO:HA | 2:1D:75:VAL:HG22 | 1.88 | 0.55 |
| 2:1D:76:ASP:OD1 | 2:1D:79:ARG:NH2 | 2.39 | 0.55 |
| 1:1K:186:THR:HG22 | 1:1K:411:ALA:HB1 | 1.89 | 0.55 |
| 1:1Q:235:GLY:HA3 | 1:1Q:366:THR:HG21 | 1.88 | 0.55 |
| 1:1W:287:PRO:HA | 1:1W:290:THR:HG22 | 1.89 | 0.55 |
| 1:2A:267:MET:HG2 | 1:2A:301:CYS:HB3 | 1.89 | 0.55 |
| 2:2L:266:HIS:ND1 | 2:2L:266:HIS:O | 2.38 | 0.55 |
| 2:2X:42:ILE:HD11 | 14:5M:139:ALA:CB | 2.36 | 0.55 |
| 1:2Y:320:ARG:HH12 | 38:8C:197:THR:C | 2.09 | 0.55 |
| 1:3A:190:HIS:CD2 | 1:3A:411:ALA:HA | 2.41 | 0.55 |
| 2:3D:213:CYS:HA | 2:3D:217:LEU:HB2 | 1.87 | 0.55 |
| 2:3H:90:GLU:HG3 | 3:3X:36:PHE:HB3 | 1.88 | 0.55 |
| 2:3R:245:ASP:OD2 | 14:5N:192:THR:CG2 | 2.55 | 0.55 |
| 2:3R:286:LEU:HD13 | 2:3R:371:VAL:HG13 | 1.88 | 0.55 |
| 3:3X:153:ASP:OD1 | 3:3X:156:HIS:N | 2.37 | 0.55 |
| 4:4C:90:GLU:OE2 | 4:4C:102:ARG:HD2 | 2.05 | 0.55 |
| 4:4G:90:GLU:OE2 | 4:4G:102:ARG:HD2 | 2.05 | 0.55 |
| 8:4V:438:ALA:HA | 8:4V:441:ASP:OD1 | 2.06 | 0.55 |
| 9:4Y:433:ARG:NH2 | 9:4Y:439:THR:OG1 | 2.40 | 0.55 |
| 9:4Z:49:ARG:O | 9:4Z:53:THR:HG23 | 2.06 | 0.55 |
| 14:5M:10:VAL:HG22 | 14:5M:620:PHE:CD1 | 2.41 | 0.55 |
| 14:5N:359:CYS:HB2 | 14:5N:364:ILE:HD13 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:82:PHE:HA | 15:5O:85:ASN:HD21 | 1.70 | 0.55 |
| 15:5O:180:ASP:HB3 | 15:5O:183:GLN:HG2 | 1.87 | 0.55 |
| 16:5Q:63:ARG:HD3 | 16:5Q:92:PHE:HA | 1.87 | 0.55 |
| 18:5X:175:THR:OG1 | 18:5X:177:PRO:HD2 | 2.06 | 0.55 |
| 18:6A:175:THR:OG1 | 18:6A:177:PRO:HD2 | 2.06 | 0.55 |
| 18:6B:175:THR:OG1 | 18:6B:177:PRO:HD2 | 2.06 | 0.55 |
| 18:6C:175:THR:OG1 | 18:6C:177:PRO:HD2 | 2.06 | 0.55 |
| 22:6J:110:ILE:O | 22:6J:113:ARG:NH1 | 2.39 | 0.55 |
| 24:6W:613:LYS:O | 24:6W:617:ASP:HB2 | 2.06 | 0.55 |
| 24:6Z:242:PHE:O | 24:6Z:246:VAL:HG23 | 2.07 | 0.55 |
| 24:6Z:569:LYS:HB3 | 24:6Z:572:ALA:HB3 | 1.87 | 0.55 |
| 35:7T:31:SER:O | 35:7T:35:LYS:HG3 | 2.07 | 0.55 |
| 38:8C:8:GLU:OE1 | 38:8C:8:GLU:N | 2.36 | 0.55 |
| 1:5:75:SER:HA | 24:6V:149:LYS:HE3 | 1.88 | 0.55 |
| 1:9:78:SER:CB | 24:6X:149:LYS:HG3 | 2.36 | 0.55 |
| 2:G5:129:CYS:SG | 2:G5:130:THR:N | 2.79 | 0.55 |
| 2:H7:183:GLU:HG3 | 2:H7:184:PRO:HD3 | 1.89 | 0.55 |
| 1:I0:218:THR:CB | 24:6X:489:ASN:N | 2.66 | 0.55 |
| 2:I1:217:LEU:HB3 | 2:I1:219:ILE:HD12 | 1.88 | 0.55 |
| 1:J4:135:VAL:HG21 | 1:J4:152:ILE:HD11 | 1.89 | 0.55 |
| 2:J9:133:GLN:HG2 | 2:J9:252:ILE:HG22 | 1.88 | 0.55 |
| 2:K1:381:SER:OG | 2:K1:382:THR:N | 2.38 | 0.55 |
| 1:L0:252:LYS:HA | 1:L0:255:VAL:HG12 | 1.87 | 0.55 |
| 1:L4:39:ASP:OD1 | 1:L4:40:SER:N | 2.38 | 0.55 |
| 1:L6:207:LEU:HB3 | 1:L6:225:LEU:HD22 | 1.87 | 0.55 |
| 1:M6:73:MET:HE1 | 1:M6:90:PHE:HB3 | 1.89 | 0.55 |
| 1:M6:145:SER:OG | 1:M6:188:SER:OG | 2.18 | 0.55 |
| 2:N1:109:THR:OG1 | 2:N1:411:GLU:OE2 | 2.19 | 0.55 |
| 2:N3:313:MET:N | 2:N3:380:ASN:O | 2.31 | 0.55 |
| 1:O4:70:PRO:N | 1:O4:92:PHE:HZ | 2.04 | 0.55 |
| 2:O5:381:SER:OG | 2:O5:382:THR:N | 2.39 | 0.55 |
| 2:O7:21:TRP:HZ2 | 2:O7:65:CYS:HB3 | 1.71 | 0.55 |
| 2:P5:42:ILE:HG21 | 27:7G:217:ILE:HG21 | 1.87 | 0.55 |
| 2:P5:47:ASP:O | 27:7G:187:ARG:NH2 | 2.39 | 0.55 |
| 1:Q4:248:ALA:HA | 1:Q4:252:LYS:HD2 | 1.89 | 0.55 |
| 1:Q8:334:GLN:HA | 1:Q8:341:PHE:HE2 | 1.71 | 0.55 |
| 2:Q9:156:ARG:HA | 2:Q9:159:VAL:HG12 | 1.89 | 0.55 |
| 1:R0:135:VAL:HG21 | 1:R0:152:ILE:HD11 | 1.88 | 0.55 |
| 2:R5:66:ILE:HD12 | 2:R5:68:LEU:HD23 | 1.89 | 0.55 |
| 2:T5:377:MET:SD | 2:T5:379:SER:HB3 | 2.47 | 0.55 |
| 1:T8:31:ASP:OD1 | 1:T8:35:THR:N | 2.32 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U3:279:GLU:HB3 | 2:U3:283:HIS:HE1 | 1.72 | 0.55 |
| 1:U8:397:TRP:CH2 | 2:U9:256:GLN:HB3 | 2.41 | 0.55 |
| 2:U9:327:ASP:OD1 | 2:U9:328:VAL:N | 2.39 | 0.55 |
| 2:V3:276:ILE:HD11 | 2:V3:371:VAL:HG22 | 1.88 | 0.55 |
| 1:W8:34:GLY:HA3 | 1:W8:58:ARG:HD3 | 1.87 | 0.55 |
| 2:W9:10:GLY:C | 2:W9:69:ASP:OD2 | 2.43 | 0.55 |
| 2:X5:3:GLU:O | 2:X5:133:GLN:N | 2.30 | 0.55 |
| 2:Y3:420:GLU:HA | 2:Y3:423:GLU:HG2 | 1.89 | 0.55 |
| 2:Y5:286:LEU:O | 2:Y5:373:ARG:NH1 | 2.39 | 0.55 |
| 2:Y5:417:GLU:HA | 2:Y5:420:GLU:HG2 | 1.89 | 0.55 |
| 1:Z0:156:ARG:HD3 | 1:Z0:164:MET:HE2 | 1.89 | 0.55 |
| 1:Z8:190:HIS:NE2 | 1:Z8:414:ASN:OD1 | 2.40 | 0.55 |
| 1:Z8:317:PHE:HE2 | 1:Z8:326:VAL:HG13 | 1.71 | 0.55 |
| 2:Z9:102:ASN:HD21 | 2:Z9:411:GLU:HG3 | 1.71 | 0.55 |
| 1:0E:139:LEU:HG | 1:0E:168:SER:OG | 2.06 | 0.55 |
| 1:0E:285:THR:HG23 | 1:0E:288:GLU:H | 1.72 | 0.55 |
| 2:0F:175:PRO:HB3 | 2:0F:390:ARG:HE | 1.71 | 0.55 |
| 1:0M:58:ARG:HD3 | 1:1C:280:GLN:HE22 | 1.70 | 0.55 |
| 2:0R:88:HIS:CE1 | 2:1H:283:HIS:HA | 2.42 | 0.55 |
| 2:1B:12:ALA:O | 2:1B:16:VAL:HG23 | 2.07 | 0.55 |
| 2:1F:9:ILE:HG13 | 2:1F:139:ASN:HB3 | 1.89 | 0.55 |
| 1:1K:287:PRO:HA | 1:1K:290:THR:HG22 | 1.88 | 0.55 |
| 2:1T:49:PHE:HB2 | 2:1T:53:PHE:HD2 | 1.71 | 0.55 |
| 1:1U:322:SER:OG | 1:1U:325:GLU:OE1 | 2.15 | 0.55 |
| 2:1Z:287:SER:N | 2:1Z:290:GLU:OE2 | 2.39 | 0.55 |
| 1:2A:358:PRO:HG2 | 1:2A:361:LEU:HB2 | 1.89 | 0.55 |
| 1:2Q:291:GLN:OE1 | 38:8A:98:TYR:CD1 | 2.60 | 0.55 |
| 2:2T:298:PRO:HB3 | 2:2T:307:PRO:CD | 2.37 | 0.55 |
| 1:3M:265:PHE:HD2 | 1:3M:422:TYR:HH | 1.55 | 0.55 |
| 2:3N:53:PHE:HB3 | 2:3N:61:HIS:HB3 | 1.88 | 0.55 |
| 2:3R:39:ASP:OD2 | 2:3R:40:LYS:N | 2.40 | 0.55 |
| 3:4F:153:ASP:OD1 | 3:4F:156:HIS:N | 2.37 | 0.55 |
| 7:4R:173:ALA:O | 7:4R:176:GLU:HG3 | 2.05 | 0.55 |
| 8:4W:284:ALA:O | 8:4W:288:THR:HG23 | 2.07 | 0.55 |
| 8:4W:437:ARG:O | 8:4W:441:ASP:HB3 | 2.06 | 0.55 |
| 9:4Z:20:THR:OG1 | 9:4Z:21:PHE:N | 2.39 | 0.55 |
| 10:5B:135:ARG:HG3 | 10:5B:139:MET:HE3 | 1.88 | 0.55 |
| 10:5C:133:ARG:O | 10:5C:137:THR:HG23 | 2.07 | 0.55 |
| 12:5F:298:ASP:HB3 | 12:7B:13:PRO:HG3 | 1.88 | 0.55 |
| 14:5L:528:ALA:HB1 | 14:5L:556:VAL:HG12 | 1.89 | 0.55 |
| 14:5M:528:ALA:HB1 | 14:5M:556:VAL:HG12 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5N:30:ILE:HG22 | 14:5N:41:ARG:HB2 | 1.88 | 0.55 |
| 17:5T:228:THR:HA | 17:5T:231:ARG:HE | 1.71 | 0.55 |
| 18:6D:175:THR:OG1 | 18:6D:177:PRO:HD2 | 2.06 | 0.55 |
| 22:6M:110:ILE:O | 22:6M:113:ARG:NH1 | 2.39 | 0.55 |
| 23:6S:27:ASP:O | 23:6S:28:LYS:HB2 | 2.07 | 0.55 |
| 24:6W:117:ARG:NH1 | 24:6W:134:GLU:OE2 | 2.39 | 0.55 |
| 24:6W:130:MET:HG3 | 24:6W:153:VAL:HG12 | 1.88 | 0.55 |
| 24:6Y:277:CYS:HA | 24:6Y:368:LEU:HA | 1.88 | 0.55 |
| 24:6Z:558:LEU:HD22 | 24:6Z:608:GLN:HB3 | 1.89 | 0.55 |
| 33:7Q:172:ARG:HG2 | 33:7Q:173:SER:H | 1.72 | 0.55 |
| 38:8A:122:LYS:HA | 38:8A:125:ASN:HD21 | 1.71 | 0.55 |
| 38:8C:110:ASN:HD21 | 38:8C:112:ILE:HB | 1.72 | 0.55 |
| 1:A3:340:TYR:HE1 | 3:4H:104:PRO:N | 2.05 | 0.55 |
| 2:G1:167:LEU:HD13 | 2:G1:200:VAL:HB | 1.88 | 0.55 |
| 2:H1:217:LEU:HB3 | 2:H1:219:ILE:HD12 | 1.89 | 0.55 |
| 2:H3:90:GLU:HB3 | 2:H3:121:ARG:HH22 | 1.72 | 0.55 |
| 2:H7:71:GLU:HG3 | 1:H8:2:ARG:NH1 | 2.20 | 0.55 |
| 1:I4:139:LEU:HD12 | 1:I4:170:VAL:HG12 | 1.88 | 0.55 |
| 2:I5:384:ILE:HA | 2:I5:387:ILE:HD12 | 1.88 | 0.55 |
| 1:J2:70:PRO:N | 1:J2:92:PHE:HZ | 2.03 | 0.55 |
| 1:J2:177:ASP:O | 2:J3:352:LYS:HA | 2.06 | 0.55 |
| 1:J6:77:ARG:HE | 29:7J:423:GLY:HA3 | 1.71 | 0.55 |
| 1:K8:404:ASP:HB3 | 1:K8:406:MET:SD | 2.47 | 0.55 |
| 1:L4:190:HIS:CD2 | 1:L4:411:ALA:HA | 2.41 | 0.55 |
| 2:M7:287:SER:HB2 | 30:7K:84:VAL:HG11 | 1.89 | 0.55 |
| 2:N1:129:CYS:SG | 2:N1:130:THR:N | 2.79 | 0.55 |
| 2:N7:364:PRO:HG3 | 27:7G:145:ARG:HE | 1.72 | 0.55 |
| 1:O6:54:ALA:HB3 | 1:O6:58:ARG:HB3 | 1.89 | 0.55 |
| 1:Q8:260:PHE:HD2 | 1:Q8:262:ARG:H | 1.53 | 0.55 |
| 2:R7:305:CYS:HB3 | 2:R7:387:ILE:HD11 | 1.89 | 0.55 |
| 1:S2:238:CYS:SG | 1:S2:318:ARG:NE | 2.80 | 0.55 |
| 1:T0:320:ARG:HH12 | 12:5F:210:THR:HA | 1.71 | 0.55 |
| 1:T2:156:ARG:HH22 | 3:4D:91:LYS:HE2 | 1.71 | 0.55 |
| 2:U1:195:LEU:HD12 | 2:U1:428:LEU:HD12 | 1.89 | 0.55 |
| 2:V1:287:SER:OG | 2:V1:288:VAL:N | 2.40 | 0.55 |
| 2:V9:21:TRP:CZ3 | 2:V9:63:PRO:HB3 | 2.41 | 0.55 |
| 2:W5:381:SER:OG | 2:W5:382:THR:N | 2.39 | 0.55 |
| 1:W6:177:ASP:O | 2:W7:352:LYS:HA | 2.07 | 0.55 |
| 1:X0:36:TYR:CE1 | 1:X0:44:LEU:HD21 | 2.42 | 0.55 |
| 1:Y0:39:ASP:OD1 | 1:Y0:40:SER:N | 2.40 | 0.55 |
| 2:Y3:206:ASN:OD1 | 41:Y4:501:GTP:N2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y6:212:PHE:HE1 | 1:Y6:220:PRO:HG3 | 1.70 | 0.55 |
| 2:Z3:8:HIS:CD2 | 2:Z3:138:PHE:HD2 | 2.24 | 0.55 |
| 2:Z5:417:GLU:HA | 2:Z5:420:GLU:HG2 | 1.88 | 0.55 |
| 1:0G:31:ASP:OD2 | 1:0G:33:THR:OG1 | 2.15 | 0.55 |
| 1:0I:165:LEU:HD22 | 1:0I:167:PHE:HE1 | 1.72 | 0.55 |
| 2:0L:167:LEU:HG | 2:0L:252:ILE:HD11 | 1.88 | 0.55 |
| 2:0P:352:LYS:NZ | 2:0P:353:CYS:O | 2.40 | 0.55 |
| 1:0U:3:GLU:HG2 | 1:0U:127:CYS:SG | 2.46 | 0.55 |
| 2:0V:292:THR:HG21 | 2:0V:331:SER:HB3 | 1.89 | 0.55 |
| 1:0Y:334:GLN:NE2 | 1:0Y:348:ASN:H | 2.04 | 0.55 |
| 2:0Z:178:SER:OG | 2:0Z:183:GLU:OE2 | 2.23 | 0.55 |
| 2:1H:388:PHE:HD1 | 2:1H:391:LEU:HD21 | 1.72 | 0.55 |
| 2:1N:90:GLU:HB3 | 2:1N:121:ARG:NH2 | 2.21 | 0.55 |
| 2:1N:306:ASP:OD1 | 2:1N:308:ARG:HB2 | 2.07 | 0.55 |
| 1:2G:244:GLY:H | 1:2G:247:ASN:HD21 | 1.54 | 0.55 |
| 1:2I:215:LEU:HB3 | 1:2I:217:LEU:HG | 1.88 | 0.55 |
| 2:2L:26:LEU:HD21 | 2:2L:363:VAL:HG12 | 1.89 | 0.55 |
| 2:2P:236:SER:O | 2:2P:243:ARG:NH2 | 2.40 | 0.55 |
| 1:2Q:306:ARG:NH1 | 38:8A:95:LYS:CA | 2.70 | 0.55 |
| 1:2S:244:GLY:HA2 | 1:2S:355:ASP:OD2 | 2.06 | 0.55 |
| 2:3F:340:THR:HG23 | 2:3F:341:ILE:HG23 | 1.89 | 0.55 |
| 2:3J:286:LEU:O | 2:3J:373:ARG:NH1 | 2.39 | 0.55 |
| 1:3M:218:THR:HB | 38:8C:227:LYS:HA | 1.89 | 0.55 |
| 2:3T:399:TYR:HE2 | 2:3T:418:PHE:HB3 | 1.72 | 0.55 |
| 3:4B:153:ASP:OD1 | 3:4B:156:HIS:N | 2.37 | 0.55 |
| 5:4L:289:LEU:O | 5:4L:293:LEU:HG | 2.07 | 0.55 |
| 6:4O:329:GLU:O | 6:4O:333:MET:HG2 | 2.07 | 0.55 |
| 14:5L:30:ILE:HG22 | 14:5L:41:ARG:HB2 | 1.88 | 0.55 |
| 14:5M:30:ILE:HG22 | 14:5M:41:ARG:HB2 | 1.88 | 0.55 |
| 16:5Q:100:ILE:O | 16:5Q:104:ILE:HG12 | 2.07 | 0.55 |
| 22:6K:204:PHE:HB3 | 22:6K:227:TYR:HE2 | 1.71 | 0.55 |
| 24:6V:135:PRO:HG2 | 24:6V:137:GLN:HE22 | 1.70 | 0.55 |
| 26:7D:23:THR:HG22 | 26:7D:24:GLN:H | 1.71 | 0.55 |
| 26:7E:23:THR:HG22 | 26:7E:24:GLN:H | 1.71 | 0.55 |
| 26:7F:23:THR:HG22 | 26:7F:24:GLN:H | 1.71 | 0.55 |
| 32:7O:30:ILE:HG13 | 32:7O:31:GLY:H | 1.72 | 0.55 |
| 37:7Y:210:THR:HG22 | 37:7Y:213:MET:HG2 | 1.88 | 0.55 |
| 2:G1:413:MET:HB3 | 2:G1:417:GLU:OE2 | 2.06 | 0.55 |
| 2:G3:119:LEU:HA | 2:G3:122:ILE:HG22 | 1.88 | 0.55 |
| 1:G4:68:LEU:HB3 | 1:G4:96:GLY:HA2 | 1.87 | 0.55 |
| 2:G7:5:ILE:HG22 | 2:G7:64:ARG:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I5:306:ASP:HB3 | 2:I5:309:HIS:HD2 | 1.70 | 0.55 |
| 1:J0:272:PRO:HB2 | 1:J0:282:ARG:HH12 | 1.72 | 0.55 |
| 2:K1:312:TYR:HD1 | 2:K1:381:SER:HB2 | 1.72 | 0.55 |
| 2:K3:27:GLU:CD | 2:K3:243:ARG:HH12 | 2.09 | 0.55 |
| 2:K7:51:THR:HG21 | 2:K7:243:ARG:HG2 | 1.89 | 0.55 |
| 1:L0:7:ILE:HB | 1:L0:135:VAL:HG22 | 1.88 | 0.55 |
| 2:L1:76:ASP:OD1 | 1:L2:46:ARG:NH2 | 2.39 | 0.55 |
| 2:M9:281:ALA:O | 2:M9:284:GLU:HG3 | 2.06 | 0.55 |
| 1:N6:8:GLN:HB2 | 1:N6:65:LEU:HD23 | 1.89 | 0.55 |
| 2:N7:121:ARG:NH2 | 2:N7:121:ARG:CG | 2.60 | 0.55 |
| 2:N7:286:LEU:O | 2:N7:373:ARG:NH1 | 2.40 | 0.55 |
| 2:N9:125:LEU:HD23 | 2:N9:125:LEU:O | 2.07 | 0.55 |
| 2:O3:276:ILE:HG23 | 2:O3:280:LYS:HB2 | 1.88 | 0.55 |
| 2:O5:222:PRO:O | 1:O6:322:SER:OG | 2.21 | 0.55 |
| 2:O7:406:HIS:HA | 2:O7:409:VAL:HG22 | 1.87 | 0.55 |
| 1:O8:276:ARG:HA | 1:O8:279:GLN:HG3 | 1.88 | 0.55 |
| 2:O9:287:SER:OG | 2:O9:290:GLU:OE1 | 2.17 | 0.55 |
| 1:P4:301:CYS:SG | 1:P4:302:ALA:N | 2.79 | 0.55 |
| 1:P8:52:ASN:OD1 | 1:P8:62:ARG:NH2 | 2.40 | 0.55 |
| 1:Q0:8:GLN:OE1 | 1:Q0:17:GLY:HA3 | 2.06 | 0.55 |
| 2:R5:220:GLU:HG2 | 2:R5:221:ARG:HG3 | 1.89 | 0.55 |
| 2:R5:333:ALA:O | 2:R5:337:THR:HG23 | 2.07 | 0.55 |
| 1:S4:107:THR:OG1 | 1:S4:401:GLU:OE2 | 2.21 | 0.55 |
| 1:S4:362:LYS:HD3 | 7:4T:174:HIS:CE1 | 2.41 | 0.55 |
| 1:S4:391:ARG:HG3 | 2:S5:346:TRP:NE1 | 2.22 | 0.55 |
| 2:U5:76:ASP:HB3 | 2:U5:79:ARG:HH11 | 1.72 | 0.55 |
| 2:V1:267:PHE:HB2 | 2:V1:384:ILE:HD12 | 1.88 | 0.55 |
| 1:W0:5:VAL:HG12 | 1:W0:133:PHE:HD1 | 1.71 | 0.55 |
| 1:W8:232:VAL:HG22 | 1:W8:270:PHE:HB2 | 1.89 | 0.55 |
| 1:X0:40:SER:HB2 | 8:4X:99:PRO:HG3 | 1.88 | 0.55 |
| 2:X3:286:LEU:HD11 | 2:X3:372:GLN:H | 1.72 | 0.55 |
| 2:X7:21:TRP:CZ3 | 2:X7:63:PRO:HB3 | 2.41 | 0.55 |
| 2:Z3:277:SER:OG | 2:Z3:280:LYS:HG2 | 2.07 | 0.55 |
| 1:Z4:86:ARG:HG2 | 1:Z4:88:ASP:H | 1.70 | 0.55 |
| 1:0E:26:ASP:O | 1:0E:359:LYS:NZ | 2.28 | 0.55 |
| 1:0E:86:ARG:HG2 | 1:0E:88:ASP:H | 1.72 | 0.55 |
| 2:0L:11:GLN:NE2 | 1:0M:245:GLN:O | 2.37 | 0.55 |
| 2:0L:239:THR:HG23 | 2:0L:243:ARG:HE | 1.71 | 0.55 |
| 2:0N:164:LYS:O | 2:0N:166:LYS:NZ | 2.40 | 0.55 |
| 1:1C:260:PHE:HB2 | 1:1C:263:LEU:HD13 | 1.88 | 0.55 |
| 1:1G:68:LEU:HG | 1:1G:147:MET:HE1 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1M:193:VAL:HG11 | 1:1M:418:LEU:HD11 | 1.88 | 0.55 |
| 1:1O:51:PHE:O | 1:1O:62:ARG:NH2 | 2.39 | 0.55 |
| 2:1P:175:PRO:HB3 | 2:1P:390:ARG:NE | 2.22 | 0.55 |
| 2:2J:178:SER:HB3 | 1:2K:347:ASN:ND2 | 2.22 | 0.55 |
| 1:2K:121:ARG:HD3 | 38:8C:50:LYS:HE2 | 1.89 | 0.55 |
| 2:2L:399:TYR:OH | 2:2L:415:GLU:OE2 | 2.24 | 0.55 |
| 2:2X:116:ASP:OD1 | 2:2X:117:LEU:N | 2.39 | 0.55 |
| 2:3B:66:ILE:HD12 | 2:3B:68:LEU:HD23 | 1.88 | 0.55 |
| 2:3J:124:LYS:HZ2 | 3:3Z:36:PHE:HD1 | 1.53 | 0.55 |
| 1:3K:139:LEU:HD12 | 1:3K:170:VAL:HG12 | 1.88 | 0.55 |
| 2:3P:285:GLN:O | 2:3P:285:GLN:HG2 | 2.05 | 0.55 |
| 5:4L:306:PHE:HA | 5:4L:309:ARG:HH11 | 1.71 | 0.55 |
| 8:4W:211:ALA:O | 8:4W:215:GLU:HG2 | 2.07 | 0.55 |
| 10:5C:200:GLU:O | 10:5C:203:GLU:HG3 | 2.06 | 0.55 |
| 14:5N:34:LEU:HG | 14:5N:35:GLY:H | 1.72 | 0.55 |
| 15:5O:99:LYS:HA | 15:5O:153:MET:HE1 | 1.87 | 0.55 |
| 15:5O:237:THR:HG21 | 15:5O:310:GLU:OE2 | 2.07 | 0.55 |
| 15:5O:343:LEU:H | 15:5O:343:LEU:HD23 | 1.72 | 0.55 |
| 20:6F:285:THR:HA | 20:6F:288:TYR:HE2 | 1.70 | 0.55 |
| 24:6T:86:PRO:HB2 | 24:6T:88:TRP:CD1 | 2.42 | 0.55 |
| 24:6V:482:ILE:HG22 | 24:6V:497:PHE:HB3 | 1.88 | 0.55 |
| 28:7X:403:LYS:O | 28:7X:403:LYS:HG3 | 2.05 | 0.55 |
| 2:4:30:ILE:N | 26:7D:45:MET:HE1 | 2.20 | 0.55 |
| 2:8:221:ARG:O | 26:7E:78:ALA:HA | 2.05 | 0.55 |
| 1:A3:245:GLN:HG3 | 26:7F:113:ARG:HH12 | 1.71 | 0.55 |
| 2:G1:384:ILE:HD12 | 2:G1:384:ILE:H | 1.72 | 0.55 |
| 2:G7:221:ARG:HG3 | 22:6O:178:GLY:HA2 | 1.87 | 0.55 |
| 2:I3:167:LEU:HD13 | 2:I3:200:VAL:HB | 1.89 | 0.55 |
| 2:I7:251:ASP:OD1 | 2:I7:254:GLU:HG2 | 2.06 | 0.55 |
| 1:I8:139:LEU:HD12 | 1:I8:170:VAL:HG12 | 1.89 | 0.55 |
| 1:I8:345:ILE:O | 1:I8:348:ASN:ND2 | 2.39 | 0.55 |
| 2:J9:56:THR:HA | 2:L5:285:GLN:HB2 | 1.89 | 0.55 |
| 2:J9:57:GLY:H | 2:L5:285:GLN:HG3 | 1.72 | 0.55 |
| 1:K0:139:LEU:HD12 | 1:K0:170:VAL:HG12 | 1.88 | 0.55 |
| 2:K3:88:HIS:CD2 | 2:L9:283:HIS:HB2 | 2.42 | 0.55 |
| 2:K3:313:MET:HB2 | 2:K3:380:ASN:HB3 | 1.87 | 0.55 |
| 2:K9:14:ILE:HD11 | 2:K9:74:VAL:HG13 | 1.89 | 0.55 |
| 2:L1:167:LEU:HD13 | 2:L1:200:VAL:HB | 1.89 | 0.55 |
| 2:L7:369:ALA:HA | 6:4P:205:GLN:HE22 | 1.72 | 0.55 |
| 2:M1:90:GLU:N | 1:N8:281:TYR:OH | 2.32 | 0.55 |
| 1:M4:117:LEU:HA | 1:M4:120:VAL:HG12 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M9:88:HIS:O | 1:O6:281:TYR:OH | 2.19 | 0.55 |
| 2:M9:286:LEU:O | 2:M9:373:ARG:NH1 | 2.40 | 0.55 |
| 2:N7:345:ASP:N | 2:N7:345:ASP:OD1 | 2.40 | 0.55 |
| 1:O2:125:GLU:OE2 | 1:O2:159:TYR:OH | 2.25 | 0.55 |
| 2:O5:264:ARG:NH2 | 2:O5:431:ASP:OD2 | 2.40 | 0.55 |
| 2:O7:6:SER:O | 2:O7:65:CYS:HA | 2.07 | 0.55 |
| 1:P6:72:THR:O | 1:P6:76:VAL:HG23 | 2.07 | 0.55 |
| 2:Q9:266:HIS:ND1 | 2:Q9:266:HIS:O | 2.39 | 0.55 |
| 2:R9:3:GLU:HB2 | 2:R9:129:CYS:SG | 2.46 | 0.55 |
| 1:S2:359:LYS:HD3 | 7:4R:361:GLN:HE22 | 1.71 | 0.55 |
| 1:S4:131:GLN:HE21 | 1:S4:250:LEU:HB3 | 1.71 | 0.55 |
| 1:S4:227:HIS:CE1 | 24:6U:11:LEU:HA | 2.41 | 0.55 |
| 1:S6:186:THR:HG22 | 1:S6:411:ALA:HB1 | 1.89 | 0.55 |
| 1:S8:309:ARG:H | 1:S8:372:THR:HG22 | 1.71 | 0.55 |
| 1:T6:27:GLU:OE2 | 1:T6:318:ARG:NH2 | 2.31 | 0.55 |
| 1:U8:20:PHE:HA | 1:U8:230:SER:HB2 | 1.89 | 0.55 |
| 1:V0:220:PRO:HG2 | 2:V1:326:LYS:HB2 | 1.89 | 0.55 |
| 1:V2:138:SER:OG | 1:V2:139:LEU:N | 2.40 | 0.55 |
| 1:V4:226:ASN:HD21 | 39:V4:501:GDP:HN1 | 1.53 | 0.55 |
| 1:X2:51:PHE:HB3 | 1:X2:59:TYR:HB3 | 1.88 | 0.55 |
| 2:Y1:301:MET:HE1 | 2:Y1:307:PRO:HD3 | 1.89 | 0.55 |
| 2:Y9:121:ARG:HD2 | 2:Y9:124:LYS:HE3 | 1.88 | 0.55 |
| 1:Z8:189:VAL:HA | 1:Z8:192:LEU:HB3 | 1.89 | 0.55 |
| 2:Z9:278:ALA:HA | 2:Z9:369:ALA:HB2 | 1.87 | 0.55 |
| 1:0E:165:LEU:HD12 | 1:0E:167:PHE:CE1 | 2.42 | 0.55 |
| 2:0J:268:MET:CE | 2:0J:380:ASN:HB2 | 2.36 | 0.55 |
| 2:0L:88:HIS:CE1 | 2:1B:283:HIS:HA | 2.42 | 0.55 |
| 2:0N:156:ARG:HA | 2:0N:159:VAL:HG12 | 1.89 | 0.55 |
| 1:0O:211:CYS:HA | 1:0O:215:LEU:HB2 | 1.89 | 0.55 |
| 1:0U:33:THR:O | 1:0U:58:ARG:NH2 | 2.40 | 0.55 |
| 2:1B:266:HIS:O | 2:1B:266:HIS:ND1 | 2.39 | 0.55 |
| 1:1G:317:PHE:HE2 | 1:1G:326:VAL:HG13 | 1.71 | 0.55 |
| 1:1K:301:CYS:SG | 1:1K:302:ALA:N | 2.80 | 0.55 |
| 2:1X:88:HIS:HB3 | 2:2N:283:HIS:ND1 | 2.22 | 0.55 |
| 2:2N:396:ASP:HA | 2:2N:399:TYR:HB3 | 1.87 | 0.55 |
| 2:2T:9:ILE:HG12 | 2:2T:68:LEU:HD11 | 1.88 | 0.55 |
| 1:2U:2:ARG:HE | 1:2U:240:LEU:HD22 | 1.72 | 0.55 |
| 1:2U:135:VAL:HG21 | 1:2U:152:ILE:HD11 | 1.89 | 0.55 |
| 2:2Z:88:HIS:CD2 | 2:2Z:90:GLU:HB3 | 2.42 | 0.55 |
| 2:3B:109:THR:OG1 | 2:3B:411:GLU:OE2 | 2.25 | 0.55 |
| 2:3D:172:TYR:CE2 | 2:3D:203:MET:HG2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3H:98:ASP:OD1 | 2:3H:99:ALA:N | 2.40 | 0.55 |
| 2:3J:116:ASP:N | 2:3J:116:ASP:OD1 | 2.40 | 0.55 |
| 1:3M:178:THR:HA | 2:3N:352:LYS:HD2 | 1.89 | 0.55 |
| 1:3O:139:LEU:HD12 | 1:3O:170:VAL:HG12 | 1.87 | 0.55 |
| 1:3Q:52:ASN:OD1 | 1:3Q:62:ARG:NH2 | 2.40 | 0.55 |
| 1:3Q:68:LEU:HD23 | 1:3Q:93:GLY:HA3 | 1.88 | 0.55 |
| 1:3S:263:LEU:O | 1:3S:370:ASN:ND2 | 2.40 | 0.55 |
| 2:3T:26:LEU:HD21 | 2:3T:363:VAL:HG12 | 1.89 | 0.55 |
| 2:3T:155:GLU:HB2 | 2:3T:197:HIS:CE1 | 2.41 | 0.55 |
| 8:4W:292:MET:O | 8:4W:295:MET:HG2 | 2.07 | 0.55 |
| 9:4Z:192:THR:O | 9:4Z:195:ARG:HG3 | 2.07 | 0.55 |
| 14:5L:34:LEU:HG | 14:5L:35:GLY:H | 1.72 | 0.55 |
| 14:5M:34:LEU:HG | 14:5M:35:GLY:H | 1.72 | 0.55 |
| 15:5P:95:LEU:HD23 | 15:5P:97:MET:H | 1.72 | 0.55 |
| 15:5P:274:ASP:OD1 | 15:5P:275:ARG:N | 2.39 | 0.55 |
| 20:6F:65:TYR:CB | 20:6F:138:ILE:HD11 | 2.36 | 0.55 |
| 22:6L:76:LYS:HE2 | 22:6L:77:PRO:HD2 | 1.89 | 0.55 |
| 24:6U:92:ASP:OD1 | 24:6U:92:ASP:N | 2.39 | 0.55 |
| 24:6X:473:TYR:CD1 | 24:6X:517:LEU:HD21 | 2.42 | 0.55 |
| 24:6Y:278:VAL:HG11 | 24:6Y:395:VAL:HG11 | 1.87 | 0.55 |
| 29:7J:316:VAL:HG12 | 29:7J:317:SER:H | 1.71 | 0.55 |
| 29:7J:448:VAL:HG22 | 29:7J:451:LYS:HB3 | 1.87 | 0.55 |
| 38:8C:81:VAL:O | 38:8C:81:VAL:HG13 | 2.07 | 0.55 |
| 1:A5:281:TYR:O | 1:T8:86:ARG:NH1 | 2.39 | 0.55 |
| 2:E5:282:TYR:CE1 | 22:6K:80:GLY:O | 2.60 | 0.55 |
| 1:H4:177:ASP:O | 2:H5:352:LYS:HA | 2.06 | 0.55 |
| 2:H9:63:PRO:HB2 | 2:H9:65:CYS:SG | 2.47 | 0.55 |
| 2:I7:156:ARG:HA | 2:I7:159:VAL:HG12 | 1.89 | 0.55 |
| 1:I8:172:SER:HB3 | 1:I8:175:VAL:HG22 | 1.89 | 0.55 |
| 1:I8:177:ASP:O | 2:I9:352:LYS:HA | 2.07 | 0.55 |
| 2:I9:73:THR:HG21 | 1:J0:2:ARG:HH22 | 1.71 | 0.55 |
| 2:J3:88:HIS:CE1 | 2:J3:121:ARG:HH22 | 2.25 | 0.55 |
| 1:J4:2:ARG:HE | 1:J4:240:LEU:HD22 | 1.71 | 0.55 |
| 2:K7:384:ILE:HA | 2:K7:387:ILE:HD12 | 1.88 | 0.55 |
| 1:K8:350:LYS:NZ | 1:K8:351:SER:O | 2.39 | 0.55 |
| 1:L0:68:LEU:HB3 | 1:L0:96:GLY:HA2 | 1.88 | 0.55 |
| 1:L2:27:GLU:OE2 | 1:L2:318:ARG:NH2 | 2.40 | 0.55 |
| 1:L2:52:ASN:OD1 | 1:L2:62:ARG:NH2 | 2.40 | 0.55 |
| 1:M0:190:HIS:CD2 | 1:M0:411:ALA:HA | 2.42 | 0.55 |
| 2:M1:189:LEU:HD11 | 2:M1:418:PHE:HE1 | 1.71 | 0.55 |
| 2:M3:73:THR:HA | 1:M4:46:ARG:HH21 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M5:8:HIS:NE2 | 2:M5:17:GLY:HA3 | 2.21 | 0.55 |
| 1:M6:46:ARG:NH1 | 37:7Y:115:CYS:HG | 2.05 | 0.55 |
| 2:N5:166:LYS:N | 2:N5:199:ASP:OD1 | 2.38 | 0.55 |
| 2:N9:210:TYR:HH | 1:O0:323:THR:HG1 | 1.53 | 0.55 |
| 2:O3:53:PHE:HB3 | 2:O3:61:HIS:HB3 | 1.89 | 0.55 |
| 1:O4:276:ARG:HD2 | 19:6E:68:PRO:O | 2.07 | 0.55 |
| 1:P6:272:PRO:HB2 | 1:P6:282:ARG:HH12 | 1.71 | 0.55 |
| 1:P8:4:ILE:HB | 1:P8:50:TYR:HE1 | 1.71 | 0.55 |
| 2:R1:161:TYR:CD1 | 13:5H:124:VAL:HG13 | 2.41 | 0.55 |
| 1:S6:113:ILE:HD13 | 1:S6:150:LEU:HD22 | 1.89 | 0.55 |
| 1:S8:157:GLU:OE2 | 3:3Z:90:ILE:HG23 | 2.06 | 0.55 |
| 2:S9:53:PHE:HB3 | 2:S9:61:HIS:HB3 | 1.89 | 0.55 |
| 1:T0:391:ARG:HD3 | 2:T1:346:TRP:NE1 | 2.22 | 0.55 |
| 1:T2:178:THR:O | 1:T2:181:GLU:HG3 | 2.06 | 0.55 |
| 1:T2:414:ASN:ND2 | 3:4D:84:LYS:HD2 | 2.22 | 0.55 |
| 2:U1:312:TYR:HB2 | 2:U1:343:PHE:HD1 | 1.71 | 0.55 |
| 1:U2:39:ASP:OD1 | 1:U2:40:SER:N | 2.38 | 0.55 |
| 1:U8:5:VAL:HG12 | 1:U8:133:PHE:HD1 | 1.72 | 0.55 |
| 1:W8:248:ALA:HA | 1:W8:252:LYS:HD2 | 1.89 | 0.55 |
| 2:W9:88:HIS:CA | 2:Y5:283:HIS:NE2 | 2.69 | 0.55 |
| 1:X0:40:SER:OG | 8:4X:97:PHE:O | 2.24 | 0.55 |
| 2:X3:53:PHE:HB3 | 2:X3:61:HIS:HB3 | 1.87 | 0.55 |
| 1:X4:172:SER:HB2 | 1:X4:205:GLU:OE1 | 2.07 | 0.55 |
| 1:X6:260:PHE:HB2 | 1:X6:263:LEU:HG | 1.89 | 0.55 |
| 2:Y1:90:GLU:H | 2:Z7:283:HIS:CE1 | 2.25 | 0.55 |
| 1:Y4:248:ALA:HA | 1:Y4:252:LYS:HD2 | 1.89 | 0.55 |
| 2:Y5:183:GLU:CD | 2:Y5:184:PRO:HD3 | 2.27 | 0.55 |
| 2:Z3:286:LEU:HD11 | 2:Z3:372:GLN:HB2 | 1.89 | 0.55 |
| 1:Z4:285:THR:HB | 1:Z4:287:PRO:HD2 | 1.89 | 0.55 |
| 1:Z6:58:ARG:HD3 | 1:0M:280:GLN:HE22 | 1.71 | 0.55 |
| 2:Z9:33:ASP:OD2 | 2:Z9:35:GLN:NE2 | 2.40 | 0.55 |
| 2:0J:121:ARG:HD2 | 2:0J:124:LYS:HE3 | 1.89 | 0.55 |
| 1:0Q:218:THR:O | 2:0R:326:LYS:NZ | 2.33 | 0.55 |
| 2:0R:164:LYS:O | 2:0R:166:LYS:NZ | 2.40 | 0.55 |
| 2:0V:3:GLU:CG | 2:0V:129:CYS:HB2 | 2.37 | 0.55 |
| 2:1B:313:MET:HB2 | 2:1B:380:ASN:HB3 | 1.88 | 0.55 |
| 2:1H:50:ASN:O | 2:1H:64:ARG:NH2 | 2.40 | 0.55 |
| 1:1M:317:PHE:HE2 | 1:1M:326:VAL:HG13 | 1.72 | 0.55 |
| 1:1Q:301:CYS:SG | 1:1Q:302:ALA:N | 2.80 | 0.55 |
| 2:1R:264:ARG:NH2 | 2:1R:431:ASP:OD2 | 2.33 | 0.55 |
| 1:1S:139:LEU:HD12 | 1:1S:170:VAL:HG22 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1X:362:VAL:HG11 | 2:1X:370:LYS:HE3 | 1.87 | 0.55 |
| 2:2B:287:SER:N | 2:2B:290:GLU:OE2 | 2.38 | 0.55 |
| 2:2F:274:PRO:HB2 | 2:2F:276:ILE:HG12 | 1.88 | 0.55 |
| 2:2H:123:ARG:NH2 | 38:8B:37:TYR:HD2 | 2.04 | 0.55 |
| 2:2J:336:LYS:O | 2:2J:339:ARG:NH2 | 2.39 | 0.55 |
| 2:2P:84:ARG:HB3 | 38:8A:188:ARG:NH1 | 2.17 | 0.55 |
| 1:2S:334:GLN:NE2 | 1:2S:348:ASN:H | 2.02 | 0.55 |
| 2:2X:129:CYS:SG | 2:2X:130:THR:N | 2.80 | 0.55 |
| 2:3P:88:HIS:HB3 | 2:3P:91:GLN:HE22 | 1.72 | 0.55 |
| 2:3T:391:LEU:HD23 | 2:3T:394:LYS:HD2 | 1.88 | 0.55 |
| 5:4L:428:THR:HG21 | 16:5Q:96:GLY:HA2 | 1.89 | 0.55 |
| 9:4Y:431:GLU:OE1 | 9:4Y:434:ARG:NH1 | 2.39 | 0.55 |
| 9:4Z:342:LYS:O | 9:4Z:346:LYS:HE3 | 2.05 | 0.55 |
| 10:5D:132:THR:HA | 10:5D:135:ARG:HB2 | 1.87 | 0.55 |
| 14:5M:365:ARG:HH22 | 14:5M:377:ARG:NH1 | 2.04 | 0.55 |
| 20:6F:22:LEU:O | 20:6F:26:ILE:HG13 | 2.07 | 0.55 |
| 21:6G:15:ASP:OD1 | 21:6G:16:GLU:HG3 | 2.06 | 0.55 |
| 22:6M:210:MET:O | 22:6M:213:THR:HG22 | 2.07 | 0.55 |
| 23:6R:28:LYS:CE | 23:6R:28:LYS:CA | 2.85 | 0.55 |
| 24:6T:562:LEU:HD13 | 24:6T:633:LEU:HD11 | 1.87 | 0.55 |
| 24:6Y:289:ARG:NH2 | 24:6Y:397:GLU:OE1 | 2.40 | 0.55 |
| 24:6Z:130:MET:HG3 | 24:6Z:153:VAL:HG12 | 1.87 | 0.55 |
| 36:7W:13:LYS:HA | 36:7W:16:GLN:HB3 | 1.88 | 0.55 |
| 38:7Z:12:LEU:HB3 | 38:7Z:18:VAL:HG21 | 1.89 | 0.55 |
| 38:8D:219:LEU:O | 38:8D:223:THR:HG22 | 2.07 | 0.55 |
| 2:8:41:THR:OG1 | 24:6W:97:ARG:NH1 | 2.06 | 0.55 |
| 2:A2:40:LYS:HZ1 | 26:7F:45:MET:CB | 1.93 | 0.55 |
| 1:A3:228:LEU:HD21 | 26:7F:136:PHE:HZ | 1.69 | 0.55 |
| 1:A3:340:TYR:HE1 | 3:4H:103:SER:C | 2.09 | 0.55 |
| 1:B1:320:ARG:NH1 | 18:5Y:53:GLY:HA3 | 2.22 | 0.55 |
| 2:D7:36:MET:HB2 | 22:6O:76:LYS:HE2 | 1.89 | 0.55 |
| 1:E2:320:ARG:NH1 | 22:6J:115:SER:HA | 2.18 | 0.55 |
| 2:G9:182:VAL:HG23 | 2:G9:186:ASN:HD21 | 1.72 | 0.55 |
| 2:H3:9:ILE:HG22 | 2:H3:146:GLY:HA2 | 1.88 | 0.55 |
| 2:H3:287:SER:OG | 2:H3:288:VAL:N | 2.40 | 0.55 |
| 1:H6:193:VAL:HG11 | 1:H6:418:LEU:HD11 | 1.88 | 0.55 |
| 2:H9:11:GLN:OE1 | 2:H9:15:GLN:NE2 | 2.41 | 0.55 |
| 2:H9:90:GLU:HB3 | 2:H9:121:ARG:HH22 | 1.71 | 0.55 |
| 2:I1:223:THR:HG23 | 2:I1:225:THR:H | 1.71 | 0.55 |
| 1:I4:51:PHE:O | 1:I4:62:ARG:NH2 | 2.39 | 0.55 |
| 2:J3:357:TYR:HB3 | 16:5Q:173:ARG:HE | 0.43 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J4:65:LEU:HD12 | 1:J4:90:PHE:CE1 | 2.41 | 0.55 |
| 1:J6:156:ARG:NH2 | 35:7T:31:SER:OG | 2.40 | 0.55 |
| 2:K1:230:LEU:O | 2:K1:234:VAL:HG23 | 2.07 | 0.55 |
| 1:L0:203:ASP:OD2 | 1:L0:302:ALA:N | 2.40 | 0.55 |
| 1:L6:173:PRO:HD2 | 1:L6:380:ARG:HH21 | 1.71 | 0.55 |
| 2:M5:405:VAL:HG13 | 2:M5:418:PHE:HE2 | 1.70 | 0.55 |
| 1:M6:139:LEU:HD12 | 1:M6:170:VAL:HG22 | 1.89 | 0.55 |
| 2:M9:84:ARG:NH1 | 29:7J:284:ASP:O | 2.39 | 0.55 |
| 1:N0:53:GLU:OE2 | 1:N0:57:GLY:N | 2.40 | 0.55 |
| 2:N3:414:GLU:HG2 | 2:N3:415:GLU:H | 1.72 | 0.55 |
| 1:N6:211:CYS:HA | 1:N6:215:LEU:HB2 | 1.89 | 0.55 |
| 2:N7:100:ALA:HA | 1:N8:252:LYS:HE3 | 1.88 | 0.55 |
| 1:O2:52:ASN:OD1 | 1:O2:62:ARG:NH2 | 2.39 | 0.55 |
| 1:O8:245:GLN:HG3 | 32:7P:64:THR:HG21 | 1.87 | 0.55 |
| 1:Q4:134:GLN:HE21 | 1:Q4:167:PHE:HE2 | 1.55 | 0.55 |
| 1:Q4:217:LEU:HD13 | 20:6F:184:ARG:HH22 | 1.72 | 0.55 |
| 1:Q6:309:ARG:NH1 | 1:Q6:339:SER:O | 2.40 | 0.55 |
| 2:Q9:8:HIS:CD2 | 2:Q9:17:GLY:HA3 | 2.42 | 0.55 |
| 2:S1:26:LEU:HD23 | 2:S1:363:VAL:HG12 | 1.89 | 0.55 |
| 1:S4:280:GLN:HB2 | 7:4T:182:ASP:OD1 | 2.07 | 0.55 |
| 1:S8:190:HIS:CD2 | 1:S8:411:ALA:HA | 2.42 | 0.55 |
| 1:S8:371:SER:OG | 1:S8:372:THR:N | 2.39 | 0.55 |
| 1:T2:110:ALA:HB1 | 3:4D:75:ARG:HE | 1.72 | 0.55 |
| 1:U8:329:GLN:HA | 1:U8:332:ASN:HD21 | 1.72 | 0.55 |
| 2:V3:11:GLN:NE2 | 1:V4:247:ASN:OD1 | 2.39 | 0.55 |
| 2:V3:26:LEU:HD21 | 2:V3:363:VAL:HG12 | 1.89 | 0.55 |
| 1:V6:232:VAL:HG22 | 1:V6:270:PHE:HB2 | 1.88 | 0.55 |
| 2:W3:222:PRO:HD2 | 1:W4:324:LYS:HE3 | 1.89 | 0.55 |
| 1:W4:30:ILE:HG22 | 1:W4:36:TYR:HA | 1.88 | 0.55 |
| 2:W7:276:ILE:CD1 | 2:W7:281:ALA:HA | 2.35 | 0.55 |
| 1:X6:265:PHE:HE2 | 1:X6:418:LEU:HD11 | 1.72 | 0.55 |
| 1:Y6:130:LEU:HB2 | 1:Y6:162:ARG:HE | 1.72 | 0.55 |
| 1:Y8:2:ARG:HB2 | 1:Y8:240:LEU:HD11 | 1.88 | 0.55 |
| 2:Z3:167:LEU:HD13 | 2:Z3:200:VAL:HB | 1.89 | 0.55 |
| 1:Z6:186:THR:OG1 | 1:Z6:187:LEU:HD12 | 2.07 | 0.55 |
| 2:Z7:65:CYS:SG | 2:Z7:66:ILE:N | 2.80 | 0.55 |
| 1:Z8:211:CYS:SG | 1:Z8:217:LEU:HB2 | 2.46 | 0.55 |
| 1:Z8:337:ASN:HB2 | 1:Z8:340:TYR:HD2 | 1.72 | 0.55 |
| 1:0A:7:ILE:HB | 1:0A:135:VAL:HG22 | 1.89 | 0.55 |
| 2:0H:271:SER:OG | 2:0H:300:SER:O | 2.19 | 0.55 |
| 1:0I:116:VAL:HA | 1:0I:119:VAL:HG12 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Y:45:GLU:HG2 | 1:0Y:46:ARG:HG2 | 1.88 | 0.55 |
| 1:0Y:335:ASN:O | 1:0Y:338:SER:OG | 2.25 | 0.55 |
| 1:1A:207:LEU:HB3 | 1:1A:225:LEU:HD22 | 1.89 | 0.55 |
| 2:1D:344:VAL:HG22 | 2:1D:346:TRP:H | 1.70 | 0.55 |
| 2:1F:227:LEU:O | 2:1F:231:ILE:HG13 | 2.06 | 0.55 |
| 1:1K:262:ARG:NH2 | 1:1K:417:ASP:OD1 | 2.40 | 0.55 |
| 1:1O:186:THR:HG22 | 1:1O:411:ALA:HB1 | 1.88 | 0.55 |
| 2:1R:276:ILE:HD11 | 2:1R:371:VAL:HG22 | 1.88 | 0.55 |
| 1:1U:135:VAL:HG21 | 1:1U:152:ILE:HD11 | 1.89 | 0.55 |
| 1:1U:287:PRO:HA | 1:1U:290:THR:HG22 | 1.89 | 0.55 |
| 1:2E:345:ILE:HB | 1:2E:348:ASN:HD21 | 1.72 | 0.55 |
| 1:2I:214:THR:O | 1:2I:275:SER:OG | 2.21 | 0.55 |
| 2:2P:265:ILE:HG13 | 2:2P:265:ILE:O | 2.07 | 0.55 |
| 2:2T:211:ASP:OD2 | 2:2T:304:LYS:NZ | 2.40 | 0.55 |
| 2:2V:205:ASP:OD2 | 2:2V:206:ASN:N | 2.39 | 0.55 |
| 2:2X:11:GLN:NE2 | 2:2X:71:GLU:OE2 | 2.40 | 0.55 |
| 1:2Y:325:GLU:O | 1:2Y:329:GLN:HG2 | 2.07 | 0.55 |
| 2:3D:251:ASP:OD1 | 2:3D:254:GLU:HG3 | 2.07 | 0.55 |
| 2:3H:289:ALA:O | 2:3H:293:ASN:ND2 | 2.39 | 0.55 |
| 2:3P:417:GLU:HA | 2:3P:420:GLU:HG2 | 1.89 | 0.55 |
| 2:3R:305:CYS:HB3 | 2:3R:387:ILE:HD11 | 1.88 | 0.55 |
| 3:4B:210:ASP:OD2 | 3:4B:213:VAL:HB | 2.06 | 0.55 |
| 7:4U:120:ASP:HB3 | 7:4U:123:LEU:HD23 | 1.88 | 0.55 |
| 7:4U:239:SER:HA | 31:7N:8:ASP:OD1 | 2.07 | 0.55 |
| 10:5A:429:LYS:O | 10:5A:432:GLU:HG3 | 2.06 | 0.55 |
| 14:5M:365:ARG:HH12 | 14:5M:377:ARG:NH1 | 2.03 | 0.55 |
| 14:5M:505:THR:OG1 | 14:5M:506:SER:N | 2.39 | 0.55 |
| 16:5Q:148:ARG:HG3 | 16:5Q:149:GLY:H | 1.72 | 0.55 |
| 22:6M:107:GLU:HA | 22:6M:107:GLU:OE2 | 2.06 | 0.55 |
| 24:6U:565:GLN:NE2 | 24:6U:602:LEU:HB2 | 2.22 | 0.55 |
| 24:6W:135:PRO:HG2 | 24:6W:137:GLN:HE22 | 1.71 | 0.55 |
| 24:6X:445:ILE:HD12 | 24:6X:445:ILE:N | 2.22 | 0.55 |
| 24:6Y:135:PRO:HG2 | 24:6Y:137:GLN:HE22 | 1.72 | 0.55 |
| 24:6Z:274:ARG:HD3 | 24:6Z:295:HIS:HE1 | 1.72 | 0.55 |
| 24:6Z:455:THR:OG1 | 24:6Z:456:ASP:N | 2.40 | 0.55 |
| 24:6Z:556:ASP:OD1 | 24:6Z:557:VAL:N | 2.39 | 0.55 |
| 29:7J:390:LEU:HG | 29:7J:391:PRO:CD | 2.36 | 0.55 |
| 28:7X:402:ARG:O | 28:7X:402:ARG:HG3 | 2.06 | 0.55 |
| 38:8C:25:ILE:HG13 | 38:8C:26:THR:N | 2.22 | 0.55 |
| 1:5:45:GLU:HG3 | 18:5Y:35:LEU:HD12 | 1.88 | 0.54 |
| 1:B5:362:LYS:HZ3 | 18:6A:24:ARG:HD3 | 1.66 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D7:280:LYS:HZ1 | 18:6D:166:HIS:HB3 | 1.72 | 0.54 |
| 1:G4:134:GLN:HE21 | 1:G4:167:PHE:HE2 | 1.55 | 0.54 |
| 1:G6:2:ARG:HB3 | 1:G6:131:GLN:HB2 | 1.89 | 0.54 |
| 2:H1:417:GLU:HA | 2:H1:420:GLU:HG2 | 1.89 | 0.54 |
| 2:H5:111:GLY:HA2 | 2:H5:114:ILE:HG22 | 1.89 | 0.54 |
| 1:H6:219:THR:OG1 | 2:H7:324:VAL:HG11 | 2.07 | 0.54 |
| 1:H6:276:ARG:CZ | 24:6V:490:THR:C | 2.76 | 0.54 |
| 1:I2:350:LYS:NZ | 1:I2:352:SER:OG | 2.40 | 0.54 |
| 2:I9:37:PRO:CB | 28:7H:401:THR:OG1 | 2.51 | 0.54 |
| 1:J2:135:VAL:HG21 | 1:J2:152:ILE:HD11 | 1.89 | 0.54 |
| 2:J5:372:GLN:NE2 | 5:4M:148:LEU:HA | 2.21 | 0.54 |
| 2:J9:79:ARG:NH1 | 2:J9:92:LEU:O | 2.40 | 0.54 |
| 1:K0:179:VAL:HG22 | 2:K1:258:ASN:HD22 | 1.71 | 0.54 |
| 1:L4:27:GLU:OE2 | 1:L4:318:ARG:NH2 | 2.40 | 0.54 |
| 2:L7:15:GLN:HG2 | 2:L7:224:TYR:HE2 | 1.72 | 0.54 |
| 2:M5:121:ARG:HA | 2:M5:121:ARG:NH1 | 2.14 | 0.54 |
| 1:M6:52:ASN:OD1 | 1:M6:62:ARG:NH2 | 2.39 | 0.54 |
| 1:O0:309:ARG:NH1 | 1:O0:339:SER:O | 2.40 | 0.54 |
| 2:P5:129:CYS:SG | 2:P5:130:THR:N | 2.79 | 0.54 |
| 2:Q9:97:GLU:OE1 | 2:Q9:105:ARG:NH2 | 2.39 | 0.54 |
| 2:R7:156:ARG:HA | 2:R7:159:VAL:HG12 | 1.89 | 0.54 |
| 2:R9:7:ILE:HD12 | 2:R9:153:LEU:HD21 | 1.88 | 0.54 |
| 2:S5:267:PHE:HB2 | 2:S5:384:ILE:HD12 | 1.89 | 0.54 |
| 1:S8:237:THR:HG23 | 1:S8:241:ARG:HE | 1.72 | 0.54 |
| 2:T1:325:PRO:HA | 2:T1:328:VAL:HG12 | 1.88 | 0.54 |
| 1:U2:418:LEU:O | 1:U2:421:GLU:HG2 | 2.07 | 0.54 |
| 2:U5:31:GLN:OE1 | 2:U5:35:GLN:NE2 | 2.36 | 0.54 |
| 1:U6:5:VAL:HG12 | 1:U6:133:PHE:HD1 | 1.70 | 0.54 |
| 1:U6:118:ASP:O | 1:U6:122:LYS:HG2 | 2.07 | 0.54 |
| 2:V7:203:MET:O | 2:V7:204:LEU:HD23 | 2.06 | 0.54 |
| 2:W9:84:ARG:HG3 | 2:W9:84:ARG:HH11 | 1.71 | 0.54 |
| 2:X3:324:VAL:HB | 2:X3:326:LYS:HZ3 | 1.72 | 0.54 |
| 2:X5:25:CYS:SG | 2:X5:86:LEU:HD11 | 2.47 | 0.54 |
| 2:X9:89:PRO:HD2 | 2:Z5:283:HIS:ND1 | 2.22 | 0.54 |
| 2:Y3:236:SER:OG | 2:Y3:243:ARG:NH2 | 2.41 | 0.54 |
| 1:Z0:273:LEU:H | 1:Z0:292:GLN:HE22 | 1.54 | 0.54 |
| 1:Z2:317:PHE:HB2 | 1:Z2:353:VAL:HG12 | 1.89 | 0.54 |
| 1:Z4:52:ASN:OD1 | 1:Z4:62:ARG:NH2 | 2.40 | 0.54 |
| 2:Z5:399:TYR:O | 2:Z5:402:ARG:NH1 | 2.40 | 0.54 |
| 1:0E:51:PHE:HB3 | 1:0E:59:TYR:HB3 | 1.88 | 0.54 |
| 1:0K:272:PRO:HB2 | 1:0K:282:ARG:HH12 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0L:56:THR:HA | 2:1B:285:GLN:HB2 | 1.89 | 0.54 |
| 1:0M:200:MET:HE3 | 1:0M:268:VAL:HG21 | 1.89 | 0.54 |
| 1:0O:121:ARG:NH2 | 1:0O:158:GLU:OE2 | 2.41 | 0.54 |
| 1:0Y:301:CYS:SG | 1:0Y:302:ALA:N | 2.80 | 0.54 |
| 1:1A:8:GLN:CD | 1:1A:17:GLY:HA3 | 2.28 | 0.54 |
| 2:1B:145:THR:OG1 | 41:1C:501:GTP:O1B | 2.23 | 0.54 |
| 1:1C:180:VAL:HG23 | 1:1C:184:ASN:ND2 | 2.22 | 0.54 |
| 2:1L:88:HIS:CG | 2:1L:89:PRO:HD2 | 2.42 | 0.54 |
| 1:1O:165:LEU:HG | 1:1O:250:LEU:HD11 | 1.89 | 0.54 |
| 2:1R:183:GLU:HG3 | 2:1R:184:PRO:HD3 | 1.89 | 0.54 |
| 1:1S:135:VAL:HG21 | 1:1S:152:ILE:HD11 | 1.89 | 0.54 |
| 1:1S:248:ALA:HA | 1:1S:252:LYS:HD2 | 1.89 | 0.54 |
| 2:1T:122:ILE:HA | 2:1T:125:LEU:HB2 | 1.88 | 0.54 |
| 1:1W:379:LYS:HG3 | 1:1W:419:VAL:HG11 | 1.89 | 0.54 |
| 2:1Z:88:HIS:HB3 | 2:1Z:91:GLN:CG | 2.31 | 0.54 |
| 2:1Z:318:MET:HE1 | 2:1Z:354:GLY:HA3 | 1.89 | 0.54 |
| 1:2A:3:GLU:HB2 | 1:2A:130:LEU:HA | 1.89 | 0.54 |
| 2:2B:264:ARG:NH2 | 2:2B:431:ASP:OD2 | 2.37 | 0.54 |
| 2:2P:287:SER:N | 2:2P:290:GLU:OE2 | 2.39 | 0.54 |
| 2:2R:248:LEU:HD22 | 2:2R:354:GLY:HA2 | 1.89 | 0.54 |
| 2:2R:417:GLU:HA | 2:2R:420:GLU:HG2 | 1.87 | 0.54 |
| 1:2U:309:ARG:NH1 | 1:2U:341:PHE:O | 2.40 | 0.54 |
| 2:2X:41:THR:HG21 | 14:5M:144:PRO:HD3 | 1.88 | 0.54 |
| 2:3B:339:ARG:HG2 | 38:8C:39:LYS:HZ2 | 1.72 | 0.54 |
| 2:3J:384:ILE:HA | 2:3J:387:ILE:HD12 | 1.89 | 0.54 |
| 3:3X:210:ASP:OD2 | 3:3X:213:VAL:HB | 2.06 | 0.54 |
| 3:4F:210:ASP:OD2 | 3:4F:213:VAL:HB | 2.06 | 0.54 |
| 3:4J:137:ARG:O | 3:4J:141:ASN:ND2 | 2.40 | 0.54 |
| 6:4O:349:ASP:O | 6:4O:353:LYS:HG3 | 2.07 | 0.54 |
| 10:5B:175:ALA:O | 10:5B:178:GLU:HG3 | 2.06 | 0.54 |
| 15:5O:56:LYS:HE2 | 15:5O:59:LEU:HD23 | 1.88 | 0.54 |
| 15:5O:226:ARG:NH1 | 15:5O:226:ARG:CB | 2.70 | 0.54 |
| 17:5S:179:GLN:OE1 | 17:5S:179:GLN:HA | 2.06 | 0.54 |
| 19:6E:72:GLU:HG2 | 19:6E:77:GLN:NE2 | 2.22 | 0.54 |
| 19:6E:201:THR:O | 19:6E:205:SER:N | 2.40 | 0.54 |
| 20:6F:379:ARG:HB3 | 20:6F:380:PRO:HD2 | 1.90 | 0.54 |
| 22:6L:177:LEU:HD23 | 22:6L:187:MET:HE2 | 1.88 | 0.54 |
| 24:6U:92:ASP:CG | 24:6U:93:ARG:H | 2.10 | 0.54 |
| 24:6Z:310:GLU:OE1 | 24:6Z:310:GLU:HA | 2.07 | 0.54 |
| 24:6Z:503:ILE:HG21 | 24:6Z:525:VAL:HG22 | 1.88 | 0.54 |
| 29:7I:23:ILE:HG12 | 29:7I:24:PRO:HD2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:7V:13:LYS:HA | 36:7V:16:GLN:HB3 | 1.88 | 0.54 |
| 37:7Y:177:ARG:HH11 | 37:7Y:177:ARG:CB | 2.20 | 0.54 |
| 1:A3:245:GLN:HG3 | 26:7F:113:ARG:NH1 | 2.21 | 0.54 |
| 1:E6:32:PRO:HG3 | 24:6W:402:LYS:HE3 | 1.89 | 0.54 |
| 1:G0:177:ASP:O | 2:G1:352:LYS:HA | 2.07 | 0.54 |
| 1:G4:379:LYS:HA | 1:G4:382:SER:HG | 1.72 | 0.54 |
| 1:G6:371:SER:OG | 1:G6:372:THR:N | 2.39 | 0.54 |
| 2:H7:267:PHE:HB2 | 2:H7:384:ILE:HD12 | 1.89 | 0.54 |
| 1:I0:2:ARG:HB3 | 1:I0:131:GLN:HB2 | 1.89 | 0.54 |
| 1:I0:371:SER:OG | 1:I0:372:THR:N | 2.40 | 0.54 |
| 2:I3:109:THR:OG1 | 2:I3:411:GLU:OE2 | 2.25 | 0.54 |
| 2:I9:31:GLN:NE2 | 2:I9:35:GLN:O | 2.40 | 0.54 |
| 2:J5:42:ILE:HG21 | 5:4L:478:ARG:NH2 | 2.22 | 0.54 |
| 2:J5:88:HIS:HB3 | 2:L1:283:HIS:ND1 | 2.23 | 0.54 |
| 1:J6:220:PRO:HD2 | 2:J7:326:LYS:HD2 | 1.88 | 0.54 |
| 2:J7:80:THR:O | 29:7J:390:LEU:HG | 2.08 | 0.54 |
| 2:K1:216:SER:OG | 2:K1:275:ILE:O | 2.24 | 0.54 |
| 1:K4:5:VAL:HG22 | 1:K4:133:PHE:HD1 | 1.71 | 0.54 |
| 2:K5:245:ASP:N | 2:K5:245:ASP:OD1 | 2.40 | 0.54 |
| 1:L4:27:GLU:CD | 1:L4:241:ARG:HH12 | 2.11 | 0.54 |
| 2:L5:265:ILE:HD11 | 2:L5:435:VAL:HG21 | 1.89 | 0.54 |
| 2:N9:175:PRO:HB3 | 2:N9:390:ARG:HE | 1.71 | 0.54 |
| 1:O2:91:VAL:HG11 | 1:O2:116:VAL:HG12 | 1.90 | 0.54 |
| 2:O3:223:THR:HG23 | 2:O3:225:THR:H | 1.72 | 0.54 |
| 1:O4:212:PHE:CZ | 2:O5:326:LYS:HD2 | 2.42 | 0.54 |
| 2:O5:407:TRP:O | 2:O5:411:GLU:HG2 | 2.07 | 0.54 |
| 2:O7:267:PHE:HB2 | 2:O7:384:ILE:HD12 | 1.89 | 0.54 |
| 1:O8:39:ASP:N | 1:O8:39:ASP:OD1 | 2.40 | 0.54 |
| 1:O8:177:ASP:O | 2:O9:352:LYS:HA | 2.06 | 0.54 |
| 2:P5:249:ASN:HD21 | 27:7G:184:LYS:N | 2.05 | 0.54 |
| 1:P6:8:GLN:OE1 | 1:P6:17:GLY:HA3 | 2.07 | 0.54 |
| 1:Q4:107:THR:OG1 | 1:Q4:108:GLU:OE1 | 2.17 | 0.54 |
| 2:Q5:114:ILE:HG21 | 2:Q5:149:LEU:HD22 | 1.88 | 0.54 |
| 2:S1:69:ASP:OD1 | 2:S1:70:LEU:N | 2.39 | 0.54 |
| 1:S2:320:ARG:NH1 | 12:5F:72:ALA:O | 2.37 | 0.54 |
| 2:S5:5:ILE:HG22 | 2:S5:64:ARG:HB3 | 1.87 | 0.54 |
| 1:S8:174:LYS:HD2 | 13:5I:14:PHE:CD2 | 2.43 | 0.54 |
| 1:T0:52:ASN:OD1 | 1:T0:62:ARG:NH2 | 2.40 | 0.54 |
| 1:T0:139:LEU:HD12 | 1:T0:170:VAL:HG12 | 1.88 | 0.54 |
| 1:T0:145:SER:HG | 1:T0:188:SER:HG | 1.56 | 0.54 |
| 1:T0:320:ARG:HE | 7:4T:349:LEU:HD21 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T1:76:ASP:HA | 2:T1:79:ARG:HD2 | 1.88 | 0.54 |
| 2:T1:394:LYS:HB2 | 1:T2:346:PRO:HG3 | 1.88 | 0.54 |
| 2:T3:369:ALA:HA | 7:4U:92:GLN:HE21 | 1.72 | 0.54 |
| 2:U1:56:THR:HA | 2:V7:285:GLN:HB2 | 1.88 | 0.54 |
| 2:U7:88:HIS:ND1 | 2:U7:89:PRO:CD | 2.69 | 0.54 |
| 2:U9:56:THR:HA | 2:W5:285:GLN:HB2 | 1.89 | 0.54 |
| 1:W0:309:ARG:H | 1:W0:372:THR:HG22 | 1.72 | 0.54 |
| 2:W1:154:LEU:HD21 | 2:W1:198:THR:HG22 | 1.89 | 0.54 |
| 1:W4:173:PRO:HG2 | 1:W4:174:LYS:HZ2 | 1.71 | 0.54 |
| 1:W6:324:LYS:O | 1:W6:328:GLU:HG2 | 2.08 | 0.54 |
| 1:X2:31:ASP:OD2 | 1:X2:33:THR:OG1 | 2.16 | 0.54 |
| 2:X5:62:VAL:HB | 2:X5:88:HIS:CE1 | 2.41 | 0.54 |
| 2:Z5:70:LEU:HG | 2:Z5:145:THR:HG23 | 1.88 | 0.54 |
| 2:Z5:287:SER:OG | 2:Z5:288:VAL:N | 2.38 | 0.54 |
| 1:0A:52:ASN:OD1 | 1:0A:62:ARG:NH2 | 2.41 | 0.54 |
| 1:0A:125:GLU:OE2 | 1:0A:159:TYR:OH | 2.24 | 0.54 |
| 2:0H:121:ARG:HD2 | 2:0H:124:LYS:HE3 | 1.88 | 0.54 |
| 2:0H:401:LYS:HD2 | 1:0I:344:TRP:CD2 | 2.42 | 0.54 |
| 2:0N:12:ALA:HB2 | 41:0O:501:GTP:C8 | 2.42 | 0.54 |
| 1:0Q:210:ILE:O | 1:0Q:214:THR:OG1 | 2.17 | 0.54 |
| 1:1C:121:ARG:NH2 | 1:1C:158:GLU:OE2 | 2.40 | 0.54 |
| 1:1C:210:ILE:O | 1:1C:214:THR:OG1 | 2.19 | 0.54 |
| 1:1C:388:MET:CE | 2:1D:348:PRO:HD2 | 2.32 | 0.54 |
| 2:1D:109:THR:HB | 2:1D:110:ILE:HD12 | 1.89 | 0.54 |
| 1:1E:242:PHE:CD1 | 1:1E:356:ILE:HG13 | 2.41 | 0.54 |
| 2:1P:119:LEU:HD11 | 2:1P:156:ARG:HD3 | 1.89 | 0.54 |
| 1:1S:221:THR:HG23 | 1:1S:223:GLY:H | 1.72 | 0.54 |
| 2:1Z:217:LEU:HD21 | 2:1Z:367:ASP:HB2 | 1.90 | 0.54 |
| 2:2F:14:ILE:HD11 | 2:2F:74:VAL:HG13 | 1.89 | 0.54 |
| 2:2J:399:TYR:O | 2:2J:402:ARG:NH1 | 2.40 | 0.54 |
| 1:2K:2:ARG:HE | 1:2K:240:LEU:HD22 | 1.72 | 0.54 |
| 1:2M:144:GLY:N | 39:2M:501:GDP:O1B | 2.40 | 0.54 |
| 2:2P:274:PRO:HB2 | 2:2P:276:ILE:HG12 | 1.87 | 0.54 |
| 2:3F:205:ASP:OD2 | 2:3F:207:GLU:N | 2.36 | 0.54 |
| 1:3O:167:PHE:CZ | 1:3O:233:MET:HG2 | 2.42 | 0.54 |
| 2:3R:202:VAL:HG22 | 2:3R:268:MET:HB2 | 1.89 | 0.54 |
| 5:4L:311:ARG:O | 5:4L:315:ARG:HG3 | 2.08 | 0.54 |
| 5:4M:249:ASP:O | 5:4M:252:GLU:HG3 | 2.06 | 0.54 |
| 6:4P:181:GLU:O | 6:4P:184:GLU:HG3 | 2.08 | 0.54 |
| 7:4R:12:ASP:OD1 | 7:4R:14:GLU:CD | 2.30 | 0.54 |
| 7:4R:357:GLU:OE1 | 12:5F:67:GLY:N | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:4V:391:GLU:HG3 | 8:4V:395:ARG:NH1 | 2.17 | 0.54 |
| 12:5F:310:VAL:HG13 | 12:5F:311:HIS:HD2 | 1.71 | 0.54 |
| 14:5N:511:THR:HG23 | 14:5N:512:PHE:O | 2.07 | 0.54 |
| 19:6E:186:THR:HG23 | 19:6E:188:MET:HG3 | 1.88 | 0.54 |
| 22:6N:209:ASN:O | 22:6N:213:THR:HG23 | 2.06 | 0.54 |
| 24:6U:559:ILE:O | 24:6U:563:LYS:HG2 | 2.06 | 0.54 |
| 24:6X:95:VAL:HG11 | 24:6X:124:TYR:CD2 | 2.41 | 0.54 |
| 24:6Y:113:ASN:OD1 | 24:6Y:114:HIS:ND1 | 2.33 | 0.54 |
| 24:7A:185:ASP:OD1 | 24:7A:186:SER:N | 2.39 | 0.54 |
| 31:7N:71:THR:OG1 | 31:7N:72:THR:N | 2.38 | 0.54 |
| 31:7N:75:PRO:HB2 | 31:7N:78:HIS:HD2 | 1.71 | 0.54 |
| 1:A7:276:ARG:NH1 | 24:6T:210:VAL:HG11 | 2.23 | 0.54 |
| 1:B8:79:GLY:HA3 | 24:6Y:221:ARG:HH22 | 1.72 | 0.54 |
| 1:G4:414:ASN:HA | 1:G4:417:ASP:OD2 | 2.07 | 0.54 |
| 1:G8:180:VAL:HG23 | 1:G8:184:ASN:ND2 | 2.22 | 0.54 |
| 2:G9:221:ARG:NH1 | 22:6P:177:LEU:O | 2.40 | 0.54 |
| 2:H5:9:ILE:HG22 | 2:H5:146:GLY:HA2 | 1.88 | 0.54 |
| 1:H6:271:THR:HG21 | 1:H6:293:MET:HG3 | 1.90 | 0.54 |
| 2:I1:132:LEU:HD22 | 2:I1:164:LYS:HD3 | 1.90 | 0.54 |
| 2:I3:296:PHE:HE1 | 2:I3:377:MET:HG3 | 1.72 | 0.54 |
| 2:J5:90:GLU:OE1 | 2:J5:121:ARG:NH1 | 2.40 | 0.54 |
| 2:K3:9:ILE:HG22 | 2:K3:68:LEU:HD21 | 1.88 | 0.54 |
| 1:L4:345:ILE:O | 1:L4:348:ASN:ND2 | 2.38 | 0.54 |
| 2:M1:217:LEU:HD11 | 2:M1:275:ILE:HD11 | 1.89 | 0.54 |
| 1:M6:41:ASP:HB2 | 37:7Y:138:ARG:HH22 | 1.72 | 0.54 |
| 2:M9:221:ARG:NE | 29:7J:308:LEU:O | 2.27 | 0.54 |
| 2:N1:35:GLN:OE1 | 2:N1:35:GLN:N | 2.40 | 0.54 |
| 2:N5:229:ARG:NH2 | 32:7O:68:SER:O | 2.41 | 0.54 |
| 2:N9:280:LYS:HA | 2:N9:283:HIS:HB3 | 1.90 | 0.54 |
| 2:O1:14:ILE:HD11 | 2:O1:74:VAL:HG13 | 1.88 | 0.54 |
| 1:O4:173:PRO:O | 1:O4:176:SER:OG | 2.26 | 0.54 |
| 2:O7:346:TRP:HZ2 | 2:O7:435:VAL:CG2 | 2.20 | 0.54 |
| 2:P3:56:THR:HA | 2:Q9:285:GLN:HB2 | 1.89 | 0.54 |
| 1:Q0:3:GLU:HG3 | 1:Q0:127:CYS:HB2 | 1.88 | 0.54 |
| 1:R0:70:PRO:N | 1:R0:92:PHE:HZ | 2.04 | 0.54 |
| 1:R2:177:ASP:N | 1:R2:181:GLU:OE2 | 2.40 | 0.54 |
| 1:R2:186:THR:HG23 | 1:R2:415:MET:HG3 | 1.89 | 0.54 |
| 2:R5:42:ILE:HA | 11:5E:242:ILE:HD12 | 1.88 | 0.54 |
| 2:R7:137:VAL:HG11 | 2:R7:154:LEU:HD11 | 1.89 | 0.54 |
| 2:R7:267:PHE:HB2 | 2:R7:384:ILE:HD12 | 1.89 | 0.54 |
| 2:S1:117:LEU:HD11 | 13:5K:87:PRO:HD2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S1:132:LEU:HD23 | 2:S1:164:LYS:HE3 | 1.90 | 0.54 |
| 2:S7:352:LYS:NZ | 2:S7:353:CYS:O | 2.40 | 0.54 |
| 2:S9:174:SER:HB3 | 2:S9:177:VAL:O | 2.06 | 0.54 |
| 1:T2:91:VAL:HG21 | 1:T2:116:VAL:HG12 | 1.89 | 0.54 |
| 1:T2:106:TYR:CE2 | 3:4D:78:PRO:HA | 2.42 | 0.54 |
| 2:T3:176:GLN:NE2 | 2:T3:207:GLU:OE2 | 2.40 | 0.54 |
| 1:T4:285:THR:OG1 | 1:T4:287:PRO:HD2 | 2.07 | 0.54 |
| 2:U1:317:LEU:HB3 | 2:U1:319:TYR:HE1 | 1.72 | 0.54 |
| 2:V1:35:GLN:HB3 | 2:V1:59:GLY:O | 2.07 | 0.54 |
| 1:V8:10:GLY:HA2 | 1:V8:143:THR:HG23 | 1.88 | 0.54 |
| 2:W1:399:TYR:O | 2:W1:402:ARG:NH1 | 2.40 | 0.54 |
| 1:X4:58:ARG:HH11 | 1:X4:84:ILE:HA | 1.72 | 0.54 |
| 1:X6:100:ASN:HB3 | 1:X6:103:LYS:HB2 | 1.90 | 0.54 |
| 1:Y0:64:ILE:HG13 | 1:Y0:120:VAL:HG22 | 1.87 | 0.54 |
| 1:Y8:263:LEU:HD13 | 1:Y8:422:TYR:CZ | 2.43 | 0.54 |
| 1:Z4:249:ASP:O | 1:Z4:253:LEU:HG | 2.07 | 0.54 |
| 1:Z6:344:TRP:CE3 | 1:Z6:345:ILE:HG13 | 2.42 | 0.54 |
| 2:0H:222:PRO:HD2 | 1:0I:324:LYS:HE3 | 1.89 | 0.54 |
| 1:0I:202:LEU:HD11 | 1:0I:300:MET:HE3 | 1.89 | 0.54 |
| 1:0I:293:MET:HE3 | 1:0I:367:PHE:HB2 | 1.89 | 0.54 |
| 2:0N:56:THR:N | 2:0N:60:LYS:O | 2.40 | 0.54 |
| 1:0Q:311:LEU:HD23 | 1:0Q:312:THR:HG23 | 1.88 | 0.54 |
| 1:0Y:31:ASP:OD2 | 1:0Y:33:THR:OG1 | 2.16 | 0.54 |
| 2:1D:240:ALA:O | 2:1D:356:ASN:ND2 | 2.40 | 0.54 |
| 1:1M:135:VAL:O | 1:1M:166:THR:HA | 2.07 | 0.54 |
| 1:1M:404:ASP:HB3 | 1:1M:406:MET:SD | 2.47 | 0.54 |
| 2:1P:88:HIS:CG | 2:2F:283:HIS:HA | 2.42 | 0.54 |
| 1:1Q:287:PRO:HA | 1:1Q:290:THR:HG22 | 1.88 | 0.54 |
| 2:1R:381:SER:OG | 2:1R:382:THR:N | 2.39 | 0.54 |
| 2:1T:317:LEU:HB3 | 2:1T:319:TYR:HE1 | 1.71 | 0.54 |
| 1:1U:317:PHE:HB3 | 1:1U:321:MET:SD | 2.47 | 0.54 |
| 1:2G:418:LEU:HG | 1:2G:422:TYR:HE2 | 1.72 | 0.54 |
| 1:2M:135:VAL:HG11 | 1:2M:152:ILE:HD11 | 1.89 | 0.54 |
| 1:2Y:5:VAL:HG22 | 1:2Y:133:PHE:HD1 | 1.72 | 0.54 |
| 2:3N:79:ARG:NH1 | 2:3N:94:SER:OG | 2.40 | 0.54 |
| 1:3O:271:THR:HG21 | 1:3O:293:MET:HG3 | 1.89 | 0.54 |
| 6:4O:97:ARG:HA | 30:7K:445:HIS:CE1 | 2.41 | 0.54 |
| 10:5C:254:MET:O | 10:5C:258:ILE:HG12 | 2.07 | 0.54 |
| 15:5O:118:PHE:HB3 | 15:5O:163:LEU:HD12 | 1.90 | 0.54 |
| 15:5O:241:LEU:HB2 | 15:5O:357:HIS:HB3 | 1.89 | 0.54 |
| 20:6F:57:LEU:HD11 | 20:6F:73:GLN:HG2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6P:138:ASP:N | 22:6P:138:ASP:OD1 | 2.40 | 0.54 |
| 24:6U:442:ASP:OD1 | 24:6U:443:LYS:HG3 | 2.07 | 0.54 |
| 24:6W:452:MET:HA | 24:6W:530:PHE:HA | 1.88 | 0.54 |
| 24:6W:591:ASP:OD1 | 24:6W:591:ASP:N | 2.41 | 0.54 |
| 24:6X:135:PRO:HG2 | 24:6X:137:GLN:HE22 | 1.73 | 0.54 |
| 29:7I:78:LYS:N | 29:7I:81:ASP:OD1 | 2.37 | 0.54 |
| 2:B4:278:ALA:HB3 | 18:6A:43:ASN:HD22 | 1.71 | 0.54 |
| 1:G2:198:GLU:HA | 1:G2:264:HIS:HB2 | 1.89 | 0.54 |
| 1:G2:218:THR:OG1 | 24:6W:418:ASP:OD1 | 2.26 | 0.54 |
| 1:G2:276:ARG:HD2 | 24:6W:410:PHE:HA | 1.89 | 0.54 |
| 1:G6:121:ARG:NH2 | 1:G6:158:GLU:OE2 | 2.39 | 0.54 |
| 1:I2:272:PRO:HB2 | 1:I2:282:ARG:HH12 | 1.71 | 0.54 |
| 2:I9:255:PHE:HA | 2:I9:259:LEU:HD13 | 1.89 | 0.54 |
| 2:I9:399:TYR:O | 2:I9:402:ARG:NH1 | 2.40 | 0.54 |
| 2:J3:88:HIS:CG | 2:J3:89:PRO:HD2 | 2.42 | 0.54 |
| 2:J5:9:ILE:HG12 | 2:J5:68:LEU:HD21 | 1.88 | 0.54 |
| 2:J7:392:ASP:OD2 | 2:J7:422:ARG:NH1 | 2.40 | 0.54 |
| 1:L2:362:LYS:HD3 | 6:4O:389:ARG:HH22 | 1.73 | 0.54 |
| 1:L6:138:SER:OG | 1:L6:139:LEU:N | 2.41 | 0.54 |
| 2:L7:129:CYS:SG | 2:L7:130:THR:N | 2.80 | 0.54 |
| 2:L7:386:GLU:O | 2:L7:390:ARG:HG3 | 2.08 | 0.54 |
| 1:M6:75:SER:HB2 | 15:5P:48:LYS:NZ | 2.22 | 0.54 |
| 2:M9:296:PHE:HE2 | 2:M9:335:ILE:HG13 | 1.72 | 0.54 |
| 2:N3:122:ILE:HA | 2:N3:125:LEU:HB2 | 1.87 | 0.54 |
| 2:O1:116:ASP:OD1 | 2:O1:156:ARG:NH1 | 2.35 | 0.54 |
| 1:O2:362:LYS:HG3 | 37:7Y:230:PRO:HA | 1.89 | 0.54 |
| 1:O2:393:ALA:HB1 | 2:O3:346:TRP:HE1 | 1.71 | 0.54 |
| 2:O9:109:THR:OG1 | 2:O9:411:GLU:OE2 | 2.20 | 0.54 |
| 1:Q4:237:THR:HG23 | 1:Q4:240:LEU:HD12 | 1.89 | 0.54 |
| 1:Q8:116:VAL:HA | 1:Q8:119:VAL:HG12 | 1.88 | 0.54 |
| 1:R0:80:PRO:HD2 | 7:4R:11:GLU:OE2 | 2.07 | 0.54 |
| 1:R0:284:LEU:HB3 | 7:4Q:352:ASN:HB3 | 1.88 | 0.54 |
| 2:R5:286:LEU:O | 2:R5:373:ARG:NH1 | 2.39 | 0.54 |
| 1:S2:94:GLN:HB2 | 13:5K:119:VAL:O | 2.07 | 0.54 |
| 1:T0:49:VAL:HG11 | 1:T0:241:ARG:HG2 | 1.89 | 0.54 |
| 2:T1:27:GLU:OE1 | 2:T1:243:ARG:NH1 | 2.41 | 0.54 |
| 1:T2:260:PHE:HB2 | 1:T2:263:LEU:HG | 1.89 | 0.54 |
| 1:T8:333:VAL:CG1 | 13:5K:102:ALA:HB3 | 2.38 | 0.54 |
| 2:V7:236:SER:O | 2:V7:243:ARG:NH2 | 2.35 | 0.54 |
| 2:V7:313:MET:HB2 | 2:V7:380:ASN:HB3 | 1.87 | 0.54 |
| 1:W4:105:HIS:CD2 | 1:W4:150:LEU:HB2 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:313:MET:HB2 | 2:W9:380:ASN:HB3 | 1.89 | 0.54 |
| 1:X2:77:ARG:O | 1:X2:83:GLN:NE2 | 2.40 | 0.54 |
| 1:X4:319:GLY:HA2 | 1:X4:357:PRO:HD3 | 1.89 | 0.54 |
| 2:X7:26:LEU:HD21 | 2:X7:363:VAL:HG12 | 1.90 | 0.54 |
| 1:Y0:3:GLU:HB2 | 1:Y0:130:LEU:HA | 1.88 | 0.54 |
| 1:Y4:130:LEU:HB2 | 1:Y4:162:ARG:HE | 1.72 | 0.54 |
| 1:Y4:249:ASP:O | 1:Y4:253:LEU:HG | 2.07 | 0.54 |
| 1:Z4:386:THR:HB | 1:Z4:390:ARG:CZ | 2.37 | 0.54 |
| 1:Z6:49:VAL:HG11 | 1:Z6:241:ARG:HG2 | 1.89 | 0.54 |
| 2:Z9:172:TYR:HH | 2:Z9:388:PHE:HZ | 1.54 | 0.54 |
| 2:0H:65:CYS:SG | 2:0H:66:ILE:N | 2.81 | 0.54 |
| 1:0M:4:ILE:HG22 | 1:0M:49:VAL:HG22 | 1.90 | 0.54 |
| 2:0N:71:GLU:HG3 | 2:0N:98:ASP:HB3 | 1.88 | 0.54 |
| 2:0R:381:SER:OG | 2:0R:382:THR:N | 2.39 | 0.54 |
| 2:2B:58:ALA:HB3 | 10:5C:211:ARG:HH22 | 1.72 | 0.54 |
| 1:2I:391:ARG:HD2 | 2:2J:346:TRP:CE2 | 2.42 | 0.54 |
| 1:2M:77:ARG:HH21 | 1:2M:90:PHE:HD2 | 1.55 | 0.54 |
| 2:2R:264:ARG:NH2 | 2:2R:431:ASP:OD2 | 2.40 | 0.54 |
| 1:2S:211:CYS:HB3 | 1:2S:217:LEU:HD12 | 1.89 | 0.54 |
| 2:2T:304:LYS:HZ3 | 38:8A:20:SER:HG | 1.50 | 0.54 |
| 2:2T:392:ASP:OD2 | 2:2T:422:ARG:NH1 | 2.40 | 0.54 |
| 2:2Z:189:LEU:HD11 | 2:2Z:418:PHE:HE1 | 1.73 | 0.54 |
| 2:3B:5:ILE:HD11 | 2:3B:135:PHE:CE1 | 2.42 | 0.54 |
| 2:3H:222:PRO:HD2 | 1:3I:324:LYS:HE3 | 1.88 | 0.54 |
| 1:3K:114:ASP:N | 1:3K:114:ASP:OD1 | 2.41 | 0.54 |
| 1:3K:214:THR:HG23 | 1:3K:297:LYS:HZ2 | 1.72 | 0.54 |
| 1:3K:335:ASN:O | 1:3K:338:SER:OG | 2.25 | 0.54 |
| 2:3L:287:SER:N | 2:3L:290:GLU:OE2 | 2.27 | 0.54 |
| 2:3R:76:ASP:OD2 | 1:3S:46:ARG:NH2 | 2.40 | 0.54 |
| 1:3S:173:PRO:HD3 | 1:3S:380:ARG:HH12 | 1.71 | 0.54 |
| 1:3S:233:MET:O | 1:3S:236:ILE:HG22 | 2.08 | 0.54 |
| 2:3T:128:ASN:HA | 3:4J:171:PRO:HB3 | 1.88 | 0.54 |
| 2:3T:284:GLU:OE1 | 2:3T:286:LEU:HG | 2.07 | 0.54 |
| 3:3V:210:ASP:OD2 | 3:3V:213:VAL:HB | 2.06 | 0.54 |
| 4:3Y:61:CYS:HB3 | 4:3Y:62:PRO:HD3 | 1.89 | 0.54 |
| 3:3Z:210:ASP:OD2 | 3:3Z:213:VAL:HB | 2.06 | 0.54 |
| 4:4A:79:ILE:HB | 4:4A:163:ARG:O | 2.07 | 0.54 |
| 3:4D:210:ASP:OD2 | 3:4D:213:VAL:HB | 2.06 | 0.54 |
| 5:4M:293:LEU:HB3 | 28:7X:306:LEU:HD21 | 1.83 | 0.54 |
| 9:4Z:367:GLU:O | 9:4Z:371:LYS:HG2 | 2.07 | 0.54 |
| 10:5B:99:LYS:O | 10:5B:103:GLU:HG2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:5E:196:VAL:HG12 | 11:5E:197:LEU:HD23 | 1.89 | 0.54 |
| 12:5F:278:VAL:H | 12:5F:292:LEU:HD23 | 1.71 | 0.54 |
| 14:5L:113:CYS:SG | 14:5L:159:SER:HB3 | 2.47 | 0.54 |
| 14:5L:349:PRO:HG2 | 14:5L:352:TYR:HB3 | 1.90 | 0.54 |
| 14:5L:509:ALA:HB3 | 14:5L:513:PHE:HZ | 1.71 | 0.54 |
| 14:5M:349:PRO:HG2 | 14:5M:352:TYR:HB3 | 1.90 | 0.54 |
| 14:5N:349:PRO:HG2 | 14:5N:352:TYR:HB3 | 1.90 | 0.54 |
| 21:6H:37:ILE:HG12 | 21:6H:40:PHE:HB3 | 1.90 | 0.54 |
| 22:6J:172:ARG:NH2 | 22:6J:215:GLY:O | 2.40 | 0.54 |
| 24:6T:282:ARG:NH1 | 24:6T:289:ARG:HD3 | 2.23 | 0.54 |
| 24:6V:271:LYS:HD2 | 24:6V:271:LYS:N | 2.23 | 0.54 |
| 24:6X:132:VAL:HG12 | 24:6X:147:PHE:HB3 | 1.89 | 0.54 |
| 24:7A:171:THR:HG22 | 24:7A:180:TYR:HD1 | 1.72 | 0.54 |
| 29:7J:316:VAL:HG13 | 29:7J:341:GLU:HA | 1.88 | 0.54 |
| 1:G4:78:SER:HB2 | 24:6X:499:GLU:H | 1.71 | 0.54 |
| 2:G5:116:ASP:N | 2:G5:116:ASP:OD1 | 2.39 | 0.54 |
| 1:G6:216:LYS:C | 24:6Y:422:ASN:HD21 | 2.09 | 0.54 |
| 2:G7:70:LEU:HG | 2:G7:145:THR:HG23 | 1.89 | 0.54 |
| 2:G7:111:GLY:HA2 | 2:G7:114:ILE:HG22 | 1.89 | 0.54 |
| 1:I0:219:THR:HA | 2:I1:326:LYS:NZ | 2.22 | 0.54 |
| 2:I1:387:ILE:HG12 | 2:I1:390:ARG:HH22 | 1.72 | 0.54 |
| 1:J2:2:ARG:HE | 1:J2:240:LEU:HD22 | 1.72 | 0.54 |
| 2:J5:129:CYS:SG | 2:J5:130:THR:N | 2.80 | 0.54 |
| 1:K4:72:THR:O | 1:K4:76:VAL:HG23 | 2.08 | 0.54 |
| 2:K5:98:ASP:OD1 | 2:K5:99:ALA:N | 2.41 | 0.54 |
| 2:L3:129:CYS:SG | 2:L3:130:THR:N | 2.80 | 0.54 |
| 1:L6:178:THR:HG23 | 1:L6:181:GLU:HG3 | 1.88 | 0.54 |
| 2:M3:129:CYS:SG | 2:M3:130:THR:N | 2.80 | 0.54 |
| 1:O2:245:GLN:HE21 | 37:7Y:237:ILE:HG13 | 1.73 | 0.54 |
| 1:O8:145:SER:OG | 1:O8:188:SER:OG | 2.16 | 0.54 |
| 1:Q2:135:VAL:HG21 | 1:Q2:152:ILE:HD11 | 1.90 | 0.54 |
| 2:R7:220:GLU:HG2 | 2:R7:221:ARG:HG3 | 1.90 | 0.54 |
| 1:T0:274:THR:HG21 | 1:T0:282:ARG:HD2 | 1.88 | 0.54 |
| 1:T2:203:ASP:N | 1:T2:203:ASP:OD2 | 2.41 | 0.54 |
| 2:T5:165:SER:HB2 | 2:T5:256:GLN:HE22 | 1.72 | 0.54 |
| 2:T5:206:ASN:OD1 | 41:T6:501:GTP:N2 | 2.41 | 0.54 |
| 1:U2:276:ARG:NH1 | 1:U2:279:GLN:HB3 | 2.19 | 0.54 |
| 2:U3:191:THR:HA | 2:U3:194:LEU:HB2 | 1.88 | 0.54 |
| 1:V2:224:ASP:OD2 | 6:4P:33:ARG:NH2 | 2.40 | 0.54 |
| 1:W4:100:ASN:HB3 | 1:W4:103:LYS:HB2 | 1.87 | 0.54 |
| 1:X2:11:GLN:HG3 | 1:X2:72:THR:CG2 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X4:51:PHE:HB3 | 1:X4:59:TYR:HB3 | 1.89 | 0.54 |
| 2:X5:5:ILE:HD11 | 2:X5:135:PHE:CE1 | 2.41 | 0.54 |
| 1:X6:161:ASP:OD1 | 1:X6:161:ASP:N | 2.41 | 0.54 |
| 2:X7:191:THR:HA | 2:X7:194:LEU:HG | 1.88 | 0.54 |
| 2:Y3:109:THR:OG1 | 2:Y3:411:GLU:OE2 | 2.22 | 0.54 |
| 1:Y4:139:LEU:HD12 | 1:Y4:170:VAL:HG12 | 1.90 | 0.54 |
| 2:Z1:377:MET:SD | 2:Z1:379:SER:HB2 | 2.47 | 0.54 |
| 1:Z2:58:ARG:HD3 | 1:0I:280:GLN:HE22 | 1.72 | 0.54 |
| 2:0B:34:GLY:HA3 | 2:0B:60:LYS:HZ2 | 1.72 | 0.54 |
| 2:0J:75:VAL:HG12 | 2:0J:79:ARG:HE | 1.73 | 0.54 |
| 1:0Y:72:THR:O | 1:0Y:76:VAL:HG23 | 2.07 | 0.54 |
| 2:0Z:381:SER:OG | 2:0Z:382:THR:N | 2.40 | 0.54 |
| 2:1B:203:MET:O | 2:1B:204:LEU:HD23 | 2.06 | 0.54 |
| 2:1B:223:THR:HG23 | 2:1B:225:THR:H | 1.71 | 0.54 |
| 1:1G:271:THR:HG1 | 1:1G:272:PRO:HA | 1.72 | 0.54 |
| 1:1S:215:LEU:HB3 | 1:1S:217:LEU:HG | 1.89 | 0.54 |
| 2:1X:9:ILE:HD11 | 2:1X:153:LEU:HD13 | 1.90 | 0.54 |
| 1:2E:215:LEU:HB3 | 1:2E:217:LEU:HG | 1.89 | 0.54 |
| 2:2F:230:LEU:HD12 | 2:2F:231:ILE:HD13 | 1.90 | 0.54 |
| 2:2F:352:LYS:NZ | 2:2F:353:CYS:O | 2.41 | 0.54 |
| 1:2G:125:GLU:O | 38:8B:56:PRO:HD3 | 2.08 | 0.54 |
| 1:2G:229:ILE:HG22 | 1:2G:233:MET:HE2 | 1.90 | 0.54 |
| 2:2J:121:ARG:NE | 2:2J:121:ARG:HA | 2.22 | 0.54 |
| 2:2N:88:HIS:ND1 | 2:3D:283:HIS:HA | 2.22 | 0.54 |
| 1:3G:99:ASN:ND2 | 2:3H:254:GLU:OE1 | 2.40 | 0.54 |
| 2:3N:124:LYS:HZ2 | 3:4D:36:PHE:HD1 | 1.54 | 0.54 |
| 1:3O:49:VAL:HG11 | 1:3O:241:ARG:HG2 | 1.89 | 0.54 |
| 1:3S:405:GLU:O | 1:3S:409:THR:HG23 | 2.08 | 0.54 |
| 4:4C:61:CYS:HB3 | 4:4C:62:PRO:HD3 | 1.89 | 0.54 |
| 4:4E:79:ILE:HB | 4:4E:163:ARG:O | 2.07 | 0.54 |
| 4:4G:61:CYS:HB3 | 4:4G:62:PRO:HD3 | 1.90 | 0.54 |
| 5:4M:316:ARG:O | 5:4M:319:GLU:HG3 | 2.07 | 0.54 |
| 14:5M:36:SER:OG | 14:5M:595:SER:HB2 | 2.07 | 0.54 |
| 14:5M:234:ALA:HB2 | 14:5M:280:ARG:HB2 | 1.89 | 0.54 |
| 14:5N:36:SER:OG | 14:5N:595:SER:HB2 | 2.07 | 0.54 |
| 15:5P:129:SER:N | 15:5P:132:GLU:OE2 | 2.36 | 0.54 |
| 16:5Q:61:ILE:HG12 | 16:5Q:98:MET:HB3 | 1.88 | 0.54 |
| 22:6J:210:MET:O | 22:6J:213:THR:OG1 | 2.24 | 0.54 |
| 24:6U:482:ILE:HG22 | 24:6U:497:PHE:HB3 | 1.90 | 0.54 |
| 24:6Z:135:PRO:HG2 | 24:6Z:137:GLN:HE22 | 1.73 | 0.54 |
| 1:G8:274:THR:HG21 | 1:G8:282:ARG:HD2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G9:287:SER:N | 2:G9:290:GLU:OE2 | 2.41 | 0.54 |
| 2:G9:305:CYS:SG | 2:G9:306:ASP:N | 2.81 | 0.54 |
| 1:I0:186:THR:HG22 | 1:I0:411:ALA:HB1 | 1.88 | 0.54 |
| 2:I3:191:THR:HA | 2:I3:194:LEU:HB3 | 1.89 | 0.54 |
| 1:I4:156:ARG:NH1 | 1:I4:197:ASP:OD1 | 2.41 | 0.54 |
| 1:J6:186:THR:HG23 | 1:J6:187:LEU:HD12 | 1.87 | 0.54 |
| 2:K9:174:SER:HB3 | 2:K9:177:VAL:O | 2.07 | 0.54 |
| 1:L0:2:ARG:HE | 1:L0:240:LEU:HD22 | 1.73 | 0.54 |
| 1:L6:306:ARG:NH1 | 28:7X:453:SER:HA | 2.23 | 0.54 |
| 2:L7:288:VAL:HG21 | 2:L7:327:ASP:HB2 | 1.90 | 0.54 |
| 2:M3:379:SER:OG | 2:M3:380:ASN:N | 2.38 | 0.54 |
| 1:N0:20:PHE:HA | 1:N0:230:SER:HB2 | 1.90 | 0.54 |
| 1:N0:91:VAL:HG11 | 1:N0:116:VAL:HG12 | 1.90 | 0.54 |
| 1:N0:227:HIS:CE1 | 30:7L:361:GLY:HA2 | 2.42 | 0.54 |
| 1:N2:309:ARG:H | 1:N2:372:THR:HG22 | 1.72 | 0.54 |
| 2:N5:192:HIS:HD2 | 2:N5:421:ALA:HA | 1.72 | 0.54 |
| 2:N7:21:TRP:CZ2 | 2:N7:65:CYS:HB2 | 2.43 | 0.54 |
| 1:O2:320:ARG:HB3 | 37:7Y:237:ILE:HD11 | 1.89 | 0.54 |
| 2:O3:90:GLU:CG | 2:O3:121:ARG:HH12 | 2.21 | 0.54 |
| 2:O3:221:ARG:NH2 | 37:7Y:71:ARG:O | 2.38 | 0.54 |
| 1:Q0:65:LEU:HD12 | 1:Q0:90:PHE:CE1 | 2.43 | 0.54 |
| 1:Q8:119:VAL:O | 1:Q8:123:GLU:HG2 | 2.07 | 0.54 |
| 1:R4:218:THR:O | 2:R5:326:LYS:NZ | 2.36 | 0.54 |
| 2:S1:217:LEU:HB3 | 2:S1:219:ILE:HD12 | 1.89 | 0.54 |
| 1:T2:11:GLN:HE22 | 2:T3:249:ASN:H | 1.55 | 0.54 |
| 2:T3:269:LEU:HD13 | 2:T3:301:MET:HE1 | 1.90 | 0.54 |
| 2:T3:401:LYS:HD2 | 1:T4:344:TRP:CD2 | 2.43 | 0.54 |
| 1:T4:390:ARG:NH1 | 1:T4:390:ARG:CB | 2.69 | 0.54 |
| 1:T6:48:ASN:O | 1:T6:62:ARG:NH1 | 2.39 | 0.54 |
| 1:U6:329:GLN:HA | 1:U6:332:ASN:HD21 | 1.73 | 0.54 |
| 2:V7:272:TYR:HD1 | 2:V7:376:CYS:HG | 1.56 | 0.54 |
| 2:W1:88:HIS:NE2 | 2:W1:90:GLU:HB3 | 2.22 | 0.54 |
| 2:W1:287:SER:OG | 2:W1:288:VAL:N | 2.41 | 0.54 |
| 2:W1:325:PRO:O | 2:W1:329:ASN:ND2 | 2.40 | 0.54 |
| 2:W5:89:PRO:HD3 | 2:Y1:283:HIS:CG | 2.42 | 0.54 |
| 1:W6:117:LEU:HD11 | 1:W6:154:LYS:HB3 | 1.90 | 0.54 |
| 1:X0:22:GLU:HG2 | 1:X0:81:TYR:HB2 | 1.89 | 0.54 |
| 1:X0:42:LEU:CD2 | 8:4X:97:PHE:HZ | 2.21 | 0.54 |
| 1:X0:58:ARG:HD3 | 8:4W:469:GLN:OE1 | 2.07 | 0.54 |
| 2:Y3:264:ARG:NH1 | 2:Y3:431:ASP:OD1 | 2.36 | 0.54 |
| 2:Z5:221:ARG:HB3 | 1:Z6:322:SER:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z8:101:TRP:HB2 | 1:Z8:184:ASN:OD1 | 2.08 | 0.54 |
| 1:0E:139:LEU:HD12 | 1:0E:170:VAL:HG22 | 1.88 | 0.54 |
| 1:0I:391:ARG:HB3 | 2:0J:346:TRP:CZ3 | 2.42 | 0.54 |
| 1:0O:139:LEU:HD12 | 1:0O:170:VAL:HG12 | 1.90 | 0.54 |
| 1:0Q:116:VAL:HA | 1:0Q:119:VAL:HG12 | 1.89 | 0.54 |
| 1:0U:350:LYS:NZ | 1:0U:351:SER:O | 2.35 | 0.54 |
| 2:0V:353:CYS:SG | 2:0V:354:GLY:N | 2.80 | 0.54 |
| 1:0W:6:HIS:CE1 | 1:0W:8:GLN:HG2 | 2.42 | 0.54 |
| 2:1B:74:VAL:O | 2:1B:78:VAL:HG23 | 2.08 | 0.54 |
| 1:1E:232:VAL:O | 1:1E:236:ILE:HG12 | 2.08 | 0.54 |
| 2:1R:121:ARG:HD2 | 2:1R:121:ARG:O | 2.07 | 0.54 |
| 1:2C:3:GLU:HB2 | 1:2C:130:LEU:HA | 1.90 | 0.54 |
| 1:2E:140:GLY:O | 1:2E:184:ASN:ND2 | 2.37 | 0.54 |
| 2:2L:22:GLU:HG2 | 2:2L:83:TYR:OH | 2.07 | 0.54 |
| 1:2M:301:CYS:SG | 1:2M:302:ALA:N | 2.81 | 0.54 |
| 2:2X:192:HIS:HD2 | 2:2X:421:ALA:HA | 1.73 | 0.54 |
| 2:2X:267:PHE:HB2 | 2:2X:384:ILE:HD12 | 1.89 | 0.54 |
| 2:3L:287:SER:OG | 2:3L:290:GLU:OE1 | 2.17 | 0.54 |
| 1:3M:175:VAL:HG22 | 2:3N:329:ASN:ND2 | 2.23 | 0.54 |
| 2:3N:210:TYR:OH | 1:3O:323:THR:OG1 | 2.24 | 0.54 |
| 2:3P:406:HIS:HA | 2:3P:409:VAL:HG22 | 1.90 | 0.54 |
| 1:3S:113:ILE:HG13 | 1:3S:117:LEU:HD23 | 1.90 | 0.54 |
| 2:3T:221:ARG:HG2 | 2:3T:221:ARG:O | 2.08 | 0.54 |
| 4:4C:79:ILE:HB | 4:4C:163:ARG:O | 2.07 | 0.54 |
| 3:4H:210:ASP:OD2 | 3:4H:213:VAL:HB | 2.06 | 0.54 |
| 3:4J:282:GLU:HB3 | 3:4J:283:GLN:NE2 | 2.22 | 0.54 |
| 6:4O:43:ASN:O | 6:4O:47:ASN:HB2 | 2.07 | 0.54 |
| 8:4W:330:ARG:O | 8:4W:334:GLU:HG2 | 2.07 | 0.54 |
| 10:5A:375:GLU:HA | 10:5A:378:ASN:HD21 | 1.72 | 0.54 |
| 14:5L:36:SER:OG | 14:5L:595:SER:HB2 | 2.07 | 0.54 |
| 14:5N:234:ALA:HB2 | 14:5N:280:ARG:HB2 | 1.89 | 0.54 |
| 17:5S:188:LYS:O | 17:5S:191:SER:OG | 2.19 | 0.54 |
| 24:6U:130:MET:HB2 | 24:6U:153:VAL:HG13 | 1.90 | 0.54 |
| 24:6W:277:CYS:HA | 24:6W:368:LEU:HA | 1.89 | 0.54 |
| 24:6W:488:ARG:CB | 24:6W:488:ARG:CZ | 2.86 | 0.54 |
| 24:6X:316:ASP:OD2 | 24:6X:317:PRO:HD3 | 2.05 | 0.54 |
| 26:7F:144:HIS:NE2 | 26:7F:146:ASN:HB3 | 2.22 | 0.54 |
| 29:7J:316:VAL:HG21 | 29:7J:326:ILE:HG21 | 1.90 | 0.54 |
| 31:7M:37:ILE:HD12 | 31:7M:37:ILE:H | 1.73 | 0.54 |
| 34:7R:99:ARG:HB2 | 35:7T:47:ASN:HD21 | 1.73 | 0.54 |
| 1:A5:280:GLN:NE2 | 1:T8:58:ARG:HG2 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:72:THR:O | 1:G4:76:VAL:HG23 | 2.08 | 0.54 |
| 2:G7:221:ARG:NH2 | 22:6O:174:GLU:O | 2.40 | 0.54 |
| 1:G8:128:ASP:OD1 | 1:G8:129:CYS:N | 2.39 | 0.54 |
| 1:H2:386:THR:O | 1:H2:390:ARG:HG3 | 2.07 | 0.54 |
| 1:H6:244:GLY:H | 1:H6:247:ASN:HD21 | 1.55 | 0.54 |
| 1:I4:257:LEU:HD21 | 1:I4:314:SER:HB3 | 1.90 | 0.54 |
| 2:I5:301:MET:HE1 | 2:I5:307:PRO:HD3 | 1.88 | 0.54 |
| 1:J0:52:ASN:OD1 | 1:J0:62:ARG:NH2 | 2.41 | 0.54 |
| 2:J3:111:GLY:O | 2:J3:115:VAL:HG22 | 2.08 | 0.54 |
| 1:J4:2:ARG:HB3 | 1:J4:131:GLN:HB2 | 1.89 | 0.54 |
| 2:J7:91:GLN:O | 2:J7:93:ILE:HG12 | 2.07 | 0.54 |
| 2:K5:264:ARG:NH2 | 2:K5:431:ASP:OD2 | 2.41 | 0.54 |
| 2:M1:90:GLU:HG3 | 2:M1:121:ARG:NH1 | 2.21 | 0.54 |
| 1:M2:86:ARG:HB3 | 2:N9:283:HIS:HE1 | 1.73 | 0.54 |
| 2:M7:5:ILE:HG22 | 2:M7:64:ARG:HB3 | 1.88 | 0.54 |
| 2:N5:121:ARG:HD2 | 2:N5:121:ARG:C | 2.28 | 0.54 |
| 1:N6:99:ASN:ND2 | 2:N7:254:GLU:OE1 | 2.41 | 0.54 |
| 2:N7:88:HIS:HE2 | 2:N7:90:GLU:HB2 | 1.73 | 0.54 |
| 1:O8:309:ARG:H | 1:O8:372:THR:HG22 | 1.72 | 0.54 |
| 2:O9:183:GLU:HG3 | 2:O9:184:PRO:HD3 | 1.89 | 0.54 |
| 2:O9:384:ILE:HA | 2:O9:387:ILE:HD12 | 1.89 | 0.54 |
| 2:P3:279:GLU:H | 2:P3:279:GLU:CD | 2.05 | 0.54 |
| 2:P7:329:ASN:O | 2:P7:332:VAL:HG12 | 2.07 | 0.54 |
| 1:Q8:244:GLY:HA3 | 1:Q8:354:CYS:HA | 1.90 | 0.54 |
| 1:R2:91:VAL:HG21 | 1:R2:116:VAL:HG22 | 1.88 | 0.54 |
| 1:R8:229:ILE:HG22 | 1:R8:233:MET:HE2 | 1.88 | 0.54 |
| 1:S0:418:LEU:HG | 1:S0:422:TYR:CE2 | 2.42 | 0.54 |
| 2:S1:287:SER:OG | 2:S1:290:GLU:OE1 | 2.26 | 0.54 |
| 1:S6:3:GLU:HB2 | 1:S6:130:LEU:HA | 1.90 | 0.54 |
| 1:S6:259:PRO:HG2 | 1:S6:263:LEU:HD23 | 1.89 | 0.54 |
| 1:S8:173:PRO:HD3 | 1:S8:380:ARG:NH1 | 2.23 | 0.54 |
| 1:U4:285:THR:HG23 | 1:U4:288:GLU:H | 1.72 | 0.54 |
| 1:U6:117:LEU:HD11 | 1:U6:154:LYS:HB3 | 1.90 | 0.54 |
| 1:U8:257:LEU:HD21 | 1:U8:314:SER:HB2 | 1.90 | 0.54 |
| 1:V2:41:ASP:HA | 1:V2:44:LEU:HD23 | 1.89 | 0.54 |
| 2:V3:77:GLU:OE2 | 1:V4:243:PRO:HB3 | 2.07 | 0.54 |
| 1:V6:205:GLU:HG2 | 1:V6:206:ALA:H | 1.73 | 0.54 |
| 1:W2:77:ARG:O | 1:W2:83:GLN:NE2 | 2.41 | 0.54 |
| 2:W7:276:ILE:HG12 | 2:W7:281:ALA:HB2 | 1.89 | 0.54 |
| 1:X2:153:SER:HA | 1:X2:195:ASN:OD1 | 2.07 | 0.54 |
| 2:X7:3:GLU:O | 2:X7:133:GLN:N | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X7:236:SER:O | 2:X7:243:ARG:NH2 | 2.40 | 0.54 |
| 2:Y1:62:VAL:HB | 2:Y1:88:HIS:CE1 | 2.42 | 0.54 |
| 2:Y1:100:ALA:O | 1:Y2:255:VAL:HG21 | 2.07 | 0.54 |
| 1:Y2:58:ARG:HH11 | 1:Y2:84:ILE:HA | 1.71 | 0.54 |
| 2:Y5:129:CYS:SG | 2:Y5:130:THR:N | 2.81 | 0.54 |
| 1:Y8:51:PHE:HB3 | 1:Y8:59:TYR:HB3 | 1.88 | 0.54 |
| 2:Z5:8:HIS:CD2 | 2:Z5:138:PHE:HD2 | 2.25 | 0.54 |
| 1:0E:31:ASP:OD2 | 1:0E:33:THR:OG1 | 2.26 | 0.54 |
| 2:0F:69:ASP:OD1 | 2:0F:70:LEU:N | 2.41 | 0.54 |
| 2:0R:198:THR:HG21 | 2:0R:201:ALA:HB2 | 1.90 | 0.54 |
| 1:0U:91:VAL:HG11 | 1:0U:116:VAL:HG12 | 1.90 | 0.54 |
| 1:1A:268:VAL:O | 1:1A:300:MET:N | 2.34 | 0.54 |
| 1:1M:163:MET:HB3 | 1:1M:250:LEU:HD22 | 1.88 | 0.54 |
| 1:1Q:52:ASN:OD1 | 1:1Q:62:ARG:NH2 | 2.40 | 0.54 |
| 1:1Q:186:THR:HG22 | 1:1Q:411:ALA:HB1 | 1.90 | 0.54 |
| 2:1T:289:ALA:O | 2:1T:293:ASN:ND2 | 2.41 | 0.54 |
| 1:1U:31:ASP:OD1 | 1:1U:35:THR:N | 2.32 | 0.54 |
| 1:1W:34:GLY:HA3 | 1:1W:58:ARG:HD2 | 1.90 | 0.54 |
| 2:2D:145:THR:OG1 | 41:2E:501:GTP:O1B | 2.25 | 0.54 |
| 2:2H:88:HIS:ND1 | 2:2H:121:ARG:NH2 | 2.56 | 0.54 |
| 2:2L:9:ILE:HG13 | 2:2L:139:ASN:HB3 | 1.90 | 0.54 |
| 1:2U:211:CYS:HA | 1:2U:215:LEU:HB2 | 1.89 | 0.54 |
| 2:2X:22:GLU:OE1 | 38:8C:203:PHE:CD1 | 2.60 | 0.54 |
| 1:3A:309:ARG:H | 1:3A:372:THR:HG22 | 1.73 | 0.54 |
| 1:3I:51:PHE:HB3 | 1:3I:59:TYR:HB3 | 1.90 | 0.54 |
| 1:3K:350:LYS:NZ | 1:3K:352:SER:OG | 2.40 | 0.54 |
| 1:3M:52:ASN:HD22 | 1:3M:52:ASN:N | 2.02 | 0.54 |
| 1:3Q:309:ARG:H | 1:3Q:372:THR:HG22 | 1.71 | 0.54 |
| 2:3T:137:VAL:HG13 | 2:3T:168:GLY:HA2 | 1.90 | 0.54 |
| 2:3T:241:SER:HA | 2:3T:356:ASN:ND2 | 2.19 | 0.54 |
| 4:3W:79:ILE:HB | 4:3W:163:ARG:O | 2.07 | 0.54 |
| 4:4I:61:CYS:HB3 | 4:4I:62:PRO:HD3 | 1.89 | 0.54 |
| 6:4O:247:GLN:O | 6:4O:251:GLU:HG2 | 2.07 | 0.54 |
| 8:4W:191:GLU:OE2 | 8:4W:192:ARG:HD2 | 2.08 | 0.54 |
| 11:5E:115:LEU:HG | 11:5E:115:LEU:O | 2.08 | 0.54 |
| 12:5F:289:TYR:CE1 | 12:5F:322:LEU:HB2 | 2.42 | 0.54 |
| 13:5K:18:ARG:NH1 | 24:6Z:35:TYR:OH | 2.41 | 0.54 |
| 14:5L:234:ALA:HB2 | 14:5L:280:ARG:HB2 | 1.89 | 0.54 |
| 14:5L:415:LYS:NZ | 23:6Q:21:THR:O | 2.41 | 0.54 |
| 14:5N:222:ALA:HB2 | 14:5N:229:LYS:HG2 | 1.88 | 0.54 |
| 16:5Q:127:ASP:O | 16:5Q:131:THR:HG23 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6P:110:ILE:O | 22:6P:113:ARG:NH1 | 2.41 | 0.54 |
| 24:6T:97:ARG:NH2 | 24:6T:99:TYR:OH | 2.41 | 0.54 |
| 24:6T:488:ARG:H | 24:6T:488:ARG:HH11 | 1.55 | 0.54 |
| 24:6V:282:ARG:NH1 | 24:6V:289:ARG:HD3 | 2.23 | 0.54 |
| 26:7F:136:PHE:HB3 | 26:7F:137:PRO:HD2 | 1.88 | 0.54 |
| 29:7I:14:LEU:HD12 | 29:7I:14:LEU:O | 2.06 | 0.54 |
| 29:7I:254:MET:CE | 30:7K:341:ARG:HD3 | 2.36 | 0.54 |
| 38:8A:91:GLN:HG2 | 38:8A:102:PHE:HD1 | 1.72 | 0.54 |
| 2:F5:145:THR:OG1 | 41:F5:501:GTP:O1B | 2.25 | 0.54 |
| 2:G1:417:GLU:HA | 2:G1:420:GLU:HG2 | 1.90 | 0.54 |
| 2:G3:222:PRO:HD2 | 1:G4:324:LYS:HE3 | 1.90 | 0.54 |
| 2:G3:229:ARG:HD3 | 2:G3:363:VAL:HG11 | 1.90 | 0.54 |
| 2:G5:98:ASP:OD1 | 2:G5:99:ALA:N | 2.41 | 0.54 |
| 2:G5:384:ILE:HD12 | 2:G5:387:ILE:HB | 1.90 | 0.54 |
| 2:H3:129:CYS:SG | 2:H3:130:THR:N | 2.81 | 0.54 |
| 2:H5:213:CYS:HA | 2:H5:217:LEU:HB2 | 1.90 | 0.54 |
| 2:I5:72:PRO:HA | 2:I5:75:VAL:HG22 | 1.89 | 0.54 |
| 1:J0:371:SER:OG | 1:J0:372:THR:N | 2.41 | 0.54 |
| 1:K0:257:LEU:HD11 | 1:K0:314:SER:HB2 | 1.89 | 0.54 |
| 1:K4:203:ASP:OD2 | 1:K4:302:ALA:N | 2.39 | 0.54 |
| 1:L0:67:ASP:OD2 | 1:L0:72:THR:OG1 | 2.25 | 0.54 |
| 2:L3:84:ARG:HH22 | 29:7J:345:PRO:CD | 2.20 | 0.54 |
| 2:L5:387:ILE:HG12 | 2:L5:390:ARG:HH22 | 1.73 | 0.54 |
| 1:M0:387:ALA:HA | 1:M0:390:ARG:HE | 1.73 | 0.54 |
| 1:M2:183:TYR:HE2 | 1:M2:394:PHE:HB2 | 1.73 | 0.54 |
| 1:M4:382:SER:OG | 1:M4:415:MET:HG2 | 2.07 | 0.54 |
| 1:N0:345:ILE:O | 1:N0:348:ASN:ND2 | 2.40 | 0.54 |
| 2:O1:90:GLU:HB2 | 2:O1:121:ARG:NH1 | 2.22 | 0.54 |
| 1:O2:285:THR:OG1 | 1:O2:287:PRO:HD2 | 2.07 | 0.54 |
| 2:O7:246:GLY:HA3 | 2:O7:356:ASN:HA | 1.90 | 0.54 |
| 2:Q5:206:ASN:OD1 | 41:Q6:501:GTP:N2 | 2.40 | 0.54 |
| 2:R1:220:GLU:HG2 | 2:R1:221:ARG:HG3 | 1.88 | 0.54 |
| 2:R3:155:GLU:HG2 | 2:R3:197:HIS:CE1 | 2.42 | 0.54 |
| 1:R4:90:PHE:HD2 | 19:6E:254:PHE:CZ | 2.26 | 0.54 |
| 2:T1:384:ILE:HA | 2:T1:387:ILE:HD12 | 1.90 | 0.54 |
| 1:T2:222:PHE:CZ | 2:T3:325:PRO:HB3 | 2.43 | 0.54 |
| 1:T2:271:THR:HG21 | 1:T2:293:MET:HG3 | 1.90 | 0.54 |
| 2:T5:129:CYS:SG | 2:T5:130:THR:N | 2.80 | 0.54 |
| 2:U3:234:VAL:O | 2:U3:237:SER:OG | 2.20 | 0.54 |
| 2:U5:287:SER:N | 2:U5:290:GLU:OE2 | 2.39 | 0.54 |
| 2:V1:129:CYS:SG | 2:V1:130:THR:N | 2.80 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W0:173:PRO:HD3 | 1:W0:380:ARG:HD3 | 1.90 | 0.54 |
| 1:W6:371:SER:OG | 1:W6:372:THR:N | 2.40 | 0.54 |
| 2:W7:195:LEU:HD21 | 2:W7:264:ARG:HH11 | 1.71 | 0.54 |
| 1:W8:392:LYS:HD2 | 1:W8:395:LEU:HD22 | 1.90 | 0.54 |
| 1:X0:225:LEU:HA | 1:X0:228:LEU:HD12 | 1.89 | 0.54 |
| 1:X6:3:GLU:HB2 | 1:X6:130:LEU:HA | 1.89 | 0.54 |
| 2:Y1:239:THR:HG23 | 2:Y1:243:ARG:HE | 1.73 | 0.54 |
| 1:Y2:285:THR:OG1 | 1:Y2:287:PRO:HD2 | 2.07 | 0.54 |
| 1:Y4:21:TRP:CZ3 | 1:Y4:61:PRO:HB3 | 2.43 | 0.54 |
| 1:Y4:69:GLU:C | 1:Y4:92:PHE:HZ | 2.12 | 0.54 |
| 1:Y8:11:GLN:NE2 | 39:Y8:501:GDP:O1A | 2.40 | 0.54 |
| 2:Z3:406:HIS:HA | 2:Z3:409:VAL:HG12 | 1.89 | 0.54 |
| 1:Z6:405:GLU:HA | 1:Z6:408:PHE:HD2 | 1.72 | 0.54 |
| 1:0G:139:LEU:HG | 1:0G:168:SER:HB2 | 1.90 | 0.54 |
| 1:0I:128:ASP:OD1 | 1:0I:129:CYS:N | 2.39 | 0.54 |
| 1:0O:358:PRO:HG2 | 1:0O:361:LEU:HB2 | 1.90 | 0.54 |
| 2:0P:244:PHE:HB2 | 2:0P:356:ASN:HD21 | 1.72 | 0.54 |
| 2:0R:185:TYR:O | 2:0R:189:LEU:HG | 2.08 | 0.54 |
| 1:0U:109:GLY:O | 1:0U:113:ILE:HG12 | 2.07 | 0.54 |
| 1:1G:248:ALA:HA | 1:1G:252:LYS:HD2 | 1.89 | 0.54 |
| 1:1O:7:ILE:HD13 | 1:1O:151:LEU:HD21 | 1.90 | 0.54 |
| 2:1R:89:PRO:HD3 | 2:2H:283:HIS:ND1 | 2.23 | 0.54 |
| 1:1U:172:SER:HB3 | 1:1U:175:VAL:HG22 | 1.88 | 0.54 |
| 2:1Z:223:THR:HA | 1:2A:323:THR:HG22 | 1.88 | 0.54 |
| 1:2A:246:LEU:O | 1:2A:352:SER:OG | 2.22 | 0.54 |
| 2:2H:65:CYS:SG | 2:2H:66:ILE:N | 2.81 | 0.54 |
| 2:2H:279:GLU:OE1 | 10:5B:167:ILE:HD13 | 2.08 | 0.54 |
| 2:2T:413:MET:HB3 | 2:2T:417:GLU:OE2 | 2.08 | 0.54 |
| 1:2U:263:LEU:HD22 | 1:2U:422:TYR:HE1 | 1.72 | 0.54 |
| 2:2V:47:ASP:OD1 | 2:2V:48:ALA:N | 2.41 | 0.54 |
| 2:2X:39:ASP:O | 2:2X:42:ILE:HG22 | 2.08 | 0.54 |
| 2:2X:200:VAL:HG13 | 2:2X:268:MET:HE2 | 1.89 | 0.54 |
| 1:2Y:193:VAL:HG12 | 1:2Y:265:PHE:HZ | 1.73 | 0.54 |
| 2:2Z:122:ILE:HD11 | 2:2Z:135:PHE:CE1 | 2.43 | 0.54 |
| 1:3A:69:GLU:C | 1:3A:92:PHE:HZ | 2.11 | 0.54 |
| 1:3A:207:LEU:HB3 | 1:3A:225:LEU:HD22 | 1.90 | 0.54 |
| 1:3C:320:ARG:HH12 | 38:8D:198:THR:CA | 2.21 | 0.54 |
| 2:3F:276:ILE:HG23 | 2:3F:280:LYS:HB2 | 1.90 | 0.54 |
| 1:3M:51:PHE:HB3 | 1:3M:59:TYR:HB3 | 1.90 | 0.54 |
| 1:3M:52:ASN:HD21 | 1:3M:62:ARG:HB2 | 1.70 | 0.54 |
| 2:3N:22:GLU:HG3 | 2:3N:83:TYR:OH | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3O:70:PRO:N | 1:3O:92:PHE:HZ | 2.06 | 0.54 |
| 1:3S:377:MET:HA | 1:3S:380:ARG:CD | 2.37 | 0.54 |
| 4:3W:61:CYS:HB3 | 4:3W:62:PRO:HD3 | 1.90 | 0.54 |
| 4:4I:79:ILE:HB | 4:4I:163:ARG:O | 2.07 | 0.54 |
| 6:4O:307:ASP:HA | 6:4O:310:TYR:CE2 | 2.43 | 0.54 |
| 7:4T:184:LEU:HD23 | 31:7M:78:HIS:CE1 | 2.41 | 0.54 |
| 15:5O:265:VAL:HG11 | 15:5O:309:LEU:HD12 | 1.90 | 0.54 |
| 15:5P:40:ILE:HD13 | 37:7Y:56:MET:HB2 | 1.90 | 0.54 |
| 16:5Q:79:ARG:HH11 | 16:5Q:81:HIS:HE1 | 1.56 | 0.54 |
| 21:6H:129:VAL:O | 21:6H:133:VAL:HG23 | 2.07 | 0.54 |
| 22:6J:333:MET:HG3 | 22:6J:334:THR:HG23 | 1.90 | 0.54 |
| 22:6M:305:VAL:HG11 | 22:6M:343:TYR:HB3 | 1.90 | 0.54 |
| 24:6X:451:LYS:HD2 | 24:6X:468:ARG:NH2 | 2.20 | 0.54 |
| 24:6Y:93:ARG:HH11 | 26:7F:48:LEU:HG | 1.73 | 0.54 |
| 27:7G:135:GLU:HA | 27:7G:139:ILE:HD13 | 1.89 | 0.54 |
| 31:7M:78:HIS:N | 31:7M:79:PRO:HD2 | 2.23 | 0.54 |
| 36:7W:19:LEU:N | 36:7W:102:MET:CE | 2.71 | 0.54 |
| 36:7W:98:VAL:O | 36:7W:102:MET:CB | 2.52 | 0.54 |
| 1:A1:281:TYR:OH | 1:T4:83:GLN:O | 2.17 | 0.54 |
| 1:A3:359:LYS:HB2 | 26:7F:131:THR:HG21 | 1.90 | 0.54 |
| 2:E9:88:HIS:NE2 | 2:G5:284:GLU:HG2 | 2.23 | 0.54 |
| 2:G9:279:GLU:H | 2:G9:279:GLU:CD | 2.05 | 0.54 |
| 1:H6:107:THR:OG1 | 1:H6:401:GLU:OE1 | 2.25 | 0.54 |
| 1:H8:218:THR:HB | 24:6W:489:ASN:H | 1.73 | 0.54 |
| 1:I2:193:VAL:HG23 | 1:I2:194:GLU:HG3 | 1.90 | 0.54 |
| 2:I3:189:LEU:HD11 | 2:I3:418:PHE:HE1 | 1.73 | 0.54 |
| 1:I4:263:LEU:HD13 | 1:I4:422:TYR:HE1 | 1.71 | 0.54 |
| 1:I8:118:ASP:OD1 | 28:7H:452:ASN:HB2 | 2.07 | 0.54 |
| 1:I8:246:LEU:HD22 | 1:I8:352:SER:HA | 1.90 | 0.54 |
| 1:J2:122:LYS:NZ | 1:J2:123:GLU:OE1 | 2.38 | 0.54 |
| 1:J4:371:SER:OG | 1:J4:372:THR:N | 2.41 | 0.54 |
| 1:K4:387:ALA:HA | 1:K4:390:ARG:HE | 1.73 | 0.54 |
| 1:K6:135:VAL:HG21 | 1:K6:152:ILE:HD11 | 1.89 | 0.54 |
| 2:L5:204:LEU:HD13 | 2:L5:231:ILE:HD12 | 1.89 | 0.54 |
| 1:L6:183:TYR:HB3 | 1:L6:398:TYR:HE2 | 1.73 | 0.54 |
| 1:N2:244:GLY:H | 1:N2:247:ASN:HD21 | 1.55 | 0.54 |
| 2:N3:208:ALA:HA | 2:N3:304:LYS:HE3 | 1.88 | 0.54 |
| 1:P4:49:VAL:HG11 | 1:P4:241:ARG:HG2 | 1.90 | 0.54 |
| 2:P9:170:THR:HG21 | 2:P9:194:LEU:HD11 | 1.89 | 0.54 |
| 1:Q2:52:ASN:OD1 | 1:Q2:62:ARG:NH2 | 2.37 | 0.54 |
| 2:Q5:9:ILE:HD13 | 2:Q5:150:GLY:HA2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q6:396:HIS:HA | 1:Q6:399:THR:HG22 | 1.90 | 0.54 |
| 1:Q8:406:MET:HA | 1:Q8:409:THR:HG22 | 1.90 | 0.54 |
| 2:Q9:394:LYS:HB2 | 1:R0:346:PRO:HG3 | 1.90 | 0.54 |
| 1:R0:124:ALA:HB1 | 1:R0:130:LEU:HD11 | 1.89 | 0.54 |
| 2:R5:55:GLU:HG3 | 2:R5:61:HIS:CE1 | 2.43 | 0.54 |
| 2:R5:66:ILE:O | 2:R5:66:ILE:HG13 | 2.08 | 0.54 |
| 2:R5:267:PHE:HB2 | 2:R5:384:ILE:HD12 | 1.90 | 0.54 |
| 1:S2:359:LYS:HD3 | 7:4R:361:GLN:NE2 | 2.23 | 0.54 |
| 1:S4:163:MET:HB3 | 1:S4:250:LEU:HD22 | 1.89 | 0.54 |
| 1:S8:125:GLU:OE2 | 1:S8:159:TYR:OH | 2.24 | 0.54 |
| 1:T0:245:GLN:HG2 | 12:5F:210:THR:HG21 | 1.89 | 0.54 |
| 1:T4:279:GLN:OE1 | 7:4U:115:ARG:HB3 | 2.07 | 0.54 |
| 1:T6:56:GLY:N | 26:7F:104:GLN:NE2 | 2.55 | 0.54 |
| 2:U3:90:GLU:HG3 | 2:U3:121:ARG:NH1 | 2.23 | 0.54 |
| 2:W1:234:VAL:HG13 | 2:W1:376:CYS:SG | 2.48 | 0.54 |
| 1:W4:382:SER:OG | 1:W4:415:MET:HG2 | 2.08 | 0.54 |
| 1:X0:40:SER:OG | 8:4X:97:PHE:CD2 | 2.51 | 0.54 |
| 2:X7:72:PRO:HG2 | 1:X8:46:ARG:HH22 | 1.73 | 0.54 |
| 2:X7:254:GLU:HB3 | 2:X7:352:LYS:HE2 | 1.89 | 0.54 |
| 1:X8:177:ASP:O | 2:X9:352:LYS:HA | 2.07 | 0.54 |
| 1:Y0:58:ARG:HH11 | 1:Y0:84:ILE:HA | 1.72 | 0.54 |
| 2:Z7:392:ASP:OD2 | 2:Z7:422:ARG:NH1 | 2.41 | 0.54 |
| 2:Z9:129:CYS:SG | 2:Z9:130:THR:N | 2.80 | 0.54 |
| 1:0E:16:ILE:HD11 | 1:0E:136:CYS:HB3 | 1.90 | 0.54 |
| 1:0K:83:GLN:O | 1:1A:281:TYR:OH | 2.17 | 0.54 |
| 2:1B:254:GLU:HA | 2:1B:257:THR:HG22 | 1.90 | 0.54 |
| 1:1C:4:ILE:HB | 1:1C:50:TYR:CE1 | 2.35 | 0.54 |
| 1:1E:26:ASP:O | 1:1E:359:LYS:NZ | 2.26 | 0.54 |
| 1:1K:144:GLY:N | 39:1K:501:GDP:O1B | 2.41 | 0.54 |
| 1:1Q:388:MET:CE | 2:1R:348:PRO:HD2 | 2.38 | 0.54 |
| 2:1V:336:LYS:O | 2:1V:339:ARG:NH2 | 2.41 | 0.54 |
| 2:1X:183:GLU:HG3 | 2:1X:184:PRO:HD3 | 1.89 | 0.54 |
| 2:1Z:269:LEU:HD23 | 2:1Z:384:ILE:HD11 | 1.90 | 0.54 |
| 1:2A:364:SER:OG | 1:2A:365:ALA:N | 2.41 | 0.54 |
| 1:2C:208:TYR:CE1 | 1:2C:225:LEU:HD11 | 2.42 | 0.54 |
| 1:2I:118:ASP:CA | 38:8C:99:THR:HG22 | 2.38 | 0.54 |
| 2:2J:220:GLU:HG2 | 2:2J:221:ARG:HG3 | 1.89 | 0.54 |
| 2:2P:88:HIS:CE1 | 2:3F:283:HIS:HA | 2.42 | 0.54 |
| 2:2V:22:GLU:HG3 | 2:2V:83:TYR:OH | 2.08 | 0.54 |
| 1:2Y:219:THR:HB | 2:2Z:324:VAL:HG11 | 1.90 | 0.54 |
| 1:3A:309:ARG:NH1 | 1:3A:339:SER:O | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3B:381:SER:OG | 2:3B:382:THR:N | 2.41 | 0.54 |
| 2:3D:194:LEU:O | 2:3D:198:THR:HG22 | 2.07 | 0.54 |
| 2:3D:264:ARG:NH2 | 2:3D:431:ASP:OD2 | 2.41 | 0.54 |
| 1:3I:7:ILE:HB | 1:3I:135:VAL:HG22 | 1.89 | 0.54 |
| 1:3O:39:ASP:OD1 | 1:3O:40:SER:N | 2.40 | 0.54 |
| 1:3S:67:ASP:OD2 | 1:3S:72:THR:OG1 | 2.20 | 0.54 |
| 1:3S:406:MET:O | 1:3S:410:GLU:HG2 | 2.07 | 0.54 |
| 2:3T:237:SER:HA | 2:3T:320:ARG:HD2 | 1.90 | 0.54 |
| 3:3X:207:ASN:O | 3:3X:209:ARG:NH2 | 2.41 | 0.54 |
| 4:3Y:79:ILE:HB | 4:3Y:163:ARG:O | 2.07 | 0.54 |
| 3:4B:207:ASN:O | 3:4B:209:ARG:NH2 | 2.41 | 0.54 |
| 4:4E:61:CYS:HB3 | 4:4E:62:PRO:HD3 | 1.90 | 0.54 |
| 3:4F:207:ASN:O | 3:4F:209:ARG:NH2 | 2.41 | 0.54 |
| 4:4G:79:ILE:HB | 4:4G:163:ARG:O | 2.07 | 0.54 |
| 8:4V:436:GLU:HA | 8:4V:439:LYS:HG2 | 1.89 | 0.54 |
| 14:5L:177:ASP:OD1 | 14:5L:177:ASP:N | 2.41 | 0.54 |
| 15:5O:122:LYS:HD2 | 15:5O:222:PHE:CE2 | 2.43 | 0.54 |
| 15:5O:237:THR:HG22 | 15:5O:312:ALA:HB2 | 1.89 | 0.54 |
| 1:3:281:TYR:OH | 1:S6:83:GLN:O | 2.14 | 0.54 |
| 2:D1:206:ASN:OD1 | 41:D1:501:GTP:N2 | 2.29 | 0.54 |
| 2:G1:317:LEU:HB3 | 2:G1:319:TYR:HE1 | 1.72 | 0.54 |
| 2:G7:227:LEU:O | 2:G7:230:LEU:HD23 | 2.08 | 0.54 |
| 2:G7:381:SER:OG | 2:G7:382:THR:N | 2.40 | 0.54 |
| 2:H1:90:GLU:O | 2:H1:121:ARG:NH1 | 2.41 | 0.54 |
| 2:H3:254:GLU:HA | 2:H3:257:THR:HG22 | 1.89 | 0.54 |
| 2:H7:33:ASP:O | 2:H7:60:LYS:NZ | 2.41 | 0.54 |
| 2:H9:49:PHE:HB2 | 2:H9:53:PHE:HD2 | 1.73 | 0.54 |
| 1:I0:211:CYS:HA | 1:I0:215:LEU:HB2 | 1.90 | 0.54 |
| 2:I1:56:THR:HG23 | 2:I1:60:LYS:HB3 | 1.89 | 0.54 |
| 2:I1:333:ALA:O | 2:I1:337:THR:HG23 | 2.08 | 0.54 |
| 1:I2:180:VAL:HG23 | 1:I2:184:ASN:ND2 | 2.20 | 0.54 |
| 2:J3:417:GLU:HA | 2:J3:420:GLU:HG2 | 1.90 | 0.54 |
| 1:J4:114:ASP:N | 1:J4:114:ASP:OD1 | 2.39 | 0.54 |
| 1:J6:86:ARG:HG2 | 1:J6:88:ASP:H | 1.73 | 0.54 |
| 1:J6:309:ARG:NH1 | 1:J6:339:SER:O | 2.41 | 0.54 |
| 1:K6:248:ALA:HA | 1:K6:252:LYS:HD2 | 1.90 | 0.54 |
| 1:L2:340:TYR:HE1 | 34:7S:242:ASN:HD21 | 1.55 | 0.54 |
| 1:L6:203:ASP:HB2 | 1:L6:205:GLU:OE1 | 2.08 | 0.54 |
| 2:L7:12:ALA:O | 2:L7:16:VAL:HG23 | 2.08 | 0.54 |
| 2:L9:313:MET:HB2 | 2:L9:380:ASN:HB3 | 1.89 | 0.54 |
| 1:M2:5:VAL:HG23 | 1:M2:62:ARG:HG2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N1:236:SER:O | 2:N1:243:ARG:NH2 | 2.41 | 0.54 |
| 1:O0:297:LYS:NZ | 27:7G:5:ALA:O | 2.33 | 0.54 |
| 2:O7:155:GLU:HG2 | 2:O7:197:HIS:CE1 | 2.43 | 0.54 |
| 1:P4:175:VAL:CG1 | 2:P5:329:ASN:HD21 | 2.19 | 0.54 |
| 1:P8:190:HIS:CD2 | 1:P8:411:ALA:HA | 2.43 | 0.54 |
| 1:Q0:113:ILE:HD11 | 1:Q0:151:LEU:HD13 | 1.90 | 0.54 |
| 1:S2:248:ALA:HA | 1:S2:252:LYS:HD2 | 1.90 | 0.54 |
| 1:S4:74:ASP:OD1 | 24:6U:33:LEU:HD12 | 2.07 | 0.54 |
| 1:S4:249:ASP:HB2 | 1:S4:252:LYS:HE2 | 1.90 | 0.54 |
| 1:S8:320:ARG:NE | 12:5F:241:GLU:OE1 | 2.41 | 0.54 |
| 2:T3:88:HIS:CE1 | 2:T3:90:GLU:HB2 | 2.42 | 0.54 |
| 1:T4:128:ASP:OD1 | 1:T4:129:CYS:N | 2.37 | 0.54 |
| 2:U7:333:ALA:O | 2:U7:337:THR:HG23 | 2.08 | 0.54 |
| 2:V3:98:ASP:OD1 | 2:V3:99:ALA:N | 2.41 | 0.54 |
| 2:V3:221:ARG:HG2 | 1:V4:325:GLU:OE2 | 2.07 | 0.54 |
| 2:W7:60:LYS:HE2 | 2:Y3:283:HIS:CE1 | 2.44 | 0.54 |
| 2:X7:174:SER:HB3 | 2:X7:177:VAL:O | 2.07 | 0.54 |
| 2:X7:267:PHE:HB3 | 2:X7:384:ILE:HG21 | 1.90 | 0.54 |
| 1:Y0:263:LEU:HD22 | 1:Y0:422:TYR:CE1 | 2.42 | 0.54 |
| 1:Y8:273:LEU:H | 1:Y8:292:GLN:NE2 | 2.04 | 0.54 |
| 1:Z0:211:CYS:SG | 1:Z0:220:PRO:HB3 | 2.47 | 0.54 |
| 2:Z1:116:ASP:N | 2:Z1:116:ASP:OD1 | 2.40 | 0.54 |
| 2:Z5:392:ASP:OD2 | 2:Z5:422:ARG:NH1 | 2.41 | 0.54 |
| 1:Z8:8:GLN:HG3 | 1:Z8:65:LEU:HA | 1.89 | 0.54 |
| 1:0A:273:LEU:H | 1:0A:292:GLN:HE22 | 1.56 | 0.54 |
| 2:0B:83:TYR:HB3 | 2:0B:86:LEU:HB3 | 1.90 | 0.54 |
| 1:0E:113:ILE:HA | 1:0E:116:VAL:HG22 | 1.90 | 0.54 |
| 1:0E:309:ARG:NH1 | 1:0E:339:SER:O | 2.41 | 0.54 |
| 2:0J:429:GLU:O | 2:0J:433:GLU:HG2 | 2.08 | 0.54 |
| 1:0K:121:ARG:NH2 | 1:0K:158:GLU:OE2 | 2.41 | 0.54 |
| 2:0L:12:ALA:HB2 | 41:0M:501:GTP:C8 | 2.43 | 0.54 |
| 2:0L:398:MET:HG2 | 1:0M:345:ILE:HG12 | 1.90 | 0.54 |
| 2:0N:250:VAL:HG13 | 2:0N:254:GLU:HG3 | 1.90 | 0.54 |
| 2:0N:305:CYS:HB3 | 2:0N:387:ILE:HD11 | 1.89 | 0.54 |
| 2:0P:156:ARG:HA | 2:0P:159:VAL:HG22 | 1.90 | 0.54 |
| 2:0P:194:LEU:O | 2:0P:198:THR:HG22 | 2.07 | 0.54 |
| 1:0Q:287:PRO:HA | 1:0Q:290:THR:HG22 | 1.89 | 0.54 |
| 2:0R:407:TRP:CD2 | 1:0S:255:VAL:HG12 | 2.43 | 0.54 |
| 1:0U:97:ALA:HA | 1:0U:103:LYS:HE3 | 1.90 | 0.54 |
| 2:0V:83:TYR:HB3 | 2:0V:86:LEU:HB3 | 1.88 | 0.54 |
| 2:0V:100:ALA:CA | 1:0W:252:LYS:HG2 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1E:33:THR:O | 1:1E:58:ARG:NH2 | 2.41 | 0.54 |
| 1:1G:183:TYR:HA | 1:1G:385:PHE:HE1 | 1.72 | 0.54 |
| 2:1H:81:GLY:O | 2:1H:84:ARG:NH1 | 2.35 | 0.54 |
| 1:1M:379:LYS:HG3 | 1:1M:419:VAL:HG21 | 1.90 | 0.54 |
| 1:1O:309:ARG:H | 1:1O:372:THR:HG22 | 1.72 | 0.54 |
| 1:1Q:56:GLY:O | 10:5A:460:ARG:NH2 | 2.41 | 0.54 |
| 2:1Z:88:HIS:CD2 | 2:2P:283:HIS:HB3 | 2.37 | 0.54 |
| 2:1Z:141:VAL:HG22 | 2:1Z:187:SER:HA | 1.89 | 0.54 |
| 1:2E:135:VAL:HG21 | 1:2E:152:ILE:HD11 | 1.90 | 0.54 |
| 2:2F:267:PHE:HB2 | 2:2F:384:ILE:HD12 | 1.90 | 0.54 |
| 2:2J:266:HIS:ND1 | 2:2J:266:HIS:O | 2.41 | 0.54 |
| 2:2L:121:ARG:O | 2:2L:121:ARG:HD3 | 2.07 | 0.54 |
| 2:2R:98:ASP:OD1 | 2:2R:99:ALA:N | 2.41 | 0.54 |
| 1:2U:391:ARG:HG3 | 2:2V:346:TRP:CD2 | 2.43 | 0.54 |
| 2:2X:90:GLU:HG3 | 2:2X:121:ARG:NH1 | 2.23 | 0.54 |
| 1:3A:391:ARG:NH1 | 2:3B:438:GLU:O | 2.41 | 0.54 |
| 2:3N:109:THR:OG1 | 2:3N:411:GLU:OE2 | 2.20 | 0.54 |
| 2:3T:235:ILE:O | 2:3T:238:LEU:HG | 2.08 | 0.54 |
| 3:3V:119:THR:HG23 | 3:3V:122:ARG:H | 1.73 | 0.54 |
| 3:3X:119:THR:HG23 | 3:3X:122:ARG:H | 1.73 | 0.54 |
| 3:3Z:119:THR:HG23 | 3:3Z:122:ARG:H | 1.73 | 0.54 |
| 4:4A:61:CYS:HB3 | 4:4A:62:PRO:HD3 | 1.90 | 0.54 |
| 3:4B:119:THR:HG23 | 3:4B:122:ARG:H | 1.73 | 0.54 |
| 3:4D:119:THR:HG23 | 3:4D:122:ARG:H | 1.73 | 0.54 |
| 3:4F:119:THR:HG23 | 3:4F:122:ARG:H | 1.73 | 0.54 |
| 6:4O:103:ARG:HH12 | 6:4O:107:ALA:HB2 | 1.71 | 0.54 |
| 7:4T:213:GLU:HG3 | 31:7M:43:VAL:HG13 | 1.90 | 0.54 |
| 10:5C:499:ILE:HD12 | 10:5C:499:ILE:C | 2.28 | 0.54 |
| 14:5M:177:ASP:OD1 | 14:5M:177:ASP:N | 2.41 | 0.54 |
| 14:5N:177:ASP:OD1 | 14:5N:177:ASP:N | 2.41 | 0.54 |
| 15:5O:289:LEU:H | 15:5O:290:PRO:CD | 2.17 | 0.54 |
| 15:5P:257:ASP:OD1 | 15:5P:258:LEU:N | 2.41 | 0.54 |
| 18:5X:178:GLN:HA | 18:5X:181:GLN:HG2 | 1.90 | 0.54 |
| 24:6Y:322:LEU:HD23 | 24:6Y:323:LYS:O | 2.08 | 0.54 |
| 31:7M:65:THR:HG21 | 31:7M:73:ARG:HD3 | 1.90 | 0.54 |
| 36:7V:76:GLN:OE1 | 36:7V:76:GLN:HA | 2.08 | 0.54 |
| 1:9:41:ASP:N | 26:7E:25:TYR:HE2 | 2.06 | 0.53 |
| 2:F1:18:ASN:ND2 | 22:6O:116:TYR:HE1 | 2.06 | 0.53 |
| 1:F6:216:LYS:HB2 | 24:6T:422:ASN:HD21 | 1.72 | 0.53 |
| 1:G4:177:ASP:N | 1:G4:181:GLU:OE2 | 2.40 | 0.53 |
| 2:G7:88:HIS:CE1 | 2:G7:90:GLU:HB2 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G7:287:SER:N | 2:G7:290:GLU:OE2 | 2.40 | 0.53 |
| 1:G8:253:LEU:HD11 | 1:G8:316:LEU:HD11 | 1.91 | 0.53 |
| 2:H3:88:HIS:HB3 | 2:H3:91:GLN:CG | 2.37 | 0.53 |
| 1:H8:244:GLY:H | 1:H8:247:ASN:HD21 | 1.54 | 0.53 |
| 2:I1:26:LEU:HD21 | 2:I1:363:VAL:HG12 | 1.90 | 0.53 |
| 1:I4:153:SER:O | 1:I4:157:GLU:HG2 | 2.08 | 0.53 |
| 1:I4:248:ALA:HA | 1:I4:252:LYS:HD2 | 1.90 | 0.53 |
| 2:I5:199:ASP:OD1 | 2:I5:256:GLN:HG2 | 2.09 | 0.53 |
| 2:I7:88:HIS:CD2 | 2:K3:283:HIS:HA | 2.44 | 0.53 |
| 1:J6:5:VAL:HG22 | 1:J6:133:PHE:HD1 | 1.72 | 0.53 |
| 1:J8:77:ARG:HH21 | 1:J8:90:PHE:HD2 | 1.56 | 0.53 |
| 1:K0:2:ARG:HH21 | 1:K0:240:LEU:HA | 1.72 | 0.53 |
| 2:K3:47:ASP:N | 2:K3:47:ASP:OD1 | 2.41 | 0.53 |
| 1:L2:69:GLU:C | 1:L2:92:PHE:HZ | 2.10 | 0.53 |
| 2:L7:221:ARG:HG2 | 2:L7:221:ARG:O | 2.08 | 0.53 |
| 1:M0:275:SER:HG | 1:M0:278:SER:HG | 1.57 | 0.53 |
| 1:M4:5:VAL:HG23 | 1:M4:62:ARG:HG2 | 1.90 | 0.53 |
| 1:M6:114:ASP:N | 1:M6:114:ASP:OD1 | 2.41 | 0.53 |
| 1:M8:107:THR:OG1 | 1:M8:401:GLU:OE2 | 2.22 | 0.53 |
| 1:M8:117:LEU:HA | 1:M8:120:VAL:HG12 | 1.88 | 0.53 |
| 1:N2:117:LEU:HA | 1:N2:120:VAL:HG12 | 1.89 | 0.53 |
| 1:O0:131:GLN:HE22 | 1:O0:249:ASP:HB3 | 1.72 | 0.53 |
| 1:O2:139:LEU:HD12 | 1:O2:170:VAL:HG12 | 1.90 | 0.53 |
| 2:O9:187:SER:O | 2:O9:191:THR:HG23 | 2.09 | 0.53 |
| 1:P4:8:GLN:OE1 | 1:P4:17:GLY:HA3 | 2.09 | 0.53 |
| 2:P7:88:HIS:HB2 | 2:R3:283:HIS:ND1 | 2.23 | 0.53 |
| 1:P8:190:HIS:CD2 | 1:P8:414:ASN:HB2 | 2.43 | 0.53 |
| 2:R7:372:GLN:NE2 | 7:4R:203:THR:HG21 | 2.22 | 0.53 |
| 1:S6:66:MET:HE3 | 1:S6:116:VAL:HG21 | 1.91 | 0.53 |
| 1:S6:417:ASP:OD1 | 1:S6:418:LEU:N | 2.41 | 0.53 |
| 1:T0:321:MET:HG2 | 1:T0:363:MET:SD | 2.48 | 0.53 |
| 1:U4:211:CYS:HB3 | 1:U4:217:LEU:HD12 | 1.90 | 0.53 |
| 1:U6:122:LYS:NZ | 1:W2:291:GLN:HB3 | 2.22 | 0.53 |
| 1:U8:177:ASP:OD2 | 2:U9:248:LEU:HD11 | 2.09 | 0.53 |
| 1:V2:4:ILE:HB | 1:V2:50:TYR:HE1 | 1.72 | 0.53 |
| 1:V2:175:VAL:HG13 | 2:V3:329:ASN:HD21 | 1.73 | 0.53 |
| 2:V3:363:VAL:HG23 | 2:V3:366:GLY:HA3 | 1.90 | 0.53 |
| 1:V4:260:PHE:HB2 | 1:V4:263:LEU:HD23 | 1.89 | 0.53 |
| 1:W0:215:LEU:HB3 | 1:W0:217:LEU:HG | 1.90 | 0.53 |
| 2:W9:14:ILE:CD1 | 2:W9:74:VAL:HG11 | 2.38 | 0.53 |
| 2:W9:225:THR:HG22 | 2:W9:229:ARG:HE | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X5:211:ASP:HB3 | 2:X5:215:ARG:HH12 | 1.73 | 0.53 |
| 1:X6:50:TYR:OH | 1:X6:237:THR:OG1 | 2.24 | 0.53 |
| 2:X7:281:ALA:HB1 | 8:4W:209:ARG:CZ | 2.39 | 0.53 |
| 1:Y6:3:GLU:HB2 | 1:Y6:130:LEU:HA | 1.89 | 0.53 |
| 1:Z0:374:ILE:O | 1:Z0:377:MET:HG3 | 2.07 | 0.53 |
| 2:Z1:286:LEU:HD11 | 2:Z1:372:GLN:HB2 | 1.89 | 0.53 |
| 1:Z2:207:LEU:HB3 | 1:Z2:225:LEU:HD22 | 1.90 | 0.53 |
| 2:Z3:49:PHE:HE2 | 2:Z3:55:GLU:HG3 | 1.72 | 0.53 |
| 1:Z4:8:GLN:OE1 | 1:Z4:136:CYS:HB3 | 2.07 | 0.53 |
| 1:Z8:166:THR:OG1 | 1:Z8:199:CYS:HB3 | 2.08 | 0.53 |
| 2:0J:384:ILE:HD12 | 2:0J:384:ILE:H | 1.73 | 0.53 |
| 2:0L:324:VAL:HG12 | 2:0L:326:LYS:H | 1.72 | 0.53 |
| 2:0R:52:PHE:CE2 | 2:0R:243:ARG:HD3 | 2.44 | 0.53 |
| 2:0V:90:GLU:O | 2:0V:121:ARG:NH1 | 2.24 | 0.53 |
| 1:0Y:26:ASP:O | 1:0Y:359:LYS:NZ | 2.33 | 0.53 |
| 1:0Y:134:GLN:HE21 | 1:0Y:167:PHE:HE2 | 1.55 | 0.53 |
| 1:1A:335:ASN:O | 1:1A:338:SER:OG | 2.26 | 0.53 |
| 2:1D:108:TYR:HB2 | 2:1D:411:GLU:OE2 | 2.08 | 0.53 |
| 2:1L:132:LEU:HD22 | 2:1L:164:LYS:HD3 | 1.90 | 0.53 |
| 2:2H:305:CYS:SG | 2:2H:383:ALA:HB1 | 2.48 | 0.53 |
| 1:2S:211:CYS:HA | 1:2S:215:LEU:HB2 | 1.90 | 0.53 |
| 1:2U:320:ARG:NH2 | 38:8B:201:LEU:HD23 | 2.22 | 0.53 |
| 1:2Y:6:HIS:CE1 | 1:2Y:136:CYS:HG | 2.26 | 0.53 |
| 2:2Z:147:SER:OG | 2:2Z:190:SER:HB2 | 2.08 | 0.53 |
| 1:3A:282:ARG:HE | 1:3A:288:GLU:CG | 2.21 | 0.53 |
| 2:3B:214:ARG:HH22 | 38:8C:17:GLY:N | 2.05 | 0.53 |
| 1:3K:11:GLN:N | 39:3K:503:GDP:O1B | 2.27 | 0.53 |
| 3:3V:207:ASN:O | 3:3V:209:ARG:NH2 | 2.41 | 0.53 |
| 3:3Z:207:ASN:O | 3:3Z:209:ARG:NH2 | 2.41 | 0.53 |
| 3:4D:207:ASN:O | 3:4D:209:ARG:NH2 | 2.41 | 0.53 |
| 3:4H:119:THR:HG23 | 3:4H:122:ARG:H | 1.73 | 0.53 |
| 3:4H:207:ASN:O | 3:4H:209:ARG:NH2 | 2.41 | 0.53 |
| 6:4O:290:GLU:OE2 | 6:4O:293:ARG:NH1 | 2.41 | 0.53 |
| 8:4W:468:MET:HE3 | 8:4W:470:TYR:CE1 | 2.42 | 0.53 |
| 14:5M:415:LYS:HZ1 | 23:6R:22:MET:HG3 | 1.72 | 0.53 |
| 15:5O:282:LEU:O | 15:5O:284:VAL:N | 2.41 | 0.53 |
| 22:6P:128:GLU:N | 22:6P:128:GLU:OE1 | 2.41 | 0.53 |
| 24:6T:96:LEU:HD22 | 24:6T:188:THR:HG22 | 1.89 | 0.53 |
| 24:6U:223:ARG:NH1 | 24:6U:223:ARG:HA | 2.22 | 0.53 |
| 24:6V:130:MET:HB3 | 24:6V:153:VAL:HG23 | 1.90 | 0.53 |
| 24:6X:473:TYR:HA | 24:6X:480:ASN:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Z:42:GLU:N | 24:6Z:42:GLU:OE1 | 2.41 | 0.53 |
| 24:6Z:88:TRP:HA | 24:6Z:126:GLU:HG2 | 1.90 | 0.53 |
| 24:7A:135:PRO:HG2 | 24:7A:137:GLN:HE22 | 1.74 | 0.53 |
| 27:7G:208:ASP:N | 27:7G:208:ASP:OD1 | 2.39 | 0.53 |
| 38:8D:62:THR:O | 38:8D:65:VAL:HG12 | 2.08 | 0.53 |
| 1:A7:280:GLN:NE2 | 24:6T:106:VAL:HA | 2.22 | 0.53 |
| 2:E7:56:THR:HG23 | 2:G3:285:GLN:HA | 1.90 | 0.53 |
| 1:G2:216:LYS:C | 24:6W:422:ASN:HD21 | 2.11 | 0.53 |
| 2:G3:274:PRO:HB2 | 2:G3:276:ILE:HG12 | 1.90 | 0.53 |
| 2:G3:333:ALA:O | 2:G3:337:THR:HG23 | 2.09 | 0.53 |
| 2:G5:71:GLU:HG3 | 1:G6:2:ARG:NH1 | 2.23 | 0.53 |
| 2:G5:187:SER:O | 2:G5:191:THR:HG23 | 2.07 | 0.53 |
| 2:G7:88:HIS:HD2 | 2:G7:89:PRO:HD2 | 1.65 | 0.53 |
| 2:H1:287:SER:OG | 2:H1:288:VAL:N | 2.41 | 0.53 |
| 2:H3:289:ALA:O | 2:H3:293:ASN:ND2 | 2.42 | 0.53 |
| 2:I5:172:TYR:CE2 | 2:I5:203:MET:HG2 | 2.43 | 0.53 |
| 2:J3:11:GLN:OE1 | 2:J3:15:GLN:NE2 | 2.41 | 0.53 |
| 2:J3:312:TYR:HD1 | 2:J3:381:SER:HB3 | 1.73 | 0.53 |
| 2:L3:121:ARG:CZ | 2:L3:124:LYS:HE3 | 2.38 | 0.53 |
| 2:M3:26:LEU:HD11 | 2:M3:364:PRO:HD3 | 1.90 | 0.53 |
| 2:M3:324:VAL:HG21 | 2:M3:326:LYS:HE3 | 1.90 | 0.53 |
| 2:M3:417:GLU:HA | 2:M3:420:GLU:HG2 | 1.90 | 0.53 |
| 1:M6:2:ARG:HE | 1:M6:240:LEU:HD22 | 1.71 | 0.53 |
| 1:M6:140:GLY:O | 1:M6:184:ASN:ND2 | 2.39 | 0.53 |
| 1:M6:287:PRO:HA | 1:M6:290:THR:HG22 | 1.89 | 0.53 |
| 1:M8:139:LEU:HD12 | 1:M8:170:VAL:HG12 | 1.89 | 0.53 |
| 1:N0:177:ASP:O | 2:N1:352:LYS:HA | 2.08 | 0.53 |
| 1:N6:52:ASN:OD1 | 1:N6:62:ARG:NH2 | 2.41 | 0.53 |
| 1:N8:20:PHE:HA | 1:N8:230:SER:OG | 2.07 | 0.53 |
| 1:O2:21:TRP:O | 1:O2:25:SER:OG | 2.21 | 0.53 |
| 2:O5:102:ASN:HB3 | 2:O5:105:ARG:HB3 | 1.90 | 0.53 |
| 1:Q4:20:PHE:HA | 1:Q4:230:SER:OG | 2.08 | 0.53 |
| 1:Q4:186:THR:HG23 | 1:Q4:187:LEU:HD12 | 1.91 | 0.53 |
| 1:Q4:406:MET:O | 1:Q4:410:GLU:HG2 | 2.08 | 0.53 |
| 1:Q8:137:HIS:NE2 | 1:Q8:166:THR:OG1 | 2.41 | 0.53 |
| 2:R1:90:GLU:HB3 | 2:R1:121:ARG:NH1 | 2.23 | 0.53 |
| 1:R4:301:CYS:SG | 1:R4:302:ALA:N | 2.81 | 0.53 |
| 2:R9:84:ARG:NH1 | 33:7Q:173:SER:HB3 | 2.23 | 0.53 |
| 1:S2:135:VAL:HG11 | 1:S2:152:ILE:HD11 | 1.90 | 0.53 |
| 2:S5:72:PRO:HD2 | 1:S6:2:ARG:NH1 | 2.24 | 0.53 |
| 1:T0:252:LYS:HA | 1:T0:255:VAL:CG1 | 2.34 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T1:145:THR:OG1 | 41:T2:501:GTP:O1B | 2.25 | 0.53 |
| 1:T6:11:GLN:HE22 | 2:T7:248:LEU:HA | 1.73 | 0.53 |
| 2:U3:336:LYS:NZ | 2:U3:348:PRO:O | 2.40 | 0.53 |
| 2:U5:76:ASP:HB3 | 2:U5:79:ARG:NH1 | 2.24 | 0.53 |
| 2:U5:81:GLY:O | 2:U5:84:ARG:HG3 | 2.08 | 0.53 |
| 2:U5:384:ILE:HA | 2:U5:387:ILE:HD12 | 1.91 | 0.53 |
| 1:V4:274:THR:HG21 | 1:V4:282:ARG:HD2 | 1.90 | 0.53 |
| 2:V9:311:LYS:HG2 | 2:V9:342:GLN:HG3 | 1.89 | 0.53 |
| 2:X9:213:CYS:HA | 2:X9:217:LEU:HD12 | 1.90 | 0.53 |
| 2:Y3:282:TYR:HD2 | 8:4W:373:ASN:HD22 | 0.62 | 0.53 |
| 2:Z1:407:TRP:HZ2 | 1:Z2:258:ILE:HB | 1.72 | 0.53 |
| 1:Z4:177:ASP:O | 2:Z5:352:LYS:HA | 2.07 | 0.53 |
| 1:Z8:86:ARG:HG2 | 1:Z8:88:ASP:H | 1.72 | 0.53 |
| 1:Z8:391:ARG:HB2 | 2:Z9:346:TRP:CD1 | 2.43 | 0.53 |
| 1:0A:27:GLU:OE1 | 1:0A:318:ARG:NH2 | 2.41 | 0.53 |
| 2:0F:195:LEU:HD21 | 2:0F:264:ARG:HG2 | 1.91 | 0.53 |
| 2:0J:181:VAL:HG12 | 1:0K:347:ASN:O | 2.08 | 0.53 |
| 1:0W:114:ASP:OD1 | 1:0W:114:ASP:N | 2.37 | 0.53 |
| 1:1E:40:SER:HB2 | 1:1E:42:LEU:HD12 | 1.91 | 0.53 |
| 2:1H:90:GLU:O | 2:1H:121:ARG:NH1 | 2.41 | 0.53 |
| 2:1L:85:GLN:O | 2:2B:283:HIS:CE1 | 2.62 | 0.53 |
| 1:1Q:335:ASN:O | 1:1Q:338:SER:OG | 2.25 | 0.53 |
| 2:1R:116:ASP:N | 2:1R:116:ASP:OD1 | 2.40 | 0.53 |
| 1:1U:3:GLU:HB2 | 1:1U:130:LEU:HA | 1.89 | 0.53 |
| 2:1V:156:ARG:HA | 2:1V:159:VAL:HG12 | 1.90 | 0.53 |
| 2:1Z:141:VAL:CG2 | 2:1Z:187:SER:HA | 2.37 | 0.53 |
| 2:1Z:157:LEU:HD22 | 2:1Z:166:LYS:HD3 | 1.90 | 0.53 |
| 2:2H:68:LEU:HA | 2:2H:93:ILE:O | 2.07 | 0.53 |
| 2:2J:213:CYS:HA | 2:2J:217:LEU:HG | 1.90 | 0.53 |
| 2:2L:317:LEU:HB3 | 2:2L:319:TYR:HE1 | 1.72 | 0.53 |
| 1:2M:371:SER:OG | 1:2M:372:THR:N | 2.41 | 0.53 |
| 2:2Z:88:HIS:NE2 | 2:2Z:90:GLU:HB3 | 2.23 | 0.53 |
| 1:3A:325:GLU:O | 1:3A:329:GLN:HG2 | 2.07 | 0.53 |
| 1:3C:332:ASN:HD21 | 38:8C:1:MET:N | 2.06 | 0.53 |
| 2:3D:90:GLU:HB3 | 2:3T:283:HIS:CE1 | 2.43 | 0.53 |
| 1:3G:88:ASP:OD1 | 3:3X:262:TYR:HB3 | 2.07 | 0.53 |
| 2:3N:8:HIS:CD2 | 2:3N:138:PHE:HD2 | 2.25 | 0.53 |
| 1:3Q:11:GLN:N | 39:3Q:501:GDP:O1B | 2.31 | 0.53 |
| 5:4M:293:LEU:HB2 | 28:7X:306:LEU:HD21 | 1.89 | 0.53 |
| 10:5C:205:GLN:O | 10:5C:208:GLU:HG3 | 2.09 | 0.53 |
| 15:5P:99:LYS:HB2 | 15:5P:204:ALA:HA | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5V:179:GLN:HA | 17:5V:179:GLN:HE21 | 1.73 | 0.53 |
| 22:6K:172:ARG:HH11 | 22:6K:215:GLY:HA3 | 1.73 | 0.53 |
| 24:6T:88:TRP:HA | 24:6T:126:GLU:HG2 | 1.90 | 0.53 |
| 24:6T:111:MET:HG2 | 24:6T:213:TYR:CE2 | 2.43 | 0.53 |
| 24:6Z:278:VAL:HG11 | 24:6Z:395:VAL:HG11 | 1.90 | 0.53 |
| 26:7E:133:PHE:CD2 | 26:7E:134:LEU:HB2 | 2.44 | 0.53 |
| 2:4:29:GLY:O | 26:7D:45:MET:HE3 | 2.07 | 0.53 |
| 1:D4:78:SER:OG | 24:6Y:323:LYS:HG3 | 2.09 | 0.53 |
| 1:E2:32:PRO:HG3 | 24:6U:402:LYS:HE3 | 1.90 | 0.53 |
| 2:G1:317:LEU:HB3 | 2:G1:319:TYR:CE1 | 2.43 | 0.53 |
| 1:G4:5:VAL:HG22 | 1:G4:62:ARG:HD3 | 1.90 | 0.53 |
| 2:G7:98:ASP:OD1 | 2:G7:99:ALA:N | 2.40 | 0.53 |
| 2:H5:88:HIS:ND1 | 2:J1:283:HIS:HA | 2.23 | 0.53 |
| 2:H5:205:ASP:OD2 | 2:H5:303:VAL:HG13 | 2.09 | 0.53 |
| 2:H7:181:VAL:HG13 | 2:H7:182:VAL:HG13 | 1.90 | 0.53 |
| 2:I3:217:LEU:HB3 | 2:I3:219:ILE:HD12 | 1.89 | 0.53 |
| 1:J6:174:LYS:HB2 | 1:J6:205:GLU:OE2 | 2.08 | 0.53 |
| 2:J9:370:LYS:HD2 | 5:4M:266:PHE:HE2 | 1.73 | 0.53 |
| 2:K7:156:ARG:HA | 2:K7:159:VAL:HG12 | 1.90 | 0.53 |
| 1:K8:216:LYS:NZ | 16:5Q:184:GLU:O | 2.41 | 0.53 |
| 1:L4:339:SER:H | 35:7U:147:ASN:ND2 | 2.06 | 0.53 |
| 1:L4:388:MET:CE | 2:L5:348:PRO:HD2 | 2.39 | 0.53 |
| 2:L7:62:VAL:HB | 2:L7:88:HIS:CE1 | 2.42 | 0.53 |
| 1:M4:3:GLU:HB2 | 1:M4:130:LEU:HA | 1.89 | 0.53 |
| 2:M7:222:PRO:HD2 | 1:M8:324:LYS:HE3 | 1.90 | 0.53 |
| 2:M9:372:GLN:HG2 | 30:7K:24:PRO:HB2 | 1.90 | 0.53 |
| 1:N0:212:PHE:HZ | 2:N1:326:LYS:HG3 | 1.73 | 0.53 |
| 2:N3:70:LEU:HD13 | 2:N3:145:THR:HG23 | 1.91 | 0.53 |
| 1:N6:117:LEU:HA | 1:N6:120:VAL:HG12 | 1.89 | 0.53 |
| 1:N8:91:VAL:HG11 | 1:N8:116:VAL:HG12 | 1.91 | 0.53 |
| 2:O3:214:ARG:NH2 | 37:7Y:84:ARG:HH12 | 2.06 | 0.53 |
| 1:O6:40:SER:HB3 | 32:7P:112:LEU:HD13 | 1.91 | 0.53 |
| 2:O9:266:HIS:ND1 | 2:O9:266:HIS:O | 2.39 | 0.53 |
| 2:P5:9:ILE:HG13 | 2:P5:139:ASN:HB3 | 1.90 | 0.53 |
| 2:P7:367:ASP:N | 2:P7:367:ASP:OD2 | 2.41 | 0.53 |
| 1:P8:207:LEU:HB3 | 1:P8:225:LEU:HD22 | 1.90 | 0.53 |
| 1:P8:273:LEU:H | 1:P8:292:GLN:HE22 | 1.56 | 0.53 |
| 1:Q4:175:VAL:HG22 | 2:Q5:329:ASN:ND2 | 2.22 | 0.53 |
| 2:R1:333:ALA:O | 2:R1:337:THR:HG23 | 2.08 | 0.53 |
| 1:R2:397:TRP:CE3 | 1:R2:397:TRP:HA | 2.42 | 0.53 |
| 1:R4:173:PRO:HB3 | 1:R4:384:GLN:HE22 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S0:274:THR:OG1 | 1:S0:282:ARG:NH1 | 2.39 | 0.53 |
| 2:S1:88:HIS:CG | 2:S1:89:PRO:CD | 2.89 | 0.53 |
| 2:T3:191:THR:O | 2:T3:195:LEU:HG | 2.08 | 0.53 |
| 2:U9:312:TYR:HB2 | 2:U9:343:PHE:HD1 | 1.72 | 0.53 |
| 1:V0:138:SER:OG | 1:V0:139:LEU:N | 2.39 | 0.53 |
| 2:V3:111:GLY:HA2 | 2:V3:114:ILE:HG22 | 1.90 | 0.53 |
| 2:V9:76:ASP:HA | 2:V9:79:ARG:HB2 | 1.90 | 0.53 |
| 1:W2:11:GLN:N | 39:W2:503:GDP:O2B | 2.39 | 0.53 |
| 1:W4:263:LEU:HD13 | 1:W4:422:TYR:HE1 | 1.73 | 0.53 |
| 1:X0:25:SER:OG | 1:X0:30:ILE:O | 2.27 | 0.53 |
| 2:X5:276:ILE:HG23 | 2:X5:280:LYS:HB2 | 1.91 | 0.53 |
| 2:X5:287:SER:N | 2:X5:290:GLU:OE2 | 2.24 | 0.53 |
| 1:Y6:47:ILE:HD12 | 1:Y6:59:TYR:CE1 | 2.43 | 0.53 |
| 2:Z1:322:ASP:OD2 | 2:Z1:373:ARG:NH2 | 2.41 | 0.53 |
| 2:Z3:232:ALA:HA | 2:Z3:235:ILE:HG22 | 1.90 | 0.53 |
| 1:Z4:195:ASN:OD1 | 1:Z4:196:ALA:N | 2.41 | 0.53 |
| 1:0C:274:THR:OG1 | 1:0C:282:ARG:NH1 | 2.41 | 0.53 |
| 1:0E:233:MET:N | 1:0E:233:MET:SD | 2.82 | 0.53 |
| 1:0I:179:VAL:HB | 2:0J:258:ASN:HD22 | 1.72 | 0.53 |
| 1:0I:290:THR:HA | 1:0I:293:MET:HB2 | 1.90 | 0.53 |
| 2:0N:90:GLU:O | 2:0N:121:ARG:NH1 | 2.41 | 0.53 |
| 1:0U:139:LEU:HG | 1:0U:168:SER:HB2 | 1.89 | 0.53 |
| 1:0W:72:THR:O | 1:0W:76:VAL:HG23 | 2.07 | 0.53 |
| 1:1C:77:ARG:HH21 | 1:1C:90:PHE:HD2 | 1.56 | 0.53 |
| 1:1G:139:LEU:HD12 | 1:1G:170:VAL:HG22 | 1.88 | 0.53 |
| 2:1L:121:ARG:C | 2:1L:121:ARG:CD | 2.76 | 0.53 |
| 2:1P:276:ILE:CG1 | 2:1P:281:ALA:HB2 | 2.39 | 0.53 |
| 2:1Z:245:ASP:OD1 | 2:1Z:245:ASP:N | 2.39 | 0.53 |
| 1:2C:14:ASN:HD22 | 1:2C:65:LEU:HD22 | 1.74 | 0.53 |
| 2:2D:50:ASN:O | 2:2D:64:ARG:NH2 | 2.42 | 0.53 |
| 2:2D:113:GLU:HG2 | 38:8A:7:ASP:HA | 1.88 | 0.53 |
| 2:2H:123:ARG:HH22 | 38:8B:37:TYR:CB | 2.21 | 0.53 |
| 2:2T:214:ARG:NH2 | 38:8A:18:VAL:HA | 2.23 | 0.53 |
| 2:2Z:213:CYS:HA | 2:2Z:217:LEU:HB2 | 1.90 | 0.53 |
| 2:2Z:381:SER:OG | 2:2Z:382:THR:N | 2.42 | 0.53 |
| 1:3A:3:GLU:HB2 | 1:3A:130:LEU:HA | 1.91 | 0.53 |
| 1:3C:139:LEU:HG | 1:3C:168:SER:OG | 2.09 | 0.53 |
| 1:3C:211:CYS:HB3 | 1:3C:217:LEU:HD12 | 1.90 | 0.53 |
| 2:3F:222:PRO:HD2 | 1:3G:324:LYS:HE3 | 1.89 | 0.53 |
| 2:3F:398:MET:HG3 | 1:3G:346:PRO:HD2 | 1.90 | 0.53 |
| 2:3J:283:HIS:HD2 | 2:3J:284:GLU:HB2 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3R:339:ARG:HH22 | 2:3R:342:GLN:HB3 | 1.73 | 0.53 |
| 3:4J:212:SER:O | 3:4J:216:ILE:HG12 | 2.07 | 0.53 |
| 15:5O:257:ASP:OD1 | 15:5O:258:LEU:N | 2.42 | 0.53 |
| 19:6E:92:ARG:HD3 | 19:6E:99:ARG:CZ | 2.38 | 0.53 |
| 26:7F:48:LEU:N | 26:7F:49:PRO:CD | 2.70 | 0.53 |
| 36:7W:76:GLN:OE1 | 36:7W:76:GLN:HA | 2.09 | 0.53 |
| 2:B4:80:THR:HG22 | 18:6A:169:LYS:O | 2.08 | 0.53 |
| 1:F6:122:LYS:HE3 | 1:H2:291:GLN:HB3 | 1.88 | 0.53 |
| 1:G2:72:THR:O | 1:G2:76:VAL:HG23 | 2.08 | 0.53 |
| 1:H2:404:ASP:HB3 | 1:H2:406:MET:SD | 2.48 | 0.53 |
| 1:H4:52:ASN:OD1 | 1:H4:62:ARG:NH1 | 2.41 | 0.53 |
| 2:H5:290:GLU:HA | 2:H5:293:ASN:HD22 | 1.73 | 0.53 |
| 2:H5:430:LYS:O | 2:H5:433:GLU:HG3 | 2.09 | 0.53 |
| 2:I3:101:ASN:ND2 | 2:I3:143:GLY:HA2 | 2.22 | 0.53 |
| 1:I8:7:ILE:HB | 1:I8:135:VAL:HG22 | 1.90 | 0.53 |
| 1:I8:271:THR:HG23 | 1:I8:365:ALA:HB3 | 1.88 | 0.53 |
| 1:J0:7:ILE:HB | 1:J0:135:VAL:HG22 | 1.89 | 0.53 |
| 1:J2:113:ILE:HG21 | 1:J2:150:LEU:HD22 | 1.91 | 0.53 |
| 2:J7:271:SER:OG | 2:J7:377:MET:HB3 | 2.09 | 0.53 |
| 2:K1:223:THR:HG22 | 2:K1:224:TYR:H | 1.74 | 0.53 |
| 2:L3:245:ASP:OD1 | 2:L3:245:ASP:N | 2.42 | 0.53 |
| 2:M3:156:ARG:HA | 2:M3:159:VAL:HG12 | 1.91 | 0.53 |
| 2:M5:57:GLY:HA3 | 1:O2:280:GLN:O | 2.09 | 0.53 |
| 1:M6:54:ALA:HA | 2:O3:285:GLN:HB2 | 1.90 | 0.53 |
| 1:M6:86:ARG:NH1 | 1:M6:123:GLU:OE2 | 2.41 | 0.53 |
| 2:M7:91:GLN:HE21 | 2:M7:125:LEU:HD21 | 1.74 | 0.53 |
| 2:M7:346:TRP:CZ3 | 2:M7:347:CYS:HB3 | 2.43 | 0.53 |
| 2:M9:259:LEU:HD11 | 2:M9:316:CYS:HB2 | 1.90 | 0.53 |
| 2:M9:287:SER:OG | 2:M9:288:VAL:N | 2.41 | 0.53 |
| 2:N1:147:SER:OG | 2:N1:148:GLY:N | 2.42 | 0.53 |
| 2:N3:386:GLU:O | 2:N3:390:ARG:HG3 | 2.09 | 0.53 |
| 1:O2:50:TYR:OH | 1:O2:237:THR:OG1 | 2.24 | 0.53 |
| 2:O5:62:VAL:HG23 | 2:O5:62:VAL:O | 2.08 | 0.53 |
| 1:O8:99:ASN:ND2 | 2:O9:254:GLU:OE1 | 2.41 | 0.53 |
| 2:P3:266:HIS:O | 2:P3:266:HIS:ND1 | 2.41 | 0.53 |
| 1:P8:20:PHE:HA | 1:P8:230:SER:HB2 | 1.90 | 0.53 |
| 1:Q6:173:PRO:HG3 | 1:Q6:380:ARG:HD2 | 1.90 | 0.53 |
| 2:R1:145:THR:OG1 | 41:R2:501:GTP:O1B | 2.25 | 0.53 |
| 2:S1:170:THR:HG21 | 2:S1:194:LEU:HD11 | 1.91 | 0.53 |
| 1:S6:39:ASP:OD1 | 1:S6:40:SER:N | 2.41 | 0.53 |
| 2:S9:79:ARG:NH1 | 2:S9:94:SER:OG | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T0:39:ASP:OD1 | 1:T0:39:ASP:N | 2.41 | 0.53 |
| 1:T0:248:ALA:HA | 1:T0:252:LYS:CD | 2.19 | 0.53 |
| 1:T2:1:MET:HA | 1:T2:1:MET:CE | 2.37 | 0.53 |
| 1:T6:80:PRO:O | 1:T6:81:TYR:HB2 | 2.09 | 0.53 |
| 2:U1:72:PRO:HD2 | 1:U2:2:ARG:NH1 | 2.24 | 0.53 |
| 2:U9:287:SER:N | 2:U9:290:GLU:OE2 | 2.36 | 0.53 |
| 1:V0:31:ASP:OD2 | 1:V0:33:THR:OG1 | 2.22 | 0.53 |
| 1:V0:322:SER:HB3 | 1:V0:325:GLU:HB2 | 1.91 | 0.53 |
| 1:V4:156:ARG:NH1 | 1:V4:197:ASP:OD2 | 2.41 | 0.53 |
| 2:V7:277:SER:OG | 2:V7:278:ALA:N | 2.42 | 0.53 |
| 1:X0:3:GLU:OE1 | 1:X0:62:ARG:NH1 | 2.41 | 0.53 |
| 2:X3:109:THR:OG1 | 2:X3:411:GLU:OE2 | 2.19 | 0.53 |
| 2:X7:121:ARG:HD2 | 2:X7:124:LYS:HE3 | 1.89 | 0.53 |
| 2:Y1:181:VAL:HG23 | 1:Y2:256:ASN:HD22 | 1.74 | 0.53 |
| 2:Y5:109:THR:OG1 | 2:Y5:411:GLU:OE2 | 2.23 | 0.53 |
| 1:Z0:179:VAL:HG22 | 2:Z1:258:ASN:HD22 | 1.73 | 0.53 |
| 1:Z2:127:CYS:SG | 1:Z2:130:LEU:HG | 2.48 | 0.53 |
| 2:Z5:86:LEU:HD12 | 2:Z5:86:LEU:O | 2.09 | 0.53 |
| 1:0C:152:ILE:HD13 | 1:0C:155:ILE:HD11 | 1.90 | 0.53 |
| 2:0F:268:MET:SD | 2:0F:380:ASN:HB2 | 2.49 | 0.53 |
| 1:0G:335:ASN:O | 1:0G:338:SER:OG | 2.27 | 0.53 |
| 2:0H:381:SER:OG | 2:0H:382:THR:N | 2.41 | 0.53 |
| 2:0N:55:GLU:O | 2:1D:285:GLN:NE2 | 2.40 | 0.53 |
| 2:0R:56:THR:HA | 2:1H:285:GLN:HB2 | 1.89 | 0.53 |
| 2:0R:203:MET:SD | 2:0R:203:MET:N | 2.82 | 0.53 |
| 2:0X:35:GLN:HB3 | 2:0X:59:GLY:O | 2.08 | 0.53 |
| 2:1D:313:MET:HB2 | 2:1D:380:ASN:HB3 | 1.90 | 0.53 |
| 2:1P:213:CYS:HB3 | 2:1P:219:ILE:HD11 | 1.90 | 0.53 |
| 2:1R:289:ALA:O | 2:1R:293:ASN:ND2 | 2.42 | 0.53 |
| 2:1T:202:VAL:HG22 | 2:1T:268:MET:HB2 | 1.89 | 0.53 |
| 2:1V:5:ILE:HG22 | 2:1V:64:ARG:HB3 | 1.90 | 0.53 |
| 2:1X:116:ASP:OD1 | 2:1X:116:ASP:N | 2.38 | 0.53 |
| 2:1Z:56:THR:O | 2:1Z:56:THR:OG1 | 2.23 | 0.53 |
| 1:2E:72:THR:O | 1:2E:76:VAL:HG23 | 2.09 | 0.53 |
| 2:2L:246:GLY:N | 2:2L:249:ASN:HD21 | 2.06 | 0.53 |
| 1:2U:245:GLN:NE2 | 38:8B:198:THR:HG21 | 2.23 | 0.53 |
| 2:2X:192:HIS:CD2 | 2:2X:421:ALA:HA | 2.44 | 0.53 |
| 2:3D:297:GLU:OE2 | 38:8D:73:TRP:HA | 2.08 | 0.53 |
| 1:3G:49:VAL:HG11 | 1:3G:241:ARG:HG2 | 1.90 | 0.53 |
| 1:3I:391:ARG:HD3 | 2:3J:346:TRP:CE2 | 2.44 | 0.53 |
| 2:3L:56:THR:OG1 | 3:4B:34:SER:HA | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3N:223:THR:HG23 | 2:3N:225:THR:H | 1.73 | 0.53 |
| 7:4U:99:GLU:OE1 | 7:4U:99:GLU:N | 2.41 | 0.53 |
| 11:5E:242:ILE:HD11 | 11:5E:247:LEU:HD23 | 1.90 | 0.53 |
| 14:5L:13:PHE:CZ | 14:5L:318:ILE:HG13 | 2.42 | 0.53 |
| 14:5L:287:GLY:HA3 | 14:5L:330:LEU:HD12 | 1.89 | 0.53 |
| 14:5M:287:GLY:HA3 | 14:5M:330:LEU:HD12 | 1.89 | 0.53 |
| 19:6E:20:LEU:HD22 | 19:6E:24:TRP:CE3 | 2.43 | 0.53 |
| 20:6F:348:GLU:OE2 | 20:6F:348:GLU:HA | 2.07 | 0.53 |
| 24:6V:277:CYS:HA | 24:6V:368:LEU:HA | 1.90 | 0.53 |
| 24:7A:88:TRP:HA | 24:7A:126:GLU:HG3 | 1.91 | 0.53 |
| 25:7C:22:GLN:HA | 25:7C:22:GLN:OE1 | 2.07 | 0.53 |
| 38:8A:164:GLU:HA | 38:8A:164:GLU:OE1 | 2.08 | 0.53 |
| 1:C8:78:SER:OG | 24:6V:323:LYS:HG3 | 2.08 | 0.53 |
| 2:G1:344:VAL:HG13 | 2:G1:347:CYS:H | 1.74 | 0.53 |
| 2:G9:393:HIS:O | 2:G9:397:LEU:HG | 2.09 | 0.53 |
| 1:H2:178:THR:OG1 | 1:H2:181:GLU:HG3 | 2.08 | 0.53 |
| 1:I2:117:LEU:HA | 1:I2:120:VAL:HG12 | 1.91 | 0.53 |
| 2:I5:21:TRP:CD1 | 2:I5:87:PHE:HZ | 2.26 | 0.53 |
| 2:J5:381:SER:OG | 2:J5:382:THR:N | 2.40 | 0.53 |
| 2:K1:269:LEU:CD1 | 2:K1:303:VAL:HB | 2.39 | 0.53 |
| 2:K1:306:ASP:HB3 | 2:K1:309:HIS:HD2 | 1.74 | 0.53 |
| 2:K1:344:VAL:HG13 | 2:K1:346:TRP:H | 1.73 | 0.53 |
| 2:L1:66:ILE:O | 2:L1:66:ILE:HG13 | 2.08 | 0.53 |
| 1:L2:117:LEU:HA | 1:L2:120:VAL:HG12 | 1.90 | 0.53 |
| 1:L4:135:VAL:HG21 | 1:L4:152:ILE:HD11 | 1.89 | 0.53 |
| 2:L5:167:LEU:HD22 | 2:L5:200:VAL:HB | 1.90 | 0.53 |
| 2:N1:9:ILE:HD11 | 2:N1:153:LEU:HD23 | 1.91 | 0.53 |
| 2:N1:11:GLN:NE2 | 1:N2:247:ASN:OD1 | 2.41 | 0.53 |
| 2:N1:90:GLU:N | 1:O8:281:TYR:OH | 2.41 | 0.53 |
| 1:N6:91:VAL:HG11 | 1:N6:116:VAL:HG12 | 1.91 | 0.53 |
| 1:N6:207:LEU:HB3 | 1:N6:225:LEU:HD22 | 1.91 | 0.53 |
| 1:N8:14:ASN:HD22 | 1:N8:65:LEU:HD22 | 1.73 | 0.53 |
| 1:O0:211:CYS:SG | 1:O0:220:PRO:HB3 | 2.48 | 0.53 |
| 1:O0:361:LEU:CD2 | 27:7G:54:HIS:HB2 | 2.39 | 0.53 |
| 2:O3:311:LYS:NZ | 2:O3:342:GLN:OE1 | 2.41 | 0.53 |
| 1:O6:309:ARG:H | 1:O6:372:THR:HG22 | 1.71 | 0.53 |
| 2:O7:240:ALA:HB1 | 2:O7:356:ASN:HD22 | 1.72 | 0.53 |
| 2:O7:394:LYS:HB2 | 1:O8:346:PRO:HG3 | 1.91 | 0.53 |
| 2:P9:333:ALA:O | 2:P9:337:THR:HG23 | 2.09 | 0.53 |
| 2:Q1:212:ILE:O | 2:Q1:216:SER:OG | 2.24 | 0.53 |
| 2:R1:166:LYS:N | 2:R1:199:ASP:OD2 | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R2:290:THR:HG21 | 1:R2:329:GLN:HE21 | 1.73 | 0.53 |
| 1:R6:301:CYS:SG | 1:R6:302:ALA:N | 2.82 | 0.53 |
| 2:S1:88:HIS:HD2 | 2:S1:89:PRO:HD3 | 1.69 | 0.53 |
| 1:S4:67:ASP:N | 1:S4:67:ASP:OD1 | 2.40 | 0.53 |
| 1:S4:194:GLU:OE1 | 1:S4:194:GLU:N | 2.41 | 0.53 |
| 2:S7:8:HIS:CD2 | 2:S7:138:PHE:HD2 | 2.26 | 0.53 |
| 2:S9:346:TRP:CH2 | 2:S9:435:VAL:HG13 | 2.43 | 0.53 |
| 1:T0:213:ARG:HH21 | 1:T0:297:LYS:HE2 | 1.74 | 0.53 |
| 2:T1:405:VAL:HG11 | 2:T1:415:GLU:OE2 | 2.08 | 0.53 |
| 2:T1:423:GLU:OE2 | 17:5T:19:ARG:NH2 | 2.24 | 0.53 |
| 2:U3:405:VAL:HG13 | 2:U3:418:PHE:HE2 | 1.72 | 0.53 |
| 2:U5:277:SER:H | 2:U5:280:LYS:HZ3 | 1.57 | 0.53 |
| 1:U6:208:TYR:CE1 | 1:U6:225:LEU:HD11 | 2.44 | 0.53 |
| 2:U7:51:THR:HG21 | 2:U7:243:ARG:HG2 | 1.90 | 0.53 |
| 1:U8:328:GLU:O | 1:U8:332:ASN:ND2 | 2.42 | 0.53 |
| 2:V3:88:HIS:CD2 | 2:V3:90:GLU:H | 2.27 | 0.53 |
| 2:V7:183:GLU:HG3 | 2:V7:184:PRO:HD3 | 1.90 | 0.53 |
| 2:V9:33:ASP:OD2 | 2:V9:35:GLN:NE2 | 2.41 | 0.53 |
| 2:V9:133:GLN:HB3 | 2:V9:252:ILE:HG21 | 1.90 | 0.53 |
| 1:W0:100:ASN:HB3 | 1:W0:103:LYS:HB2 | 1.89 | 0.53 |
| 1:W0:375:GLN:HB2 | 1:W0:419:VAL:HG13 | 1.91 | 0.53 |
| 2:W3:81:GLY:O | 2:W3:84:ARG:NH1 | 2.42 | 0.53 |
| 2:W9:203:MET:O | 2:W9:204:LEU:HD23 | 2.08 | 0.53 |
| 1:X6:2:ARG:NE | 1:X6:240:LEU:HD22 | 2.23 | 0.53 |
| 1:Y0:33:THR:O | 1:Y0:58:ARG:NH2 | 2.41 | 0.53 |
| 1:Y0:52:ASN:OD1 | 1:Y0:62:ARG:NH2 | 2.41 | 0.53 |
| 1:Y0:101:TRP:HE3 | 1:Y0:403:MET:HE1 | 1.72 | 0.53 |
| 2:Y1:244:PHE:HB2 | 2:Y1:356:ASN:HD21 | 1.73 | 0.53 |
| 2:Y1:399:TYR:O | 2:Y1:402:ARG:NH1 | 2.41 | 0.53 |
| 1:Y2:49:VAL:HG11 | 1:Y2:241:ARG:HG2 | 1.90 | 0.53 |
| 1:Y2:52:ASN:OD1 | 1:Y2:62:ARG:NH2 | 2.40 | 0.53 |
| 1:Y8:207:LEU:HB3 | 1:Y8:225:LEU:HD22 | 1.89 | 0.53 |
| 2:Y9:276:ILE:HG23 | 2:Y9:280:LYS:HB3 | 1.91 | 0.53 |
| 2:Z1:223:THR:HG23 | 2:Z1:225:THR:H | 1.72 | 0.53 |
| 2:0F:297:GLU:HG2 | 2:0F:298:PRO:HD2 | 1.90 | 0.53 |
| 2:0H:274:PRO:HG3 | 2:0H:286:LEU:HD11 | 1.91 | 0.53 |
| 2:0J:387:ILE:HD12 | 2:0J:390:ARG:HH22 | 1.73 | 0.53 |
| 2:0L:65:CYS:SG | 2:0L:66:ILE:N | 2.82 | 0.53 |
| 1:0Q:139:LEU:HG | 1:0Q:168:SER:HB2 | 1.89 | 0.53 |
| 1:1C:134:GLN:HE21 | 1:1C:167:PHE:HE2 | 1.56 | 0.53 |
| 2:1D:88:HIS:HD2 | 2:1D:121:ARG:NH2 | 2.06 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1F:223:THR:HG23 | 2:1F:225:THR:H | 1.73 | 0.53 |
| 2:1H:98:ASP:CG | 2:1H:100:ALA:H | 2.12 | 0.53 |
| 2:1R:178:SER:HB3 | 2:1R:183:GLU:OE2 | 2.09 | 0.53 |
| 2:1V:93:ILE:HG22 | 2:1V:93:ILE:O | 2.08 | 0.53 |
| 1:2C:345:ILE:HB | 1:2C:348:ASN:HD21 | 1.73 | 0.53 |
| 2:2P:392:ASP:OD1 | 2:2P:422:ARG:NH1 | 2.42 | 0.53 |
| 1:2Q:7:ILE:HB | 1:2Q:135:VAL:HG12 | 1.91 | 0.53 |
| 1:2S:114:ASP:OD2 | 1:2S:115:SER:N | 2.41 | 0.53 |
| 2:2V:336:LYS:O | 2:2V:339:ARG:NH2 | 2.42 | 0.53 |
| 2:2Z:392:ASP:OD2 | 2:2Z:422:ARG:NH1 | 2.41 | 0.53 |
| 1:3G:276:ARG:HH22 | 17:5S:216:GLU:HG2 | 1.73 | 0.53 |
| 2:3P:100:ALA:HB1 | 1:3Q:252:LYS:HB3 | 1.91 | 0.53 |
| 2:3P:132:LEU:HD23 | 2:3P:164:LYS:HE3 | 1.91 | 0.53 |
| 6:4O:118:SER:O | 6:4O:122:VAL:HG23 | 2.08 | 0.53 |
| 7:4Q:324:GLN:HA | 24:6T:22:LEU:HD23 | 1.90 | 0.53 |
| 7:4R:11:GLU:N | 7:4R:11:GLU:OE1 | 2.41 | 0.53 |
| 10:5B:234:LEU:O | 10:5B:238:GLU:HG2 | 2.09 | 0.53 |
| 12:5G:370:ARG:HA | 12:5G:376:ARG:O | 2.08 | 0.53 |
| 14:5M:13:PHE:CZ | 14:5M:318:ILE:HG13 | 2.42 | 0.53 |
| 15:5O:4:ASN:N | 15:5O:4:ASN:OD1 | 2.41 | 0.53 |
| 20:6F:125:LYS:HE3 | 20:6F:344:LEU:HD21 | 1.90 | 0.53 |
| 22:6J:17:ILE:HG22 | 22:6J:19:GLY:H | 1.74 | 0.53 |
| 24:7A:113:ASN:OD1 | 24:7A:114:HIS:ND1 | 2.35 | 0.53 |
| 2:C9:36:MET:HB2 | 22:6K:76:LYS:HE3 | 1.89 | 0.53 |
| 1:E0:204:ASN:HD21 | 39:E0:501:GDP:HN22 | 1.54 | 0.53 |
| 2:F5:221:ARG:HB2 | 22:6I:178:GLY:HA2 | 1.90 | 0.53 |
| 1:G6:3:GLU:OE1 | 1:G6:62:ARG:NH1 | 2.37 | 0.53 |
| 2:H5:267:PHE:HB2 | 2:H5:384:ILE:HD12 | 1.90 | 0.53 |
| 2:H9:98:ASP:OD1 | 2:H9:99:ALA:N | 2.42 | 0.53 |
| 2:I1:189:LEU:HD11 | 2:I1:418:PHE:HE1 | 1.74 | 0.53 |
| 2:J7:216:SER:O | 2:J7:280:LYS:HE2 | 2.09 | 0.53 |
| 2:J7:274:PRO:HB2 | 2:J7:276:ILE:HG12 | 1.91 | 0.53 |
| 1:J8:139:LEU:HD12 | 1:J8:170:VAL:HG12 | 1.91 | 0.53 |
| 2:K3:111:GLY:HA2 | 2:K3:114:ILE:HG22 | 1.91 | 0.53 |
| 1:L2:285:THR:OG1 | 1:L2:287:PRO:HD2 | 2.07 | 0.53 |
| 1:L6:205:GLU:H | 1:L6:205:GLU:CD | 2.12 | 0.53 |
| 2:L9:90:GLU:HG3 | 2:L9:121:ARG:HH12 | 1.74 | 0.53 |
| 2:L9:311:LYS:NZ | 2:L9:343:PHE:O | 2.36 | 0.53 |
| 1:M6:334:GLN:HE22 | 1:M6:348:ASN:H | 1.56 | 0.53 |
| 1:N0:393:ALA:O | 1:N0:395:LEU:N | 2.42 | 0.53 |
| 2:N3:331:SER:O | 2:N3:334:THR:OG1 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N6:204:ASN:HD21 | 39:N6:503:GDP:HN22 | 1.57 | 0.53 |
| 1:O2:113:ILE:HA | 1:O2:116:VAL:HG22 | 1.91 | 0.53 |
| 2:O3:177:VAL:HG11 | 2:O3:207:GLU:HB2 | 1.90 | 0.53 |
| 2:O3:322:ASP:HB3 | 37:7Y:188:LEU:HD11 | 1.90 | 0.53 |
| 1:O4:107:THR:OG1 | 1:O4:108:GLU:OE2 | 2.21 | 0.53 |
| 1:O4:320:ARG:NH2 | 37:7Y:67:ILE:O | 2.42 | 0.53 |
| 2:P3:116:ASP:OD1 | 2:P3:117:LEU:N | 2.42 | 0.53 |
| 1:P4:190:HIS:NE2 | 1:P4:414:ASN:OD1 | 2.42 | 0.53 |
| 2:P5:317:LEU:HB3 | 2:P5:319:TYR:HE1 | 1.73 | 0.53 |
| 1:Q2:304:ASP:OD2 | 1:Q2:306:ARG:NH2 | 2.42 | 0.53 |
| 2:R5:265:ILE:HD11 | 2:R5:435:VAL:HG21 | 1.91 | 0.53 |
| 2:R7:405:VAL:HG13 | 17:5U:112:VAL:HG11 | 1.91 | 0.53 |
| 2:R9:58:ALA:HB3 | 7:4U:146:ILE:HG21 | 1.91 | 0.53 |
| 1:S2:207:LEU:HD13 | 1:S2:225:LEU:HB3 | 1.91 | 0.53 |
| 1:S8:222:PHE:CD2 | 2:S9:247:ALA:HB1 | 2.44 | 0.53 |
| 2:T1:170:THR:HG21 | 2:T1:194:LEU:HD11 | 1.90 | 0.53 |
| 2:T3:51:THR:HG21 | 2:T3:243:ARG:HG2 | 1.90 | 0.53 |
| 2:T3:269:LEU:HD21 | 2:T3:384:ILE:HG13 | 1.91 | 0.53 |
| 2:U3:216:SER:O | 2:U3:280:LYS:NZ | 2.41 | 0.53 |
| 2:U9:27:GLU:OE1 | 2:U9:243:ARG:NH1 | 2.42 | 0.53 |
| 1:V6:4:ILE:HD12 | 1:V6:132:GLY:C | 2.29 | 0.53 |
| 2:V9:90:GLU:CD | 2:V9:90:GLU:H | 2.11 | 0.53 |
| 2:W3:88:HIS:HD2 | 2:X9:283:HIS:HB3 | 1.73 | 0.53 |
| 2:W9:88:HIS:HB3 | 2:W9:91:GLN:H | 1.72 | 0.53 |
| 1:X0:285:THR:HG23 | 1:X0:287:PRO:HD2 | 1.89 | 0.53 |
| 2:X9:129:CYS:SG | 2:X9:130:THR:N | 2.81 | 0.53 |
| 1:Y4:100:ASN:HB3 | 1:Y4:103:LYS:HB2 | 1.91 | 0.53 |
| 2:Z1:176:GLN:HE22 | 2:Z1:304:LYS:HE2 | 1.73 | 0.53 |
| 2:Z1:313:MET:HE2 | 2:Z1:380:ASN:HD22 | 1.74 | 0.53 |
| 2:Z7:188:VAL:HG23 | 2:Z7:189:LEU:HD12 | 1.91 | 0.53 |
| 1:Z8:5:VAL:HG22 | 1:Z8:62:ARG:HD3 | 1.89 | 0.53 |
| 2:0F:313:MET:HG3 | 2:0F:346:TRP:HH2 | 1.73 | 0.53 |
| 2:0H:9:ILE:HG22 | 2:0H:146:GLY:HA2 | 1.89 | 0.53 |
| 1:0I:67:ASP:N | 1:0I:67:ASP:OD1 | 2.41 | 0.53 |
| 1:0I:163:MET:HB3 | 1:0I:250:LEU:HD22 | 1.90 | 0.53 |
| 2:0J:175:PRO:HB3 | 2:0J:390:ARG:HE | 1.74 | 0.53 |
| 1:0O:7:ILE:HB | 1:0O:135:VAL:HG12 | 1.90 | 0.53 |
| 1:0O:69:GLU:C | 1:0O:92:PHE:HZ | 2.12 | 0.53 |
| 1:0Q:83:GLN:O | 1:1G:281:TYR:OH | 2.18 | 0.53 |
| 1:0Q:309:ARG:NH1 | 1:0Q:339:SER:O | 2.42 | 0.53 |
| 2:0R:25:CYS:SG | 2:0R:86:LEU:HD21 | 2.49 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0R:417:GLU:HA | 2:0R:420:GLU:HG2 | 1.91 | 0.53 |
| 2:0X:176:GLN:HE22 | 2:0X:304:LYS:HE2 | 1.73 | 0.53 |
| 2:0X:368:LEU:H | 2:0X:368:LEU:HD23 | 1.74 | 0.53 |
| 1:1C:350:LYS:NZ | 1:1C:351:SER:O | 2.42 | 0.53 |
| 2:1D:57:GLY:N | 2:1T:285:GLN:OE1 | 2.39 | 0.53 |
| 2:1F:4:VAL:HG23 | 2:1F:134:GLY:O | 2.08 | 0.53 |
| 1:1G:8:GLN:CD | 1:1G:17:GLY:HA3 | 2.29 | 0.53 |
| 2:1N:267:PHE:HB2 | 2:1N:384:ILE:HD12 | 1.91 | 0.53 |
| 2:1V:259:LEU:HD21 | 2:1V:316:CYS:HB2 | 1.90 | 0.53 |
| 2:1Z:88:HIS:CD2 | 2:1Z:89:PRO:CD | 2.71 | 0.53 |
| 1:2C:208:TYR:HE1 | 1:2C:225:LEU:HD11 | 1.74 | 0.53 |
| 2:2D:287:SER:OG | 2:2D:288:VAL:N | 2.41 | 0.53 |
| 2:2F:381:SER:OG | 2:2F:382:THR:N | 2.41 | 0.53 |
| 1:2G:173:PRO:HD2 | 1:2G:380:ARG:NE | 2.24 | 0.53 |
| 1:2I:27:GLU:OE1 | 1:2I:241:ARG:NH1 | 2.39 | 0.53 |
| 1:2I:114:ASP:HB3 | 38:8C:101:ASP:CG | 2.29 | 0.53 |
| 1:2I:114:ASP:OD1 | 38:8C:93:LYS:NZ | 2.20 | 0.53 |
| 1:2M:45:GLU:OE1 | 1:2M:46:ARG:HG2 | 2.08 | 0.53 |
| 1:2Y:317:PHE:HB3 | 1:2Y:321:MET:CE | 2.38 | 0.53 |
| 1:3C:77:ARG:HG3 | 1:3C:77:ARG:HH11 | 1.73 | 0.53 |
| 1:3C:128:ASP:OD1 | 1:3C:129:CYS:N | 2.37 | 0.53 |
| 2:3D:49:PHE:HB2 | 2:3D:53:PHE:HD2 | 1.74 | 0.53 |
| 2:3F:288:VAL:O | 2:3F:292:THR:HG23 | 2.09 | 0.53 |
| 2:3J:223:THR:HG22 | 2:3J:224:TYR:H | 1.73 | 0.53 |
| 2:3L:132:LEU:HD23 | 2:3L:164:LYS:HE3 | 1.89 | 0.53 |
| 2:3N:287:SER:N | 2:3N:290:GLU:OE2 | 2.21 | 0.53 |
| 1:3S:248:ALA:HA | 1:3S:252:LYS:HD2 | 1.91 | 0.53 |
| 10:5C:488:GLY:HA2 | 10:5C:491:ARG:HH11 | 1.73 | 0.53 |
| 13:5H:11:GLU:OE1 | 13:5H:11:GLU:N | 2.33 | 0.53 |
| 13:5I:11:GLU:OE1 | 13:5I:11:GLU:N | 2.33 | 0.53 |
| 13:5K:11:GLU:OE1 | 13:5K:11:GLU:N | 2.33 | 0.53 |
| 14:5L:563:ARG:HG2 | 14:5L:607:LYS:HZ1 | 1.74 | 0.53 |
| 14:5M:563:ARG:HG2 | 14:5M:607:LYS:HZ1 | 1.74 | 0.53 |
| 14:5N:13:PHE:CZ | 14:5N:318:ILE:HG13 | 2.42 | 0.53 |
| 14:5N:287:GLY:HA3 | 14:5N:330:LEU:HD12 | 1.89 | 0.53 |
| 17:5S:3:GLU:OE1 | 17:5S:3:GLU:N | 2.42 | 0.53 |
| 20:6F:112:PRO:O | 20:6F:150:HIS:HB3 | 2.09 | 0.53 |
| 22:6K:108:ARG:NH2 | 24:6V:282:ARG:O | 2.41 | 0.53 |
| 24:6V:97:ARG:H | 24:6V:188:THR:CG2 | 2.20 | 0.53 |
| 24:6V:452:MET:HA | 24:6V:530:PHE:HA | 1.90 | 0.53 |
| 24:6Y:95:VAL:HG22 | 24:6Y:124:TYR:HA | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:7K:339:ASP:N | 30:7K:339:ASP:OD1 | 2.39 | 0.53 |
| 30:7K:382:LEU:HD11 | 30:7K:434:ARG:O | 2.09 | 0.53 |
| 31:7M:45:GLU:O | 31:7M:48:MET:HG3 | 2.08 | 0.53 |
| 32:7P:30:ILE:HG13 | 32:7P:31:GLY:H | 1.73 | 0.53 |
| 37:7Y:40:VAL:HA | 37:7Y:43:TYR:CE2 | 2.44 | 0.53 |
| 1:B5:360:GLY:HA3 | 24:6X:110:ASN:HA | 1.90 | 0.53 |
| 2:C7:322:ASP:OD2 | 24:6U:261:ARG:NH1 | 2.41 | 0.53 |
| 2:G3:305:CYS:HB3 | 2:G3:387:ILE:HD11 | 1.91 | 0.53 |
| 1:G4:86:ARG:NH1 | 1:G4:89:ASN:OD1 | 2.42 | 0.53 |
| 2:G5:109:THR:OG1 | 2:G5:411:GLU:OE2 | 2.26 | 0.53 |
| 1:J0:113:ILE:HA | 1:J0:116:VAL:HG12 | 1.91 | 0.53 |
| 2:K1:21:TRP:CZ2 | 2:K1:65:CYS:HB2 | 2.43 | 0.53 |
| 2:K3:203:MET:O | 2:K3:204:LEU:HD23 | 2.08 | 0.53 |
| 2:K3:384:ILE:HA | 2:K3:387:ILE:HD12 | 1.91 | 0.53 |
| 2:K7:109:THR:OG1 | 2:K7:411:GLU:OE2 | 2.22 | 0.53 |
| 1:K8:65:LEU:HD12 | 1:K8:90:PHE:CE1 | 2.44 | 0.53 |
| 2:K9:85:GLN:OE1 | 2:K9:85:GLN:HA | 2.08 | 0.53 |
| 1:L6:391:ARG:HH12 | 2:L7:435:VAL:HA | 1.74 | 0.53 |
| 1:M4:309:ARG:H | 1:M4:372:THR:HG22 | 1.74 | 0.53 |
| 2:M7:176:GLN:HE22 | 2:M7:304:LYS:HE2 | 1.74 | 0.53 |
| 2:M9:305:CYS:HB3 | 2:M9:387:ILE:HD11 | 1.90 | 0.53 |
| 1:N6:77:ARG:NH2 | 27:7G:166:CYS:HB3 | 2.23 | 0.53 |
| 1:O2:285:THR:HG23 | 1:O2:288:GLU:H | 1.73 | 0.53 |
| 2:P3:18:ASN:HD21 | 2:P3:78:VAL:HG22 | 1.73 | 0.53 |
| 1:Q0:180:VAL:HG23 | 1:Q0:184:ASN:HD21 | 1.74 | 0.53 |
| 1:R6:207:LEU:HB3 | 1:R6:225:LEU:HD22 | 1.91 | 0.53 |
| 2:R7:71:GLU:HB3 | 2:R7:98:ASP:OD2 | 2.08 | 0.53 |
| 1:S6:178:THR:OG1 | 1:S6:181:GLU:HG3 | 2.09 | 0.53 |
| 2:S7:79:ARG:O | 2:S7:84:ARG:HG2 | 2.08 | 0.53 |
| 2:T1:265:ILE:HD11 | 2:T1:435:VAL:HG21 | 1.91 | 0.53 |
| 1:T4:371:SER:OG | 1:T4:372:THR:N | 2.41 | 0.53 |
| 2:U7:2:ARG:HA | 2:U7:133:GLN:HE21 | 1.73 | 0.53 |
| 2:U7:88:HIS:CE1 | 2:U7:89:PRO:HD2 | 2.42 | 0.53 |
| 1:U8:190:HIS:CD2 | 1:U8:411:ALA:HA | 2.44 | 0.53 |
| 2:V1:47:ASP:N | 2:V1:47:ASP:OD1 | 2.42 | 0.53 |
| 2:V1:417:GLU:HA | 2:V1:420:GLU:HG3 | 1.90 | 0.53 |
| 2:V3:212:ILE:HG23 | 2:V3:275:ILE:HD12 | 1.91 | 0.53 |
| 1:V6:3:GLU:HG2 | 1:V6:127:CYS:SG | 2.49 | 0.53 |
| 1:V6:60:VAL:HG21 | 1:V6:86:ARG:NH2 | 2.24 | 0.53 |
| 2:V7:91:GLN:HG3 | 2:X3:283:HIS:HE1 | 1.74 | 0.53 |
| 2:W5:107:HIS:CD2 | 2:W5:152:LEU:HB2 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X8:411:ALA:O | 1:X8:415:MET:HG2 | 2.09 | 0.53 |
| 2:X9:313:MET:SD | 2:X9:380:ASN:ND2 | 2.82 | 0.53 |
| 2:Y5:76:ASP:HA | 2:Y5:79:ARG:HB2 | 1.90 | 0.53 |
| 1:Z2:262:ARG:HH21 | 1:Z2:418:LEU:HD13 | 1.74 | 0.53 |
| 1:Z4:344:TRP:CE3 | 1:Z4:345:ILE:HG13 | 2.43 | 0.53 |
| 1:Z6:190:HIS:CD2 | 1:Z6:411:ALA:HA | 2.43 | 0.53 |
| 1:Z8:131:GLN:HE21 | 1:Z8:250:LEU:HB2 | 1.72 | 0.53 |
| 2:Z9:336:LYS:O | 2:Z9:339:ARG:NH2 | 2.41 | 0.53 |
| 1:0A:19:LYS:NZ | 1:0A:227:HIS:HD2 | 2.07 | 0.53 |
| 1:0A:250:LEU:HD12 | 1:0A:250:LEU:H | 1.73 | 0.53 |
| 2:0H:20:CYS:SG | 2:0H:21:TRP:N | 2.82 | 0.53 |
| 2:0L:306:ASP:HB3 | 2:0L:309:HIS:HD2 | 1.72 | 0.53 |
| 2:0N:11:GLN:HE22 | 1:0O:246:LEU:HA | 1.74 | 0.53 |
| 2:0P:115:VAL:HG21 | 2:0P:152:LEU:HD22 | 1.90 | 0.53 |
| 2:0R:266:HIS:ND1 | 2:0R:266:HIS:O | 2.42 | 0.53 |
| 1:0U:392:LYS:HE3 | 1:0U:395:LEU:CD2 | 2.39 | 0.53 |
| 1:0W:77:ARG:HE | 1:0W:90:PHE:HE2 | 1.56 | 0.53 |
| 1:0W:289:LEU:O | 1:0W:293:MET:HG3 | 2.08 | 0.53 |
| 2:0Z:379:SER:OG | 2:0Z:380:ASN:N | 2.42 | 0.53 |
| 1:1E:1:MET:HE1 | 1:1E:2:ARG:CG | 2.38 | 0.53 |
| 1:1E:128:ASP:OD1 | 1:1E:129:CYS:N | 2.37 | 0.53 |
| 2:1H:353:CYS:SG | 2:1H:354:GLY:N | 2.82 | 0.53 |
| 2:1X:181:VAL:HG23 | 2:1X:182:VAL:HG13 | 1.90 | 0.53 |
| 2:1X:317:LEU:HD11 | 2:1X:351:PHE:HD1 | 1.72 | 0.53 |
| 2:1Z:236:SER:O | 2:1Z:243:ARG:NH2 | 2.42 | 0.53 |
| 1:2G:70:PRO:N | 1:2G:92:PHE:HZ | 2.06 | 0.53 |
| 2:2L:183:GLU:HG3 | 2:2L:184:PRO:HD3 | 1.91 | 0.53 |
| 2:2L:399:TYR:O | 2:2L:402:ARG:NH1 | 2.41 | 0.53 |
| 2:2X:245:ASP:HB3 | 38:8C:216:ARG:HG2 | 1.90 | 0.53 |
| 2:2X:358:GLN:NE2 | 38:8C:212:PRO:HB2 | 2.23 | 0.53 |
| 2:3D:427:ALA:HA | 2:3D:430:LYS:HE2 | 1.89 | 0.53 |
| 2:3F:47:ASP:N | 2:3F:47:ASP:OD1 | 2.41 | 0.53 |
| 2:3F:164:LYS:O | 2:3F:166:LYS:NZ | 2.42 | 0.53 |
| 2:3H:236:SER:O | 2:3H:243:ARG:NH2 | 2.42 | 0.53 |
| 1:3I:134:GLN:HE21 | 1:3I:167:PHE:HE2 | 1.57 | 0.53 |
| 2:3N:210:TYR:HH | 1:3O:323:THR:HG1 | 1.54 | 0.53 |
| 1:3O:172:SER:HB2 | 1:3O:380:ARG:HH22 | 1.72 | 0.53 |
| 1:3S:94:GLN:NE2 | 3:4J:139:SER:O | 2.40 | 0.53 |
| 4:4C:23:GLU:OE1 | 23:6R:7:VAL:HG21 | 2.09 | 0.53 |
| 5:4L:323:LEU:O | 5:4L:327:LYS:HG2 | 2.08 | 0.53 |
| 7:4R:101:ASP:OD1 | 7:4R:101:ASP:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:5B:186:LEU:O | 10:5B:189:GLU:HG3 | 2.09 | 0.53 |
| 10:5B:261:LYS:HB2 | 10:5B:265:LYS:NZ | 2.24 | 0.53 |
| 12:5G:324:GLY:HA3 | 12:5G:332:ASN:HB3 | 1.91 | 0.53 |
| 14:5L:97:HIS:HB3 | 14:5L:99:MET:SD | 2.48 | 0.53 |
| 14:5M:97:HIS:HB3 | 14:5M:99:MET:SD | 2.48 | 0.53 |
| 17:5T:3:GLU:N | 17:5T:3:GLU:OE1 | 2.42 | 0.53 |
| 17:5U:3:GLU:N | 17:5U:3:GLU:OE1 | 2.42 | 0.53 |
| 20:6F:200:VAL:HG13 | 20:6F:230:CYS:HB3 | 1.90 | 0.53 |
| 24:6T:574:ARG:O | 24:6T:578:ILE:HG12 | 2.09 | 0.53 |
| 24:6V:505:LYS:HB3 | 24:6V:506:PRO:HD2 | 1.91 | 0.53 |
| 24:6W:123:TYR:HE2 | 24:6W:163:PRO:HG3 | 1.74 | 0.53 |
| 32:7P:106:GLU:N | 32:7P:106:GLU:OE1 | 2.41 | 0.53 |
| 35:7T:168:ILE:O | 35:7T:171:GLU:HG3 | 2.09 | 0.53 |
| 38:8A:36:GLU:OE2 | 38:8A:37:TYR:N | 2.42 | 0.53 |
| 1:A1:337:ASN:HD22 | 3:4F:69:TYR:HD2 | 1.56 | 0.53 |
| 2:G7:155:GLU:O | 2:G7:158:SER:OG | 2.22 | 0.53 |
| 1:G8:335:ASN:O | 1:G8:338:SER:OG | 2.26 | 0.53 |
| 2:H7:387:ILE:HG12 | 2:H7:390:ARG:HH22 | 1.73 | 0.53 |
| 1:I0:248:ALA:HA | 1:I0:252:LYS:HD2 | 1.90 | 0.53 |
| 2:I3:267:PHE:HB2 | 2:I3:384:ILE:HD12 | 1.90 | 0.53 |
| 2:I5:111:GLY:O | 2:I5:115:VAL:HG12 | 2.08 | 0.53 |
| 1:J4:135:VAL:HG12 | 1:J4:137:HIS:HD2 | 1.73 | 0.53 |
| 2:J7:264:ARG:NH2 | 2:J7:431:ASP:OD2 | 2.42 | 0.53 |
| 1:J8:232:VAL:HG11 | 1:J8:268:VAL:HG21 | 1.91 | 0.53 |
| 2:K3:213:CYS:HA | 2:K3:217:LEU:HB2 | 1.90 | 0.53 |
| 1:K4:219:THR:HB | 2:K5:324:VAL:HG11 | 1.91 | 0.53 |
| 2:L7:153:LEU:O | 2:L7:157:LEU:HG | 2.09 | 0.53 |
| 2:M3:392:ASP:OD2 | 2:M3:425:LEU:HB3 | 2.09 | 0.53 |
| 1:M6:88:ASP:OD1 | 37:7Y:86:ASN:ND2 | 2.39 | 0.53 |
| 1:M8:335:ASN:O | 1:M8:338:SER:OG | 2.26 | 0.53 |
| 2:N1:11:GLN:OE1 | 2:N1:15:GLN:NE2 | 2.41 | 0.53 |
| 1:N6:77:ARG:HD2 | 27:7G:165:PHE:CZ | 2.44 | 0.53 |
| 1:N8:125:GLU:OE2 | 1:N8:159:TYR:OH | 2.26 | 0.53 |
| 2:O1:222:PRO:HD2 | 1:O2:324:LYS:HE3 | 1.91 | 0.53 |
| 1:O4:412:GLU:OE2 | 1:O4:416:ASN:ND2 | 2.40 | 0.53 |
| 2:P5:41:THR:HB | 27:7G:220:MET:O | 2.09 | 0.53 |
| 1:P8:177:ASP:O | 2:P9:352:LYS:HA | 2.09 | 0.53 |
| 2:Q1:270:SER:HB2 | 2:Q1:302:MET:HB2 | 1.89 | 0.53 |
| 1:Q2:379:LYS:HG3 | 1:Q2:419:VAL:HG21 | 1.91 | 0.53 |
| 2:Q9:155:GLU:HG2 | 2:Q9:197:HIS:CE1 | 2.43 | 0.53 |
| 2:R3:9:ILE:HG22 | 2:R3:146:GLY:HA2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:350:LYS:NZ | 1:R6:351:SER:O | 2.41 | 0.53 |
| 2:R7:372:GLN:HE22 | 7:4R:203:THR:HG21 | 1.74 | 0.53 |
| 1:S4:182:PRO:O | 1:S4:186:THR:HG22 | 2.09 | 0.53 |
| 1:S8:220:PRO:HD2 | 2:S9:326:LYS:HG2 | 1.89 | 0.53 |
| 2:S9:5:ILE:HG22 | 2:S9:64:ARG:HB3 | 1.91 | 0.53 |
| 1:T8:213:ARG:HH21 | 1:T8:297:LYS:HE3 | 1.73 | 0.53 |
| 1:T8:336:LYS:HE3 | 13:5K:101:LYS:HB3 | 1.91 | 0.53 |
| 1:U4:273:LEU:H | 1:U4:292:GLN:HE22 | 1.56 | 0.53 |
| 2:U5:276:ILE:HD11 | 2:U5:371:VAL:HG22 | 1.91 | 0.53 |
| 1:V6:112:LEU:O | 1:V6:115:SER:OG | 2.25 | 0.53 |
| 1:V6:199:CYS:SG | 1:V6:265:PHE:HD1 | 2.32 | 0.53 |
| 1:V8:325:GLU:O | 1:V8:329:GLN:HB2 | 2.08 | 0.53 |
| 2:W3:181:VAL:HG23 | 2:W3:182:VAL:HG13 | 1.91 | 0.53 |
| 1:W4:135:VAL:HG11 | 1:W4:152:ILE:HD11 | 1.90 | 0.53 |
| 2:X3:239:THR:HG23 | 2:X3:243:ARG:HE | 1.72 | 0.53 |
| 2:X5:133:GLN:HB3 | 2:X5:252:ILE:HG21 | 1.91 | 0.53 |
| 1:X6:385:PHE:HZ | 1:X6:408:PHE:HD1 | 1.57 | 0.53 |
| 2:X7:358:GLN:NE2 | 2:X7:359:PRO:O | 2.41 | 0.53 |
| 1:Y0:153:SER:HA | 1:Y0:195:ASN:ND2 | 2.24 | 0.53 |
| 1:Y8:192:LEU:HD12 | 1:Y8:196:ALA:HB3 | 1.91 | 0.53 |
| 1:Z4:207:LEU:HB3 | 1:Z4:225:LEU:HD22 | 1.90 | 0.53 |
| 1:Z6:86:ARG:HG2 | 1:Z6:88:ASP:H | 1.73 | 0.53 |
| 1:0E:12:CYS:SG | 1:0E:138:SER:HB3 | 2.49 | 0.53 |
| 1:0I:51:PHE:HB3 | 1:0I:59:TYR:HB3 | 1.91 | 0.53 |
| 2:0J:56:THR:HA | 2:0Z:285:GLN:HB2 | 1.89 | 0.53 |
| 2:0N:274:PRO:HG3 | 2:0N:286:LEU:HD11 | 1.90 | 0.53 |
| 2:0N:384:ILE:H | 2:0N:384:ILE:HD12 | 1.73 | 0.53 |
| 2:0P:213:CYS:HA | 2:0P:217:LEU:HB2 | 1.90 | 0.53 |
| 2:0X:213:CYS:HA | 2:0X:217:LEU:HB2 | 1.90 | 0.53 |
| 2:0X:267:PHE:HB2 | 2:0X:384:ILE:HD12 | 1.91 | 0.53 |
| 2:0Z:56:THR:CB | 2:1P:285:GLN:HB2 | 2.38 | 0.53 |
| 2:1F:157:LEU:HD22 | 2:1F:166:LYS:HD3 | 1.91 | 0.53 |
| 2:1H:12:ALA:HB2 | 41:1H:501:GTP:C8 | 2.43 | 0.53 |
| 2:1H:120:ASP:O | 2:1H:124:LYS:HG2 | 2.09 | 0.53 |
| 1:1M:253:LEU:O | 1:1M:257:LEU:HG | 2.09 | 0.53 |
| 2:1R:317:LEU:HB3 | 2:1R:319:TYR:HE1 | 1.73 | 0.53 |
| 2:1R:428:LEU:HG | 2:1R:432:PHE:CE2 | 2.44 | 0.53 |
| 1:1S:5:VAL:HG22 | 1:1S:133:PHE:HD1 | 1.73 | 0.53 |
| 1:2A:360:GLY:HA2 | 10:5A:296:ILE:HD12 | 1.91 | 0.53 |
| 2:2B:133:GLN:HB3 | 2:2B:252:ILE:HG21 | 1.90 | 0.53 |
| 2:2B:381:SER:OG | 2:2B:382:THR:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2G:186:THR:HG22 | 1:2G:411:ALA:HB1 | 1.91 | 0.53 |
| 2:2H:123:ARG:NH2 | 38:8B:37:TYR:HA | 2.07 | 0.53 |
| 2:2H:286:LEU:N | 2:2H:286:LEU:HD22 | 2.23 | 0.53 |
| 2:2P:333:ALA:O | 2:2P:337:THR:HG23 | 2.09 | 0.53 |
| 1:2Q:121:ARG:O | 1:2Q:125:GLU:HG2 | 2.08 | 0.53 |
| 2:3F:306:ASP:HB3 | 2:3F:309:HIS:HD2 | 1.72 | 0.53 |
| 2:3H:312:TYR:HB2 | 2:3H:343:PHE:CD1 | 2.44 | 0.53 |
| 2:3T:387:ILE:HG12 | 2:3T:390:ARG:HH22 | 1.74 | 0.53 |
| 3:4J:184:LEU:CD1 | 3:4J:223:LYS:HG3 | 2.38 | 0.53 |
| 6:4O:293:ARG:O | 6:4O:297:GLU:HG2 | 2.09 | 0.53 |
| 6:4O:355:GLU:O | 6:4O:358:LYS:HG3 | 2.08 | 0.53 |
| 14:5M:415:LYS:CE | 23:6R:22:MET:CG | 2.87 | 0.53 |
| 14:5N:97:HIS:HB3 | 14:5N:99:MET:SD | 2.48 | 0.53 |
| 22:6I:46:SER:OG | 22:6I:48:GLU:OE2 | 2.24 | 0.53 |
| 22:6L:108:ARG:NH2 | 24:6W:282:ARG:O | 2.42 | 0.53 |
| 24:6Y:555:THR:O | 24:6Y:559:ILE:HG12 | 2.09 | 0.53 |
| 1:1:306:ARG:CZ | 3:3V:59:LEU:HB3 | 2.39 | 0.53 |
| 2:8:357:TYR:HB3 | 24:6W:150:ARG:HH12 | 1.73 | 0.53 |
| 2:D7:280:LYS:HE3 | 18:6D:166:HIS:HB3 | 1.90 | 0.53 |
| 1:G0:218:THR:OG1 | 24:6V:418:ASP:OD1 | 2.19 | 0.53 |
| 1:G2:175:VAL:HG22 | 1:G2:205:GLU:HB2 | 1.90 | 0.53 |
| 1:G2:211:CYS:HA | 1:G2:215:LEU:HB2 | 1.91 | 0.53 |
| 1:H2:8:GLN:O | 1:H2:66:MET:HG3 | 2.08 | 0.53 |
| 1:H2:91:VAL:HG11 | 1:H2:116:VAL:HG12 | 1.91 | 0.53 |
| 1:H2:167:PHE:CE2 | 1:H2:233:MET:HG2 | 2.44 | 0.53 |
| 1:H4:364:SER:OG | 1:H4:365:ALA:N | 2.40 | 0.53 |
| 2:H5:289:ALA:O | 2:H5:293:ASN:ND2 | 2.42 | 0.53 |
| 1:H8:135:VAL:O | 1:H8:166:THR:HA | 2.09 | 0.53 |
| 2:I3:399:TYR:O | 2:I3:402:ARG:NH1 | 2.42 | 0.53 |
| 2:I9:195:LEU:HD21 | 2:I9:264:ARG:HH11 | 1.73 | 0.53 |
| 2:J1:284:GLU:OE1 | 2:J1:285:GLN:N | 2.42 | 0.53 |
| 1:K0:418:LEU:O | 1:K0:421:GLU:HG2 | 2.08 | 0.53 |
| 1:K8:50:TYR:CE2 | 1:K8:241:ARG:HD3 | 2.44 | 0.53 |
| 1:L2:175:VAL:HG22 | 2:L3:329:ASN:HD21 | 1.74 | 0.53 |
| 2:L3:167:LEU:HD11 | 2:L3:252:ILE:HG23 | 1.91 | 0.53 |
| 1:M6:190:HIS:CD2 | 1:M6:411:ALA:HA | 2.44 | 0.53 |
| 1:N0:276:ARG:HH12 | 30:7L:366:PRO:CB | 2.22 | 0.53 |
| 2:N9:76:ASP:HA | 2:N9:79:ARG:HD2 | 1.90 | 0.53 |
| 2:O7:28:HIS:CE1 | 2:O7:49:PHE:HA | 2.44 | 0.53 |
| 2:O7:236:SER:OG | 2:O7:243:ARG:NH2 | 2.42 | 0.53 |
| 2:P3:278:ALA:HA | 2:P3:369:ALA:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:317:LEU:HB3 | 2:P3:319:TYR:HE1 | 1.74 | 0.53 |
| 1:Q0:248:ALA:CB | 1:Q0:252:LYS:HE2 | 2.39 | 0.53 |
| 2:Q3:217:LEU:HB3 | 2:Q3:219:ILE:HD12 | 1.89 | 0.53 |
| 1:Q4:11:GLN:HA | 1:Q4:72:THR:HG21 | 1.89 | 0.53 |
| 1:R2:248:ALA:HA | 1:R2:252:LYS:HD2 | 1.91 | 0.53 |
| 2:R3:242:LEU:HD11 | 2:R3:252:ILE:HG12 | 1.89 | 0.53 |
| 1:R4:178:THR:OG1 | 1:R4:181:GLU:HG3 | 2.08 | 0.53 |
| 1:R4:418:LEU:O | 1:R4:421:GLU:HG2 | 2.08 | 0.53 |
| 1:S4:268:VAL:HG23 | 1:S4:368:ILE:HG13 | 1.91 | 0.53 |
| 1:T2:358:PRO:HG2 | 1:T2:361:LEU:HD12 | 1.90 | 0.53 |
| 1:T6:56:GLY:CA | 26:7F:104:GLN:HE22 | 2.22 | 0.53 |
| 1:T6:274:THR:OG1 | 1:T6:279:GLN:HG2 | 2.08 | 0.53 |
| 2:U1:27:GLU:OE1 | 2:U1:243:ARG:NH1 | 2.41 | 0.53 |
| 2:U5:50:ASN:O | 2:U5:64:ARG:NH2 | 2.41 | 0.53 |
| 1:U6:124:ALA:HB1 | 1:U6:130:LEU:HD11 | 1.90 | 0.53 |
| 1:V4:49:VAL:HG11 | 1:V4:241:ARG:HG2 | 1.90 | 0.53 |
| 2:W1:72:PRO:HD2 | 1:W2:2:ARG:HH12 | 1.74 | 0.53 |
| 1:W8:184:ASN:OD1 | 1:W8:398:TYR:OH | 2.26 | 0.53 |
| 1:X4:150:LEU:O | 1:X4:153:SER:OG | 2.23 | 0.53 |
| 2:X5:165:SER:HA | 2:X5:199:ASP:OD2 | 2.09 | 0.53 |
| 1:Y2:248:ALA:CA | 1:Y2:252:LYS:HD3 | 2.37 | 0.53 |
| 1:Z2:83:GLN:O | 1:0I:281:TYR:OH | 2.18 | 0.53 |
| 2:Z5:344:VAL:HG21 | 2:Z5:346:TRP:CE3 | 2.44 | 0.53 |
| 2:Z9:417:GLU:HA | 2:Z9:420:GLU:HG2 | 1.91 | 0.53 |
| 2:0H:244:PHE:HB2 | 2:0H:356:ASN:HD21 | 1.74 | 0.53 |
| 2:0H:306:ASP:HB3 | 2:0H:309:HIS:HD2 | 1.73 | 0.53 |
| 2:0J:333:ALA:O | 2:0J:337:THR:HG23 | 2.09 | 0.53 |
| 1:0K:193:VAL:HG11 | 1:0K:418:LEU:HD11 | 1.91 | 0.53 |
| 1:0K:391:ARG:HD3 | 2:0L:346:TRP:CB | 2.38 | 0.53 |
| 1:0O:165:LEU:HD22 | 1:0O:167:PHE:CE1 | 2.43 | 0.53 |
| 2:0P:217:LEU:HB3 | 2:0P:219:ILE:HD12 | 1.91 | 0.53 |
| 1:1C:397:TRP:HA | 1:1C:397:TRP:HE3 | 1.72 | 0.53 |
| 2:1D:236:SER:O | 2:1D:243:ARG:NH2 | 2.42 | 0.53 |
| 1:1E:377:MET:SD | 1:1E:380:ARG:NH2 | 2.80 | 0.53 |
| 1:1K:208:TYR:CE1 | 1:1K:225:LEU:HD21 | 2.43 | 0.53 |
| 1:1M:80:PRO:HD3 | 9:4Z:90:ILE:HG21 | 1.89 | 0.53 |
| 1:1S:100:ASN:HB3 | 1:1S:103:LYS:HB2 | 1.90 | 0.53 |
| 1:1U:39:ASP:OD1 | 1:1U:40:SER:N | 2.42 | 0.53 |
| 1:1W:99:ASN:ND2 | 2:1X:254:GLU:OE1 | 2.42 | 0.53 |
| 1:2E:95:THR:HG21 | 38:8B:83:ARG:CZ | 2.33 | 0.53 |
| 2:2F:317:LEU:HB3 | 2:2F:319:TYR:HE1 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2G:134:GLN:HE21 | 1:2G:167:PHE:HE2 | 1.57 | 0.53 |
| 2:2H:123:ARG:NH2 | 38:8B:37:TYR:CD2 | 2.77 | 0.53 |
| 2:2H:183:GLU:HG3 | 2:2H:184:PRO:HD3 | 1.91 | 0.53 |
| 2:2H:195:LEU:HD11 | 2:2H:264:ARG:HH11 | 1.73 | 0.53 |
| 1:3C:22:GLU:HG2 | 1:3C:81:TYR:HB2 | 1.91 | 0.53 |
| 2:3D:9:ILE:HG22 | 2:3D:146:GLY:HA2 | 1.90 | 0.53 |
| 2:3F:292:THR:HG22 | 2:3F:319:TYR:OH | 2.09 | 0.53 |
| 1:3G:274:THR:HB | 1:3G:282:ARG:HH11 | 1.73 | 0.53 |
| 2:3H:269:LEU:HD11 | 2:3H:305:CYS:SG | 2.49 | 0.53 |
| 1:3K:49:VAL:HG11 | 1:3K:241:ARG:HG2 | 1.91 | 0.53 |
| 2:3N:280:LYS:O | 2:3N:283:HIS:HB3 | 2.09 | 0.53 |
| 1:3S:113:ILE:HA | 1:3S:116:VAL:HG12 | 1.90 | 0.53 |
| 1:3S:309:ARG:NH1 | 1:3S:339:SER:O | 2.41 | 0.53 |
| 2:3T:116:ASP:N | 2:3T:116:ASP:OD1 | 2.42 | 0.53 |
| 3:4F:236:VAL:HG13 | 3:4F:237:PRO:HD3 | 1.91 | 0.53 |
| 8:4W:249:ALA:HA | 8:4W:252:LYS:HE2 | 1.91 | 0.53 |
| 10:5A:372:MET:O | 10:5A:375:GLU:HG3 | 2.08 | 0.53 |
| 10:5C:493:GLU:HA | 10:5C:496:LYS:HG2 | 1.91 | 0.53 |
| 12:5F:31:PHE:HB2 | 12:5G:363:MET:HB3 | 1.91 | 0.53 |
| 12:5G:273:ARG:O | 12:5G:295:ARG:NH2 | 2.41 | 0.53 |
| 15:5O:29:TYR:N | 15:5O:29:TYR:CD1 | 2.76 | 0.53 |
| 15:5O:337:VAL:O | 25:7C:102:ARG:NH1 | 2.39 | 0.53 |
| 15:5P:128:LEU:O | 15:5P:154:SER:OG | 2.25 | 0.53 |
| 18:6B:38:GLY:HA2 | 18:6B:83:HIS:NE2 | 2.24 | 0.53 |
| 18:6C:38:GLY:HA2 | 18:6C:83:HIS:NE2 | 2.24 | 0.53 |
| 19:6E:131:GLU:O | 19:6E:135:THR:HG23 | 2.09 | 0.53 |
| 20:6F:113:ARG:NH2 | 20:6F:247:TYR:CG | 2.77 | 0.53 |
| 24:6U:246:VAL:O | 24:6U:250:LEU:HG | 2.08 | 0.53 |
| 24:6Y:503:ILE:HG21 | 24:6Y:525:VAL:HG22 | 1.89 | 0.53 |
| 29:7I:262:LEU:HB3 | 30:7K:356:ASN:HB2 | 1.91 | 0.53 |
| 31:7M:56:HIS:O | 31:7M:60:ILE:HG23 | 2.09 | 0.53 |
| 2:C1:58:ALA:HB3 | 24:6Z:263:ARG:HB2 | 1.90 | 0.53 |
| 2:G1:176:GLN:HE22 | 2:G1:304:LYS:HE2 | 1.73 | 0.53 |
| 1:G8:235:GLY:HA3 | 1:G8:366:THR:HG21 | 1.91 | 0.53 |
| 1:H8:173:PRO:HG3 | 1:H8:380:ARG:HD2 | 1.91 | 0.53 |
| 2:I1:278:ALA:HA | 2:I1:369:ALA:HB2 | 1.90 | 0.53 |
| 2:J3:98:ASP:OD1 | 2:J3:99:ALA:N | 2.42 | 0.53 |
| 2:J3:287:SER:OG | 2:J3:288:VAL:N | 2.39 | 0.53 |
| 2:J9:51:THR:HG23 | 2:J9:52:PHE:HD2 | 1.74 | 0.53 |
| 1:K6:309:ARG:H | 1:K6:372:THR:HG22 | 1.73 | 0.53 |
| 2:K7:33:ASP:O | 2:K7:60:LYS:NZ | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K7:399:TYR:O | 2:K7:402:ARG:NH1 | 2.42 | 0.53 |
| 1:K8:371:SER:OG | 1:K8:372:THR:N | 2.42 | 0.53 |
| 2:L1:69:ASP:OD1 | 2:L1:70:LEU:N | 2.41 | 0.53 |
| 2:M5:51:THR:HG21 | 2:M5:243:ARG:HG2 | 1.90 | 0.53 |
| 2:M9:389:SER:N | 2:M9:429:GLU:OE2 | 2.42 | 0.53 |
| 2:N3:372:GLN:NE2 | 30:7L:277:ALA:O | 2.42 | 0.53 |
| 2:N9:319:TYR:HB3 | 2:N9:323:VAL:HG21 | 1.90 | 0.53 |
| 2:O3:3:GLU:OE2 | 2:O3:50:ASN:ND2 | 2.42 | 0.53 |
| 2:O3:177:VAL:CG1 | 2:O3:207:GLU:HB2 | 2.39 | 0.53 |
| 1:O8:45:GLU:OE1 | 1:O8:46:ARG:NE | 2.41 | 0.53 |
| 1:Q0:167:PHE:CE2 | 1:Q0:233:MET:HG3 | 2.44 | 0.53 |
| 2:R1:313:MET:N | 2:R1:380:ASN:O | 2.38 | 0.53 |
| 1:R2:222:PHE:CD2 | 2:R3:247:ALA:HB1 | 2.44 | 0.53 |
| 2:R7:333:ALA:O | 2:R7:337:THR:HG23 | 2.09 | 0.53 |
| 1:S4:373:ALA:O | 1:S4:376:GLU:HG3 | 2.08 | 0.53 |
| 2:S5:174:SER:OG | 2:S5:207:GLU:OE1 | 2.27 | 0.53 |
| 2:S5:384:ILE:HA | 2:S5:387:ILE:HD12 | 1.91 | 0.53 |
| 2:S7:66:ILE:O | 2:S7:66:ILE:HG13 | 2.09 | 0.53 |
| 2:S7:90:GLU:HG2 | 2:S7:121:ARG:NH1 | 2.24 | 0.53 |
| 2:S7:102:ASN:HB3 | 2:S7:105:ARG:HB3 | 1.91 | 0.53 |
| 1:T0:67:ASP:OD2 | 1:T0:72:THR:OG1 | 2.19 | 0.53 |
| 1:T2:371:SER:OG | 1:T2:372:THR:N | 2.42 | 0.53 |
| 1:T2:390:ARG:NH2 | 13:5J:54:ILE:HD11 | 2.24 | 0.53 |
| 2:T5:265:ILE:HG21 | 2:T5:313:MET:HE1 | 1.91 | 0.53 |
| 2:T7:27:GLU:HG3 | 2:T7:361:THR:HG21 | 1.90 | 0.53 |
| 2:T7:88:HIS:ND1 | 2:T7:91:GLN:HG2 | 2.24 | 0.53 |
| 1:T8:190:HIS:CD2 | 1:T8:411:ALA:HA | 2.45 | 0.53 |
| 1:U2:68:LEU:HB3 | 1:U2:96:GLY:HA2 | 1.91 | 0.53 |
| 1:U2:285:THR:HG23 | 1:U2:288:GLU:H | 1.73 | 0.53 |
| 1:V6:198:GLU:HA | 1:V6:264:HIS:HB2 | 1.91 | 0.53 |
| 1:V6:207:LEU:HD11 | 1:V6:229:ILE:HD11 | 1.90 | 0.53 |
| 1:V6:342:VAL:HG12 | 1:V6:348:ASN:ND2 | 2.20 | 0.53 |
| 2:V7:76:ASP:OD2 | 1:V8:46:ARG:NH2 | 2.42 | 0.53 |
| 1:W2:166:THR:HG23 | 1:W2:199:CYS:HB2 | 1.90 | 0.53 |
| 2:Y3:322:ASP:OD2 | 2:Y3:373:ARG:NH2 | 2.42 | 0.53 |
| 2:Y9:315:CYS:SG | 2:Y9:316:CYS:N | 2.82 | 0.53 |
| 1:Z0:39:ASP:OD1 | 1:Z0:40:SER:N | 2.41 | 0.53 |
| 1:Z2:165:LEU:HD12 | 1:Z2:166:THR:H | 1.74 | 0.53 |
| 2:Z3:49:PHE:CE2 | 2:Z3:55:GLU:HG3 | 2.43 | 0.53 |
| 1:Z8:309:ARG:H | 1:Z8:372:THR:HG22 | 1.74 | 0.53 |
| 2:0H:198:THR:HG21 | 2:0H:201:ALA:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0O:87:PRO:HA | 1:0O:90:PHE:CD2 | 2.44 | 0.53 |
| 1:0O:371:SER:OG | 1:0O:372:THR:N | 2.42 | 0.53 |
| 2:0P:60:LYS:NZ | 2:1F:282:TYR:O | 2.33 | 0.53 |
| 1:0U:345:ILE:O | 1:0U:348:ASN:ND2 | 2.38 | 0.53 |
| 1:1G:309:ARG:NH1 | 1:1G:339:SER:O | 2.42 | 0.53 |
| 2:1L:405:VAL:HG23 | 2:1L:418:PHE:HE2 | 1.74 | 0.53 |
| 1:1M:385:PHE:HZ | 1:1M:408:PHE:HD1 | 1.57 | 0.53 |
| 2:1N:175:PRO:HB3 | 2:1N:390:ARG:NE | 2.24 | 0.53 |
| 1:1Q:215:LEU:HB3 | 1:1Q:217:LEU:HG | 1.91 | 0.53 |
| 1:1S:385:PHE:HZ | 1:1S:408:PHE:HD2 | 1.55 | 0.53 |
| 2:2H:387:ILE:HG12 | 2:2H:390:ARG:HH22 | 1.74 | 0.53 |
| 1:2I:259:PRO:HG3 | 1:2I:311:LEU:HD21 | 1.91 | 0.53 |
| 1:2I:391:ARG:HB2 | 2:2J:346:TRP:CD1 | 2.44 | 0.53 |
| 2:2L:277:SER:OG | 2:2L:278:ALA:N | 2.41 | 0.53 |
| 1:2W:306:ARG:HH21 | 38:8B:46:ALA:HA | 1.74 | 0.53 |
| 1:3A:177:ASP:O | 2:3B:352:LYS:HA | 2.09 | 0.53 |
| 1:3A:189:VAL:O | 1:3A:193:VAL:HG23 | 2.08 | 0.53 |
| 1:3A:274:THR:OG1 | 1:3A:279:GLN:NE2 | 2.41 | 0.53 |
| 1:3G:77:ARG:NH2 | 3:3X:19:LEU:O | 2.41 | 0.53 |
| 2:3P:220:GLU:H | 2:3P:220:GLU:CD | 2.13 | 0.53 |
| 1:3S:131:GLN:HE21 | 1:3S:250:LEU:HB2 | 1.73 | 0.53 |
| 3:3X:236:VAL:HG13 | 3:3X:237:PRO:HD3 | 1.91 | 0.53 |
| 6:4O:408:ARG:HH22 | 29:7J:430:ASN:ND2 | 2.07 | 0.53 |
| 9:4Z:212:LEU:HB3 | 9:4Z:216:ARG:NH2 | 2.24 | 0.53 |
| 10:5B:82:ALA:O | 10:5B:85:ARG:HG2 | 2.09 | 0.53 |
| 12:5F:294:PRO:HD2 | 12:5F:297:LEU:HD22 | 1.91 | 0.53 |
| 13:5J:11:GLU:OE1 | 13:5J:11:GLU:N | 2.33 | 0.53 |
| 14:5N:563:ARG:HG2 | 14:5N:607:LYS:HZ1 | 1.74 | 0.53 |
| 17:5V:143:ASN:OD1 | 17:5V:146:ARG:NH2 | 2.40 | 0.53 |
| 18:6A:38:GLY:HA2 | 18:6A:83:HIS:NE2 | 2.24 | 0.53 |
| 18:6D:38:GLY:HA2 | 18:6D:83:HIS:NE2 | 2.24 | 0.53 |
| 21:6H:75:ASN:HD22 | 21:6H:115:TYR:HE2 | 1.57 | 0.53 |
| 22:6L:138:ASP:N | 22:6L:138:ASP:OD2 | 2.39 | 0.53 |
| 22:6O:63:PRO:HB2 | 24:6Z:399:ILE:HG13 | 1.90 | 0.53 |
| 22:6P:201:ARG:HB3 | 22:6P:237:TYR:HB3 | 1.91 | 0.53 |
| 24:6U:613:LYS:O | 24:6U:617:ASP:HB2 | 2.09 | 0.53 |
| 24:6W:124:TYR:CE2 | 24:6W:150:ARG:HG3 | 2.44 | 0.53 |
| 29:7I:265:VAL:HG22 | 29:7I:266:MET:H | 1.73 | 0.53 |
| 30:7K:336:ILE:HD12 | 30:7K:353:ASN:HD21 | 1.74 | 0.53 |
| 31:7N:66:HIS:CD2 | 31:7N:77:GLY:H | 2.27 | 0.53 |
| 33:7Q:139:GLU:HG3 | 33:7Q:140:TYR:N | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:7U:228:ARG:HA | 35:7U:231:THR:HG22 | 1.91 | 0.53 |
| 1:D4:204:ASN:HD21 | 39:D4:501:GDP:N2 | 2.02 | 0.52 |
| 2:E3:145:THR:OG1 | 41:E4:501:GTP:O2G | 2.24 | 0.52 |
| 1:F2:276:ARG:HH12 | 22:6O:65:ARG:NH2 | 2.06 | 0.52 |
| 1:G2:9:GLY:HA2 | 1:G2:66:MET:SD | 2.49 | 0.52 |
| 1:G2:211:CYS:SG | 1:G2:220:PRO:HB3 | 2.49 | 0.52 |
| 1:H2:334:GLN:NE2 | 1:H2:348:ASN:H | 2.06 | 0.52 |
| 1:H2:335:ASN:O | 1:H2:338:SER:OG | 2.27 | 0.52 |
| 2:H3:132:LEU:HD23 | 2:H3:164:LYS:HD3 | 1.91 | 0.52 |
| 2:H9:183:GLU:HG3 | 2:H9:184:PRO:HD3 | 1.92 | 0.52 |
| 2:I3:417:GLU:HA | 2:I3:420:GLU:HG2 | 1.90 | 0.52 |
| 2:I7:116:ASP:OD1 | 2:I7:117:LEU:N | 2.41 | 0.52 |
| 1:J2:249:ASP:O | 1:J2:253:LEU:HG | 2.09 | 0.52 |
| 1:J4:52:ASN:OD1 | 1:J4:62:ARG:NH2 | 2.42 | 0.52 |
| 1:J6:49:VAL:HG11 | 1:J6:241:ARG:HG2 | 1.91 | 0.52 |
| 1:K0:94:GLN:CD | 28:7X:448:THR:HG21 | 2.28 | 0.52 |
| 2:K3:381:SER:OG | 2:K3:382:THR:N | 2.42 | 0.52 |
| 2:K5:244:PHE:HB2 | 2:K5:356:ASN:HD21 | 1.73 | 0.52 |
| 2:K7:145:THR:OG1 | 41:K7:501:GTP:O1B | 2.25 | 0.52 |
| 2:L3:84:ARG:NH1 | 29:7J:345:PRO:CA | 2.61 | 0.52 |
| 2:L7:231:ILE:O | 2:L7:235:ILE:HG12 | 2.09 | 0.52 |
| 1:M0:285:THR:HG23 | 1:M0:288:GLU:H | 1.74 | 0.52 |
| 1:M6:177:ASP:O | 2:M7:352:LYS:HA | 2.08 | 0.52 |
| 2:N3:191:THR:O | 2:N3:195:LEU:HG | 2.09 | 0.52 |
| 1:O4:177:ASP:O | 2:O5:352:LYS:HA | 2.08 | 0.52 |
| 2:O5:414:GLU:HG2 | 2:O5:417:GLU:OE2 | 2.08 | 0.52 |
| 1:R0:207:LEU:HB3 | 1:R0:225:LEU:HD22 | 1.91 | 0.52 |
| 2:R7:250:VAL:HG23 | 2:R7:254:GLU:HG3 | 1.91 | 0.52 |
| 1:R8:207:LEU:HB3 | 1:R8:225:LEU:HD22 | 1.90 | 0.52 |
| 1:S4:112:LEU:O | 1:S4:116:VAL:HG23 | 2.08 | 0.52 |
| 1:T2:337:ASN:HD21 | 17:5T:48:THR:N | 2.07 | 0.52 |
| 1:T6:88:ASP:N | 1:T6:88:ASP:OD1 | 2.42 | 0.52 |
| 1:U4:177:ASP:O | 2:U5:352:LYS:HA | 2.10 | 0.52 |
| 2:U9:9:ILE:HG13 | 2:U9:139:ASN:HB3 | 1.90 | 0.52 |
| 2:V7:311:LYS:HG2 | 2:V7:342:GLN:HG3 | 1.90 | 0.52 |
| 1:W4:139:LEU:HD12 | 1:W4:170:VAL:HG12 | 1.90 | 0.52 |
| 2:W7:287:SER:OG | 2:W7:288:VAL:N | 2.42 | 0.52 |
| 2:W9:70:LEU:HD11 | 2:W9:110:ILE:CG2 | 2.39 | 0.52 |
| 1:X0:69:GLU:C | 1:X0:92:PHE:HZ | 2.12 | 0.52 |
| 2:X3:7:ILE:HG22 | 2:X3:66:ILE:HB | 1.91 | 0.52 |
| 1:X6:248:ALA:HA | 1:X6:252:LYS:HD2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X9:286:LEU:HD12 | 2:X9:286:LEU:H | 1.73 | 0.52 |
| 2:Z3:85:GLN:O | 2:Z3:88:HIS:NE2 | 2.42 | 0.52 |
| 1:Z4:131:GLN:HG2 | 1:Z4:250:LEU:HD13 | 1.90 | 0.52 |
| 1:Z6:190:HIS:NE2 | 1:Z6:410:GLU:HG2 | 2.24 | 0.52 |
| 1:0A:207:LEU:HG | 1:0A:225:LEU:HD22 | 1.91 | 0.52 |
| 2:0B:268:MET:CE | 2:0B:380:ASN:HB2 | 2.38 | 0.52 |
| 1:0C:309:ARG:H | 1:0C:372:THR:HG22 | 1.74 | 0.52 |
| 2:0N:177:VAL:HG21 | 2:0N:207:GLU:HB2 | 1.90 | 0.52 |
| 2:0P:12:ALA:HB2 | 41:0Q:501:GTP:C8 | 2.44 | 0.52 |
| 2:0R:56:THR:HG23 | 2:1H:285:GLN:HB2 | 1.91 | 0.52 |
| 2:1H:313:MET:HB2 | 2:1H:380:ASN:HB3 | 1.91 | 0.52 |
| 2:1L:98:ASP:OD1 | 2:1L:99:ALA:N | 2.42 | 0.52 |
| 2:1R:203:MET:HE3 | 2:1R:267:PHE:HD1 | 1.72 | 0.52 |
| 1:1U:165:LEU:HD21 | 1:1U:250:LEU:CD2 | 2.34 | 0.52 |
| 2:1X:75:VAL:HG11 | 2:1X:94:SER:HB3 | 1.90 | 0.52 |
| 1:2A:178:THR:HG23 | 1:2A:181:GLU:HG3 | 1.89 | 0.52 |
| 1:2E:405:GLU:HA | 1:2E:408:PHE:HD2 | 1.74 | 0.52 |
| 1:2G:345:ILE:O | 1:2G:348:ASN:ND2 | 2.42 | 0.52 |
| 1:2S:244:GLY:H | 1:2S:247:ASN:HD21 | 1.58 | 0.52 |
| 1:2U:260:PHE:HB2 | 1:2U:263:LEU:HG | 1.90 | 0.52 |
| 1:2W:107:THR:OG1 | 1:2W:108:GLU:OE1 | 2.25 | 0.52 |
| 1:2Y:138:SER:OG | 1:2Y:139:LEU:N | 2.42 | 0.52 |
| 1:3A:70:PRO:N | 1:3A:92:PHE:HZ | 2.06 | 0.52 |
| 1:3G:334:GLN:HE22 | 1:3G:348:ASN:H | 1.56 | 0.52 |
| 1:3K:7:ILE:HB | 1:3K:135:VAL:HG12 | 1.91 | 0.52 |
| 1:3M:78:SER:OG | 14:5M:192:THR:O | 2.19 | 0.52 |
| 1:3M:177:ASP:OD2 | 2:3N:248:LEU:HD11 | 2.09 | 0.52 |
| 3:3V:236:VAL:HG13 | 3:3V:237:PRO:HD3 | 1.91 | 0.52 |
| 3:4B:236:VAL:HG13 | 3:4B:237:PRO:HD3 | 1.91 | 0.52 |
| 6:4N:477:VAL:HG23 | 6:4N:478:LEU:HD22 | 1.90 | 0.52 |
| 7:4R:183:LEU:O | 7:4R:187:THR:HG23 | 2.09 | 0.52 |
| 18:5X:38:GLY:HA2 | 18:5X:83:HIS:NE2 | 2.24 | 0.52 |
| 18:5Y:38:GLY:HA2 | 18:5Y:83:HIS:NE2 | 2.24 | 0.52 |
| 21:6H:106:ARG:HE | 24:6X:80:ASP:N | 2.07 | 0.52 |
| 22:6P:307:ARG:NH2 | 22:6P:326:PHE:HB2 | 2.23 | 0.52 |
| 24:6U:41:ARG:HA | 24:6U:41:ARG:NE | 2.20 | 0.52 |
| 24:6Z:97:ARG:HD2 | 24:6Z:122:TYR:HE1 | 1.73 | 0.52 |
| 29:7I:254:MET:CE | 30:7K:341:ARG:CD | 2.87 | 0.52 |
| 30:7K:41:TRP:O | 30:7K:41:TRP:CG | 2.62 | 0.52 |
| 1:A5:414:ASN:HD21 | 3:4J:240:ARG:HE | 1.55 | 0.52 |
| 2:G9:97:GLU:HB3 | 2:G9:105:ARG:HH22 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H1:57:GLY:O | 2:I7:285:GLN:NE2 | 2.42 | 0.52 |
| 2:H1:240:ALA:HA | 2:H1:243:ARG:HB2 | 1.90 | 0.52 |
| 2:H1:331:SER:O | 2:H1:335:ILE:HG13 | 2.08 | 0.52 |
| 2:H5:145:THR:OG1 | 41:H6:501:GTP:O1B | 2.26 | 0.52 |
| 1:H8:186:THR:HG22 | 1:H8:411:ALA:HB1 | 1.91 | 0.52 |
| 2:H9:179:THR:O | 1:I0:350:LYS:HD2 | 2.09 | 0.52 |
| 2:I3:387:ILE:HG12 | 2:I3:390:ARG:HH22 | 1.73 | 0.52 |
| 2:I7:370:LYS:HZ3 | 5:4L:263:LEU:HB2 | 1.75 | 0.52 |
| 1:J2:391:ARG:HH12 | 2:J3:435:VAL:HA | 1.74 | 0.52 |
| 2:J5:282:TYR:HE1 | 5:4M:159:ILE:CD1 | 2.20 | 0.52 |
| 1:J6:135:VAL:HG12 | 1:J6:137:HIS:HD2 | 1.74 | 0.52 |
| 2:J9:175:PRO:HB3 | 2:J9:390:ARG:HE | 1.74 | 0.52 |
| 2:K5:206:ASN:OD1 | 41:K6:501:GTP:N2 | 2.40 | 0.52 |
| 2:K5:219:ILE:HD12 | 29:7I:14:LEU:HD11 | 1.90 | 0.52 |
| 2:L7:138:PHE:HZ | 2:L7:235:ILE:HG21 | 1.75 | 0.52 |
| 2:L7:228:ASN:HA | 2:L7:231:ILE:HD12 | 1.90 | 0.52 |
| 1:M4:380:ARG:HA | 1:M4:383:GLU:OE2 | 2.09 | 0.52 |
| 2:M5:183:GLU:HG3 | 2:M5:184:PRO:HD3 | 1.91 | 0.52 |
| 2:M9:278:ALA:HA | 2:M9:369:ALA:HB2 | 1.90 | 0.52 |
| 2:N5:18:ASN:ND2 | 2:N5:78:VAL:HG22 | 2.23 | 0.52 |
| 2:N5:217:LEU:HD13 | 2:N5:367:ASP:OD2 | 2.09 | 0.52 |
| 2:N9:27:GLU:CD | 2:N9:243:ARG:HH12 | 2.13 | 0.52 |
| 2:O3:129:CYS:SG | 2:O3:130:THR:N | 2.81 | 0.52 |
| 2:O3:225:THR:HG21 | 19:6E:90:THR:OG1 | 2.10 | 0.52 |
| 2:P3:100:ALA:HA | 1:P4:252:LYS:HE2 | 1.91 | 0.52 |
| 2:P3:145:THR:OG1 | 41:P4:501:GTP:O1B | 2.27 | 0.52 |
| 1:Q2:198:GLU:HA | 1:Q2:264:HIS:HB2 | 1.91 | 0.52 |
| 1:R2:67:ASP:OD2 | 1:R2:72:THR:OG1 | 2.26 | 0.52 |
| 1:S4:210:ILE:O | 1:S4:214:THR:OG1 | 2.27 | 0.52 |
| 1:S6:343:GLU:HG3 | 1:S6:344:TRP:N | 2.24 | 0.52 |
| 2:S7:294:ALA:HA | 2:S7:297:GLU:HG2 | 1.92 | 0.52 |
| 2:S7:409:VAL:HA | 2:S7:413:MET:O | 2.09 | 0.52 |
| 1:U6:11:GLN:HE21 | 1:U6:15:GLN:HE22 | 1.57 | 0.52 |
| 2:U9:224:TYR:O | 2:U9:228:ASN:ND2 | 2.39 | 0.52 |
| 2:U9:312:TYR:HB2 | 2:U9:343:PHE:CD1 | 2.44 | 0.52 |
| 2:V1:207:GLU:HB3 | 2:V1:304:LYS:HE3 | 1.92 | 0.52 |
| 1:V2:173:PRO:HD2 | 1:V2:380:ARG:NE | 2.24 | 0.52 |
| 1:V6:279:GLN:HA | 1:V6:282:ARG:HG2 | 1.90 | 0.52 |
| 1:W0:105:HIS:CD2 | 1:W0:150:LEU:HB2 | 2.43 | 0.52 |
| 2:W9:181:VAL:HG23 | 2:W9:182:VAL:HG13 | 1.91 | 0.52 |
| 2:X3:327:ASP:N | 2:X3:327:ASP:OD1 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X4:344:TRP:CE3 | 1:X4:345:ILE:HG13 | 2.43 | 0.52 |
| 1:X8:139:LEU:HD12 | 1:X8:170:VAL:HG12 | 1.90 | 0.52 |
| 1:Y0:125:GLU:OE2 | 1:Y0:159:TYR:OH | 2.26 | 0.52 |
| 1:Y2:99:ASN:HD21 | 2:Y3:352:LYS:HE2 | 1.74 | 0.52 |
| 2:Y5:191:THR:HA | 2:Y5:194:LEU:HG | 1.91 | 0.52 |
| 1:Y6:2:ARG:HE | 1:Y6:240:LEU:HD22 | 1.75 | 0.52 |
| 1:Y8:342:VAL:HB | 1:Y8:344:TRP:CZ3 | 2.44 | 0.52 |
| 2:Z5:210:TYR:HE1 | 2:Z5:227:LEU:HD11 | 1.74 | 0.52 |
| 1:0A:204:ASN:ND2 | 39:0A:503:GDP:HN22 | 2.07 | 0.52 |
| 1:0G:101:TRP:HB2 | 1:0G:184:ASN:OD1 | 2.09 | 0.52 |
| 1:0G:358:PRO:HG2 | 1:0G:361:LEU:HD13 | 1.92 | 0.52 |
| 2:0H:383:ALA:O | 2:0H:387:ILE:HG12 | 2.09 | 0.52 |
| 1:0K:388:MET:CE | 1:0K:388:MET:CA | 2.86 | 0.52 |
| 1:0U:179:VAL:HB | 2:0V:258:ASN:HD22 | 1.74 | 0.52 |
| 2:0V:30:ILE:HG12 | 2:0V:36:MET:HG2 | 1.90 | 0.52 |
| 2:1B:90:GLU:HG2 | 2:1B:121:ARG:HH22 | 1.74 | 0.52 |
| 2:1B:183:GLU:HG3 | 2:1B:184:PRO:HD3 | 1.92 | 0.52 |
| 2:1H:227:LEU:O | 2:1H:231:ILE:HG12 | 2.09 | 0.52 |
| 1:1O:107:THR:OG1 | 1:1O:401:GLU:OE2 | 2.23 | 0.52 |
| 2:1V:63:PRO:HB2 | 2:1V:65:CYS:SG | 2.49 | 0.52 |
| 2:1X:287:SER:OG | 2:1X:288:VAL:N | 2.43 | 0.52 |
| 2:2B:161:TYR:HD1 | 38:8A:80:TYR:HB3 | 1.72 | 0.52 |
| 2:2F:227:LEU:O | 2:2F:231:ILE:HG12 | 2.09 | 0.52 |
| 1:2M:5:VAL:HG12 | 1:2M:62:ARG:HD3 | 1.91 | 0.52 |
| 2:2T:129:CYS:SG | 2:2T:130:THR:N | 2.83 | 0.52 |
| 2:2T:333:ALA:O | 2:2T:337:THR:HG23 | 2.09 | 0.52 |
| 2:2V:381:SER:OG | 2:2V:382:THR:N | 2.43 | 0.52 |
| 2:2X:183:GLU:HG3 | 2:2X:184:PRO:HD3 | 1.90 | 0.52 |
| 1:2Y:34:GLY:HA3 | 1:2Y:58:ARG:NH1 | 2.24 | 0.52 |
| 1:2Y:183:TYR:HB3 | 1:2Y:398:TYR:HE2 | 1.74 | 0.52 |
| 2:2Z:26:LEU:HD22 | 2:2Z:363:VAL:HG12 | 1.92 | 0.52 |
| 1:3G:350:LYS:NZ | 1:3G:351:SER:O | 2.42 | 0.52 |
| 1:3G:382:SER:HB2 | 1:3G:415:MET:HG2 | 1.91 | 0.52 |
| 1:3I:211:CYS:HB2 | 1:3I:217:LEU:HD12 | 1.92 | 0.52 |
| 2:3L:238:LEU:HD22 | 2:3L:378:ILE:HD11 | 1.90 | 0.52 |
| 1:3S:362:LYS:CE | 38:8D:166:GLU:CB | 2.85 | 0.52 |
| 3:3Z:236:VAL:HG13 | 3:3Z:237:PRO:HD3 | 1.91 | 0.52 |
| 5:4M:15:MET:O | 5:4M:19:GLU:HG2 | 2.09 | 0.52 |
| 6:4P:158:ILE:HD11 | 29:7J:233:LYS:HD3 | 1.91 | 0.52 |
| 10:5A:447:ARG:NE | 10:5A:447:ARG:HA | 2.24 | 0.52 |
| 10:5C:494:LEU:HD12 | 10:5C:494:LEU:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5P:22:TRP:CD1 | 15:5P:22:TRP:N | 2.76 | 0.52 |
| 18:5Z:38:GLY:HA2 | 18:5Z:83:HIS:NE2 | 2.24 | 0.52 |
| 22:6L:329:LEU:HD13 | 22:6L:346:PHE:HZ | 1.74 | 0.52 |
| 24:6T:541:THR:HG22 | 24:6T:614:ARG:HH22 | 1.74 | 0.52 |
| 24:6U:481:LEU:HD23 | 24:6U:481:LEU:C | 2.30 | 0.52 |
| 24:6W:482:ILE:HD13 | 24:6W:498:LEU:HB3 | 1.91 | 0.52 |
| 24:6X:274:ARG:NE | 24:6X:372:ASP:OD2 | 2.37 | 0.52 |
| 30:7K:41:TRP:O | 30:7K:41:TRP:CD2 | 2.62 | 0.52 |
| 36:7W:98:VAL:HA | 36:7W:101:VAL:HG12 | 1.90 | 0.52 |
| 1:G4:391:ARG:NH2 | 2:G5:435:VAL:HA | 2.24 | 0.52 |
| 2:G9:420:GLU:HA | 2:G9:423:GLU:HG3 | 1.91 | 0.52 |
| 1:H6:33:THR:O | 1:H6:58:ARG:NH2 | 2.43 | 0.52 |
| 1:I0:135:VAL:HG21 | 1:I0:152:ILE:HD11 | 1.92 | 0.52 |
| 2:I7:191:THR:HA | 2:I7:194:LEU:HB2 | 1.90 | 0.52 |
| 2:I9:276:ILE:HG23 | 2:I9:280:LYS:HB2 | 1.91 | 0.52 |
| 2:J3:379:SER:OG | 2:J3:380:ASN:N | 2.41 | 0.52 |
| 1:J6:176:SER:HB3 | 2:J7:349:THR:OG1 | 2.09 | 0.52 |
| 2:J7:121:ARG:C | 2:J7:121:ARG:CD | 2.77 | 0.52 |
| 1:K0:379:LYS:O | 1:K0:383:GLU:HG2 | 2.09 | 0.52 |
| 2:K3:372:GLN:HE22 | 6:4O:141:VAL:HA | 1.73 | 0.52 |
| 2:K5:167:LEU:HD11 | 2:K5:252:ILE:HG23 | 1.89 | 0.52 |
| 1:L2:113:ILE:HD13 | 1:L2:150:LEU:HD22 | 1.91 | 0.52 |
| 1:L4:56:GLY:HA2 | 29:7J:331:TYR:CB | 2.27 | 0.52 |
| 1:M4:135:VAL:HG21 | 1:M4:152:ILE:HD11 | 1.92 | 0.52 |
| 1:M8:219:THR:HB | 2:M9:324:VAL:HG11 | 1.89 | 0.52 |
| 1:O0:405:GLU:HA | 1:O0:408:PHE:HD2 | 1.75 | 0.52 |
| 2:O5:287:SER:N | 2:O5:290:GLU:OE2 | 2.42 | 0.52 |
| 2:P3:8:HIS:CD2 | 2:P3:138:PHE:HD2 | 2.27 | 0.52 |
| 2:P3:105:ARG:O | 2:P3:109:THR:OG1 | 2.23 | 0.52 |
| 1:Q0:114:ASP:OD2 | 1:Q0:115:SER:N | 2.43 | 0.52 |
| 1:Q0:219:THR:O | 1:Q0:219:THR:OG1 | 2.28 | 0.52 |
| 1:R0:172:SER:OG | 1:R0:205:GLU:OE1 | 2.13 | 0.52 |
| 1:R2:180:VAL:HG23 | 1:R2:184:ASN:HD21 | 1.74 | 0.52 |
| 1:R4:325:GLU:HA | 1:R4:328:GLU:HG2 | 1.91 | 0.52 |
| 2:S9:166:LYS:N | 2:S9:199:ASP:OD2 | 2.42 | 0.52 |
| 2:T1:14:ILE:HD11 | 2:T1:69:ASP:HB2 | 1.90 | 0.52 |
| 2:T1:339:ARG:HH21 | 2:T1:342:GLN:HB3 | 1.74 | 0.52 |
| 2:U3:414:GLU:HG2 | 2:U3:416:GLY:H | 1.75 | 0.52 |
| 2:U7:406:HIS:HA | 2:U7:409:VAL:HG22 | 1.90 | 0.52 |
| 2:V9:88:HIS:CG | 2:X5:283:HIS:HB2 | 2.44 | 0.52 |
| 1:W2:273:LEU:O | 1:W2:292:GLN:NE2 | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:88:HIS:CA | 2:Y5:283:HIS:CE1 | 2.84 | 0.52 |
| 1:X2:290:THR:HB | 1:X2:329:GLN:HE21 | 1.74 | 0.52 |
| 1:X4:113:ILE:HG21 | 1:X4:150:LEU:HD22 | 1.91 | 0.52 |
| 1:X6:240:LEU:HD11 | 1:X6:250:LEU:HD11 | 1.90 | 0.52 |
| 1:X6:273:LEU:H | 1:X6:292:GLN:HE22 | 1.57 | 0.52 |
| 2:X9:21:TRP:CZ2 | 2:X9:65:CYS:HB2 | 2.44 | 0.52 |
| 2:Y9:8:HIS:CD2 | 2:Y9:138:PHE:HD2 | 2.27 | 0.52 |
| 1:Z0:86:ARG:HH21 | 1:0G:282:ARG:HA | 1.73 | 0.52 |
| 1:Z0:105:HIS:NE2 | 1:Z0:150:LEU:HD13 | 2.24 | 0.52 |
| 1:Z4:91:VAL:HG21 | 1:Z4:116:VAL:HG22 | 1.89 | 0.52 |
| 1:Z8:237:THR:HG23 | 1:Z8:241:ARG:HH21 | 1.74 | 0.52 |
| 1:0A:51:PHE:HB3 | 1:0A:59:TYR:HB3 | 1.91 | 0.52 |
| 1:0E:173:PRO:HG2 | 1:0E:174:LYS:HZ3 | 1.74 | 0.52 |
| 1:0I:237:THR:HG23 | 1:0I:241:ARG:HH21 | 1.75 | 0.52 |
| 1:0O:388:MET:HE1 | 2:0P:348:PRO:HD3 | 1.91 | 0.52 |
| 1:0S:193:VAL:HG12 | 1:0S:265:PHE:HZ | 1.74 | 0.52 |
| 2:0X:322:ASP:HB3 | 2:0X:373:ARG:HH21 | 1.73 | 0.52 |
| 2:0Z:264:ARG:NH2 | 2:0Z:431:ASP:OD2 | 2.43 | 0.52 |
| 1:1E:404:ASP:HB3 | 1:1E:406:MET:SD | 2.49 | 0.52 |
| 1:1K:97:ALA:HA | 1:1K:103:LYS:HE3 | 1.91 | 0.52 |
| 2:1R:120:ASP:O | 2:1R:123:ARG:HB3 | 2.09 | 0.52 |
| 1:1W:290:THR:HA | 1:1W:293:MET:HB2 | 1.90 | 0.52 |
| 2:1Z:195:LEU:HD11 | 2:1Z:264:ARG:HH11 | 1.74 | 0.52 |
| 1:2A:32:PRO:O | 1:2A:83:GLN:NE2 | 2.43 | 0.52 |
| 1:2C:113:ILE:HG13 | 1:2C:150:LEU:HD23 | 1.90 | 0.52 |
| 2:2D:282:TYR:HH | 10:5A:380:ARG:HB3 | 1.69 | 0.52 |
| 2:2F:392:ASP:OD2 | 2:2F:422:ARG:NH1 | 2.42 | 0.52 |
| 1:2I:5:VAL:HG22 | 1:2I:133:PHE:HD1 | 1.74 | 0.52 |
| 2:2J:9:ILE:HD11 | 2:2J:153:LEU:HD23 | 1.91 | 0.52 |
| 2:2J:236:SER:O | 2:2J:243:ARG:NH2 | 2.43 | 0.52 |
| 2:2L:301:MET:HE1 | 2:2L:307:PRO:HD3 | 1.92 | 0.52 |
| 1:2M:185:ALA:O | 1:2M:189:VAL:HG12 | 2.09 | 0.52 |
| 2:2V:129:CYS:SG | 2:2V:130:THR:N | 2.83 | 0.52 |
| 2:2V:297:GLU:CD | 38:8B:74:ILE:H | 2.13 | 0.52 |
| 1:2W:371:SER:OG | 1:2W:372:THR:N | 2.42 | 0.52 |
| 2:2X:290:GLU:OE1 | 2:2X:290:GLU:N | 2.32 | 0.52 |
| 1:2Y:263:LEU:HD13 | 1:2Y:422:TYR:CE1 | 2.43 | 0.52 |
| 2:3B:264:ARG:NH2 | 2:3B:431:ASP:OD2 | 2.41 | 0.52 |
| 1:3C:245:GLN:NE2 | 38:8D:198:THR:HG21 | 2.24 | 0.52 |
| 2:3D:27:GLU:OE1 | 2:3D:243:ARG:NH1 | 2.42 | 0.52 |
| 2:3D:109:THR:OG1 | 2:3D:411:GLU:OE2 | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3I:77:ARG:CZ | 3:3Z:19:LEU:HA | 2.39 | 0.52 |
| 2:3R:183:GLU:CD | 2:3R:184:PRO:HD3 | 2.30 | 0.52 |
| 3:4D:236:VAL:HG13 | 3:4D:237:PRO:HD3 | 1.91 | 0.52 |
| 3:4H:236:VAL:HG13 | 3:4H:237:PRO:HD3 | 1.91 | 0.52 |
| 5:4L:326:GLU:O | 5:4L:330:GLU:HG3 | 2.09 | 0.52 |
| 5:4M:50:VAL:O | 5:4M:54:VAL:HG23 | 2.09 | 0.52 |
| 8:4W:176:GLU:O | 8:4W:179:GLU:HG3 | 2.10 | 0.52 |
| 14:5L:415:LYS:HG2 | 23:6Q:23:ILE:HD11 | 1.92 | 0.52 |
| 14:5N:507:LEU:HD11 | 14:5N:525:LEU:HD12 | 1.91 | 0.52 |
| 15:5O:73:LEU:CD2 | 15:5O:73:LEU:N | 2.72 | 0.52 |
| 17:5S:183:ARG:HA | 17:5S:186:LYS:CE | 2.40 | 0.52 |
| 22:6J:274:GLU:O | 22:6J:277:SER:OG | 2.20 | 0.52 |
| 22:6L:51:ILE:HA | 22:6L:54:ARG:HD3 | 1.91 | 0.52 |
| 22:6L:137:GLU:HA | 22:6L:140:VAL:HG12 | 1.91 | 0.52 |
| 24:6V:476:MET:HG2 | 24:6V:477:ASP:OD2 | 2.10 | 0.52 |
| 24:6Z:282:ARG:NH1 | 24:6Z:289:ARG:HD3 | 2.24 | 0.52 |
| 27:7G:199:ASN:HD22 | 27:7G:213:TRP:HE1 | 1.56 | 0.52 |
| 38:8B:95:LYS:HA | 38:8B:100:SER:HB2 | 1.91 | 0.52 |
| 38:8C:92:GLU:CD | 38:8C:94:LYS:HE3 | 2.29 | 0.52 |
| 1:5:217:LEU:HD11 | 26:7D:136:PHE:HB3 | 1.91 | 0.52 |
| 2:A2:264:ARG:NH2 | 4:4G:118:ILE:HD13 | 2.24 | 0.52 |
| 1:A3:33:THR:HG21 | 18:6C:101:LYS:HE2 | 1.91 | 0.52 |
| 1:A3:44:LEU:CD1 | 18:6C:36:ASN:HB3 | 2.39 | 0.52 |
| 2:A8:145:THR:OG1 | 41:A9:501:GTP:O1B | 2.27 | 0.52 |
| 2:E7:282:TYR:CD1 | 22:6L:82:LEU:HD21 | 2.44 | 0.52 |
| 2:G5:145:THR:OG1 | 41:G5:501:GTP:O1B | 2.27 | 0.52 |
| 2:G7:287:SER:OG | 2:G7:290:GLU:OE1 | 2.22 | 0.52 |
| 2:G7:379:SER:OG | 2:G7:380:ASN:N | 2.42 | 0.52 |
| 1:H4:11:GLN:N | 39:H4:501:GDP:O2B | 2.38 | 0.52 |
| 1:H4:135:VAL:HG12 | 1:H4:137:HIS:HD2 | 1.74 | 0.52 |
| 1:H6:178:THR:OG1 | 1:H6:181:GLU:HG3 | 2.09 | 0.52 |
| 1:I2:113:ILE:HA | 1:I2:116:VAL:HG22 | 1.90 | 0.52 |
| 2:I7:345:ASP:N | 2:I7:345:ASP:OD2 | 2.43 | 0.52 |
| 1:I8:68:LEU:HD11 | 1:I8:147:MET:HE1 | 1.92 | 0.52 |
| 1:J0:39:ASP:OD2 | 28:7H:410:HIS:NE2 | 2.41 | 0.52 |
| 2:J5:69:ASP:OD1 | 2:J5:70:LEU:N | 2.43 | 0.52 |
| 1:J8:404:ASP:HB3 | 1:J8:406:MET:SD | 2.50 | 0.52 |
| 2:K3:109:THR:OG1 | 2:K3:411:GLU:OE2 | 2.24 | 0.52 |
| 2:K3:277:SER:OG | 2:K3:278:ALA:N | 2.41 | 0.52 |
| 2:L5:187:SER:O | 2:L5:191:THR:HG23 | 2.09 | 0.52 |
| 2:L9:9:ILE:HG22 | 2:L9:146:GLY:HA2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M0:243:PRO:HG2 | 29:7I:109:THR:HG21 | 1.92 | 0.52 |
| 2:M5:250:VAL:HB | 2:M5:254:GLU:HG3 | 1.90 | 0.52 |
| 1:N2:274:THR:HB | 1:N2:282:ARG:HH11 | 1.73 | 0.52 |
| 1:N6:175:VAL:HG12 | 1:N6:205:GLU:HG2 | 1.92 | 0.52 |
| 1:N8:134:GLN:HE21 | 1:N8:167:PHE:HE2 | 1.58 | 0.52 |
| 2:N9:202:VAL:HG22 | 2:N9:268:MET:HB2 | 1.92 | 0.52 |
| 2:O1:259:LEU:HD11 | 2:O1:316:CYS:HB2 | 1.92 | 0.52 |
| 2:O3:214:ARG:NE | 37:7Y:84:ARG:HH22 | 2.06 | 0.52 |
| 2:O5:285:GLN:HE22 | 19:6E:10:SER:HB3 | 1.75 | 0.52 |
| 1:O8:190:HIS:HD2 | 1:O8:411:ALA:HA | 1.75 | 0.52 |
| 1:P4:248:ALA:HA | 1:P4:252:LYS:HD2 | 1.91 | 0.52 |
| 1:P4:309:ARG:H | 1:P4:372:THR:HG22 | 1.75 | 0.52 |
| 2:R9:414:GLU:HG2 | 2:R9:417:GLU:OE1 | 2.10 | 0.52 |
| 1:S0:211:CYS:SG | 1:S0:217:LEU:HB2 | 2.49 | 0.52 |
| 2:T1:58:ALA:HB3 | 24:6W:86:PRO:HB3 | 1.91 | 0.52 |
| 2:T1:203:MET:HB2 | 2:T1:303:VAL:HG21 | 1.91 | 0.52 |
| 2:T1:266:HIS:ND1 | 2:T1:266:HIS:O | 2.43 | 0.52 |
| 1:T2:172:SER:HB3 | 1:T2:175:VAL:HG12 | 1.90 | 0.52 |
| 1:T2:175:VAL:O | 1:T2:175:VAL:HG13 | 2.10 | 0.52 |
| 1:T8:334:GLN:HE22 | 1:T8:348:ASN:H | 1.57 | 0.52 |
| 1:V6:2:ARG:CZ | 1:V6:131:GLN:HG3 | 2.40 | 0.52 |
| 1:V6:311:LEU:HD11 | 1:V6:372:THR:HB | 1.91 | 0.52 |
| 2:W1:399:TYR:OH | 2:W1:415:GLU:OE2 | 2.20 | 0.52 |
| 2:W7:331:SER:O | 2:W7:334:THR:OG1 | 2.17 | 0.52 |
| 2:W9:287:SER:OG | 2:W9:288:VAL:N | 2.43 | 0.52 |
| 2:X3:258:ASN:CB | 2:X3:352:LYS:HG3 | 2.40 | 0.52 |
| 2:X3:281:ALA:HB3 | 8:4V:427:VAL:HG21 | 1.90 | 0.52 |
| 2:X9:286:LEU:O | 2:X9:373:ARG:NH1 | 2.39 | 0.52 |
| 1:Y0:67:ASP:N | 1:Y0:67:ASP:OD1 | 2.41 | 0.52 |
| 1:Y0:150:LEU:O | 1:Y0:153:SER:OG | 2.22 | 0.52 |
| 1:Y2:263:LEU:HD22 | 1:Y2:422:TYR:HE1 | 1.74 | 0.52 |
| 2:Y3:90:GLU:H | 2:Z9:283:HIS:HE1 | 1.56 | 0.52 |
| 2:Y9:297:GLU:HG2 | 2:Y9:299:ALA:H | 1.75 | 0.52 |
| 1:Z0:116:VAL:HA | 1:Z0:119:VAL:HG12 | 1.91 | 0.52 |
| 1:Z0:117:LEU:HD11 | 1:Z0:154:LYS:HD3 | 1.91 | 0.52 |
| 2:Z1:216:SER:OG | 2:Z1:217:LEU:N | 2.42 | 0.52 |
| 2:Z3:9:ILE:HG22 | 2:Z3:146:GLY:HA2 | 1.91 | 0.52 |
| 1:Z4:260:PHE:HB2 | 1:Z4:263:LEU:HG | 1.92 | 0.52 |
| 1:Z4:294:TRP:CD1 | 1:Z4:333:VAL:HG21 | 2.45 | 0.52 |
| 2:Z5:181:VAL:HG22 | 1:Z6:256:ASN:HD22 | 1.73 | 0.52 |
| 2:Z7:259:LEU:HD21 | 2:Z7:316:CYS:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z9:69:ASP:OD1 | 2:Z9:70:LEU:N | 2.43 | 0.52 |
| 2:Z9:313:MET:HE2 | 2:Z9:380:ASN:HD22 | 1.73 | 0.52 |
| 1:0A:152:ILE:HD13 | 1:0A:155:ILE:HD11 | 1.91 | 0.52 |
| 1:0C:116:VAL:HA | 1:0C:119:VAL:HG22 | 1.91 | 0.52 |
| 1:0G:391:ARG:HD3 | 2:0H:346:TRP:CE2 | 2.45 | 0.52 |
| 2:0N:407:TRP:NE1 | 1:0O:258:ILE:O | 2.35 | 0.52 |
| 1:0O:204:ASN:HD21 | 39:0O:502:GDP:HN22 | 1.58 | 0.52 |
| 1:0S:317:PHE:HB2 | 1:0S:353:VAL:HG23 | 1.92 | 0.52 |
| 1:0U:134:GLN:HE21 | 1:0U:167:PHE:HE2 | 1.56 | 0.52 |
| 1:0U:182:PRO:CG | 1:0U:388:MET:HE3 | 2.40 | 0.52 |
| 1:0Y:180:VAL:HG23 | 1:0Y:184:ASN:ND2 | 2.23 | 0.52 |
| 1:1A:52:ASN:OD1 | 1:1A:62:ARG:NH2 | 2.42 | 0.52 |
| 2:1B:7:ILE:HD11 | 2:1B:137:VAL:HG12 | 1.90 | 0.52 |
| 1:1C:345:ILE:O | 1:1C:348:ASN:ND2 | 2.42 | 0.52 |
| 2:1H:254:GLU:HA | 2:1H:257:THR:HG22 | 1.91 | 0.52 |
| 1:1Q:140:GLY:O | 1:1Q:184:ASN:ND2 | 2.42 | 0.52 |
| 1:1Q:396:HIS:H | 1:1Q:396:HIS:HD2 | 1.57 | 0.52 |
| 1:1W:138:SER:OG | 1:1W:139:LEU:N | 2.42 | 0.52 |
| 2:2F:290:GLU:HA | 2:2F:293:ASN:HD22 | 1.74 | 0.52 |
| 2:2J:90:GLU:HG3 | 2:2J:121:ARG:NH1 | 2.24 | 0.52 |
| 2:2J:392:ASP:OD2 | 2:2J:422:ARG:NH1 | 2.42 | 0.52 |
| 1:2K:207:LEU:HB3 | 1:2K:225:LEU:HD22 | 1.91 | 0.52 |
| 1:2M:167:PHE:CE2 | 1:2M:233:MET:HG2 | 2.44 | 0.52 |
| 1:2M:200:MET:HE3 | 1:2M:268:VAL:HG22 | 1.90 | 0.52 |
| 2:2R:287:SER:OG | 2:2R:288:VAL:N | 2.43 | 0.52 |
| 2:3F:56:THR:OG1 | 3:3V:33:GLY:O | 2.27 | 0.52 |
| 1:3G:3:GLU:HB2 | 1:3G:130:LEU:HA | 1.92 | 0.52 |
| 1:3G:90:PHE:HB2 | 3:3X:19:LEU:HD13 | 1.89 | 0.52 |
| 2:3H:199:ASP:OD1 | 2:3H:256:GLN:HG2 | 2.09 | 0.52 |
| 1:3K:248:ALA:HA | 1:3K:252:LYS:HD2 | 1.92 | 0.52 |
| 1:3K:282:ARG:NH2 | 1:3K:288:GLU:OE1 | 2.42 | 0.52 |
| 1:3M:382:SER:HB2 | 1:3M:415:MET:HG2 | 1.91 | 0.52 |
| 1:3O:70:PRO:HG2 | 2:3P:2:ARG:HH11 | 1.75 | 0.52 |
| 2:3T:183:GLU:HB3 | 2:3T:184:PRO:HD3 | 1.91 | 0.52 |
| 3:3X:252:LYS:HD3 | 3:3X:270:LEU:HD21 | 1.92 | 0.52 |
| 3:4F:252:LYS:HD3 | 3:4F:270:LEU:HD21 | 1.92 | 0.52 |
| 3:4H:161:PHE:HB3 | 3:4H:180:VAL:HG23 | 1.91 | 0.52 |
| 5:4L:466:LEU:N | 5:4L:466:LEU:HD23 | 2.25 | 0.52 |
| 5:4M:76:LEU:CD2 | 15:5P:288:VAL:HG21 | 2.15 | 0.52 |
| 7:4S:9:PRO:HD2 | 7:4S:12:ASP:HB2 | 1.91 | 0.52 |
| 7:4U:195:VAL:O | 7:4U:199:VAL:HG13 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5L:251:GLY:O | 14:5L:267:THR:OG1 | 2.28 | 0.52 |
| 14:5L:302:MET:SD | 14:5L:307:PHE:HE1 | 2.33 | 0.52 |
| 14:5M:251:GLY:O | 14:5M:267:THR:OG1 | 2.27 | 0.52 |
| 15:5P:14:LEU:CD2 | 15:5P:14:LEU:N | 2.73 | 0.52 |
| 21:6G:69:TYR:O | 21:6G:73:VAL:HG23 | 2.08 | 0.52 |
| 22:6L:274:GLU:O | 22:6L:277:SER:OG | 2.22 | 0.52 |
| 24:6V:626:ILE:O | 24:6V:630:LEU:HG | 2.10 | 0.52 |
| 24:6W:556:ASP:OD1 | 24:6W:557:VAL:N | 2.42 | 0.52 |
| 28:7H:398:ASP:O | 28:7H:401:THR:HG22 | 2.08 | 0.52 |
| 30:7K:382:LEU:HB3 | 30:7K:434:ARG:HH21 | 1.74 | 0.52 |
| 1:3:423:GLN:HE22 | 3:3X:107:ALA:HB1 | 1.74 | 0.52 |
| 2:6:42:ILE:HD13 | 24:6V:93:ARG:HE | 1.74 | 0.52 |
| 1:A1:340:TYR:CD1 | 3:4F:104:PRO:HD3 | 2.44 | 0.52 |
| 1:A3:40:SER:HA | 26:7F:122:VAL:HB | 1.91 | 0.52 |
| 1:A9:80:PRO:HD2 | 24:6U:221:ARG:HH12 | 1.72 | 0.52 |
| 1:B1:279:GLN:NE2 | 24:6V:108:GLU:O | 2.42 | 0.52 |
| 1:G0:78:SER:O | 24:6V:498:LEU:HD12 | 2.09 | 0.52 |
| 2:G9:104:ALA:H | 2:G9:408:TYR:HE1 | 1.56 | 0.52 |
| 2:G9:114:ILE:HB | 2:G9:149:LEU:HD11 | 1.91 | 0.52 |
| 2:G9:259:LEU:HB3 | 2:G9:268:MET:HE2 | 1.91 | 0.52 |
| 2:H1:278:ALA:HA | 2:H1:369:ALA:HB2 | 1.90 | 0.52 |
| 2:H3:88:HIS:CD2 | 2:H3:121:ARG:HH21 | 2.12 | 0.52 |
| 2:H9:278:ALA:HA | 2:H9:369:ALA:HB2 | 1.92 | 0.52 |
| 1:I8:113:ILE:HG21 | 1:I8:150:LEU:HD22 | 1.91 | 0.52 |
| 2:J1:98:ASP:OD1 | 2:J1:99:ALA:N | 2.43 | 0.52 |
| 2:J3:117:LEU:HA | 2:J3:120:ASP:OD1 | 2.09 | 0.52 |
| 1:J6:72:THR:O | 1:J6:76:VAL:HG23 | 2.10 | 0.52 |
| 1:J6:204:ASN:OD1 | 39:J6:502:GDP:O2' | 2.27 | 0.52 |
| 2:J7:56:THR:HG23 | 2:J7:60:LYS:HB3 | 1.92 | 0.52 |
| 1:K4:69:GLU:C | 1:K4:92:PHE:HZ | 2.13 | 0.52 |
| 2:K5:53:PHE:HB3 | 2:K5:61:HIS:HB3 | 1.91 | 0.52 |
| 2:K5:242:LEU:HD11 | 2:K5:252:ILE:HG12 | 1.90 | 0.52 |
| 2:L1:203:MET:O | 2:L1:204:LEU:HD23 | 2.09 | 0.52 |
| 1:L2:248:ALA:HA | 1:L2:252:LYS:HD2 | 1.91 | 0.52 |
| 2:L5:109:THR:OG1 | 2:L5:411:GLU:OE2 | 2.21 | 0.52 |
| 2:L9:331:SER:O | 2:L9:334:THR:OG1 | 2.22 | 0.52 |
| 1:M2:78:SER:HA | 15:5O:48:LYS:CG | 2.38 | 0.52 |
| 2:M3:116:ASP:N | 2:M3:116:ASP:OD1 | 2.41 | 0.52 |
| 1:M4:52:ASN:OD1 | 1:M4:62:ARG:NH2 | 2.43 | 0.52 |
| 1:N6:125:GLU:OE2 | 1:N6:159:TYR:OH | 2.28 | 0.52 |
| 2:O3:14:ILE:HD11 | 2:O3:74:VAL:HG13 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O5:364:PRO:HB2 | 32:7P:127:ASP:OD2 | 2.09 | 0.52 |
| 1:P4:170:VAL:HG11 | 1:P4:377:MET:HE2 | 1.91 | 0.52 |
| 2:P7:10:GLY:O | 2:P7:13:GLY:N | 2.43 | 0.52 |
| 1:Q2:392:LYS:HD2 | 1:Q2:395:LEU:HD22 | 1.92 | 0.52 |
| 2:Q5:170:THR:HG21 | 2:Q5:194:LEU:HD11 | 1.92 | 0.52 |
| 1:R8:36:TYR:HD2 | 21:6H:163:THR:HG21 | 1.74 | 0.52 |
| 1:S8:125:GLU:OE1 | 3:3Z:65:SER:OG | 2.20 | 0.52 |
| 1:T0:213:ARG:HH22 | 13:5I:117:ASN:HD21 | 1.57 | 0.52 |
| 1:T0:397:TRP:NE1 | 2:T1:256:GLN:O | 2.42 | 0.52 |
| 2:T1:90:GLU:HG2 | 2:T1:121:ARG:NH1 | 2.25 | 0.52 |
| 1:T8:2:ARG:HB3 | 1:T8:131:GLN:HB2 | 1.91 | 0.52 |
| 1:U2:49:VAL:HG11 | 1:U2:241:ARG:HG2 | 1.91 | 0.52 |
| 1:V2:33:THR:O | 1:V2:58:ARG:NH2 | 2.42 | 0.52 |
| 2:V7:242:LEU:HD11 | 2:V7:252:ILE:HG12 | 1.92 | 0.52 |
| 1:W6:183:TYR:HB3 | 1:W6:398:TYR:HE2 | 1.74 | 0.52 |
| 1:X2:50:TYR:OH | 1:X2:237:THR:OG1 | 2.06 | 0.52 |
| 2:X9:166:LYS:N | 2:X9:199:ASP:OD2 | 2.43 | 0.52 |
| 2:Y3:100:ALA:HA | 1:Y4:252:LYS:HE3 | 1.91 | 0.52 |
| 1:Y6:153:SER:HA | 1:Y6:195:ASN:OD1 | 2.09 | 0.52 |
| 1:Y8:91:VAL:HG11 | 1:Y8:119:VAL:HG11 | 1.90 | 0.52 |
| 1:Y8:210:ILE:O | 1:Y8:214:THR:OG1 | 2.22 | 0.52 |
| 1:Y8:404:ASP:HB2 | 1:Y8:406:MET:SD | 2.48 | 0.52 |
| 2:Y9:75:VAL:HG11 | 2:Y9:94:SER:HB2 | 1.91 | 0.52 |
| 1:Z0:8:GLN:HG2 | 1:Z0:17:GLY:HA3 | 1.91 | 0.52 |
| 1:Z2:190:HIS:CD2 | 1:Z2:414:ASN:HB2 | 2.43 | 0.52 |
| 1:0A:190:HIS:NE2 | 1:0A:414:ASN:OD1 | 2.42 | 0.52 |
| 2:0J:322:ASP:HB2 | 2:0J:373:ARG:HH21 | 1.74 | 0.52 |
| 1:0M:260:PHE:HB2 | 1:0M:263:LEU:HG | 1.91 | 0.52 |
| 2:0N:90:GLU:HB2 | 2:1D:283:HIS:CE1 | 2.43 | 0.52 |
| 1:0S:51:PHE:HB3 | 1:0S:59:TYR:HB3 | 1.92 | 0.52 |
| 1:0U:393:ALA:C | 1:0U:395:LEU:N | 2.63 | 0.52 |
| 2:0X:119:LEU:HD11 | 2:0X:156:ARG:HD3 | 1.90 | 0.52 |
| 2:1D:317:LEU:HB3 | 2:1D:319:TYR:CE1 | 2.45 | 0.52 |
| 2:1L:9:ILE:HD13 | 2:1L:150:GLY:HA2 | 1.90 | 0.52 |
| 1:1M:35:THR:OG1 | 1:1M:37:HIS:NE2 | 2.42 | 0.52 |
| 2:1T:90:GLU:O | 2:1T:121:ARG:NH1 | 2.32 | 0.52 |
| 2:2B:177:VAL:HG13 | 1:2C:327:ASP:OD1 | 2.09 | 0.52 |
| 1:2C:193:VAL:HG23 | 1:2C:194:GLU:OE2 | 2.08 | 0.52 |
| 2:2F:305:CYS:SG | 2:2F:383:ALA:HB1 | 2.49 | 0.52 |
| 2:2H:66:ILE:HG13 | 2:2H:91:GLN:O | 2.10 | 0.52 |
| 1:2I:177:ASP:OD1 | 1:2I:178:THR:HG23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2J:121:ARG:HE | 2:2J:124:LYS:HD3 | 1.74 | 0.52 |
| 2:2J:176:GLN:HG2 | 2:2J:177:VAL:HG23 | 1.90 | 0.52 |
| 1:2M:244:GLY:H | 1:2M:247:ASN:HD21 | 1.57 | 0.52 |
| 1:2Q:345:ILE:HB | 1:2Q:348:ASN:HD21 | 1.74 | 0.52 |
| 1:2U:22:GLU:HG3 | 1:2U:81:TYR:CD2 | 2.45 | 0.52 |
| 1:3C:201:VAL:HG12 | 1:3C:266:PHE:O | 2.08 | 0.52 |
| 2:3F:198:THR:HG21 | 2:3F:201:ALA:HB2 | 1.90 | 0.52 |
| 2:3H:301:MET:HE1 | 2:3H:307:PRO:HD3 | 1.91 | 0.52 |
| 2:3J:392:ASP:OD2 | 2:3J:422:ARG:NH1 | 2.42 | 0.52 |
| 1:3K:320:ARG:HH21 | 38:8B:171:ASP:HB3 | 1.74 | 0.52 |
| 2:3N:129:CYS:SG | 2:3N:130:THR:N | 2.83 | 0.52 |
| 3:3V:161:PHE:HB3 | 3:3V:180:VAL:HG23 | 1.91 | 0.52 |
| 3:3Z:161:PHE:HB3 | 3:3Z:180:VAL:HG23 | 1.91 | 0.52 |
| 3:4B:252:LYS:HD3 | 3:4B:270:LEU:HD21 | 1.92 | 0.52 |
| 3:4D:161:PHE:HB3 | 3:4D:180:VAL:HG23 | 1.91 | 0.52 |
| 4:4E:109:GLN:HE22 | 4:4E:120:THR:HB | 1.74 | 0.52 |
| 5:4L:300:GLU:O | 5:4L:304:LEU:HG | 2.09 | 0.52 |
| 5:4L:328:GLU:O | 5:4L:332:THR:HG23 | 2.09 | 0.52 |
| 5:4L:443:GLU:O | 5:4L:447:GLU:HG3 | 2.09 | 0.52 |
| 7:4Q:367:ARG:HG2 | 7:4R:10:ASN:OD1 | 2.08 | 0.52 |
| 7:4S:6:ALA:C | 7:4S:8:VAL:H | 2.12 | 0.52 |
| 7:4T:292:GLU:HA | 7:4T:295:GLU:HG3 | 1.90 | 0.52 |
| 10:5B:135:ARG:O | 10:5B:139:MET:HG2 | 2.09 | 0.52 |
| 12:5F:148:MET:N | 12:5F:148:MET:SD | 2.82 | 0.52 |
| 14:5M:302:MET:SD | 14:5M:307:PHE:HE1 | 2.33 | 0.52 |
| 14:5N:251:GLY:O | 14:5N:267:THR:OG1 | 2.28 | 0.52 |
| 14:5N:302:MET:SD | 14:5N:307:PHE:HE1 | 2.33 | 0.52 |
| 20:6F:206:PRO:O | 20:6F:211:ARG:NH2 | 2.42 | 0.52 |
| 24:6U:322:LEU:HD23 | 24:6U:323:LYS:O | 2.09 | 0.52 |
| 24:6Y:480:ASN:ND2 | 24:6Y:503:ILE:HD12 | 2.21 | 0.52 |
| 24:7A:6:PRO:HG2 | 31:7N:83:THR:HG23 | 1.92 | 0.52 |
| 29:7J:393:HIS:CE1 | 29:7J:402:LEU:HD22 | 2.44 | 0.52 |
| 31:7M:45:GLU:OE1 | 31:7M:45:GLU:N | 2.29 | 0.52 |
| 35:7T:57:GLU:HA | 35:7T:60:PHE:CE1 | 2.45 | 0.52 |
| 35:7U:221:GLN:NE2 | 35:7U:224:GLU:OE2 | 2.42 | 0.52 |
| 37:7Y:61:VAL:O | 37:7Y:64:TRP:N | 2.43 | 0.52 |
| 2:A2:206:ASN:OD1 | 41:A2:501:GTP:N2 | 2.42 | 0.52 |
| 1:G6:166:THR:OG1 | 1:G6:199:CYS:SG | 2.67 | 0.52 |
| 1:G6:180:VAL:HG23 | 1:G6:184:ASN:HD21 | 1.74 | 0.52 |
| 1:G6:207:LEU:HB3 | 1:G6:225:LEU:HD22 | 1.91 | 0.52 |
| 2:G9:23:LEU:O | 2:G9:27:GLU:HG3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G9:156:ARG:HA | 2:G9:159:VAL:HG22 | 1.91 | 0.52 |
| 2:H3:55:GLU:HG2 | 2:H3:61:HIS:CE1 | 2.44 | 0.52 |
| 2:H7:287:SER:OG | 2:H7:288:VAL:N | 2.42 | 0.52 |
| 2:H9:204:LEU:HD23 | 2:H9:231:ILE:HD12 | 1.91 | 0.52 |
| 1:I0:122:LYS:HZ2 | 1:J6:291:GLN:HB3 | 1.75 | 0.52 |
| 2:I7:34:GLY:HA3 | 2:I7:60:LYS:NZ | 2.24 | 0.52 |
| 1:J4:173:PRO:HD2 | 1:J4:380:ARG:HH21 | 1.74 | 0.52 |
| 2:J9:306:ASP:HB3 | 2:J9:309:HIS:HD2 | 1.75 | 0.52 |
| 2:J9:313:MET:HE1 | 2:J9:435:VAL:HG11 | 1.92 | 0.52 |
| 2:K3:217:LEU:HG | 2:K3:367:ASP:OD2 | 2.10 | 0.52 |
| 1:L0:77:ARG:HE | 1:L0:90:PHE:HE2 | 1.57 | 0.52 |
| 2:L1:204:LEU:HD13 | 2:L1:231:ILE:HD12 | 1.91 | 0.52 |
| 2:L3:387:ILE:HG12 | 2:L3:390:ARG:HH22 | 1.74 | 0.52 |
| 1:L4:58:ARG:HD3 | 1:N0:280:GLN:HE22 | 1.74 | 0.52 |
| 2:M5:14:ILE:O | 2:M5:18:ASN:HB2 | 2.09 | 0.52 |
| 2:M5:205:ASP:OD1 | 2:M5:303:VAL:HA | 2.10 | 0.52 |
| 2:N5:8:HIS:CD2 | 2:N5:138:PHE:HD2 | 2.27 | 0.52 |
| 2:N7:81:GLY:O | 2:N7:84:ARG:NH1 | 2.43 | 0.52 |
| 1:O8:138:SER:OG | 1:O8:139:LEU:N | 2.43 | 0.52 |
| 2:O9:167:LEU:HD13 | 2:O9:200:VAL:HB | 1.91 | 0.52 |
| 1:P4:4:ILE:HB | 1:P4:50:TYR:HE1 | 1.74 | 0.52 |
| 1:P4:156:ARG:NH1 | 1:P4:197:ASP:OD1 | 2.42 | 0.52 |
| 1:Q2:45:GLU:HG3 | 1:Q2:46:ARG:HG2 | 1.90 | 0.52 |
| 1:Q4:217:LEU:HA | 20:6F:184:ARG:HH12 | 1.74 | 0.52 |
| 2:Q9:2:ARG:N | 2:Q9:3:GLU:OE2 | 2.43 | 0.52 |
| 2:R5:394:LYS:HB2 | 1:R6:346:PRO:HG3 | 1.91 | 0.52 |
| 1:T0:350:LYS:NZ | 1:T0:351:SER:O | 2.39 | 0.52 |
| 2:T1:105:ARG:O | 2:T1:109:THR:OG1 | 2.22 | 0.52 |
| 2:T3:176:GLN:OE1 | 2:T3:176:GLN:N | 2.43 | 0.52 |
| 1:T4:155:ILE:HG13 | 1:T4:164:MET:HE1 | 1.92 | 0.52 |
| 1:T4:418:LEU:HG | 1:T4:422:TYR:HE2 | 1.74 | 0.52 |
| 2:U1:292:THR:HG21 | 2:U1:331:SER:HB3 | 1.92 | 0.52 |
| 2:U3:98:ASP:OD1 | 2:U3:99:ALA:N | 2.43 | 0.52 |
| 2:U5:72:PRO:HD2 | 1:U6:2:ARG:NH1 | 2.25 | 0.52 |
| 1:U8:121:ARG:NH2 | 1:U8:158:GLU:OE2 | 2.33 | 0.52 |
| 2:U9:88:HIS:HA | 2:W5:283:HIS:CD2 | 2.45 | 0.52 |
| 2:U9:133:GLN:HB3 | 2:U9:252:ILE:HG21 | 1.92 | 0.52 |
| 2:U9:213:CYS:HA | 2:U9:217:LEU:HB3 | 1.91 | 0.52 |
| 1:V2:178:THR:OG1 | 1:V2:181:GLU:HG3 | 2.09 | 0.52 |
| 2:V7:119:LEU:HA | 2:V7:122:ILE:HG22 | 1.91 | 0.52 |
| 1:V8:248:ALA:HA | 1:V8:252:LYS:HD2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V9:53:PHE:HB3 | 2:V9:61:HIS:HB3 | 1.92 | 0.52 |
| 1:W0:145:SER:OG | 1:W0:188:SER:OG | 2.14 | 0.52 |
| 1:W6:170:VAL:N | 1:W6:202:LEU:O | 2.36 | 0.52 |
| 1:X2:50:TYR:CE2 | 1:X2:241:ARG:HD3 | 2.44 | 0.52 |
| 1:X2:174:LYS:HG3 | 1:X2:380:ARG:NH2 | 2.24 | 0.52 |
| 2:X3:322:ASP:OD2 | 2:X3:373:ARG:NH2 | 2.42 | 0.52 |
| 1:X4:67:ASP:OD1 | 1:X4:67:ASP:N | 2.42 | 0.52 |
| 2:X5:8:HIS:HE1 | 2:X5:21:TRP:HE1 | 1.58 | 0.52 |
| 1:Y0:328:GLU:OE2 | 1:Y0:332:ASN:ND2 | 2.42 | 0.52 |
| 2:Y5:34:GLY:HA3 | 2:Y5:60:LYS:HZ2 | 1.74 | 0.52 |
| 1:Y6:58:ARG:HD3 | 1:Y6:59:TYR:N | 2.24 | 0.52 |
| 2:Y9:69:ASP:OD1 | 2:Y9:70:LEU:N | 2.43 | 0.52 |
| 2:Z1:56:THR:HG22 | 2:0H:285:GLN:HB2 | 1.92 | 0.52 |
| 1:Z4:67:ASP:OD2 | 1:Z4:72:THR:OG1 | 2.27 | 0.52 |
| 2:Z5:5:ILE:HD13 | 2:Z5:125:LEU:HG | 1.92 | 0.52 |
| 1:Z8:405:GLU:HA | 1:Z8:408:PHE:HD2 | 1.75 | 0.52 |
| 2:0F:227:LEU:O | 2:0F:231:ILE:HG12 | 2.10 | 0.52 |
| 2:0J:12:ALA:O | 2:0J:16:VAL:HG23 | 2.10 | 0.52 |
| 2:0J:82:THR:O | 2:0J:84:ARG:NH1 | 2.42 | 0.52 |
| 2:0L:156:ARG:HA | 2:0L:159:VAL:HG12 | 1.92 | 0.52 |
| 2:0L:381:SER:OG | 2:0L:382:THR:N | 2.42 | 0.52 |
| 2:1D:116:ASP:N | 2:1D:116:ASP:OD1 | 2.40 | 0.52 |
| 1:1W:3:GLU:HB2 | 1:1W:130:LEU:HA | 1.92 | 0.52 |
| 1:1W:100:ASN:HB3 | 1:1W:103:LYS:HB2 | 1.90 | 0.52 |
| 2:1X:187:SER:O | 2:1X:191:THR:HG23 | 2.08 | 0.52 |
| 2:1Z:246:GLY:HA3 | 2:1Z:356:ASN:HA | 1.91 | 0.52 |
| 2:1Z:279:GLU:OE1 | 10:5A:275:ASN:ND2 | 2.43 | 0.52 |
| 2:1Z:331:SER:O | 2:1Z:335:ILE:HG13 | 2.10 | 0.52 |
| 1:2E:12:CYS:SG | 1:2E:13:GLY:N | 2.82 | 0.52 |
| 1:2E:286:VAL:HG12 | 1:2E:329:GLN:HG3 | 1.91 | 0.52 |
| 2:2H:3:GLU:HB2 | 2:2H:129:CYS:SG | 2.50 | 0.52 |
| 1:2I:135:VAL:HB | 1:2I:166:THR:HG22 | 1.92 | 0.52 |
| 1:2I:335:ASN:O | 1:2I:338:SER:OG | 2.28 | 0.52 |
| 1:2K:156:ARG:NH1 | 1:2K:197:ASP:OD1 | 2.43 | 0.52 |
| 2:2P:368:LEU:O | 10:5C:166:GLN:NE2 | 2.37 | 0.52 |
| 1:2W:244:GLY:H | 1:2W:247:ASN:HD21 | 1.58 | 0.52 |
| 1:2Y:56:GLY:HA3 | 38:8C:161:GLN:CD | 2.29 | 0.52 |
| 1:3A:418:LEU:O | 1:3A:421:GLU:HG2 | 2.08 | 0.52 |
| 2:3B:276:ILE:HD11 | 2:3B:280:LYS:HB3 | 1.92 | 0.52 |
| 2:3D:214:ARG:HH22 | 38:8D:66:TYR:HD1 | 1.55 | 0.52 |
| 2:3H:90:GLU:HG2 | 2:3H:121:ARG:HH22 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3O:77:ARG:CZ | 3:4F:18:LYS:HB3 | 2.40 | 0.52 |
| 1:3O:219:THR:HB | 2:3P:324:VAL:HG11 | 1.91 | 0.52 |
| 2:3T:13:GLY:O | 2:3T:16:VAL:HG22 | 2.09 | 0.52 |
| 3:3V:252:LYS:HD3 | 3:3V:270:LEU:HD21 | 1.92 | 0.52 |
| 4:4A:109:GLN:HE22 | 4:4A:120:THR:HB | 1.74 | 0.52 |
| 3:4D:252:LYS:HD3 | 3:4D:270:LEU:HD21 | 1.92 | 0.52 |
| 3:4H:252:LYS:HD3 | 3:4H:270:LEU:HD21 | 1.92 | 0.52 |
| 8:4W:392:ALA:HA | 8:4W:395:ARG:HE | 1.74 | 0.52 |
| 15:5P:20:ILE:HD11 | 19:6E:104:TYR:CE1 | 2.45 | 0.52 |
| 19:6E:181:THR:O | 19:6E:185:GLU:HG2 | 2.10 | 0.52 |
| 20:6F:375:PRO:HG3 | 20:6F:383:ARG:HB2 | 1.92 | 0.52 |
| 21:6H:51:ARG:HE | 21:6H:89:ILE:HG21 | 1.74 | 0.52 |
| 21:6H:106:ARG:HB3 | 24:6X:81:THR:HG23 | 1.92 | 0.52 |
| 22:6N:122:ALA:HB3 | 22:6N:128:GLU:HG3 | 1.91 | 0.52 |
| 22:6O:45:PRO:HB2 | 22:6O:52:TYR:HB2 | 1.91 | 0.52 |
| 24:6V:253:PRO:HB2 | 24:6V:256:LEU:HD13 | 1.90 | 0.52 |
| 24:6X:322:LEU:HD23 | 24:6X:323:LYS:O | 2.09 | 0.52 |
| 24:6Y:450:VAL:HB | 24:6Y:469:PHE:CE2 | 2.45 | 0.52 |
| 24:6Z:124:TYR:N | 24:6Z:124:TYR:HD1 | 2.06 | 0.52 |
| 38:8A:158:MET:O | 38:8A:162:VAL:HG23 | 2.10 | 0.52 |
| 1:1:306:ARG:NH2 | 3:3V:60:PRO:HD2 | 2.24 | 0.52 |
| 2:A2:42:ILE:CD1 | 24:6Y:93:ARG:CZ | 2.68 | 0.52 |
| 2:G1:238:LEU:HD11 | 2:G1:255:PHE:CZ | 2.44 | 0.52 |
| 1:G2:216:LYS:O | 24:6W:422:ASN:ND2 | 2.43 | 0.52 |
| 2:G5:276:ILE:CD1 | 2:G5:281:ALA:HA | 2.39 | 0.52 |
| 1:G6:3:GLU:HB2 | 1:G6:130:LEU:HD13 | 1.91 | 0.52 |
| 2:G9:183:GLU:HG2 | 2:G9:184:PRO:HD3 | 1.92 | 0.52 |
| 2:G9:421:ALA:O | 2:G9:425:LEU:HG | 2.10 | 0.52 |
| 2:H3:133:GLN:HB3 | 2:H3:252:ILE:HD11 | 1.91 | 0.52 |
| 2:H3:318:MET:HB2 | 2:H3:376:CYS:HB3 | 1.90 | 0.52 |
| 1:H8:39:ASP:N | 1:H8:39:ASP:OD1 | 2.38 | 0.52 |
| 2:H9:69:ASP:OD1 | 2:H9:70:LEU:N | 2.42 | 0.52 |
| 1:I4:260:PHE:HB2 | 1:I4:263:LEU:HD23 | 1.91 | 0.52 |
| 2:I9:189:LEU:HD11 | 2:I9:418:PHE:HE1 | 1.74 | 0.52 |
| 1:J0:215:LEU:HB3 | 1:J0:217:LEU:HG | 1.91 | 0.52 |
| 1:J4:5:VAL:HG23 | 1:J4:62:ARG:HG2 | 1.92 | 0.52 |
| 2:J7:266:HIS:ND1 | 2:J7:266:HIS:O | 2.42 | 0.52 |
| 1:K4:198:GLU:HA | 1:K4:264:HIS:HB2 | 1.92 | 0.52 |
| 2:K5:9:ILE:HG22 | 2:K5:146:GLY:HA2 | 1.91 | 0.52 |
| 1:K6:186:THR:HG22 | 1:K6:411:ALA:HB1 | 1.92 | 0.52 |
| 1:L0:382:SER:HB3 | 1:L0:415:MET:HG2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M2:54:ALA:HA | 2:N9:285:GLN:HB2 | 1.92 | 0.52 |
| 1:N0:371:SER:OG | 1:N0:372:THR:N | 2.43 | 0.52 |
| 1:N2:2:ARG:HE | 1:N2:240:LEU:HD22 | 1.75 | 0.52 |
| 1:O0:276:ARG:HA | 1:O0:279:GLN:HG3 | 1.90 | 0.52 |
| 1:O2:309:ARG:H | 1:O2:372:THR:HG22 | 1.73 | 0.52 |
| 1:O4:294:TRP:CD1 | 1:O4:333:VAL:HG21 | 2.45 | 0.52 |
| 2:O7:407:TRP:O | 2:O7:411:GLU:HG2 | 2.10 | 0.52 |
| 1:O8:274:THR:HG21 | 1:O8:282:ARG:HD2 | 1.91 | 0.52 |
| 1:P6:404:ASP:HB2 | 1:P6:406:MET:SD | 2.50 | 0.52 |
| 1:Q2:31:ASP:OD1 | 1:Q2:35:THR:N | 2.36 | 0.52 |
| 1:R0:404:ASP:OD2 | 1:R0:405:GLU:N | 2.43 | 0.52 |
| 1:S2:183:TYR:HA | 1:S2:385:PHE:HE2 | 1.73 | 0.52 |
| 2:T1:90:GLU:HG2 | 2:T1:121:ARG:HH12 | 1.74 | 0.52 |
| 1:T4:290:THR:HG21 | 1:T4:329:GLN:HE21 | 1.75 | 0.52 |
| 2:U5:90:GLU:O | 2:U5:121:ARG:NH1 | 2.39 | 0.52 |
| 2:V7:8:HIS:HB2 | 2:V7:67:PHE:HD1 | 1.74 | 0.52 |
| 1:W6:68:LEU:HD23 | 1:W6:93:GLY:HA3 | 1.92 | 0.52 |
| 2:W7:88:HIS:CD2 | 2:W7:121:ARG:HH22 | 2.28 | 0.52 |
| 1:W8:204:ASN:OD1 | 39:W8:503:GDP:O2' | 2.28 | 0.52 |
| 2:W9:384:ILE:HA | 2:W9:387:ILE:HD12 | 1.91 | 0.52 |
| 1:X8:21:TRP:O | 1:X8:25:SER:OG | 2.21 | 0.52 |
| 2:Y5:195:LEU:HD21 | 2:Y5:428:LEU:HD12 | 1.90 | 0.52 |
| 1:Y6:192:LEU:HD22 | 1:Y6:196:ALA:HB2 | 1.92 | 0.52 |
| 1:Z0:311:LEU:HD23 | 1:Z0:312:THR:HG23 | 1.91 | 0.52 |
| 1:0C:182:PRO:HG2 | 1:0C:388:MET:HE2 | 1.92 | 0.52 |
| 1:0C:262:ARG:HH21 | 1:0C:418:LEU:HD13 | 1.73 | 0.52 |
| 2:0F:9:ILE:HG22 | 2:0F:146:GLY:HA2 | 1.91 | 0.52 |
| 2:0F:171:VAL:HG22 | 2:0F:204:LEU:HD11 | 1.92 | 0.52 |
| 2:0J:217:LEU:HD13 | 2:0J:367:ASP:OD2 | 2.10 | 0.52 |
| 2:0J:244:PHE:HB2 | 2:0J:356:ASN:HD21 | 1.74 | 0.52 |
| 2:0N:296:PHE:HE2 | 2:0N:335:ILE:HD12 | 1.74 | 0.52 |
| 2:0P:296:PHE:HE2 | 2:0P:335:ILE:HD12 | 1.74 | 0.52 |
| 2:0R:109:THR:OG1 | 2:0R:411:GLU:OE2 | 2.25 | 0.52 |
| 1:0U:393:ALA:C | 1:0U:395:LEU:H | 2.13 | 0.52 |
| 1:0Y:66:MET:HE1 | 1:0Y:147:MET:HB3 | 1.91 | 0.52 |
| 2:0Z:69:ASP:OD2 | 2:0Z:70:LEU:N | 2.43 | 0.52 |
| 2:1F:111:GLY:O | 2:1F:115:VAL:HG12 | 2.09 | 0.52 |
| 2:1H:187:SER:O | 2:1H:191:THR:HG23 | 2.10 | 0.52 |
| 1:1K:189:VAL:O | 1:1K:193:VAL:HG13 | 2.10 | 0.52 |
| 1:1O:233:MET:HA | 1:1O:236:ILE:HD12 | 1.92 | 0.52 |
| 1:1Q:130:LEU:HB2 | 1:1Q:162:ARG:HE | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1U:213:ARG:HE | 1:1U:297:LYS:HE3 | 1.73 | 0.52 |
| 2:1V:288:VAL:O | 2:1V:292:THR:HG23 | 2.08 | 0.52 |
| 1:1W:34:GLY:HA3 | 1:1W:58:ARG:CD | 2.40 | 0.52 |
| 2:1X:413:MET:HB3 | 2:1X:417:GLU:OE2 | 2.10 | 0.52 |
| 1:2A:69:GLU:O | 1:2A:72:THR:OG1 | 2.27 | 0.52 |
| 2:2B:417:GLU:HA | 2:2B:420:GLU:HG2 | 1.91 | 0.52 |
| 2:2H:394:LYS:HB2 | 1:2I:346:PRO:HG3 | 1.92 | 0.52 |
| 2:2J:317:LEU:HB3 | 2:2J:319:TYR:HE1 | 1.75 | 0.52 |
| 2:2T:214:ARG:CZ | 38:8A:18:VAL:HA | 2.39 | 0.52 |
| 1:3A:382:SER:HB3 | 1:3A:415:MET:HG2 | 1.91 | 0.52 |
| 2:3D:362:VAL:HG21 | 10:5D:220:GLN:HE22 | 1.75 | 0.52 |
| 2:3L:119:LEU:HA | 2:3L:122:ILE:HG22 | 1.91 | 0.52 |
| 2:3N:66:ILE:HG23 | 2:3N:125:LEU:HD11 | 1.92 | 0.52 |
| 2:3P:311:LYS:HG2 | 2:3P:342:GLN:HG3 | 1.90 | 0.52 |
| 2:3R:220:GLU:HB3 | 38:8D:177:HIS:HB2 | 1.92 | 0.52 |
| 2:3T:255:PHE:HA | 2:3T:259:LEU:HD13 | 1.92 | 0.52 |
| 4:3W:109:GLN:HE22 | 4:3W:120:THR:HB | 1.74 | 0.52 |
| 3:3Z:252:LYS:HD3 | 3:3Z:270:LEU:HD21 | 1.92 | 0.52 |
| 5:4M:76:LEU:HA | 15:5P:361:LEU:HD21 | 1.92 | 0.52 |
| 6:4O:415:HIS:O | 6:4O:418:GLU:HG2 | 2.10 | 0.52 |
| 7:4R:283:GLU:OE2 | 20:6F:390:ARG:NH2 | 2.43 | 0.52 |
| 12:5G:309:THR:OG1 | 12:5G:314:GLN:OE1 | 2.25 | 0.52 |
| 15:5O:241:LEU:HD23 | 15:5O:308:ALA:HB2 | 1.90 | 0.52 |
| 17:5S:144:LYS:HA | 17:5S:147:VAL:HG12 | 1.91 | 0.52 |
| 17:5S:182:VAL:O | 17:5S:186:LYS:HG2 | 2.09 | 0.52 |
| 17:5V:224:ARG:NH2 | 17:5V:224:ARG:CB | 2.73 | 0.52 |
| 18:5Z:5:VAL:HG11 | 18:5Z:62:GLU:HG2 | 1.89 | 0.52 |
| 21:6H:51:ARG:NE | 21:6H:89:ILE:HG21 | 2.24 | 0.52 |
| 24:6T:119:VAL:HG21 | 24:6T:179:PHE:HD1 | 1.74 | 0.52 |
| 24:6X:451:LYS:HB3 | 24:6X:468:ARG:HH11 | 1.74 | 0.52 |
| 29:7I:4:LYS:H | 29:7I:4:LYS:CD | 1.98 | 0.52 |
| 29:7I:31:PRO:HB2 | 29:7I:33:THR:HG22 | 1.91 | 0.52 |
| 33:7Q:179:GLN:N | 33:7Q:180:PRO:HD2 | 2.25 | 0.52 |
| 34:7S:216:MET:O | 34:7S:220:VAL:HG23 | 2.09 | 0.52 |
| 36:7V:76:GLN:O | 36:7V:80:THR:HG22 | 2.09 | 0.52 |
| 36:7W:76:GLN:O | 36:7W:80:THR:HG22 | 2.09 | 0.52 |
| 38:8D:91:GLN:HG3 | 38:8D:92:GLU:N | 2.25 | 0.52 |
| 2:A2:30:ILE:N | 26:7F:45:MET:HE1 | 2.23 | 0.52 |
| 1:C0:276:ARG:O | 24:6Z:115:ARG:NH2 | 2.34 | 0.52 |
| 1:C8:226:ASN:OD1 | 39:C8:502:GDP:N1 | 2.28 | 0.52 |
| 2:E1:15:GLN:OE1 | 41:E1:501:GTP:N7 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E5:282:TYR:CG | 22:6K:82:LEU:CD2 | 2.54 | 0.52 |
| 1:G2:212:PHE:CZ | 2:G3:326:LYS:HG3 | 2.45 | 0.52 |
| 2:G3:318:MET:HB2 | 2:G3:376:CYS:HB3 | 1.90 | 0.52 |
| 2:G5:88:HIS:ND1 | 2:I1:283:HIS:HA | 2.24 | 0.52 |
| 2:G5:381:SER:OG | 2:G5:382:THR:N | 2.42 | 0.52 |
| 1:G6:218:THR:HB | 24:6Y:418:ASP:OD1 | 2.09 | 0.52 |
| 2:G7:217:LEU:HD22 | 2:G7:367:ASP:HB2 | 1.91 | 0.52 |
| 1:H4:128:ASP:OD1 | 1:H4:129:CYS:N | 2.42 | 0.52 |
| 2:H7:191:THR:HA | 2:H7:194:LEU:HB3 | 1.91 | 0.52 |
| 2:H7:274:PRO:HB2 | 2:H7:276:ILE:HG12 | 1.92 | 0.52 |
| 2:J1:109:THR:OG1 | 2:J1:411:GLU:OE2 | 2.23 | 0.52 |
| 1:J2:77:ARG:HG3 | 16:5Q:180:VAL:CG2 | 2.40 | 0.52 |
| 2:J3:241:SER:OG | 2:J3:250:VAL:O | 2.23 | 0.52 |
| 2:K1:22:GLU:OE1 | 28:7X:420:TYR:HB3 | 2.09 | 0.52 |
| 2:K1:287:SER:OG | 2:K1:288:VAL:N | 2.42 | 0.52 |
| 2:K3:210:TYR:CE1 | 2:K3:227:LEU:HD11 | 2.42 | 0.52 |
| 1:K8:257:LEU:HA | 1:K8:312:THR:HG21 | 1.92 | 0.52 |
| 2:L7:4:VAL:HG12 | 2:L7:133:GLN:HB2 | 1.90 | 0.52 |
| 1:M2:87:PRO:HD2 | 2:N9:283:HIS:HB2 | 1.91 | 0.52 |
| 2:M3:79:ARG:NH1 | 2:M3:92:LEU:O | 2.42 | 0.52 |
| 1:M4:414:ASN:HA | 1:M4:417:ASP:OD2 | 2.10 | 0.52 |
| 2:M9:379:SER:OG | 2:M9:380:ASN:N | 2.43 | 0.52 |
| 2:N1:195:LEU:HD21 | 2:N1:264:ARG:HH11 | 1.75 | 0.52 |
| 2:N3:229:ARG:HH12 | 2:N3:368:LEU:HD12 | 1.74 | 0.52 |
| 2:N3:336:LYS:O | 2:N3:339:ARG:NH2 | 2.42 | 0.52 |
| 1:N6:337:ASN:HB2 | 1:N6:340:TYR:HD2 | 1.74 | 0.52 |
| 2:N7:129:CYS:SG | 2:N7:130:THR:N | 2.83 | 0.52 |
| 1:N8:39:ASP:OD1 | 1:N8:40:SER:N | 2.42 | 0.52 |
| 1:O0:139:LEU:HD12 | 1:O0:170:VAL:HG12 | 1.92 | 0.52 |
| 2:O3:9:ILE:HG22 | 2:O3:146:GLY:HA2 | 1.91 | 0.52 |
| 2:O3:322:ASP:OD1 | 2:O3:322:ASP:N | 2.42 | 0.52 |
| 1:O4:86:ARG:HG2 | 1:O4:88:ASP:H | 1.74 | 0.52 |
| 2:P3:137:VAL:HG11 | 2:P3:154:LEU:HD11 | 1.92 | 0.52 |
| 2:P7:259:LEU:HD21 | 2:P7:316:CYS:HB2 | 1.91 | 0.52 |
| 1:P8:39:ASP:OD1 | 21:6G:167:ARG:NH2 | 2.42 | 0.52 |
| 1:P8:292:GLN:HG2 | 1:P8:298:ASN:OD1 | 2.10 | 0.52 |
| 1:P8:334:GLN:HE22 | 1:P8:348:ASN:H | 1.56 | 0.52 |
| 1:R0:80:PRO:HB3 | 12:7B:9:GLY:HA3 | 1.92 | 0.52 |
| 1:R0:140:GLY:O | 1:R0:184:ASN:ND2 | 2.43 | 0.52 |
| 1:R0:183:TYR:HE2 | 1:R0:394:PHE:HB2 | 1.73 | 0.52 |
| 2:R3:33:ASP:O | 2:R3:60:LYS:NZ | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R5:212:ILE:O | 2:R5:216:SER:OG | 2.26 | 0.52 |
| 2:R9:333:ALA:O | 2:R9:337:THR:HG23 | 2.09 | 0.52 |
| 2:S1:3:GLU:HB2 | 2:S1:129:CYS:SG | 2.50 | 0.52 |
| 2:T1:430:LYS:HE2 | 17:5T:23:HIS:HB2 | 1.92 | 0.52 |
| 1:T4:301:CYS:SG | 1:T4:302:ALA:N | 2.83 | 0.52 |
| 2:T7:176:GLN:HE22 | 2:T7:207:GLU:HG2 | 1.75 | 0.52 |
| 1:T8:100:ASN:HB3 | 1:T8:103:LYS:HB2 | 1.92 | 0.52 |
| 1:U8:49:VAL:HG11 | 1:U8:241:ARG:HG2 | 1.91 | 0.52 |
| 1:V8:33:THR:O | 1:V8:58:ARG:NH2 | 2.43 | 0.52 |
| 2:W1:31:GLN:HE21 | 2:W1:37:PRO:HG3 | 1.74 | 0.52 |
| 2:W3:107:HIS:CD2 | 2:W3:152:LEU:HB2 | 2.44 | 0.52 |
| 1:X2:58:ARG:HH11 | 1:X2:84:ILE:HA | 1.74 | 0.52 |
| 2:X5:253:THR:O | 2:X5:257:THR:HG23 | 2.09 | 0.52 |
| 1:X6:204:ASN:ND2 | 39:X6:502:GDP:HN22 | 2.03 | 0.52 |
| 2:X7:399:TYR:O | 2:X7:402:ARG:NH1 | 2.43 | 0.52 |
| 2:X9:12:ALA:HB2 | 41:Y0:501:GTP:C8 | 2.45 | 0.52 |
| 1:Y2:171:PRO:O | 1:Y2:380:ARG:NH2 | 2.43 | 0.52 |
| 2:Z1:392:ASP:OD2 | 2:Z1:422:ARG:NH1 | 2.43 | 0.52 |
| 1:Z2:2:ARG:HB3 | 1:Z2:131:GLN:HB2 | 1.91 | 0.52 |
| 1:Z4:66:MET:HE1 | 1:Z4:147:MET:HG3 | 1.92 | 0.52 |
| 2:Z5:407:TRP:HZ2 | 1:Z6:258:ILE:HB | 1.75 | 0.52 |
| 2:Z7:133:GLN:HG3 | 2:Z7:242:LEU:HD11 | 1.92 | 0.52 |
| 1:0C:330:MET:HA | 1:0C:333:VAL:HG12 | 1.92 | 0.52 |
| 1:0G:54:ALA:HA | 1:0W:283:ALA:HB2 | 1.92 | 0.52 |
| 1:0G:165:LEU:HB3 | 1:0G:167:PHE:CZ | 2.44 | 0.52 |
| 1:0G:201:VAL:O | 1:0G:202:LEU:HD23 | 2.09 | 0.52 |
| 2:0P:25:CYS:SG | 2:0P:86:LEU:HD11 | 2.49 | 0.52 |
| 2:0R:34:GLY:HA3 | 2:0R:60:LYS:HZ2 | 1.75 | 0.52 |
| 1:0S:156:ARG:NH1 | 1:0S:160:PRO:O | 2.43 | 0.52 |
| 1:0U:293:MET:SD | 1:0U:367:PHE:HB2 | 2.50 | 0.52 |
| 1:0W:220:PRO:HD2 | 2:0X:326:LYS:HG2 | 1.90 | 0.52 |
| 1:1C:248:ALA:HA | 1:1C:252:LYS:HD2 | 1.91 | 0.52 |
| 1:1M:24:VAL:HG21 | 1:1M:50:TYR:CD2 | 2.45 | 0.52 |
| 2:1N:98:ASP:OD1 | 2:1N:99:ALA:N | 2.42 | 0.52 |
| 2:2B:123:ARG:NH2 | 2:2B:160:ASP:OD2 | 2.43 | 0.52 |
| 2:2H:251:ASP:OD1 | 2:2H:253:THR:OG1 | 2.26 | 0.52 |
| 2:2H:277:SER:OG | 2:2H:278:ALA:N | 2.42 | 0.52 |
| 2:2J:53:PHE:HB3 | 2:2J:61:HIS:HB3 | 1.92 | 0.52 |
| 1:2K:140:GLY:O | 1:2K:184:ASN:ND2 | 2.36 | 0.52 |
| 2:2N:123:ARG:NH1 | 38:8D:75:SER:O | 2.43 | 0.52 |
| 2:2N:195:LEU:HD11 | 2:2N:264:ARG:HD2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:204:LEU:HD23 | 2:2N:231:ILE:HD12 | 1.91 | 0.52 |
| 1:2Q:233:MET:O | 1:2Q:237:THR:HG22 | 2.10 | 0.52 |
| 1:2W:5:VAL:HG22 | 1:2W:133:PHE:HD1 | 1.74 | 0.52 |
| 1:2W:91:VAL:HG11 | 1:2W:116:VAL:HG23 | 1.91 | 0.52 |
| 1:3A:178:THR:OG1 | 1:3A:179:VAL:N | 2.43 | 0.52 |
| 2:3D:301:MET:HE1 | 2:3D:307:PRO:HD3 | 1.91 | 0.52 |
| 1:3I:113:ILE:HA | 1:3I:116:VAL:HG12 | 1.91 | 0.52 |
| 2:3J:50:ASN:O | 2:3J:64:ARG:NH2 | 2.43 | 0.52 |
| 2:3J:56:THR:OG1 | 3:3Z:34:SER:HA | 2.10 | 0.52 |
| 1:3K:371:SER:OG | 1:3K:372:THR:N | 2.42 | 0.52 |
| 1:3O:52:ASN:OD1 | 1:3O:52:ASN:N | 2.43 | 0.52 |
| 2:3R:333:ALA:O | 2:3R:337:THR:HG23 | 2.09 | 0.52 |
| 3:4D:149:ILE:HA | 3:4D:152:LEU:HD12 | 1.92 | 0.52 |
| 3:4F:161:PHE:HB3 | 3:4F:180:VAL:HG23 | 1.91 | 0.52 |
| 4:4I:109:GLN:HE22 | 4:4I:120:THR:HB | 1.74 | 0.52 |
| 5:4L:325:MET:O | 5:4L:329:ARG:HG2 | 2.10 | 0.52 |
| 7:4R:308:ARG:CZ | 20:6F:215:GLU:HG3 | 2.40 | 0.52 |
| 8:4W:146:ALA:O | 8:4W:150:THR:HG23 | 2.09 | 0.52 |
| 9:4Z:205:ARG:O | 9:4Z:209:GLU:HG2 | 2.10 | 0.52 |
| 10:5A:421:VAL:O | 10:5A:425:THR:HG23 | 2.10 | 0.52 |
| 10:5B:261:LYS:O | 10:5B:265:LYS:HG2 | 2.10 | 0.52 |
| 10:5C:166:GLN:O | 10:5C:169:GLU:HG2 | 2.09 | 0.52 |
| 12:5F:58:ARG:HD2 | 12:5G:316:GLN:HB2 | 1.92 | 0.52 |
| 12:5F:135:ARG:HH21 | 21:6H:148:HIS:HB3 | 1.75 | 0.52 |
| 14:5M:225:ARG:HG2 | 14:5M:225:ARG:NH1 | 2.23 | 0.52 |
| 15:5P:6:ARG:HG2 | 15:5P:29:TYR:CE1 | 2.45 | 0.52 |
| 15:5P:98:ILE:HG22 | 15:5P:159:VAL:HB | 1.91 | 0.52 |
| 15:5P:331:ASP:OD2 | 15:5P:334:LEU:HD13 | 2.09 | 0.52 |
| 17:5T:144:LYS:HA | 17:5T:147:VAL:HG12 | 1.91 | 0.52 |
| 17:5U:144:LYS:HA | 17:5U:147:VAL:HG12 | 1.91 | 0.52 |
| 22:6L:172:ARG:HH22 | 22:6L:176:LYS:HE2 | 1.74 | 0.52 |
| 22:6L:210:MET:O | 22:6L:213:THR:OG1 | 2.27 | 0.52 |
| 24:6W:41:ARG:NE | 24:6W:41:ARG:CA | 2.73 | 0.52 |
| 24:6Y:274:ARG:HD3 | 24:6Y:295:HIS:HE1 | 1.74 | 0.52 |
| 27:7G:13:ILE:HG13 | 27:7G:13:ILE:O | 2.10 | 0.52 |
| 38:8A:206:PRO:HG3 | 38:8A:209:HIS:CE1 | 2.44 | 0.52 |
| 1:B1:80:PRO:HD2 | 24:6V:221:ARG:HH12 | 1.75 | 0.52 |
| 1:C4:143:THR:N | 39:C4:501:GDP:O2B | 2.41 | 0.52 |
| 2:F9:221:ARG:NH2 | 22:6K:174:GLU:O | 2.42 | 0.52 |
| 1:G6:190:HIS:NE2 | 1:G6:414:ASN:OD1 | 2.43 | 0.52 |
| 1:G6:414:ASN:HA | 1:G6:417:ASP:OD2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H5:204:LEU:HD13 | 2:H5:231:ILE:HD12 | 1.91 | 0.52 |
| 1:H8:178:THR:OG1 | 1:H8:181:GLU:HG3 | 2.10 | 0.52 |
| 2:I3:301:MET:HE1 | 2:I3:307:PRO:HD3 | 1.92 | 0.52 |
| 2:I7:333:ALA:O | 2:I7:337:THR:HG23 | 2.10 | 0.52 |
| 1:I8:404:ASP:HB3 | 1:I8:406:MET:SD | 2.50 | 0.52 |
| 2:I9:90:GLU:HB3 | 2:I9:121:ARG:NH2 | 2.22 | 0.52 |
| 1:J8:7:ILE:HB | 1:J8:135:VAL:HG22 | 1.91 | 0.52 |
| 1:J8:57:GLY:HA2 | 29:7J:379:ASN:HD21 | 1.75 | 0.52 |
| 1:J8:113:ILE:HD13 | 1:J8:150:LEU:HD22 | 1.91 | 0.52 |
| 2:J9:60:LYS:NZ | 2:L5:282:TYR:HA | 2.25 | 0.52 |
| 2:K3:14:ILE:HD11 | 2:K3:74:VAL:HG13 | 1.91 | 0.52 |
| 1:L4:248:ALA:HA | 1:L4:252:LYS:HD2 | 1.91 | 0.52 |
| 2:M3:176:GLN:NE2 | 2:M3:207:GLU:OE2 | 2.43 | 0.52 |
| 2:M5:187:SER:O | 2:M5:191:THR:HG23 | 2.10 | 0.52 |
| 1:M6:75:SER:CB | 15:5P:48:LYS:CE | 2.88 | 0.52 |
| 1:M8:324:LYS:O | 1:M8:328:GLU:HG3 | 2.10 | 0.52 |
| 2:N3:103:PHE:CE1 | 2:N3:148:GLY:HA2 | 2.45 | 0.52 |
| 2:N9:250:VAL:HG23 | 2:N9:254:GLU:HG3 | 1.91 | 0.52 |
| 1:O8:233:MET:O | 1:O8:236:ILE:HG22 | 2.10 | 0.52 |
| 1:Q6:272:PRO:HB2 | 1:Q6:282:ARG:HH12 | 1.75 | 0.52 |
| 1:R0:177:ASP:O | 2:R1:352:LYS:HA | 2.10 | 0.52 |
| 2:R9:253:THR:O | 2:R9:257:THR:OG1 | 2.28 | 0.52 |
| 1:S4:309:ARG:H | 1:S4:372:THR:HG22 | 1.75 | 0.52 |
| 1:S4:371:SER:OG | 1:S4:372:THR:N | 2.43 | 0.52 |
| 1:S6:121:ARG:O | 3:3X:65:SER:OG | 2.28 | 0.52 |
| 1:S6:397:TRP:CZ2 | 2:S7:256:GLN:HB3 | 2.45 | 0.52 |
| 2:S9:90:GLU:C | 2:S9:121:ARG:HH12 | 2.13 | 0.52 |
| 2:S9:407:TRP:CG | 1:T0:255:VAL:HG23 | 2.44 | 0.52 |
| 1:T2:12:CYS:SG | 1:T2:13:GLY:N | 2.83 | 0.52 |
| 2:U5:327:ASP:OD1 | 2:U5:328:VAL:N | 2.43 | 0.52 |
| 2:U7:223:THR:HG23 | 2:U7:225:THR:HG22 | 1.91 | 0.52 |
| 1:V0:49:VAL:HG11 | 1:V0:241:ARG:HG2 | 1.92 | 0.52 |
| 2:V3:90:GLU:HB3 | 2:V3:121:ARG:HH22 | 1.75 | 0.52 |
| 1:V6:175:VAL:HG11 | 1:V6:204:ASN:HB2 | 1.91 | 0.52 |
| 1:W0:211:CYS:HA | 1:W0:215:LEU:HB2 | 1.90 | 0.52 |
| 1:X0:248:ALA:HA | 1:X0:252:LYS:HD2 | 1.92 | 0.52 |
| 2:X3:136:LEU:HD12 | 2:X3:167:LEU:HB2 | 1.92 | 0.52 |
| 1:X6:260:PHE:HD2 | 1:X6:263:LEU:HD12 | 1.73 | 0.52 |
| 1:Y4:328:GLU:OE2 | 1:Y4:332:ASN:ND2 | 2.43 | 0.52 |
| 2:Y5:65:CYS:SG | 2:Y5:66:ILE:N | 2.83 | 0.52 |
| 1:Z0:27:GLU:OE1 | 1:Z0:318:ARG:NH2 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z2:273:LEU:H | 1:Z2:292:GLN:HE22 | 1.58 | 0.52 |
| 2:Z7:216:SER:OG | 2:Z7:217:LEU:N | 2.43 | 0.52 |
| 2:Z7:269:LEU:N | 2:Z7:379:SER:O | 2.42 | 0.52 |
| 1:Z8:344:TRP:CE3 | 1:Z8:345:ILE:HG13 | 2.44 | 0.52 |
| 2:0B:8:HIS:CD2 | 2:0B:138:PHE:HD2 | 2.28 | 0.52 |
| 2:0L:204:LEU:HD23 | 2:0L:231:ILE:HD12 | 1.91 | 0.52 |
| 1:0O:163:MET:HB3 | 1:0O:250:LEU:HD22 | 1.92 | 0.52 |
| 1:0Q:12:CYS:O | 1:0Q:16:ILE:HG12 | 2.09 | 0.52 |
| 2:0V:55:GLU:HG2 | 2:0V:61:HIS:CE1 | 2.44 | 0.52 |
| 2:0X:56:THR:HG23 | 2:1N:285:GLN:HB2 | 1.92 | 0.52 |
| 2:0X:118:ALA:O | 2:0X:122:ILE:HG12 | 2.09 | 0.52 |
| 1:0Y:177:ASP:N | 1:0Y:181:GLU:OE2 | 2.42 | 0.52 |
| 1:1A:6:HIS:CE1 | 1:1A:8:GLN:HG2 | 2.45 | 0.52 |
| 2:1B:33:ASP:OD2 | 2:1B:35:GLN:NE2 | 2.43 | 0.52 |
| 2:1F:377:MET:O | 2:1F:378:ILE:HD13 | 2.10 | 0.52 |
| 1:1M:5:VAL:HG22 | 1:1M:133:PHE:HD1 | 1.74 | 0.52 |
| 1:1S:418:LEU:O | 1:1S:421:GLU:HG2 | 2.09 | 0.52 |
| 1:1U:218:THR:O | 2:1V:326:LYS:HE2 | 2.10 | 0.52 |
| 2:1V:191:THR:HA | 2:1V:194:LEU:HB3 | 1.92 | 0.52 |
| 1:2A:309:ARG:NH1 | 1:2A:339:SER:O | 2.43 | 0.52 |
| 2:2F:96:LYS:HZ2 | 38:8B:62:THR:HG21 | 1.74 | 0.52 |
| 1:2G:139:LEU:HD12 | 1:2G:170:VAL:HG12 | 1.92 | 0.52 |
| 2:2J:56:THR:HG23 | 2:2J:60:LYS:HB3 | 1.92 | 0.52 |
| 1:2M:397:TRP:HE1 | 2:2N:260:VAL:HG13 | 1.74 | 0.52 |
| 2:2T:90:GLU:O | 2:2T:121:ARG:NH1 | 2.32 | 0.52 |
| 2:2T:326:LYS:HG3 | 2:2T:327:ASP:N | 2.24 | 0.52 |
| 1:2U:177:ASP:O | 2:2V:352:LYS:HA | 2.10 | 0.52 |
| 2:2V:9:ILE:HD13 | 2:2V:150:GLY:HA2 | 1.91 | 0.52 |
| 2:2Z:239:THR:HG23 | 2:2Z:243:ARG:HH21 | 1.75 | 0.52 |
| 2:2Z:274:PRO:HB2 | 2:2Z:276:ILE:HG12 | 1.92 | 0.52 |
| 2:3B:21:TRP:CZ2 | 2:3B:65:CYS:HB3 | 2.45 | 0.52 |
| 2:3B:415:GLU:OE2 | 2:3B:419:SER:OG | 2.27 | 0.52 |
| 1:3C:51:PHE:HB3 | 1:3C:59:TYR:HB3 | 1.91 | 0.52 |
| 2:3D:47:ASP:OD1 | 2:3D:48:ALA:N | 2.43 | 0.52 |
| 1:3I:309:ARG:H | 1:3I:372:THR:HG22 | 1.75 | 0.52 |
| 2:3J:236:SER:O | 2:3J:243:ARG:NH2 | 2.42 | 0.52 |
| 2:3L:5:ILE:HD11 | 2:3L:135:PHE:CE1 | 2.45 | 0.52 |
| 1:3S:391:ARG:HD3 | 2:3T:346:TRP:CZ2 | 2.45 | 0.52 |
| 2:3T:317:LEU:HD23 | 2:3T:377:MET:HG3 | 1.91 | 0.52 |
| 3:3V:149:ILE:HA | 3:3V:152:LEU:HD12 | 1.92 | 0.52 |
| 3:3X:161:PHE:HB3 | 3:3X:180:VAL:HG23 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3Z:149:ILE:HA | 3:3Z:152:LEU:HD12 | 1.92 | 0.52 |
| 3:4B:161:PHE:HB3 | 3:4B:180:VAL:HG23 | 1.91 | 0.52 |
| 4:4C:109:GLN:HE22 | 4:4C:120:THR:HB | 1.74 | 0.52 |
| 3:4F:149:ILE:HA | 3:4F:152:LEU:HD12 | 1.92 | 0.52 |
| 4:4G:109:GLN:HE22 | 4:4G:120:THR:HB | 1.74 | 0.52 |
| 3:4H:149:ILE:HA | 3:4H:152:LEU:HD12 | 1.92 | 0.52 |
| 3:4J:243:LEU:N | 3:4J:244:PRO:HD2 | 2.25 | 0.52 |
| 6:4O:181:GLU:O | 6:4O:184:GLU:HG3 | 2.09 | 0.52 |
| 6:4O:309:MET:O | 6:4O:313:VAL:HG23 | 2.10 | 0.52 |
| 8:4W:402:VAL:O | 8:4W:405:GLU:HG3 | 2.10 | 0.52 |
| 10:5A:406:LEU:HA | 10:5A:409:ASN:ND2 | 2.24 | 0.52 |
| 12:5F:41:ALA:HB3 | 12:5F:44:ILE:CG2 | 2.38 | 0.52 |
| 14:5L:113:CYS:H | 14:5L:159:SER:HB3 | 1.73 | 0.52 |
| 14:5L:403:ASP:OD2 | 14:5L:405:LYS:HD2 | 2.10 | 0.52 |
| 14:5M:403:ASP:OD2 | 14:5M:405:LYS:HD2 | 2.10 | 0.52 |
| 14:5N:189:THR:OG1 | 14:5N:189:THR:O | 2.22 | 0.52 |
| 15:5P:180:ASP:OD1 | 15:5P:183:GLN:N | 2.33 | 0.52 |
| 22:6I:42:THR:HA | 22:6I:51:ILE:HD13 | 1.92 | 0.52 |
| 22:6K:238:LEU:HD21 | 22:6K:243:LEU:HD22 | 1.90 | 0.52 |
| 22:6L:137:GLU:O | 22:6L:141:LYS:HG2 | 2.10 | 0.52 |
| 22:6N:28:GLN:HG3 | 22:6N:29:GLU:OE2 | 2.10 | 0.52 |
| 22:6N:31:TYR:O | 22:6N:32:LYS:HG3 | 2.10 | 0.52 |
| 24:6T:242:PHE:O | 24:6T:246:VAL:HG23 | 2.10 | 0.52 |
| 24:6U:513:THR:HG23 | 24:6U:515:LEU:H | 1.74 | 0.52 |
| 24:6X:450:VAL:HG13 | 24:6X:469:PHE:O | 2.10 | 0.52 |
| 24:6Y:86:PRO:HD2 | 24:6Y:89:VAL:HG11 | 1.92 | 0.52 |
| 26:7F:58:ILE:HD13 | 26:7F:82:PRO:HB2 | 1.92 | 0.52 |
| 29:7J:316:VAL:HG12 | 29:7J:317:SER:N | 2.25 | 0.52 |
| 35:7U:121:ALA:O | 35:7U:124:GLN:HG3 | 2.10 | 0.52 |
| 2:4:283:HIS:HE1 | 2:S7:85:GLN:O | 1.93 | 0.52 |
| 2:8:221:ARG:C | 26:7E:77:ILE:O | 2.44 | 0.52 |
| 2:A4:324:VAL:CG1 | 26:7F:142:PHE:HZ | 2.23 | 0.52 |
| 1:C0:358:PRO:O | 18:6C:22:ARG:NH2 | 2.43 | 0.52 |
| 2:F3:26:LEU:HD21 | 22:6O:90:ALA:HB1 | 1.91 | 0.52 |
| 2:G3:392:ASP:OD2 | 2:G3:422:ARG:NH1 | 2.43 | 0.52 |
| 1:G6:134:GLN:HE21 | 1:G6:167:PHE:HE2 | 1.58 | 0.52 |
| 1:G6:218:THR:O | 2:G7:326:LYS:HE2 | 2.10 | 0.52 |
| 2:H1:227:LEU:O | 2:H1:230:LEU:HG | 2.10 | 0.52 |
| 2:H3:90:GLU:HB3 | 2:H3:121:ARG:NH2 | 2.25 | 0.52 |
| 2:H5:280:LYS:HA | 2:H5:283:HIS:HB3 | 1.92 | 0.52 |
| 1:I0:219:THR:HG21 | 24:6X:488:ARG:CD | 2.35 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I3:35:GLN:HB3 | 2:I3:59:GLY:O | 2.09 | 0.52 |
| 2:I7:222:PRO:HD2 | 1:I8:324:LYS:HE3 | 1.92 | 0.52 |
| 2:J1:9:ILE:HG22 | 2:J1:146:GLY:HA2 | 1.90 | 0.52 |
| 1:J4:35:THR:HG21 | 5:4M:120:ARG:HH11 | 1.74 | 0.52 |
| 1:J6:207:LEU:HB3 | 1:J6:225:LEU:HD22 | 1.92 | 0.52 |
| 2:J7:121:ARG:HD2 | 2:J7:121:ARG:O | 2.10 | 0.52 |
| 2:J9:14:ILE:HD11 | 2:J9:74:VAL:HG22 | 1.92 | 0.52 |
| 1:K0:5:VAL:HG12 | 1:K0:133:PHE:HD1 | 1.74 | 0.52 |
| 2:K3:129:CYS:SG | 2:K3:130:THR:N | 2.83 | 0.52 |
| 2:K7:88:HIS:HD1 | 2:M3:283:HIS:CB | 2.23 | 0.52 |
| 2:L3:98:ASP:OD1 | 2:L3:99:ALA:N | 2.42 | 0.52 |
| 1:L4:60:VAL:HG11 | 1:N0:281:TYR:HB3 | 1.91 | 0.52 |
| 1:M0:6:HIS:NE2 | 1:M0:136:CYS:SG | 2.79 | 0.52 |
| 2:O1:327:ASP:N | 2:O1:327:ASP:OD2 | 2.35 | 0.52 |
| 1:O4:245:GLN:HG2 | 19:6E:86:THR:HG21 | 1.92 | 0.52 |
| 1:O8:153:SER:HA | 1:O8:195:ASN:HD22 | 1.75 | 0.52 |
| 2:O9:236:SER:O | 2:O9:243:ARG:NH2 | 2.43 | 0.52 |
| 2:P7:90:GLU:HG2 | 2:P7:121:ARG:HH12 | 1.72 | 0.52 |
| 2:Q3:122:ILE:O | 2:Q3:125:LEU:HB2 | 2.09 | 0.52 |
| 1:R8:173:PRO:HB3 | 1:R8:384:GLN:HE22 | 1.74 | 0.52 |
| 1:R8:177:ASP:O | 2:R9:352:LYS:HA | 2.10 | 0.52 |
| 2:R9:119:LEU:HA | 2:R9:122:ILE:HG22 | 1.91 | 0.52 |
| 2:R9:223:THR:OG1 | 1:S0:245:GLN:NE2 | 2.43 | 0.52 |
| 2:S1:156:ARG:HA | 2:S1:159:VAL:HG12 | 1.91 | 0.52 |
| 1:S4:336:LYS:HD3 | 17:5R:48:THR:HG23 | 1.91 | 0.52 |
| 2:S5:324:VAL:HG23 | 2:S5:326:LYS:HG3 | 1.92 | 0.52 |
| 2:S5:434:GLU:OE1 | 13:5H:60:HIS:ND1 | 2.43 | 0.52 |
| 1:S8:5:VAL:HG22 | 1:S8:62:ARG:HD3 | 1.92 | 0.52 |
| 1:T8:183:TYR:HE2 | 1:T8:394:PHE:HB2 | 1.75 | 0.52 |
| 2:U3:287:SER:OG | 2:U3:288:VAL:N | 2.42 | 0.52 |
| 1:U6:175:VAL:HG12 | 2:U7:329:ASN:HD21 | 1.75 | 0.52 |
| 2:U9:90:GLU:HB3 | 2:U9:121:ARG:HH22 | 1.73 | 0.52 |
| 1:V2:177:ASP:O | 2:V3:352:LYS:HA | 2.10 | 0.52 |
| 1:V6:60:VAL:HG11 | 1:X2:281:TYR:HB3 | 1.92 | 0.52 |
| 2:V7:33:ASP:HA | 2:V7:85:GLN:HB2 | 1.91 | 0.52 |
| 2:V9:154:LEU:HD11 | 2:V9:166:LYS:HD2 | 1.92 | 0.52 |
| 1:W0:171:PRO:HB3 | 1:W0:181:GLU:OE2 | 2.10 | 0.52 |
| 1:W2:309:ARG:H | 1:W2:372:THR:HG22 | 1.75 | 0.52 |
| 2:W7:33:ASP:OD2 | 2:W7:35:GLN:NE2 | 2.43 | 0.52 |
| 2:X3:286:LEU:O | 2:X3:373:ARG:NH1 | 2.42 | 0.52 |
| 1:X4:122:LYS:O | 1:X4:126:SER:OG | 2.22 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X4:205:GLU:HG2 | 1:X4:206:ALA:N | 2.25 | 0.52 |
| 2:X7:282:TYR:CE2 | 2:X7:283:HIS:CE1 | 2.98 | 0.52 |
| 1:Y4:49:VAL:HG13 | 1:Y4:50:TYR:HD2 | 1.75 | 0.52 |
| 2:Y9:27:GLU:CD | 2:Y9:243:ARG:HH12 | 2.13 | 0.52 |
| 1:Z4:198:GLU:HA | 1:Z4:264:HIS:HB2 | 1.92 | 0.52 |
| 2:Z5:21:TRP:CZ3 | 2:Z5:63:PRO:HB3 | 2.45 | 0.52 |
| 2:Z7:252:ILE:HA | 2:Z7:255:PHE:CE2 | 2.45 | 0.52 |
| 1:0E:24:VAL:HA | 1:0E:27:GLU:HG2 | 1.92 | 0.52 |
| 1:0K:207:LEU:HB3 | 1:0K:225:LEU:HD22 | 1.92 | 0.52 |
| 2:0L:227:LEU:O | 2:0L:231:ILE:HG12 | 2.09 | 0.52 |
| 2:0N:175:PRO:HB3 | 2:0N:390:ARG:NE | 2.25 | 0.52 |
| 2:0N:213:CYS:SG | 2:0N:219:ILE:HB | 2.50 | 0.52 |
| 1:0Q:27:GLU:OE2 | 1:0Q:318:ARG:NH2 | 2.43 | 0.52 |
| 1:0Q:249:ASP:OD1 | 1:0Q:250:LEU:N | 2.43 | 0.52 |
| 1:0Q:265:PHE:HB3 | 1:0Q:374:ILE:HD13 | 1.92 | 0.52 |
| 1:0Q:286:VAL:HG23 | 1:0Q:287:PRO:HD3 | 1.91 | 0.52 |
| 1:0S:204:ASN:ND2 | 39:0S:502:GDP:N3 | 2.49 | 0.52 |
| 2:0V:183:GLU:HG3 | 2:0V:184:PRO:HD3 | 1.91 | 0.52 |
| 2:0V:212:ILE:O | 2:0V:216:SER:OG | 2.26 | 0.52 |
| 1:0W:301:CYS:SG | 1:0W:302:ALA:N | 2.83 | 0.52 |
| 1:1A:199:CYS:SG | 1:1A:200:MET:N | 2.82 | 0.52 |
| 2:1F:115:VAL:HG22 | 2:1F:119:LEU:HD23 | 1.92 | 0.52 |
| 2:1L:26:LEU:HD21 | 2:1L:363:VAL:HG12 | 1.91 | 0.52 |
| 1:1M:207:LEU:HB3 | 1:1M:225:LEU:HD22 | 1.92 | 0.52 |
| 2:1N:83:TYR:HB3 | 2:1N:86:LEU:CB | 2.40 | 0.52 |
| 2:1N:313:MET:SD | 2:1N:346:TRP:CZ2 | 3.01 | 0.52 |
| 2:1P:362:VAL:HG13 | 2:1P:370:LYS:HD3 | 1.92 | 0.52 |
| 1:1Q:385:PHE:HZ | 1:1Q:408:PHE:HD1 | 1.56 | 0.52 |
| 2:1R:145:THR:OG1 | 41:1S:501:GTP:O1B | 2.27 | 0.52 |
| 2:1T:116:ASP:N | 2:1T:116:ASP:OD1 | 2.40 | 0.52 |
| 2:1X:383:ALA:HA | 2:1X:386:GLU:OE1 | 2.09 | 0.52 |
| 2:1Z:258:ASN:HD22 | 2:1Z:352:LYS:NZ | 2.08 | 0.52 |
| 1:2C:5:VAL:HG12 | 1:2C:133:PHE:HD1 | 1.74 | 0.52 |
| 1:2C:211:CYS:HA | 1:2C:215:LEU:HB2 | 1.91 | 0.52 |
| 2:2J:195:LEU:O | 2:2J:266:HIS:NE2 | 2.36 | 0.52 |
| 2:2P:344:VAL:HG22 | 2:2P:346:TRP:H | 1.75 | 0.52 |
| 1:2Q:107:THR:OG1 | 1:2Q:108:GLU:OE1 | 2.20 | 0.52 |
| 1:2Q:328:GLU:CD | 38:7Z:1:MET:HB2 | 2.31 | 0.52 |
| 2:2Z:178:SER:HB3 | 2:2Z:183:GLU:OE2 | 2.10 | 0.52 |
| 2:3B:156:ARG:HA | 2:3B:159:VAL:HG12 | 1.92 | 0.52 |
| 1:3G:178:THR:OG1 | 1:3G:181:GLU:HG3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3O:145:SER:HG | 1:3O:188:SER:HG | 1.58 | 0.52 |
| 3:3X:149:ILE:HA | 3:3X:152:LEU:HD12 | 1.92 | 0.52 |
| 3:4B:149:ILE:HA | 3:4B:152:LEU:HD12 | 1.92 | 0.52 |
| 14:5M:415:LYS:CE | 23:6R:22:MET:CB | 2.68 | 0.52 |
| 14:5N:403:ASP:OD2 | 14:5N:405:LYS:HD2 | 2.10 | 0.52 |
| 15:5O:15:ASP:OD1 | 15:5O:15:ASP:N | 2.28 | 0.52 |
| 15:5O:167:GLY:O | 15:5O:171:LYS:HG2 | 2.10 | 0.52 |
| 16:5Q:63:ARG:NE | 16:5Q:95:SER:O | 2.30 | 0.52 |
| 17:5T:116:LYS:HG2 | 17:5T:117:PRO:HD2 | 1.92 | 0.52 |
| 21:6G:52:GLN:HG3 | 21:6G:55:TRP:HE1 | 1.74 | 0.52 |
| 22:6M:31:TYR:O | 22:6M:32:LYS:HG3 | 2.10 | 0.52 |
| 24:6T:482:ILE:N | 24:6T:482:ILE:CD1 | 2.72 | 0.52 |
| 24:6U:279:TRP:CZ2 | 24:6U:364:ARG:HG3 | 2.45 | 0.52 |
| 24:6U:555:THR:O | 24:6U:558:LEU:HG | 2.10 | 0.52 |
| 24:6Z:123:TYR:CE2 | 24:6Z:163:PRO:HG3 | 2.44 | 0.52 |
| 28:7H:316:ASN:O | 28:7H:320:THR:HG23 | 2.09 | 0.52 |
| 29:7J:390:LEU:CG | 29:7J:391:PRO:CD | 2.88 | 0.52 |
| 38:8A:82:ASP:CB | 38:8A:112:ILE:HG21 | 2.33 | 0.52 |
| 1:3:45:GLU:HG2 | 18:5X:35:LEU:HD12 | 1.92 | 0.51 |
| 2:E7:282:TYR:OH | 22:6L:82:LEU:N | 2.43 | 0.51 |
| 2:F7:221:ARG:NH1 | 22:6J:177:LEU:O | 2.43 | 0.51 |
| 1:H4:214:THR:O | 1:H4:275:SER:OG | 2.27 | 0.51 |
| 1:I2:391:ARG:HD3 | 2:I3:346:TRP:NE1 | 2.21 | 0.51 |
| 2:I3:287:SER:OG | 2:I3:288:VAL:N | 2.43 | 0.51 |
| 1:I4:276:ARG:HH11 | 24:6Z:491:GLY:CA | 2.23 | 0.51 |
| 1:J0:91:VAL:HG11 | 1:J0:116:VAL:HG23 | 1.92 | 0.51 |
| 2:J1:116:ASP:N | 2:J1:116:ASP:OD1 | 2.41 | 0.51 |
| 1:J4:40:SER:OG | 1:J4:41:ASP:N | 2.43 | 0.51 |
| 1:J8:219:THR:HA | 2:J9:326:LYS:NZ | 2.25 | 0.51 |
| 1:K0:248:ALA:HA | 1:K0:252:LYS:HD2 | 1.92 | 0.51 |
| 2:K1:34:GLY:HA3 | 2:K1:60:LYS:HZ2 | 1.75 | 0.51 |
| 2:K3:278:ALA:HA | 2:K3:369:ALA:HB2 | 1.92 | 0.51 |
| 2:K5:344:VAL:HG22 | 2:K5:346:TRP:H | 1.75 | 0.51 |
| 2:K7:213:CYS:SG | 2:K7:219:ILE:HB | 2.50 | 0.51 |
| 2:K9:129:CYS:SG | 2:K9:130:THR:N | 2.83 | 0.51 |
| 2:L3:155:GLU:HB3 | 2:L3:197:HIS:CE1 | 2.44 | 0.51 |
| 2:L9:88:HIS:CE1 | 1:N6:280:GLN:HB2 | 2.44 | 0.51 |
| 2:M1:84:ARG:HH12 | 27:7G:112:THR:HA | 1.75 | 0.51 |
| 2:M7:88:HIS:O | 1:O4:281:TYR:OH | 2.27 | 0.51 |
| 1:M8:260:PHE:HB2 | 1:M8:263:LEU:HD23 | 1.91 | 0.51 |
| 1:M8:282:ARG:HH21 | 1:M8:288:GLU:HB3 | 1.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N0:404:ASP:HB3 | 1:N0:406:MET:SD | 2.51 | 0.51 |
| 2:N1:405:VAL:HG13 | 2:N1:418:PHE:HE2 | 1.75 | 0.51 |
| 2:N3:209:ILE:HD13 | 2:N3:227:LEU:CD1 | 2.40 | 0.51 |
| 1:O2:45:GLU:HG3 | 1:O2:46:ARG:HG2 | 1.92 | 0.51 |
| 1:O4:334:GLN:HE22 | 1:O4:348:ASN:H | 1.58 | 0.51 |
| 2:Q3:327:ASP:OD1 | 2:Q3:328:VAL:N | 2.44 | 0.51 |
| 1:Q4:5:VAL:HB | 1:Q4:133:PHE:HD1 | 1.75 | 0.51 |
| 1:Q4:12:CYS:HB3 | 1:Q4:138:SER:HB3 | 1.92 | 0.51 |
| 2:S1:118:ALA:O | 2:S1:122:ILE:HG13 | 2.11 | 0.51 |
| 1:S4:128:ASP:OD1 | 1:S4:129:CYS:N | 2.42 | 0.51 |
| 2:S9:176:GLN:N | 2:S9:176:GLN:OE1 | 2.43 | 0.51 |
| 1:T4:193:VAL:HG13 | 1:T4:194:GLU:HG2 | 1.91 | 0.51 |
| 2:T5:170:THR:HG21 | 2:T5:194:LEU:HD11 | 1.92 | 0.51 |
| 2:T5:191:THR:HA | 2:T5:194:LEU:HB3 | 1.92 | 0.51 |
| 2:T7:66:ILE:HD12 | 2:T7:68:LEU:HD23 | 1.92 | 0.51 |
| 2:U1:11:GLN:NE2 | 1:U2:247:ASN:OD1 | 2.43 | 0.51 |
| 2:U1:187:SER:O | 2:U1:191:THR:HG23 | 2.11 | 0.51 |
| 1:U6:282:ARG:HH21 | 1:U6:284:LEU:HD13 | 1.75 | 0.51 |
| 1:U6:334:GLN:HE22 | 1:U6:348:ASN:H | 1.58 | 0.51 |
| 1:V2:220:PRO:HD2 | 2:V3:326:LYS:HD3 | 1.91 | 0.51 |
| 2:W9:317:LEU:HB3 | 2:W9:319:TYR:HE1 | 1.74 | 0.51 |
| 2:W9:363:VAL:HG23 | 2:W9:366:GLY:HA3 | 1.93 | 0.51 |
| 1:X2:273:LEU:H | 1:X2:292:GLN:NE2 | 2.06 | 0.51 |
| 1:X4:199:CYS:HG | 1:X4:265:PHE:HD1 | 1.58 | 0.51 |
| 1:X6:344:TRP:CE3 | 1:X6:345:ILE:HG13 | 2.45 | 0.51 |
| 1:Y0:371:SER:OG | 1:Y0:372:THR:N | 2.42 | 0.51 |
| 2:Y3:244:PHE:HB2 | 2:Y3:356:ASN:HD21 | 1.74 | 0.51 |
| 2:Y9:203:MET:HB2 | 2:Y9:303:VAL:HG21 | 1.92 | 0.51 |
| 2:Y9:275:ILE:HD12 | 2:Y9:368:LEU:HD21 | 1.91 | 0.51 |
| 1:Z4:250:LEU:HD12 | 1:Z4:250:LEU:H | 1.74 | 0.51 |
| 1:Z6:309:ARG:NH1 | 1:Z6:339:SER:O | 2.43 | 0.51 |
| 1:0G:134:GLN:HE21 | 1:0G:167:PHE:HE2 | 1.58 | 0.51 |
| 1:0G:287:PRO:HA | 1:0G:290:THR:HG22 | 1.91 | 0.51 |
| 1:0G:337:ASN:HB3 | 1:0G:340:TYR:HD2 | 1.75 | 0.51 |
| 2:0N:313:MET:CG | 2:0N:346:TRP:CH2 | 2.93 | 0.51 |
| 1:0O:54:ALA:HB3 | 1:0O:58:ARG:HB3 | 1.91 | 0.51 |
| 1:0Q:134:GLN:HE21 | 1:0Q:167:PHE:HE2 | 1.57 | 0.51 |
| 2:1B:269:LEU:HD21 | 2:1B:383:ALA:HB3 | 1.92 | 0.51 |
| 2:1F:74:VAL:O | 2:1F:78:VAL:HG23 | 2.09 | 0.51 |
| 2:1H:313:MET:SD | 2:1H:344:VAL:HG11 | 2.51 | 0.51 |
| 2:1N:3:GLU:HB2 | 2:1N:129:CYS:SG | 2.50 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1N:417:GLU:HA | 2:1N:420:GLU:HG2 | 1.92 | 0.51 |
| 2:1V:98:ASP:OD1 | 2:1V:99:ALA:N | 2.43 | 0.51 |
| 2:1Z:254:GLU:O | 2:1Z:258:ASN:ND2 | 2.43 | 0.51 |
| 1:2C:210:ILE:O | 1:2C:214:THR:OG1 | 2.23 | 0.51 |
| 2:2D:392:ASP:OD2 | 2:2D:422:ARG:NH1 | 2.43 | 0.51 |
| 2:2D:428:LEU:HG | 2:2D:432:PHE:CE2 | 2.43 | 0.51 |
| 1:2K:274:THR:HG21 | 1:2K:282:ARG:HD2 | 1.92 | 0.51 |
| 1:2K:309:ARG:H | 1:2K:372:THR:HG22 | 1.73 | 0.51 |
| 2:2N:325:PRO:HA | 2:2N:328:VAL:HG22 | 1.91 | 0.51 |
| 1:2Q:173:PRO:HD2 | 1:2Q:380:ARG:NH1 | 2.25 | 0.51 |
| 1:2U:198:GLU:HA | 1:2U:264:HIS:HB2 | 1.91 | 0.51 |
| 2:2V:14:ILE:HD11 | 2:2V:74:VAL:HG13 | 1.92 | 0.51 |
| 2:2X:313:MET:HE1 | 2:2X:435:VAL:HG11 | 1.91 | 0.51 |
| 2:3R:156:ARG:HA | 2:3R:159:VAL:HG12 | 1.92 | 0.51 |
| 2:3T:8:HIS:CD2 | 2:3T:138:PHE:HD2 | 2.29 | 0.51 |
| 4:3Y:109:GLN:HE22 | 4:3Y:120:THR:HB | 1.74 | 0.51 |
| 3:4D:35:CYS:SG | 3:4D:36:PHE:N | 2.83 | 0.51 |
| 6:4N:474:PRO:HG3 | 6:4O:138:LYS:HB3 | 1.92 | 0.51 |
| 12:5G:340:ILE:HD11 | 12:5G:369:ALA:HB1 | 1.92 | 0.51 |
| 15:5O:56:LYS:N | 15:5O:56:LYS:CD | 2.73 | 0.51 |
| 15:5O:321:GLU:OE2 | 15:5O:324:ARG:NH2 | 2.43 | 0.51 |
| 15:5P:172:TRP:HE1 | 15:5P:207:GLY:HA3 | 1.75 | 0.51 |
| 19:6E:71:ILE:O | 19:6E:71:ILE:HG13 | 2.08 | 0.51 |
| 22:6P:53:THR:O | 22:6P:57:THR:OG1 | 2.27 | 0.51 |
| 22:6P:114:THR:O | 22:6P:118:VAL:HG23 | 2.10 | 0.51 |
| 24:6Z:187:PHE:O | 24:6Z:190:GLU:HG3 | 2.10 | 0.51 |
| 24:6Z:322:LEU:HD23 | 24:6Z:323:LYS:O | 2.10 | 0.51 |
| 24:6Z:452:MET:HA | 24:6Z:530:PHE:HA | 1.91 | 0.51 |
| 26:7D:58:ILE:HD11 | 26:7D:82:PRO:HB2 | 1.91 | 0.51 |
| 30:7K:207:ASP:OD2 | 30:7K:210:GLN:HG3 | 2.10 | 0.51 |
| 36:7W:99:GLU:O | 36:7W:103:ASN:OD1 | 2.27 | 0.51 |
| 37:7Y:177:ARG:HH12 | 37:7Y:184:ALA:HB1 | 1.74 | 0.51 |
| 2:2:85:GLN:HE21 | 18:5X:78:LEU:HD22 | 1.74 | 0.51 |
| 2:2:434:GLU:OE2 | 4:3W:100:ARG:NH1 | 2.20 | 0.51 |
| 2:G3:289:ALA:O | 2:G3:293:ASN:ND2 | 2.43 | 0.51 |
| 1:G6:58:ARG:HD3 | 1:I2:280:GLN:HE22 | 1.75 | 0.51 |
| 1:G6:219:THR:HG22 | 24:6Y:418:ASP:OD1 | 2.09 | 0.51 |
| 1:G8:216:LYS:HB3 | 24:6Z:422:ASN:OD1 | 2.09 | 0.51 |
| 2:G9:55:GLU:HG2 | 2:G9:61:HIS:CE1 | 2.45 | 0.51 |
| 2:G9:116:ASP:OD1 | 2:G9:116:ASP:N | 2.38 | 0.51 |
| 2:G9:282:TYR:HE2 | 22:6P:217:GLN:HE22 | 1.57 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G9:394:LYS:HA | 2:G9:397:LEU:HD12 | 1.93 | 0.51 |
| 2:H3:116:ASP:N | 2:H3:116:ASP:OD1 | 2.43 | 0.51 |
| 2:H3:306:ASP:HB3 | 2:H3:309:HIS:HD2 | 1.74 | 0.51 |
| 2:H9:287:SER:OG | 2:H9:288:VAL:N | 2.43 | 0.51 |
| 1:I2:77:ARG:HH21 | 1:I2:90:PHE:HD2 | 1.57 | 0.51 |
| 2:I3:116:ASP:N | 2:I3:116:ASP:OD1 | 2.44 | 0.51 |
| 2:I5:287:SER:OG | 2:I5:288:VAL:N | 2.43 | 0.51 |
| 1:J2:274:THR:O | 1:J2:276:ARG:NH1 | 2.40 | 0.51 |
| 2:J3:88:HIS:CE1 | 2:J3:121:ARG:NH2 | 2.78 | 0.51 |
| 2:J9:29:GLY:HA3 | 2:J9:40:LYS:HZ2 | 1.76 | 0.51 |
| 2:J9:58:ALA:HB1 | 6:4O:474:PRO:HB3 | 1.92 | 0.51 |
| 2:J9:305:CYS:HB3 | 2:J9:387:ILE:HD11 | 1.92 | 0.51 |
| 2:L1:381:SER:OG | 2:L1:382:THR:N | 2.42 | 0.51 |
| 2:L5:405:VAL:HG13 | 2:L5:418:PHE:HE2 | 1.75 | 0.51 |
| 2:L7:211:ASP:OD2 | 2:L7:304:LYS:HD3 | 2.09 | 0.51 |
| 1:M4:220:PRO:HD2 | 2:M5:326:LYS:HD3 | 1.92 | 0.51 |
| 1:M6:3:GLU:HB2 | 1:M6:130:LEU:HA | 1.91 | 0.51 |
| 2:N1:277:SER:OG | 2:N1:278:ALA:N | 2.43 | 0.51 |
| 1:O0:361:LEU:HD21 | 27:7G:54:HIS:HB2 | 1.91 | 0.51 |
| 2:O1:170:THR:HG21 | 2:O1:194:LEU:HD11 | 1.91 | 0.51 |
| 1:P6:180:VAL:HG23 | 1:P6:184:ASN:HD21 | 1.76 | 0.51 |
| 1:P6:287:PRO:HA | 1:P6:290:THR:HG22 | 1.92 | 0.51 |
| 2:Q1:115:VAL:HG22 | 2:Q1:119:LEU:HD23 | 1.92 | 0.51 |
| 1:Q2:317:PHE:HE2 | 1:Q2:326:VAL:HG13 | 1.75 | 0.51 |
| 1:Q4:301:CYS:HB2 | 1:Q4:377:MET:CE | 2.40 | 0.51 |
| 2:Q9:337:THR:O | 2:Q9:339:ARG:NH1 | 2.43 | 0.51 |
| 1:R8:253:LEU:HD21 | 1:R8:316:LEU:HD21 | 1.92 | 0.51 |
| 2:R9:192:HIS:HD2 | 2:R9:421:ALA:HA | 1.75 | 0.51 |
| 1:S2:153:SER:O | 1:S2:157:GLU:HG2 | 2.09 | 0.51 |
| 1:S4:180:VAL:HG23 | 1:S4:184:ASN:HD21 | 1.75 | 0.51 |
| 1:S8:2:ARG:HE | 1:S8:240:LEU:HD22 | 1.75 | 0.51 |
| 2:S9:381:SER:OG | 2:S9:382:THR:N | 2.43 | 0.51 |
| 2:T3:372:GLN:NE2 | 7:4U:84:THR:HG21 | 2.24 | 0.51 |
| 1:T6:110:ALA:HB1 | 3:4H:75:ARG:NE | 2.25 | 0.51 |
| 2:T7:15:GLN:HB3 | 2:T7:228:ASN:HD21 | 1.75 | 0.51 |
| 1:U6:114:ASP:OD1 | 1:U6:115:SER:N | 2.44 | 0.51 |
| 2:U7:399:TYR:O | 2:U7:402:ARG:NH1 | 2.43 | 0.51 |
| 1:V2:285:THR:OG1 | 1:V2:287:PRO:HD2 | 2.10 | 0.51 |
| 2:V7:320:ARG:NH2 | 2:V7:359:PRO:O | 2.43 | 0.51 |
| 2:V9:417:GLU:HA | 2:V9:420:GLU:HG2 | 1.92 | 0.51 |
| 2:W3:399:TYR:OH | 2:W3:415:GLU:OE2 | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W8:140:GLY:O | 1:W8:184:ASN:ND2 | 2.32 | 0.51 |
| 1:W8:273:LEU:H | 1:W8:292:GLN:HE22 | 1.58 | 0.51 |
| 1:X0:113:ILE:HA | 1:X0:116:VAL:HG12 | 1.92 | 0.51 |
| 1:X2:178:THR:HA | 2:X3:352:LYS:HD2 | 1.93 | 0.51 |
| 2:X3:129:CYS:SG | 2:X3:130:THR:N | 2.83 | 0.51 |
| 2:X5:286:LEU:HD11 | 2:X5:372:GLN:H | 1.75 | 0.51 |
| 1:Y2:177:ASP:O | 2:Y3:352:LYS:HA | 2.09 | 0.51 |
| 2:Y3:62:VAL:HG12 | 2:Y3:88:HIS:HD2 | 1.75 | 0.51 |
| 2:Y5:90:GLU:HB2 | 2:0B:283:HIS:CE1 | 2.46 | 0.51 |
| 1:Z0:7:ILE:HD13 | 1:Z0:135:VAL:HG22 | 1.92 | 0.51 |
| 1:Z4:183:TYR:OH | 1:Z4:388:MET:HB3 | 2.11 | 0.51 |
| 2:Z5:324:VAL:HG13 | 2:Z5:327:ASP:H | 1.74 | 0.51 |
| 2:0F:101:ASN:OD1 | 1:0G:252:LYS:HE3 | 2.10 | 0.51 |
| 1:0G:405:GLU:HA | 1:0G:408:PHE:HD2 | 1.74 | 0.51 |
| 2:0H:28:HIS:CE1 | 2:0H:49:PHE:HA | 2.46 | 0.51 |
| 2:0J:33:ASP:OD2 | 2:0J:35:GLN:NE2 | 2.43 | 0.51 |
| 2:0L:213:CYS:SG | 2:0L:219:ILE:HB | 2.50 | 0.51 |
| 1:0Q:274:THR:HG21 | 1:0Q:282:ARG:HD2 | 1.92 | 0.51 |
| 2:1D:9:ILE:HG23 | 2:1D:68:LEU:HD11 | 1.92 | 0.51 |
| 1:1M:193:VAL:HG12 | 1:1M:265:PHE:HZ | 1.73 | 0.51 |
| 2:1N:178:SER:HB3 | 2:1N:183:GLU:OE2 | 2.10 | 0.51 |
| 2:1X:156:ARG:HA | 2:1X:159:VAL:HG22 | 1.92 | 0.51 |
| 2:1X:189:LEU:HD11 | 2:1X:418:PHE:HE1 | 1.73 | 0.51 |
| 2:2B:161:TYR:CE1 | 38:8A:80:TYR:HB3 | 2.46 | 0.51 |
| 2:2F:204:LEU:CD2 | 2:2F:231:ILE:HD12 | 2.41 | 0.51 |
| 2:2H:47:ASP:N | 2:2H:47:ASP:OD1 | 2.44 | 0.51 |
| 1:2M:49:VAL:HG11 | 1:2M:241:ARG:HG2 | 1.92 | 0.51 |
| 2:2P:305:CYS:HB3 | 2:2P:387:ILE:HD11 | 1.92 | 0.51 |
| 2:2R:47:ASP:N | 2:2R:47:ASP:OD1 | 2.42 | 0.51 |
| 1:3K:177:ASP:O | 2:3L:352:LYS:HA | 2.10 | 0.51 |
| 1:3Q:68:LEU:HD12 | 1:3Q:143:THR:HG22 | 1.92 | 0.51 |
| 2:3T:250:VAL:HB | 2:3T:254:GLU:HG3 | 1.92 | 0.51 |
| 3:3V:35:CYS:SG | 3:3V:36:PHE:N | 2.83 | 0.51 |
| 3:3X:35:CYS:SG | 3:3X:36:PHE:N | 2.83 | 0.51 |
| 3:4B:35:CYS:SG | 3:4B:36:PHE:N | 2.83 | 0.51 |
| 3:4H:35:CYS:SG | 3:4H:36:PHE:N | 2.83 | 0.51 |
| 5:4M:198:ASP:OD2 | 5:4M:202:ARG:NE | 2.43 | 0.51 |
| 10:5A:472:GLN:HB2 | 10:5A:476:ARG:HH21 | 1.74 | 0.51 |
| 14:5L:188:ALA:CA | 14:5L:226:VAL:HG12 | 2.31 | 0.51 |
| 14:5L:354:GLU:HA | 14:5L:369:LEU:HB3 | 1.92 | 0.51 |
| 14:5N:354:GLU:HA | 14:5N:369:LEU:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6I:281:LYS:HB2 | 22:6I:282:LYS:NZ | 2.25 | 0.51 |
| 24:6U:9:PRO:HB2 | 24:6U:14:TYR:CE2 | 2.45 | 0.51 |
| 24:6V:592:ASP:OD1 | 24:6V:593:LEU:HD12 | 2.09 | 0.51 |
| 24:6X:445:ILE:N | 24:6X:445:ILE:CD1 | 2.72 | 0.51 |
| 24:6Z:345:ASP:OD1 | 24:6Z:346:GLN:N | 2.44 | 0.51 |
| 28:7H:411:PRO:HA | 28:7H:414:GLN:NE2 | 2.24 | 0.51 |
| 34:7S:255:LEU:HA | 35:7U:209:MET:HE1 | 1.92 | 0.51 |
| 28:7X:411:PRO:HA | 28:7X:414:GLN:NE2 | 2.24 | 0.51 |
| 38:8A:12:LEU:HD11 | 38:8A:24:TYR:OH | 2.10 | 0.51 |
| 38:8B:172:GLY:O | 38:8B:173:ALA:C | 2.48 | 0.51 |
| 2:8:264:ARG:NH2 | 4:4C:118:ILE:HD13 | 2.24 | 0.51 |
| 1:A3:40:SER:O | 26:7F:25:TYR:HE2 | 1.92 | 0.51 |
| 1:F6:216:LYS:HB2 | 24:6T:422:ASN:ND2 | 2.24 | 0.51 |
| 1:G4:282:ARG:HH11 | 1:G4:288:GLU:HG3 | 1.75 | 0.51 |
| 2:G9:229:ARG:HD3 | 2:G9:363:VAL:HG21 | 1.92 | 0.51 |
| 2:H5:189:LEU:HD11 | 2:H5:418:PHE:HE1 | 1.75 | 0.51 |
| 1:H6:335:ASN:O | 1:H6:338:SER:OG | 2.27 | 0.51 |
| 1:H8:248:ALA:HA | 1:H8:252:LYS:HD2 | 1.92 | 0.51 |
| 1:J0:126:SER:HA | 29:7I:6:PRO:HG2 | 1.93 | 0.51 |
| 1:J6:67:ASP:N | 1:J6:67:ASP:OD1 | 2.43 | 0.51 |
| 2:J9:132:LEU:HD22 | 2:J9:164:LYS:HD3 | 1.92 | 0.51 |
| 1:K0:114:ASP:OD1 | 1:K0:114:ASP:N | 2.43 | 0.51 |
| 1:K4:139:LEU:HD12 | 1:K4:170:VAL:HG22 | 1.93 | 0.51 |
| 1:K8:391:ARG:HD3 | 2:K9:346:TRP:CE2 | 2.45 | 0.51 |
| 2:K9:417:GLU:HA | 2:K9:420:GLU:HG2 | 1.93 | 0.51 |
| 1:L2:121:ARG:O | 1:L2:125:GLU:HG2 | 2.11 | 0.51 |
| 1:L4:272:PRO:HB2 | 1:L4:282:ARG:HH12 | 1.74 | 0.51 |
| 2:L5:174:SER:HA | 2:L5:205:ASP:OD1 | 2.10 | 0.51 |
| 2:L5:370:LYS:HD3 | 6:4P:147:GLU:OE2 | 2.11 | 0.51 |
| 1:L6:113:ILE:HA | 1:L6:116:VAL:HG22 | 1.92 | 0.51 |
| 1:M2:309:ARG:H | 1:M2:372:THR:HG22 | 1.74 | 0.51 |
| 1:M6:30:ILE:HG22 | 1:M6:36:TYR:HA | 1.93 | 0.51 |
| 1:M6:75:SER:HA | 15:5P:48:LYS:HE2 | 1.85 | 0.51 |
| 1:M6:138:SER:OG | 1:M6:139:LEU:N | 2.41 | 0.51 |
| 2:N1:280:LYS:HD2 | 30:7L:318:TYR:CD2 | 2.45 | 0.51 |
| 1:N2:3:GLU:HB2 | 1:N2:130:LEU:HA | 1.91 | 0.51 |
| 2:N3:121:ARG:NH1 | 2:N3:125:LEU:HG | 2.25 | 0.51 |
| 2:N5:187:SER:O | 2:N5:190:SER:OG | 2.24 | 0.51 |
| 2:N7:14:ILE:HD11 | 2:N7:74:VAL:HG13 | 1.92 | 0.51 |
| 2:N7:116:ASP:OD1 | 2:N7:156:ARG:NH1 | 2.43 | 0.51 |
| 2:N7:269:LEU:N | 2:N7:379:SER:O | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O1:278:ALA:HA | 2:O1:369:ALA:HB2 | 1.93 | 0.51 |
| 1:O6:393:ALA:HB2 | 2:O7:346:TRP:CZ3 | 2.45 | 0.51 |
| 2:P3:238:LEU:HD11 | 2:P3:255:PHE:HZ | 1.75 | 0.51 |
| 2:Q3:32:PRO:HG2 | 20:6F:356:GLN:HE22 | 1.74 | 0.51 |
| 2:Q9:428:LEU:HG | 2:Q9:432:PHE:CE2 | 2.45 | 0.51 |
| 2:R1:155:GLU:HG2 | 2:R1:197:HIS:CE1 | 2.46 | 0.51 |
| 2:R1:324:VAL:HG23 | 2:R1:326:LYS:H | 1.75 | 0.51 |
| 1:R4:54:ALA:O | 7:4T:351:ARG:NH1 | 2.43 | 0.51 |
| 1:R4:117:LEU:HA | 1:R4:120:VAL:HG12 | 1.92 | 0.51 |
| 1:R4:317:PHE:HB3 | 1:R4:321:MET:SD | 2.50 | 0.51 |
| 2:R7:14:ILE:HD11 | 2:R7:74:VAL:HG13 | 1.92 | 0.51 |
| 2:R9:223:THR:HG23 | 2:R9:225:THR:H | 1.74 | 0.51 |
| 2:R9:282:TYR:OH | 20:6F:333:ARG:HD3 | 2.10 | 0.51 |
| 1:S2:8:GLN:CD | 1:S2:17:GLY:HA3 | 2.30 | 0.51 |
| 1:S2:424:GLN:HE21 | 17:5V:104:PHE:HD2 | 1.58 | 0.51 |
| 1:S4:134:GLN:HE21 | 1:S4:167:PHE:HE2 | 1.59 | 0.51 |
| 1:S4:186:THR:HG21 | 1:S4:385:PHE:CD2 | 2.45 | 0.51 |
| 2:S7:389:SER:HB2 | 17:5S:25:SER:OG | 2.11 | 0.51 |
| 2:S9:26:LEU:HD23 | 2:S9:363:VAL:HG12 | 1.93 | 0.51 |
| 1:T2:99:ASN:ND2 | 2:T3:258:ASN:OD1 | 2.37 | 0.51 |
| 2:T3:7:ILE:HD12 | 2:T3:153:LEU:HD21 | 1.91 | 0.51 |
| 2:T3:130:THR:HG21 | 24:6Y:35:TYR:O | 2.09 | 0.51 |
| 1:T4:114:ASP:OD1 | 1:T4:115:SER:N | 2.43 | 0.51 |
| 1:T6:53:GLU:HB3 | 1:T6:59:TYR:CD1 | 2.46 | 0.51 |
| 1:T8:291:GLN:HG3 | 13:5K:100:MET:HE1 | 1.93 | 0.51 |
| 2:U5:336:LYS:HD3 | 2:U5:351:PHE:CE2 | 2.45 | 0.51 |
| 1:V8:246:LEU:HD22 | 1:V8:352:SER:HA | 1.92 | 0.51 |
| 1:W8:177:ASP:O | 2:W9:352:LYS:HA | 2.11 | 0.51 |
| 2:X3:12:ALA:HB2 | 41:X4:501:GTP:C8 | 2.45 | 0.51 |
| 1:X6:208:TYR:CE1 | 1:X6:225:LEU:HD11 | 2.45 | 0.51 |
| 1:Y0:249:ASP:OD1 | 1:Y0:250:LEU:N | 2.44 | 0.51 |
| 2:Y1:83:TYR:HB3 | 2:Y1:86:LEU:HB3 | 1.91 | 0.51 |
| 2:Y1:129:CYS:SG | 2:Y1:130:THR:N | 2.83 | 0.51 |
| 2:Z1:244:PHE:HB2 | 2:Z1:356:ASN:HD21 | 1.75 | 0.51 |
| 1:Z2:205:GLU:HG2 | 1:Z2:206:ALA:H | 1.74 | 0.51 |
| 1:Z2:257:LEU:HD11 | 1:Z2:314:SER:HB3 | 1.92 | 0.51 |
| 1:Z6:198:GLU:HA | 1:Z6:264:HIS:HB2 | 1.92 | 0.51 |
| 2:0B:271:SER:OG | 2:0B:377:MET:HB3 | 2.10 | 0.51 |
| 2:0F:63:PRO:HB2 | 2:0F:65:CYS:SG | 2.51 | 0.51 |
| 2:0F:156:ARG:HA | 2:0F:159:VAL:HG12 | 1.92 | 0.51 |
| 2:0H:109:THR:HB | 2:0H:110:ILE:HD12 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0I:31:ASP:OD1 | 1:0I:35:THR:N | 2.27 | 0.51 |
| 1:0U:77:ARG:HH21 | 1:0U:90:PHE:HD2 | 1.56 | 0.51 |
| 1:0U:398:TYR:HB3 | 1:0U:403:MET:HE3 | 1.93 | 0.51 |
| 2:0V:305:CYS:HB3 | 2:0V:387:ILE:HD11 | 1.92 | 0.51 |
| 1:1E:210:ILE:O | 1:1E:214:THR:OG1 | 2.23 | 0.51 |
| 2:1L:175:PRO:HB3 | 2:1L:390:ARG:HE | 1.75 | 0.51 |
| 1:1S:3:GLU:HB2 | 1:1S:130:LEU:HA | 1.92 | 0.51 |
| 1:1S:172:SER:OG | 1:1S:380:ARG:NH2 | 2.40 | 0.51 |
| 1:1U:114:ASP:N | 1:1U:114:ASP:OD1 | 2.41 | 0.51 |
| 1:1W:404:ASP:HB3 | 1:1W:406:MET:SD | 2.49 | 0.51 |
| 2:1Z:384:ILE:HD12 | 2:1Z:384:ILE:H | 1.75 | 0.51 |
| 1:2A:2:ARG:HB3 | 1:2A:131:GLN:HB2 | 1.92 | 0.51 |
| 1:2G:2:ARG:HB3 | 1:2G:131:GLN:HB2 | 1.92 | 0.51 |
| 1:2G:69:GLU:C | 1:2G:92:PHE:HZ | 2.14 | 0.51 |
| 1:2K:49:VAL:HG11 | 1:2K:241:ARG:HG2 | 1.92 | 0.51 |
| 1:2M:123:GLU:O | 1:2M:126:SER:OG | 2.28 | 0.51 |
| 2:2N:217:LEU:HD11 | 2:2N:367:ASP:HB3 | 1.92 | 0.51 |
| 1:2Q:306:ARG:HD3 | 38:8A:96:GLY:CA | 2.21 | 0.51 |
| 2:2T:261:PRO:HG3 | 2:2T:313:MET:HE2 | 1.92 | 0.51 |
| 1:2U:212:PHE:CE1 | 2:2V:326:LYS:HD3 | 2.46 | 0.51 |
| 1:2U:273:LEU:H | 1:2U:292:GLN:HE22 | 1.59 | 0.51 |
| 1:2W:297:LYS:HZ3 | 38:8B:46:ALA:HB3 | 1.75 | 0.51 |
| 1:2Y:340:TYR:HE2 | 38:8C:95:LYS:O | 1.91 | 0.51 |
| 1:3A:274:THR:HG23 | 1:3A:282:ARG:HH11 | 1.75 | 0.51 |
| 2:3F:72:PRO:HG3 | 1:3G:1:MET:HG2 | 1.91 | 0.51 |
| 2:3N:127:ASP:OD2 | 3:4D:125:TYR:OH | 2.26 | 0.51 |
| 1:3Q:94:GLN:NE2 | 3:4H:139:SER:O | 2.44 | 0.51 |
| 1:3Q:316:LEU:HD13 | 1:3Q:352:SER:HB2 | 1.92 | 0.51 |
| 1:3S:99:ASN:ND2 | 2:3T:254:GLU:OE1 | 2.43 | 0.51 |
| 2:3T:50:ASN:O | 2:3T:64:ARG:NH2 | 2.44 | 0.51 |
| 2:3T:276:ILE:HG23 | 2:3T:280:LYS:HB2 | 1.93 | 0.51 |
| 2:3T:296:PHE:HE2 | 2:3T:335:ILE:HD13 | 1.74 | 0.51 |
| 3:3Z:35:CYS:SG | 3:3Z:36:PHE:N | 2.83 | 0.51 |
| 3:4F:35:CYS:SG | 3:4F:36:PHE:N | 2.83 | 0.51 |
| 5:4M:293:LEU:CB | 28:7X:306:LEU:HD23 | 2.40 | 0.51 |
| 10:5A:292:GLU:O | 10:5A:296:ILE:HG12 | 2.11 | 0.51 |
| 10:5C:233:GLU:O | 10:5C:237:GLN:HG3 | 2.09 | 0.51 |
| 14:5M:354:GLU:HA | 14:5M:369:LEU:HB3 | 1.92 | 0.51 |
| 15:5O:145:PHE:CE1 | 15:5O:200:LYS:NZ | 2.77 | 0.51 |
| 15:5P:176:ILE:O | 15:5P:191:SER:OG | 2.28 | 0.51 |
| 19:6E:20:LEU:HD22 | 19:6E:24:TRP:CD2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6J:323:ASP:OD1 | 22:6J:324:LYS:N | 2.43 | 0.51 |
| 22:6N:291:GLU:HB2 | 22:6N:347:CYS:SG | 2.50 | 0.51 |
| 24:6U:505:LYS:HB3 | 24:6U:506:PRO:HD2 | 1.92 | 0.51 |
| 24:6X:451:LYS:HD2 | 24:6X:468:ARG:HH12 | 0.34 | 0.51 |
| 34:7R:153:LEU:HD12 | 35:7T:101:LEU:HD23 | 1.92 | 0.51 |
| 36:7V:90:GLU:O | 36:7V:92:ARG:NH2 | 2.44 | 0.51 |
| 2:G5:65:CYS:SG | 2:G5:66:ILE:N | 2.83 | 0.51 |
| 2:G5:69:ASP:OD1 | 2:G5:70:LEU:N | 2.43 | 0.51 |
| 1:G6:391:ARG:HH11 | 2:G7:346:TRP:HE1 | 1.57 | 0.51 |
| 2:G7:7:ILE:HG22 | 2:G7:66:ILE:HB | 1.91 | 0.51 |
| 2:G7:306:ASP:OD2 | 2:G7:309:HIS:N | 2.44 | 0.51 |
| 1:G8:214:THR:O | 1:G8:275:SER:OG | 2.29 | 0.51 |
| 2:H3:170:THR:OG1 | 2:H3:203:MET:SD | 2.69 | 0.51 |
| 1:I0:218:THR:CB | 24:6X:489:ASN:CA | 2.89 | 0.51 |
| 2:I1:69:ASP:OD1 | 2:I1:70:LEU:N | 2.42 | 0.51 |
| 2:I1:116:ASP:N | 2:I1:116:ASP:OD1 | 2.42 | 0.51 |
| 2:I5:391:LEU:HA | 2:I5:394:LYS:HE3 | 1.92 | 0.51 |
| 2:I7:227:LEU:O | 2:I7:231:ILE:HG12 | 2.10 | 0.51 |
| 1:J4:203:ASP:N | 1:J4:203:ASP:OD1 | 2.41 | 0.51 |
| 2:J5:176:GLN:NE2 | 2:J5:207:GLU:OE1 | 2.44 | 0.51 |
| 1:J8:112:LEU:O | 1:J8:115:SER:OG | 2.23 | 0.51 |
| 2:J9:28:HIS:O | 2:J9:40:LYS:NZ | 2.40 | 0.51 |
| 2:K3:80:THR:HB | 29:7I:167:ILE:HB | 1.93 | 0.51 |
| 2:K5:90:GLU:H | 2:M1:283:HIS:CE1 | 2.28 | 0.51 |
| 1:K8:396:HIS:HA | 1:K8:399:THR:OG1 | 2.10 | 0.51 |
| 2:K9:281:ALA:C | 2:K9:283:HIS:N | 2.63 | 0.51 |
| 2:L5:147:SER:HB2 | 2:L5:190:SER:OG | 2.09 | 0.51 |
| 2:L9:9:ILE:HD11 | 2:L9:153:LEU:HD23 | 1.92 | 0.51 |
| 2:M5:392:ASP:OD2 | 2:M5:422:ARG:NH1 | 2.43 | 0.51 |
| 2:N7:88:HIS:NE2 | 2:N7:90:GLU:HB2 | 2.25 | 0.51 |
| 1:O2:317:PHE:HB3 | 1:O2:321:MET:HE1 | 1.91 | 0.51 |
| 2:O5:50:ASN:ND2 | 37:7Y:17:GLU:OE2 | 2.43 | 0.51 |
| 2:O7:100:ALA:HA | 1:O8:252:LYS:HE3 | 1.93 | 0.51 |
| 1:P4:113:ILE:HD11 | 1:P4:151:LEU:HD13 | 1.93 | 0.51 |
| 1:P4:170:VAL:HG11 | 1:P4:377:MET:CE | 2.39 | 0.51 |
| 2:P5:72:PRO:HD2 | 1:P6:2:ARG:NH1 | 2.26 | 0.51 |
| 2:P5:98:ASP:N | 2:P5:98:ASP:OD1 | 2.40 | 0.51 |
| 1:P6:391:ARG:HG3 | 2:P7:346:TRP:NE1 | 2.25 | 0.51 |
| 2:Q3:27:GLU:OE1 | 2:Q3:243:ARG:NH1 | 2.43 | 0.51 |
| 2:Q9:195:LEU:HD21 | 2:Q9:264:ARG:HH21 | 1.74 | 0.51 |
| 1:R0:95:THR:HG21 | 1:R0:108:GLU:HG2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R3:5:ILE:HG22 | 2:R3:64:ARG:HB3 | 1.93 | 0.51 |
| 1:R6:19:LYS:HA | 1:R6:22:GLU:OE1 | 2.09 | 0.51 |
| 1:R6:193:VAL:HG23 | 1:R6:194:GLU:HG2 | 1.91 | 0.51 |
| 2:R7:145:THR:HG23 | 2:R7:149:LEU:HD21 | 1.93 | 0.51 |
| 2:R7:166:LYS:N | 2:R7:199:ASP:OD2 | 2.41 | 0.51 |
| 1:R8:121:ARG:NH2 | 1:R8:158:GLU:OE2 | 2.40 | 0.51 |
| 1:S0:273:LEU:H | 1:S0:292:GLN:HE22 | 1.59 | 0.51 |
| 1:S2:80:PRO:HB3 | 12:5F:9:GLY:HA3 | 1.92 | 0.51 |
| 1:S6:139:LEU:HD12 | 1:S6:170:VAL:HG12 | 1.91 | 0.51 |
| 1:T0:287:PRO:HD3 | 1:T0:325:GLU:OE2 | 2.10 | 0.51 |
| 2:T5:430:LYS:HE2 | 17:5U:23:HIS:HB2 | 1.91 | 0.51 |
| 2:U1:363:VAL:HG23 | 2:U1:366:GLY:HA3 | 1.93 | 0.51 |
| 1:U8:22:GLU:HG2 | 1:U8:81:TYR:HB2 | 1.93 | 0.51 |
| 1:V6:50:TYR:HE2 | 1:V6:241:ARG:HE | 1.57 | 0.51 |
| 2:W1:60:LYS:NZ | 2:W1:86:LEU:HA | 2.26 | 0.51 |
| 2:W1:89:PRO:HD3 | 2:X7:283:HIS:CG | 2.46 | 0.51 |
| 2:W5:108:TYR:HA | 2:W5:112:LYS:HE3 | 1.91 | 0.51 |
| 2:W5:331:SER:O | 2:W5:334:THR:OG1 | 2.21 | 0.51 |
| 1:W8:11:GLN:N | 39:W8:503:GDP:O2B | 2.43 | 0.51 |
| 2:W9:88:HIS:CE1 | 2:W9:90:GLU:HB2 | 2.46 | 0.51 |
| 2:X5:358:GLN:NE2 | 2:X5:359:PRO:O | 2.43 | 0.51 |
| 1:X6:238:CYS:SG | 1:X6:316:LEU:HD21 | 2.50 | 0.51 |
| 1:X8:344:TRP:CE3 | 1:X8:345:ILE:HG13 | 2.45 | 0.51 |
| 2:X9:422:ARG:NH1 | 2:X9:426:ALA:HB2 | 2.25 | 0.51 |
| 2:Y5:90:GLU:O | 2:Y5:121:ARG:NH1 | 2.43 | 0.51 |
| 1:Z0:11:GLN:NE2 | 39:Z0:502:GDP:O1A | 2.43 | 0.51 |
| 1:Z4:252:LYS:HE2 | 1:Z4:350:LYS:CE | 2.41 | 0.51 |
| 1:Z6:83:GLN:N | 1:Z6:83:GLN:OE1 | 2.44 | 0.51 |
| 2:Z7:221:ARG:HB3 | 1:Z8:322:SER:HB2 | 1.93 | 0.51 |
| 1:0E:244:GLY:HA3 | 1:0E:354:CYS:HA | 1.91 | 0.51 |
| 2:0F:221:ARG:HB3 | 1:0G:322:SER:OG | 2.10 | 0.51 |
| 1:0I:382:SER:HB3 | 1:0I:415:MET:HG2 | 1.91 | 0.51 |
| 1:0K:183:TYR:CE1 | 1:0K:388:MET:HB3 | 2.45 | 0.51 |
| 2:0L:170:THR:HG21 | 2:0L:194:LEU:HD11 | 1.93 | 0.51 |
| 2:0L:312:TYR:CE2 | 2:0L:341:ILE:HG21 | 2.46 | 0.51 |
| 1:0U:113:ILE:HG13 | 1:0U:150:LEU:HD22 | 1.93 | 0.51 |
| 1:0U:128:ASP:OD1 | 1:0U:129:CYS:N | 2.40 | 0.51 |
| 1:0W:396:HIS:CE1 | 1:0W:397:TRP:CE2 | 2.99 | 0.51 |
| 1:0Y:257:LEU:HD21 | 1:0Y:314:SER:HB3 | 1.93 | 0.51 |
| 2:1D:245:ASP:N | 2:1D:245:ASP:OD2 | 2.42 | 0.51 |
| 1:1G:114:ASP:N | 1:1G:114:ASP:OD1 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1L:90:GLU:C | 2:1L:121:ARG:HH12 | 2.14 | 0.51 |
| 1:1W:3:GLU:HG3 | 1:1W:127:CYS:HB3 | 1.92 | 0.51 |
| 2:2B:287:SER:OG | 2:2B:288:VAL:N | 2.42 | 0.51 |
| 1:2C:135:VAL:HG21 | 1:2C:152:ILE:HD11 | 1.92 | 0.51 |
| 1:2G:177:ASP:O | 2:2H:352:LYS:HA | 2.10 | 0.51 |
| 1:2M:122:LYS:HE3 | 1:3C:291:GLN:HB3 | 1.93 | 0.51 |
| 1:2M:134:GLN:HE21 | 1:2M:167:PHE:HE2 | 1.57 | 0.51 |
| 2:2P:174:SER:OG | 2:2P:207:GLU:OE1 | 2.19 | 0.51 |
| 1:2Q:31:ASP:OD1 | 1:2Q:35:THR:N | 2.38 | 0.51 |
| 1:2S:130:LEU:HB2 | 1:2S:162:ARG:HE | 1.75 | 0.51 |
| 1:2W:325:GLU:HG2 | 38:8B:57:LEU:HD23 | 1.92 | 0.51 |
| 1:2Y:309:ARG:NH1 | 1:2Y:341:PHE:O | 2.44 | 0.51 |
| 1:2Y:340:TYR:CZ | 38:8C:95:LYS:O | 2.62 | 0.51 |
| 2:2Z:183:GLU:HG3 | 2:2Z:184:PRO:HD3 | 1.92 | 0.51 |
| 2:3F:211:ASP:OD1 | 2:3F:214:ARG:NH2 | 2.43 | 0.51 |
| 2:3P:287:SER:OG | 2:3P:288:VAL:N | 2.43 | 0.51 |
| 4:3W:22:LEU:N | 3:3X:258:ASP:OD2 | 2.40 | 0.51 |
| 3:4B:16:ASN:HD22 | 3:4B:22:LYS:HD2 | 1.75 | 0.51 |
| 3:4J:176:ALA:O | 3:4J:180:VAL:HG23 | 2.10 | 0.51 |
| 6:4O:454:LEU:O | 6:4O:457:GLU:HG3 | 2.11 | 0.51 |
| 12:5F:161:ARG:HG2 | 24:6X:46:ALA:HB1 | 1.93 | 0.51 |
| 14:5L:55:HIS:CE1 | 14:5L:86:ILE:HD13 | 2.45 | 0.51 |
| 14:5M:55:HIS:CE1 | 14:5M:86:ILE:HD13 | 2.45 | 0.51 |
| 14:5M:395:SER:O | 14:5M:411:PRO:HD3 | 2.11 | 0.51 |
| 14:5N:55:HIS:CE1 | 14:5N:86:ILE:HD13 | 2.45 | 0.51 |
| 15:5O:67:THR:HA | 15:5O:72:GLN:HA | 1.92 | 0.51 |
| 21:6H:79:VAL:HG21 | 21:6H:91:THR:OG1 | 2.11 | 0.51 |
| 22:6I:31:TYR:O | 22:6I:32:LYS:HG3 | 2.10 | 0.51 |
| 22:6K:31:TYR:O | 22:6K:32:LYS:HG3 | 2.11 | 0.51 |
| 22:6P:278:GLN:O | 22:6P:282:LYS:HG2 | 2.10 | 0.51 |
| 23:6R:62:GLN:NE2 | 23:6R:63:PRO:O | 2.43 | 0.51 |
| 24:6U:32:THR:OG1 | 24:6U:47:GLN:O | 2.28 | 0.51 |
| 24:6V:213:TYR:HH | 24:6V:217:PHE:HE2 | 1.57 | 0.51 |
| 24:6Y:14:TYR:N | 24:6Y:14:TYR:HD2 | 2.09 | 0.51 |
| 24:6Z:117:ARG:NH1 | 24:6Z:134:GLU:OE2 | 2.43 | 0.51 |
| 27:7G:165:PHE:O | 27:7G:169:SER:HB3 | 2.11 | 0.51 |
| 32:7P:89:ASN:OD1 | 32:7P:90:GLN:N | 2.38 | 0.51 |
| 38:8D:209:HIS:CD2 | 38:8D:209:HIS:N | 2.77 | 0.51 |
| 2:8:279:GLU:HG3 | 26:7E:82:PRO:HG2 | 1.92 | 0.51 |
| 1:9:39:ASP:O | 26:7E:25:TYR:CD2 | 2.64 | 0.51 |
| 2:A4:282:TYR:OH | 24:6Z:89:VAL:HG21 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G2:8:GLN:CD | 1:G2:17:GLY:HA3 | 2.31 | 0.51 |
| 2:G5:398:MET:HG2 | 1:G6:345:ILE:HG12 | 1.92 | 0.51 |
| 2:G9:90:GLU:O | 2:G9:121:ARG:NH1 | 2.35 | 0.51 |
| 2:G9:223:THR:H | 2:G9:226:ASN:ND2 | 2.07 | 0.51 |
| 2:H3:9:ILE:HG12 | 2:H3:68:LEU:HD21 | 1.93 | 0.51 |
| 1:H4:72:THR:O | 1:H4:76:VAL:HG23 | 2.09 | 0.51 |
| 2:H7:14:ILE:HD11 | 2:H7:74:VAL:HG13 | 1.93 | 0.51 |
| 2:H7:66:ILE:HG13 | 2:H7:66:ILE:O | 2.11 | 0.51 |
| 1:I0:219:THR:HG23 | 24:6X:488:ARG:CG | 2.41 | 0.51 |
| 2:I1:176:GLN:HE22 | 2:I1:304:LYS:HE2 | 1.75 | 0.51 |
| 2:K5:119:LEU:HA | 2:K5:122:ILE:HG22 | 1.92 | 0.51 |
| 2:L1:297:GLU:OE1 | 2:L1:298:PRO:HD2 | 2.10 | 0.51 |
| 1:L4:113:ILE:HD11 | 1:L4:151:LEU:HD13 | 1.93 | 0.51 |
| 2:L7:210:TYR:HE1 | 2:L7:227:LEU:HD11 | 1.76 | 0.51 |
| 2:L9:73:THR:HA | 1:M0:46:ARG:HH21 | 1.76 | 0.51 |
| 2:M1:72:PRO:HG3 | 1:M2:1:MET:HG2 | 1.92 | 0.51 |
| 2:N3:203:MET:HE3 | 2:N3:267:PHE:HD1 | 1.75 | 0.51 |
| 2:N5:9:ILE:HG22 | 2:N5:146:GLY:HA2 | 1.93 | 0.51 |
| 2:N5:222:PRO:HD2 | 1:N6:324:LYS:HE3 | 1.91 | 0.51 |
| 2:N7:388:PHE:HB3 | 2:N7:425:LEU:HD21 | 1.91 | 0.51 |
| 2:N9:177:VAL:HB | 2:N9:207:GLU:HG3 | 1.92 | 0.51 |
| 2:O1:276:ILE:HG23 | 2:O1:280:LYS:HB2 | 1.92 | 0.51 |
| 2:O1:408:TYR:HB3 | 2:O1:413:MET:HE2 | 1.91 | 0.51 |
| 1:O2:393:ALA:O | 1:O2:394:PHE:HB2 | 2.10 | 0.51 |
| 2:O3:280:LYS:HD3 | 37:7Y:87:VAL:HG11 | 1.91 | 0.51 |
| 2:P5:41:THR:HA | 27:7G:221:PRO:HA | 1.93 | 0.51 |
| 2:P9:259:LEU:HD11 | 2:P9:316:CYS:HB2 | 1.91 | 0.51 |
| 1:Q2:33:THR:O | 1:Q2:58:ARG:NH2 | 2.44 | 0.51 |
| 1:Q2:248:ALA:HA | 1:Q2:252:LYS:HD2 | 1.92 | 0.51 |
| 2:Q5:194:LEU:O | 2:Q5:198:THR:HG22 | 2.11 | 0.51 |
| 1:Q8:99:ASN:ND2 | 2:Q9:254:GLU:OE1 | 2.43 | 0.51 |
| 2:Q9:274:PRO:HB2 | 2:Q9:276:ILE:HG12 | 1.93 | 0.51 |
| 2:R3:18:ASN:HD21 | 21:6G:59:GLN:HE21 | 1.58 | 0.51 |
| 2:R3:210:TYR:HH | 1:R4:323:THR:HG1 | 1.57 | 0.51 |
| 2:R5:415:GLU:OE1 | 17:5T:73:PRO:HG3 | 2.09 | 0.51 |
| 1:R8:249:ASP:OD1 | 1:R8:252:LYS:N | 2.34 | 0.51 |
| 1:S4:260:PHE:HB2 | 1:S4:263:LEU:HD23 | 1.92 | 0.51 |
| 1:S4:267:MET:SD | 1:S4:303:ALA:HB3 | 2.51 | 0.51 |
| 2:S5:5:ILE:HD11 | 2:S5:135:PHE:CE2 | 2.45 | 0.51 |
| 1:T0:173:PRO:HA | 1:T0:176:SER:OG | 2.10 | 0.51 |
| 1:T4:31:ASP:OD1 | 1:T4:35:THR:N | 2.36 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U5:279:GLU:HB3 | 2:U5:283:HIS:NE2 | 2.25 | 0.51 |
| 2:U7:121:ARG:HD2 | 2:U7:125:LEU:HG | 1.91 | 0.51 |
| 1:U8:153:SER:O | 1:U8:157:GLU:HG2 | 2.10 | 0.51 |
| 1:V0:3:GLU:HG2 | 1:V0:127:CYS:SG | 2.49 | 0.51 |
| 1:V2:232:VAL:HG13 | 1:V2:268:VAL:HG11 | 1.92 | 0.51 |
| 1:V8:121:ARG:NH2 | 1:V8:158:GLU:OE2 | 2.42 | 0.51 |
| 1:V8:309:ARG:NH1 | 1:V8:341:PHE:O | 2.44 | 0.51 |
| 1:W2:67:ASP:N | 1:W2:67:ASP:OD1 | 2.44 | 0.51 |
| 2:W9:274:PRO:HD3 | 2:W9:374:ALA:HA | 1.92 | 0.51 |
| 1:X4:178:THR:OG1 | 2:X5:258:ASN:OD1 | 2.28 | 0.51 |
| 2:X9:279:GLU:OE1 | 2:X9:279:GLU:N | 2.43 | 0.51 |
| 1:Y0:232:VAL:HG11 | 1:Y0:268:VAL:HG11 | 1.93 | 0.51 |
| 1:Y0:325:GLU:O | 1:Y0:329:GLN:HG2 | 2.10 | 0.51 |
| 2:Y1:70:LEU:HB2 | 2:Y1:98:ASP:HA | 1.91 | 0.51 |
| 1:Y4:30:ILE:HD12 | 1:Y4:59:TYR:HD2 | 1.75 | 0.51 |
| 1:Y8:139:LEU:HD21 | 1:Y8:168:SER:HB2 | 1.92 | 0.51 |
| 1:Z0:206:ALA:O | 1:Z0:210:ILE:HG12 | 2.11 | 0.51 |
| 2:Z3:181:VAL:HG12 | 1:Z4:347:ASN:O | 2.11 | 0.51 |
| 2:Z3:394:LYS:HD2 | 1:Z4:346:PRO:HG3 | 1.91 | 0.51 |
| 1:Z4:83:GLN:O | 1:0K:281:TYR:OH | 2.17 | 0.51 |
| 1:Z6:414:ASN:HA | 1:Z6:417:ASP:OD2 | 2.11 | 0.51 |
| 2:Z9:338:LYS:HZ3 | 2:Z9:339:ARG:H | 1.57 | 0.51 |
| 1:0I:21:TRP:CZ3 | 1:0I:61:PRO:HB3 | 2.45 | 0.51 |
| 1:0I:358:PRO:HG2 | 1:0I:361:LEU:HD13 | 1.92 | 0.51 |
| 1:0K:135:VAL:HG11 | 1:0K:152:ILE:HD11 | 1.92 | 0.51 |
| 1:0K:384:GLN:O | 1:0K:388:MET:HE2 | 2.11 | 0.51 |
| 2:0R:174:SER:HB2 | 2:0R:177:VAL:O | 2.11 | 0.51 |
| 1:0W:212:PHE:HZ | 2:0X:326:LYS:HB2 | 1.76 | 0.51 |
| 1:1A:242:PHE:CD1 | 1:1A:356:ILE:HG13 | 2.45 | 0.51 |
| 1:1E:179:VAL:HG22 | 2:1F:258:ASN:HD22 | 1.76 | 0.51 |
| 1:1E:246:LEU:HD22 | 1:1E:352:SER:HA | 1.93 | 0.51 |
| 1:1E:311:LEU:HD23 | 1:1E:312:THR:HG23 | 1.93 | 0.51 |
| 1:1G:39:ASP:OD1 | 1:1G:39:ASP:N | 2.44 | 0.51 |
| 1:1G:207:LEU:HB3 | 1:1G:225:LEU:HD22 | 1.92 | 0.51 |
| 2:1L:92:LEU:N | 2:1L:92:LEU:HD23 | 2.25 | 0.51 |
| 2:1N:2:ARG:HA | 2:1N:133:GLN:HE21 | 1.75 | 0.51 |
| 1:1O:248:ALA:HB1 | 1:1O:252:LYS:HD3 | 1.93 | 0.51 |
| 1:1S:2:ARG:HB3 | 1:1S:131:GLN:HB2 | 1.93 | 0.51 |
| 1:1S:244:GLY:H | 1:1S:247:ASN:HD21 | 1.59 | 0.51 |
| 1:1W:186:THR:HG22 | 1:1W:411:ALA:HB1 | 1.92 | 0.51 |
| 2:1X:145:THR:OG1 | 41:1X:501:GTP:O1B | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2M:220:PRO:HG2 | 2:2N:326:LYS:HB2 | 1.92 | 0.51 |
| 2:2P:129:CYS:SG | 2:2P:130:THR:N | 2.84 | 0.51 |
| 2:2R:181:VAL:HG12 | 1:2S:347:ASN:O | 2.11 | 0.51 |
| 2:2V:334:THR:HA | 2:2V:337:THR:HG22 | 1.93 | 0.51 |
| 1:3C:3:GLU:HB2 | 1:3C:130:LEU:HA | 1.93 | 0.51 |
| 1:3I:260:PHE:HB2 | 1:3I:263:LEU:HD23 | 1.93 | 0.51 |
| 2:3L:296:PHE:CE2 | 2:3L:335:ILE:HD13 | 2.45 | 0.51 |
| 1:3M:292:GLN:HG2 | 1:3M:298:ASN:HD22 | 1.76 | 0.51 |
| 1:3S:203:ASP:O | 1:3S:207:LEU:HG | 2.10 | 0.51 |
| 3:4F:16:ASN:HD22 | 3:4F:22:LYS:HD2 | 1.75 | 0.51 |
| 5:4L:281:GLU:O | 5:4L:284:LEU:HG | 2.10 | 0.51 |
| 5:4M:111:ALA:O | 5:4M:115:THR:HG23 | 2.11 | 0.51 |
| 6:4O:212:ALA:O | 6:4O:215:LEU:HG | 2.10 | 0.51 |
| 9:4Z:66:VAL:HA | 9:4Z:69:ASP:OD2 | 2.11 | 0.51 |
| 12:5F:304:ARG:HB3 | 12:5F:356:THR:HB | 1.91 | 0.51 |
| 14:5L:395:SER:O | 14:5L:411:PRO:HD3 | 2.11 | 0.51 |
| 14:5M:219:LEU:CD1 | 14:5M:228:PHE:HE2 | 2.18 | 0.51 |
| 14:5N:395:SER:O | 14:5N:411:PRO:HD3 | 2.11 | 0.51 |
| 22:6O:208:ARG:O | 22:6O:212:GLU:HG2 | 2.10 | 0.51 |
| 23:6Q:62:GLN:NE2 | 23:6Q:63:PRO:O | 2.43 | 0.51 |
| 23:6S:62:GLN:NE2 | 23:6S:63:PRO:O | 2.43 | 0.51 |
| 24:6T:97:ARG:H | 24:6T:188:THR:CG2 | 2.21 | 0.51 |
| 24:6T:117:ARG:NH1 | 24:6T:134:GLU:OE2 | 2.42 | 0.51 |
| 24:6V:503:ILE:HG21 | 24:6V:525:VAL:HG22 | 1.91 | 0.51 |
| 24:6Y:452:MET:HA | 24:6Y:530:PHE:HA | 1.92 | 0.51 |
| 25:7C:110:ARG:NH1 | 30:7K:251:LYS:HD3 | 2.25 | 0.51 |
| 36:7W:90:GLU:O | 36:7W:92:ARG:NH2 | 2.44 | 0.51 |
| 38:8B:44:ARG:HB2 | 38:8B:47:PHE:CD2 | 2.45 | 0.51 |
| 1:A1:420:SER:OG | 3:4F:209:ARG:NH1 | 2.44 | 0.51 |
| 1:A5:423:GLN:HE22 | 3:4J:109:ALA:N | 2.08 | 0.51 |
| 2:G3:90:GLU:HB2 | 2:G3:121:ARG:HH22 | 1.75 | 0.51 |
| 1:G4:28:HIS:NE2 | 1:G4:241:ARG:HD2 | 2.26 | 0.51 |
| 2:G5:227:LEU:O | 2:G5:231:ILE:HG13 | 2.11 | 0.51 |
| 2:H1:167:LEU:HD23 | 2:H1:200:VAL:HB | 1.93 | 0.51 |
| 2:H1:254:GLU:HB3 | 2:H1:258:ASN:HD21 | 1.75 | 0.51 |
| 2:H1:379:SER:OG | 2:H1:380:ASN:N | 2.43 | 0.51 |
| 1:I0:64:ILE:HD11 | 1:I0:123:GLU:HG3 | 1.91 | 0.51 |
| 1:I0:207:LEU:HB3 | 1:I0:225:LEU:HD22 | 1.91 | 0.51 |
| 2:I5:181:VAL:HG13 | 2:I5:182:VAL:HG23 | 1.92 | 0.51 |
| 2:J1:21:TRP:CZ3 | 2:J1:63:PRO:HB3 | 2.45 | 0.51 |
| 2:J3:246:GLY:HA3 | 2:J3:356:ASN:HA | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J3:280:LYS:HA | 2:J3:283:HIS:HB3 | 1.93 | 0.51 |
| 2:J5:22:GLU:O | 2:J5:26:LEU:HG | 2.10 | 0.51 |
| 1:K0:391:ARG:HB3 | 2:K1:346:TRP:CZ3 | 2.46 | 0.51 |
| 1:K6:117:LEU:HA | 1:K6:120:VAL:HG12 | 1.92 | 0.51 |
| 2:L3:84:ARG:NH2 | 29:7J:345:PRO:HD3 | 2.26 | 0.51 |
| 1:M0:244:GLY:H | 1:M0:247:ASN:HD21 | 1.58 | 0.51 |
| 2:M7:30:ILE:HG12 | 2:M7:36:MET:SD | 2.50 | 0.51 |
| 1:M8:358:PRO:HG2 | 1:M8:361:LEU:HD12 | 1.92 | 0.51 |
| 2:M9:39:ASP:OD1 | 2:M9:40:LYS:N | 2.44 | 0.51 |
| 2:M9:66:ILE:HG13 | 2:M9:66:ILE:O | 2.10 | 0.51 |
| 2:N3:2:ARG:HA | 2:N3:133:GLN:HE21 | 1.75 | 0.51 |
| 2:N5:11:GLN:NE2 | 1:N6:245:GLN:O | 2.43 | 0.51 |
| 1:O0:396:HIS:H | 1:O0:396:HIS:CD2 | 2.28 | 0.51 |
| 1:O2:79:GLY:HA3 | 37:7Y:191:ARG:NH2 | 2.19 | 0.51 |
| 1:P4:8:GLN:CD | 1:P4:17:GLY:HA3 | 2.31 | 0.51 |
| 2:P7:65:CYS:SG | 2:P7:66:ILE:N | 2.84 | 0.51 |
| 2:P7:66:ILE:O | 2:P7:66:ILE:HG13 | 2.10 | 0.51 |
| 1:Q2:176:SER:HB3 | 2:Q3:349:THR:HG23 | 1.93 | 0.51 |
| 1:Q6:117:LEU:HA | 1:Q6:120:VAL:HG12 | 1.93 | 0.51 |
| 1:R0:183:TYR:OH | 1:R0:388:MET:HB3 | 2.10 | 0.51 |
| 2:R3:55:GLU:HG2 | 2:R3:61:HIS:CE1 | 2.46 | 0.51 |
| 2:R3:216:SER:OG | 2:R3:217:LEU:N | 2.43 | 0.51 |
| 1:R6:362:LYS:HB2 | 7:4R:174:HIS:CE1 | 2.46 | 0.51 |
| 2:R7:402:ARG:HB3 | 2:R7:405:VAL:HG11 | 1.92 | 0.51 |
| 1:R8:62:ARG:HG3 | 1:R8:123:GLU:OE2 | 2.11 | 0.51 |
| 1:R8:371:SER:OG | 1:R8:372:THR:N | 2.44 | 0.51 |
| 1:S0:156:ARG:NH1 | 1:S0:197:ASP:OD1 | 2.43 | 0.51 |
| 2:S5:201:ALA:O | 2:S5:268:MET:HE2 | 2.11 | 0.51 |
| 2:S5:278:ALA:HA | 2:S5:369:ALA:HB2 | 1.93 | 0.51 |
| 2:S5:305:CYS:HB3 | 2:S5:387:ILE:HD11 | 1.92 | 0.51 |
| 1:T0:371:SER:OG | 1:T0:372:THR:N | 2.43 | 0.51 |
| 1:T6:135:VAL:HG11 | 1:T6:152:ILE:HD11 | 1.93 | 0.51 |
| 1:U2:201:VAL:HG12 | 1:U2:266:PHE:O | 2.10 | 0.51 |
| 2:U5:9:ILE:HG22 | 2:U5:146:GLY:HA2 | 1.93 | 0.51 |
| 2:U7:363:VAL:HG23 | 2:U7:366:GLY:HA3 | 1.92 | 0.51 |
| 1:U8:166:THR:OG1 | 1:U8:199:CYS:SG | 2.69 | 0.51 |
| 1:V0:3:GLU:OE1 | 1:V0:62:ARG:NH1 | 2.44 | 0.51 |
| 2:V3:379:SER:OG | 2:V3:380:ASN:N | 2.43 | 0.51 |
| 1:V4:7:ILE:HB | 1:V4:135:VAL:HG22 | 1.93 | 0.51 |
| 1:V8:317:PHE:HB3 | 1:V8:321:MET:SD | 2.51 | 0.51 |
| 1:W2:22:GLU:HG2 | 1:W2:81:TYR:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W3:384:ILE:HA | 2:W3:387:ILE:HD12 | 1.92 | 0.51 |
| 1:X0:6:HIS:NE2 | 1:X0:136:CYS:SG | 2.70 | 0.51 |
| 2:X5:52:PHE:CZ | 2:X5:239:THR:HG21 | 2.42 | 0.51 |
| 2:X9:5:ILE:HD11 | 2:X9:135:PHE:CE1 | 2.46 | 0.51 |
| 2:X9:255:PHE:HB3 | 2:X9:259:LEU:HD12 | 1.91 | 0.51 |
| 1:Y0:49:VAL:HG11 | 1:Y0:241:ARG:HG2 | 1.91 | 0.51 |
| 1:Y0:165:LEU:HD11 | 1:Y0:200:MET:SD | 2.50 | 0.51 |
| 2:Y5:31:GLN:HB2 | 2:Y5:33:ASP:OD1 | 2.11 | 0.51 |
| 1:Y6:2:ARG:HH21 | 1:Y6:240:LEU:HA | 1.76 | 0.51 |
| 1:Y6:86:ARG:HG2 | 1:Y6:88:ASP:H | 1.75 | 0.51 |
| 1:Y8:247:ASN:O | 1:Y8:252:LYS:NZ | 2.43 | 0.51 |
| 2:Z1:287:SER:OG | 2:Z1:288:VAL:N | 2.44 | 0.51 |
| 1:Z2:135:VAL:HB | 1:Z2:166:THR:HG22 | 1.93 | 0.51 |
| 1:Z6:138:SER:HA | 1:Z6:169:VAL:HG22 | 1.92 | 0.51 |
| 2:Z7:302:MET:N | 2:Z7:302:MET:SD | 2.83 | 0.51 |
| 1:0E:31:ASP:OD1 | 1:0E:35:THR:N | 2.23 | 0.51 |
| 1:0E:198:GLU:HA | 1:0E:264:HIS:HD2 | 1.76 | 0.51 |
| 1:0M:287:PRO:HA | 1:0M:290:THR:HG22 | 1.91 | 0.51 |
| 1:0Q:52:ASN:OD1 | 1:0Q:62:ARG:NH2 | 2.43 | 0.51 |
| 2:0R:213:CYS:HA | 2:0R:217:LEU:HB2 | 1.92 | 0.51 |
| 2:0V:167:LEU:HB3 | 2:0V:169:PHE:CE1 | 2.45 | 0.51 |
| 2:0V:312:TYR:O | 2:0V:344:VAL:HG13 | 2.09 | 0.51 |
| 1:0W:67:ASP:OD1 | 1:0W:68:LEU:N | 2.43 | 0.51 |
| 1:0W:364:SER:OG | 1:0W:365:ALA:N | 2.43 | 0.51 |
| 2:0Z:182:VAL:HG23 | 2:0Z:186:ASN:ND2 | 2.25 | 0.51 |
| 2:0Z:305:CYS:HB3 | 2:0Z:387:ILE:HD11 | 1.92 | 0.51 |
| 2:1D:274:PRO:HB2 | 2:1D:276:ILE:HG12 | 1.93 | 0.51 |
| 1:1E:235:GLY:HA3 | 1:1E:366:THR:HG21 | 1.93 | 0.51 |
| 2:1Z:53:PHE:HB3 | 2:1Z:61:HIS:HB3 | 1.91 | 0.51 |
| 2:1Z:262:TYR:HD1 | 2:1Z:265:ILE:H | 1.57 | 0.51 |
| 2:2D:287:SER:N | 2:2D:290:GLU:OE2 | 2.42 | 0.51 |
| 2:2H:278:ALA:HA | 2:2H:369:ALA:HB2 | 1.92 | 0.51 |
| 2:2P:282:TYR:CZ | 10:5C:163:ARG:HB3 | 2.46 | 0.51 |
| 1:2U:208:TYR:CE1 | 1:2U:225:LEU:HD11 | 2.44 | 0.51 |
| 1:3A:375:GLN:HB2 | 1:3A:419:VAL:HG13 | 1.93 | 0.51 |
| 2:3J:399:TYR:O | 2:3J:402:ARG:NH1 | 2.43 | 0.51 |
| 2:3T:328:VAL:O | 2:3T:332:VAL:HG13 | 2.11 | 0.51 |
| 3:3X:16:ASN:HD22 | 3:3X:22:LYS:HD2 | 1.75 | 0.51 |
| 4:4G:23:GLU:OE1 | 23:6S:7:VAL:HG21 | 2.10 | 0.51 |
| 3:4J:134:VAL:HG12 | 3:4J:136:HIS:H | 1.76 | 0.51 |
| 5:4M:91:LEU:HD13 | 30:7K:109:TRP:CZ3 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:39:TRP:HH2 | 14:5L:524:GLN:OE1 | 1.94 | 0.51 |
| 10:5A:360:GLN:HG3 | 10:5A:363:ARG:HH12 | 1.76 | 0.51 |
| 20:6F:8:ASN:OD1 | 20:6F:9:ALA:N | 2.43 | 0.51 |
| 22:6P:210:MET:O | 22:6P:214:PHE:HD2 | 1.94 | 0.51 |
| 22:6P:283:ILE:HD12 | 22:6P:350:PHE:CG | 2.46 | 0.51 |
| 31:7N:29:GLU:HG3 | 31:7N:30:TYR:N | 2.26 | 0.51 |
| 35:7T:122:LYS:O | 35:7T:126:THR:HG23 | 2.11 | 0.51 |
| 38:8A:8:GLU:OE1 | 38:8A:8:GLU:N | 2.33 | 0.51 |
| 1:3:423:GLN:NE2 | 3:3X:107:ALA:O | 2.43 | 0.51 |
| 1:A3:41:ASP:H | 26:7F:122:VAL:CG2 | 2.22 | 0.51 |
| 1:A5:280:GLN:HE22 | 1:T8:58:ARG:HG2 | 1.74 | 0.51 |
| 1:B5:79:GLY:HA3 | 24:6X:221:ARG:HH22 | 1.74 | 0.51 |
| 1:C2:39:ASP:O | 18:6D:119:ARG:NH1 | 2.43 | 0.51 |
| 1:D2:204:ASN:HD21 | 39:D2:501:GDP:HN22 | 1.59 | 0.51 |
| 2:G1:305:CYS:HB3 | 2:G1:387:ILE:HD11 | 1.92 | 0.51 |
| 2:G3:27:GLU:CD | 2:G3:243:ARG:HH12 | 2.14 | 0.51 |
| 2:G3:155:GLU:HB2 | 2:G3:197:HIS:CE1 | 2.45 | 0.51 |
| 2:G3:252:ILE:HD12 | 2:G3:255:PHE:HE2 | 1.75 | 0.51 |
| 2:G3:255:PHE:HE1 | 2:G3:316:CYS:HG | 1.57 | 0.51 |
| 2:G7:182:VAL:HG23 | 2:G7:186:ASN:ND2 | 2.24 | 0.51 |
| 1:G8:287:PRO:HA | 1:G8:290:THR:HG22 | 1.93 | 0.51 |
| 2:G9:336:LYS:O | 2:G9:339:ARG:NH2 | 2.43 | 0.51 |
| 1:H4:389:PHE:O | 1:H4:392:LYS:NZ | 2.33 | 0.51 |
| 2:H7:56:THR:HA | 2:J3:285:GLN:HB2 | 1.93 | 0.51 |
| 1:I0:364:SER:OG | 1:I0:365:ALA:N | 2.42 | 0.51 |
| 1:I2:178:THR:HG23 | 1:I2:181:GLU:HG3 | 1.93 | 0.51 |
| 1:I4:335:ASN:O | 1:I4:338:SER:OG | 2.29 | 0.51 |
| 2:J1:27:GLU:OE1 | 2:J1:243:ARG:NH1 | 2.38 | 0.51 |
| 2:K1:205:ASP:OD1 | 2:K1:303:VAL:HG13 | 2.11 | 0.51 |
| 1:K8:135:VAL:HG21 | 1:K8:152:ILE:HD11 | 1.93 | 0.51 |
| 1:L4:186:THR:HG22 | 1:L4:411:ALA:HB1 | 1.93 | 0.51 |
| 2:L5:267:PHE:HB2 | 2:L5:384:ILE:HD12 | 1.92 | 0.51 |
| 1:L6:125:GLU:OE2 | 1:L6:159:TYR:OH | 2.27 | 0.51 |
| 2:M5:58:ALA:HB2 | 37:7Y:214:ASP:CB | 2.41 | 0.51 |
| 1:M8:361:LEU:HA | 30:7K:41:TRP:CE3 | 2.45 | 0.51 |
| 2:M9:8:HIS:HB2 | 2:M9:14:ILE:HG22 | 1.92 | 0.51 |
| 1:N0:177:ASP:OD1 | 2:N1:248:LEU:HD11 | 2.10 | 0.51 |
| 2:N5:332:VAL:HA | 2:N5:335:ILE:HD12 | 1.93 | 0.51 |
| 1:N8:8:GLN:CD | 1:N8:17:GLY:HA3 | 2.30 | 0.51 |
| 2:O1:62:VAL:O | 2:O1:62:VAL:HG23 | 2.10 | 0.51 |
| 1:O8:405:GLU:N | 1:O8:405:GLU:OE1 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:240:ALA:HB1 | 2:P3:356:ASN:HD22 | 1.75 | 0.51 |
| 2:P9:47:ASP:OD2 | 2:P9:50:ASN:HB2 | 2.10 | 0.51 |
| 2:Q1:166:LYS:N | 2:Q1:199:ASP:OD2 | 2.43 | 0.51 |
| 2:Q1:297:GLU:N | 2:Q1:297:GLU:OE1 | 2.43 | 0.51 |
| 1:R0:156:ARG:NH1 | 1:R0:197:ASP:OD2 | 2.43 | 0.51 |
| 2:R5:121:ARG:CZ | 2:R5:124:LYS:HE3 | 2.40 | 0.51 |
| 2:S1:14:ILE:HD11 | 2:S1:74:VAL:HG13 | 1.92 | 0.51 |
| 2:S5:69:ASP:OD2 | 2:S5:70:LEU:N | 2.41 | 0.51 |
| 2:S5:250:VAL:HG11 | 2:S5:352:LYS:NZ | 2.26 | 0.51 |
| 1:T0:45:GLU:HG3 | 1:T0:46:ARG:HG2 | 1.92 | 0.51 |
| 1:T6:260:PHE:HB2 | 1:T6:263:LEU:HD23 | 1.93 | 0.51 |
| 2:U3:379:SER:OG | 2:U3:380:ASN:N | 2.43 | 0.51 |
| 2:V1:333:ALA:O | 2:V1:337:THR:HG23 | 2.10 | 0.51 |
| 2:V3:122:ILE:HD13 | 2:V3:157:LEU:HD21 | 1.91 | 0.51 |
| 2:V7:72:PRO:HD2 | 1:V8:2:ARG:HH12 | 1.75 | 0.51 |
| 2:W1:88:HIS:HB3 | 2:W1:91:GLN:HG3 | 1.92 | 0.51 |
| 1:W4:414:ASN:HA | 1:W4:417:ASP:OD2 | 2.11 | 0.51 |
| 1:W6:248:ALA:HA | 1:W6:252:LYS:HD3 | 1.93 | 0.51 |
| 2:W7:109:THR:OG1 | 2:W7:411:GLU:OE2 | 2.23 | 0.51 |
| 2:W9:292:THR:HG22 | 2:W9:319:TYR:OH | 2.11 | 0.51 |
| 2:X3:33:ASP:OD2 | 2:X3:35:GLN:NE2 | 2.43 | 0.51 |
| 2:X3:76:ASP:HA | 2:X3:79:ARG:HB2 | 1.92 | 0.51 |
| 2:X3:208:ALA:O | 2:X3:212:ILE:HG12 | 2.11 | 0.51 |
| 2:Y1:9:ILE:HG12 | 2:Y1:68:LEU:HD21 | 1.93 | 0.51 |
| 1:Y2:327:ASP:N | 1:Y2:327:ASP:OD2 | 2.42 | 0.51 |
| 1:Z4:325:GLU:HA | 1:Z4:328:GLU:HG3 | 1.92 | 0.51 |
| 2:Z5:3:GLU:HB2 | 2:Z5:129:CYS:SG | 2.51 | 0.51 |
| 2:Z5:191:THR:HA | 2:Z5:194:LEU:HB3 | 1.93 | 0.51 |
| 1:Z6:418:LEU:O | 1:Z6:421:GLU:HG2 | 2.10 | 0.51 |
| 2:0L:285:GLN:OE1 | 2:0L:287:SER:OG | 2.27 | 0.51 |
| 1:0M:268:VAL:O | 1:0M:300:MET:N | 2.27 | 0.51 |
| 1:0O:8:GLN:CD | 1:0O:17:GLY:HA3 | 2.31 | 0.51 |
| 1:0Q:248:ALA:HA | 1:0Q:252:LYS:HD2 | 1.93 | 0.51 |
| 2:0X:69:ASP:OD1 | 2:0X:70:LEU:N | 2.41 | 0.51 |
| 2:1F:318:MET:HB2 | 2:1F:376:CYS:HB3 | 1.93 | 0.51 |
| 2:1H:209:ILE:HG21 | 2:1H:227:LEU:HG | 1.92 | 0.51 |
| 2:1H:280:LYS:HA | 2:1H:283:HIS:HB3 | 1.92 | 0.51 |
| 1:1O:180:VAL:HG23 | 1:1O:184:ASN:ND2 | 2.26 | 0.51 |
| 2:1P:178:SER:HB2 | 1:1Q:347:ASN:OD1 | 2.11 | 0.51 |
| 2:1R:132:LEU:HD22 | 2:1R:164:LYS:HD3 | 1.92 | 0.51 |
| 2:1T:320:ARG:NH2 | 2:1T:359:PRO:O | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1T:333:ALA:O | 2:1T:337:THR:HG23 | 2.11 | 0.51 |
| 1:1U:113:ILE:HD11 | 1:1U:151:LEU:HA | 1.93 | 0.51 |
| 1:1W:317:PHE:HE2 | 1:1W:326:VAL:HG13 | 1.75 | 0.51 |
| 2:1Z:287:SER:OG | 2:1Z:288:VAL:N | 2.43 | 0.51 |
| 2:2D:70:LEU:HB3 | 2:2D:97:GLU:O | 2.11 | 0.51 |
| 1:2E:16:ILE:HD11 | 1:2E:136:CYS:HB3 | 1.92 | 0.51 |
| 2:2F:280:LYS:HA | 2:2F:283:HIS:HB3 | 1.93 | 0.51 |
| 2:2N:161:TYR:CE1 | 38:8D:80:TYR:HB2 | 2.22 | 0.51 |
| 2:2N:278:ALA:HA | 2:2N:369:ALA:HB2 | 1.93 | 0.51 |
| 1:2Q:276:ARG:O | 1:2Q:276:ARG:NH1 | 2.44 | 0.51 |
| 1:2S:350:LYS:HZ3 | 1:2S:352:SER:HB3 | 1.75 | 0.51 |
| 2:2T:384:ILE:HA | 2:2T:387:ILE:HD12 | 1.93 | 0.51 |
| 2:2Z:79:ARG:NH1 | 2:2Z:92:LEU:O | 2.43 | 0.51 |
| 2:2Z:308:ARG:HH22 | 38:8C:72:ASP:CB | 2.13 | 0.51 |
| 2:3D:88:HIS:CG | 2:3T:283:HIS:HA | 2.45 | 0.51 |
| 1:3M:39:ASP:OD1 | 1:3M:39:ASP:N | 2.43 | 0.51 |
| 1:3M:211:CYS:SG | 1:3M:217:LEU:HB2 | 2.51 | 0.51 |
| 3:3V:16:ASN:HD22 | 3:3V:22:LYS:HD2 | 1.75 | 0.51 |
| 9:4Z:184:ALA:O | 9:4Z:188:THR:HG23 | 2.11 | 0.51 |
| 10:5A:330:ALA:HA | 10:5A:333:GLU:OE1 | 2.11 | 0.51 |
| 10:5B:240:LEU:O | 10:5B:243:LEU:HG | 2.11 | 0.51 |
| 10:5C:196:LEU:O | 10:5C:200:GLU:HG2 | 2.11 | 0.51 |
| 10:5C:235:ARG:HA | 10:5C:238:GLU:HG3 | 1.92 | 0.51 |
| 14:5M:578:LYS:HA | 14:5M:589:PHE:HB3 | 1.92 | 0.51 |
| 20:6F:344:LEU:HD11 | 20:6F:375:PRO:HB3 | 1.91 | 0.51 |
| 20:6F:382:THR:HG23 | 20:6F:383:ARG:HG3 | 1.92 | 0.51 |
| 21:6G:149:LEU:HD11 | 21:6G:152:ALA:HA | 1.93 | 0.51 |
| 22:6L:31:TYR:O | 22:6L:32:LYS:HG3 | 2.11 | 0.51 |
| 22:6P:248:MET:HE1 | 22:6P:256:TYR:HB2 | 1.92 | 0.51 |
| 24:6U:142:ILE:HG13 | 24:6U:144:GLN:HG3 | 1.91 | 0.51 |
| 24:6V:97:ARG:NH2 | 24:6V:99:TYR:OH | 2.40 | 0.51 |
| 34:7S:272:LYS:HA | 34:7S:275:GLU:OE1 | 2.10 | 0.51 |
| 35:7U:232:THR:O | 35:7U:236:GLU:HG2 | 2.10 | 0.51 |
| 38:8B:110:ASN:O | 38:8B:114:THR:HG23 | 2.11 | 0.51 |
| 2:4:42:ILE:HG21 | 24:6U:93:ARG:HH11 | 1.74 | 0.51 |
| 2:B0:229:ARG:NH2 | 18:5Y:50:SER:OG | 2.41 | 0.51 |
| 1:D6:226:ASN:ND2 | 39:D6:501:GDP:O6 | 2.30 | 0.51 |
| 2:G1:219:ILE:CG2 | 22:6L:175:ALA:HB1 | 2.41 | 0.51 |
| 1:G2:31:ASP:OD2 | 1:G2:33:THR:OG1 | 2.28 | 0.51 |
| 1:G4:77:ARG:O | 1:G4:82:GLY:HA3 | 2.10 | 0.51 |
| 2:G5:174:SER:HB3 | 2:G5:207:GLU:OE1 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G7:344:VAL:HG22 | 2:G7:346:TRP:H | 1.75 | 0.51 |
| 2:H1:324:VAL:HG23 | 2:H1:326:LYS:HG3 | 1.93 | 0.51 |
| 2:H7:90:GLU:HG3 | 2:H7:121:ARG:NH1 | 2.24 | 0.51 |
| 2:H7:109:THR:OG1 | 2:H7:411:GLU:OE2 | 2.23 | 0.51 |
| 1:I2:139:LEU:HG | 1:I2:168:SER:HB3 | 1.93 | 0.51 |
| 1:I4:172:SER:OG | 1:I4:380:ARG:NH1 | 2.44 | 0.51 |
| 1:I4:183:TYR:OH | 1:I4:388:MET:HB3 | 2.10 | 0.51 |
| 2:I9:370:LYS:HD2 | 5:4L:317:TYR:CE2 | 2.46 | 0.51 |
| 1:J4:175:VAL:HG13 | 2:J5:329:ASN:HD21 | 1.76 | 0.51 |
| 2:K1:119:LEU:HA | 2:K1:122:ILE:HG22 | 1.91 | 0.51 |
| 1:L4:262:ARG:NH2 | 1:L4:417:ASP:OD1 | 2.44 | 0.51 |
| 2:L9:90:GLU:HG3 | 2:L9:121:ARG:NH1 | 2.25 | 0.51 |
| 2:M3:287:SER:OG | 2:M3:288:VAL:N | 2.43 | 0.51 |
| 2:M5:79:ARG:NH1 | 2:M5:92:LEU:O | 2.44 | 0.51 |
| 2:M7:287:SER:OG | 2:M7:288:VAL:N | 2.44 | 0.51 |
| 2:M9:280:LYS:NZ | 29:7J:320:PRO:HB2 | 2.26 | 0.51 |
| 2:N7:296:PHE:CE2 | 2:N7:335:ILE:HG12 | 2.46 | 0.51 |
| 1:N8:204:ASN:HD21 | 39:N8:502:GDP:HN22 | 1.58 | 0.51 |
| 2:O5:3:GLU:HB2 | 2:O5:129:CYS:SG | 2.51 | 0.51 |
| 1:Q8:173:PRO:HD2 | 1:Q8:380:ARG:NE | 2.25 | 0.51 |
| 2:Q9:170:THR:HG21 | 2:Q9:194:LEU:HD11 | 1.93 | 0.51 |
| 2:R1:156:ARG:HA | 2:R1:159:VAL:HG12 | 1.93 | 0.51 |
| 1:R2:112:LEU:O | 1:R2:116:VAL:HG23 | 2.10 | 0.51 |
| 1:R2:301:CYS:SG | 1:R2:302:ALA:N | 2.84 | 0.51 |
| 1:R4:90:PHE:HD2 | 19:6E:254:PHE:HZ | 1.57 | 0.51 |
| 1:R6:70:PRO:HG2 | 2:R7:2:ARG:NH2 | 2.26 | 0.51 |
| 1:R6:248:ALA:HA | 1:R6:252:LYS:HD2 | 1.93 | 0.51 |
| 1:R8:139:LEU:HD12 | 1:R8:170:VAL:HG12 | 1.93 | 0.51 |
| 1:S0:67:ASP:OD2 | 1:S0:72:THR:OG1 | 2.28 | 0.51 |
| 1:S2:156:ARG:NH1 | 1:S2:197:ASP:OD1 | 2.44 | 0.51 |
| 1:S6:288:GLU:OE1 | 1:S6:289:LEU:HD12 | 2.11 | 0.51 |
| 2:S7:51:THR:HG21 | 2:S7:243:ARG:HG2 | 1.93 | 0.51 |
| 2:T1:333:ALA:O | 2:T1:337:THR:HG23 | 2.11 | 0.51 |
| 2:T3:147:SER:OG | 2:T3:190:SER:HB3 | 2.11 | 0.51 |
| 1:T4:14:ASN:HD21 | 1:T4:65:LEU:HB3 | 1.75 | 0.51 |
| 2:U1:129:CYS:SG | 2:U1:130:THR:N | 2.83 | 0.51 |
| 1:U4:70:PRO:N | 1:U4:92:PHE:HZ | 2.08 | 0.51 |
| 1:U6:175:VAL:HG12 | 2:U7:329:ASN:ND2 | 2.25 | 0.51 |
| 1:V0:167:PHE:CZ | 1:V0:233:MET:HG2 | 2.46 | 0.51 |
| 2:W1:147:SER:OG | 2:W1:190:SER:HB2 | 2.11 | 0.51 |
| 1:W4:240:LEU:HD11 | 1:W4:250:LEU:HD23 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W5:9:ILE:HG22 | 2:W5:146:GLY:HA2 | 1.93 | 0.51 |
| 2:X5:12:ALA:HB2 | 41:X6:501:GTP:C8 | 2.46 | 0.51 |
| 1:X6:354:CYS:SG | 1:X6:355:ASP:N | 2.84 | 0.51 |
| 2:X7:31:GLN:HE21 | 2:X7:37:PRO:HG3 | 1.76 | 0.51 |
| 2:X7:88:HIS:HB3 | 2:Z3:283:HIS:ND1 | 2.25 | 0.51 |
| 1:X8:250:LEU:HD12 | 1:X8:250:LEU:N | 2.25 | 0.51 |
| 2:Y3:278:ALA:HA | 2:Y3:369:ALA:HB2 | 1.91 | 0.51 |
| 2:Y5:12:ALA:HB2 | 41:Y6:501:GTP:C8 | 2.45 | 0.51 |
| 1:Y6:205:GLU:HG2 | 1:Y6:206:ALA:N | 2.25 | 0.51 |
| 2:Y9:133:GLN:HB3 | 2:Y9:252:ILE:HD11 | 1.93 | 0.51 |
| 2:Y9:332:VAL:HA | 2:Y9:335:ILE:HG22 | 1.93 | 0.51 |
| 1:Z0:8:GLN:HB3 | 1:Z0:13:GLY:O | 2.11 | 0.51 |
| 1:Z0:49:VAL:HG21 | 1:Z0:241:ARG:HG2 | 1.93 | 0.51 |
| 1:Z0:272:PRO:O | 1:Z0:273:LEU:HD23 | 2.11 | 0.51 |
| 2:Z1:27:GLU:OE2 | 2:Z1:243:ARG:NH1 | 2.44 | 0.51 |
| 2:Z3:233:GLN:OE1 | 2:Z3:272:TYR:OH | 2.26 | 0.51 |
| 2:Z5:121:ARG:NE | 2:Z5:121:ARG:HA | 2.26 | 0.51 |
| 1:Z6:113:ILE:HA | 1:Z6:116:VAL:HG22 | 1.93 | 0.51 |
| 2:Z7:8:HIS:CD2 | 2:Z7:138:PHE:HD2 | 2.27 | 0.51 |
| 2:0B:296:PHE:CE2 | 2:0B:335:ILE:HG12 | 2.45 | 0.51 |
| 1:0C:171:PRO:HG3 | 1:0C:181:GLU:HB3 | 1.92 | 0.51 |
| 1:0E:2:ARG:HB2 | 1:0E:240:LEU:HD11 | 1.93 | 0.51 |
| 1:0G:173:PRO:HB3 | 1:0G:384:GLN:HE22 | 1.76 | 0.51 |
| 1:0G:237:THR:HG23 | 1:0G:241:ARG:HH21 | 1.76 | 0.51 |
| 1:0I:286:VAL:O | 1:0I:290:THR:HG23 | 2.11 | 0.51 |
| 1:0I:309:ARG:H | 1:0I:372:THR:HG22 | 1.76 | 0.51 |
| 2:0N:217:LEU:HD21 | 2:0N:368:LEU:HD23 | 1.92 | 0.51 |
| 2:0N:271:SER:OG | 2:0N:300:SER:O | 2.24 | 0.51 |
| 1:0O:66:MET:SD | 1:0O:116:VAL:HG11 | 2.50 | 0.51 |
| 2:0P:288:VAL:HG13 | 2:0P:319:TYR:HE2 | 1.76 | 0.51 |
| 2:0X:90:GLU:O | 2:0X:121:ARG:NH1 | 2.35 | 0.51 |
| 1:1C:50:TYR:CE2 | 1:1C:241:ARG:HD3 | 2.45 | 0.51 |
| 2:1R:109:THR:OG1 | 2:1R:411:GLU:OE2 | 2.29 | 0.51 |
| 2:1V:175:PRO:HB3 | 2:1V:390:ARG:HE | 1.76 | 0.51 |
| 1:1W:7:ILE:HD13 | 1:1W:151:LEU:HD21 | 1.92 | 0.51 |
| 2:1Z:129:CYS:SG | 2:1Z:130:THR:N | 2.84 | 0.51 |
| 1:2A:139:LEU:HD12 | 1:2A:170:VAL:HG12 | 1.92 | 0.51 |
| 1:2I:178:THR:HG22 | 2:2J:352:LYS:HE2 | 1.93 | 0.51 |
| 1:2M:173:PRO:HD2 | 1:2M:380:ARG:NE | 2.17 | 0.51 |
| 2:2N:287:SER:OG | 2:2N:288:VAL:N | 2.43 | 0.51 |
| 2:2R:394:LYS:HB2 | 1:2S:346:PRO:HG3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2X:248:LEU:HD22 | 2:2X:354:GLY:HA2 | 1.92 | 0.51 |
| 1:2Y:189:VAL:O | 1:2Y:193:VAL:HG13 | 2.11 | 0.51 |
| 1:2Y:207:LEU:HB3 | 1:2Y:225:LEU:HD22 | 1.93 | 0.51 |
| 1:3A:178:THR:HG23 | 1:3A:181:GLU:HG3 | 1.91 | 0.51 |
| 1:3G:173:PRO:HD2 | 1:3G:380:ARG:NH1 | 2.26 | 0.51 |
| 2:3H:183:GLU:CD | 2:3H:184:PRO:HD3 | 2.31 | 0.51 |
| 1:3I:139:LEU:HA | 1:3I:145:SER:OG | 2.11 | 0.51 |
| 1:3K:203:ASP:OD2 | 1:3K:302:ALA:N | 2.43 | 0.51 |
| 2:3L:21:TRP:CZ2 | 2:3L:65:CYS:HB3 | 2.45 | 0.51 |
| 1:3O:274:THR:O | 1:3O:279:GLN:NE2 | 2.41 | 0.51 |
| 2:3R:79:ARG:O | 2:3R:84:ARG:HG2 | 2.11 | 0.51 |
| 2:3T:71:GLU:CG | 2:3T:98:ASP:HB3 | 2.40 | 0.51 |
| 3:3Z:16:ASN:HD22 | 3:3Z:22:LYS:HD2 | 1.75 | 0.51 |
| 14:5L:210:TYR:HE1 | 14:5L:220:GLN:HB2 | 1.72 | 0.51 |
| 14:5L:578:LYS:HA | 14:5L:589:PHE:HB3 | 1.92 | 0.51 |
| 15:5P:334:LEU:HD23 | 15:5P:334:LEU:C | 2.31 | 0.51 |
| 18:5Z:106:GLU:OE1 | 18:5Z:106:GLU:N | 2.38 | 0.51 |
| 18:5Z:210:GLU:N | 18:5Z:210:GLU:OE1 | 2.44 | 0.51 |
| 21:6H:104:THR:HG23 | 21:6H:113:PRO:HA | 1.93 | 0.51 |
| 23:6Q:28:LYS:NZ | 23:6Q:50:ALA:HA | 2.26 | 0.51 |
| 24:6V:456:ASP:N | 24:6V:456:ASP:OD1 | 2.43 | 0.51 |
| 24:6X:50:ASP:OD1 | 24:6X:51:LEU:N | 2.43 | 0.51 |
| 24:6X:536:ASP:OD1 | 24:6X:537:GLU:N | 2.44 | 0.51 |
| 24:7A:151:HIS:CE1 | 24:7A:153:VAL:HG22 | 2.46 | 0.51 |
| 38:8A:213:GLU:HG2 | 38:8A:214:HIS:H | 1.76 | 0.51 |
| 1:D6:219:THR:HG22 | 24:6Z:254:SER:HB3 | 1.93 | 0.51 |
| 2:G3:220:GLU:OE1 | 2:G3:220:GLU:N | 2.44 | 0.51 |
| 1:G4:31:ASP:OD1 | 1:G4:35:THR:N | 2.35 | 0.51 |
| 1:G6:122:LYS:O | 1:G6:126:SER:OG | 2.21 | 0.51 |
| 1:G6:287:PRO:HA | 1:G6:290:THR:HG22 | 1.93 | 0.51 |
| 2:G7:116:ASP:N | 2:G7:116:ASP:OD1 | 2.43 | 0.51 |
| 2:G7:333:ALA:O | 2:G7:337:THR:HG23 | 2.11 | 0.51 |
| 2:H1:9:ILE:HD13 | 2:H1:150:GLY:HA2 | 1.92 | 0.51 |
| 2:H1:207:GLU:HG2 | 2:H1:304:LYS:HD2 | 1.93 | 0.51 |
| 1:H4:113:ILE:HD11 | 1:H4:151:LEU:HA | 1.93 | 0.51 |
| 1:H6:153:SER:O | 1:H6:157:GLU:HG2 | 2.11 | 0.51 |
| 2:I7:34:GLY:HA3 | 2:I7:60:LYS:HZ2 | 1.76 | 0.51 |
| 2:J1:287:SER:OG | 2:J1:288:VAL:N | 2.44 | 0.51 |
| 2:J3:52:PHE:HZ | 2:J3:239:THR:HG21 | 1.75 | 0.51 |
| 1:J4:107:THR:OG1 | 1:J4:401:GLU:OE2 | 2.20 | 0.51 |
| 2:K1:88:HIS:HB3 | 2:L7:283:HIS:CG | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K3:289:ALA:O | 2:K3:293:ASN:ND2 | 2.44 | 0.51 |
| 2:L9:88:HIS:HB2 | 1:N6:281:TYR:CE1 | 2.46 | 0.51 |
| 2:M1:11:GLN:NE2 | 1:M2:247:ASN:OD1 | 2.44 | 0.51 |
| 2:M5:8:HIS:CD2 | 2:M5:17:GLY:HA3 | 2.46 | 0.51 |
| 2:M9:237:SER:HA | 2:M9:320:ARG:HD2 | 1.93 | 0.51 |
| 1:N0:41:ASP:N | 1:N0:41:ASP:OD1 | 2.43 | 0.51 |
| 1:N8:309:ARG:NH1 | 1:N8:339:SER:O | 2.44 | 0.51 |
| 1:O0:232:VAL:O | 1:O0:236:ILE:HG12 | 2.11 | 0.51 |
| 2:O5:287:SER:OG | 2:O5:288:VAL:N | 2.44 | 0.51 |
| 2:O7:346:TRP:HZ2 | 2:O7:435:VAL:HG23 | 1.76 | 0.51 |
| 2:P3:259:LEU:HD11 | 2:P3:316:CYS:HB2 | 1.92 | 0.51 |
| 2:P3:313:MET:N | 2:P3:380:ASN:O | 2.38 | 0.51 |
| 2:P5:7:ILE:HD11 | 2:P5:137:VAL:HG12 | 1.91 | 0.51 |
| 2:P9:53:PHE:HB3 | 2:P9:61:HIS:HB3 | 1.92 | 0.51 |
| 2:Q1:66:ILE:HG13 | 2:Q1:66:ILE:O | 2.10 | 0.51 |
| 2:Q3:399:TYR:OH | 2:Q3:415:GLU:OE1 | 2.23 | 0.51 |
| 1:R0:101:TRP:HD1 | 1:R0:145:SER:HG | 1.57 | 0.51 |
| 1:R6:67:ASP:N | 1:R6:67:ASP:OD1 | 2.44 | 0.51 |
| 1:S4:337:ASN:HD21 | 17:5R:48:THR:N | 2.07 | 0.51 |
| 1:S8:135:VAL:HG11 | 1:S8:152:ILE:HD11 | 1.93 | 0.51 |
| 1:S8:375:GLN:HB3 | 1:S8:422:TYR:CD2 | 2.43 | 0.51 |
| 1:T0:108:GLU:OE1 | 1:T0:108:GLU:N | 2.44 | 0.51 |
| 2:T3:342:GLN:HE21 | 13:5J:74:ASN:HD21 | 1.59 | 0.51 |
| 2:T5:296:PHE:CD2 | 2:T5:335:ILE:HD13 | 2.46 | 0.51 |
| 1:T6:244:GLY:HA2 | 1:T6:355:ASP:OD2 | 2.11 | 0.51 |
| 2:T7:70:LEU:HG | 2:T7:145:THR:HG23 | 1.92 | 0.51 |
| 1:V0:391:ARG:HD3 | 2:V1:346:TRP:CH2 | 2.45 | 0.51 |
| 2:V9:147:SER:OG | 2:V9:190:SER:HB2 | 2.11 | 0.51 |
| 2:W3:205:ASP:OD2 | 2:W3:304:LYS:N | 2.43 | 0.51 |
| 2:W3:331:SER:O | 2:W3:334:THR:OG1 | 2.20 | 0.51 |
| 2:W7:90:GLU:CB | 2:W7:121:ARG:HH12 | 2.18 | 0.51 |
| 1:W8:183:TYR:HB3 | 1:W8:398:TYR:HE2 | 1.76 | 0.51 |
| 1:X2:12:CYS:O | 1:X2:16:ILE:HG13 | 2.10 | 0.51 |
| 1:X2:284:LEU:HG | 1:X2:362:LYS:HD2 | 1.93 | 0.51 |
| 1:X4:178:THR:HB | 2:X5:352:LYS:HE3 | 1.93 | 0.51 |
| 1:X4:237:THR:HG23 | 1:X4:241:ARG:HH21 | 1.75 | 0.51 |
| 1:Y2:322:SER:OG | 1:Y2:325:GLU:HG3 | 2.11 | 0.51 |
| 1:Y4:190:HIS:HE2 | 1:Y4:410:GLU:HG3 | 1.76 | 0.51 |
| 1:Y8:114:ASP:OD1 | 1:Y8:114:ASP:N | 2.42 | 0.51 |
| 1:Z0:372:THR:O | 1:Z0:375:GLN:HG3 | 2.10 | 0.51 |
| 2:Z5:313:MET:SD | 2:Z5:380:ASN:ND2 | 2.84 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0J:271:SER:HB2 | 2:0J:301:MET:SD | 2.51 | 0.51 |
| 2:0J:338:LYS:HZ2 | 2:0J:339:ARG:H | 1.59 | 0.51 |
| 2:0J:362:VAL:HG13 | 2:0J:370:LYS:HD2 | 1.91 | 0.51 |
| 1:0S:311:LEU:HD23 | 1:0S:312:THR:HG22 | 1.92 | 0.51 |
| 1:0U:317:PHE:HE2 | 1:0U:326:VAL:HG13 | 1.74 | 0.51 |
| 1:0W:173:PRO:HB3 | 1:0W:384:GLN:HE22 | 1.75 | 0.51 |
| 2:0X:12:ALA:O | 2:0X:16:VAL:HG23 | 2.10 | 0.51 |
| 2:0X:290:GLU:HA | 2:0X:293:ASN:HD22 | 1.75 | 0.51 |
| 2:0X:301:MET:HE1 | 2:0X:307:PRO:HD3 | 1.93 | 0.51 |
| 1:1C:301:CYS:SG | 1:1C:302:ALA:N | 2.83 | 0.51 |
| 2:1F:12:ALA:O | 2:1F:16:VAL:HG23 | 2.10 | 0.51 |
| 2:1F:65:CYS:SG | 2:1F:66:ILE:N | 2.84 | 0.51 |
| 2:1H:156:ARG:HA | 2:1H:159:VAL:HG12 | 1.93 | 0.51 |
| 2:1N:116:ASP:OD1 | 2:1N:117:LEU:N | 2.42 | 0.51 |
| 1:1Q:325:GLU:N | 1:1Q:325:GLU:OE1 | 2.44 | 0.51 |
| 2:1R:205:ASP:OD2 | 2:1R:206:ASN:N | 2.44 | 0.51 |
| 1:1S:286:VAL:HG22 | 1:1S:321:MET:HE3 | 1.93 | 0.51 |
| 2:1T:72:PRO:HG3 | 1:1U:1:MET:HG2 | 1.92 | 0.51 |
| 2:1V:317:LEU:HB3 | 2:1V:319:TYR:HE1 | 1.75 | 0.51 |
| 1:1W:5:VAL:HG23 | 1:1W:62:ARG:HG2 | 1.92 | 0.51 |
| 2:1Z:262:TYR:CE1 | 2:1Z:264:ARG:HB2 | 2.45 | 0.51 |
| 1:2A:115:SER:HA | 1:2A:118:ASP:OD1 | 2.11 | 0.51 |
| 2:2B:14:ILE:HD11 | 2:2B:74:VAL:HG13 | 1.92 | 0.51 |
| 1:2C:173:PRO:CD | 1:2C:380:ARG:HE | 2.24 | 0.51 |
| 1:2G:91:VAL:HG11 | 1:2G:116:VAL:HG23 | 1.93 | 0.51 |
| 2:2H:213:CYS:SG | 2:2H:219:ILE:HB | 2.51 | 0.51 |
| 1:2K:86:ARG:HG2 | 1:2K:88:ASP:H | 1.75 | 0.51 |
| 2:2T:406:HIS:HA | 2:2T:409:VAL:HG22 | 1.92 | 0.51 |
| 2:2V:5:ILE:HG22 | 2:2V:64:ARG:HB3 | 1.93 | 0.51 |
| 1:3A:5:VAL:HG12 | 1:3A:133:PHE:HD1 | 1.75 | 0.51 |
| 1:3A:86:ARG:HG2 | 1:3A:88:ASP:H | 1.76 | 0.51 |
| 2:3B:211:ASP:OD1 | 38:8C:18:VAL:HG13 | 2.11 | 0.51 |
| 2:3F:218:ASP:O | 38:8A:175:ARG:HG3 | 2.11 | 0.51 |
| 1:3M:77:ARG:CZ | 3:4D:19:LEU:HA | 2.40 | 0.51 |
| 1:3Q:65:LEU:HD13 | 1:3Q:90:PHE:CD1 | 2.46 | 0.51 |
| 2:3T:65:CYS:SG | 2:3T:66:ILE:N | 2.83 | 0.51 |
| 3:4D:16:ASN:HD22 | 3:4D:22:LYS:HD2 | 1.75 | 0.51 |
| 3:4H:16:ASN:HD22 | 3:4H:22:LYS:HD2 | 1.75 | 0.51 |
| 3:4J:182:ASP:O | 3:4J:186:VAL:HG22 | 2.10 | 0.51 |
| 5:4M:199:ARG:O | 5:4M:203:GLU:HG2 | 2.11 | 0.51 |
| 7:4U:91:GLN:NE2 | 21:6H:74:LEU:HD21 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:5C:478:LEU:HD11 | 10:5C:495:GLU:CA | 2.34 | 0.51 |
| 12:5F:362:ASP:OD1 | 12:5F:362:ASP:C | 2.49 | 0.51 |
| 14:5L:32:TYR:OH | 14:5L:41:ARG:HD2 | 2.10 | 0.51 |
| 14:5M:32:TYR:OH | 14:5M:41:ARG:HD2 | 2.10 | 0.51 |
| 15:5P:279:ALA:HA | 15:5P:298:VAL:CG2 | 2.41 | 0.51 |
| 18:5X:210:GLU:N | 18:5X:210:GLU:OE1 | 2.44 | 0.51 |
| 18:5Y:210:GLU:N | 18:5Y:210:GLU:OE1 | 2.44 | 0.51 |
| 18:6A:210:GLU:N | 18:6A:210:GLU:OE1 | 2.44 | 0.51 |
| 18:6C:106:GLU:OE1 | 18:6C:106:GLU:N | 2.38 | 0.51 |
| 18:6D:210:GLU:N | 18:6D:210:GLU:OE1 | 2.44 | 0.51 |
| 21:6H:136:GLN:NE2 | 21:6H:170:LEU:HB3 | 2.26 | 0.51 |
| 22:6K:108:ARG:HH22 | 24:6V:283:THR:C | 2.13 | 0.51 |
| 24:6T:481:LEU:HB3 | 24:6T:500:ARG:HB3 | 1.93 | 0.51 |
| 24:6U:92:ASP:OD2 | 26:7D:49:PRO:HD2 | 2.10 | 0.51 |
| 24:6W:507:ARG:NH2 | 24:6W:507:ARG:HA | 2.26 | 0.51 |
| 24:6X:132:VAL:HB | 24:6X:148:ILE:HB | 1.93 | 0.51 |
| 24:6Y:435:LEU:HD12 | 24:6Y:435:LEU:H | 1.74 | 0.51 |
| 24:6Z:171:THR:HG22 | 24:6Z:180:TYR:HD1 | 1.75 | 0.51 |
| 24:6Z:183:ASP:OD1 | 24:6Z:184:ALA:N | 2.43 | 0.51 |
| 24:7A:5:ALA:HA | 31:7N:84:TYR:CD1 | 2.46 | 0.51 |
| 30:7K:344:ARG:HB2 | 30:7K:344:ARG:NH2 | 2.26 | 0.51 |
| 31:7M:64:HIS:O | 31:7M:76:THR:CG2 | 2.58 | 0.51 |
| 1:A3:413:SER:HA | 3:4H:203:LYS:HZ1 | 1.76 | 0.51 |
| 1:G6:190:HIS:HD2 | 1:G6:411:ALA:HA | 1.74 | 0.51 |
| 1:G6:276:ARG:HD2 | 24:6Y:410:PHE:HA | 1.93 | 0.51 |
| 2:G7:288:VAL:HG11 | 2:G7:323:VAL:HG13 | 1.92 | 0.51 |
| 2:G9:88:HIS:HB3 | 2:I5:283:HIS:ND1 | 2.25 | 0.51 |
| 2:G9:236:SER:O | 2:G9:243:ARG:NH2 | 2.44 | 0.51 |
| 1:H4:167:PHE:CZ | 1:H4:233:MET:HG2 | 2.45 | 0.51 |
| 2:H5:399:TYR:O | 2:H5:402:ARG:NH1 | 2.44 | 0.51 |
| 1:H8:404:ASP:OD1 | 1:H8:405:GLU:N | 2.38 | 0.51 |
| 2:H9:9:ILE:HG22 | 2:H9:146:GLY:HA2 | 1.93 | 0.51 |
| 2:H9:26:LEU:HD23 | 2:H9:363:VAL:HG12 | 1.93 | 0.51 |
| 1:I0:113:ILE:HD13 | 1:I0:150:LEU:HD22 | 1.92 | 0.51 |
| 2:I7:305:CYS:HB3 | 2:I7:387:ILE:HD11 | 1.92 | 0.51 |
| 1:J0:40:SER:CB | 28:7H:413:TYR:HD1 | 2.24 | 0.51 |
| 2:J1:72:PRO:HG3 | 1:J2:1:MET:HG2 | 1.93 | 0.51 |
| 1:J2:41:ASP:HA | 1:J2:44:LEU:HD23 | 1.93 | 0.51 |
| 2:J3:76:ASP:OD2 | 1:J4:46:ARG:NH2 | 2.44 | 0.51 |
| 2:K5:267:PHE:HB2 | 2:K5:384:ILE:HD12 | 1.92 | 0.51 |
| 1:K6:7:ILE:HB | 1:K6:135:VAL:HG22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K6:139:LEU:HD12 | 1:K6:170:VAL:HG12 | 1.93 | 0.51 |
| 1:K6:371:SER:OG | 1:K6:372:THR:N | 2.43 | 0.51 |
| 2:K9:88:HIS:CD2 | 2:M5:283:HIS:HB3 | 2.46 | 0.51 |
| 1:L2:203:ASP:OD2 | 1:L2:302:ALA:N | 2.44 | 0.51 |
| 2:N1:137:VAL:HG22 | 2:N1:168:GLY:HA2 | 1.92 | 0.51 |
| 1:N6:91:VAL:HG21 | 1:N6:116:VAL:HG12 | 1.93 | 0.51 |
| 1:N6:273:LEU:H | 1:N6:292:GLN:HE22 | 1.58 | 0.51 |
| 2:N7:53:PHE:HB3 | 2:N7:61:HIS:HB3 | 1.93 | 0.51 |
| 2:N7:203:MET:HB2 | 2:N7:303:VAL:HG21 | 1.92 | 0.51 |
| 2:N7:242:LEU:HD11 | 2:N7:252:ILE:HG12 | 1.93 | 0.51 |
| 1:O6:406:MET:O | 1:O6:410:GLU:HG2 | 2.10 | 0.51 |
| 1:O8:371:SER:OG | 1:O8:372:THR:N | 2.44 | 0.51 |
| 2:P3:386:GLU:OE1 | 2:P3:390:ARG:NH1 | 2.43 | 0.51 |
| 2:P7:205:ASP:OD2 | 2:P7:206:ASN:N | 2.43 | 0.51 |
| 2:Q5:166:LYS:N | 2:Q5:199:ASP:OD2 | 2.44 | 0.51 |
| 1:Q8:163:MET:SD | 1:Q8:164:MET:N | 2.84 | 0.51 |
| 1:R8:135:VAL:HG12 | 1:R8:137:HIS:HD2 | 1.76 | 0.51 |
| 2:S1:21:TRP:CZ2 | 2:S1:65:CYS:HB3 | 2.45 | 0.51 |
| 1:S2:2:ARG:HE | 1:S2:240:LEU:HD22 | 1.76 | 0.51 |
| 1:S4:249:ASP:HB2 | 1:S4:252:LYS:CE | 2.40 | 0.51 |
| 2:T3:145:THR:OG1 | 41:T4:501:GTP:O1B | 2.29 | 0.51 |
| 1:U4:309:ARG:H | 1:U4:372:THR:HG22 | 1.76 | 0.51 |
| 1:U4:317:PHE:HE2 | 1:U4:326:VAL:HG13 | 1.75 | 0.51 |
| 2:U7:47:ASP:N | 2:U7:47:ASP:OD1 | 2.44 | 0.51 |
| 2:U7:317:LEU:HB3 | 2:U7:319:TYR:HE1 | 1.75 | 0.51 |
| 2:V3:100:ALA:CA | 1:V4:252:LYS:HG2 | 2.40 | 0.51 |
| 1:V6:170:VAL:HG22 | 1:V6:203:ASP:HB3 | 1.93 | 0.51 |
| 2:V7:79:ARG:NH1 | 2:V7:92:LEU:O | 2.43 | 0.51 |
| 2:V7:274:PRO:HD3 | 2:V7:374:ALA:HA | 1.93 | 0.51 |
| 2:W1:207:GLU:HB3 | 2:W1:304:LYS:HG3 | 1.93 | 0.51 |
| 2:W1:429:GLU:O | 2:W1:433:GLU:HG2 | 2.10 | 0.51 |
| 2:W5:65:CYS:SG | 2:W5:66:ILE:N | 2.84 | 0.51 |
| 2:W7:88:HIS:HB3 | 2:W7:91:GLN:CB | 2.40 | 0.51 |
| 1:X2:123:GLU:O | 1:X2:126:SER:OG | 2.29 | 0.51 |
| 2:Y1:203:MET:HB2 | 2:Y1:303:VAL:HG21 | 1.93 | 0.51 |
| 1:Y4:97:ALA:HA | 1:Y4:103:LYS:HE3 | 1.93 | 0.51 |
| 2:Y5:154:LEU:HD12 | 2:Y5:157:LEU:HD23 | 1.92 | 0.51 |
| 2:Y5:156:ARG:O | 2:Y5:159:VAL:HG22 | 2.11 | 0.51 |
| 1:Z0:293:MET:HE2 | 1:Z0:367:PHE:HB3 | 1.91 | 0.51 |
| 1:Z2:397:TRP:HE1 | 2:Z3:260:VAL:HB | 1.76 | 0.51 |
| 1:Z6:325:GLU:HA | 1:Z6:328:GLU:HG3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:245:ASP:OD1 | 2:Z7:245:ASP:N | 2.44 | 0.51 |
| 1:Z8:242:PHE:HB2 | 1:Z8:354:CYS:SG | 2.51 | 0.51 |
| 2:Z9:181:VAL:HG12 | 1:0A:347:ASN:O | 2.11 | 0.51 |
| 2:Z9:300:SER:OG | 2:Z9:300:SER:O | 2.28 | 0.51 |
| 2:Z9:383:ALA:O | 2:Z9:387:ILE:HG12 | 2.10 | 0.51 |
| 1:0G:165:LEU:HD22 | 1:0G:167:PHE:CE1 | 2.46 | 0.51 |
| 1:0G:252:LYS:HE2 | 1:0G:350:LYS:CE | 2.41 | 0.51 |
| 2:0H:145:THR:OG1 | 41:0I:501:GTP:O1B | 2.28 | 0.51 |
| 1:0K:5:VAL:HG23 | 1:0K:62:ARG:HG2 | 1.92 | 0.51 |
| 2:0L:392:ASP:OD2 | 2:0L:422:ARG:NH1 | 2.44 | 0.51 |
| 1:0M:101:TRP:HB2 | 1:0M:184:ASN:OD1 | 2.11 | 0.51 |
| 1:0M:248:ALA:HA | 1:0M:252:LYS:HD2 | 1.93 | 0.51 |
| 1:0M:393:ALA:CB | 2:0N:346:TRP:NE1 | 2.37 | 0.51 |
| 2:0N:88:HIS:ND1 | 2:1D:283:HIS:HA | 2.26 | 0.51 |
| 1:0Q:235:GLY:HA3 | 1:0Q:366:THR:HG21 | 1.92 | 0.51 |
| 1:0U:8:GLN:O | 1:0U:66:MET:HG2 | 2.11 | 0.51 |
| 1:0Y:207:LEU:HB3 | 1:0Y:225:LEU:HD22 | 1.92 | 0.51 |
| 1:0Y:260:PHE:HB2 | 1:0Y:263:LEU:HD23 | 1.93 | 0.51 |
| 2:1B:336:LYS:O | 2:1B:339:ARG:NH2 | 2.43 | 0.51 |
| 1:1E:236:ILE:HD12 | 1:1E:368:ILE:HD11 | 1.93 | 0.51 |
| 2:1L:204:LEU:HD23 | 2:1L:231:ILE:HD12 | 1.93 | 0.51 |
| 1:1M:177:ASP:O | 2:1N:352:LYS:HA | 2.11 | 0.51 |
| 1:1O:189:VAL:HA | 1:1O:192:LEU:HB2 | 1.92 | 0.51 |
| 2:1T:111:GLY:HA2 | 2:1T:114:ILE:HG22 | 1.93 | 0.51 |
| 1:1U:72:THR:O | 1:1U:76:VAL:HG23 | 2.11 | 0.51 |
| 2:1Z:191:THR:HG23 | 2:1Z:425:LEU:HD21 | 1.93 | 0.51 |
| 1:2A:335:ASN:O | 1:2A:338:SER:OG | 2.29 | 0.51 |
| 2:2B:116:ASP:N | 2:2B:116:ASP:OD1 | 2.44 | 0.51 |
| 1:2M:404:ASP:HB3 | 1:2M:406:MET:SD | 2.51 | 0.51 |
| 2:2R:399:TYR:O | 2:2R:402:ARG:NH1 | 2.43 | 0.51 |
| 2:2T:187:SER:O | 2:2T:191:THR:HG23 | 2.11 | 0.51 |
| 1:3A:309:ARG:NH1 | 1:3A:341:PHE:O | 2.42 | 0.51 |
| 1:3G:114:ASP:N | 1:3G:114:ASP:OD1 | 2.44 | 0.51 |
| 1:3I:140:GLY:O | 1:3I:184:ASN:ND2 | 2.34 | 0.51 |
| 1:3I:161:ASP:OD1 | 1:3I:162:ARG:NH1 | 2.44 | 0.51 |
| 1:3K:4:ILE:HD11 | 1:3K:134:GLN:HB2 | 1.92 | 0.51 |
| 1:3O:128:ASP:OD1 | 1:3O:129:CYS:N | 2.39 | 0.51 |
| 1:3S:86:ARG:HB3 | 1:3S:89:ASN:OD1 | 2.11 | 0.51 |
| 2:3T:316:CYS:HB3 | 2:3T:378:ILE:HG22 | 1.92 | 0.51 |
| 3:4J:188:GLY:H | 3:4J:190:LYS:NZ | 2.09 | 0.51 |
| 6:4N:458:GLU:OE1 | 6:4O:126:ARG:NE | 2.35 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:328:ASP:HB3 | 9:4Z:331:ARG:NH2 | 2.26 | 0.51 |
| 12:5F:35:PRO:HD2 | 12:5G:383:ARG:CZ | 2.41 | 0.51 |
| 12:5F:108:ASN:HA | 33:7Q:179:GLN:NE2 | 2.26 | 0.51 |
| 14:5N:578:LYS:HA | 14:5N:589:PHE:HB3 | 1.92 | 0.51 |
| 18:5Z:103:PRO:HD3 | 24:6W:178:ASN:HB3 | 1.93 | 0.51 |
| 18:6A:5:VAL:HG13 | 18:6A:62:GLU:HG2 | 1.91 | 0.51 |
| 18:6A:39:TYR:CZ | 26:7E:24:GLN:OE1 | 2.64 | 0.51 |
| 18:6B:210:GLU:N | 18:6B:210:GLU:OE1 | 2.44 | 0.51 |
| 18:6C:210:GLU:N | 18:6C:210:GLU:OE1 | 2.44 | 0.51 |
| 18:6D:106:GLU:OE1 | 18:6D:106:GLU:N | 2.38 | 0.51 |
| 24:6V:152:ARG:HD3 | 24:6V:160:PHE:CG | 2.46 | 0.51 |
| 24:6W:536:ASP:OD1 | 24:6W:537:GLU:N | 2.44 | 0.51 |
| 24:6Y:122:TYR:HB2 | 24:6Y:131:HIS:HB3 | 1.92 | 0.51 |
| 24:6Y:378:TRP:O | 24:6Y:382:ASN:ND2 | 2.39 | 0.51 |
| 27:7G:73:GLU:O | 27:7G:77:LEU:HD23 | 2.11 | 0.51 |
| 2:2:85:GLN:NE2 | 18:5X:78:LEU:HD13 | 2.25 | 0.50 |
| 2:B7:223:THR:HG23 | 18:6B:51:MET:HE3 | 1.93 | 0.50 |
| 2:C5:44:GLY:HA3 | 24:6T:306:LEU:HD11 | 1.93 | 0.50 |
| 1:C6:358:PRO:HB2 | 24:6U:336:THR:HG21 | 1.91 | 0.50 |
| 2:E1:85:GLN:HE22 | 22:6J:213:THR:HG22 | 1.77 | 0.50 |
| 1:G2:211:CYS:SG | 1:G2:217:LEU:HB2 | 2.52 | 0.50 |
| 1:G2:361:LEU:HD23 | 1:G2:364:SER:HB2 | 1.92 | 0.50 |
| 1:G4:167:PHE:CE2 | 1:G4:233:MET:HG2 | 2.47 | 0.50 |
| 2:G5:7:ILE:HG23 | 2:G5:137:VAL:HG12 | 1.93 | 0.50 |
| 2:H1:101:ASN:ND2 | 2:H1:143:GLY:HA2 | 2.27 | 0.50 |
| 1:H6:396:HIS:H | 1:H6:396:HIS:CD2 | 2.29 | 0.50 |
| 1:H6:404:ASP:HB3 | 1:H6:406:MET:SD | 2.50 | 0.50 |
| 2:I1:115:VAL:O | 2:I1:119:LEU:HG | 2.11 | 0.50 |
| 1:J2:77:ARG:HG3 | 16:5Q:180:VAL:HG21 | 1.92 | 0.50 |
| 1:K0:215:LEU:HB3 | 1:K0:217:LEU:HG | 1.92 | 0.50 |
| 1:K6:2:ARG:HE | 1:K6:240:LEU:HD22 | 1.75 | 0.50 |
| 1:K8:14:ASN:HD22 | 1:K8:65:LEU:HD22 | 1.75 | 0.50 |
| 1:K8:131:GLN:HE21 | 1:K8:250:LEU:HB2 | 1.76 | 0.50 |
| 1:L6:117:LEU:HA | 1:L6:120:VAL:HG12 | 1.92 | 0.50 |
| 2:L9:10:GLY:HA2 | 2:L9:145:THR:HG23 | 1.92 | 0.50 |
| 2:L9:277:SER:OG | 2:L9:278:ALA:N | 2.44 | 0.50 |
| 2:M9:5:ILE:HG22 | 2:M9:64:ARG:HB3 | 1.93 | 0.50 |
| 1:N0:272:PRO:CB | 1:N0:282:ARG:HH22 | 2.23 | 0.50 |
| 1:N2:121:ARG:NH2 | 1:N2:158:GLU:OE2 | 2.42 | 0.50 |
| 2:N5:129:CYS:SG | 2:N5:130:THR:N | 2.84 | 0.50 |
| 1:N8:49:VAL:O | 1:N8:62:ARG:NH1 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O5:113:GLU:OE1 | 2:O5:113:GLU:N | 2.44 | 0.50 |
| 2:O5:217:LEU:HG | 2:O5:275:ILE:HG22 | 1.93 | 0.50 |
| 2:O7:90:GLU:HA | 2:O7:90:GLU:OE2 | 2.12 | 0.50 |
| 1:O8:211:CYS:HA | 1:O8:215:LEU:HB2 | 1.93 | 0.50 |
| 1:P4:257:LEU:HD21 | 1:P4:314:SER:HB3 | 1.92 | 0.50 |
| 2:P5:66:ILE:O | 2:P5:66:ILE:HG13 | 2.10 | 0.50 |
| 1:Q6:237:THR:HG22 | 1:Q6:237:THR:O | 2.11 | 0.50 |
| 1:Q6:417:ASP:HA | 1:Q6:420:SER:HB3 | 1.93 | 0.50 |
| 1:Q8:46:ARG:HH21 | 1:Q8:240:LEU:HB3 | 1.75 | 0.50 |
| 1:R0:215:LEU:HB3 | 1:R0:217:LEU:HG | 1.93 | 0.50 |
| 1:R6:278:SER:O | 1:R6:278:SER:OG | 2.30 | 0.50 |
| 2:S7:330:ALA:O | 2:S7:334:THR:HG23 | 2.10 | 0.50 |
| 1:T4:134:GLN:HE21 | 1:T4:167:PHE:HE2 | 1.58 | 0.50 |
| 1:T6:6:HIS:CE1 | 1:T6:8:GLN:HG2 | 2.46 | 0.50 |
| 1:U4:67:ASP:OD2 | 1:U4:72:THR:OG1 | 2.26 | 0.50 |
| 2:U7:84:ARG:HG3 | 2:U7:84:ARG:HH11 | 1.75 | 0.50 |
| 1:V8:70:PRO:N | 1:V8:92:PHE:HZ | 2.09 | 0.50 |
| 2:W1:111:GLY:O | 2:W1:115:VAL:HG22 | 2.11 | 0.50 |
| 2:W3:31:GLN:HE21 | 2:W3:37:PRO:HG3 | 1.76 | 0.50 |
| 2:W3:68:LEU:HA | 2:W3:93:ILE:O | 2.11 | 0.50 |
| 1:W6:285:THR:HG22 | 1:W6:288:GLU:HG2 | 1.92 | 0.50 |
| 1:W8:6:HIS:NE2 | 1:W8:136:CYS:SG | 2.74 | 0.50 |
| 2:W9:245:ASP:N | 2:W9:245:ASP:OD1 | 2.41 | 0.50 |
| 2:X3:88:HIS:HB3 | 2:Y9:283:HIS:CE1 | 2.46 | 0.50 |
| 1:X4:238:CYS:SG | 1:X4:239:CYS:N | 2.84 | 0.50 |
| 1:Y4:140:GLY:HA3 | 1:Y4:181:GLU:OE1 | 2.11 | 0.50 |
| 1:Y8:309:ARG:NH1 | 1:Y8:343:GLU:OE2 | 2.44 | 0.50 |
| 2:Z1:69:ASP:OD1 | 2:Z1:70:LEU:N | 2.42 | 0.50 |
| 2:Z1:381:SER:OG | 2:Z1:382:THR:N | 2.44 | 0.50 |
| 1:Z4:4:ILE:HD11 | 1:Z4:240:LEU:HD22 | 1.93 | 0.50 |
| 1:Z6:207:LEU:HD11 | 1:Z6:229:ILE:HD11 | 1.92 | 0.50 |
| 1:Z8:86:ARG:HD3 | 1:Z8:88:ASP:HB2 | 1.93 | 0.50 |
| 1:Z8:395:LEU:O | 1:Z8:399:THR:HG23 | 2.11 | 0.50 |
| 2:0B:31:GLN:HB2 | 2:0B:33:ASP:OD1 | 2.11 | 0.50 |
| 1:0C:20:PHE:HA | 1:0C:230:SER:OG | 2.11 | 0.50 |
| 2:0H:257:THR:OG1 | 2:0H:258:ASN:N | 2.42 | 0.50 |
| 1:0K:68:LEU:HD21 | 1:0K:112:LEU:HD22 | 1.92 | 0.50 |
| 2:0L:174:SER:HA | 2:0L:205:ASP:OD1 | 2.11 | 0.50 |
| 1:0O:388:MET:HG3 | 1:0O:393:ALA:HB3 | 1.94 | 0.50 |
| 2:0P:191:THR:HA | 2:0P:194:LEU:HB3 | 1.94 | 0.50 |
| 1:0S:143:THR:O | 1:0S:147:MET:HE2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0U:384:GLN:HB3 | 2:0V:348:PRO:HG3 | 1.93 | 0.50 |
| 2:0Z:227:LEU:O | 2:0Z:231:ILE:HG12 | 2.11 | 0.50 |
| 1:1E:192:LEU:HD22 | 1:1E:265:PHE:HE1 | 1.77 | 0.50 |
| 2:1N:83:TYR:HB3 | 2:1N:86:LEU:HB3 | 1.93 | 0.50 |
| 2:1N:109:THR:OG1 | 2:1N:411:GLU:OE2 | 2.27 | 0.50 |
| 1:1O:97:ALA:HA | 1:1O:103:LYS:HE3 | 1.93 | 0.50 |
| 2:1X:227:LEU:O | 2:1X:231:ILE:HG12 | 2.11 | 0.50 |
| 2:1Z:286:LEU:H | 2:1Z:286:LEU:HD23 | 1.76 | 0.50 |
| 1:2A:111:GLU:HG2 | 1:2A:112:LEU:HD22 | 1.93 | 0.50 |
| 2:2B:123:ARG:HD2 | 38:8A:75:SER:HB3 | 1.92 | 0.50 |
| 1:2G:25:SER:OG | 1:2G:30:ILE:HG13 | 2.11 | 0.50 |
| 2:2H:69:ASP:OD1 | 2:2H:70:LEU:N | 2.44 | 0.50 |
| 2:2H:81:GLY:O | 2:2H:84:ARG:NH1 | 2.43 | 0.50 |
| 1:2I:94:GLN:OE1 | 38:8C:116:GLN:NE2 | 2.44 | 0.50 |
| 1:2U:199:CYS:HB2 | 1:2U:265:PHE:HD1 | 1.76 | 0.50 |
| 1:2W:190:HIS:CD2 | 1:2W:411:ALA:HA | 2.46 | 0.50 |
| 1:3A:113:ILE:HA | 1:3A:116:VAL:HG12 | 1.92 | 0.50 |
| 2:3B:236:SER:OG | 2:3B:243:ARG:NH2 | 2.44 | 0.50 |
| 1:3M:77:ARG:NE | 3:4D:19:LEU:HA | 2.26 | 0.50 |
| 2:3T:195:LEU:HD21 | 2:3T:264:ARG:HH11 | 1.75 | 0.50 |
| 3:3X:90:ILE:O | 3:3X:93:LYS:HB2 | 2.12 | 0.50 |
| 3:4J:122:ARG:NH2 | 3:4J:167:GLU:OE2 | 2.44 | 0.50 |
| 3:4J:123:ARG:O | 3:4J:126:GLU:HG3 | 2.10 | 0.50 |
| 5:4L:290:GLN:NE2 | 28:7H:309:ALA:HB1 | 2.11 | 0.50 |
| 6:4O:406:GLN:O | 6:4O:410:MET:HG3 | 2.11 | 0.50 |
| 9:4Y:377:VAL:O | 9:4Y:381:LEU:HD23 | 2.11 | 0.50 |
| 10:5A:283:GLU:HA | 10:5A:286:LYS:HE2 | 1.93 | 0.50 |
| 10:5C:334:ARG:HH11 | 10:5C:338:LYS:CD | 2.24 | 0.50 |
| 14:5L:188:ALA:CA | 14:5L:226:VAL:CG1 | 2.86 | 0.50 |
| 14:5N:32:TYR:OH | 14:5N:41:ARG:HD2 | 2.10 | 0.50 |
| 15:5P:34:GLU:OE2 | 15:5P:49:ARG:CG | 2.55 | 0.50 |
| 18:6A:106:GLU:OE1 | 18:6A:106:GLU:N | 2.38 | 0.50 |
| 22:6I:114:THR:HG23 | 22:6I:117:GLY:H | 1.76 | 0.50 |
| 24:6Z:130:MET:CE | 24:6Z:174:ILE:CD1 | 2.89 | 0.50 |
| 28:7H:314:GLN:HA | 28:7H:317:GLU:OE1 | 2.11 | 0.50 |
| 34:7R:128:LEU:HD21 | 35:7T:76:LEU:HB3 | 1.94 | 0.50 |
| 2:6:324:VAL:CG1 | 26:7D:142:PHE:HZ | 2.23 | 0.50 |
| 1:7:405:GLU:HG2 | 4:4C:97:LYS:NZ | 2.26 | 0.50 |
| 1:A3:379:LYS:NZ | 3:4H:49:HIS:O | 2.44 | 0.50 |
| 1:A9:276:ARG:O | 24:6U:115:ARG:NH2 | 2.44 | 0.50 |
| 1:D2:177:ASP:OD1 | 39:D2:501:GDP:H3' | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G1:387:ILE:HG12 | 2:G1:390:ARG:HH22 | 1.75 | 0.50 |
| 2:G5:101:ASN:OD1 | 1:G6:252:LYS:HE3 | 2.10 | 0.50 |
| 2:G7:156:ARG:HA | 2:G7:159:VAL:HG12 | 1.93 | 0.50 |
| 2:H7:102:ASN:HB3 | 2:H7:105:ARG:HB3 | 1.93 | 0.50 |
| 2:I5:100:ALA:O | 2:I5:102:ASN:ND2 | 2.44 | 0.50 |
| 2:I9:287:SER:OG | 2:I9:288:VAL:N | 2.44 | 0.50 |
| 1:J2:11:GLN:N | 39:J2:502:GDP:O1B | 2.35 | 0.50 |
| 2:J3:48:ALA:CB | 16:5Q:174:THR:OG1 | 2.57 | 0.50 |
| 1:J8:219:THR:HA | 2:J9:326:LYS:HZ1 | 1.75 | 0.50 |
| 2:K9:384:ILE:HA | 2:K9:387:ILE:HD12 | 1.93 | 0.50 |
| 1:L0:371:SER:OG | 1:L0:372:THR:N | 2.43 | 0.50 |
| 1:L2:207:LEU:HB3 | 1:L2:225:LEU:HD22 | 1.93 | 0.50 |
| 1:L2:391:ARG:HD2 | 2:L3:346:TRP:CE2 | 2.46 | 0.50 |
| 2:L7:173:PRO:HG3 | 2:L7:183:GLU:OE2 | 2.12 | 0.50 |
| 2:L9:129:CYS:SG | 2:L9:130:THR:N | 2.83 | 0.50 |
| 1:M0:386:THR:O | 1:M0:390:ARG:HG3 | 2.10 | 0.50 |
| 2:M1:269:LEU:HG | 2:M1:384:ILE:HD11 | 1.94 | 0.50 |
| 2:M1:306:ASP:HB3 | 2:M1:309:HIS:HD2 | 1.77 | 0.50 |
| 1:M2:215:LEU:HB3 | 1:M2:217:LEU:HG | 1.92 | 0.50 |
| 2:M5:176:GLN:HE22 | 2:M5:304:LYS:HE2 | 1.76 | 0.50 |
| 2:N1:90:GLU:HG3 | 2:N1:121:ARG:NH1 | 2.26 | 0.50 |
| 2:P3:221:ARG:HB3 | 1:P4:322:SER:OG | 2.12 | 0.50 |
| 1:P6:4:ILE:HB | 1:P6:50:TYR:HE1 | 1.76 | 0.50 |
| 1:P8:42:LEU:HD22 | 1:P8:356:ILE:HD11 | 1.93 | 0.50 |
| 2:P9:206:ASN:OD1 | 41:P9:501:GTP:N2 | 2.44 | 0.50 |
| 1:Q0:212:PHE:HZ | 2:Q1:326:LYS:HG3 | 1.77 | 0.50 |
| 2:Q5:56:THR:CG2 | 2:Q5:60:LYS:HB3 | 2.40 | 0.50 |
| 2:R7:290:GLU:HA | 2:R7:293:ASN:HD22 | 1.76 | 0.50 |
| 1:R8:391:ARG:HD3 | 2:R9:346:TRP:CZ2 | 2.45 | 0.50 |
| 1:S0:207:LEU:HB3 | 1:S0:225:LEU:HD22 | 1.94 | 0.50 |
| 2:S1:110:ILE:O | 2:S1:113:GLU:HG2 | 2.11 | 0.50 |
| 1:S4:198:GLU:HB3 | 1:S4:258:ILE:HD11 | 1.92 | 0.50 |
| 1:S4:263:LEU:HD13 | 1:S4:422:TYR:HE1 | 1.77 | 0.50 |
| 1:S4:409:THR:HB | 13:5H:50:ARG:HD3 | 1.93 | 0.50 |
| 2:S5:381:SER:OG | 2:S5:382:THR:N | 2.43 | 0.50 |
| 2:S7:334:THR:HG21 | 13:5H:135:ASN:ND2 | 2.26 | 0.50 |
| 1:S8:336:LYS:HE3 | 17:5S:40:GLN:HG3 | 1.93 | 0.50 |
| 1:T0:292:GLN:HG2 | 1:T0:298:ASN:HD22 | 1.76 | 0.50 |
| 2:T1:175:PRO:O | 2:T1:394:LYS:NZ | 2.44 | 0.50 |
| 1:T2:91:VAL:HG12 | 1:T2:112:LEU:HD11 | 1.94 | 0.50 |
| 1:T4:113:ILE:HD11 | 1:T4:151:LEU:HD13 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T4:276:ARG:NH1 | 21:6H:39:ASN:OD1 | 2.44 | 0.50 |
| 1:T6:1:MET:HE2 | 26:7F:67:GLN:NE2 | 2.26 | 0.50 |
| 1:T6:49:VAL:HG13 | 1:T6:50:TYR:CD2 | 2.46 | 0.50 |
| 1:T6:359:LYS:HE2 | 33:7Q:136:TYR:OH | 2.11 | 0.50 |
| 1:T8:278:SER:O | 1:T8:278:SER:OG | 2.26 | 0.50 |
| 1:U4:7:ILE:HB | 1:U4:135:VAL:HG22 | 1.93 | 0.50 |
| 1:U8:263:LEU:HD22 | 1:U8:422:TYR:CE1 | 2.46 | 0.50 |
| 1:V0:36:TYR:CZ | 1:V0:44:LEU:HD21 | 2.46 | 0.50 |
| 1:W0:113:ILE:HA | 1:W0:116:VAL:HG12 | 1.92 | 0.50 |
| 2:W1:34:GLY:HA3 | 2:W1:60:LYS:CE | 2.41 | 0.50 |
| 1:W2:211:CYS:HA | 1:W2:215:LEU:HB2 | 1.93 | 0.50 |
| 1:W4:173:PRO:HD2 | 1:W4:380:ARG:CZ | 2.41 | 0.50 |
| 1:W4:325:GLU:O | 1:W4:329:GLN:HB2 | 2.12 | 0.50 |
| 2:W5:398:MET:HG3 | 1:W6:346:PRO:HD2 | 1.93 | 0.50 |
| 1:W6:301:CYS:SG | 1:W6:302:ALA:N | 2.84 | 0.50 |
| 1:W8:412:GLU:OE2 | 1:W8:416:ASN:ND2 | 2.42 | 0.50 |
| 2:X9:240:ALA:HB1 | 2:X9:356:ASN:HD22 | 1.76 | 0.50 |
| 1:Y0:98:GLY:HA3 | 2:Y1:254:GLU:OE2 | 2.11 | 0.50 |
| 2:Y1:318:MET:HE1 | 2:Y1:320:ARG:HG3 | 1.93 | 0.50 |
| 1:Y2:139:LEU:HD12 | 1:Y2:170:VAL:HG12 | 1.92 | 0.50 |
| 1:Y8:254:ALA:O | 1:Y8:258:ILE:HG12 | 2.11 | 0.50 |
| 1:Z0:12:CYS:HB2 | 39:Z0:502:GDP:C8 | 2.46 | 0.50 |
| 1:Z0:396:HIS:HA | 1:Z0:399:THR:HG22 | 1.93 | 0.50 |
| 2:Z1:74:VAL:O | 2:Z1:78:VAL:HG23 | 2.12 | 0.50 |
| 2:Z1:275:ILE:HD12 | 2:Z1:368:LEU:HD21 | 1.91 | 0.50 |
| 1:Z6:105:HIS:CE1 | 1:Z6:150:LEU:HD13 | 2.46 | 0.50 |
| 2:Z9:324:VAL:HG13 | 2:Z9:326:LYS:HG2 | 1.92 | 0.50 |
| 2:0B:33:ASP:OD2 | 2:0B:35:GLN:NE2 | 2.44 | 0.50 |
| 1:0E:396:HIS:HA | 1:0E:399:THR:OG1 | 2.10 | 0.50 |
| 1:0I:8:GLN:CD | 1:0I:17:GLY:HA3 | 2.31 | 0.50 |
| 2:0J:338:LYS:HZ1 | 2:0J:340:THR:N | 2.09 | 0.50 |
| 1:0K:101:TRP:HB2 | 1:0K:184:ASN:OD1 | 2.11 | 0.50 |
| 1:0M:318:ARG:HD3 | 1:0M:358:PRO:HD3 | 1.93 | 0.50 |
| 1:0O:198:GLU:HA | 1:0O:264:HIS:HB2 | 1.94 | 0.50 |
| 2:0R:56:THR:HB | 2:0R:60:LYS:HB3 | 1.93 | 0.50 |
| 2:0R:116:ASP:N | 2:0R:116:ASP:OD1 | 2.40 | 0.50 |
| 1:0S:385:PHE:HA | 1:0S:388:MET:HE2 | 1.93 | 0.50 |
| 1:0Y:55:THR:CG2 | 1:1O:284:LEU:HD23 | 2.41 | 0.50 |
| 1:1A:8:GLN:O | 1:1A:66:MET:HG3 | 2.12 | 0.50 |
| 2:1D:90:GLU:C | 2:1D:121:ARG:HH12 | 2.14 | 0.50 |
| 1:1E:8:GLN:CD | 1:1E:17:GLY:HA3 | 2.32 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1F:176:GLN:HE22 | 2:1F:304:LYS:HE2 | 1.76 | 0.50 |
| 2:1F:222:PRO:HD2 | 1:1G:324:LYS:HE3 | 1.92 | 0.50 |
| 2:1P:189:LEU:HD11 | 2:1P:418:PHE:HE1 | 1.75 | 0.50 |
| 1:1S:391:ARG:NH1 | 2:1T:434:GLU:O | 2.43 | 0.50 |
| 1:1W:177:ASP:O | 2:1X:352:LYS:HA | 2.11 | 0.50 |
| 2:1X:238:LEU:HD12 | 2:1X:239:THR:HG23 | 1.93 | 0.50 |
| 1:2A:177:ASP:O | 2:2B:352:LYS:HA | 2.11 | 0.50 |
| 1:2E:337:ASN:HB3 | 1:2E:340:TYR:HD2 | 1.76 | 0.50 |
| 2:2J:335:ILE:HG23 | 2:2J:341:ILE:HD11 | 1.94 | 0.50 |
| 2:2L:129:CYS:SG | 2:2L:130:THR:N | 2.84 | 0.50 |
| 1:2W:328:GLU:HB3 | 38:8B:67:PHE:CE1 | 2.46 | 0.50 |
| 2:3B:102:ASN:HB3 | 2:3B:105:ARG:HB3 | 1.93 | 0.50 |
| 2:3B:339:ARG:CG | 38:8C:39:LYS:NZ | 2.72 | 0.50 |
| 2:3F:406:HIS:HA | 2:3F:409:VAL:HG22 | 1.92 | 0.50 |
| 2:3H:51:THR:HG21 | 2:3H:243:ARG:HG2 | 1.94 | 0.50 |
| 1:3I:128:ASP:OD1 | 1:3I:129:CYS:N | 2.40 | 0.50 |
| 1:3K:67:ASP:OD1 | 1:3K:67:ASP:N | 2.43 | 0.50 |
| 2:3L:10:GLY:O | 2:3L:14:ILE:HG13 | 2.12 | 0.50 |
| 2:3T:195:LEU:HD11 | 2:3T:264:ARG:HB3 | 1.92 | 0.50 |
| 2:3T:305:CYS:HB3 | 2:3T:387:ILE:HD11 | 1.92 | 0.50 |
| 3:4F:90:ILE:O | 3:4F:93:LYS:HB2 | 2.12 | 0.50 |
| 12:5G:273:ARG:NH2 | 12:5G:297:LEU:O | 2.44 | 0.50 |
| 12:5G:379:ARG:HB3 | 12:5G:387:VAL:HG23 | 1.94 | 0.50 |
| 15:5O:93:ARG:NE | 15:5O:162:GLU:OE1 | 2.39 | 0.50 |
| 15:5O:169:ILE:CD1 | 15:5O:208:SER:O | 2.58 | 0.50 |
| 15:5P:370:ASN:O | 15:5P:374:THR:OG1 | 2.25 | 0.50 |
| 18:6B:106:GLU:OE1 | 18:6B:106:GLU:N | 2.38 | 0.50 |
| 21:6H:128:ALA:O | 21:6H:132:VAL:HG23 | 2.11 | 0.50 |
| 22:6N:209:ASN:OD1 | 22:6N:210:MET:N | 2.44 | 0.50 |
| 24:6V:96:LEU:HB2 | 24:6V:123:TYR:HB3 | 1.93 | 0.50 |
| 24:6X:452:MET:HA | 24:6X:530:PHE:HA | 1.93 | 0.50 |
| 29:7J:167:ILE:HD13 | 29:7J:167:ILE:O | 2.11 | 0.50 |
| 33:7Q:137:LEU:HB3 | 33:7Q:142:ASP:OD2 | 2.11 | 0.50 |
| 34:7R:106:ILE:HD11 | 35:7T:54:LEU:HB2 | 1.92 | 0.50 |
| 35:7U:146:TYR:CZ | 35:7U:150:ILE:HD11 | 2.46 | 0.50 |
| 2:8:11:GLN:HB3 | 41:8:501:GTP:PA | 2.50 | 0.50 |
| 1:B1:79:GLY:HA3 | 24:6V:221:ARG:HH22 | 1.77 | 0.50 |
| 2:E7:223:THR:HG23 | 22:6M:32:LYS:HB3 | 1.94 | 0.50 |
| 2:F1:18:ASN:HD21 | 22:6O:116:TYR:HE1 | 1.59 | 0.50 |
| 1:G0:58:ARG:HD3 | 1:H6:280:GLN:HE22 | 1.75 | 0.50 |
| 1:G2:3:GLU:HB2 | 1:G2:130:LEU:HD13 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G8:309:ARG:H | 1:G8:372:THR:HG22 | 1.76 | 0.50 |
| 2:G9:330:ALA:O | 2:G9:334:THR:HG23 | 2.11 | 0.50 |
| 1:H4:137:HIS:NE2 | 1:H4:166:THR:OG1 | 2.44 | 0.50 |
| 1:H4:263:LEU:HD13 | 1:H4:422:TYR:CE1 | 2.46 | 0.50 |
| 1:H8:2:ARG:HB3 | 1:H8:131:GLN:HB2 | 1.93 | 0.50 |
| 1:H8:289:LEU:HD23 | 1:H8:365:ALA:HB2 | 1.94 | 0.50 |
| 1:I0:178:THR:HG23 | 1:I0:181:GLU:HG3 | 1.94 | 0.50 |
| 2:I3:72:PRO:HD2 | 1:I4:2:ARG:NH1 | 2.26 | 0.50 |
| 1:J2:391:ARG:NH1 | 2:J3:435:VAL:HA | 2.27 | 0.50 |
| 2:J5:267:PHE:HB2 | 2:J5:384:ILE:HD12 | 1.93 | 0.50 |
| 2:K1:21:TRP:CD1 | 2:K1:87:PHE:HZ | 2.30 | 0.50 |
| 1:K8:91:VAL:HG11 | 1:K8:116:VAL:HG12 | 1.93 | 0.50 |
| 2:K9:281:ALA:O | 2:K9:283:HIS:N | 2.45 | 0.50 |
| 1:L0:77:ARG:HH21 | 1:L0:90:PHE:HD2 | 1.59 | 0.50 |
| 1:L0:260:PHE:HB2 | 1:L0:263:LEU:HD23 | 1.91 | 0.50 |
| 1:L4:233:MET:O | 1:L4:236:ILE:HG22 | 2.12 | 0.50 |
| 2:M1:250:VAL:HG13 | 2:M1:254:GLU:HG3 | 1.93 | 0.50 |
| 2:M9:282:TYR:HD1 | 30:7K:25:ALA:HB1 | 1.74 | 0.50 |
| 2:M9:371:VAL:HG12 | 2:M9:373:ARG:H | 1.76 | 0.50 |
| 1:N0:285:THR:OG1 | 1:N0:287:PRO:HD2 | 2.10 | 0.50 |
| 2:N3:208:ALA:CB | 2:N3:304:LYS:HE3 | 2.41 | 0.50 |
| 1:O0:67:ASP:OD1 | 1:O0:67:ASP:N | 2.44 | 0.50 |
| 1:O2:292:GLN:HG2 | 1:O2:298:ASN:ND2 | 2.26 | 0.50 |
| 2:O7:88:HIS:CD2 | 2:O7:90:GLU:HB3 | 2.45 | 0.50 |
| 2:O9:121:ARG:HD2 | 2:O9:124:LYS:HE3 | 1.93 | 0.50 |
| 1:P4:161:ASP:N | 1:P4:161:ASP:OD1 | 2.43 | 0.50 |
| 2:P5:116:ASP:OD1 | 2:P5:117:LEU:N | 2.44 | 0.50 |
| 1:P6:135:VAL:HG21 | 1:P6:152:ILE:HD11 | 1.94 | 0.50 |
| 1:P8:287:PRO:HA | 1:P8:290:THR:HG22 | 1.91 | 0.50 |
| 2:P9:220:GLU:HG2 | 2:P9:221:ARG:HG3 | 1.93 | 0.50 |
| 1:Q8:177:ASP:N | 1:Q8:181:GLU:OE2 | 2.45 | 0.50 |
| 2:R1:21:TRP:CZ3 | 2:R1:63:PRO:HB3 | 2.46 | 0.50 |
| 1:R2:389:PHE:O | 1:R2:392:LYS:NZ | 2.30 | 0.50 |
| 1:R6:139:LEU:HD12 | 1:R6:170:VAL:HG12 | 1.94 | 0.50 |
| 1:R6:148:GLY:O | 1:R6:152:ILE:HG12 | 2.12 | 0.50 |
| 2:S1:320:ARG:O | 2:S1:373:ARG:HA | 2.11 | 0.50 |
| 1:S2:51:PHE:HB3 | 1:S2:59:TYR:HB3 | 1.93 | 0.50 |
| 2:T1:53:PHE:HB3 | 2:T1:61:HIS:HB3 | 1.93 | 0.50 |
| 2:T3:53:PHE:HB3 | 2:T3:61:HIS:HB3 | 1.93 | 0.50 |
| 2:T3:326:LYS:NZ | 24:6X:37:ASN:HD21 | 2.09 | 0.50 |
| 1:T6:412:GLU:OE1 | 13:5K:51:THR:HG23 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U2:375:GLN:NE2 | 1:U2:376:GLU:OE1 | 2.43 | 0.50 |
| 2:U3:129:CYS:SG | 2:U3:130:THR:N | 2.84 | 0.50 |
| 2:U7:264:ARG:NH2 | 2:U7:431:ASP:OD2 | 2.45 | 0.50 |
| 2:U7:340:THR:HG23 | 2:U7:341:ILE:HG23 | 1.94 | 0.50 |
| 2:V9:56:THR:HG23 | 2:V9:60:LYS:HB3 | 1.94 | 0.50 |
| 1:X0:232:VAL:HG22 | 1:X0:270:PHE:HB2 | 1.93 | 0.50 |
| 1:X2:121:ARG:HG2 | 1:X2:125:GLU:OE1 | 2.11 | 0.50 |
| 1:X4:21:TRP:CZ3 | 1:X4:61:PRO:HB3 | 2.47 | 0.50 |
| 1:X6:30:ILE:HG13 | 1:X6:35:THR:C | 2.31 | 0.50 |
| 2:X7:56:THR:HG22 | 2:Z3:285:GLN:HB3 | 1.93 | 0.50 |
| 2:X9:222:PRO:HD2 | 1:Y0:324:LYS:HE3 | 1.93 | 0.50 |
| 2:Y1:172:TYR:CE2 | 2:Y1:203:MET:HG2 | 2.46 | 0.50 |
| 2:Y5:223:THR:HG22 | 2:Y5:224:TYR:N | 2.26 | 0.50 |
| 2:Y9:50:ASN:O | 2:Y9:64:ARG:NH2 | 2.43 | 0.50 |
| 1:Z2:249:ASP:O | 1:Z2:253:LEU:HG | 2.11 | 0.50 |
| 2:Z9:27:GLU:OE2 | 2:Z9:243:ARG:NH1 | 2.43 | 0.50 |
| 2:Z9:208:ALA:O | 2:Z9:212:ILE:HG12 | 2.11 | 0.50 |
| 1:0A:189:VAL:HA | 1:0A:192:LEU:HB3 | 1.93 | 0.50 |
| 1:0E:8:GLN:NE2 | 1:0E:63:ALA:HB1 | 2.25 | 0.50 |
| 1:0E:83:GLN:O | 1:0U:281:TYR:OH | 2.22 | 0.50 |
| 1:0G:165:LEU:HD13 | 1:0G:167:PHE:CZ | 2.44 | 0.50 |
| 2:0H:50:ASN:O | 2:0H:64:ARG:NH2 | 2.45 | 0.50 |
| 2:0J:178:SER:HB2 | 1:0K:347:ASN:OD1 | 2.12 | 0.50 |
| 1:0K:386:THR:O | 1:0K:390:ARG:HG3 | 2.12 | 0.50 |
| 1:0S:12:CYS:O | 1:0S:16:ILE:HG12 | 2.12 | 0.50 |
| 1:0W:156:ARG:NH1 | 1:0W:197:ASP:OD1 | 2.44 | 0.50 |
| 1:0Y:8:GLN:CD | 1:0Y:17:GLY:HA3 | 2.31 | 0.50 |
| 2:0Z:5:ILE:HG22 | 2:0Z:64:ARG:HB3 | 1.93 | 0.50 |
| 2:1B:69:ASP:OD1 | 2:1B:70:LEU:N | 2.44 | 0.50 |
| 1:1C:397:TRP:HZ2 | 2:1D:260:VAL:CG2 | 2.25 | 0.50 |
| 2:1D:88:HIS:NE2 | 2:1D:90:GLU:HB2 | 2.27 | 0.50 |
| 2:1L:333:ALA:O | 2:1L:337:THR:HG23 | 2.11 | 0.50 |
| 1:1M:7:ILE:HB | 1:1M:135:VAL:HG22 | 1.92 | 0.50 |
| 2:1N:317:LEU:HB3 | 2:1N:319:TYR:HE1 | 1.76 | 0.50 |
| 2:1Z:63:PRO:O | 2:1Z:91:GLN:NE2 | 2.43 | 0.50 |
| 2:1Z:269:LEU:O | 2:1Z:378:ILE:HD12 | 2.10 | 0.50 |
| 2:2D:69:ASP:OD1 | 2:2D:70:LEU:N | 2.44 | 0.50 |
| 1:2E:116:VAL:HA | 1:2E:119:VAL:HG12 | 1.94 | 0.50 |
| 2:2P:286:LEU:O | 2:2P:373:ARG:NH1 | 2.44 | 0.50 |
| 1:2Q:280:GLN:OE1 | 10:5C:192:ARG:NH1 | 2.44 | 0.50 |
| 1:2S:282:ARG:HH21 | 1:2S:288:GLU:CD | 2.15 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2T:287:SER:OG | 2:2T:288:VAL:N | 2.45 | 0.50 |
| 1:3A:125:GLU:OE2 | 1:3A:159:TYR:OH | 2.30 | 0.50 |
| 1:3A:391:ARG:HD2 | 2:3B:346:TRP:CG | 2.45 | 0.50 |
| 2:3D:11:GLN:OE1 | 2:3D:15:GLN:NE2 | 2.44 | 0.50 |
| 1:3G:128:ASP:OD1 | 1:3G:129:CYS:N | 2.39 | 0.50 |
| 2:3H:280:LYS:HA | 2:3H:283:HIS:HB3 | 1.93 | 0.50 |
| 2:3L:223:THR:HG22 | 2:3L:224:TYR:N | 2.26 | 0.50 |
| 2:3N:405:VAL:HG13 | 2:3N:418:PHE:HE2 | 1.76 | 0.50 |
| 2:3P:179:THR:O | 1:3Q:350:LYS:HD2 | 2.11 | 0.50 |
| 3:3V:90:ILE:O | 3:3V:93:LYS:HB2 | 2.12 | 0.50 |
| 3:3Z:90:ILE:O | 3:3Z:93:LYS:HB2 | 2.12 | 0.50 |
| 3:4B:90:ILE:O | 3:4B:93:LYS:HB2 | 2.12 | 0.50 |
| 4:4C:50:MET:HG3 | 4:4C:159:ASN:HD22 | 1.77 | 0.50 |
| 3:4D:90:ILE:O | 3:4D:93:LYS:HB2 | 2.12 | 0.50 |
| 3:4H:90:ILE:O | 3:4H:93:LYS:HB2 | 2.12 | 0.50 |
| 7:4R:301:ARG:NH2 | 7:4R:301:ARG:CG | 2.60 | 0.50 |
| 9:4Y:355:ALA:O | 9:4Y:359:ARG:HG2 | 2.12 | 0.50 |
| 9:4Z:196:LYS:O | 9:4Z:199:GLU:HG3 | 2.11 | 0.50 |
| 10:5B:250:LYS:O | 10:5B:254:MET:HG3 | 2.11 | 0.50 |
| 15:5O:95:LEU:HD11 | 15:5O:221:TRP:HD1 | 1.75 | 0.50 |
| 15:5P:336:ARG:HA | 15:5P:345:ALA:HB1 | 1.92 | 0.50 |
| 18:5X:214:TYR:O | 18:5X:218:SER:OG | 2.28 | 0.50 |
| 18:5Y:106:GLU:OE1 | 18:5Y:106:GLU:N | 2.38 | 0.50 |
| 18:5Y:214:TYR:O | 18:5Y:218:SER:OG | 2.29 | 0.50 |
| 19:6E:182:PHE:O | 19:6E:186:THR:HG22 | 2.12 | 0.50 |
| 22:6O:146:LEU:HD23 | 22:6O:234:GLY:HA2 | 1.94 | 0.50 |
| 23:6R:28:LYS:HE2 | 23:6R:28:LYS:CA | 2.35 | 0.50 |
| 24:6X:185:ASP:OD1 | 24:6X:186:SER:N | 2.43 | 0.50 |
| 27:7G:109:ILE:HG13 | 27:7G:113:ILE:HB | 1.93 | 0.50 |
| 31:7M:63:ARG:O | 31:7M:76:THR:HG21 | 2.11 | 0.50 |
| 36:7V:46:LEU:HD22 | 36:7V:48:HIS:ND1 | 2.26 | 0.50 |
| 36:7W:46:LEU:HD22 | 36:7W:48:HIS:ND1 | 2.26 | 0.50 |
| 38:8A:82:ASP:OD1 | 38:8A:82:ASP:N | 2.37 | 0.50 |
| 1:A3:40:SER:C | 26:7F:25:TYR:CE2 | 2.84 | 0.50 |
| 2:E9:88:HIS:HE1 | 2:G5:280:LYS:HA | 1.74 | 0.50 |
| 2:I1:147:SER:HB2 | 2:I1:190:SER:OG | 2.11 | 0.50 |
| 1:I2:173:PRO:HG2 | 1:I2:174:LYS:HZ2 | 1.76 | 0.50 |
| 1:I2:358:PRO:HG2 | 1:I2:361:LEU:HB2 | 1.93 | 0.50 |
| 2:I3:363:VAL:HG23 | 2:I3:366:GLY:HA3 | 1.94 | 0.50 |
| 1:I4:174:LYS:HD2 | 1:I4:174:LYS:H | 1.76 | 0.50 |
| 2:I7:387:ILE:HG12 | 2:I7:390:ARG:HH22 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I8:215:LEU:HB3 | 1:I8:217:LEU:HG | 1.91 | 0.50 |
| 1:J4:33:THR:HG21 | 5:4M:120:ARG:CD | 2.42 | 0.50 |
| 2:J5:98:ASP:OD1 | 2:J5:99:ALA:N | 2.44 | 0.50 |
| 2:J7:50:ASN:O | 2:J7:64:ARG:NH2 | 2.44 | 0.50 |
| 2:K1:156:ARG:HA | 2:K1:159:VAL:HG12 | 1.94 | 0.50 |
| 1:K6:131:GLN:HE21 | 1:K6:250:LEU:HB2 | 1.77 | 0.50 |
| 1:K8:7:ILE:HB | 1:K8:135:VAL:HG22 | 1.92 | 0.50 |
| 1:L2:350:LYS:NZ | 1:L2:351:SER:O | 2.41 | 0.50 |
| 2:L3:53:PHE:HB3 | 2:L3:61:HIS:HB3 | 1.94 | 0.50 |
| 1:L6:350:LYS:NZ | 1:L6:351:SER:O | 2.42 | 0.50 |
| 2:L9:333:ALA:O | 2:L9:337:THR:HG23 | 2.12 | 0.50 |
| 1:M2:396:HIS:H | 1:M2:396:HIS:CD2 | 2.30 | 0.50 |
| 1:M8:244:GLY:H | 1:M8:247:ASN:HD21 | 1.60 | 0.50 |
| 2:O5:79:ARG:NH1 | 2:O5:94:SER:OG | 2.44 | 0.50 |
| 2:O9:109:THR:HB | 2:O9:110:ILE:HD12 | 1.94 | 0.50 |
| 1:P8:382:SER:HB2 | 1:P8:415:MET:HG2 | 1.93 | 0.50 |
| 2:P9:5:ILE:HD11 | 2:P9:135:PHE:HE1 | 1.75 | 0.50 |
| 2:Q1:27:GLU:HG3 | 2:Q1:361:THR:HG21 | 1.94 | 0.50 |
| 2:Q1:56:THR:OG1 | 2:R7:285:GLN:N | 2.45 | 0.50 |
| 1:Q8:36:TYR:HD1 | 1:Q8:59:TYR:HE2 | 1.59 | 0.50 |
| 1:R0:22:GLU:HG3 | 1:R0:81:TYR:CD1 | 2.47 | 0.50 |
| 2:R3:6:SER:O | 2:R3:65:CYS:HA | 2.10 | 0.50 |
| 1:S8:67:ASP:N | 1:S8:67:ASP:OD1 | 2.44 | 0.50 |
| 1:T4:362:LYS:HG3 | 1:T4:363:MET:HG3 | 1.93 | 0.50 |
| 2:T5:33:ASP:O | 2:T5:60:LYS:NZ | 2.41 | 0.50 |
| 1:T6:113:ILE:HD11 | 1:T6:151:LEU:HD13 | 1.94 | 0.50 |
| 2:T7:339:ARG:HH21 | 13:5K:24:VAL:CG1 | 2.24 | 0.50 |
| 2:U1:287:SER:OG | 2:U1:288:VAL:N | 2.44 | 0.50 |
| 1:U6:282:ARG:NH2 | 1:U6:284:LEU:HD13 | 2.27 | 0.50 |
| 2:V9:76:ASP:OD1 | 1:W0:46:ARG:NH2 | 2.45 | 0.50 |
| 2:V9:287:SER:N | 2:V9:290:GLU:OE2 | 2.20 | 0.50 |
| 2:V9:297:GLU:OE2 | 2:V9:308:ARG:NH2 | 2.43 | 0.50 |
| 1:W2:317:PHE:HE2 | 1:W2:326:VAL:HG13 | 1.75 | 0.50 |
| 1:W4:211:CYS:HA | 1:W4:215:LEU:HB2 | 1.94 | 0.50 |
| 1:W4:233:MET:O | 1:W4:237:THR:HG22 | 2.12 | 0.50 |
| 2:Y3:22:GLU:HG2 | 2:Y3:83:TYR:CE2 | 2.45 | 0.50 |
| 2:Y3:88:HIS:CE1 | 2:Z9:283:HIS:HA | 2.46 | 0.50 |
| 2:Y3:115:VAL:HG21 | 2:Y3:152:LEU:HD23 | 1.92 | 0.50 |
| 2:Y3:180:ALA:HB1 | 1:Y4:256:ASN:HD21 | 1.76 | 0.50 |
| 2:Y5:254:GLU:OE2 | 2:Y5:254:GLU:N | 2.44 | 0.50 |
| 1:Y8:327:ASP:O | 1:Y8:331:LEU:HG | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z1:8:HIS:CD2 | 2:Z1:138:PHE:HD2 | 2.29 | 0.50 |
| 1:Z2:86:ARG:HG2 | 1:Z2:88:ASP:H | 1.76 | 0.50 |
| 1:Z2:272:PRO:O | 1:Z2:273:LEU:HD23 | 2.12 | 0.50 |
| 1:Z4:239:CYS:HB2 | 1:Z4:316:LEU:HD11 | 1.94 | 0.50 |
| 2:Z5:15:GLN:HB3 | 2:Z5:228:ASN:ND2 | 2.25 | 0.50 |
| 1:0I:91:VAL:HG21 | 1:0I:116:VAL:HG12 | 1.93 | 0.50 |
| 1:0I:244:GLY:H | 1:0I:247:ASN:HD21 | 1.60 | 0.50 |
| 1:0K:123:GLU:O | 1:0K:126:SER:OG | 2.29 | 0.50 |
| 1:0K:371:SER:OG | 1:0K:372:THR:N | 2.44 | 0.50 |
| 2:0N:344:VAL:CG1 | 2:0N:347:CYS:HB3 | 2.41 | 0.50 |
| 1:0O:173:PRO:HB3 | 1:0O:384:GLN:HE22 | 1.77 | 0.50 |
| 2:0P:164:LYS:O | 2:0P:166:LYS:NZ | 2.45 | 0.50 |
| 1:0Y:167:PHE:HD1 | 1:0Y:200:MET:HB3 | 1.76 | 0.50 |
| 2:1F:217:LEU:HB3 | 2:1F:219:ILE:HD12 | 1.93 | 0.50 |
| 1:1K:193:VAL:HG12 | 1:1K:265:PHE:HZ | 1.76 | 0.50 |
| 2:1L:83:TYR:HB3 | 2:1L:86:LEU:HB3 | 1.93 | 0.50 |
| 2:1N:291:ILE:HD12 | 2:1N:375:VAL:HG23 | 1.92 | 0.50 |
| 1:2E:186:THR:HG22 | 1:2E:411:ALA:HB1 | 1.94 | 0.50 |
| 2:2H:279:GLU:OE2 | 2:2H:279:GLU:HA | 2.11 | 0.50 |
| 1:2K:286:VAL:HG21 | 1:2K:325:GLU:HB3 | 1.92 | 0.50 |
| 2:2L:212:ILE:O | 2:2L:216:SER:OG | 2.29 | 0.50 |
| 2:2L:284:GLU:HG3 | 2:2L:285:GLN:N | 2.26 | 0.50 |
| 2:2N:320:ARG:NH2 | 2:2N:358:GLN:OE1 | 2.44 | 0.50 |
| 2:2P:259:LEU:HD11 | 2:2P:316:CYS:HB2 | 1.92 | 0.50 |
| 1:2U:114:ASP:N | 1:2U:114:ASP:OD2 | 2.44 | 0.50 |
| 1:2Y:221:THR:HG23 | 1:2Y:223:GLY:H | 1.76 | 0.50 |
| 2:2Z:279:GLU:H | 2:2Z:279:GLU:CD | 2.11 | 0.50 |
| 1:3A:199:CYS:HG | 1:3A:265:PHE:HD1 | 1.58 | 0.50 |
| 2:3P:91:GLN:HE21 | 3:4F:36:PHE:HE2 | 1.59 | 0.50 |
| 2:3P:217:LEU:HB3 | 2:3P:219:ILE:HD12 | 1.92 | 0.50 |
| 1:3S:115:SER:O | 1:3S:119:VAL:HG23 | 2.12 | 0.50 |
| 2:3T:287:SER:OG | 2:3T:288:VAL:N | 2.44 | 0.50 |
| 3:3X:13:THR:O | 3:3X:17:VAL:HG13 | 2.11 | 0.50 |
| 4:4A:50:MET:HG3 | 4:4A:159:ASN:HD22 | 1.77 | 0.50 |
| 3:4B:13:THR:O | 3:4B:17:VAL:HG13 | 2.11 | 0.50 |
| 4:4E:50:MET:HG3 | 4:4E:159:ASN:HD22 | 1.77 | 0.50 |
| 3:4F:13:THR:O | 3:4F:17:VAL:HG13 | 2.11 | 0.50 |
| 14:5L:485:VAL:HG13 | 14:5L:518:TYR:OH | 2.11 | 0.50 |
| 14:5L:520:PRO:HD3 | 14:5L:561:VAL:HG11 | 1.94 | 0.50 |
| 15:5P:283:GLU:OE1 | 15:5P:283:GLU:N | 2.44 | 0.50 |
| 15:5P:327:ALA:HA | 15:5P:343:LEU:CD2 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5S:140:LEU:O | 17:5S:144:LYS:HG3 | 2.11 | 0.50 |
| 17:5T:140:LEU:O | 17:5T:144:LYS:HG3 | 2.11 | 0.50 |
| 18:5Z:214:TYR:O | 18:5Z:218:SER:OG | 2.29 | 0.50 |
| 18:6B:214:TYR:O | 18:6B:218:SER:OG | 2.28 | 0.50 |
| 22:6K:204:PHE:CB | 22:6K:227:TYR:HE2 | 2.24 | 0.50 |
| 22:6L:177:LEU:HD21 | 22:6L:187:MET:CG | 2.41 | 0.50 |
| 22:6M:130:LEU:HD23 | 22:6M:209:ASN:ND2 | 2.22 | 0.50 |
| 22:6P:183:ASN:OD1 | 22:6P:184:ALA:N | 2.45 | 0.50 |
| 24:6T:123:TYR:HE2 | 24:6T:163:PRO:HG3 | 1.75 | 0.50 |
| 24:6T:183:ASP:OD1 | 24:6T:184:ALA:N | 2.44 | 0.50 |
| 24:6V:371:ALA:HB1 | 24:6V:375:THR:OG1 | 2.11 | 0.50 |
| 24:6W:563:LYS:HA | 24:6W:566:VAL:HG12 | 1.94 | 0.50 |
| 24:6Y:123:TYR:HD1 | 24:6Y:130:MET:SD | 2.33 | 0.50 |
| 34:7S:205:LEU:HD12 | 36:7W:91:PRO:HG3 | 1.92 | 0.50 |
| 38:8C:163:PHE:O | 38:8C:164:GLU:HB3 | 2.11 | 0.50 |
| 2:C9:220:GLU:HB3 | 18:5Z:160:ASP:OD1 | 2.10 | 0.50 |
| 1:E4:32:PRO:HG2 | 24:6V:403:PRO:HD2 | 1.93 | 0.50 |
| 1:G2:86:ARG:NH1 | 1:G2:89:ASN:OD1 | 2.45 | 0.50 |
| 2:G5:220:GLU:N | 2:G5:220:GLU:OE2 | 2.45 | 0.50 |
| 1:H6:218:THR:CB | 24:6V:488:ARG:HB3 | 2.40 | 0.50 |
| 2:I3:98:ASP:OD1 | 2:I3:99:ALA:N | 2.45 | 0.50 |
| 2:I7:132:LEU:HD22 | 2:I7:164:LYS:HD3 | 1.93 | 0.50 |
| 1:I8:70:PRO:N | 1:I8:92:PHE:HZ | 2.09 | 0.50 |
| 2:J1:280:LYS:HA | 2:J1:283:HIS:HB3 | 1.92 | 0.50 |
| 2:J5:294:ALA:HA | 2:J5:297:GLU:OE1 | 2.11 | 0.50 |
| 1:J8:248:ALA:HA | 1:J8:252:LYS:HD2 | 1.93 | 0.50 |
| 2:K1:21:TRP:NE1 | 2:K1:65:CYS:SG | 2.84 | 0.50 |
| 2:K9:278:ALA:HA | 2:K9:369:ALA:HB2 | 1.94 | 0.50 |
| 1:L0:392:LYS:HD2 | 1:L0:395:LEU:HD22 | 1.93 | 0.50 |
| 2:L3:288:VAL:HG13 | 2:L3:319:TYR:HE2 | 1.77 | 0.50 |
| 2:L5:116:ASP:N | 2:L5:116:ASP:OD1 | 2.42 | 0.50 |
| 1:M2:5:VAL:HG12 | 1:M2:133:PHE:HD1 | 1.77 | 0.50 |
| 1:M6:117:LEU:HA | 1:M6:120:VAL:HG12 | 1.93 | 0.50 |
| 1:M8:211:CYS:HA | 1:M8:215:LEU:HB2 | 1.93 | 0.50 |
| 2:N7:198:THR:HG21 | 2:N7:201:ALA:HB2 | 1.92 | 0.50 |
| 2:N7:429:GLU:O | 2:N7:433:GLU:HG2 | 2.11 | 0.50 |
| 2:N9:287:SER:OG | 2:N9:288:VAL:N | 2.44 | 0.50 |
| 2:O1:203:MET:HB2 | 2:O1:303:VAL:HG21 | 1.92 | 0.50 |
| 1:O4:207:LEU:HB3 | 1:O4:225:LEU:HD22 | 1.92 | 0.50 |
| 2:O9:335:ILE:HG23 | 2:O9:341:ILE:HD11 | 1.94 | 0.50 |
| 2:P5:4:VAL:HG23 | 2:P5:134:GLY:O | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:319:GLY:O | 1:Q0:321:MET:HG3 | 2.11 | 0.50 |
| 2:Q3:333:ALA:O | 2:Q3:337:THR:HG23 | 2.12 | 0.50 |
| 1:Q4:153:SER:HA | 1:Q4:195:ASN:ND2 | 2.27 | 0.50 |
| 2:Q5:212:ILE:O | 2:Q5:216:SER:OG | 2.28 | 0.50 |
| 2:Q5:430:LYS:O | 2:Q5:434:GLU:HG2 | 2.12 | 0.50 |
| 1:Q6:134:GLN:HE21 | 1:Q6:167:PHE:HE2 | 1.59 | 0.50 |
| 1:Q6:139:LEU:HD12 | 1:Q6:170:VAL:HG12 | 1.93 | 0.50 |
| 1:R0:121:ARG:NH2 | 1:R0:158:GLU:OE2 | 2.39 | 0.50 |
| 1:R4:52:ASN:OD1 | 1:R4:62:ARG:NH2 | 2.44 | 0.50 |
| 1:S2:359:LYS:HG3 | 12:5F:66:LYS:HG2 | 1.92 | 0.50 |
| 2:S5:223:THR:OG1 | 2:S5:224:TYR:N | 2.45 | 0.50 |
| 1:S6:65:LEU:HD12 | 1:S6:90:PHE:CE1 | 2.46 | 0.50 |
| 2:S7:72:PRO:HD2 | 1:S8:2:ARG:HH12 | 1.75 | 0.50 |
| 1:S8:83:GLN:OE1 | 1:S8:83:GLN:N | 2.35 | 0.50 |
| 1:T4:4:ILE:HB | 1:T4:50:TYR:HE1 | 1.75 | 0.50 |
| 1:T4:186:THR:HG22 | 1:T4:411:ALA:HB1 | 1.93 | 0.50 |
| 1:T6:306:ARG:HD3 | 17:5U:49:MET:HB2 | 1.92 | 0.50 |
| 1:U4:173:PRO:HD2 | 1:U4:380:ARG:NE | 2.27 | 0.50 |
| 2:U7:100:ALA:CA | 1:U8:252:LYS:HG2 | 2.40 | 0.50 |
| 2:U7:175:PRO:HB3 | 2:U7:390:ARG:HD2 | 1.94 | 0.50 |
| 2:V3:72:PRO:HD2 | 1:V4:2:ARG:HH12 | 1.76 | 0.50 |
| 2:V7:253:THR:O | 2:V7:257:THR:HG23 | 2.11 | 0.50 |
| 1:V8:173:PRO:HD2 | 1:V8:380:ARG:NH1 | 2.25 | 0.50 |
| 2:V9:5:ILE:HD11 | 2:V9:135:PHE:CE1 | 2.46 | 0.50 |
| 2:W1:167:LEU:HD13 | 2:W1:200:VAL:HB | 1.94 | 0.50 |
| 2:W3:90:GLU:CG | 2:W3:121:ARG:HD3 | 2.40 | 0.50 |
| 2:W3:90:GLU:HG3 | 2:W3:121:ARG:HD3 | 1.93 | 0.50 |
| 1:W6:70:PRO:N | 1:W6:92:PHE:HZ | 2.09 | 0.50 |
| 1:W8:31:ASP:HB2 | 1:W8:32:PRO:HD2 | 1.94 | 0.50 |
| 2:X3:2:ARG:HD2 | 2:X3:242:LEU:HD22 | 1.93 | 0.50 |
| 2:X3:3:GLU:O | 2:X3:133:GLN:N | 2.40 | 0.50 |
| 2:X5:70:LEU:HB3 | 2:X5:97:GLU:O | 2.12 | 0.50 |
| 2:X9:183:GLU:CD | 2:X9:184:PRO:HD3 | 2.32 | 0.50 |
| 1:Y0:83:GLN:O | 1:Z6:281:TYR:OH | 2.25 | 0.50 |
| 1:Y4:249:ASP:OD1 | 1:Y4:252:LYS:N | 2.39 | 0.50 |
| 2:Y5:188:VAL:HA | 2:Y5:191:THR:HG22 | 1.94 | 0.50 |
| 2:Y5:203:MET:HG3 | 2:Y5:303:VAL:HG21 | 1.93 | 0.50 |
| 1:Y8:86:ARG:HG2 | 1:Y8:88:ASP:H | 1.77 | 0.50 |
| 1:Z4:122:LYS:O | 1:Z4:126:SER:OG | 2.21 | 0.50 |
| 2:Z5:174:SER:OG | 2:Z5:175:PRO:HD2 | 2.12 | 0.50 |
| 1:Z8:204:ASN:ND2 | 39:Z8:501:GDP:HN22 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0E:6:HIS:HE1 | 1:0E:8:GLN:HG3 | 1.76 | 0.50 |
| 2:0F:208:ALA:O | 2:0F:212:ILE:HG12 | 2.11 | 0.50 |
| 1:0W:275:SER:O | 1:0W:279:GLN:HG3 | 2.10 | 0.50 |
| 2:0X:14:ILE:HD11 | 2:0X:74:VAL:HG22 | 1.93 | 0.50 |
| 2:1B:345:ASP:N | 2:1B:345:ASP:OD1 | 2.45 | 0.50 |
| 2:1F:320:ARG:NH2 | 2:1F:359:PRO:O | 2.45 | 0.50 |
| 2:1H:191:THR:HA | 2:1H:194:LEU:HB3 | 1.93 | 0.50 |
| 1:1O:113:ILE:O | 1:1O:117:LEU:HG | 2.12 | 0.50 |
| 1:1Q:42:LEU:HA | 1:1Q:45:GLU:OE2 | 2.11 | 0.50 |
| 2:1T:383:ALA:HA | 2:1T:386:GLU:HG2 | 1.94 | 0.50 |
| 1:2A:114:ASP:OD1 | 1:2A:114:ASP:N | 2.41 | 0.50 |
| 1:2A:150:LEU:O | 1:2A:153:SER:OG | 2.25 | 0.50 |
| 2:2B:156:ARG:HA | 2:2B:159:VAL:HG12 | 1.94 | 0.50 |
| 1:2E:276:ARG:HH12 | 10:5A:413:GLU:CG | 2.24 | 0.50 |
| 2:2H:88:HIS:HD1 | 2:2H:121:ARG:NH2 | 2.09 | 0.50 |
| 1:2I:274:THR:OG1 | 1:2I:279:GLN:HG2 | 2.12 | 0.50 |
| 1:2I:309:ARG:NH1 | 1:2I:339:SER:O | 2.44 | 0.50 |
| 1:2I:418:LEU:HG | 1:2I:422:TYR:HE2 | 1.77 | 0.50 |
| 2:2N:137:VAL:HG22 | 2:2N:168:GLY:HA2 | 1.93 | 0.50 |
| 1:2S:167:PHE:CE2 | 1:2S:233:MET:HG2 | 2.47 | 0.50 |
| 1:2S:208:TYR:HE1 | 1:2S:225:LEU:HD11 | 1.76 | 0.50 |
| 2:2T:9:ILE:HG22 | 2:2T:146:GLY:HA2 | 1.94 | 0.50 |
| 2:2T:48:ALA:HB2 | 38:8B:215:ALA:HB1 | 1.94 | 0.50 |
| 2:2V:108:TYR:O | 2:2V:112:LYS:HG2 | 2.11 | 0.50 |
| 2:2V:217:LEU:HD21 | 2:2V:368:LEU:HD23 | 1.94 | 0.50 |
| 2:3B:346:TRP:CZ3 | 2:3B:347:CYS:HB2 | 2.46 | 0.50 |
| 1:3C:117:LEU:HD21 | 1:3C:121:ARG:HH22 | 1.77 | 0.50 |
| 1:3I:272:PRO:HB2 | 1:3I:282:ARG:HH12 | 1.76 | 0.50 |
| 2:3N:9:ILE:HG22 | 2:3N:146:GLY:HA2 | 1.92 | 0.50 |
| 2:3P:119:LEU:HA | 2:3P:122:ILE:HG22 | 1.93 | 0.50 |
| 1:3S:7:ILE:HD13 | 1:3S:151:LEU:HD21 | 1.94 | 0.50 |
| 1:3S:266:PHE:HE1 | 1:3S:370:ASN:HD22 | 1.58 | 0.50 |
| 4:3W:50:MET:HG3 | 4:3W:159:ASN:HD22 | 1.77 | 0.50 |
| 4:3Y:50:MET:HG3 | 4:3Y:159:ASN:HD22 | 1.77 | 0.50 |
| 3:3Z:13:THR:O | 3:3Z:17:VAL:HG13 | 2.11 | 0.50 |
| 4:4G:50:MET:HG3 | 4:4G:159:ASN:HD22 | 1.77 | 0.50 |
| 4:4I:50:MET:HG3 | 4:4I:159:ASN:HD22 | 1.77 | 0.50 |
| 3:4J:154:TYR:HD2 | 3:4J:158:LEU:HD11 | 1.77 | 0.50 |
| 10:5B:173:MET:O | 10:5B:176:GLU:HG3 | 2.12 | 0.50 |
| 11:5E:185:ASP:HB3 | 11:5E:188:THR:HG23 | 1.93 | 0.50 |
| 14:5M:485:VAL:HG13 | 14:5M:518:TYR:OH | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:520:PRO:HD3 | 14:5M:561:VAL:HG11 | 1.94 | 0.50 |
| 14:5N:186:THR:O | 14:5N:186:THR:OG1 | 2.29 | 0.50 |
| 14:5N:415:LYS:HG2 | 23:6S:23:ILE:CD1 | 2.40 | 0.50 |
| 14:5N:485:VAL:HG13 | 14:5N:518:TYR:OH | 2.11 | 0.50 |
| 14:5N:520:PRO:HD3 | 14:5N:561:VAL:HG11 | 1.94 | 0.50 |
| 15:5O:6:ARG:CD | 15:5O:27:PHE:CE2 | 2.90 | 0.50 |
| 15:5O:22:TRP:NE1 | 15:5O:24:TYR:CE1 | 2.80 | 0.50 |
| 15:5P:20:ILE:HD11 | 19:6E:104:TYR:CZ | 2.47 | 0.50 |
| 15:5P:213:THR:O | 15:5P:217:GLU:HG3 | 2.12 | 0.50 |
| 16:5Q:36:THR:O | 16:5Q:40:THR:HG23 | 2.12 | 0.50 |
| 17:5U:140:LEU:O | 17:5U:144:LYS:HG3 | 2.11 | 0.50 |
| 18:6A:214:TYR:O | 18:6A:218:SER:OG | 2.29 | 0.50 |
| 18:6D:214:TYR:O | 18:6D:218:SER:OG | 2.29 | 0.50 |
| 19:6E:12:ASN:O | 19:6E:38:ARG:NH1 | 2.44 | 0.50 |
| 20:6F:75:VAL:HB | 20:6F:82:VAL:HG12 | 1.93 | 0.50 |
| 22:6M:323:ASP:O | 22:6M:327:GLU:HG3 | 2.11 | 0.50 |
| 22:6P:31:TYR:O | 22:6P:32:LYS:HG3 | 2.12 | 0.50 |
| 24:6U:123:TYR:CE2 | 24:6U:163:PRO:HG3 | 2.47 | 0.50 |
| 24:6V:450:VAL:HB | 24:6V:469:PHE:CE2 | 2.47 | 0.50 |
| 24:6X:88:TRP:HA | 24:6X:126:GLU:HG3 | 1.94 | 0.50 |
| 24:6X:376:LYS:HA | 24:6X:390:MET:HE2 | 1.92 | 0.50 |
| 24:6Y:88:TRP:CZ3 | 24:6Y:89:VAL:HB | 2.46 | 0.50 |
| 24:6Y:93:ARG:HD3 | 26:7F:45:MET:O | 2.12 | 0.50 |
| 24:6Z:123:TYR:HE2 | 24:6Z:163:PRO:HG3 | 1.75 | 0.50 |
| 26:7E:58:ILE:H | 26:7E:58:ILE:CD1 | 2.16 | 0.50 |
| 28:7H:429:ASP:OD1 | 28:7H:429:ASP:N | 2.44 | 0.50 |
| 29:7J:383:GLY:HA2 | 29:7J:386:HIS:HD2 | 1.77 | 0.50 |
| 28:7X:429:ASP:OD1 | 28:7X:429:ASP:N | 2.44 | 0.50 |
| 38:8C:83:ARG:HD3 | 38:8C:83:ARG:H | 1.76 | 0.50 |
| 1:3:78:SER:CB | 24:6U:149:LYS:HG3 | 2.39 | 0.50 |
| 2:4:29:GLY:C | 26:7D:45:MET:HE1 | 2.30 | 0.50 |
| 2:G1:364:PRO:HB2 | 22:6L:165:MET:SD | 2.51 | 0.50 |
| 1:G2:54:ALA:HB3 | 1:G2:58:ARG:HB3 | 1.93 | 0.50 |
| 2:H7:91:GLN:NE2 | 2:J3:283:HIS:HE1 | 2.08 | 0.50 |
| 2:I1:251:ASP:OD1 | 2:I1:254:GLU:HG2 | 2.12 | 0.50 |
| 1:I4:407:GLU:N | 1:I4:407:GLU:OE1 | 2.41 | 0.50 |
| 1:I8:179:VAL:HG12 | 2:I9:258:ASN:HD22 | 1.77 | 0.50 |
| 1:I8:317:PHE:HB3 | 1:I8:321:MET:SD | 2.51 | 0.50 |
| 1:J2:152:ILE:HD12 | 1:J2:164:MET:SD | 2.51 | 0.50 |
| 2:J3:21:TRP:CZ3 | 2:J3:63:PRO:HB3 | 2.47 | 0.50 |
| 2:J3:84:ARG:HB3 | 16:5Q:138:ARG:HG2 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J5:306:ASP:OD1 | 2:J5:308:ARG:HB2 | 2.10 | 0.50 |
| 2:J7:213:CYS:HA | 2:J7:217:LEU:HB2 | 1.92 | 0.50 |
| 2:K3:187:SER:O | 2:K3:191:THR:HG23 | 2.12 | 0.50 |
| 1:L0:99:ASN:ND2 | 2:L1:254:GLU:OE1 | 2.34 | 0.50 |
| 2:L3:65:CYS:O | 2:L3:91:GLN:HG2 | 2.11 | 0.50 |
| 2:L3:88:HIS:HE1 | 2:M9:284:GLU:HB3 | 1.76 | 0.50 |
| 1:L6:183:TYR:OH | 1:L6:388:MET:HB3 | 2.11 | 0.50 |
| 2:L9:244:PHE:HB2 | 2:L9:356:ASN:HD21 | 1.76 | 0.50 |
| 1:M2:274:THR:HG22 | 1:M2:282:ARG:HH11 | 1.77 | 0.50 |
| 1:M6:51:PHE:O | 37:7Y:110:TYR:OH | 2.28 | 0.50 |
| 2:N1:223:THR:OG1 | 1:N2:245:GLN:NE2 | 2.31 | 0.50 |
| 2:N3:65:CYS:SG | 2:N3:66:ILE:N | 2.85 | 0.50 |
| 2:N5:65:CYS:SG | 2:N5:66:ILE:N | 2.85 | 0.50 |
| 2:N9:25:CYS:HA | 2:N9:30:ILE:HG22 | 1.92 | 0.50 |
| 1:O2:39:ASP:OD2 | 1:O2:40:SER:N | 2.44 | 0.50 |
| 1:O4:70:PRO:HG2 | 2:O5:2:ARG:HH11 | 1.77 | 0.50 |
| 2:O7:176:GLN:HE22 | 2:O7:304:LYS:HE2 | 1.77 | 0.50 |
| 2:O7:405:VAL:HG11 | 2:O7:415:GLU:OE2 | 2.12 | 0.50 |
| 1:O8:405:GLU:HA | 1:O8:408:PHE:HD2 | 1.75 | 0.50 |
| 1:P4:65:LEU:HD12 | 1:P4:90:PHE:CE1 | 2.47 | 0.50 |
| 1:P4:304:ASP:OD2 | 1:P4:306:ARG:NH1 | 2.45 | 0.50 |
| 1:Q2:384:GLN:HG2 | 2:Q3:348:PRO:CB | 2.42 | 0.50 |
| 2:R3:394:LYS:HB2 | 1:R4:346:PRO:HG3 | 1.93 | 0.50 |
| 1:S2:134:GLN:HE21 | 1:S2:167:PHE:HE2 | 1.60 | 0.50 |
| 1:S2:424:GLN:HE21 | 17:5V:104:PHE:HB2 | 1.77 | 0.50 |
| 1:S4:337:ASN:OD1 | 17:5R:49:MET:HG2 | 2.11 | 0.50 |
| 2:S5:405:VAL:HG11 | 2:S5:415:GLU:OE2 | 2.10 | 0.50 |
| 1:T0:157:GLU:OE1 | 3:4B:90:ILE:HD12 | 2.12 | 0.50 |
| 1:T0:404:ASP:OD2 | 1:T0:405:GLU:N | 2.45 | 0.50 |
| 2:T3:27:GLU:OE1 | 2:T3:243:ARG:NH2 | 2.44 | 0.50 |
| 2:U5:317:LEU:HB3 | 2:U5:319:TYR:HE1 | 1.75 | 0.50 |
| 2:U7:195:LEU:HD21 | 2:U7:264:ARG:HH11 | 1.76 | 0.50 |
| 2:U7:305:CYS:HB3 | 2:U7:387:ILE:HD11 | 1.94 | 0.50 |
| 2:U9:222:PRO:CD | 1:V0:324:LYS:HE3 | 2.41 | 0.50 |
| 2:V1:66:ILE:O | 2:V1:66:ILE:HG13 | 2.10 | 0.50 |
| 2:V1:200:VAL:HG13 | 2:V1:268:MET:CE | 2.41 | 0.50 |
| 1:V2:7:ILE:HB | 1:V2:135:VAL:HG12 | 1.92 | 0.50 |
| 1:W0:86:ARG:HG2 | 1:W0:88:ASP:H | 1.77 | 0.50 |
| 1:W0:101:TRP:HE3 | 1:W0:403:MET:HE1 | 1.76 | 0.50 |
| 1:W4:203:ASP:OD2 | 1:W4:302:ALA:N | 2.43 | 0.50 |
| 2:W9:333:ALA:O | 2:W9:337:THR:HG23 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X2:412:GLU:O | 1:X2:416:ASN:ND2 | 2.45 | 0.50 |
| 1:X8:51:PHE:HB3 | 1:X8:59:TYR:HB3 | 1.93 | 0.50 |
| 2:Y1:191:THR:HA | 2:Y1:194:LEU:HB2 | 1.93 | 0.50 |
| 1:Y8:285:THR:HG23 | 1:Y8:288:GLU:H | 1.76 | 0.50 |
| 2:Z1:9:ILE:HG22 | 2:Z1:68:LEU:HD11 | 1.93 | 0.50 |
| 1:Z2:211:CYS:HA | 1:Z2:215:LEU:HB2 | 1.94 | 0.50 |
| 2:Z3:101:ASN:OD1 | 1:Z4:252:LYS:HE3 | 2.12 | 0.50 |
| 2:Z3:246:GLY:HA3 | 2:Z3:356:ASN:HA | 1.93 | 0.50 |
| 2:Z5:251:ASP:OD2 | 2:Z5:252:ILE:HD12 | 2.11 | 0.50 |
| 2:Z7:380:ASN:OD1 | 2:Z7:381:SER:N | 2.44 | 0.50 |
| 1:0A:117:LEU:HD11 | 1:0A:154:LYS:HD2 | 1.93 | 0.50 |
| 1:0I:404:ASP:HB3 | 1:0I:406:MET:SD | 2.51 | 0.50 |
| 1:0K:311:LEU:HD23 | 1:0K:312:THR:HG22 | 1.94 | 0.50 |
| 1:0M:344:TRP:CE3 | 1:0M:345:ILE:HG13 | 2.46 | 0.50 |
| 1:0Q:62:ARG:HG3 | 1:0Q:123:GLU:OE2 | 2.11 | 0.50 |
| 1:0S:105:HIS:CD2 | 1:0S:150:LEU:HD13 | 2.47 | 0.50 |
| 2:0V:254:GLU:HB3 | 2:0V:352:LYS:HE2 | 1.93 | 0.50 |
| 1:0W:113:ILE:HG21 | 1:0W:150:LEU:HD22 | 1.93 | 0.50 |
| 2:0Z:288:VAL:HG11 | 2:0Z:328:VAL:HG12 | 1.92 | 0.50 |
| 1:1C:174:LYS:HG3 | 1:1C:380:ARG:NH2 | 2.26 | 0.50 |
| 2:1D:288:VAL:O | 2:1D:292:THR:OG1 | 2.25 | 0.50 |
| 1:1E:389:PHE:O | 1:1E:392:LYS:NZ | 2.31 | 0.50 |
| 2:1F:145:THR:OG1 | 41:1G:501:GTP:O1B | 2.29 | 0.50 |
| 2:1H:98:ASP:OD1 | 2:1H:99:ALA:N | 2.44 | 0.50 |
| 1:1K:396:HIS:CD2 | 1:1K:396:HIS:H | 2.30 | 0.50 |
| 2:1L:145:THR:OG1 | 41:1L:501:GTP:O1B | 2.29 | 0.50 |
| 2:1L:287:SER:OG | 2:1L:288:VAL:N | 2.44 | 0.50 |
| 2:1P:361:THR:HA | 2:1P:370:LYS:NZ | 2.27 | 0.50 |
| 1:2A:67:ASP:N | 1:2A:67:ASP:OD1 | 2.42 | 0.50 |
| 2:2F:129:CYS:SG | 2:2F:130:THR:N | 2.85 | 0.50 |
| 2:2J:90:GLU:OE1 | 2:2J:90:GLU:CA | 2.56 | 0.50 |
| 2:2J:161:TYR:CE1 | 38:8C:80:TYR:CB | 2.94 | 0.50 |
| 2:2N:88:HIS:HB3 | 2:3D:283:HIS:CG | 2.46 | 0.50 |
| 2:2P:5:ILE:HG22 | 2:2P:64:ARG:HB3 | 1.93 | 0.50 |
| 2:2P:372:GLN:HE22 | 10:5C:156:TYR:HA | 1.77 | 0.50 |
| 2:2R:129:CYS:SG | 2:2R:130:THR:N | 2.85 | 0.50 |
| 2:2X:346:TRP:CZ3 | 2:2X:347:CYS:HB2 | 2.47 | 0.50 |
| 2:3B:6:SER:O | 2:3B:65:CYS:HA | 2.12 | 0.50 |
| 2:3B:66:ILE:HG13 | 2:3B:66:ILE:O | 2.10 | 0.50 |
| 2:3D:65:CYS:SG | 2:3D:66:ILE:N | 2.84 | 0.50 |
| 1:3G:139:LEU:HD12 | 1:3G:170:VAL:HG12 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3K:34:GLY:O | 1:3K:58:ARG:HA | 2.12 | 0.50 |
| 1:3M:140:GLY:O | 1:3M:184:ASN:ND2 | 2.44 | 0.50 |
| 1:3S:309:ARG:NH1 | 1:3S:341:PHE:O | 2.41 | 0.50 |
| 1:3S:362:LYS:HE2 | 38:8D:166:GLU:HG2 | 1.89 | 0.50 |
| 2:3T:5:ILE:HG22 | 2:3T:64:ARG:HB3 | 1.92 | 0.50 |
| 4:3W:126:ASP:OD1 | 4:3W:130:ASN:ND2 | 2.45 | 0.50 |
| 4:4A:126:ASP:OD1 | 4:4A:130:ASN:ND2 | 2.45 | 0.50 |
| 4:4C:6:PHE:CE2 | 4:4C:8:SER:HB2 | 2.47 | 0.50 |
| 4:4C:126:ASP:OD1 | 4:4C:130:ASN:ND2 | 2.45 | 0.50 |
| 4:4E:126:ASP:OD1 | 4:4E:130:ASN:ND2 | 2.45 | 0.50 |
| 5:4L:284:LEU:O | 5:4L:288:ILE:HG12 | 2.11 | 0.50 |
| 7:4U:77:ARG:HE | 24:6Y:19:PRO:HG3 | 1.77 | 0.50 |
| 8:4V:460:ALA:O | 8:4V:464:VAL:HG22 | 2.11 | 0.50 |
| 9:4Z:28:LEU:HD22 | 9:4Z:31:LEU:HD13 | 1.94 | 0.50 |
| 12:5F:286:SER:OG | 12:5F:287:ASP:N | 2.43 | 0.50 |
| 13:5K:126:VAL:HG12 | 13:5K:127:PRO:HD2 | 1.94 | 0.50 |
| 14:5L:24:HIS:CD2 | 14:5L:25:PRO:HD2 | 2.47 | 0.50 |
| 16:5Q:59:THR:HB | 16:5Q:100:ILE:HG22 | 1.93 | 0.50 |
| 18:5X:106:GLU:OE1 | 18:5X:106:GLU:N | 2.38 | 0.50 |
| 18:6C:214:TYR:O | 18:6C:218:SER:OG | 2.29 | 0.50 |
| 19:6E:243:ASN:OD1 | 19:6E:244:THR:N | 2.44 | 0.50 |
| 22:6M:295:LYS:HD3 | 22:6M:343:TYR:OH | 2.12 | 0.50 |
| 24:6V:416:ILE:HD12 | 24:6V:416:ILE:H | 1.75 | 0.50 |
| 24:6X:123:TYR:CE2 | 24:6X:163:PRO:HG3 | 2.46 | 0.50 |
| 30:7K:36:LYS:O | 30:7K:40:THR:HG23 | 2.11 | 0.50 |
| 30:7K:56:ARG:HD3 | 30:7K:57:GLN:H | 1.75 | 0.50 |
| 30:7K:382:LEU:HD21 | 30:7K:434:ARG:HB3 | 1.94 | 0.50 |
| 30:7L:377:GLU:HA | 30:7L:380:VAL:HG12 | 1.93 | 0.50 |
| 28:7X:399:VAL:HG23 | 28:7X:427:GLN:OE1 | 2.11 | 0.50 |
| 2:6:324:VAL:HG11 | 26:7D:142:PHE:HZ | 1.76 | 0.50 |
| 2:B7:278:ALA:HB3 | 18:6B:43:ASN:ND2 | 2.21 | 0.50 |
| 1:E6:276:ARG:CZ | 24:6W:314:GLY:H | 2.24 | 0.50 |
| 1:G6:404:ASP:HB2 | 1:G6:406:MET:SD | 2.51 | 0.50 |
| 2:H7:271:SER:HB2 | 2:H7:301:MET:HA | 1.93 | 0.50 |
| 2:H9:101:ASN:ND2 | 2:H9:143:GLY:HA2 | 2.27 | 0.50 |
| 1:I2:139:LEU:HD12 | 1:I2:170:VAL:HG12 | 1.94 | 0.50 |
| 2:I5:49:PHE:HD2 | 2:I5:53:PHE:HB2 | 1.77 | 0.50 |
| 1:J4:5:VAL:HG12 | 1:J4:133:PHE:CD1 | 2.46 | 0.50 |
| 2:J5:379:SER:OG | 2:J5:380:ASN:N | 2.45 | 0.50 |
| 1:J6:364:SER:OG | 1:J6:365:ALA:N | 2.43 | 0.50 |
| 2:J9:8:HIS:CD2 | 2:J9:138:PHE:HD2 | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J9:21:TRP:CZ2 | 2:J9:65:CYS:HB3 | 2.46 | 0.50 |
| 2:J9:282:TYR:HD1 | 5:4M:263:LEU:CD1 | 2.24 | 0.50 |
| 2:K3:217:LEU:HB3 | 2:K3:219:ILE:HD12 | 1.94 | 0.50 |
| 2:K5:327:ASP:N | 2:K5:327:ASP:OD1 | 2.44 | 0.50 |
| 2:L3:206:ASN:OD1 | 41:L4:501:GTP:N2 | 2.44 | 0.50 |
| 2:L3:287:SER:OG | 2:L3:288:VAL:N | 2.45 | 0.50 |
| 1:L4:175:VAL:HG22 | 2:L5:329:ASN:HD21 | 1.76 | 0.50 |
| 1:M2:130:LEU:HB2 | 1:M2:162:ARG:HE | 1.77 | 0.50 |
| 2:M5:88:HIS:HD2 | 2:M5:89:PRO:CD | 2.24 | 0.50 |
| 2:N3:227:LEU:O | 2:N3:231:ILE:HG12 | 2.11 | 0.50 |
| 2:N7:405:VAL:HG13 | 2:N7:418:PHE:HE2 | 1.77 | 0.50 |
| 2:O1:429:GLU:O | 2:O1:433:GLU:HG2 | 2.11 | 0.50 |
| 1:O4:139:LEU:HD12 | 1:O4:170:VAL:HG12 | 1.92 | 0.50 |
| 2:O9:14:ILE:HD11 | 2:O9:74:VAL:HG13 | 1.94 | 0.50 |
| 2:P3:5:ILE:HG22 | 2:P3:64:ARG:HB3 | 1.94 | 0.50 |
| 2:P3:338:LYS:HZ2 | 2:P3:339:ARG:H | 1.59 | 0.50 |
| 2:P3:392:ASP:OD2 | 2:P3:422:ARG:NH1 | 2.45 | 0.50 |
| 2:P5:402:ARG:NE | 2:P5:415:GLU:OE2 | 2.44 | 0.50 |
| 2:Q5:92:LEU:N | 2:Q5:92:LEU:HD23 | 2.27 | 0.50 |
| 1:Q6:204:ASN:HD21 | 39:Q6:502:GDP:HN22 | 1.59 | 0.50 |
| 1:Q8:418:LEU:O | 1:Q8:421:GLU:HG2 | 2.12 | 0.50 |
| 1:R2:141:GLY:O | 1:R2:145:SER:OG | 2.15 | 0.50 |
| 2:R3:170:THR:HG21 | 2:R3:194:LEU:HD11 | 1.94 | 0.50 |
| 2:R5:336:LYS:O | 2:R5:339:ARG:NH2 | 2.45 | 0.50 |
| 2:R7:69:ASP:OD1 | 2:R7:70:LEU:N | 2.45 | 0.50 |
| 1:S4:186:THR:HG21 | 1:S4:385:PHE:CE2 | 2.46 | 0.50 |
| 1:S8:94:GLN:HB3 | 24:6W:35:TYR:CD1 | 2.47 | 0.50 |
| 2:T3:9:ILE:HD13 | 2:T3:150:GLY:HA2 | 1.93 | 0.50 |
| 2:T5:51:THR:HG21 | 2:T5:243:ARG:HG2 | 1.92 | 0.50 |
| 1:T6:186:THR:HG22 | 1:T6:411:ALA:HB1 | 1.93 | 0.50 |
| 2:U5:217:LEU:HB3 | 2:U5:219:ILE:HD12 | 1.93 | 0.50 |
| 2:U5:264:ARG:NH2 | 2:U5:431:ASP:OD2 | 2.26 | 0.50 |
| 2:U9:88:HIS:HB3 | 2:U9:91:GLN:CG | 2.42 | 0.50 |
| 2:V1:277:SER:OG | 2:V1:280:LYS:NZ | 2.41 | 0.50 |
| 2:V3:172:TYR:N | 2:V3:204:LEU:O | 2.44 | 0.50 |
| 1:W0:202:LEU:CD2 | 1:W0:229:ILE:CD1 | 2.81 | 0.50 |
| 2:W1:246:GLY:HA3 | 2:W1:356:ASN:HA | 1.94 | 0.50 |
| 1:W6:375:GLN:HB2 | 1:W6:419:VAL:HG13 | 1.92 | 0.50 |
| 2:W9:224:TYR:H | 1:X0:245:GLN:HE22 | 1.60 | 0.50 |
| 2:X5:192:HIS:NE2 | 2:X5:420:GLU:OE2 | 2.44 | 0.50 |
| 1:X8:266:PHE:CE1 | 1:X8:370:ASN:HB2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y2:249:ASP:O | 1:Y2:253:LEU:HG | 2.12 | 0.50 |
| 1:Y4:58:ARG:HH11 | 1:Y4:84:ILE:HA | 1.75 | 0.50 |
| 1:Z0:113:ILE:HA | 1:Z0:116:VAL:HG12 | 1.94 | 0.50 |
| 2:Z3:116:ASP:N | 2:Z3:116:ASP:OD1 | 2.43 | 0.50 |
| 1:Z4:21:TRP:CH2 | 1:Z4:61:PRO:HB3 | 2.46 | 0.50 |
| 2:Z5:259:LEU:HD21 | 2:Z5:316:CYS:HB2 | 1.94 | 0.50 |
| 1:Z6:67:ASP:OD1 | 1:Z6:67:ASP:N | 2.44 | 0.50 |
| 2:0B:213:CYS:HA | 2:0B:217:LEU:HB2 | 1.94 | 0.50 |
| 2:0F:392:ASP:OD2 | 2:0F:422:ARG:NH1 | 2.44 | 0.50 |
| 2:0H:353:CYS:SG | 2:0H:354:GLY:N | 2.85 | 0.50 |
| 1:0K:12:CYS:O | 1:0K:16:ILE:HG12 | 2.12 | 0.50 |
| 1:0O:193:VAL:HG11 | 1:0O:418:LEU:HD11 | 1.94 | 0.50 |
| 2:0P:407:TRP:NE1 | 1:0Q:258:ILE:O | 2.38 | 0.50 |
| 1:0S:260:PHE:HB2 | 1:0S:263:LEU:HG | 1.94 | 0.50 |
| 1:0Y:268:VAL:O | 1:0Y:300:MET:N | 2.42 | 0.50 |
| 1:1C:371:SER:OG | 1:1C:372:THR:N | 2.45 | 0.50 |
| 2:1D:176:GLN:HG2 | 2:1D:177:VAL:N | 2.27 | 0.50 |
| 2:1H:69:ASP:OD2 | 2:1H:71:GLU:N | 2.40 | 0.50 |
| 2:1L:116:ASP:OD1 | 2:1L:117:LEU:N | 2.43 | 0.50 |
| 2:1L:133:GLN:HB3 | 2:1L:252:ILE:HG21 | 1.93 | 0.50 |
| 2:1P:203:MET:HE3 | 2:1P:267:PHE:HD1 | 1.77 | 0.50 |
| 1:1Q:290:THR:HG21 | 1:1Q:329:GLN:HG3 | 1.92 | 0.50 |
| 2:1T:3:GLU:HG3 | 2:1T:51:THR:HA | 1.93 | 0.50 |
| 1:1U:174:LYS:HD2 | 1:1U:174:LYS:H | 1.77 | 0.50 |
| 2:1V:179:THR:O | 1:1W:350:LYS:HD2 | 2.12 | 0.50 |
| 1:2A:289:LEU:HD11 | 1:2A:363:MET:HG2 | 1.94 | 0.50 |
| 2:2B:277:SER:OG | 2:2B:278:ALA:N | 2.43 | 0.50 |
| 1:2E:253:LEU:HD11 | 1:2E:316:LEU:HD21 | 1.94 | 0.50 |
| 2:2N:306:ASP:HB3 | 2:2N:309:HIS:HD2 | 1.76 | 0.50 |
| 1:2Q:207:LEU:HB3 | 1:2Q:225:LEU:HD22 | 1.92 | 0.50 |
| 1:2W:140:GLY:O | 1:2W:184:ASN:ND2 | 2.35 | 0.50 |
| 1:3C:205:GLU:OE1 | 1:3C:205:GLU:N | 2.39 | 0.50 |
| 2:3F:116:ASP:N | 2:3F:116:ASP:OD1 | 2.42 | 0.50 |
| 2:3H:367:ASP:OD1 | 2:3H:367:ASP:N | 2.45 | 0.50 |
| 1:3K:213:ARG:HB2 | 1:3K:297:LYS:HZ2 | 1.76 | 0.50 |
| 1:3K:391:ARG:NH2 | 2:3L:435:VAL:HA | 2.26 | 0.50 |
| 1:3M:53:GLU:HG2 | 1:3M:59:TYR:CE1 | 2.47 | 0.50 |
| 1:3M:122:LYS:NZ | 3:4D:262:TYR:HA | 2.27 | 0.50 |
| 2:3N:287:SER:OG | 2:3N:288:VAL:N | 2.45 | 0.50 |
| 2:3T:135:PHE:O | 2:3T:136:LEU:HD12 | 2.11 | 0.50 |
| 3:3V:13:THR:O | 3:3V:17:VAL:HG13 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:3Y:101:ARG:NH1 | 4:3Y:116:PRO:O | 2.44 | 0.50 |
| 4:3Y:126:ASP:OD1 | 4:3Y:130:ASN:ND2 | 2.45 | 0.50 |
| 4:4A:8:SER:OG | 4:4A:9:GLY:N | 2.44 | 0.50 |
| 4:4A:101:ARG:NH1 | 4:4A:116:PRO:O | 2.44 | 0.50 |
| 4:4C:8:SER:OG | 4:4C:9:GLY:N | 2.44 | 0.50 |
| 3:4D:13:THR:O | 3:4D:17:VAL:HG13 | 2.11 | 0.50 |
| 4:4E:6:PHE:CE2 | 4:4E:8:SER:HB2 | 2.47 | 0.50 |
| 4:4E:101:ARG:NH1 | 4:4E:116:PRO:O | 2.44 | 0.50 |
| 4:4G:8:SER:OG | 4:4G:9:GLY:N | 2.44 | 0.50 |
| 3:4H:13:THR:O | 3:4H:17:VAL:HG13 | 2.11 | 0.50 |
| 5:4M:98:PRO:HB3 | 5:4M:102:ARG:HH21 | 1.77 | 0.50 |
| 5:4M:293:LEU:HB2 | 28:7X:306:LEU:CD2 | 2.39 | 0.50 |
| 9:4Z:360:THR:O | 9:4Z:363:LEU:HG | 2.12 | 0.50 |
| 10:5B:203:GLU:O | 10:5B:207:VAL:HG23 | 2.12 | 0.50 |
| 11:5E:103:VAL:HB | 11:5E:104:PRO:HD3 | 1.93 | 0.50 |
| 13:5J:126:VAL:HG12 | 13:5J:127:PRO:HD2 | 1.94 | 0.50 |
| 14:5L:356:PHE:HZ | 14:5L:369:LEU:HD13 | 1.76 | 0.50 |
| 14:5M:24:HIS:CD2 | 14:5M:25:PRO:HD2 | 2.47 | 0.50 |
| 14:5M:356:PHE:HZ | 14:5M:369:LEU:HD13 | 1.76 | 0.50 |
| 14:5N:24:HIS:CD2 | 14:5N:25:PRO:HD2 | 2.47 | 0.50 |
| 15:5O:52:TYR:CE2 | 15:5O:55:LEU:CD2 | 2.93 | 0.50 |
| 15:5O:102:ALA:HB2 | 15:5O:204:ALA:CB | 2.42 | 0.50 |
| 24:6T:18:LEU:O | 24:6T:20:GLN:NE2 | 2.45 | 0.50 |
| 24:6U:371:ALA:HB1 | 24:6U:375:THR:OG1 | 2.12 | 0.50 |
| 24:6Z:316:ASP:OD2 | 24:6Z:317:PRO:HD2 | 2.12 | 0.50 |
| 24:7A:213:TYR:HH | 24:7A:217:PHE:HE2 | 1.59 | 0.50 |
| 30:7K:161:ALA:HA | 30:7K:164:VAL:HG12 | 1.93 | 0.50 |
| 35:7U:175:SER:OG | 35:7U:179:ARG:NH2 | 2.44 | 0.50 |
| 37:7Y:164:HIS:O | 37:7Y:168:THR:HG23 | 2.11 | 0.50 |
| 1:A3:273:LEU:CD2 | 26:7F:134:LEU:HD21 | 2.41 | 0.50 |
| 2:B7:80:THR:HG22 | 18:6B:169:LYS:O | 2.11 | 0.50 |
| 1:C8:11:GLN:N | 39:C8:502:GDP:O1B | 2.45 | 0.50 |
| 1:D0:47:ILE:HD11 | 22:6L:23:TYR:CD1 | 2.46 | 0.50 |
| 2:H1:246:GLY:HA3 | 2:H1:356:ASN:HA | 1.94 | 0.50 |
| 2:H5:21:TRP:CD1 | 2:H5:87:PHE:HZ | 2.29 | 0.50 |
| 2:H5:203:MET:HE1 | 2:H5:267:PHE:HD1 | 1.77 | 0.50 |
| 2:I1:85:GLN:HA | 2:J7:283:HIS:HE1 | 1.77 | 0.50 |
| 2:I3:72:PRO:HD2 | 1:I4:2:ARG:HH12 | 1.77 | 0.50 |
| 2:I3:155:GLU:O | 2:I3:158:SER:OG | 2.29 | 0.50 |
| 2:I5:115:VAL:HG22 | 2:I5:119:LEU:HD13 | 1.94 | 0.50 |
| 2:I5:381:SER:OG | 2:I5:382:THR:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I7:50:ASN:O | 2:I7:64:ARG:NH2 | 2.45 | 0.50 |
| 1:I8:19:LYS:O | 1:I8:23:VAL:HG23 | 2.12 | 0.50 |
| 1:J0:25:SER:OG | 1:J0:30:ILE:O | 2.30 | 0.50 |
| 2:J1:53:PHE:HB3 | 2:J1:61:HIS:HB3 | 1.92 | 0.50 |
| 2:J1:156:ARG:HA | 2:J1:159:VAL:HG22 | 1.94 | 0.50 |
| 1:K0:165:LEU:HD21 | 1:K0:250:LEU:HD11 | 1.93 | 0.50 |
| 2:K1:312:TYR:CD1 | 2:K1:381:SER:HB2 | 2.46 | 0.50 |
| 2:K1:392:ASP:OD1 | 2:K1:425:LEU:HD22 | 2.12 | 0.50 |
| 1:L6:334:GLN:NE2 | 1:L6:348:ASN:H | 2.08 | 0.50 |
| 1:M0:67:ASP:N | 1:M0:67:ASP:OD1 | 2.43 | 0.50 |
| 2:M1:69:ASP:OD1 | 2:M1:71:GLU:N | 2.45 | 0.50 |
| 1:M4:140:GLY:O | 1:M4:184:ASN:ND2 | 2.44 | 0.50 |
| 1:M4:273:LEU:H | 1:M4:292:GLN:HE22 | 1.59 | 0.50 |
| 2:M7:53:PHE:HB3 | 2:M7:61:HIS:HB3 | 1.93 | 0.50 |
| 1:N6:77:ARG:HD3 | 1:N6:90:PHE:CE2 | 2.47 | 0.50 |
| 1:N8:358:PRO:HG2 | 1:N8:361:LEU:HD12 | 1.94 | 0.50 |
| 1:O0:3:GLU:HB2 | 1:O0:130:LEU:HD13 | 1.92 | 0.50 |
| 1:O2:322:SER:O | 1:O2:325:GLU:HG2 | 2.11 | 0.50 |
| 2:O3:222:PRO:HD2 | 1:O4:324:LYS:HE3 | 1.93 | 0.50 |
| 1:O6:175:VAL:HG22 | 2:O7:329:ASN:HD21 | 1.76 | 0.50 |
| 2:P7:313:MET:N | 2:P7:380:ASN:O | 2.40 | 0.50 |
| 1:P8:358:PRO:HG2 | 1:P8:361:LEU:HD13 | 1.93 | 0.50 |
| 2:P9:315:CYS:SG | 2:P9:316:CYS:N | 2.85 | 0.50 |
| 1:Q0:167:PHE:HE2 | 1:Q0:233:MET:HG3 | 1.77 | 0.50 |
| 1:Q0:292:GLN:HG2 | 1:Q0:298:ASN:ND2 | 2.27 | 0.50 |
| 1:R0:238:CYS:SG | 1:R0:318:ARG:NE | 2.85 | 0.50 |
| 1:R2:102:ALA:HB1 | 1:R2:401:GLU:CB | 2.41 | 0.50 |
| 2:R3:129:CYS:SG | 2:R3:130:THR:N | 2.85 | 0.50 |
| 1:R4:37:HIS:HE1 | 11:5E:160:ARG:HG3 | 1.76 | 0.50 |
| 1:R4:382:SER:HB2 | 1:R4:415:MET:HG2 | 1.94 | 0.50 |
| 2:R5:300:SER:O | 2:R5:300:SER:OG | 2.29 | 0.50 |
| 2:R7:119:LEU:HA | 2:R7:122:ILE:HG22 | 1.92 | 0.50 |
| 1:R8:263:LEU:HD11 | 1:R8:425:TYR:CD2 | 2.46 | 0.50 |
| 2:S1:33:ASP:O | 2:S1:60:LYS:NZ | 2.43 | 0.50 |
| 2:S5:326:LYS:NZ | 24:6T:37:ASN:HD21 | 2.09 | 0.50 |
| 1:S6:396:HIS:HA | 1:S6:399:THR:HG22 | 1.94 | 0.50 |
| 1:S6:397:TRP:HZ2 | 2:S7:256:GLN:HB3 | 1.77 | 0.50 |
| 2:S7:156:ARG:HA | 2:S7:159:VAL:HG12 | 1.94 | 0.50 |
| 1:S8:134:GLN:HE21 | 1:S8:167:PHE:HE2 | 1.60 | 0.50 |
| 2:T5:53:PHE:HB3 | 2:T5:61:HIS:HB3 | 1.94 | 0.50 |
| 1:T6:36:TYR:CE2 | 1:T6:44:LEU:HD11 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T8:20:PHE:HA | 1:T8:230:SER:OG | 2.12 | 0.50 |
| 1:T8:176:SER:OG | 1:T8:181:GLU:OE1 | 2.22 | 0.50 |
| 1:U6:36:TYR:CZ | 1:U6:44:LEU:HD21 | 2.46 | 0.50 |
| 1:V2:275:SER:O | 1:V2:279:GLN:HG3 | 2.11 | 0.50 |
| 1:V6:19:LYS:HE2 | 1:V6:227:HIS:HB2 | 1.94 | 0.50 |
| 1:V6:105:HIS:CD2 | 1:V6:150:LEU:HB2 | 2.46 | 0.50 |
| 2:W1:107:HIS:CD2 | 2:W1:152:LEU:HB2 | 2.47 | 0.50 |
| 2:W5:254:GLU:HB3 | 2:W5:352:LYS:HE2 | 1.93 | 0.50 |
| 1:W8:285:THR:HG23 | 1:W8:287:PRO:HD2 | 1.93 | 0.50 |
| 1:X0:42:LEU:CB | 8:4X:97:PHE:CE1 | 2.92 | 0.50 |
| 1:X2:52:ASN:OD1 | 1:X2:62:ARG:NH2 | 2.45 | 0.50 |
| 1:X4:418:LEU:O | 1:X4:421:GLU:HG2 | 2.12 | 0.50 |
| 1:X8:20:PHE:HA | 1:X8:230:SER:OG | 2.11 | 0.50 |
| 1:X8:274:THR:HB | 1:X8:282:ARG:HH11 | 1.75 | 0.50 |
| 2:Y3:18:ASN:O | 2:Y3:22:GLU:HG3 | 2.12 | 0.50 |
| 1:Y8:31:ASP:OD2 | 1:Y8:33:THR:OG1 | 2.19 | 0.50 |
| 2:Y9:210:TYR:CE1 | 2:Y9:227:LEU:HD21 | 2.47 | 0.50 |
| 2:Z1:115:VAL:HG23 | 2:Z1:153:LEU:HD13 | 1.93 | 0.50 |
| 1:Z2:31:ASP:OD2 | 1:Z2:33:THR:OG1 | 2.24 | 0.50 |
| 1:Z4:190:HIS:CD2 | 1:Z4:414:ASN:HB2 | 2.46 | 0.50 |
| 1:Z8:20:PHE:HA | 1:Z8:230:SER:OG | 2.10 | 0.50 |
| 1:0E:391:ARG:CG | 2:0F:346:TRP:HB3 | 2.42 | 0.50 |
| 2:0F:213:CYS:HA | 2:0F:217:LEU:HB2 | 1.94 | 0.50 |
| 2:0H:90:GLU:H | 2:0X:283:HIS:CE1 | 2.29 | 0.50 |
| 2:0H:246:GLY:HA3 | 2:0H:356:ASN:HA | 1.93 | 0.50 |
| 1:0I:55:THR:O | 1:0I:58:ARG:HG2 | 2.12 | 0.50 |
| 1:0O:49:VAL:HG11 | 1:0O:241:ARG:HG2 | 1.92 | 0.50 |
| 2:0P:176:GLN:HG2 | 2:0P:177:VAL:H | 1.77 | 0.50 |
| 1:0U:72:THR:O | 1:0U:76:VAL:HG23 | 2.12 | 0.50 |
| 1:0U:263:LEU:HD22 | 1:0U:422:TYR:HE1 | 1.77 | 0.50 |
| 2:0V:209:ILE:HG21 | 2:0V:227:LEU:HG | 1.93 | 0.50 |
| 2:0Z:58:ALA:C | 9:4Z:165:ARG:CZ | 2.79 | 0.50 |
| 2:0Z:88:HIS:HD2 | 2:0Z:89:PRO:CD | 2.14 | 0.50 |
| 2:0Z:176:GLN:HG2 | 2:0Z:177:VAL:HG23 | 1.94 | 0.50 |
| 1:1A:67:ASP:OD2 | 1:1A:72:THR:OG1 | 2.18 | 0.50 |
| 1:1C:361:LEU:HD12 | 1:1C:362:LYS:N | 2.26 | 0.50 |
| 2:1D:353:CYS:SG | 2:1D:354:GLY:N | 2.85 | 0.50 |
| 1:1G:31:ASP:OD1 | 1:1G:35:THR:N | 2.34 | 0.50 |
| 2:1H:305:CYS:SG | 2:1H:383:ALA:HB1 | 2.52 | 0.50 |
| 1:1K:72:THR:O | 1:1K:76:VAL:HG23 | 2.12 | 0.50 |
| 1:1U:8:GLN:O | 1:1U:66:MET:HG3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1V:264:ARG:NH2 | 2:1V:431:ASP:OD2 | 2.43 | 0.50 |
| 1:2C:114:ASP:N | 1:2C:114:ASP:OD1 | 2.44 | 0.50 |
| 1:2I:211:CYS:HA | 1:2I:215:LEU:HB2 | 1.94 | 0.50 |
| 2:2N:196:GLU:OE2 | 2:2N:197:HIS:NE2 | 2.45 | 0.50 |
| 1:2S:39:ASP:OD2 | 1:2S:39:ASP:N | 2.43 | 0.50 |
| 1:2U:5:VAL:HG23 | 1:2U:62:ARG:HG2 | 1.93 | 0.50 |
| 1:2W:177:ASP:O | 2:2X:352:LYS:HA | 2.11 | 0.50 |
| 2:2Z:21:TRP:CZ2 | 2:2Z:65:CYS:HB2 | 2.47 | 0.50 |
| 2:2Z:306:ASP:HB3 | 2:2Z:309:HIS:HD2 | 1.76 | 0.50 |
| 1:3A:371:SER:OG | 1:3A:372:THR:N | 2.44 | 0.50 |
| 1:3C:98:GLY:HA3 | 2:3D:253:THR:HG23 | 1.93 | 0.50 |
| 1:3C:245:GLN:HE21 | 38:8D:198:THR:CG2 | 2.25 | 0.50 |
| 2:3F:90:GLU:HG2 | 2:3F:121:ARG:HH22 | 1.77 | 0.50 |
| 2:3N:345:ASP:OD2 | 2:3N:346:TRP:HD1 | 1.95 | 0.50 |
| 2:3T:155:GLU:O | 2:3T:159:VAL:HG13 | 2.12 | 0.50 |
| 2:3T:259:LEU:HD23 | 2:3T:268:MET:HG2 | 1.93 | 0.50 |
| 4:3W:8:SER:OG | 4:3W:9:GLY:N | 2.44 | 0.50 |
| 4:3Y:8:SER:OG | 4:3Y:9:GLY:N | 2.44 | 0.50 |
| 4:4A:6:PHE:CE2 | 4:4A:8:SER:HB2 | 2.47 | 0.50 |
| 4:4C:101:ARG:NH1 | 4:4C:116:PRO:O | 2.44 | 0.50 |
| 4:4G:101:ARG:NH1 | 4:4G:116:PRO:O | 2.44 | 0.50 |
| 4:4G:126:ASP:OD1 | 4:4G:130:ASN:ND2 | 2.45 | 0.50 |
| 4:4I:126:ASP:OD1 | 4:4I:130:ASN:ND2 | 2.45 | 0.50 |
| 9:4Y:433:ARG:NH1 | 9:4Y:443:GLU:OE2 | 2.44 | 0.50 |
| 9:4Y:442:MET:N | 9:4Y:442:MET:SD | 2.85 | 0.50 |
| 9:4Z:96:ASP:OD1 | 9:4Z:97:ARG:N | 2.45 | 0.50 |
| 13:5H:126:VAL:HG12 | 13:5H:127:PRO:HD2 | 1.94 | 0.50 |
| 13:5I:126:VAL:HG12 | 13:5I:127:PRO:HD2 | 1.94 | 0.50 |
| 14:5N:356:PHE:HZ | 14:5N:369:LEU:HD13 | 1.76 | 0.50 |
| 15:5O:56:LYS:CE | 15:5O:56:LYS:N | 2.73 | 0.50 |
| 15:5O:99:LYS:CD | 15:5O:203:ASN:O | 2.60 | 0.50 |
| 19:6E:8:TYR:HE1 | 19:6E:10:SER:HG | 1.58 | 0.50 |
| 22:6L:65:ARG:HE | 22:6L:101:ASN:HB2 | 1.76 | 0.50 |
| 22:6P:266:LYS:HA | 22:6P:269:GLU:CG | 2.41 | 0.50 |
| 24:6T:452:MET:HA | 24:6T:530:PHE:HA | 1.93 | 0.50 |
| 24:6U:97:ARG:H | 24:6U:188:THR:CG2 | 2.24 | 0.50 |
| 24:6U:280:ASP:HA | 24:6U:289:ARG:HB2 | 1.92 | 0.50 |
| 24:6U:498:LEU:HD23 | 24:6U:503:ILE:HD11 | 1.94 | 0.50 |
| 24:6W:536:ASP:HB3 | 24:6W:539:THR:HG23 | 1.94 | 0.50 |
| 24:6X:97:ARG:H | 24:6X:188:THR:CG2 | 2.24 | 0.50 |
| 28:7H:306:LEU:O | 28:7H:310:ARG:HG3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:7K:307:ASP:N | 30:7K:307:ASP:OD1 | 2.43 | 0.50 |
| 31:7M:68:HIS:CD2 | 31:7M:69:LYS:HG2 | 2.47 | 0.50 |
| 33:7Q:119:SER:OG | 33:7Q:120:SER:N | 2.45 | 0.50 |
| 35:7U:199:PHE:HD1 | 35:7U:202:ARG:HH12 | 1.60 | 0.50 |
| 37:7Y:46:ARG:O | 37:7Y:48:PRO:HD3 | 2.12 | 0.50 |
| 37:7Y:177:ARG:CB | 37:7Y:177:ARG:NH1 | 2.75 | 0.50 |
| 2:E7:62:VAL:HG22 | 2:G3:283:HIS:HD2 | 1.77 | 0.50 |
| 2:F9:145:THR:OG1 | 41:G0:501:GTP:O1B | 2.30 | 0.50 |
| 2:G3:167:LEU:HD13 | 2:G3:200:VAL:HB | 1.94 | 0.50 |
| 2:G5:217:LEU:HD22 | 2:G5:367:ASP:HB2 | 1.94 | 0.50 |
| 2:G7:274:PRO:HB2 | 2:G7:276:ILE:HG12 | 1.94 | 0.50 |
| 1:G8:91:VAL:HG21 | 1:G8:116:VAL:HG12 | 1.94 | 0.50 |
| 1:H2:301:CYS:SG | 1:H2:302:ALA:N | 2.84 | 0.50 |
| 2:H9:353:CYS:SG | 2:H9:354:GLY:N | 2.84 | 0.50 |
| 2:I3:213:CYS:HA | 2:I3:217:LEU:HB2 | 1.94 | 0.50 |
| 1:I4:276:ARG:NH1 | 24:6Z:491:GLY:HA3 | 2.26 | 0.50 |
| 2:I9:379:SER:OG | 2:I9:380:ASN:N | 2.45 | 0.50 |
| 2:J3:88:HIS:CD2 | 2:K9:283:HIS:HB3 | 2.45 | 0.50 |
| 2:J9:11:GLN:OE1 | 2:J9:15:GLN:NE2 | 2.44 | 0.50 |
| 2:K3:90:GLU:OE2 | 2:L9:283:HIS:NE2 | 2.45 | 0.50 |
| 1:K4:86:ARG:HG2 | 1:K4:88:ASP:H | 1.77 | 0.50 |
| 2:L1:96:LYS:HD2 | 1:L2:129:CYS:SG | 2.52 | 0.50 |
| 2:M1:265:ILE:HD11 | 2:M1:435:VAL:HG21 | 1.93 | 0.50 |
| 1:M6:39:ASP:OD1 | 1:M6:39:ASP:N | 2.45 | 0.50 |
| 2:M9:178:SER:HB3 | 2:M9:183:GLU:OE2 | 2.11 | 0.50 |
| 2:M9:251:ASP:OD2 | 2:M9:253:THR:HG22 | 2.11 | 0.50 |
| 2:N7:297:GLU:OE1 | 32:7O:15:VAL:HG23 | 2.12 | 0.50 |
| 2:O3:414:GLU:N | 2:O3:414:GLU:OE1 | 2.45 | 0.50 |
| 1:O6:226:ASN:OD1 | 39:O6:502:GDP:N1 | 2.41 | 0.50 |
| 2:O7:259:LEU:HD11 | 2:O7:316:CYS:HB2 | 1.94 | 0.50 |
| 2:P3:413:MET:HB3 | 2:P3:417:GLU:OE2 | 2.11 | 0.50 |
| 2:P7:306:ASP:HB3 | 2:P7:309:HIS:HD2 | 1.75 | 0.50 |
| 1:Q0:3:GLU:HB2 | 1:Q0:130:LEU:HA | 1.93 | 0.50 |
| 1:Q0:252:LYS:HE3 | 1:Q0:350:LYS:HE3 | 1.94 | 0.50 |
| 2:Q1:9:ILE:HG22 | 2:Q1:146:GLY:HA2 | 1.92 | 0.50 |
| 1:Q2:179:VAL:HB | 2:Q3:258:ASN:HD22 | 1.77 | 0.50 |
| 1:Q2:204:ASN:HD21 | 39:Q2:502:GDP:HN22 | 1.59 | 0.50 |
| 2:Q3:413:MET:HB3 | 2:Q3:417:GLU:OE2 | 2.11 | 0.50 |
| 2:Q9:26:LEU:HD22 | 2:Q9:363:VAL:HG12 | 1.94 | 0.50 |
| 1:R4:237:THR:O | 1:R4:237:THR:HG22 | 2.11 | 0.50 |
| 2:R5:14:ILE:HD11 | 2:R5:74:VAL:HG13 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R5:212:ILE:HG23 | 2:R5:275:ILE:HD12 | 1.93 | 0.50 |
| 2:R7:72:PRO:HD2 | 1:R8:2:ARG:NH1 | 2.27 | 0.50 |
| 1:S2:117:LEU:HA | 1:S2:120:VAL:HG12 | 1.94 | 0.50 |
| 2:S7:237:SER:HA | 2:S7:320:ARG:HD2 | 1.93 | 0.50 |
| 1:S8:11:GLN:NE2 | 2:S9:249:ASN:OD1 | 2.44 | 0.50 |
| 2:T3:239:THR:HG23 | 2:T3:243:ARG:NH1 | 2.26 | 0.50 |
| 1:T4:221:THR:HG21 | 31:7N:117:TRP:CZ2 | 2.47 | 0.50 |
| 2:T5:386:GLU:HG2 | 17:5U:27:PHE:HB3 | 1.93 | 0.50 |
| 2:T7:69:ASP:OD1 | 2:T7:70:LEU:N | 2.41 | 0.50 |
| 2:U1:79:ARG:NH1 | 2:U1:94:SER:OG | 2.45 | 0.50 |
| 1:U6:105:HIS:CD2 | 1:U6:150:LEU:HB2 | 2.46 | 0.50 |
| 2:U7:200:VAL:HG13 | 2:U7:268:MET:CE | 2.42 | 0.50 |
| 1:V2:165:LEU:HD21 | 1:V2:250:LEU:CD1 | 2.40 | 0.50 |
| 1:V8:232:VAL:HG22 | 1:V8:270:PHE:HB2 | 1.93 | 0.50 |
| 1:W4:21:TRP:CZ3 | 1:W4:61:PRO:HB3 | 2.47 | 0.50 |
| 1:W4:328:GLU:O | 1:W4:332:ASN:ND2 | 2.44 | 0.50 |
| 2:W5:154:LEU:HD21 | 2:W5:198:THR:HG22 | 1.93 | 0.50 |
| 1:X4:204:ASN:ND2 | 39:X4:502:GDP:HN22 | 2.10 | 0.50 |
| 2:X5:187:SER:O | 2:X5:190:SER:OG | 2.27 | 0.50 |
| 2:X5:330:ALA:O | 2:X5:334:THR:HG23 | 2.11 | 0.50 |
| 1:X6:246:LEU:HD22 | 1:X6:352:SER:HA | 1.93 | 0.50 |
| 2:Y5:426:ALA:O | 2:Y5:430:LYS:HG3 | 2.12 | 0.50 |
| 1:Y6:333:VAL:HG23 | 1:Y6:336:LYS:HE2 | 1.94 | 0.50 |
| 2:Y9:175:PRO:HB3 | 2:Y9:390:ARG:HH21 | 1.77 | 0.50 |
| 1:Z0:51:PHE:HB3 | 1:Z0:59:TYR:HB3 | 1.93 | 0.50 |
| 2:Z1:157:LEU:HD13 | 2:Z1:166:LYS:HD3 | 1.94 | 0.50 |
| 1:Z4:379:LYS:HD3 | 1:Z4:419:VAL:HG21 | 1.94 | 0.50 |
| 2:Z7:220:GLU:OE2 | 2:Z7:221:ARG:NH1 | 2.45 | 0.50 |
| 2:Z9:15:GLN:HB3 | 2:Z9:228:ASN:ND2 | 2.26 | 0.50 |
| 1:0C:8:GLN:NE2 | 1:0C:14:ASN:HA | 2.27 | 0.50 |
| 2:0J:246:GLY:HA3 | 2:0J:356:ASN:HA | 1.94 | 0.50 |
| 1:0Q:237:THR:HG23 | 1:0Q:241:ARG:HE | 1.76 | 0.50 |
| 1:0S:182:PRO:HG3 | 1:0S:384:GLN:HG3 | 1.93 | 0.50 |
| 1:0U:72:THR:O | 1:0U:75:SER:OG | 2.26 | 0.50 |
| 1:0U:86:ARG:HG2 | 1:0U:88:ASP:H | 1.76 | 0.50 |
| 2:0V:108:TYR:HB2 | 2:0V:411:GLU:OE1 | 2.11 | 0.50 |
| 2:0X:183:GLU:HG3 | 2:0X:184:PRO:HD3 | 1.94 | 0.50 |
| 2:0X:203:MET:O | 2:0X:204:LEU:HD23 | 2.12 | 0.50 |
| 2:1B:88:HIS:CD2 | 2:1R:283:HIS:HB3 | 2.47 | 0.50 |
| 2:1H:111:GLY:HA2 | 2:1H:114:ILE:HG22 | 1.94 | 0.50 |
| 1:1M:50:TYR:CE2 | 1:1M:241:ARG:HD3 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1M:178:THR:OG1 | 1:1M:181:GLU:HG3 | 2.12 | 0.50 |
| 1:1U:31:ASP:HB3 | 1:1U:37:HIS:HD2 | 1.76 | 0.50 |
| 1:2C:77:ARG:HE | 1:2C:90:PHE:HE2 | 1.60 | 0.50 |
| 1:2E:167:PHE:CE2 | 1:2E:233:MET:HG2 | 2.47 | 0.50 |
| 2:2H:110:ILE:HD11 | 38:8B:6:LEU:HD23 | 1.94 | 0.50 |
| 2:2J:417:GLU:HA | 2:2J:420:GLU:HG2 | 1.93 | 0.50 |
| 2:2P:8:HIS:CD2 | 2:2P:138:PHE:HD2 | 2.30 | 0.50 |
| 2:2P:239:THR:HG23 | 2:2P:243:ARG:HE | 1.77 | 0.50 |
| 2:2R:223:THR:HG22 | 2:2R:224:TYR:N | 2.26 | 0.50 |
| 2:2T:339:ARG:HB2 | 38:8A:35:GLU:OE1 | 2.11 | 0.50 |
| 1:2U:309:ARG:NH1 | 1:2U:339:SER:O | 2.45 | 0.50 |
| 1:3A:67:ASP:OD1 | 1:3A:68:LEU:N | 2.42 | 0.50 |
| 2:3B:214:ARG:HH22 | 38:8C:16:LYS:HB3 | 1.76 | 0.50 |
| 1:3C:334:GLN:NE2 | 1:3C:348:ASN:H | 2.05 | 0.50 |
| 2:3D:90:GLU:H | 2:3T:283:HIS:CE1 | 2.30 | 0.50 |
| 2:3J:213:CYS:HA | 2:3J:217:LEU:HB2 | 1.94 | 0.50 |
| 1:3K:232:VAL:HG11 | 1:3K:268:VAL:HG11 | 1.94 | 0.50 |
| 1:3K:285:THR:HG23 | 1:3K:288:GLU:H | 1.77 | 0.50 |
| 1:3O:280:GLN:HG2 | 38:8C:162:VAL:HG13 | 1.94 | 0.50 |
| 1:3Q:183:TYR:OH | 1:3Q:388:MET:HB3 | 2.12 | 0.50 |
| 1:3S:53:GLU:OE2 | 1:3S:57:GLY:N | 2.45 | 0.50 |
| 4:4E:8:SER:OG | 4:4E:9:GLY:N | 2.44 | 0.50 |
| 4:4I:8:SER:OG | 4:4I:9:GLY:N | 2.44 | 0.50 |
| 4:4I:101:ARG:NH1 | 4:4I:116:PRO:O | 2.44 | 0.50 |
| 3:4J:184:LEU:HD11 | 3:4J:223:LYS:HG3 | 1.93 | 0.50 |
| 5:4L:244:ASP:N | 5:4L:244:ASP:OD2 | 2.44 | 0.50 |
| 7:4S:3:ARG:NH1 | 7:4S:3:ARG:CG | 2.73 | 0.50 |
| 8:4W:463:THR:CG2 | 8:4X:128:LEU:HD13 | 2.37 | 0.50 |
| 9:4Z:237:VAL:HG13 | 9:4Z:238:GLU:OE2 | 2.10 | 0.50 |
| 11:5E:205:GLU:O | 11:5E:209:ILE:HG12 | 2.12 | 0.50 |
| 13:5J:55:VAL:HG13 | 13:5J:56:ASP:O | 2.12 | 0.50 |
| 14:5L:426:LYS:N | 14:5L:446:GLU:OE1 | 2.44 | 0.50 |
| 14:5L:480:SER:OG | 14:5L:482:ASP:OD1 | 2.28 | 0.50 |
| 14:5M:426:LYS:N | 14:5M:446:GLU:OE1 | 2.44 | 0.50 |
| 14:5N:127:ASN:N | 14:5N:127:ASN:HD22 | 2.10 | 0.50 |
| 14:5N:149:PHE:HD2 | 38:8D:229:ASN:HD21 | 1.59 | 0.50 |
| 14:5N:426:LYS:N | 14:5N:446:GLU:OE1 | 2.44 | 0.50 |
| 14:5N:480:SER:OG | 14:5N:482:ASP:OD1 | 2.28 | 0.50 |
| 15:5O:38:VAL:HG23 | 15:5O:38:VAL:O | 2.12 | 0.50 |
| 15:5P:128:LEU:HB3 | 15:5P:132:GLU:HG2 | 1.94 | 0.50 |
| 20:6F:56:GLU:OE2 | 20:6F:56:GLU:N | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:6F:159:ASP:N | 20:6F:301:PRO:O | 2.33 | 0.50 |
| 24:6T:345:ASP:OD2 | 24:6T:346:GLN:N | 2.45 | 0.50 |
| 24:6U:183:ASP:OD1 | 24:6U:184:ALA:N | 2.44 | 0.50 |
| 24:6Z:402:LYS:HE3 | 24:6Z:403:PRO:HD2 | 1.94 | 0.50 |
| 26:7E:50:SER:N | 26:7E:55:THR:OG1 | 2.42 | 0.50 |
| 32:7P:208:MET:HB3 | 32:7P:209:PRO:HD2 | 1.94 | 0.50 |
| 37:7Y:141:THR:HG22 | 37:7Y:142:ARG:N | 2.27 | 0.50 |
| 38:8C:92:GLU:HG3 | 38:8C:94:LYS:HE3 | 1.93 | 0.50 |
| 1:3:83:GLN:HB2 | 24:6U:177:ARG:HH22 | 1.77 | 0.49 |
| 1:7:33:THR:HG21 | 18:5Z:101:LYS:HE2 | 1.94 | 0.49 |
| 1:7:55:THR:HG21 | 24:6W:107:VAL:HG21 | 1.93 | 0.49 |
| 1:A3:282:ARG:C | 1:T6:54:ALA:HB1 | 2.32 | 0.49 |
| 1:D6:143:THR:N | 39:D6:501:GDP:O1B | 2.44 | 0.49 |
| 1:E2:11:GLN:N | 39:E2:501:GDP:O2B | 2.29 | 0.49 |
| 1:F6:218:THR:N | 24:6T:418:ASP:OD2 | 2.41 | 0.49 |
| 2:G1:362:VAL:HG13 | 2:G1:370:LYS:HD2 | 1.94 | 0.49 |
| 2:G3:68:LEU:HA | 2:G3:93:ILE:O | 2.12 | 0.49 |
| 2:G7:88:HIS:CD2 | 2:G7:89:PRO:CD | 2.91 | 0.49 |
| 2:G9:212:ILE:O | 2:G9:216:SER:OG | 2.29 | 0.49 |
| 2:G9:245:ASP:N | 2:G9:245:ASP:OD1 | 2.45 | 0.49 |
| 2:G9:338:LYS:HG3 | 2:G9:340:THR:HG22 | 1.93 | 0.49 |
| 2:H1:129:CYS:SG | 2:H1:130:THR:N | 2.85 | 0.49 |
| 1:H8:304:ASP:OD1 | 1:H8:306:ARG:NE | 2.39 | 0.49 |
| 2:I1:109:THR:OG1 | 2:I1:411:GLU:OE2 | 2.29 | 0.49 |
| 2:I1:280:LYS:HA | 2:I1:283:HIS:HB3 | 1.93 | 0.49 |
| 1:I2:185:ALA:O | 1:I2:189:VAL:HG12 | 2.12 | 0.49 |
| 2:I3:129:CYS:SG | 2:I3:130:THR:N | 2.85 | 0.49 |
| 2:I7:119:LEU:HA | 2:I7:122:ILE:HG12 | 1.94 | 0.49 |
| 1:J0:131:GLN:HE21 | 1:J0:250:LEU:HB3 | 1.75 | 0.49 |
| 2:J3:53:PHE:HB3 | 2:J3:61:HIS:HB3 | 1.94 | 0.49 |
| 2:J5:176:GLN:HE22 | 2:J5:304:LYS:HE2 | 1.76 | 0.49 |
| 2:J5:245:ASP:HA | 5:4L:477:ARG:HH21 | 1.77 | 0.49 |
| 2:J9:311:LYS:NZ | 2:J9:343:PHE:O | 2.40 | 0.49 |
| 2:K1:276:ILE:HG23 | 2:K1:280:LYS:HB2 | 1.93 | 0.49 |
| 2:K3:223:THR:HA | 1:K4:323:THR:HG22 | 1.94 | 0.49 |
| 2:L3:276:ILE:CD1 | 2:L3:281:ALA:CA | 2.86 | 0.49 |
| 1:L4:2:ARG:HB3 | 1:L4:131:GLN:HB2 | 1.93 | 0.49 |
| 1:M0:117:LEU:HA | 1:M0:120:VAL:HG12 | 1.94 | 0.49 |
| 1:M2:7:ILE:HB | 1:M2:135:VAL:HG12 | 1.92 | 0.49 |
| 2:M3:69:ASP:OD1 | 2:M3:71:GLU:N | 2.45 | 0.49 |
| 2:M3:387:ILE:HG12 | 2:M3:390:ARG:HH22 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M7:116:ASP:N | 2:M7:116:ASP:OD1 | 2.45 | 0.49 |
| 2:M7:221:ARG:HG2 | 2:M7:221:ARG:O | 2.11 | 0.49 |
| 1:N0:317:PHE:HB3 | 1:N0:321:MET:SD | 2.52 | 0.49 |
| 1:N6:68:LEU:HB3 | 1:N6:96:GLY:HA2 | 1.94 | 0.49 |
| 2:N9:7:ILE:HD11 | 2:N9:137:VAL:HG22 | 1.94 | 0.49 |
| 2:O9:277:SER:OG | 2:O9:278:ALA:N | 2.44 | 0.49 |
| 1:P4:117:LEU:HA | 1:P4:120:VAL:HG12 | 1.93 | 0.49 |
| 2:P5:241:SER:HB2 | 2:P5:249:ASN:HB2 | 1.93 | 0.49 |
| 1:Q6:66:MET:SD | 1:Q6:147:MET:HG2 | 2.52 | 0.49 |
| 1:Q8:44:LEU:HA | 1:Q8:47:ILE:HD11 | 1.93 | 0.49 |
| 1:R0:186:THR:HG22 | 1:R0:411:ALA:HB1 | 1.92 | 0.49 |
| 1:R4:320:ARG:HH21 | 7:4R:102:ILE:HD11 | 1.76 | 0.49 |
| 2:R9:69:ASP:OD2 | 2:R9:70:LEU:N | 2.45 | 0.49 |
| 1:S8:52:ASN:OD1 | 1:S8:62:ARG:NH2 | 2.45 | 0.49 |
| 1:T4:122:LYS:HA | 3:4F:65:SER:OG | 2.12 | 0.49 |
| 2:T5:88:HIS:HD2 | 2:T5:121:ARG:HH12 | 1.58 | 0.49 |
| 2:U1:210:TYR:CE1 | 1:U2:324:LYS:HB2 | 2.47 | 0.49 |
| 1:U2:273:LEU:O | 1:U2:292:GLN:NE2 | 2.43 | 0.49 |
| 1:V8:77:ARG:O | 1:V8:83:GLN:NE2 | 2.45 | 0.49 |
| 2:V9:234:VAL:HG13 | 2:V9:376:CYS:SG | 2.52 | 0.49 |
| 1:W0:309:ARG:NH1 | 1:W0:339:SER:O | 2.45 | 0.49 |
| 2:W1:221:ARG:HG2 | 1:W2:325:GLU:OE2 | 2.12 | 0.49 |
| 2:W3:265:ILE:HD11 | 2:W3:435:VAL:HG21 | 1.93 | 0.49 |
| 1:X2:101:TRP:HE3 | 1:X2:403:MET:HE1 | 1.77 | 0.49 |
| 1:X2:404:ASP:OD2 | 1:X2:405:GLU:N | 2.44 | 0.49 |
| 1:X8:309:ARG:NH1 | 1:X8:339:SER:O | 2.45 | 0.49 |
| 2:Y1:173:PRO:HB3 | 2:Y1:183:GLU:HG2 | 1.93 | 0.49 |
| 1:Y2:130:LEU:HB2 | 1:Y2:162:ARG:HE | 1.76 | 0.49 |
| 1:Y2:207:LEU:HB3 | 1:Y2:225:LEU:HD22 | 1.93 | 0.49 |
| 2:Y3:22:GLU:HG2 | 2:Y3:83:TYR:OH | 2.12 | 0.49 |
| 2:Y3:132:LEU:HD23 | 2:Y3:164:LYS:HE3 | 1.93 | 0.49 |
| 2:Y3:305:CYS:HB3 | 2:Y3:387:ILE:HD11 | 1.94 | 0.49 |
| 2:Y9:24:TYR:HE1 | 2:Y9:236:SER:OG | 1.95 | 0.49 |
| 2:Y9:286:LEU:HG | 2:Y9:373:ARG:NH1 | 2.27 | 0.49 |
| 1:Z0:21:TRP:HA | 1:Z0:24:VAL:HG12 | 1.94 | 0.49 |
| 1:0A:379:LYS:HD3 | 1:0A:419:VAL:HG21 | 1.93 | 0.49 |
| 1:0A:404:ASP:HB3 | 1:0A:406:MET:SD | 2.52 | 0.49 |
| 2:0H:100:ALA:HA | 1:0I:252:LYS:HE2 | 1.94 | 0.49 |
| 1:0K:393:ALA:C | 1:0K:395:LEU:N | 2.65 | 0.49 |
| 1:0Q:8:GLN:CD | 1:0Q:17:GLY:HA3 | 2.32 | 0.49 |
| 1:0Q:12:CYS:HB2 | 39:0Q:502:GDP:C8 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0U:334:GLN:NE2 | 1:0U:348:ASN:H | 2.09 | 0.49 |
| 1:0W:97:ALA:HA | 1:0W:103:LYS:HE3 | 1.94 | 0.49 |
| 1:0Y:272:PRO:O | 1:0Y:273:LEU:HD23 | 2.12 | 0.49 |
| 1:1A:7:ILE:HB | 1:1A:135:VAL:HG22 | 1.93 | 0.49 |
| 1:1G:374:ILE:HD11 | 1:1G:422:TYR:CZ | 2.47 | 0.49 |
| 1:1M:144:GLY:N | 39:1M:501:GDP:O1B | 2.44 | 0.49 |
| 2:1N:230:LEU:HD12 | 2:1N:231:ILE:HD13 | 1.92 | 0.49 |
| 1:1O:114:ASP:N | 1:1O:114:ASP:OD1 | 2.43 | 0.49 |
| 1:1S:192:LEU:HD22 | 1:1S:196:ALA:HB2 | 1.92 | 0.49 |
| 1:1U:385:PHE:HZ | 1:1U:408:PHE:HD1 | 1.60 | 0.49 |
| 1:2C:215:LEU:HB3 | 1:2C:217:LEU:HG | 1.94 | 0.49 |
| 1:2E:273:LEU:H | 1:2E:292:GLN:HE22 | 1.60 | 0.49 |
| 1:2M:335:ASN:O | 1:2M:338:SER:OG | 2.30 | 0.49 |
| 2:2P:53:PHE:HB3 | 2:2P:61:HIS:HB3 | 1.94 | 0.49 |
| 2:2P:261:PRO:HG2 | 2:2P:265:ILE:HD11 | 1.94 | 0.49 |
| 1:2Q:212:PHE:HZ | 38:8A:117:TRP:HB3 | 1.77 | 0.49 |
| 2:2X:69:ASP:OD1 | 2:2X:70:LEU:N | 2.45 | 0.49 |
| 2:2Z:286:LEU:O | 2:2Z:373:ARG:NH1 | 2.45 | 0.49 |
| 1:3A:244:GLY:HA2 | 1:3A:355:ASP:OD2 | 2.13 | 0.49 |
| 2:3D:5:ILE:HD11 | 2:3D:135:PHE:CE2 | 2.48 | 0.49 |
| 1:3G:72:THR:O | 1:3G:76:VAL:HG23 | 2.11 | 0.49 |
| 2:3H:127:ASP:OD2 | 3:3X:175:LEU:HD11 | 2.11 | 0.49 |
| 1:3K:404:ASP:OD1 | 1:3K:405:GLU:N | 2.44 | 0.49 |
| 1:3Q:335:ASN:O | 1:3Q:338:SER:OG | 2.28 | 0.49 |
| 1:3S:7:ILE:HB | 1:3S:135:VAL:HG12 | 1.93 | 0.49 |
| 4:3W:6:PHE:CE2 | 4:3W:8:SER:HB2 | 2.47 | 0.49 |
| 4:3W:101:ARG:NH1 | 4:3W:116:PRO:O | 2.44 | 0.49 |
| 4:3Y:6:PHE:CE2 | 4:3Y:8:SER:HB2 | 2.47 | 0.49 |
| 3:4B:154:TYR:HD2 | 3:4B:158:LEU:HD11 | 1.76 | 0.49 |
| 4:4G:6:PHE:CE2 | 4:4G:8:SER:HB2 | 2.47 | 0.49 |
| 4:4I:6:PHE:CE2 | 4:4I:8:SER:HB2 | 2.47 | 0.49 |
| 3:4J:181:GLU:OE2 | 3:4J:223:LYS:HG2 | 2.12 | 0.49 |
| 5:4M:79:LYS:HE2 | 15:5P:324:ARG:HH12 | 1.77 | 0.49 |
| 9:4Z:328:ASP:HA | 9:4Z:331:ARG:HE | 1.77 | 0.49 |
| 10:5A:262:ILE:HA | 10:5A:265:LYS:HE3 | 1.94 | 0.49 |
| 12:5F:13:PRO:HB3 | 12:5G:300:PRO:HG2 | 1.93 | 0.49 |
| 13:5H:55:VAL:HG13 | 13:5H:56:ASP:O | 2.12 | 0.49 |
| 13:5I:55:VAL:HG13 | 13:5I:56:ASP:O | 2.12 | 0.49 |
| 14:5L:127:ASN:N | 14:5L:127:ASN:HD22 | 2.10 | 0.49 |
| 14:5L:377:ARG:HH21 | 23:6Q:52:LEU:HD11 | 1.77 | 0.49 |
| 14:5M:217:ASP:HB3 | 14:5M:237:ASN:ND2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:480:SER:OG | 14:5M:482:ASP:OD1 | 2.28 | 0.49 |
| 14:5M:511:THR:OG1 | 14:5M:531:ASP:CG | 2.49 | 0.49 |
| 14:5N:532:ARG:HB3 | 14:5N:552:ASP:HA | 1.94 | 0.49 |
| 15:5O:127:LYS:NZ | 15:5O:155:SER:O | 2.42 | 0.49 |
| 17:5S:114:LEU:N | 17:5S:114:LEU:CD2 | 2.75 | 0.49 |
| 18:5X:70:TYR:HB3 | 18:5X:81:VAL:HG23 | 1.94 | 0.49 |
| 18:5X:205:HIS:CE1 | 18:5X:207:ASP:HB2 | 2.47 | 0.49 |
| 18:5Y:205:HIS:CE1 | 18:5Y:207:ASP:HB2 | 2.47 | 0.49 |
| 18:5Z:70:TYR:HB3 | 18:5Z:81:VAL:HG23 | 1.94 | 0.49 |
| 18:6A:205:HIS:CE1 | 18:6A:207:ASP:HB2 | 2.47 | 0.49 |
| 18:6C:70:TYR:HB3 | 18:6C:81:VAL:HG23 | 1.94 | 0.49 |
| 18:6D:70:TYR:HB3 | 18:6D:81:VAL:HG23 | 1.94 | 0.49 |
| 18:6D:205:HIS:CE1 | 18:6D:207:ASP:HB2 | 2.47 | 0.49 |
| 22:6I:165:MET:HE2 | 22:6I:218:LEU:HD23 | 1.94 | 0.49 |
| 22:6N:203:HIS:HB3 | 22:6N:206:ASP:OD2 | 2.11 | 0.49 |
| 22:6O:108:ARG:NH2 | 24:6Z:282:ARG:O | 2.42 | 0.49 |
| 30:7K:179:ARG:NH1 | 30:7K:190:GLN:OE1 | 2.45 | 0.49 |
| 31:7N:114:GLU:O | 31:7N:116:THR:HG23 | 2.11 | 0.49 |
| 32:7P:100:ARG:NH2 | 32:7P:108:PRO:HG3 | 2.27 | 0.49 |
| 37:7Y:105:ASP:OD2 | 37:7Y:106:GLY:N | 2.44 | 0.49 |
| 37:7Y:216:THR:HG23 | 37:7Y:221:ARG:NH2 | 2.27 | 0.49 |
| 1:D2:56:GLY:H | 22:6M:54:ARG:HD2 | 1.76 | 0.49 |
| 1:E0:177:ASP:OD2 | 39:E0:501:GDP:H3' | 2.12 | 0.49 |
| 2:E5:56:THR:HA | 2:G1:285:GLN:HG2 | 1.94 | 0.49 |
| 2:G1:392:ASP:OD1 | 2:G1:422:ARG:NH1 | 2.45 | 0.49 |
| 2:G7:209:ILE:HD13 | 2:G7:231:ILE:HD11 | 1.93 | 0.49 |
| 2:H1:315:CYS:SG | 2:H1:379:SER:HB2 | 2.52 | 0.49 |
| 1:H2:418:LEU:O | 1:H2:421:GLU:HG2 | 2.11 | 0.49 |
| 2:H7:205:ASP:H | 2:H7:303:VAL:HG22 | 1.76 | 0.49 |
| 2:I1:363:VAL:HG23 | 2:I1:366:GLY:HA3 | 1.94 | 0.49 |
| 1:I2:86:ARG:HG2 | 1:I2:88:ASP:H | 1.77 | 0.49 |
| 1:I4:219:THR:HA | 2:I5:326:LYS:NZ | 2.27 | 0.49 |
| 1:I8:83:GLN:O | 1:K4:281:TYR:OH | 2.25 | 0.49 |
| 1:J0:382:SER:HB2 | 1:J0:415:MET:HG2 | 1.93 | 0.49 |
| 1:J2:212:PHE:HE1 | 2:J3:326:LYS:HG3 | 1.77 | 0.49 |
| 2:J5:8:HIS:CD2 | 2:J5:138:PHE:HD2 | 2.29 | 0.49 |
| 2:K1:34:GLY:HA3 | 2:K1:60:LYS:NZ | 2.27 | 0.49 |
| 2:K1:133:GLN:NE2 | 2:K1:252:ILE:HG22 | 2.27 | 0.49 |
| 2:K1:236:SER:O | 2:K1:243:ARG:NH2 | 2.42 | 0.49 |
| 2:K5:129:CYS:SG | 2:K5:130:THR:N | 2.84 | 0.49 |
| 1:L2:177:ASP:OD2 | 39:L2:502:GDP:H3' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L6:173:PRO:CD | 1:L6:380:ARG:HE | 2.25 | 0.49 |
| 1:M2:418:LEU:HG | 1:M2:422:TYR:CE2 | 2.34 | 0.49 |
| 2:M3:236:SER:O | 2:M3:243:ARG:NH2 | 2.41 | 0.49 |
| 2:M7:156:ARG:HA | 2:M7:159:VAL:HG12 | 1.94 | 0.49 |
| 1:N2:91:VAL:HG11 | 1:N2:116:VAL:HG12 | 1.94 | 0.49 |
| 1:N2:228:LEU:O | 1:N2:232:VAL:HG23 | 2.13 | 0.49 |
| 2:N3:198:THR:HG21 | 2:N3:201:ALA:HB2 | 1.93 | 0.49 |
| 2:N5:191:THR:HA | 2:N5:194:LEU:HB3 | 1.93 | 0.49 |
| 2:N7:394:LYS:HB2 | 1:N8:346:PRO:HG3 | 1.94 | 0.49 |
| 2:O1:3:GLU:HB2 | 2:O1:129:CYS:SG | 2.52 | 0.49 |
| 1:O4:276:ARG:HG3 | 19:6E:30:LEU:HD13 | 1.94 | 0.49 |
| 2:O7:9:ILE:HD13 | 2:O7:150:GLY:HA2 | 1.94 | 0.49 |
| 2:O7:88:HIS:HD2 | 2:O7:90:GLU:H | 1.58 | 0.49 |
| 2:O7:262:TYR:HE2 | 2:O7:346:TRP:CH2 | 2.30 | 0.49 |
| 2:O9:285:GLN:HE22 | 32:7P:23:GLU:H | 1.60 | 0.49 |
| 1:P4:276:ARG:HA | 1:P4:279:GLN:HB2 | 1.93 | 0.49 |
| 2:P5:384:ILE:HD12 | 2:P5:384:ILE:H | 1.77 | 0.49 |
| 1:P8:49:VAL:HG11 | 1:P8:241:ARG:HG2 | 1.93 | 0.49 |
| 2:P9:414:GLU:HG2 | 2:P9:417:GLU:OE1 | 2.12 | 0.49 |
| 1:Q4:354:CYS:SG | 1:Q4:355:ASP:N | 2.85 | 0.49 |
| 1:Q8:176:SER:HB2 | 2:Q9:349:THR:OG1 | 2.12 | 0.49 |
| 1:R0:31:ASP:OD1 | 1:R0:35:THR:N | 2.43 | 0.49 |
| 1:R0:31:ASP:OD2 | 1:R0:35:THR:OG1 | 2.29 | 0.49 |
| 1:R2:49:VAL:HG11 | 1:R2:241:ARG:HG2 | 1.93 | 0.49 |
| 1:R4:31:ASP:HB2 | 1:R4:32:PRO:HD2 | 1.93 | 0.49 |
| 1:R6:189:VAL:O | 1:R6:193:VAL:HG13 | 2.11 | 0.49 |
| 2:R7:90:GLU:CB | 2:R7:121:ARG:HH12 | 2.23 | 0.49 |
| 2:R7:408:TYR:HB3 | 2:R7:413:MET:HE2 | 1.93 | 0.49 |
| 2:R9:105:ARG:O | 2:R9:109:THR:OG1 | 2.30 | 0.49 |
| 2:R9:413:MET:HB3 | 2:R9:417:GLU:OE2 | 2.12 | 0.49 |
| 2:S1:88:HIS:NE2 | 2:S1:89:PRO:HD2 | 2.11 | 0.49 |
| 1:S4:290:THR:HA | 1:S4:293:MET:HB2 | 1.93 | 0.49 |
| 2:S7:26:LEU:HD22 | 2:S7:363:VAL:HG12 | 1.94 | 0.49 |
| 2:S7:267:PHE:CD2 | 2:S7:432:PHE:HZ | 2.30 | 0.49 |
| 1:T0:186:THR:HG22 | 1:T0:411:ALA:HB1 | 1.94 | 0.49 |
| 2:T1:5:ILE:HG22 | 2:T1:64:ARG:HB3 | 1.94 | 0.49 |
| 2:T1:151:SER:O | 2:T1:155:GLU:HG3 | 2.12 | 0.49 |
| 2:T3:250:VAL:HG21 | 2:T3:352:LYS:HE3 | 1.94 | 0.49 |
| 1:T4:161:ASP:OD2 | 1:T4:162:ARG:NH1 | 2.45 | 0.49 |
| 2:T7:175:PRO:HB3 | 2:T7:390:ARG:NE | 2.26 | 0.49 |
| 2:T7:264:ARG:NH2 | 2:T7:431:ASP:OD1 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U5:427:ALA:HA | 2:U5:430:LYS:HD2 | 1.94 | 0.49 |
| 2:V3:246:GLY:H | 2:V3:249:ASN:HD21 | 1.60 | 0.49 |
| 1:V8:382:SER:HB3 | 1:V8:415:MET:HG2 | 1.93 | 0.49 |
| 1:W0:329:GLN:O | 1:W0:333:VAL:HG23 | 2.12 | 0.49 |
| 2:W7:284:GLU:HG2 | 2:W7:285:GLN:N | 2.27 | 0.49 |
| 2:W9:84:ARG:HH11 | 2:W9:84:ARG:CG | 2.25 | 0.49 |
| 2:X3:31:GLN:HB2 | 2:X3:33:ASP:OD1 | 2.12 | 0.49 |
| 2:X7:133:GLN:HB3 | 2:X7:252:ILE:HG21 | 1.94 | 0.49 |
| 2:Y3:65:CYS:SG | 2:Y3:66:ILE:N | 2.85 | 0.49 |
| 1:Y6:58:ARG:CG | 1:Y6:58:ARG:NH2 | 2.62 | 0.49 |
| 2:Z1:90:GLU:HB2 | 2:0H:283:HIS:CE1 | 2.47 | 0.49 |
| 2:Z5:9:ILE:HG12 | 2:Z5:68:LEU:HD11 | 1.93 | 0.49 |
| 2:Z5:88:HIS:CE1 | 2:Z5:90:GLU:HG2 | 2.47 | 0.49 |
| 2:Z7:69:ASP:OD1 | 2:Z7:70:LEU:N | 2.45 | 0.49 |
| 1:Z8:3:GLU:O | 1:Z8:131:GLN:N | 2.37 | 0.49 |
| 1:Z8:273:LEU:H | 1:Z8:292:GLN:HE22 | 1.60 | 0.49 |
| 1:0C:382:SER:O | 1:0C:386:THR:HG23 | 2.12 | 0.49 |
| 2:0J:28:HIS:CE1 | 2:0J:49:PHE:HA | 2.48 | 0.49 |
| 2:0J:51:THR:HG21 | 2:0J:243:ARG:HG2 | 1.94 | 0.49 |
| 2:0J:245:ASP:N | 2:0J:245:ASP:OD1 | 2.43 | 0.49 |
| 1:0O:405:GLU:HA | 1:0O:408:PHE:HD2 | 1.77 | 0.49 |
| 2:0V:203:MET:CE | 2:0V:267:PHE:HB3 | 2.43 | 0.49 |
| 2:0V:277:SER:OG | 2:0V:278:ALA:N | 2.46 | 0.49 |
| 2:0V:344:VAL:HB | 2:0V:346:TRP:CD1 | 2.47 | 0.49 |
| 2:0X:317:LEU:HB3 | 2:0X:319:TYR:CE1 | 2.47 | 0.49 |
| 2:1F:278:ALA:HA | 2:1F:369:ALA:HB2 | 1.93 | 0.49 |
| 2:1L:109:THR:OG1 | 2:1L:411:GLU:OE2 | 2.31 | 0.49 |
| 1:1O:301:CYS:SG | 1:1O:302:ALA:N | 2.85 | 0.49 |
| 2:1T:271:SER:OG | 2:1T:377:MET:HB3 | 2.12 | 0.49 |
| 2:1X:103:PHE:HB3 | 2:1X:408:TYR:HE2 | 1.76 | 0.49 |
| 2:2D:335:ILE:HG23 | 2:2D:341:ILE:HD11 | 1.94 | 0.49 |
| 1:2E:45:GLU:HG2 | 1:2E:46:ARG:HG2 | 1.94 | 0.49 |
| 2:2N:182:VAL:HG22 | 2:2N:185:TYR:HB2 | 1.94 | 0.49 |
| 1:3C:165:LEU:HD11 | 1:3C:250:LEU:HD11 | 1.93 | 0.49 |
| 1:3C:212:PHE:HZ | 38:8D:117:TRP:HB3 | 1.76 | 0.49 |
| 2:3H:156:ARG:HA | 2:3H:159:VAL:HG12 | 1.94 | 0.49 |
| 2:3J:399:TYR:OH | 2:3J:415:GLU:OE2 | 2.29 | 0.49 |
| 2:3L:417:GLU:HA | 2:3L:420:GLU:HG2 | 1.94 | 0.49 |
| 1:3O:211:CYS:SG | 1:3O:217:LEU:HB2 | 2.52 | 0.49 |
| 2:3R:399:TYR:OH | 2:3R:415:GLU:OE2 | 2.21 | 0.49 |
| 1:3S:153:SER:HA | 1:3S:195:ASN:ND2 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3T:185:TYR:HA | 2:3T:395:PHE:CE1 | 2.47 | 0.49 |
| 3:3X:154:TYR:HD2 | 3:3X:158:LEU:HD11 | 1.76 | 0.49 |
| 3:4F:154:TYR:HD2 | 3:4F:158:LEU:HD11 | 1.76 | 0.49 |
| 3:4J:192:LEU:HD11 | 3:4J:230:LEU:HD21 | 1.93 | 0.49 |
| 5:4M:166:ARG:O | 5:4M:169:GLU:HG3 | 2.12 | 0.49 |
| 6:4O:459:ARG:NH2 | 6:4O:483:ASP:OD1 | 2.41 | 0.49 |
| 14:5L:217:ASP:HB3 | 14:5L:237:ASN:ND2 | 2.27 | 0.49 |
| 14:5L:532:ARG:HB3 | 14:5L:552:ASP:HA | 1.94 | 0.49 |
| 14:5M:127:ASN:N | 14:5M:127:ASN:HD22 | 2.10 | 0.49 |
| 14:5N:217:ASP:HB3 | 14:5N:237:ASN:ND2 | 2.27 | 0.49 |
| 15:5O:10:ILE:HG12 | 15:5O:77:GLU:O | 2.12 | 0.49 |
| 17:5T:177:ASP:HA | 17:5T:180:GLN:HE21 | 1.77 | 0.49 |
| 18:5Y:70:TYR:HB3 | 18:5Y:81:VAL:HG23 | 1.94 | 0.49 |
| 18:5Z:205:HIS:CE1 | 18:5Z:207:ASP:HB2 | 2.47 | 0.49 |
| 18:6A:70:TYR:HB3 | 18:6A:81:VAL:HG23 | 1.94 | 0.49 |
| 18:6B:70:TYR:HB3 | 18:6B:81:VAL:HG23 | 1.94 | 0.49 |
| 18:6B:205:HIS:CE1 | 18:6B:207:ASP:HB2 | 2.47 | 0.49 |
| 18:6C:205:HIS:CE1 | 18:6C:207:ASP:HB2 | 2.47 | 0.49 |
| 19:6E:92:ARG:CG | 19:6E:99:ARG:NE | 2.73 | 0.49 |
| 22:6P:307:ARG:O | 22:6P:311:VAL:HG23 | 2.11 | 0.49 |
| 24:6W:123:TYR:HD1 | 24:6W:130:MET:SD | 2.35 | 0.49 |
| 24:6Y:435:LEU:HA | 24:6Y:438:LEU:HB2 | 1.93 | 0.49 |
| 1:7:436:PHE:HE1 | 3:4B:110:TYR:CE1 | 2.29 | 0.49 |
| 1:B8:80:PRO:HD2 | 24:6Y:221:ARG:HH12 | 1.77 | 0.49 |
| 2:E1:221:ARG:HH22 | 22:6J:28:GLN:HA | 1.78 | 0.49 |
| 2:G1:320:ARG:HD3 | 2:G1:360:PRO:HG3 | 1.94 | 0.49 |
| 1:G2:68:LEU:HB3 | 1:G2:96:GLY:HA2 | 1.94 | 0.49 |
| 1:G4:122:LYS:HE3 | 1:I0:291:GLN:HB3 | 1.94 | 0.49 |
| 2:G5:212:ILE:O | 2:G5:216:SER:OG | 2.27 | 0.49 |
| 2:G5:388:PHE:HB3 | 2:G5:425:LEU:HD11 | 1.93 | 0.49 |
| 1:G6:7:ILE:HB | 1:G6:135:VAL:HG12 | 1.93 | 0.49 |
| 2:G7:219:ILE:HG23 | 22:6O:175:ALA:HB1 | 1.93 | 0.49 |
| 1:G8:8:GLN:CD | 1:G8:17:GLY:HA3 | 2.33 | 0.49 |
| 1:G8:404:ASP:HB3 | 1:G8:406:MET:SD | 2.53 | 0.49 |
| 1:G8:414:ASN:HA | 1:G8:417:ASP:OD2 | 2.11 | 0.49 |
| 2:H1:209:ILE:HG23 | 2:H1:230:LEU:HD21 | 1.93 | 0.49 |
| 1:H4:121:ARG:NH2 | 1:H4:158:GLU:OE2 | 2.39 | 0.49 |
| 1:H6:19:LYS:O | 1:H6:23:VAL:HG23 | 2.12 | 0.49 |
| 1:H8:203:ASP:N | 1:H8:203:ASP:OD2 | 2.45 | 0.49 |
| 1:H8:272:PRO:HD3 | 1:H8:364:SER:HA | 1.93 | 0.49 |
| 2:H9:267:PHE:HB2 | 2:H9:384:ILE:HD12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I1:213:CYS:HA | 2:I1:217:LEU:HB2 | 1.93 | 0.49 |
| 2:I1:236:SER:O | 2:I1:243:ARG:NH2 | 2.45 | 0.49 |
| 2:I1:274:PRO:HB2 | 2:I1:276:ILE:HG12 | 1.94 | 0.49 |
| 1:I2:207:LEU:HB3 | 1:I2:225:LEU:HD22 | 1.94 | 0.49 |
| 1:I4:334:GLN:NE2 | 1:I4:348:ASN:H | 2.10 | 0.49 |
| 2:J1:88:HIS:CD2 | 2:K7:283:HIS:HA | 2.47 | 0.49 |
| 1:J4:54:ALA:HB3 | 1:J4:58:ARG:HB3 | 1.93 | 0.49 |
| 1:J4:178:THR:OG1 | 1:J4:181:GLU:HG3 | 2.11 | 0.49 |
| 2:K5:287:SER:OG | 2:K5:288:VAL:N | 2.45 | 0.49 |
| 1:L2:186:THR:HG22 | 1:L2:411:ALA:HB1 | 1.94 | 0.49 |
| 2:L3:76:ASP:OD2 | 1:L4:46:ARG:NH2 | 2.45 | 0.49 |
| 2:L5:201:ALA:O | 2:L5:268:MET:HE2 | 2.12 | 0.49 |
| 2:L5:345:ASP:N | 2:L5:345:ASP:OD1 | 2.46 | 0.49 |
| 1:M2:325:GLU:HA | 1:M2:328:GLU:OE1 | 2.11 | 0.49 |
| 2:M3:229:ARG:HH11 | 2:M3:363:VAL:HG21 | 1.77 | 0.49 |
| 2:M7:51:THR:HG23 | 2:M7:52:PHE:CD2 | 2.47 | 0.49 |
| 1:M8:257:LEU:HD21 | 1:M8:314:SER:HB3 | 1.95 | 0.49 |
| 1:M8:361:LEU:HD23 | 30:7K:41:TRP:CE3 | 2.47 | 0.49 |
| 2:N9:114:ILE:HG21 | 2:N9:149:LEU:HD22 | 1.94 | 0.49 |
| 2:O3:12:ALA:HB2 | 41:O4:501:GTP:C8 | 2.48 | 0.49 |
| 2:O3:414:GLU:HG2 | 2:O3:416:GLY:H | 1.76 | 0.49 |
| 2:O5:69:ASP:OD1 | 2:O5:70:LEU:N | 2.46 | 0.49 |
| 2:O7:319:TYR:HB3 | 2:O7:323:VAL:HG11 | 1.93 | 0.49 |
| 2:P5:170:THR:HG21 | 2:P5:194:LEU:HD11 | 1.95 | 0.49 |
| 2:P7:114:ILE:HD12 | 2:P7:117:LEU:HD21 | 1.95 | 0.49 |
| 1:Q6:12:CYS:HB3 | 1:Q6:138:SER:HB2 | 1.94 | 0.49 |
| 1:Q6:311:LEU:HD23 | 1:Q6:312:THR:HG23 | 1.92 | 0.49 |
| 1:Q8:253:LEU:O | 1:Q8:257:LEU:HB2 | 2.12 | 0.49 |
| 2:R5:176:GLN:HG2 | 2:R5:177:VAL:N | 2.28 | 0.49 |
| 2:R9:88:HIS:NE2 | 2:T5:283:HIS:HB3 | 2.28 | 0.49 |
| 2:S1:110:ILE:HA | 2:S1:113:GLU:OE1 | 2.12 | 0.49 |
| 1:S2:424:GLN:NE2 | 17:5V:104:PHE:H | 2.10 | 0.49 |
| 2:S5:205:ASP:OD1 | 2:S5:303:VAL:HG13 | 2.12 | 0.49 |
| 1:S6:156:ARG:NH1 | 1:S6:197:ASP:OD1 | 2.45 | 0.49 |
| 2:S7:72:PRO:HD2 | 1:S8:2:ARG:NH1 | 2.27 | 0.49 |
| 2:S7:123:ARG:NH2 | 2:S7:160:ASP:OD1 | 2.45 | 0.49 |
| 1:T0:285:THR:HB | 1:T0:287:PRO:HD2 | 1.94 | 0.49 |
| 1:T0:309:ARG:H | 1:T0:372:THR:HG22 | 1.76 | 0.49 |
| 1:T2:174:LYS:HB2 | 1:T2:205:GLU:OE1 | 2.12 | 0.49 |
| 1:T4:391:ARG:O | 1:T4:391:ARG:CG | 2.59 | 0.49 |
| 1:T6:167:PHE:CE1 | 1:T6:233:MET:HG2 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T8:28:HIS:NE2 | 1:T8:241:ARG:HD2 | 2.27 | 0.49 |
| 2:U1:53:PHE:HA | 2:U1:62:VAL:O | 2.11 | 0.49 |
| 2:U1:72:PRO:HD2 | 1:U2:2:ARG:HH12 | 1.77 | 0.49 |
| 1:U2:6:HIS:NE2 | 1:U2:136:CYS:SG | 2.85 | 0.49 |
| 1:U2:117:LEU:HA | 1:U2:120:VAL:HG12 | 1.94 | 0.49 |
| 1:U4:221:THR:HG23 | 1:U4:223:GLY:H | 1.76 | 0.49 |
| 1:U4:263:LEU:HD22 | 1:U4:422:TYR:HE1 | 1.77 | 0.49 |
| 2:U7:121:ARG:CD | 2:U7:121:ARG:C | 2.78 | 0.49 |
| 2:V1:55:GLU:HA | 2:V1:60:LYS:O | 2.12 | 0.49 |
| 1:V2:309:ARG:O | 1:V2:372:THR:HG22 | 2.12 | 0.49 |
| 2:V7:20:CYS:SG | 2:V7:21:TRP:N | 2.84 | 0.49 |
| 2:V7:76:ASP:HA | 2:V7:79:ARG:HB2 | 1.95 | 0.49 |
| 2:V9:79:ARG:NH1 | 2:V9:92:LEU:O | 2.43 | 0.49 |
| 2:W1:88:HIS:NE2 | 2:W1:90:GLU:HB2 | 2.27 | 0.49 |
| 2:W9:90:GLU:CB | 2:W9:121:ARG:HH12 | 2.26 | 0.49 |
| 2:X7:332:VAL:HA | 2:X7:335:ILE:HG22 | 1.93 | 0.49 |
| 1:X8:105:HIS:NE2 | 1:X8:150:LEU:HD13 | 2.27 | 0.49 |
| 1:Y6:111:GLU:HG2 | 1:Y6:112:LEU:HD22 | 1.94 | 0.49 |
| 1:Y8:286:VAL:O | 1:Y8:290:THR:OG1 | 2.26 | 0.49 |
| 1:Z4:3:GLU:HB2 | 1:Z4:130:LEU:HA | 1.95 | 0.49 |
| 2:Z5:380:ASN:OD1 | 2:Z5:381:SER:N | 2.45 | 0.49 |
| 2:Z7:157:LEU:HD22 | 2:Z7:166:LYS:HD3 | 1.94 | 0.49 |
| 1:Z8:260:PHE:HB2 | 1:Z8:263:LEU:HD23 | 1.94 | 0.49 |
| 2:0B:71:GLU:HB3 | 2:0B:98:ASP:OD2 | 2.12 | 0.49 |
| 2:0B:166:LYS:N | 2:0B:199:ASP:OD2 | 2.45 | 0.49 |
| 1:0E:385:PHE:HZ | 1:0E:408:PHE:HD1 | 1.61 | 0.49 |
| 1:0I:397:TRP:NE1 | 2:0J:260:VAL:O | 2.43 | 0.49 |
| 2:0J:69:ASP:OD1 | 2:0J:70:LEU:N | 2.42 | 0.49 |
| 1:0K:52:ASN:OD1 | 1:0K:62:ARG:NH2 | 2.46 | 0.49 |
| 1:0K:232:VAL:HG21 | 1:0K:300:MET:CE | 2.42 | 0.49 |
| 1:0O:8:GLN:O | 1:0O:66:MET:HB2 | 2.12 | 0.49 |
| 2:0P:109:THR:OG1 | 2:0P:411:GLU:OE2 | 2.28 | 0.49 |
| 2:0P:274:PRO:HB2 | 2:0P:276:ILE:HG12 | 1.95 | 0.49 |
| 1:0S:86:ARG:HD3 | 1:0S:88:ASP:HB2 | 1.94 | 0.49 |
| 1:0U:15:GLN:O | 1:0U:19:LYS:HG2 | 2.12 | 0.49 |
| 1:0U:114:ASP:OD1 | 1:0U:115:SER:N | 2.45 | 0.49 |
| 1:0Y:135:VAL:HG21 | 1:0Y:152:ILE:HD11 | 1.94 | 0.49 |
| 1:1A:256:ASN:ND2 | 1:1A:350:LYS:HD3 | 2.27 | 0.49 |
| 1:1E:113:ILE:HD12 | 1:1E:150:LEU:HG | 1.94 | 0.49 |
| 1:1E:248:ALA:HA | 1:1E:252:LYS:CD | 2.33 | 0.49 |
| 1:1G:388:MET:SD | 2:1H:348:PRO:HD3 | 2.53 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1K:165:LEU:HG | 1:1K:250:LEU:HD11 | 1.93 | 0.49 |
| 1:1K:385:PHE:HZ | 1:1K:408:PHE:HD1 | 1.60 | 0.49 |
| 1:1O:16:ILE:HG22 | 1:1O:226:ASN:OD1 | 2.12 | 0.49 |
| 1:1O:282:ARG:NH2 | 1:1O:288:GLU:OE1 | 2.45 | 0.49 |
| 2:1T:5:ILE:HG22 | 2:1T:64:ARG:HB3 | 1.94 | 0.49 |
| 2:1V:50:ASN:O | 2:1V:64:ARG:NH2 | 2.44 | 0.49 |
| 2:1V:379:SER:OG | 2:1V:380:ASN:N | 2.45 | 0.49 |
| 1:2A:5:VAL:HG22 | 1:2A:133:PHE:HD1 | 1.77 | 0.49 |
| 1:2A:113:ILE:HG12 | 1:2A:150:LEU:HG | 1.93 | 0.49 |
| 1:2C:212:PHE:HZ | 2:2D:326:LYS:HG3 | 1.77 | 0.49 |
| 1:2I:285:THR:OG1 | 1:2I:287:PRO:HD2 | 2.13 | 0.49 |
| 2:2J:9:ILE:HG22 | 2:2J:146:GLY:HA2 | 1.94 | 0.49 |
| 2:2J:275:ILE:O | 2:2J:275:ILE:HG13 | 2.12 | 0.49 |
| 1:2S:317:PHE:HE2 | 1:2S:326:VAL:HG13 | 1.77 | 0.49 |
| 1:2U:167:PHE:CE2 | 1:2U:233:MET:HG2 | 2.48 | 0.49 |
| 1:3A:193:VAL:HG22 | 1:3A:265:PHE:CZ | 2.45 | 0.49 |
| 2:3B:287:SER:OG | 2:3B:288:VAL:N | 2.45 | 0.49 |
| 2:3J:287:SER:OG | 2:3J:288:VAL:N | 2.45 | 0.49 |
| 2:3P:261:PRO:HG3 | 2:3P:313:MET:HE2 | 1.94 | 0.49 |
| 2:3P:327:ASP:N | 2:3P:327:ASP:OD1 | 2.45 | 0.49 |
| 1:3Q:130:LEU:HB2 | 1:3Q:162:ARG:HE | 1.77 | 0.49 |
| 4:3Y:14:LEU:HD23 | 4:3Y:162:ILE:HD11 | 1.94 | 0.49 |
| 3:3Z:154:TYR:HD2 | 3:3Z:158:LEU:HD11 | 1.76 | 0.49 |
| 4:4G:14:LEU:HD23 | 4:4G:162:ILE:HD11 | 1.94 | 0.49 |
| 4:4I:15:TYR:CE2 | 4:4I:17:ILE:HB | 2.47 | 0.49 |
| 7:4U:111:ASP:OD1 | 7:4U:112:MET:N | 2.45 | 0.49 |
| 13:5K:55:VAL:HG13 | 13:5K:56:ASP:O | 2.12 | 0.49 |
| 14:5M:532:ARG:HB3 | 14:5M:552:ASP:HA | 1.94 | 0.49 |
| 15:5O:32:SER:HB3 | 15:5O:49:ARG:HH12 | 1.77 | 0.49 |
| 15:5P:172:TRP:NE1 | 15:5P:176:ILE:HD11 | 2.27 | 0.49 |
| 16:5Q:63:ARG:NH1 | 16:5Q:91:ASP:O | 2.40 | 0.49 |
| 17:5V:219:LEU:O | 17:5V:223:GLU:HG3 | 2.12 | 0.49 |
| 17:5V:224:ARG:O | 17:5V:228:THR:HG23 | 2.11 | 0.49 |
| 20:6F:135:ASP:OD2 | 20:6F:136:ASP:N | 2.45 | 0.49 |
| 22:6I:53:THR:O | 22:6I:57:THR:OG1 | 2.29 | 0.49 |
| 22:6L:177:LEU:HD23 | 22:6L:187:MET:HE3 | 1.94 | 0.49 |
| 22:6O:314:CYS:HA | 22:6O:317:VAL:HG12 | 1.94 | 0.49 |
| 22:6P:203:HIS:HB3 | 22:6P:206:ASP:OD2 | 2.12 | 0.49 |
| 24:6U:480:ASN:HD21 | 24:6U:503:ILE:HD12 | 1.77 | 0.49 |
| 24:6V:123:TYR:CE2 | 24:6V:163:PRO:HG3 | 2.48 | 0.49 |
| 24:6W:456:ASP:N | 24:6W:456:ASP:OD1 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:276:TRP:CD1 | 24:6X:293:VAL:HG12 | 2.48 | 0.49 |
| 24:6Y:571:ASP:N | 24:6Y:571:ASP:OD1 | 2.45 | 0.49 |
| 26:7D:59:ARG:HH21 | 26:7D:59:ARG:CB | 2.21 | 0.49 |
| 30:7K:108:ARG:NH2 | 37:7Y:142:ARG:HD3 | 2.27 | 0.49 |
| 38:7Z:33:LYS:HD3 | 38:7Z:34:ALA:N | 2.27 | 0.49 |
| 38:8C:80:TYR:CD2 | 38:8C:80:TYR:C | 2.86 | 0.49 |
| 2:G3:297:GLU:OE1 | 2:G3:297:GLU:N | 2.44 | 0.49 |
| 1:G4:32:PRO:HD2 | 24:6X:527:ASN:ND2 | 2.25 | 0.49 |
| 1:G6:219:THR:H | 24:6Y:418:ASP:CG | 2.16 | 0.49 |
| 1:G6:389:PHE:O | 1:G6:392:LYS:NZ | 2.39 | 0.49 |
| 2:G7:277:SER:OG | 2:G7:278:ALA:N | 2.44 | 0.49 |
| 2:G9:188:VAL:HG13 | 2:G9:425:LEU:HD11 | 1.93 | 0.49 |
| 1:H6:11:GLN:N | 39:H6:502:GDP:O2B | 2.41 | 0.49 |
| 1:H6:114:ASP:N | 1:H6:114:ASP:OD1 | 2.44 | 0.49 |
| 1:H8:95:THR:OG1 | 1:H8:96:GLY:N | 2.46 | 0.49 |
| 2:H9:155:GLU:HB2 | 2:H9:197:HIS:CE1 | 2.48 | 0.49 |
| 1:I4:391:ARG:NH2 | 2:I5:434:GLU:OE2 | 2.46 | 0.49 |
| 2:I5:81:GLY:O | 2:I5:84:ARG:NH1 | 2.43 | 0.49 |
| 2:I5:116:ASP:N | 2:I5:116:ASP:OD1 | 2.44 | 0.49 |
| 2:I9:56:THR:HG23 | 2:I9:60:LYS:HB3 | 1.94 | 0.49 |
| 2:J3:312:TYR:HB2 | 2:J3:343:PHE:HD1 | 1.78 | 0.49 |
| 2:J5:111:GLY:HA2 | 2:J5:114:ILE:HG22 | 1.94 | 0.49 |
| 2:K7:287:SER:N | 2:K7:290:GLU:OE2 | 2.45 | 0.49 |
| 1:L0:317:PHE:HB3 | 1:L0:321:MET:SD | 2.52 | 0.49 |
| 2:L5:222:PRO:HD2 | 1:L6:324:LYS:HE3 | 1.94 | 0.49 |
| 1:M0:320:ARG:HH12 | 29:7I:110:THR:HA | 1.77 | 0.49 |
| 1:M8:404:ASP:HB3 | 1:M8:406:MET:SD | 2.52 | 0.49 |
| 2:N9:191:THR:HA | 2:N9:194:LEU:HB3 | 1.94 | 0.49 |
| 2:O1:88:HIS:ND1 | 2:O1:89:PRO:CD | 2.72 | 0.49 |
| 2:P5:269:LEU:HD21 | 2:P5:384:ILE:HG13 | 1.93 | 0.49 |
| 1:P6:318:ARG:HD3 | 1:P6:358:PRO:HD3 | 1.95 | 0.49 |
| 2:P7:111:GLY:HA2 | 2:P7:114:ILE:HG22 | 1.95 | 0.49 |
| 1:Q2:278:SER:O | 1:Q2:278:SER:OG | 2.28 | 0.49 |
| 2:Q5:282:TYR:N | 2:Q5:282:TYR:CD2 | 2.79 | 0.49 |
| 1:Q6:273:LEU:H | 1:Q6:292:GLN:HE22 | 1.60 | 0.49 |
| 2:Q9:248:LEU:HD22 | 2:Q9:354:GLY:HA2 | 1.94 | 0.49 |
| 1:R0:42:LEU:HD12 | 12:7B:70:LEU:HD21 | 1.94 | 0.49 |
| 1:R4:2:ARG:HB3 | 1:R4:131:GLN:HB2 | 1.94 | 0.49 |
| 2:R5:62:VAL:HG21 | 2:R5:88:HIS:HB2 | 1.93 | 0.49 |
| 2:R9:81:GLY:HA3 | 12:5F:106:TYR:HE2 | 1.77 | 0.49 |
| 1:S4:5:VAL:HG23 | 1:S4:62:ARG:HG2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S7:325:PRO:HA | 2:S7:328:VAL:HG12 | 1.94 | 0.49 |
| 1:T0:273:LEU:H | 1:T0:292:GLN:HE22 | 1.59 | 0.49 |
| 1:T4:49:VAL:HG11 | 1:T4:241:ARG:HG2 | 1.93 | 0.49 |
| 2:T5:5:ILE:HD11 | 2:T5:135:PHE:CE1 | 2.47 | 0.49 |
| 2:T7:18:ASN:HD21 | 31:7N:30:TYR:HE1 | 1.59 | 0.49 |
| 2:T7:176:GLN:NE2 | 2:T7:207:GLU:HG2 | 2.28 | 0.49 |
| 1:T8:4:ILE:HB | 1:T8:50:TYR:HE1 | 1.77 | 0.49 |
| 1:U8:317:PHE:HE2 | 1:U8:326:VAL:HG13 | 1.75 | 0.49 |
| 1:V0:114:ASP:OD1 | 1:V0:115:SER:N | 2.45 | 0.49 |
| 1:V6:48:ASN:O | 1:V6:62:ARG:NH1 | 2.41 | 0.49 |
| 1:W0:111:GLU:N | 1:W0:111:GLU:OE2 | 2.46 | 0.49 |
| 2:W3:54:SER:OG | 2:W3:64:ARG:NH2 | 2.46 | 0.49 |
| 2:W7:234:VAL:HG13 | 2:W7:376:CYS:SG | 2.52 | 0.49 |
| 1:W8:325:GLU:O | 1:W8:329:GLN:HB2 | 2.12 | 0.49 |
| 1:X4:389:PHE:O | 1:X4:392:LYS:NZ | 2.36 | 0.49 |
| 2:X7:203:MET:HE3 | 2:X7:387:ILE:HG21 | 1.95 | 0.49 |
| 1:X8:234:SER:O | 1:X8:241:ARG:NH2 | 2.45 | 0.49 |
| 2:X9:53:PHE:HB3 | 2:X9:61:HIS:HB3 | 1.95 | 0.49 |
| 1:Y0:330:MET:HA | 1:Y0:333:VAL:HG12 | 1.94 | 0.49 |
| 2:Y3:22:GLU:HG2 | 2:Y3:83:TYR:CZ | 2.48 | 0.49 |
| 1:Z0:396:HIS:H | 1:Z0:396:HIS:CD2 | 2.31 | 0.49 |
| 1:Z2:20:PHE:HA | 1:Z2:230:SER:OG | 2.12 | 0.49 |
| 1:Z2:179:VAL:HG23 | 1:Z2:180:VAL:HG13 | 1.95 | 0.49 |
| 1:Z6:167:PHE:HE1 | 1:Z6:200:MET:HG3 | 1.77 | 0.49 |
| 1:Z8:12:CYS:O | 1:Z8:16:ILE:HG12 | 2.12 | 0.49 |
| 2:Z9:121:ARG:HD2 | 2:Z9:124:LYS:HE3 | 1.94 | 0.49 |
| 2:0B:313:MET:HE2 | 2:0B:380:ASN:HD22 | 1.78 | 0.49 |
| 1:0E:6:HIS:HA | 1:0E:134:GLN:HB3 | 1.95 | 0.49 |
| 1:0E:8:GLN:OE1 | 1:0E:65:LEU:HA | 2.12 | 0.49 |
| 1:0E:139:LEU:HD22 | 1:0E:188:SER:OG | 2.12 | 0.49 |
| 2:0F:379:SER:OG | 2:0F:380:ASN:N | 2.46 | 0.49 |
| 1:0G:165:LEU:HD22 | 1:0G:167:PHE:HE1 | 1.77 | 0.49 |
| 1:0G:276:ARG:CZ | 1:0G:279:GLN:HB3 | 2.42 | 0.49 |
| 2:0H:175:PRO:HB3 | 2:0H:390:ARG:NE | 2.27 | 0.49 |
| 2:0N:76:ASP:OD1 | 2:0N:79:ARG:HD2 | 2.12 | 0.49 |
| 2:0N:88:HIS:CE1 | 2:1D:283:HIS:HA | 2.48 | 0.49 |
| 1:0O:112:LEU:O | 1:0O:115:SER:OG | 2.26 | 0.49 |
| 1:0O:139:LEU:HG | 1:0O:168:SER:HB2 | 1.94 | 0.49 |
| 1:0U:186:THR:HG22 | 1:0U:411:ALA:HB1 | 1.95 | 0.49 |
| 2:0V:88:HIS:ND1 | 2:1L:283:HIS:HB3 | 2.28 | 0.49 |
| 2:0V:280:LYS:HA | 2:0V:283:HIS:HB3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1B:182:VAL:HG23 | 2:1B:186:ASN:HD21 | 1.77 | 0.49 |
| 2:1F:71:GLU:HB2 | 1:1G:2:ARG:HH12 | 1.77 | 0.49 |
| 2:1F:92:LEU:N | 2:1F:92:LEU:HD23 | 2.28 | 0.49 |
| 2:1F:167:LEU:HG | 2:1F:252:ILE:HD11 | 1.95 | 0.49 |
| 2:1H:56:THR:HG23 | 2:1H:60:LYS:HB3 | 1.94 | 0.49 |
| 2:1H:396:ASP:HA | 2:1H:422:ARG:HH22 | 1.77 | 0.49 |
| 1:1M:318:ARG:HB3 | 1:1M:357:PRO:HA | 1.94 | 0.49 |
| 2:1N:266:HIS:O | 2:1N:266:HIS:ND1 | 2.42 | 0.49 |
| 2:1N:381:SER:OG | 2:1N:382:THR:N | 2.45 | 0.49 |
| 2:1P:21:TRP:CZ2 | 2:1P:65:CYS:HB2 | 2.46 | 0.49 |
| 2:1P:145:THR:OG1 | 41:1Q:501:GTP:O1B | 2.29 | 0.49 |
| 1:1Q:144:GLY:N | 39:1Q:502:GDP:O1B | 2.43 | 0.49 |
| 1:1U:317:PHE:HE2 | 1:1U:326:VAL:HG13 | 1.77 | 0.49 |
| 1:1W:235:GLY:HA3 | 1:1W:366:THR:HG21 | 1.94 | 0.49 |
| 2:1Z:278:ALA:HA | 2:1Z:369:ALA:HB2 | 1.94 | 0.49 |
| 1:2A:83:GLN:OE1 | 1:2A:83:GLN:N | 2.44 | 0.49 |
| 2:2F:90:GLU:O | 2:2F:121:ARG:NH1 | 2.39 | 0.49 |
| 2:2F:213:CYS:HA | 2:2F:217:LEU:HB2 | 1.94 | 0.49 |
| 2:2J:161:TYR:HE1 | 38:8C:80:TYR:CB | 2.25 | 0.49 |
| 2:2P:282:TYR:OH | 10:5C:164:ASP:N | 2.46 | 0.49 |
| 2:2R:360:PRO:O | 2:2R:370:LYS:NZ | 2.44 | 0.49 |
| 1:2U:207:LEU:HB3 | 1:2U:225:LEU:HD22 | 1.95 | 0.49 |
| 1:2U:345:ILE:HB | 1:2U:348:ASN:HD21 | 1.78 | 0.49 |
| 2:2V:287:SER:OG | 2:2V:288:VAL:N | 2.46 | 0.49 |
| 2:2X:279:GLU:H | 2:2X:279:GLU:CD | 2.09 | 0.49 |
| 1:3G:309:ARG:H | 1:3G:372:THR:HG22 | 1.77 | 0.49 |
| 1:3I:183:TYR:HB3 | 1:3I:398:TYR:HE2 | 1.77 | 0.49 |
| 1:3O:177:ASP:N | 1:3O:181:GLU:OE2 | 2.46 | 0.49 |
| 1:3S:133:PHE:HE2 | 1:3S:155:ILE:HD12 | 1.77 | 0.49 |
| 1:3S:246:LEU:O | 1:3S:352:SER:OG | 2.22 | 0.49 |
| 1:3S:310:TYR:O | 1:3S:342:VAL:HG23 | 2.11 | 0.49 |
| 3:3V:154:TYR:HD2 | 3:3V:158:LEU:HD11 | 1.76 | 0.49 |
| 4:3W:14:LEU:HD23 | 4:3W:162:ILE:HD11 | 1.94 | 0.49 |
| 4:3W:15:TYR:CE2 | 4:3W:17:ILE:HB | 2.47 | 0.49 |
| 3:4D:154:TYR:HD2 | 3:4D:158:LEU:HD11 | 1.76 | 0.49 |
| 4:4G:15:TYR:CE2 | 4:4G:17:ILE:HB | 2.47 | 0.49 |
| 4:4I:14:LEU:HD23 | 4:4I:162:ILE:HD11 | 1.94 | 0.49 |
| 5:4M:305:ALA:HA | 5:4M:308:GLU:HG3 | 1.94 | 0.49 |
| 10:5B:240:LEU:HD23 | 10:5B:243:LEU:HD21 | 1.94 | 0.49 |
| 17:5U:177:ASP:O | 17:5U:180:GLN:HG3 | 2.11 | 0.49 |
| 22:6P:206:ASP:HA | 22:6P:209:ASN:ND2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:563:LYS:HA | 24:6U:566:VAL:HG12 | 1.94 | 0.49 |
| 24:6W:505:LYS:N | 24:6W:510:GLU:O | 2.42 | 0.49 |
| 29:7I:159:ARG:O | 29:7I:163:THR:HG23 | 2.12 | 0.49 |
| 34:7S:201:LEU:HD21 | 36:7W:91:PRO:HB3 | 1.94 | 0.49 |
| 1:3:262:ARG:NH1 | 3:3X:240:ARG:HH11 | 2.09 | 0.49 |
| 2:4:280:LYS:NZ | 26:7D:64:PRO:HG2 | 2.18 | 0.49 |
| 2:8:30:ILE:N | 26:7E:45:MET:CE | 2.74 | 0.49 |
| 2:D7:143:GLY:HA3 | 41:D7:501:GTP:O3A | 2.11 | 0.49 |
| 2:G3:51:THR:HG21 | 2:G3:243:ARG:HG2 | 1.95 | 0.49 |
| 2:G5:417:GLU:HA | 2:G5:420:GLU:HG2 | 1.94 | 0.49 |
| 1:G6:334:GLN:HE22 | 1:G6:347:ASN:HA | 1.78 | 0.49 |
| 2:G7:264:ARG:NH2 | 2:G7:431:ASP:OD2 | 2.45 | 0.49 |
| 2:H1:328:VAL:O | 2:H1:332:VAL:HG12 | 2.12 | 0.49 |
| 2:H3:353:CYS:SG | 2:H3:354:GLY:N | 2.85 | 0.49 |
| 1:I0:117:LEU:HA | 1:I0:120:VAL:HG12 | 1.94 | 0.49 |
| 1:I4:95:THR:HG23 | 1:I4:96:GLY:N | 2.27 | 0.49 |
| 2:J3:119:LEU:HA | 2:J3:122:ILE:HG22 | 1.95 | 0.49 |
| 1:J6:233:MET:O | 1:J6:237:THR:HG22 | 2.12 | 0.49 |
| 2:J7:204:LEU:HD23 | 2:J7:231:ILE:HD12 | 1.92 | 0.49 |
| 2:J7:320:ARG:NH2 | 2:J7:359:PRO:O | 2.45 | 0.49 |
| 2:K1:133:GLN:NE2 | 2:K1:252:ILE:H | 2.11 | 0.49 |
| 2:L3:72:PRO:HB2 | 29:7J:323:THR:HG21 | 1.94 | 0.49 |
| 2:L3:226:ASN:HD21 | 29:7J:360:GLN:HE22 | 1.58 | 0.49 |
| 2:L7:246:GLY:HA3 | 2:L7:356:ASN:HA | 1.94 | 0.49 |
| 1:M0:105:HIS:CD2 | 1:M0:150:LEU:HB2 | 2.48 | 0.49 |
| 1:M0:364:SER:OG | 1:M0:365:ALA:N | 2.46 | 0.49 |
| 1:M2:20:PHE:HA | 1:M2:230:SER:HB2 | 1.95 | 0.49 |
| 2:M3:254:GLU:HB3 | 2:M3:352:LYS:HE2 | 1.94 | 0.49 |
| 2:N3:70:LEU:HB3 | 2:N3:98:ASP:HA | 1.93 | 0.49 |
| 2:N7:51:THR:HG21 | 2:N7:243:ARG:HG2 | 1.93 | 0.49 |
| 2:N7:322:ASP:N | 2:N7:322:ASP:OD1 | 2.42 | 0.49 |
| 2:N9:286:LEU:O | 2:N9:373:ARG:NH1 | 2.45 | 0.49 |
| 2:P3:90:GLU:HB2 | 2:P3:121:ARG:HH22 | 1.77 | 0.49 |
| 2:P7:175:PRO:HB3 | 2:P7:390:ARG:NE | 2.28 | 0.49 |
| 2:P7:379:SER:OG | 2:P7:380:ASN:N | 2.44 | 0.49 |
| 1:Q2:334:GLN:HE22 | 1:Q2:348:ASN:H | 1.61 | 0.49 |
| 2:Q3:93:ILE:HD11 | 2:Q3:121:ARG:HD2 | 1.95 | 0.49 |
| 1:Q4:67:ASP:N | 1:Q4:67:ASP:OD1 | 2.45 | 0.49 |
| 1:Q8:180:VAL:HG23 | 1:Q8:184:ASN:HD21 | 1.77 | 0.49 |
| 2:R5:199:ASP:HA | 17:5T:84:ARG:HH22 | 1.78 | 0.49 |
| 1:S2:317:PHE:HB3 | 1:S2:321:MET:SD | 2.52 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:100:ASN:HB3 | 1:S4:103:LYS:HB2 | 1.94 | 0.49 |
| 2:S5:319:TYR:HB3 | 2:S5:323:VAL:HG21 | 1.94 | 0.49 |
| 1:S6:213:ARG:HH12 | 13:5H:117:ASN:CG | 2.16 | 0.49 |
| 1:S8:91:VAL:HG11 | 1:S8:116:VAL:HG22 | 1.95 | 0.49 |
| 2:S9:266:HIS:ND1 | 2:S9:266:HIS:O | 2.45 | 0.49 |
| 2:T5:333:ALA:O | 2:T5:337:THR:HG23 | 2.12 | 0.49 |
| 2:T7:114:ILE:HG21 | 2:T7:149:LEU:HD22 | 1.93 | 0.49 |
| 2:U3:9:ILE:HG13 | 2:U3:139:ASN:HB3 | 1.94 | 0.49 |
| 2:U3:66:ILE:HG13 | 2:U3:66:ILE:O | 2.12 | 0.49 |
| 2:U3:305:CYS:HB3 | 2:U3:387:ILE:HD11 | 1.93 | 0.49 |
| 1:U4:114:ASP:N | 1:U4:114:ASP:OD2 | 2.44 | 0.49 |
| 2:U5:177:VAL:HG13 | 1:U6:327:ASP:HB3 | 1.95 | 0.49 |
| 1:U6:285:THR:HG23 | 1:U6:287:PRO:HD2 | 1.95 | 0.49 |
| 1:V4:178:THR:HG23 | 1:V4:181:GLU:HG3 | 1.94 | 0.49 |
| 1:V6:27:GLU:OE2 | 1:V6:234:SER:OG | 2.25 | 0.49 |
| 1:V6:322:SER:OG | 1:V6:325:GLU:HB2 | 2.11 | 0.49 |
| 1:V6:327:ASP:O | 1:V6:331:LEU:HG | 2.13 | 0.49 |
| 2:V7:5:ILE:HD11 | 2:V7:135:PHE:CE1 | 2.48 | 0.49 |
| 2:W1:199:ASP:OD1 | 2:W1:256:GLN:HG2 | 2.13 | 0.49 |
| 1:W2:5:VAL:HG12 | 1:W2:133:PHE:HD1 | 1.77 | 0.49 |
| 1:W4:107:THR:OG1 | 1:W4:401:GLU:OE2 | 2.18 | 0.49 |
| 2:W7:417:GLU:HA | 2:W7:420:GLU:HG2 | 1.94 | 0.49 |
| 2:W9:7:ILE:HG22 | 2:W9:137:VAL:CG1 | 2.28 | 0.49 |
| 1:X0:209:ASP:OD1 | 1:X0:213:ARG:HD3 | 2.13 | 0.49 |
| 2:X5:108:TYR:O | 2:X5:112:LYS:NZ | 2.32 | 0.49 |
| 1:X8:203:ASP:OD2 | 1:X8:302:ALA:N | 2.45 | 0.49 |
| 2:X9:392:ASP:OD1 | 2:X9:422:ARG:NE | 2.46 | 0.49 |
| 1:Y4:39:ASP:OD1 | 1:Y4:39:ASP:N | 2.45 | 0.49 |
| 1:Z2:386:THR:O | 1:Z2:390:ARG:HG3 | 2.12 | 0.49 |
| 2:Z3:21:TRP:CZ3 | 2:Z3:63:PRO:HB3 | 2.48 | 0.49 |
| 2:Z5:69:ASP:OD1 | 2:Z5:70:LEU:N | 2.45 | 0.49 |
| 2:Z7:174:SER:OG | 2:Z7:207:GLU:OE1 | 2.29 | 0.49 |
| 1:0E:246:LEU:O | 1:0E:352:SER:OG | 2.23 | 0.49 |
| 2:0H:88:HIS:HB3 | 2:0X:283:HIS:CE1 | 2.46 | 0.49 |
| 1:0I:405:GLU:HA | 1:0I:408:PHE:HD2 | 1.77 | 0.49 |
| 1:0O:259:PRO:HG3 | 1:0O:311:LEU:HD21 | 1.94 | 0.49 |
| 1:0O:337:ASN:HB3 | 1:0O:340:TYR:HD2 | 1.77 | 0.49 |
| 2:0P:344:VAL:O | 2:0P:344:VAL:HG12 | 2.13 | 0.49 |
| 1:0S:215:LEU:HB3 | 1:0S:217:LEU:HG | 1.93 | 0.49 |
| 2:0V:4:VAL:HG23 | 2:0V:134:GLY:O | 2.13 | 0.49 |
| 2:0V:435:VAL:CG1 | 2:0V:435:VAL:O | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0W:70:PRO:N | 1:0W:92:PHE:HZ | 2.11 | 0.49 |
| 2:0X:407:TRP:HZ2 | 1:0Y:258:ILE:HB | 1.77 | 0.49 |
| 1:1A:68:LEU:HD11 | 1:1A:147:MET:HE1 | 1.95 | 0.49 |
| 1:1A:173:PRO:HB3 | 1:1A:384:GLN:HE22 | 1.76 | 0.49 |
| 1:1U:235:GLY:HA3 | 1:1U:366:THR:HG21 | 1.93 | 0.49 |
| 2:1X:312:TYR:HD1 | 2:1X:381:SER:HB2 | 1.76 | 0.49 |
| 1:2A:396:HIS:HA | 1:2A:399:THR:HG22 | 1.95 | 0.49 |
| 2:2B:325:PRO:HA | 2:2B:328:VAL:HG22 | 1.94 | 0.49 |
| 2:2H:111:GLY:O | 2:2H:115:VAL:HG22 | 2.13 | 0.49 |
| 2:2J:137:VAL:HG11 | 2:2J:154:LEU:HD11 | 1.94 | 0.49 |
| 2:2L:66:ILE:HD12 | 2:2L:121:ARG:HG2 | 1.93 | 0.49 |
| 2:2L:290:GLU:HA | 2:2L:293:ASN:HD22 | 1.76 | 0.49 |
| 2:2P:69:ASP:OD1 | 2:2P:71:GLU:HG2 | 2.11 | 0.49 |
| 2:2V:60:LYS:HE2 | 2:2V:88:HIS:CE1 | 2.47 | 0.49 |
| 2:2X:276:ILE:HD11 | 2:2X:280:LYS:HD3 | 1.93 | 0.49 |
| 2:2Z:10:GLY:HA2 | 2:2Z:145:THR:HG23 | 1.94 | 0.49 |
| 2:3B:294:ALA:O | 2:3B:300:SER:OG | 2.28 | 0.49 |
| 1:3G:406:MET:O | 1:3G:410:GLU:HG2 | 2.13 | 0.49 |
| 2:3H:244:PHE:HB2 | 2:3H:356:ASN:HD21 | 1.76 | 0.49 |
| 1:3I:94:GLN:NE2 | 3:3Z:139:SER:O | 2.44 | 0.49 |
| 2:3P:5:ILE:HD11 | 2:3P:135:PHE:CE1 | 2.48 | 0.49 |
| 2:3P:388:PHE:HB3 | 2:3P:425:LEU:HD21 | 1.95 | 0.49 |
| 2:3R:221:ARG:N | 38:8D:174:SER:O | 2.38 | 0.49 |
| 4:3Y:15:TYR:CE2 | 4:3Y:17:ILE:HB | 2.47 | 0.49 |
| 3:4H:154:TYR:HD2 | 3:4H:158:LEU:HD11 | 1.76 | 0.49 |
| 6:4O:65:LYS:CB | 6:4O:66:ARG:HH21 | 2.25 | 0.49 |
| 6:4O:69:ARG:O | 6:4O:73:GLU:HG2 | 2.12 | 0.49 |
| 6:4O:130:ASP:OD1 | 6:4O:130:ASP:N | 2.43 | 0.49 |
| 7:4U:119:ASP:OD1 | 7:4U:119:ASP:N | 2.42 | 0.49 |
| 9:4Z:356:TRP:O | 9:4Z:360:THR:HG23 | 2.12 | 0.49 |
| 10:5B:215:ALA:O | 10:5B:218:SER:OG | 2.26 | 0.49 |
| 10:5C:156:TYR:O | 10:5C:160:VAL:HG23 | 2.12 | 0.49 |
| 13:5K:75:PHE:HA | 17:5V:126:GLN:NE2 | 2.27 | 0.49 |
| 14:5L:105:LYS:O | 14:5L:123:GLY:N | 2.45 | 0.49 |
| 14:5L:494:ILE:HD13 | 14:5L:494:ILE:N | 2.28 | 0.49 |
| 14:5M:105:LYS:O | 14:5M:123:GLY:N | 2.45 | 0.49 |
| 14:5N:105:LYS:O | 14:5N:123:GLY:N | 2.45 | 0.49 |
| 15:5O:376:LEU:N | 15:5O:377:PRO:CD | 2.75 | 0.49 |
| 22:6K:138:ASP:HA | 22:6K:141:LYS:HE2 | 1.93 | 0.49 |
| 22:6M:108:ARG:CD | 24:6X:285:MET:SD | 2.93 | 0.49 |
| 24:6T:123:TYR:CE2 | 24:6T:163:PRO:HG3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:185:ASP:OD1 | 24:6U:186:SER:N | 2.44 | 0.49 |
| 24:6X:123:TYR:HE2 | 24:6X:163:PRO:HG3 | 1.77 | 0.49 |
| 24:6X:505:LYS:HB3 | 24:6X:506:PRO:HD2 | 1.94 | 0.49 |
| 24:6Y:117:ARG:NH1 | 24:6Y:134:GLU:OE2 | 2.44 | 0.49 |
| 24:6Y:505:LYS:N | 24:6Y:510:GLU:O | 2.44 | 0.49 |
| 24:6Y:558:LEU:HD21 | 24:6Y:612:LEU:HD11 | 1.93 | 0.49 |
| 24:6Z:456:ASP:N | 24:6Z:456:ASP:OD1 | 2.45 | 0.49 |
| 29:7I:254:MET:HE1 | 30:7K:341:ARG:CD | 2.40 | 0.49 |
| 30:7K:93:ASN:ND2 | 30:7K:96:GLU:OE1 | 2.45 | 0.49 |
| 38:8B:159:TYR:CD2 | 38:8B:159:TYR:C | 2.85 | 0.49 |
| 38:8D:117:TRP:O | 38:8D:121:LEU:HG | 2.13 | 0.49 |
| 2:A2:223:THR:HG22 | 26:7F:78:ALA:HB2 | 1.89 | 0.49 |
| 2:B0:279:GLU:CD | 18:5Y:43:ASN:HD21 | 2.15 | 0.49 |
| 1:B8:362:LYS:CE | 18:6B:24:ARG:HD3 | 2.41 | 0.49 |
| 2:G3:116:ASP:N | 2:G3:116:ASP:OD1 | 2.44 | 0.49 |
| 2:G5:66:ILE:HG13 | 2:G5:91:GLN:O | 2.13 | 0.49 |
| 1:G6:219:THR:O | 1:G6:219:THR:HG23 | 2.12 | 0.49 |
| 2:H1:305:CYS:HB3 | 2:H1:387:ILE:HD11 | 1.95 | 0.49 |
| 1:H2:387:ALA:HA | 1:H2:390:ARG:HE | 1.78 | 0.49 |
| 2:H5:236:SER:O | 2:H5:243:ARG:NH2 | 2.46 | 0.49 |
| 2:H7:5:ILE:HG22 | 2:H7:64:ARG:HB3 | 1.93 | 0.49 |
| 2:I1:287:SER:OG | 2:I1:288:VAL:N | 2.46 | 0.49 |
| 2:I3:145:THR:OG1 | 41:I4:501:GTP:O1B | 2.28 | 0.49 |
| 2:I3:333:ALA:O | 2:I3:337:THR:HG23 | 2.13 | 0.49 |
| 2:J1:398:MET:HG3 | 1:J2:346:PRO:HD2 | 1.94 | 0.49 |
| 2:J3:320:ARG:NH2 | 2:J3:359:PRO:O | 2.46 | 0.49 |
| 1:J6:272:PRO:HB2 | 1:J6:282:ARG:HH12 | 1.76 | 0.49 |
| 2:J9:69:ASP:OD2 | 2:J9:71:GLU:N | 2.45 | 0.49 |
| 2:J9:76:ASP:HA | 2:J9:79:ARG:HB2 | 1.95 | 0.49 |
| 1:K0:292:GLN:O | 1:K0:298:ASN:ND2 | 2.40 | 0.49 |
| 2:K7:342:GLN:H | 35:7T:169:MET:HE2 | 1.77 | 0.49 |
| 2:K7:417:GLU:HA | 2:K7:420:GLU:HG2 | 1.95 | 0.49 |
| 1:K8:52:ASN:HA | 30:7K:186:HIS:HE1 | 1.77 | 0.49 |
| 2:K9:392:ASP:OD2 | 2:K9:422:ARG:NH1 | 2.45 | 0.49 |
| 2:L1:7:ILE:HG12 | 2:L1:137:VAL:HG12 | 1.95 | 0.49 |
| 2:L3:76:ASP:HA | 2:L3:79:ARG:HB2 | 1.93 | 0.49 |
| 1:L6:101:TRP:HD1 | 1:L6:145:SER:HG | 1.59 | 0.49 |
| 2:L9:406:HIS:HA | 2:L9:409:VAL:HG22 | 1.94 | 0.49 |
| 1:M0:125:GLU:OE2 | 1:M0:159:TYR:OH | 2.28 | 0.49 |
| 2:M5:111:GLY:HA2 | 2:M5:114:ILE:HG22 | 1.92 | 0.49 |
| 2:N5:287:SER:OG | 2:N5:288:VAL:N | 2.44 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N6:77:ARG:HH22 | 27:7G:166:CYS:HB3 | 1.77 | 0.49 |
| 2:O7:5:ILE:HD11 | 2:O7:135:PHE:CE1 | 2.48 | 0.49 |
| 2:O7:267:PHE:HB2 | 2:O7:384:ILE:CD1 | 2.41 | 0.49 |
| 2:P3:286:LEU:HD22 | 2:P3:371:VAL:HG13 | 1.93 | 0.49 |
| 2:P3:338:LYS:NZ | 2:P3:339:ARG:H | 2.11 | 0.49 |
| 2:P9:71:GLU:HB3 | 2:P9:98:ASP:OD1 | 2.12 | 0.49 |
| 2:Q1:379:SER:OG | 2:Q1:380:ASN:N | 2.45 | 0.49 |
| 1:Q8:22:GLU:HG2 | 1:Q8:81:TYR:CD2 | 2.47 | 0.49 |
| 1:Q8:220:PRO:HD2 | 2:Q9:326:LYS:CD | 2.42 | 0.49 |
| 1:Q8:291:GLN:HG3 | 1:Q8:292:GLN:N | 2.27 | 0.49 |
| 1:Q8:311:LEU:HD12 | 1:Q8:342:VAL:HG21 | 1.93 | 0.49 |
| 2:R7:175:PRO:HB3 | 2:R7:390:ARG:NE | 2.27 | 0.49 |
| 2:R7:405:VAL:CG1 | 17:5U:112:VAL:HG11 | 2.43 | 0.49 |
| 1:S4:11:GLN:HA | 1:S4:72:THR:HG21 | 1.95 | 0.49 |
| 2:S7:105:ARG:CA | 2:S7:411:GLU:HG2 | 2.42 | 0.49 |
| 2:S9:70:LEU:HD12 | 2:S9:99:ALA:HB2 | 1.94 | 0.49 |
| 1:T0:113:ILE:HD11 | 1:T0:151:LEU:HD13 | 1.95 | 0.49 |
| 1:T4:42:LEU:HD23 | 21:6H:94:THR:OG1 | 2.11 | 0.49 |
| 2:U1:98:ASP:OD1 | 2:U1:99:ALA:N | 2.46 | 0.49 |
| 1:U8:5:VAL:HG12 | 1:U8:133:PHE:CD1 | 2.47 | 0.49 |
| 2:U9:137:VAL:HG22 | 2:U9:168:GLY:HA2 | 1.94 | 0.49 |
| 2:V1:176:GLN:HB2 | 2:V1:207:GLU:OE2 | 2.13 | 0.49 |
| 1:V4:3:GLU:HB2 | 1:V4:130:LEU:HA | 1.93 | 0.49 |
| 1:V8:5:VAL:HG12 | 1:V8:133:PHE:CD1 | 2.48 | 0.49 |
| 2:W7:60:LYS:NZ | 2:Y3:283:HIS:ND1 | 2.49 | 0.49 |
| 2:W7:88:HIS:HB3 | 2:W7:91:GLN:CG | 2.43 | 0.49 |
| 2:W7:177:VAL:N | 2:W7:207:GLU:OE2 | 2.32 | 0.49 |
| 2:W7:224:TYR:H | 1:W8:245:GLN:HE22 | 1.60 | 0.49 |
| 2:W7:258:ASN:HB2 | 2:W7:259:LEU:HD12 | 1.93 | 0.49 |
| 2:W9:399:TYR:OH | 2:W9:415:GLU:OE2 | 2.30 | 0.49 |
| 1:X4:31:ASP:OD2 | 1:X4:33:THR:OG1 | 2.21 | 0.49 |
| 1:X6:311:LEU:HD11 | 1:X6:372:THR:HG23 | 1.94 | 0.49 |
| 2:X7:206:ASN:OD1 | 41:X7:501:GTP:N2 | 2.45 | 0.49 |
| 1:X8:330:MET:N | 1:X8:330:MET:SD | 2.86 | 0.49 |
| 2:X9:52:PHE:HZ | 2:X9:239:THR:HG21 | 1.77 | 0.49 |
| 1:Y0:49:VAL:O | 1:Y0:62:ARG:NH1 | 2.45 | 0.49 |
| 1:Y2:67:ASP:N | 1:Y2:67:ASP:OD1 | 2.43 | 0.49 |
| 2:Y3:195:LEU:HD21 | 2:Y3:428:LEU:HD12 | 1.95 | 0.49 |
| 2:Y5:90:GLU:HB3 | 2:Y5:121:ARG:HH12 | 1.76 | 0.49 |
| 1:Y6:203:ASP:HB2 | 1:Y6:205:GLU:OE1 | 2.12 | 0.49 |
| 1:Z0:198:GLU:HG3 | 1:Z0:266:PHE:HE2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z1:33:ASP:OD2 | 2:Z1:35:GLN:NE2 | 2.46 | 0.49 |
| 2:Z1:276:ILE:HG23 | 2:Z1:280:LYS:HB3 | 1.94 | 0.49 |
| 1:Z2:388:MET:HG3 | 1:Z2:393:ALA:HB3 | 1.94 | 0.49 |
| 1:Z4:167:PHE:HD1 | 1:Z4:200:MET:HB2 | 1.77 | 0.49 |
| 2:Z5:232:ALA:HA | 2:Z5:235:ILE:HG22 | 1.95 | 0.49 |
| 2:Z7:275:ILE:HD12 | 2:Z7:368:LEU:HD21 | 1.93 | 0.49 |
| 1:0E:55:THR:H | 1:0E:58:ARG:HB3 | 1.78 | 0.49 |
| 2:0F:111:GLY:HA2 | 2:0F:114:ILE:HG22 | 1.94 | 0.49 |
| 1:0K:206:ALA:O | 1:0K:210:ILE:HG13 | 2.13 | 0.49 |
| 2:0L:195:LEU:HD13 | 2:0L:428:LEU:HD21 | 1.95 | 0.49 |
| 2:0L:278:ALA:HA | 2:0L:369:ALA:HB2 | 1.95 | 0.49 |
| 2:0N:429:GLU:O | 2:0N:433:GLU:HG2 | 2.13 | 0.49 |
| 1:0O:113:ILE:HD11 | 1:0O:151:LEU:HA | 1.93 | 0.49 |
| 2:0R:145:THR:OG1 | 41:0S:501:GTP:O1B | 2.30 | 0.49 |
| 1:0S:116:VAL:HA | 1:0S:119:VAL:HG12 | 1.93 | 0.49 |
| 2:0V:287:SER:N | 2:0V:290:GLU:OE2 | 2.46 | 0.49 |
| 1:0W:210:ILE:O | 1:0W:214:THR:OG1 | 2.30 | 0.49 |
| 1:1C:318:ARG:NE | 1:1C:356:ILE:O | 2.43 | 0.49 |
| 1:1C:395:LEU:HG | 1:1C:399:THR:OG1 | 2.13 | 0.49 |
| 2:1D:24:TYR:O | 2:1D:27:GLU:HG2 | 2.12 | 0.49 |
| 2:1F:26:LEU:HD23 | 2:1F:363:VAL:HG12 | 1.94 | 0.49 |
| 2:1F:69:ASP:OD2 | 2:1F:70:LEU:N | 2.45 | 0.49 |
| 1:1G:388:MET:CA | 1:1G:388:MET:CE | 2.85 | 0.49 |
| 1:1K:193:VAL:HG12 | 1:1K:265:PHE:CZ | 2.47 | 0.49 |
| 1:1M:114:ASP:OD1 | 1:1M:114:ASP:N | 2.46 | 0.49 |
| 1:1S:167:PHE:CE2 | 1:1S:233:MET:HG2 | 2.46 | 0.49 |
| 1:1S:317:PHE:HB3 | 1:1S:321:MET:SD | 2.52 | 0.49 |
| 2:1T:189:LEU:HD11 | 2:1T:418:PHE:HE1 | 1.76 | 0.49 |
| 2:1X:277:SER:OG | 2:1X:278:ALA:N | 2.45 | 0.49 |
| 1:2E:2:ARG:HE | 1:2E:240:LEU:HD22 | 1.77 | 0.49 |
| 1:2G:204:ASN:HD21 | 39:2G:502:GDP:HN22 | 1.60 | 0.49 |
| 2:2N:22:GLU:O | 2:2N:26:LEU:HG | 2.11 | 0.49 |
| 2:2N:227:LEU:O | 2:2N:231:ILE:HG12 | 2.13 | 0.49 |
| 1:2U:273:LEU:H | 1:2U:292:GLN:NE2 | 2.09 | 0.49 |
| 2:2V:145:THR:OG1 | 41:2W:501:GTP:O1B | 2.30 | 0.49 |
| 1:3C:5:VAL:HG12 | 1:3C:62:ARG:HD3 | 1.94 | 0.49 |
| 2:3F:221:ARG:HD2 | 1:3G:325:GLU:OE1 | 2.12 | 0.49 |
| 1:3I:114:ASP:N | 1:3I:114:ASP:OD1 | 2.45 | 0.49 |
| 2:3L:72:PRO:HG3 | 1:3M:1:MET:HG3 | 1.93 | 0.49 |
| 1:3M:177:ASP:O | 2:3N:352:LYS:HA | 2.12 | 0.49 |
| 1:3M:391:ARG:NH1 | 2:3N:346:TRP:CE3 | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3N:394:LYS:HB2 | 1:3O:346:PRO:HG3 | 1.95 | 0.49 |
| 2:3R:42:ILE:HG13 | 2:3R:43:GLY:N | 2.28 | 0.49 |
| 1:3S:216:LYS:HB2 | 1:3S:275:SER:HG | 1.77 | 0.49 |
| 4:4A:15:TYR:CE2 | 4:4A:17:ILE:HB | 2.47 | 0.49 |
| 4:4C:14:LEU:HD23 | 4:4C:162:ILE:HD11 | 1.94 | 0.49 |
| 4:4E:14:LEU:HD23 | 4:4E:162:ILE:HD11 | 1.94 | 0.49 |
| 4:4E:15:TYR:CE2 | 4:4E:17:ILE:HB | 2.47 | 0.49 |
| 6:4O:186:GLU:O | 6:4O:190:LYS:HG2 | 2.11 | 0.49 |
| 6:4P:196:VAL:O | 6:4P:200:MET:HG2 | 2.12 | 0.49 |
| 7:4T:261:ASP:OD2 | 7:4T:262:HIS:N | 2.45 | 0.49 |
| 9:4Z:348:GLU:HB3 | 9:4Z:352:TYR:CZ | 2.46 | 0.49 |
| 10:5A:297:ALA:O | 10:5A:300:ILE:HG12 | 2.13 | 0.49 |
| 11:5E:75:LEU:O | 11:5E:79:GLN:HG3 | 2.13 | 0.49 |
| 12:5F:383:ARG:HH22 | 12:7B:32:GLN:HG2 | 1.77 | 0.49 |
| 14:5L:378:ILE:HG22 | 23:6Q:55:VAL:HB | 1.95 | 0.49 |
| 15:5O:196:PHE:O | 15:5O:204:ALA:HB2 | 2.13 | 0.49 |
| 17:5T:179:GLN:O | 17:5T:182:VAL:HG22 | 2.12 | 0.49 |
| 18:5Y:101:LYS:O | 24:6V:178:ASN:ND2 | 2.30 | 0.49 |
| 22:6N:314:CYS:SG | 22:6N:321:LEU:HB2 | 2.53 | 0.49 |
| 12:7B:39:PHE:HB3 | 12:7B:44:ILE:HG21 | 1.93 | 0.49 |
| 27:7G:42:THR:HG23 | 27:7G:45:GLU:H | 1.78 | 0.49 |
| 27:7G:105:LEU:HD11 | 27:7G:116:ASN:ND2 | 2.28 | 0.49 |
| 29:7I:161:GLU:OE2 | 29:7I:165:ARG:HD3 | 2.12 | 0.49 |
| 31:7N:45:GLU:N | 31:7N:45:GLU:OE2 | 2.43 | 0.49 |
| 38:8B:172:GLY:O | 38:8B:174:SER:N | 2.46 | 0.49 |
| 38:8D:91:GLN:HG3 | 38:8D:92:GLU:H | 1.78 | 0.49 |
| 2:A2:423:GLU:CD | 4:4G:108:TYR:HH | 2.03 | 0.49 |
| 1:B1:39:ASP:OD1 | 18:5Y:20:LYS:HE2 | 2.11 | 0.49 |
| 1:C6:143:THR:N | 39:C6:501:GDP:O1B | 2.45 | 0.49 |
| 1:E4:33:THR:HG23 | 24:6V:403:PRO:HB2 | 1.93 | 0.49 |
| 1:E4:320:ARG:NH2 | 22:6K:31:TYR:OH | 2.45 | 0.49 |
| 2:G1:27:GLU:CD | 2:G1:243:ARG:HH12 | 2.15 | 0.49 |
| 1:H2:35:THR:HG22 | 28:7H:312:LEU:CD2 | 2.41 | 0.49 |
| 1:H2:337:ASN:HB3 | 1:H2:340:TYR:HD2 | 1.77 | 0.49 |
| 2:H3:205:ASP:OD1 | 2:H3:303:VAL:HG13 | 2.13 | 0.49 |
| 1:H6:377:MET:O | 1:H6:380:ARG:HG2 | 2.13 | 0.49 |
| 2:H7:71:GLU:HB2 | 2:H7:98:ASP:OD1 | 2.13 | 0.49 |
| 2:H7:289:ALA:O | 2:H7:292:THR:OG1 | 2.28 | 0.49 |
| 2:H7:399:TYR:OH | 2:H7:415:GLU:OE1 | 2.15 | 0.49 |
| 2:I5:88:HIS:ND1 | 2:K1:283:HIS:O | 2.46 | 0.49 |
| 2:I7:288:VAL:O | 2:I7:292:THR:HG23 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I9:8:HIS:CD2 | 2:I9:138:PHE:HD2 | 2.30 | 0.49 |
| 1:J4:22:GLU:HG3 | 1:J4:81:TYR:CD1 | 2.47 | 0.49 |
| 2:J7:205:ASP:OD2 | 2:J7:206:ASN:N | 2.46 | 0.49 |
| 2:J7:417:GLU:HA | 2:J7:420:GLU:HG2 | 1.95 | 0.49 |
| 2:K1:405:VAL:O | 2:K1:409:VAL:HG23 | 2.13 | 0.49 |
| 2:K5:352:LYS:NZ | 2:K5:353:CYS:O | 2.44 | 0.49 |
| 2:L1:201:ALA:O | 2:L1:268:MET:HE2 | 2.12 | 0.49 |
| 2:L5:170:THR:HG21 | 2:L5:194:LEU:HD11 | 1.95 | 0.49 |
| 2:L5:278:ALA:HA | 2:L5:369:ALA:HB2 | 1.95 | 0.49 |
| 1:M2:49:VAL:HG11 | 1:M2:241:ARG:HG2 | 1.94 | 0.49 |
| 2:M5:305:CYS:HB3 | 2:M5:387:ILE:HD11 | 1.94 | 0.49 |
| 1:N2:360:GLY:O | 30:7L:304:GLN:NE2 | 2.46 | 0.49 |
| 2:N7:9:ILE:HD13 | 2:N7:150:GLY:HA2 | 1.94 | 0.49 |
| 2:N7:90:GLU:N | 2:N7:90:GLU:OE2 | 2.45 | 0.49 |
| 1:O0:373:ALA:O | 1:O0:376:GLU:HG3 | 2.13 | 0.49 |
| 1:O2:278:SER:O | 1:O2:279:GLN:C | 2.50 | 0.49 |
| 1:O6:55:THR:OG1 | 20:6F:94:THR:HG21 | 2.12 | 0.49 |
| 2:P9:174:SER:HB3 | 2:P9:177:VAL:O | 2.12 | 0.49 |
| 2:Q3:56:THR:HA | 2:R9:285:GLN:HB3 | 1.94 | 0.49 |
| 2:Q3:209:ILE:HG23 | 2:Q3:230:LEU:HD11 | 1.95 | 0.49 |
| 1:Q6:344:TRP:CE3 | 1:Q6:345:ILE:HG13 | 2.48 | 0.49 |
| 1:Q8:268:VAL:O | 1:Q8:300:MET:N | 2.38 | 0.49 |
| 2:R1:96:LYS:HG2 | 1:R2:1:MET:HE3 | 1.95 | 0.49 |
| 2:R1:264:ARG:NH1 | 2:R1:431:ASP:OD1 | 2.46 | 0.49 |
| 2:R1:313:MET:HB2 | 2:R1:380:ASN:HB3 | 1.94 | 0.49 |
| 2:R1:327:ASP:N | 2:R1:327:ASP:OD1 | 2.45 | 0.49 |
| 1:R4:145:SER:OG | 1:R4:188:SER:OG | 2.29 | 0.49 |
| 2:S1:242:LEU:HD11 | 2:S1:252:ILE:HG12 | 1.95 | 0.49 |
| 1:S2:118:ASP:OD2 | 13:5K:106:TYR:N | 2.46 | 0.49 |
| 1:S4:91:VAL:HG21 | 1:S4:116:VAL:HG22 | 1.94 | 0.49 |
| 1:S6:276:ARG:HB3 | 7:4T:242:MET:HB3 | 1.95 | 0.49 |
| 1:T2:12:CYS:SG | 1:T2:138:SER:HB2 | 2.53 | 0.49 |
| 1:T2:219:THR:O | 1:T2:219:THR:OG1 | 2.31 | 0.49 |
| 2:T3:337:THR:HG23 | 13:5J:21:ASN:ND2 | 2.28 | 0.49 |
| 2:T5:24:TYR:O | 2:T5:27:GLU:HG2 | 2.13 | 0.49 |
| 1:T6:50:TYR:CE2 | 1:T6:241:ARG:HD3 | 2.48 | 0.49 |
| 2:T7:254:GLU:HG2 | 2:T7:352:LYS:HE2 | 1.93 | 0.49 |
| 1:U4:49:VAL:HG11 | 1:U4:241:ARG:HG2 | 1.95 | 0.49 |
| 2:U7:101:ASN:ND2 | 2:U7:143:GLY:HA2 | 2.27 | 0.49 |
| 2:V1:166:LYS:N | 2:V1:199:ASP:OD2 | 2.39 | 0.49 |
| 2:V3:187:SER:O | 2:V3:191:THR:HG23 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V3:200:VAL:HG13 | 2:V3:268:MET:CE | 2.43 | 0.49 |
| 2:V3:292:THR:HG1 | 2:V3:319:TYR:HH | 1.59 | 0.49 |
| 2:V9:109:THR:OG1 | 2:V9:411:GLU:OE2 | 2.20 | 0.49 |
| 2:V9:306:ASP:HB3 | 2:V9:309:HIS:HD2 | 1.78 | 0.49 |
| 2:V9:399:TYR:O | 2:V9:402:ARG:NH1 | 2.45 | 0.49 |
| 1:W0:220:PRO:HD2 | 2:W1:326:LYS:CD | 2.42 | 0.49 |
| 1:W2:167:PHE:CZ | 1:W2:233:MET:HG2 | 2.48 | 0.49 |
| 1:W6:67:ASP:N | 1:W6:67:ASP:OD1 | 2.45 | 0.49 |
| 1:W8:5:VAL:HG23 | 1:W8:62:ARG:HG2 | 1.94 | 0.49 |
| 1:X0:58:ARG:HG2 | 1:Y6:280:GLN:HE22 | 1.77 | 0.49 |
| 1:X4:50:TYR:OH | 1:X4:237:THR:OG1 | 2.20 | 0.49 |
| 1:X6:324:LYS:NZ | 1:X6:325:GLU:OE2 | 2.41 | 0.49 |
| 2:X7:76:ASP:HA | 2:X7:79:ARG:HB2 | 1.95 | 0.49 |
| 1:Y0:58:ARG:NH1 | 1:Y0:83:GLN:O | 2.46 | 0.49 |
| 1:Z2:54:ALA:HB3 | 1:Z2:58:ARG:HB3 | 1.94 | 0.49 |
| 2:Z3:313:MET:HE2 | 2:Z3:380:ASN:HD22 | 1.78 | 0.49 |
| 1:Z6:165:LEU:HD11 | 1:Z6:200:MET:HG2 | 1.95 | 0.49 |
| 2:Z7:33:ASP:O | 2:Z7:60:LYS:NZ | 2.45 | 0.49 |
| 2:Z9:167:LEU:HD13 | 2:Z9:200:VAL:HB | 1.93 | 0.49 |
| 1:0A:249:ASP:O | 1:0A:253:LEU:HG | 2.13 | 0.49 |
| 2:0F:381:SER:OG | 2:0F:382:THR:N | 2.44 | 0.49 |
| 2:0H:211:ASP:OD1 | 2:0H:214:ARG:NH2 | 2.40 | 0.49 |
| 1:0I:391:ARG:HD3 | 2:0J:346:TRP:CE2 | 2.47 | 0.49 |
| 1:0M:12:CYS:HB2 | 39:0M:502:GDP:C8 | 2.48 | 0.49 |
| 2:0R:288:VAL:HA | 2:0R:291:ILE:HD11 | 1.94 | 0.49 |
| 1:0S:222:PHE:HA | 1:0S:225:LEU:HD13 | 1.93 | 0.49 |
| 2:0V:277:SER:H | 2:0V:280:LYS:HB2 | 1.78 | 0.49 |
| 1:0W:95:THR:OG1 | 1:0W:108:GLU:OE1 | 2.30 | 0.49 |
| 1:0W:186:THR:HG22 | 1:0W:411:ALA:HB1 | 1.95 | 0.49 |
| 1:0Y:287:PRO:HA | 1:0Y:290:THR:HG22 | 1.95 | 0.49 |
| 2:0Z:223:THR:HG23 | 2:0Z:225:THR:H | 1.77 | 0.49 |
| 2:1B:317:LEU:HB3 | 2:1B:319:TYR:HE1 | 1.77 | 0.49 |
| 1:1C:21:TRP:O | 1:1C:25:SER:OG | 2.22 | 0.49 |
| 2:1D:261:PRO:HB3 | 2:1D:346:TRP:HH2 | 1.78 | 0.49 |
| 2:1D:318:MET:HB2 | 2:1D:376:CYS:HB3 | 1.94 | 0.49 |
| 1:1E:248:ALA:CB | 1:1E:252:LYS:HD3 | 2.43 | 0.49 |
| 2:1L:417:GLU:HA | 2:1L:420:GLU:HG2 | 1.95 | 0.49 |
| 1:1M:3:GLU:HB2 | 1:1M:130:LEU:HA | 1.94 | 0.49 |
| 2:1P:116:ASP:N | 2:1P:116:ASP:OD1 | 2.43 | 0.49 |
| 1:1Q:371:SER:OG | 1:1Q:372:THR:N | 2.46 | 0.49 |
| 2:1T:11:GLN:OE1 | 2:1T:15:GLN:NE2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1U:325:GLU:OE1 | 1:1U:325:GLU:N | 2.40 | 0.49 |
| 2:2D:236:SER:O | 2:2D:243:ARG:NH2 | 2.45 | 0.49 |
| 1:2S:336:LYS:NZ | 38:8A:55:ALA:HB2 | 2.27 | 0.49 |
| 1:2U:194:GLU:N | 1:2U:194:GLU:OE1 | 2.46 | 0.49 |
| 1:2U:317:PHE:HE2 | 1:2U:326:VAL:HG13 | 1.78 | 0.49 |
| 1:2Y:309:ARG:H | 1:2Y:372:THR:HG22 | 1.78 | 0.49 |
| 1:3A:233:MET:O | 1:3A:237:THR:HG22 | 2.12 | 0.49 |
| 2:3D:205:ASP:OD1 | 2:3D:206:ASN:N | 2.46 | 0.49 |
| 1:3I:31:ASP:OD2 | 14:5L:240:MET:HA | 2.12 | 0.49 |
| 2:3P:356:ASN:OD1 | 2:3P:357:TYR:N | 2.46 | 0.49 |
| 1:3S:170:VAL:HB | 1:3S:171:PRO:HD2 | 1.94 | 0.49 |
| 2:3T:420:GLU:HA | 2:3T:423:GLU:HG3 | 1.95 | 0.49 |
| 4:4A:14:LEU:HD23 | 4:4A:162:ILE:HD11 | 1.94 | 0.49 |
| 4:4C:15:TYR:CE2 | 4:4C:17:ILE:HB | 2.47 | 0.49 |
| 7:4S:6:ALA:O | 7:4S:8:VAL:N | 2.46 | 0.49 |
| 7:4U:55:PHE:O | 7:4U:59:THR:HG23 | 2.13 | 0.49 |
| 8:4V:391:GLU:OE2 | 8:4V:395:ARG:HG3 | 2.13 | 0.49 |
| 10:5C:259:GLU:HA | 10:5C:262:ILE:HG12 | 1.94 | 0.49 |
| 10:5C:431:LYS:O | 10:5C:435:LEU:HG | 2.12 | 0.49 |
| 14:5L:219:LEU:HD22 | 14:5L:228:PHE:CE2 | 2.46 | 0.49 |
| 14:5L:540:TYR:CD2 | 14:5L:540:TYR:C | 2.85 | 0.49 |
| 14:5N:156:PHE:CZ | 14:5N:223:LEU:HD22 | 2.47 | 0.49 |
| 15:5O:24:TYR:HE2 | 15:5O:46:PHE:CE2 | 2.31 | 0.49 |
| 20:6F:149:LEU:HD23 | 20:6F:149:LEU:H | 1.78 | 0.49 |
| 22:6M:323:ASP:OD1 | 22:6M:324:LYS:N | 2.45 | 0.49 |
| 24:6T:371:ALA:HB1 | 24:6T:375:THR:OG1 | 2.13 | 0.49 |
| 24:6U:36:VAL:HG22 | 24:6U:45:LEU:HD11 | 1.94 | 0.49 |
| 24:6U:185:ASP:O | 24:6U:188:THR:OG1 | 2.28 | 0.49 |
| 24:6W:365:ASP:OD1 | 24:6W:365:ASP:N | 2.43 | 0.49 |
| 24:6X:518:TYR:CD1 | 24:6X:521:ALA:HB2 | 2.48 | 0.49 |
| 24:6Y:88:TRP:HA | 24:6Y:126:GLU:HG3 | 1.95 | 0.49 |
| 24:6Y:95:VAL:O | 24:6Y:187:PHE:CD2 | 2.66 | 0.49 |
| 38:8C:158:MET:O | 38:8C:162:VAL:HG23 | 2.12 | 0.49 |
| 2:A0:282:TYR:HE1 | 24:6X:88:TRP:CH2 | 2.29 | 0.49 |
| 1:A3:215:LEU:CD1 | 26:7F:136:PHE:CE2 | 2.96 | 0.49 |
| 2:D1:279:GLU:CD | 18:6A:167:SER:HA | 2.32 | 0.49 |
| 1:E4:219:THR:N | 24:6V:312:ASN:OD1 | 2.21 | 0.49 |
| 2:G5:56:THR:HA | 2:I1:285:GLN:HG2 | 1.95 | 0.49 |
| 2:G5:221:ARG:HB3 | 1:G6:322:SER:OG | 2.13 | 0.49 |
| 2:G7:417:GLU:HA | 2:G7:420:GLU:HG2 | 1.93 | 0.49 |
| 2:G9:56:THR:HA | 2:I5:285:GLN:HB2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H1:72:PRO:HD2 | 1:H2:2:ARG:NH1 | 2.28 | 0.49 |
| 1:H8:315:ALA:HB1 | 1:H8:317:PHE:CE1 | 2.47 | 0.49 |
| 2:I1:14:ILE:HD11 | 2:I1:74:VAL:HG13 | 1.94 | 0.49 |
| 2:I9:49:PHE:HB2 | 2:I9:53:PHE:HD2 | 1.78 | 0.49 |
| 1:J2:5:VAL:HB | 1:J2:133:PHE:HD1 | 1.77 | 0.49 |
| 1:J4:375:GLN:HB2 | 1:J4:419:VAL:HG13 | 1.95 | 0.49 |
| 2:J5:101:ASN:HD22 | 2:J5:143:GLY:HA2 | 1.77 | 0.49 |
| 2:J7:196:GLU:OE2 | 2:J7:197:HIS:NE2 | 2.46 | 0.49 |
| 2:J9:90:GLU:HB3 | 2:L5:283:HIS:CE1 | 2.48 | 0.49 |
| 2:K3:9:ILE:HG13 | 2:K3:139:ASN:HB3 | 1.95 | 0.49 |
| 2:K3:417:GLU:HA | 2:K3:420:GLU:HG2 | 1.94 | 0.49 |
| 1:K4:5:VAL:HG12 | 1:K4:62:ARG:HD3 | 1.94 | 0.49 |
| 1:K6:167:PHE:CE2 | 1:K6:233:MET:HG2 | 2.47 | 0.49 |
| 1:L2:285:THR:HG23 | 1:L2:288:GLU:H | 1.78 | 0.49 |
| 1:M6:320:ARG:NH2 | 37:7Y:146:GLU:OE2 | 2.46 | 0.49 |
| 2:N1:90:GLU:O | 2:N1:121:ARG:NH1 | 2.40 | 0.49 |
| 1:N6:145:SER:OG | 1:N6:146:GLY:N | 2.46 | 0.49 |
| 1:N6:153:SER:HA | 1:N6:195:ASN:HD22 | 1.78 | 0.49 |
| 2:O1:250:VAL:HB | 2:O1:254:GLU:HG3 | 1.95 | 0.49 |
| 2:O5:292:THR:HG1 | 2:O5:319:TYR:HH | 1.59 | 0.49 |
| 2:O7:5:ILE:HG22 | 2:O7:64:ARG:HB3 | 1.94 | 0.49 |
| 2:P5:65:CYS:SG | 2:P5:66:ILE:N | 2.85 | 0.49 |
| 2:P5:88:HIS:CG | 2:P5:89:PRO:HD2 | 2.40 | 0.49 |
| 2:P5:90:GLU:HB2 | 2:P5:121:ARG:NH1 | 2.26 | 0.49 |
| 1:P6:23:VAL:HG11 | 1:P6:230:SER:HB3 | 1.95 | 0.49 |
| 2:P7:388:PHE:HB3 | 2:P7:425:LEU:HD21 | 1.94 | 0.49 |
| 1:Q0:128:ASP:N | 1:Q0:128:ASP:OD1 | 2.44 | 0.49 |
| 2:Q1:116:ASP:OD2 | 2:Q1:117:LEU:N | 2.46 | 0.49 |
| 1:Q2:207:LEU:HB3 | 1:Q2:225:LEU:HD22 | 1.93 | 0.49 |
| 1:Q8:228:LEU:O | 1:Q8:232:VAL:HG23 | 2.12 | 0.49 |
| 2:Q9:267:PHE:HB2 | 2:Q9:384:ILE:HD12 | 1.94 | 0.49 |
| 1:R4:220:PRO:HD2 | 2:R5:326:LYS:HD2 | 1.95 | 0.49 |
| 2:R5:9:ILE:HD11 | 2:R5:153:LEU:HD23 | 1.95 | 0.49 |
| 2:R7:336:LYS:O | 2:R7:339:ARG:NH2 | 2.46 | 0.49 |
| 2:R9:417:GLU:HA | 2:R9:420:GLU:HG2 | 1.94 | 0.49 |
| 1:S0:51:PHE:HB3 | 1:S0:59:TYR:HB3 | 1.95 | 0.49 |
| 2:T1:81:GLY:O | 2:T1:84:ARG:NH1 | 2.45 | 0.49 |
| 1:T4:177:ASP:O | 2:T5:352:LYS:HA | 2.12 | 0.49 |
| 1:U2:207:LEU:HB3 | 1:U2:225:LEU:HD22 | 1.93 | 0.49 |
| 1:U4:285:THR:OG1 | 1:U4:287:PRO:HD2 | 2.12 | 0.49 |
| 2:V3:333:ALA:O | 2:V3:337:THR:HG23 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V6:50:TYR:OH | 1:V6:237:THR:HB | 2.12 | 0.49 |
| 1:V6:263:LEU:HD13 | 1:V6:422:TYR:CE1 | 2.47 | 0.49 |
| 1:V8:25:SER:OG | 1:V8:30:ILE:O | 2.30 | 0.49 |
| 1:V8:152:ILE:HD11 | 1:V8:164:MET:HG2 | 1.95 | 0.49 |
| 2:V9:9:ILE:HD11 | 2:V9:153:LEU:HD23 | 1.95 | 0.49 |
| 1:W4:387:ALA:HA | 1:W4:390:ARG:HH21 | 1.77 | 0.49 |
| 2:W5:147:SER:OG | 2:W5:190:SER:HB2 | 2.12 | 0.49 |
| 1:W6:167:PHE:CZ | 1:W6:233:MET:HG2 | 2.47 | 0.49 |
| 1:W8:309:ARG:H | 1:W8:372:THR:HG22 | 1.78 | 0.49 |
| 1:X2:224:ASP:OD1 | 1:X2:225:LEU:N | 2.46 | 0.49 |
| 1:X4:8:GLN:HG2 | 1:X4:17:GLY:HA3 | 1.95 | 0.49 |
| 1:X4:207:LEU:HB3 | 1:X4:225:LEU:HD22 | 1.95 | 0.49 |
| 1:X4:273:LEU:H | 1:X4:292:GLN:NE2 | 2.11 | 0.49 |
| 2:X5:6:SER:HB2 | 2:X5:136:LEU:HD21 | 1.95 | 0.49 |
| 2:X7:12:ALA:HB2 | 41:X7:501:GTP:C8 | 2.48 | 0.49 |
| 1:Y4:27:GLU:OE2 | 1:Y4:318:ARG:NH2 | 2.41 | 0.49 |
| 1:Y8:68:LEU:HB3 | 1:Y8:96:GLY:HA2 | 1.93 | 0.49 |
| 1:Y8:260:PHE:CD2 | 1:Y8:263:LEU:HD23 | 2.47 | 0.49 |
| 2:Z1:338:LYS:HZ2 | 2:Z1:340:THR:H | 1.60 | 0.49 |
| 1:Z2:5:VAL:HG13 | 1:Z2:123:GLU:OE2 | 2.13 | 0.49 |
| 1:Z2:414:ASN:O | 1:Z2:418:LEU:HB2 | 2.13 | 0.49 |
| 1:Z4:130:LEU:HG | 1:Z4:132:GLY:N | 2.27 | 0.49 |
| 1:0A:8:GLN:HG2 | 1:0A:17:GLY:HA3 | 1.93 | 0.49 |
| 1:0C:173:PRO:HB3 | 1:0C:384:GLN:HE22 | 1.78 | 0.49 |
| 1:0K:265:PHE:HB2 | 1:0K:374:ILE:HD13 | 1.95 | 0.49 |
| 1:0K:337:ASN:HB3 | 1:0K:340:TYR:HD2 | 1.78 | 0.49 |
| 1:0M:350:LYS:HZ3 | 1:0M:352:SER:HB3 | 1.78 | 0.49 |
| 2:0N:205:ASP:OD1 | 2:0N:207:GLU:N | 2.46 | 0.49 |
| 1:0Q:3:GLU:O | 1:0Q:131:GLN:N | 2.41 | 0.49 |
| 2:0R:76:ASP:HA | 2:0R:79:ARG:HD2 | 1.94 | 0.49 |
| 2:0R:305:CYS:HB3 | 2:0R:387:ILE:HD11 | 1.94 | 0.49 |
| 1:0S:314:SER:HA | 1:0S:350:LYS:O | 2.13 | 0.49 |
| 1:0U:268:VAL:HG13 | 1:0U:300:MET:HB2 | 1.95 | 0.49 |
| 2:0X:417:GLU:HA | 2:0X:420:GLU:HG2 | 1.95 | 0.49 |
| 1:1A:392:LYS:HD2 | 1:1A:395:LEU:HD22 | 1.95 | 0.49 |
| 1:1A:418:LEU:HG | 1:1A:422:TYR:HE2 | 1.78 | 0.49 |
| 1:1C:309:ARG:NH1 | 1:1C:341:PHE:O | 2.45 | 0.49 |
| 1:1E:259:PRO:HG3 | 1:1E:311:LEU:HD21 | 1.95 | 0.49 |
| 1:1G:127:CYS:SG | 1:1G:128:ASP:N | 2.86 | 0.49 |
| 2:1H:343:PHE:N | 2:1H:343:PHE:CD2 | 2.81 | 0.49 |
| 1:1K:114:ASP:N | 1:1K:114:ASP:OD1 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1L:203:MET:C | 2:1L:204:LEU:HD12 | 2.33 | 0.49 |
| 1:1M:350:LYS:NZ | 1:1M:351:SER:O | 2.38 | 0.49 |
| 1:1Q:66:MET:SD | 1:1Q:147:MET:HG3 | 2.53 | 0.49 |
| 1:1S:193:VAL:HG23 | 1:1S:194:GLU:OE1 | 2.13 | 0.49 |
| 1:1U:350:LYS:NZ | 1:1U:351:SER:O | 2.45 | 0.49 |
| 2:1X:175:PRO:HB3 | 2:1X:390:ARG:HE | 1.78 | 0.49 |
| 2:2B:213:CYS:HA | 2:2B:217:LEU:HB2 | 1.95 | 0.49 |
| 1:2E:207:LEU:HB3 | 1:2E:225:LEU:HD22 | 1.95 | 0.49 |
| 2:2F:417:GLU:HA | 2:2F:420:GLU:HG2 | 1.95 | 0.49 |
| 2:2J:290:GLU:HA | 2:2J:293:ASN:HD22 | 1.78 | 0.49 |
| 2:2N:65:CYS:SG | 2:2N:66:ILE:N | 2.86 | 0.49 |
| 2:2P:2:ARG:HG3 | 2:2P:242:LEU:HD12 | 1.95 | 0.49 |
| 2:2P:277:SER:OG | 2:2P:278:ALA:N | 2.45 | 0.49 |
| 1:2Q:317:PHE:HE2 | 1:2Q:326:VAL:HG13 | 1.77 | 0.49 |
| 1:2Q:404:ASP:HB3 | 1:2Q:406:MET:SD | 2.53 | 0.49 |
| 2:2R:21:TRP:CZ2 | 2:2R:65:CYS:HB2 | 2.47 | 0.49 |
| 2:2R:251:ASP:N | 2:2R:254:GLU:OE2 | 2.45 | 0.49 |
| 1:3A:68:LEU:HD23 | 1:3A:93:GLY:HA3 | 1.95 | 0.49 |
| 2:3F:333:ALA:O | 2:3F:337:THR:HG23 | 2.13 | 0.49 |
| 2:3L:27:GLU:OE1 | 2:3L:243:ARG:NH1 | 2.46 | 0.49 |
| 1:3M:391:ARG:HH11 | 2:3N:346:TRP:CB | 2.25 | 0.49 |
| 1:3O:90:PHE:CD2 | 3:4F:19:LEU:HD22 | 2.48 | 0.49 |
| 1:3S:362:LYS:HE2 | 38:8D:166:GLU:HB3 | 1.95 | 0.49 |
| 10:5B:265:LYS:O | 10:5B:269:GLU:HG2 | 2.12 | 0.49 |
| 10:5D:132:THR:HG1 | 14:5N:81:PHE:HE1 | 1.58 | 0.49 |
| 12:5F:290:PHE:HE2 | 12:5F:305:GLN:HG3 | 1.78 | 0.49 |
| 14:5L:28:ARG:O | 14:5L:28:ARG:HG3 | 2.13 | 0.49 |
| 22:6J:16:LYS:HD3 | 22:6J:20:TYR:CE2 | 2.47 | 0.49 |
| 22:6K:145:SER:OG | 22:6K:148:ASN:ND2 | 2.46 | 0.49 |
| 22:6L:313:GLY:O | 22:6L:317:VAL:HG23 | 2.13 | 0.49 |
| 22:6N:266:LYS:O | 22:6N:269:GLU:HG3 | 2.12 | 0.49 |
| 22:6P:45:PRO:HB3 | 22:6P:51:ILE:HG23 | 1.93 | 0.49 |
| 24:6T:45:LEU:H | 24:6T:45:LEU:HD23 | 1.78 | 0.49 |
| 24:6U:536:ASP:HB3 | 24:6U:539:THR:HG23 | 1.95 | 0.49 |
| 24:6W:488:ARG:NH1 | 24:6W:488:ARG:CB | 2.73 | 0.49 |
| 24:6X:22:LEU:H | 24:6X:22:LEU:HD23 | 1.77 | 0.49 |
| 24:6Y:469:PHE:HB3 | 24:6Y:484:GLU:HB3 | 1.95 | 0.49 |
| 24:6Y:499:GLU:OE1 | 24:6Y:499:GLU:N | 2.42 | 0.49 |
| 12:7B:46:ASP:HB3 | 12:7B:48:PRO:HD2 | 1.94 | 0.49 |
| 26:7E:59:ARG:HG2 | 26:7E:59:ARG:NH1 | 2.28 | 0.49 |
| 34:7R:208:ARG:NH1 | 36:7V:90:GLU:OE2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8B:165:LYS:H | 38:8B:165:LYS:CD | 1.95 | 0.49 |
| 38:8C:8:GLU:O | 38:8C:12:LEU:HG | 2.13 | 0.49 |
| 2:A2:218:ASP:OD1 | 26:7F:81:LYS:HB2 | 2.13 | 0.49 |
| 2:F3:12:ALA:HB2 | 41:F3:501:GTP:C8 | 2.47 | 0.49 |
| 2:G1:298:PRO:HA | 2:G1:301:MET:HG3 | 1.95 | 0.49 |
| 1:G2:67:ASP:N | 1:G2:67:ASP:OD1 | 2.44 | 0.49 |
| 2:G5:379:SER:OG | 2:G5:380:ASN:N | 2.45 | 0.49 |
| 1:G6:3:GLU:CD | 1:G6:62:ARG:HH12 | 2.16 | 0.49 |
| 1:G6:233:MET:O | 1:G6:237:THR:HG22 | 2.13 | 0.49 |
| 1:G6:345:ILE:O | 1:G6:348:ASN:ND2 | 2.45 | 0.49 |
| 1:G8:260:PHE:HB2 | 1:G8:263:LEU:HD23 | 1.94 | 0.49 |
| 2:G9:387:ILE:O | 2:G9:391:LEU:HG | 2.13 | 0.49 |
| 2:H3:85:GLN:O | 2:I9:283:HIS:CE1 | 2.66 | 0.49 |
| 2:H3:278:ALA:CA | 2:H3:369:ALA:HB2 | 2.39 | 0.49 |
| 2:H5:119:LEU:HA | 2:H5:122:ILE:HG22 | 1.94 | 0.49 |
| 1:H6:117:LEU:HA | 1:H6:120:VAL:HG12 | 1.94 | 0.49 |
| 1:H6:203:ASP:OD1 | 1:H6:204:ASN:N | 2.46 | 0.49 |
| 1:H6:337:ASN:HB3 | 1:H6:340:TYR:HD2 | 1.78 | 0.49 |
| 2:I5:49:PHE:HB2 | 2:I5:53:PHE:HD2 | 1.76 | 0.49 |
| 2:J1:223:THR:HG23 | 1:J2:323:THR:HG23 | 1.95 | 0.49 |
| 1:J8:309:ARG:NH1 | 1:J8:339:SER:O | 2.46 | 0.49 |
| 2:L3:12:ALA:HB2 | 41:L4:501:GTP:C8 | 2.48 | 0.49 |
| 2:L3:278:ALA:HA | 2:L3:369:ALA:HB2 | 1.94 | 0.49 |
| 2:L3:311:LYS:HE2 | 2:L3:344:VAL:HA | 1.94 | 0.49 |
| 2:M1:280:LYS:O | 2:M1:283:HIS:HB3 | 2.11 | 0.49 |
| 1:M2:322:SER:HB3 | 1:M2:325:GLU:HB2 | 1.94 | 0.49 |
| 1:M6:80:PRO:CB | 15:5P:69:PHE:CE1 | 2.96 | 0.49 |
| 1:M8:114:ASP:N | 1:M8:114:ASP:OD1 | 2.45 | 0.49 |
| 2:M9:33:ASP:CG | 30:7K:10:ARG:HH21 | 2.15 | 0.49 |
| 2:M9:280:LYS:HZ1 | 29:7J:320:PRO:HB2 | 1.78 | 0.49 |
| 1:N2:273:LEU:H | 1:N2:292:GLN:HE22 | 1.59 | 0.49 |
| 2:N3:292:THR:HG22 | 2:N3:319:TYR:OH | 2.12 | 0.49 |
| 1:N6:113:ILE:HA | 1:N6:116:VAL:HG22 | 1.95 | 0.49 |
| 2:N7:334:THR:HA | 2:N7:337:THR:HG22 | 1.95 | 0.49 |
| 2:O1:21:TRP:CZ2 | 2:O1:65:CYS:HB2 | 2.47 | 0.49 |
| 1:O2:207:LEU:HB3 | 1:O2:225:LEU:HD22 | 1.95 | 0.49 |
| 1:O2:292:GLN:HG2 | 1:O2:298:ASN:HD22 | 1.78 | 0.49 |
| 1:O2:356:ILE:HD12 | 37:7Y:234:HIS:HA | 1.94 | 0.49 |
| 2:O3:394:LYS:HB2 | 1:O4:346:PRO:HG3 | 1.93 | 0.49 |
| 1:O6:125:GLU:OE2 | 1:O6:159:TYR:OH | 2.31 | 0.49 |
| 2:O7:223:THR:OG1 | 1:O8:245:GLN:NE2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:333:ALA:O | 2:P3:337:THR:HG23 | 2.12 | 0.49 |
| 2:P7:53:PHE:HB3 | 2:P7:61:HIS:HB3 | 1.95 | 0.49 |
| 2:P9:56:THR:HA | 2:R5:285:GLN:HB3 | 1.95 | 0.49 |
| 1:Q4:180:VAL:HG23 | 1:Q4:184:ASN:ND2 | 2.28 | 0.49 |
| 2:Q9:408:TYR:HB3 | 2:Q9:413:MET:HE2 | 1.93 | 0.49 |
| 2:R1:223:THR:HG22 | 2:R1:224:TYR:N | 2.27 | 0.49 |
| 2:R1:425:LEU:O | 2:R1:429:GLU:HG2 | 2.12 | 0.49 |
| 1:R2:238:CYS:SG | 1:R2:318:ARG:NE | 2.85 | 0.49 |
| 2:R3:237:SER:HA | 2:R3:320:ARG:HD2 | 1.95 | 0.49 |
| 1:R4:167:PHE:CE2 | 1:R4:233:MET:HG2 | 2.47 | 0.49 |
| 1:R8:210:ILE:O | 1:R8:214:THR:OG1 | 2.28 | 0.49 |
| 1:S0:180:VAL:HG23 | 1:S0:184:ASN:HD21 | 1.78 | 0.49 |
| 1:S2:189:VAL:O | 1:S2:193:VAL:HG13 | 2.13 | 0.49 |
| 2:S5:195:LEU:HD21 | 2:S5:264:ARG:NH2 | 2.28 | 0.49 |
| 1:S8:11:GLN:HE22 | 2:S9:249:ASN:H | 1.61 | 0.49 |
| 1:S8:238:CYS:SG | 1:S8:318:ARG:NE | 2.85 | 0.49 |
| 1:S8:248:ALA:HA | 1:S8:252:LYS:HD2 | 1.95 | 0.49 |
| 1:S8:271:THR:HG21 | 1:S8:293:MET:HG3 | 1.94 | 0.49 |
| 1:T0:14:ASN:HD22 | 1:T0:65:LEU:HD22 | 1.78 | 0.49 |
| 2:T1:3:GLU:HB2 | 2:T1:129:CYS:SG | 2.53 | 0.49 |
| 2:T1:66:ILE:O | 2:T1:66:ILE:HG13 | 2.13 | 0.49 |
| 1:U2:41:ASP:N | 1:U2:41:ASP:OD1 | 2.44 | 0.49 |
| 1:U6:53:GLU:N | 1:U6:53:GLU:OE2 | 2.46 | 0.49 |
| 2:U9:222:PRO:HD2 | 1:V0:324:LYS:HE3 | 1.93 | 0.49 |
| 1:V0:272:PRO:HD2 | 1:V0:361:LEU:HD21 | 1.95 | 0.49 |
| 1:V2:10:GLY:O | 1:V2:14:ASN:HB2 | 2.13 | 0.49 |
| 1:V6:237:THR:OG1 | 1:V6:241:ARG:NH2 | 2.37 | 0.49 |
| 2:W1:89:PRO:CB | 2:X7:280:LYS:HZ1 | 2.24 | 0.49 |
| 1:W2:203:ASP:OD2 | 1:W2:302:ALA:N | 2.46 | 0.49 |
| 1:W4:173:PRO:O | 2:W5:336:LYS:NZ | 2.46 | 0.49 |
| 2:X3:201:ALA:O | 2:X3:268:MET:HE2 | 2.13 | 0.49 |
| 1:X8:130:LEU:HB2 | 1:X8:162:ARG:HE | 1.77 | 0.49 |
| 2:Y3:12:ALA:HB2 | 41:Y4:501:GTP:C8 | 2.48 | 0.49 |
| 2:Y9:115:VAL:HG23 | 2:Y9:153:LEU:HD22 | 1.93 | 0.49 |
| 2:Z1:12:ALA:O | 2:Z1:16:VAL:HG23 | 2.12 | 0.49 |
| 2:Z1:21:TRP:CZ3 | 2:Z1:63:PRO:HB3 | 2.48 | 0.49 |
| 1:Z2:405:GLU:HA | 1:Z2:408:PHE:HD2 | 1.77 | 0.49 |
| 2:Z3:12:ALA:O | 2:Z3:16:VAL:HG23 | 2.13 | 0.49 |
| 2:Z3:407:TRP:HZ2 | 1:Z4:258:ILE:HB | 1.77 | 0.49 |
| 1:Z8:134:GLN:HE21 | 1:Z8:167:PHE:HE2 | 1.61 | 0.49 |
| 1:Z8:263:LEU:HD13 | 1:Z8:422:TYR:CZ | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0C:67:ASP:N | 1:0C:67:ASP:OD1 | 2.45 | 0.49 |
| 1:0E:20:PHE:O | 1:0E:24:VAL:HG23 | 2.13 | 0.49 |
| 1:0E:237:THR:HG23 | 1:0E:241:ARG:HE | 1.78 | 0.49 |
| 2:0J:30:ILE:HG12 | 2:0J:36:MET:HG2 | 1.95 | 0.49 |
| 1:0O:165:LEU:HD22 | 1:0O:167:PHE:HE1 | 1.77 | 0.49 |
| 1:0Q:382:SER:HB3 | 1:0Q:415:MET:HG2 | 1.95 | 0.49 |
| 2:0R:286:LEU:HD23 | 2:0R:286:LEU:H | 1.78 | 0.49 |
| 1:0U:375:GLN:HB3 | 1:0U:422:TYR:CD2 | 2.47 | 0.49 |
| 2:0X:49:PHE:HB2 | 2:0X:53:PHE:HD2 | 1.77 | 0.49 |
| 2:0Z:176:GLN:HG2 | 2:0Z:177:VAL:N | 2.28 | 0.49 |
| 1:1A:27:GLU:OE1 | 1:1A:241:ARG:NH2 | 2.39 | 0.49 |
| 1:1A:210:ILE:O | 1:1A:214:THR:OG1 | 2.20 | 0.49 |
| 2:1B:66:ILE:O | 2:1B:66:ILE:HG13 | 2.13 | 0.49 |
| 2:1D:5:ILE:HG22 | 2:1D:64:ARG:HB3 | 1.95 | 0.49 |
| 2:1H:57:GLY:H | 2:1X:285:GLN:HB2 | 1.78 | 0.49 |
| 2:1H:182:VAL:HG23 | 2:1H:186:ASN:HD21 | 1.77 | 0.49 |
| 2:1N:317:LEU:HB3 | 2:1N:319:TYR:CE1 | 2.48 | 0.49 |
| 2:1P:285:GLN:HG2 | 2:1P:286:LEU:H | 1.78 | 0.49 |
| 1:1Q:388:MET:HE2 | 2:1R:348:PRO:HD2 | 1.93 | 0.49 |
| 2:1T:176:GLN:HG2 | 2:1T:177:VAL:HG13 | 1.95 | 0.49 |
| 2:1V:111:GLY:HA2 | 2:1V:149:LEU:HD13 | 1.94 | 0.49 |
| 1:1W:121:ARG:NH2 | 1:1W:158:GLU:OE2 | 2.43 | 0.49 |
| 2:2F:287:SER:OG | 2:2F:288:VAL:N | 2.44 | 0.49 |
| 2:2H:119:LEU:HA | 2:2H:122:ILE:HG22 | 1.95 | 0.49 |
| 2:2J:27:GLU:OE1 | 2:2J:243:ARG:NH1 | 2.45 | 0.49 |
| 2:2J:56:THR:HA | 2:2Z:285:GLN:HB2 | 1.93 | 0.49 |
| 1:2K:121:ARG:NH2 | 1:2K:158:GLU:OE2 | 2.36 | 0.49 |
| 2:2L:120:ASP:OD2 | 38:8C:24:TYR:HB3 | 2.13 | 0.49 |
| 2:2N:123:ARG:O | 2:2N:127:ASP:N | 2.41 | 0.49 |
| 2:2P:183:GLU:HG3 | 2:2P:184:PRO:HD3 | 1.95 | 0.49 |
| 1:2Q:174:LYS:HE3 | 38:8A:109:THR:HG21 | 1.94 | 0.49 |
| 2:2R:223:THR:HG22 | 2:2R:224:TYR:H | 1.78 | 0.49 |
| 2:2T:319:TYR:HB3 | 2:2T:323:VAL:HG21 | 1.95 | 0.49 |
| 2:2Z:109:THR:OG1 | 2:2Z:411:GLU:OE2 | 2.29 | 0.49 |
| 1:3C:2:ARG:HE | 1:3C:240:LEU:HD22 | 1.78 | 0.49 |
| 1:3C:77:ARG:HG3 | 1:3C:77:ARG:NH1 | 2.28 | 0.49 |
| 2:3D:113:GLU:OE1 | 2:3D:114:ILE:HB | 2.13 | 0.49 |
| 2:3F:156:ARG:HA | 2:3F:159:VAL:HG12 | 1.95 | 0.49 |
| 1:3O:276:ARG:NH2 | 17:5U:223:GLU:OE1 | 2.46 | 0.49 |
| 1:3S:203:ASP:OD2 | 1:3S:302:ALA:N | 2.45 | 0.49 |
| 2:3T:163:LYS:HE3 | 3:4J:137:ARG:HG2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3T:417:GLU:O | 2:3T:420:GLU:HG2 | 2.13 | 0.49 |
| 3:4J:267:TYR:HB3 | 3:4J:273:LEU:HD11 | 1.93 | 0.49 |
| 10:5C:404:ARG:NH1 | 38:8C:194:GLU:HB3 | 2.28 | 0.49 |
| 11:5E:218:ASP:N | 11:5E:218:ASP:OD1 | 2.46 | 0.49 |
| 14:5L:127:ASN:OD1 | 14:5L:149:PHE:HA | 2.12 | 0.49 |
| 14:5L:207:GLU:HG3 | 14:5L:208:TYR:CD2 | 2.48 | 0.49 |
| 14:5L:482:ASP:HA | 14:5L:498:LEU:HB3 | 1.95 | 0.49 |
| 14:5M:28:ARG:O | 14:5M:28:ARG:HG3 | 2.13 | 0.49 |
| 14:5M:482:ASP:HA | 14:5M:498:LEU:HB3 | 1.95 | 0.49 |
| 14:5M:519:HIS:ND1 | 14:5M:520:PRO:HD2 | 2.26 | 0.49 |
| 14:5N:28:ARG:O | 14:5N:28:ARG:HG3 | 2.13 | 0.49 |
| 14:5N:180:ASN:OD1 | 14:5N:180:ASN:N | 2.25 | 0.49 |
| 15:5O:81:GLU:O | 15:5O:84:ARG:HB3 | 2.13 | 0.49 |
| 15:5O:226:ARG:CG | 15:5O:226:ARG:NH1 | 2.58 | 0.49 |
| 15:5P:92:GLU:O | 15:5P:164:VAL:HA | 2.13 | 0.49 |
| 16:5Q:60:HIS:HA | 16:5Q:98:MET:O | 2.13 | 0.49 |
| 18:5X:13:ARG:NH1 | 18:5X:207:ASP:OD1 | 2.45 | 0.49 |
| 18:5Z:13:ARG:NH1 | 18:5Z:207:ASP:OD1 | 2.45 | 0.49 |
| 18:6D:13:ARG:NH1 | 18:6D:207:ASP:OD1 | 2.45 | 0.49 |
| 20:6F:125:LYS:CE | 20:6F:344:LEU:HD21 | 2.43 | 0.49 |
| 21:6H:200:LEU:O | 21:6H:204:VAL:HG23 | 2.13 | 0.49 |
| 22:6J:114:THR:HG23 | 22:6J:117:GLY:H | 1.78 | 0.49 |
| 22:6M:54:ARG:HA | 24:6X:285:MET:HG3 | 1.95 | 0.49 |
| 24:6W:371:ALA:HB1 | 24:6W:375:THR:OG1 | 2.13 | 0.49 |
| 24:6W:503:ILE:HG21 | 24:6W:525:VAL:HG22 | 1.93 | 0.49 |
| 28:7H:319:ARG:HH21 | 28:7H:326:LEU:HD21 | 1.77 | 0.49 |
| 38:8A:31:GLU:CD | 38:8A:33:LYS:HB3 | 2.32 | 0.49 |
| 38:8B:167:ASP:OD1 | 38:8B:168:PRO:HD2 | 2.13 | 0.49 |
| 2:8:280:LYS:HG2 | 2:T1:89:PRO:CG | 2.42 | 0.49 |
| 1:A7:276:ARG:HH22 | 24:6T:210:VAL:HG21 | 1.78 | 0.49 |
| 1:B8:142:GLY:N | 39:B8:501:GDP:O2B | 2.45 | 0.49 |
| 2:F7:60:LYS:CE | 2:H3:283:HIS:CD2 | 2.96 | 0.49 |
| 2:G1:333:ALA:O | 2:G1:337:THR:HG23 | 2.13 | 0.49 |
| 2:G3:170:THR:HG21 | 2:G3:194:LEU:HD11 | 1.95 | 0.49 |
| 1:G4:130:LEU:HD23 | 1:G4:162:ARG:HG3 | 1.94 | 0.49 |
| 2:G7:4:VAL:HG23 | 2:G7:134:GLY:O | 2.13 | 0.49 |
| 2:G7:325:PRO:HA | 2:G7:328:VAL:HG12 | 1.94 | 0.49 |
| 2:H1:274:PRO:HB2 | 2:H1:276:ILE:HG12 | 1.95 | 0.49 |
| 2:H9:317:LEU:HD11 | 2:H9:351:PHE:CD2 | 2.45 | 0.49 |
| 2:H9:417:GLU:HA | 2:H9:420:GLU:HG2 | 1.94 | 0.49 |
| 1:I0:215:LEU:HB3 | 1:I0:217:LEU:HG | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I5:271:SER:N | 2:I5:377:MET:O | 2.45 | 0.49 |
| 1:I8:301:CYS:SG | 1:I8:302:ALA:N | 2.86 | 0.49 |
| 2:I9:267:PHE:HB2 | 2:I9:384:ILE:HD12 | 1.94 | 0.49 |
| 2:I9:432:PHE:HA | 2:I9:435:VAL:HG12 | 1.93 | 0.49 |
| 1:J4:190:HIS:CD2 | 1:J4:411:ALA:HA | 2.48 | 0.49 |
| 2:J9:279:GLU:HA | 5:4M:267:ASN:ND2 | 2.28 | 0.49 |
| 1:K0:395:LEU:O | 1:K0:399:THR:HG23 | 2.13 | 0.49 |
| 2:K1:339:ARG:HE | 2:K1:342:GLN:HE21 | 1.61 | 0.49 |
| 1:K4:336:LYS:HE2 | 28:7H:458:SER:O | 2.13 | 0.49 |
| 1:L0:345:ILE:HB | 1:L0:348:ASN:HD21 | 1.77 | 0.49 |
| 2:L7:191:THR:HA | 2:L7:194:LEU:HB2 | 1.95 | 0.49 |
| 1:M0:135:VAL:HG11 | 1:M0:152:ILE:HD11 | 1.95 | 0.49 |
| 1:M2:6:HIS:NE2 | 1:M2:136:CYS:SG | 2.86 | 0.49 |
| 2:M3:205:ASP:OD1 | 2:M3:206:ASN:N | 2.45 | 0.49 |
| 2:M9:394:LYS:HB2 | 1:N0:346:PRO:HG3 | 1.94 | 0.49 |
| 1:N0:74:ASP:O | 1:N0:78:SER:OG | 2.28 | 0.49 |
| 2:N3:66:ILE:HD12 | 2:N3:68:LEU:HD11 | 1.94 | 0.49 |
| 1:N8:392:LYS:HB2 | 1:N8:395:LEU:HD22 | 1.95 | 0.49 |
| 2:O7:88:HIS:CD2 | 2:O7:89:PRO:HD2 | 2.48 | 0.49 |
| 1:P4:6:HIS:CE1 | 1:P4:8:GLN:HG3 | 2.48 | 0.49 |
| 1:Q4:317:PHE:HB3 | 1:Q4:321:MET:SD | 2.53 | 0.49 |
| 2:Q9:56:THR:HG23 | 2:Q9:60:LYS:HB3 | 1.94 | 0.49 |
| 1:R0:309:ARG:H | 1:R0:372:THR:HG22 | 1.78 | 0.49 |
| 1:R4:392:LYS:HD2 | 1:R4:395:LEU:HD22 | 1.95 | 0.49 |
| 2:S1:371:VAL:HG22 | 2:S1:373:ARG:H | 1.78 | 0.49 |
| 1:T2:218:THR:HG22 | 24:6X:41:ARG:NH2 | 2.28 | 0.49 |
| 1:T6:204:ASN:HD21 | 39:T6:502:GDP:HN22 | 1.60 | 0.49 |
| 1:T8:329:GLN:O | 1:T8:333:VAL:HG13 | 2.13 | 0.49 |
| 2:U3:301:MET:HE1 | 2:U3:307:PRO:HD3 | 1.95 | 0.49 |
| 1:U4:22:GLU:HG2 | 1:U4:81:TYR:HB2 | 1.94 | 0.49 |
| 1:U4:310:TYR:N | 1:U4:340:TYR:O | 2.37 | 0.49 |
| 1:V0:325:GLU:O | 1:V0:329:GLN:HG2 | 2.12 | 0.49 |
| 1:V2:325:GLU:O | 1:V2:329:GLN:HG2 | 2.13 | 0.49 |
| 1:V4:232:VAL:HG13 | 1:V4:268:VAL:HG11 | 1.95 | 0.49 |
| 1:V6:2:ARG:HB2 | 1:V6:46:ARG:NH2 | 2.21 | 0.49 |
| 1:V6:330:MET:SD | 1:V6:351:SER:HB3 | 2.52 | 0.49 |
| 2:V7:245:ASP:N | 2:V7:245:ASP:OD1 | 2.46 | 0.49 |
| 2:W3:21:TRP:CZ3 | 2:W3:63:PRO:HB3 | 2.47 | 0.49 |
| 2:W3:311:LYS:HG2 | 2:W3:342:GLN:HG3 | 1.94 | 0.49 |
| 1:W6:5:VAL:HG12 | 1:W6:133:PHE:CD1 | 2.48 | 0.49 |
| 1:W6:273:LEU:H | 1:W6:292:GLN:HE22 | 1.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W6:375:GLN:HB3 | 1:W6:422:TYR:HD2 | 1.77 | 0.49 |
| 2:W7:5:ILE:HD11 | 2:W7:135:PHE:CE1 | 2.47 | 0.49 |
| 1:X2:423:GLN:NE2 | 1:X2:426:GLN:OE1 | 2.44 | 0.49 |
| 1:Y0:165:LEU:HA | 1:Y0:165:LEU:HD12 | 1.58 | 0.49 |
| 2:Y5:27:GLU:OE1 | 2:Y5:243:ARG:NH1 | 2.46 | 0.49 |
| 1:Y8:121:ARG:NH2 | 1:Y8:158:GLU:OE2 | 2.38 | 0.49 |
| 1:Z0:257:LEU:HD21 | 1:Z0:314:SER:HB2 | 1.93 | 0.49 |
| 2:Z3:208:ALA:O | 2:Z3:212:ILE:HG12 | 2.13 | 0.49 |
| 2:Z5:115:VAL:HG23 | 2:Z5:153:LEU:HD22 | 1.95 | 0.49 |
| 1:Z6:294:TRP:CG | 1:Z6:333:VAL:HG21 | 2.47 | 0.49 |
| 1:Z6:334:GLN:HE22 | 1:Z6:347:ASN:H | 1.61 | 0.49 |
| 2:0B:89:PRO:HD2 | 2:0R:283:HIS:ND1 | 2.28 | 0.49 |
| 1:0C:5:VAL:HG23 | 1:0C:62:ARG:HG2 | 1.95 | 0.49 |
| 1:0C:21:TRP:CZ3 | 1:0C:61:PRO:HB3 | 2.48 | 0.49 |
| 1:0C:83:GLN:O | 1:0S:281:TYR:OH | 2.26 | 0.49 |
| 2:0F:198:THR:HG21 | 2:0F:201:ALA:HB2 | 1.95 | 0.49 |
| 2:0F:344:VAL:HB | 2:0F:346:TRP:CE2 | 2.48 | 0.49 |
| 2:0H:208:ALA:O | 2:0H:212:ILE:HG12 | 2.13 | 0.49 |
| 2:0J:32:PRO:HA | 2:0J:86:LEU:HD12 | 1.94 | 0.49 |
| 1:0K:21:TRP:CH2 | 1:0K:61:PRO:HB3 | 2.48 | 0.49 |
| 1:0K:259:PRO:HG3 | 1:0K:311:LEU:HD21 | 1.94 | 0.49 |
| 1:0O:27:GLU:OE2 | 1:0O:358:PRO:HA | 2.12 | 0.49 |
| 1:0O:379:LYS:HD3 | 1:0O:419:VAL:HG21 | 1.94 | 0.49 |
| 2:0X:406:HIS:HA | 2:0X:409:VAL:HG22 | 1.95 | 0.49 |
| 2:1B:88:HIS:NE2 | 2:1R:283:HIS:HB3 | 2.27 | 0.49 |
| 2:1D:174:SER:HB3 | 2:1D:177:VAL:O | 2.13 | 0.49 |
| 2:1D:223:THR:HG23 | 2:1D:225:THR:H | 1.78 | 0.49 |
| 1:1G:3:GLU:OE1 | 1:1G:5:VAL:HG23 | 2.13 | 0.49 |
| 1:1K:109:GLY:HA2 | 1:1K:113:ILE:HG13 | 1.93 | 0.49 |
| 1:1K:210:ILE:O | 1:1K:214:THR:OG1 | 2.30 | 0.49 |
| 2:1N:246:GLY:HA2 | 2:1N:357:TYR:CD2 | 2.48 | 0.49 |
| 1:1S:404:ASP:HB3 | 1:1S:406:MET:SD | 2.53 | 0.49 |
| 2:1X:14:ILE:HD13 | 2:1X:69:ASP:OD2 | 2.11 | 0.49 |
| 2:1Z:316:CYS:HB3 | 2:1Z:378:ILE:HG23 | 1.94 | 0.49 |
| 1:2A:134:GLN:HE21 | 1:2A:167:PHE:HE2 | 1.59 | 0.49 |
| 1:2E:239:CYS:SG | 1:2E:248:ALA:N | 2.84 | 0.49 |
| 1:2G:68:LEU:HD23 | 1:2G:93:GLY:HA3 | 1.95 | 0.49 |
| 1:2G:78:SER:O | 10:5B:135:ARG:NH2 | 2.37 | 0.49 |
| 2:2J:121:ARG:HG3 | 2:2J:121:ARG:HH11 | 1.78 | 0.49 |
| 1:2K:72:THR:O | 1:2K:76:VAL:HG23 | 2.12 | 0.49 |
| 2:2L:156:ARG:HH22 | 38:8C:29:GLY:HA2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2M:177:ASP:O | 2:2N:352:LYS:HA | 2.13 | 0.49 |
| 2:2N:81:GLY:O | 2:2N:84:ARG:NH1 | 2.38 | 0.49 |
| 2:2P:317:LEU:HB3 | 2:2P:319:TYR:HE1 | 1.78 | 0.49 |
| 1:2Q:212:PHE:CZ | 38:8A:117:TRP:HB3 | 2.48 | 0.49 |
| 1:2S:113:ILE:HA | 1:2S:116:VAL:HG22 | 1.94 | 0.49 |
| 1:2S:175:VAL:HG23 | 2:2T:329:ASN:ND2 | 2.28 | 0.49 |
| 1:2Y:358:PRO:HG2 | 1:2Y:361:LEU:HD12 | 1.95 | 0.49 |
| 2:3H:115:VAL:HG11 | 2:3H:152:LEU:HD23 | 1.94 | 0.49 |
| 2:3L:8:HIS:CD2 | 2:3L:138:PHE:HD2 | 2.31 | 0.49 |
| 1:3O:175:VAL:HG22 | 2:3P:329:ASN:HD21 | 1.77 | 0.49 |
| 2:3R:5:ILE:HD11 | 2:3R:135:PHE:CE1 | 2.47 | 0.49 |
| 2:3T:167:LEU:HA | 2:3T:200:VAL:HG23 | 1.95 | 0.49 |
| 5:4M:148:LEU:O | 5:4M:152:ILE:HG12 | 2.13 | 0.49 |
| 6:4O:146:LYS:O | 6:4O:149:SER:OG | 2.26 | 0.49 |
| 6:4O:275:ALA:O | 6:4O:279:LYS:HG3 | 2.13 | 0.49 |
| 6:4O:469:LEU:H | 6:4O:469:LEU:HD23 | 1.78 | 0.49 |
| 8:4W:104:MET:N | 8:4W:105:PRO:HD2 | 2.28 | 0.49 |
| 9:4Y:425:ALA:HB1 | 9:4Y:446:LEU:HD11 | 1.95 | 0.49 |
| 9:4Z:291:HIS:O | 9:4Z:294:GLU:HG3 | 2.12 | 0.49 |
| 9:4Z:372:LEU:HD23 | 9:4Z:373:LYS:HD3 | 1.94 | 0.49 |
| 10:5B:120:GLU:HG2 | 10:5C:359:ARG:HH22 | 1.77 | 0.49 |
| 12:5F:24:TYR:HE1 | 12:5G:264:ARG:HD3 | 1.77 | 0.49 |
| 12:5F:39:PHE:HD2 | 12:5F:44:ILE:HD13 | 1.78 | 0.49 |
| 14:5L:340:ASN:OD1 | 14:5L:341:ASP:N | 2.46 | 0.49 |
| 14:5L:519:HIS:ND1 | 14:5L:520:PRO:HD2 | 2.26 | 0.49 |
| 14:5M:127:ASN:OD1 | 14:5M:149:PHE:HA | 2.12 | 0.49 |
| 14:5M:273:SER:O | 14:5M:274:THR:OG1 | 2.28 | 0.49 |
| 14:5N:163:LEU:HD12 | 14:5N:171:MET:HE1 | 1.94 | 0.49 |
| 14:5N:207:GLU:HG3 | 14:5N:208:TYR:CD2 | 2.48 | 0.49 |
| 14:5N:482:ASP:HA | 14:5N:498:LEU:HB3 | 1.95 | 0.49 |
| 14:5N:519:HIS:ND1 | 14:5N:520:PRO:HD2 | 2.26 | 0.49 |
| 15:5O:23:LYS:CB | 15:5O:40:ILE:HD12 | 2.43 | 0.49 |
| 15:5O:294:PHE:CD2 | 15:5O:294:PHE:C | 2.86 | 0.49 |
| 15:5O:373:PHE:C | 15:5O:377:PRO:HG3 | 2.33 | 0.49 |
| 18:6A:13:ARG:NH1 | 18:6A:207:ASP:OD1 | 2.45 | 0.49 |
| 18:6C:13:ARG:NH1 | 18:6C:207:ASP:OD1 | 2.45 | 0.49 |
| 21:6H:44:ILE:HG22 | 21:6H:162:MET:HB3 | 1.94 | 0.49 |
| 22:6O:48:GLU:HA | 22:6O:113:ARG:HE | 1.78 | 0.49 |
| 22:6P:153:SER:O | 22:6P:157:VAL:HG12 | 2.13 | 0.49 |
| 24:6T:536:ASP:OD1 | 24:6T:537:GLU:N | 2.46 | 0.49 |
| 28:7H:361:TRP:HA | 28:7H:361:TRP:CE3 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:7K:173:GLU:CD | 30:7K:173:GLU:H | 2.15 | 0.49 |
| 31:7N:78:HIS:N | 31:7N:79:PRO:HD2 | 2.27 | 0.49 |
| 32:7P:136:HIS:CD2 | 32:7P:141:VAL:HG11 | 2.48 | 0.49 |
| 36:7W:24:ASN:N | 36:7W:24:ASN:OD1 | 2.45 | 0.49 |
| 28:7X:319:ARG:HA | 28:7X:329:ALA:HB2 | 1.94 | 0.49 |
| 2:6:285:GLN:HG2 | 2:S9:57:GLY:H | 1.78 | 0.48 |
| 1:A1:423:GLN:HB3 | 3:4F:109:ALA:HB2 | 1.95 | 0.48 |
| 1:A3:40:SER:O | 26:7F:25:TYR:CE2 | 2.64 | 0.48 |
| 2:C5:12:ALA:HB2 | 41:C5:501:GTP:C8 | 2.48 | 0.48 |
| 2:E9:12:ALA:HB2 | 41:F0:501:GTP:C8 | 2.47 | 0.48 |
| 2:E9:33:ASP:OD2 | 22:6N:131:ARG:NH1 | 2.45 | 0.48 |
| 2:F3:229:ARG:NH2 | 22:6P:119:ASP:O | 2.46 | 0.48 |
| 2:H1:227:LEU:O | 2:H1:231:ILE:HG12 | 2.13 | 0.48 |
| 1:H2:20:PHE:O | 1:H2:24:VAL:HG23 | 2.12 | 0.48 |
| 2:H3:68:LEU:HA | 2:H3:93:ILE:O | 2.13 | 0.48 |
| 1:H6:276:ARG:NH1 | 24:6V:489:ASN:C | 2.66 | 0.48 |
| 2:I1:183:GLU:HG3 | 2:I1:184:PRO:HD3 | 1.95 | 0.48 |
| 2:I5:69:ASP:OD2 | 2:I5:71:GLU:N | 2.46 | 0.48 |
| 2:I7:312:TYR:HB2 | 2:I7:343:PHE:HD1 | 1.78 | 0.48 |
| 2:I9:155:GLU:HB2 | 2:I9:197:HIS:CE1 | 2.48 | 0.48 |
| 2:J3:254:GLU:N | 2:J3:254:GLU:OE1 | 2.46 | 0.48 |
| 2:J7:31:GLN:HE21 | 2:J7:37:PRO:HG3 | 1.78 | 0.48 |
| 2:K1:88:HIS:HB3 | 2:L7:283:HIS:ND1 | 2.28 | 0.48 |
| 2:K1:185:TYR:CE1 | 2:K1:398:MET:HG3 | 2.48 | 0.48 |
| 1:K6:334:GLN:HE22 | 1:K6:348:ASN:H | 1.61 | 0.48 |
| 1:K8:72:THR:O | 1:K8:76:VAL:HG23 | 2.13 | 0.48 |
| 2:L5:363:VAL:HG23 | 2:L5:366:GLY:HA3 | 1.94 | 0.48 |
| 2:L9:312:TYR:HB2 | 2:L9:343:PHE:CD1 | 2.47 | 0.48 |
| 1:M0:178:THR:HG22 | 1:M0:181:GLU:HG3 | 1.95 | 0.48 |
| 2:M3:331:SER:O | 2:M3:334:THR:OG1 | 2.21 | 0.48 |
| 2:M5:121:ARG:HD3 | 2:M5:121:ARG:O | 2.13 | 0.48 |
| 2:N3:103:PHE:CD2 | 2:N3:189:LEU:HB3 | 2.48 | 0.48 |
| 2:N7:2:ARG:NH2 | 27:7G:162:LYS:HB3 | 2.27 | 0.48 |
| 2:N9:53:PHE:HB3 | 2:N9:61:HIS:HB3 | 1.95 | 0.48 |
| 2:N9:174:SER:OG | 2:N9:207:GLU:OE1 | 2.30 | 0.48 |
| 2:O3:177:VAL:HG23 | 1:O4:327:ASP:CG | 2.32 | 0.48 |
| 2:Q3:4:VAL:HG23 | 2:Q3:134:GLY:O | 2.12 | 0.48 |
| 1:Q4:304:ASP:OD2 | 1:Q4:306:ARG:NH1 | 2.46 | 0.48 |
| 1:Q6:114:ASP:OD1 | 1:Q6:115:SER:N | 2.44 | 0.48 |
| 1:Q6:288:GLU:OE2 | 1:Q6:291:GLN:NE2 | 2.46 | 0.48 |
| 1:R4:74:ASP:OD2 | 19:6E:252:THR:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:418:LEU:O | 1:R6:421:GLU:HG2 | 2.13 | 0.48 |
| 2:R7:291:ILE:HD12 | 2:R7:375:VAL:HG23 | 1.95 | 0.48 |
| 2:R9:34:GLY:HA3 | 2:R9:60:LYS:HD3 | 1.95 | 0.48 |
| 1:S0:70:PRO:HG2 | 2:S1:2:ARG:NH2 | 2.27 | 0.48 |
| 1:S0:173:PRO:HA | 1:S0:176:SER:HB2 | 1.93 | 0.48 |
| 1:S8:117:LEU:HA | 1:S8:120:VAL:HG12 | 1.95 | 0.48 |
| 2:S9:174:SER:HA | 2:S9:205:ASP:OD2 | 2.13 | 0.48 |
| 2:T1:371:VAL:HG22 | 2:T1:373:ARG:H | 1.78 | 0.48 |
| 1:T2:5:VAL:HG22 | 1:T2:62:ARG:HD3 | 1.94 | 0.48 |
| 1:T4:108:GLU:N | 1:T4:108:GLU:OE1 | 2.46 | 0.48 |
| 1:T6:74:ASP:C | 1:T6:76:VAL:H | 2.17 | 0.48 |
| 1:T6:386:THR:HB | 13:5K:51:THR:HG21 | 1.95 | 0.48 |
| 1:T8:190:HIS:CD2 | 1:T8:414:ASN:HB2 | 2.47 | 0.48 |
| 2:U5:51:THR:HG21 | 2:U5:243:ARG:HG2 | 1.94 | 0.48 |
| 1:U8:67:ASP:N | 1:U8:67:ASP:OD1 | 2.45 | 0.48 |
| 2:V1:69:ASP:OD1 | 2:V1:71:GLU:N | 2.45 | 0.48 |
| 1:V2:5:VAL:HG12 | 1:V2:133:PHE:HD1 | 1.78 | 0.48 |
| 2:V3:14:ILE:HD11 | 2:V3:74:VAL:HG13 | 1.94 | 0.48 |
| 2:V7:90:GLU:HG3 | 2:V7:121:ARG:NH1 | 2.28 | 0.48 |
| 1:V8:208:TYR:CE1 | 1:V8:225:LEU:HD11 | 2.48 | 0.48 |
| 1:W0:248:ALA:HA | 1:W0:252:LYS:HD2 | 1.95 | 0.48 |
| 2:W5:9:ILE:HD11 | 2:W5:153:LEU:HD23 | 1.95 | 0.48 |
| 2:W5:88:HIS:ND1 | 2:Y1:283:HIS:HB3 | 2.28 | 0.48 |
| 2:X9:214:ARG:HE | 2:X9:215:ARG:HG2 | 1.78 | 0.48 |
| 1:Y0:204:ASN:HD21 | 39:Y0:502:GDP:HN22 | 1.60 | 0.48 |
| 1:Y8:1:MET:SD | 1:Y8:2:ARG:NH1 | 2.86 | 0.48 |
| 1:Z0:86:ARG:HG2 | 1:Z0:88:ASP:H | 1.77 | 0.48 |
| 2:Z1:387:ILE:HD12 | 2:Z1:390:ARG:HH22 | 1.77 | 0.48 |
| 2:Z3:5:ILE:HD13 | 2:Z3:125:LEU:HD23 | 1.95 | 0.48 |
| 2:Z5:433:GLU:OE1 | 2:Z5:433:GLU:HA | 2.12 | 0.48 |
| 1:Z8:107:THR:OG1 | 1:Z8:401:GLU:OE2 | 2.24 | 0.48 |
| 1:Z8:113:ILE:HD13 | 1:Z8:150:LEU:HD22 | 1.95 | 0.48 |
| 2:Z9:246:GLY:HA3 | 2:Z9:356:ASN:HA | 1.94 | 0.48 |
| 2:0B:206:ASN:OD1 | 41:0C:501:GTP:N2 | 2.40 | 0.48 |
| 2:0F:121:ARG:HD2 | 2:0F:124:LYS:HE3 | 1.95 | 0.48 |
| 2:0F:402:ARG:NH2 | 2:0F:415:GLU:OE2 | 2.45 | 0.48 |
| 1:0G:3:GLU:O | 1:0G:131:GLN:N | 2.44 | 0.48 |
| 1:0K:67:ASP:OD2 | 1:0K:72:THR:OG1 | 2.22 | 0.48 |
| 2:0N:333:ALA:O | 2:0N:337:THR:HG23 | 2.13 | 0.48 |
| 1:0O:246:LEU:O | 1:0O:352:SER:OG | 2.25 | 0.48 |
| 1:0S:257:LEU:HA | 1:0S:312:THR:HG21 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0U:39:ASP:OD1 | 1:0U:39:ASP:N | 2.42 | 0.48 |
| 1:0W:310:TYR:N | 1:0W:340:TYR:O | 2.39 | 0.48 |
| 2:0X:7:ILE:HD12 | 2:0X:153:LEU:HD21 | 1.94 | 0.48 |
| 2:0X:333:ALA:O | 2:0X:337:THR:HG23 | 2.12 | 0.48 |
| 1:0Y:114:ASP:N | 1:0Y:114:ASP:OD1 | 2.44 | 0.48 |
| 2:0Z:14:ILE:HD11 | 2:0Z:74:VAL:HG13 | 1.96 | 0.48 |
| 1:1C:3:GLU:OE1 | 1:1C:62:ARG:NH1 | 2.42 | 0.48 |
| 2:1D:417:GLU:HA | 2:1D:420:GLU:HG2 | 1.93 | 0.48 |
| 1:1K:178:THR:CG2 | 1:1K:181:GLU:HG3 | 2.43 | 0.48 |
| 1:1Q:7:ILE:HB | 1:1Q:135:VAL:HG22 | 1.94 | 0.48 |
| 1:1Q:39:ASP:OD1 | 1:1Q:40:SER:N | 2.45 | 0.48 |
| 2:1T:222:PRO:CD | 1:1U:324:LYS:HE3 | 2.42 | 0.48 |
| 2:1V:202:VAL:HG22 | 2:1V:268:MET:HB2 | 1.95 | 0.48 |
| 2:1V:290:GLU:HA | 2:1V:293:ASN:HD22 | 1.77 | 0.48 |
| 1:2A:211:CYS:SG | 1:2A:220:PRO:HB3 | 2.53 | 0.48 |
| 1:2C:257:LEU:HA | 1:2C:312:THR:HG21 | 1.93 | 0.48 |
| 1:2C:379:LYS:HG3 | 1:2C:419:VAL:HG21 | 1.95 | 0.48 |
| 2:2F:76:ASP:OD2 | 1:2G:46:ARG:NH2 | 2.46 | 0.48 |
| 2:2H:414:GLU:HG2 | 2:2H:416:GLY:H | 1.77 | 0.48 |
| 2:2P:201:ALA:O | 2:2P:268:MET:HE2 | 2.12 | 0.48 |
| 2:2R:387:ILE:HG12 | 2:2R:390:ARG:HH22 | 1.78 | 0.48 |
| 1:2S:3:GLU:HG3 | 1:2S:127:CYS:SG | 2.53 | 0.48 |
| 2:2T:170:THR:HG21 | 2:2T:194:LEU:HD11 | 1.94 | 0.48 |
| 1:2U:396:HIS:HA | 1:2U:399:THR:OG1 | 2.13 | 0.48 |
| 1:2Y:67:ASP:N | 1:2Y:67:ASP:OD1 | 2.46 | 0.48 |
| 1:2Y:260:PHE:HB2 | 1:2Y:263:LEU:HD23 | 1.95 | 0.48 |
| 1:3G:34:GLY:HA3 | 1:3G:58:ARG:CD | 2.43 | 0.48 |
| 2:3J:122:ILE:HD13 | 2:3J:125:LEU:HD12 | 1.95 | 0.48 |
| 2:3N:88:HIS:H | 2:3N:91:GLN:NE2 | 2.11 | 0.48 |
| 2:3P:414:GLU:HG2 | 2:3P:416:GLY:H | 1.78 | 0.48 |
| 1:3S:276:ARG:NH2 | 17:5V:219:LEU:HB3 | 2.28 | 0.48 |
| 6:4P:118:SER:HA | 6:4P:121:GLU:OE1 | 2.12 | 0.48 |
| 10:5A:351:GLN:O | 10:5A:355:GLU:HG2 | 2.13 | 0.48 |
| 10:5D:222:LYS:O | 10:5D:225:GLU:HG3 | 2.13 | 0.48 |
| 14:5M:207:GLU:HG3 | 14:5M:208:TYR:CD2 | 2.48 | 0.48 |
| 14:5M:340:ASN:OD1 | 14:5M:341:ASP:N | 2.46 | 0.48 |
| 14:5N:127:ASN:OD1 | 14:5N:149:PHE:HA | 2.12 | 0.48 |
| 14:5N:340:ASN:OD1 | 14:5N:341:ASP:N | 2.46 | 0.48 |
| 15:5O:31:GLU:OE1 | 15:5O:32:SER:N | 2.46 | 0.48 |
| 15:5O:123:LEU:HD13 | 15:5O:161:MET:HB3 | 1.95 | 0.48 |
| 17:5V:137:PRO:HG2 | 17:5V:140:LEU:HG | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:5Y:13:ARG:NH1 | 18:5Y:207:ASP:OD1 | 2.45 | 0.48 |
| 18:6B:13:ARG:NH1 | 18:6B:207:ASP:OD1 | 2.45 | 0.48 |
| 22:6L:219:ASP:OD1 | 22:6L:222:SER:OG | 2.21 | 0.48 |
| 22:6M:63:PRO:HA | 22:6M:66:ASP:OD2 | 2.13 | 0.48 |
| 24:6U:242:PHE:O | 24:6U:246:VAL:HG23 | 2.13 | 0.48 |
| 24:6V:132:VAL:HB | 24:6V:148:ILE:HB | 1.95 | 0.48 |
| 24:6V:434:ASP:OD1 | 24:6V:437:LYS:HB3 | 2.13 | 0.48 |
| 36:7V:24:ASN:N | 36:7V:24:ASN:OD1 | 2.45 | 0.48 |
| 37:7Y:190:LYS:O | 37:7Y:191:ARG:HB2 | 2.13 | 0.48 |
| 2:A2:29:GLY:CA | 26:7F:45:MET:HE1 | 2.35 | 0.48 |
| 2:G7:189:LEU:HD11 | 2:G7:418:PHE:HE1 | 1.77 | 0.48 |
| 1:G8:207:LEU:HB3 | 1:G8:225:LEU:HD22 | 1.94 | 0.48 |
| 1:H4:67:ASP:N | 1:H4:67:ASP:OD1 | 2.45 | 0.48 |
| 1:H6:237:THR:O | 1:H6:237:THR:HG22 | 2.13 | 0.48 |
| 1:H6:246:LEU:HD22 | 1:H6:352:SER:HA | 1.94 | 0.48 |
| 1:H8:199:CYS:HB2 | 1:H8:265:PHE:CD1 | 2.48 | 0.48 |
| 2:I1:108:TYR:O | 2:I1:112:LYS:NZ | 2.35 | 0.48 |
| 2:I3:183:GLU:HG3 | 2:I3:184:PRO:HD3 | 1.95 | 0.48 |
| 2:I5:192:HIS:HD2 | 2:I5:421:ALA:HA | 1.78 | 0.48 |
| 2:I7:72:PRO:HG3 | 1:I8:1:MET:HG2 | 1.94 | 0.48 |
| 2:I7:76:ASP:HA | 2:I7:79:ARG:HB2 | 1.94 | 0.48 |
| 2:J3:294:ALA:HA | 2:J3:297:GLU:OE1 | 2.12 | 0.48 |
| 1:K0:67:ASP:HB3 | 1:K0:92:PHE:HE1 | 1.77 | 0.48 |
| 2:K1:203:MET:O | 2:K1:204:LEU:HD23 | 2.13 | 0.48 |
| 1:M8:262:ARG:NH2 | 1:M8:417:ASP:OD1 | 2.46 | 0.48 |
| 2:M9:271:SER:OG | 2:M9:301:MET:SD | 2.71 | 0.48 |
| 1:N2:382:SER:HB2 | 1:N2:415:MET:HG2 | 1.95 | 0.48 |
| 2:N3:119:LEU:HD11 | 2:N3:160:ASP:OD2 | 2.12 | 0.48 |
| 2:N3:373:ARG:NH2 | 30:7L:280:GLN:O | 2.39 | 0.48 |
| 1:N6:107:THR:OG1 | 1:N6:108:GLU:OE1 | 2.23 | 0.48 |
| 2:N7:12:ALA:HB2 | 41:N8:501:GTP:C8 | 2.48 | 0.48 |
| 2:N7:91:GLN:O | 2:N7:92:LEU:HD23 | 2.12 | 0.48 |
| 1:N8:113:ILE:HA | 1:N8:116:VAL:HG22 | 1.94 | 0.48 |
| 1:N8:179:VAL:H | 2:N9:258:ASN:ND2 | 2.11 | 0.48 |
| 2:O1:137:VAL:HG22 | 2:O1:168:GLY:HA2 | 1.95 | 0.48 |
| 2:O3:384:ILE:HD12 | 2:O3:384:ILE:H | 1.78 | 0.48 |
| 1:O8:67:ASP:N | 1:O8:67:ASP:OD1 | 2.47 | 0.48 |
| 1:O8:184:ASN:OD1 | 1:O8:398:TYR:OH | 2.29 | 0.48 |
| 1:P6:137:HIS:HE1 | 1:P6:139:LEU:HD21 | 1.78 | 0.48 |
| 2:Q3:174:SER:HB3 | 2:Q3:177:VAL:O | 2.13 | 0.48 |
| 1:Q4:130:LEU:HB2 | 1:Q4:162:ARG:HE | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:49:VAL:HG11 | 1:R4:241:ARG:HG2 | 1.96 | 0.48 |
| 2:R7:4:VAL:HG23 | 2:R7:134:GLY:O | 2.13 | 0.48 |
| 2:S1:238:LEU:HD22 | 2:S1:378:ILE:HD11 | 1.96 | 0.48 |
| 2:S1:275:ILE:HG23 | 2:S1:368:LEU:HD21 | 1.95 | 0.48 |
| 2:S7:266:HIS:ND1 | 2:S7:266:HIS:O | 2.46 | 0.48 |
| 1:T0:178:THR:OG1 | 1:T0:181:GLU:HG3 | 2.13 | 0.48 |
| 2:T1:65:CYS:O | 2:T1:91:GLN:NE2 | 2.46 | 0.48 |
| 2:U1:216:SER:OG | 2:U1:275:ILE:O | 2.30 | 0.48 |
| 1:U2:167:PHE:CE2 | 1:U2:233:MET:HG2 | 2.49 | 0.48 |
| 1:U4:161:ASP:OD2 | 1:U4:162:ARG:NH1 | 2.46 | 0.48 |
| 2:U5:224:TYR:H | 1:U6:245:GLN:NE2 | 2.11 | 0.48 |
| 1:U8:417:ASP:OD1 | 1:U8:418:LEU:N | 2.46 | 0.48 |
| 1:V2:361:LEU:HD12 | 1:V2:362:LYS:H | 1.77 | 0.48 |
| 2:V3:317:LEU:HB3 | 2:V3:319:TYR:HE1 | 1.77 | 0.48 |
| 1:V6:169:VAL:HG13 | 1:V6:203:ASP:HA | 1.95 | 0.48 |
| 1:V6:173:PRO:HD2 | 1:V6:380:ARG:NH1 | 2.27 | 0.48 |
| 2:W9:102:ASN:HB3 | 2:W9:105:ARG:HG3 | 1.95 | 0.48 |
| 2:X3:280:LYS:HA | 2:X3:283:HIS:HB3 | 1.95 | 0.48 |
| 1:X4:111:GLU:HG2 | 1:X4:112:LEU:HD22 | 1.94 | 0.48 |
| 2:Y9:336:LYS:O | 2:Y9:339:ARG:NH2 | 2.45 | 0.48 |
| 2:Z1:225:THR:HG22 | 2:Z1:229:ARG:HE | 1.78 | 0.48 |
| 2:Z1:239:THR:HG23 | 2:Z1:243:ARG:HH21 | 1.78 | 0.48 |
| 1:Z2:166:THR:OG1 | 1:Z2:199:CYS:SG | 2.58 | 0.48 |
| 2:Z5:21:TRP:CZ2 | 2:Z5:65:CYS:HB2 | 2.48 | 0.48 |
| 2:Z9:262:TYR:CD2 | 2:Z9:265:ILE:HD12 | 2.48 | 0.48 |
| 1:0C:51:PHE:HB3 | 1:0C:59:TYR:HB3 | 1.95 | 0.48 |
| 2:0F:235:ILE:HD12 | 2:0F:238:LEU:HD11 | 1.95 | 0.48 |
| 2:0F:398:MET:HE1 | 1:0G:345:ILE:HG23 | 1.94 | 0.48 |
| 2:0J:212:ILE:O | 2:0J:216:SER:OG | 2.26 | 0.48 |
| 1:0M:244:GLY:HA3 | 1:0M:354:CYS:HA | 1.95 | 0.48 |
| 1:0O:318:ARG:HA | 1:0O:354:CYS:SG | 2.53 | 0.48 |
| 2:0R:74:VAL:O | 2:0R:78:VAL:HG23 | 2.14 | 0.48 |
| 2:0R:318:MET:HB2 | 2:0R:376:CYS:HB3 | 1.94 | 0.48 |
| 1:0S:66:MET:HB3 | 1:0S:147:MET:HE1 | 1.94 | 0.48 |
| 1:0W:317:PHE:HE2 | 1:0W:326:VAL:HG13 | 1.77 | 0.48 |
| 1:1A:175:VAL:HG13 | 2:1B:329:ASN:HD21 | 1.78 | 0.48 |
| 2:1B:386:GLU:OE1 | 2:1B:387:ILE:HG13 | 2.12 | 0.48 |
| 2:1H:99:ALA:HA | 2:1H:105:ARG:HD3 | 1.94 | 0.48 |
| 1:1K:391:ARG:HD3 | 2:1L:346:TRP:NE1 | 2.28 | 0.48 |
| 2:1L:66:ILE:HD12 | 2:1L:68:LEU:HD23 | 1.96 | 0.48 |
| 1:1O:116:VAL:HA | 1:1O:119:VAL:HG12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1R:9:ILE:HD13 | 2:1R:150:GLY:HA2 | 1.94 | 0.48 |
| 2:1R:71:GLU:HB3 | 2:1R:98:ASP:OD1 | 2.14 | 0.48 |
| 2:1V:115:VAL:HG22 | 2:1V:119:LEU:HD23 | 1.94 | 0.48 |
| 1:1W:50:TYR:CE2 | 1:1W:237:THR:HG21 | 2.48 | 0.48 |
| 2:1Z:241:SER:OG | 2:1Z:250:VAL:N | 2.45 | 0.48 |
| 1:2E:364:SER:OG | 1:2E:365:ALA:N | 2.43 | 0.48 |
| 2:2L:65:CYS:SG | 2:2L:66:ILE:N | 2.86 | 0.48 |
| 1:2W:99:ASN:ND2 | 2:2X:254:GLU:OE1 | 2.46 | 0.48 |
| 2:2X:119:LEU:HD11 | 2:2X:156:ARG:HD3 | 1.94 | 0.48 |
| 1:2Y:177:ASP:N | 1:2Y:181:GLU:OE2 | 2.46 | 0.48 |
| 1:3A:265:PHE:HE2 | 1:3A:418:LEU:HD11 | 1.78 | 0.48 |
| 1:3C:35:THR:HG22 | 38:8D:161:GLN:OE1 | 2.13 | 0.48 |
| 1:3C:173:PRO:CD | 1:3C:380:ARG:HE | 2.26 | 0.48 |
| 1:3C:325:GLU:O | 1:3C:329:GLN:HB2 | 2.13 | 0.48 |
| 2:3D:234:VAL:HG13 | 2:3D:376:CYS:SG | 2.54 | 0.48 |
| 2:3D:246:GLY:HA3 | 2:3D:356:ASN:HA | 1.95 | 0.48 |
| 1:3G:65:LEU:HD12 | 1:3G:90:PHE:CD1 | 2.48 | 0.48 |
| 1:3G:280:GLN:HG2 | 38:8A:162:VAL:HG13 | 1.94 | 0.48 |
| 2:3H:250:VAL:HB | 2:3H:254:GLU:HG3 | 1.95 | 0.48 |
| 1:3I:217:LEU:HD22 | 38:8B:229:ASN:H | 1.78 | 0.48 |
| 1:3K:263:LEU:HG | 1:3K:422:TYR:HE1 | 1.77 | 0.48 |
| 2:3N:182:VAL:HG12 | 2:3N:185:TYR:HB2 | 1.95 | 0.48 |
| 1:3O:5:VAL:HG22 | 1:3O:133:PHE:CD1 | 2.47 | 0.48 |
| 1:3S:211:CYS:HG | 1:3S:217:LEU:HB2 | 1.78 | 0.48 |
| 2:3T:132:LEU:HD23 | 2:3T:164:LYS:HE3 | 1.94 | 0.48 |
| 10:5A:406:LEU:HA | 10:5A:409:ASN:HD21 | 1.77 | 0.48 |
| 12:5F:137:THR:HG23 | 12:5F:140:GLN:H | 1.78 | 0.48 |
| 14:5L:174:TRP:CE2 | 14:5L:185:PRO:HB3 | 2.48 | 0.48 |
| 14:5L:218:VAL:O | 14:5L:232:GLY:N | 2.46 | 0.48 |
| 14:5M:415:LYS:HE2 | 23:6R:22:MET:SD | 2.52 | 0.48 |
| 14:5M:507:LEU:HD11 | 14:5M:525:LEU:HD12 | 1.95 | 0.48 |
| 14:5N:492:SER:HB3 | 14:5N:508:PHE:CE1 | 2.47 | 0.48 |
| 18:5Y:5:VAL:HG13 | 18:5Y:62:GLU:HG2 | 1.95 | 0.48 |
| 19:6E:36:VAL:HG11 | 19:6E:40:LEU:HA | 1.95 | 0.48 |
| 22:6O:23:TYR:HE2 | 22:6O:25:GLN:HA | 1.78 | 0.48 |
| 24:6T:461:SER:OG | 24:6T:464:ASP:OD2 | 2.29 | 0.48 |
| 24:6U:23:SER:HB3 | 24:6U:27:PHE:CZ | 2.48 | 0.48 |
| 24:6U:132:VAL:HB | 24:6U:148:ILE:HB | 1.95 | 0.48 |
| 24:6V:280:ASP:HA | 24:6V:289:ARG:HB2 | 1.95 | 0.48 |
| 24:6W:322:LEU:HD23 | 24:6W:323:LYS:O | 2.13 | 0.48 |
| 24:6Y:127:ASP:OD2 | 24:6Y:127:ASP:N | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Z:97:ARG:H | 24:6Z:188:THR:CG2 | 2.25 | 0.48 |
| 27:7G:189:GLU:N | 27:7G:189:GLU:OE2 | 2.45 | 0.48 |
| 34:7R:212:GLU:OE1 | 35:7T:167:ARG:NH1 | 2.37 | 0.48 |
| 37:7Y:128:TYR:C | 37:7Y:128:TYR:CD2 | 2.85 | 0.48 |
| 38:7Z:2:ASN:HB3 | 38:7Z:5:LYS:HB2 | 1.95 | 0.48 |
| 2:A2:18:ASN:O | 26:7F:114:PRO:HB2 | 2.13 | 0.48 |
| 1:E2:33:THR:HG21 | 22:6J:262:TYR:HB2 | 1.95 | 0.48 |
| 1:G4:58:ARG:HD3 | 1:I0:280:GLN:HE22 | 1.79 | 0.48 |
| 2:G5:155:GLU:O | 2:G5:159:VAL:HG23 | 2.13 | 0.48 |
| 2:G7:208:ALA:O | 2:G7:212:ILE:HG12 | 2.13 | 0.48 |
| 2:H1:108:TYR:O | 2:H1:112:LYS:NZ | 2.34 | 0.48 |
| 1:H4:186:THR:HG22 | 1:H4:411:ALA:HB1 | 1.94 | 0.48 |
| 1:H6:72:THR:O | 1:H6:76:VAL:HG23 | 2.12 | 0.48 |
| 1:I4:113:ILE:HD13 | 1:I4:150:LEU:HD22 | 1.95 | 0.48 |
| 2:I5:173:PRO:HB3 | 2:I5:183:GLU:OE1 | 2.12 | 0.48 |
| 2:J1:399:TYR:O | 2:J1:402:ARG:NH1 | 2.46 | 0.48 |
| 1:J6:115:SER:HA | 1:J6:118:ASP:OD1 | 2.12 | 0.48 |
| 2:K1:49:PHE:HB2 | 2:K1:53:PHE:HB2 | 1.95 | 0.48 |
| 2:K3:31:GLN:HE22 | 29:7I:247:GLY:HA3 | 1.78 | 0.48 |
| 2:K3:266:HIS:ND1 | 2:K3:266:HIS:O | 2.45 | 0.48 |
| 2:K5:170:THR:HG21 | 2:K5:194:LEU:HD11 | 1.95 | 0.48 |
| 2:L1:277:SER:OG | 2:L1:278:ALA:N | 2.45 | 0.48 |
| 2:L5:53:PHE:HB3 | 2:L5:61:HIS:HB3 | 1.95 | 0.48 |
| 2:L7:71:GLU:N | 2:L7:71:GLU:OE1 | 2.46 | 0.48 |
| 2:L7:230:LEU:O | 2:L7:234:VAL:HG23 | 2.13 | 0.48 |
| 2:L7:320:ARG:O | 2:L7:373:ARG:HA | 2.12 | 0.48 |
| 2:M3:98:ASP:OD1 | 2:M3:99:ALA:N | 2.45 | 0.48 |
| 1:M4:105:HIS:CD2 | 1:M4:150:LEU:HB2 | 2.48 | 0.48 |
| 2:M5:8:HIS:HE2 | 2:M5:17:GLY:HA3 | 1.79 | 0.48 |
| 2:M5:121:ARG:HD3 | 2:M5:121:ARG:C | 2.33 | 0.48 |
| 1:N0:39:ASP:OD1 | 1:N0:39:ASP:N | 2.46 | 0.48 |
| 1:N2:86:ARG:HD2 | 2:O9:283:HIS:CE1 | 2.48 | 0.48 |
| 2:N7:8:HIS:CD2 | 2:N7:138:PHE:HD2 | 2.31 | 0.48 |
| 2:N7:183:GLU:HG2 | 2:N7:184:PRO:HD3 | 1.96 | 0.48 |
| 1:O2:4:ILE:HB | 1:O2:50:TYR:HE1 | 1.78 | 0.48 |
| 2:O7:21:TRP:CZ3 | 2:O7:63:PRO:HB3 | 2.47 | 0.48 |
| 1:O8:10:GLY:HA2 | 1:O8:143:THR:HG23 | 1.95 | 0.48 |
| 1:Q2:190:HIS:HD2 | 1:Q2:414:ASN:HB2 | 1.78 | 0.48 |
| 2:Q3:155:GLU:O | 2:Q3:159:VAL:HG23 | 2.13 | 0.48 |
| 2:Q3:170:THR:HG21 | 2:Q3:194:LEU:HD11 | 1.95 | 0.48 |
| 1:Q4:139:LEU:HD12 | 1:Q4:170:VAL:HG12 | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q8:100:ASN:HB3 | 1:Q8:103:LYS:HB2 | 1.95 | 0.48 |
| 1:Q8:293:MET:SD | 1:Q8:367:PHE:HB2 | 2.53 | 0.48 |
| 1:R0:19:LYS:O | 1:R0:23:VAL:HG13 | 2.14 | 0.48 |
| 2:R1:188:VAL:O | 2:R1:191:THR:HG22 | 2.13 | 0.48 |
| 2:R1:259:LEU:HD11 | 2:R1:316:CYS:HB2 | 1.95 | 0.48 |
| 1:R2:309:ARG:NH1 | 1:R2:339:SER:O | 2.46 | 0.48 |
| 1:R6:70:PRO:CD | 1:R6:92:PHE:HZ | 2.27 | 0.48 |
| 2:R9:27:GLU:CD | 2:R9:243:ARG:HH12 | 2.17 | 0.48 |
| 1:S6:257:LEU:HD21 | 1:S6:314:SER:HB2 | 1.94 | 0.48 |
| 2:S9:207:GLU:OE2 | 13:5I:90:PRO:HG3 | 2.13 | 0.48 |
| 2:S9:305:CYS:HB3 | 2:S9:387:ILE:HD11 | 1.94 | 0.48 |
| 1:T0:183:TYR:HE2 | 1:T0:394:PHE:HB2 | 1.78 | 0.48 |
| 1:T6:108:GLU:HB3 | 1:T6:147:MET:HE1 | 1.95 | 0.48 |
| 2:V1:317:LEU:HB3 | 2:V1:319:TYR:HE1 | 1.77 | 0.48 |
| 1:W0:70:PRO:N | 1:W0:92:PHE:HZ | 2.11 | 0.48 |
| 1:W0:237:THR:HG23 | 1:W0:241:ARG:HE | 1.78 | 0.48 |
| 2:W1:224:TYR:H | 1:W2:245:GLN:NE2 | 2.11 | 0.48 |
| 1:W2:135:VAL:O | 1:W2:166:THR:HA | 2.13 | 0.48 |
| 2:W9:109:THR:HG22 | 2:W9:110:ILE:CD1 | 2.43 | 0.48 |
| 1:X0:49:VAL:HG11 | 1:X0:241:ARG:HG2 | 1.94 | 0.48 |
| 2:Y5:154:LEU:HD12 | 2:Y5:157:LEU:CD2 | 2.43 | 0.48 |
| 1:Y8:250:LEU:O | 1:Y8:253:LEU:HG | 2.12 | 0.48 |
| 2:Z1:251:ASP:OD1 | 2:Z1:252:ILE:HD12 | 2.14 | 0.48 |
| 1:Z2:207:LEU:HD13 | 1:Z2:225:LEU:HB3 | 1.94 | 0.48 |
| 1:Z4:8:GLN:HG3 | 1:Z4:17:GLY:HA3 | 1.94 | 0.48 |
| 1:Z4:174:LYS:HD3 | 1:Z4:205:GLU:OE2 | 2.14 | 0.48 |
| 1:Z8:69:GLU:HG2 | 1:Z8:72:THR:HG23 | 1.95 | 0.48 |
| 1:Z8:139:LEU:HG | 1:Z8:168:SER:HB3 | 1.96 | 0.48 |
| 1:0A:334:GLN:HE22 | 1:0A:347:ASN:H | 1.61 | 0.48 |
| 2:0F:320:ARG:O | 2:0F:373:ARG:HA | 2.13 | 0.48 |
| 1:0G:16:ILE:HD11 | 1:0G:136:CYS:HB3 | 1.95 | 0.48 |
| 1:0G:86:ARG:NH1 | 1:0G:89:ASN:OD1 | 2.47 | 0.48 |
| 1:0G:404:ASP:HB3 | 1:0G:406:MET:SD | 2.53 | 0.48 |
| 2:0H:15:GLN:HB3 | 2:0H:228:ASN:ND2 | 2.28 | 0.48 |
| 1:0I:52:ASN:OD1 | 1:0I:62:ARG:NH2 | 2.45 | 0.48 |
| 1:0K:2:ARG:HB3 | 1:0K:131:GLN:HB2 | 1.95 | 0.48 |
| 1:0K:207:LEU:HD11 | 1:0K:229:ILE:HD11 | 1.94 | 0.48 |
| 1:0M:91:VAL:HG11 | 1:0M:116:VAL:HG12 | 1.95 | 0.48 |
| 1:0Q:8:GLN:NE2 | 1:0Q:14:ASN:HA | 2.25 | 0.48 |
| 1:0S:248:ALA:HA | 1:0S:252:LYS:HD2 | 1.93 | 0.48 |
| 1:1A:135:VAL:O | 1:1A:166:THR:HA | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:204:ASN:HD21 | 39:1A:503:GDP:N2 | 2.09 | 0.48 |
| 2:1D:99:ALA:HA | 2:1D:105:ARG:HD3 | 1.95 | 0.48 |
| 1:1O:58:ARG:HG2 | 1:2E:280:GLN:HE22 | 1.78 | 0.48 |
| 2:1P:88:HIS:HB3 | 2:2F:283:HIS:CG | 2.48 | 0.48 |
| 2:1P:345:ASP:N | 2:1P:345:ASP:OD1 | 2.45 | 0.48 |
| 1:1U:21:TRP:HA | 1:1U:24:VAL:HG12 | 1.95 | 0.48 |
| 1:1U:396:HIS:HA | 1:1U:399:THR:OG1 | 2.13 | 0.48 |
| 1:1W:68:LEU:HB3 | 1:1W:96:GLY:HA2 | 1.95 | 0.48 |
| 2:1Z:116:ASP:N | 2:1Z:116:ASP:OD1 | 2.47 | 0.48 |
| 2:1Z:227:LEU:O | 2:1Z:231:ILE:HG12 | 2.13 | 0.48 |
| 2:2B:9:ILE:HG13 | 2:2B:68:LEU:HD21 | 1.94 | 0.48 |
| 2:2B:129:CYS:SG | 2:2B:130:THR:N | 2.86 | 0.48 |
| 1:2E:121:ARG:HD2 | 38:8B:98:TYR:O | 2.13 | 0.48 |
| 2:2F:201:ALA:O | 2:2F:268:MET:HE1 | 2.13 | 0.48 |
| 2:2F:286:LEU:O | 2:2F:373:ARG:NH1 | 2.47 | 0.48 |
| 1:2G:5:VAL:HG22 | 1:2G:133:PHE:HD1 | 1.78 | 0.48 |
| 1:2G:177:ASP:OD1 | 2:2H:248:LEU:HD11 | 2.13 | 0.48 |
| 2:2J:245:ASP:OD1 | 2:2J:245:ASP:N | 2.45 | 0.48 |
| 2:2L:333:ALA:O | 2:2L:337:THR:HG23 | 2.13 | 0.48 |
| 1:2M:244:GLY:HA2 | 1:2M:355:ASP:OD1 | 2.13 | 0.48 |
| 2:2N:56:THR:HB | 2:2N:60:LYS:HB3 | 1.94 | 0.48 |
| 1:2Q:91:VAL:HG11 | 1:2Q:116:VAL:HG12 | 1.96 | 0.48 |
| 2:3B:183:GLU:HG3 | 2:3B:184:PRO:HD3 | 1.95 | 0.48 |
| 2:3B:282:TYR:HD2 | 2:3B:282:TYR:H | 1.61 | 0.48 |
| 1:3I:118:ASP:OD1 | 1:3I:121:ARG:NH1 | 2.46 | 0.48 |
| 2:3J:88:HIS:HB3 | 2:3J:90:GLU:CD | 2.34 | 0.48 |
| 2:3R:35:GLN:N | 2:3R:35:GLN:OE1 | 2.46 | 0.48 |
| 2:3T:390:ARG:HG2 | 2:3T:394:LYS:NZ | 2.28 | 0.48 |
| 4:4E:22:LEU:H | 3:4F:258:ASP:CG | 2.16 | 0.48 |
| 4:4E:115:LYS:HB3 | 4:4E:116:PRO:HD2 | 1.94 | 0.48 |
| 7:4U:240:SER:N | 31:7N:8:ASP:OD1 | 2.45 | 0.48 |
| 8:4W:349:GLN:O | 8:4W:353:GLU:HG2 | 2.13 | 0.48 |
| 9:4Z:25:ARG:HB3 | 14:5L:540:TYR:CD1 | 2.44 | 0.48 |
| 9:4Z:194:ARG:O | 9:4Z:198:LEU:HG | 2.13 | 0.48 |
| 10:5B:177:GLU:O | 10:5B:180:GLU:HG3 | 2.13 | 0.48 |
| 14:5L:273:SER:O | 14:5L:274:THR:OG1 | 2.28 | 0.48 |
| 14:5N:594:HIS:N | 14:5N:620:PHE:HE2 | 2.01 | 0.48 |
| 15:5O:182:ASN:ND2 | 15:5O:185:ARG:HH21 | 2.11 | 0.48 |
| 17:5U:179:GLN:OE1 | 17:5U:179:GLN:HA | 2.14 | 0.48 |
| 22:6L:159:GLU:CD | 22:6L:159:GLU:H | 2.15 | 0.48 |
| 22:6L:177:LEU:HD23 | 22:6L:177:LEU:HA | 1.73 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6N:23:TYR:HE2 | 22:6N:25:GLN:HA | 1.77 | 0.48 |
| 22:6N:89:THR:HG22 | 22:6N:91:ILE:H | 1.79 | 0.48 |
| 22:6O:159:GLU:H | 22:6O:159:GLU:CD | 2.16 | 0.48 |
| 22:6P:314:CYS:HA | 22:6P:317:VAL:HG22 | 1.95 | 0.48 |
| 24:6T:480:ASN:HD21 | 24:6T:503:ILE:HD12 | 1.78 | 0.48 |
| 24:6T:505:LYS:HD2 | 24:6T:510:GLU:HB3 | 1.95 | 0.48 |
| 24:6V:126:GLU:HG2 | 24:6V:127:ASP:OD2 | 2.14 | 0.48 |
| 24:6X:513:THR:O | 24:6X:517:LEU:HD11 | 2.14 | 0.48 |
| 24:6Z:152:ARG:HD3 | 24:6Z:160:PHE:CG | 2.48 | 0.48 |
| 30:7L:272:LEU:HD13 | 30:7L:278:PHE:HE1 | 1.78 | 0.48 |
| 31:7N:53:ILE:O | 31:7N:57:ILE:HG13 | 2.14 | 0.48 |
| 35:7U:124:GLN:O | 35:7U:128:VAL:HG13 | 2.13 | 0.48 |
| 2:A2:29:GLY:CA | 26:7F:45:MET:HE3 | 2.36 | 0.48 |
| 2:A2:370:LYS:HG3 | 24:6Y:88:TRP:HZ3 | 1.77 | 0.48 |
| 1:A3:282:ARG:C | 1:T6:54:ALA:CB | 2.81 | 0.48 |
| 1:G0:216:LYS:HB2 | 24:6V:422:ASN:ND2 | 2.28 | 0.48 |
| 1:G2:5:VAL:HG23 | 1:G2:62:ARG:HG2 | 1.95 | 0.48 |
| 2:G5:71:GLU:HG3 | 1:G6:2:ARG:HH12 | 1.78 | 0.48 |
| 2:G5:205:ASP:OD1 | 2:G5:207:GLU:HG2 | 2.14 | 0.48 |
| 1:G8:183:TYR:HA | 1:G8:385:PHE:HE1 | 1.78 | 0.48 |
| 2:G9:422:ARG:HH12 | 2:G9:426:ALA:HB2 | 1.78 | 0.48 |
| 2:H1:71:GLU:HG2 | 2:H1:98:ASP:HB2 | 1.95 | 0.48 |
| 1:H2:190:HIS:NE2 | 1:H2:410:GLU:HG3 | 2.28 | 0.48 |
| 1:H6:177:ASP:O | 2:H7:352:LYS:HA | 2.12 | 0.48 |
| 2:I1:211:ASP:OD1 | 2:I1:214:ARG:NH2 | 2.47 | 0.48 |
| 1:I2:174:LYS:H | 1:I2:174:LYS:HD2 | 1.78 | 0.48 |
| 2:I5:148:GLY:O | 2:I5:151:SER:OG | 2.21 | 0.48 |
| 2:J1:222:PRO:CD | 1:J2:324:LYS:HE3 | 2.44 | 0.48 |
| 2:J1:234:VAL:HG13 | 2:J1:376:CYS:SG | 2.53 | 0.48 |
| 1:J2:301:CYS:SG | 1:J2:302:ALA:N | 2.85 | 0.48 |
| 2:J3:340:THR:HG23 | 2:J3:341:ILE:HG23 | 1.95 | 0.48 |
| 1:J4:211:CYS:HA | 1:J4:215:LEU:HB2 | 1.95 | 0.48 |
| 1:J6:121:ARG:NH2 | 1:J6:158:GLU:OE2 | 2.44 | 0.48 |
| 2:J7:413:MET:HB3 | 2:J7:417:GLU:OE2 | 2.14 | 0.48 |
| 1:J8:257:LEU:HD21 | 1:J8:314:SER:HB2 | 1.95 | 0.48 |
| 2:J9:60:LYS:HZ3 | 2:L5:282:TYR:HA | 1.78 | 0.48 |
| 1:K0:21:TRP:CZ2 | 1:K0:63:ALA:HB2 | 2.49 | 0.48 |
| 2:K3:198:THR:HG21 | 2:K3:201:ALA:HB2 | 1.95 | 0.48 |
| 1:K4:31:ASP:OD1 | 1:K4:35:THR:N | 2.35 | 0.48 |
| 1:K4:233:MET:O | 1:K4:236:ILE:HG22 | 2.12 | 0.48 |
| 2:K5:286:LEU:O | 2:K5:373:ARG:NH1 | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K7:187:SER:O | 2:K7:191:THR:HG23 | 2.13 | 0.48 |
| 2:K7:201:ALA:O | 2:K7:268:MET:HE2 | 2.13 | 0.48 |
| 2:K9:90:GLU:HB3 | 2:K9:121:ARG:NH1 | 2.27 | 0.48 |
| 2:L1:312:TYR:HD1 | 2:L1:381:SER:HB2 | 1.78 | 0.48 |
| 1:L2:178:THR:HG23 | 1:L2:181:GLU:HG3 | 1.95 | 0.48 |
| 2:L5:51:THR:HG21 | 2:L5:243:ARG:HG2 | 1.94 | 0.48 |
| 1:L6:12:CYS:SG | 1:L6:13:GLY:N | 2.86 | 0.48 |
| 1:L6:130:LEU:HD21 | 1:L6:133:PHE:CE1 | 2.48 | 0.48 |
| 2:L7:70:LEU:HD22 | 2:L7:110:ILE:HD12 | 1.95 | 0.48 |
| 2:M1:326:LYS:HG3 | 2:M1:327:ASP:N | 2.28 | 0.48 |
| 1:M2:183:TYR:OH | 1:M2:388:MET:HB3 | 2.14 | 0.48 |
| 2:M3:60:LYS:HD3 | 1:O0:280:GLN:HB3 | 1.96 | 0.48 |
| 1:M4:173:PRO:HD3 | 1:M4:380:ARG:CZ | 2.43 | 0.48 |
| 2:M7:88:HIS:HB2 | 1:O4:281:TYR:CE1 | 2.48 | 0.48 |
| 2:M9:11:GLN:NE2 | 1:N0:247:ASN:OD1 | 2.46 | 0.48 |
| 2:M9:14:ILE:HD11 | 2:M9:74:VAL:HG13 | 1.95 | 0.48 |
| 2:M9:39:ASP:OD2 | 32:7P:139:LYS:NZ | 2.46 | 0.48 |
| 2:N1:76:ASP:HA | 2:N1:79:ARG:HB2 | 1.94 | 0.48 |
| 1:N2:114:ASP:N | 1:N2:114:ASP:OD1 | 2.45 | 0.48 |
| 2:N7:21:TRP:CZ3 | 2:N7:63:PRO:HB3 | 2.48 | 0.48 |
| 1:N8:122:LYS:O | 1:N8:126:SER:OG | 2.22 | 0.48 |
| 2:N9:8:HIS:CD2 | 2:N9:138:PHE:HD2 | 2.31 | 0.48 |
| 1:O0:181:GLU:HG2 | 1:O0:182:PRO:HD3 | 1.95 | 0.48 |
| 2:O5:121:ARG:HA | 2:O5:121:ARG:HD3 | 1.59 | 0.48 |
| 1:O6:179:VAL:HB | 2:O7:258:ASN:HD22 | 1.78 | 0.48 |
| 1:O6:273:LEU:H | 1:O6:292:GLN:HE22 | 1.61 | 0.48 |
| 1:O6:393:ALA:CB | 2:O7:346:TRP:CZ3 | 2.95 | 0.48 |
| 1:O8:114:ASP:OD2 | 1:O8:115:SER:N | 2.46 | 0.48 |
| 2:P3:88:HIS:ND1 | 2:Q9:283:HIS:HB2 | 2.29 | 0.48 |
| 1:P8:54:ALA:HB3 | 1:P8:58:ARG:HB3 | 1.95 | 0.48 |
| 1:Q2:167:PHE:HE2 | 1:Q2:233:MET:HG3 | 1.79 | 0.48 |
| 2:Q5:223:THR:H | 2:Q5:226:ASN:ND2 | 2.10 | 0.48 |
| 2:Q9:90:GLU:N | 2:Q9:90:GLU:OE1 | 2.45 | 0.48 |
| 1:R0:87:PRO:HD3 | 1:S6:281:TYR:CD2 | 2.48 | 0.48 |
| 2:R3:12:ALA:O | 2:R3:16:VAL:HG23 | 2.14 | 0.48 |
| 2:R5:6:SER:O | 2:R5:65:CYS:HB2 | 2.14 | 0.48 |
| 1:R6:176:SER:HB3 | 2:R7:349:THR:OG1 | 2.14 | 0.48 |
| 2:S7:97:GLU:N | 2:S7:97:GLU:OE2 | 2.46 | 0.48 |
| 2:T3:88:HIS:CD2 | 2:T3:91:GLN:HG3 | 2.47 | 0.48 |
| 2:T3:434:GLU:OE2 | 13:5J:67:LYS:NZ | 2.46 | 0.48 |
| 2:U1:2:ARG:HA | 2:U1:133:GLN:HE21 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U4:286:VAL:HG12 | 1:U4:329:GLN:HG3 | 1.95 | 0.48 |
| 2:U5:379:SER:OG | 2:U5:380:ASN:N | 2.47 | 0.48 |
| 2:U9:66:ILE:O | 2:U9:66:ILE:HG13 | 2.13 | 0.48 |
| 2:V7:358:GLN:NE2 | 2:V7:359:PRO:HD2 | 2.29 | 0.48 |
| 2:V9:274:PRO:HD3 | 2:V9:374:ALA:HA | 1.94 | 0.48 |
| 2:W1:129:CYS:SG | 2:W1:130:THR:N | 2.86 | 0.48 |
| 2:W5:245:ASP:N | 2:W5:245:ASP:OD1 | 2.44 | 0.48 |
| 1:X2:141:GLY:HA3 | 39:X2:501:GDP:PB | 2.53 | 0.48 |
| 1:X6:130:LEU:HB2 | 1:X6:162:ARG:HE | 1.79 | 0.48 |
| 2:X7:98:ASP:OD2 | 1:X8:252:LYS:HE2 | 2.13 | 0.48 |
| 1:X8:183:TYR:HE2 | 1:X8:394:PHE:HB2 | 1.78 | 0.48 |
| 1:Y0:164:MET:SD | 1:Y0:196:ALA:HA | 2.53 | 0.48 |
| 2:Y5:431:ASP:O | 2:Y5:434:GLU:HG3 | 2.13 | 0.48 |
| 2:Y9:222:PRO:HD2 | 1:Z0:324:LYS:HE3 | 1.95 | 0.48 |
| 2:Z1:246:GLY:HA3 | 2:Z1:356:ASN:HA | 1.94 | 0.48 |
| 1:Z2:177:ASP:O | 2:Z3:352:LYS:HA | 2.13 | 0.48 |
| 1:Z6:163:MET:HB3 | 1:Z6:250:LEU:HD22 | 1.96 | 0.48 |
| 1:Z8:52:ASN:OD1 | 1:Z8:62:ARG:NH2 | 2.46 | 0.48 |
| 1:Z8:267:MET:HG2 | 1:Z8:299:MET:SD | 2.53 | 0.48 |
| 2:Z9:116:ASP:OD1 | 2:Z9:116:ASP:N | 2.45 | 0.48 |
| 1:0E:100:ASN:H | 1:0E:142:GLY:HA3 | 1.77 | 0.48 |
| 1:0E:260:PHE:HB2 | 1:0E:263:LEU:HD13 | 1.95 | 0.48 |
| 2:0F:81:GLY:O | 2:0F:84:ARG:NH1 | 2.43 | 0.48 |
| 2:0H:7:ILE:HD11 | 2:0H:137:VAL:HG12 | 1.96 | 0.48 |
| 2:0H:298:PRO:HA | 2:0H:301:MET:HG2 | 1.96 | 0.48 |
| 2:0J:88:HIS:HB3 | 2:0Z:283:HIS:CE1 | 2.49 | 0.48 |
| 2:0L:288:VAL:HG13 | 2:0L:319:TYR:HE2 | 1.78 | 0.48 |
| 2:0N:325:PRO:HA | 2:0N:328:VAL:HG12 | 1.94 | 0.48 |
| 1:0Q:116:VAL:O | 1:0Q:120:VAL:HG22 | 2.13 | 0.48 |
| 2:0R:271:SER:OG | 2:0R:377:MET:HB3 | 2.14 | 0.48 |
| 1:0W:229:ILE:HG22 | 1:0W:233:MET:HE2 | 1.95 | 0.48 |
| 1:1A:202:LEU:HD13 | 1:1A:300:MET:HB3 | 1.95 | 0.48 |
| 2:1B:156:ARG:HA | 2:1B:159:VAL:HG12 | 1.96 | 0.48 |
| 1:1E:21:TRP:HA | 1:1E:24:VAL:HG12 | 1.95 | 0.48 |
| 2:1F:111:GLY:HA2 | 2:1F:114:ILE:HG22 | 1.96 | 0.48 |
| 2:1L:63:PRO:HB2 | 2:1L:65:CYS:SG | 2.53 | 0.48 |
| 1:1M:273:LEU:H | 1:1M:292:GLN:HE22 | 1.61 | 0.48 |
| 2:1N:55:GLU:HG3 | 2:1N:55:GLU:O | 2.13 | 0.48 |
| 2:1N:269:LEU:HD11 | 2:1N:384:ILE:HG23 | 1.95 | 0.48 |
| 1:1Q:246:LEU:HD22 | 1:1Q:352:SER:HA | 1.95 | 0.48 |
| 2:1T:266:HIS:ND1 | 2:1T:266:HIS:O | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:176:SER:OG | 2:2B:349:THR:HB | 2.13 | 0.48 |
| 2:2D:98:ASP:OD1 | 2:2D:99:ALA:N | 2.46 | 0.48 |
| 2:2D:119:LEU:HD21 | 38:8A:27:HIS:CE1 | 2.49 | 0.48 |
| 2:2D:286:LEU:HD13 | 2:2D:371:VAL:HG13 | 1.96 | 0.48 |
| 1:2Q:263:LEU:HD13 | 1:2Q:422:TYR:CE1 | 2.46 | 0.48 |
| 1:2U:382:SER:HB2 | 1:2U:415:MET:HG2 | 1.95 | 0.48 |
| 2:2V:210:TYR:HB3 | 38:8B:67:PHE:HE2 | 1.79 | 0.48 |
| 1:2W:139:LEU:HD12 | 1:2W:170:VAL:HG12 | 1.95 | 0.48 |
| 2:2Z:394:LYS:HB2 | 1:3A:346:PRO:HG3 | 1.95 | 0.48 |
| 2:3B:205:ASP:OD1 | 2:3B:206:ASN:N | 2.44 | 0.48 |
| 1:3C:116:VAL:HA | 1:3C:119:VAL:HG12 | 1.95 | 0.48 |
| 2:3D:5:ILE:HG22 | 2:3D:64:ARG:HB3 | 1.94 | 0.48 |
| 2:3F:8:HIS:CD2 | 2:3F:138:PHE:HD2 | 2.30 | 0.48 |
| 2:3H:261:PRO:HG3 | 2:3H:313:MET:HE2 | 1.95 | 0.48 |
| 2:3J:156:ARG:HA | 2:3J:159:VAL:HG12 | 1.96 | 0.48 |
| 1:3K:117:LEU:HD11 | 1:3K:154:LYS:HB3 | 1.95 | 0.48 |
| 2:3L:217:LEU:HB3 | 2:3L:219:ILE:HD12 | 1.95 | 0.48 |
| 2:3N:296:PHE:CE2 | 2:3N:335:ILE:HD13 | 2.43 | 0.48 |
| 1:3S:152:ILE:HD12 | 1:3S:164:MET:SD | 2.53 | 0.48 |
| 2:3T:5:ILE:HD11 | 2:3T:135:PHE:CE1 | 2.48 | 0.48 |
| 4:3W:115:LYS:HB3 | 4:3W:116:PRO:HD2 | 1.94 | 0.48 |
| 4:4I:115:LYS:HB3 | 4:4I:116:PRO:HD2 | 1.94 | 0.48 |
| 6:4O:390:MET:SD | 6:4O:391:LEU:N | 2.86 | 0.48 |
| 6:4O:415:HIS:HA | 6:4O:418:GLU:OE1 | 2.13 | 0.48 |
| 8:4W:221:GLU:O | 8:4W:224:LEU:HG | 2.14 | 0.48 |
| 10:5C:426:LEU:O | 10:5C:429:LYS:HG3 | 2.13 | 0.48 |
| 12:5G:281:VAL:HG13 | 12:5G:286:SER:HA | 1.96 | 0.48 |
| 14:5L:415:LYS:NZ | 23:6Q:22:MET:HB2 | 2.28 | 0.48 |
| 14:5M:174:TRP:CE2 | 14:5M:185:PRO:HB3 | 2.48 | 0.48 |
| 14:5M:452:TRP:CZ3 | 14:5M:461:LEU:HB2 | 2.47 | 0.48 |
| 14:5N:174:TRP:CE2 | 14:5N:185:PRO:HB3 | 2.48 | 0.48 |
| 14:5N:273:SER:O | 14:5N:274:THR:OG1 | 2.28 | 0.48 |
| 15:5O:95:LEU:HD13 | 15:5O:217:GLU:HB2 | 1.95 | 0.48 |
| 15:5O:172:TRP:HE1 | 15:5O:207:GLY:CA | 2.27 | 0.48 |
| 15:5P:244:PRO:HA | 15:5P:247:VAL:HG22 | 1.95 | 0.48 |
| 18:6B:5:VAL:CG1 | 18:6B:62:GLU:HG2 | 2.44 | 0.48 |
| 22:6J:263:SER:HB2 | 22:6J:265:ASP:OD1 | 2.13 | 0.48 |
| 22:6J:291:GLU:O | 22:6J:295:LYS:HD3 | 2.13 | 0.48 |
| 22:6O:277:SER:OG | 22:6O:281:LYS:NZ | 2.34 | 0.48 |
| 24:6T:365:ASP:OD1 | 24:6T:365:ASP:N | 2.42 | 0.48 |
| 24:6V:591:ASP:N | 24:6V:591:ASP:OD1 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Y:111:MET:HG2 | 24:6Y:213:TYR:CE2 | 2.48 | 0.48 |
| 30:7K:30:LYS:HD3 | 30:7K:31:LEU:O | 2.13 | 0.48 |
| 30:7K:326:ASP:OD2 | 30:7K:329:ARG:NE | 2.45 | 0.48 |
| 34:7S:188:ILE:HG13 | 35:7U:143:TYR:CE1 | 2.45 | 0.48 |
| 34:7S:255:LEU:HD11 | 35:7U:205:ALA:HB1 | 1.95 | 0.48 |
| 36:7V:38:GLU:HA | 36:7V:41:GLU:OE1 | 2.13 | 0.48 |
| 38:8B:170:PHE:O | 38:8B:172:GLY:N | 2.46 | 0.48 |
| 38:8D:188:ARG:HG3 | 38:8D:189:ASP:N | 2.28 | 0.48 |
| 1:G2:78:SER:HB2 | 24:6W:499:GLU:HG2 | 1.96 | 0.48 |
| 2:G5:399:TYR:O | 2:G5:402:ARG:NH1 | 2.46 | 0.48 |
| 1:G6:216:LYS:HB3 | 24:6Y:422:ASN:OD1 | 2.13 | 0.48 |
| 1:G6:238:CYS:SG | 1:G6:318:ARG:NE | 2.85 | 0.48 |
| 1:G8:114:ASP:OD1 | 1:G8:114:ASP:N | 2.46 | 0.48 |
| 2:G9:51:THR:HG23 | 2:G9:52:PHE:CD2 | 2.49 | 0.48 |
| 1:H2:139:LEU:HG | 1:H2:168:SER:HB2 | 1.95 | 0.48 |
| 2:H3:264:ARG:NH2 | 2:H3:431:ASP:OD2 | 2.47 | 0.48 |
| 2:H9:116:ASP:OD1 | 2:H9:116:ASP:N | 2.46 | 0.48 |
| 2:I3:141:VAL:HG13 | 2:I3:170:THR:HG21 | 1.95 | 0.48 |
| 2:J1:336:LYS:O | 2:J1:339:ARG:NH2 | 2.46 | 0.48 |
| 1:J2:112:LEU:O | 1:J2:116:VAL:HG13 | 2.13 | 0.48 |
| 2:J7:394:LYS:HB2 | 1:J8:346:PRO:HG3 | 1.94 | 0.48 |
| 1:J8:101:TRP:HE3 | 1:J8:403:MET:HE1 | 1.78 | 0.48 |
| 2:J9:5:ILE:HD11 | 2:J9:135:PHE:CE2 | 2.48 | 0.48 |
| 2:K1:84:ARG:HH12 | 28:7X:407:LYS:HB2 | 1.77 | 0.48 |
| 2:K3:305:CYS:HB3 | 2:K3:387:ILE:HD11 | 1.96 | 0.48 |
| 2:K9:187:SER:O | 2:K9:191:THR:HG23 | 2.12 | 0.48 |
| 2:L3:244:PHE:HB2 | 2:L3:356:ASN:HD21 | 1.77 | 0.48 |
| 1:L4:8:GLN:OE1 | 1:L4:17:GLY:HA3 | 2.14 | 0.48 |
| 2:L5:156:ARG:HA | 2:L5:159:VAL:HG22 | 1.96 | 0.48 |
| 2:L7:191:THR:O | 2:L7:195:LEU:HG | 2.14 | 0.48 |
| 1:M6:207:LEU:HB3 | 1:M6:225:LEU:HD22 | 1.96 | 0.48 |
| 2:M7:305:CYS:HB3 | 2:M7:387:ILE:HD11 | 1.96 | 0.48 |
| 2:N5:90:GLU:HB2 | 2:N5:121:ARG:HH22 | 1.77 | 0.48 |
| 1:N8:105:HIS:NE2 | 1:N8:150:LEU:HD13 | 2.29 | 0.48 |
| 2:O5:205:ASP:OD2 | 2:O5:206:ASN:N | 2.45 | 0.48 |
| 2:O7:88:HIS:CD2 | 2:O7:90:GLU:H | 2.31 | 0.48 |
| 2:P3:2:ARG:HA | 2:P3:133:GLN:HE21 | 1.78 | 0.48 |
| 2:P3:182:VAL:HG22 | 1:P4:256:ASN:HD21 | 1.78 | 0.48 |
| 1:P4:204:ASN:HD21 | 39:P4:503:GDP:HN22 | 1.61 | 0.48 |
| 2:Q1:417:GLU:HA | 2:Q1:420:GLU:HG2 | 1.96 | 0.48 |
| 1:Q2:177:ASP:O | 2:Q3:352:LYS:HA | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q5:392:ASP:HB2 | 2:Q5:425:LEU:HD22 | 1.95 | 0.48 |
| 1:Q8:86:ARG:HG2 | 1:Q8:88:ASP:H | 1.77 | 0.48 |
| 1:R2:210:ILE:O | 1:R2:214:THR:OG1 | 2.25 | 0.48 |
| 2:R3:132:LEU:HD23 | 2:R3:164:LYS:HE2 | 1.95 | 0.48 |
| 2:R5:155:GLU:HG2 | 2:R5:197:HIS:CE1 | 2.48 | 0.48 |
| 1:S0:178:THR:HB | 1:S0:181:GLU:HG3 | 1.94 | 0.48 |
| 1:S4:257:LEU:HD11 | 1:S4:314:SER:HB2 | 1.94 | 0.48 |
| 2:S7:301:MET:HE1 | 2:S7:307:PRO:HD3 | 1.96 | 0.48 |
| 1:S8:386:THR:HG21 | 13:5I:47:ARG:HD3 | 1.96 | 0.48 |
| 2:S9:102:ASN:HB3 | 2:S9:105:ARG:HB3 | 1.96 | 0.48 |
| 1:T2:134:GLN:HE21 | 1:T2:167:PHE:HE2 | 1.62 | 0.48 |
| 1:T4:405:GLU:HA | 1:T4:408:PHE:HD2 | 1.78 | 0.48 |
| 2:T5:236:SER:OG | 2:T5:243:ARG:NH2 | 2.46 | 0.48 |
| 2:U3:47:ASP:OD1 | 2:U3:48:ALA:N | 2.46 | 0.48 |
| 1:U4:113:ILE:HD12 | 1:U4:150:LEU:HG | 1.95 | 0.48 |
| 1:U4:117:LEU:HA | 1:U4:120:VAL:HG12 | 1.95 | 0.48 |
| 1:U6:217:LEU:HD23 | 1:U6:276:ARG:HH22 | 1.77 | 0.48 |
| 1:U8:112:LEU:O | 1:U8:116:VAL:HG13 | 2.13 | 0.48 |
| 2:U9:47:ASP:N | 2:U9:47:ASP:OD1 | 2.45 | 0.48 |
| 1:V2:117:LEU:HA | 1:V2:120:VAL:HG12 | 1.96 | 0.48 |
| 2:V7:179:THR:O | 1:V8:350:LYS:HG2 | 2.13 | 0.48 |
| 1:V8:204:ASN:OD1 | 39:V8:502:GDP:O2' | 2.31 | 0.48 |
| 2:W3:195:LEU:HD11 | 2:W3:428:LEU:HD12 | 1.95 | 0.48 |
| 1:W8:262:ARG:NH2 | 1:W8:417:ASP:OD1 | 2.46 | 0.48 |
| 1:X0:86:ARG:HB3 | 1:X0:89:ASN:OD1 | 2.13 | 0.48 |
| 1:X0:317:PHE:HB3 | 1:X0:321:MET:SD | 2.54 | 0.48 |
| 1:X2:198:GLU:HB2 | 1:X2:266:PHE:CE2 | 2.48 | 0.48 |
| 2:X3:121:ARG:HE | 2:X3:124:LYS:NZ | 2.11 | 0.48 |
| 2:X3:251:ASP:H | 2:X3:254:GLU:HG2 | 1.79 | 0.48 |
| 1:X4:86:ARG:HG2 | 1:X4:88:ASP:H | 1.78 | 0.48 |
| 2:X7:205:ASP:OD2 | 2:X7:207:GLU:N | 2.45 | 0.48 |
| 2:X9:60:LYS:HE2 | 2:Z5:282:TYR:CZ | 2.49 | 0.48 |
| 2:X9:101:ASN:OD1 | 1:Y0:252:LYS:HG3 | 2.12 | 0.48 |
| 1:Y0:128:ASP:OD1 | 1:Y0:129:CYS:N | 2.43 | 0.48 |
| 1:Y0:273:LEU:H | 1:Y0:292:GLN:HE22 | 1.61 | 0.48 |
| 1:Y4:99:ASN:HD22 | 2:Y5:258:ASN:HD21 | 1.62 | 0.48 |
| 1:Y4:354:CYS:SG | 1:Y4:355:ASP:N | 2.86 | 0.48 |
| 1:Y8:268:VAL:HG12 | 1:Y8:368:ILE:HD13 | 1.96 | 0.48 |
| 1:Z4:274:THR:OG1 | 1:Z4:282:ARG:NH1 | 2.46 | 0.48 |
| 1:Z6:270:PHE:O | 1:Z6:298:ASN:ND2 | 2.41 | 0.48 |
| 1:0A:139:LEU:HD21 | 1:0A:168:SER:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0E:207:LEU:HD11 | 1:0E:229:ILE:HD11 | 1.95 | 0.48 |
| 1:0E:332:ASN:HA | 1:0E:335:ASN:HD21 | 1.79 | 0.48 |
| 2:0F:417:GLU:HA | 2:0F:420:GLU:HG2 | 1.94 | 0.48 |
| 2:0J:222:PRO:HD2 | 1:0K:324:LYS:HE3 | 1.94 | 0.48 |
| 1:0M:52:ASN:OD1 | 1:0M:62:ARG:NH2 | 2.46 | 0.48 |
| 2:0N:109:THR:HB | 2:0N:110:ILE:HD12 | 1.95 | 0.48 |
| 2:0N:174:SER:HB2 | 2:0N:177:VAL:HB | 1.95 | 0.48 |
| 2:0N:251:ASP:OD2 | 2:0N:253:THR:N | 2.47 | 0.48 |
| 1:0O:62:ARG:HG3 | 1:0O:123:GLU:OE2 | 2.13 | 0.48 |
| 2:0R:33:ASP:O | 2:0R:60:LYS:NZ | 2.46 | 0.48 |
| 2:0R:34:GLY:HA2 | 2:0R:86:LEU:HD13 | 1.96 | 0.48 |
| 1:0S:21:TRP:HA | 1:0S:24:VAL:HG12 | 1.95 | 0.48 |
| 2:0X:397:LEU:HD11 | 1:0Y:344:TRP:HA | 1.95 | 0.48 |
| 1:0Y:72:THR:O | 1:0Y:75:SER:OG | 2.27 | 0.48 |
| 2:1B:220:GLU:HG2 | 2:1B:221:ARG:HG3 | 1.95 | 0.48 |
| 2:1D:90:GLU:HB3 | 2:1D:121:ARG:NH1 | 2.28 | 0.48 |
| 2:1D:280:LYS:HA | 2:1D:283:HIS:HB3 | 1.94 | 0.48 |
| 2:1D:346:TRP:CZ3 | 2:1D:347:CYS:HB2 | 2.49 | 0.48 |
| 2:1F:155:GLU:O | 2:1F:159:VAL:HG23 | 2.12 | 0.48 |
| 2:1F:271:SER:HA | 2:1F:302:MET:HG2 | 1.95 | 0.48 |
| 2:1H:103:PHE:HB3 | 2:1H:408:TYR:HE2 | 1.78 | 0.48 |
| 1:1K:128:ASP:OD1 | 1:1K:128:ASP:N | 2.46 | 0.48 |
| 1:1M:285:THR:HG23 | 1:1M:287:PRO:HD2 | 1.95 | 0.48 |
| 1:1M:396:HIS:H | 1:1M:396:HIS:CD2 | 2.31 | 0.48 |
| 1:1S:114:ASP:N | 1:1S:114:ASP:OD1 | 2.46 | 0.48 |
| 2:2N:271:SER:OG | 2:2N:377:MET:HB3 | 2.13 | 0.48 |
| 2:2R:90:GLU:HG3 | 2:2R:121:ARG:NH1 | 2.27 | 0.48 |
| 2:2R:242:LEU:HD11 | 2:2R:252:ILE:HG12 | 1.95 | 0.48 |
| 1:2W:336:LYS:HZ1 | 38:8B:55:ALA:HB2 | 1.76 | 0.48 |
| 2:2X:42:ILE:HD11 | 14:5M:139:ALA:HB1 | 1.95 | 0.48 |
| 2:2X:409:VAL:HA | 2:2X:413:MET:O | 2.13 | 0.48 |
| 1:2Y:306:ARG:HD3 | 38:8C:96:GLY:HA3 | 1.89 | 0.48 |
| 2:2Z:297:GLU:CG | 38:8C:74:ILE:CG2 | 2.87 | 0.48 |
| 1:3A:190:HIS:HD2 | 1:3A:411:ALA:HA | 1.78 | 0.48 |
| 1:3K:214:THR:HG23 | 1:3K:297:LYS:NZ | 2.27 | 0.48 |
| 1:3K:282:ARG:HH21 | 1:3K:288:GLU:CD | 2.17 | 0.48 |
| 2:3L:21:TRP:CZ3 | 2:3L:63:PRO:HB3 | 2.49 | 0.48 |
| 1:3Q:406:MET:O | 1:3Q:410:GLU:HG2 | 2.13 | 0.48 |
| 2:3R:65:CYS:SG | 2:3R:66:ILE:N | 2.87 | 0.48 |
| 4:4A:115:LYS:HB3 | 4:4A:116:PRO:HD2 | 1.95 | 0.48 |
| 6:4O:484:VAL:O | 6:4O:487:ILE:HG22 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:158:ARG:O | 9:4Z:162:MET:HG3 | 2.13 | 0.48 |
| 9:4Z:350:ALA:O | 9:4Z:353:LEU:HG | 2.13 | 0.48 |
| 10:5A:325:THR:O | 10:5A:328:LEU:HG | 2.13 | 0.48 |
| 10:5B:243:LEU:O | 10:5B:246:ILE:HG22 | 2.13 | 0.48 |
| 14:5N:452:TRP:CZ3 | 14:5N:461:LEU:HB2 | 2.47 | 0.48 |
| 15:5O:56:LYS:N | 15:5O:56:LYS:HD3 | 2.29 | 0.48 |
| 15:5O:181:SER:OG | 15:5O:185:ARG:NH2 | 2.46 | 0.48 |
| 20:6F:73:GLN:HE22 | 20:6F:114:ASN:HB3 | 1.78 | 0.48 |
| 21:6G:14:LEU:HD13 | 21:6G:131:TYR:CE2 | 2.47 | 0.48 |
| 21:6H:107:GLY:HA3 | 21:6H:110:TRP:NE1 | 2.28 | 0.48 |
| 22:6O:31:TYR:O | 22:6O:32:LYS:HG3 | 2.13 | 0.48 |
| 24:6W:88:TRP:HA | 24:6W:126:GLU:HG3 | 1.96 | 0.48 |
| 24:6W:469:PHE:HB3 | 24:6W:484:GLU:CB | 2.42 | 0.48 |
| 24:6X:365:ASP:OD1 | 24:6X:365:ASP:N | 2.43 | 0.48 |
| 24:6X:473:TYR:CD2 | 24:6X:473:TYR:C | 2.86 | 0.48 |
| 24:7A:185:ASP:O | 24:7A:188:THR:OG1 | 2.28 | 0.48 |
| 27:7G:4:TYR:HD1 | 27:7G:6:HIS:H | 1.61 | 0.48 |
| 28:7H:317:GLU:O | 28:7H:321:MET:HG2 | 2.14 | 0.48 |
| 31:7M:56:HIS:O | 31:7M:59:THR:HG22 | 2.12 | 0.48 |
| 35:7T:220:GLN:O | 35:7T:224:GLU:HG2 | 2.13 | 0.48 |
| 1:1:337:ASN:HD21 | 3:3V:69:TYR:N | 1.90 | 0.48 |
| 2:C5:43:GLY:H | 24:6T:272:VAL:HG21 | 1.78 | 0.48 |
| 2:C9:100:ALA:N | 41:C9:501:GTP:O3G | 2.46 | 0.48 |
| 1:E2:320:ARG:NH2 | 22:6J:31:TYR:OH | 2.47 | 0.48 |
| 1:E8:217:LEU:HB3 | 24:6X:312:ASN:OD1 | 2.12 | 0.48 |
| 2:G1:287:SER:OG | 2:G1:288:VAL:N | 2.47 | 0.48 |
| 1:G2:237:THR:HG22 | 1:G2:237:THR:O | 2.14 | 0.48 |
| 2:G7:71:GLU:HG2 | 2:G7:73:THR:H | 1.78 | 0.48 |
| 2:G7:353:CYS:SG | 2:G7:354:GLY:N | 2.86 | 0.48 |
| 2:H3:69:ASP:OD2 | 2:H3:70:LEU:N | 2.45 | 0.48 |
| 2:H5:333:ALA:O | 2:H5:337:THR:HG23 | 2.13 | 0.48 |
| 1:H8:218:THR:H | 24:6W:489:ASN:HA | 1.78 | 0.48 |
| 1:I8:50:TYR:CE2 | 1:I8:241:ARG:HD3 | 2.48 | 0.48 |
| 2:I9:76:ASP:HA | 2:I9:79:ARG:HB2 | 1.94 | 0.48 |
| 2:J1:8:HIS:CD2 | 2:J1:138:PHE:HD2 | 2.31 | 0.48 |
| 2:J1:274:PRO:HB2 | 2:J1:276:ILE:HG12 | 1.96 | 0.48 |
| 1:J4:153:SER:OG | 1:J4:195:ASN:OD1 | 2.29 | 0.48 |
| 1:J8:186:THR:HG22 | 1:J8:411:ALA:HB1 | 1.96 | 0.48 |
| 2:K1:318:MET:O | 2:K1:375:VAL:HA | 2.13 | 0.48 |
| 2:K9:90:GLU:HB3 | 2:K9:121:ARG:HH12 | 1.79 | 0.48 |
| 2:K9:201:ALA:O | 2:K9:268:MET:HE2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L3:9:ILE:HG12 | 2:L3:68:LEU:HD21 | 1.96 | 0.48 |
| 2:L3:223:THR:HG23 | 2:L3:225:THR:H | 1.78 | 0.48 |
| 1:L6:320:ARG:HH12 | 29:7J:226:THR:HA | 1.78 | 0.48 |
| 2:M1:236:SER:O | 2:M1:243:ARG:NH2 | 2.47 | 0.48 |
| 1:M2:214:THR:HG23 | 1:M2:215:LEU:HD22 | 1.94 | 0.48 |
| 1:M4:396:HIS:H | 1:M4:396:HIS:CD2 | 2.31 | 0.48 |
| 2:M5:55:GLU:HG2 | 37:7Y:226:VAL:HG11 | 1.95 | 0.48 |
| 1:M6:1:MET:CE | 37:7Y:116:MET:HA | 2.42 | 0.48 |
| 2:M9:90:GLU:HB2 | 1:O6:281:TYR:HE2 | 1.78 | 0.48 |
| 2:N3:121:ARG:HH11 | 2:N3:124:LYS:HG3 | 1.78 | 0.48 |
| 2:N3:213:CYS:HA | 2:N3:217:LEU:HB2 | 1.95 | 0.48 |
| 2:N7:145:THR:OG1 | 41:N8:501:GTP:O1B | 2.32 | 0.48 |
| 1:N8:219:THR:O | 1:N8:219:THR:OG1 | 2.32 | 0.48 |
| 2:N9:9:ILE:HG22 | 2:N9:146:GLY:HA2 | 1.96 | 0.48 |
| 2:O5:70:LEU:HG | 2:O5:145:THR:HG23 | 1.95 | 0.48 |
| 1:O6:130:LEU:HB2 | 1:O6:162:ARG:HE | 1.78 | 0.48 |
| 2:P5:405:VAL:HG23 | 2:P5:418:PHE:HE2 | 1.78 | 0.48 |
| 2:P7:72:PRO:HD2 | 1:P8:2:ARG:NH1 | 2.27 | 0.48 |
| 2:P9:167:LEU:HD13 | 2:P9:200:VAL:HB | 1.96 | 0.48 |
| 1:Q0:8:GLN:CD | 1:Q0:17:GLY:HA3 | 2.34 | 0.48 |
| 1:Q0:49:VAL:HG11 | 1:Q0:241:ARG:HG2 | 1.96 | 0.48 |
| 2:Q1:72:PRO:HG3 | 1:Q2:1:MET:HG2 | 1.95 | 0.48 |
| 1:Q6:259:PRO:HG3 | 1:Q6:311:LEU:HD21 | 1.96 | 0.48 |
| 2:Q9:405:VAL:CG2 | 17:5S:112:VAL:HG11 | 2.42 | 0.48 |
| 1:R4:189:VAL:O | 1:R4:193:VAL:HG13 | 2.14 | 0.48 |
| 2:R7:12:ALA:O | 2:R7:16:VAL:HG23 | 2.14 | 0.48 |
| 1:R8:317:PHE:HB3 | 1:R8:321:MET:SD | 2.54 | 0.48 |
| 2:R9:26:LEU:HD22 | 2:R9:363:VAL:HG12 | 1.96 | 0.48 |
| 2:S7:259:LEU:HD11 | 2:S7:316:CYS:HB2 | 1.96 | 0.48 |
| 1:S8:244:GLY:HA2 | 1:S8:355:ASP:OD1 | 2.14 | 0.48 |
| 2:T1:97:GLU:OE1 | 2:T1:97:GLU:N | 2.46 | 0.48 |
| 1:T2:113:ILE:HA | 1:T2:116:VAL:HG22 | 1.96 | 0.48 |
| 1:T6:375:GLN:HE22 | 1:T6:423:GLN:NE2 | 2.11 | 0.48 |
| 1:T8:14:ASN:HD21 | 1:T8:65:LEU:HB3 | 1.79 | 0.48 |
| 2:V1:27:GLU:OE1 | 2:V1:243:ARG:NH1 | 2.47 | 0.48 |
| 2:V1:27:GLU:HG2 | 2:V1:361:THR:HG21 | 1.95 | 0.48 |
| 1:V6:86:ARG:HG2 | 1:V6:88:ASP:H | 1.78 | 0.48 |
| 2:V7:384:ILE:HA | 2:V7:387:ILE:HD12 | 1.96 | 0.48 |
| 1:X2:294:TRP:HE1 | 1:X2:330:MET:HE1 | 1.79 | 0.48 |
| 2:X5:172:TYR:CE2 | 2:X5:203:MET:HG2 | 2.49 | 0.48 |
| 1:X6:263:LEU:HD21 | 1:X6:421:GLU:OE1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X7:239:THR:HG23 | 2:X7:243:ARG:HE | 1.77 | 0.48 |
| 2:X9:60:LYS:HE3 | 2:X9:88:HIS:NE2 | 2.28 | 0.48 |
| 1:Y6:260:PHE:HB2 | 1:Y6:263:LEU:HD23 | 1.96 | 0.48 |
| 1:Y8:101:TRP:HB2 | 1:Y8:184:ASN:OD1 | 2.12 | 0.48 |
| 2:Y9:34:GLY:HA3 | 2:Y9:60:LYS:NZ | 2.28 | 0.48 |
| 2:Y9:157:LEU:HG | 2:Y9:166:LYS:HD3 | 1.95 | 0.48 |
| 1:Z2:24:VAL:HG12 | 1:Z2:27:GLU:OE2 | 2.14 | 0.48 |
| 1:Z4:382:SER:O | 1:Z4:386:THR:HG23 | 2.14 | 0.48 |
| 2:Z9:334:THR:HA | 2:Z9:337:THR:HG22 | 1.96 | 0.48 |
| 1:0A:69:GLU:HG2 | 1:0A:72:THR:HG23 | 1.96 | 0.48 |
| 2:0B:312:TYR:HB2 | 2:0B:343:PHE:CD1 | 2.48 | 0.48 |
| 2:0F:30:ILE:HG12 | 2:0F:36:MET:HG2 | 1.96 | 0.48 |
| 1:0G:385:PHE:HZ | 1:0G:408:PHE:HD1 | 1.62 | 0.48 |
| 2:0H:2:ARG:HA | 2:0H:133:GLN:HE21 | 1.78 | 0.48 |
| 2:0H:90:GLU:H | 2:0X:283:HIS:HE1 | 1.60 | 0.48 |
| 1:0O:284:LEU:HG | 1:0O:362:LYS:HD3 | 1.96 | 0.48 |
| 1:0S:2:ARG:NE | 1:0S:240:LEU:HD22 | 2.28 | 0.48 |
| 2:0X:203:MET:SD | 2:0X:267:PHE:HB3 | 2.54 | 0.48 |
| 1:0Y:311:LEU:HD21 | 1:0Y:372:THR:HB | 1.96 | 0.48 |
| 1:1C:396:HIS:H | 1:1C:396:HIS:CD2 | 2.31 | 0.48 |
| 2:1F:387:ILE:HG12 | 2:1F:390:ARG:NH2 | 2.28 | 0.48 |
| 2:1L:50:ASN:O | 2:1L:64:ARG:NH2 | 2.46 | 0.48 |
| 2:1N:65:CYS:SG | 2:1N:66:ILE:N | 2.86 | 0.48 |
| 1:1O:198:GLU:HB3 | 1:1O:258:ILE:HD11 | 1.95 | 0.48 |
| 2:1P:333:ALA:O | 2:1P:337:THR:HG23 | 2.14 | 0.48 |
| 2:1R:88:HIS:HD2 | 2:1R:90:GLU:H | 1.59 | 0.48 |
| 2:2B:276:ILE:CG2 | 2:2B:281:ALA:HB2 | 2.43 | 0.48 |
| 2:2B:387:ILE:HG12 | 2:2B:390:ARG:HH22 | 1.78 | 0.48 |
| 2:2D:118:ALA:O | 2:2D:122:ILE:HG13 | 2.14 | 0.48 |
| 1:2E:117:LEU:HA | 1:2E:120:VAL:HG12 | 1.96 | 0.48 |
| 1:2E:324:LYS:HA | 1:2E:327:ASP:OD1 | 2.13 | 0.48 |
| 1:2G:207:LEU:HB3 | 1:2G:225:LEU:HD22 | 1.95 | 0.48 |
| 2:2L:47:ASP:OD1 | 2:2L:48:ALA:N | 2.47 | 0.48 |
| 2:2N:49:PHE:HB2 | 2:2N:53:PHE:HD2 | 1.79 | 0.48 |
| 2:2N:102:ASN:ND2 | 2:2N:105:ARG:HB2 | 2.28 | 0.48 |
| 2:2P:47:ASP:N | 2:2P:47:ASP:OD1 | 2.46 | 0.48 |
| 1:2Q:135:VAL:HG21 | 1:2Q:152:ILE:HD11 | 1.95 | 0.48 |
| 1:2Q:177:ASP:O | 2:2R:352:LYS:HA | 2.14 | 0.48 |
| 2:2T:298:PRO:HA | 2:2T:301:MET:HG3 | 1.95 | 0.48 |
| 1:2Y:320:ARG:NH1 | 38:8C:197:THR:O | 2.40 | 0.48 |
| 2:3D:119:LEU:HD11 | 2:3D:156:ARG:HB3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3D:211:ASP:OD2 | 38:8D:67:PHE:HB2 | 2.13 | 0.48 |
| 2:3F:214:ARG:HA | 2:3F:219:ILE:O | 2.14 | 0.48 |
| 2:3F:320:ARG:NH2 | 2:3F:359:PRO:O | 2.47 | 0.48 |
| 2:3N:21:TRP:CZ2 | 2:3N:65:CYS:HB3 | 2.49 | 0.48 |
| 1:3O:117:LEU:HD21 | 1:3O:121:ARG:HH22 | 1.79 | 0.48 |
| 10:5A:360:GLN:HA | 10:5A:363:ARG:NH2 | 2.28 | 0.48 |
| 10:5B:313:GLU:O | 10:5B:316:ARG:HG3 | 2.13 | 0.48 |
| 12:5F:316:GLN:HB2 | 12:7B:58:ARG:HD2 | 1.96 | 0.48 |
| 14:5L:36:SER:HA | 14:5L:59:VAL:HG12 | 1.94 | 0.48 |
| 14:5L:452:TRP:CZ3 | 14:5L:461:LEU:HB2 | 2.47 | 0.48 |
| 14:5L:594:HIS:N | 14:5L:620:PHE:HE2 | 2.01 | 0.48 |
| 14:5M:36:SER:HA | 14:5M:59:VAL:HG12 | 1.94 | 0.48 |
| 14:5M:594:HIS:N | 14:5M:620:PHE:HE2 | 2.01 | 0.48 |
| 14:5N:36:SER:HA | 14:5N:59:VAL:HG12 | 1.94 | 0.48 |
| 15:5O:185:ARG:NH1 | 15:5O:197:GLY:O | 2.42 | 0.48 |
| 15:5O:264:GLU:OE2 | 15:5O:314:ARG:HG3 | 2.13 | 0.48 |
| 15:5O:320:VAL:HG21 | 15:5O:362:PRO:HA | 1.96 | 0.48 |
| 20:6F:131:GLU:H | 20:6F:131:GLU:CD | 2.16 | 0.48 |
| 20:6F:285:THR:HA | 20:6F:288:TYR:CD2 | 2.48 | 0.48 |
| 22:6L:53:THR:O | 22:6L:57:THR:OG1 | 2.31 | 0.48 |
| 22:6M:203:HIS:CD2 | 22:6M:204:PHE:H | 2.32 | 0.48 |
| 22:6N:290:LEU:O | 22:6N:294:LEU:HG | 2.13 | 0.48 |
| 24:6U:540:LEU:HD13 | 24:6U:614:ARG:HD2 | 1.95 | 0.48 |
| 24:6V:415:THR:HG23 | 24:6V:418:ASP:H | 1.78 | 0.48 |
| 24:6W:376:LYS:O | 24:6W:380:LYS:HG3 | 2.14 | 0.48 |
| 24:6W:602:LEU:HG | 24:6W:604:PHE:HD1 | 1.79 | 0.48 |
| 24:6X:450:VAL:CG1 | 24:6X:469:PHE:O | 2.62 | 0.48 |
| 24:6Z:559:ILE:O | 24:6Z:563:LYS:HG2 | 2.13 | 0.48 |
| 32:7O:70:THR:OG1 | 32:7O:72:GLU:HG3 | 2.14 | 0.48 |
| 34:7R:232:ASP:O | 34:7R:236:THR:HG23 | 2.14 | 0.48 |
| 34:7S:149:LYS:HA | 34:7S:152:VAL:HG12 | 1.95 | 0.48 |
| 35:7T:84:ALA:O | 35:7T:87:ILE:HG22 | 2.13 | 0.48 |
| 38:8B:58:LYS:HD2 | 38:8B:58:LYS:H | 1.79 | 0.48 |
| 38:8C:10:ALA:HA | 38:8C:17:GLY:HA2 | 1.96 | 0.48 |
| 38:8D:83:ARG:HD2 | 38:8D:113:ARG:HD3 | 1.96 | 0.48 |
| 2:6:372:GLN:NE2 | 24:6V:88:TRP:CE2 | 2.80 | 0.48 |
| 1:B8:39:ASP:O | 18:6B:119:ARG:NH1 | 2.46 | 0.48 |
| 1:E4:35:THR:HG21 | 22:6K:260:VAL:H | 1.77 | 0.48 |
| 2:G5:47:ASP:OD1 | 2:G5:47:ASP:N | 2.46 | 0.48 |
| 1:G6:72:THR:O | 1:G6:76:VAL:HG13 | 2.14 | 0.48 |
| 1:G6:78:SER:OG | 24:6Y:499:GLU:OE2 | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G8:66:MET:HE1 | 1:G8:147:MET:HG2 | 1.96 | 0.48 |
| 1:G8:313:ALA:HA | 1:G8:369:GLY:HA2 | 1.94 | 0.48 |
| 1:H4:301:CYS:SG | 1:H4:302:ALA:N | 2.86 | 0.48 |
| 2:H9:264:ARG:NH2 | 2:H9:431:ASP:OD2 | 2.46 | 0.48 |
| 1:I0:386:THR:O | 1:I0:390:ARG:HG3 | 2.13 | 0.48 |
| 1:I2:52:ASN:OD1 | 1:I2:62:ARG:NH2 | 2.42 | 0.48 |
| 1:I2:219:THR:HB | 2:I3:324:VAL:HG11 | 1.95 | 0.48 |
| 1:I2:371:SER:OG | 1:I2:372:THR:N | 2.46 | 0.48 |
| 1:I4:52:ASN:OD1 | 1:I4:62:ARG:NH2 | 2.45 | 0.48 |
| 2:I5:188:VAL:HG23 | 2:I5:425:LEU:HD12 | 1.95 | 0.48 |
| 2:I9:9:ILE:HD13 | 2:I9:150:GLY:HA2 | 1.94 | 0.48 |
| 2:I9:9:ILE:HG12 | 2:I9:68:LEU:HD21 | 1.96 | 0.48 |
| 1:J2:60:VAL:HG23 | 1:J2:84:ILE:O | 2.14 | 0.48 |
| 1:J2:86:ARG:HG2 | 1:J2:88:ASP:H | 1.77 | 0.48 |
| 2:J3:109:THR:OG1 | 2:J3:411:GLU:OE2 | 2.21 | 0.48 |
| 1:J6:385:PHE:HE2 | 1:J6:412:GLU:HG3 | 1.79 | 0.48 |
| 2:J7:73:THR:HG23 | 1:J8:2:ARG:HH12 | 1.78 | 0.48 |
| 2:K5:15:GLN:HA | 2:K5:18:ASN:HD21 | 1.79 | 0.48 |
| 2:K7:9:ILE:HG22 | 2:K7:146:GLY:HA2 | 1.95 | 0.48 |
| 1:K8:107:THR:OG1 | 1:K8:108:GLU:OE1 | 2.24 | 0.48 |
| 2:K9:66:ILE:HG13 | 2:K9:66:ILE:O | 2.14 | 0.48 |
| 1:L0:70:PRO:N | 1:L0:92:PHE:HZ | 2.12 | 0.48 |
| 2:L3:90:GLU:HB3 | 2:L3:121:ARG:NH1 | 2.29 | 0.48 |
| 1:L6:345:ILE:HB | 1:L6:348:ASN:HD21 | 1.79 | 0.48 |
| 2:L7:236:SER:O | 2:L7:243:ARG:NH2 | 2.47 | 0.48 |
| 2:L9:241:SER:OG | 2:L9:250:VAL:O | 2.25 | 0.48 |
| 2:M1:223:THR:HG23 | 2:M1:225:THR:H | 1.78 | 0.48 |
| 2:M7:183:GLU:HG3 | 2:M7:184:PRO:HD3 | 1.95 | 0.48 |
| 1:N2:204:ASN:OD1 | 39:N2:501:GDP:O2' | 2.30 | 0.48 |
| 2:N3:103:PHE:CD1 | 2:N3:148:GLY:HA2 | 2.48 | 0.48 |
| 2:N3:277:SER:OG | 2:N3:278:ALA:N | 2.46 | 0.48 |
| 2:N7:276:ILE:HD11 | 2:N7:280:LYS:HB3 | 1.95 | 0.48 |
| 2:N7:327:ASP:N | 2:N7:327:ASP:OD1 | 2.47 | 0.48 |
| 2:O3:214:ARG:CZ | 37:7Y:84:ARG:HH22 | 2.27 | 0.48 |
| 2:O5:65:CYS:SG | 2:O5:66:ILE:N | 2.86 | 0.48 |
| 2:O5:286:LEU:HD13 | 2:O5:371:VAL:HG23 | 1.95 | 0.48 |
| 2:O7:313:MET:HE3 | 2:O7:346:TRP:CH2 | 2.48 | 0.48 |
| 2:P5:41:THR:CA | 27:7G:220:MET:O | 2.61 | 0.48 |
| 2:P5:313:MET:N | 2:P5:380:ASN:O | 2.43 | 0.48 |
| 1:P8:172:SER:OG | 1:P8:205:GLU:OE1 | 2.20 | 0.48 |
| 1:Q0:45:GLU:HG3 | 1:Q0:46:ARG:HG2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:292:GLN:HG2 | 1:Q0:298:ASN:HD22 | 1.78 | 0.48 |
| 2:Q3:306:ASP:OD2 | 2:V1:282:TYR:OH | 2.22 | 0.48 |
| 1:Q6:309:ARG:H | 1:Q6:372:THR:HG22 | 1.79 | 0.48 |
| 2:Q9:205:ASP:OD2 | 2:Q9:303:VAL:HG13 | 2.14 | 0.48 |
| 1:R0:87:PRO:HD3 | 1:S6:281:TYR:CE2 | 2.49 | 0.48 |
| 2:R1:175:PRO:HG2 | 2:R1:176:GLN:OE1 | 2.14 | 0.48 |
| 2:R3:207:GLU:HG3 | 2:R3:304:LYS:HD2 | 1.95 | 0.48 |
| 1:R8:272:PRO:HB2 | 1:R8:282:ARG:HH22 | 1.79 | 0.48 |
| 2:R9:220:GLU:HG2 | 2:R9:221:ARG:HG3 | 1.96 | 0.48 |
| 2:R9:277:SER:OG | 2:R9:278:ALA:N | 2.45 | 0.48 |
| 1:S0:405:GLU:OE1 | 1:S0:406:MET:HG2 | 2.13 | 0.48 |
| 1:S4:414:ASN:ND2 | 3:3V:84:LYS:HD2 | 2.29 | 0.48 |
| 1:S6:320:ARG:HH12 | 31:7M:29:GLU:HB3 | 1.78 | 0.48 |
| 2:S9:105:ARG:O | 2:S9:109:THR:OG1 | 2.32 | 0.48 |
| 1:T0:244:GLY:HA2 | 1:T0:355:ASP:OD1 | 2.13 | 0.48 |
| 2:T3:7:ILE:HD11 | 2:T3:137:VAL:HG12 | 1.95 | 0.48 |
| 2:T3:379:SER:OG | 2:T3:380:ASN:N | 2.46 | 0.48 |
| 2:T7:317:LEU:HB3 | 2:T7:319:TYR:HE1 | 1.78 | 0.48 |
| 2:U1:217:LEU:HG | 2:U1:275:ILE:HG22 | 1.96 | 0.48 |
| 1:U2:334:GLN:HE22 | 1:U2:348:ASN:H | 1.60 | 0.48 |
| 2:U3:2:ARG:HA | 2:U3:133:GLN:HE21 | 1.79 | 0.48 |
| 1:U6:218:THR:O | 2:U7:326:LYS:HE2 | 2.14 | 0.48 |
| 2:V3:11:GLN:OE1 | 2:V3:15:GLN:NE2 | 2.46 | 0.48 |
| 2:W9:70:LEU:CD1 | 2:W9:110:ILE:HG21 | 2.44 | 0.48 |
| 2:W9:288:VAL:O | 2:W9:292:THR:HG23 | 2.13 | 0.48 |
| 2:X3:52:PHE:CE2 | 2:X3:243:ARG:HD3 | 2.48 | 0.48 |
| 1:X4:22:GLU:OE1 | 1:X4:80:PRO:HG2 | 2.14 | 0.48 |
| 2:X5:217:LEU:HD21 | 2:X5:367:ASP:HB2 | 1.95 | 0.48 |
| 2:X7:265:ILE:HD11 | 2:X7:435:VAL:HG21 | 1.96 | 0.48 |
| 2:X9:102:ASN:HB3 | 2:X9:105:ARG:HB3 | 1.95 | 0.48 |
| 1:Y0:257:LEU:HA | 1:Y0:312:THR:HG21 | 1.94 | 0.48 |
| 2:Y3:282:TYR:CE2 | 8:4W:373:ASN:CG | 2.86 | 0.48 |
| 2:Y5:108:TYR:HA | 2:Y5:112:LYS:NZ | 2.29 | 0.48 |
| 2:Y5:253:THR:O | 2:Y5:257:THR:HG23 | 2.14 | 0.48 |
| 2:Y9:223:THR:HG23 | 2:Y9:225:THR:H | 1.78 | 0.48 |
| 2:Y9:286:LEU:HD11 | 2:Y9:372:GLN:HB2 | 1.94 | 0.48 |
| 1:Z2:122:LYS:O | 1:Z2:126:SER:OG | 2.18 | 0.48 |
| 1:Z2:205:GLU:HG2 | 1:Z2:206:ALA:N | 2.29 | 0.48 |
| 1:Z4:74:ASP:OD1 | 1:Z4:75:SER:N | 2.47 | 0.48 |
| 1:Z4:273:LEU:H | 1:Z4:292:GLN:HE22 | 1.62 | 0.48 |
| 2:Z9:4:VAL:HG12 | 2:Z9:133:GLN:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z9:34:GLY:HA3 | 2:Z9:60:LYS:NZ | 2.29 | 0.48 |
| 2:Z9:269:LEU:N | 2:Z9:379:SER:O | 2.47 | 0.48 |
| 1:0A:49:VAL:HG21 | 1:0A:241:ARG:HG2 | 1.96 | 0.48 |
| 1:0A:242:PHE:HB2 | 1:0A:354:CYS:SG | 2.54 | 0.48 |
| 1:0A:285:THR:HB | 1:0A:287:PRO:HD2 | 1.95 | 0.48 |
| 1:0A:344:TRP:CE3 | 1:0A:345:ILE:HG13 | 2.48 | 0.48 |
| 2:0B:3:GLU:HG3 | 2:0B:51:THR:HA | 1.95 | 0.48 |
| 2:0B:31:GLN:HE21 | 2:0B:37:PRO:HG3 | 1.78 | 0.48 |
| 2:0B:90:GLU:HB2 | 2:0B:121:ARG:HH22 | 1.78 | 0.48 |
| 2:0B:225:THR:HG22 | 2:0B:229:ARG:HE | 1.78 | 0.48 |
| 2:0H:280:LYS:HA | 2:0H:283:HIS:HB3 | 1.94 | 0.48 |
| 2:0L:75:VAL:HG21 | 2:0L:94:SER:HB2 | 1.95 | 0.48 |
| 2:0N:407:TRP:CG | 1:0O:255:VAL:HG23 | 2.49 | 0.48 |
| 1:0S:153:SER:HA | 1:0S:195:ASN:ND2 | 2.29 | 0.48 |
| 1:0U:406:MET:SD | 1:0U:406:MET:N | 2.86 | 0.48 |
| 2:0V:9:ILE:HG23 | 2:0V:68:LEU:HD11 | 1.95 | 0.48 |
| 2:0X:90:GLU:HG3 | 2:0X:121:ARG:NH1 | 2.28 | 0.48 |
| 1:1A:67:ASP:N | 1:1A:67:ASP:OD1 | 2.45 | 0.48 |
| 2:1B:242:LEU:HD12 | 2:1B:252:ILE:HG13 | 1.94 | 0.48 |
| 1:1C:203:ASP:OD2 | 1:1C:204:ASN:N | 2.47 | 0.48 |
| 1:1C:236:ILE:HG23 | 1:1C:237:THR:HG23 | 1.96 | 0.48 |
| 2:1F:169:PHE:CD1 | 2:1F:235:ILE:HD11 | 2.49 | 0.48 |
| 1:1O:5:VAL:HG22 | 1:1O:133:PHE:HD1 | 1.79 | 0.48 |
| 2:1P:111:GLY:HA2 | 2:1P:114:ILE:HG22 | 1.95 | 0.48 |
| 2:1P:306:ASP:HB3 | 2:1P:309:HIS:CD2 | 2.48 | 0.48 |
| 2:1T:417:GLU:HA | 2:1T:420:GLU:HG2 | 1.96 | 0.48 |
| 2:1V:121:ARG:CG | 2:1V:121:ARG:NH1 | 2.56 | 0.48 |
| 1:2A:131:GLN:HE21 | 1:2A:250:LEU:HB2 | 1.78 | 0.48 |
| 1:2I:83:GLN:O | 1:2Y:281:TYR:OH | 2.24 | 0.48 |
| 1:2K:317:PHE:HB2 | 1:2K:353:VAL:HG22 | 1.96 | 0.48 |
| 2:2L:33:ASP:OD2 | 2:2L:35:GLN:NE2 | 2.47 | 0.48 |
| 2:2N:156:ARG:HA | 2:2N:159:VAL:HG22 | 1.96 | 0.48 |
| 1:2S:309:ARG:H | 1:2S:372:THR:HG22 | 1.79 | 0.48 |
| 2:2T:69:ASP:OD2 | 2:2T:71:GLU:N | 2.46 | 0.48 |
| 2:2X:399:TYR:O | 2:2X:402:ARG:NH1 | 2.46 | 0.48 |
| 1:3A:10:GLY:HA2 | 1:3A:143:THR:HG23 | 1.95 | 0.48 |
| 2:3B:91:GLN:O | 2:3B:93:ILE:HG12 | 2.14 | 0.48 |
| 1:3C:274:THR:HG23 | 1:3C:279:GLN:HG2 | 1.95 | 0.48 |
| 1:3C:309:ARG:NH1 | 1:3C:339:SER:O | 2.46 | 0.48 |
| 2:3D:267:PHE:HB2 | 2:3D:384:ILE:HD12 | 1.94 | 0.48 |
| 1:3I:218:THR:OG1 | 38:8B:227:LYS:HA | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3J:72:PRO:HG2 | 1:3K:46:ARG:HH22 | 1.79 | 0.48 |
| 2:3J:333:ALA:O | 2:3J:337:THR:HG23 | 2.13 | 0.48 |
| 2:3R:132:LEU:HD23 | 2:3R:164:LYS:HE3 | 1.96 | 0.48 |
| 1:3S:67:ASP:N | 1:3S:67:ASP:OD1 | 2.46 | 0.48 |
| 1:3S:111:GLU:HG3 | 3:4J:139:SER:HB2 | 1.95 | 0.48 |
| 4:4C:115:LYS:HB3 | 4:4C:116:PRO:HD2 | 1.94 | 0.48 |
| 6:4O:358:LYS:HB2 | 6:4O:362:ARG:HH21 | 1.78 | 0.48 |
| 7:4R:86:ALA:O | 7:4R:90:GLN:HG2 | 2.14 | 0.48 |
| 9:4Z:297:ARG:HA | 9:4Z:300:ARG:HD2 | 1.96 | 0.48 |
| 10:5C:406:LEU:O | 10:5C:410:ARG:HG3 | 2.13 | 0.48 |
| 14:5M:166:ALA:HB3 | 14:5M:170:ASN:H | 1.78 | 0.48 |
| 16:5Q:27:PHE:CD2 | 16:5Q:110:LEU:HD21 | 2.49 | 0.48 |
| 21:6H:56:LYS:HD3 | 21:6H:61:HIS:HB2 | 1.96 | 0.48 |
| 21:6H:106:ARG:HG3 | 24:6X:80:ASP:HB2 | 1.94 | 0.48 |
| 22:6M:314:CYS:HA | 22:6M:317:VAL:HG12 | 1.95 | 0.48 |
| 24:6T:290:ARG:HG3 | 24:6T:291:PRO:HD2 | 1.95 | 0.48 |
| 24:6X:358:PHE:CE1 | 24:6X:367:TYR:HB2 | 2.49 | 0.48 |
| 30:7L:377:GLU:OE2 | 30:7L:377:GLU:N | 2.44 | 0.48 |
| 34:7R:203:TYR:O | 34:7R:207:GLU:HG2 | 2.14 | 0.48 |
| 36:7W:38:GLU:HA | 36:7W:41:GLU:OE1 | 2.13 | 0.48 |
| 38:8A:8:GLU:O | 38:8A:12:LEU:HB2 | 2.12 | 0.48 |
| 38:8D:108:PHE:HE1 | 38:8D:113:ARG:HH11 | 1.61 | 0.48 |
| 2:4:280:LYS:HZ2 | 26:7D:64:PRO:CG | 2.04 | 0.48 |
| 1:B8:360:GLY:HA3 | 24:6Y:110:ASN:HA | 1.95 | 0.48 |
| 2:F7:219:ILE:HG23 | 22:6J:175:ALA:HB1 | 1.96 | 0.48 |
| 1:G0:219:THR:N | 24:6V:418:ASP:OD1 | 2.44 | 0.48 |
| 1:G4:292:GLN:HG2 | 1:G4:298:ASN:ND2 | 2.29 | 0.48 |
| 2:G5:74:VAL:O | 2:G5:78:VAL:HG23 | 2.13 | 0.48 |
| 1:G6:199:CYS:HB2 | 1:G6:265:PHE:HD1 | 1.79 | 0.48 |
| 1:G8:49:VAL:HG11 | 1:G8:241:ARG:HG2 | 1.95 | 0.48 |
| 2:G9:227:LEU:O | 2:G9:231:ILE:HG12 | 2.13 | 0.48 |
| 2:G9:266:HIS:O | 2:G9:266:HIS:ND1 | 2.46 | 0.48 |
| 2:G9:364:PRO:O | 22:6P:168:THR:HG21 | 2.14 | 0.48 |
| 2:H1:381:SER:OG | 2:H1:382:THR:N | 2.47 | 0.48 |
| 1:H8:135:VAL:HG21 | 1:H8:152:ILE:HD11 | 1.95 | 0.48 |
| 1:I2:156:ARG:NH1 | 1:I2:197:ASP:OD2 | 2.47 | 0.48 |
| 2:I7:274:PRO:HB2 | 2:I7:276:ILE:HG12 | 1.95 | 0.48 |
| 2:I7:370:LYS:NZ | 5:4L:263:LEU:HD13 | 2.29 | 0.48 |
| 1:J2:145:SER:OG | 1:J2:188:SER:OG | 2.24 | 0.48 |
| 2:J9:3:GLU:HG3 | 2:J9:51:THR:HA | 1.95 | 0.48 |
| 1:K8:244:GLY:H | 1:K8:247:ASN:HD21 | 1.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L2:233:MET:O | 1:L2:237:THR:HG22 | 2.13 | 0.48 |
| 1:L4:11:GLN:HB3 | 39:L4:502:GDP:O1A | 2.14 | 0.48 |
| 1:L6:114:ASP:N | 1:L6:114:ASP:OD2 | 2.44 | 0.48 |
| 2:L7:192:HIS:NE2 | 2:L7:424:ASP:OD2 | 2.46 | 0.48 |
| 2:L9:51:THR:HG21 | 2:L9:243:ARG:HG2 | 1.95 | 0.48 |
| 1:M2:371:SER:OG | 1:M2:372:THR:N | 2.46 | 0.48 |
| 2:M3:46:ASP:OD2 | 2:M3:46:ASP:N | 2.38 | 0.48 |
| 2:M3:333:ALA:O | 2:M3:337:THR:HG23 | 2.14 | 0.48 |
| 1:M4:273:LEU:H | 1:M4:292:GLN:NE2 | 2.12 | 0.48 |
| 1:M4:304:ASP:OD1 | 1:M4:306:ARG:NH1 | 2.47 | 0.48 |
| 2:M9:313:MET:N | 2:M9:380:ASN:O | 2.33 | 0.48 |
| 2:N1:90:GLU:HG3 | 2:N1:121:ARG:HH12 | 1.77 | 0.48 |
| 1:N2:20:PHE:HA | 1:N2:230:SER:HB2 | 1.96 | 0.48 |
| 2:N5:62:VAL:HG21 | 2:P3:283:HIS:O | 2.13 | 0.48 |
| 1:O8:3:GLU:HG3 | 1:O8:127:CYS:HB2 | 1.96 | 0.48 |
| 1:O8:145:SER:HG | 1:O8:188:SER:HG | 1.56 | 0.48 |
| 2:P5:58:ALA:HB3 | 7:4R:31:LYS:HE3 | 1.94 | 0.48 |
| 1:P8:248:ALA:HA | 1:P8:252:LYS:HD2 | 1.96 | 0.48 |
| 2:P9:377:MET:SD | 2:P9:379:SER:OG | 2.71 | 0.48 |
| 1:Q2:153:SER:O | 1:Q2:157:GLU:HG2 | 2.14 | 0.48 |
| 2:Q3:425:LEU:O | 2:Q3:429:GLU:HG2 | 2.14 | 0.48 |
| 2:Q5:90:GLU:CB | 2:Q5:121:ARG:HH12 | 2.26 | 0.48 |
| 1:Q6:233:MET:O | 1:Q6:236:ILE:HG22 | 2.14 | 0.48 |
| 1:Q8:414:ASN:HD21 | 17:5R:63:ALA:HA | 1.79 | 0.48 |
| 1:R0:5:VAL:HG23 | 1:R0:62:ARG:HG2 | 1.95 | 0.48 |
| 1:R0:248:ALA:HA | 1:R0:252:LYS:HD2 | 1.96 | 0.48 |
| 1:R6:226:ASN:OD1 | 39:R6:503:GDP:N1 | 2.34 | 0.48 |
| 1:S0:232:VAL:O | 1:S0:236:ILE:HG12 | 2.13 | 0.48 |
| 1:S2:50:TYR:OH | 1:S2:237:THR:HG21 | 2.14 | 0.48 |
| 1:S8:362:LYS:HE3 | 7:4T:303:GLN:NE2 | 2.27 | 0.48 |
| 1:S8:383:GLU:HG2 | 13:5I:47:ARG:HH12 | 1.79 | 0.48 |
| 2:S9:100:ALA:HA | 1:T0:252:LYS:HE2 | 1.94 | 0.48 |
| 2:T3:306:ASP:HB3 | 2:T3:309:HIS:CD2 | 2.49 | 0.48 |
| 1:T6:183:TYR:HD2 | 1:T6:398:TYR:HE2 | 1.61 | 0.48 |
| 2:U5:332:VAL:O | 2:U5:336:LYS:HG2 | 2.14 | 0.48 |
| 1:U6:317:PHE:HE2 | 1:U6:326:VAL:HG13 | 1.79 | 0.48 |
| 1:U8:175:VAL:O | 1:U8:175:VAL:HG23 | 2.14 | 0.48 |
| 2:V3:72:PRO:HD2 | 1:V4:2:ARG:NH1 | 2.29 | 0.48 |
| 2:W1:88:HIS:ND1 | 2:X7:283:HIS:HB3 | 2.28 | 0.48 |
| 1:W2:282:ARG:NH2 | 1:W2:288:GLU:OE2 | 2.39 | 0.48 |
| 1:W6:3:GLU:HG3 | 1:W6:127:CYS:SG | 2.53 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:21:TRP:CZ3 | 2:W9:63:PRO:HB3 | 2.49 | 0.48 |
| 1:X0:207:LEU:HD11 | 1:X0:229:ILE:HD11 | 1.95 | 0.48 |
| 1:X0:325:GLU:O | 1:X0:329:GLN:HB2 | 2.14 | 0.48 |
| 1:X2:177:ASP:OD1 | 39:X2:501:GDP:H3' | 2.13 | 0.48 |
| 1:X2:193:VAL:HG12 | 1:X2:265:PHE:HZ | 1.79 | 0.48 |
| 2:X5:296:PHE:HZ | 2:X5:351:PHE:HE1 | 1.60 | 0.48 |
| 2:X5:370:LYS:HD2 | 8:4W:154:ILE:HG21 | 1.96 | 0.48 |
| 2:X9:76:ASP:HA | 2:X9:79:ARG:HB2 | 1.96 | 0.48 |
| 2:X9:100:ALA:HA | 1:Y0:252:LYS:HE3 | 1.96 | 0.48 |
| 1:Y4:204:ASN:HD21 | 39:Y4:502:GDP:HN22 | 1.60 | 0.48 |
| 2:Y5:330:ALA:O | 2:Y5:334:THR:HG23 | 2.13 | 0.48 |
| 1:Y6:49:VAL:HG11 | 1:Y6:241:ARG:HG2 | 1.96 | 0.48 |
| 1:Y8:405:GLU:HA | 1:Y8:408:PHE:HD2 | 1.79 | 0.48 |
| 2:Z3:417:GLU:HA | 2:Z3:420:GLU:HG2 | 1.96 | 0.48 |
| 1:Z6:266:PHE:CD1 | 1:Z6:370:ASN:HB2 | 2.48 | 0.48 |
| 1:Z6:266:PHE:CE1 | 1:Z6:370:ASN:HB2 | 2.49 | 0.48 |
| 1:Z6:345:ILE:O | 1:Z6:348:ASN:ND2 | 2.47 | 0.48 |
| 2:Z7:90:GLU:HB2 | 2:Z7:121:ARG:HH22 | 1.79 | 0.48 |
| 2:Z9:312:TYR:HB2 | 2:Z9:343:PHE:CD1 | 2.49 | 0.48 |
| 1:0E:388:MET:SD | 1:0E:393:ALA:HB3 | 2.54 | 0.48 |
| 2:0F:202:VAL:HG22 | 2:0F:268:MET:HB2 | 1.95 | 0.48 |
| 2:0H:60:LYS:NZ | 2:0X:282:TYR:O | 2.33 | 0.48 |
| 2:0H:205:ASP:OD2 | 2:0H:304:LYS:N | 2.37 | 0.48 |
| 2:0V:278:ALA:HA | 2:0V:369:ALA:HB2 | 1.95 | 0.48 |
| 1:0W:242:PHE:CD1 | 1:0W:356:ILE:HG13 | 2.48 | 0.48 |
| 2:0X:3:GLU:HB2 | 2:0X:129:CYS:SG | 2.54 | 0.48 |
| 2:0X:116:ASP:N | 2:0X:116:ASP:OD1 | 2.46 | 0.48 |
| 1:0Y:50:TYR:CE2 | 1:0Y:241:ARG:HD3 | 2.48 | 0.48 |
| 2:0Z:397:LEU:HD23 | 1:1A:346:PRO:HD3 | 1.95 | 0.48 |
| 2:1D:85:GLN:OE1 | 2:1D:85:GLN:HA | 2.14 | 0.48 |
| 1:1M:101:TRP:HE3 | 1:1M:403:MET:HE1 | 1.78 | 0.48 |
| 2:1N:370:LYS:HB3 | 9:4Z:110:VAL:HG13 | 1.96 | 0.48 |
| 1:1Q:317:PHE:HB3 | 1:1Q:321:MET:SD | 2.53 | 0.48 |
| 2:1R:317:LEU:HB3 | 2:1R:319:TYR:CE1 | 2.49 | 0.48 |
| 2:1T:11:GLN:NE2 | 1:1U:247:ASN:OD1 | 2.47 | 0.48 |
| 2:1T:129:CYS:SG | 2:1T:130:THR:N | 2.86 | 0.48 |
| 2:1T:298:PRO:HA | 2:1T:301:MET:HG3 | 1.96 | 0.48 |
| 1:1W:48:ASN:N | 1:1W:48:ASN:OD1 | 2.47 | 0.48 |
| 1:1W:121:ARG:O | 1:1W:125:GLU:HG3 | 2.14 | 0.48 |
| 2:1Z:244:PHE:HB2 | 2:1Z:356:ASN:HD21 | 1.78 | 0.48 |
| 1:2A:72:THR:O | 1:2A:76:VAL:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:114:ASP:HB2 | 38:8A:101:ASP:CB | 2.42 | 0.48 |
| 2:2D:114:ILE:HG21 | 2:2D:149:LEU:HD22 | 1.96 | 0.48 |
| 2:2N:14:ILE:HD11 | 2:2N:74:VAL:HG22 | 1.95 | 0.48 |
| 1:2S:49:VAL:HG11 | 1:2S:241:ARG:HG2 | 1.95 | 0.48 |
| 2:2T:326:LYS:HG3 | 2:2T:327:ASP:H | 1.79 | 0.48 |
| 1:2U:332:ASN:HD22 | 38:8A:1:MET:HA | 1.78 | 0.48 |
| 2:2X:287:SER:OG | 2:2X:290:GLU:OE1 | 2.24 | 0.48 |
| 2:2Z:102:ASN:HB3 | 2:2Z:105:ARG:HB3 | 1.95 | 0.48 |
| 1:3C:170:VAL:HG22 | 1:3C:202:LEU:O | 2.13 | 0.48 |
| 2:3D:116:ASP:OD1 | 2:3D:116:ASP:N | 2.47 | 0.48 |
| 2:3F:236:SER:OG | 2:3F:243:ARG:NH2 | 2.47 | 0.48 |
| 1:3G:202:LEU:HD23 | 1:3G:229:ILE:HG12 | 1.95 | 0.48 |
| 1:3K:183:TYR:HE2 | 1:3K:394:PHE:HB2 | 1.78 | 0.48 |
| 1:3K:193:VAL:HG13 | 1:3K:194:GLU:HG3 | 1.95 | 0.48 |
| 1:3M:100:ASN:HB3 | 1:3M:103:LYS:HB2 | 1.96 | 0.48 |
| 4:4G:115:LYS:HB3 | 4:4G:116:PRO:HD2 | 1.94 | 0.48 |
| 5:4M:79:LYS:CE | 15:5P:324:ARG:HH12 | 2.26 | 0.48 |
| 6:4O:34:ILE:HG13 | 6:4O:35:ALA:N | 2.29 | 0.48 |
| 7:4R:17:LYS:HB3 | 27:7G:230:GLN:HG2 | 1.95 | 0.48 |
| 7:4U:98:ARG:HG2 | 21:6H:62:SER:HA | 1.94 | 0.48 |
| 9:4Y:387:ARG:O | 9:4Y:391:ILE:HG12 | 2.13 | 0.48 |
| 9:4Z:357:SER:O | 9:4Z:360:THR:OG1 | 2.26 | 0.48 |
| 10:5A:298:ASP:O | 10:5A:301:LEU:HG | 2.14 | 0.48 |
| 14:5L:166:ALA:HB3 | 14:5L:170:ASN:H | 1.78 | 0.48 |
| 14:5L:367:TRP:CZ3 | 14:5L:374:GLU:HB2 | 2.49 | 0.48 |
| 14:5M:367:TRP:CZ3 | 14:5M:374:GLU:HB2 | 2.49 | 0.48 |
| 14:5N:367:TRP:CZ3 | 14:5N:374:GLU:HB2 | 2.49 | 0.48 |
| 14:5N:558:ALA:HB3 | 14:5N:571:GLY:HA3 | 1.94 | 0.48 |
| 22:6J:168:THR:HA | 22:6J:171:GLU:OE1 | 2.13 | 0.48 |
| 22:6L:220:ASP:OD1 | 22:6L:221:ASP:N | 2.46 | 0.48 |
| 22:6N:146:LEU:HD12 | 22:6N:146:LEU:H | 1.79 | 0.48 |
| 22:6O:209:ASN:O | 22:6O:213:THR:HG23 | 2.12 | 0.48 |
| 24:6U:505:LYS:N | 24:6U:510:GLU:O | 2.45 | 0.48 |
| 24:6X:425:SER:OG | 24:6X:427:VAL:O | 2.29 | 0.48 |
| 26:7D:59:ARG:HB2 | 26:7D:59:ARG:CZ | 2.44 | 0.48 |
| 38:8B:26:THR:O | 38:8B:35:GLU:HG2 | 2.13 | 0.48 |
| 38:8D:171:ASP:OD1 | 38:8D:171:ASP:N | 2.46 | 0.48 |
| 2:F3:27:GLU:HA | 22:6O:91:ILE:HD11 | 1.95 | 0.48 |
| 2:F7:56:THR:HG21 | 2:H3:283:HIS:O | 2.14 | 0.48 |
| 1:F8:78:SER:OG | 24:6U:499:GLU:OE2 | 2.31 | 0.48 |
| 1:G6:378:PHE:HA | 1:G6:381:VAL:HG12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G7:51:THR:HG21 | 2:G7:243:ARG:HG2 | 1.96 | 0.48 |
| 2:G7:101:ASN:OD1 | 1:G8:252:LYS:HE3 | 2.13 | 0.48 |
| 1:G8:117:LEU:HA | 1:G8:120:VAL:HG12 | 1.94 | 0.48 |
| 2:G9:135:PHE:HD2 | 2:G9:166:LYS:HG2 | 1.78 | 0.48 |
| 2:G9:384:ILE:HD12 | 2:G9:387:ILE:HB | 1.96 | 0.48 |
| 1:H6:23:VAL:HG21 | 1:H6:230:SER:OG | 2.13 | 0.48 |
| 2:I5:170:THR:OG1 | 2:I5:203:MET:HG3 | 2.14 | 0.48 |
| 1:I8:95:THR:OG1 | 1:I8:96:GLY:N | 2.47 | 0.48 |
| 1:J0:375:GLN:HB2 | 1:J0:419:VAL:HG13 | 1.96 | 0.48 |
| 2:J7:287:SER:OG | 2:J7:288:VAL:N | 2.46 | 0.48 |
| 1:J8:114:ASP:N | 1:J8:114:ASP:OD1 | 2.47 | 0.48 |
| 2:J9:49:PHE:HE1 | 6:4O:475:ARG:NH1 | 2.12 | 0.48 |
| 2:J9:129:CYS:SG | 2:J9:130:THR:N | 2.87 | 0.48 |
| 1:K0:45:GLU:HG3 | 1:K0:46:ARG:HG2 | 1.96 | 0.48 |
| 1:K0:393:ALA:HB2 | 2:K1:346:TRP:HE3 | 1.78 | 0.48 |
| 2:K7:324:VAL:HG23 | 2:K7:326:LYS:H | 1.79 | 0.48 |
| 1:K8:139:LEU:HD12 | 1:K8:170:VAL:HG22 | 1.95 | 0.48 |
| 1:L2:273:LEU:H | 1:L2:292:GLN:HE22 | 1.60 | 0.48 |
| 1:L4:190:HIS:HD2 | 1:L4:411:ALA:HA | 1.78 | 0.48 |
| 2:L7:208:ALA:HB1 | 2:L7:301:MET:O | 2.14 | 0.48 |
| 1:M8:273:LEU:H | 1:M8:292:GLN:NE2 | 2.12 | 0.48 |
| 2:N3:56:THR:HG21 | 2:N3:88:HIS:CE1 | 2.49 | 0.48 |
| 1:O2:355:ASP:OD1 | 37:7Y:236:THR:HG23 | 2.14 | 0.48 |
| 1:O4:145:SER:OG | 1:O4:146:GLY:N | 2.47 | 0.48 |
| 2:O5:114:ILE:HG21 | 2:O5:149:LEU:HD22 | 1.96 | 0.48 |
| 1:P8:170:VAL:HG21 | 1:P8:377:MET:SD | 2.54 | 0.48 |
| 2:P9:22:GLU:OE1 | 2:P9:229:ARG:NH1 | 2.46 | 0.48 |
| 2:Q9:8:HIS:CD2 | 2:Q9:138:PHE:HD2 | 2.31 | 0.48 |
| 1:R0:139:LEU:HD12 | 1:R0:170:VAL:HG12 | 1.94 | 0.48 |
| 1:R2:237:THR:HG22 | 1:R2:250:LEU:HD21 | 1.96 | 0.48 |
| 2:R9:217:LEU:HD21 | 2:R9:368:LEU:HD23 | 1.96 | 0.48 |
| 1:S0:21:TRP:O | 1:S0:25:SER:OG | 2.30 | 0.48 |
| 2:S7:58:ALA:HB3 | 24:6U:86:PRO:HB3 | 1.95 | 0.48 |
| 1:S8:135:VAL:HG22 | 1:S8:137:HIS:HD2 | 1.79 | 0.48 |
| 1:T2:135:VAL:HG21 | 1:T2:152:ILE:HD11 | 1.95 | 0.48 |
| 2:T3:238:LEU:HD22 | 2:T3:378:ILE:HD11 | 1.96 | 0.48 |
| 2:T7:8:HIS:CD2 | 2:T7:138:PHE:HD2 | 2.31 | 0.48 |
| 1:U2:322:SER:HB3 | 1:U2:325:GLU:HB3 | 1.95 | 0.48 |
| 1:U8:191:GLN:HG3 | 1:U8:195:ASN:OD1 | 2.14 | 0.48 |
| 1:V4:285:THR:H | 1:V4:288:GLU:CG | 2.26 | 0.48 |
| 1:V6:139:LEU:HD12 | 1:V6:170:VAL:HG12 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W0:3:GLU:HG3 | 1:W0:127:CYS:HB2 | 1.95 | 0.48 |
| 1:W0:232:VAL:HG22 | 1:W0:270:PHE:HB2 | 1.96 | 0.48 |
| 2:W1:3:GLU:OE2 | 2:W1:50:ASN:ND2 | 2.47 | 0.48 |
| 1:X0:244:GLY:H | 1:X0:247:ASN:HD21 | 1.61 | 0.48 |
| 1:X2:267:MET:HG3 | 1:X2:301:CYS:SG | 2.53 | 0.48 |
| 2:X3:181:VAL:HG23 | 1:X4:256:ASN:HD22 | 1.78 | 0.48 |
| 2:X5:332:VAL:HA | 2:X5:335:ILE:HG22 | 1.96 | 0.48 |
| 1:X6:311:LEU:CD1 | 1:X6:372:THR:HG23 | 2.44 | 0.48 |
| 1:X8:181:GLU:HG3 | 1:X8:182:PRO:CD | 2.42 | 0.48 |
| 1:Y0:203:ASP:OD2 | 1:Y0:302:ALA:N | 2.47 | 0.48 |
| 1:Y6:212:PHE:CE1 | 1:Y6:220:PRO:HG3 | 2.47 | 0.48 |
| 1:Y6:309:ARG:NH1 | 1:Y6:341:PHE:O | 2.47 | 0.48 |
| 1:Y8:152:ILE:HD13 | 1:Y8:155:ILE:HD11 | 1.96 | 0.48 |
| 2:Z1:31:GLN:HB2 | 2:Z1:33:ASP:OD1 | 2.14 | 0.48 |
| 2:Z1:296:PHE:HE2 | 2:Z1:335:ILE:HG21 | 1.79 | 0.48 |
| 1:Z2:87:PRO:HA | 1:Z2:90:PHE:CD2 | 2.49 | 0.48 |
| 2:Z5:21:TRP:CH2 | 2:Z5:63:PRO:HB3 | 2.49 | 0.48 |
| 2:Z5:192:HIS:HD2 | 2:Z5:421:ALA:HA | 1.78 | 0.48 |
| 1:Z6:107:THR:OG1 | 1:Z6:401:GLU:OE2 | 2.24 | 0.48 |
| 1:Z6:404:ASP:HB2 | 1:Z6:406:MET:SD | 2.53 | 0.48 |
| 2:Z9:286:LEU:O | 2:Z9:373:ARG:NH1 | 2.47 | 0.48 |
| 1:0C:2:ARG:HE | 1:0C:240:LEU:HD22 | 1.78 | 0.48 |
| 1:0C:113:ILE:HA | 1:0C:116:VAL:HG22 | 1.96 | 0.48 |
| 1:0C:122:LYS:HD2 | 1:0S:292:GLN:HE22 | 1.76 | 0.48 |
| 1:0C:238:CYS:SG | 1:0C:316:LEU:HD21 | 2.53 | 0.48 |
| 1:0M:139:LEU:HG | 1:0M:168:SER:HB2 | 1.96 | 0.48 |
| 2:0N:398:MET:HG3 | 1:0O:346:PRO:HD2 | 1.96 | 0.48 |
| 2:0P:116:ASP:N | 2:0P:116:ASP:OD1 | 2.45 | 0.48 |
| 1:0Q:135:VAL:HB | 1:0Q:166:THR:HG22 | 1.95 | 0.48 |
| 2:0R:111:GLY:HA2 | 2:0R:114:ILE:HG22 | 1.96 | 0.48 |
| 1:0U:272:PRO:HB2 | 1:0U:282:ARG:HH12 | 1.78 | 0.48 |
| 1:0W:374:ILE:HD12 | 1:0W:378:PHE:HE2 | 1.78 | 0.48 |
| 1:0Y:27:GLU:OE1 | 1:0Y:241:ARG:NH1 | 2.39 | 0.48 |
| 1:1C:8:GLN:CD | 1:1C:17:GLY:HA3 | 2.35 | 0.48 |
| 2:1F:305:CYS:HB3 | 2:1F:387:ILE:HD11 | 1.96 | 0.48 |
| 1:1G:31:ASP:OD2 | 1:1G:33:THR:OG1 | 2.32 | 0.48 |
| 2:1N:195:LEU:HD23 | 2:1N:196:GLU:HB3 | 1.96 | 0.48 |
| 2:1N:277:SER:H | 2:1N:280:LYS:HB2 | 1.79 | 0.48 |
| 2:1R:318:MET:HB2 | 2:1R:376:CYS:HB3 | 1.95 | 0.48 |
| 1:2I:115:SER:HA | 1:2I:118:ASP:OD1 | 2.14 | 0.48 |
| 1:2M:67:ASP:CG | 1:2M:68:LEU:N | 2.67 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:155:GLU:O | 2:2N:158:SER:OG | 2.28 | 0.48 |
| 2:2R:274:PRO:HB2 | 2:2R:276:ILE:HG12 | 1.95 | 0.48 |
| 1:2S:304:ASP:OD1 | 38:8A:46:ALA:HB2 | 2.14 | 0.48 |
| 2:2V:236:SER:OG | 2:2V:243:ARG:NH2 | 2.47 | 0.48 |
| 1:2Y:2:ARG:HE | 1:2Y:240:LEU:HD22 | 1.78 | 0.48 |
| 1:2Y:198:GLU:HB3 | 1:2Y:258:ILE:HD11 | 1.95 | 0.48 |
| 2:3B:331:SER:O | 2:3B:334:THR:OG1 | 2.27 | 0.48 |
| 1:3G:219:THR:HB | 2:3H:324:VAL:HG11 | 1.94 | 0.48 |
| 1:3O:11:GLN:NE2 | 2:3P:249:ASN:OD1 | 2.42 | 0.48 |
| 1:3O:172:SER:HB2 | 1:3O:380:ARG:NH2 | 2.29 | 0.48 |
| 2:3P:180:ALA:HA | 1:3Q:350:LYS:HD2 | 1.96 | 0.48 |
| 2:3P:333:ALA:O | 2:3P:337:THR:HG23 | 2.13 | 0.48 |
| 4:3Y:115:LYS:HB3 | 4:3Y:116:PRO:HD2 | 1.94 | 0.48 |
| 5:4L:309:ARG:HB2 | 5:4L:309:ARG:NH1 | 2.29 | 0.48 |
| 6:4P:167:ARG:HA | 6:4P:170:ASN:ND2 | 2.28 | 0.48 |
| 8:4W:117:VAL:O | 8:4W:120:SER:OG | 2.23 | 0.48 |
| 8:4W:157:THR:O | 8:4W:161:MET:HG2 | 2.14 | 0.48 |
| 12:5F:115:ARG:NH2 | 12:5F:116:ALA:O | 2.46 | 0.48 |
| 14:5L:112:SER:N | 14:5L:155:PHE:CD2 | 2.78 | 0.48 |
| 14:5N:166:ALA:HB3 | 14:5N:170:ASN:H | 1.78 | 0.48 |
| 15:5O:96:ALA:HB3 | 15:5O:163:LEU:HD23 | 1.96 | 0.48 |
| 18:6C:61:LYS:HD2 | 18:6C:61:LYS:HA | 1.73 | 0.48 |
| 22:6I:278:GLN:O | 22:6I:282:LYS:HG2 | 2.14 | 0.48 |
| 22:6M:16:LYS:HG2 | 22:6M:20:TYR:CE2 | 2.49 | 0.48 |
| 24:6U:436:HIS:O | 24:6U:440:ASN:ND2 | 2.47 | 0.48 |
| 24:6Z:111:MET:HB3 | 24:6Z:112:GLU:OE1 | 2.14 | 0.48 |
| 38:8B:73:TRP:CD1 | 38:8B:75:SER:HB2 | 2.44 | 0.48 |
| 1:5:41:ASP:N | 26:7D:25:TYR:HE2 | 2.11 | 0.48 |
| 2:A2:42:ILE:HG21 | 26:7F:45:MET:O | 2.12 | 0.48 |
| 2:A2:285:GLN:HB2 | 2:T5:56:THR:HA | 1.96 | 0.48 |
| 1:A3:215:LEU:HD11 | 26:7F:136:PHE:HE2 | 1.70 | 0.48 |
| 1:B8:279:GLN:HE22 | 24:6Y:109:SER:HB2 | 1.78 | 0.48 |
| 1:D6:216:LYS:HG2 | 24:6Z:245:TYR:CZ | 2.48 | 0.48 |
| 1:F2:217:LEU:HB3 | 24:6Z:312:ASN:OD1 | 2.12 | 0.48 |
| 2:G1:289:ALA:O | 2:G1:293:ASN:ND2 | 2.46 | 0.48 |
| 1:G4:289:LEU:HD23 | 1:G4:365:ALA:HB2 | 1.96 | 0.48 |
| 1:G6:391:ARG:NH1 | 2:G7:346:TRP:HE1 | 2.11 | 0.48 |
| 2:G7:73:THR:O | 2:G7:77:GLU:HG2 | 2.13 | 0.48 |
| 1:G8:216:LYS:C | 24:6Z:422:ASN:HD21 | 2.16 | 0.48 |
| 2:G9:230:LEU:HD11 | 2:G9:275:ILE:HD11 | 1.96 | 0.48 |
| 2:H7:147:SER:OG | 2:H7:190:SER:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H8:404:ASP:HB3 | 1:H8:406:MET:SD | 2.54 | 0.48 |
| 1:I4:140:GLY:O | 1:I4:184:ASN:ND2 | 2.45 | 0.48 |
| 1:I4:286:VAL:HB | 1:I4:287:PRO:HD3 | 1.95 | 0.48 |
| 1:I8:175:VAL:HG23 | 1:I8:175:VAL:O | 2.14 | 0.48 |
| 1:I8:373:ALA:O | 1:I8:376:GLU:HG2 | 2.14 | 0.48 |
| 1:J0:95:THR:OG1 | 1:J0:96:GLY:N | 2.47 | 0.48 |
| 2:J3:358:GLN:HE22 | 16:5Q:172:ARG:HG2 | 1.75 | 0.48 |
| 2:J5:306:ASP:HB3 | 2:J5:309:HIS:HD2 | 1.79 | 0.48 |
| 2:J7:34:GLY:HA3 | 2:J7:60:LYS:NZ | 2.28 | 0.48 |
| 2:J7:384:ILE:HA | 2:J7:387:ILE:HD12 | 1.96 | 0.48 |
| 2:J9:179:THR:O | 1:K0:350:LYS:HD2 | 2.14 | 0.48 |
| 2:K3:330:ALA:O | 2:K3:334:THR:HG23 | 2.14 | 0.48 |
| 1:K4:70:PRO:N | 1:K4:92:PHE:HZ | 2.12 | 0.48 |
| 2:K9:85:GLN:OE1 | 30:7K:134:HIS:CE1 | 2.63 | 0.48 |
| 2:L3:88:HIS:CE1 | 2:M9:284:GLU:HB3 | 2.49 | 0.48 |
| 1:L4:11:GLN:HE21 | 1:L4:15:GLN:HE22 | 1.61 | 0.48 |
| 2:L5:384:ILE:HA | 2:L5:387:ILE:HD12 | 1.96 | 0.48 |
| 2:L7:383:ALA:HA | 2:L7:386:GLU:OE1 | 2.14 | 0.48 |
| 2:M1:116:ASP:OD1 | 2:M1:116:ASP:N | 2.45 | 0.48 |
| 1:M2:396:HIS:HA | 1:M2:399:THR:HG22 | 1.96 | 0.48 |
| 2:M5:346:TRP:CH2 | 2:M5:435:VAL:HG13 | 2.49 | 0.48 |
| 1:M6:73:MET:HE3 | 1:M6:90:PHE:HB3 | 1.96 | 0.48 |
| 1:M8:418:LEU:HG | 1:M8:422:TYR:HE2 | 1.79 | 0.48 |
| 1:N0:178:THR:OG1 | 1:N0:181:GLU:HG3 | 2.13 | 0.48 |
| 2:N3:3:GLU:HG3 | 2:N3:51:THR:HA | 1.95 | 0.48 |
| 2:N5:70:LEU:HG | 2:N5:145:THR:HG23 | 1.95 | 0.48 |
| 1:N6:86:ARG:HG2 | 1:N6:88:ASP:H | 1.79 | 0.48 |
| 2:N7:264:ARG:HH21 | 2:U3:339:ARG:NH1 | 2.12 | 0.48 |
| 2:N7:392:ASP:OD2 | 2:N7:422:ARG:NH1 | 2.47 | 0.48 |
| 1:O8:236:ILE:HG23 | 1:O8:237:THR:HG23 | 1.94 | 0.48 |
| 2:O9:286:LEU:HD13 | 2:O9:371:VAL:HG23 | 1.96 | 0.48 |
| 2:P7:381:SER:OG | 2:P7:382:THR:N | 2.47 | 0.48 |
| 2:Q3:72:PRO:HD2 | 1:Q4:2:ARG:NH1 | 2.29 | 0.48 |
| 1:Q8:67:ASP:N | 1:Q8:67:ASP:OD1 | 2.46 | 0.48 |
| 2:Q9:259:LEU:HD11 | 2:Q9:316:CYS:HB2 | 1.95 | 0.48 |
| 1:R6:244:GLY:HA2 | 1:R6:355:ASP:OD1 | 2.12 | 0.48 |
| 1:S0:309:ARG:NH1 | 1:S0:339:SER:O | 2.46 | 0.48 |
| 2:S5:207:GLU:OE2 | 13:5H:90:PRO:HG3 | 2.14 | 0.48 |
| 2:S7:116:ASP:OD1 | 2:S7:117:LEU:N | 2.46 | 0.48 |
| 1:T2:3:GLU:HG3 | 1:T2:127:CYS:HB2 | 1.96 | 0.48 |
| 1:T2:110:ALA:HB1 | 3:4D:75:ARG:NE | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T5:132:LEU:HB3 | 2:T5:164:LYS:HE3 | 1.96 | 0.48 |
| 2:T5:174:SER:OG | 2:T5:175:PRO:HD2 | 2.14 | 0.48 |
| 1:T6:213:ARG:NE | 1:T6:297:LYS:HD2 | 2.29 | 0.48 |
| 2:U1:72:PRO:HG3 | 1:U2:1:MET:HG3 | 1.94 | 0.48 |
| 2:U1:272:TYR:HD2 | 2:U1:275:ILE:HG13 | 1.78 | 0.48 |
| 1:U2:173:PRO:HG2 | 1:U2:174:LYS:NZ | 2.29 | 0.48 |
| 2:U3:90:GLU:HG3 | 2:U3:121:ARG:HH12 | 1.78 | 0.48 |
| 2:U3:317:LEU:HB3 | 2:U3:319:TYR:HE1 | 1.79 | 0.48 |
| 2:U5:137:VAL:HG22 | 2:U5:168:GLY:HA2 | 1.96 | 0.48 |
| 2:U9:2:ARG:HA | 2:U9:133:GLN:HE21 | 1.79 | 0.48 |
| 2:V1:196:GLU:OE2 | 2:V1:197:HIS:NE2 | 2.47 | 0.48 |
| 2:V3:79:ARG:HG2 | 2:V3:92:LEU:HD13 | 1.95 | 0.48 |
| 2:V7:80:THR:OG1 | 8:4W:106:VAL:HG11 | 2.13 | 0.48 |
| 2:W3:189:LEU:HD11 | 2:W3:418:PHE:HE1 | 1.79 | 0.48 |
| 2:W5:145:THR:OG1 | 41:W5:501:GTP:O1B | 2.31 | 0.48 |
| 2:W7:246:GLY:HA2 | 2:W7:357:TYR:CD2 | 2.49 | 0.48 |
| 2:W9:84:ARG:HB2 | 2:W9:84:ARG:CZ | 2.43 | 0.48 |
| 2:W9:324:VAL:HG12 | 2:W9:326:LYS:HG2 | 1.96 | 0.48 |
| 1:X0:33:THR:HA | 8:4W:471:SER:HB2 | 1.95 | 0.48 |
| 1:X2:181:GLU:OE2 | 2:X3:349:THR:HG21 | 2.13 | 0.48 |
| 1:X4:4:ILE:HB | 1:X4:50:TYR:HE1 | 1.79 | 0.48 |
| 2:X7:166:LYS:N | 2:X7:199:ASP:OD2 | 2.47 | 0.48 |
| 2:X7:286:LEU:HD11 | 2:X7:372:GLN:H | 1.79 | 0.48 |
| 2:X9:287:SER:OG | 2:X9:288:VAL:N | 2.46 | 0.48 |
| 1:Y2:309:ARG:O | 1:Y2:371:SER:OG | 2.25 | 0.48 |
| 1:Y8:259:PRO:HG3 | 1:Y8:311:LEU:HD21 | 1.96 | 0.48 |
| 2:Y9:21:TRP:CH2 | 2:Y9:63:PRO:HB3 | 2.49 | 0.48 |
| 2:Y9:116:ASP:N | 2:Y9:116:ASP:OD1 | 2.42 | 0.48 |
| 2:Z1:88:HIS:HB3 | 2:0H:283:HIS:ND1 | 2.29 | 0.48 |
| 2:Z1:338:LYS:HZ2 | 2:Z1:340:THR:N | 2.12 | 0.48 |
| 1:Z2:2:ARG:HB2 | 1:Z2:240:LEU:HD11 | 1.95 | 0.48 |
| 1:Z2:51:PHE:HB3 | 1:Z2:59:TYR:HB3 | 1.96 | 0.48 |
| 2:Z3:241:SER:OG | 2:Z3:318:MET:SD | 2.72 | 0.48 |
| 1:Z4:115:SER:O | 1:Z4:119:VAL:HG23 | 2.14 | 0.48 |
| 1:Z6:179:VAL:H | 2:Z7:258:ASN:ND2 | 2.11 | 0.48 |
| 2:Z9:119:LEU:HA | 2:Z9:122:ILE:HG22 | 1.96 | 0.48 |
| 2:0B:387:ILE:HD12 | 2:0B:390:ARG:HH22 | 1.79 | 0.48 |
| 2:0H:9:ILE:HD13 | 2:0H:150:GLY:HA2 | 1.95 | 0.48 |
| 2:0H:417:GLU:HA | 2:0H:420:GLU:HG2 | 1.96 | 0.48 |
| 2:0J:15:GLN:HB3 | 2:0J:228:ASN:HD21 | 1.78 | 0.48 |
| 2:0L:30:ILE:HG12 | 2:0L:36:MET:HG2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0L:90:GLU:HB3 | 2:0L:121:ARG:HH22 | 1.79 | 0.48 |
| 2:0N:116:ASP:N | 2:0N:116:ASP:OD1 | 2.45 | 0.48 |
| 2:0N:417:GLU:HA | 2:0N:420:GLU:HG2 | 1.96 | 0.48 |
| 1:0O:207:LEU:HB3 | 1:0O:225:LEU:HD22 | 1.94 | 0.48 |
| 1:0Q:388:MET:HG3 | 1:0Q:393:ALA:HB3 | 1.95 | 0.48 |
| 2:0R:2:ARG:HA | 2:0R:133:GLN:HE21 | 1.79 | 0.48 |
| 1:0W:177:ASP:O | 2:0X:352:LYS:HA | 2.14 | 0.48 |
| 2:0X:205:ASP:OD1 | 2:0X:303:VAL:HG13 | 2.14 | 0.48 |
| 2:0Z:271:SER:HA | 2:0Z:302:MET:HG2 | 1.95 | 0.48 |
| 2:0Z:274:PRO:HB2 | 2:0Z:276:ILE:HG12 | 1.96 | 0.48 |
| 2:1D:50:ASN:O | 2:1D:64:ARG:NH2 | 2.47 | 0.48 |
| 2:1H:74:VAL:O | 2:1H:78:VAL:HG23 | 2.13 | 0.48 |
| 1:1K:178:THR:HG23 | 1:1K:181:GLU:HG3 | 1.95 | 0.48 |
| 1:1O:145:SER:OG | 1:1O:146:GLY:N | 2.46 | 0.48 |
| 2:1T:278:ALA:HA | 2:1T:369:ALA:HB2 | 1.96 | 0.48 |
| 1:1U:317:PHE:CE2 | 1:1U:326:VAL:HG13 | 2.49 | 0.48 |
| 1:1W:107:THR:OG1 | 1:1W:401:GLU:OE2 | 2.28 | 0.48 |
| 1:1W:273:LEU:H | 1:1W:292:GLN:HE22 | 1.62 | 0.48 |
| 2:1X:63:PRO:HB2 | 2:1X:65:CYS:SG | 2.54 | 0.48 |
| 2:1X:71:GLU:HG3 | 2:1X:73:THR:HG23 | 1.96 | 0.48 |
| 2:2B:5:ILE:HG22 | 2:2B:64:ARG:HB3 | 1.94 | 0.48 |
| 2:2D:290:GLU:HA | 2:2D:293:ASN:HD22 | 1.79 | 0.48 |
| 1:2G:335:ASN:O | 1:2G:338:SER:OG | 2.32 | 0.48 |
| 2:2H:120:ASP:OD1 | 38:8B:24:TYR:CG | 2.67 | 0.48 |
| 1:2I:173:PRO:HG2 | 1:2I:380:ARG:HH21 | 1.79 | 0.48 |
| 2:2J:413:MET:HB3 | 2:2J:417:GLU:OE1 | 2.13 | 0.48 |
| 1:2M:148:GLY:O | 1:2M:152:ILE:HG12 | 2.13 | 0.48 |
| 1:2Q:391:ARG:HG3 | 2:2R:346:TRP:CE2 | 2.49 | 0.48 |
| 1:3C:12:CYS:SG | 1:3C:13:GLY:N | 2.87 | 0.48 |
| 1:3C:86:ARG:HG2 | 1:3C:88:ASP:H | 1.77 | 0.48 |
| 2:3D:246:GLY:HA2 | 2:3D:357:TYR:HD2 | 1.79 | 0.48 |
| 2:3H:182:VAL:HG12 | 2:3H:185:TYR:HB2 | 1.95 | 0.48 |
| 1:3K:276:ARG:HH22 | 17:5T:216:GLU:HG2 | 1.79 | 0.48 |
| 2:3L:156:ARG:HA | 2:3L:159:VAL:HG12 | 1.96 | 0.48 |
| 2:3N:333:ALA:O | 2:3N:337:THR:HG23 | 2.14 | 0.48 |
| 2:3R:14:ILE:HD11 | 2:3R:74:VAL:HG22 | 1.96 | 0.48 |
| 2:3R:294:ALA:O | 2:3R:300:SER:OG | 2.31 | 0.48 |
| 1:3S:166:THR:OG1 | 1:3S:199:CYS:HB2 | 2.13 | 0.48 |
| 5:4L:474:TRP:NE1 | 5:4L:476:GLY:HA3 | 2.29 | 0.48 |
| 7:4U:10:ASN:HB3 | 7:4U:11:GLU:OE2 | 2.14 | 0.48 |
| 14:5L:495:LEU:HD13 | 14:5L:505:THR:HG23 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5O:31:GLU:OE1 | 15:5O:32:SER:HB2 | 2.14 | 0.48 |
| 16:5Q:131:THR:HA | 16:5Q:134:VAL:HG12 | 1.95 | 0.48 |
| 18:5Z:61:LYS:HD2 | 18:5Z:61:LYS:HA | 1.73 | 0.48 |
| 21:6G:73:VAL:HA | 21:6G:78:ILE:HD11 | 1.95 | 0.48 |
| 22:6J:31:TYR:O | 22:6J:32:LYS:HG3 | 2.14 | 0.48 |
| 22:6L:16:LYS:HG2 | 22:6L:20:TYR:CE2 | 2.49 | 0.48 |
| 22:6N:307:ARG:HH21 | 22:6N:326:PHE:HD2 | 1.60 | 0.48 |
| 22:6O:190:LEU:HG | 22:6O:191:PHE:CD2 | 2.48 | 0.48 |
| 23:6Q:65:LEU:HD12 | 23:6Q:65:LEU:HA | 1.79 | 0.48 |
| 24:6T:126:GLU:OE2 | 24:6T:127:ASP:HB2 | 2.14 | 0.48 |
| 24:6U:43:ASP:OD1 | 24:6U:43:ASP:N | 2.46 | 0.48 |
| 24:6U:212:VAL:O | 24:6U:216:THR:HG23 | 2.13 | 0.48 |
| 24:6V:569:LYS:O | 24:6V:573:VAL:HG13 | 2.14 | 0.48 |
| 24:6W:142:ILE:HG13 | 24:6W:144:GLN:HG3 | 1.95 | 0.48 |
| 24:6W:274:ARG:NE | 24:6W:372:ASP:OD2 | 2.41 | 0.48 |
| 24:6W:506:PRO:HB3 | 24:6W:524:GLU:OE1 | 2.12 | 0.48 |
| 24:6W:566:VAL:CG2 | 24:6W:573:VAL:HG11 | 2.44 | 0.48 |
| 24:6Y:371:ALA:HB1 | 24:6Y:375:THR:OG1 | 2.13 | 0.48 |
| 27:7G:113:ILE:HG21 | 27:7G:116:ASN:HD21 | 1.78 | 0.48 |
| 29:7J:129:SER:HB2 | 29:7J:137:VAL:CG2 | 2.43 | 0.48 |
| 29:7J:439:SER:O | 29:7J:443:LEU:HG | 2.13 | 0.48 |
| 30:7K:124:GLU:N | 30:7K:125:PRO:HD3 | 2.29 | 0.48 |
| 30:7K:302:ASP:OD1 | 30:7K:303:GLU:N | 2.47 | 0.48 |
| 31:7M:80:PRO:O | 31:7M:83:THR:OG1 | 2.29 | 0.48 |
| 37:7Y:83:PRO:HA | 37:7Y:86:ASN:OD1 | 2.14 | 0.48 |
| 37:7Y:177:ARG:HB2 | 37:7Y:177:ARG:NH1 | 2.27 | 0.48 |
| 38:8B:28:THR:O | 38:8B:28:THR:OG1 | 2.30 | 0.48 |
| 2:4:280:LYS:HZ2 | 26:7D:64:PRO:CB | 2.23 | 0.47 |
| 2:D7:58:ALA:HB1 | 22:6O:77:PRO:HB2 | 1.95 | 0.47 |
| 1:D8:11:GLN:N | 39:D8:501:GDP:O2B | 2.36 | 0.47 |
| 2:G1:399:TYR:O | 2:G1:402:ARG:NH1 | 2.47 | 0.47 |
| 1:G4:219:THR:HB | 2:G5:324:VAL:HG11 | 1.95 | 0.47 |
| 2:G5:75:VAL:HG11 | 2:G5:94:SER:HB2 | 1.95 | 0.47 |
| 1:G6:191:GLN:HG3 | 1:G6:195:ASN:OD1 | 2.13 | 0.47 |
| 2:H3:167:LEU:HD13 | 2:H3:200:VAL:HB | 1.95 | 0.47 |
| 1:H6:77:ARG:HE | 1:H6:90:PHE:HE2 | 1.62 | 0.47 |
| 1:H6:95:THR:OG1 | 1:H6:96:GLY:N | 2.47 | 0.47 |
| 1:I0:173:PRO:HB3 | 1:I0:384:GLN:HE22 | 1.79 | 0.47 |
| 2:I1:324:VAL:HG21 | 2:I1:326:LYS:NZ | 2.28 | 0.47 |
| 1:I2:218:THR:HG21 | 24:6Y:488:ARG:HA | 1.95 | 0.47 |
| 1:I4:396:HIS:CE1 | 1:I4:397:TRP:CE2 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I9:119:LEU:O | 2:I9:122:ILE:HG22 | 2.14 | 0.47 |
| 2:I9:165:SER:HA | 2:I9:199:ASP:OD2 | 2.14 | 0.47 |
| 2:J1:223:THR:HG22 | 2:J1:224:TYR:N | 2.29 | 0.47 |
| 2:J9:217:LEU:HB3 | 2:J9:219:ILE:HD12 | 1.96 | 0.47 |
| 2:K3:8:HIS:CD2 | 2:K3:138:PHE:HD2 | 2.32 | 0.47 |
| 1:K4:186:THR:HG22 | 1:K4:411:ALA:HB1 | 1.96 | 0.47 |
| 2:L5:76:ASP:OD1 | 1:L6:46:ARG:NH2 | 2.47 | 0.47 |
| 1:L6:362:LYS:HB2 | 6:4P:169:PHE:HE2 | 1.79 | 0.47 |
| 2:L7:383:ALA:O | 2:L7:387:ILE:HG23 | 2.14 | 0.47 |
| 1:M0:375:GLN:HB2 | 1:M0:419:VAL:HG13 | 1.94 | 0.47 |
| 2:M1:21:TRP:CZ3 | 2:M1:63:PRO:HB3 | 2.49 | 0.47 |
| 1:M4:260:PHE:HB2 | 1:M4:263:LEU:HD23 | 1.94 | 0.47 |
| 1:N0:260:PHE:HB2 | 1:N0:263:LEU:HD23 | 1.96 | 0.47 |
| 2:N1:91:GLN:HE21 | 2:N1:125:LEU:HD21 | 1.79 | 0.47 |
| 2:N9:333:ALA:O | 2:N9:337:THR:HG23 | 2.14 | 0.47 |
| 1:O2:101:TRP:HB2 | 1:O2:184:ASN:OD1 | 2.13 | 0.47 |
| 1:O2:391:ARG:HA | 1:O2:391:ARG:HH21 | 1.79 | 0.47 |
| 2:O3:91:GLN:O | 2:O3:92:LEU:HD23 | 2.14 | 0.47 |
| 2:O7:90:GLU:HG3 | 2:O7:121:ARG:HH11 | 1.79 | 0.47 |
| 2:O7:172:TYR:HE2 | 2:O7:203:MET:HE2 | 1.78 | 0.47 |
| 2:O9:90:GLU:N | 2:O9:90:GLU:OE1 | 2.46 | 0.47 |
| 2:O9:264:ARG:NH2 | 2:O9:431:ASP:OD2 | 2.47 | 0.47 |
| 1:P4:3:GLU:HB2 | 1:P4:130:LEU:HD13 | 1.94 | 0.47 |
| 2:P7:33:ASP:N | 2:P7:33:ASP:OD1 | 2.44 | 0.47 |
| 1:P8:5:VAL:HG23 | 1:P8:62:ARG:HG2 | 1.95 | 0.47 |
| 1:Q2:325:GLU:HA | 1:Q2:328:GLU:HG2 | 1.96 | 0.47 |
| 2:Q3:313:MET:HE3 | 2:Q3:344:VAL:HG11 | 1.96 | 0.47 |
| 1:Q8:414:ASN:HA | 1:Q8:417:ASP:OD2 | 2.14 | 0.47 |
| 2:Q9:413:MET:O | 17:5S:117:PRO:HG3 | 2.14 | 0.47 |
| 2:R1:6:SER:O | 2:R1:65:CYS:HB2 | 2.13 | 0.47 |
| 1:R2:172:SER:HB3 | 1:R2:175:VAL:HG22 | 1.95 | 0.47 |
| 2:R5:102:ASN:HB3 | 2:R5:105:ARG:HB3 | 1.96 | 0.47 |
| 2:R7:304:LYS:HA | 2:R7:304:LYS:HD2 | 1.67 | 0.47 |
| 2:U3:137:VAL:HG22 | 2:U3:168:GLY:HA2 | 1.95 | 0.47 |
| 2:U3:286:LEU:HD11 | 2:U3:372:GLN:HB2 | 1.96 | 0.47 |
| 2:U3:333:ALA:O | 2:U3:337:THR:HG23 | 2.14 | 0.47 |
| 1:U4:77:ARG:HE | 1:U4:90:PHE:HE2 | 1.60 | 0.47 |
| 1:U6:317:PHE:CE2 | 1:U6:326:VAL:HG13 | 2.49 | 0.47 |
| 1:U8:107:THR:OG1 | 1:U8:401:GLU:OE2 | 2.22 | 0.47 |
| 1:V0:282:ARG:HH22 | 1:V0:284:LEU:HG | 1.80 | 0.47 |
| 1:V0:361:LEU:HD12 | 1:V0:362:LYS:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V2:221:THR:HG23 | 1:V2:223:GLY:H | 1.79 | 0.47 |
| 2:V9:301:MET:HE1 | 2:V9:307:PRO:HD3 | 1.96 | 0.47 |
| 1:W2:49:VAL:HG11 | 1:W2:241:ARG:HG2 | 1.96 | 0.47 |
| 2:W5:68:LEU:HA | 2:W5:93:ILE:O | 2.14 | 0.47 |
| 2:W5:301:MET:HE1 | 2:W5:307:PRO:HD3 | 1.95 | 0.47 |
| 2:W9:58:ALA:HB3 | 8:4W:421:THR:HG22 | 1.95 | 0.47 |
| 2:X3:207:GLU:HB3 | 2:X3:304:LYS:HG3 | 1.94 | 0.47 |
| 2:X3:356:ASN:OD1 | 2:X3:357:TYR:N | 2.47 | 0.47 |
| 1:X4:203:ASP:HB2 | 1:X4:205:GLU:OE2 | 2.14 | 0.47 |
| 1:X4:257:LEU:HD23 | 1:X4:312:THR:HG23 | 1.96 | 0.47 |
| 2:X5:8:HIS:CE1 | 2:X5:21:TRP:HE1 | 2.31 | 0.47 |
| 1:X6:86:ARG:HG2 | 1:X6:88:ASP:H | 1.78 | 0.47 |
| 1:Y0:187:LEU:O | 1:Y0:191:GLN:HG2 | 2.14 | 0.47 |
| 1:Y8:67:ASP:N | 1:Y8:67:ASP:OD1 | 2.47 | 0.47 |
| 1:Y8:317:PHE:HE2 | 1:Y8:326:VAL:HG13 | 1.78 | 0.47 |
| 1:Y8:396:HIS:CE1 | 1:Y8:397:TRP:CE2 | 3.02 | 0.47 |
| 1:Z0:116:VAL:O | 1:Z0:120:VAL:HG22 | 2.14 | 0.47 |
| 1:Z0:151:LEU:O | 1:Z0:155:ILE:HG12 | 2.13 | 0.47 |
| 2:Z1:72:PRO:HG3 | 1:Z2:1:MET:HG3 | 1.95 | 0.47 |
| 2:Z5:90:GLU:HG3 | 2:Z5:91:GLN:N | 2.28 | 0.47 |
| 2:Z9:207:GLU:OE1 | 2:Z9:304:LYS:HD2 | 2.14 | 0.47 |
| 1:0A:114:ASP:OD1 | 1:0A:114:ASP:N | 2.45 | 0.47 |
| 2:0B:32:PRO:HB3 | 2:0B:83:TYR:CE1 | 2.49 | 0.47 |
| 2:0B:275:ILE:HD12 | 2:0B:368:LEU:HD21 | 1.96 | 0.47 |
| 2:0H:290:GLU:HA | 2:0H:293:ASN:HD22 | 1.79 | 0.47 |
| 1:0I:183:TYR:O | 1:0I:187:LEU:HD13 | 2.13 | 0.47 |
| 2:0J:9:ILE:HD13 | 2:0J:137:VAL:HG23 | 1.96 | 0.47 |
| 2:0J:21:TRP:CZ2 | 2:0J:65:CYS:HB2 | 2.49 | 0.47 |
| 2:0J:115:VAL:HG21 | 2:0J:156:ARG:HD3 | 1.96 | 0.47 |
| 2:0J:320:ARG:HD3 | 2:0J:360:PRO:HG3 | 1.96 | 0.47 |
| 1:0K:301:CYS:SG | 1:0K:302:ALA:N | 2.87 | 0.47 |
| 2:0N:171:VAL:HG22 | 2:0N:204:LEU:HD11 | 1.96 | 0.47 |
| 2:0P:320:ARG:O | 2:0P:373:ARG:HA | 2.14 | 0.47 |
| 2:0R:246:GLY:HA3 | 2:0R:356:ASN:HA | 1.96 | 0.47 |
| 2:0V:49:PHE:HD2 | 2:0V:53:PHE:HB2 | 1.79 | 0.47 |
| 2:0V:239:THR:HG23 | 2:0V:243:ARG:HE | 1.77 | 0.47 |
| 1:0W:334:GLN:NE2 | 1:0W:348:ASN:H | 2.09 | 0.47 |
| 1:0Y:310:TYR:N | 1:0Y:340:TYR:O | 2.39 | 0.47 |
| 1:1A:130:LEU:O | 1:1A:162:ARG:HD2 | 2.14 | 0.47 |
| 1:1C:315:ALA:HB1 | 1:1C:317:PHE:CE1 | 2.49 | 0.47 |
| 2:1D:178:SER:HB2 | 2:1D:183:GLU:OE2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1D:407:TRP:CG | 1:1E:255:VAL:HG23 | 2.49 | 0.47 |
| 2:1F:4:VAL:HG13 | 2:1F:52:PHE:HE1 | 1.77 | 0.47 |
| 1:1G:169:VAL:HG11 | 1:1G:204:ASN:OD1 | 2.14 | 0.47 |
| 2:1H:399:TYR:OH | 2:1H:415:GLU:OE1 | 2.22 | 0.47 |
| 1:1K:314:SER:HB3 | 1:1K:368:ILE:HG23 | 1.96 | 0.47 |
| 1:1K:404:ASP:HB3 | 1:1K:406:MET:SD | 2.53 | 0.47 |
| 1:1Q:396:HIS:CD2 | 1:1Q:396:HIS:N | 2.82 | 0.47 |
| 1:1S:95:THR:OG1 | 1:1S:96:GLY:N | 2.47 | 0.47 |
| 2:1V:116:ASP:N | 2:1V:116:ASP:OD1 | 2.47 | 0.47 |
| 2:1V:119:LEU:HA | 2:1V:122:ILE:HG12 | 1.96 | 0.47 |
| 1:1W:114:ASP:N | 1:1W:114:ASP:OD1 | 2.45 | 0.47 |
| 2:1Z:240:ALA:HB1 | 2:1Z:356:ASN:HD22 | 1.78 | 0.47 |
| 2:2F:47:ASP:OD1 | 2:2F:48:ALA:N | 2.46 | 0.47 |
| 1:2I:55:THR:HG21 | 1:2Y:284:LEU:HD23 | 1.95 | 0.47 |
| 2:2L:175:PRO:HB3 | 2:2L:390:ARG:HE | 1.79 | 0.47 |
| 2:2L:198:THR:HG21 | 2:2L:201:ALA:HB2 | 1.95 | 0.47 |
| 2:2L:276:ILE:HG21 | 2:2L:281:ALA:CB | 2.43 | 0.47 |
| 2:2T:8:HIS:CD2 | 2:2T:138:PHE:HD2 | 2.32 | 0.47 |
| 1:2U:287:PRO:HA | 1:2U:290:THR:HG22 | 1.96 | 0.47 |
| 1:2U:404:ASP:HB2 | 1:2U:406:MET:SD | 2.54 | 0.47 |
| 2:2X:335:ILE:HG23 | 2:2X:341:ILE:HD11 | 1.95 | 0.47 |
| 2:2Z:214:ARG:HH21 | 38:8C:65:VAL:HB | 1.79 | 0.47 |
| 2:3B:129:CYS:SG | 2:3B:130:THR:N | 2.87 | 0.47 |
| 2:3H:327:ASP:N | 2:3H:327:ASP:OD1 | 2.47 | 0.47 |
| 1:3I:263:LEU:HD13 | 1:3I:422:TYR:HE1 | 1.79 | 0.47 |
| 1:3K:182:PRO:O | 1:3K:186:THR:HG23 | 2.14 | 0.47 |
| 2:3P:220:GLU:HB3 | 23:6S:85:PHE:CE1 | 2.49 | 0.47 |
| 1:3Q:114:ASP:N | 1:3Q:114:ASP:OD1 | 2.47 | 0.47 |
| 5:4M:293:LEU:HB3 | 28:7X:306:LEU:HD23 | 1.91 | 0.47 |
| 7:4T:233:MET:O | 7:4T:237:ILE:HG12 | 2.14 | 0.47 |
| 10:5A:334:ARG:NH2 | 10:5A:337:ASP:OD1 | 2.39 | 0.47 |
| 10:5B:310:LEU:O | 10:5B:314:LYS:HG2 | 2.14 | 0.47 |
| 14:5L:604:THR:HG22 | 14:5L:609:ARG:O | 2.14 | 0.47 |
| 14:5N:528:ALA:HB1 | 14:5N:556:VAL:HG12 | 1.95 | 0.47 |
| 15:5O:7:TYR:CE2 | 15:5O:30:PRO:HG3 | 2.49 | 0.47 |
| 17:5S:31:THR:HB | 17:5S:36:PHE:CE2 | 2.49 | 0.47 |
| 17:5U:31:THR:HB | 17:5U:36:PHE:CE2 | 2.49 | 0.47 |
| 18:6D:61:LYS:HD2 | 18:6D:61:LYS:HA | 1.73 | 0.47 |
| 21:6G:129:VAL:O | 21:6G:133:VAL:HG23 | 2.14 | 0.47 |
| 22:6M:190:LEU:HG | 22:6M:191:PHE:CD2 | 2.49 | 0.47 |
| 22:6P:20:TYR:CZ | 22:6P:22:GLY:HA3 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6T:482:ILE:HB | 24:6T:498:LEU:HB3 | 1.95 | 0.47 |
| 24:6T:512:TYR:CE1 | 24:6T:523:ILE:HG23 | 2.49 | 0.47 |
| 24:6V:92:ASP:OD2 | 24:6V:93:ARG:N | 2.46 | 0.47 |
| 24:6V:558:LEU:HD13 | 24:6V:608:GLN:HB3 | 1.95 | 0.47 |
| 24:6X:505:LYS:N | 24:6X:510:GLU:O | 2.45 | 0.47 |
| 24:6X:518:TYR:CG | 24:6X:521:ALA:HB2 | 2.49 | 0.47 |
| 24:6Y:335:ASN:OD1 | 24:6Y:337:THR:OG1 | 2.22 | 0.47 |
| 24:6Z:602:LEU:C | 24:6Z:603:LYS:HD3 | 2.34 | 0.47 |
| 25:7C:110:ARG:HH12 | 30:7K:251:LYS:HD3 | 1.77 | 0.47 |
| 29:7I:44:GLU:O | 29:7I:45:HIS:HB3 | 2.14 | 0.47 |
| 30:7L:350:ASN:ND2 | 30:7L:352:CYS:O | 2.47 | 0.47 |
| 31:7M:66:HIS:CD2 | 31:7M:76:THR:HA | 2.48 | 0.47 |
| 28:7X:349:ALA:O | 28:7X:353:LEU:HG | 2.13 | 0.47 |
| 2:2:282:TYR:HE1 | 24:6T:88:TRP:CZ2 | 2.32 | 0.47 |
| 2:A0:206:ASN:OD1 | 41:A1:501:GTP:N2 | 2.46 | 0.47 |
| 1:B5:276:ARG:O | 24:6X:115:ARG:NH2 | 2.44 | 0.47 |
| 2:E7:62:VAL:HG21 | 2:G3:283:HIS:O | 2.14 | 0.47 |
| 1:G4:183:TYR:CZ | 1:G4:388:MET:HG2 | 2.49 | 0.47 |
| 2:H1:88:HIS:ND1 | 2:I7:283:HIS:HA | 2.29 | 0.47 |
| 1:H4:153:SER:O | 1:H4:157:GLU:HG2 | 2.14 | 0.47 |
| 1:H6:121:ARG:NH2 | 1:H6:158:GLU:OE2 | 2.41 | 0.47 |
| 2:H9:4:VAL:HG23 | 2:H9:134:GLY:O | 2.14 | 0.47 |
| 2:H9:145:THR:OG1 | 41:I0:501:GTP:O1B | 2.30 | 0.47 |
| 2:H9:326:LYS:HG3 | 2:H9:327:ASP:N | 2.30 | 0.47 |
| 1:I0:219:THR:HG23 | 24:6X:488:ARG:HG2 | 1.96 | 0.47 |
| 2:I9:191:THR:HA | 2:I9:194:LEU:HB3 | 1.95 | 0.47 |
| 1:J0:199:CYS:SG | 1:J0:265:PHE:HD1 | 2.37 | 0.47 |
| 2:J5:156:ARG:HA | 2:J5:159:VAL:HG22 | 1.96 | 0.47 |
| 1:J6:26:ASP:O | 1:J6:359:LYS:NZ | 2.33 | 0.47 |
| 1:K6:25:SER:HB2 | 1:K6:30:ILE:HG13 | 1.96 | 0.47 |
| 1:K6:125:GLU:OE2 | 1:K6:159:TYR:OH | 2.28 | 0.47 |
| 1:K8:325:GLU:HA | 1:K8:328:GLU:OE1 | 2.14 | 0.47 |
| 2:K9:90:GLU:HB3 | 2:K9:121:ARG:CZ | 2.44 | 0.47 |
| 2:K9:176:GLN:HE22 | 2:K9:304:LYS:HE2 | 1.79 | 0.47 |
| 1:L0:8:GLN:OE1 | 1:L0:17:GLY:HA3 | 2.14 | 0.47 |
| 2:L7:224:TYR:HA | 2:L7:227:LEU:HD22 | 1.95 | 0.47 |
| 2:M3:49:PHE:CE2 | 2:M3:61:HIS:HE1 | 2.31 | 0.47 |
| 2:M5:413:MET:HB3 | 2:M5:417:GLU:OE2 | 2.14 | 0.47 |
| 2:M9:119:LEU:HA | 2:M9:122:ILE:HG22 | 1.96 | 0.47 |
| 1:N0:173:PRO:HD2 | 1:N0:380:ARG:CZ | 2.44 | 0.47 |
| 2:N7:83:TYR:HB3 | 2:N7:86:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N8:139:LEU:HD22 | 1:N8:170:VAL:HG12 | 1.95 | 0.47 |
| 1:N8:204:ASN:ND2 | 39:N8:502:GDP:HN22 | 2.12 | 0.47 |
| 1:N8:350:LYS:HZ3 | 1:N8:351:SER:C | 2.17 | 0.47 |
| 2:N9:306:ASP:HB3 | 2:N9:309:HIS:HD2 | 1.79 | 0.47 |
| 1:O2:108:GLU:N | 1:O2:108:GLU:OE1 | 2.47 | 0.47 |
| 2:O3:32:PRO:HG3 | 19:6E:94:PRO:CD | 2.44 | 0.47 |
| 1:O6:30:ILE:HD12 | 1:O6:59:TYR:HB2 | 1.95 | 0.47 |
| 2:O7:399:TYR:OH | 2:O7:415:GLU:OE1 | 2.20 | 0.47 |
| 1:O8:245:GLN:CG | 32:7P:64:THR:HG21 | 2.44 | 0.47 |
| 2:P7:175:PRO:HG2 | 2:P7:176:GLN:OE1 | 2.14 | 0.47 |
| 1:P8:128:ASP:N | 1:P8:128:ASP:OD1 | 2.46 | 0.47 |
| 2:Q5:282:TYR:N | 2:Q5:282:TYR:HD2 | 2.11 | 0.47 |
| 1:Q6:49:VAL:HG11 | 1:Q6:241:ARG:HG2 | 1.96 | 0.47 |
| 2:Q9:392:ASP:OD2 | 2:Q9:422:ARG:NH1 | 2.48 | 0.47 |
| 2:R1:47:ASP:OD1 | 2:R1:50:ASN:HB2 | 2.14 | 0.47 |
| 2:R3:76:ASP:O | 2:R3:80:THR:HG22 | 2.14 | 0.47 |
| 1:R4:177:ASP:O | 2:R5:352:LYS:HA | 2.13 | 0.47 |
| 2:R7:325:PRO:HA | 2:R7:328:VAL:HG12 | 1.95 | 0.47 |
| 1:R8:167:PHE:CZ | 1:R8:233:MET:HG2 | 2.49 | 0.47 |
| 1:S0:36:TYR:CG | 1:S0:44:LEU:HD21 | 2.49 | 0.47 |
| 1:S0:49:VAL:HG11 | 1:S0:241:ARG:HG2 | 1.96 | 0.47 |
| 1:S4:125:GLU:HB2 | 3:3V:65:SER:OG | 2.15 | 0.47 |
| 2:S9:66:ILE:O | 2:S9:66:ILE:HG13 | 2.14 | 0.47 |
| 1:T0:276:ARG:HB3 | 7:4T:359:PHE:CG | 2.49 | 0.47 |
| 2:T5:322:ASP:OD2 | 2:T5:373:ARG:NH2 | 2.46 | 0.47 |
| 1:T6:273:LEU:H | 1:T6:292:GLN:HE22 | 1.61 | 0.47 |
| 2:T7:339:ARG:HH21 | 13:5K:24:VAL:HG13 | 1.79 | 0.47 |
| 1:T8:6:HIS:CE1 | 1:T8:8:GLN:HG2 | 2.49 | 0.47 |
| 1:T8:328:GLU:HB3 | 13:5K:89:TRP:HH2 | 1.79 | 0.47 |
| 2:U1:3:GLU:HG3 | 2:U1:51:THR:HA | 1.95 | 0.47 |
| 1:U4:5:VAL:HG22 | 1:U4:133:PHE:HD1 | 1.79 | 0.47 |
| 2:U5:90:GLU:HB3 | 2:U5:121:ARG:HH22 | 1.78 | 0.47 |
| 1:U8:286:VAL:HG12 | 1:U8:329:GLN:HG3 | 1.96 | 0.47 |
| 2:U9:223:THR:OG1 | 2:U9:224:TYR:N | 2.48 | 0.47 |
| 2:V3:116:ASP:OD1 | 2:V3:117:LEU:N | 2.47 | 0.47 |
| 2:V9:5:ILE:HD11 | 2:V9:135:PHE:HE1 | 1.79 | 0.47 |
| 1:W2:375:GLN:HB3 | 1:W2:422:TYR:HD2 | 1.78 | 0.47 |
| 1:W2:412:GLU:OE1 | 1:W2:416:ASN:ND2 | 2.46 | 0.47 |
| 2:W3:246:GLY:HA2 | 2:W3:357:TYR:CD2 | 2.49 | 0.47 |
| 2:W7:27:GLU:OE1 | 2:W7:243:ARG:NH1 | 2.47 | 0.47 |
| 2:W9:109:THR:HG22 | 2:W9:110:ILE:HD13 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:430:LYS:HD2 | 2:W9:433:GLU:OE2 | 2.14 | 0.47 |
| 1:X2:395:LEU:O | 1:X2:399:THR:HG23 | 2.14 | 0.47 |
| 1:X6:14:ASN:HD22 | 1:X6:72:THR:HB | 1.80 | 0.47 |
| 2:X7:407:TRP:CD2 | 1:X8:255:VAL:HG12 | 2.48 | 0.47 |
| 2:X9:327:ASP:N | 2:X9:327:ASP:OD1 | 2.45 | 0.47 |
| 2:Y1:21:TRP:CZ2 | 2:Y1:65:CYS:HB2 | 2.49 | 0.47 |
| 1:Z2:21:TRP:CZ3 | 1:Z2:61:PRO:HB3 | 2.50 | 0.47 |
| 1:Z2:237:THR:HG23 | 1:Z2:241:ARG:HH21 | 1.79 | 0.47 |
| 2:Z3:259:LEU:HD21 | 2:Z3:316:CYS:HB2 | 1.95 | 0.47 |
| 1:Z6:66:MET:HE3 | 1:Z6:116:VAL:HG11 | 1.96 | 0.47 |
| 2:Z7:428:LEU:HA | 2:Z7:431:ASP:OD1 | 2.14 | 0.47 |
| 2:0B:100:ALA:HA | 1:0C:252:LYS:HE2 | 1.95 | 0.47 |
| 1:0C:311:LEU:O | 1:0C:348:ASN:ND2 | 2.47 | 0.47 |
| 2:0F:3:GLU:HB2 | 2:0F:129:CYS:SG | 2.54 | 0.47 |
| 1:0G:200:MET:SD | 1:0G:268:VAL:HG21 | 2.53 | 0.47 |
| 2:0H:338:LYS:HZ2 | 2:0H:339:ARG:H | 1.62 | 0.47 |
| 1:0K:100:ASN:HB3 | 1:0K:103:LYS:HB2 | 1.95 | 0.47 |
| 1:0O:4:ILE:HG22 | 1:0O:49:VAL:HG22 | 1.94 | 0.47 |
| 1:0O:113:ILE:HD13 | 1:0O:154:LYS:HG3 | 1.95 | 0.47 |
| 2:0P:111:GLY:HA2 | 2:0P:114:ILE:HG22 | 1.96 | 0.47 |
| 2:0R:174:SER:HB3 | 2:0R:207:GLU:OE1 | 2.14 | 0.47 |
| 2:0R:296:PHE:CE2 | 2:0R:335:ILE:HG12 | 2.49 | 0.47 |
| 1:0S:249:ASP:OD1 | 1:0S:252:LYS:N | 2.39 | 0.47 |
| 1:0U:2:ARG:HE | 1:0U:240:LEU:HD21 | 1.78 | 0.47 |
| 2:0V:116:ASP:N | 2:0V:116:ASP:OD1 | 2.45 | 0.47 |
| 2:0X:63:PRO:HB2 | 2:0X:65:CYS:SG | 2.54 | 0.47 |
| 2:1B:9:ILE:HG22 | 2:1B:146:GLY:HA2 | 1.97 | 0.47 |
| 1:1E:161:ASP:OD2 | 1:1E:162:ARG:HG2 | 2.14 | 0.47 |
| 2:1H:176:GLN:NE2 | 2:1H:207:GLU:HG2 | 2.28 | 0.47 |
| 2:1N:348:PRO:HG2 | 2:1N:349:THR:HG22 | 1.97 | 0.47 |
| 2:1R:156:ARG:HA | 2:1R:159:VAL:HG12 | 1.96 | 0.47 |
| 1:1S:7:ILE:HB | 1:1S:135:VAL:HG22 | 1.96 | 0.47 |
| 2:1T:187:SER:O | 2:1T:191:THR:HG23 | 2.14 | 0.47 |
| 2:1T:305:CYS:HB3 | 2:1T:387:ILE:HD11 | 1.96 | 0.47 |
| 2:1X:129:CYS:SG | 2:1X:130:THR:N | 2.86 | 0.47 |
| 2:1X:166:LYS:N | 2:1X:199:ASP:OD2 | 2.47 | 0.47 |
| 1:2A:167:PHE:CE2 | 1:2A:233:MET:HG2 | 2.49 | 0.47 |
| 2:2H:123:ARG:O | 2:2H:127:ASP:N | 2.43 | 0.47 |
| 1:2I:375:GLN:HB2 | 1:2I:419:VAL:HG13 | 1.96 | 0.47 |
| 2:2J:289:ALA:O | 2:2J:293:ASN:ND2 | 2.48 | 0.47 |
| 2:2J:325:PRO:HA | 2:2J:328:VAL:HG22 | 1.94 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2P:90:GLU:O | 2:2P:121:ARG:NH1 | 2.46 | 0.47 |
| 1:2Q:276:ARG:HH22 | 10:5C:192:ARG:NH1 | 2.12 | 0.47 |
| 1:2Q:325:GLU:O | 1:2Q:329:GLN:HB2 | 2.14 | 0.47 |
| 2:2R:66:ILE:O | 2:2R:66:ILE:HG13 | 2.13 | 0.47 |
| 2:2R:69:ASP:OD1 | 2:2R:71:GLU:N | 2.47 | 0.47 |
| 1:2U:77:ARG:HH11 | 17:5T:201:LEU:HG | 1.77 | 0.47 |
| 1:2Y:91:VAL:HG11 | 1:2Y:116:VAL:HG12 | 1.95 | 0.47 |
| 2:3B:236:SER:O | 2:3B:243:ARG:NH2 | 2.45 | 0.47 |
| 2:3D:198:THR:HG21 | 2:3D:201:ALA:HB2 | 1.95 | 0.47 |
| 2:3J:305:CYS:HB3 | 2:3J:387:ILE:HD11 | 1.95 | 0.47 |
| 2:3P:246:GLY:HA3 | 2:3P:356:ASN:HA | 1.95 | 0.47 |
| 1:3Q:354:CYS:SG | 1:3Q:355:ASP:N | 2.87 | 0.47 |
| 5:4L:370:ALA:HA | 5:4L:373:GLN:OE1 | 2.14 | 0.47 |
| 6:4O:89:ARG:HH12 | 30:7K:452:LEU:N | 2.10 | 0.47 |
| 8:4W:227:LYS:O | 8:4W:230:GLU:HG3 | 2.14 | 0.47 |
| 13:5J:18:ARG:HB3 | 24:6X:38:GLY:HA2 | 1.95 | 0.47 |
| 14:5M:208:TYR:HD1 | 14:5M:222:ALA:HA | 1.78 | 0.47 |
| 14:5M:229:LYS:O | 14:5M:230:ASN:C | 2.51 | 0.47 |
| 14:5M:604:THR:HG22 | 14:5M:609:ARG:O | 2.14 | 0.47 |
| 14:5N:604:THR:HG22 | 14:5N:609:ARG:O | 2.14 | 0.47 |
| 15:5O:109:ILE:HG23 | 15:5O:192:LEU:HD21 | 1.96 | 0.47 |
| 16:5Q:148:ARG:HG3 | 16:5Q:149:GLY:N | 2.29 | 0.47 |
| 17:5U:212:LYS:O | 17:5U:216:GLU:HG3 | 2.14 | 0.47 |
| 17:5V:144:LYS:HA | 17:5V:147:VAL:HG22 | 1.96 | 0.47 |
| 17:5V:200:SER:OG | 17:5V:201:LEU:N | 2.47 | 0.47 |
| 22:6O:238:LEU:H | 22:6O:238:LEU:HD23 | 1.78 | 0.47 |
| 22:6P:281:LYS:HB2 | 22:6P:282:LYS:NZ | 2.29 | 0.47 |
| 24:6T:450:VAL:HB | 24:6T:469:PHE:CE2 | 2.49 | 0.47 |
| 24:6X:463:THR:O | 24:6X:467:ARG:CG | 2.57 | 0.47 |
| 24:7A:183:ASP:OD1 | 24:7A:184:ALA:N | 2.47 | 0.47 |
| 26:7D:80:ARG:HG3 | 26:7D:82:PRO:HD2 | 1.96 | 0.47 |
| 26:7E:80:ARG:HG3 | 26:7E:82:PRO:HD2 | 1.96 | 0.47 |
| 26:7F:80:ARG:HG3 | 26:7F:82:PRO:HD2 | 1.96 | 0.47 |
| 29:7I:57:LYS:HB3 | 29:7I:61:LYS:NZ | 2.28 | 0.47 |
| 30:7K:410:LEU:O | 30:7K:413:GLU:HG3 | 2.14 | 0.47 |
| 2:2:370:LYS:HG3 | 24:6T:88:TRP:HZ3 | 1.78 | 0.47 |
| 1:5:337:ASN:HD21 | 3:3Z:69:TYR:N | 1.84 | 0.47 |
| 1:A9:77:ARG:NH1 | 24:6U:242:PHE:HB2 | 2.29 | 0.47 |
| 2:B2:222:PRO:HA | 18:5Z:51:MET:HE1 | 1.97 | 0.47 |
| 2:F1:88:HIS:HB3 | 2:G7:283:HIS:ND1 | 2.29 | 0.47 |
| 2:F9:322:ASP:OD2 | 24:6U:433:ARG:NH1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G2:65:LEU:HD12 | 1:G2:90:PHE:HE1 | 1.77 | 0.47 |
| 2:G7:318:MET:HB2 | 2:G7:376:CYS:HB3 | 1.95 | 0.47 |
| 1:G8:107:THR:OG1 | 1:G8:401:GLU:OE2 | 2.23 | 0.47 |
| 2:H1:203:MET:O | 2:H1:204:LEU:HD12 | 2.15 | 0.47 |
| 2:H7:145:THR:OG1 | 41:H8:501:GTP:O1B | 2.31 | 0.47 |
| 2:H7:220:GLU:O | 1:H8:324:LYS:NZ | 2.35 | 0.47 |
| 2:H9:109:THR:OG1 | 2:H9:411:GLU:OE2 | 2.32 | 0.47 |
| 2:I1:11:GLN:NE2 | 1:I2:247:ASN:OD1 | 2.48 | 0.47 |
| 1:I4:70:PRO:HG2 | 2:I5:2:ARG:HH11 | 1.79 | 0.47 |
| 1:I4:327:ASP:N | 1:I4:327:ASP:OD2 | 2.44 | 0.47 |
| 1:I8:334:GLN:HE22 | 1:I8:348:ASN:H | 1.61 | 0.47 |
| 1:J2:190:HIS:HD2 | 1:J2:414:ASN:HB2 | 1.78 | 0.47 |
| 1:J2:212:PHE:CE1 | 2:J3:326:LYS:HG3 | 2.49 | 0.47 |
| 1:J4:178:THR:HG22 | 2:J5:352:LYS:HZ3 | 1.80 | 0.47 |
| 1:J6:86:ARG:NH1 | 1:J6:123:GLU:OE2 | 2.47 | 0.47 |
| 1:K0:52:ASN:OD1 | 1:K0:62:ARG:NH2 | 2.47 | 0.47 |
| 2:K1:31:GLN:HB2 | 2:K1:33:ASP:OD1 | 2.14 | 0.47 |
| 2:K1:288:VAL:HG11 | 2:K1:327:ASP:CB | 2.44 | 0.47 |
| 1:L0:391:ARG:HD3 | 2:L1:346:TRP:CZ2 | 2.48 | 0.47 |
| 2:L1:97:GLU:N | 2:L1:97:GLU:OE2 | 2.48 | 0.47 |
| 1:L2:244:GLY:HA2 | 1:L2:355:ASP:OD2 | 2.15 | 0.47 |
| 1:L4:382:SER:HB2 | 1:L4:415:MET:HG2 | 1.94 | 0.47 |
| 2:M3:187:SER:O | 2:M3:191:THR:HG23 | 2.15 | 0.47 |
| 2:M5:89:PRO:HG3 | 37:7Y:124:ARG:CZ | 2.44 | 0.47 |
| 1:M6:32:PRO:HD3 | 1:M6:81:TYR:CZ | 2.50 | 0.47 |
| 1:M6:80:PRO:HB3 | 15:5P:69:PHE:CE1 | 2.50 | 0.47 |
| 1:M6:178:THR:HG23 | 1:M6:181:GLU:HG3 | 1.96 | 0.47 |
| 1:M8:282:ARG:NH2 | 1:M8:288:GLU:HB3 | 2.29 | 0.47 |
| 1:O0:117:LEU:HA | 1:O0:120:VAL:HG12 | 1.96 | 0.47 |
| 1:O4:208:TYR:CE1 | 1:O4:225:LEU:HD11 | 2.49 | 0.47 |
| 1:O8:239:CYS:SG | 1:O8:248:ALA:N | 2.85 | 0.47 |
| 2:P5:249:ASN:ND2 | 27:7G:184:LYS:O | 2.47 | 0.47 |
| 1:P6:100:ASN:HB3 | 1:P6:103:LYS:HB2 | 1.96 | 0.47 |
| 2:Q1:100:ALA:HA | 1:Q2:252:LYS:HE2 | 1.96 | 0.47 |
| 1:Q6:111:GLU:OE1 | 1:Q6:111:GLU:N | 2.47 | 0.47 |
| 1:Q8:178:THR:OG1 | 1:Q8:181:GLU:HG3 | 2.14 | 0.47 |
| 2:R3:372:GLN:HE22 | 7:4R:84:THR:HG21 | 1.77 | 0.47 |
| 2:R5:4:VAL:HG23 | 2:R5:134:GLY:O | 2.14 | 0.47 |
| 2:R5:47:ASP:OD2 | 19:6E:256:LYS:NZ | 2.30 | 0.47 |
| 2:R5:55:GLU:HG3 | 2:R5:61:HIS:HE1 | 1.79 | 0.47 |
| 2:R5:121:ARG:NH1 | 2:R5:124:LYS:HE3 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:11:GLN:HE22 | 2:R7:249:ASN:H | 1.62 | 0.47 |
| 1:R6:317:PHE:HE2 | 1:R6:326:VAL:HG13 | 1.80 | 0.47 |
| 2:R7:289:ALA:O | 2:R7:293:ASN:ND2 | 2.48 | 0.47 |
| 2:S5:184:PRO:O | 2:S5:188:VAL:HG23 | 2.14 | 0.47 |
| 1:T2:31:ASP:HB2 | 1:T2:32:PRO:HD2 | 1.96 | 0.47 |
| 1:T2:301:CYS:SG | 1:T2:302:ALA:N | 2.87 | 0.47 |
| 2:T5:166:LYS:N | 2:T5:199:ASP:OD1 | 2.48 | 0.47 |
| 1:T6:39:ASP:OD1 | 1:T6:40:SER:N | 2.47 | 0.47 |
| 2:T7:204:LEU:HD23 | 2:T7:302:MET:HB3 | 1.96 | 0.47 |
| 1:U6:169:VAL:HG13 | 1:U6:203:ASP:HA | 1.95 | 0.47 |
| 1:U6:282:ARG:HG2 | 1:U6:283:ALA:O | 2.14 | 0.47 |
| 2:U7:119:LEU:HA | 2:U7:122:ILE:HG22 | 1.97 | 0.47 |
| 1:V0:67:ASP:N | 1:V0:67:ASP:OD1 | 2.47 | 0.47 |
| 2:V7:33:ASP:OD2 | 2:V7:35:GLN:NE2 | 2.47 | 0.47 |
| 2:V7:132:LEU:HD22 | 2:V7:164:LYS:HD3 | 1.97 | 0.47 |
| 1:W6:186:THR:HG22 | 1:W6:411:ALA:HB1 | 1.96 | 0.47 |
| 1:W6:260:PHE:HB2 | 1:W6:263:LEU:CD1 | 2.45 | 0.47 |
| 2:W9:14:ILE:CG1 | 2:W9:74:VAL:HG21 | 2.43 | 0.47 |
| 1:X2:178:THR:HA | 2:X3:352:LYS:HD3 | 1.95 | 0.47 |
| 1:X2:250:LEU:HD12 | 1:X2:250:LEU:H | 1.78 | 0.47 |
| 2:X3:332:VAL:HA | 2:X3:335:ILE:HG12 | 1.95 | 0.47 |
| 2:X3:417:GLU:HA | 2:X3:420:GLU:HG2 | 1.96 | 0.47 |
| 2:X5:240:ALA:HB1 | 2:X5:356:ASN:HD22 | 1.80 | 0.47 |
| 1:Y6:6:HIS:HA | 1:Y6:134:GLN:O | 2.13 | 0.47 |
| 1:Y8:396:HIS:HA | 1:Y8:399:THR:OG1 | 2.14 | 0.47 |
| 1:Z0:64:ILE:HD11 | 1:Z0:123:GLU:OE1 | 2.14 | 0.47 |
| 2:Z7:67:PHE:C | 2:Z7:68:LEU:HD12 | 2.34 | 0.47 |
| 2:Z7:280:LYS:O | 2:Z7:283:HIS:HB3 | 2.14 | 0.47 |
| 1:Z8:414:ASN:HA | 1:Z8:417:ASP:OD2 | 2.14 | 0.47 |
| 1:0A:358:PRO:HG2 | 1:0A:361:LEU:HB2 | 1.96 | 0.47 |
| 2:0B:259:LEU:HB3 | 2:0B:268:MET:HE3 | 1.96 | 0.47 |
| 2:0B:333:ALA:O | 2:0B:337:THR:HG23 | 2.14 | 0.47 |
| 1:0C:17:GLY:HA2 | 1:0C:20:PHE:HB3 | 1.97 | 0.47 |
| 2:0H:12:ALA:HB2 | 41:0I:501:GTP:C8 | 2.49 | 0.47 |
| 1:0K:179:VAL:HA | 2:0L:349:THR:HG23 | 1.95 | 0.47 |
| 1:0K:237:THR:HG23 | 1:0K:241:ARG:HE | 1.79 | 0.47 |
| 2:0L:53:PHE:HB3 | 2:0L:61:HIS:HB3 | 1.96 | 0.47 |
| 2:0L:138:PHE:CZ | 2:0L:235:ILE:HG13 | 2.49 | 0.47 |
| 2:0N:12:ALA:O | 2:0N:16:VAL:HG23 | 2.14 | 0.47 |
| 2:0N:56:THR:HB | 2:0N:60:LYS:HG2 | 1.97 | 0.47 |
| 1:0Y:395:LEU:HD23 | 1:0Y:395:LEU:HA | 1.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0Z:287:SER:N | 2:0Z:290:GLU:OE2 | 2.43 | 0.47 |
| 1:1A:31:ASP:OD1 | 1:1A:35:THR:N | 2.38 | 0.47 |
| 2:1B:182:VAL:HG23 | 2:1B:186:ASN:ND2 | 2.29 | 0.47 |
| 2:1F:333:ALA:O | 2:1F:337:THR:HG23 | 2.14 | 0.47 |
| 1:1G:8:GLN:O | 1:1G:66:MET:HG3 | 2.14 | 0.47 |
| 1:1G:334:GLN:NE2 | 1:1G:348:ASN:H | 2.10 | 0.47 |
| 1:1K:99:ASN:ND2 | 2:1L:254:GLU:OE2 | 2.47 | 0.47 |
| 2:1R:50:ASN:O | 2:1R:64:ARG:NH2 | 2.46 | 0.47 |
| 2:1T:217:LEU:HD11 | 2:1T:275:ILE:HD11 | 1.96 | 0.47 |
| 2:2B:164:LYS:HE3 | 38:8A:80:TYR:HE2 | 1.78 | 0.47 |
| 1:2C:337:ASN:HB3 | 1:2C:340:TYR:HD2 | 1.79 | 0.47 |
| 2:2F:90:GLU:C | 2:2F:121:ARG:HH12 | 2.17 | 0.47 |
| 1:2K:144:GLY:N | 39:2K:502:GDP:O1B | 2.46 | 0.47 |
| 1:2K:350:LYS:NZ | 1:2K:351:SER:O | 2.41 | 0.47 |
| 2:2N:66:ILE:HG13 | 2:2N:91:GLN:O | 2.14 | 0.47 |
| 1:2Q:220:PRO:HG2 | 2:2R:326:LYS:HB2 | 1.97 | 0.47 |
| 1:2S:237:THR:HG23 | 1:2S:241:ARG:HE | 1.78 | 0.47 |
| 1:2W:328:GLU:HB3 | 38:8B:67:PHE:HE1 | 1.79 | 0.47 |
| 2:2X:298:PRO:HG2 | 38:8B:23:SER:O | 2.14 | 0.47 |
| 1:3A:5:VAL:HG23 | 1:3A:62:ARG:HG2 | 1.96 | 0.47 |
| 1:3C:371:SER:OG | 1:3C:372:THR:N | 2.47 | 0.47 |
| 2:3D:133:GLN:HB3 | 2:3D:252:ILE:CG2 | 2.44 | 0.47 |
| 2:3F:176:GLN:HE22 | 2:3F:304:LYS:HE2 | 1.79 | 0.47 |
| 2:3J:223:THR:HG22 | 2:3J:224:TYR:N | 2.29 | 0.47 |
| 2:3P:174:SER:HB3 | 2:3P:177:VAL:O | 2.14 | 0.47 |
| 1:3Q:322:SER:OG | 1:3Q:325:GLU:OE1 | 2.32 | 0.47 |
| 2:3T:47:ASP:OD1 | 2:3T:48:ALA:N | 2.47 | 0.47 |
| 3:3V:10:PHE:HB3 | 3:3V:140:LYS:NZ | 2.29 | 0.47 |
| 3:3Z:10:PHE:HB3 | 3:3Z:140:LYS:NZ | 2.29 | 0.47 |
| 3:3Z:75:ARG:HG2 | 3:3Z:76:PRO:HD2 | 1.96 | 0.47 |
| 3:4B:10:PHE:HB3 | 3:4B:140:LYS:NZ | 2.29 | 0.47 |
| 3:4B:63:SER:OG | 3:4B:66:THR:O | 2.29 | 0.47 |
| 3:4D:10:PHE:HB3 | 3:4D:140:LYS:NZ | 2.29 | 0.47 |
| 3:4D:75:ARG:HG2 | 3:4D:76:PRO:HD2 | 1.96 | 0.47 |
| 3:4H:10:PHE:HB3 | 3:4H:140:LYS:NZ | 2.29 | 0.47 |
| 6:4O:199:ARG:O | 6:4O:203:GLU:HG2 | 2.14 | 0.47 |
| 6:4O:261:GLU:O | 6:4O:265:GLU:HG2 | 2.14 | 0.47 |
| 6:4O:284:TYR:O | 6:4O:287:SER:OG | 2.31 | 0.47 |
| 6:4P:85:TYR:O | 6:4P:88:GLU:HG3 | 2.14 | 0.47 |
| 10:5B:158:LYS:O | 10:5B:162:ILE:HG12 | 2.14 | 0.47 |
| 15:5O:61:PHE:CE1 | 15:5O:64:SER:HB3 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5T:31:THR:HB | 17:5T:36:PHE:CE2 | 2.50 | 0.47 |
| 20:6F:238:LEU:HD21 | 20:6F:251:LEU:HD13 | 1.95 | 0.47 |
| 21:6H:117:PRO:O | 21:6H:123:LEU:HD12 | 2.14 | 0.47 |
| 22:6L:17:ILE:HG22 | 22:6L:19:GLY:H | 1.79 | 0.47 |
| 22:6M:46:SER:O | 22:6M:49:SER:OG | 2.31 | 0.47 |
| 22:6M:162:LEU:HD11 | 22:6M:225:ALA:HB1 | 1.96 | 0.47 |
| 23:6R:65:LEU:HD12 | 23:6R:65:LEU:HA | 1.79 | 0.47 |
| 24:6T:503:ILE:HG21 | 24:6T:525:VAL:HG22 | 1.95 | 0.47 |
| 24:6T:570:GLU:N | 24:6T:570:GLU:OE1 | 2.41 | 0.47 |
| 24:6T:602:LEU:HG | 24:6T:604:PHE:HD1 | 1.80 | 0.47 |
| 24:6W:338:LEU:HD22 | 24:6W:341:LYS:HZ1 | 1.79 | 0.47 |
| 24:6Y:282:ARG:NH1 | 24:6Y:289:ARG:HD3 | 2.29 | 0.47 |
| 24:6Z:247:GLU:HG3 | 24:6Z:252:LYS:HB2 | 1.97 | 0.47 |
| 27:7G:202:GLY:HA3 | 27:7G:234:PHE:HE2 | 1.79 | 0.47 |
| 29:7I:169:THR:HB | 29:7I:172:VAL:HG21 | 1.95 | 0.47 |
| 37:7Y:63:ASP:OD1 | 37:7Y:71:ARG:N | 2.48 | 0.47 |
| 38:8D:76:ASP:OD2 | 38:8D:77:LYS:HD3 | 2.15 | 0.47 |
| 1:B8:277:GLY:HA2 | 24:6Y:142:ILE:HG13 | 1.95 | 0.47 |
| 1:G2:167:PHE:CE2 | 1:G2:233:MET:HG2 | 2.50 | 0.47 |
| 1:G2:238:CYS:SG | 1:G2:318:ARG:NE | 2.87 | 0.47 |
| 1:G8:7:ILE:HD13 | 1:G8:64:ILE:HB | 1.96 | 0.47 |
| 2:G9:317:LEU:HB3 | 2:G9:319:TYR:HE1 | 1.78 | 0.47 |
| 1:H4:113:ILE:HD13 | 1:H4:150:LEU:CD2 | 2.45 | 0.47 |
| 1:H4:215:LEU:HB3 | 1:H4:217:LEU:HG | 1.95 | 0.47 |
| 2:H7:4:VAL:HG23 | 2:H7:134:GLY:O | 2.14 | 0.47 |
| 2:H7:353:CYS:SG | 2:H7:354:GLY:N | 2.86 | 0.47 |
| 2:H9:72:PRO:HD2 | 1:I0:2:ARG:NH1 | 2.30 | 0.47 |
| 2:I1:172:TYR:CE2 | 2:I1:203:MET:HG2 | 2.50 | 0.47 |
| 1:I4:178:THR:OG1 | 1:I4:181:GLU:HG3 | 2.14 | 0.47 |
| 1:I4:392:LYS:HA | 1:I4:395:LEU:HD12 | 1.97 | 0.47 |
| 2:I7:287:SER:OG | 2:I7:290:GLU:OE1 | 2.25 | 0.47 |
| 2:J1:262:TYR:HE2 | 2:J1:346:TRP:HZ3 | 1.61 | 0.47 |
| 1:J2:178:THR:HG22 | 1:J2:180:VAL:H | 1.79 | 0.47 |
| 1:J4:263:LEU:HD21 | 1:J4:311:LEU:HD13 | 1.95 | 0.47 |
| 2:J9:89:PRO:HD2 | 2:L5:283:HIS:ND1 | 2.30 | 0.47 |
| 1:K0:135:VAL:HG21 | 1:K0:152:ILE:HD11 | 1.96 | 0.47 |
| 2:K1:129:CYS:SG | 2:K1:130:THR:N | 2.88 | 0.47 |
| 1:K4:175:VAL:O | 1:K4:175:VAL:HG23 | 2.14 | 0.47 |
| 2:K5:7:ILE:HG12 | 2:K5:137:VAL:HG12 | 1.95 | 0.47 |
| 1:K8:382:SER:HB3 | 1:K8:415:MET:HG2 | 1.96 | 0.47 |
| 2:L1:305:CYS:HB3 | 2:L1:387:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L7:413:MET:HE3 | 2:L7:414:GLU:H | 1.78 | 0.47 |
| 1:M4:201:VAL:HG13 | 1:M4:301:CYS:SG | 2.55 | 0.47 |
| 1:N0:48:ASN:N | 1:N0:48:ASN:OD1 | 2.46 | 0.47 |
| 2:N3:108:TYR:HB3 | 2:N3:411:GLU:OE2 | 2.14 | 0.47 |
| 2:N5:76:ASP:O | 2:N5:80:THR:HG23 | 2.14 | 0.47 |
| 2:N5:240:ALA:HB1 | 2:N5:356:ASN:HD22 | 1.80 | 0.47 |
| 1:N8:7:ILE:HB | 1:N8:135:VAL:HG22 | 1.96 | 0.47 |
| 2:N9:155:GLU:HG3 | 2:N9:197:HIS:NE2 | 2.29 | 0.47 |
| 1:O0:86:ARG:HG2 | 1:O0:88:ASP:H | 1.78 | 0.47 |
| 2:P3:65:CYS:SG | 2:P3:66:ILE:N | 2.87 | 0.47 |
| 1:P4:318:ARG:HA | 1:P4:354:CYS:O | 2.14 | 0.47 |
| 2:P5:41:THR:HA | 27:7G:220:MET:O | 2.13 | 0.47 |
| 2:P9:195:LEU:HD21 | 2:P9:264:ARG:HH11 | 1.79 | 0.47 |
| 1:Q4:117:LEU:HA | 1:Q4:120:VAL:HG12 | 1.96 | 0.47 |
| 1:Q6:204:ASN:ND2 | 39:Q6:502:GDP:HN22 | 2.12 | 0.47 |
| 1:Q8:26:ASP:OD2 | 24:6T:10:LYS:HG3 | 2.15 | 0.47 |
| 1:R0:153:SER:O | 1:R0:157:GLU:HG2 | 2.13 | 0.47 |
| 1:R2:180:VAL:HG23 | 1:R2:184:ASN:ND2 | 2.29 | 0.47 |
| 1:R2:272:PRO:HD3 | 1:R2:364:SER:HA | 1.96 | 0.47 |
| 2:R3:288:VAL:HG21 | 2:R3:323:VAL:HG23 | 1.96 | 0.47 |
| 2:R9:90:GLU:HB2 | 2:R9:121:ARG:HH12 | 1.79 | 0.47 |
| 2:S1:300:SER:O | 2:S1:300:SER:OG | 2.31 | 0.47 |
| 2:S7:394:LYS:HB2 | 1:S8:346:PRO:HG3 | 1.96 | 0.47 |
| 1:S8:208:TYR:CE1 | 1:S8:225:LEU:HD11 | 2.49 | 0.47 |
| 2:S9:12:ALA:O | 2:S9:16:VAL:HG23 | 2.14 | 0.47 |
| 2:T1:11:GLN:OE1 | 2:T1:74:VAL:HG11 | 2.14 | 0.47 |
| 2:T3:284:GLU:HG2 | 2:T3:285:GLN:N | 2.29 | 0.47 |
| 1:T8:279:GLN:OE1 | 7:4U:236:THR:HG23 | 2.14 | 0.47 |
| 1:U6:49:VAL:HG11 | 1:U6:241:ARG:HG2 | 1.95 | 0.47 |
| 1:U6:286:VAL:O | 1:U6:290:THR:HG23 | 2.14 | 0.47 |
| 2:U9:305:CYS:HB3 | 2:U9:387:ILE:HD11 | 1.96 | 0.47 |
| 2:U9:336:LYS:HE3 | 2:U9:351:PHE:HD2 | 1.79 | 0.47 |
| 1:V6:212:PHE:HZ | 2:V7:326:LYS:HB2 | 1.80 | 0.47 |
| 1:V6:220:PRO:HD2 | 2:V7:326:LYS:HD2 | 1.96 | 0.47 |
| 2:V7:251:ASP:OD1 | 2:V7:254:GLU:HG2 | 2.13 | 0.47 |
| 2:V7:407:TRP:CD2 | 1:V8:255:VAL:HG12 | 2.50 | 0.47 |
| 2:W3:277:SER:OG | 2:W3:278:ALA:N | 2.47 | 0.47 |
| 2:W7:53:PHE:HD1 | 2:W7:63:PRO:HA | 1.78 | 0.47 |
| 2:W9:101:ASN:OD1 | 2:W9:186:ASN:ND2 | 2.47 | 0.47 |
| 2:W9:211:ASP:OD1 | 2:W9:214:ARG:NH2 | 2.41 | 0.47 |
| 1:X0:327:ASP:N | 1:X0:327:ASP:OD2 | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X7:174:SER:HA | 2:X7:205:ASP:OD1 | 2.14 | 0.47 |
| 2:X9:51:THR:HG21 | 2:X9:243:ARG:HG2 | 1.96 | 0.47 |
| 2:X9:90:GLU:H | 2:Z5:283:HIS:CE1 | 2.32 | 0.47 |
| 2:Y3:267:PHE:HB3 | 2:Y3:384:ILE:HG21 | 1.97 | 0.47 |
| 2:Y5:26:LEU:HD21 | 2:Y5:363:VAL:HG22 | 1.97 | 0.47 |
| 1:Y8:294:TRP:CD1 | 1:Y8:333:VAL:HG21 | 2.49 | 0.47 |
| 2:Y9:404:PHE:CE1 | 1:Z0:259:PRO:HB3 | 2.48 | 0.47 |
| 1:Z0:10:GLY:O | 1:Z0:14:ASN:HB2 | 2.14 | 0.47 |
| 1:Z0:311:LEU:HD22 | 1:Z0:370:ASN:ND2 | 2.29 | 0.47 |
| 1:Z2:396:HIS:CE1 | 1:Z2:397:TRP:CE2 | 3.02 | 0.47 |
| 1:Z2:404:ASP:HB3 | 1:Z2:406:MET:SD | 2.54 | 0.47 |
| 2:Z3:53:PHE:HB3 | 2:Z3:61:HIS:HB3 | 1.96 | 0.47 |
| 2:Z3:202:VAL:HG22 | 2:Z3:268:MET:HB2 | 1.97 | 0.47 |
| 1:Z6:4:ILE:HD11 | 1:Z6:134:GLN:HB2 | 1.96 | 0.47 |
| 1:0A:397:TRP:HE1 | 2:0B:260:VAL:HB | 1.80 | 0.47 |
| 2:0B:33:ASP:O | 2:0B:60:LYS:NZ | 2.47 | 0.47 |
| 1:0E:249:ASP:OD1 | 1:0E:252:LYS:N | 2.39 | 0.47 |
| 2:0F:205:ASP:OD2 | 2:0F:207:GLU:N | 2.48 | 0.47 |
| 2:0J:338:LYS:NZ | 2:0J:339:ARG:H | 2.11 | 0.47 |
| 2:0L:90:GLU:HG2 | 2:0L:121:ARG:HH12 | 1.79 | 0.47 |
| 2:0L:387:ILE:HD12 | 2:0L:390:ARG:NH2 | 2.29 | 0.47 |
| 1:0O:293:MET:SD | 1:0O:367:PHE:HB2 | 2.55 | 0.47 |
| 1:0Q:165:LEU:HD22 | 1:0Q:167:PHE:CE1 | 2.49 | 0.47 |
| 2:0R:88:HIS:HB3 | 2:1H:283:HIS:CE1 | 2.49 | 0.47 |
| 1:0S:73:MET:HE3 | 1:0S:77:ARG:HG3 | 1.95 | 0.47 |
| 1:0U:375:GLN:HB3 | 1:0U:422:TYR:HD2 | 1.79 | 0.47 |
| 1:0W:165:LEU:HD21 | 1:0W:250:LEU:HD11 | 1.96 | 0.47 |
| 2:0Z:145:THR:OG1 | 41:1A:501:GTP:O1B | 2.32 | 0.47 |
| 2:0Z:415:GLU:OE1 | 2:0Z:415:GLU:N | 2.45 | 0.47 |
| 2:1B:9:ILE:HG23 | 2:1B:68:LEU:HD11 | 1.97 | 0.47 |
| 1:1C:397:TRP:HZ2 | 2:1D:260:VAL:HG21 | 1.79 | 0.47 |
| 2:1H:116:ASP:N | 2:1H:116:ASP:OD1 | 2.45 | 0.47 |
| 2:1P:9:ILE:HD11 | 2:1P:153:LEU:HD23 | 1.96 | 0.47 |
| 2:1P:76:ASP:OD2 | 1:1Q:46:ARG:NH2 | 2.47 | 0.47 |
| 2:1R:33:ASP:OD1 | 2:1R:34:GLY:N | 2.47 | 0.47 |
| 1:1S:35:THR:OG1 | 1:1S:37:HIS:NE2 | 2.48 | 0.47 |
| 1:1S:417:ASP:HA | 1:1S:420:SER:OG | 2.13 | 0.47 |
| 1:1U:72:THR:O | 1:1U:75:SER:OG | 2.27 | 0.47 |
| 2:1V:49:PHE:HB2 | 2:1V:53:PHE:HD2 | 1.80 | 0.47 |
| 1:2A:235:GLY:HA3 | 1:2A:366:THR:HG21 | 1.96 | 0.47 |
| 1:2C:68:LEU:HB3 | 1:2C:96:GLY:HA2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2C:186:THR:HG22 | 1:2C:411:ALA:HB1 | 1.95 | 0.47 |
| 2:2H:109:THR:OG1 | 2:2H:411:GLU:OE2 | 2.26 | 0.47 |
| 2:2P:214:ARG:NH1 | 38:7Z:18:VAL:HA | 2.29 | 0.47 |
| 1:2W:404:ASP:OD1 | 1:2W:405:GLU:N | 2.47 | 0.47 |
| 1:3A:53:GLU:HA | 1:3A:53:GLU:OE2 | 2.14 | 0.47 |
| 1:3A:170:VAL:HG22 | 1:3A:202:LEU:O | 2.15 | 0.47 |
| 2:3B:90:GLU:HG2 | 2:3B:121:ARG:HH12 | 1.79 | 0.47 |
| 2:3B:115:VAL:HG21 | 2:3B:152:LEU:HD23 | 1.96 | 0.47 |
| 2:3B:214:ARG:NH2 | 38:8C:16:LYS:HB3 | 2.28 | 0.47 |
| 2:3B:262:TYR:HB2 | 2:3B:265:ILE:HD12 | 1.95 | 0.47 |
| 1:3C:53:GLU:OE1 | 1:3C:53:GLU:HA | 2.15 | 0.47 |
| 1:3C:86:ARG:HB3 | 1:3C:89:ASN:OD1 | 2.14 | 0.47 |
| 1:3C:320:ARG:HH12 | 38:8D:198:THR:N | 2.13 | 0.47 |
| 2:3F:221:ARG:NE | 38:8A:174:SER:OG | 2.46 | 0.47 |
| 1:3G:211:CYS:HA | 1:3G:215:LEU:HB2 | 1.96 | 0.47 |
| 2:3L:301:MET:HE1 | 2:3L:307:PRO:HD3 | 1.97 | 0.47 |
| 1:3M:334:GLN:HE22 | 1:3M:347:ASN:HA | 1.80 | 0.47 |
| 1:3Q:309:ARG:NH1 | 1:3Q:341:PHE:O | 2.47 | 0.47 |
| 3:3V:63:SER:OG | 3:3V:66:THR:O | 2.29 | 0.47 |
| 3:3X:10:PHE:HB3 | 3:3X:140:LYS:NZ | 2.29 | 0.47 |
| 3:3X:63:SER:OG | 3:3X:66:THR:O | 2.29 | 0.47 |
| 3:4F:10:PHE:HB3 | 3:4F:140:LYS:NZ | 2.29 | 0.47 |
| 3:4F:63:SER:OG | 3:4F:66:THR:O | 2.29 | 0.47 |
| 7:4R:123:LEU:HA | 7:4R:123:LEU:HD13 | 1.70 | 0.47 |
| 7:4R:254:SER:OG | 7:4R:255:ALA:N | 2.47 | 0.47 |
| 7:4U:24:TRP:HD1 | 11:5E:248:LEU:HG | 1.80 | 0.47 |
| 7:4U:199:VAL:HG12 | 31:7N:60:ILE:HD12 | 1.97 | 0.47 |
| 9:4Z:234:LEU:O | 9:4Z:238:GLU:HG2 | 2.14 | 0.47 |
| 12:5G:331:ASN:ND2 | 31:7N:18:THR:HG22 | 2.30 | 0.47 |
| 17:5S:212:LYS:O | 17:5S:216:GLU:HG3 | 2.14 | 0.47 |
| 17:5T:212:LYS:O | 17:5T:216:GLU:HG3 | 2.14 | 0.47 |
| 18:5X:24:ARG:HG3 | 18:5X:27:ASP:OD1 | 2.15 | 0.47 |
| 18:5Z:24:ARG:HG3 | 18:5Z:27:ASP:OD1 | 2.15 | 0.47 |
| 18:6A:61:LYS:HA | 18:6A:61:LYS:HD2 | 1.73 | 0.47 |
| 18:6B:61:LYS:HA | 18:6B:61:LYS:HD2 | 1.73 | 0.47 |
| 18:6D:24:ARG:HG3 | 18:6D:27:ASP:OD1 | 2.15 | 0.47 |
| 22:6K:28:GLN:HG3 | 22:6K:29:GLU:OE1 | 2.14 | 0.47 |
| 24:6V:11:LEU:HD23 | 24:6V:14:TYR:CE2 | 2.49 | 0.47 |
| 24:6V:183:ASP:OD1 | 24:6V:184:ALA:N | 2.47 | 0.47 |
| 24:6W:112:GLU:HB2 | 24:6W:209:PRO:HG2 | 1.97 | 0.47 |
| 24:6X:591:ASP:N | 24:6X:591:ASP:OD1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:9:281:TYR:OH | 1:T2:83:GLN:O | 2.27 | 0.47 |
| 1:D2:78:SER:CB | 24:6X:323:LYS:HG3 | 2.43 | 0.47 |
| 1:D4:74:ASP:OD2 | 24:6Y:319:PRO:HD2 | 2.13 | 0.47 |
| 2:G1:220:GLU:OE1 | 2:G1:220:GLU:N | 2.47 | 0.47 |
| 2:G3:12:ALA:HB2 | 41:G4:501:GTP:C8 | 2.49 | 0.47 |
| 1:G6:7:ILE:HD13 | 1:G6:151:LEU:HD21 | 1.96 | 0.47 |
| 2:G7:56:THR:HA | 2:I3:285:GLN:HB2 | 1.95 | 0.47 |
| 1:G8:68:LEU:HB3 | 1:G8:96:GLY:HA2 | 1.97 | 0.47 |
| 2:G9:334:THR:HA | 2:G9:337:THR:HG22 | 1.96 | 0.47 |
| 2:H7:194:LEU:O | 2:H7:198:THR:HG22 | 2.14 | 0.47 |
| 1:H8:53:GLU:OE2 | 1:H8:57:GLY:N | 2.47 | 0.47 |
| 2:H9:102:ASN:HD22 | 2:H9:105:ARG:HB2 | 1.79 | 0.47 |
| 2:I1:320:ARG:NH2 | 2:I1:359:PRO:O | 2.46 | 0.47 |
| 1:I2:190:HIS:CD2 | 1:I2:411:ALA:HA | 2.50 | 0.47 |
| 1:I8:69:GLU:C | 1:I8:92:PHE:HZ | 2.18 | 0.47 |
| 1:J0:60:VAL:HG23 | 1:J0:84:ILE:O | 2.14 | 0.47 |
| 2:J3:88:HIS:ND1 | 2:J3:121:ARG:NH2 | 2.63 | 0.47 |
| 2:J7:352:LYS:NZ | 2:J7:353:CYS:O | 2.48 | 0.47 |
| 2:L3:21:TRP:CZ2 | 2:L3:65:CYS:HB3 | 2.49 | 0.47 |
| 1:L4:117:LEU:HA | 1:L4:120:VAL:HG12 | 1.97 | 0.47 |
| 1:L6:130:LEU:HB3 | 1:L6:162:ARG:HE | 1.80 | 0.47 |
| 1:L6:220:PRO:HG2 | 2:L7:326:LYS:HB2 | 1.95 | 0.47 |
| 2:L9:287:SER:OG | 2:L9:290:GLU:OE1 | 2.24 | 0.47 |
| 1:M0:178:THR:OG1 | 2:M1:258:ASN:ND2 | 2.47 | 0.47 |
| 2:M5:34:GLY:O | 2:M5:60:LYS:HA | 2.14 | 0.47 |
| 1:M6:309:ARG:H | 1:M6:372:THR:HG22 | 1.79 | 0.47 |
| 2:M7:14:ILE:HD11 | 2:M7:74:VAL:HG13 | 1.96 | 0.47 |
| 2:N1:189:LEU:HD11 | 2:N1:418:PHE:HE1 | 1.80 | 0.47 |
| 1:N2:359:LYS:HE2 | 29:7J:105:PHE:HB2 | 1.95 | 0.47 |
| 1:O2:274:THR:HG22 | 1:O2:282:ARG:HD2 | 1.95 | 0.47 |
| 1:O2:320:ARG:HH22 | 37:7Y:240:SER:HB3 | 1.79 | 0.47 |
| 1:O4:69:GLU:C | 1:O4:92:PHE:HZ | 2.17 | 0.47 |
| 2:O7:264:ARG:NH2 | 2:O7:431:ASP:OD1 | 2.47 | 0.47 |
| 1:O8:131:GLN:HE21 | 1:O8:250:LEU:HD13 | 1.80 | 0.47 |
| 2:P3:79:ARG:O | 2:P3:84:ARG:HG2 | 2.15 | 0.47 |
| 2:P3:183:GLU:HG3 | 2:P3:184:PRO:HD3 | 1.97 | 0.47 |
| 1:Q4:51:PHE:HB3 | 1:Q4:59:TYR:HB3 | 1.97 | 0.47 |
| 2:Q5:62:VAL:HG21 | 2:S1:283:HIS:O | 2.14 | 0.47 |
| 2:Q5:320:ARG:HD3 | 2:Q5:360:PRO:HG3 | 1.95 | 0.47 |
| 2:Q9:278:ALA:HA | 2:Q9:369:ALA:HB2 | 1.97 | 0.47 |
| 2:Q9:306:ASP:OD1 | 2:Q9:308:ARG:NH1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R2:149:THR:HG23 | 1:R2:191:GLN:HG2 | 1.97 | 0.47 |
| 1:R2:397:TRP:HA | 1:R2:397:TRP:HE3 | 1.78 | 0.47 |
| 1:R4:238:CYS:SG | 1:R4:318:ARG:NE | 2.88 | 0.47 |
| 2:R5:7:ILE:HD12 | 2:R5:153:LEU:HD21 | 1.96 | 0.47 |
| 2:R5:100:ALA:HA | 1:R6:252:LYS:HE2 | 1.96 | 0.47 |
| 2:R5:175:PRO:HG2 | 2:R5:176:GLN:OE1 | 2.14 | 0.47 |
| 1:R8:190:HIS:HD2 | 1:R8:414:ASN:HB2 | 1.78 | 0.47 |
| 1:S2:314:SER:HA | 1:S2:350:LYS:O | 2.15 | 0.47 |
| 2:S9:333:ALA:O | 2:S9:337:THR:HG23 | 2.14 | 0.47 |
| 1:T4:45:GLU:HG3 | 1:T4:46:ARG:HG2 | 1.96 | 0.47 |
| 2:U1:51:THR:HG21 | 2:U1:243:ARG:HG2 | 1.96 | 0.47 |
| 1:U4:229:ILE:HG22 | 1:U4:233:MET:SD | 2.54 | 0.47 |
| 2:U5:224:TYR:CZ | 1:U6:323:THR:HG21 | 2.50 | 0.47 |
| 1:W0:53:GLU:OE2 | 1:W0:57:GLY:N | 2.47 | 0.47 |
| 2:W3:9:ILE:HD11 | 2:W3:153:LEU:HD23 | 1.97 | 0.47 |
| 1:W4:22:GLU:HG2 | 1:W4:81:TYR:CD1 | 2.50 | 0.47 |
| 2:X3:265:ILE:HD11 | 2:X3:435:VAL:HG21 | 1.97 | 0.47 |
| 2:X5:352:LYS:HD2 | 2:X5:353:CYS:N | 2.29 | 0.47 |
| 1:X6:49:VAL:HG21 | 1:X6:241:ARG:HG2 | 1.97 | 0.47 |
| 1:X6:185:ALA:O | 1:X6:189:VAL:HG12 | 2.15 | 0.47 |
| 1:X8:52:ASN:OD1 | 1:X8:62:ARG:NH2 | 2.47 | 0.47 |
| 2:X9:5:ILE:HD11 | 2:X9:135:PHE:HE1 | 1.77 | 0.47 |
| 2:X9:62:VAL:HB | 2:X9:88:HIS:CE1 | 2.50 | 0.47 |
| 2:Y3:33:ASP:O | 2:Y3:60:LYS:NZ | 2.47 | 0.47 |
| 1:Y6:21:TRP:HA | 1:Y6:24:VAL:HG22 | 1.96 | 0.47 |
| 2:Y9:7:ILE:HG23 | 2:Y9:66:ILE:HG13 | 1.97 | 0.47 |
| 1:Z0:404:ASP:HB3 | 1:Z0:406:MET:SD | 2.55 | 0.47 |
| 2:Z1:194:LEU:O | 2:Z1:198:THR:HG22 | 2.14 | 0.47 |
| 2:Z7:238:LEU:HD11 | 2:Z7:255:PHE:HE1 | 1.80 | 0.47 |
| 1:Z8:177:ASP:O | 2:Z9:352:LYS:HA | 2.14 | 0.47 |
| 2:Z9:188:VAL:HG23 | 2:Z9:189:LEU:HD12 | 1.97 | 0.47 |
| 1:0G:382:SER:HB3 | 1:0G:415:MET:HG2 | 1.95 | 0.47 |
| 1:0K:139:LEU:HD12 | 1:0K:170:VAL:HG12 | 1.96 | 0.47 |
| 1:0K:374:ILE:HD11 | 1:0K:422:TYR:CZ | 2.49 | 0.47 |
| 1:0O:117:LEU:HA | 1:0O:120:VAL:HG12 | 1.96 | 0.47 |
| 2:0R:397:LEU:HD11 | 1:0S:344:TRP:HA | 1.96 | 0.47 |
| 1:0S:135:VAL:HG11 | 1:0S:152:ILE:HD11 | 1.95 | 0.47 |
| 1:0S:272:PRO:HB2 | 1:0S:282:ARG:HH12 | 1.79 | 0.47 |
| 1:0S:382:SER:OG | 1:0S:415:MET:HG2 | 2.15 | 0.47 |
| 1:0U:421:GLU:HA | 1:0U:424:GLN:HB3 | 1.96 | 0.47 |
| 2:0V:66:ILE:HG13 | 2:0V:66:ILE:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0V:368:LEU:H | 2:0V:368:LEU:HD23 | 1.79 | 0.47 |
| 2:0X:176:GLN:HG2 | 2:0X:177:VAL:N | 2.28 | 0.47 |
| 1:1A:5:VAL:HG23 | 1:1A:62:ARG:HG2 | 1.96 | 0.47 |
| 2:1P:250:VAL:HG23 | 2:1P:254:GLU:HG3 | 1.95 | 0.47 |
| 2:1P:312:TYR:HB2 | 2:1P:343:PHE:HD1 | 1.79 | 0.47 |
| 2:1R:5:ILE:HD11 | 2:1R:135:PHE:HE1 | 1.79 | 0.47 |
| 2:1R:259:LEU:HD21 | 2:1R:316:CYS:HB2 | 1.95 | 0.47 |
| 2:1V:317:LEU:HB3 | 2:1V:319:TYR:CE1 | 2.49 | 0.47 |
| 1:1W:377:MET:SD | 1:1W:380:ARG:NH2 | 2.87 | 0.47 |
| 2:1X:178:SER:OG | 2:1X:180:ALA:O | 2.31 | 0.47 |
| 2:1X:382:THR:O | 2:1X:385:GLY:N | 2.47 | 0.47 |
| 2:2B:245:ASP:OD1 | 2:2B:245:ASP:N | 2.43 | 0.47 |
| 2:2B:394:LYS:HB2 | 1:2C:346:PRO:HG3 | 1.97 | 0.47 |
| 1:2C:178:THR:OG1 | 1:2C:179:VAL:N | 2.47 | 0.47 |
| 2:2D:187:SER:O | 2:2D:191:THR:HG23 | 2.14 | 0.47 |
| 2:2D:333:ALA:O | 2:2D:337:THR:HG23 | 2.14 | 0.47 |
| 1:2E:210:ILE:O | 1:2E:214:THR:OG1 | 2.24 | 0.47 |
| 2:2F:66:ILE:O | 2:2F:66:ILE:HG13 | 2.14 | 0.47 |
| 2:2H:259:LEU:HD11 | 2:2H:316:CYS:HB2 | 1.96 | 0.47 |
| 1:2M:183:TYR:HA | 1:2M:385:PHE:HE1 | 1.79 | 0.47 |
| 2:2N:50:ASN:O | 2:2N:64:ARG:NH2 | 2.47 | 0.47 |
| 2:2N:111:GLY:O | 2:2N:115:VAL:HG12 | 2.13 | 0.47 |
| 2:2P:90:GLU:HG2 | 2:3F:280:LYS:NZ | 2.29 | 0.47 |
| 1:2Q:213:ARG:HE | 1:2Q:297:LYS:HZ2 | 1.61 | 0.47 |
| 1:2Q:332:ASN:OD1 | 38:7Z:1:MET:HA | 2.14 | 0.47 |
| 2:2R:175:PRO:HB3 | 2:2R:390:ARG:NE | 2.29 | 0.47 |
| 1:2S:178:THR:OG1 | 1:2S:179:VAL:N | 2.47 | 0.47 |
| 1:2S:179:VAL:HG23 | 1:2S:180:VAL:HG13 | 1.96 | 0.47 |
| 2:2X:11:GLN:NE2 | 1:2Y:247:ASN:OD1 | 2.47 | 0.47 |
| 2:2Z:47:ASP:N | 2:2Z:47:ASP:OD1 | 2.46 | 0.47 |
| 1:3A:49:VAL:HG11 | 1:3A:241:ARG:HG2 | 1.95 | 0.47 |
| 2:3B:231:ILE:O | 2:3B:234:VAL:HG12 | 2.14 | 0.47 |
| 1:3C:306:ARG:NH2 | 38:8D:99:THR:H | 2.10 | 0.47 |
| 2:3D:6:SER:HG | 2:3D:21:TRP:HZ2 | 1.63 | 0.47 |
| 2:3J:246:GLY:N | 2:3J:249:ASN:HD21 | 2.09 | 0.47 |
| 3:3V:75:ARG:HG2 | 3:3V:76:PRO:HD2 | 1.96 | 0.47 |
| 3:3Z:63:SER:OG | 3:3Z:66:THR:O | 2.29 | 0.47 |
| 4:4E:136:LEU:O | 4:4E:140:THR:OG1 | 2.32 | 0.47 |
| 3:4H:75:ARG:HG2 | 3:4H:76:PRO:HD2 | 1.96 | 0.47 |
| 7:4R:308:ARG:NH2 | 20:6F:215:GLU:HG3 | 2.29 | 0.47 |
| 8:4W:150:THR:O | 8:4W:154:ILE:HG12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Y:448:LYS:HA | 9:4Y:448:LYS:HD2 | 1.67 | 0.47 |
| 11:5E:110:GLN:H | 11:5E:110:GLN:CD | 2.17 | 0.47 |
| 12:5F:56:THR:HG23 | 12:5F:57:THR:N | 2.29 | 0.47 |
| 12:5G:302:SER:OG | 12:5G:358:HIS:ND1 | 2.46 | 0.47 |
| 13:5K:70:LYS:HE2 | 13:5K:70:LYS:HB3 | 1.43 | 0.47 |
| 14:5L:461:LEU:HG | 14:5L:462:GLU:O | 2.15 | 0.47 |
| 14:5M:461:LEU:HG | 14:5M:462:GLU:O | 2.15 | 0.47 |
| 14:5N:461:LEU:HG | 14:5N:462:GLU:O | 2.15 | 0.47 |
| 15:5P:21:LEU:HB2 | 19:6E:105:VAL:HG11 | 1.96 | 0.47 |
| 15:5P:145:PHE:O | 15:5P:149:LEU:HG | 2.14 | 0.47 |
| 18:5X:61:LYS:HD2 | 18:5X:61:LYS:HA | 1.73 | 0.47 |
| 18:6A:24:ARG:HG3 | 18:6A:27:ASP:OD1 | 2.15 | 0.47 |
| 18:6C:24:ARG:HG3 | 18:6C:27:ASP:OD1 | 2.15 | 0.47 |
| 22:6P:307:ARG:HG3 | 22:6P:326:PHE:CE1 | 2.49 | 0.47 |
| 24:6U:92:ASP:CG | 24:6U:93:ARG:N | 2.66 | 0.47 |
| 24:6U:132:VAL:HG12 | 24:6U:147:PHE:HB3 | 1.96 | 0.47 |
| 24:6X:106:VAL:HG22 | 24:6X:107:VAL:H | 1.78 | 0.47 |
| 24:6X:505:LYS:NZ | 24:6X:510:GLU:HG3 | 2.29 | 0.47 |
| 30:7K:251:LYS:O | 30:7K:255:THR:HG22 | 2.14 | 0.47 |
| 30:7K:316:GLU:HG2 | 30:7K:319:ARG:HH12 | 1.78 | 0.47 |
| 30:7K:346:ARG:HH21 | 30:7K:350:ASN:HD22 | 1.62 | 0.47 |
| 38:8C:117:TRP:O | 38:8C:121:LEU:HG | 2.15 | 0.47 |
| 1:5:40:SER:O | 26:7D:25:TYR:HE2 | 1.89 | 0.47 |
| 1:D6:79:GLY:HA2 | 24:6Z:323:LYS:HG3 | 1.95 | 0.47 |
| 1:E2:56:GLY:HA2 | 22:6J:254:ALA:HB3 | 1.96 | 0.47 |
| 1:F8:216:LYS:HB3 | 24:6U:422:ASN:OD1 | 2.15 | 0.47 |
| 2:G1:216:SER:OG | 2:G1:217:LEU:N | 2.48 | 0.47 |
| 2:G3:212:ILE:O | 2:G3:216:SER:OG | 2.31 | 0.47 |
| 1:G4:6:HIS:CE1 | 1:G4:8:GLN:HG2 | 2.49 | 0.47 |
| 1:G4:404:ASP:HB3 | 1:G4:406:MET:SD | 2.55 | 0.47 |
| 1:G6:95:THR:HG23 | 1:G6:96:GLY:N | 2.29 | 0.47 |
| 1:G6:232:VAL:CG1 | 1:G6:268:VAL:HG11 | 2.45 | 0.47 |
| 2:G9:52:PHE:HE2 | 2:G9:243:ARG:HG3 | 1.79 | 0.47 |
| 1:H2:107:THR:OG1 | 1:H2:108:GLU:OE1 | 2.21 | 0.47 |
| 2:H3:414:GLU:HG2 | 2:H3:417:GLU:OE1 | 2.14 | 0.47 |
| 2:H7:71:GLU:HG2 | 2:H7:73:THR:H | 1.79 | 0.47 |
| 1:I0:35:THR:HA | 1:I0:57:GLY:O | 2.15 | 0.47 |
| 1:I4:218:THR:OG1 | 24:6Z:488:ARG:HB2 | 2.14 | 0.47 |
| 2:I7:398:MET:HG3 | 1:I8:346:PRO:HD2 | 1.96 | 0.47 |
| 1:I8:145:SER:HG | 1:I8:188:SER:HG | 1.63 | 0.47 |
| 1:J4:245:GLN:HG2 | 16:5Q:153:THR:HG21 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J5:53:PHE:HB3 | 2:J5:61:HIS:HB3 | 1.96 | 0.47 |
| 1:J6:271:THR:OG1 | 1:J6:365:ALA:HB3 | 2.14 | 0.47 |
| 1:J6:385:PHE:CE2 | 1:J6:412:GLU:HG3 | 2.49 | 0.47 |
| 1:J8:285:THR:OG1 | 1:J8:288:GLU:HG2 | 2.15 | 0.47 |
| 1:J8:371:SER:OG | 1:J8:372:THR:N | 2.48 | 0.47 |
| 2:K3:259:LEU:HD11 | 2:K3:316:CYS:HB2 | 1.97 | 0.47 |
| 1:K4:16:ILE:HD11 | 1:K4:229:ILE:HB | 1.95 | 0.47 |
| 2:K5:9:ILE:HD13 | 2:K5:150:GLY:HA2 | 1.96 | 0.47 |
| 2:K9:88:HIS:ND1 | 2:K9:89:PRO:HD2 | 2.30 | 0.47 |
| 1:L2:173:PRO:HB3 | 1:L2:384:GLN:HE22 | 1.79 | 0.47 |
| 1:L2:185:ALA:O | 1:L2:189:VAL:HG22 | 2.15 | 0.47 |
| 1:L6:44:LEU:O | 1:L6:47:ILE:HG12 | 2.14 | 0.47 |
| 2:L9:8:HIS:CD2 | 2:L9:17:GLY:HA3 | 2.49 | 0.47 |
| 2:M3:255:PHE:HA | 2:M3:259:LEU:HD13 | 1.96 | 0.47 |
| 2:M9:72:PRO:HD2 | 1:N0:2:ARG:HH12 | 1.79 | 0.47 |
| 2:N3:288:VAL:HG11 | 2:N3:327:ASP:HB2 | 1.96 | 0.47 |
| 2:N7:167:LEU:HD12 | 2:N7:200:VAL:HB | 1.96 | 0.47 |
| 1:O2:232:VAL:O | 1:O2:236:ILE:HG12 | 2.14 | 0.47 |
| 1:O4:35:THR:OG1 | 1:O4:37:HIS:NE2 | 2.45 | 0.47 |
| 1:O4:404:ASP:HB2 | 1:O4:406:MET:SD | 2.53 | 0.47 |
| 2:O7:203:MET:CE | 2:O7:267:PHE:HB3 | 2.45 | 0.47 |
| 2:O9:297:GLU:HG3 | 2:O9:299:ALA:H | 1.80 | 0.47 |
| 2:P5:242:LEU:HD11 | 2:P5:252:ILE:HG12 | 1.97 | 0.47 |
| 2:P5:278:ALA:HA | 2:P5:369:ALA:HB2 | 1.96 | 0.47 |
| 1:P8:317:PHE:HB3 | 1:P8:321:MET:SD | 2.55 | 0.47 |
| 2:P9:12:ALA:HB2 | 41:P9:501:GTP:C8 | 2.49 | 0.47 |
| 2:P9:286:LEU:HD13 | 2:P9:371:VAL:HG13 | 1.96 | 0.47 |
| 1:Q0:391:ARG:HB2 | 2:Q1:346:TRP:CZ3 | 2.49 | 0.47 |
| 2:Q3:247:ALA:HB2 | 2:Q3:357:TYR:OH | 2.15 | 0.47 |
| 1:Q4:156:ARG:NH1 | 1:Q4:197:ASP:OD1 | 2.48 | 0.47 |
| 2:Q9:9:ILE:HG22 | 2:Q9:146:GLY:HA2 | 1.97 | 0.47 |
| 2:R5:191:THR:HA | 2:R5:194:LEU:HB3 | 1.95 | 0.47 |
| 1:R6:293:MET:HE1 | 1:R6:317:PHE:CE1 | 2.45 | 0.47 |
| 2:R7:117:LEU:HD22 | 13:5J:95:THR:HG21 | 1.97 | 0.47 |
| 2:R9:4:VAL:HG23 | 2:R9:134:GLY:O | 2.15 | 0.47 |
| 2:S5:177:VAL:HG23 | 1:S6:327:ASP:HB3 | 1.96 | 0.47 |
| 2:S5:242:LEU:HD11 | 2:S5:252:ILE:HG12 | 1.97 | 0.47 |
| 2:S7:183:GLU:CD | 2:S7:184:PRO:HD3 | 2.35 | 0.47 |
| 2:T1:21:TRP:CZ2 | 2:T1:65:CYS:HB3 | 2.49 | 0.47 |
| 1:T2:222:PHE:CD2 | 2:T3:247:ALA:HB1 | 2.50 | 0.47 |
| 2:T5:394:LYS:HB2 | 1:T6:346:PRO:HG3 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T6:91:VAL:HG21 | 1:T6:116:VAL:HG22 | 1.96 | 0.47 |
| 1:T6:121:ARG:NE | 1:T6:158:GLU:OE2 | 2.38 | 0.47 |
| 2:U5:156:ARG:HA | 2:U5:159:VAL:HG12 | 1.95 | 0.47 |
| 2:V1:222:PRO:HD2 | 1:V2:324:LYS:HE3 | 1.96 | 0.47 |
| 2:V3:216:SER:OG | 2:V3:275:ILE:O | 2.32 | 0.47 |
| 1:V6:4:ILE:HG22 | 1:V6:49:VAL:CG2 | 2.44 | 0.47 |
| 1:V8:417:ASP:HA | 1:V8:420:SER:OG | 2.15 | 0.47 |
| 1:W4:286:VAL:HG22 | 1:W4:321:MET:HE2 | 1.97 | 0.47 |
| 2:W7:176:GLN:HB3 | 1:W8:331:LEU:HD11 | 1.97 | 0.47 |
| 1:X0:262:ARG:NH2 | 1:X0:417:ASP:OD1 | 2.48 | 0.47 |
| 1:X2:394:PHE:CE2 | 2:X3:261:PRO:HB3 | 2.49 | 0.47 |
| 2:X5:129:CYS:SG | 2:X5:130:THR:N | 2.87 | 0.47 |
| 1:X8:418:LEU:O | 1:X8:421:GLU:HG2 | 2.14 | 0.47 |
| 2:X9:147:SER:OG | 2:X9:190:SER:HB2 | 2.14 | 0.47 |
| 2:X9:181:VAL:H | 1:Y0:256:ASN:ND2 | 2.12 | 0.47 |
| 1:Y4:273:LEU:H | 1:Y4:292:GLN:HE22 | 1.63 | 0.47 |
| 2:Y5:32:PRO:HB3 | 2:Y5:83:TYR:CE1 | 2.49 | 0.47 |
| 2:Y5:179:THR:HG21 | 1:Y6:246:LEU:HD11 | 1.95 | 0.47 |
| 1:Y8:273:LEU:N | 1:Y8:292:GLN:HE22 | 2.09 | 0.47 |
| 1:Z0:11:GLN:HG2 | 1:Z0:12:CYS:N | 2.29 | 0.47 |
| 1:Z0:121:ARG:NH2 | 1:Z0:158:GLU:OE2 | 2.39 | 0.47 |
| 1:Z0:186:THR:OG1 | 1:Z0:187:LEU:HD12 | 2.14 | 0.47 |
| 1:Z0:248:ALA:HA | 1:Z0:252:LYS:HD2 | 1.96 | 0.47 |
| 2:Z3:121:ARG:HD3 | 2:Z3:124:LYS:HE3 | 1.95 | 0.47 |
| 1:Z6:202:LEU:HD23 | 1:Z6:229:ILE:CD1 | 2.44 | 0.47 |
| 1:Z6:372:THR:O | 1:Z6:375:GLN:HG3 | 2.15 | 0.47 |
| 1:Z8:274:THR:HG21 | 1:Z8:282:ARG:HD3 | 1.97 | 0.47 |
| 1:Z8:404:ASP:OD1 | 1:Z8:405:GLU:N | 2.44 | 0.47 |
| 2:0B:332:VAL:HA | 2:0B:335:ILE:HG22 | 1.95 | 0.47 |
| 1:0E:203:ASP:N | 1:0E:203:ASP:OD1 | 2.48 | 0.47 |
| 1:0E:286:VAL:CG2 | 1:0E:287:PRO:HD3 | 2.43 | 0.47 |
| 2:0F:21:TRP:CZ3 | 2:0F:63:PRO:HB3 | 2.49 | 0.47 |
| 1:0G:244:GLY:HA3 | 1:0G:354:CYS:HA | 1.95 | 0.47 |
| 2:0N:346:TRP:CD1 | 2:0N:346:TRP:O | 2.67 | 0.47 |
| 1:0O:267:MET:HG3 | 1:0O:299:MET:HE2 | 1.97 | 0.47 |
| 1:0Q:337:ASN:HB2 | 1:0Q:340:TYR:CD2 | 2.49 | 0.47 |
| 1:0U:242:PHE:CD1 | 1:0U:356:ILE:HG13 | 2.50 | 0.47 |
| 2:0V:203:MET:O | 2:0V:204:LEU:HD12 | 2.14 | 0.47 |
| 2:0X:305:CYS:SG | 2:0X:383:ALA:HB1 | 2.54 | 0.47 |
| 1:0Y:385:PHE:HZ | 1:0Y:408:PHE:HD1 | 1.61 | 0.47 |
| 2:0Z:344:VAL:HG22 | 2:0Z:346:TRP:H | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:180:VAL:HG23 | 1:1A:184:ASN:ND2 | 2.29 | 0.47 |
| 1:1C:186:THR:HG22 | 1:1C:411:ALA:HB1 | 1.96 | 0.47 |
| 2:1D:177:VAL:HG13 | 1:1E:327:ASP:HB2 | 1.97 | 0.47 |
| 2:1D:346:TRP:O | 2:1D:346:TRP:CE3 | 2.65 | 0.47 |
| 2:1F:394:LYS:HB2 | 1:1G:346:PRO:HG3 | 1.96 | 0.47 |
| 1:1G:183:TYR:OH | 1:1G:388:MET:HB3 | 2.15 | 0.47 |
| 1:1G:202:LEU:HD13 | 1:1G:229:ILE:HD13 | 1.95 | 0.47 |
| 2:1L:200:VAL:HG13 | 2:1L:268:MET:CE | 2.44 | 0.47 |
| 1:1Q:174:LYS:HB2 | 1:1Q:205:GLU:OE2 | 2.15 | 0.47 |
| 2:1R:280:LYS:HA | 2:1R:283:HIS:HB2 | 1.97 | 0.47 |
| 2:1T:221:ARG:HA | 1:1U:325:GLU:OE2 | 2.14 | 0.47 |
| 2:1Z:204:LEU:HD23 | 2:1Z:231:ILE:HD12 | 1.96 | 0.47 |
| 2:2F:278:ALA:HB2 | 10:5A:437:GLN:HE22 | 1.79 | 0.47 |
| 1:2G:165:LEU:HD23 | 1:2G:165:LEU:HA | 1.76 | 0.47 |
| 2:2H:21:TRP:CZ2 | 2:2H:65:CYS:HB2 | 2.49 | 0.47 |
| 1:2K:177:ASP:OD1 | 2:2L:248:LEU:HD11 | 2.15 | 0.47 |
| 2:2L:145:THR:OG1 | 41:2L:501:GTP:O1B | 2.29 | 0.47 |
| 2:2N:333:ALA:O | 2:2N:337:THR:HG23 | 2.14 | 0.47 |
| 2:2P:297:GLU:HG2 | 38:7Z:25:ILE:HD12 | 1.95 | 0.47 |
| 2:2P:317:LEU:HD23 | 2:2P:377:MET:HG2 | 1.96 | 0.47 |
| 1:2S:77:ARG:NH2 | 38:8B:220:VAL:HA | 2.23 | 0.47 |
| 2:2V:85:GLN:HG3 | 14:5M:503:ARG:HH22 | 1.79 | 0.47 |
| 2:2X:104:ALA:HB1 | 2:2X:411:GLU:HB3 | 1.96 | 0.47 |
| 2:2X:174:SER:OG | 2:2X:207:GLU:OE1 | 2.31 | 0.47 |
| 2:2X:282:TYR:HH | 10:5C:384:GLN:HE21 | 1.48 | 0.47 |
| 1:2Y:354:CYS:SG | 1:2Y:355:ASP:N | 2.87 | 0.47 |
| 2:3B:49:PHE:HB2 | 2:3B:53:PHE:CZ | 2.50 | 0.47 |
| 2:3D:277:SER:OG | 2:3D:278:ALA:N | 2.47 | 0.47 |
| 1:3I:249:ASP:O | 1:3I:253:LEU:HG | 2.15 | 0.47 |
| 1:3M:389:PHE:HZ | 1:3M:405:GLU:HG2 | 1.80 | 0.47 |
| 2:3N:221:ARG:NH1 | 38:8C:176:THR:OG1 | 2.48 | 0.47 |
| 1:3O:77:ARG:NH2 | 3:4F:18:LYS:HB3 | 2.30 | 0.47 |
| 1:3Q:108:GLU:HA | 1:3Q:111:GLU:OE2 | 2.15 | 0.47 |
| 1:3Q:201:VAL:HG22 | 1:3Q:266:PHE:O | 2.14 | 0.47 |
| 1:3Q:274:THR:OG1 | 1:3Q:282:ARG:NH1 | 2.48 | 0.47 |
| 4:3W:136:LEU:O | 4:3W:140:THR:OG1 | 2.32 | 0.47 |
| 4:4A:136:LEU:O | 4:4A:140:THR:OG1 | 2.32 | 0.47 |
| 3:4H:63:SER:OG | 3:4H:66:THR:O | 2.29 | 0.47 |
| 5:4M:293:LEU:CD1 | 28:7X:305:ALA:CB | 2.83 | 0.47 |
| 6:4O:358:LYS:HD2 | 6:4O:362:ARG:HE | 1.79 | 0.47 |
| 6:4O:411:ARG:NH1 | 29:7J:436:GLU:HG2 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:4W:458:GLU:HA | 8:4W:461:VAL:CG1 | 2.45 | 0.47 |
| 9:4Z:206:ARG:NE | 9:4Z:206:ARG:HA | 2.29 | 0.47 |
| 10:5A:477:LYS:HD2 | 10:5B:150:MET:HB3 | 1.97 | 0.47 |
| 10:5B:110:GLU:HA | 10:5B:113:LYS:HD3 | 1.97 | 0.47 |
| 12:5G:347:PRO:HG2 | 12:5G:350:VAL:HG21 | 1.96 | 0.47 |
| 14:5L:218:VAL:HG12 | 14:5L:281:LYS:HZ2 | 1.78 | 0.47 |
| 15:5O:34:GLU:CG | 15:5O:49:ARG:CZ | 2.81 | 0.47 |
| 15:5P:68:VAL:HG22 | 15:5P:69:PHE:HD2 | 1.79 | 0.47 |
| 18:5Y:24:ARG:HG3 | 18:5Y:27:ASP:OD1 | 2.15 | 0.47 |
| 18:6B:24:ARG:HG3 | 18:6B:27:ASP:OD1 | 2.15 | 0.47 |
| 22:6I:248:MET:HG2 | 22:6I:253:PHE:HA | 1.96 | 0.47 |
| 22:6O:265:ASP:HA | 22:6O:268:ASP:OD1 | 2.15 | 0.47 |
| 24:6U:112:GLU:HB2 | 24:6U:209:PRO:HG2 | 1.96 | 0.47 |
| 24:6X:80:ASP:O | 24:6X:81:THR:OG1 | 2.26 | 0.47 |
| 24:6X:602:LEU:HG | 24:6X:604:PHE:HD1 | 1.80 | 0.47 |
| 24:6Y:558:LEU:HD13 | 24:6Y:608:GLN:HB3 | 1.96 | 0.47 |
| 36:7V:22:ALA:HA | 36:7V:25:THR:HG22 | 1.95 | 0.47 |
| 1:5:42:LEU:HD21 | 26:7D:121:LYS:HE3 | 1.95 | 0.47 |
| 2:B4:206:ASN:ND2 | 41:B5:501:GTP:O2' | 2.46 | 0.47 |
| 2:B7:222:PRO:HA | 18:6B:51:MET:HE1 | 1.94 | 0.47 |
| 2:B9:223:THR:HG22 | 18:6C:51:MET:HE3 | 1.96 | 0.47 |
| 1:C4:11:GLN:N | 39:C4:501:GDP:O1B | 2.38 | 0.47 |
| 1:D0:11:GLN:N | 39:D0:501:GDP:O2B | 2.47 | 0.47 |
| 1:D0:204:ASN:HD21 | 39:D0:501:GDP:N2 | 2.09 | 0.47 |
| 1:G4:114:ASP:N | 1:G4:114:ASP:OD1 | 2.47 | 0.47 |
| 1:G4:145:SER:OG | 1:G4:146:GLY:N | 2.48 | 0.47 |
| 2:G5:90:GLU:HB2 | 2:G5:121:ARG:HH22 | 1.78 | 0.47 |
| 1:G8:156:ARG:NH1 | 1:G8:160:PRO:O | 2.48 | 0.47 |
| 1:G8:316:LEU:HB2 | 1:G8:366:THR:OG1 | 2.15 | 0.47 |
| 2:G9:381:SER:OG | 2:G9:382:THR:N | 2.46 | 0.47 |
| 1:H2:191:GLN:HG3 | 1:H2:195:ASN:OD1 | 2.15 | 0.47 |
| 1:H2:374:ILE:HD11 | 1:H2:422:TYR:CE1 | 2.50 | 0.47 |
| 1:H4:199:CYS:HB2 | 1:H4:265:PHE:HD1 | 1.79 | 0.47 |
| 1:H4:276:ARG:HB2 | 24:6U:463:THR:HG21 | 1.97 | 0.47 |
| 2:H5:66:ILE:O | 2:H5:66:ILE:HG13 | 2.15 | 0.47 |
| 1:H6:414:ASN:O | 1:H6:418:LEU:HG | 2.14 | 0.47 |
| 2:H7:255:PHE:HA | 2:H7:259:LEU:HD13 | 1.97 | 0.47 |
| 1:H8:117:LEU:HA | 1:H8:120:VAL:HG12 | 1.96 | 0.47 |
| 1:I0:219:THR:CG2 | 24:6X:488:ARG:CG | 2.92 | 0.47 |
| 2:I1:4:VAL:HG23 | 2:I1:134:GLY:O | 2.15 | 0.47 |
| 1:I2:77:ARG:HE | 1:I2:90:PHE:HE2 | 1.62 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I2:203:ASP:N | 1:I2:203:ASP:OD1 | 2.47 | 0.47 |
| 2:I3:201:ALA:O | 2:I3:268:MET:HE2 | 2.15 | 0.47 |
| 2:I5:11:GLN:OE1 | 2:I5:15:GLN:NE2 | 2.47 | 0.47 |
| 1:I8:51:PHE:O | 1:I8:62:ARG:NH2 | 2.48 | 0.47 |
| 2:I9:52:PHE:CZ | 2:I9:239:THR:HG21 | 2.50 | 0.47 |
| 2:I9:88:HIS:CG | 2:I9:89:PRO:HD2 | 2.49 | 0.47 |
| 2:I9:203:MET:C | 2:I9:204:LEU:HD12 | 2.35 | 0.47 |
| 2:I9:216:SER:OG | 2:I9:217:LEU:N | 2.45 | 0.47 |
| 2:J1:179:THR:O | 1:J2:350:LYS:HD2 | 2.14 | 0.47 |
| 2:J3:204:LEU:HD23 | 2:J3:231:ILE:HD12 | 1.95 | 0.47 |
| 1:J4:65:LEU:HD12 | 1:J4:90:PHE:HE1 | 1.79 | 0.47 |
| 1:J4:207:LEU:HB3 | 1:J4:225:LEU:HD22 | 1.97 | 0.47 |
| 1:J4:285:THR:HG22 | 1:J4:288:GLU:OE1 | 2.15 | 0.47 |
| 2:J5:30:ILE:HG12 | 2:J5:36:MET:HG2 | 1.95 | 0.47 |
| 2:J5:51:THR:HG21 | 2:J5:243:ARG:HG2 | 1.95 | 0.47 |
| 1:J6:107:THR:OG1 | 1:J6:401:GLU:OE2 | 2.22 | 0.47 |
| 1:J6:246:LEU:HD22 | 1:J6:352:SER:HA | 1.95 | 0.47 |
| 2:J9:417:GLU:HA | 2:J9:420:GLU:HG2 | 1.97 | 0.47 |
| 1:K0:278:SER:O | 1:K0:278:SER:OG | 2.31 | 0.47 |
| 2:K1:97:GLU:OE2 | 2:K1:105:ARG:NH2 | 2.48 | 0.47 |
| 1:K6:140:GLY:O | 1:K6:184:ASN:ND2 | 2.47 | 0.47 |
| 1:K6:271:THR:OG1 | 1:K6:365:ALA:HB3 | 2.14 | 0.47 |
| 2:K7:330:ALA:O | 2:K7:334:THR:HG23 | 2.15 | 0.47 |
| 1:K8:5:VAL:HG12 | 1:K8:133:PHE:HD1 | 1.80 | 0.47 |
| 2:K9:405:VAL:HG13 | 2:K9:418:PHE:HE2 | 1.79 | 0.47 |
| 2:L1:4:VAL:HG23 | 2:L1:134:GLY:O | 2.15 | 0.47 |
| 2:L1:47:ASP:OD1 | 2:L1:48:ALA:N | 2.47 | 0.47 |
| 2:L1:399:TYR:O | 2:L1:402:ARG:NH1 | 2.48 | 0.47 |
| 2:L3:89:PRO:CG | 29:7J:320:PRO:HG3 | 2.43 | 0.47 |
| 1:L4:344:TRP:CE3 | 1:L4:345:ILE:HG13 | 2.49 | 0.47 |
| 1:L4:414:ASN:HA | 1:L4:417:ASP:OD2 | 2.15 | 0.47 |
| 2:L5:287:SER:OG | 2:L5:288:VAL:N | 2.48 | 0.47 |
| 1:L6:41:ASP:HA | 1:L6:44:LEU:HD23 | 1.96 | 0.47 |
| 1:L6:52:ASN:OD1 | 1:L6:62:ARG:NH2 | 2.47 | 0.47 |
| 1:L6:362:LYS:HA | 6:4P:169:PHE:CZ | 2.50 | 0.47 |
| 2:L7:104:ALA:HB1 | 2:L7:411:GLU:OE2 | 2.14 | 0.47 |
| 2:L9:399:TYR:O | 2:L9:402:ARG:NH1 | 2.48 | 0.47 |
| 1:M0:111:GLU:N | 1:M0:111:GLU:OE1 | 2.48 | 0.47 |
| 2:M1:119:LEU:HA | 2:M1:122:ILE:HG22 | 1.95 | 0.47 |
| 1:M2:359:LYS:NZ | 30:7K:230:GLN:OE1 | 2.48 | 0.47 |
| 1:M4:391:ARG:HD3 | 2:M5:346:TRP:NE1 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M5:70:LEU:HD13 | 2:M5:110:ILE:HG21 | 1.96 | 0.47 |
| 2:M5:96:LYS:NZ | 37:7Y:98:PHE:HA | 2.30 | 0.47 |
| 2:M5:236:SER:O | 2:M5:243:ARG:NH2 | 2.46 | 0.47 |
| 2:M7:65:CYS:SG | 2:M7:87:PHE:HE1 | 2.38 | 0.47 |
| 1:N2:1:MET:SD | 1:N2:1:MET:N | 2.86 | 0.47 |
| 1:N2:364:SER:OG | 1:N2:365:ALA:N | 2.48 | 0.47 |
| 2:N5:167:LEU:HD13 | 2:N5:200:VAL:HB | 1.95 | 0.47 |
| 2:N9:68:LEU:HA | 2:N9:93:ILE:O | 2.15 | 0.47 |
| 1:O0:248:ALA:HA | 1:O0:252:LYS:HD2 | 1.97 | 0.47 |
| 1:O0:270:PHE:HD2 | 1:O0:273:LEU:HD21 | 1.79 | 0.47 |
| 2:O3:5:ILE:HG22 | 2:O3:64:ARG:HB3 | 1.97 | 0.47 |
| 1:O4:208:TYR:CD1 | 2:O5:326:LYS:HE2 | 2.49 | 0.47 |
| 1:O4:391:ARG:HB2 | 2:O5:346:TRP:CD1 | 2.50 | 0.47 |
| 2:O7:313:MET:HE1 | 2:O7:346:TRP:HH2 | 1.74 | 0.47 |
| 2:O9:296:PHE:CE2 | 2:O9:335:ILE:HD13 | 2.50 | 0.47 |
| 1:P4:190:HIS:HD2 | 1:P4:411:ALA:HA | 1.79 | 0.47 |
| 1:P6:219:THR:O | 1:P6:219:THR:OG1 | 2.30 | 0.47 |
| 2:P7:332:VAL:O | 2:P7:336:LYS:HG3 | 2.15 | 0.47 |
| 2:P9:209:ILE:HG23 | 2:P9:230:LEU:HD11 | 1.96 | 0.47 |
| 2:P9:300:SER:O | 2:P9:300:SER:OG | 2.30 | 0.47 |
| 1:Q0:145:SER:OG | 1:Q0:188:SER:OG | 2.27 | 0.47 |
| 1:Q2:317:PHE:HB3 | 1:Q2:321:MET:SD | 2.55 | 0.47 |
| 2:Q3:167:LEU:HD21 | 2:Q3:256:GLN:HE22 | 1.79 | 0.47 |
| 2:Q3:222:PRO:HD2 | 1:Q4:324:LYS:HE3 | 1.96 | 0.47 |
| 1:Q4:382:SER:HB2 | 1:Q4:415:MET:HG2 | 1.97 | 0.47 |
| 2:Q5:53:PHE:HB3 | 2:Q5:61:HIS:HB3 | 1.97 | 0.47 |
| 2:Q5:73:THR:OG1 | 2:Q5:74:VAL:N | 2.46 | 0.47 |
| 1:Q6:78:SER:OG | 1:Q6:79:GLY:N | 2.48 | 0.47 |
| 1:Q6:175:VAL:O | 1:Q6:175:VAL:HG23 | 2.15 | 0.47 |
| 2:Q9:275:ILE:HG23 | 2:Q9:368:LEU:HD21 | 1.95 | 0.47 |
| 2:R1:192:HIS:O | 2:R1:192:HIS:ND1 | 2.42 | 0.47 |
| 2:R3:9:ILE:HD13 | 2:R3:150:GLY:HA2 | 1.97 | 0.47 |
| 2:R3:175:PRO:HG2 | 2:R3:176:GLN:OE1 | 2.15 | 0.47 |
| 2:R3:250:VAL:HG23 | 2:R3:254:GLU:HG3 | 1.96 | 0.47 |
| 2:R5:88:HIS:CD2 | 2:R5:89:PRO:CD | 2.94 | 0.47 |
| 1:R6:165:LEU:HG | 1:R6:250:LEU:HD21 | 1.95 | 0.47 |
| 2:R9:40:LYS:HE3 | 2:R9:42:ILE:HD11 | 1.97 | 0.47 |
| 2:R9:45:GLY:HA3 | 7:4R:257:ARG:NH2 | 2.30 | 0.47 |
| 2:R9:84:ARG:HH21 | 33:7Q:172:ARG:HA | 1.80 | 0.47 |
| 1:S0:8:GLN:OE1 | 1:S0:17:GLY:HA3 | 2.14 | 0.47 |
| 1:S2:69:GLU:HG3 | 7:4S:3:ARG:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:171:PRO:O | 1:S4:380:ARG:NH2 | 2.48 | 0.47 |
| 2:S5:419:SER:O | 2:S5:423:GLU:HG3 | 2.15 | 0.47 |
| 2:S7:9:ILE:HD13 | 2:S7:150:GLY:HA2 | 1.97 | 0.47 |
| 2:S7:287:SER:OG | 2:S7:288:VAL:N | 2.48 | 0.47 |
| 1:S8:77:ARG:NH1 | 24:6W:47:GLN:O | 2.42 | 0.47 |
| 1:S8:226:ASN:OD1 | 39:S8:502:GDP:N1 | 2.45 | 0.47 |
| 1:S8:260:PHE:HB2 | 1:S8:263:LEU:HG | 1.97 | 0.47 |
| 1:S8:292:GLN:HG2 | 1:S8:298:ASN:ND2 | 2.30 | 0.47 |
| 2:S9:196:GLU:OE2 | 2:S9:197:HIS:NE2 | 2.48 | 0.47 |
| 1:T2:203:ASP:OD1 | 1:T2:302:ALA:N | 2.47 | 0.47 |
| 1:T4:390:ARG:CB | 1:T4:390:ARG:HH11 | 2.28 | 0.47 |
| 1:T6:1:MET:HE1 | 26:7F:67:GLN:HE21 | 1.78 | 0.47 |
| 1:T8:383:GLU:OE2 | 1:T8:384:GLN:HG3 | 2.15 | 0.47 |
| 2:U1:333:ALA:O | 2:U1:337:THR:HG23 | 2.14 | 0.47 |
| 1:U2:53:GLU:OE2 | 1:U2:57:GLY:N | 2.47 | 0.47 |
| 1:U2:173:PRO:HG2 | 1:U2:174:LYS:HZ2 | 1.79 | 0.47 |
| 1:U4:207:LEU:HB3 | 1:U4:225:LEU:HD22 | 1.95 | 0.47 |
| 1:U6:107:THR:OG1 | 1:U6:108:GLU:OE1 | 2.22 | 0.47 |
| 1:U6:239:CYS:SG | 1:U6:240:LEU:HD12 | 2.55 | 0.47 |
| 1:U6:285:THR:HG22 | 1:U6:288:GLU:OE2 | 2.14 | 0.47 |
| 2:U7:56:THR:HB | 2:W3:285:GLN:HB2 | 1.96 | 0.47 |
| 1:U8:208:TYR:HA | 1:U8:211:CYS:SG | 2.55 | 0.47 |
| 2:U9:79:ARG:O | 2:U9:84:ARG:HG2 | 2.15 | 0.47 |
| 1:V0:137:HIS:ND1 | 1:V0:138:SER:O | 2.46 | 0.47 |
| 2:V1:9:ILE:HD13 | 2:V1:150:GLY:HA2 | 1.95 | 0.47 |
| 2:V1:121:ARG:HE | 2:V1:125:LEU:HG | 1.78 | 0.47 |
| 2:V1:183:GLU:HG3 | 2:V1:184:PRO:HD3 | 1.96 | 0.47 |
| 2:V1:187:SER:O | 2:V1:191:THR:HG23 | 2.15 | 0.47 |
| 1:V2:6:HIS:NE2 | 1:V2:136:CYS:SG | 2.87 | 0.47 |
| 1:V2:229:ILE:HG22 | 1:V2:233:MET:SD | 2.55 | 0.47 |
| 1:V6:205:GLU:HG2 | 1:V6:206:ALA:N | 2.30 | 0.47 |
| 1:V6:235:GLY:HA2 | 1:V6:318:ARG:NH1 | 2.24 | 0.47 |
| 1:W2:31:ASP:OD1 | 1:W2:31:ASP:N | 2.47 | 0.47 |
| 2:W3:9:ILE:HG22 | 2:W3:146:GLY:HA2 | 1.96 | 0.47 |
| 2:W3:91:GLN:NE2 | 2:W3:125:LEU:HD21 | 2.29 | 0.47 |
| 2:W3:253:THR:O | 2:W3:257:THR:HG23 | 2.15 | 0.47 |
| 1:W4:135:VAL:O | 1:W4:166:THR:HA | 2.14 | 0.47 |
| 1:W6:139:LEU:HG | 1:W6:168:SER:HB3 | 1.96 | 0.47 |
| 1:W6:198:GLU:HB3 | 1:W6:258:ILE:HD11 | 1.95 | 0.47 |
| 2:W7:251:ASP:OD1 | 2:W7:252:ILE:N | 2.44 | 0.47 |
| 2:X3:83:TYR:HB3 | 2:X3:86:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X3:90:GLU:HB2 | 2:Y9:283:HIS:CE1 | 2.50 | 0.47 |
| 2:X3:282:TYR:HA | 8:4V:424:LYS:HE2 | 1.97 | 0.47 |
| 1:X6:67:ASP:N | 1:X6:67:ASP:OD1 | 2.48 | 0.47 |
| 2:X7:53:PHE:HB3 | 2:X7:61:HIS:HB3 | 1.96 | 0.47 |
| 1:X8:244:GLY:HA3 | 1:X8:354:CYS:HA | 1.97 | 0.47 |
| 2:X9:34:GLY:HA3 | 2:X9:60:LYS:NZ | 2.30 | 0.47 |
| 2:X9:179:THR:HG21 | 1:Y0:246:LEU:HD11 | 1.96 | 0.47 |
| 2:X9:201:ALA:O | 2:X9:268:MET:HE2 | 2.14 | 0.47 |
| 2:X9:417:GLU:OE2 | 2:X9:417:GLU:N | 2.43 | 0.47 |
| 1:Y0:179:VAL:HG13 | 2:Y1:349:THR:O | 2.14 | 0.47 |
| 2:Y1:429:GLU:O | 2:Y1:433:GLU:HG2 | 2.15 | 0.47 |
| 2:Y3:25:CYS:SG | 2:Y3:86:LEU:HD11 | 2.55 | 0.47 |
| 2:Y3:31:GLN:HB2 | 2:Y3:33:ASP:OD1 | 2.15 | 0.47 |
| 1:Y4:395:LEU:O | 1:Y4:399:THR:HG23 | 2.15 | 0.47 |
| 2:Y5:51:THR:HG21 | 2:Y5:243:ARG:HG2 | 1.96 | 0.47 |
| 2:Y5:157:LEU:HD12 | 2:Y5:157:LEU:O | 2.14 | 0.47 |
| 2:Y5:384:ILE:HA | 2:Y5:387:ILE:HD12 | 1.97 | 0.47 |
| 1:Y8:183:TYR:OH | 1:Y8:388:MET:HG2 | 2.15 | 0.47 |
| 2:Y9:72:PRO:HG3 | 1:Z0:1:MET:HG3 | 1.97 | 0.47 |
| 2:Y9:118:ALA:HB3 | 2:Y9:153:LEU:HD11 | 1.95 | 0.47 |
| 2:Y9:297:GLU:HG3 | 2:Y9:298:PRO:HD2 | 1.97 | 0.47 |
| 1:Z0:6:HIS:O | 1:Z0:64:ILE:HD12 | 2.15 | 0.47 |
| 1:Z0:86:ARG:NH2 | 1:0G:281:TYR:O | 2.47 | 0.47 |
| 1:Z2:8:GLN:OE1 | 1:Z2:8:GLN:N | 2.48 | 0.47 |
| 1:Z2:389:PHE:HZ | 1:Z2:405:GLU:HG2 | 1.79 | 0.47 |
| 2:Z5:240:ALA:HB1 | 2:Z5:356:ASN:HD22 | 1.79 | 0.47 |
| 1:Z6:54:ALA:HB3 | 1:Z6:58:ARG:HB3 | 1.97 | 0.47 |
| 1:Z8:86:ARG:NH2 | 1:0O:281:TYR:O | 2.48 | 0.47 |
| 1:Z8:130:LEU:HG | 1:Z8:132:GLY:N | 2.29 | 0.47 |
| 1:Z8:249:ASP:OD2 | 1:Z8:250:LEU:HD12 | 2.15 | 0.47 |
| 2:Z9:268:MET:CE | 2:Z9:378:ILE:HG22 | 2.45 | 0.47 |
| 1:0A:31:ASP:OD2 | 1:0A:33:THR:OG1 | 2.26 | 0.47 |
| 2:0B:290:GLU:HA | 2:0B:293:ASN:OD1 | 2.15 | 0.47 |
| 2:0F:232:ALA:HA | 2:0F:235:ILE:HG22 | 1.96 | 0.47 |
| 2:0F:352:LYS:NZ | 2:0F:353:CYS:O | 2.48 | 0.47 |
| 1:0G:166:THR:OG1 | 1:0G:199:CYS:SG | 2.71 | 0.47 |
| 1:0G:334:GLN:HE22 | 1:0G:347:ASN:H | 1.63 | 0.47 |
| 2:0H:90:GLU:HB2 | 2:0H:121:ARG:HH22 | 1.79 | 0.47 |
| 2:0H:171:VAL:HG22 | 2:0H:204:LEU:HD11 | 1.97 | 0.47 |
| 2:0H:259:LEU:HD21 | 2:0H:316:CYS:HB2 | 1.97 | 0.47 |
| 2:0J:167:LEU:HB3 | 2:0J:169:PHE:CE1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0J:300:SER:O | 2:0J:300:SER:OG | 2.27 | 0.47 |
| 1:0K:183:TYR:O | 1:0K:187:LEU:HD13 | 2.15 | 0.47 |
| 1:0K:318:ARG:HA | 1:0K:354:CYS:SG | 2.55 | 0.47 |
| 2:0L:88:HIS:HB3 | 2:1B:283:HIS:CE1 | 2.49 | 0.47 |
| 2:0L:88:HIS:HB3 | 2:1B:283:HIS:ND1 | 2.28 | 0.47 |
| 2:0L:290:GLU:HA | 2:0L:293:ASN:ND2 | 2.30 | 0.47 |
| 2:0L:389:SER:O | 2:0L:393:HIS:ND1 | 2.47 | 0.47 |
| 1:0M:183:TYR:O | 1:0M:187:LEU:HD13 | 2.15 | 0.47 |
| 1:0M:206:ALA:O | 1:0M:210:ILE:HG13 | 2.14 | 0.47 |
| 2:0N:290:GLU:HA | 2:0N:293:ASN:HD22 | 1.79 | 0.47 |
| 2:0N:313:MET:SD | 2:0N:346:TRP:HH2 | 2.38 | 0.47 |
| 1:0O:248:ALA:HA | 1:0O:252:LYS:HD2 | 1.95 | 0.47 |
| 1:0O:389:PHE:O | 1:0O:392:LYS:NZ | 2.30 | 0.47 |
| 2:0P:417:GLU:HA | 2:0P:420:GLU:HG2 | 1.95 | 0.47 |
| 1:0Q:8:GLN:O | 1:0Q:66:MET:HB2 | 2.14 | 0.47 |
| 2:0R:9:ILE:HB | 2:0R:139:ASN:HB3 | 1.97 | 0.47 |
| 2:0R:121:ARG:HD2 | 2:0R:124:LYS:HE3 | 1.95 | 0.47 |
| 2:0R:276:ILE:HG23 | 2:0R:280:LYS:HB3 | 1.96 | 0.47 |
| 1:0S:53:GLU:HB2 | 1:0S:59:TYR:CE2 | 2.49 | 0.47 |
| 1:0U:2:ARG:HE | 1:0U:240:LEU:CD2 | 2.28 | 0.47 |
| 1:0U:273:LEU:H | 1:0U:292:GLN:NE2 | 2.13 | 0.47 |
| 1:1A:385:PHE:HZ | 1:1A:408:PHE:HD1 | 1.63 | 0.47 |
| 2:1B:83:TYR:HB3 | 2:1B:86:LEU:HB3 | 1.97 | 0.47 |
| 2:1B:123:ARG:HD2 | 2:1B:123:ARG:HA | 1.74 | 0.47 |
| 2:1D:4:VAL:HG23 | 2:1D:134:GLY:O | 2.14 | 0.47 |
| 2:1D:60:LYS:NZ | 2:1T:282:TYR:HA | 2.30 | 0.47 |
| 2:1F:212:ILE:O | 2:1F:216:SER:OG | 2.23 | 0.47 |
| 2:1F:235:ILE:HD13 | 2:1F:238:LEU:HD21 | 1.96 | 0.47 |
| 1:1G:337:ASN:HB3 | 1:1G:340:TYR:HD2 | 1.80 | 0.47 |
| 2:1H:161:TYR:HB3 | 2:1H:164:LYS:HD2 | 1.96 | 0.47 |
| 2:1H:312:TYR:O | 2:1H:344:VAL:HG22 | 2.14 | 0.47 |
| 1:1K:6:HIS:CE1 | 1:1K:8:GLN:HG2 | 2.50 | 0.47 |
| 1:1K:139:LEU:HD12 | 1:1K:170:VAL:HG12 | 1.97 | 0.47 |
| 1:1K:414:ASN:HA | 1:1K:417:ASP:OD2 | 2.15 | 0.47 |
| 1:1M:51:PHE:O | 1:1M:62:ARG:NH2 | 2.48 | 0.47 |
| 1:1O:135:VAL:HG21 | 1:1O:152:ILE:HD11 | 1.95 | 0.47 |
| 2:1P:178:SER:HB3 | 2:1P:183:GLU:OE2 | 2.14 | 0.47 |
| 2:1R:4:VAL:HG23 | 2:1R:134:GLY:O | 2.14 | 0.47 |
| 2:1R:57:GLY:HA3 | 10:5B:156:TYR:CZ | 2.50 | 0.47 |
| 2:1T:275:ILE:HD12 | 2:1T:368:LEU:HD11 | 1.97 | 0.47 |
| 1:1U:16:ILE:HG22 | 1:1U:226:ASN:OD1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1U:100:ASN:HB3 | 1:1U:103:LYS:HB2 | 1.96 | 0.47 |
| 2:1V:222:PRO:CD | 1:1W:324:LYS:HE3 | 2.45 | 0.47 |
| 1:1W:152:ILE:HG23 | 1:1W:164:MET:SD | 2.54 | 0.47 |
| 2:1X:155:GLU:O | 2:1X:158:SER:OG | 2.24 | 0.47 |
| 2:1X:212:ILE:O | 2:1X:216:SER:OG | 2.28 | 0.47 |
| 1:2A:274:THR:OG1 | 1:2A:279:GLN:OE1 | 2.24 | 0.47 |
| 2:2B:306:ASP:HB3 | 2:2B:309:HIS:HD2 | 1.80 | 0.47 |
| 1:2C:139:LEU:HD12 | 1:2C:170:VAL:HG12 | 1.97 | 0.47 |
| 1:2C:177:ASP:O | 2:2D:352:LYS:HA | 2.14 | 0.47 |
| 1:2C:314:SER:HA | 1:2C:350:LYS:O | 2.14 | 0.47 |
| 2:2D:100:ALA:HA | 1:2E:252:LYS:HE3 | 1.96 | 0.47 |
| 2:2H:282:TYR:CE1 | 10:5B:167:ILE:HD11 | 2.49 | 0.47 |
| 1:2I:139:LEU:HD12 | 1:2I:170:VAL:HG12 | 1.96 | 0.47 |
| 1:2K:75:SER:O | 1:2K:78:SER:OG | 2.32 | 0.47 |
| 1:2K:121:ARG:CZ | 38:8C:50:LYS:HG2 | 2.44 | 0.47 |
| 1:2M:385:PHE:HZ | 1:2M:408:PHE:HD1 | 1.63 | 0.47 |
| 2:2P:426:ALA:O | 2:2P:430:LYS:HG2 | 2.15 | 0.47 |
| 1:2Q:280:GLN:HG3 | 1:2Q:281:TYR:CD2 | 2.49 | 0.47 |
| 1:2S:306:ARG:NH2 | 38:8A:51:GLN:HA | 2.25 | 0.47 |
| 2:2T:156:ARG:HA | 2:2T:159:VAL:HG12 | 1.97 | 0.47 |
| 2:2T:204:LEU:HD23 | 2:2T:302:MET:HB3 | 1.95 | 0.47 |
| 2:2X:161:TYR:O | 2:2X:163:LYS:NZ | 2.47 | 0.47 |
| 2:2X:415:GLU:HA | 2:2X:418:PHE:HD2 | 1.78 | 0.47 |
| 1:2Y:161:ASP:OD2 | 1:2Y:161:ASP:N | 2.48 | 0.47 |
| 2:2Z:203:MET:O | 2:2Z:204:LEU:HD23 | 2.14 | 0.47 |
| 2:3B:265:ILE:CD1 | 2:3B:435:VAL:HG21 | 2.45 | 0.47 |
| 2:3D:287:SER:OG | 2:3D:288:VAL:N | 2.46 | 0.47 |
| 2:3F:5:ILE:HD11 | 2:3F:135:PHE:CE1 | 2.50 | 0.47 |
| 1:3I:317:PHE:CE2 | 1:3I:326:VAL:HG13 | 2.50 | 0.47 |
| 1:3I:404:ASP:HB2 | 1:3I:406:MET:SD | 2.54 | 0.47 |
| 2:3J:3:GLU:HB2 | 2:3J:129:CYS:SG | 2.55 | 0.47 |
| 1:3K:77:ARG:NE | 3:4B:19:LEU:HA | 2.29 | 0.47 |
| 1:3K:101:TRP:HE3 | 1:3K:403:MET:HE1 | 1.80 | 0.47 |
| 1:3K:211:CYS:HA | 1:3K:215:LEU:HB2 | 1.95 | 0.47 |
| 2:3N:14:ILE:HD11 | 2:3N:74:VAL:HG13 | 1.96 | 0.47 |
| 1:3O:2:ARG:HH21 | 1:3O:240:LEU:HA | 1.80 | 0.47 |
| 1:3O:116:VAL:HA | 1:3O:119:VAL:HG12 | 1.97 | 0.47 |
| 2:3P:76:ASP:HA | 2:3P:79:ARG:HB2 | 1.96 | 0.47 |
| 1:3Q:53:GLU:OE2 | 1:3Q:57:GLY:N | 2.48 | 0.47 |
| 3:3V:44:ALA:O | 3:3V:118:ASN:ND2 | 2.47 | 0.47 |
| 3:3X:75:ARG:HG2 | 3:3X:76:PRO:HD2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:3Y:126:ASP:OD1 | 4:3Y:126:ASP:N | 2.46 | 0.47 |
| 3:4B:75:ARG:HG2 | 3:4B:76:PRO:HD2 | 1.96 | 0.47 |
| 4:4C:126:ASP:OD1 | 4:4C:126:ASP:N | 2.46 | 0.47 |
| 3:4D:63:SER:OG | 3:4D:66:THR:O | 2.29 | 0.47 |
| 3:4D:132:ILE:HD11 | 3:4D:161:PHE:CZ | 2.50 | 0.47 |
| 3:4F:75:ARG:HG2 | 3:4F:76:PRO:HD2 | 1.96 | 0.47 |
| 4:4I:136:LEU:O | 4:4I:140:THR:OG1 | 2.32 | 0.47 |
| 3:4J:200:ILE:HD12 | 3:4J:200:ILE:H | 1.79 | 0.47 |
| 5:4L:325:MET:HB3 | 5:4L:329:ARG:HH12 | 1.79 | 0.47 |
| 5:4M:293:LEU:HD11 | 28:7X:305:ALA:HB1 | 1.97 | 0.47 |
| 6:4O:316:GLU:O | 6:4O:320:GLU:HG2 | 2.15 | 0.47 |
| 6:4O:352:ARG:NH1 | 6:4O:355:GLU:OE1 | 2.48 | 0.47 |
| 7:4Q:321:LYS:HA | 7:4Q:324:GLN:CD | 2.35 | 0.47 |
| 10:5B:82:ALA:HA | 10:5B:85:ARG:HE | 1.79 | 0.47 |
| 10:5C:243:LEU:O | 10:5C:247:GLU:HG2 | 2.15 | 0.47 |
| 10:5C:486:VAL:O | 10:5C:491:ARG:NH1 | 2.39 | 0.47 |
| 11:5E:187:PRO:HA | 11:5E:190:VAL:HG12 | 1.96 | 0.47 |
| 12:5F:271:LEU:HD21 | 12:7B:23:MET:HG2 | 1.94 | 0.47 |
| 14:5L:112:SER:CB | 14:5L:159:SER:HB2 | 2.42 | 0.47 |
| 14:5L:451:VAL:HG13 | 14:5L:462:GLU:HB2 | 1.95 | 0.47 |
| 14:5L:465:MET:N | 14:5L:465:MET:SD | 2.88 | 0.47 |
| 14:5M:451:VAL:HG13 | 14:5M:462:GLU:HB2 | 1.95 | 0.47 |
| 14:5N:451:VAL:HG13 | 14:5N:462:GLU:HB2 | 1.95 | 0.47 |
| 14:5N:489:SER:HB3 | 14:5N:512:PHE:CD2 | 2.50 | 0.47 |
| 14:5N:511:THR:HG23 | 14:5N:512:PHE:N | 2.28 | 0.47 |
| 15:5P:56:LYS:NZ | 15:5P:249:ASP:OD2 | 2.48 | 0.47 |
| 15:5P:157:ARG:NH2 | 15:5P:266:THR:HG23 | 2.29 | 0.47 |
| 16:5Q:173:ARG:NH1 | 16:5Q:173:ARG:CG | 2.73 | 0.47 |
| 17:5S:132:ASP:N | 17:5S:132:ASP:OD1 | 2.47 | 0.47 |
| 17:5T:132:ASP:OD1 | 17:5T:132:ASP:N | 2.47 | 0.47 |
| 17:5U:132:ASP:OD1 | 17:5U:132:ASP:N | 2.47 | 0.47 |
| 18:5Y:61:LYS:HD2 | 18:5Y:61:LYS:HA | 1.73 | 0.47 |
| 18:6A:82:ASP:N | 18:6A:82:ASP:OD1 | 2.47 | 0.47 |
| 18:6B:82:ASP:N | 18:6B:82:ASP:OD1 | 2.48 | 0.47 |
| 18:6C:82:ASP:N | 18:6C:82:ASP:OD1 | 2.48 | 0.47 |
| 21:6H:44:ILE:CG2 | 21:6H:162:MET:HB3 | 2.44 | 0.47 |
| 21:6H:149:LEU:H | 21:6H:149:LEU:HD23 | 1.79 | 0.47 |
| 22:6I:276:LEU:HD23 | 22:6I:279:LEU:HD12 | 1.97 | 0.47 |
| 22:6I:291:GLU:HA | 22:6I:294:LEU:HG | 1.96 | 0.47 |
| 22:6N:124:PHE:HB2 | 22:6N:127:THR:HG23 | 1.96 | 0.47 |
| 22:6O:286:VAL:O | 22:6O:286:VAL:HG12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:6Q:24:LYS:HG2 | 23:6Q:25:GLU:HG2 | 1.97 | 0.47 |
| 23:6R:4:LYS:HA | 23:6R:4:LYS:HD2 | 1.45 | 0.47 |
| 24:6T:107:VAL:HG12 | 24:6T:108:GLU:N | 2.26 | 0.47 |
| 24:6T:536:ASP:HB3 | 24:6T:539:THR:HG23 | 1.97 | 0.47 |
| 24:6Z:505:LYS:NZ | 24:6Z:506:PRO:HD2 | 2.30 | 0.47 |
| 26:7E:50:SER:HA | 26:7E:56:LEU:HD23 | 1.96 | 0.47 |
| 32:7P:114:THR:HG22 | 32:7P:117:GLN:OE1 | 2.15 | 0.47 |
| 34:7R:159:ASP:OD2 | 35:7T:108:LEU:HD11 | 2.14 | 0.47 |
| 36:7W:22:ALA:HA | 36:7W:25:THR:HG22 | 1.95 | 0.47 |
| 38:8A:104:LYS:HE2 | 38:8A:107:GLU:OE1 | 2.15 | 0.47 |
| 2:2:11:GLN:HB3 | 41:3:501:GTP:PA | 2.54 | 0.47 |
| 2:8:44:GLY:HA3 | 24:6W:124:TYR:OH | 2.13 | 0.47 |
| 1:A7:360:GLY:HA3 | 24:6T:110:ASN:HA | 1.96 | 0.47 |
| 2:F1:56:THR:HA | 2:G7:285:GLN:HG2 | 1.96 | 0.47 |
| 2:F7:55:GLU:O | 2:H3:285:GLN:NE2 | 2.48 | 0.47 |
| 2:G1:276:ILE:HG23 | 2:G1:280:LYS:HB2 | 1.96 | 0.47 |
| 2:G1:290:GLU:OE1 | 2:G1:290:GLU:N | 2.31 | 0.47 |
| 1:G2:177:ASP:N | 1:G2:181:GLU:OE2 | 2.47 | 0.47 |
| 2:G3:205:ASP:OD2 | 2:G3:207:GLU:N | 2.48 | 0.47 |
| 2:G3:239:THR:HG23 | 2:G3:243:ARG:HE | 1.80 | 0.47 |
| 2:G3:264:ARG:NH2 | 2:G3:431:ASP:OD2 | 2.47 | 0.47 |
| 1:G4:177:ASP:OD1 | 39:G4:502:GDP:H3' | 2.15 | 0.47 |
| 1:G6:91:VAL:HG11 | 1:G6:116:VAL:HG22 | 1.97 | 0.47 |
| 2:G7:198:THR:HG21 | 2:G7:201:ALA:HB2 | 1.97 | 0.47 |
| 2:G9:9:ILE:HG13 | 2:G9:139:ASN:HB3 | 1.96 | 0.47 |
| 2:G9:279:GLU:HG2 | 2:G9:280:LYS:H | 1.79 | 0.47 |
| 2:G9:317:LEU:HB3 | 2:G9:319:TYR:CE1 | 2.50 | 0.47 |
| 2:H3:85:GLN:O | 2:I9:283:HIS:HE1 | 1.97 | 0.47 |
| 2:H3:98:ASP:OD1 | 2:H3:99:ALA:N | 2.48 | 0.47 |
| 1:H4:371:SER:OG | 1:H4:372:THR:N | 2.48 | 0.47 |
| 1:H4:375:GLN:HB2 | 1:H4:419:VAL:HG13 | 1.96 | 0.47 |
| 1:H6:67:ASP:OD2 | 1:H6:68:LEU:N | 2.48 | 0.47 |
| 1:H8:391:ARG:HH22 | 2:H9:435:VAL:HA | 1.79 | 0.47 |
| 1:I0:219:THR:O | 1:I0:219:THR:OG1 | 2.31 | 0.47 |
| 2:I1:88:HIS:CD2 | 2:I1:89:PRO:CD | 2.96 | 0.47 |
| 2:I1:379:SER:OG | 2:I1:380:ASN:N | 2.45 | 0.47 |
| 1:I2:252:LYS:CA | 1:I2:255:VAL:HG12 | 2.36 | 0.47 |
| 2:I3:75:VAL:HG21 | 2:I3:94:SER:HB2 | 1.96 | 0.47 |
| 1:I4:20:PHE:O | 1:I4:24:VAL:HG23 | 2.15 | 0.47 |
| 1:I4:290:THR:HA | 1:I4:293:MET:HB2 | 1.95 | 0.47 |
| 2:I5:174:SER:OG | 2:I5:207:GLU:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J0:173:PRO:HD2 | 1:J0:380:ARG:CZ | 2.44 | 0.47 |
| 1:J0:221:THR:OG1 | 1:J0:222:PHE:N | 2.47 | 0.47 |
| 1:J2:354:CYS:SG | 1:J2:355:ASP:N | 2.87 | 0.47 |
| 1:J6:3:GLU:HB2 | 1:J6:130:LEU:HA | 1.96 | 0.47 |
| 2:J7:129:CYS:SG | 2:J7:130:THR:N | 2.88 | 0.47 |
| 2:J9:346:TRP:CZ3 | 2:J9:347:CYS:HB2 | 2.50 | 0.47 |
| 1:K0:382:SER:HB3 | 1:K0:415:MET:HG2 | 1.96 | 0.47 |
| 2:K1:210:TYR:HE1 | 2:K1:227:LEU:HD11 | 1.80 | 0.47 |
| 2:K1:312:TYR:HB2 | 2:K1:343:PHE:CD1 | 2.50 | 0.47 |
| 2:K1:383:ALA:HA | 2:K1:386:GLU:OE1 | 2.15 | 0.47 |
| 1:K4:117:LEU:HA | 1:K4:120:VAL:HG12 | 1.96 | 0.47 |
| 1:K4:183:TYR:OH | 1:K4:388:MET:HB3 | 2.15 | 0.47 |
| 2:K7:250:VAL:HG23 | 2:K7:254:GLU:HG3 | 1.95 | 0.47 |
| 1:L0:3:GLU:HB2 | 1:L0:130:LEU:HD13 | 1.97 | 0.47 |
| 2:L1:121:ARG:O | 2:L1:121:ARG:HD2 | 2.15 | 0.47 |
| 1:L4:274:THR:OG1 | 1:L4:279:GLN:OE1 | 2.30 | 0.47 |
| 1:M2:239:CYS:SG | 1:M2:248:ALA:N | 2.79 | 0.47 |
| 2:M3:35:GLN:HA | 2:M3:59:GLY:O | 2.14 | 0.47 |
| 2:M3:223:THR:HA | 1:M4:323:THR:HG22 | 1.95 | 0.47 |
| 1:M4:6:HIS:NE2 | 1:M4:136:CYS:SG | 2.77 | 0.47 |
| 1:M8:177:ASP:N | 1:M8:181:GLU:OE2 | 2.48 | 0.47 |
| 1:M8:253:LEU:HD23 | 1:M8:253:LEU:HA | 1.84 | 0.47 |
| 2:M9:333:ALA:O | 2:M9:337:THR:HG23 | 2.15 | 0.47 |
| 2:N1:342:GLN:HG3 | 2:N1:342:GLN:O | 2.14 | 0.47 |
| 1:N2:245:GLN:CG | 29:7J:110:THR:HG21 | 2.44 | 0.47 |
| 1:N2:283:ALA:O | 1:N2:288:GLU:HG2 | 2.15 | 0.47 |
| 1:N2:322:SER:HB3 | 1:N2:325:GLU:HB2 | 1.96 | 0.47 |
| 1:N2:395:LEU:O | 1:N2:399:THR:HG23 | 2.15 | 0.47 |
| 1:N6:253:LEU:HD23 | 1:N6:253:LEU:HA | 1.75 | 0.47 |
| 2:O1:27:GLU:CD | 2:O1:243:ARG:HH12 | 2.18 | 0.47 |
| 2:O3:420:GLU:O | 2:O3:423:GLU:HG3 | 2.15 | 0.47 |
| 2:O9:271:SER:HB2 | 2:O9:377:MET:HE2 | 1.97 | 0.47 |
| 1:P4:404:ASP:OD1 | 1:P4:405:GLU:N | 2.48 | 0.47 |
| 2:Q1:3:GLU:HB2 | 2:Q1:129:CYS:SG | 2.55 | 0.47 |
| 2:Q3:86:LEU:HG | 2:Q3:86:LEU:O | 2.14 | 0.47 |
| 1:Q4:207:LEU:HB3 | 1:Q4:225:LEU:HD22 | 1.97 | 0.47 |
| 1:Q4:213:ARG:NH1 | 6:4P:52:TYR:OH | 2.48 | 0.47 |
| 2:Q5:115:VAL:HG22 | 2:Q5:119:LEU:HD23 | 1.96 | 0.47 |
| 2:Q5:155:GLU:O | 2:Q5:159:VAL:HG23 | 2.14 | 0.47 |
| 2:Q9:155:GLU:O | 2:Q9:158:SER:OG | 2.30 | 0.47 |
| 2:R3:90:GLU:OE1 | 2:R3:90:GLU:N | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:289:LEU:HD23 | 1:R4:365:ALA:HB2 | 1.97 | 0.47 |
| 1:R4:358:PRO:HG2 | 1:R4:361:LEU:HB2 | 1.95 | 0.47 |
| 2:R7:164:LYS:HD3 | 2:R7:164:LYS:HA | 1.74 | 0.47 |
| 1:S0:67:ASP:N | 1:S0:67:ASP:OD1 | 2.47 | 0.47 |
| 1:S0:238:CYS:SG | 1:S0:318:ARG:NE | 2.87 | 0.47 |
| 2:S5:3:GLU:HB2 | 2:S5:129:CYS:SG | 2.55 | 0.47 |
| 1:S8:172:SER:OG | 1:S8:173:PRO:HD2 | 2.14 | 0.47 |
| 1:T0:144:GLY:N | 39:T0:501:GDP:O1B | 2.41 | 0.47 |
| 2:T1:132:LEU:HD23 | 2:T1:164:LYS:HD3 | 1.97 | 0.47 |
| 1:T6:324:LYS:HE2 | 17:5U:38:PHE:HE1 | 1.78 | 0.47 |
| 2:T7:88:HIS:HB3 | 2:T7:91:GLN:HG3 | 1.97 | 0.47 |
| 1:T8:19:LYS:O | 1:T8:23:VAL:HG23 | 2.15 | 0.47 |
| 1:U2:293:MET:HG3 | 1:U2:367:PHE:HB2 | 1.95 | 0.47 |
| 2:U3:88:HIS:HB3 | 2:V9:283:HIS:CG | 2.50 | 0.47 |
| 2:U3:223:THR:OG1 | 2:U3:224:TYR:N | 2.48 | 0.47 |
| 1:U6:50:TYR:OH | 1:U6:237:THR:HG21 | 2.14 | 0.47 |
| 1:U6:68:LEU:HB3 | 1:U6:96:GLY:HA2 | 1.97 | 0.47 |
| 1:U8:155:ILE:HG22 | 1:U8:164:MET:HE1 | 1.96 | 0.47 |
| 2:U9:187:SER:O | 2:U9:191:THR:HG23 | 2.14 | 0.47 |
| 2:V1:90:GLU:HG3 | 2:V1:121:ARG:NH1 | 2.28 | 0.47 |
| 1:V2:114:ASP:N | 1:V2:114:ASP:OD1 | 2.47 | 0.47 |
| 1:V6:330:MET:HA | 1:V6:333:VAL:HG12 | 1.97 | 0.47 |
| 1:V8:175:VAL:HG21 | 1:V8:204:ASN:HB2 | 1.96 | 0.47 |
| 2:V9:331:SER:O | 2:V9:334:THR:OG1 | 2.24 | 0.47 |
| 1:W2:107:THR:OG1 | 1:W2:401:GLU:OE2 | 2.12 | 0.47 |
| 2:W3:276:ILE:HD11 | 2:W3:284:GLU:HG2 | 1.96 | 0.47 |
| 2:W5:274:PRO:HD3 | 2:W5:374:ALA:HA | 1.97 | 0.47 |
| 1:W6:170:VAL:HG22 | 1:W6:202:LEU:O | 2.15 | 0.47 |
| 2:W7:21:TRP:CZ3 | 2:W7:63:PRO:HB3 | 2.49 | 0.47 |
| 2:W9:223:THR:OG1 | 1:X0:245:GLN:NE2 | 2.47 | 0.47 |
| 2:W9:331:SER:O | 2:W9:334:THR:OG1 | 2.23 | 0.47 |
| 1:X0:114:ASP:N | 1:X0:114:ASP:OD1 | 2.47 | 0.47 |
| 2:X7:253:THR:O | 2:X7:257:THR:HG23 | 2.14 | 0.47 |
| 2:Y3:205:ASP:OD2 | 2:Y3:207:GLU:N | 2.47 | 0.47 |
| 2:Y5:52:PHE:CE2 | 2:Y5:243:ARG:HD3 | 2.50 | 0.47 |
| 2:Y5:311:LYS:HG2 | 2:Y5:342:GLN:HG3 | 1.96 | 0.47 |
| 1:Y6:237:THR:O | 1:Y6:241:ARG:NE | 2.48 | 0.47 |
| 1:Y8:178:THR:HG22 | 2:Y9:258:ASN:HD21 | 1.80 | 0.47 |
| 1:Y8:326:VAL:HG12 | 1:Y8:330:MET:CE | 2.45 | 0.47 |
| 2:Z3:75:VAL:O | 2:Z3:79:ARG:HG3 | 2.14 | 0.47 |
| 2:Z5:305:CYS:HB3 | 2:Z5:387:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z6:51:PHE:HB3 | 1:Z6:59:TYR:HB3 | 1.97 | 0.47 |
| 1:Z8:177:ASP:OD2 | 39:Z8:501:GDP:H3' | 2.14 | 0.47 |
| 1:0A:68:LEU:HB3 | 1:0A:96:GLY:HA2 | 1.97 | 0.47 |
| 1:0A:186:THR:OG1 | 1:0A:187:LEU:HD12 | 2.15 | 0.47 |
| 1:0C:114:ASP:N | 1:0C:114:ASP:OD1 | 2.47 | 0.47 |
| 1:0G:396:HIS:CE1 | 1:0G:397:TRP:CE2 | 3.03 | 0.47 |
| 1:0O:314:SER:HA | 1:0O:350:LYS:O | 2.14 | 0.47 |
| 2:0P:234:VAL:HG22 | 2:0P:272:TYR:CD1 | 2.49 | 0.47 |
| 1:0Q:239:CYS:SG | 1:0Q:248:ALA:N | 2.79 | 0.47 |
| 1:0S:66:MET:HB3 | 1:0S:147:MET:CE | 2.45 | 0.47 |
| 1:0U:180:VAL:HG23 | 1:0U:184:ASN:ND2 | 2.26 | 0.47 |
| 1:0U:262:ARG:NH2 | 1:0U:417:ASP:OD1 | 2.48 | 0.47 |
| 2:0X:362:VAL:HG22 | 2:0X:370:LYS:HE2 | 1.96 | 0.47 |
| 2:1D:434:GLU:CD | 2:1D:434:GLU:C | 2.72 | 0.47 |
| 1:1G:210:ILE:O | 1:1G:214:THR:OG1 | 2.25 | 0.47 |
| 1:1G:271:THR:OG1 | 1:1G:272:PRO:HA | 2.15 | 0.47 |
| 2:1L:205:ASP:OD1 | 2:1L:303:VAL:HG13 | 2.15 | 0.47 |
| 2:1L:406:HIS:HA | 2:1L:409:VAL:HG22 | 1.96 | 0.47 |
| 2:1R:192:HIS:HD2 | 2:1R:421:ALA:HA | 1.79 | 0.47 |
| 1:1S:275:SER:O | 1:1S:279:GLN:HG3 | 2.15 | 0.47 |
| 2:1Z:23:LEU:O | 2:1Z:26:LEU:HG | 2.14 | 0.47 |
| 2:1Z:83:TYR:HB3 | 2:1Z:86:LEU:HB3 | 1.96 | 0.47 |
| 2:1Z:262:TYR:HB3 | 2:1Z:265:ILE:HB | 1.97 | 0.47 |
| 1:2A:391:ARG:NH2 | 2:2B:346:TRP:HB2 | 2.30 | 0.47 |
| 2:2B:116:ASP:HB2 | 38:8A:73:TRP:CZ3 | 2.50 | 0.47 |
| 2:2F:156:ARG:HA | 2:2F:159:VAL:HG12 | 1.97 | 0.47 |
| 1:2I:22:GLU:HG2 | 1:2I:81:TYR:CD1 | 2.49 | 0.47 |
| 1:2I:111:GLU:N | 1:2I:111:GLU:OE1 | 2.48 | 0.47 |
| 1:2K:113:ILE:HA | 1:2K:116:VAL:HG22 | 1.96 | 0.47 |
| 1:2M:274:THR:OG1 | 1:2M:282:ARG:NH1 | 2.46 | 0.47 |
| 2:2T:214:ARG:HH22 | 38:8A:19:PHE:H | 1.63 | 0.47 |
| 2:2V:312:TYR:HD1 | 2:2V:381:SER:HB2 | 1.80 | 0.47 |
| 1:2Y:306:ARG:HD2 | 38:8C:96:GLY:HA2 | 1.90 | 0.47 |
| 1:3A:117:LEU:HA | 1:3A:120:VAL:HG12 | 1.97 | 0.47 |
| 2:3B:54:SER:HB3 | 2:3B:64:ARG:NH1 | 2.30 | 0.47 |
| 2:3B:220:GLU:HG2 | 2:3B:221:ARG:HG3 | 1.96 | 0.47 |
| 2:3D:107:HIS:CD2 | 2:3D:152:LEU:HB2 | 2.50 | 0.47 |
| 2:3F:109:THR:OG1 | 2:3F:411:GLU:OE2 | 2.30 | 0.47 |
| 2:3L:195:LEU:HD23 | 2:3L:195:LEU:HA | 1.71 | 0.47 |
| 2:3P:14:ILE:HD11 | 2:3P:74:VAL:HG13 | 1.96 | 0.47 |
| 1:3S:314:SER:HB3 | 1:3S:368:ILE:HG23 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3T:21:TRP:CZ2 | 2:3T:65:CYS:HB2 | 2.50 | 0.47 |
| 2:3T:202:VAL:HG22 | 2:3T:378:ILE:HD11 | 1.97 | 0.47 |
| 2:3T:414:GLU:HG2 | 2:3T:416:GLY:H | 1.79 | 0.47 |
| 3:3Z:132:ILE:HD11 | 3:3Z:161:PHE:CZ | 2.50 | 0.47 |
| 3:4B:132:ILE:HD11 | 3:4B:161:PHE:CZ | 2.50 | 0.47 |
| 4:4C:136:LEU:O | 4:4C:140:THR:OG1 | 2.32 | 0.47 |
| 4:4G:136:LEU:O | 4:4G:140:THR:OG1 | 2.32 | 0.47 |
| 6:4O:251:GLU:HA | 6:4O:254:ASP:OD2 | 2.14 | 0.47 |
| 7:4U:187:THR:HG21 | 31:7N:78:HIS:NE2 | 2.30 | 0.47 |
| 8:4W:248:ALA:HA | 8:4W:251:ARG:HD2 | 1.96 | 0.47 |
| 10:5D:231:GLN:O | 10:5D:235:ARG:HG3 | 2.15 | 0.47 |
| 13:5K:18:ARG:HB3 | 24:6Z:38:GLY:HA2 | 1.97 | 0.47 |
| 14:5M:5:LEU:HD11 | 14:5M:623:ASP:O | 2.15 | 0.47 |
| 14:5M:465:MET:N | 14:5M:465:MET:SD | 2.88 | 0.47 |
| 14:5N:5:LEU:HD11 | 14:5N:623:ASP:O | 2.15 | 0.47 |
| 14:5N:36:SER:HB2 | 14:5N:57:ASP:O | 2.15 | 0.47 |
| 14:5N:465:MET:N | 14:5N:465:MET:SD | 2.88 | 0.47 |
| 15:5O:227:TYR:CD1 | 15:5O:227:TYR:C | 2.86 | 0.47 |
| 15:5P:327:ALA:HA | 15:5P:343:LEU:HD21 | 1.95 | 0.47 |
| 17:5S:230:GLU:OE2 | 17:5S:231:ARG:N | 2.48 | 0.47 |
| 17:5U:230:GLU:OE2 | 17:5U:231:ARG:N | 2.48 | 0.47 |
| 18:5X:180:ARG:CG | 18:5X:180:ARG:NH2 | 2.73 | 0.47 |
| 18:5X:183:LEU:HG | 18:5X:189:TRP:CZ3 | 2.50 | 0.47 |
| 18:5Y:82:ASP:N | 18:5Y:82:ASP:OD1 | 2.48 | 0.47 |
| 18:6D:82:ASP:N | 18:6D:82:ASP:OD1 | 2.48 | 0.47 |
| 19:6E:15:ASP:OD1 | 19:6E:43:SER:HB3 | 2.15 | 0.47 |
| 19:6E:77:GLN:OE1 | 37:7Y:47:ASN:HB2 | 2.15 | 0.47 |
| 22:6P:190:LEU:HG | 22:6P:191:PHE:CD2 | 2.49 | 0.47 |
| 23:6Q:69:GLN:H | 23:6Q:69:GLN:CD | 2.15 | 0.47 |
| 23:6R:69:GLN:H | 23:6R:69:GLN:CD | 2.15 | 0.47 |
| 24:6T:372:ASP:O | 24:6T:375:THR:OG1 | 2.22 | 0.47 |
| 24:6T:434:ASP:OD2 | 24:6T:437:LYS:HB3 | 2.15 | 0.47 |
| 24:6V:274:ARG:HD3 | 24:6V:295:HIS:HE1 | 1.80 | 0.47 |
| 24:6W:183:ASP:OD1 | 24:6W:184:ALA:N | 2.47 | 0.47 |
| 24:6W:299:GLU:HG3 | 24:6W:300:ASP:CG | 2.34 | 0.47 |
| 24:6Y:345:ASP:OD2 | 24:6Y:346:GLN:N | 2.48 | 0.47 |
| 24:6Z:299:GLU:HG3 | 24:6Z:300:ASP:CG | 2.35 | 0.47 |
| 27:7G:75:LYS:HA | 27:7G:78:THR:HG22 | 1.97 | 0.47 |
| 30:7K:383:ARG:HD3 | 30:7K:387:GLU:OE2 | 2.15 | 0.47 |
| 33:7Q:139:GLU:HG3 | 33:7Q:140:TYR:H | 1.80 | 0.47 |
| 37:7Y:92:TYR:OH | 37:7Y:108:PRO:HD2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8A:73:TRP:CD1 | 38:8A:75:SER:HB2 | 2.49 | 0.47 |
| 38:8A:93:LYS:HD2 | 38:8A:93:LYS:C | 2.35 | 0.47 |
| 38:8C:206:PRO:HG2 | 38:8C:209:HIS:CE1 | 2.50 | 0.47 |
| 1:A1:333:VAL:CG2 | 3:4F:67:LEU:HD13 | 2.44 | 0.47 |
| 1:A7:280:GLN:NE2 | 24:6T:104:GLU:OE2 | 2.48 | 0.47 |
| 2:D5:280:LYS:NZ | 18:6C:166:HIS:HB3 | 2.30 | 0.47 |
| 1:F6:219:THR:N | 24:6T:418:ASP:OD1 | 2.48 | 0.47 |
| 2:G1:11:GLN:NE2 | 1:G2:245:GLN:O | 2.37 | 0.47 |
| 1:G4:309:ARG:NH1 | 1:G4:339:SER:O | 2.47 | 0.47 |
| 2:G9:90:GLU:HB2 | 2:I5:283:HIS:CE1 | 2.49 | 0.47 |
| 1:H2:257:LEU:HD21 | 1:H2:314:SER:HB3 | 1.97 | 0.47 |
| 2:H3:90:GLU:HB3 | 2:H3:121:ARG:CZ | 2.44 | 0.47 |
| 1:H4:135:VAL:O | 1:H4:166:THR:HA | 2.15 | 0.47 |
| 2:H5:379:SER:OG | 2:H5:380:ASN:N | 2.48 | 0.47 |
| 1:H8:7:ILE:HB | 1:H8:135:VAL:HG22 | 1.95 | 0.47 |
| 2:H9:306:ASP:HB3 | 2:H9:309:HIS:HD2 | 1.80 | 0.47 |
| 2:I1:5:ILE:HG22 | 2:I1:64:ARG:HB3 | 1.97 | 0.47 |
| 1:I4:177:ASP:O | 2:I5:352:LYS:HA | 2.15 | 0.47 |
| 1:I4:414:ASN:HA | 1:I4:417:ASP:OD2 | 2.15 | 0.47 |
| 2:I9:151:SER:HB2 | 2:I9:193:SER:OG | 2.15 | 0.47 |
| 2:I9:387:ILE:HG12 | 2:I9:390:ARG:HH22 | 1.80 | 0.47 |
| 1:J0:49:VAL:HG11 | 1:J0:241:ARG:HG2 | 1.97 | 0.47 |
| 2:J1:312:TYR:HB2 | 2:J1:343:PHE:CD1 | 2.50 | 0.47 |
| 1:J4:268:VAL:HG23 | 1:J4:300:MET:HB2 | 1.96 | 0.47 |
| 2:J5:223:THR:OG1 | 2:J5:224:TYR:N | 2.48 | 0.47 |
| 2:J7:201:ALA:O | 2:J7:268:MET:HE2 | 2.14 | 0.47 |
| 2:J9:287:SER:OG | 2:J9:288:VAL:N | 2.48 | 0.47 |
| 2:K1:22:GLU:O | 2:K1:26:LEU:HG | 2.14 | 0.47 |
| 2:K5:261:PRO:HG3 | 2:K5:313:MET:HE2 | 1.97 | 0.47 |
| 1:L0:117:LEU:HD11 | 1:L0:154:LYS:HB3 | 1.97 | 0.47 |
| 2:L1:387:ILE:HG12 | 2:L1:390:ARG:HH22 | 1.80 | 0.47 |
| 1:L4:190:HIS:CD2 | 1:L4:414:ASN:HB2 | 2.50 | 0.47 |
| 1:L4:397:TRP:CH2 | 2:L5:256:GLN:HB3 | 2.50 | 0.47 |
| 2:L7:237:SER:HA | 2:L7:320:ARG:HD2 | 1.96 | 0.47 |
| 2:M1:2:ARG:HA | 2:M1:133:GLN:HE21 | 1.80 | 0.47 |
| 1:M2:208:TYR:CE1 | 1:M2:225:LEU:HD11 | 2.50 | 0.47 |
| 2:M3:278:ALA:HA | 2:M3:369:ALA:HB2 | 1.97 | 0.47 |
| 2:M5:222:PRO:HD2 | 1:M6:324:LYS:HE3 | 1.97 | 0.47 |
| 1:M6:49:VAL:HG11 | 1:M6:241:ARG:HG2 | 1.96 | 0.47 |
| 1:M8:139:LEU:HG | 1:M8:168:SER:HB3 | 1.97 | 0.47 |
| 2:N3:121:ARG:NH1 | 2:N3:124:LYS:HG3 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N3:312:TYR:HD1 | 2:N3:381:SER:HB2 | 1.80 | 0.47 |
| 2:N3:313:MET:HB2 | 2:N3:380:ASN:HB3 | 1.97 | 0.47 |
| 2:N7:330:ALA:O | 2:N7:334:THR:HG23 | 2.14 | 0.47 |
| 2:N9:81:GLY:O | 2:N9:84:ARG:NH1 | 2.48 | 0.47 |
| 1:O0:202:LEU:HD23 | 1:O0:229:ILE:HG12 | 1.97 | 0.47 |
| 2:O3:116:ASP:OD1 | 2:O3:117:LEU:N | 2.44 | 0.47 |
| 1:O4:171:PRO:O | 1:O4:380:ARG:NH2 | 2.48 | 0.47 |
| 2:P3:394:LYS:HB2 | 1:P4:346:PRO:HG3 | 1.97 | 0.47 |
| 1:P4:58:ARG:HD3 | 1:R0:280:GLN:HE22 | 1.80 | 0.47 |
| 1:P6:5:VAL:HB | 1:P6:133:PHE:HD1 | 1.79 | 0.47 |
| 1:P6:207:LEU:HB3 | 1:P6:225:LEU:HD22 | 1.96 | 0.47 |
| 2:P7:51:THR:HG21 | 2:P7:243:ARG:HG2 | 1.97 | 0.47 |
| 2:P7:398:MET:HG2 | 1:P8:345:ILE:HD13 | 1.97 | 0.47 |
| 2:P9:66:ILE:O | 2:P9:66:ILE:HG13 | 2.15 | 0.47 |
| 1:Q0:311:LEU:HD23 | 1:Q0:311:LEU:HA | 1.72 | 0.47 |
| 1:Q2:128:ASP:OD1 | 1:Q2:128:ASP:N | 2.44 | 0.47 |
| 1:Q8:170:VAL:HG12 | 1:Q8:202:LEU:O | 2.14 | 0.47 |
| 2:Q9:69:ASP:OD2 | 2:Q9:71:GLU:N | 2.47 | 0.47 |
| 1:R2:25:SER:O | 1:R2:30:ILE:HG12 | 2.14 | 0.47 |
| 1:R2:208:TYR:CE1 | 1:R2:225:LEU:HD11 | 2.50 | 0.47 |
| 2:R3:205:ASP:OD2 | 2:R3:303:VAL:HG13 | 2.15 | 0.47 |
| 1:S0:173:PRO:HD2 | 1:S0:380:ARG:CZ | 2.45 | 0.47 |
| 1:S2:164:MET:O | 1:S2:197:ASP:HB2 | 2.15 | 0.47 |
| 2:T5:344:VAL:HG13 | 2:T5:347:CYS:H | 1.79 | 0.47 |
| 1:T6:222:PHE:CD2 | 2:T7:247:ALA:HB1 | 2.50 | 0.47 |
| 1:T6:278:SER:O | 1:T6:278:SER:OG | 2.30 | 0.47 |
| 1:T8:67:ASP:N | 1:T8:67:ASP:OD1 | 2.47 | 0.47 |
| 1:T8:117:LEU:HB3 | 1:T8:121:ARG:HH22 | 1.80 | 0.47 |
| 1:U6:377:MET:O | 1:U6:381:VAL:HG23 | 2.15 | 0.47 |
| 1:V0:170:VAL:HG12 | 1:V0:202:LEU:O | 2.14 | 0.47 |
| 1:V0:397:TRP:HE1 | 2:V1:260:VAL:HG23 | 1.80 | 0.47 |
| 2:V1:89:PRO:HG2 | 2:W7:279:GLU:OE1 | 2.15 | 0.47 |
| 1:W2:100:ASN:HB3 | 1:W2:103:LYS:HB2 | 1.96 | 0.47 |
| 1:W4:309:ARG:NH1 | 1:W4:339:SER:O | 2.47 | 0.47 |
| 1:W6:178:THR:HG23 | 1:W6:181:GLU:HG3 | 1.97 | 0.47 |
| 1:W8:32:PRO:HD3 | 1:W8:81:TYR:CZ | 2.50 | 0.47 |
| 2:W9:70:LEU:CD1 | 2:W9:95:GLY:HA3 | 2.45 | 0.47 |
| 1:X4:178:THR:HA | 2:X5:352:LYS:HD3 | 1.97 | 0.47 |
| 1:X6:33:THR:O | 1:X6:58:ARG:NH2 | 2.47 | 0.47 |
| 1:X8:330:MET:HB3 | 1:X8:349:VAL:HG11 | 1.96 | 0.47 |
| 1:Y0:386:THR:O | 1:Y0:390:ARG:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y2:24:VAL:HG21 | 1:Y2:50:TYR:HD2 | 1.80 | 0.47 |
| 1:Y2:91:VAL:HG21 | 1:Y2:119:VAL:HG21 | 1.96 | 0.47 |
| 1:Y2:273:LEU:H | 1:Y2:292:GLN:NE2 | 2.12 | 0.47 |
| 1:Y4:317:PHE:HB3 | 1:Y4:321:MET:HE3 | 1.96 | 0.47 |
| 1:Z0:294:TRP:CG | 1:Z0:333:VAL:HG21 | 2.50 | 0.47 |
| 2:Z3:15:GLN:HB3 | 2:Z3:228:ASN:ND2 | 2.27 | 0.47 |
| 2:Z3:21:TRP:CH2 | 2:Z3:63:PRO:HB3 | 2.50 | 0.47 |
| 2:Z3:139:ASN:O | 2:Z3:171:VAL:HG23 | 2.15 | 0.47 |
| 1:Z6:31:ASP:OD2 | 1:Z6:33:THR:OG1 | 2.24 | 0.47 |
| 2:0B:55:GLU:OE2 | 2:0B:59:GLY:N | 2.47 | 0.47 |
| 2:0B:288:VAL:HG13 | 2:0B:319:TYR:HE2 | 1.79 | 0.47 |
| 1:0E:204:ASN:OD1 | 39:0E:501:GDP:O2' | 2.33 | 0.47 |
| 1:0G:39:ASP:OD1 | 1:0G:39:ASP:N | 2.42 | 0.47 |
| 2:0H:72:PRO:HG3 | 1:0I:1:MET:HG3 | 1.96 | 0.47 |
| 1:0M:229:ILE:O | 1:0M:233:MET:HG3 | 2.14 | 0.47 |
| 1:0O:270:PHE:N | 1:0O:298:ASN:OD1 | 2.47 | 0.47 |
| 2:0R:65:CYS:SG | 2:0R:66:ILE:N | 2.87 | 0.47 |
| 1:0U:210:ILE:O | 1:0U:214:THR:OG1 | 2.22 | 0.47 |
| 1:0Y:21:TRP:HA | 1:0Y:24:VAL:HG22 | 1.97 | 0.47 |
| 2:0Z:194:LEU:O | 2:0Z:198:THR:HG22 | 2.14 | 0.47 |
| 2:1D:402:ARG:HA | 2:1D:402:ARG:HD3 | 1.72 | 0.47 |
| 1:1E:45:GLU:HG2 | 1:1E:46:ARG:HG2 | 1.97 | 0.47 |
| 1:1E:135:VAL:HG12 | 1:1E:137:HIS:HD2 | 1.80 | 0.47 |
| 1:1G:392:LYS:HB3 | 1:1G:395:LEU:HD22 | 1.97 | 0.47 |
| 1:1K:334:GLN:HE22 | 1:1K:348:ASN:H | 1.61 | 0.47 |
| 1:1O:213:ARG:NE | 1:1O:297:LYS:HZ2 | 2.12 | 0.47 |
| 1:1O:275:SER:O | 1:1O:279:GLN:HG3 | 2.15 | 0.47 |
| 2:1T:71:GLU:HB3 | 2:1T:98:ASP:OD2 | 2.15 | 0.47 |
| 1:1U:68:LEU:HB3 | 1:1U:96:GLY:HA2 | 1.97 | 0.47 |
| 1:1U:327:ASP:OD1 | 1:1U:328:GLU:N | 2.48 | 0.47 |
| 2:1V:333:ALA:O | 2:1V:337:THR:HG23 | 2.15 | 0.47 |
| 2:1V:387:ILE:HG12 | 2:1V:390:ARG:HH22 | 1.79 | 0.47 |
| 1:1W:31:ASP:OD1 | 1:1W:35:THR:N | 2.41 | 0.47 |
| 2:1X:333:ALA:O | 2:1X:337:THR:HG23 | 2.15 | 0.47 |
| 1:2A:170:VAL:HG22 | 1:2A:202:LEU:O | 2.15 | 0.47 |
| 2:2B:290:GLU:HA | 2:2B:293:ASN:HD22 | 1.78 | 0.47 |
| 2:2F:289:ALA:O | 2:2F:293:ASN:ND2 | 2.48 | 0.47 |
| 2:2H:336:LYS:O | 2:2H:339:ARG:NH2 | 2.48 | 0.47 |
| 1:2Q:69:GLU:OE2 | 1:2Q:96:GLY:HA2 | 2.15 | 0.47 |
| 1:2Q:337:ASN:OD1 | 38:8A:97:PHE:HD1 | 1.97 | 0.47 |
| 2:2T:274:PRO:HB2 | 2:2T:276:ILE:HG12 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2Y:148:GLY:O | 1:2Y:152:ILE:HG12 | 2.15 | 0.47 |
| 2:3B:277:SER:HB3 | 2:3B:279:GLU:OE2 | 2.15 | 0.47 |
| 1:3C:86:ARG:NH1 | 1:3C:89:ASN:OD1 | 2.44 | 0.47 |
| 1:3C:148:GLY:O | 1:3C:152:ILE:HG12 | 2.14 | 0.47 |
| 2:3D:156:ARG:HA | 2:3D:159:VAL:HG12 | 1.97 | 0.47 |
| 1:3G:244:GLY:H | 1:3G:247:ASN:HD21 | 1.63 | 0.47 |
| 1:3O:53:GLU:HG2 | 1:3O:59:TYR:CE1 | 2.49 | 0.47 |
| 1:3O:404:ASP:OD2 | 1:3O:405:GLU:N | 2.47 | 0.47 |
| 1:3Q:167:PHE:CZ | 1:3Q:233:MET:HG2 | 2.49 | 0.47 |
| 1:3Q:330:MET:HA | 1:3Q:333:VAL:HG12 | 1.97 | 0.47 |
| 2:3T:425:LEU:C | 2:3T:425:LEU:CD2 | 2.81 | 0.47 |
| 3:3V:132:ILE:HD11 | 3:3V:161:PHE:CZ | 2.50 | 0.47 |
| 3:3X:132:ILE:HD11 | 3:3X:161:PHE:CZ | 2.50 | 0.47 |
| 3:4F:132:ILE:HD11 | 3:4F:161:PHE:CZ | 2.50 | 0.47 |
| 3:4H:132:ILE:HD11 | 3:4H:161:PHE:CZ | 2.50 | 0.47 |
| 5:4L:253:ARG:O | 5:4L:257:LYS:HG3 | 2.15 | 0.47 |
| 5:4L:260:ALA:O | 5:4L:263:LEU:HG | 2.15 | 0.47 |
| 5:4M:141:ASP:OD2 | 5:4M:142:GLU:N | 2.48 | 0.47 |
| 5:4M:250:VAL:O | 5:4M:254:GLU:HG2 | 2.15 | 0.47 |
| 5:4M:320:GLN:HB3 | 28:7X:428:LEU:CD1 | 2.44 | 0.47 |
| 7:4R:191:GLU:OE1 | 24:6X:16:VAL:HG21 | 2.14 | 0.47 |
| 7:4R:327:ARG:O | 7:4R:330:GLU:HG3 | 2.15 | 0.47 |
| 7:4S:42:LYS:HB3 | 7:4S:46:GLN:NE2 | 2.30 | 0.47 |
| 9:4Y:355:ALA:O | 9:4Y:358:THR:HG22 | 2.14 | 0.47 |
| 9:4Y:392:LYS:HD3 | 9:4Y:392:LYS:HA | 1.76 | 0.47 |
| 9:4Z:188:THR:O | 9:4Z:191:GLU:HG3 | 2.15 | 0.47 |
| 10:5B:82:ALA:O | 10:5B:86:GLU:HG2 | 2.15 | 0.47 |
| 10:5C:338:LYS:HB3 | 10:5C:338:LYS:HE3 | 1.73 | 0.47 |
| 11:5E:112:ARG:HA | 11:5E:112:ARG:HD2 | 1.30 | 0.47 |
| 12:5F:207:ASP:OD1 | 12:5F:207:ASP:N | 2.47 | 0.47 |
| 14:5L:5:LEU:HD11 | 14:5L:623:ASP:O | 2.15 | 0.47 |
| 14:5M:36:SER:HB2 | 14:5M:57:ASP:O | 2.15 | 0.47 |
| 14:5N:205:ASN:N | 14:5N:205:ASN:OD1 | 2.48 | 0.47 |
| 15:5O:34:GLU:OE2 | 15:5O:49:ARG:HA | 2.15 | 0.47 |
| 15:5O:308:ALA:HB3 | 15:5O:372:PHE:CE2 | 2.50 | 0.47 |
| 17:5S:30:LYS:H | 17:5S:30:LYS:HG3 | 1.44 | 0.47 |
| 18:5X:82:ASP:N | 18:5X:82:ASP:OD1 | 2.48 | 0.47 |
| 18:5X:183:LEU:HD23 | 18:5X:191:VAL:HG11 | 1.97 | 0.47 |
| 18:5Z:82:ASP:N | 18:5Z:82:ASP:OD1 | 2.48 | 0.47 |
| 18:5Z:183:LEU:HD23 | 18:5Z:191:VAL:HG11 | 1.97 | 0.47 |
| 18:6C:183:LEU:HD23 | 18:6C:191:VAL:HG11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:6D:183:LEU:HG | 18:6D:189:TRP:CZ3 | 2.50 | 0.47 |
| 20:6F:113:ARG:HH22 | 20:6F:247:TYR:CB | 2.27 | 0.47 |
| 20:6F:197:PHE:O | 20:6F:200:VAL:HG12 | 2.15 | 0.47 |
| 22:6J:20:TYR:CZ | 22:6J:22:GLY:HA3 | 2.49 | 0.47 |
| 22:6K:122:ALA:HB1 | 22:6K:127:THR:OG1 | 2.15 | 0.47 |
| 24:6U:124:TYR:CE2 | 24:6U:150:ARG:HG3 | 2.50 | 0.47 |
| 24:6V:481:LEU:HB3 | 24:6V:500:ARG:HB3 | 1.97 | 0.47 |
| 24:6X:183:ASP:OD1 | 24:6X:184:ALA:N | 2.47 | 0.47 |
| 24:6X:444:ILE:C | 24:6X:445:ILE:CD1 | 2.77 | 0.47 |
| 24:6Z:273:LEU:HD11 | 24:6Z:298:LEU:HD21 | 1.97 | 0.47 |
| 31:7M:29:GLU:HG3 | 31:7M:30:TYR:N | 2.30 | 0.47 |
| 34:7R:205:LEU:HD22 | 35:7T:160:ILE:HD13 | 1.96 | 0.47 |
| 28:7X:317:GLU:O | 28:7X:320:THR:OG1 | 2.28 | 0.47 |
| 38:8B:8:GLU:CD | 38:8B:21:LYS:HD3 | 2.36 | 0.47 |
| 1:9:204:ASN:OD1 | 39:9:501:GDP:O2' | 2.20 | 0.47 |
| 2:B0:80:THR:HG22 | 18:5Y:169:LYS:O | 2.14 | 0.47 |
| 2:E3:369:ALA:HB1 | 22:6J:82:LEU:HD13 | 1.96 | 0.47 |
| 1:G2:128:ASP:OD1 | 1:G2:128:ASP:N | 2.48 | 0.47 |
| 2:G3:269:LEU:HG | 2:G3:384:ILE:HD11 | 1.97 | 0.47 |
| 1:G4:378:PHE:HA | 1:G4:381:VAL:HG12 | 1.96 | 0.47 |
| 1:G8:173:PRO:HG2 | 1:G8:380:ARG:HH21 | 1.80 | 0.47 |
| 2:H5:69:ASP:OD1 | 2:H5:70:LEU:N | 2.47 | 0.47 |
| 1:H8:99:ASN:ND2 | 1:H8:178:THR:HG21 | 2.29 | 0.47 |
| 1:H8:203:ASP:OD2 | 1:H8:301:CYS:HA | 2.15 | 0.47 |
| 2:I5:9:ILE:HG13 | 2:I5:9:ILE:O | 2.15 | 0.47 |
| 2:I5:21:TRP:CZ2 | 2:I5:65:CYS:HB2 | 2.50 | 0.47 |
| 2:I5:121:ARG:HD2 | 2:I5:124:LYS:HE3 | 1.97 | 0.47 |
| 2:I5:156:ARG:HA | 2:I5:159:VAL:HG12 | 1.97 | 0.47 |
| 2:I7:344:VAL:HG13 | 2:I7:346:TRP:H | 1.80 | 0.47 |
| 1:J0:86:ARG:HG2 | 1:J0:88:ASP:H | 1.79 | 0.47 |
| 1:J0:100:ASN:HB3 | 1:J0:103:LYS:HB2 | 1.97 | 0.47 |
| 2:J5:121:ARG:HD2 | 2:J5:124:LYS:HE3 | 1.96 | 0.47 |
| 2:J9:271:SER:OG | 2:J9:300:SER:O | 2.26 | 0.47 |
| 2:K3:121:ARG:HA | 2:K3:121:ARG:HD2 | 1.62 | 0.47 |
| 1:K4:396:HIS:HE1 | 1:K4:397:TRP:CZ2 | 2.33 | 0.47 |
| 1:K6:183:TYR:O | 1:K6:187:LEU:HD13 | 2.15 | 0.47 |
| 2:K9:157:LEU:HA | 2:K9:157:LEU:HD23 | 1.78 | 0.47 |
| 1:L0:325:GLU:O | 1:L0:329:GLN:HG2 | 2.15 | 0.47 |
| 1:L4:177:ASP:O | 2:L5:352:LYS:HA | 2.15 | 0.47 |
| 2:L7:116:ASP:OD1 | 2:L7:117:LEU:N | 2.46 | 0.47 |
| 1:M2:113:ILE:HG23 | 1:M2:117:LEU:HD23 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M4:87:PRO:HD2 | 2:O1:283:HIS:ND1 | 2.30 | 0.47 |
| 1:M8:149:THR:O | 1:M8:152:ILE:HG22 | 2.14 | 0.47 |
| 2:N1:72:PRO:HD2 | 1:N2:2:ARG:HH12 | 1.80 | 0.47 |
| 1:N2:371:SER:OG | 1:N2:372:THR:N | 2.48 | 0.47 |
| 2:N5:336:LYS:O | 2:N5:339:ARG:NH2 | 2.48 | 0.47 |
| 1:N6:278:SER:HB2 | 1:N6:281:TYR:HD2 | 1.80 | 0.47 |
| 1:N8:139:LEU:CD1 | 1:N8:168:SER:HB3 | 2.45 | 0.47 |
| 1:O0:3:GLU:HG3 | 1:O0:127:CYS:HB2 | 1.96 | 0.47 |
| 2:O1:175:PRO:HB3 | 2:O1:390:ARG:HE | 1.80 | 0.47 |
| 2:O3:65:CYS:SG | 2:O3:66:ILE:N | 2.88 | 0.47 |
| 2:P5:251:ASP:OD1 | 27:7G:184:LYS:HD2 | 2.14 | 0.47 |
| 2:Q1:4:VAL:HG23 | 2:Q1:134:GLY:O | 2.14 | 0.47 |
| 2:Q5:21:TRP:CZ2 | 2:Q5:65:CYS:HB2 | 2.50 | 0.47 |
| 2:R1:56:THR:HG23 | 2:R1:60:LYS:HB3 | 1.97 | 0.47 |
| 1:R2:3:GLU:HG3 | 1:R2:127:CYS:SG | 2.55 | 0.47 |
| 1:S2:11:GLN:N | 39:S2:502:GDP:O1B | 2.31 | 0.47 |
| 1:S6:117:LEU:HD23 | 1:S6:117:LEU:HA | 1.77 | 0.47 |
| 1:T0:6:HIS:NE2 | 1:T0:136:CYS:SG | 2.88 | 0.47 |
| 2:T7:289:ALA:O | 2:T7:293:ASN:ND2 | 2.48 | 0.47 |
| 1:U2:208:TYR:HA | 1:U2:211:CYS:SG | 2.55 | 0.47 |
| 1:U4:2:ARG:HB3 | 1:U4:131:GLN:HB2 | 1.97 | 0.47 |
| 2:U7:399:TYR:OH | 2:U7:415:GLU:OE2 | 2.33 | 0.47 |
| 2:V1:209:ILE:HG23 | 2:V1:230:LEU:HD11 | 1.96 | 0.47 |
| 2:V1:292:THR:HG1 | 2:V1:319:TYR:HH | 1.63 | 0.47 |
| 2:V9:244:PHE:HB2 | 2:V9:356:ASN:HD21 | 1.79 | 0.47 |
| 2:W3:320:ARG:NH2 | 2:W3:359:PRO:O | 2.45 | 0.47 |
| 2:W3:394:LYS:HB2 | 1:W4:346:PRO:HG3 | 1.97 | 0.47 |
| 2:W7:224:TYR:CZ | 1:W8:323:THR:HG21 | 2.50 | 0.47 |
| 2:W9:251:ASP:OD1 | 2:W9:252:ILE:N | 2.48 | 0.47 |
| 2:X5:76:ASP:HA | 2:X5:79:ARG:HB2 | 1.96 | 0.47 |
| 1:X6:263:LEU:HD22 | 1:X6:422:TYR:CE1 | 2.50 | 0.47 |
| 1:Y4:33:THR:O | 1:Y4:58:ARG:NH2 | 2.48 | 0.47 |
| 1:Y6:5:VAL:HG12 | 1:Y6:133:PHE:HD1 | 1.80 | 0.47 |
| 1:Y8:65:LEU:HD12 | 1:Y8:90:PHE:CD1 | 2.50 | 0.47 |
| 1:Z0:125:GLU:OE2 | 1:Z0:159:TYR:OH | 2.24 | 0.47 |
| 1:Z2:21:TRP:CH2 | 1:Z2:61:PRO:HB3 | 2.50 | 0.47 |
| 2:Z3:33:ASP:O | 2:Z3:60:LYS:NZ | 2.47 | 0.47 |
| 1:Z6:11:GLN:NE2 | 39:Z6:502:GDP:O2A | 2.49 | 0.47 |
| 1:Z6:58:ARG:HD3 | 1:0M:280:GLN:NE2 | 2.29 | 0.47 |
| 1:Z8:207:LEU:HD21 | 1:Z8:229:ILE:HD11 | 1.97 | 0.47 |
| 2:Z9:181:VAL:HG22 | 1:0A:256:ASN:HD22 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0B:70:LEU:HG | 2:0B:145:THR:HG23 | 1.97 | 0.47 |
| 2:0B:276:ILE:HG23 | 2:0B:280:LYS:HB3 | 1.97 | 0.47 |
| 1:0C:388:MET:HB2 | 1:0C:388:MET:HE3 | 1.67 | 0.47 |
| 1:0G:290:THR:HA | 1:0G:293:MET:HB2 | 1.97 | 0.47 |
| 2:0H:27:GLU:CD | 2:0H:243:ARG:HH12 | 2.19 | 0.47 |
| 2:0H:183:GLU:CD | 2:0H:184:PRO:HD3 | 2.35 | 0.47 |
| 2:0J:232:ALA:HA | 2:0J:235:ILE:HG22 | 1.97 | 0.47 |
| 1:0K:66:MET:SD | 1:0K:116:VAL:HG11 | 2.55 | 0.47 |
| 1:0M:404:ASP:HB3 | 1:0M:406:MET:SD | 2.55 | 0.47 |
| 2:0N:208:ALA:O | 2:0N:212:ILE:HG13 | 2.15 | 0.47 |
| 1:0O:179:VAL:HB | 2:0P:258:ASN:HD22 | 1.79 | 0.47 |
| 2:0P:333:ALA:O | 2:0P:337:THR:HG23 | 2.15 | 0.47 |
| 2:0R:406:HIS:CG | 1:0S:261:PRO:HD3 | 2.49 | 0.47 |
| 1:1A:95:THR:OG1 | 1:1A:96:GLY:N | 2.48 | 0.47 |
| 1:1E:334:GLN:HE22 | 1:1E:348:ASN:H | 1.62 | 0.47 |
| 2:1L:370:LYS:HG3 | 9:4Y:381:LEU:HD13 | 1.96 | 0.47 |
| 2:1P:246:GLY:HA2 | 2:1P:357:TYR:CD2 | 2.50 | 0.47 |
| 2:1P:317:LEU:HB3 | 2:1P:319:TYR:CE1 | 2.49 | 0.47 |
| 2:1T:238:LEU:HD12 | 2:1T:239:THR:HG23 | 1.97 | 0.47 |
| 1:1U:8:GLN:CD | 1:1U:17:GLY:HA3 | 2.35 | 0.47 |
| 1:1U:207:LEU:HD13 | 1:1U:225:LEU:HB3 | 1.96 | 0.47 |
| 2:1V:14:ILE:HG12 | 2:1V:67:PHE:HB3 | 1.97 | 0.47 |
| 2:2F:203:MET:C | 2:2F:204:LEU:HD12 | 2.36 | 0.47 |
| 1:2G:20:PHE:HB2 | 1:2G:233:MET:HE3 | 1.97 | 0.47 |
| 1:2G:309:ARG:NH1 | 1:2G:341:PHE:O | 2.48 | 0.47 |
| 2:2H:88:HIS:HD1 | 2:2H:91:GLN:HG3 | 1.79 | 0.47 |
| 2:2H:274:PRO:HB2 | 2:2H:276:ILE:HG12 | 1.96 | 0.47 |
| 1:2I:212:PHE:CE1 | 2:2J:326:LYS:HE3 | 2.50 | 0.47 |
| 1:2I:244:GLY:HA2 | 1:2I:355:ASP:OD1 | 2.15 | 0.47 |
| 2:2J:277:SER:OG | 2:2J:278:ALA:N | 2.46 | 0.47 |
| 1:2K:177:ASP:O | 2:2L:352:LYS:HA | 2.14 | 0.47 |
| 2:2L:250:VAL:HG23 | 2:2L:254:GLU:HG3 | 1.97 | 0.47 |
| 2:2N:7:ILE:HG13 | 2:2N:9:ILE:HD11 | 1.97 | 0.47 |
| 2:2N:161:TYR:HD1 | 38:8D:80:TYR:HB3 | 1.74 | 0.47 |
| 2:2N:317:LEU:HB3 | 2:2N:319:TYR:HE1 | 1.79 | 0.47 |
| 2:2P:66:ILE:O | 2:2P:66:ILE:HG13 | 2.14 | 0.47 |
| 2:2P:88:HIS:ND1 | 2:3F:283:HIS:HA | 2.30 | 0.47 |
| 1:2Q:306:ARG:O | 38:8A:94:LYS:HE2 | 2.15 | 0.47 |
| 2:2R:420:GLU:HA | 2:2R:423:GLU:HG3 | 1.97 | 0.47 |
| 1:2U:256:ASN:O | 1:2U:312:THR:HG21 | 2.15 | 0.47 |
| 2:2X:22:GLU:OE1 | 38:8C:203:PHE:HE1 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3B:259:LEU:HD11 | 2:3B:316:CYS:HB2 | 1.97 | 0.47 |
| 1:3C:337:ASN:CG | 38:8D:97:PHE:HA | 2.36 | 0.47 |
| 2:3H:47:ASP:N | 2:3H:47:ASP:OD1 | 2.48 | 0.47 |
| 1:3K:77:ARG:NH2 | 3:4B:18:LYS:HB3 | 2.27 | 0.47 |
| 2:3L:333:ALA:O | 2:3L:337:THR:HG23 | 2.14 | 0.47 |
| 2:3N:117:LEU:HD13 | 4:4E:6:PHE:HB2 | 1.97 | 0.47 |
| 2:3P:221:ARG:NE | 1:3Q:325:GLU:OE2 | 2.48 | 0.47 |
| 1:3Q:116:VAL:HA | 1:3Q:119:VAL:HG12 | 1.96 | 0.47 |
| 1:3Q:257:LEU:HD23 | 1:3Q:312:THR:HG22 | 1.96 | 0.47 |
| 3:3X:28:ASN:ND2 | 3:3X:115:ASN:H | 2.12 | 0.47 |
| 4:4A:126:ASP:OD1 | 4:4A:126:ASP:N | 2.46 | 0.47 |
| 4:4E:126:ASP:OD1 | 4:4E:126:ASP:N | 2.46 | 0.47 |
| 12:5G:264:ARG:NH2 | 31:7N:13:LEU:HD11 | 2.30 | 0.47 |
| 14:5L:36:SER:HB2 | 14:5L:57:ASP:O | 2.15 | 0.47 |
| 14:5L:205:ASN:N | 14:5L:205:ASN:OD1 | 2.48 | 0.47 |
| 14:5L:493:CYS:SG | 14:5L:513:PHE:CG | 3.08 | 0.47 |
| 14:5M:205:ASN:N | 14:5M:205:ASN:OD1 | 2.48 | 0.47 |
| 14:5N:385:CYS:HB2 | 14:5N:401:TRP:CH2 | 2.50 | 0.47 |
| 18:5Y:183:LEU:HD23 | 18:5Y:191:VAL:HG11 | 1.97 | 0.47 |
| 18:5Y:183:LEU:HG | 18:5Y:189:TRP:CZ3 | 2.50 | 0.47 |
| 18:5Z:183:LEU:HG | 18:5Z:189:TRP:CZ3 | 2.50 | 0.47 |
| 18:6A:183:LEU:HD23 | 18:6A:191:VAL:HG11 | 1.97 | 0.47 |
| 18:6B:183:LEU:HD23 | 18:6B:191:VAL:HG11 | 1.97 | 0.47 |
| 18:6D:183:LEU:HD23 | 18:6D:191:VAL:HG11 | 1.97 | 0.47 |
| 19:6E:107:THR:O | 19:6E:107:THR:HG22 | 2.14 | 0.47 |
| 20:6F:86:ASP:HB3 | 20:6F:247:TYR:CE1 | 2.49 | 0.47 |
| 22:6I:185:PHE:HE1 | 22:6I:193:MET:SD | 2.38 | 0.47 |
| 22:6I:187:MET:SD | 22:6I:256:TYR:HB2 | 2.55 | 0.47 |
| 22:6K:96:LYS:HD3 | 22:6K:97:PRO:CD | 2.45 | 0.47 |
| 23:6S:69:GLN:H | 23:6S:69:GLN:CD | 2.15 | 0.47 |
| 24:6W:507:ARG:HA | 24:6W:507:ARG:CZ | 2.45 | 0.47 |
| 24:6X:156:ASP:N | 24:6X:156:ASP:OD2 | 2.48 | 0.47 |
| 25:7C:21:LEU:O | 25:7C:24:GLN:HB3 | 2.15 | 0.47 |
| 26:7D:115:GLU:HB3 | 26:7D:116:GLN:HG3 | 1.96 | 0.47 |
| 29:7I:264:ARG:HD2 | 29:7I:265:VAL:H | 1.79 | 0.47 |
| 34:7R:92:LEU:HD13 | 35:7T:36:GLN:HE21 | 1.80 | 0.47 |
| 35:7U:144:VAL:HG13 | 35:7U:148:GLN:HE21 | 1.80 | 0.47 |
| 1:5:224:ASP:OD2 | 26:7D:137:PRO:CD | 2.64 | 0.46 |
| 2:A0:44:GLY:HA3 | 24:6X:131:HIS:CD2 | 2.49 | 0.46 |
| 1:E0:33:THR:HG23 | 24:6T:403:PRO:HB2 | 1.97 | 0.46 |
| 2:G1:189:LEU:HD11 | 2:G1:418:PHE:HE1 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G2:95:THR:OG1 | 1:G2:96:GLY:N | 2.48 | 0.46 |
| 1:G6:396:HIS:CD2 | 2:G7:263:PRO:HD3 | 2.50 | 0.46 |
| 1:G8:239:CYS:SG | 1:G8:248:ALA:N | 2.84 | 0.46 |
| 1:H2:208:TYR:HA | 1:H2:211:CYS:SG | 2.55 | 0.46 |
| 1:H2:374:ILE:HD12 | 1:H2:378:PHE:HE2 | 1.80 | 0.46 |
| 2:H7:333:ALA:O | 2:H7:337:THR:HG23 | 2.15 | 0.46 |
| 1:I2:392:LYS:HD2 | 1:I2:395:LEU:HD22 | 1.97 | 0.46 |
| 2:I3:353:CYS:SG | 2:I3:354:GLY:N | 2.89 | 0.46 |
| 1:I4:77:ARG:HE | 1:I4:90:PHE:HE2 | 1.63 | 0.46 |
| 2:I5:319:TYR:CD1 | 2:I5:375:VAL:HG22 | 2.50 | 0.46 |
| 2:I5:362:VAL:HA | 2:I5:368:LEU:HD11 | 1.97 | 0.46 |
| 2:J7:250:VAL:HB | 2:J7:254:GLU:HG3 | 1.98 | 0.46 |
| 2:K3:88:HIS:HB2 | 2:L9:283:HIS:ND1 | 2.31 | 0.46 |
| 2:K3:90:GLU:OE1 | 2:K3:90:GLU:N | 2.44 | 0.46 |
| 2:K3:116:ASP:OD2 | 2:K3:117:LEU:N | 2.47 | 0.46 |
| 1:K4:44:LEU:O | 1:K4:47:ILE:HG12 | 2.15 | 0.46 |
| 1:L2:145:SER:OG | 1:L2:146:GLY:N | 2.48 | 0.46 |
| 2:L3:70:LEU:HD12 | 2:L3:99:ALA:HB2 | 1.97 | 0.46 |
| 2:L3:73:THR:CG2 | 1:L4:2:ARG:HH22 | 2.28 | 0.46 |
| 1:L4:67:ASP:OD2 | 1:L4:72:THR:OG1 | 2.31 | 0.46 |
| 2:L9:98:ASP:OD2 | 2:L9:99:ALA:N | 2.48 | 0.46 |
| 1:M0:7:ILE:O | 1:M0:135:VAL:HA | 2.15 | 0.46 |
| 2:M1:76:ASP:HA | 2:M1:79:ARG:HB2 | 1.97 | 0.46 |
| 1:M2:167:PHE:CZ | 1:M2:233:MET:HG2 | 2.50 | 0.46 |
| 2:M7:372:GLN:HG3 | 30:7K:83:GLY:HA3 | 1.96 | 0.46 |
| 1:M8:95:THR:OG1 | 1:M8:96:GLY:N | 2.48 | 0.46 |
| 1:M8:178:THR:OG1 | 1:M8:181:GLU:HG3 | 2.14 | 0.46 |
| 1:N0:50:TYR:OH | 1:N0:237:THR:HG21 | 2.15 | 0.46 |
| 1:N2:317:PHE:HB3 | 1:N2:321:MET:SD | 2.55 | 0.46 |
| 2:N3:122:ILE:HD11 | 2:N3:157:LEU:HD21 | 1.97 | 0.46 |
| 2:N3:250:VAL:HG13 | 2:N3:254:GLU:HG3 | 1.98 | 0.46 |
| 2:N7:417:GLU:HA | 2:N7:420:GLU:HG2 | 1.97 | 0.46 |
| 2:N9:56:THR:HG22 | 2:P7:285:GLN:CB | 2.42 | 0.46 |
| 2:O1:397:LEU:HD23 | 2:O1:397:LEU:HA | 1.82 | 0.46 |
| 1:O2:362:LYS:NZ | 37:7Y:227:GLY:HA3 | 2.30 | 0.46 |
| 2:O3:188:VAL:O | 2:O3:191:THR:HG22 | 2.14 | 0.46 |
| 1:O4:77:ARG:O | 37:7Y:29:SER:HB2 | 2.14 | 0.46 |
| 2:O5:225:THR:HB | 32:7P:130:VAL:HG11 | 1.97 | 0.46 |
| 2:O7:54:SER:OG | 2:O7:64:ARG:NE | 2.49 | 0.46 |
| 2:P5:413:MET:HB3 | 2:P5:417:GLU:OE2 | 2.14 | 0.46 |
| 2:Q5:306:ASP:OD2 | 2:Q5:308:ARG:HB2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q6:1:MET:HB3 | 1:Q6:2:ARG:H | 1.57 | 0.46 |
| 1:Q6:207:LEU:HB3 | 1:Q6:225:LEU:HD22 | 1.98 | 0.46 |
| 1:Q8:294:TRP:HZ3 | 1:Q8:367:PHE:CZ | 2.33 | 0.46 |
| 2:Q9:72:PRO:HD2 | 1:R0:2:ARG:NH1 | 2.30 | 0.46 |
| 1:R0:121:ARG:HG2 | 1:R0:125:GLU:OE1 | 2.15 | 0.46 |
| 2:R1:392:ASP:OD2 | 2:R1:422:ARG:NH1 | 2.48 | 0.46 |
| 2:R3:72:PRO:HD2 | 1:R4:2:ARG:NH1 | 2.30 | 0.46 |
| 1:R6:35:THR:HA | 1:R6:57:GLY:O | 2.15 | 0.46 |
| 2:R9:79:ARG:O | 2:R9:84:ARG:HG2 | 2.15 | 0.46 |
| 2:R9:399:TYR:O | 2:R9:402:ARG:NH1 | 2.47 | 0.46 |
| 1:S2:311:LEU:HD23 | 1:S2:311:LEU:HA | 1.70 | 0.46 |
| 1:S4:52:ASN:OD1 | 1:S4:62:ARG:NH2 | 2.48 | 0.46 |
| 1:S4:219:THR:OG1 | 24:6U:17:CYS:SG | 2.68 | 0.46 |
| 2:S5:9:ILE:HD13 | 2:S5:150:GLY:HA2 | 1.97 | 0.46 |
| 2:S5:96:LYS:HG2 | 1:S6:1:MET:HE1 | 1.96 | 0.46 |
| 2:T1:9:ILE:HG22 | 2:T1:146:GLY:HA2 | 1.96 | 0.46 |
| 1:T2:208:TYR:CE1 | 1:T2:225:LEU:HD11 | 2.50 | 0.46 |
| 2:T3:210:TYR:HH | 1:T4:323:THR:HG1 | 1.57 | 0.46 |
| 2:T5:183:GLU:CD | 2:T5:184:PRO:HD3 | 2.36 | 0.46 |
| 2:T5:269:LEU:HD22 | 2:T5:303:VAL:HG11 | 1.97 | 0.46 |
| 1:T6:301:CYS:SG | 1:T6:302:ALA:N | 2.89 | 0.46 |
| 2:T7:333:ALA:O | 2:T7:337:THR:HG23 | 2.14 | 0.46 |
| 2:U5:76:ASP:HA | 2:U5:79:ARG:HB2 | 1.97 | 0.46 |
| 2:U7:72:PRO:HD2 | 1:U8:2:ARG:HH12 | 1.80 | 0.46 |
| 1:U8:296:ALA:HB3 | 1:U8:297:LYS:HZ2 | 1.80 | 0.46 |
| 1:V0:173:PRO:HD2 | 1:V0:380:ARG:CZ | 2.45 | 0.46 |
| 1:V4:285:THR:HG23 | 1:V4:288:GLU:H | 1.79 | 0.46 |
| 1:W0:273:LEU:H | 1:W0:292:GLN:HE22 | 1.62 | 0.46 |
| 1:W4:205:GLU:OE1 | 1:W4:205:GLU:N | 2.35 | 0.46 |
| 2:W5:305:CYS:HB3 | 2:W5:387:ILE:HD11 | 1.97 | 0.46 |
| 2:W9:6:SER:O | 2:W9:65:CYS:HA | 2.16 | 0.46 |
| 2:X7:21:TRP:CZ2 | 2:X7:65:CYS:HB3 | 2.50 | 0.46 |
| 2:X7:109:THR:OG1 | 2:X7:411:GLU:OE2 | 2.22 | 0.46 |
| 2:X7:239:THR:HG23 | 2:X7:243:ARG:HH21 | 1.79 | 0.46 |
| 1:Y6:222:PHE:HA | 1:Y6:225:LEU:HD12 | 1.97 | 0.46 |
| 1:Y6:309:ARG:O | 1:Y6:371:SER:OG | 2.27 | 0.46 |
| 2:Y9:30:ILE:HG12 | 2:Y9:36:MET:HG2 | 1.97 | 0.46 |
| 1:Z2:417:ASP:HA | 1:Z2:420:SER:OG | 2.15 | 0.46 |
| 1:0A:155:ILE:HG13 | 1:0A:164:MET:HE1 | 1.97 | 0.46 |
| 2:0B:34:GLY:HA3 | 2:0B:60:LYS:NZ | 2.31 | 0.46 |
| 1:0G:19:LYS:O | 1:0G:23:VAL:HG23 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0H:213:CYS:HA | 2:0H:217:LEU:HB2 | 1.97 | 0.46 |
| 2:0H:406:HIS:CG | 1:0I:261:PRO:HD3 | 2.50 | 0.46 |
| 2:0N:145:THR:OG1 | 41:0O:501:GTP:O1B | 2.33 | 0.46 |
| 1:0W:8:GLN:CD | 1:0W:17:GLY:HA3 | 2.35 | 0.46 |
| 1:0W:112:LEU:HB3 | 1:0W:147:MET:HE1 | 1.98 | 0.46 |
| 1:0W:204:ASN:HD21 | 39:0W:502:GDP:HN22 | 1.62 | 0.46 |
| 2:1B:5:ILE:HG22 | 2:1B:64:ARG:HB3 | 1.96 | 0.46 |
| 1:1C:95:THR:OG1 | 1:1C:108:GLU:OE2 | 2.33 | 0.46 |
| 2:1D:49:PHE:HD2 | 2:1D:53:PHE:HB2 | 1.80 | 0.46 |
| 1:1G:273:LEU:H | 1:1G:292:GLN:HE22 | 1.62 | 0.46 |
| 1:1K:212:PHE:O | 1:1K:216:LYS:HD2 | 2.15 | 0.46 |
| 2:1L:76:ASP:HA | 2:1L:79:ARG:HB2 | 1.96 | 0.46 |
| 1:1O:67:ASP:N | 1:1O:67:ASP:OD1 | 2.48 | 0.46 |
| 2:1R:387:ILE:HG12 | 2:1R:390:ARG:HH12 | 1.80 | 0.46 |
| 1:1S:418:LEU:HG | 1:1S:422:TYR:CE2 | 2.43 | 0.46 |
| 2:1T:157:LEU:HD23 | 2:1T:157:LEU:HA | 1.81 | 0.46 |
| 1:1U:5:VAL:HG23 | 1:1U:62:ARG:HG2 | 1.98 | 0.46 |
| 1:1U:52:ASN:OD1 | 1:1U:62:ARG:NH2 | 2.48 | 0.46 |
| 1:1U:295:ASP:OD1 | 1:1U:297:LYS:HG2 | 2.15 | 0.46 |
| 2:1V:198:THR:HG21 | 2:1V:201:ALA:HB2 | 1.97 | 0.46 |
| 1:1W:35:THR:OG1 | 1:1W:37:HIS:NE2 | 2.44 | 0.46 |
| 2:1X:381:SER:OG | 2:1X:382:THR:N | 2.48 | 0.46 |
| 1:2G:27:GLU:OE1 | 1:2G:241:ARG:NH1 | 2.47 | 0.46 |
| 1:2G:337:ASN:HB3 | 1:2G:340:TYR:HD2 | 1.78 | 0.46 |
| 2:2J:5:ILE:HG22 | 2:2J:64:ARG:HD3 | 1.97 | 0.46 |
| 2:2L:213:CYS:SG | 2:2L:219:ILE:HB | 2.55 | 0.46 |
| 2:2L:305:CYS:HB3 | 2:2L:387:ILE:HD11 | 1.96 | 0.46 |
| 2:2P:9:ILE:HD13 | 2:2P:150:GLY:HA2 | 1.96 | 0.46 |
| 2:2P:90:GLU:HB2 | 2:2P:121:ARG:HH22 | 1.79 | 0.46 |
| 2:2P:166:LYS:N | 2:2P:199:ASP:OD1 | 2.48 | 0.46 |
| 2:2P:417:GLU:HA | 2:2P:420:GLU:CG | 2.43 | 0.46 |
| 2:2T:9:ILE:HD13 | 2:2T:150:GLY:HA2 | 1.96 | 0.46 |
| 2:2T:21:TRP:CZ2 | 2:2T:65:CYS:HB2 | 2.49 | 0.46 |
| 1:2W:39:ASP:CG | 10:5C:346:ARG:HH12 | 2.18 | 0.46 |
| 1:2Y:183:TYR:O | 1:2Y:187:LEU:HD13 | 2.15 | 0.46 |
| 2:2Z:72:PRO:HD2 | 1:3A:2:ARG:NH1 | 2.30 | 0.46 |
| 2:2Z:199:ASP:OD2 | 2:2Z:199:ASP:N | 2.43 | 0.46 |
| 1:3A:271:THR:OG1 | 1:3A:365:ALA:HB3 | 2.15 | 0.46 |
| 1:3C:49:VAL:HG11 | 1:3C:241:ARG:HG2 | 1.97 | 0.46 |
| 1:3C:301:CYS:O | 38:8D:105:ARG:NH1 | 2.48 | 0.46 |
| 2:3F:230:LEU:O | 2:3F:234:VAL:HG23 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3G:233:MET:O | 1:3G:237:THR:HG22 | 2.15 | 0.46 |
| 2:3J:335:ILE:HG23 | 2:3J:341:ILE:HD11 | 1.97 | 0.46 |
| 1:3S:108:GLU:N | 1:3S:108:GLU:OE1 | 2.48 | 0.46 |
| 3:3V:28:ASN:ND2 | 3:3V:115:ASN:H | 2.13 | 0.46 |
| 4:3W:54:VAL:HG11 | 4:3W:86:TYR:HB2 | 1.97 | 0.46 |
| 3:4B:28:ASN:ND2 | 3:4B:115:ASN:H | 2.12 | 0.46 |
| 4:4G:54:VAL:HG11 | 4:4G:86:TYR:HB2 | 1.97 | 0.46 |
| 4:4G:126:ASP:OD1 | 4:4G:126:ASP:N | 2.46 | 0.46 |
| 3:4H:28:ASN:ND2 | 3:4H:115:ASN:H | 2.13 | 0.46 |
| 6:4P:91:LYS:HA | 6:4P:91:LYS:HD3 | 1.75 | 0.46 |
| 10:5A:406:LEU:HD21 | 10:5A:410:ARG:CZ | 2.45 | 0.46 |
| 10:5B:275:ASN:O | 10:5B:278:GLN:HG3 | 2.15 | 0.46 |
| 11:5E:14:TRP:CH2 | 11:5E:103:VAL:HG22 | 2.50 | 0.46 |
| 14:5L:112:SER:HB2 | 14:5L:159:SER:CB | 2.40 | 0.46 |
| 14:5L:238:VAL:HG23 | 14:5L:240:MET:O | 2.15 | 0.46 |
| 14:5M:244:ALA:HB1 | 14:5M:297:ILE:HG13 | 1.96 | 0.46 |
| 14:5M:315:MET:HG3 | 14:5M:315:MET:O | 2.14 | 0.46 |
| 14:5N:238:VAL:HG23 | 14:5N:240:MET:O | 2.15 | 0.46 |
| 15:5O:12:GLU:OE1 | 15:5O:74:LYS:HG2 | 2.15 | 0.46 |
| 15:5O:65:VAL:HA | 15:5O:74:LYS:HA | 1.96 | 0.46 |
| 17:5S:174:SER:CB | 17:5S:175:PRO:HD2 | 2.43 | 0.46 |
| 17:5T:30:LYS:H | 17:5T:30:LYS:HG3 | 1.44 | 0.46 |
| 18:6A:183:LEU:HG | 18:6A:189:TRP:CZ3 | 2.50 | 0.46 |
| 18:6B:183:LEU:HG | 18:6B:189:TRP:CZ3 | 2.50 | 0.46 |
| 18:6C:183:LEU:HG | 18:6C:189:TRP:CZ3 | 2.50 | 0.46 |
| 19:6E:65:ALA:O | 19:6E:66:THR:HG22 | 2.14 | 0.46 |
| 20:6F:149:LEU:HD21 | 20:6F:167:VAL:HG23 | 1.98 | 0.46 |
| 21:6G:15:ASP:OD1 | 21:6G:16:GLU:N | 2.48 | 0.46 |
| 22:6L:289:ASP:HA | 22:6L:292:ARG:HD2 | 1.97 | 0.46 |
| 23:6Q:4:LYS:HA | 23:6Q:4:LYS:HD2 | 1.45 | 0.46 |
| 23:6Q:27:ASP:HB3 | 23:6Q:54:ASN:OD1 | 2.14 | 0.46 |
| 24:6T:113:ASN:OD1 | 24:6T:114:HIS:ND1 | 2.46 | 0.46 |
| 24:6V:304:GLU:OE2 | 24:6V:306:LEU:HG | 2.15 | 0.46 |
| 24:6Y:123:TYR:CE2 | 24:6Y:163:PRO:HG3 | 2.50 | 0.46 |
| 24:6Z:556:ASP:O | 24:6Z:560:ARG:HG3 | 2.15 | 0.46 |
| 24:7A:117:ARG:NH1 | 24:7A:134:GLU:OE2 | 2.48 | 0.46 |
| 26:7E:115:GLU:HB3 | 26:7E:116:GLN:HG3 | 1.96 | 0.46 |
| 29:7J:269:GLY:O | 30:7L:368:ARG:NH2 | 2.43 | 0.46 |
| 28:7X:351:ARG:O | 28:7X:355:ASN:ND2 | 2.48 | 0.46 |
| 38:8C:83:ARG:CZ | 38:8C:85:ARG:HD2 | 2.43 | 0.46 |
| 1:1:379:LYS:HZ1 | 3:3V:49:HIS:CD2 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A5:78:SER:OG | 24:7A:149:LYS:HG3 | 2.15 | 0.46 |
| 1:A9:280:GLN:HE22 | 24:6U:106:VAL:HA | 1.79 | 0.46 |
| 2:E5:88:HIS:CE1 | 2:G1:283:HIS:HA | 2.49 | 0.46 |
| 2:E7:88:HIS:ND1 | 2:G3:283:HIS:HB3 | 2.30 | 0.46 |
| 1:G0:216:LYS:HB2 | 24:6V:422:ASN:HD22 | 1.80 | 0.46 |
| 2:G3:9:ILE:HG23 | 2:G3:68:LEU:HD11 | 1.97 | 0.46 |
| 2:G9:185:TYR:HA | 2:G9:395:PHE:HE1 | 1.81 | 0.46 |
| 2:H3:72:PRO:HD2 | 1:H4:2:ARG:NH1 | 2.29 | 0.46 |
| 2:H3:119:LEU:HA | 2:H3:122:ILE:HG22 | 1.97 | 0.46 |
| 1:I0:177:ASP:O | 2:I1:352:LYS:HA | 2.16 | 0.46 |
| 1:I2:9:GLY:HA2 | 1:I2:66:MET:HE3 | 1.98 | 0.46 |
| 1:I2:382:SER:HB2 | 1:I2:415:MET:HG2 | 1.97 | 0.46 |
| 2:I3:317:LEU:HB3 | 2:I3:319:TYR:CE1 | 2.50 | 0.46 |
| 1:I8:3:GLU:HG3 | 1:I8:127:CYS:SG | 2.56 | 0.46 |
| 2:I9:76:ASP:HA | 2:I9:79:ARG:HD2 | 1.96 | 0.46 |
| 1:J2:210:ILE:O | 1:J2:214:THR:OG1 | 2.25 | 0.46 |
| 1:J4:19:LYS:NZ | 1:J4:227:HIS:HD2 | 2.13 | 0.46 |
| 2:J5:255:PHE:HA | 2:J5:259:LEU:HD13 | 1.97 | 0.46 |
| 2:K1:383:ALA:O | 2:K1:387:ILE:HG13 | 2.15 | 0.46 |
| 2:K3:137:VAL:HG22 | 2:K3:168:GLY:HA2 | 1.96 | 0.46 |
| 2:K9:250:VAL:HG23 | 2:K9:254:GLU:HG3 | 1.98 | 0.46 |
| 1:L4:22:GLU:HG2 | 1:L4:81:TYR:CD1 | 2.50 | 0.46 |
| 2:M1:98:ASP:OD1 | 2:M1:99:ALA:N | 2.48 | 0.46 |
| 1:M6:134:GLN:HE21 | 1:M6:167:PHE:HE2 | 1.62 | 0.46 |
| 1:N0:218:THR:HG21 | 30:7L:353:ASN:HB3 | 1.96 | 0.46 |
| 2:N1:100:ALA:HA | 1:N2:252:LYS:HE2 | 1.97 | 0.46 |
| 1:N2:86:ARG:HB2 | 1:N2:89:ASN:HB2 | 1.97 | 0.46 |
| 2:N3:214:ARG:NH2 | 2:N3:215:ARG:HB2 | 2.31 | 0.46 |
| 1:N6:39:ASP:OD1 | 1:N6:40:SER:N | 2.48 | 0.46 |
| 2:N9:287:SER:N | 2:N9:290:GLU:OE2 | 2.48 | 0.46 |
| 2:N9:296:PHE:HE2 | 2:N9:335:ILE:HG21 | 1.81 | 0.46 |
| 1:O0:68:LEU:HB3 | 1:O0:96:GLY:HA2 | 1.97 | 0.46 |
| 1:O0:344:TRP:CE3 | 1:O0:345:ILE:HG13 | 2.50 | 0.46 |
| 2:O1:122:ILE:HA | 2:O1:125:LEU:HB2 | 1.97 | 0.46 |
| 1:O2:175:VAL:HG11 | 1:O2:208:TYR:HE2 | 1.79 | 0.46 |
| 2:O3:62:VAL:HG23 | 2:O3:62:VAL:O | 2.15 | 0.46 |
| 1:O4:309:ARG:NH1 | 1:O4:341:PHE:O | 2.48 | 0.46 |
| 1:P4:180:VAL:HG23 | 1:P4:184:ASN:ND2 | 2.29 | 0.46 |
| 1:P4:238:CYS:SG | 1:P4:318:ARG:NE | 2.89 | 0.46 |
| 1:P4:286:VAL:HG21 | 1:P4:325:GLU:HB3 | 1.98 | 0.46 |
| 1:P6:31:ASP:OD2 | 1:P6:33:THR:OG1 | 2.25 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P8:111:GLU:N | 1:P8:111:GLU:OE1 | 2.48 | 0.46 |
| 2:P9:288:VAL:HG13 | 2:P9:319:TYR:HE2 | 1.81 | 0.46 |
| 1:Q0:207:LEU:HB3 | 1:Q0:225:LEU:HD22 | 1.95 | 0.46 |
| 1:Q2:244:GLY:HA2 | 1:Q2:355:ASP:OD1 | 2.15 | 0.46 |
| 2:Q9:305:CYS:HB3 | 2:Q9:387:ILE:HD11 | 1.96 | 0.46 |
| 1:R4:70:PRO:HA | 1:R4:92:PHE:HZ | 1.79 | 0.46 |
| 1:R4:135:VAL:O | 1:R4:166:THR:HA | 2.16 | 0.46 |
| 1:R4:219:THR:O | 1:R4:219:THR:OG1 | 2.31 | 0.46 |
| 1:R6:227:HIS:CE1 | 24:6X:11:LEU:HA | 2.50 | 0.46 |
| 1:R6:237:THR:HG22 | 1:R6:237:THR:O | 2.15 | 0.46 |
| 1:R8:100:ASN:HB3 | 1:R8:103:LYS:HB2 | 1.96 | 0.46 |
| 2:R9:33:ASP:O | 2:R9:60:LYS:NZ | 2.38 | 0.46 |
| 2:R9:370:LYS:O | 7:4R:278:GLN:NE2 | 2.48 | 0.46 |
| 2:S1:73:THR:OG1 | 2:S1:74:VAL:N | 2.49 | 0.46 |
| 1:S4:317:PHE:HB3 | 1:S4:321:MET:HE3 | 1.98 | 0.46 |
| 1:S6:358:PRO:HG2 | 1:S6:361:LEU:HD12 | 1.97 | 0.46 |
| 2:S9:245:ASP:HB3 | 24:6W:29:LYS:HD2 | 1.98 | 0.46 |
| 2:T7:254:GLU:O | 2:T7:257:THR:N | 2.46 | 0.46 |
| 2:T7:278:ALA:HA | 2:T7:369:ALA:HB2 | 1.96 | 0.46 |
| 2:U3:325:PRO:HA | 2:U3:328:VAL:HG22 | 1.97 | 0.46 |
| 1:U4:414:ASN:HA | 1:U4:417:ASP:OD2 | 2.15 | 0.46 |
| 2:U7:35:GLN:HB3 | 2:U7:59:GLY:O | 2.14 | 0.46 |
| 2:U9:72:PRO:HG3 | 1:V0:1:MET:HG3 | 1.97 | 0.46 |
| 2:V1:211:ASP:OD1 | 2:V1:215:ARG:NH1 | 2.48 | 0.46 |
| 1:V4:212:PHE:HE1 | 1:V4:220:PRO:HG3 | 1.81 | 0.46 |
| 1:V6:418:LEU:O | 1:V6:421:GLU:HG2 | 2.15 | 0.46 |
| 2:V7:88:HIS:CG | 2:X3:283:HIS:HA | 2.50 | 0.46 |
| 2:V9:5:ILE:HG22 | 2:V9:64:ARG:HB3 | 1.96 | 0.46 |
| 1:W0:56:GLY:HA2 | 8:4W:173:LYS:HD3 | 1.98 | 0.46 |
| 1:W2:32:PRO:HD3 | 1:W2:81:TYR:CZ | 2.50 | 0.46 |
| 2:W3:26:LEU:HD21 | 2:W3:363:VAL:HG12 | 1.97 | 0.46 |
| 1:W4:272:PRO:HB2 | 1:W4:282:ARG:HH12 | 1.80 | 0.46 |
| 2:W5:139:ASN:O | 2:W5:170:THR:HA | 2.16 | 0.46 |
| 2:X3:25:CYS:SG | 2:X3:86:LEU:HD11 | 2.55 | 0.46 |
| 2:X3:70:LEU:HD13 | 2:X3:95:GLY:HA3 | 1.97 | 0.46 |
| 1:X8:49:VAL:HG11 | 1:X8:241:ARG:HG2 | 1.95 | 0.46 |
| 2:Y1:116:ASP:N | 2:Y1:116:ASP:OD1 | 2.48 | 0.46 |
| 1:Y2:177:ASP:OD2 | 39:Y2:501:GDP:H3' | 2.14 | 0.46 |
| 1:Y8:117:LEU:HD13 | 1:Y8:121:ARG:HH22 | 1.81 | 0.46 |
| 1:Y8:358:PRO:HG2 | 1:Y8:361:LEU:HB2 | 1.97 | 0.46 |
| 2:Y9:70:LEU:HB2 | 2:Y9:98:ASP:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y9:405:VAL:HG23 | 2:Y9:418:PHE:HE2 | 1.80 | 0.46 |
| 2:Z5:429:GLU:O | 2:Z5:433:GLU:HG2 | 2.15 | 0.46 |
| 1:Z8:51:PHE:HB3 | 1:Z8:59:TYR:HB3 | 1.96 | 0.46 |
| 2:Z9:202:VAL:HG22 | 2:Z9:268:MET:HB2 | 1.96 | 0.46 |
| 2:0B:53:PHE:HA | 2:0B:62:VAL:O | 2.16 | 0.46 |
| 1:0C:314:SER:OG | 1:0C:350:LYS:HB3 | 2.15 | 0.46 |
| 1:0E:21:TRP:CZ3 | 1:0E:61:PRO:HB3 | 2.51 | 0.46 |
| 1:0E:53:GLU:HB2 | 1:0E:59:TYR:CE1 | 2.50 | 0.46 |
| 2:0H:132:LEU:HD12 | 2:0H:132:LEU:H | 1.80 | 0.46 |
| 2:0L:71:GLU:N | 2:0L:71:GLU:OE2 | 2.49 | 0.46 |
| 2:0L:208:ALA:O | 2:0L:212:ILE:HG12 | 2.15 | 0.46 |
| 1:0M:21:TRP:CH2 | 1:0M:61:PRO:HB3 | 2.51 | 0.46 |
| 2:0N:288:VAL:HG13 | 2:0N:319:TYR:HE2 | 1.80 | 0.46 |
| 2:0N:298:PRO:HA | 2:0N:301:MET:HG2 | 1.97 | 0.46 |
| 2:0N:311:LYS:HD2 | 2:0N:436:GLY:HA2 | 1.98 | 0.46 |
| 2:0R:60:LYS:NZ | 2:0R:85:GLN:O | 2.46 | 0.46 |
| 2:0V:175:PRO:HB3 | 2:0V:390:ARG:HE | 1.80 | 0.46 |
| 2:0X:202:VAL:HG22 | 2:0X:268:MET:HB2 | 1.98 | 0.46 |
| 2:0X:298:PRO:HA | 2:0X:301:MET:HG3 | 1.96 | 0.46 |
| 2:0Z:3:GLU:HB2 | 2:0Z:129:CYS:SG | 2.56 | 0.46 |
| 2:0Z:286:LEU:O | 2:0Z:373:ARG:NH1 | 2.48 | 0.46 |
| 2:1B:65:CYS:SG | 2:1B:66:ILE:N | 2.88 | 0.46 |
| 2:1D:65:CYS:SG | 2:1D:66:ILE:N | 2.88 | 0.46 |
| 2:1D:90:GLU:HB3 | 2:1D:121:ARG:CZ | 2.46 | 0.46 |
| 2:1D:260:VAL:O | 2:1D:260:VAL:HG23 | 2.15 | 0.46 |
| 1:1G:180:VAL:O | 1:1G:180:VAL:HG12 | 2.15 | 0.46 |
| 1:1K:154:LYS:O | 1:1K:158:GLU:HG3 | 2.16 | 0.46 |
| 1:1K:209:ASP:N | 1:1K:209:ASP:OD1 | 2.48 | 0.46 |
| 1:1O:387:ALA:HA | 1:1O:390:ARG:HH21 | 1.78 | 0.46 |
| 2:1P:74:VAL:O | 2:1P:78:VAL:HG23 | 2.15 | 0.46 |
| 2:1P:266:HIS:ND1 | 2:1P:266:HIS:O | 2.48 | 0.46 |
| 1:1W:301:CYS:SG | 1:1W:302:ALA:N | 2.89 | 0.46 |
| 1:2E:284:LEU:HA | 1:2E:284:LEU:HD23 | 1.74 | 0.46 |
| 1:2E:418:LEU:O | 1:2E:422:TYR:HD2 | 1.98 | 0.46 |
| 2:2F:71:GLU:HB3 | 2:2F:98:ASP:HB2 | 1.97 | 0.46 |
| 2:2J:147:SER:OG | 2:2J:190:SER:HB3 | 2.15 | 0.46 |
| 1:2K:1:MET:O | 1:2K:129:CYS:HB3 | 2.15 | 0.46 |
| 1:2K:52:ASN:OD1 | 1:2K:62:ARG:NH2 | 2.48 | 0.46 |
| 2:2N:73:THR:O | 2:2N:77:GLU:HG3 | 2.15 | 0.46 |
| 1:2S:105:HIS:CD2 | 1:2S:150:LEU:HB2 | 2.50 | 0.46 |
| 1:2U:306:ARG:NE | 38:8B:97:PHE:HD2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2X:62:VAL:HG22 | 2:2X:88:HIS:CD2 | 2.50 | 0.46 |
| 2:2Z:223:THR:HG23 | 2:2Z:225:THR:H | 1.80 | 0.46 |
| 1:3C:332:ASN:OD1 | 38:8C:1:MET:HA | 2.15 | 0.46 |
| 2:3D:120:ASP:HA | 2:3D:123:ARG:HB3 | 1.97 | 0.46 |
| 2:3D:214:ARG:HD2 | 2:3D:220:GLU:OE2 | 2.15 | 0.46 |
| 1:3G:271:THR:HG21 | 1:3G:293:MET:HG3 | 1.96 | 0.46 |
| 2:3J:8:HIS:CD2 | 2:3J:138:PHE:HD2 | 2.34 | 0.46 |
| 1:3K:90:PHE:HB2 | 3:4B:19:LEU:HD13 | 1.97 | 0.46 |
| 1:3O:72:THR:O | 1:3O:76:VAL:HG23 | 2.14 | 0.46 |
| 2:3R:174:SER:OG | 2:3R:175:PRO:HD2 | 2.15 | 0.46 |
| 1:3S:158:GLU:HG2 | 1:3S:159:TYR:CE1 | 2.50 | 0.46 |
| 3:3X:270:LEU:H | 3:3X:270:LEU:HD23 | 1.78 | 0.46 |
| 4:3Y:54:VAL:HG11 | 4:3Y:86:TYR:HB2 | 1.97 | 0.46 |
| 3:3Z:28:ASN:ND2 | 3:3Z:115:ASN:H | 2.13 | 0.46 |
| 3:3Z:270:LEU:H | 3:3Z:270:LEU:HD23 | 1.78 | 0.46 |
| 4:4C:54:VAL:HG11 | 4:4C:86:TYR:HB2 | 1.97 | 0.46 |
| 3:4D:28:ASN:ND2 | 3:4D:115:ASN:H | 2.13 | 0.46 |
| 3:4D:270:LEU:H | 3:4D:270:LEU:HD23 | 1.78 | 0.46 |
| 3:4F:28:ASN:ND2 | 3:4F:115:ASN:H | 2.13 | 0.46 |
| 3:4H:270:LEU:HD23 | 3:4H:270:LEU:H | 1.78 | 0.46 |
| 4:4I:54:VAL:HG11 | 4:4I:86:TYR:HB2 | 1.97 | 0.46 |
| 5:4M:17:GLU:O | 5:4M:20:GLU:HG3 | 2.15 | 0.46 |
| 5:4M:66:GLU:OE2 | 5:4M:70:ASN:ND2 | 2.48 | 0.46 |
| 6:4O:328:GLU:O | 6:4O:332:ASN:ND2 | 2.48 | 0.46 |
| 7:4R:112:MET:CG | 7:4R:113:PRO:HD2 | 2.29 | 0.46 |
| 10:5C:260:LYS:HE3 | 10:5C:261:LYS:HZ1 | 1.80 | 0.46 |
| 12:5F:280:PHE:CD1 | 12:5F:290:PHE:HB2 | 2.51 | 0.46 |
| 13:5H:22:TRP:CE3 | 13:5H:22:TRP:HA | 2.51 | 0.46 |
| 13:5J:22:TRP:CE3 | 13:5J:22:TRP:HA | 2.51 | 0.46 |
| 13:5K:22:TRP:CE3 | 13:5K:22:TRP:HA | 2.51 | 0.46 |
| 14:5L:147:THR:O | 38:8B:227:LYS:HD2 | 2.16 | 0.46 |
| 14:5L:219:LEU:HD23 | 14:5L:231:THR:HA | 1.97 | 0.46 |
| 14:5L:315:MET:HG3 | 14:5L:315:MET:O | 2.14 | 0.46 |
| 14:5M:238:VAL:HG23 | 14:5M:240:MET:O | 2.15 | 0.46 |
| 14:5N:315:MET:O | 14:5N:315:MET:HG3 | 2.14 | 0.46 |
| 14:5N:556:VAL:HG13 | 14:5N:571:GLY:O | 2.15 | 0.46 |
| 18:5Y:5:VAL:HG11 | 18:5Y:62:GLU:HG2 | 1.97 | 0.46 |
| 19:6E:92:ARG:NE | 19:6E:92:ARG:HA | 2.30 | 0.46 |
| 22:6M:59:PRO:CB | 22:6M:108:ARG:NH2 | 2.74 | 0.46 |
| 22:6M:201:ARG:HB3 | 22:6M:237:TYR:HB3 | 1.98 | 0.46 |
| 22:6P:171:GLU:HA | 22:6P:174:GLU:OE1 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:14:TYR:CD2 | 24:6U:14:TYR:N | 2.82 | 0.46 |
| 24:6X:502:LYS:HB3 | 24:6X:511:ILE:HD12 | 1.96 | 0.46 |
| 24:6Z:570:GLU:OE2 | 24:6Z:570:GLU:N | 2.46 | 0.46 |
| 24:6Z:574:ARG:O | 24:6Z:578:ILE:HG12 | 2.15 | 0.46 |
| 26:7F:138:THR:HG23 | 26:7F:139:PRO:CD | 2.44 | 0.46 |
| 26:7F:146:ASN:ND2 | 26:7F:146:ASN:N | 2.61 | 0.46 |
| 27:7G:48:THR:O | 27:7G:52:VAL:HG22 | 2.15 | 0.46 |
| 37:7Y:139:ARG:HG2 | 37:7Y:139:ARG:HH11 | 1.80 | 0.46 |
| 38:8B:213:GLU:HG3 | 38:8B:214:HIS:N | 2.30 | 0.46 |
| 38:8C:112:ILE:O | 38:8C:116:GLN:HG3 | 2.15 | 0.46 |
| 2:B2:226:ASN:ND2 | 18:5Z:51:MET:SD | 2.88 | 0.46 |
| 2:D5:285:GLN:NE2 | 24:6Y:253:PRO:HG2 | 2.28 | 0.46 |
| 1:E2:77:ARG:HH12 | 24:6U:426:LEU:N | 2.12 | 0.46 |
| 2:F7:322:ASP:OD2 | 24:6T:433:ARG:NH2 | 2.47 | 0.46 |
| 1:G4:125:GLU:OE2 | 1:I0:336:LYS:NZ | 2.37 | 0.46 |
| 1:G6:272:PRO:HD3 | 1:G6:364:SER:HA | 1.97 | 0.46 |
| 1:G8:186:THR:HG22 | 1:G8:411:ALA:HB1 | 1.96 | 0.46 |
| 2:G9:101:ASN:N | 41:G9:501:GTP:O3G | 2.47 | 0.46 |
| 2:H7:317:LEU:HB3 | 2:H7:319:TYR:CE1 | 2.43 | 0.46 |
| 1:H8:257:LEU:HD21 | 1:H8:314:SER:HB2 | 1.97 | 0.46 |
| 1:H8:391:ARG:NH2 | 2:H9:435:VAL:HA | 2.31 | 0.46 |
| 2:I3:9:ILE:HG22 | 2:I3:146:GLY:HA2 | 1.97 | 0.46 |
| 1:J0:114:ASP:OD2 | 1:J0:115:SER:N | 2.49 | 0.46 |
| 1:J0:178:THR:HA | 2:J1:352:LYS:HD2 | 1.97 | 0.46 |
| 1:J0:317:PHE:HB3 | 1:J0:321:MET:SD | 2.56 | 0.46 |
| 1:J2:364:SER:OG | 1:J2:365:ALA:N | 2.48 | 0.46 |
| 2:J3:66:ILE:HG22 | 2:J3:91:GLN:HB3 | 1.98 | 0.46 |
| 2:J3:123:ARG:HH22 | 35:7T:118:ILE:HD13 | 1.79 | 0.46 |
| 2:J3:312:TYR:HB2 | 2:J3:343:PHE:CD1 | 2.50 | 0.46 |
| 1:J6:268:VAL:HG23 | 1:J6:300:MET:HB2 | 1.97 | 0.46 |
| 2:J7:65:CYS:SG | 2:J7:66:ILE:N | 2.88 | 0.46 |
| 1:J8:204:ASN:OD1 | 39:J8:502:GDP:O2' | 2.34 | 0.46 |
| 2:J9:334:THR:HA | 2:J9:337:THR:HG22 | 1.97 | 0.46 |
| 2:K1:223:THR:HG22 | 2:K1:224:TYR:N | 2.29 | 0.46 |
| 2:K1:431:ASP:O | 2:K1:435:VAL:HG22 | 2.15 | 0.46 |
| 2:K3:312:TYR:HD1 | 2:K3:381:SER:HB2 | 1.81 | 0.46 |
| 2:K5:414:GLU:N | 2:K5:414:GLU:OE1 | 2.49 | 0.46 |
| 1:K6:396:HIS:HE1 | 1:K6:397:TRP:CZ2 | 2.34 | 0.46 |
| 2:K7:309:HIS:CG | 35:7T:165:ARG:HE | 2.33 | 0.46 |
| 1:K8:324:LYS:HD3 | 1:K8:328:GLU:OE1 | 2.16 | 0.46 |
| 2:L1:145:THR:OG1 | 41:L2:501:GTP:O1B | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L6:391:ARG:HG3 | 2:L7:262:TYR:OH | 2.15 | 0.46 |
| 2:L9:17:GLY:HA2 | 2:L9:20:CYS:HB3 | 1.97 | 0.46 |
| 2:L9:286:LEU:HD12 | 2:L9:286:LEU:HA | 1.81 | 0.46 |
| 1:M0:67:ASP:OD2 | 1:M0:72:THR:OG1 | 2.34 | 0.46 |
| 1:M0:173:PRO:HD2 | 1:M0:380:ARG:CZ | 2.45 | 0.46 |
| 2:M1:255:PHE:HA | 2:M1:259:LEU:HD13 | 1.96 | 0.46 |
| 2:M5:96:LYS:HZ1 | 37:7Y:98:PHE:HA | 1.80 | 0.46 |
| 2:N3:114:ILE:HB | 2:N3:149:LEU:HD21 | 1.97 | 0.46 |
| 2:N5:124:LYS:HA | 2:N5:127:ASP:OD1 | 2.16 | 0.46 |
| 2:N5:330:ALA:O | 2:N5:334:THR:HG23 | 2.14 | 0.46 |
| 2:O5:121:ARG:HD2 | 2:O5:121:ARG:O | 2.14 | 0.46 |
| 2:O5:280:LYS:HA | 2:O5:283:HIS:HB3 | 1.98 | 0.46 |
| 2:O7:172:TYR:CE2 | 2:O7:203:MET:HG2 | 2.51 | 0.46 |
| 2:Q3:62:VAL:CG2 | 2:Q3:88:HIS:HB2 | 2.45 | 0.46 |
| 2:Q3:367:ASP:OD1 | 2:Q3:368:LEU:HD12 | 2.16 | 0.46 |
| 1:Q6:237:THR:HG23 | 1:Q6:240:LEU:HD12 | 1.96 | 0.46 |
| 1:Q8:159:TYR:HB3 | 1:Q8:162:ARG:HD2 | 1.96 | 0.46 |
| 2:Q9:175:PRO:HG2 | 2:Q9:176:GLN:OE1 | 2.15 | 0.46 |
| 1:R0:60:VAL:HG23 | 1:R0:84:ILE:O | 2.15 | 0.46 |
| 1:R2:189:VAL:O | 1:R2:193:VAL:HG13 | 2.14 | 0.46 |
| 2:R3:153:LEU:O | 2:R3:157:LEU:HB2 | 2.16 | 0.46 |
| 1:R4:70:PRO:CA | 1:R4:92:PHE:HZ | 2.28 | 0.46 |
| 2:R7:242:LEU:HD11 | 2:R7:252:ILE:HG12 | 1.96 | 0.46 |
| 2:R9:176:GLN:HG2 | 2:R9:177:VAL:N | 2.29 | 0.46 |
| 1:S0:186:THR:HG22 | 1:S0:411:ALA:HB1 | 1.97 | 0.46 |
| 2:S1:266:HIS:O | 2:S1:266:HIS:ND1 | 2.47 | 0.46 |
| 1:S2:54:ALA:HB3 | 1:S2:58:ARG:HB3 | 1.97 | 0.46 |
| 1:S6:292:GLN:HG2 | 1:S6:298:ASN:ND2 | 2.29 | 0.46 |
| 1:S6:325:GLU:O | 1:S6:329:GLN:HG2 | 2.15 | 0.46 |
| 2:S7:45:GLY:HA2 | 7:4T:257:ARG:NE | 2.30 | 0.46 |
| 1:S8:6:HIS:HD2 | 1:S8:134:GLN:OE1 | 1.99 | 0.46 |
| 2:S9:70:LEU:HG | 2:S9:145:THR:HG23 | 1.96 | 0.46 |
| 2:T3:384:ILE:HA | 2:T3:387:ILE:HD12 | 1.97 | 0.46 |
| 1:T4:279:GLN:HE22 | 7:4U:129:GLN:HB3 | 1.81 | 0.46 |
| 1:T6:2:ARG:HB3 | 1:T6:131:GLN:HB2 | 1.97 | 0.46 |
| 2:U1:66:ILE:O | 2:U1:66:ILE:HG13 | 2.15 | 0.46 |
| 1:U2:218:THR:O | 2:U3:326:LYS:HE2 | 2.15 | 0.46 |
| 1:U2:412:GLU:OE1 | 1:U2:416:ASN:ND2 | 2.48 | 0.46 |
| 2:U3:72:PRO:HD2 | 1:U4:2:ARG:NH1 | 2.30 | 0.46 |
| 2:U3:116:ASP:OD2 | 2:U3:117:LEU:N | 2.48 | 0.46 |
| 2:U7:32:PRO:HB3 | 2:U7:83:TYR:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U8:350:LYS:NZ | 1:U8:352:SER:OG | 2.48 | 0.46 |
| 2:U9:428:LEU:HG | 2:U9:432:PHE:CE2 | 2.50 | 0.46 |
| 1:V2:53:GLU:OE2 | 1:V2:58:ARG:N | 2.45 | 0.46 |
| 1:V4:173:PRO:HD2 | 1:V4:380:ARG:NH1 | 2.31 | 0.46 |
| 1:W0:335:ASN:O | 1:W0:338:SER:OG | 2.32 | 0.46 |
| 1:W4:167:PHE:CZ | 1:W4:233:MET:HG2 | 2.51 | 0.46 |
| 1:W4:249:ASP:OD1 | 1:W4:250:LEU:N | 2.47 | 0.46 |
| 2:W7:50:ASN:O | 2:W7:64:ARG:NH2 | 2.48 | 0.46 |
| 1:W8:145:SER:OG | 1:W8:188:SER:OG | 2.24 | 0.46 |
| 1:X2:6:HIS:CD2 | 1:X2:134:GLN:HG3 | 2.50 | 0.46 |
| 2:X9:180:ALA:HB1 | 1:Y0:256:ASN:HD21 | 1.79 | 0.46 |
| 1:Y2:2:ARG:HH21 | 1:Y2:240:LEU:HA | 1.81 | 0.46 |
| 2:Y3:52:PHE:CE2 | 2:Y3:243:ARG:HD3 | 2.50 | 0.46 |
| 1:Y8:103:LYS:NZ | 1:Y8:108:GLU:OE2 | 2.46 | 0.46 |
| 1:Z0:181:GLU:HG3 | 1:Z0:182:PRO:CD | 2.45 | 0.46 |
| 1:Z2:117:LEU:HD11 | 1:Z2:154:LYS:HE3 | 1.97 | 0.46 |
| 1:Z2:186:THR:OG1 | 1:Z2:187:LEU:HD12 | 2.15 | 0.46 |
| 1:Z4:189:VAL:HA | 1:Z4:192:LEU:HB3 | 1.98 | 0.46 |
| 1:Z4:404:ASP:HB2 | 1:Z4:406:MET:SD | 2.55 | 0.46 |
| 2:Z7:407:TRP:NE1 | 1:Z8:258:ILE:O | 2.38 | 0.46 |
| 1:Z8:325:GLU:HA | 1:Z8:328:GLU:HG3 | 1.96 | 0.46 |
| 1:Z8:391:ARG:NH2 | 2:Z9:434:GLU:O | 2.43 | 0.46 |
| 2:Z9:12:ALA:O | 2:Z9:16:VAL:HG23 | 2.15 | 0.46 |
| 2:0F:298:PRO:HA | 2:0F:301:MET:HG2 | 1.98 | 0.46 |
| 2:0L:174:SER:HB3 | 2:0L:177:VAL:O | 2.15 | 0.46 |
| 2:0L:178:SER:OG | 2:0L:183:GLU:OE2 | 2.29 | 0.46 |
| 1:0Q:153:SER:O | 1:0Q:157:GLU:HG2 | 2.14 | 0.46 |
| 2:0R:55:GLU:O | 2:1H:285:GLN:NE2 | 2.48 | 0.46 |
| 1:0S:152:ILE:HG22 | 1:0S:195:ASN:OD1 | 2.15 | 0.46 |
| 1:0U:233:MET:O | 1:0U:237:THR:HG22 | 2.16 | 0.46 |
| 1:0U:393:ALA:HB2 | 2:0V:262:TYR:OH | 2.16 | 0.46 |
| 2:0V:431:ASP:O | 2:0V:434:GLU:HG3 | 2.15 | 0.46 |
| 1:1A:404:ASP:HB3 | 1:1A:406:MET:SD | 2.55 | 0.46 |
| 1:1K:389:PHE:O | 1:1K:392:LYS:NZ | 2.36 | 0.46 |
| 2:1L:3:GLU:HB2 | 2:1L:129:CYS:SG | 2.55 | 0.46 |
| 2:1N:55:GLU:O | 2:1N:55:GLU:CG | 2.63 | 0.46 |
| 1:1O:68:LEU:HB3 | 1:1O:96:GLY:HA2 | 1.97 | 0.46 |
| 2:1P:177:VAL:HG13 | 1:1Q:327:ASP:HB3 | 1.96 | 0.46 |
| 1:1Q:114:ASP:N | 1:1Q:114:ASP:OD1 | 2.47 | 0.46 |
| 1:1Q:135:VAL:HG21 | 1:1Q:152:ILE:HD11 | 1.98 | 0.46 |
| 1:1W:396:HIS:CE1 | 1:1W:397:TRP:CE2 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1X:155:GLU:HG2 | 2:1X:197:HIS:NE2 | 2.31 | 0.46 |
| 1:2A:31:ASP:OD2 | 1:2A:33:THR:OG1 | 2.21 | 0.46 |
| 2:2H:271:SER:OG | 2:2H:300:SER:O | 2.33 | 0.46 |
| 1:2K:345:ILE:O | 1:2K:348:ASN:ND2 | 2.47 | 0.46 |
| 2:2N:111:GLY:HA2 | 2:2N:114:ILE:HG22 | 1.96 | 0.46 |
| 2:2P:214:ARG:HH22 | 38:7Z:19:PHE:H | 1.63 | 0.46 |
| 1:2Q:306:ARG:NH1 | 38:8A:99:THR:O | 2.47 | 0.46 |
| 1:3A:114:ASP:OD1 | 1:3A:115:SER:N | 2.49 | 0.46 |
| 2:3D:109:THR:O | 2:3D:112:LYS:HE2 | 2.16 | 0.46 |
| 2:3F:132:LEU:HD22 | 2:3F:164:LYS:HD3 | 1.97 | 0.46 |
| 2:3H:84:ARG:HE | 23:6Q:15:ARG:HH22 | 1.62 | 0.46 |
| 1:3I:293:MET:HE1 | 1:3I:317:PHE:HE1 | 1.79 | 0.46 |
| 1:3I:395:LEU:O | 1:3I:399:THR:HG23 | 2.16 | 0.46 |
| 1:3K:91:VAL:HG11 | 1:3K:116:VAL:HG23 | 1.96 | 0.46 |
| 2:3N:21:TRP:CZ3 | 2:3N:63:PRO:HB3 | 2.50 | 0.46 |
| 2:3N:244:PHE:HB2 | 2:3N:356:ASN:HD21 | 1.79 | 0.46 |
| 1:3O:389:PHE:O | 1:3O:392:LYS:NZ | 2.37 | 0.46 |
| 1:3Q:217:LEU:HA | 38:8D:226:ARG:O | 2.15 | 0.46 |
| 1:3S:266:PHE:CD1 | 1:3S:370:ASN:HB2 | 2.50 | 0.46 |
| 3:3V:270:LEU:H | 3:3V:270:LEU:HD23 | 1.78 | 0.46 |
| 4:3W:126:ASP:OD1 | 4:3W:126:ASP:N | 2.46 | 0.46 |
| 4:4E:54:VAL:HG11 | 4:4E:86:TYR:HB2 | 1.97 | 0.46 |
| 5:4M:293:LEU:HA | 5:4M:296:GLU:OE2 | 2.15 | 0.46 |
| 10:5C:190:ILE:HA | 10:5C:193:VAL:HG22 | 1.97 | 0.46 |
| 10:5C:285:MET:HE1 | 38:8B:201:LEU:HD21 | 1.96 | 0.46 |
| 13:5I:22:TRP:CE3 | 13:5I:22:TRP:HA | 2.51 | 0.46 |
| 14:5L:244:ALA:HB1 | 14:5L:297:ILE:HG13 | 1.96 | 0.46 |
| 14:5L:578:LYS:HA | 14:5L:589:PHE:CB | 2.45 | 0.46 |
| 14:5L:579:LEU:HD23 | 14:5L:588:TYR:HD2 | 1.79 | 0.46 |
| 14:5M:399:SER:OG | 14:5M:401:TRP:NE1 | 2.48 | 0.46 |
| 14:5M:578:LYS:HA | 14:5M:589:PHE:CB | 2.45 | 0.46 |
| 14:5M:579:LEU:HD23 | 14:5M:588:TYR:HD2 | 1.79 | 0.46 |
| 14:5N:578:LYS:HA | 14:5N:589:PHE:CB | 2.45 | 0.46 |
| 14:5N:579:LEU:HD23 | 14:5N:588:TYR:HD2 | 1.79 | 0.46 |
| 15:5O:210:ALA:HB3 | 15:5O:213:THR:CG2 | 2.45 | 0.46 |
| 15:5P:330:LEU:HD23 | 15:5P:330:LEU:O | 2.15 | 0.46 |
| 17:5U:30:LYS:H | 17:5U:30:LYS:HG3 | 1.44 | 0.46 |
| 21:6H:109:THR:CA | 24:6X:82:ALA:HB3 | 2.44 | 0.46 |
| 22:6J:172:ARG:NH1 | 22:6J:215:GLY:HA3 | 2.30 | 0.46 |
| 22:6N:201:ARG:HB3 | 22:6N:237:TYR:HB3 | 1.98 | 0.46 |
| 22:6O:271:ARG:HH12 | 22:6O:275:LEU:CG | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6V:142:ILE:HD12 | 24:6V:142:ILE:H | 1.80 | 0.46 |
| 24:6V:482:ILE:HB | 24:6V:498:LEU:HB3 | 1.96 | 0.46 |
| 24:6W:18:LEU:HD12 | 24:6W:18:LEU:N | 2.31 | 0.46 |
| 24:6Y:183:ASP:OD1 | 24:6Y:184:ALA:N | 2.48 | 0.46 |
| 24:6Y:290:ARG:HG3 | 24:6Y:291:PRO:HD2 | 1.96 | 0.46 |
| 24:6Y:482:ILE:HG22 | 24:6Y:497:PHE:HB3 | 1.97 | 0.46 |
| 29:7I:41:LYS:HA | 29:7I:41:LYS:HD3 | 1.82 | 0.46 |
| 37:7Y:225:TRP:CD1 | 37:7Y:226:VAL:HG13 | 2.51 | 0.46 |
| 1:7:281:TYR:OH | 1:T0:83:GLN:O | 2.24 | 0.46 |
| 2:D3:12:ALA:HB2 | 41:D3:501:GTP:C8 | 2.50 | 0.46 |
| 2:E9:81:GLY:HA3 | 22:6N:116:TYR:CE2 | 2.47 | 0.46 |
| 1:G2:174:LYS:HB3 | 1:G2:174:LYS:HE2 | 1.76 | 0.46 |
| 1:G2:178:THR:OG1 | 2:G3:258:ASN:ND2 | 2.48 | 0.46 |
| 1:G2:190:HIS:HD2 | 1:G2:414:ASN:HB2 | 1.78 | 0.46 |
| 2:G3:379:SER:OG | 2:G3:380:ASN:N | 2.48 | 0.46 |
| 2:H5:51:THR:HG23 | 2:H5:52:PHE:CD2 | 2.50 | 0.46 |
| 2:H5:182:VAL:HG23 | 2:H5:186:ASN:HD21 | 1.80 | 0.46 |
| 2:H9:3:GLU:HB2 | 2:H9:129:CYS:SG | 2.55 | 0.46 |
| 1:I0:176:SER:HB3 | 2:I1:349:THR:OG1 | 2.16 | 0.46 |
| 2:I3:83:TYR:HB3 | 2:I3:86:LEU:HB3 | 1.96 | 0.46 |
| 1:I4:276:ARG:HH11 | 24:6Z:491:GLY:HA3 | 1.81 | 0.46 |
| 2:I5:105:ARG:O | 2:I5:109:THR:OG1 | 2.27 | 0.46 |
| 2:I9:21:TRP:CZ3 | 2:I9:63:PRO:HB3 | 2.50 | 0.46 |
| 1:J0:135:VAL:HG12 | 1:J0:137:HIS:HD2 | 1.79 | 0.46 |
| 1:J2:10:GLY:HA2 | 1:J2:67:ASP:OD2 | 2.15 | 0.46 |
| 1:J2:49:VAL:HG11 | 1:J2:241:ARG:HG2 | 1.98 | 0.46 |
| 1:J2:121:ARG:NH2 | 1:J2:158:GLU:OE2 | 2.39 | 0.46 |
| 2:J7:121:ARG:C | 2:J7:121:ARG:HD2 | 2.36 | 0.46 |
| 2:J7:362:VAL:HG11 | 5:4M:212:GLN:NE2 | 2.30 | 0.46 |
| 2:K1:269:LEU:N | 2:K1:379:SER:O | 2.36 | 0.46 |
| 1:K4:284:LEU:HD22 | 1:K4:362:LYS:HB3 | 1.96 | 0.46 |
| 2:K5:387:ILE:HG12 | 2:K5:390:ARG:HH22 | 1.79 | 0.46 |
| 2:L7:33:ASP:O | 2:L7:60:LYS:NZ | 2.47 | 0.46 |
| 2:M1:384:ILE:HA | 2:M1:387:ILE:HD12 | 1.97 | 0.46 |
| 1:M6:178:THR:CG2 | 1:M6:181:GLU:HG3 | 2.45 | 0.46 |
| 1:M6:324:LYS:O | 1:M6:328:GLU:HG3 | 2.15 | 0.46 |
| 2:M7:326:LYS:HG3 | 2:M7:327:ASP:N | 2.31 | 0.46 |
| 2:M7:328:VAL:O | 2:M7:332:VAL:HG22 | 2.16 | 0.46 |
| 2:N1:22:GLU:O | 2:N1:26:LEU:HD23 | 2.16 | 0.46 |
| 2:N1:301:MET:HE1 | 2:N1:307:PRO:HD3 | 1.97 | 0.46 |
| 2:N5:306:ASP:HB3 | 2:N5:309:HIS:CD2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O0:274:THR:HG21 | 1:O0:282:ARG:HD3 | 1.98 | 0.46 |
| 1:O2:337:ASN:HB2 | 1:O2:340:TYR:HD2 | 1.80 | 0.46 |
| 2:O5:265:ILE:HD11 | 2:O5:435:VAL:HG21 | 1.97 | 0.46 |
| 2:O7:88:HIS:HD2 | 2:O7:90:GLU:HB3 | 1.79 | 0.46 |
| 1:P4:135:VAL:HG21 | 1:P4:152:ILE:HD11 | 1.97 | 0.46 |
| 2:P7:145:THR:OG1 | 41:P8:501:GTP:O1B | 2.33 | 0.46 |
| 1:Q0:245:GLN:HG2 | 19:6E:148:THR:HG21 | 1.98 | 0.46 |
| 1:Q2:174:LYS:HE2 | 1:Q2:174:LYS:HB3 | 1.78 | 0.46 |
| 1:Q4:287:PRO:HG3 | 1:Q4:329:GLN:OE1 | 2.15 | 0.46 |
| 1:Q6:8:GLN:CD | 1:Q6:17:GLY:HA3 | 2.36 | 0.46 |
| 2:R1:178:SER:HB3 | 2:R1:183:GLU:OE2 | 2.15 | 0.46 |
| 2:R3:370:LYS:HD2 | 7:4R:87:PHE:CD2 | 2.50 | 0.46 |
| 1:R8:24:VAL:HG11 | 1:R8:50:TYR:CD2 | 2.50 | 0.46 |
| 2:S1:417:GLU:HA | 2:S1:420:GLU:HG2 | 1.97 | 0.46 |
| 2:S9:183:GLU:CD | 2:S9:184:PRO:HD3 | 2.36 | 0.46 |
| 2:S9:407:TRP:CE2 | 1:T0:255:VAL:HA | 2.50 | 0.46 |
| 1:T2:77:ARG:NH1 | 24:6Y:47:GLN:O | 2.48 | 0.46 |
| 1:T2:328:GLU:HB3 | 17:5T:38:PHE:CZ | 2.50 | 0.46 |
| 1:T4:320:ARG:NE | 7:4U:101:ASP:OD2 | 2.46 | 0.46 |
| 1:T6:50:TYR:O | 1:T6:61:PRO:HA | 2.15 | 0.46 |
| 2:T7:90:GLU:CD | 2:T7:121:ARG:HD3 | 2.35 | 0.46 |
| 1:T8:3:GLU:O | 1:T8:131:GLN:HB3 | 2.15 | 0.46 |
| 1:U4:263:LEU:HD22 | 1:U4:422:TYR:CE1 | 2.50 | 0.46 |
| 2:U5:251:ASP:OD2 | 2:U5:253:THR:N | 2.49 | 0.46 |
| 1:U6:20:PHE:CD1 | 1:U6:233:MET:HE2 | 2.51 | 0.46 |
| 1:U8:7:ILE:HB | 1:U8:135:VAL:HG22 | 1.96 | 0.46 |
| 2:U9:76:ASP:OD2 | 1:V0:46:ARG:NH2 | 2.48 | 0.46 |
| 2:U9:422:ARG:NH1 | 2:U9:426:ALA:HB2 | 2.29 | 0.46 |
| 1:V0:282:ARG:HG2 | 1:V0:283:ALA:O | 2.14 | 0.46 |
| 1:V2:317:PHE:HE2 | 1:V2:326:VAL:HG13 | 1.79 | 0.46 |
| 2:V3:72:PRO:HG3 | 1:V4:1:MET:HG3 | 1.97 | 0.46 |
| 2:W1:76:ASP:O | 2:W1:80:THR:HG22 | 2.16 | 0.46 |
| 2:W3:27:GLU:HG2 | 2:W3:361:THR:HG21 | 1.98 | 0.46 |
| 2:W7:22:GLU:O | 2:W7:26:LEU:HD23 | 2.16 | 0.46 |
| 2:W7:414:GLU:HG2 | 2:W7:417:GLU:OE1 | 2.15 | 0.46 |
| 1:X0:58:ARG:HB2 | 8:4W:469:GLN:HE22 | 1.80 | 0.46 |
| 1:X4:354:CYS:SG | 1:X4:355:ASP:N | 2.89 | 0.46 |
| 1:X6:22:GLU:HG3 | 1:X6:81:TYR:CD1 | 2.50 | 0.46 |
| 1:Y0:19:LYS:HB3 | 1:Y0:19:LYS:HE3 | 1.74 | 0.46 |
| 2:Y1:51:THR:HG21 | 2:Y1:243:ARG:HG2 | 1.97 | 0.46 |
| 2:Y5:116:ASP:N | 2:Y5:116:ASP:OD1 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y8:322:SER:O | 1:Y8:326:VAL:HG23 | 2.15 | 0.46 |
| 2:Z1:157:LEU:HD22 | 2:Z1:166:LYS:HD3 | 1.97 | 0.46 |
| 2:Z3:286:LEU:HG | 2:Z3:373:ARG:NH1 | 2.31 | 0.46 |
| 2:Z5:90:GLU:CD | 2:Z5:124:LYS:HZ1 | 2.18 | 0.46 |
| 2:Z5:345:ASP:N | 2:Z5:345:ASP:OD1 | 2.49 | 0.46 |
| 1:Z6:212:PHE:HE1 | 1:Z6:220:PRO:HG3 | 1.81 | 0.46 |
| 1:Z8:257:LEU:HD11 | 1:Z8:314:SER:HB3 | 1.98 | 0.46 |
| 1:Z8:297:LYS:HD3 | 1:Z8:297:LYS:HA | 1.62 | 0.46 |
| 2:Z9:65:CYS:SG | 2:Z9:66:ILE:N | 2.89 | 0.46 |
| 1:0E:379:LYS:HA | 1:0E:382:SER:OG | 2.16 | 0.46 |
| 2:0H:398:MET:SD | 1:0I:345:ILE:HG23 | 2.56 | 0.46 |
| 1:0K:314:SER:HA | 1:0K:350:LYS:O | 2.15 | 0.46 |
| 2:0L:9:ILE:HB | 2:0L:139:ASN:HB3 | 1.96 | 0.46 |
| 2:0L:176:GLN:HG2 | 2:0L:177:VAL:N | 2.31 | 0.46 |
| 2:0L:417:GLU:HA | 2:0L:420:GLU:HG2 | 1.97 | 0.46 |
| 2:0N:195:LEU:CD2 | 2:0N:196:GLU:HG2 | 2.45 | 0.46 |
| 1:0Q:207:LEU:HB3 | 1:0Q:225:LEU:HD22 | 1.98 | 0.46 |
| 1:0Q:335:ASN:O | 1:0Q:338:SER:OG | 2.32 | 0.46 |
| 1:0Y:161:ASP:OD2 | 1:0Y:161:ASP:N | 2.42 | 0.46 |
| 2:1B:367:ASP:OD2 | 2:1B:367:ASP:N | 2.48 | 0.46 |
| 1:1C:6:HIS:CE1 | 1:1C:8:GLN:HG2 | 2.50 | 0.46 |
| 1:1E:114:ASP:N | 1:1E:114:ASP:OD1 | 2.47 | 0.46 |
| 2:1P:405:VAL:HG23 | 2:1P:418:PHE:HE2 | 1.81 | 0.46 |
| 1:1S:8:GLN:CD | 1:1S:17:GLY:HA3 | 2.36 | 0.46 |
| 2:1X:367:ASP:OD1 | 2:1X:367:ASP:N | 2.48 | 0.46 |
| 1:2I:233:MET:O | 1:2I:236:ILE:HG22 | 2.15 | 0.46 |
| 2:2P:119:LEU:HD21 | 2:2P:156:ARG:HB3 | 1.97 | 0.46 |
| 1:2S:345:ILE:HB | 1:2S:348:ASN:HD21 | 1.81 | 0.46 |
| 2:2V:90:GLU:HG3 | 2:2V:121:ARG:CZ | 2.46 | 0.46 |
| 2:2X:358:GLN:HE21 | 38:8C:214:HIS:H | 1.63 | 0.46 |
| 1:2Y:178:THR:HA | 2:2Z:352:LYS:HD3 | 1.97 | 0.46 |
| 2:2Z:297:GLU:OE2 | 38:8C:74:ILE:CB | 2.64 | 0.46 |
| 1:3C:320:ARG:HH12 | 38:8D:198:THR:HA | 1.80 | 0.46 |
| 1:3C:406:MET:O | 1:3C:410:GLU:HG2 | 2.16 | 0.46 |
| 2:3D:88:HIS:ND1 | 2:3T:283:HIS:HA | 2.30 | 0.46 |
| 2:3F:102:ASN:HB3 | 2:3F:105:ARG:HB3 | 1.97 | 0.46 |
| 1:3G:391:ARG:HH12 | 2:3H:434:GLU:HG2 | 1.80 | 0.46 |
| 1:3K:178:THR:HG22 | 1:3K:180:VAL:H | 1.80 | 0.46 |
| 1:3K:330:MET:HA | 1:3K:333:VAL:HG12 | 1.97 | 0.46 |
| 2:3N:399:TYR:O | 2:3N:402:ARG:NH1 | 2.48 | 0.46 |
| 1:3O:170:VAL:HG21 | 1:3O:377:MET:SD | 2.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:3Y:2:PHE:HZ | 23:6Q:3:LEU:HD12 | 1.80 | 0.46 |
| 4:3Y:136:LEU:O | 4:3Y:140:THR:OG1 | 2.32 | 0.46 |
| 4:4A:54:VAL:HG11 | 4:4A:86:TYR:HB2 | 1.97 | 0.46 |
| 3:4B:270:LEU:H | 3:4B:270:LEU:HD23 | 1.78 | 0.46 |
| 3:4F:270:LEU:H | 3:4F:270:LEU:HD23 | 1.78 | 0.46 |
| 7:4U:27:ILE:O | 7:4U:27:ILE:HG13 | 2.16 | 0.46 |
| 8:4W:225:SER:HA | 8:4W:228:ARG:HD3 | 1.97 | 0.46 |
| 10:5C:474:LYS:NZ | 10:5C:495:GLU:O | 2.41 | 0.46 |
| 12:5F:138:THR:O | 12:5F:142:THR:HG23 | 2.16 | 0.46 |
| 14:5M:454:ILE:O | 14:5M:456:ARG:NH2 | 2.49 | 0.46 |
| 14:5N:244:ALA:HB1 | 14:5N:297:ILE:HG13 | 1.96 | 0.46 |
| 14:5N:454:ILE:O | 14:5N:456:ARG:NH2 | 2.48 | 0.46 |
| 15:5O:95:LEU:HD11 | 15:5O:221:TRP:CD1 | 2.50 | 0.46 |
| 17:5U:189:TRP:HZ3 | 17:5U:223:GLU:HG3 | 1.79 | 0.46 |
| 21:6H:26:VAL:HG11 | 21:6H:128:ALA:HB1 | 1.96 | 0.46 |
| 22:6J:171:GLU:HA | 22:6J:174:GLU:OE1 | 2.15 | 0.46 |
| 22:6P:186:ARG:O | 22:6P:189:LYS:HB2 | 2.15 | 0.46 |
| 24:6T:456:ASP:N | 24:6T:456:ASP:OD1 | 2.48 | 0.46 |
| 24:6T:627:GLU:O | 24:6T:630:LEU:HG | 2.14 | 0.46 |
| 24:6W:90:GLU:HG2 | 24:6W:91:ASN:ND2 | 2.30 | 0.46 |
| 24:6W:97:ARG:H | 24:6W:188:THR:CG2 | 2.27 | 0.46 |
| 24:6W:156:ASP:OD1 | 24:6W:157:ASP:N | 2.49 | 0.46 |
| 24:6X:107:VAL:HG12 | 24:6X:108:GLU:N | 2.27 | 0.46 |
| 24:6X:416:ILE:HD12 | 24:6X:416:ILE:H | 1.80 | 0.46 |
| 24:6X:445:ILE:HG13 | 24:6X:474:PHE:CE1 | 2.49 | 0.46 |
| 24:6X:489:ASN:ND2 | 24:6X:489:ASN:O | 2.48 | 0.46 |
| 24:6X:519:VAL:CG1 | 24:6X:533:LEU:O | 2.57 | 0.46 |
| 24:6Y:505:LYS:HD2 | 24:6Y:510:GLU:HB3 | 1.96 | 0.46 |
| 24:6Y:536:ASP:HB3 | 24:6Y:539:THR:HG23 | 1.98 | 0.46 |
| 24:6Y:602:LEU:HG | 24:6Y:604:PHE:HD1 | 1.79 | 0.46 |
| 24:6Z:244:ALA:CB | 24:6Z:257:LEU:HD11 | 2.44 | 0.46 |
| 24:6Z:482:ILE:HB | 24:6Z:498:LEU:HB3 | 1.97 | 0.46 |
| 24:7A:97:ARG:H | 24:7A:188:THR:CG2 | 2.26 | 0.46 |
| 29:7J:117:ASN:O | 29:7J:121:ASN:HB2 | 2.15 | 0.46 |
| 35:7U:95:LYS:HA | 35:7U:98:ASP:OD2 | 2.14 | 0.46 |
| 38:8C:83:ARG:N | 38:8C:83:ARG:CD | 2.79 | 0.46 |
| 2:2:33:ASP:HB3 | 18:5X:77:THR:HG21 | 1.97 | 0.46 |
| 1:9:78:SER:HB2 | 24:6X:149:LYS:HG3 | 1.96 | 0.46 |
| 2:A0:282:TYR:HE1 | 24:6X:88:TRP:HH2 | 1.63 | 0.46 |
| 2:E9:18:ASN:HD21 | 22:6N:116:TYR:HE1 | 1.63 | 0.46 |
| 2:G3:279:GLU:HG2 | 2:G3:280:LYS:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G3:286:LEU:O | 2:G3:373:ARG:NH1 | 2.49 | 0.46 |
| 1:G4:286:VAL:O | 1:G4:290:THR:HG23 | 2.15 | 0.46 |
| 1:G6:209:ASP:OD1 | 1:G6:210:ILE:N | 2.48 | 0.46 |
| 2:G7:102:ASN:ND2 | 2:G7:105:ARG:HB2 | 2.29 | 0.46 |
| 2:H1:109:THR:OG1 | 2:H1:411:GLU:OE2 | 2.29 | 0.46 |
| 1:H2:33:THR:O | 1:H2:58:ARG:NH2 | 2.49 | 0.46 |
| 2:H5:3:GLU:HB2 | 2:H5:129:CYS:SG | 2.56 | 0.46 |
| 2:H5:312:TYR:HB2 | 2:H5:343:PHE:HD1 | 1.79 | 0.46 |
| 1:H6:175:VAL:HG22 | 2:H7:329:ASN:HD21 | 1.81 | 0.46 |
| 1:H6:248:ALA:HA | 1:H6:252:LYS:HD2 | 1.96 | 0.46 |
| 1:I2:396:HIS:H | 1:I2:396:HIS:CD2 | 2.34 | 0.46 |
| 2:I3:113:GLU:N | 2:I3:113:GLU:OE1 | 2.48 | 0.46 |
| 1:I4:69:GLU:OE2 | 1:I4:96:GLY:HA2 | 2.15 | 0.46 |
| 1:J0:177:ASP:O | 2:J1:352:LYS:HA | 2.15 | 0.46 |
| 2:J3:305:CYS:HB3 | 2:J3:387:ILE:HD11 | 1.98 | 0.46 |
| 1:J4:244:GLY:H | 1:J4:247:ASN:HD21 | 1.64 | 0.46 |
| 2:J5:409:VAL:HA | 2:J5:413:MET:O | 2.15 | 0.46 |
| 1:J6:7:ILE:HB | 1:J6:135:VAL:HG22 | 1.98 | 0.46 |
| 2:J7:17:GLY:HA2 | 2:J7:20:CYS:HB3 | 1.97 | 0.46 |
| 2:J7:281:ALA:HA | 2:J7:284:GLU:CG | 2.41 | 0.46 |
| 2:J9:326:LYS:HG3 | 2:J9:327:ASP:H | 1.80 | 0.46 |
| 2:J9:406:HIS:HA | 2:J9:409:VAL:HG22 | 1.97 | 0.46 |
| 1:K8:274:THR:OG1 | 1:K8:279:GLN:OE1 | 2.28 | 0.46 |
| 2:K9:11:GLN:HB3 | 41:K9:501:GTP:PA | 2.56 | 0.46 |
| 2:K9:51:THR:HG21 | 2:K9:243:ARG:HG2 | 1.96 | 0.46 |
| 1:L2:224:ASP:OD2 | 29:7J:431:SER:OG | 2.34 | 0.46 |
| 2:M1:137:VAL:HG22 | 2:M1:168:GLY:HA2 | 1.98 | 0.46 |
| 2:M1:417:GLU:HA | 2:M1:420:GLU:HG2 | 1.98 | 0.46 |
| 2:M3:5:ILE:HG22 | 2:M3:64:ARG:HB3 | 1.98 | 0.46 |
| 2:M5:384:ILE:HA | 2:M5:387:ILE:HD12 | 1.96 | 0.46 |
| 1:N0:5:VAL:HG23 | 1:N0:62:ARG:HG2 | 1.96 | 0.46 |
| 1:N0:216:LYS:HB2 | 1:N0:275:SER:OG | 2.15 | 0.46 |
| 2:N1:223:THR:HG23 | 2:N1:225:THR:H | 1.81 | 0.46 |
| 2:N1:286:LEU:HD12 | 2:N1:286:LEU:HA | 1.78 | 0.46 |
| 1:N2:128:ASP:N | 1:N2:128:ASP:OD1 | 2.48 | 0.46 |
| 2:N3:52:PHE:CE2 | 2:N3:243:ARG:HD3 | 2.51 | 0.46 |
| 2:N7:185:TYR:HE1 | 2:N7:398:MET:HG2 | 1.80 | 0.46 |
| 1:O4:67:ASP:OD1 | 1:O4:68:LEU:N | 2.42 | 0.46 |
| 1:O4:385:PHE:HZ | 1:O4:408:PHE:HB3 | 1.79 | 0.46 |
| 1:O6:49:VAL:HG11 | 1:O6:241:ARG:HG2 | 1.98 | 0.46 |
| 1:O6:91:VAL:HG11 | 1:O6:116:VAL:HG23 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:4:VAL:HG23 | 2:P3:134:GLY:O | 2.15 | 0.46 |
| 2:P5:279:GLU:OE2 | 2:P5:279:GLU:HA | 2.16 | 0.46 |
| 2:P9:5:ILE:HG22 | 2:P9:64:ARG:HD3 | 1.97 | 0.46 |
| 1:Q4:319:GLY:O | 1:Q4:321:MET:HG3 | 2.15 | 0.46 |
| 1:Q8:30:ILE:HG21 | 1:Q8:59:TYR:HD2 | 1.79 | 0.46 |
| 1:R0:173:PRO:HG2 | 1:R0:174:LYS:NZ | 2.31 | 0.46 |
| 1:R4:68:LEU:HD13 | 1:R4:108:GLU:OE2 | 2.16 | 0.46 |
| 1:S2:95:THR:HG23 | 1:S2:96:GLY:N | 2.31 | 0.46 |
| 1:S4:3:GLU:HB2 | 1:S4:130:LEU:HA | 1.97 | 0.46 |
| 2:S9:178:SER:OG | 2:S9:183:GLU:OE2 | 2.28 | 0.46 |
| 2:S9:239:THR:HG23 | 2:S9:243:ARG:HE | 1.81 | 0.46 |
| 2:S9:300:SER:O | 2:S9:300:SER:OG | 2.30 | 0.46 |
| 1:T0:209:ASP:OD2 | 13:5I:114:LEU:HB3 | 2.15 | 0.46 |
| 1:U2:7:ILE:O | 1:U2:135:VAL:HA | 2.15 | 0.46 |
| 1:U2:60:VAL:HG23 | 1:U2:84:ILE:O | 2.16 | 0.46 |
| 1:U2:396:HIS:HE1 | 1:U2:397:TRP:CZ2 | 2.33 | 0.46 |
| 1:U4:304:ASP:HB3 | 1:U4:307:HIS:ND1 | 2.31 | 0.46 |
| 1:U6:170:VAL:HG12 | 1:U6:202:LEU:O | 2.15 | 0.46 |
| 1:U6:173:PRO:HG2 | 1:U6:174:LYS:NZ | 2.31 | 0.46 |
| 1:U6:270:PHE:HD2 | 1:U6:273:LEU:HD21 | 1.80 | 0.46 |
| 1:V2:7:ILE:O | 1:V2:135:VAL:HA | 2.16 | 0.46 |
| 2:V3:175:PRO:HB3 | 2:V3:390:ARG:NE | 2.29 | 0.46 |
| 1:V4:114:ASP:OD1 | 1:V4:115:SER:N | 2.48 | 0.46 |
| 1:W4:7:ILE:HG23 | 1:W4:64:ILE:HG23 | 1.98 | 0.46 |
| 1:W8:208:TYR:CE1 | 1:W8:225:LEU:HD11 | 2.51 | 0.46 |
| 2:W9:8:HIS:CD2 | 2:W9:17:GLY:HA3 | 2.51 | 0.46 |
| 1:X0:208:TYR:CE1 | 1:X0:225:LEU:HD11 | 2.51 | 0.46 |
| 1:X4:309:ARG:O | 1:X4:371:SER:OG | 2.29 | 0.46 |
| 1:X4:395:LEU:O | 1:X4:399:THR:HG23 | 2.14 | 0.46 |
| 1:X4:412:GLU:O | 1:X4:416:ASN:ND2 | 2.48 | 0.46 |
| 1:X8:3:GLU:HB2 | 1:X8:130:LEU:HA | 1.98 | 0.46 |
| 1:Y0:327:ASP:HA | 1:Y0:330:MET:HE1 | 1.98 | 0.46 |
| 1:Y0:361:LEU:HA | 8:4W:292:MET:CE | 2.46 | 0.46 |
| 2:Y1:5:ILE:HD11 | 2:Y1:135:PHE:CE1 | 2.50 | 0.46 |
| 1:Y2:150:LEU:O | 1:Y2:153:SER:OG | 2.30 | 0.46 |
| 1:Y4:70:PRO:N | 1:Y4:92:PHE:HZ | 2.12 | 0.46 |
| 1:Z0:66:MET:HE1 | 1:Z0:151:LEU:HD21 | 1.98 | 0.46 |
| 1:Z2:66:MET:HE2 | 1:Z2:147:MET:CG | 2.46 | 0.46 |
| 2:Z5:269:LEU:HD21 | 2:Z5:301:MET:SD | 2.56 | 0.46 |
| 1:Z8:412:GLU:O | 1:Z8:415:MET:HG2 | 2.16 | 0.46 |
| 2:0B:232:ALA:HA | 2:0B:235:ILE:HG22 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0F:246:GLY:HA3 | 2:0F:356:ASN:HA | 1.97 | 0.46 |
| 1:0G:118:ASP:O | 1:0G:122:LYS:HG2 | 2.16 | 0.46 |
| 2:0H:74:VAL:O | 2:0H:78:VAL:HG23 | 2.15 | 0.46 |
| 2:0J:330:ALA:O | 2:0J:334:THR:HG23 | 2.15 | 0.46 |
| 2:0L:198:THR:OG1 | 2:0L:200:VAL:O | 2.34 | 0.46 |
| 1:0M:372:THR:HG21 | 1:0M:426:GLN:HB2 | 1.98 | 0.46 |
| 1:0O:165:LEU:HD13 | 1:0O:167:PHE:HZ | 1.81 | 0.46 |
| 2:0P:407:TRP:HZ2 | 1:0Q:258:ILE:HB | 1.81 | 0.46 |
| 2:0R:189:LEU:HD11 | 2:0R:418:PHE:HE1 | 1.81 | 0.46 |
| 1:0S:246:LEU:O | 1:0S:352:SER:OG | 2.29 | 0.46 |
| 1:0U:391:ARG:NH2 | 2:0V:435:VAL:HA | 2.31 | 0.46 |
| 1:0U:414:ASN:HA | 1:0U:417:ASP:OD2 | 2.16 | 0.46 |
| 2:0V:320:ARG:O | 2:0V:373:ARG:HA | 2.16 | 0.46 |
| 1:0W:350:LYS:NZ | 1:0W:352:SER:HG | 2.12 | 0.46 |
| 2:0X:217:LEU:HB3 | 2:0X:219:ILE:CD1 | 2.46 | 0.46 |
| 1:0Y:210:ILE:O | 1:0Y:214:THR:OG1 | 2.24 | 0.46 |
| 1:0Y:382:SER:HB3 | 1:0Y:415:MET:HG2 | 1.98 | 0.46 |
| 2:1B:204:LEU:HD22 | 2:1B:302:MET:HB3 | 1.98 | 0.46 |
| 1:1E:203:ASP:OD1 | 1:1E:204:ASN:N | 2.49 | 0.46 |
| 1:1E:252:LYS:HE2 | 1:1E:350:LYS:HE2 | 1.96 | 0.46 |
| 1:1G:83:GLN:O | 1:1W:281:TYR:OH | 2.31 | 0.46 |
| 1:1K:69:GLU:C | 1:1K:92:PHE:HZ | 2.19 | 0.46 |
| 1:1M:276:ARG:NH1 | 1:1M:279:GLN:HE22 | 2.13 | 0.46 |
| 2:1T:50:ASN:O | 2:1T:64:ARG:NH2 | 2.47 | 0.46 |
| 2:1X:420:GLU:O | 2:1X:424:ASP:HB2 | 2.15 | 0.46 |
| 2:1Z:318:MET:HB2 | 2:1Z:376:CYS:HB3 | 1.97 | 0.46 |
| 1:2E:284:LEU:HD13 | 1:2E:362:LYS:HE2 | 1.98 | 0.46 |
| 1:2G:140:GLY:O | 1:2G:184:ASN:ND2 | 2.48 | 0.46 |
| 2:2H:90:GLU:OE1 | 2:2X:280:LYS:HD2 | 2.15 | 0.46 |
| 2:2J:26:LEU:HD21 | 2:2J:363:VAL:HG12 | 1.97 | 0.46 |
| 2:2L:72:PRO:HD2 | 1:2M:2:ARG:NH1 | 2.31 | 0.46 |
| 2:2P:331:SER:O | 2:2P:334:THR:OG1 | 2.27 | 0.46 |
| 2:2T:308:ARG:NH2 | 38:8A:28:THR:CG2 | 2.61 | 0.46 |
| 1:2U:201:VAL:HG12 | 1:2U:266:PHE:O | 2.15 | 0.46 |
| 1:2W:86:ARG:HB3 | 1:2W:89:ASN:OD1 | 2.16 | 0.46 |
| 1:2Y:117:LEU:HA | 1:2Y:120:VAL:HG12 | 1.98 | 0.46 |
| 2:3D:137:VAL:HG22 | 2:3D:168:GLY:HA2 | 1.98 | 0.46 |
| 1:3G:317:PHE:HE2 | 1:3G:326:VAL:HG13 | 1.80 | 0.46 |
| 1:3K:58:ARG:NH1 | 1:3K:84:ILE:HA | 2.30 | 0.46 |
| 1:3K:263:LEU:HG | 1:3K:422:TYR:CE1 | 2.49 | 0.46 |
| 2:3L:200:VAL:HG13 | 2:3L:268:MET:CE | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3L:213:CYS:HA | 2:3L:217:LEU:HB2 | 1.98 | 0.46 |
| 1:3M:233:MET:O | 1:3M:236:ILE:HG22 | 2.16 | 0.46 |
| 2:3N:320:ARG:HE | 2:3N:320:ARG:HB3 | 1.61 | 0.46 |
| 1:3O:60:VAL:HG23 | 1:3O:60:VAL:O | 2.15 | 0.46 |
| 2:3P:56:THR:HG1 | 3:4F:34:SER:HA | 1.78 | 0.46 |
| 2:3R:135:PHE:HB2 | 2:3R:166:LYS:HG2 | 1.96 | 0.46 |
| 1:3S:218:THR:OG1 | 17:5V:213:GLU:OE2 | 2.34 | 0.46 |
| 2:3T:6:SER:O | 2:3T:65:CYS:HA | 2.15 | 0.46 |
| 4:4I:126:ASP:OD1 | 4:4I:126:ASP:N | 2.46 | 0.46 |
| 7:4R:286:LYS:HD3 | 20:6F:339:GLU:OE2 | 2.16 | 0.46 |
| 10:5A:291:GLU:O | 10:5A:294:LEU:HG | 2.15 | 0.46 |
| 10:5C:364:ALA:HA | 10:5C:367:GLU:OE2 | 2.16 | 0.46 |
| 13:5K:99:ASN:H | 13:5K:99:ASN:HD22 | 1.63 | 0.46 |
| 14:5L:208:TYR:HD1 | 14:5L:222:ALA:HA | 1.81 | 0.46 |
| 14:5L:399:SER:OG | 14:5L:401:TRP:NE1 | 2.48 | 0.46 |
| 14:5L:454:ILE:O | 14:5L:456:ARG:NH2 | 2.49 | 0.46 |
| 14:5L:512:PHE:N | 14:5L:512:PHE:CD2 | 2.84 | 0.46 |
| 15:5O:238:THR:HG23 | 15:5O:311:VAL:HB | 1.98 | 0.46 |
| 22:6I:204:PHE:CE2 | 22:6I:205:GLU:HG2 | 2.50 | 0.46 |
| 22:6O:29:GLU:HG2 | 22:6O:29:GLU:O | 2.16 | 0.46 |
| 22:6O:218:LEU:HD23 | 22:6O:223:LEU:HD12 | 1.98 | 0.46 |
| 23:6S:4:LYS:HA | 23:6S:4:LYS:HD2 | 1.45 | 0.46 |
| 24:6T:537:GLU:O | 24:6T:541:THR:HG23 | 2.15 | 0.46 |
| 24:6U:456:ASP:N | 24:6U:456:ASP:OD1 | 2.48 | 0.46 |
| 24:6V:6:PRO:N | 24:6V:7:PRO:HD2 | 2.27 | 0.46 |
| 24:6V:263:ARG:HG3 | 24:6V:263:ARG:HH21 | 1.81 | 0.46 |
| 24:6W:95:VAL:HG22 | 24:6W:124:TYR:HA | 1.98 | 0.46 |
| 24:6W:505:LYS:HD2 | 24:6W:510:GLU:HB3 | 1.96 | 0.46 |
| 24:6Y:296:TYR:OH | 24:6Y:301:ASP:OD1 | 2.24 | 0.46 |
| 24:6Z:279:TRP:CZ2 | 24:6Z:364:ARG:HG3 | 2.50 | 0.46 |
| 30:7K:132:ARG:HB3 | 30:7K:134:HIS:CD2 | 2.51 | 0.46 |
| 35:7U:230:LEU:HD23 | 35:7U:230:LEU:HA | 1.80 | 0.46 |
| 28:7X:398:ASP:O | 28:7X:401:THR:HG22 | 2.15 | 0.46 |
| 37:7Y:210:THR:H | 37:7Y:213:MET:HE3 | 1.81 | 0.46 |
| 38:8A:197:THR:HG23 | 38:8A:200:ALA:CB | 2.45 | 0.46 |
| 2:C9:206:ASN:OD1 | 41:C9:501:GTP:N2 | 2.47 | 0.46 |
| 1:E0:280:GLN:CD | 24:6T:286:TYR:HB2 | 2.36 | 0.46 |
| 2:F1:12:ALA:HB2 | 41:F1:501:GTP:C8 | 2.50 | 0.46 |
| 2:G1:15:GLN:HB3 | 2:G1:228:ASN:HD21 | 1.79 | 0.46 |
| 1:G2:414:ASN:HA | 1:G2:417:ASP:OD2 | 2.16 | 0.46 |
| 1:G4:117:LEU:HA | 1:G4:120:VAL:HG12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:177:ASP:O | 2:G5:352:LYS:HA | 2.15 | 0.46 |
| 1:G6:135:VAL:HG21 | 1:G6:152:ILE:HD11 | 1.98 | 0.46 |
| 2:G9:187:SER:O | 2:G9:191:THR:HG23 | 2.15 | 0.46 |
| 2:H1:212:ILE:HG23 | 2:H1:275:ILE:HD12 | 1.97 | 0.46 |
| 1:H2:337:ASN:HB3 | 1:H2:340:TYR:CD2 | 2.51 | 0.46 |
| 1:H4:201:VAL:HG21 | 1:H4:374:ILE:HD11 | 1.98 | 0.46 |
| 2:H7:200:VAL:HG13 | 2:H7:268:MET:HE3 | 1.98 | 0.46 |
| 2:I1:121:ARG:HD2 | 2:I1:121:ARG:O | 2.16 | 0.46 |
| 1:I8:203:ASP:N | 1:I8:203:ASP:OD1 | 2.48 | 0.46 |
| 1:I8:379:LYS:HG3 | 1:I8:419:VAL:HG21 | 1.96 | 0.46 |
| 2:J3:8:HIS:CD2 | 2:J3:138:PHE:HD2 | 2.34 | 0.46 |
| 2:J3:246:GLY:HA2 | 2:J3:357:TYR:CD2 | 2.51 | 0.46 |
| 1:K0:414:ASN:HA | 1:K0:417:ASP:OD2 | 2.15 | 0.46 |
| 1:K4:77:ARG:HH21 | 1:K4:90:PHE:HD2 | 1.63 | 0.46 |
| 2:K5:392:ASP:OD2 | 2:K5:422:ARG:NH1 | 2.48 | 0.46 |
| 1:K6:49:VAL:HG11 | 1:K6:241:ARG:HG2 | 1.97 | 0.46 |
| 1:L0:309:ARG:NH1 | 1:L0:339:SER:O | 2.48 | 0.46 |
| 1:L2:27:GLU:CD | 1:L2:241:ARG:HH12 | 2.18 | 0.46 |
| 1:L2:334:GLN:HE22 | 1:L2:347:ASN:N | 2.14 | 0.46 |
| 2:L3:156:ARG:HA | 2:L3:159:VAL:HG12 | 1.97 | 0.46 |
| 1:L4:139:LEU:HD12 | 1:L4:170:VAL:HG12 | 1.97 | 0.46 |
| 2:L9:8:HIS:CD2 | 2:L9:138:PHE:HD2 | 2.33 | 0.46 |
| 1:M2:218:THR:O | 2:M3:326:LYS:HE2 | 2.15 | 0.46 |
| 1:M2:228:LEU:HD12 | 1:M2:228:LEU:HA | 1.79 | 0.46 |
| 2:M7:119:LEU:O | 2:M7:122:ILE:HG22 | 2.16 | 0.46 |
| 2:M7:250:VAL:HB | 2:M7:254:GLU:HG3 | 1.97 | 0.46 |
| 1:N0:135:VAL:HG21 | 1:N0:152:ILE:HD11 | 1.96 | 0.46 |
| 1:N2:391:ARG:NH2 | 2:N3:435:VAL:HA | 2.29 | 0.46 |
| 2:N3:217:LEU:HD11 | 2:N3:275:ILE:HD11 | 1.98 | 0.46 |
| 2:N5:189:LEU:HD11 | 2:N5:418:PHE:HE1 | 1.81 | 0.46 |
| 1:N6:164:MET:O | 1:N6:197:ASP:HB2 | 2.16 | 0.46 |
| 1:N6:232:VAL:HG11 | 1:N6:268:VAL:HG11 | 1.96 | 0.46 |
| 2:N7:187:SER:O | 2:N7:190:SER:OG | 2.27 | 0.46 |
| 1:N8:138:SER:HA | 1:N8:169:VAL:HG22 | 1.96 | 0.46 |
| 2:N9:56:THR:HG21 | 2:P7:283:HIS:O | 2.15 | 0.46 |
| 1:O2:117:LEU:HD23 | 1:O2:117:LEU:HA | 1.84 | 0.46 |
| 1:O4:43:GLN:O | 1:O4:47:ILE:HG23 | 2.16 | 0.46 |
| 1:O6:183:TYR:O | 1:O6:187:LEU:HD13 | 2.15 | 0.46 |
| 2:O7:9:ILE:HG12 | 2:O7:68:LEU:HD21 | 1.97 | 0.46 |
| 2:O9:121:ARG:HD2 | 2:O9:121:ARG:HA | 1.71 | 0.46 |
| 2:P3:399:TYR:O | 2:P3:402:ARG:NH1 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P4:153:SER:O | 1:P4:157:GLU:HG2 | 2.16 | 0.46 |
| 2:P7:287:SER:OG | 2:P7:288:VAL:N | 2.49 | 0.46 |
| 1:Q6:198:GLU:HA | 1:Q6:264:HIS:HB2 | 1.97 | 0.46 |
| 2:R1:285:GLN:HG2 | 7:4R:27:ILE:HG21 | 1.97 | 0.46 |
| 1:R2:94:GLN:NE2 | 13:5I:18:ARG:HG2 | 2.31 | 0.46 |
| 1:R6:172:SER:HB2 | 1:R6:203:ASP:OD1 | 2.16 | 0.46 |
| 1:R6:190:HIS:CD2 | 1:R6:414:ASN:HD22 | 2.34 | 0.46 |
| 1:R8:391:ARG:HB3 | 2:R9:346:TRP:CZ3 | 2.51 | 0.46 |
| 2:R9:274:PRO:HD3 | 2:R9:374:ALA:HA | 1.97 | 0.46 |
| 1:S2:268:VAL:HG23 | 1:S2:300:MET:HB2 | 1.97 | 0.46 |
| 1:S4:263:LEU:HD13 | 1:S4:422:TYR:CE1 | 2.50 | 0.46 |
| 2:S5:358:GLN:OE1 | 2:S5:359:PRO:HD2 | 2.15 | 0.46 |
| 2:S7:370:LYS:HD2 | 7:4T:277:ALA:HB3 | 1.98 | 0.46 |
| 1:S8:1:MET:HE2 | 1:S8:128:ASP:OD2 | 2.16 | 0.46 |
| 1:S8:172:SER:HB3 | 1:S8:175:VAL:HG12 | 1.98 | 0.46 |
| 1:T0:284:LEU:HB3 | 7:4T:352:ASN:HB2 | 1.97 | 0.46 |
| 2:T1:327:ASP:CG | 7:4U:25:ARG:HH12 | 2.13 | 0.46 |
| 1:T6:52:ASN:O | 1:T6:60:VAL:HG22 | 2.15 | 0.46 |
| 1:T8:207:LEU:HB3 | 1:T8:225:LEU:HD22 | 1.98 | 0.46 |
| 2:U3:142:GLY:O | 2:U3:186:ASN:ND2 | 2.32 | 0.46 |
| 2:V1:205:ASP:OD1 | 2:V1:303:VAL:HG13 | 2.16 | 0.46 |
| 1:V2:100:ASN:HB3 | 1:V2:103:LYS:HB2 | 1.97 | 0.46 |
| 2:V3:330:ALA:O | 2:V3:334:THR:HG23 | 2.15 | 0.46 |
| 1:V4:3:GLU:HG2 | 1:V4:129:CYS:O | 2.15 | 0.46 |
| 1:V4:95:THR:OG1 | 1:V4:96:GLY:N | 2.47 | 0.46 |
| 2:W5:88:HIS:HB3 | 2:W5:91:GLN:CD | 2.36 | 0.46 |
| 2:W5:286:LEU:HD23 | 2:W5:286:LEU:HA | 1.75 | 0.46 |
| 1:W6:414:ASN:HA | 1:W6:417:ASP:OD2 | 2.15 | 0.46 |
| 2:W7:238:LEU:HD12 | 2:W7:238:LEU:HA | 1.75 | 0.46 |
| 2:X5:322:ASP:OD2 | 2:X5:373:ARG:NH2 | 2.48 | 0.46 |
| 1:X6:260:PHE:CD2 | 1:X6:263:LEU:HD12 | 2.49 | 0.46 |
| 1:X6:290:THR:HG21 | 1:X6:329:GLN:HG3 | 1.98 | 0.46 |
| 2:X7:31:GLN:HB2 | 2:X7:33:ASP:OD1 | 2.16 | 0.46 |
| 2:X7:229:ARG:HD3 | 2:X7:363:VAL:HG21 | 1.98 | 0.46 |
| 2:X9:3:GLU:O | 2:X9:133:GLN:N | 2.41 | 0.46 |
| 1:Y0:86:ARG:HG2 | 1:Y0:88:ASP:H | 1.79 | 0.46 |
| 1:Y2:198:GLU:HA | 1:Y2:264:HIS:CD2 | 2.51 | 0.46 |
| 2:Y3:201:ALA:O | 2:Y3:268:MET:HE2 | 2.16 | 0.46 |
| 2:Y3:245:ASP:HA | 2:Y3:249:ASN:HD21 | 1.81 | 0.46 |
| 2:Y5:107:HIS:CD2 | 2:Y5:152:LEU:HB2 | 2.51 | 0.46 |
| 2:Y9:148:GLY:O | 2:Y9:151:SER:OG | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z0:265:PHE:HB3 | 1:Z0:374:ILE:HG12 | 1.98 | 0.46 |
| 2:Z1:33:ASP:O | 2:Z1:60:LYS:NZ | 2.47 | 0.46 |
| 1:0A:294:TRP:CG | 1:0A:333:VAL:HG21 | 2.49 | 0.46 |
| 1:0A:391:ARG:HG3 | 2:0B:346:TRP:CE2 | 2.51 | 0.46 |
| 2:0B:69:ASP:OD1 | 2:0B:70:LEU:N | 2.47 | 0.46 |
| 1:0I:272:PRO:O | 1:0I:273:LEU:HD23 | 2.15 | 0.46 |
| 2:0L:325:PRO:HA | 2:0L:328:VAL:HG12 | 1.98 | 0.46 |
| 1:0M:253:LEU:HD11 | 1:0M:316:LEU:HD11 | 1.98 | 0.46 |
| 2:0P:298:PRO:HA | 2:0P:301:MET:HG3 | 1.98 | 0.46 |
| 1:0Q:2:ARG:HB3 | 1:0Q:131:GLN:HB2 | 1.97 | 0.46 |
| 2:0R:233:GLN:O | 2:0R:237:SER:OG | 2.25 | 0.46 |
| 1:0S:313:ALA:HB3 | 1:0S:349:VAL:HG22 | 1.97 | 0.46 |
| 1:0S:375:GLN:HE22 | 1:0S:423:GLN:HB2 | 1.81 | 0.46 |
| 2:0X:5:ILE:HG22 | 2:0X:64:ARG:HB3 | 1.97 | 0.46 |
| 1:0Y:113:ILE:HD11 | 1:0Y:151:LEU:HB2 | 1.96 | 0.46 |
| 2:0Z:217:LEU:HB3 | 2:0Z:219:ILE:CD1 | 2.46 | 0.46 |
| 2:1B:212:ILE:O | 2:1B:216:SER:OG | 2.26 | 0.46 |
| 1:1E:317:PHE:HE2 | 1:1E:326:VAL:HG13 | 1.81 | 0.46 |
| 2:1F:26:LEU:HD21 | 2:1F:364:PRO:HD2 | 1.98 | 0.46 |
| 1:1G:180:VAL:HG13 | 1:1G:183:TYR:HB2 | 1.98 | 0.46 |
| 1:1K:41:ASP:N | 1:1K:41:ASP:OD2 | 2.47 | 0.46 |
| 1:1W:271:THR:HB | 1:1W:365:ALA:HB3 | 1.96 | 0.46 |
| 2:1Z:31:GLN:HB2 | 2:1Z:33:ASP:OD1 | 2.16 | 0.46 |
| 2:2B:3:GLU:HG3 | 2:2B:51:THR:HA | 1.97 | 0.46 |
| 2:2B:151:SER:HB2 | 2:2B:193:SER:OG | 2.16 | 0.46 |
| 2:2D:305:CYS:HB3 | 2:2D:387:ILE:HD11 | 1.98 | 0.46 |
| 2:2H:185:TYR:HE1 | 2:2H:398:MET:HE3 | 1.81 | 0.46 |
| 2:2J:305:CYS:HB3 | 2:2J:387:ILE:HD11 | 1.97 | 0.46 |
| 1:2K:178:THR:OG1 | 1:2K:179:VAL:N | 2.49 | 0.46 |
| 2:2P:17:GLY:HA2 | 2:2P:20:CYS:SG | 2.56 | 0.46 |
| 2:2P:145:THR:OG1 | 41:2Q:501:GTP:O1B | 2.33 | 0.46 |
| 2:2P:205:ASP:OD2 | 2:2P:206:ASN:N | 2.48 | 0.46 |
| 2:2P:279:GLU:H | 2:2P:279:GLU:HG3 | 1.57 | 0.46 |
| 1:2Q:244:GLY:H | 1:2Q:247:ASN:HD21 | 1.62 | 0.46 |
| 2:2R:7:ILE:HG13 | 2:2R:137:VAL:HG13 | 1.97 | 0.46 |
| 1:2S:31:ASP:OD2 | 1:2S:33:THR:OG1 | 2.29 | 0.46 |
| 1:2S:140:GLY:O | 1:2S:184:ASN:ND2 | 2.49 | 0.46 |
| 2:2T:157:LEU:HD23 | 2:2T:157:LEU:HA | 1.73 | 0.46 |
| 2:2X:62:VAL:HG13 | 2:2X:88:HIS:HD2 | 1.80 | 0.46 |
| 2:3B:244:PHE:CE1 | 38:8D:212:PRO:HG3 | 2.51 | 0.46 |
| 2:3B:291:ILE:HD12 | 2:3B:375:VAL:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3C:161:ASP:OD1 | 1:3C:161:ASP:N | 2.47 | 0.46 |
| 2:3D:32:PRO:HB3 | 2:3D:83:TYR:CE1 | 2.51 | 0.46 |
| 2:3H:340:THR:HG23 | 2:3H:341:ILE:HG23 | 1.98 | 0.46 |
| 2:3L:3:GLU:HB2 | 2:3L:129:CYS:SG | 2.56 | 0.46 |
| 1:3O:395:LEU:O | 1:3O:399:THR:HG23 | 2.16 | 0.46 |
| 2:3R:430:LYS:HA | 2:3R:433:GLU:OE2 | 2.16 | 0.46 |
| 4:4G:172:TYR:HA | 4:4G:176:GLU:OE2 | 2.16 | 0.46 |
| 3:4J:170:GLU:N | 3:4J:171:PRO:HD2 | 2.31 | 0.46 |
| 5:4L:396:GLN:O | 5:4L:399:GLU:HG3 | 2.16 | 0.46 |
| 6:4P:53:ASP:OD2 | 6:4P:54:THR:N | 2.48 | 0.46 |
| 7:4U:136:LEU:O | 7:4U:137:THR:HG22 | 2.15 | 0.46 |
| 7:4U:166:ALA:HA | 33:7Q:161:TYR:OH | 2.15 | 0.46 |
| 8:4W:217:ARG:O | 8:4W:220:ARG:HG3 | 2.16 | 0.46 |
| 10:5D:136:ALA:O | 10:5D:140:MET:HG2 | 2.15 | 0.46 |
| 11:5E:33:ASP:O | 11:5E:37:GLU:HG2 | 2.15 | 0.46 |
| 11:5E:173:ALA:O | 11:5E:176:VAL:HG12 | 2.14 | 0.46 |
| 13:5H:99:ASN:HD22 | 13:5H:99:ASN:H | 1.63 | 0.46 |
| 14:5L:132:TRP:CZ3 | 14:5L:139:ALA:HB2 | 2.51 | 0.46 |
| 14:5L:230:ASN:N | 14:5L:230:ASN:OD1 | 2.48 | 0.46 |
| 14:5M:132:TRP:CZ3 | 14:5M:139:ALA:HB2 | 2.51 | 0.46 |
| 14:5N:132:TRP:CZ3 | 14:5N:139:ALA:HB2 | 2.51 | 0.46 |
| 15:5P:109:ILE:O | 15:5P:113:ILE:HG12 | 2.15 | 0.46 |
| 15:5P:112:ALA:O | 15:5P:115:GLN:HG2 | 2.14 | 0.46 |
| 18:6C:173:HIS:HB3 | 18:6C:211:PHE:HB3 | 1.98 | 0.46 |
| 22:6N:308:HIS:CD2 | 24:6Y:560:ARG:HH12 | 2.34 | 0.46 |
| 22:6O:145:SER:HB2 | 22:6O:148:ASN:OD1 | 2.16 | 0.46 |
| 24:6T:97:ARG:HD2 | 24:6T:122:TYR:HE1 | 1.80 | 0.46 |
| 24:6T:299:GLU:HG3 | 24:6T:300:ASP:CG | 2.36 | 0.46 |
| 24:6T:474:PHE:HD2 | 24:6T:500:ARG:HH21 | 1.64 | 0.46 |
| 24:6T:555:THR:HG22 | 24:6T:612:LEU:HD22 | 1.97 | 0.46 |
| 24:6U:96:LEU:HD22 | 24:6U:188:THR:HG22 | 1.98 | 0.46 |
| 24:6V:88:TRP:CE3 | 24:6V:89:VAL:HG13 | 2.50 | 0.46 |
| 24:6V:505:LYS:HG3 | 24:6V:510:GLU:O | 2.15 | 0.46 |
| 24:6X:108:GLU:H | 24:6X:108:GLU:HG2 | 1.59 | 0.46 |
| 24:6X:445:ILE:HG21 | 24:6X:447:ARG:HE | 1.81 | 0.46 |
| 24:6X:519:VAL:HG23 | 24:6X:607:HIS:ND1 | 2.30 | 0.46 |
| 12:7B:56:THR:OG1 | 12:7B:57:THR:N | 2.48 | 0.46 |
| 29:7J:88:THR:OG1 | 29:7J:89:GLY:N | 2.48 | 0.46 |
| 38:8B:2:ASN:HB3 | 38:8B:5:LYS:HB2 | 1.97 | 0.46 |
| 2:8:29:GLY:O | 26:7E:45:MET:HE3 | 2.13 | 0.46 |
| 2:8:280:LYS:HG2 | 2:T1:89:PRO:HG3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B4:223:THR:HG22 | 18:6A:51:MET:HE3 | 1.95 | 0.46 |
| 2:C5:41:THR:HG21 | 24:6T:274:ARG:CZ | 2.45 | 0.46 |
| 1:E2:276:ARG:HD3 | 22:6J:103:ALA:HB3 | 1.97 | 0.46 |
| 2:F1:88:HIS:HB3 | 2:G7:283:HIS:CG | 2.51 | 0.46 |
| 1:G6:271:THR:HG21 | 1:G6:293:MET:HG3 | 1.98 | 0.46 |
| 2:G7:399:TYR:O | 2:G7:402:ARG:NH1 | 2.48 | 0.46 |
| 1:G8:91:VAL:HG11 | 1:G8:119:VAL:HG11 | 1.97 | 0.46 |
| 1:G8:175:VAL:HG23 | 1:G8:175:VAL:O | 2.16 | 0.46 |
| 2:H1:62:VAL:HG23 | 2:H1:88:HIS:HD2 | 1.81 | 0.46 |
| 2:H3:93:ILE:HD12 | 2:H3:117:LEU:CD2 | 2.45 | 0.46 |
| 2:H3:155:GLU:HB2 | 2:H3:197:HIS:CE1 | 2.51 | 0.46 |
| 1:H4:180:VAL:HG23 | 1:H4:184:ASN:ND2 | 2.31 | 0.46 |
| 2:H9:88:HIS:CG | 2:J5:283:HIS:HB3 | 2.51 | 0.46 |
| 1:I2:50:TYR:OH | 1:I2:237:THR:HB | 2.16 | 0.46 |
| 1:I2:149:THR:O | 1:I2:152:ILE:HG22 | 2.15 | 0.46 |
| 1:I2:274:THR:OG1 | 1:I2:282:ARG:NH1 | 2.48 | 0.46 |
| 1:I4:107:THR:OG1 | 1:I4:108:GLU:OE1 | 2.17 | 0.46 |
| 2:I5:163:LYS:HD2 | 2:I5:163:LYS:HA | 1.75 | 0.46 |
| 2:I7:21:TRP:CZ2 | 2:I7:65:CYS:HB2 | 2.51 | 0.46 |
| 2:I7:292:THR:OG1 | 2:I7:331:SER:OG | 2.33 | 0.46 |
| 1:J2:71:GLY:HA2 | 16:5Q:175:LEU:CD2 | 2.44 | 0.46 |
| 2:J7:55:GLU:HG2 | 2:J7:61:HIS:CE1 | 2.51 | 0.46 |
| 2:J7:88:HIS:CE1 | 2:J7:90:GLU:H | 2.33 | 0.46 |
| 1:K0:177:ASP:O | 2:K1:352:LYS:HA | 2.15 | 0.46 |
| 2:K5:88:HIS:CE1 | 2:M1:283:HIS:HA | 2.50 | 0.46 |
| 2:K9:116:ASP:OD1 | 2:K9:117:LEU:N | 2.48 | 0.46 |
| 1:L6:173:PRO:O | 1:L6:176:SER:OG | 2.31 | 0.46 |
| 2:L7:155:GLU:O | 2:L7:158:SER:OG | 2.30 | 0.46 |
| 2:L7:245:ASP:N | 2:L7:245:ASP:OD1 | 2.48 | 0.46 |
| 2:L9:27:GLU:OE2 | 2:L9:243:ARG:NH1 | 2.44 | 0.46 |
| 1:M0:283:ALA:O | 1:M0:288:GLU:HG2 | 2.14 | 0.46 |
| 1:M0:309:ARG:NH1 | 1:M0:339:SER:O | 2.48 | 0.46 |
| 2:M1:179:THR:O | 1:M2:350:LYS:HG2 | 2.16 | 0.46 |
| 1:M2:101:TRP:HE3 | 1:M2:403:MET:HE1 | 1.81 | 0.46 |
| 2:M5:156:ARG:HA | 2:M5:159:VAL:HG12 | 1.98 | 0.46 |
| 1:M6:125:GLU:CG | 37:7Y:93:LYS:HG3 | 2.45 | 0.46 |
| 2:M9:145:THR:OG1 | 41:N0:501:GTP:O1B | 2.34 | 0.46 |
| 1:N0:49:VAL:HG11 | 1:N0:241:ARG:HG2 | 1.96 | 0.46 |
| 2:N1:237:SER:HA | 2:N1:320:ARG:HD2 | 1.97 | 0.46 |
| 2:N5:242:LEU:HD11 | 2:N5:252:ILE:HG12 | 1.97 | 0.46 |
| 1:N8:8:GLN:OE1 | 1:N8:17:GLY:HA3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N8:175:VAL:HB | 2:N9:329:ASN:HD21 | 1.81 | 0.46 |
| 1:N8:396:HIS:H | 1:N8:396:HIS:CD2 | 2.32 | 0.46 |
| 2:O1:288:VAL:HG13 | 2:O1:319:TYR:HE2 | 1.80 | 0.46 |
| 2:O3:26:LEU:HD13 | 2:O3:363:VAL:HG12 | 1.98 | 0.46 |
| 1:O6:6:HIS:CE1 | 1:O6:8:GLN:HG2 | 2.51 | 0.46 |
| 1:P4:190:HIS:CD2 | 1:P4:411:ALA:HA | 2.51 | 0.46 |
| 1:P4:213:ARG:HE | 1:P4:297:LYS:HE3 | 1.80 | 0.46 |
| 1:P6:95:THR:HG23 | 1:P6:96:GLY:H | 1.80 | 0.46 |
| 2:Q1:206:ASN:OD1 | 41:Q2:501:GTP:N2 | 2.49 | 0.46 |
| 1:Q4:186:THR:HG21 | 1:Q4:385:PHE:CD1 | 2.51 | 0.46 |
| 2:Q5:217:LEU:HD21 | 2:Q5:368:LEU:HD23 | 1.97 | 0.46 |
| 2:Q9:52:PHE:HZ | 2:Q9:239:THR:HG21 | 1.81 | 0.46 |
| 1:R4:207:LEU:HB3 | 1:R4:225:LEU:HD22 | 1.98 | 0.46 |
| 1:R4:272:PRO:HB2 | 1:R4:282:ARG:HH12 | 1.80 | 0.46 |
| 1:R4:359:LYS:HA | 21:6G:55:TRP:HZ2 | 1.80 | 0.46 |
| 2:R5:21:TRP:CZ3 | 2:R5:63:PRO:HB3 | 2.50 | 0.46 |
| 1:R6:344:TRP:CE3 | 1:R6:345:ILE:HG13 | 2.51 | 0.46 |
| 1:R8:180:VAL:HG22 | 2:R9:258:ASN:HD21 | 1.79 | 0.46 |
| 2:S1:325:PRO:HA | 2:S1:328:VAL:HG12 | 1.97 | 0.46 |
| 1:S6:207:LEU:HB3 | 1:S6:225:LEU:HD22 | 1.98 | 0.46 |
| 2:S7:21:TRP:CZ2 | 2:S7:65:CYS:HB3 | 2.50 | 0.46 |
| 1:S8:317:PHE:HE2 | 1:S8:326:VAL:HG13 | 1.81 | 0.46 |
| 2:S9:286:LEU:O | 2:S9:373:ARG:NH1 | 2.49 | 0.46 |
| 1:T2:69:GLU:HG2 | 1:T2:96:GLY:HA2 | 1.97 | 0.46 |
| 1:T2:337:ASN:HD21 | 17:5T:48:THR:H | 1.64 | 0.46 |
| 2:T3:116:ASP:N | 2:T3:116:ASP:OD1 | 2.49 | 0.46 |
| 2:T3:250:VAL:HG23 | 2:T3:254:GLU:HG3 | 1.98 | 0.46 |
| 1:T4:100:ASN:HB3 | 1:T4:103:LYS:HB2 | 1.97 | 0.46 |
| 2:T7:33:ASP:N | 2:T7:33:ASP:OD1 | 2.48 | 0.46 |
| 2:U1:119:LEU:HD21 | 2:U1:156:ARG:HB3 | 1.98 | 0.46 |
| 2:U1:291:ILE:HA | 2:U1:294:ALA:HB3 | 1.97 | 0.46 |
| 1:U4:271:THR:O | 1:U4:365:ALA:N | 2.47 | 0.46 |
| 2:U5:90:GLU:HG3 | 2:U5:121:ARG:NH1 | 2.31 | 0.46 |
| 2:U7:279:GLU:HG2 | 2:U7:280:LYS:HD2 | 1.98 | 0.46 |
| 2:U9:254:GLU:OE1 | 2:U9:254:GLU:N | 2.48 | 0.46 |
| 2:U9:317:LEU:HB3 | 2:U9:319:TYR:HE1 | 1.80 | 0.46 |
| 2:V1:406:HIS:HA | 2:V1:409:VAL:HG22 | 1.98 | 0.46 |
| 1:V4:335:ASN:O | 1:V4:338:SER:OG | 2.33 | 0.46 |
| 1:V6:167:PHE:CE2 | 1:V6:233:MET:HG2 | 2.51 | 0.46 |
| 2:V9:60:LYS:HE2 | 2:V9:88:HIS:CE1 | 2.51 | 0.46 |
| 1:W4:184:ASN:OD1 | 1:W4:398:TYR:OH | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W5:88:HIS:CD2 | 2:W5:121:ARG:HH22 | 2.34 | 0.46 |
| 2:W7:9:ILE:HG23 | 2:W7:68:LEU:HD11 | 1.97 | 0.46 |
| 2:W9:398:MET:HG3 | 1:X0:346:PRO:HD2 | 1.98 | 0.46 |
| 1:X4:288:GLU:OE1 | 1:X4:289:LEU:HD12 | 2.16 | 0.46 |
| 1:X6:105:HIS:NE2 | 1:X6:150:LEU:HD13 | 2.30 | 0.46 |
| 1:X6:207:LEU:HB3 | 1:X6:225:LEU:HD22 | 1.97 | 0.46 |
| 1:X6:266:PHE:CE1 | 1:X6:370:ASN:HB2 | 2.51 | 0.46 |
| 2:X7:245:ASP:OD1 | 2:X7:245:ASP:N | 2.45 | 0.46 |
| 2:X9:70:LEU:HA | 2:X9:95:GLY:HA3 | 1.98 | 0.46 |
| 1:Y2:251:ARG:O | 1:Y2:255:VAL:HG22 | 2.16 | 0.46 |
| 2:Y3:271:SER:OG | 2:Y3:377:MET:HB3 | 2.16 | 0.46 |
| 2:Y3:333:ALA:O | 2:Y3:337:THR:HG23 | 2.16 | 0.46 |
| 1:Y4:170:VAL:HG22 | 1:Y4:202:LEU:O | 2.15 | 0.46 |
| 1:Y6:395:LEU:O | 1:Y6:399:THR:HG23 | 2.15 | 0.46 |
| 1:Z0:2:ARG:HB3 | 1:Z0:131:GLN:HB2 | 1.98 | 0.46 |
| 1:Z0:156:ARG:HD2 | 1:Z0:156:ARG:HA | 1.56 | 0.46 |
| 1:Z2:86:ARG:HH21 | 1:0I:282:ARG:HA | 1.81 | 0.46 |
| 2:Z3:88:HIS:HB3 | 2:0J:283:HIS:ND1 | 2.31 | 0.46 |
| 1:Z4:131:GLN:HE21 | 1:Z4:250:LEU:HB2 | 1.81 | 0.46 |
| 1:Z4:249:ASP:OD1 | 1:Z4:252:LYS:N | 2.44 | 0.46 |
| 2:Z5:12:ALA:O | 2:Z5:16:VAL:HG23 | 2.15 | 0.46 |
| 1:Z6:67:ASP:OD2 | 1:Z6:72:THR:OG1 | 2.33 | 0.46 |
| 2:Z7:322:ASP:OD2 | 2:Z7:373:ARG:NH2 | 2.45 | 0.46 |
| 1:Z8:11:GLN:NE2 | 39:Z8:501:GDP:O3B | 2.49 | 0.46 |
| 1:0A:311:LEU:HD23 | 1:0A:312:THR:HG23 | 1.97 | 0.46 |
| 1:0C:418:LEU:O | 1:0C:421:GLU:HG2 | 2.16 | 0.46 |
| 1:0G:175:VAL:O | 1:0G:175:VAL:HG23 | 2.16 | 0.46 |
| 1:0G:297:LYS:HD3 | 1:0G:297:LYS:HA | 1.75 | 0.46 |
| 2:0H:333:ALA:O | 2:0H:337:THR:HG23 | 2.16 | 0.46 |
| 1:0K:7:ILE:O | 1:0K:135:VAL:HA | 2.15 | 0.46 |
| 1:0K:286:VAL:HG23 | 1:0K:287:PRO:HD3 | 1.96 | 0.46 |
| 2:0L:407:TRP:CE2 | 1:0M:255:VAL:HA | 2.51 | 0.46 |
| 1:0Q:86:ARG:HD3 | 1:0Q:88:ASP:HB2 | 1.98 | 0.46 |
| 1:0Q:112:LEU:O | 1:0Q:116:VAL:HG23 | 2.15 | 0.46 |
| 2:0R:8:HIS:CD2 | 2:0R:138:PHE:HD2 | 2.34 | 0.46 |
| 2:0R:66:ILE:HG13 | 2:0R:122:ILE:HG22 | 1.98 | 0.46 |
| 2:0R:398:MET:HG2 | 1:0S:346:PRO:HD2 | 1.97 | 0.46 |
| 1:0S:116:VAL:O | 1:0S:120:VAL:HG12 | 2.16 | 0.46 |
| 2:0V:227:LEU:O | 2:0V:231:ILE:HG12 | 2.16 | 0.46 |
| 2:0V:344:VAL:HB | 2:0V:346:TRP:NE1 | 2.31 | 0.46 |
| 1:0W:203:ASP:OD2 | 1:0W:204:ASN:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0W:311:LEU:HD23 | 1:0W:312:THR:HG23 | 1.98 | 0.46 |
| 2:0X:50:ASN:O | 2:0X:64:ARG:NH2 | 2.49 | 0.46 |
| 2:0Z:288:VAL:O | 2:0Z:292:THR:OG1 | 2.32 | 0.46 |
| 1:1A:345:ILE:O | 1:1A:348:ASN:ND2 | 2.48 | 0.46 |
| 2:1H:5:ILE:HG22 | 2:1H:64:ARG:HB3 | 1.98 | 0.46 |
| 2:1H:49:PHE:HD2 | 2:1H:53:PHE:HB2 | 1.80 | 0.46 |
| 2:1H:384:ILE:HG23 | 2:1H:432:PHE:CZ | 2.51 | 0.46 |
| 1:1K:334:GLN:NE2 | 1:1K:348:ASN:H | 2.13 | 0.46 |
| 2:1L:19:ALA:O | 2:1L:22:GLU:HG3 | 2.16 | 0.46 |
| 2:1L:121:ARG:HH11 | 2:1L:121:ARG:CG | 2.00 | 0.46 |
| 2:1R:66:ILE:O | 2:1R:66:ILE:HG13 | 2.15 | 0.46 |
| 1:2C:138:SER:OG | 1:2C:139:LEU:N | 2.48 | 0.46 |
| 1:2C:334:GLN:HE22 | 1:2C:347:ASN:HA | 1.81 | 0.46 |
| 2:2F:119:LEU:HD11 | 38:8B:73:TRP:CZ2 | 2.51 | 0.46 |
| 2:2F:287:SER:N | 2:2F:290:GLU:OE2 | 2.41 | 0.46 |
| 2:2F:312:TYR:HB2 | 2:2F:343:PHE:HD1 | 1.80 | 0.46 |
| 1:2G:371:SER:OG | 1:2G:372:THR:N | 2.49 | 0.46 |
| 1:2I:389:PHE:HZ | 1:2I:405:GLU:HG3 | 1.81 | 0.46 |
| 2:2L:261:PRO:HG3 | 2:2L:313:MET:HE2 | 1.98 | 0.46 |
| 2:2P:214:ARG:NH2 | 38:7Z:18:VAL:HA | 2.31 | 0.46 |
| 2:2T:76:ASP:OD2 | 1:2U:46:ARG:NH2 | 2.48 | 0.46 |
| 2:2V:112:LYS:HG3 | 2:2V:113:GLU:OE2 | 2.15 | 0.46 |
| 2:2X:250:VAL:HG23 | 2:2X:254:GLU:HG3 | 1.97 | 0.46 |
| 2:2Z:137:VAL:HG22 | 2:2Z:168:GLY:HA2 | 1.98 | 0.46 |
| 1:3A:77:ARG:HH22 | 38:8D:220:VAL:HG23 | 1.80 | 0.46 |
| 2:3H:124:LYS:HZ2 | 3:3X:36:PHE:HD1 | 1.64 | 0.46 |
| 2:3H:345:ASP:N | 2:3H:345:ASP:OD1 | 2.48 | 0.46 |
| 2:3J:236:SER:OG | 2:3J:243:ARG:NH2 | 2.49 | 0.46 |
| 1:3K:68:LEU:HD21 | 1:3K:112:LEU:HD22 | 1.98 | 0.46 |
| 1:3K:285:THR:OG1 | 1:3K:287:PRO:HD2 | 2.15 | 0.46 |
| 1:3K:292:GLN:HG2 | 1:3K:298:ASN:ND2 | 2.30 | 0.46 |
| 1:3K:387:ALA:HA | 1:3K:390:ARG:HE | 1.80 | 0.46 |
| 2:3N:239:THR:HG23 | 2:3N:243:ARG:HE | 1.80 | 0.46 |
| 2:3T:417:GLU:HA | 2:3T:420:GLU:HG2 | 1.97 | 0.46 |
| 4:3Y:172:TYR:HA | 4:3Y:176:GLU:OE2 | 2.16 | 0.46 |
| 3:3Z:158:LEU:HD12 | 3:3Z:194:VAL:HG11 | 1.98 | 0.46 |
| 3:3Z:229:ASP:HB3 | 3:3Z:230:LEU:HD23 | 1.97 | 0.46 |
| 3:4D:158:LEU:HD12 | 3:4D:194:VAL:HG11 | 1.98 | 0.46 |
| 3:4F:229:ASP:HB3 | 3:4F:230:LEU:HD23 | 1.97 | 0.46 |
| 3:4H:158:LEU:HD12 | 3:4H:194:VAL:HG11 | 1.98 | 0.46 |
| 5:4M:293:LEU:HD13 | 5:4M:296:GLU:OE2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:4O:103:ARG:O | 6:4O:103:ARG:NH1 | 2.42 | 0.46 |
| 6:4O:182:ALA:O | 6:4O:186:GLU:HG2 | 2.16 | 0.46 |
| 8:4W:341:ALA:O | 8:4W:344:GLU:HG2 | 2.16 | 0.46 |
| 9:4Y:400:ARG:HA | 9:4Y:403:GLU:OE1 | 2.15 | 0.46 |
| 10:5C:312:ALA:O | 10:5C:315:GLU:HG3 | 2.15 | 0.46 |
| 12:5F:32:GLN:N | 12:5F:32:GLN:OE1 | 2.49 | 0.46 |
| 13:5I:99:ASN:H | 13:5I:99:ASN:HD22 | 1.63 | 0.46 |
| 13:5J:99:ASN:H | 13:5J:99:ASN:HD22 | 1.63 | 0.46 |
| 14:5N:221:ILE:HA | 14:5N:228:PHE:HA | 1.97 | 0.46 |
| 15:5O:280:GLU:OE1 | 27:7G:90:MET:HG3 | 2.16 | 0.46 |
| 15:5P:54:GLU:HB3 | 15:5P:55:LEU:HD23 | 1.97 | 0.46 |
| 17:5R:53:ASP:N | 17:5R:53:ASP:OD2 | 2.49 | 0.46 |
| 18:5Y:180:ARG:O | 18:5Y:184:THR:HG23 | 2.15 | 0.46 |
| 18:5Z:173:HIS:HB3 | 18:5Z:211:PHE:HB3 | 1.98 | 0.46 |
| 18:6A:173:HIS:HB3 | 18:6A:211:PHE:HB3 | 1.98 | 0.46 |
| 18:6A:180:ARG:O | 18:6A:184:THR:HG23 | 2.15 | 0.46 |
| 18:6B:173:HIS:HB3 | 18:6B:211:PHE:HB3 | 1.98 | 0.46 |
| 18:6B:180:ARG:O | 18:6B:184:THR:HG23 | 2.15 | 0.46 |
| 18:6D:173:HIS:HB3 | 18:6D:211:PHE:HB3 | 1.98 | 0.46 |
| 20:6F:370:LEU:CD2 | 20:6F:384:LEU:HB2 | 2.44 | 0.46 |
| 21:6G:24:TYR:OH | 21:6G:90:THR:HG21 | 2.16 | 0.46 |
| 21:6H:89:ILE:HG12 | 21:6H:93:HIS:HB2 | 1.97 | 0.46 |
| 22:6I:220:ASP:OD1 | 22:6I:221:ASP:N | 2.48 | 0.46 |
| 22:6J:172:ARG:HH12 | 22:6J:215:GLY:HA3 | 1.79 | 0.46 |
| 22:6M:289:ASP:OD2 | 22:6M:289:ASP:N | 2.49 | 0.46 |
| 24:6T:252:LYS:HE3 | 24:6T:256:LEU:HB2 | 1.98 | 0.46 |
| 24:6W:8:ILE:HG13 | 24:6W:9:PRO:HD2 | 1.97 | 0.46 |
| 24:6W:37:ASN:HD22 | 24:6W:37:ASN:N | 2.14 | 0.46 |
| 24:6X:480:ASN:OD1 | 24:6X:480:ASN:N | 2.41 | 0.46 |
| 24:6X:505:LYS:HD2 | 24:6X:510:GLU:HB3 | 1.97 | 0.46 |
| 24:6X:556:ASP:OD1 | 24:6X:557:VAL:N | 2.48 | 0.46 |
| 24:6X:565:GLN:OE1 | 24:6X:602:LEU:HB2 | 2.16 | 0.46 |
| 24:6Y:94:LYS:HB3 | 24:6Y:187:PHE:HZ | 1.79 | 0.46 |
| 24:6Y:507:ARG:HA | 24:6Y:507:ARG:NH2 | 2.31 | 0.46 |
| 24:6Y:569:LYS:HB2 | 24:6Y:572:ALA:HB3 | 1.97 | 0.46 |
| 24:6Z:487:VAL:CG1 | 24:6Z:490:THR:HG23 | 2.45 | 0.46 |
| 31:7M:39:LEU:HD22 | 31:7M:43:VAL:HG11 | 1.97 | 0.46 |
| 32:7O:74:LYS:O | 32:7O:75:THR:HG22 | 2.16 | 0.46 |
| 38:8D:159:TYR:CD1 | 38:8D:159:TYR:C | 2.88 | 0.46 |
| 1:D4:47:ILE:HD11 | 22:6N:23:TYR:CD2 | 2.49 | 0.46 |
| 2:E9:358:GLN:NE2 | 22:6M:94:SER:OG | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F5:88:HIS:HB3 | 2:H1:283:HIS:ND1 | 2.31 | 0.46 |
| 2:G5:56:THR:HG23 | 2:G5:60:LYS:HE2 | 1.98 | 0.46 |
| 1:G6:117:LEU:HD11 | 1:G6:154:LYS:HB3 | 1.97 | 0.46 |
| 1:G8:173:PRO:O | 1:G8:176:SER:OG | 2.34 | 0.46 |
| 1:G8:345:ILE:HB | 1:G8:348:ASN:HD21 | 1.80 | 0.46 |
| 1:I4:208:TYR:HA | 1:I4:211:CYS:SG | 2.55 | 0.46 |
| 2:I7:22:GLU:HG3 | 2:I7:83:TYR:OH | 2.16 | 0.46 |
| 2:I7:76:ASP:OD2 | 1:I8:46:ARG:NH2 | 2.49 | 0.46 |
| 1:I8:114:ASP:N | 1:I8:114:ASP:OD1 | 2.48 | 0.46 |
| 2:I9:178:SER:HB2 | 1:J0:347:ASN:CG | 2.35 | 0.46 |
| 2:J1:2:ARG:HA | 2:J1:133:GLN:HE21 | 1.81 | 0.46 |
| 2:J1:278:ALA:HA | 2:J1:369:ALA:HB2 | 1.97 | 0.46 |
| 1:J6:130:LEU:HB2 | 1:J6:162:ARG:HE | 1.81 | 0.46 |
| 2:L1:352:LYS:NZ | 2:L1:353:CYS:O | 2.47 | 0.46 |
| 1:L2:2:ARG:HB3 | 1:L2:131:GLN:HB2 | 1.98 | 0.46 |
| 1:L2:39:ASP:OD1 | 1:L2:39:ASP:N | 2.41 | 0.46 |
| 2:L3:370:LYS:HE2 | 2:L3:370:LYS:HB2 | 1.60 | 0.46 |
| 2:L5:333:ALA:O | 2:L5:337:THR:HG23 | 2.15 | 0.46 |
| 1:L6:339:SER:OG | 34:7S:140:ASN:ND2 | 2.48 | 0.46 |
| 2:L7:149:LEU:HA | 2:L7:152:LEU:HB3 | 1.98 | 0.46 |
| 2:L9:384:ILE:HA | 2:L9:387:ILE:HD12 | 1.98 | 0.46 |
| 1:M0:345:ILE:O | 1:M0:348:ASN:ND2 | 2.49 | 0.46 |
| 1:M2:3:GLU:HB2 | 1:M2:130:LEU:HA | 1.98 | 0.46 |
| 2:M3:189:LEU:HD11 | 2:M3:418:PHE:HE1 | 1.81 | 0.46 |
| 1:M4:391:ARG:HD3 | 2:M5:346:TRP:HE1 | 1.81 | 0.46 |
| 2:M9:69:ASP:OD1 | 2:M9:71:GLU:HG2 | 2.15 | 0.46 |
| 2:N3:191:THR:HA | 2:N3:194:LEU:HB3 | 1.98 | 0.46 |
| 2:N7:79:ARG:NH1 | 2:N7:94:SER:OG | 2.49 | 0.46 |
| 2:N7:192:HIS:ND1 | 2:N7:192:HIS:O | 2.48 | 0.46 |
| 1:O2:219:THR:O | 1:O2:219:THR:OG1 | 2.33 | 0.46 |
| 2:O3:333:ALA:O | 2:O3:337:THR:HG23 | 2.16 | 0.46 |
| 2:O7:305:CYS:HB3 | 2:O7:387:ILE:HD11 | 1.98 | 0.46 |
| 1:O8:11:GLN:N | 39:O8:503:GDP:O1B | 2.35 | 0.46 |
| 1:Q0:86:ARG:NH1 | 1:Q0:89:ASN:OD1 | 2.48 | 0.46 |
| 2:Q1:240:ALA:HB1 | 2:Q1:356:ASN:HD22 | 1.81 | 0.46 |
| 2:Q3:133:GLN:HB3 | 2:Q3:252:ILE:HG21 | 1.98 | 0.46 |
| 1:Q4:371:SER:OG | 1:Q4:372:THR:N | 2.49 | 0.46 |
| 2:Q5:245:ASP:N | 2:Q5:245:ASP:OD1 | 2.49 | 0.46 |
| 2:Q5:265:ILE:HD11 | 2:Q5:435:VAL:HG21 | 1.97 | 0.46 |
| 2:Q5:333:ALA:O | 2:Q5:337:THR:HG23 | 2.16 | 0.46 |
| 1:Q8:152:ILE:HD12 | 1:Q8:164:MET:SD | 2.56 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R1:279:GLU:N | 2:R1:279:GLU:OE1 | 2.48 | 0.46 |
| 2:R5:62:VAL:O | 2:R5:62:VAL:HG13 | 2.16 | 0.46 |
| 1:R6:177:ASP:N | 1:R6:181:GLU:OE2 | 2.48 | 0.46 |
| 1:R8:95:THR:HG23 | 1:R8:96:GLY:H | 1.80 | 0.46 |
| 2:R9:102:ASN:HB3 | 2:R9:105:ARG:HB3 | 1.98 | 0.46 |
| 2:S1:91:GLN:HG2 | 2:S1:121:ARG:NH2 | 2.30 | 0.46 |
| 2:S9:68:LEU:HA | 2:S9:93:ILE:O | 2.15 | 0.46 |
| 1:T2:173:PRO:HB3 | 1:T2:384:GLN:NE2 | 2.30 | 0.46 |
| 1:T4:232:VAL:HG13 | 1:T4:268:VAL:HG11 | 1.98 | 0.46 |
| 1:T6:56:GLY:N | 26:7F:104:GLN:HE22 | 2.13 | 0.46 |
| 2:U1:49:PHE:HB2 | 2:U1:53:PHE:HD2 | 1.80 | 0.46 |
| 1:U2:105:HIS:NE2 | 1:U2:150:LEU:HD13 | 2.31 | 0.46 |
| 1:U4:177:ASP:OD1 | 2:U5:248:LEU:HD11 | 2.16 | 0.46 |
| 1:U6:52:ASN:OD1 | 1:U6:62:ARG:NH2 | 2.49 | 0.46 |
| 1:U6:201:VAL:HG12 | 1:U6:266:PHE:O | 2.16 | 0.46 |
| 1:U6:207:LEU:HB3 | 1:U6:225:LEU:HD22 | 1.98 | 0.46 |
| 1:V0:233:MET:O | 1:V0:237:THR:HG22 | 2.16 | 0.46 |
| 1:V2:3:GLU:HG2 | 1:V2:129:CYS:O | 2.15 | 0.46 |
| 1:V4:207:LEU:HB3 | 1:V4:225:LEU:HD22 | 1.98 | 0.46 |
| 1:V6:178:THR:HA | 2:V7:352:LYS:HD2 | 1.97 | 0.46 |
| 2:V7:280:LYS:O | 2:V7:283:HIS:HB3 | 2.15 | 0.46 |
| 1:V8:249:ASP:O | 1:V8:253:LEU:HG | 2.16 | 0.46 |
| 2:V9:5:ILE:O | 2:V9:136:LEU:HD23 | 2.16 | 0.46 |
| 1:W0:67:ASP:N | 1:W0:67:ASP:OD1 | 2.49 | 0.46 |
| 1:W0:304:ASP:HB3 | 1:W0:307:HIS:CG | 2.51 | 0.46 |
| 2:W9:96:LYS:O | 2:W9:97:GLU:HG3 | 2.15 | 0.46 |
| 1:X2:309:ARG:H | 1:X2:372:THR:HG22 | 1.81 | 0.46 |
| 2:X3:5:ILE:HD13 | 2:X3:125:LEU:HD23 | 1.98 | 0.46 |
| 2:X3:70:LEU:HD23 | 2:X3:145:THR:HG23 | 1.97 | 0.46 |
| 1:X4:101:TRP:CZ3 | 1:X4:187:LEU:HD23 | 2.51 | 0.46 |
| 2:X5:21:TRP:CZ2 | 2:X5:65:CYS:HB2 | 2.51 | 0.46 |
| 2:X5:392:ASP:OD2 | 2:X5:422:ARG:NH1 | 2.49 | 0.46 |
| 1:X6:6:HIS:HA | 1:X6:134:GLN:O | 2.16 | 0.46 |
| 1:X6:273:LEU:H | 1:X6:292:GLN:NE2 | 2.14 | 0.46 |
| 1:X6:279:GLN:NE2 | 8:4W:184:VAL:HG22 | 2.25 | 0.46 |
| 1:Y2:273:LEU:H | 1:Y2:292:GLN:HE22 | 1.63 | 0.46 |
| 1:Z0:190:HIS:HD2 | 1:Z0:414:ASN:HB2 | 1.81 | 0.46 |
| 2:Z1:185:TYR:HE1 | 2:Z1:398:MET:HG2 | 1.81 | 0.46 |
| 1:Z2:70:PRO:HG2 | 2:Z3:2:ARG:HH11 | 1.80 | 0.46 |
| 1:Z2:379:LYS:HA | 1:Z2:382:SER:OG | 2.15 | 0.46 |
| 1:Z4:337:ASN:HB2 | 1:Z4:340:TYR:HD2 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z5:187:SER:O | 2:Z5:190:SER:OG | 2.23 | 0.46 |
| 1:Z6:130:LEU:HG | 1:Z6:132:GLY:N | 2.31 | 0.46 |
| 1:Z6:389:PHE:O | 1:Z6:392:LYS:NZ | 2.36 | 0.46 |
| 1:Z8:235:GLY:O | 1:Z8:316:LEU:HD23 | 2.16 | 0.46 |
| 2:0B:65:CYS:SG | 2:0B:66:ILE:N | 2.89 | 0.46 |
| 1:0C:139:LEU:HD12 | 1:0C:170:VAL:HA | 1.98 | 0.46 |
| 1:0C:244:GLY:HA3 | 1:0C:354:CYS:HA | 1.97 | 0.46 |
| 1:0E:332:ASN:HA | 1:0E:335:ASN:ND2 | 2.30 | 0.46 |
| 2:0F:276:ILE:HG23 | 2:0F:280:LYS:HB3 | 1.97 | 0.46 |
| 2:0P:217:LEU:HB3 | 2:0P:219:ILE:CD1 | 2.46 | 0.46 |
| 1:0Q:183:TYR:HB3 | 1:0Q:398:TYR:HE2 | 1.80 | 0.46 |
| 2:0R:353:CYS:SG | 2:0R:354:GLY:N | 2.89 | 0.46 |
| 2:0V:129:CYS:SG | 2:0V:132:LEU:HD12 | 2.56 | 0.46 |
| 2:0V:176:GLN:HG2 | 2:0V:177:VAL:N | 2.30 | 0.46 |
| 1:0W:418:LEU:O | 1:0W:421:GLU:HG2 | 2.16 | 0.46 |
| 2:0X:111:GLY:O | 2:0X:115:VAL:HG12 | 2.16 | 0.46 |
| 2:0X:241:SER:OG | 2:0X:250:VAL:O | 2.29 | 0.46 |
| 2:0X:253:THR:O | 2:0X:256:GLN:HB3 | 2.16 | 0.46 |
| 2:0X:362:VAL:HG12 | 2:0X:368:LEU:HG | 1.98 | 0.46 |
| 2:1B:4:VAL:HG23 | 2:1B:134:GLY:O | 2.16 | 0.46 |
| 1:1C:66:MET:SD | 1:1C:91:VAL:HG13 | 2.56 | 0.46 |
| 1:1C:392:LYS:HB3 | 1:1C:395:LEU:HD22 | 1.98 | 0.46 |
| 2:1D:199:ASP:HB3 | 2:1D:256:GLN:HE22 | 1.77 | 0.46 |
| 2:1F:123:ARG:NH1 | 2:1F:160:ASP:OD2 | 2.49 | 0.46 |
| 2:1H:71:GLU:HG2 | 2:1H:73:THR:HG22 | 1.98 | 0.46 |
| 2:1H:377:MET:O | 2:1H:378:ILE:HD13 | 2.15 | 0.46 |
| 2:1H:404:PHE:HB3 | 2:1H:407:TRP:CD1 | 2.51 | 0.46 |
| 1:1O:50:TYR:CE2 | 1:1O:241:ARG:HD3 | 2.50 | 0.46 |
| 2:1P:223:THR:HG22 | 2:1P:224:TYR:N | 2.30 | 0.46 |
| 2:1X:286:LEU:O | 2:1X:373:ARG:NH1 | 2.48 | 0.46 |
| 1:2C:209:ASP:N | 1:2C:209:ASP:OD1 | 2.48 | 0.46 |
| 1:2C:279:GLN:HE22 | 1:2C:282:ARG:HD3 | 1.81 | 0.46 |
| 1:2C:418:LEU:HG | 1:2C:422:TYR:CE2 | 2.38 | 0.46 |
| 1:2E:189:VAL:O | 1:2E:193:VAL:HG13 | 2.16 | 0.46 |
| 1:2E:257:LEU:HA | 1:2E:312:THR:HG21 | 1.96 | 0.46 |
| 2:2L:325:PRO:HA | 2:2L:328:VAL:HG22 | 1.97 | 0.46 |
| 2:2N:124:LYS:HA | 2:2N:127:ASP:HB2 | 1.98 | 0.46 |
| 1:2Q:186:THR:HG23 | 1:2Q:415:MET:HG3 | 1.97 | 0.46 |
| 1:2Q:306:ARG:CD | 38:8A:96:GLY:CA | 2.67 | 0.46 |
| 2:2R:333:ALA:O | 2:2R:337:THR:HG23 | 2.15 | 0.46 |
| 2:2T:305:CYS:CB | 2:2T:387:ILE:HD11 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2U:403:MET:HB2 | 1:2U:403:MET:HE3 | 1.70 | 0.46 |
| 2:2V:271:SER:OG | 2:2V:301:MET:HG2 | 2.16 | 0.46 |
| 2:2Z:56:THR:HA | 2:3P:285:GLN:HB2 | 1.98 | 0.46 |
| 2:3B:121:ARG:HD2 | 2:3B:121:ARG:O | 2.16 | 0.46 |
| 2:3D:66:ILE:HD12 | 2:3D:68:LEU:HD23 | 1.98 | 0.46 |
| 2:3F:236:SER:O | 2:3F:243:ARG:NH2 | 2.48 | 0.46 |
| 1:3G:30:ILE:CD1 | 1:3G:59:TYR:HB2 | 2.46 | 0.46 |
| 1:3G:156:ARG:NH1 | 1:3G:197:ASP:OD2 | 2.49 | 0.46 |
| 1:3G:209:ASP:N | 1:3G:209:ASP:OD1 | 2.47 | 0.46 |
| 2:3J:72:PRO:HD2 | 1:3K:2:ARG:NH1 | 2.31 | 0.46 |
| 2:3J:336:LYS:HZ1 | 2:3J:349:THR:HA | 1.81 | 0.46 |
| 1:3K:100:ASN:HB3 | 1:3K:103:LYS:HB2 | 1.98 | 0.46 |
| 1:3K:108:GLU:HA | 1:3K:111:GLU:OE2 | 2.16 | 0.46 |
| 1:3O:178:THR:OG1 | 1:3O:181:GLU:HG3 | 2.16 | 0.46 |
| 2:3P:414:GLU:N | 2:3P:414:GLU:OE1 | 2.48 | 0.46 |
| 1:3S:239:CYS:SG | 1:3S:248:ALA:N | 2.87 | 0.46 |
| 2:3T:79:ARG:O | 2:3T:84:ARG:HG2 | 2.15 | 0.46 |
| 3:3V:158:LEU:HD12 | 3:3V:194:VAL:HG11 | 1.98 | 0.46 |
| 3:4B:158:LEU:HD12 | 3:4B:194:VAL:HG11 | 1.98 | 0.46 |
| 3:4D:229:ASP:HB3 | 3:4D:230:LEU:HD23 | 1.97 | 0.46 |
| 3:4F:158:LEU:HD12 | 3:4F:194:VAL:HG11 | 1.98 | 0.46 |
| 4:4I:172:TYR:HA | 4:4I:176:GLU:OE2 | 2.16 | 0.46 |
| 6:4O:89:ARG:HH12 | 30:7K:452:LEU:H | 1.62 | 0.46 |
| 6:4O:377:ALA:HA | 6:4O:380:ARG:NE | 2.30 | 0.46 |
| 6:4O:465:GLU:OE2 | 6:4P:139:ILE:HD13 | 2.15 | 0.46 |
| 7:4T:357:GLU:OE2 | 7:4T:357:GLU:N | 2.49 | 0.46 |
| 9:4Z:367:GLU:HB3 | 9:4Z:371:LYS:NZ | 2.31 | 0.46 |
| 14:5L:455:GLY:N | 14:5L:458:SER:O | 2.47 | 0.46 |
| 14:5L:577:VAL:HG23 | 14:5L:594:HIS:CE1 | 2.49 | 0.46 |
| 14:5M:455:GLY:N | 14:5M:458:SER:O | 2.47 | 0.46 |
| 15:5O:226:ARG:HG2 | 15:5O:226:ARG:NH1 | 2.16 | 0.46 |
| 15:5P:146:VAL:HA | 15:5P:149:LEU:HG | 1.97 | 0.46 |
| 17:5S:181:LEU:C | 17:5S:181:LEU:CD2 | 2.83 | 0.46 |
| 18:5X:173:HIS:HB3 | 18:5X:211:PHE:HB3 | 1.98 | 0.46 |
| 18:5Y:173:HIS:HB3 | 18:5Y:211:PHE:HB3 | 1.98 | 0.46 |
| 18:5Z:180:ARG:O | 18:5Z:184:THR:HG23 | 2.15 | 0.46 |
| 18:6C:180:ARG:O | 18:6C:184:THR:HG23 | 2.15 | 0.46 |
| 22:6I:170:ARG:NE | 22:6I:174:GLU:OE2 | 2.48 | 0.46 |
| 22:6J:220:ASP:OD2 | 22:6J:221:ASP:N | 2.48 | 0.46 |
| 22:6M:53:THR:HA | 22:6M:57:THR:CG2 | 2.45 | 0.46 |
| 22:6M:307:ARG:O | 22:6M:311:VAL:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:33:LEU:HD12 | 24:6U:33:LEU:H | 1.80 | 0.46 |
| 24:6U:290:ARG:HG3 | 24:6U:291:PRO:HD2 | 1.97 | 0.46 |
| 24:6U:512:TYR:CZ | 24:6U:523:ILE:HG23 | 2.51 | 0.46 |
| 24:6Y:103:LYS:HG2 | 24:6Y:116:ILE:HG12 | 1.97 | 0.46 |
| 30:7K:360:ALA:O | 30:7K:364:LEU:HD23 | 2.16 | 0.46 |
| 33:7Q:137:LEU:HD23 | 33:7Q:137:LEU:HA | 1.82 | 0.46 |
| 2:A0:282:TYR:OH | 24:6X:89:VAL:HG21 | 2.15 | 0.46 |
| 1:A7:276:ARG:NH2 | 24:6T:210:VAL:HG21 | 2.30 | 0.46 |
| 1:D6:47:ILE:HD11 | 22:6O:23:TYR:CD2 | 2.50 | 0.46 |
| 2:E5:279:GLU:OE2 | 22:6L:36:VAL:HG23 | 2.16 | 0.46 |
| 2:G5:12:ALA:HB2 | 41:G5:501:GTP:C8 | 2.51 | 0.46 |
| 2:H1:201:ALA:O | 2:H1:268:MET:HE2 | 2.16 | 0.46 |
| 2:H1:298:PRO:HA | 2:H1:301:MET:HG3 | 1.98 | 0.46 |
| 2:H3:83:TYR:HB3 | 2:H3:86:LEU:HB3 | 1.97 | 0.46 |
| 1:H4:238:CYS:SG | 1:H4:318:ARG:NE | 2.88 | 0.46 |
| 2:I1:119:LEU:O | 2:I1:122:ILE:HG22 | 2.16 | 0.46 |
| 1:I2:4:ILE:HB | 1:I2:50:TYR:CE1 | 2.51 | 0.46 |
| 1:I2:405:GLU:OE1 | 1:I2:405:GLU:N | 2.49 | 0.46 |
| 2:I3:217:LEU:HB3 | 2:I3:219:ILE:CD1 | 2.46 | 0.46 |
| 2:I7:111:GLY:HA2 | 2:I7:114:ILE:HG22 | 1.97 | 0.46 |
| 2:I7:204:LEU:HD23 | 2:I7:231:ILE:HD12 | 1.98 | 0.46 |
| 1:J0:40:SER:CB | 28:7H:413:TYR:CD1 | 2.98 | 0.46 |
| 2:J1:155:GLU:O | 2:J1:158:SER:OG | 2.31 | 0.46 |
| 2:K1:211:ASP:OD2 | 2:K1:215:ARG:NH1 | 2.48 | 0.46 |
| 1:K6:70:PRO:N | 1:K6:92:PHE:HZ | 2.12 | 0.46 |
| 1:K6:345:ILE:HB | 1:K6:348:ASN:HD21 | 1.80 | 0.46 |
| 2:K7:52:PHE:CE2 | 2:K7:243:ARG:HD3 | 2.51 | 0.46 |
| 1:K8:293:MET:HG3 | 1:K8:367:PHE:HB2 | 1.98 | 0.46 |
| 1:L2:404:ASP:HB3 | 1:L2:406:MET:SD | 2.55 | 0.46 |
| 1:L4:204:ASN:ND2 | 39:L4:502:GDP:HN22 | 2.14 | 0.46 |
| 1:L6:77:ARG:HH21 | 1:L6:90:PHE:HD2 | 1.63 | 0.46 |
| 1:L6:306:ARG:HH12 | 28:7X:453:SER:HA | 1.78 | 0.46 |
| 2:L7:394:LYS:HA | 2:L7:397:LEU:HG | 1.97 | 0.46 |
| 2:L9:22:GLU:O | 2:L9:26:LEU:HD23 | 2.16 | 0.46 |
| 1:M0:207:LEU:HB3 | 1:M0:225:LEU:HD22 | 1.98 | 0.46 |
| 1:M0:273:LEU:H | 1:M0:292:GLN:NE2 | 2.14 | 0.46 |
| 2:M5:9:ILE:HD13 | 2:M5:150:GLY:HA2 | 1.98 | 0.46 |
| 2:M5:287:SER:OG | 2:M5:288:VAL:N | 2.48 | 0.46 |
| 1:M6:274:THR:HG21 | 1:M6:282:ARG:HD2 | 1.98 | 0.46 |
| 2:M7:79:ARG:CB | 19:6E:24:TRP:HH2 | 2.27 | 0.46 |
| 2:M7:137:VAL:HG22 | 2:M7:168:GLY:HA2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M8:418:LEU:O | 1:M8:422:TYR:HD2 | 1.99 | 0.46 |
| 1:N0:46:ARG:CZ | 20:6F:12:LEU:HD11 | 2.46 | 0.46 |
| 1:N0:324:LYS:O | 1:N0:328:GLU:HG3 | 2.16 | 0.46 |
| 2:N1:221:ARG:NH2 | 30:7L:309:ASP:HB3 | 2.30 | 0.46 |
| 1:N2:70:PRO:HG2 | 2:N3:2:ARG:HH11 | 1.80 | 0.46 |
| 1:N2:314:SER:OG | 1:N2:368:ILE:HB | 2.16 | 0.46 |
| 2:N7:170:THR:HG21 | 2:N7:194:LEU:HD11 | 1.98 | 0.46 |
| 2:N9:222:PRO:HD2 | 1:O0:324:LYS:HE3 | 1.96 | 0.46 |
| 1:O2:42:LEU:HD13 | 1:O2:356:ILE:HD11 | 1.97 | 0.46 |
| 2:O3:109:THR:OG1 | 2:O3:110:ILE:HD12 | 2.15 | 0.46 |
| 2:O3:114:ILE:HG21 | 2:O3:149:LEU:HD22 | 1.98 | 0.46 |
| 2:O3:246:GLY:HA2 | 2:O3:357:TYR:CD2 | 2.51 | 0.46 |
| 2:O5:324:VAL:HG12 | 2:O5:327:ASP:OD1 | 2.16 | 0.46 |
| 1:O6:65:LEU:HD13 | 1:O6:90:PHE:CE1 | 2.51 | 0.46 |
| 2:O7:384:ILE:HA | 2:O7:387:ILE:HD12 | 1.98 | 0.46 |
| 1:R0:54:ALA:HB3 | 1:R0:58:ARG:HB3 | 1.97 | 0.46 |
| 1:R0:117:LEU:HD11 | 1:R0:154:LYS:HB3 | 1.97 | 0.46 |
| 2:R5:56:THR:CG2 | 2:R5:60:LYS:HB3 | 2.38 | 0.46 |
| 1:R8:58:ARG:HH22 | 21:6H:41:LYS:HB2 | 1.81 | 0.46 |
| 2:R9:47:ASP:OD1 | 2:R9:50:ASN:HB2 | 2.16 | 0.46 |
| 2:R9:183:GLU:HG3 | 2:R9:184:PRO:HD3 | 1.98 | 0.46 |
| 2:S1:79:ARG:O | 2:S1:84:ARG:HG2 | 2.16 | 0.46 |
| 2:S1:155:GLU:OE1 | 2:S1:197:HIS:HE1 | 1.98 | 0.46 |
| 1:S4:172:SER:OG | 1:S4:173:PRO:HD2 | 2.15 | 0.46 |
| 1:S6:192:LEU:HD23 | 1:S6:192:LEU:HA | 1.78 | 0.46 |
| 1:S6:359:LYS:HE2 | 31:7M:26:TRP:HZ2 | 1.80 | 0.46 |
| 2:S9:8:HIS:CD2 | 2:S9:138:PHE:HD2 | 2.34 | 0.46 |
| 2:S9:73:THR:OG1 | 2:S9:74:VAL:N | 2.49 | 0.46 |
| 2:S9:156:ARG:HA | 2:S9:159:VAL:HG22 | 1.98 | 0.46 |
| 2:S9:211:ASP:OD1 | 2:S9:214:ARG:NH1 | 2.48 | 0.46 |
| 1:T0:36:TYR:CG | 1:T0:44:LEU:HD21 | 2.50 | 0.46 |
| 1:T0:272:PRO:HB2 | 1:T0:282:ARG:HH12 | 1.81 | 0.46 |
| 1:T2:317:PHE:HE2 | 1:T2:326:VAL:HG13 | 1.81 | 0.46 |
| 2:T3:274:PRO:HD3 | 2:T3:374:ALA:HA | 1.98 | 0.46 |
| 1:T6:226:ASN:HA | 1:T6:229:ILE:HB | 1.97 | 0.46 |
| 1:U2:211:CYS:HB2 | 1:U2:217:LEU:HD12 | 1.98 | 0.46 |
| 2:U3:88:HIS:CE1 | 2:V9:283:HIS:HA | 2.50 | 0.46 |
| 1:U4:100:ASN:HB3 | 1:U4:103:LYS:HB2 | 1.98 | 0.46 |
| 1:U4:375:GLN:HB3 | 1:U4:422:TYR:CD2 | 2.45 | 0.46 |
| 2:U5:203:MET:HE1 | 2:U5:267:PHE:CB | 2.44 | 0.46 |
| 1:V2:338:SER:O | 1:V2:338:SER:OG | 2.28 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V7:58:ALA:HB3 | 8:4V:421:THR:HG23 | 1.97 | 0.46 |
| 2:V9:9:ILE:HD13 | 2:V9:150:GLY:HA2 | 1.98 | 0.46 |
| 1:W6:418:LEU:O | 1:W6:421:GLU:HG2 | 2.16 | 0.46 |
| 2:W7:51:THR:HG21 | 2:W7:243:ARG:HG2 | 1.97 | 0.46 |
| 2:W7:207:GLU:OE1 | 2:W7:304:LYS:HD3 | 2.16 | 0.46 |
| 2:W7:301:MET:HE1 | 2:W7:307:PRO:HD3 | 1.97 | 0.46 |
| 2:W7:312:TYR:HD2 | 2:W7:315:CYS:SG | 2.39 | 0.46 |
| 2:W9:79:ARG:HG3 | 2:W9:92:LEU:HD23 | 1.96 | 0.46 |
| 1:X2:287:PRO:HA | 1:X2:329:GLN:NE2 | 2.31 | 0.46 |
| 1:X4:20:PHE:HA | 1:X4:230:SER:OG | 2.16 | 0.46 |
| 1:X6:183:TYR:O | 1:X6:187:LEU:HD13 | 2.16 | 0.46 |
| 2:X7:6:SER:OG | 2:X7:136:LEU:HB2 | 2.15 | 0.46 |
| 1:X8:100:ASN:HB3 | 1:X8:103:LYS:HB2 | 1.98 | 0.46 |
| 2:Y1:89:PRO:HD2 | 2:Z7:283:HIS:ND1 | 2.31 | 0.46 |
| 2:Y1:224:TYR:HD1 | 2:Y1:227:LEU:HD12 | 1.80 | 0.46 |
| 1:Y2:309:ARG:H | 1:Y2:372:THR:HG22 | 1.81 | 0.46 |
| 1:Y4:165:LEU:HD11 | 1:Y4:250:LEU:HD13 | 1.98 | 0.46 |
| 2:Y5:88:HIS:CE1 | 2:0B:283:HIS:HA | 2.51 | 0.46 |
| 1:Y8:317:PHE:CE2 | 1:Y8:326:VAL:HG13 | 2.51 | 0.46 |
| 2:Y9:137:VAL:HG23 | 2:Y9:168:GLY:HA2 | 1.98 | 0.46 |
| 2:Z1:296:PHE:CE2 | 2:Z1:335:ILE:HD13 | 2.51 | 0.46 |
| 1:Z8:172:SER:HB3 | 1:Z8:205:GLU:OE2 | 2.16 | 0.46 |
| 1:0C:170:VAL:HG12 | 1:0C:202:LEU:O | 2.16 | 0.46 |
| 1:0E:198:GLU:HA | 1:0E:264:HIS:CD2 | 2.51 | 0.46 |
| 2:0J:205:ASP:OD1 | 2:0J:206:ASN:N | 2.49 | 0.46 |
| 2:0J:208:ALA:O | 2:0J:212:ILE:HG12 | 2.15 | 0.46 |
| 2:0L:145:THR:OG1 | 41:0M:501:GTP:O1B | 2.32 | 0.46 |
| 2:0L:252:ILE:HD12 | 2:0L:255:PHE:CD2 | 2.50 | 0.46 |
| 2:0N:121:ARG:HD2 | 2:0N:124:LYS:HE3 | 1.97 | 0.46 |
| 1:0Q:40:SER:OG | 1:0Q:42:LEU:HG | 2.16 | 0.46 |
| 1:0Q:67:ASP:OD2 | 1:0Q:72:THR:OG1 | 2.23 | 0.46 |
| 2:0R:274:PRO:HB2 | 2:0R:276:ILE:HG12 | 1.98 | 0.46 |
| 1:0S:182:PRO:HG2 | 1:0S:388:MET:CE | 2.46 | 0.46 |
| 2:0V:290:GLU:HA | 2:0V:293:ASN:HD22 | 1.80 | 0.46 |
| 2:0X:176:GLN:NE2 | 2:0X:304:LYS:HE2 | 2.30 | 0.46 |
| 2:0X:260:VAL:HG23 | 2:0X:260:VAL:O | 2.16 | 0.46 |
| 1:0Y:86:ARG:HG2 | 1:0Y:88:ASP:H | 1.80 | 0.46 |
| 1:0Y:248:ALA:HA | 1:0Y:252:LYS:HD2 | 1.97 | 0.46 |
| 2:0Z:417:GLU:HA | 2:0Z:420:GLU:HG2 | 1.98 | 0.46 |
| 2:1D:93:ILE:HD12 | 2:1D:117:LEU:HD21 | 1.98 | 0.46 |
| 1:1E:1:MET:CE | 1:1E:2:ARG:HG3 | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1E:165:LEU:HD13 | 1:1E:167:PHE:CZ | 2.50 | 0.46 |
| 1:1E:244:GLY:H | 1:1E:247:ASN:HD21 | 1.64 | 0.46 |
| 2:1F:224:TYR:O | 2:1F:228:ASN:ND2 | 2.39 | 0.46 |
| 1:1G:97:ALA:HA | 1:1G:103:LYS:HE3 | 1.97 | 0.46 |
| 2:1L:88:HIS:CG | 2:1L:89:PRO:CD | 2.99 | 0.46 |
| 2:1L:266:HIS:O | 2:1L:266:HIS:ND1 | 2.47 | 0.46 |
| 1:1M:8:GLN:O | 1:1M:66:MET:HG3 | 2.15 | 0.46 |
| 1:1M:317:PHE:HB3 | 1:1M:321:MET:SD | 2.55 | 0.46 |
| 2:1N:121:ARG:HD2 | 2:1N:124:LYS:HE3 | 1.98 | 0.46 |
| 2:1X:298:PRO:HA | 2:1X:301:MET:HG3 | 1.98 | 0.46 |
| 1:2C:75:SER:O | 1:2C:78:SER:OG | 2.29 | 0.46 |
| 1:2C:201:VAL:HG22 | 1:2C:266:PHE:O | 2.16 | 0.46 |
| 2:2H:123:ARG:NH2 | 38:8B:37:TYR:CB | 2.78 | 0.46 |
| 1:2I:301:CYS:SG | 1:2I:302:ALA:N | 2.88 | 0.46 |
| 2:2J:58:ALA:O | 10:5C:431:LYS:HE3 | 2.15 | 0.46 |
| 1:2M:170:VAL:HG22 | 1:2M:202:LEU:O | 2.16 | 0.46 |
| 2:2N:251:ASP:OD1 | 2:2N:253:THR:HG22 | 2.15 | 0.46 |
| 2:2R:251:ASP:OD2 | 2:2R:253:THR:N | 2.48 | 0.46 |
| 1:2S:333:VAL:HG22 | 38:8A:54:THR:HG22 | 1.98 | 0.46 |
| 2:2T:51:THR:HG21 | 2:2T:243:ARG:HG2 | 1.98 | 0.46 |
| 1:2U:117:LEU:HG | 1:2U:121:ARG:NH2 | 2.31 | 0.46 |
| 2:2V:88:HIS:HB2 | 2:3L:283:HIS:ND1 | 2.30 | 0.46 |
| 1:2W:273:LEU:H | 1:2W:292:GLN:NE2 | 2.14 | 0.46 |
| 1:2W:325:GLU:O | 1:2W:329:GLN:HG2 | 2.16 | 0.46 |
| 2:2X:195:LEU:HD11 | 2:2X:428:LEU:HD22 | 1.98 | 0.46 |
| 1:2Y:68:LEU:HG | 1:2Y:147:MET:HE1 | 1.98 | 0.46 |
| 1:3A:376:GLU:HA | 1:3A:379:LYS:HD2 | 1.98 | 0.46 |
| 1:3C:212:PHE:CZ | 38:8D:117:TRP:HB3 | 2.51 | 0.46 |
| 1:3C:236:ILE:HG23 | 1:3C:237:THR:HG23 | 1.98 | 0.46 |
| 2:3D:280:LYS:O | 2:3D:283:HIS:HB3 | 2.16 | 0.46 |
| 2:3F:88:HIS:HE1 | 3:3V:34:SER:CB | 2.29 | 0.46 |
| 2:3H:417:GLU:HA | 2:3H:420:GLU:HG2 | 1.98 | 0.46 |
| 2:3J:21:TRP:CZ2 | 2:3J:65:CYS:HB3 | 2.51 | 0.46 |
| 2:3J:221:ARG:HG2 | 38:8B:177:HIS:HA | 1.98 | 0.46 |
| 1:3K:210:ILE:HA | 1:3K:297:LYS:HZ3 | 1.79 | 0.46 |
| 1:3Q:100:ASN:HB3 | 1:3Q:103:LYS:HB2 | 1.96 | 0.46 |
| 2:3T:114:ILE:HG21 | 2:3T:149:LEU:HD22 | 1.98 | 0.46 |
| 2:3T:116:ASP:O | 2:3T:119:LEU:HG | 2.15 | 0.46 |
| 3:3V:229:ASP:HB3 | 3:3V:230:LEU:HD23 | 1.97 | 0.46 |
| 4:3W:172:TYR:HA | 4:3W:176:GLU:OE2 | 2.16 | 0.46 |
| 3:3X:158:LEU:HD12 | 3:3X:194:VAL:HG11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4A:172:TYR:HA | 4:4A:176:GLU:OE2 | 2.16 | 0.46 |
| 3:4B:229:ASP:HB3 | 3:4B:230:LEU:HD23 | 1.97 | 0.46 |
| 4:4C:172:TYR:HA | 4:4C:176:GLU:OE2 | 2.16 | 0.46 |
| 3:4D:7:GLY:C | 3:4D:140:LYS:HE2 | 2.37 | 0.46 |
| 4:4E:172:TYR:HA | 4:4E:176:GLU:OE2 | 2.16 | 0.46 |
| 3:4H:7:GLY:C | 3:4H:140:LYS:HE2 | 2.37 | 0.46 |
| 3:4H:229:ASP:HB3 | 3:4H:230:LEU:HD23 | 1.97 | 0.46 |
| 5:4M:292:ALA:O | 5:4M:296:GLU:HG3 | 2.16 | 0.46 |
| 6:4O:208:GLU:O | 6:4O:211:GLU:HG3 | 2.15 | 0.46 |
| 8:4W:356:ALA:O | 8:4W:360:GLU:HG2 | 2.16 | 0.46 |
| 10:5A:451:HIS:O | 10:5A:454:GLU:HG2 | 2.16 | 0.46 |
| 10:5B:247:GLU:O | 10:5B:251:GLU:HG3 | 2.16 | 0.46 |
| 10:5B:257:GLN:HG3 | 10:5B:261:LYS:HZ2 | 1.81 | 0.46 |
| 12:5F:336:GLY:HA3 | 12:5F:380:TRP:CZ2 | 2.50 | 0.46 |
| 14:5L:478:LYS:HD3 | 14:5L:483:GLU:HB2 | 1.98 | 0.46 |
| 14:5N:78:TYR:HB3 | 14:5N:81:PHE:CD2 | 2.51 | 0.46 |
| 14:5N:455:GLY:N | 14:5N:458:SER:O | 2.47 | 0.46 |
| 14:5N:577:VAL:HG23 | 14:5N:594:HIS:CE1 | 2.49 | 0.46 |
| 15:5P:99:LYS:HD2 | 15:5P:203:ASN:O | 2.16 | 0.46 |
| 15:5P:332:PRO:HG3 | 15:5P:350:ASP:CA | 2.45 | 0.46 |
| 18:6D:180:ARG:O | 18:6D:184:THR:HG23 | 2.15 | 0.46 |
| 22:6K:201:ARG:HB3 | 22:6K:237:TYR:HB3 | 1.97 | 0.46 |
| 23:6S:54:ASN:N | 23:6S:54:ASN:OD1 | 2.47 | 0.46 |
| 24:6U:345:ASP:N | 24:6U:345:ASP:OD2 | 2.47 | 0.46 |
| 38:7Z:21:LYS:HG2 | 38:7Z:22:THR:N | 2.29 | 0.46 |
| 2:2:415:GLU:OE2 | 4:3W:86:TYR:OH | 2.16 | 0.46 |
| 1:G2:15:GLN:HB3 | 1:G2:226:ASN:HD21 | 1.81 | 0.46 |
| 2:G5:9:ILE:CG1 | 2:G5:139:ASN:HB3 | 2.45 | 0.46 |
| 2:G5:298:PRO:HA | 2:G5:301:MET:HG2 | 1.97 | 0.46 |
| 2:G5:333:ALA:O | 2:G5:337:THR:HG23 | 2.15 | 0.46 |
| 1:G6:169:VAL:HG12 | 1:G6:202:LEU:HB2 | 1.97 | 0.46 |
| 1:G8:58:ARG:HD3 | 1:I4:280:GLN:HE22 | 1.81 | 0.46 |
| 1:G8:167:PHE:CE2 | 1:G8:233:MET:HG2 | 2.51 | 0.46 |
| 2:G9:193:SER:HB3 | 2:G9:197:HIS:CE1 | 2.50 | 0.46 |
| 2:H1:2:ARG:HA | 2:H1:133:GLN:HE21 | 1.81 | 0.46 |
| 2:H9:143:GLY:O | 2:H9:147:SER:OG | 2.23 | 0.46 |
| 1:I0:39:ASP:OD1 | 1:I0:39:ASP:N | 2.46 | 0.46 |
| 2:I3:331:SER:O | 2:I3:334:THR:N | 2.49 | 0.46 |
| 1:I4:112:LEU:O | 1:I4:115:SER:OG | 2.31 | 0.46 |
| 2:I5:191:THR:HA | 2:I5:194:LEU:HB3 | 1.97 | 0.46 |
| 2:I5:402:ARG:NH2 | 2:I5:415:GLU:HG2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I5:430:LYS:HD3 | 2:I5:430:LYS:O | 2.15 | 0.46 |
| 2:I9:230:LEU:HD12 | 2:I9:231:ILE:HD13 | 1.97 | 0.46 |
| 1:J0:70:PRO:N | 1:J0:92:PHE:HZ | 2.14 | 0.46 |
| 1:J0:135:VAL:HG21 | 1:J0:152:ILE:HD11 | 1.98 | 0.46 |
| 2:J3:90:GLU:HB3 | 2:J3:121:ARG:NH1 | 2.22 | 0.46 |
| 2:J5:328:VAL:O | 2:J5:332:VAL:HG23 | 2.16 | 0.46 |
| 2:J7:155:GLU:HG3 | 2:J7:197:HIS:NE2 | 2.31 | 0.46 |
| 1:K0:334:GLN:HE22 | 1:K0:348:ASN:H | 1.64 | 0.46 |
| 2:K3:420:GLU:HA | 2:K3:423:GLU:HG3 | 1.98 | 0.46 |
| 2:L5:35:GLN:N | 2:L5:35:GLN:OE1 | 2.49 | 0.46 |
| 2:M3:305:CYS:HB3 | 2:M3:387:ILE:HD11 | 1.98 | 0.46 |
| 2:M5:69:ASP:OD2 | 2:M5:71:GLU:N | 2.49 | 0.46 |
| 1:M6:125:GLU:HB3 | 37:7Y:93:LYS:HA | 1.98 | 0.46 |
| 2:M7:236:SER:O | 2:M7:243:ARG:NH2 | 2.49 | 0.46 |
| 2:M9:72:PRO:HG3 | 1:N0:1:MET:HG2 | 1.98 | 0.46 |
| 1:N0:7:ILE:HB | 1:N0:135:VAL:HG22 | 1.98 | 0.46 |
| 1:N2:178:THR:OG1 | 1:N2:181:GLU:HG3 | 2.16 | 0.46 |
| 2:N3:229:ARG:HE | 2:N3:363:VAL:CG2 | 2.29 | 0.46 |
| 1:N6:344:TRP:CE3 | 1:N6:345:ILE:HG13 | 2.51 | 0.46 |
| 2:N9:85:GLN:O | 2:P7:283:HIS:CE1 | 2.64 | 0.46 |
| 1:O0:174:LYS:NZ | 27:7G:7:ASN:OD1 | 2.43 | 0.46 |
| 2:O1:62:VAL:HA | 2:O1:63:PRO:HD3 | 1.80 | 0.46 |
| 1:O4:185:ALA:O | 1:O4:189:VAL:HG12 | 2.16 | 0.46 |
| 2:O5:183:GLU:HG3 | 2:O5:184:PRO:HD3 | 1.98 | 0.46 |
| 2:O7:69:ASP:OD1 | 2:O7:70:LEU:N | 2.47 | 0.46 |
| 1:O8:86:ARG:HG2 | 1:O8:88:ASP:H | 1.80 | 0.46 |
| 2:O9:9:ILE:HD13 | 2:O9:150:GLY:HA2 | 1.97 | 0.46 |
| 2:O9:253:THR:HA | 2:O9:256:GLN:HG2 | 1.98 | 0.46 |
| 2:P3:175:PRO:HB3 | 2:P3:390:ARG:NE | 2.31 | 0.46 |
| 2:P7:73:THR:OG1 | 2:P7:74:VAL:N | 2.49 | 0.46 |
| 1:P8:301:CYS:SG | 1:P8:302:ALA:N | 2.88 | 0.46 |
| 2:P9:345:ASP:OD1 | 2:P9:346:TRP:N | 2.49 | 0.46 |
| 1:Q2:214:THR:OG1 | 1:Q2:215:LEU:N | 2.49 | 0.46 |
| 2:Q3:392:ASP:OD2 | 2:Q3:422:ARG:NH1 | 2.48 | 0.46 |
| 1:Q4:128:ASP:OD1 | 1:Q4:129:CYS:N | 2.43 | 0.46 |
| 2:Q5:177:VAL:HG13 | 1:Q6:327:ASP:HB3 | 1.98 | 0.46 |
| 1:Q8:114:ASP:OD2 | 1:Q8:115:SER:N | 2.47 | 0.46 |
| 2:Q9:217:LEU:HD21 | 2:Q9:368:LEU:HD23 | 1.98 | 0.46 |
| 1:R0:314:SER:HA | 1:R0:350:LYS:O | 2.16 | 0.46 |
| 2:S1:259:LEU:HD21 | 2:S1:316:CYS:HB2 | 1.98 | 0.46 |
| 2:S1:367:ASP:HA | 7:4R:342:ARG:HH12 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:391:ARG:HG3 | 2:S5:346:TRP:CE2 | 2.51 | 0.46 |
| 2:S7:227:LEU:O | 2:S7:231:ILE:HG12 | 2.15 | 0.46 |
| 1:S8:287:PRO:HA | 1:S8:290:THR:HG22 | 1.98 | 0.46 |
| 1:S8:334:GLN:NE2 | 1:S8:348:ASN:H | 2.13 | 0.46 |
| 1:T2:391:ARG:O | 2:T3:262:TYR:OH | 2.34 | 0.46 |
| 1:T6:31:ASP:OD1 | 1:T6:33:THR:HG22 | 2.16 | 0.46 |
| 1:T6:173:PRO:HD3 | 1:T6:380:ARG:NH1 | 2.31 | 0.46 |
| 1:T6:273:LEU:O | 1:T6:292:GLN:NE2 | 2.47 | 0.46 |
| 2:T7:203:MET:HE1 | 2:T7:267:PHE:HD1 | 1.81 | 0.46 |
| 1:U2:232:VAL:O | 1:U2:236:ILE:HG12 | 2.16 | 0.46 |
| 1:U4:316:LEU:HD23 | 1:U4:352:SER:HB3 | 1.98 | 0.46 |
| 1:U6:325:GLU:O | 1:U6:329:GLN:HG2 | 2.16 | 0.46 |
| 2:U7:66:ILE:O | 2:U7:66:ILE:HG13 | 2.16 | 0.46 |
| 2:U9:9:ILE:HD12 | 2:U9:150:GLY:HA3 | 1.98 | 0.46 |
| 1:V0:208:TYR:CE1 | 1:V0:225:LEU:HD11 | 2.51 | 0.46 |
| 1:V0:276:ARG:NH1 | 1:V0:279:GLN:HB3 | 2.31 | 0.46 |
| 2:V1:22:GLU:HB2 | 2:V1:83:TYR:HE2 | 1.81 | 0.46 |
| 1:V2:371:SER:OG | 1:V2:372:THR:N | 2.49 | 0.46 |
| 2:V3:287:SER:N | 2:V3:290:GLU:OE2 | 2.48 | 0.46 |
| 1:V4:172:SER:OG | 1:V4:380:ARG:NH1 | 2.49 | 0.46 |
| 1:V6:20:PHE:O | 1:V6:24:VAL:HG23 | 2.16 | 0.46 |
| 1:W2:5:VAL:HG23 | 1:W2:62:ARG:HG2 | 1.97 | 0.46 |
| 1:X2:114:ASP:N | 1:X2:114:ASP:OD1 | 2.49 | 0.46 |
| 2:X5:90:GLU:HB2 | 2:Z1:283:HIS:CE1 | 2.51 | 0.46 |
| 2:X7:23:LEU:O | 2:X7:27:GLU:HG2 | 2.15 | 0.46 |
| 1:Y0:51:PHE:HB3 | 1:Y0:59:TYR:HB3 | 1.98 | 0.46 |
| 1:Y2:2:ARG:HE | 1:Y2:240:LEU:HD22 | 1.80 | 0.46 |
| 2:Y3:88:HIS:HB3 | 2:Z9:283:HIS:CG | 2.51 | 0.46 |
| 2:Y3:313:MET:SD | 2:Y3:380:ASN:ND2 | 2.89 | 0.46 |
| 1:Y6:418:LEU:O | 1:Y6:421:GLU:HG3 | 2.16 | 0.46 |
| 1:Z2:198:GLU:HA | 1:Z2:264:HIS:HB2 | 1.98 | 0.46 |
| 2:Z3:209:ILE:HG21 | 2:Z3:227:LEU:HG | 1.98 | 0.46 |
| 2:Z5:19:ALA:O | 2:Z5:22:GLU:HG3 | 2.16 | 0.46 |
| 2:Z5:56:THR:HA | 2:0L:285:GLN:CG | 2.46 | 0.46 |
| 2:Z7:236:SER:HA | 2:Z7:239:THR:HG22 | 1.98 | 0.46 |
| 2:Z7:394:LYS:HD2 | 1:Z8:346:PRO:HG3 | 1.98 | 0.46 |
| 1:Z8:358:PRO:HG2 | 1:Z8:361:LEU:HB2 | 1.96 | 0.46 |
| 1:0C:240:LEU:HD11 | 1:0C:250:LEU:CD1 | 2.46 | 0.46 |
| 2:0F:28:HIS:CE1 | 2:0F:49:PHE:HA | 2.50 | 0.46 |
| 2:0F:90:GLU:HB2 | 2:0V:283:HIS:CE1 | 2.50 | 0.46 |
| 2:0F:116:ASP:N | 2:0F:116:ASP:OD1 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0O:418:LEU:O | 1:0O:421:GLU:HG2 | 2.16 | 0.46 |
| 2:0R:286:LEU:HD11 | 2:0R:372:GLN:HB2 | 1.98 | 0.46 |
| 2:0R:403:ALA:HB2 | 1:0S:344:TRP:HZ3 | 1.81 | 0.46 |
| 2:0V:108:TYR:HA | 2:0V:112:LYS:HE2 | 1.99 | 0.46 |
| 2:0Z:267:PHE:HB2 | 2:0Z:384:ILE:HD12 | 1.98 | 0.46 |
| 1:1C:68:LEU:HG | 1:1C:147:MET:HE1 | 1.98 | 0.46 |
| 1:1E:166:THR:OG1 | 1:1E:199:CYS:SG | 2.73 | 0.46 |
| 2:1F:72:PRO:HD2 | 1:1G:2:ARG:NH1 | 2.30 | 0.46 |
| 2:1F:147:SER:OG | 2:1F:148:GLY:N | 2.49 | 0.46 |
| 1:1G:27:GLU:OE1 | 1:1G:318:ARG:NH2 | 2.48 | 0.46 |
| 1:1G:242:PHE:CD1 | 1:1G:356:ILE:HG13 | 2.50 | 0.46 |
| 1:1Q:8:GLN:CD | 1:1Q:17:GLY:HA3 | 2.37 | 0.46 |
| 1:1W:215:LEU:HB3 | 1:1W:217:LEU:HG | 1.98 | 0.46 |
| 2:1Z:90:GLU:HB3 | 2:1Z:121:ARG:HH22 | 1.81 | 0.46 |
| 2:2B:120:ASP:OD1 | 38:8A:73:TRP:CE2 | 2.68 | 0.46 |
| 2:2B:204:LEU:HD22 | 2:2B:231:ILE:HD12 | 1.98 | 0.46 |
| 2:2B:428:LEU:HG | 2:2B:432:PHE:HE2 | 1.81 | 0.46 |
| 2:2D:406:HIS:HA | 2:2D:409:VAL:HG12 | 1.98 | 0.46 |
| 2:2F:69:ASP:OD1 | 2:2F:70:LEU:N | 2.45 | 0.46 |
| 2:2F:90:GLU:H | 2:2V:283:HIS:CE1 | 2.34 | 0.46 |
| 2:2L:238:LEU:HD12 | 2:2L:318:MET:HG3 | 1.98 | 0.46 |
| 2:2L:274:PRO:HB2 | 2:2L:276:ILE:CG1 | 2.46 | 0.46 |
| 1:2Q:173:PRO:HD2 | 1:2Q:380:ARG:CZ | 2.46 | 0.46 |
| 2:2T:201:ALA:O | 2:2T:268:MET:HE2 | 2.16 | 0.46 |
| 2:2T:312:TYR:HB2 | 2:2T:343:PHE:HD1 | 1.80 | 0.46 |
| 2:2X:214:ARG:NH2 | 38:8B:18:VAL:HG13 | 2.31 | 0.46 |
| 1:2Y:396:HIS:HE1 | 1:2Y:397:TRP:CZ2 | 2.33 | 0.46 |
| 2:3B:241:SER:OG | 2:3B:250:VAL:O | 2.28 | 0.46 |
| 2:3B:414:GLU:HG2 | 2:3B:417:GLU:OE1 | 2.15 | 0.46 |
| 2:3D:244:PHE:HB2 | 2:3D:356:ASN:HD21 | 1.81 | 0.46 |
| 1:3G:138:SER:OG | 1:3G:139:LEU:N | 2.48 | 0.46 |
| 1:3K:192:LEU:HD23 | 1:3K:192:LEU:HA | 1.81 | 0.46 |
| 2:3L:178:SER:HB2 | 2:3L:183:GLU:OE2 | 2.15 | 0.46 |
| 2:3P:223:THR:HG22 | 1:3Q:322:SER:HA | 1.98 | 0.46 |
| 2:3P:251:ASP:OD1 | 2:3P:251:ASP:N | 2.43 | 0.46 |
| 1:3S:121:ARG:O | 1:3S:125:GLU:OE1 | 2.34 | 0.46 |
| 2:3T:393:HIS:O | 2:3T:397:LEU:HG | 2.16 | 0.46 |
| 3:3X:229:ASP:HB3 | 3:3X:230:LEU:HD23 | 1.97 | 0.46 |
| 3:3Z:7:GLY:C | 3:3Z:140:LYS:HE2 | 2.37 | 0.46 |
| 5:4M:13:GLN:OE1 | 5:4M:16:ARG:NH2 | 2.49 | 0.46 |
| 5:4M:321:LEU:HA | 5:4M:324:MET:HG2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:4O:80:MET:O | 6:4O:84:LEU:HG | 2.16 | 0.46 |
| 7:4U:199:VAL:HG12 | 31:7N:60:ILE:CD1 | 2.46 | 0.46 |
| 10:5A:458:ARG:NH1 | 10:5A:458:ARG:HB3 | 2.30 | 0.46 |
| 10:5B:87:ALA:O | 10:5B:90:LYS:HG3 | 2.15 | 0.46 |
| 10:5B:111:GLU:O | 10:5B:115:GLN:HG2 | 2.16 | 0.46 |
| 11:5E:115:LEU:HD13 | 11:5E:120:PHE:HD2 | 1.82 | 0.46 |
| 14:5L:188:ALA:HA | 14:5L:226:VAL:HG11 | 1.94 | 0.46 |
| 14:5M:577:VAL:HG23 | 14:5M:594:HIS:CE1 | 2.50 | 0.46 |
| 14:5N:478:LYS:HD3 | 14:5N:483:GLU:HB2 | 1.98 | 0.46 |
| 15:5O:8:CYS:HA | 15:5O:26:LEU:O | 2.16 | 0.46 |
| 15:5O:55:LEU:N | 15:5O:55:LEU:HD23 | 2.31 | 0.46 |
| 15:5O:66:VAL:O | 15:5O:73:LEU:HD23 | 2.16 | 0.46 |
| 15:5O:291:ALA:CB | 15:5O:297:MET:HE1 | 2.23 | 0.46 |
| 15:5P:303:SER:O | 15:5P:303:SER:OG | 2.27 | 0.46 |
| 22:6I:342:ASP:O | 22:6I:346:PHE:HB2 | 2.16 | 0.46 |
| 22:6L:54:ARG:HA | 24:6W:285:MET:SD | 2.56 | 0.46 |
| 23:6Q:54:ASN:OD1 | 23:6Q:54:ASN:N | 2.47 | 0.46 |
| 24:6T:386:THR:OG1 | 24:6T:388:GLU:HG3 | 2.16 | 0.46 |
| 24:6U:592:ASP:N | 24:6U:592:ASP:OD1 | 2.48 | 0.46 |
| 24:6V:112:GLU:HB2 | 24:6V:209:PRO:HG2 | 1.98 | 0.46 |
| 24:6V:615:ARG:HG2 | 24:6V:616:LEU:HD23 | 1.98 | 0.46 |
| 24:6Z:435:LEU:O | 24:6Z:439:MET:HG2 | 2.16 | 0.46 |
| 24:6Z:469:PHE:CE2 | 24:6Z:482:ILE:HG23 | 2.51 | 0.46 |
| 24:6Z:484:GLU:HG2 | 24:6Z:495:GLY:O | 2.16 | 0.46 |
| 25:7C:6:ARG:O | 25:7C:10:GLU:HG2 | 2.15 | 0.46 |
| 30:7L:357:GLU:HG2 | 30:7L:358:PRO:HD2 | 1.98 | 0.46 |
| 34:7R:90:LEU:HA | 34:7R:93:GLU:HG3 | 1.97 | 0.46 |
| 34:7R:103:LEU:O | 34:7R:107:LYS:HG2 | 2.16 | 0.46 |
| 34:7R:206:GLY:HA2 | 34:7R:209:THR:HG22 | 1.98 | 0.46 |
| 37:7Y:59:PRO:O | 37:7Y:62:GLN:HB2 | 2.15 | 0.46 |
| 37:7Y:87:VAL:O | 37:7Y:87:VAL:HG13 | 2.16 | 0.46 |
| 38:8D:220:VAL:HG13 | 38:8D:221:ARG:N | 2.31 | 0.46 |
| 1:A7:204:ASN:OD1 | 39:A7:501:GDP:O2' | 2.34 | 0.45 |
| 1:C6:11:GLN:HB3 | 39:C6:501:GDP:O1A | 2.15 | 0.45 |
| 2:F9:39:ASP:O | 24:6U:537:GLU:HB2 | 2.14 | 0.45 |
| 1:G6:244:GLY:HA2 | 1:G6:355:ASP:OD1 | 2.17 | 0.45 |
| 2:G7:153:LEU:HD23 | 2:G7:153:LEU:HA | 1.80 | 0.45 |
| 2:H1:216:SER:OG | 2:H1:217:LEU:N | 2.49 | 0.45 |
| 2:H3:56:THR:HG21 | 2:I9:283:HIS:O | 2.17 | 0.45 |
| 1:H4:315:ALA:HB1 | 1:H4:317:PHE:CE1 | 2.51 | 0.45 |
| 2:H5:200:VAL:HG13 | 2:H5:268:MET:HE3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H6:260:PHE:HB2 | 1:H6:263:LEU:HD23 | 1.97 | 0.45 |
| 1:I2:91:VAL:CG1 | 1:I2:116:VAL:HG12 | 2.46 | 0.45 |
| 2:I3:248:LEU:HD22 | 2:I3:354:GLY:HA2 | 1.98 | 0.45 |
| 2:I3:317:LEU:HB3 | 2:I3:319:TYR:HE1 | 1.82 | 0.45 |
| 2:I3:323:VAL:HG22 | 2:I3:373:ARG:HD3 | 1.98 | 0.45 |
| 1:I4:149:THR:O | 1:I4:152:ILE:HG22 | 2.15 | 0.45 |
| 2:I7:222:PRO:CD | 1:I8:324:LYS:HE3 | 2.46 | 0.45 |
| 2:I7:245:ASP:N | 2:I7:245:ASP:OD1 | 2.49 | 0.45 |
| 2:I7:311:LYS:HE3 | 2:I7:344:VAL:HA | 1.98 | 0.45 |
| 2:I7:415:GLU:N | 2:I7:415:GLU:OE1 | 2.49 | 0.45 |
| 1:I8:421:GLU:HA | 1:I8:424:GLN:HB3 | 1.98 | 0.45 |
| 1:J4:33:THR:HG21 | 5:4M:120:ARG:HD3 | 1.97 | 0.45 |
| 2:J5:320:ARG:HE | 2:J5:320:ARG:HB3 | 1.53 | 0.45 |
| 2:J7:14:ILE:HD11 | 2:J7:74:VAL:HG13 | 1.97 | 0.45 |
| 1:K0:289:LEU:HD23 | 1:K0:365:ALA:HB2 | 1.97 | 0.45 |
| 2:K1:384:ILE:HD12 | 2:K1:387:ILE:HD12 | 1.98 | 0.45 |
| 1:K4:274:THR:OG1 | 1:K4:279:GLN:OE1 | 2.32 | 0.45 |
| 2:K5:21:TRP:CZ2 | 2:K5:65:CYS:HB2 | 2.51 | 0.45 |
| 1:L4:74:ASP:O | 1:L4:78:SER:OG | 2.26 | 0.45 |
| 2:L5:328:VAL:HG11 | 2:L5:355:ILE:HD11 | 1.97 | 0.45 |
| 2:L9:102:ASN:HB3 | 2:L9:105:ARG:HB3 | 1.98 | 0.45 |
| 1:M0:140:GLY:O | 1:M0:184:ASN:ND2 | 2.37 | 0.45 |
| 2:M5:33:ASP:N | 2:M5:33:ASP:OD1 | 2.48 | 0.45 |
| 2:M9:102:ASN:HB3 | 2:M9:105:ARG:HB3 | 1.98 | 0.45 |
| 2:M9:276:ILE:HG22 | 2:M9:281:ALA:HB2 | 1.98 | 0.45 |
| 2:N1:100:ALA:HB1 | 1:N2:252:LYS:HB3 | 1.98 | 0.45 |
| 1:N2:172:SER:OG | 1:N2:380:ARG:NH2 | 2.50 | 0.45 |
| 1:O0:22:GLU:HG2 | 1:O0:81:TYR:CD2 | 2.51 | 0.45 |
| 1:O0:412:GLU:O | 1:O0:416:ASN:ND2 | 2.49 | 0.45 |
| 1:O4:285:THR:HG23 | 1:O4:287:PRO:HD2 | 1.97 | 0.45 |
| 1:O8:68:LEU:HD13 | 1:O8:108:GLU:HG2 | 1.98 | 0.45 |
| 2:O9:52:PHE:CE2 | 2:O9:243:ARG:HD3 | 2.50 | 0.45 |
| 2:P3:53:PHE:O | 2:P3:64:ARG:NH2 | 2.50 | 0.45 |
| 1:P4:259:PRO:HG3 | 1:P4:311:LEU:HD21 | 1.99 | 0.45 |
| 2:P5:15:GLN:HB3 | 2:P5:228:ASN:ND2 | 2.30 | 0.45 |
| 1:P6:405:GLU:HA | 1:P6:408:PHE:HD2 | 1.80 | 0.45 |
| 2:P7:176:GLN:HG2 | 2:P7:177:VAL:N | 2.31 | 0.45 |
| 1:P8:8:GLN:OE1 | 1:P8:17:GLY:HA3 | 2.16 | 0.45 |
| 1:Q0:317:PHE:HB3 | 1:Q0:321:MET:SD | 2.56 | 0.45 |
| 2:Q1:210:TYR:HH | 2:Q1:224:TYR:HE1 | 1.64 | 0.45 |
| 1:Q8:190:HIS:HD2 | 1:Q8:414:ASN:HB2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q9:110:ILE:HA | 2:Q9:113:GLU:OE1 | 2.16 | 0.45 |
| 1:R0:397:TRP:CZ2 | 2:R1:256:GLN:HB3 | 2.52 | 0.45 |
| 2:R1:416:GLY:HA3 | 17:5S:76:PRO:HG3 | 1.97 | 0.45 |
| 2:R5:69:ASP:OD1 | 2:R5:70:LEU:N | 2.45 | 0.45 |
| 2:R7:7:ILE:HD12 | 2:R7:153:LEU:HD21 | 1.97 | 0.45 |
| 2:R7:73:THR:OG1 | 2:R7:74:VAL:N | 2.49 | 0.45 |
| 2:R7:176:GLN:HG2 | 2:R7:177:VAL:N | 2.31 | 0.45 |
| 1:S0:58:ARG:NH2 | 1:T6:280:GLN:OE1 | 2.49 | 0.45 |
| 2:S1:298:PRO:HB3 | 2:S1:307:PRO:HD2 | 1.97 | 0.45 |
| 1:S2:328:GLU:O | 1:S2:332:ASN:ND2 | 2.49 | 0.45 |
| 1:S4:287:PRO:HA | 1:S4:290:THR:HG22 | 1.98 | 0.45 |
| 1:S4:330:MET:HA | 1:S4:333:VAL:HG12 | 1.98 | 0.45 |
| 1:S8:100:ASN:HB3 | 1:S8:103:LYS:HB2 | 1.97 | 0.45 |
| 2:S9:137:VAL:HG22 | 2:S9:168:GLY:HA2 | 1.98 | 0.45 |
| 1:T2:190:HIS:HD2 | 1:T2:414:ASN:HB2 | 1.80 | 0.45 |
| 2:T3:113:GLU:N | 2:T3:113:GLU:OE1 | 2.49 | 0.45 |
| 2:T5:14:ILE:O | 2:T5:18:ASN:HB2 | 2.16 | 0.45 |
| 1:T6:325:GLU:HA | 1:T6:328:GLU:HG2 | 1.97 | 0.45 |
| 1:U2:229:ILE:HG22 | 1:U2:233:MET:SD | 2.56 | 0.45 |
| 1:U2:279:GLN:NE2 | 1:U2:282:ARG:HH21 | 2.13 | 0.45 |
| 2:U7:27:GLU:OE1 | 2:U7:243:ARG:NH1 | 2.49 | 0.45 |
| 2:U7:223:THR:OG1 | 2:U7:224:TYR:N | 2.50 | 0.45 |
| 1:U8:173:PRO:HD2 | 1:U8:174:LYS:HZ3 | 1.80 | 0.45 |
| 2:U9:119:LEU:HA | 2:U9:122:ILE:HG22 | 1.98 | 0.45 |
| 1:V2:45:GLU:HG2 | 1:V2:46:ARG:HG2 | 1.97 | 0.45 |
| 1:V2:361:LEU:HG | 1:V2:363:MET:H | 1.80 | 0.45 |
| 1:V6:5:VAL:HG22 | 1:V6:133:PHE:HD1 | 1.80 | 0.45 |
| 1:V6:77:ARG:O | 1:V6:83:GLN:NE2 | 2.45 | 0.45 |
| 1:V6:290:THR:HG21 | 1:V6:329:GLN:NE2 | 2.31 | 0.45 |
| 2:V9:275:ILE:HG13 | 2:V9:275:ILE:O | 2.16 | 0.45 |
| 2:W3:157:LEU:HD23 | 2:W3:157:LEU:HA | 1.80 | 0.45 |
| 1:W4:31:ASP:OD1 | 1:W4:34:GLY:N | 2.48 | 0.45 |
| 2:W9:11:GLN:O | 2:W9:14:ILE:HG12 | 2.16 | 0.45 |
| 1:X0:22:GLU:HG2 | 1:X0:81:TYR:HD2 | 1.82 | 0.45 |
| 1:X0:44:LEU:HD13 | 1:X0:47:ILE:HD11 | 1.97 | 0.45 |
| 1:X0:167:PHE:CZ | 1:X0:233:MET:HG2 | 2.51 | 0.45 |
| 1:X2:266:PHE:HB3 | 1:X2:368:ILE:HD11 | 1.98 | 0.45 |
| 2:X3:167:LEU:HG | 2:X3:252:ILE:HD11 | 1.97 | 0.45 |
| 1:X4:3:GLU:HG3 | 1:X4:127:CYS:SG | 2.56 | 0.45 |
| 1:X4:179:VAL:HG13 | 2:X5:349:THR:O | 2.16 | 0.45 |
| 2:X5:72:PRO:HG3 | 1:X6:1:MET:HG2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X5:183:GLU:CD | 2:X5:184:PRO:HD3 | 2.36 | 0.45 |
| 2:X7:90:GLU:CD | 2:Z3:280:LYS:HE2 | 2.37 | 0.45 |
| 2:X9:284:GLU:HG2 | 2:X9:285:GLN:N | 2.30 | 0.45 |
| 2:Y1:11:GLN:HB3 | 41:Y1:501:GTP:O2A | 2.15 | 0.45 |
| 2:Y1:188:VAL:HA | 2:Y1:191:THR:HG22 | 1.98 | 0.45 |
| 1:Y2:21:TRP:CZ3 | 1:Y2:61:PRO:HB3 | 2.51 | 0.45 |
| 1:Y2:295:ASP:OD1 | 1:Y2:297:LYS:N | 2.45 | 0.45 |
| 1:Y4:6:HIS:HA | 1:Y4:134:GLN:O | 2.16 | 0.45 |
| 1:Y6:58:ARG:HH11 | 1:Y6:84:ILE:HG22 | 1.80 | 0.45 |
| 1:Y6:322:SER:HB3 | 1:Y6:325:GLU:HG3 | 1.97 | 0.45 |
| 1:Y8:285:THR:HG23 | 1:Y8:287:PRO:HD2 | 1.98 | 0.45 |
| 1:Z2:141:GLY:HA3 | 39:Z2:503:GDP:PB | 2.56 | 0.45 |
| 2:Z7:107:HIS:HD2 | 2:Z7:151:SER:OG | 1.98 | 0.45 |
| 1:Z8:329:GLN:HA | 1:Z8:332:ASN:HD21 | 1.81 | 0.45 |
| 2:Z9:28:HIS:CE1 | 2:Z9:49:PHE:HA | 2.50 | 0.45 |
| 2:0B:187:SER:O | 2:0B:190:SER:OG | 2.20 | 0.45 |
| 1:0E:153:SER:O | 1:0E:157:GLU:HG2 | 2.16 | 0.45 |
| 2:0H:407:TRP:CG | 1:0I:255:VAL:HG23 | 2.51 | 0.45 |
| 1:0I:274:THR:HG21 | 1:0I:282:ARG:HD2 | 1.97 | 0.45 |
| 2:0N:66:ILE:O | 2:0N:66:ILE:HG13 | 2.15 | 0.45 |
| 1:0O:67:ASP:OD1 | 1:0O:68:LEU:N | 2.45 | 0.45 |
| 1:0O:174:LYS:HE2 | 1:0O:174:LYS:HB3 | 1.77 | 0.45 |
| 2:0P:246:GLY:HA3 | 2:0P:356:ASN:HA | 1.98 | 0.45 |
| 1:0Q:114:ASP:N | 1:0Q:114:ASP:OD1 | 2.49 | 0.45 |
| 2:0R:319:TYR:HB3 | 2:0R:323:VAL:HG21 | 1.98 | 0.45 |
| 1:0S:232:VAL:HG11 | 1:0S:268:VAL:HG11 | 1.98 | 0.45 |
| 1:0U:124:ALA:HB1 | 1:0U:130:LEU:HD21 | 1.97 | 0.45 |
| 1:1A:167:PHE:CE2 | 1:1A:233:MET:HG2 | 2.52 | 0.45 |
| 1:1A:344:TRP:O | 1:1A:345:ILE:HD13 | 2.16 | 0.45 |
| 1:1C:414:ASN:HA | 1:1C:417:ASP:OD2 | 2.17 | 0.45 |
| 2:1F:178:SER:HB3 | 2:1F:183:GLU:OE2 | 2.16 | 0.45 |
| 1:1G:4:ILE:HA | 1:1G:132:GLY:O | 2.16 | 0.45 |
| 2:1H:167:LEU:HD21 | 2:1H:252:ILE:HG23 | 1.96 | 0.45 |
| 2:1N:50:ASN:O | 2:1N:64:ARG:NH2 | 2.49 | 0.45 |
| 1:1O:219:THR:O | 1:1O:219:THR:OG1 | 2.33 | 0.45 |
| 2:1P:3:GLU:HB2 | 2:1P:129:CYS:SG | 2.55 | 0.45 |
| 2:1P:179:THR:O | 1:1Q:350:LYS:HA | 2.16 | 0.45 |
| 1:1Q:83:GLN:OE1 | 1:1Q:83:GLN:N | 2.39 | 0.45 |
| 1:1U:128:ASP:N | 1:1U:128:ASP:OD1 | 2.42 | 0.45 |
| 2:1X:317:LEU:HB3 | 2:1X:319:TYR:CE1 | 2.44 | 0.45 |
| 2:1Z:12:ALA:O | 2:1Z:16:VAL:HG23 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:309:ARG:H | 1:2A:372:THR:HG22 | 1.81 | 0.45 |
| 1:2A:404:ASP:HB3 | 1:2A:406:MET:SD | 2.56 | 0.45 |
| 2:2B:246:GLY:HA3 | 2:2B:356:ASN:HA | 1.98 | 0.45 |
| 2:2B:289:ALA:O | 2:2B:293:ASN:ND2 | 2.49 | 0.45 |
| 2:2B:315:CYS:SG | 2:2B:316:CYS:N | 2.88 | 0.45 |
| 1:2I:2:ARG:HB3 | 1:2I:131:GLN:HB2 | 1.98 | 0.45 |
| 2:2J:287:SER:N | 2:2J:290:GLU:OE2 | 2.49 | 0.45 |
| 1:2K:139:LEU:HD12 | 1:2K:170:VAL:HG12 | 1.97 | 0.45 |
| 1:2M:183:TYR:HA | 1:2M:385:PHE:CE1 | 2.51 | 0.45 |
| 2:2R:14:ILE:HD11 | 2:2R:74:VAL:HG13 | 1.98 | 0.45 |
| 1:2S:154:LYS:HD3 | 1:2S:154:LYS:HA | 1.80 | 0.45 |
| 2:2T:2:ARG:HA | 2:2T:133:GLN:HE21 | 1.80 | 0.45 |
| 1:2Y:167:PHE:CE2 | 1:2Y:233:MET:HG2 | 2.50 | 0.45 |
| 1:3A:396:HIS:HE1 | 1:3A:397:TRP:CZ2 | 2.34 | 0.45 |
| 1:3C:183:TYR:HB3 | 1:3C:398:TYR:HE2 | 1.81 | 0.45 |
| 2:3D:47:ASP:HA | 2:3D:50:ASN:ND2 | 2.31 | 0.45 |
| 1:3G:34:GLY:HA3 | 1:3G:58:ARG:HD2 | 1.97 | 0.45 |
| 1:3K:95:THR:HG23 | 1:3K:96:GLY:N | 2.31 | 0.45 |
| 1:3M:22:GLU:HG3 | 1:3M:81:TYR:CD1 | 2.51 | 0.45 |
| 2:3P:111:GLY:O | 2:3P:115:VAL:HG22 | 2.15 | 0.45 |
| 2:3R:76:ASP:O | 2:3R:80:THR:HG22 | 2.16 | 0.45 |
| 1:3S:181:GLU:HB2 | 1:3S:182:PRO:HD3 | 1.98 | 0.45 |
| 3:3V:7:GLY:C | 3:3V:140:LYS:HE2 | 2.37 | 0.45 |
| 3:3X:7:GLY:C | 3:3X:140:LYS:HE2 | 2.37 | 0.45 |
| 4:4E:117:PHE:HB2 | 4:4E:118:ILE:HD12 | 1.97 | 0.45 |
| 3:4F:7:GLY:C | 3:4F:140:LYS:HE2 | 2.37 | 0.45 |
| 6:4O:449:ASP:OD2 | 6:4O:452:ARG:NH1 | 2.49 | 0.45 |
| 7:4R:113:PRO:HG2 | 21:6G:40:PHE:CE1 | 2.51 | 0.45 |
| 7:4U:123:LEU:HD11 | 7:4U:129:GLN:HB2 | 1.98 | 0.45 |
| 9:4Z:360:THR:O | 9:4Z:364:LYS:HG3 | 2.17 | 0.45 |
| 10:5C:227:GLU:HA | 10:5C:230:ARG:HE | 1.80 | 0.45 |
| 11:5E:165:LEU:HD12 | 11:5E:192:ALA:HB2 | 1.98 | 0.45 |
| 12:5F:312:ASP:OD1 | 12:5F:312:ASP:N | 2.48 | 0.45 |
| 14:5L:78:TYR:HB3 | 14:5L:81:PHE:CD2 | 2.51 | 0.45 |
| 14:5M:78:TYR:HB3 | 14:5M:81:PHE:CD2 | 2.51 | 0.45 |
| 15:5P:60:LEU:HG | 15:5P:61:PHE:H | 1.81 | 0.45 |
| 17:5U:108:ASN:O | 17:5U:112:VAL:HG23 | 2.16 | 0.45 |
| 21:6H:106:ARG:HB2 | 24:6X:81:THR:H | 1.80 | 0.45 |
| 22:6N:129:GLN:OE1 | 22:6N:129:GLN:N | 2.48 | 0.45 |
| 22:6P:55:THR:OG1 | 22:6P:56:GLN:HG3 | 2.15 | 0.45 |
| 22:6P:281:LYS:N | 22:6P:281:LYS:HD3 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:113:ASN:OD1 | 24:6U:114:HIS:ND1 | 2.40 | 0.45 |
| 24:6X:279:TRP:CZ2 | 24:6X:364:ARG:HG3 | 2.51 | 0.45 |
| 24:6X:386:THR:OG1 | 24:6X:388:GLU:HG3 | 2.16 | 0.45 |
| 24:6Y:558:LEU:HD22 | 24:6Y:612:LEU:HD21 | 1.98 | 0.45 |
| 24:6Z:290:ARG:HG3 | 24:6Z:291:PRO:HD2 | 1.97 | 0.45 |
| 29:7J:438:VAL:HG22 | 29:7J:443:LEU:HD21 | 1.98 | 0.45 |
| 38:8B:86:TYR:N | 38:8B:86:TYR:CD2 | 2.84 | 0.45 |
| 2:B2:59:GLY:CA | 24:6V:263:ARG:HH12 | 2.28 | 0.45 |
| 2:C5:47:ASP:OD2 | 24:6T:319:PRO:HG3 | 2.16 | 0.45 |
| 2:C9:143:GLY:HA3 | 41:C9:501:GTP:O2B | 2.16 | 0.45 |
| 2:D5:285:GLN:HE21 | 24:6Y:256:LEU:HD12 | 1.80 | 0.45 |
| 2:G1:175:PRO:HB3 | 2:G1:390:ARG:NE | 2.30 | 0.45 |
| 1:G2:232:VAL:HG11 | 1:G2:268:VAL:HG11 | 1.97 | 0.45 |
| 2:G7:205:ASP:OD1 | 2:G7:206:ASN:N | 2.49 | 0.45 |
| 2:G9:175:PRO:HG2 | 2:G9:176:GLN:OE1 | 2.16 | 0.45 |
| 2:G9:275:ILE:HG23 | 2:G9:275:ILE:O | 2.17 | 0.45 |
| 1:H6:113:ILE:HG21 | 1:H6:150:LEU:HD22 | 1.97 | 0.45 |
| 1:I0:325:GLU:O | 1:I0:329:GLN:HB2 | 2.16 | 0.45 |
| 2:I7:151:SER:HB2 | 2:I7:193:SER:OG | 2.17 | 0.45 |
| 2:J1:183:GLU:HG3 | 2:J1:184:PRO:HD3 | 1.98 | 0.45 |
| 1:J2:421:GLU:HA | 1:J2:424:GLN:HB3 | 1.98 | 0.45 |
| 2:J3:2:ARG:CZ | 16:5Q:175:LEU:HD23 | 2.46 | 0.45 |
| 1:J6:221:THR:HG23 | 1:J6:223:GLY:H | 1.81 | 0.45 |
| 1:J8:173:PRO:O | 1:J8:176:SER:OG | 2.33 | 0.45 |
| 2:J9:90:GLU:HG3 | 2:J9:121:ARG:CZ | 2.47 | 0.45 |
| 2:J9:345:ASP:OD1 | 2:J9:346:TRP:N | 2.49 | 0.45 |
| 1:K0:416:ASN:O | 1:K0:420:SER:OG | 2.31 | 0.45 |
| 2:K3:392:ASP:OD2 | 2:K3:422:ARG:NH1 | 2.49 | 0.45 |
| 1:K4:386:THR:O | 1:K4:390:ARG:HG3 | 2.16 | 0.45 |
| 1:K8:294:TRP:CE2 | 1:K8:333:VAL:HG11 | 2.51 | 0.45 |
| 2:K9:11:GLN:NE2 | 1:L0:247:ASN:OD1 | 2.48 | 0.45 |
| 1:L0:145:SER:OG | 1:L0:146:GLY:N | 2.49 | 0.45 |
| 2:L3:175:PRO:HG2 | 2:L3:176:GLN:OE1 | 2.16 | 0.45 |
| 2:L7:315:CYS:SG | 2:L7:379:SER:OG | 2.60 | 0.45 |
| 1:M0:88:ASP:HB3 | 2:N7:283:HIS:CE1 | 2.51 | 0.45 |
| 2:M5:9:ILE:HG22 | 2:M5:146:GLY:HA2 | 1.99 | 0.45 |
| 2:M5:66:ILE:HD12 | 2:M5:68:LEU:HD23 | 1.97 | 0.45 |
| 1:M6:245:GLN:HG2 | 37:7Y:146:GLU:HG2 | 1.98 | 0.45 |
| 2:M7:79:ARG:HB2 | 19:6E:24:TRP:HH2 | 1.80 | 0.45 |
| 2:M7:205:ASP:OD2 | 2:M7:206:ASN:N | 2.45 | 0.45 |
| 2:M9:35:GLN:NE2 | 2:M9:40:LYS:HZ2 | 2.11 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M9:35:GLN:NE2 | 2:M9:40:LYS:NZ | 2.62 | 0.45 |
| 2:M9:129:CYS:SG | 2:M9:130:THR:N | 2.89 | 0.45 |
| 1:N0:135:VAL:HG12 | 1:N0:137:HIS:HD2 | 1.81 | 0.45 |
| 2:N1:177:VAL:HG13 | 1:N2:327:ASP:HB3 | 1.97 | 0.45 |
| 1:N2:126:SER:O | 32:7P:22:ASN:ND2 | 2.48 | 0.45 |
| 1:N6:27:GLU:OE1 | 1:N6:318:ARG:NH2 | 2.46 | 0.45 |
| 1:N8:417:ASP:OD2 | 1:N8:418:LEU:N | 2.49 | 0.45 |
| 1:O0:277:GLY:HA2 | 27:7G:31:PHE:CD2 | 2.49 | 0.45 |
| 1:O2:317:PHE:HB3 | 1:O2:321:MET:CE | 2.46 | 0.45 |
| 2:O3:325:PRO:HA | 2:O3:328:VAL:HG12 | 1.97 | 0.45 |
| 2:O5:88:HIS:CE1 | 2:O5:89:PRO:HD2 | 2.51 | 0.45 |
| 2:O5:285:GLN:NE2 | 19:6E:10:SER:HB3 | 2.31 | 0.45 |
| 2:O7:32:PRO:HB3 | 2:O7:83:TYR:HE1 | 1.81 | 0.45 |
| 2:P3:170:THR:HG21 | 2:P3:194:LEU:HD11 | 1.98 | 0.45 |
| 1:P4:5:VAL:HB | 1:P4:133:PHE:HD1 | 1.80 | 0.45 |
| 1:P4:128:ASP:OD1 | 1:P4:128:ASP:N | 2.47 | 0.45 |
| 1:Q0:131:GLN:HE21 | 1:Q0:250:LEU:HB2 | 1.81 | 0.45 |
| 2:Q1:430:LYS:HE3 | 2:Q1:434:GLU:OE2 | 2.15 | 0.45 |
| 2:Q3:66:ILE:HG13 | 2:Q3:66:ILE:O | 2.16 | 0.45 |
| 1:Q4:153:SER:HA | 1:Q4:195:ASN:HD22 | 1.81 | 0.45 |
| 2:Q5:66:ILE:O | 2:Q5:66:ILE:HG13 | 2.17 | 0.45 |
| 2:Q9:155:GLU:HG2 | 2:Q9:197:HIS:ND1 | 2.31 | 0.45 |
| 1:R2:176:SER:O | 1:R2:176:SER:OG | 2.32 | 0.45 |
| 1:R2:418:LEU:HG | 1:R2:422:TYR:HE2 | 1.80 | 0.45 |
| 1:R6:371:SER:OG | 1:R6:372:THR:N | 2.48 | 0.45 |
| 1:R8:154:LYS:HA | 1:R8:157:GLU:OE1 | 2.17 | 0.45 |
| 1:R8:292:GLN:HG2 | 1:R8:298:ASN:ND2 | 2.31 | 0.45 |
| 2:R9:247:ALA:HB2 | 2:R9:357:TYR:OH | 2.16 | 0.45 |
| 2:R9:265:ILE:HD11 | 2:R9:435:VAL:HG21 | 1.98 | 0.45 |
| 1:S0:8:GLN:CD | 1:S0:17:GLY:HA3 | 2.37 | 0.45 |
| 1:S0:176:SER:OG | 2:S1:349:THR:HB | 2.16 | 0.45 |
| 1:S0:211:CYS:SG | 1:S0:220:PRO:HB3 | 2.56 | 0.45 |
| 1:S2:183:TYR:HA | 1:S2:385:PHE:CE2 | 2.51 | 0.45 |
| 2:S5:66:ILE:O | 2:S5:66:ILE:HG13 | 2.16 | 0.45 |
| 2:S9:414:GLU:H | 2:S9:414:GLU:CD | 2.15 | 0.45 |
| 2:T5:76:ASP:OD2 | 1:T6:46:ARG:NH2 | 2.49 | 0.45 |
| 1:T8:16:ILE:HD11 | 1:T8:136:CYS:HB3 | 1.97 | 0.45 |
| 2:U1:101:ASN:ND2 | 2:U1:143:GLY:HA2 | 2.31 | 0.45 |
| 2:U3:102:ASN:HB3 | 2:U3:105:ARG:HB3 | 1.98 | 0.45 |
| 2:U5:2:ARG:HA | 2:U5:133:GLN:HE21 | 1.82 | 0.45 |
| 2:U5:129:CYS:SG | 2:U5:130:THR:N | 2.89 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U6:371:SER:OG | 1:U6:372:THR:N | 2.49 | 0.45 |
| 1:U8:113:ILE:HG21 | 1:U8:150:LEU:HD22 | 1.98 | 0.45 |
| 1:U8:282:ARG:HD3 | 1:U8:282:ARG:H | 1.81 | 0.45 |
| 1:V4:279:GLN:HA | 1:V4:282:ARG:HD3 | 1.98 | 0.45 |
| 1:V6:262:ARG:NH2 | 1:V6:414:ASN:OD1 | 2.49 | 0.45 |
| 1:V8:192:LEU:HD22 | 1:V8:196:ALA:HB2 | 1.98 | 0.45 |
| 1:V8:287:PRO:HA | 1:V8:290:THR:HG22 | 1.98 | 0.45 |
| 1:W0:175:VAL:HG13 | 2:W1:329:ASN:OD1 | 2.16 | 0.45 |
| 1:X0:173:PRO:HD2 | 1:X0:380:ARG:NH1 | 2.30 | 0.45 |
| 1:X2:6:HIS:HD2 | 1:X2:134:GLN:HG3 | 1.80 | 0.45 |
| 2:X3:223:THR:O | 2:X3:227:LEU:HG | 2.16 | 0.45 |
| 1:X4:240:LEU:HD11 | 1:X4:250:LEU:HD11 | 1.98 | 0.45 |
| 2:X5:70:LEU:HA | 2:X5:95:GLY:HA3 | 1.98 | 0.45 |
| 1:X6:3:GLU:HG3 | 1:X6:127:CYS:SG | 2.56 | 0.45 |
| 2:X7:129:CYS:SG | 2:X7:130:THR:N | 2.88 | 0.45 |
| 2:Y1:223:THR:HG23 | 2:Y1:225:THR:H | 1.81 | 0.45 |
| 1:Z4:393:ALA:O | 1:Z4:394:PHE:HB2 | 2.15 | 0.45 |
| 2:Z7:21:TRP:CH2 | 2:Z7:63:PRO:HB3 | 2.50 | 0.45 |
| 1:0A:86:ARG:HD3 | 1:0A:88:ASP:HB2 | 1.99 | 0.45 |
| 2:0B:9:ILE:CG1 | 2:0B:139:ASN:HB3 | 2.47 | 0.45 |
| 1:0C:390:ARG:HB3 | 1:0C:391:ARG:HH11 | 1.82 | 0.45 |
| 1:0E:12:CYS:HB3 | 39:0E:501:GDP:C8 | 2.51 | 0.45 |
| 1:0E:116:VAL:O | 1:0E:120:VAL:HG12 | 2.17 | 0.45 |
| 1:0G:203:ASP:OD2 | 1:0G:204:ASN:N | 2.49 | 0.45 |
| 1:0I:327:ASP:HA | 1:0I:330:MET:HE2 | 1.99 | 0.45 |
| 1:0M:20:PHE:HA | 1:0M:230:SER:OG | 2.16 | 0.45 |
| 1:0M:237:THR:HG23 | 1:0M:241:ARG:HH21 | 1.82 | 0.45 |
| 2:0N:195:LEU:HD11 | 2:0N:428:LEU:HD21 | 1.98 | 0.45 |
| 1:0Q:358:PRO:HG2 | 1:0Q:361:LEU:HB2 | 1.98 | 0.45 |
| 2:0V:5:ILE:HG22 | 2:0V:64:ARG:HB3 | 1.98 | 0.45 |
| 1:0W:95:THR:OG1 | 1:0W:96:GLY:N | 2.49 | 0.45 |
| 1:0W:148:GLY:O | 1:0W:152:ILE:HG13 | 2.16 | 0.45 |
| 1:0W:167:PHE:CE2 | 1:0W:233:MET:HG2 | 2.51 | 0.45 |
| 1:1C:95:THR:OG1 | 1:1C:96:GLY:N | 2.48 | 0.45 |
| 2:1D:379:SER:OG | 2:1D:380:ASN:N | 2.49 | 0.45 |
| 1:1G:388:MET:HE1 | 2:1H:346:TRP:C | 2.35 | 0.45 |
| 2:1H:123:ARG:HB3 | 2:1H:124:LYS:HZ2 | 1.80 | 0.45 |
| 1:1M:198:GLU:HB3 | 1:1M:258:ILE:HD11 | 1.98 | 0.45 |
| 2:1N:237:SER:HA | 2:1N:320:ARG:HD2 | 1.98 | 0.45 |
| 2:1N:248:LEU:HD22 | 2:1N:354:GLY:HA2 | 1.97 | 0.45 |
| 2:1N:345:ASP:OD1 | 2:1N:346:TRP:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1R:313:MET:HE2 | 2:1R:313:MET:HB3 | 1.77 | 0.45 |
| 1:1S:208:TYR:OH | 2:1T:325:PRO:HB2 | 2.16 | 0.45 |
| 2:1T:175:PRO:HG2 | 2:1T:176:GLN:OE1 | 2.15 | 0.45 |
| 2:1T:271:SER:HB3 | 2:1T:301:MET:HA | 1.98 | 0.45 |
| 1:1U:292:GLN:HG2 | 1:1U:298:ASN:ND2 | 2.31 | 0.45 |
| 2:1V:5:ILE:HD11 | 2:1V:135:PHE:CE1 | 2.49 | 0.45 |
| 1:1W:309:ARG:H | 1:1W:372:THR:HG22 | 1.81 | 0.45 |
| 2:1Z:120:ASP:HB3 | 38:7Z:27:HIS:CD2 | 2.50 | 0.45 |
| 2:2D:175:PRO:HB3 | 2:2D:390:ARG:NE | 2.31 | 0.45 |
| 1:2I:53:GLU:HB3 | 1:2I:59:TYR:CE1 | 2.50 | 0.45 |
| 1:2K:358:PRO:HG2 | 1:2K:361:LEU:HB2 | 1.98 | 0.45 |
| 2:2N:211:ASP:OD1 | 2:2N:215:ARG:NH1 | 2.46 | 0.45 |
| 1:2U:178:THR:HG22 | 1:2U:181:GLU:HG3 | 1.98 | 0.45 |
| 2:2V:340:THR:N | 38:8B:78:ASP:OD2 | 2.48 | 0.45 |
| 1:2W:236:ILE:HG23 | 1:2W:237:THR:HG23 | 1.97 | 0.45 |
| 1:2W:382:SER:HB3 | 1:2W:415:MET:HG2 | 1.99 | 0.45 |
| 2:2X:21:TRP:CZ2 | 2:2X:65:CYS:HB2 | 2.51 | 0.45 |
| 2:2X:66:ILE:HG13 | 2:2X:66:ILE:O | 2.17 | 0.45 |
| 2:2Z:119:LEU:HA | 2:2Z:122:ILE:HG22 | 1.99 | 0.45 |
| 2:2Z:282:TYR:CE1 | 10:5C:435:LEU:HD23 | 2.47 | 0.45 |
| 2:3B:214:ARG:HH22 | 38:8C:16:LYS:C | 2.20 | 0.45 |
| 2:3B:244:PHE:HE1 | 38:8D:212:PRO:HG3 | 1.81 | 0.45 |
| 2:3D:70:LEU:HB3 | 2:3D:97:GLU:O | 2.16 | 0.45 |
| 2:3D:420:GLU:HA | 2:3D:423:GLU:HG3 | 1.98 | 0.45 |
| 1:3G:286:VAL:CG2 | 1:3G:287:PRO:HD3 | 2.46 | 0.45 |
| 2:3H:26:LEU:HD21 | 2:3H:363:VAL:HG13 | 1.97 | 0.45 |
| 1:3I:116:VAL:HA | 1:3I:119:VAL:HG12 | 1.98 | 0.45 |
| 1:3K:228:LEU:O | 1:3K:232:VAL:HG23 | 2.16 | 0.45 |
| 1:3O:292:GLN:HG2 | 1:3O:298:ASN:ND2 | 2.31 | 0.45 |
| 2:3P:296:PHE:CE2 | 2:3P:335:ILE:HD13 | 2.51 | 0.45 |
| 1:3S:6:HIS:CE1 | 1:3S:8:GLN:HG2 | 2.51 | 0.45 |
| 2:3T:408:TYR:CD1 | 2:3T:418:PHE:HZ | 2.34 | 0.45 |
| 3:3V:46:ALA:CB | 3:3V:166:ARG:HD2 | 2.46 | 0.45 |
| 4:4A:117:PHE:HB2 | 4:4A:118:ILE:HD12 | 1.97 | 0.45 |
| 4:4I:117:PHE:HB2 | 4:4I:118:ILE:HD12 | 1.97 | 0.45 |
| 3:4J:188:GLY:H | 3:4J:190:LYS:HZ1 | 1.62 | 0.45 |
| 9:4Z:381:LEU:O | 9:4Z:385:GLN:NE2 | 2.49 | 0.45 |
| 12:5F:342:ASN:O | 12:5F:376:ARG:NH1 | 2.48 | 0.45 |
| 12:5F:386:ILE:HD11 | 12:7B:38:PRO:O | 2.16 | 0.45 |
| 14:5L:189:THR:OG1 | 14:5L:227:LEU:HD12 | 2.15 | 0.45 |
| 14:5M:478:LYS:HD3 | 14:5M:483:GLU:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5N:57:ASP:OD1 | 14:5N:58:LYS:N | 2.47 | 0.45 |
| 14:5N:412:GLN:HG2 | 17:5U:9:LEU:HD13 | 1.98 | 0.45 |
| 15:5O:125:ILE:HG12 | 15:5O:159:VAL:HG13 | 1.98 | 0.45 |
| 15:5P:148:ARG:HH21 | 15:5P:151:ASP:CB | 2.30 | 0.45 |
| 19:6E:224:THR:HA | 19:6E:227:VAL:HG12 | 1.99 | 0.45 |
| 22:6J:16:LYS:HB2 | 22:6J:39:GLN:HE22 | 1.81 | 0.45 |
| 22:6J:219:ASP:N | 22:6J:219:ASP:OD1 | 2.39 | 0.45 |
| 22:6K:197:ASP:O | 22:6K:199:SER:N | 2.50 | 0.45 |
| 22:6L:183:ASN:OD1 | 22:6L:184:ALA:N | 2.50 | 0.45 |
| 22:6N:111:PRO:HD2 | 22:6N:112:PHE:CE2 | 2.51 | 0.45 |
| 24:6V:103:LYS:HG2 | 24:6V:116:ILE:HG12 | 1.98 | 0.45 |
| 24:6V:106:VAL:HG22 | 24:6V:107:VAL:H | 1.80 | 0.45 |
| 24:6W:130:MET:HG3 | 24:6W:153:VAL:CG1 | 2.46 | 0.45 |
| 24:6X:443:LYS:O | 24:6X:445:ILE:HD13 | 2.17 | 0.45 |
| 25:7C:18:TYR:O | 25:7C:22:GLN:HG2 | 2.15 | 0.45 |
| 25:7C:22:GLN:OE1 | 25:7C:22:GLN:CA | 2.64 | 0.45 |
| 34:7R:109:VAL:HG21 | 35:7T:58:ASN:HD21 | 1.82 | 0.45 |
| 35:7T:184:LEU:O | 35:7T:188:MET:HG2 | 2.16 | 0.45 |
| 38:8B:8:GLU:O | 38:8B:12:LEU:N | 2.50 | 0.45 |
| 38:8C:110:ASN:ND2 | 38:8C:112:ILE:HB | 2.31 | 0.45 |
| 38:8D:80:TYR:CD2 | 38:8D:80:TYR:C | 2.89 | 0.45 |
| 2:2:196:GLU:OE2 | 4:3W:113:ARG:NH1 | 2.45 | 0.45 |
| 2:C7:12:ALA:HB2 | 41:C8:501:GTP:C8 | 2.51 | 0.45 |
| 2:E5:282:TYR:CZ | 22:6K:80:GLY:O | 2.69 | 0.45 |
| 1:F2:204:ASN:ND2 | 39:F2:501:GDP:HN22 | 2.14 | 0.45 |
| 2:G3:102:ASN:ND2 | 2:G3:105:ARG:HB2 | 2.31 | 0.45 |
| 1:G4:183:TYR:HA | 1:G4:385:PHE:HE1 | 1.81 | 0.45 |
| 1:G4:274:THR:HG21 | 1:G4:282:ARG:HE | 1.81 | 0.45 |
| 2:G7:371:VAL:HG22 | 2:G7:373:ARG:H | 1.81 | 0.45 |
| 1:G8:121:ARG:NH2 | 1:G8:158:GLU:OE2 | 2.43 | 0.45 |
| 1:G8:211:CYS:O | 1:G8:216:LYS:N | 2.49 | 0.45 |
| 2:G9:269:LEU:HD11 | 2:G9:379:SER:HB2 | 1.97 | 0.45 |
| 2:H1:11:GLN:HB3 | 41:H2:501:GTP:PA | 2.56 | 0.45 |
| 1:H2:207:LEU:HB3 | 1:H2:225:LEU:HD22 | 1.98 | 0.45 |
| 2:H5:287:SER:OG | 2:H5:288:VAL:N | 2.49 | 0.45 |
| 1:H6:7:ILE:HB | 1:H6:135:VAL:HG22 | 1.98 | 0.45 |
| 2:I5:312:TYR:O | 2:I5:344:VAL:HG13 | 2.17 | 0.45 |
| 1:I8:135:VAL:HG12 | 1:I8:137:HIS:HD2 | 1.81 | 0.45 |
| 1:I8:154:LYS:O | 1:I8:157:GLU:HG2 | 2.16 | 0.45 |
| 1:J0:334:GLN:NE2 | 1:J0:348:ASN:OD1 | 2.50 | 0.45 |
| 2:J1:124:LYS:HA | 2:J1:127:ASP:OD1 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J2:7:ILE:HB | 1:J2:135:VAL:HG22 | 1.98 | 0.45 |
| 2:J5:179:THR:O | 1:J6:350:LYS:HD2 | 2.17 | 0.45 |
| 1:J6:177:ASP:O | 2:J7:352:LYS:HD2 | 2.15 | 0.45 |
| 2:J9:267:PHE:HB2 | 2:J9:384:ILE:HD12 | 1.98 | 0.45 |
| 2:K7:88:HIS:CE1 | 2:K7:90:GLU:HG3 | 2.52 | 0.45 |
| 2:L3:8:HIS:O | 2:L3:68:LEU:HD23 | 2.16 | 0.45 |
| 1:L4:239:CYS:HA | 1:L4:354:CYS:SG | 2.57 | 0.45 |
| 2:L7:66:ILE:O | 2:L7:66:ILE:HG13 | 2.16 | 0.45 |
| 2:L7:377:MET:SD | 2:L7:379:SER:OG | 2.75 | 0.45 |
| 1:M0:317:PHE:HB3 | 1:M0:321:MET:SD | 2.57 | 0.45 |
| 1:M6:317:PHE:HB3 | 1:M6:321:MET:SD | 2.56 | 0.45 |
| 2:N1:420:GLU:HA | 2:N1:423:GLU:HG3 | 1.97 | 0.45 |
| 2:N3:9:ILE:HD11 | 2:N3:139:ASN:HB3 | 1.98 | 0.45 |
| 2:N5:327:ASP:OD2 | 2:N5:327:ASP:N | 2.47 | 0.45 |
| 1:N6:113:ILE:HD11 | 1:N6:151:LEU:HB2 | 1.99 | 0.45 |
| 1:N6:173:PRO:HG3 | 1:N6:380:ARG:HD3 | 1.98 | 0.45 |
| 1:O0:379:LYS:HA | 1:O0:382:SER:OG | 2.16 | 0.45 |
| 1:O6:20:PHE:HA | 1:O6:230:SER:OG | 2.16 | 0.45 |
| 2:O9:267:PHE:HB3 | 2:O9:384:ILE:HG21 | 1.98 | 0.45 |
| 1:P4:246:LEU:HD22 | 1:P4:352:SER:HA | 1.98 | 0.45 |
| 1:P6:54:ALA:HB3 | 1:P6:58:ARG:HB3 | 1.98 | 0.45 |
| 2:P7:217:LEU:HB3 | 2:P7:219:ILE:HD12 | 1.98 | 0.45 |
| 1:P8:101:TRP:HB2 | 1:P8:184:ASN:OD1 | 2.17 | 0.45 |
| 1:Q0:41:ASP:OD2 | 1:Q0:41:ASP:N | 2.49 | 0.45 |
| 2:Q1:339:ARG:CD | 5:4M:18:LEU:HD21 | 2.46 | 0.45 |
| 2:Q3:174:SER:OG | 2:Q3:175:PRO:HD2 | 2.17 | 0.45 |
| 1:Q4:180:VAL:HG23 | 1:Q4:184:ASN:HD21 | 1.81 | 0.45 |
| 2:Q5:51:THR:HG21 | 2:Q5:243:ARG:HG2 | 1.98 | 0.45 |
| 2:Q5:344:VAL:HG22 | 2:Q5:346:TRP:H | 1.82 | 0.45 |
| 1:Q6:51:PHE:HB3 | 1:Q6:59:TYR:HB3 | 1.98 | 0.45 |
| 1:Q8:10:GLY:HA2 | 1:Q8:143:THR:HG23 | 1.97 | 0.45 |
| 1:R2:92:PHE:HE2 | 24:6V:35:TYR:CD1 | 2.23 | 0.45 |
| 1:R4:248:ALA:HA | 1:R4:252:LYS:HD2 | 1.97 | 0.45 |
| 2:R5:39:ASP:OD1 | 11:5E:125:ARG:N | 2.48 | 0.45 |
| 1:R6:232:VAL:O | 1:R6:236:ILE:HG12 | 2.16 | 0.45 |
| 2:R7:66:ILE:O | 2:R7:66:ILE:HG13 | 2.16 | 0.45 |
| 2:R9:415:GLU:HA | 2:R9:418:PHE:HD2 | 1.79 | 0.45 |
| 1:S0:189:VAL:O | 1:S0:193:VAL:HG13 | 2.15 | 0.45 |
| 1:S4:175:VAL:O | 1:S4:175:VAL:HG13 | 2.17 | 0.45 |
| 1:S4:203:ASP:OD2 | 1:S4:302:ALA:N | 2.50 | 0.45 |
| 2:S5:216:SER:HB3 | 2:S5:275:ILE:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S5:289:ALA:O | 2:S5:293:ASN:ND2 | 2.49 | 0.45 |
| 2:S5:394:LYS:HB2 | 1:S6:346:PRO:HG3 | 1.99 | 0.45 |
| 1:S6:49:VAL:HG11 | 1:S6:241:ARG:HG2 | 1.98 | 0.45 |
| 2:S9:155:GLU:HB2 | 2:S9:197:HIS:CE1 | 2.51 | 0.45 |
| 2:S9:279:GLU:HA | 7:4T:336:GLN:HE21 | 1.80 | 0.45 |
| 2:S9:339:ARG:HB3 | 13:5I:26:ALA:HB2 | 1.98 | 0.45 |
| 2:T1:15:GLN:HB3 | 2:T1:228:ASN:HD21 | 1.81 | 0.45 |
| 1:T2:244:GLY:HA2 | 1:T2:355:ASP:OD2 | 2.16 | 0.45 |
| 2:T3:90:GLU:OE2 | 2:T3:90:GLU:CA | 2.61 | 0.45 |
| 1:T6:54:ALA:HB1 | 1:T6:55:THR:HG23 | 1.98 | 0.45 |
| 1:T8:3:GLU:HB2 | 1:T8:130:LEU:HA | 1.98 | 0.45 |
| 1:T8:227:HIS:HE1 | 31:7N:3:ILE:HA | 1.81 | 0.45 |
| 2:U1:312:TYR:HB2 | 2:U1:343:PHE:CD1 | 2.50 | 0.45 |
| 2:U3:65:CYS:SG | 2:U3:66:ILE:N | 2.89 | 0.45 |
| 1:U4:113:ILE:CD1 | 1:U4:150:LEU:HG | 2.46 | 0.45 |
| 2:U5:216:SER:OG | 2:U5:275:ILE:O | 2.30 | 0.45 |
| 2:U7:325:PRO:HA | 2:U7:328:VAL:HG12 | 1.97 | 0.45 |
| 2:V7:167:LEU:HD13 | 2:V7:200:VAL:HB | 1.98 | 0.45 |
| 2:V7:387:ILE:HG12 | 2:V7:390:ARG:HH22 | 1.82 | 0.45 |
| 2:W1:275:ILE:O | 2:W1:275:ILE:HG13 | 2.16 | 0.45 |
| 1:W2:172:SER:OG | 1:W2:173:PRO:HD2 | 2.17 | 0.45 |
| 1:W2:418:LEU:O | 1:W2:421:GLU:HG2 | 2.16 | 0.45 |
| 1:W4:5:VAL:HG12 | 1:W4:133:PHE:CD1 | 2.51 | 0.45 |
| 1:W4:183:TYR:HB3 | 1:W4:398:TYR:HE2 | 1.80 | 0.45 |
| 2:W5:90:GLU:HB3 | 2:W5:121:ARG:HH12 | 1.79 | 0.45 |
| 2:W5:284:GLU:OE1 | 2:W5:284:GLU:CA | 2.60 | 0.45 |
| 1:W8:21:TRP:CZ3 | 1:W8:61:PRO:HB3 | 2.52 | 0.45 |
| 2:X3:156:ARG:HA | 2:X3:159:VAL:HG12 | 1.99 | 0.45 |
| 2:X5:9:ILE:HG22 | 2:X5:146:GLY:HA2 | 1.98 | 0.45 |
| 2:X5:70:LEU:HD11 | 2:X5:149:LEU:CD2 | 2.46 | 0.45 |
| 2:X9:324:VAL:HG22 | 2:X9:326:LYS:H | 1.82 | 0.45 |
| 2:Y5:154:LEU:HA | 2:Y5:157:LEU:HD23 | 1.97 | 0.45 |
| 1:Y6:114:ASP:N | 1:Y6:114:ASP:OD1 | 2.47 | 0.45 |
| 1:Z2:155:ILE:HG23 | 1:Z2:164:MET:HE1 | 1.97 | 0.45 |
| 2:Z3:119:LEU:HA | 2:Z3:122:ILE:HG22 | 1.98 | 0.45 |
| 1:Z4:51:PHE:HB3 | 1:Z4:59:TYR:HB3 | 1.98 | 0.45 |
| 1:Z6:117:LEU:HD23 | 1:Z6:117:LEU:HA | 1.83 | 0.45 |
| 1:Z6:361:LEU:HD23 | 1:Z6:361:LEU:HA | 1.84 | 0.45 |
| 2:Z7:28:HIS:CE1 | 2:Z7:49:PHE:HA | 2.51 | 0.45 |
| 2:Z7:102:ASN:ND2 | 2:Z7:411:GLU:HG3 | 2.26 | 0.45 |
| 1:Z8:87:PRO:HA | 1:Z8:90:PHE:CD2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0F:177:VAL:HB | 1:0G:327:ASP:OD2 | 2.16 | 0.45 |
| 2:0H:3:GLU:HG3 | 2:0H:51:THR:HA | 1.99 | 0.45 |
| 1:0K:237:THR:HG23 | 1:0K:241:ARG:HH21 | 1.82 | 0.45 |
| 1:0K:238:CYS:SG | 1:0K:318:ARG:NE | 2.89 | 0.45 |
| 1:0K:244:GLY:HA3 | 1:0K:354:CYS:HA | 1.99 | 0.45 |
| 2:0L:344:VAL:O | 2:0L:344:VAL:CG1 | 2.64 | 0.45 |
| 2:0N:297:GLU:OE2 | 2:0N:299:ALA:HB3 | 2.15 | 0.45 |
| 2:0P:15:GLN:HB3 | 2:0P:228:ASN:ND2 | 2.31 | 0.45 |
| 2:0P:223:THR:OG1 | 1:0Q:245:GLN:NE2 | 2.49 | 0.45 |
| 1:0Q:244:GLY:HA3 | 1:0Q:354:CYS:HA | 1.97 | 0.45 |
| 2:0R:90:GLU:HB2 | 2:1H:283:HIS:CE1 | 2.51 | 0.45 |
| 2:0Z:4:VAL:HG23 | 2:0Z:134:GLY:O | 2.15 | 0.45 |
| 2:0Z:65:CYS:SG | 2:0Z:66:ILE:N | 2.89 | 0.45 |
| 1:1C:257:LEU:HD21 | 1:1C:314:SER:OG | 2.16 | 0.45 |
| 1:1G:128:ASP:OD1 | 1:1G:129:CYS:N | 2.49 | 0.45 |
| 1:1M:326:VAL:O | 1:1M:330:MET:HG2 | 2.17 | 0.45 |
| 2:1R:406:HIS:HA | 2:1R:409:VAL:HG22 | 1.98 | 0.45 |
| 1:1S:174:LYS:HD3 | 1:1S:205:GLU:OE2 | 2.17 | 0.45 |
| 1:1U:221:THR:OG1 | 1:1U:222:PHE:N | 2.49 | 0.45 |
| 2:1X:370:LYS:NZ | 9:4Z:387:ARG:HB3 | 2.32 | 0.45 |
| 1:2A:207:LEU:HB3 | 1:2A:225:LEU:HD22 | 1.98 | 0.45 |
| 1:2A:240:LEU:HD21 | 1:2A:249:ASP:HB2 | 1.98 | 0.45 |
| 2:2B:133:GLN:HB3 | 2:2B:252:ILE:CG2 | 2.46 | 0.45 |
| 1:2E:128:ASP:OD1 | 1:2E:129:CYS:N | 2.47 | 0.45 |
| 2:2H:279:GLU:OE2 | 10:5B:167:ILE:HD13 | 2.16 | 0.45 |
| 2:2H:420:GLU:HA | 2:2H:423:GLU:HG3 | 1.99 | 0.45 |
| 1:2K:276:ARG:HB3 | 10:5B:249:LEU:HD11 | 1.98 | 0.45 |
| 2:2P:244:PHE:HB2 | 2:2P:356:ASN:HD21 | 1.81 | 0.45 |
| 2:2P:287:SER:OG | 2:2P:288:VAL:N | 2.50 | 0.45 |
| 2:2P:297:GLU:CD | 38:7Z:25:ILE:H | 2.19 | 0.45 |
| 1:2Q:55:THR:H | 1:2Q:58:ARG:HB3 | 1.81 | 0.45 |
| 1:2Y:178:THR:HG22 | 1:2Y:181:GLU:HG3 | 1.98 | 0.45 |
| 2:2Z:91:GLN:HA | 2:2Z:121:ARG:HH12 | 1.81 | 0.45 |
| 2:3B:213:CYS:HA | 2:3B:217:LEU:HB2 | 1.97 | 0.45 |
| 2:3D:101:ASN:N | 41:3D:501:GTP:O3G | 2.40 | 0.45 |
| 2:3D:269:LEU:HB2 | 2:3D:379:SER:OG | 2.17 | 0.45 |
| 2:3F:157:LEU:HD23 | 2:3F:157:LEU:HA | 1.85 | 0.45 |
| 2:3F:223:THR:HG23 | 2:3F:225:THR:H | 1.82 | 0.45 |
| 2:3H:246:GLY:HA2 | 2:3H:357:TYR:CD2 | 2.51 | 0.45 |
| 1:3M:145:SER:OG | 1:3M:188:SER:OG | 2.33 | 0.45 |
| 1:3M:203:ASP:O | 1:3M:207:LEU:HG | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3N:11:GLN:HB3 | 41:3O:501:GTP:O2A | 2.15 | 0.45 |
| 2:3N:182:VAL:HG12 | 2:3N:182:VAL:O | 2.16 | 0.45 |
| 1:3O:3:GLU:HB2 | 1:3O:130:LEU:HA | 1.99 | 0.45 |
| 1:3O:203:ASP:OD2 | 1:3O:302:ALA:N | 2.49 | 0.45 |
| 1:3O:208:TYR:HB3 | 2:3P:326:LYS:HE2 | 1.98 | 0.45 |
| 1:3S:177:ASP:O | 2:3T:352:LYS:HA | 2.17 | 0.45 |
| 2:3T:102:ASN:HD21 | 2:3T:411:GLU:HG3 | 1.82 | 0.45 |
| 4:3W:117:PHE:HB2 | 4:3W:118:ILE:HD12 | 1.97 | 0.45 |
| 3:3Z:38:THR:HG21 | 4:4A:3:LYS:HB2 | 1.99 | 0.45 |
| 3:4B:7:GLY:C | 3:4B:140:LYS:HE2 | 2.37 | 0.45 |
| 3:4D:173:ARG:O | 3:4D:177:VAL:HG23 | 2.16 | 0.45 |
| 4:4G:117:PHE:HB2 | 4:4G:118:ILE:HD12 | 1.97 | 0.45 |
| 6:4O:388:GLN:O | 6:4O:391:LEU:HG | 2.16 | 0.45 |
| 6:4O:459:ARG:HH22 | 6:4O:483:ASP:CG | 2.19 | 0.45 |
| 7:4S:12:ASP:OD1 | 7:4S:13:PRO:CD | 2.45 | 0.45 |
| 12:5G:299:SER:OG | 12:5G:300:PRO:HD3 | 2.15 | 0.45 |
| 15:5P:162:GLU:HB2 | 15:5P:222:PHE:CE1 | 2.44 | 0.45 |
| 16:5Q:38:THR:HG21 | 16:5Q:73:ILE:HG13 | 1.99 | 0.45 |
| 16:5Q:84:ASP:O | 16:5Q:88:THR:HG22 | 2.16 | 0.45 |
| 17:5S:82:LYS:HA | 17:5S:82:LYS:HD3 | 1.76 | 0.45 |
| 22:6J:187:MET:SD | 22:6J:256:TYR:HB2 | 2.56 | 0.45 |
| 22:6N:166:ILE:HD11 | 22:6N:226:LEU:HD11 | 1.97 | 0.45 |
| 22:6P:188:ARG:HG3 | 22:6P:193:MET:HB2 | 1.97 | 0.45 |
| 24:6T:106:VAL:HG12 | 24:6T:113:ASN:C | 2.37 | 0.45 |
| 24:6U:123:TYR:HD1 | 24:6U:130:MET:SD | 2.39 | 0.45 |
| 24:6U:602:LEU:HG | 24:6U:604:PHE:HD1 | 1.82 | 0.45 |
| 24:6V:151:HIS:NE2 | 24:6V:175:TYR:OH | 2.47 | 0.45 |
| 24:6V:214:ARG:HH21 | 24:6V:223:ARG:NH2 | 2.14 | 0.45 |
| 24:6V:271:LYS:HB3 | 24:6V:298:LEU:HD12 | 1.97 | 0.45 |
| 24:6W:185:ASP:OD1 | 24:6W:186:SER:N | 2.48 | 0.45 |
| 24:6X:444:ILE:HD13 | 24:6X:542:TYR:HE1 | 1.79 | 0.45 |
| 24:6Y:304:GLU:OE1 | 24:6Y:306:LEU:HG | 2.17 | 0.45 |
| 24:6Z:341:LYS:HB3 | 24:6Z:341:LYS:HE3 | 1.74 | 0.45 |
| 24:6Z:451:LYS:HD2 | 24:6Z:468:ARG:CZ | 2.46 | 0.45 |
| 24:6Z:487:VAL:HG11 | 24:6Z:490:THR:HG23 | 1.98 | 0.45 |
| 24:7A:123:TYR:CE2 | 24:7A:163:PRO:HG3 | 2.51 | 0.45 |
| 27:7G:91:TYR:CE1 | 27:7G:99:ARG:HG2 | 2.44 | 0.45 |
| 29:7J:414:HIS:HA | 29:7J:417:TYR:CD1 | 2.51 | 0.45 |
| 30:7K:42:ASN:HB3 | 30:7K:45:ARG:NH2 | 2.31 | 0.45 |
| 30:7K:62:GLU:HB3 | 30:7K:63:PRO:HD2 | 1.98 | 0.45 |
| 38:8C:8:GLU:CG | 38:8C:21:LYS:HD3 | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:8:365:GLY:CA | 26:7E:38:ASN:OD1 | 2.64 | 0.45 |
| 2:C5:367:ASP:OD1 | 18:5X:181:GLN:HB2 | 2.16 | 0.45 |
| 1:E4:276:ARG:HG3 | 24:6V:315:ARG:HH12 | 1.82 | 0.45 |
| 2:G1:213:CYS:SG | 2:G1:219:ILE:HB | 2.57 | 0.45 |
| 1:G2:392:LYS:HG3 | 1:G2:395:LEU:CD2 | 2.45 | 0.45 |
| 2:G5:387:ILE:HD12 | 2:G5:390:ARG:HH22 | 1.81 | 0.45 |
| 1:G6:32:PRO:HD3 | 1:G6:81:TYR:CZ | 2.51 | 0.45 |
| 1:G8:224:ASP:OD2 | 1:G8:225:LEU:N | 2.48 | 0.45 |
| 2:G9:23:LEU:HG | 2:G9:27:GLU:OE1 | 2.16 | 0.45 |
| 2:H1:90:GLU:HB2 | 2:I7:283:HIS:CE1 | 2.52 | 0.45 |
| 2:H1:90:GLU:N | 2:H1:90:GLU:OE1 | 2.49 | 0.45 |
| 1:H4:193:VAL:HG13 | 1:H4:194:GLU:HG2 | 1.99 | 0.45 |
| 2:H9:156:ARG:HA | 2:H9:159:VAL:HG12 | 1.97 | 0.45 |
| 2:H9:178:SER:OG | 1:I0:347:ASN:HB3 | 2.16 | 0.45 |
| 2:I3:141:VAL:HG13 | 2:I3:170:THR:CG2 | 2.46 | 0.45 |
| 2:I5:155:GLU:O | 2:I5:158:SER:OG | 2.33 | 0.45 |
| 2:I5:387:ILE:O | 2:I5:391:LEU:HG | 2.15 | 0.45 |
| 2:I7:217:LEU:HB3 | 2:I7:219:ILE:HD12 | 1.98 | 0.45 |
| 1:J0:289:LEU:O | 1:J0:293:MET:HG3 | 2.17 | 0.45 |
| 2:J1:151:SER:HB2 | 2:J1:193:SER:OG | 2.17 | 0.45 |
| 2:J1:267:PHE:HB2 | 2:J1:384:ILE:HD12 | 1.98 | 0.45 |
| 1:J6:114:ASP:N | 1:J6:114:ASP:OD1 | 2.49 | 0.45 |
| 2:K1:50:ASN:O | 2:K1:64:ARG:NH2 | 2.49 | 0.45 |
| 2:K5:194:LEU:O | 2:K5:198:THR:HG22 | 2.16 | 0.45 |
| 2:K7:292:THR:HG21 | 2:K7:331:SER:HB3 | 1.98 | 0.45 |
| 2:L1:319:TYR:HB3 | 2:L1:323:VAL:HG11 | 1.97 | 0.45 |
| 2:L3:88:HIS:CD2 | 2:L3:90:GLU:H | 2.35 | 0.45 |
| 1:L6:145:SER:OG | 1:L6:146:GLY:N | 2.49 | 0.45 |
| 1:L6:211:CYS:HA | 1:L6:215:LEU:HB2 | 1.97 | 0.45 |
| 2:L9:365:GLY:HA3 | 29:7I:118:ALA:HB1 | 1.98 | 0.45 |
| 2:M1:66:ILE:O | 2:M1:66:ILE:HG13 | 2.16 | 0.45 |
| 1:M4:125:GLU:OE2 | 1:M4:159:TYR:OH | 2.34 | 0.45 |
| 1:M4:362:LYS:CD | 30:7K:173:GLU:HG3 | 2.47 | 0.45 |
| 2:N7:196:GLU:OE2 | 2:N7:196:GLU:N | 2.43 | 0.45 |
| 1:O6:271:THR:OG1 | 1:O6:365:ALA:HB3 | 2.17 | 0.45 |
| 1:O8:181:GLU:OE2 | 2:O9:349:THR:HG21 | 2.16 | 0.45 |
| 1:O8:207:LEU:HB3 | 1:O8:225:LEU:HD22 | 1.98 | 0.45 |
| 2:P3:306:ASP:OD2 | 2:P3:308:ARG:HB2 | 2.15 | 0.45 |
| 1:P4:175:VAL:O | 1:P4:175:VAL:HG23 | 2.16 | 0.45 |
| 1:P6:125:GLU:OE2 | 1:R2:291:GLN:NE2 | 2.49 | 0.45 |
| 2:P9:115:VAL:HG22 | 2:P9:119:LEU:HD23 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:203:ASP:OD2 | 1:Q0:204:ASN:N | 2.50 | 0.45 |
| 2:Q1:9:ILE:HD13 | 2:Q1:150:GLY:HA2 | 1.99 | 0.45 |
| 1:Q2:73:MET:HE1 | 1:Q2:90:PHE:HB3 | 1.98 | 0.45 |
| 1:Q8:327:ASP:OD1 | 1:Q8:328:GLU:N | 2.49 | 0.45 |
| 1:R4:111:GLU:HG3 | 13:5I:119:VAL:HG11 | 1.99 | 0.45 |
| 2:R5:53:PHE:O | 2:R5:64:ARG:NH2 | 2.49 | 0.45 |
| 1:S2:362:LYS:HB2 | 7:4R:353:LYS:H | 1.81 | 0.45 |
| 1:S4:224:ASP:HB3 | 24:6U:12:PRO:HB3 | 1.98 | 0.45 |
| 1:S6:69:GLU:C | 1:S6:92:PHE:HZ | 2.20 | 0.45 |
| 2:S7:319:TYR:HB3 | 2:S7:323:VAL:HG21 | 1.98 | 0.45 |
| 1:S8:50:TYR:CD2 | 1:S8:241:ARG:HD3 | 2.51 | 0.45 |
| 1:S8:271:THR:HG23 | 1:S8:365:ALA:HB3 | 1.99 | 0.45 |
| 2:T1:324:VAL:N | 7:4U:25:ARG:HH21 | 2.06 | 0.45 |
| 1:T4:152:ILE:HD13 | 1:T4:155:ILE:HD11 | 1.98 | 0.45 |
| 2:T5:119:LEU:HD11 | 2:T5:156:ARG:HB2 | 1.98 | 0.45 |
| 1:T6:342:VAL:HG11 | 1:T6:345:ILE:HD12 | 1.99 | 0.45 |
| 1:T8:273:LEU:H | 1:T8:292:GLN:HE22 | 1.64 | 0.45 |
| 2:U3:76:ASP:O | 2:U3:80:THR:HG23 | 2.16 | 0.45 |
| 2:U3:277:SER:H | 2:U3:280:LYS:HZ2 | 1.63 | 0.45 |
| 2:U5:8:HIS:CD2 | 2:U5:17:GLY:HA3 | 2.51 | 0.45 |
| 2:V1:60:LYS:HA | 2:V1:60:LYS:HD2 | 1.61 | 0.45 |
| 1:V2:97:ALA:HA | 1:V2:103:LYS:HE3 | 1.99 | 0.45 |
| 1:V6:46:ARG:HG2 | 1:V6:241:ARG:HA | 1.97 | 0.45 |
| 1:V8:149:THR:HA | 1:V8:152:ILE:HG22 | 1.97 | 0.45 |
| 2:V9:27:GLU:OE1 | 2:V9:243:ARG:NH1 | 2.49 | 0.45 |
| 2:W1:187:SER:O | 2:W1:191:THR:HG23 | 2.16 | 0.45 |
| 1:W4:166:THR:HG23 | 1:W4:199:CYS:HB2 | 1.99 | 0.45 |
| 1:W6:342:VAL:HG21 | 1:W6:345:ILE:HD12 | 1.98 | 0.45 |
| 2:W9:116:ASP:N | 2:W9:116:ASP:OD1 | 2.45 | 0.45 |
| 1:X2:8:GLN:OE1 | 1:X2:8:GLN:N | 2.49 | 0.45 |
| 2:X3:305:CYS:CB | 2:X3:387:ILE:HD11 | 2.42 | 0.45 |
| 1:X6:192:LEU:HD23 | 1:X6:192:LEU:HA | 1.80 | 0.45 |
| 1:X8:2:ARG:NE | 1:X8:240:LEU:HD22 | 2.31 | 0.45 |
| 2:X9:417:GLU:HA | 2:X9:420:GLU:HG2 | 1.97 | 0.45 |
| 1:Y0:224:ASP:N | 1:Y0:224:ASP:OD1 | 2.44 | 0.45 |
| 2:Y1:14:ILE:HD11 | 2:Y1:74:VAL:HG13 | 1.97 | 0.45 |
| 2:Y1:384:ILE:HA | 2:Y1:387:ILE:HD12 | 1.98 | 0.45 |
| 2:Y1:407:TRP:CD2 | 1:Y2:255:VAL:HG12 | 2.52 | 0.45 |
| 2:Y3:3:GLU:O | 2:Y3:133:GLN:N | 2.41 | 0.45 |
| 2:Y5:88:HIS:ND1 | 2:0B:283:HIS:HA | 2.30 | 0.45 |
| 1:Y6:224:ASP:OD1 | 1:Y6:225:LEU:HG | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y8:274:THR:OG1 | 1:Y8:282:ARG:NH1 | 2.49 | 0.45 |
| 1:Z0:294:TRP:CD1 | 1:Z0:333:VAL:HG21 | 2.51 | 0.45 |
| 2:Z1:107:HIS:O | 2:Z1:152:LEU:HD12 | 2.17 | 0.45 |
| 1:Z2:189:VAL:HA | 1:Z2:192:LEU:HB3 | 1.99 | 0.45 |
| 1:Z2:324:LYS:NZ | 1:Z2:325:GLU:OE2 | 2.41 | 0.45 |
| 2:Z3:344:VAL:HG22 | 2:Z3:346:TRP:H | 1.80 | 0.45 |
| 2:Z5:334:THR:HA | 2:Z5:337:THR:HG22 | 1.98 | 0.45 |
| 2:0B:116:ASP:OD1 | 2:0B:117:LEU:HD12 | 2.15 | 0.45 |
| 1:0E:175:VAL:HG13 | 1:0E:175:VAL:O | 2.17 | 0.45 |
| 1:0E:178:THR:HG22 | 1:0E:179:VAL:H | 1.81 | 0.45 |
| 1:0E:183:TYR:O | 1:0E:187:LEU:HD13 | 2.15 | 0.45 |
| 1:0G:172:SER:OG | 1:0G:380:ARG:NH2 | 2.49 | 0.45 |
| 2:0H:387:ILE:HD12 | 2:0H:390:ARG:HH22 | 1.81 | 0.45 |
| 2:0L:396:ASP:HB2 | 2:0L:422:ARG:HH21 | 1.80 | 0.45 |
| 1:0M:375:GLN:HB3 | 1:0M:422:TYR:HD2 | 1.82 | 0.45 |
| 2:0N:215:ARG:NH1 | 2:0N:299:ALA:HB1 | 2.31 | 0.45 |
| 1:0O:178:THR:HG22 | 2:0P:352:LYS:HE2 | 1.98 | 0.45 |
| 1:0Q:272:PRO:O | 1:0Q:273:LEU:HD23 | 2.16 | 0.45 |
| 2:0R:33:ASP:OD2 | 2:0R:35:GLN:NE2 | 2.49 | 0.45 |
| 2:0R:290:GLU:HA | 2:0R:293:ASN:HD22 | 1.81 | 0.45 |
| 1:0S:375:GLN:HA | 1:0S:378:PHE:HD2 | 1.81 | 0.45 |
| 1:0Y:242:PHE:CD1 | 1:0Y:356:ILE:HG13 | 2.50 | 0.45 |
| 2:0Z:73:THR:HA | 1:1A:46:ARG:NH2 | 2.30 | 0.45 |
| 2:0Z:134:GLY:HA2 | 2:0Z:164:LYS:HG3 | 1.99 | 0.45 |
| 1:1G:297:LYS:HA | 1:1G:297:LYS:HD3 | 1.70 | 0.45 |
| 2:1H:109:THR:HB | 2:1H:110:ILE:HD12 | 1.97 | 0.45 |
| 1:1K:48:ASN:N | 1:1K:48:ASN:OD1 | 2.49 | 0.45 |
| 1:1M:21:TRP:HA | 1:1M:24:VAL:HG12 | 1.97 | 0.45 |
| 2:1N:49:PHE:HB2 | 2:1N:53:PHE:HD2 | 1.81 | 0.45 |
| 2:1P:330:ALA:O | 2:1P:334:THR:HG23 | 2.16 | 0.45 |
| 2:1V:289:ALA:O | 2:1V:293:ASN:ND2 | 2.50 | 0.45 |
| 2:1X:431:ASP:O | 2:1X:435:VAL:HG22 | 2.16 | 0.45 |
| 2:1Z:76:ASP:HA | 2:1Z:79:ARG:HB2 | 1.97 | 0.45 |
| 2:2B:108:TYR:O | 2:2B:112:LYS:HG2 | 2.16 | 0.45 |
| 2:2F:12:ALA:HB2 | 41:2G:501:GTP:C8 | 2.51 | 0.45 |
| 2:2F:245:ASP:OD1 | 2:2F:245:ASP:N | 2.49 | 0.45 |
| 2:2J:55:GLU:OE1 | 2:2J:59:GLY:N | 2.49 | 0.45 |
| 2:2J:274:PRO:HB2 | 2:2J:276:ILE:HG12 | 1.97 | 0.45 |
| 1:2K:152:ILE:HD12 | 1:2K:164:MET:SD | 2.57 | 0.45 |
| 1:2K:334:GLN:HE22 | 1:2K:348:ASN:H | 1.62 | 0.45 |
| 1:2Q:392:LYS:HD2 | 1:2Q:395:LEU:HD22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2R:317:LEU:HB3 | 2:2R:319:TYR:HE1 | 1.81 | 0.45 |
| 1:2W:309:ARG:H | 1:2W:372:THR:HG22 | 1.81 | 0.45 |
| 2:2Z:97:GLU:N | 2:2Z:97:GLU:OE1 | 2.49 | 0.45 |
| 1:3G:117:LEU:HD23 | 1:3G:117:LEU:HA | 1.83 | 0.45 |
| 1:3G:122:LYS:HD3 | 3:3X:262:TYR:HA | 1.98 | 0.45 |
| 1:3I:68:LEU:HD21 | 1:3I:112:LEU:HD22 | 1.97 | 0.45 |
| 1:3I:203:ASP:OD1 | 1:3I:205:GLU:N | 2.48 | 0.45 |
| 2:3J:301:MET:HE1 | 2:3J:307:PRO:HD3 | 1.98 | 0.45 |
| 1:3M:276:ARG:NH1 | 38:8C:236:CYS:SG | 2.89 | 0.45 |
| 2:3P:23:LEU:HD11 | 2:3P:233:GLN:NE2 | 2.32 | 0.45 |
| 1:3Q:22:GLU:HG3 | 1:3Q:81:TYR:CD1 | 2.52 | 0.45 |
| 1:3Q:86:ARG:HB3 | 1:3Q:89:ASN:OD1 | 2.17 | 0.45 |
| 1:3Q:173:PRO:HG3 | 1:3Q:380:ARG:HD2 | 1.99 | 0.45 |
| 2:3R:100:ALA:HA | 1:3S:252:LYS:HE3 | 1.99 | 0.45 |
| 4:3Y:117:PHE:HB2 | 4:3Y:118:ILE:HD12 | 1.97 | 0.45 |
| 3:3Z:173:ARG:O | 3:3Z:177:VAL:HG23 | 2.16 | 0.45 |
| 3:4H:173:ARG:O | 3:4H:177:VAL:HG23 | 2.16 | 0.45 |
| 6:4N:469:LEU:H | 6:4N:469:LEU:HD23 | 1.81 | 0.45 |
| 10:5A:413:GLU:O | 10:5A:416:GLU:HG3 | 2.17 | 0.45 |
| 14:5L:331:LYS:HE2 | 14:5L:331:LYS:HB2 | 1.76 | 0.45 |
| 17:5S:183:ARG:HA | 17:5S:186:LYS:HE3 | 1.97 | 0.45 |
| 20:6F:343:SER:C | 20:6F:344:LEU:HD22 | 2.37 | 0.45 |
| 21:6H:106:ARG:CB | 24:6X:81:THR:HG23 | 2.46 | 0.45 |
| 22:6I:185:PHE:O | 22:6I:188:ARG:N | 2.49 | 0.45 |
| 22:6O:102:ILE:O | 22:6O:102:ILE:HG13 | 2.16 | 0.45 |
| 23:6Q:24:LYS:HE2 | 23:6Q:56:ILE:HG22 | 1.98 | 0.45 |
| 24:6V:505:LYS:N | 24:6V:510:GLU:O | 2.47 | 0.45 |
| 24:6V:602:LEU:HG | 24:6V:604:PHE:HD1 | 1.82 | 0.45 |
| 24:6V:627:GLU:H | 24:6V:627:GLU:CD | 2.19 | 0.45 |
| 24:6W:451:LYS:HE3 | 24:6W:451:LYS:HB2 | 1.86 | 0.45 |
| 24:6X:371:ALA:HB1 | 24:6X:375:THR:OG1 | 2.16 | 0.45 |
| 24:6Z:615:ARG:HG2 | 24:6Z:616:LEU:HD23 | 1.98 | 0.45 |
| 30:7K:216:VAL:O | 30:7K:216:VAL:HG13 | 2.16 | 0.45 |
| 30:7L:436:CYS:HB3 | 30:7L:439:THR:HG22 | 1.98 | 0.45 |
| 34:7S:213:HIS:HE1 | 35:7U:166:GLU:HG2 | 1.80 | 0.45 |
| 34:7S:257:ARG:HH11 | 34:7S:261:MET:HG2 | 1.81 | 0.45 |
| 38:8A:93:LYS:C | 38:8A:93:LYS:CD | 2.85 | 0.45 |
| 38:8A:208:GLU:HG3 | 38:8A:210:HIS:CE1 | 2.50 | 0.45 |
| 2:A2:221:ARG:HB3 | 26:7F:77:ILE:O | 2.17 | 0.45 |
| 1:A3:215:LEU:HD12 | 26:7F:136:PHE:CD2 | 2.51 | 0.45 |
| 1:C0:320:ARG:NH1 | 18:6C:53:GLY:HA3 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D0:320:ARG:NH2 | 18:5Z:188:ASP:OD1 | 2.50 | 0.45 |
| 2:G1:12:ALA:HB2 | 41:G1:501:GTP:C8 | 2.51 | 0.45 |
| 2:G3:111:GLY:HA2 | 2:G3:114:ILE:HG22 | 1.98 | 0.45 |
| 2:G3:181:VAL:O | 2:G3:184:PRO:HD2 | 2.17 | 0.45 |
| 1:G4:183:TYR:HD2 | 1:G4:398:TYR:HE2 | 1.65 | 0.45 |
| 2:G5:71:GLU:HG2 | 2:G5:73:THR:H | 1.81 | 0.45 |
| 1:G6:219:THR:N | 24:6Y:418:ASP:OD1 | 2.49 | 0.45 |
| 2:H1:222:PRO:O | 1:H2:322:SER:OG | 2.27 | 0.45 |
| 2:H1:414:GLU:HG2 | 2:H1:416:GLY:H | 1.82 | 0.45 |
| 1:H2:199:CYS:SG | 1:H2:265:PHE:HE1 | 2.39 | 0.45 |
| 2:H3:111:GLY:HA2 | 2:H3:114:ILE:HG22 | 1.98 | 0.45 |
| 1:H6:276:ARG:CZ | 24:6V:490:THR:CA | 2.95 | 0.45 |
| 1:I0:192:LEU:HD23 | 1:I0:192:LEU:HA | 1.80 | 0.45 |
| 1:I4:398:TYR:O | 1:I4:401:GLU:HG3 | 2.15 | 0.45 |
| 2:I5:115:VAL:HG23 | 2:I5:153:LEU:HB3 | 1.99 | 0.45 |
| 2:I9:290:GLU:HA | 2:I9:293:ASN:HD22 | 1.81 | 0.45 |
| 2:J5:109:THR:O | 35:7T:42:LYS:HE3 | 2.16 | 0.45 |
| 2:J7:80:THR:O | 29:7J:391:PRO:HD3 | 2.17 | 0.45 |
| 1:J8:199:CYS:SG | 1:J8:200:MET:N | 2.89 | 0.45 |
| 1:J8:286:VAL:HG22 | 1:J8:321:MET:HE2 | 1.98 | 0.45 |
| 2:K3:312:TYR:HB2 | 2:K3:343:PHE:CD1 | 2.52 | 0.45 |
| 2:K5:11:GLN:HB3 | 41:K6:501:GTP:PA | 2.56 | 0.45 |
| 2:K7:12:ALA:HB2 | 41:K7:501:GTP:C8 | 2.51 | 0.45 |
| 2:K7:50:ASN:O | 2:K7:64:ARG:NH2 | 2.50 | 0.45 |
| 2:K7:79:ARG:O | 2:K7:84:ARG:HG2 | 2.16 | 0.45 |
| 1:K8:285:THR:HG23 | 1:K8:288:GLU:OE1 | 2.17 | 0.45 |
| 1:L0:65:LEU:HD12 | 1:L0:90:PHE:CE1 | 2.51 | 0.45 |
| 1:L0:138:SER:O | 1:L0:139:LEU:HD23 | 2.17 | 0.45 |
| 1:L0:233:MET:O | 1:L0:236:ILE:HG22 | 2.17 | 0.45 |
| 1:L4:67:ASP:N | 1:L4:67:ASP:OD1 | 2.49 | 0.45 |
| 2:M1:187:SER:O | 2:M1:191:THR:HG23 | 2.16 | 0.45 |
| 2:M3:213:CYS:HA | 2:M3:217:LEU:HB2 | 1.99 | 0.45 |
| 2:M3:285:GLN:HG3 | 30:7K:215:ALA:HB2 | 1.98 | 0.45 |
| 1:M4:237:THR:HG22 | 1:M4:237:THR:O | 2.16 | 0.45 |
| 2:M5:76:ASP:O | 2:M5:80:THR:HG23 | 2.16 | 0.45 |
| 2:M5:116:ASP:N | 2:M5:116:ASP:OD1 | 2.50 | 0.45 |
| 1:N2:180:VAL:HG23 | 1:N2:184:ASN:HD21 | 1.81 | 0.45 |
| 1:N2:245:GLN:HG2 | 29:7J:110:THR:HG21 | 1.98 | 0.45 |
| 2:N5:317:LEU:HB3 | 2:N5:319:TYR:HE1 | 1.81 | 0.45 |
| 2:N7:3:GLU:HB2 | 2:N7:129:CYS:SG | 2.57 | 0.45 |
| 2:N7:308:ARG:HE | 32:7O:15:VAL:HG21 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N9:406:HIS:HA | 2:N9:409:VAL:HG12 | 1.98 | 0.45 |
| 1:O2:6:HIS:CE1 | 1:O2:8:GLN:HG2 | 2.52 | 0.45 |
| 1:O2:393:ALA:CB | 2:O3:346:TRP:NE1 | 2.78 | 0.45 |
| 2:O3:9:ILE:HD13 | 2:O3:150:GLY:HA2 | 1.98 | 0.45 |
| 1:O6:207:LEU:HD23 | 1:O6:225:LEU:HB3 | 1.99 | 0.45 |
| 2:O7:12:ALA:HB2 | 41:O8:501:GTP:C8 | 2.51 | 0.45 |
| 1:P4:70:PRO:N | 1:P4:92:PHE:HZ | 2.15 | 0.45 |
| 1:P4:134:GLN:HE21 | 1:P4:167:PHE:HE2 | 1.65 | 0.45 |
| 1:P4:382:SER:OG | 1:P4:412:GLU:OE1 | 2.34 | 0.45 |
| 2:P5:275:ILE:HD12 | 2:P5:368:LEU:HD21 | 1.97 | 0.45 |
| 1:P6:65:LEU:HD12 | 1:P6:90:PHE:CE1 | 2.51 | 0.45 |
| 1:P8:272:PRO:HD3 | 1:P8:364:SER:HA | 1.97 | 0.45 |
| 1:Q0:177:ASP:N | 1:Q0:181:GLU:OE2 | 2.50 | 0.45 |
| 1:Q2:175:VAL:HG22 | 2:Q3:329:ASN:ND2 | 2.32 | 0.45 |
| 2:Q5:62:VAL:HG13 | 2:S1:283:HIS:HD1 | 1.82 | 0.45 |
| 1:Q6:107:THR:OG1 | 1:Q6:108:GLU:OE1 | 2.23 | 0.45 |
| 2:Q9:33:ASP:OD1 | 2:Q9:33:ASP:N | 2.48 | 0.45 |
| 2:Q9:121:ARG:HD2 | 2:Q9:121:ARG:HA | 1.67 | 0.45 |
| 2:R1:108:TYR:HA | 2:R1:112:LYS:NZ | 2.31 | 0.45 |
| 2:R3:8:HIS:CD2 | 2:R3:17:GLY:HA3 | 2.52 | 0.45 |
| 2:R3:122:ILE:HD13 | 2:R3:122:ILE:HA | 1.80 | 0.45 |
| 1:R8:2:ARG:HB3 | 1:R8:131:GLN:HB2 | 1.97 | 0.45 |
| 2:R9:81:GLY:HA3 | 12:5F:106:TYR:CE2 | 2.50 | 0.45 |
| 1:S4:152:ILE:HD12 | 1:S4:164:MET:SD | 2.57 | 0.45 |
| 2:S7:53:PHE:HB3 | 2:S7:61:HIS:HB3 | 1.98 | 0.45 |
| 2:S7:56:THR:HG23 | 2:S7:60:LYS:HB3 | 1.99 | 0.45 |
| 2:S7:109:THR:HB | 2:S7:110:ILE:HD12 | 1.97 | 0.45 |
| 2:T3:245:ASP:N | 2:T3:245:ASP:OD1 | 2.48 | 0.45 |
| 1:T4:219:THR:O | 1:T4:219:THR:OG1 | 2.33 | 0.45 |
| 2:T5:83:TYR:HB3 | 2:T5:86:LEU:HB3 | 1.98 | 0.45 |
| 1:T6:32:PRO:HG2 | 31:7N:70:GLU:HG2 | 1.98 | 0.45 |
| 1:T6:229:ILE:O | 1:T6:233:MET:HG3 | 2.16 | 0.45 |
| 1:T8:14:ASN:HD22 | 1:T8:65:LEU:HD23 | 1.82 | 0.45 |
| 1:T8:26:ASP:OD1 | 31:7N:6:PRO:HA | 2.17 | 0.45 |
| 1:U8:114:ASP:N | 1:U8:114:ASP:OD1 | 2.49 | 0.45 |
| 2:U9:304:LYS:HA | 2:U9:304:LYS:HD2 | 1.86 | 0.45 |
| 2:V1:223:THR:OG1 | 2:V1:224:TYR:N | 2.50 | 0.45 |
| 1:V2:310:TYR:N | 1:V2:340:TYR:O | 2.31 | 0.45 |
| 2:V3:73:THR:O | 2:V3:77:GLU:HG3 | 2.15 | 0.45 |
| 2:V7:176:GLN:HB3 | 1:V8:331:LEU:HD11 | 1.99 | 0.45 |
| 1:V8:34:GLY:HA3 | 1:V8:58:ARG:NH2 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V8:64:ILE:O | 1:V8:64:ILE:HG13 | 2.17 | 0.45 |
| 2:V9:430:LYS:HA | 2:V9:430:LYS:HD3 | 1.65 | 0.45 |
| 1:W2:414:ASN:HA | 1:W2:417:ASP:OD2 | 2.16 | 0.45 |
| 2:W3:21:TRP:CZ2 | 2:W3:65:CYS:HB2 | 2.50 | 0.45 |
| 1:W6:383:GLU:HA | 1:W6:386:THR:HG22 | 1.97 | 0.45 |
| 2:W7:167:LEU:HD13 | 2:W7:200:VAL:HB | 1.98 | 0.45 |
| 2:W7:420:GLU:HA | 2:W7:423:GLU:HG3 | 1.99 | 0.45 |
| 1:W8:153:SER:OG | 1:W8:195:ASN:OD1 | 2.33 | 0.45 |
| 1:X0:11:GLN:N | 39:X0:502:GDP:O2B | 2.39 | 0.45 |
| 1:X2:294:TRP:CG | 1:X2:333:VAL:HG21 | 2.51 | 0.45 |
| 2:X7:182:VAL:HG12 | 2:X7:185:TYR:HB2 | 1.98 | 0.45 |
| 2:Y1:184:PRO:O | 2:Y1:188:VAL:HG22 | 2.16 | 0.45 |
| 2:Y5:240:ALA:HB1 | 2:Y5:356:ASN:HD22 | 1.82 | 0.45 |
| 2:Y5:279:GLU:HG2 | 2:Y5:280:LYS:N | 2.32 | 0.45 |
| 1:Y8:235:GLY:HA3 | 1:Y8:366:THR:HG21 | 1.98 | 0.45 |
| 2:Y9:206:ASN:HA | 2:Y9:209:ILE:HG22 | 1.98 | 0.45 |
| 1:Z0:87:PRO:HA | 1:Z0:90:PHE:CD2 | 2.52 | 0.45 |
| 1:Z2:192:LEU:HD21 | 1:Z2:199:CYS:SG | 2.56 | 0.45 |
| 2:Z3:185:TYR:HE1 | 2:Z3:398:MET:HG3 | 1.82 | 0.45 |
| 2:Z3:280:LYS:HA | 2:Z3:280:LYS:HE3 | 1.97 | 0.45 |
| 2:Z5:296:PHE:HE2 | 2:Z5:335:ILE:HG21 | 1.81 | 0.45 |
| 1:Z8:58:ARG:HA | 1:Z8:58:ARG:HD2 | 1.81 | 0.45 |
| 2:Z9:157:LEU:HD13 | 2:Z9:166:LYS:HD3 | 1.99 | 0.45 |
| 2:Z9:276:ILE:HG23 | 2:Z9:280:LYS:HB3 | 1.99 | 0.45 |
| 1:0C:294:TRP:CD1 | 1:0C:333:VAL:HG21 | 2.52 | 0.45 |
| 1:0C:327:ASP:OD1 | 1:0C:328:GLU:N | 2.49 | 0.45 |
| 2:0H:407:TRP:CE2 | 1:0I:255:VAL:HA | 2.51 | 0.45 |
| 2:0N:102:ASN:ND2 | 2:0N:411:GLU:HG3 | 2.20 | 0.45 |
| 2:0P:69:ASP:OD1 | 2:0P:70:LEU:N | 2.45 | 0.45 |
| 2:0P:76:ASP:OD2 | 2:0P:79:ARG:HD2 | 2.16 | 0.45 |
| 1:0Q:23:VAL:HG21 | 1:0Q:230:SER:HB3 | 1.98 | 0.45 |
| 1:0S:3:GLU:HG3 | 1:0S:127:CYS:HB2 | 1.97 | 0.45 |
| 1:0W:54:ALA:N | 1:0W:58:ARG:O | 2.50 | 0.45 |
| 2:0X:274:PRO:HB2 | 2:0X:276:ILE:HG12 | 1.99 | 0.45 |
| 1:0Y:95:THR:OG1 | 1:0Y:96:GLY:N | 2.50 | 0.45 |
| 1:0Y:361:LEU:HD23 | 1:0Y:362:LYS:N | 2.31 | 0.45 |
| 2:1B:306:ASP:OD2 | 2:1B:309:HIS:N | 2.46 | 0.45 |
| 2:1B:317:LEU:HB3 | 2:1B:319:TYR:CE1 | 2.51 | 0.45 |
| 2:1D:75:VAL:HG21 | 2:1D:94:SER:HB2 | 1.99 | 0.45 |
| 2:1H:88:HIS:HB3 | 2:1H:90:GLU:CD | 2.36 | 0.45 |
| 2:1H:311:LYS:O | 2:1H:313:MET:HE2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1K:290:THR:HA | 1:1K:293:MET:HB3 | 1.99 | 0.45 |
| 2:1L:76:ASP:OD2 | 1:1M:46:ARG:NH2 | 2.50 | 0.45 |
| 1:1M:123:GLU:O | 1:1M:126:SER:OG | 2.31 | 0.45 |
| 2:1P:285:GLN:HG2 | 2:1P:286:LEU:N | 2.31 | 0.45 |
| 2:1Z:332:VAL:O | 2:1Z:336:LYS:HG2 | 2.17 | 0.45 |
| 2:2F:116:ASP:N | 2:2F:116:ASP:OD1 | 2.50 | 0.45 |
| 2:2F:317:LEU:HB3 | 2:2F:319:TYR:CE1 | 2.52 | 0.45 |
| 2:2F:326:LYS:HG3 | 2:2F:327:ASP:N | 2.31 | 0.45 |
| 1:2G:10:GLY:HA2 | 1:2G:143:THR:HG23 | 1.98 | 0.45 |
| 2:2H:176:GLN:HE22 | 2:2H:304:LYS:HD2 | 1.82 | 0.45 |
| 1:2I:175:VAL:HG22 | 1:2I:205:GLU:HB2 | 1.99 | 0.45 |
| 2:2J:66:ILE:O | 2:2J:66:ILE:HG13 | 2.16 | 0.45 |
| 1:2M:309:ARG:H | 1:2M:372:THR:HG22 | 1.80 | 0.45 |
| 2:2N:331:SER:O | 2:2N:334:THR:OG1 | 2.25 | 0.45 |
| 2:2P:56:THR:HB | 2:2P:60:LYS:HB3 | 1.98 | 0.45 |
| 1:2S:95:THR:HG23 | 1:2S:96:GLY:H | 1.82 | 0.45 |
| 2:2X:72:PRO:HD2 | 1:2Y:2:ARG:NH1 | 2.31 | 0.45 |
| 2:2X:280:LYS:O | 2:2X:280:LYS:HG2 | 2.16 | 0.45 |
| 1:2Y:5:VAL:HG12 | 1:2Y:62:ARG:HD3 | 1.97 | 0.45 |
| 1:3A:34:GLY:O | 1:3A:58:ARG:HD3 | 2.16 | 0.45 |
| 1:3A:77:ARG:HH12 | 38:8D:220:VAL:HA | 1.81 | 0.45 |
| 1:3A:385:PHE:HZ | 1:3A:408:PHE:HB3 | 1.81 | 0.45 |
| 1:3C:317:PHE:HE2 | 1:3C:326:VAL:HG13 | 1.81 | 0.45 |
| 2:3D:147:SER:OG | 2:3D:148:GLY:N | 2.49 | 0.45 |
| 2:3D:417:GLU:HA | 2:3D:420:GLU:HG3 | 1.97 | 0.45 |
| 2:3H:76:ASP:O | 2:3H:80:THR:HG23 | 2.17 | 0.45 |
| 1:3M:260:PHE:HB2 | 1:3M:263:LEU:HG | 1.97 | 0.45 |
| 1:3O:19:LYS:NZ | 1:3O:227:HIS:HD2 | 2.14 | 0.45 |
| 1:3O:77:ARG:HH12 | 3:4F:18:LYS:HB3 | 1.80 | 0.45 |
| 2:3P:68:LEU:HD11 | 2:3P:149:LEU:HD11 | 1.98 | 0.45 |
| 2:3T:269:LEU:N | 2:3T:379:SER:O | 2.43 | 0.45 |
| 2:3T:296:PHE:CE2 | 2:3T:335:ILE:HD13 | 2.52 | 0.45 |
| 3:3V:173:ARG:O | 3:3V:177:VAL:HG23 | 2.16 | 0.45 |
| 3:3X:173:ARG:O | 3:3X:177:VAL:HG23 | 2.16 | 0.45 |
| 3:4B:173:ARG:O | 3:4B:177:VAL:HG23 | 2.16 | 0.45 |
| 4:4C:117:PHE:HB2 | 4:4C:118:ILE:HD12 | 1.97 | 0.45 |
| 10:5B:301:LEU:HA | 10:5B:304:GLU:CD | 2.37 | 0.45 |
| 12:5G:280:PHE:CD1 | 12:5G:290:PHE:HB2 | 2.51 | 0.45 |
| 14:5L:57:ASP:OD1 | 14:5L:58:LYS:N | 2.47 | 0.45 |
| 14:5M:57:ASP:OD1 | 14:5M:58:LYS:N | 2.47 | 0.45 |
| 15:5O:367:LEU:HA | 15:5O:370:ASN:HD21 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5V:211:ARG:O | 17:5V:215:MET:HG3 | 2.17 | 0.45 |
| 22:6I:188:ARG:HD3 | 22:6I:192:LYS:HB2 | 1.98 | 0.45 |
| 22:6L:48:GLU:HA | 22:6L:113:ARG:HE | 1.82 | 0.45 |
| 22:6N:132:SER:HB2 | 22:6N:209:ASN:HB3 | 1.98 | 0.45 |
| 24:6T:152:ARG:HD3 | 24:6T:160:PHE:CG | 2.52 | 0.45 |
| 24:6V:473:TYR:OH | 24:6V:478:ASP:OD1 | 2.31 | 0.45 |
| 24:6W:573:VAL:HG23 | 24:6W:600:ALA:HB1 | 1.97 | 0.45 |
| 24:6X:519:VAL:HG21 | 24:6X:610:ILE:HD12 | 1.97 | 0.45 |
| 24:6X:562:LEU:HD23 | 24:6X:562:LEU:HA | 1.72 | 0.45 |
| 24:6Y:243:LYS:O | 24:6Y:247:GLU:HG2 | 2.16 | 0.45 |
| 24:6Y:512:TYR:CZ | 24:6Y:523:ILE:HG13 | 2.52 | 0.45 |
| 24:6Z:592:ASP:N | 24:6Z:592:ASP:OD1 | 2.47 | 0.45 |
| 38:8B:170:PHE:O | 38:8B:170:PHE:CD2 | 2.70 | 0.45 |
| 1:A1:75:SER:O | 24:6Y:149:LYS:NZ | 2.50 | 0.45 |
| 1:G2:290:THR:HG1 | 1:G2:294:TRP:HD1 | 1.64 | 0.45 |
| 1:G4:385:PHE:HZ | 1:G4:408:PHE:HD1 | 1.64 | 0.45 |
| 2:G5:363:VAL:HG13 | 2:G5:366:GLY:HA3 | 1.97 | 0.45 |
| 2:G7:91:GLN:HE22 | 2:G7:125:LEU:HD11 | 1.81 | 0.45 |
| 2:G7:229:ARG:HD3 | 2:G7:363:VAL:HG11 | 1.99 | 0.45 |
| 2:G9:182:VAL:HG23 | 2:G9:186:ASN:ND2 | 2.30 | 0.45 |
| 2:H5:403:ALA:HB2 | 1:H6:344:TRP:HZ3 | 1.82 | 0.45 |
| 1:H6:49:VAL:HG11 | 1:H6:241:ARG:HG2 | 1.99 | 0.45 |
| 1:H6:276:ARG:CZ | 24:6V:490:THR:HA | 2.45 | 0.45 |
| 2:H7:271:SER:OG | 2:H7:272:TYR:N | 2.48 | 0.45 |
| 1:I0:95:THR:OG1 | 1:I0:96:GLY:N | 2.49 | 0.45 |
| 1:I4:167:PHE:CE2 | 1:I4:233:MET:HG2 | 2.51 | 0.45 |
| 2:I7:203:MET:C | 2:I7:204:LEU:HD12 | 2.36 | 0.45 |
| 2:I9:156:ARG:HA | 2:I9:159:VAL:HG22 | 1.98 | 0.45 |
| 1:J4:203:ASP:OD1 | 1:J4:301:CYS:HA | 2.16 | 0.45 |
| 1:J4:317:PHE:HB3 | 1:J4:321:MET:SD | 2.56 | 0.45 |
| 2:J5:205:ASP:OD1 | 2:J5:207:GLU:N | 2.46 | 0.45 |
| 2:J5:370:LYS:HD2 | 5:4M:155:ARG:N | 2.31 | 0.45 |
| 1:K0:177:ASP:O | 2:K1:352:LYS:HD2 | 2.17 | 0.45 |
| 1:K0:309:ARG:H | 1:K0:372:THR:CG2 | 2.29 | 0.45 |
| 2:K1:404:PHE:HE2 | 2:K1:407:TRP:CE3 | 2.34 | 0.45 |
| 2:K3:370:LYS:HD2 | 6:4O:147:GLU:OE1 | 2.17 | 0.45 |
| 1:K4:6:HIS:CE1 | 1:K4:8:GLN:HG2 | 2.51 | 0.45 |
| 1:K4:178:THR:CG2 | 1:K4:181:GLU:HG3 | 2.47 | 0.45 |
| 2:K5:14:ILE:HD11 | 2:K5:74:VAL:HG13 | 1.99 | 0.45 |
| 2:K9:394:LYS:HB2 | 1:L0:346:PRO:HG3 | 1.98 | 0.45 |
| 1:L4:36:TYR:C | 29:7J:335:GLU:OE2 | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L4:175:VAL:HG22 | 2:L5:329:ASN:ND2 | 2.31 | 0.45 |
| 1:L6:2:ARG:HB3 | 1:L6:131:GLN:HB2 | 1.99 | 0.45 |
| 1:L6:362:LYS:HA | 6:4P:169:PHE:HZ | 1.82 | 0.45 |
| 2:L9:75:VAL:HG21 | 2:L9:94:SER:HB2 | 1.99 | 0.45 |
| 2:L9:100:ALA:HA | 1:M0:252:LYS:HE3 | 1.99 | 0.45 |
| 1:M2:335:ASN:O | 1:M2:338:SER:OG | 2.33 | 0.45 |
| 2:M3:222:PRO:HD2 | 1:M4:324:LYS:HE3 | 1.99 | 0.45 |
| 2:M5:312:TYR:HB2 | 2:M5:343:PHE:CD1 | 2.52 | 0.45 |
| 1:M8:316:LEU:HD13 | 1:M8:352:SER:HB3 | 1.98 | 0.45 |
| 2:M9:175:PRO:HB3 | 2:M9:390:ARG:NE | 2.32 | 0.45 |
| 2:M9:330:ALA:O | 2:M9:334:THR:HG23 | 2.17 | 0.45 |
| 2:N1:49:PHE:HB2 | 2:N1:53:PHE:HD2 | 1.81 | 0.45 |
| 2:N1:66:ILE:HG13 | 2:N1:66:ILE:O | 2.17 | 0.45 |
| 2:N1:389:SER:N | 2:N1:429:GLU:OE2 | 2.49 | 0.45 |
| 1:N6:108:GLU:HA | 1:N6:111:GLU:OE1 | 2.16 | 0.45 |
| 2:N9:183:GLU:CD | 2:N9:184:PRO:HD3 | 2.36 | 0.45 |
| 1:O0:134:GLN:HE21 | 1:O0:167:PHE:HE2 | 1.65 | 0.45 |
| 2:O3:221:ARG:NE | 37:7Y:70:THR:OG1 | 2.50 | 0.45 |
| 1:O4:101:TRP:HB2 | 1:O4:184:ASN:OD1 | 2.16 | 0.45 |
| 1:P4:217:LEU:O | 27:7G:171:LYS:NZ | 2.48 | 0.45 |
| 2:P5:8:HIS:CD2 | 2:P5:138:PHE:HD2 | 2.35 | 0.45 |
| 2:P5:51:THR:HG21 | 2:P5:243:ARG:HG2 | 1.98 | 0.45 |
| 2:P5:176:GLN:HG2 | 2:P5:177:VAL:N | 2.32 | 0.45 |
| 1:P8:167:PHE:CE2 | 1:P8:233:MET:HG2 | 2.51 | 0.45 |
| 2:Q1:269:LEU:HD13 | 2:Q1:301:MET:HE3 | 1.98 | 0.45 |
| 2:Q1:327:ASP:OD1 | 2:Q1:328:VAL:N | 2.50 | 0.45 |
| 2:Q5:336:LYS:O | 2:Q5:339:ARG:NH2 | 2.46 | 0.45 |
| 2:Q9:27:GLU:HG3 | 2:Q9:361:THR:HG21 | 1.99 | 0.45 |
| 1:S2:219:THR:O | 1:S2:219:THR:OG1 | 2.32 | 0.45 |
| 1:S4:150:LEU:HD11 | 3:3V:76:PRO:HG3 | 1.98 | 0.45 |
| 1:S6:60:VAL:HG21 | 1:S6:86:ARG:HH21 | 1.81 | 0.45 |
| 1:S6:100:ASN:HB3 | 1:S6:103:LYS:HB2 | 1.99 | 0.45 |
| 1:S8:35:THR:HA | 1:S8:57:GLY:O | 2.16 | 0.45 |
| 1:S8:110:ALA:HB1 | 3:3Z:75:ARG:NE | 2.32 | 0.45 |
| 2:S9:105:ARG:HB2 | 2:S9:411:GLU:CG | 2.47 | 0.45 |
| 1:T0:170:VAL:HG21 | 1:T0:377:MET:SD | 2.56 | 0.45 |
| 2:T3:183:GLU:CD | 2:T3:184:PRO:HD3 | 2.37 | 0.45 |
| 1:T6:1:MET:CE | 26:7F:67:GLN:HE21 | 2.29 | 0.45 |
| 1:T6:77:ARG:HH22 | 24:7A:46:ALA:HB1 | 1.80 | 0.45 |
| 2:T7:88:HIS:HD2 | 2:T7:89:PRO:CD | 2.17 | 0.45 |
| 2:V1:116:ASP:OD1 | 2:V1:117:LEU:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V6:2:ARG:NH2 | 1:V6:249:ASP:HB3 | 2.32 | 0.45 |
| 1:V6:328:GLU:OE1 | 1:V6:332:ASN:ND2 | 2.49 | 0.45 |
| 1:W0:101:TRP:CE3 | 1:W0:403:MET:HE1 | 2.52 | 0.45 |
| 1:W2:263:LEU:HD23 | 1:W2:422:TYR:HE1 | 1.80 | 0.45 |
| 1:W4:5:VAL:HG23 | 1:W4:62:ARG:HG2 | 1.99 | 0.45 |
| 1:W4:101:TRP:HE3 | 1:W4:403:MET:HE1 | 1.81 | 0.45 |
| 2:W7:187:SER:O | 2:W7:191:THR:HG23 | 2.16 | 0.45 |
| 1:W8:3:GLU:HG3 | 1:W8:127:CYS:SG | 2.57 | 0.45 |
| 2:W9:33:ASP:OD2 | 2:W9:35:GLN:NE2 | 2.44 | 0.45 |
| 1:X2:397:TRP:HE1 | 2:X3:260:VAL:HB | 1.81 | 0.45 |
| 1:X4:148:GLY:O | 1:X4:152:ILE:HG12 | 2.16 | 0.45 |
| 1:X4:164:MET:SD | 1:X4:196:ALA:HA | 2.56 | 0.45 |
| 2:X7:33:ASP:OD2 | 2:X7:35:GLN:NE2 | 2.44 | 0.45 |
| 2:X7:72:PRO:HD2 | 1:X8:2:ARG:HH12 | 1.82 | 0.45 |
| 1:Y0:21:TRP:CZ3 | 1:Y0:61:PRO:HB3 | 2.52 | 0.45 |
| 2:Y1:245:ASP:OD1 | 2:Y1:245:ASP:N | 2.37 | 0.45 |
| 1:Y2:154:LYS:HD2 | 1:Y2:154:LYS:N | 2.31 | 0.45 |
| 2:Y3:21:TRP:CZ3 | 2:Y3:63:PRO:HB3 | 2.52 | 0.45 |
| 1:Y8:183:TYR:HB3 | 1:Y8:398:TYR:HE2 | 1.82 | 0.45 |
| 1:Z2:62:ARG:HG2 | 1:Z2:123:GLU:OE2 | 2.17 | 0.45 |
| 1:Z2:115:SER:HA | 1:Z2:118:ASP:OD2 | 2.16 | 0.45 |
| 1:Z4:409:THR:HA | 1:Z4:412:GLU:OE1 | 2.16 | 0.45 |
| 2:Z5:166:LYS:N | 2:Z5:199:ASP:OD2 | 2.50 | 0.45 |
| 2:Z7:292:THR:HG1 | 2:Z7:319:TYR:HH | 1.63 | 0.45 |
| 2:Z9:176:GLN:HG2 | 2:Z9:177:VAL:N | 2.32 | 0.45 |
| 1:0A:274:THR:OG1 | 1:0A:278:SER:OG | 2.34 | 0.45 |
| 2:0B:344:VAL:HG22 | 2:0B:346:TRP:H | 1.81 | 0.45 |
| 1:0C:68:LEU:HD21 | 1:0C:108:GLU:HG2 | 1.99 | 0.45 |
| 1:0C:134:GLN:HE21 | 1:0C:167:PHE:HZ | 1.64 | 0.45 |
| 2:0F:306:ASP:HB3 | 2:0F:309:HIS:HD2 | 1.80 | 0.45 |
| 2:0H:147:SER:OG | 2:0H:148:GLY:N | 2.50 | 0.45 |
| 2:0H:320:ARG:O | 2:0H:373:ARG:HA | 2.17 | 0.45 |
| 1:0I:204:ASN:HD22 | 1:0I:207:LEU:HD12 | 1.82 | 0.45 |
| 1:0K:39:ASP:OD1 | 1:0K:39:ASP:N | 2.48 | 0.45 |
| 1:0K:117:LEU:O | 1:0K:121:ARG:HB2 | 2.17 | 0.45 |
| 1:0K:204:ASN:ND2 | 39:0K:502:GDP:HN22 | 2.15 | 0.45 |
| 1:0Q:404:ASP:HB3 | 1:0Q:406:MET:SD | 2.57 | 0.45 |
| 1:0U:314:SER:HA | 1:0U:350:LYS:O | 2.16 | 0.45 |
| 1:0W:6:HIS:HE1 | 1:0W:8:GLN:HG2 | 1.80 | 0.45 |
| 1:0W:272:PRO:O | 1:0W:273:LEU:HD23 | 2.16 | 0.45 |
| 2:0X:56:THR:HG23 | 2:1N:285:GLN:CB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Y:309:ARG:H | 1:0Y:372:THR:HG22 | 1.82 | 0.45 |
| 1:1C:35:THR:HA | 1:1C:57:GLY:O | 2.17 | 0.45 |
| 2:1D:427:ALA:HA | 2:1D:430:LYS:HE2 | 1.98 | 0.45 |
| 1:1G:219:THR:O | 1:1G:219:THR:OG1 | 2.35 | 0.45 |
| 1:1M:286:VAL:HG12 | 1:1M:321:MET:HE3 | 1.98 | 0.45 |
| 1:1O:248:ALA:HA | 1:1O:252:LYS:CD | 2.39 | 0.45 |
| 2:1P:69:ASP:OD1 | 2:1P:70:LEU:N | 2.47 | 0.45 |
| 1:1S:135:VAL:O | 1:1S:166:THR:HA | 2.16 | 0.45 |
| 2:1T:246:GLY:N | 2:1T:249:ASN:HD21 | 2.12 | 0.45 |
| 1:1U:12:CYS:O | 1:1U:16:ILE:HG23 | 2.17 | 0.45 |
| 1:1W:86:ARG:HB3 | 1:1W:89:ASN:ND2 | 2.31 | 0.45 |
| 2:1Z:250:VAL:HG23 | 2:1Z:254:GLU:CD | 2.37 | 0.45 |
| 1:2C:404:ASP:HB3 | 1:2C:406:MET:SD | 2.57 | 0.45 |
| 2:2F:130:THR:O | 38:8B:116:GLN:NE2 | 2.49 | 0.45 |
| 1:2G:404:ASP:OD1 | 1:2G:405:GLU:N | 2.41 | 0.45 |
| 1:2I:167:PHE:CE2 | 1:2I:233:MET:HG2 | 2.51 | 0.45 |
| 2:2N:47:ASP:N | 2:2N:47:ASP:OD1 | 2.50 | 0.45 |
| 1:2Q:5:VAL:HG12 | 1:2Q:133:PHE:HD1 | 1.80 | 0.45 |
| 1:2S:113:ILE:HG13 | 1:2S:114:ASP:N | 2.32 | 0.45 |
| 2:2T:286:LEU:HA | 2:2T:286:LEU:HD13 | 1.81 | 0.45 |
| 2:2X:122:ILE:HG22 | 2:2X:125:LEU:HD12 | 1.98 | 0.45 |
| 1:2Y:293:MET:HE1 | 1:2Y:317:PHE:HE1 | 1.82 | 0.45 |
| 2:3D:199:ASP:OD2 | 2:3D:256:GLN:HG2 | 2.17 | 0.45 |
| 2:3D:413:MET:HB3 | 2:3D:417:GLU:OE2 | 2.17 | 0.45 |
| 2:3H:174:SER:HB3 | 2:3H:177:VAL:O | 2.17 | 0.45 |
| 2:3J:199:ASP:OD1 | 2:3J:200:VAL:N | 2.50 | 0.45 |
| 2:3J:276:ILE:HD12 | 2:3J:280:LYS:HB3 | 1.98 | 0.45 |
| 2:3L:220:GLU:HG2 | 2:3L:221:ARG:HG3 | 1.98 | 0.45 |
| 1:3M:391:ARG:HD2 | 2:3N:346:TRP:CB | 2.27 | 0.45 |
| 1:3M:391:ARG:NH1 | 2:3N:346:TRP:HE3 | 2.13 | 0.45 |
| 2:3P:210:TYR:HH | 1:3Q:323:THR:HG1 | 1.56 | 0.45 |
| 2:3R:288:VAL:HG11 | 2:3R:327:ASP:HB2 | 1.97 | 0.45 |
| 2:3R:346:TRP:CZ3 | 2:3R:347:CYS:HB2 | 2.52 | 0.45 |
| 1:3S:139:LEU:HD12 | 1:3S:170:VAL:HG12 | 1.99 | 0.45 |
| 1:3S:183:TYR:O | 1:3S:187:LEU:HD13 | 2.17 | 0.45 |
| 3:4J:192:LEU:O | 3:4J:195:ILE:HG22 | 2.17 | 0.45 |
| 8:4W:466:ARG:HD3 | 8:4W:466:ARG:C | 2.37 | 0.45 |
| 9:4Z:259:ASP:OD2 | 9:4Z:263:ARG:NH2 | 2.50 | 0.45 |
| 12:5F:382:GLN:HG2 | 12:5F:383:ARG:CD | 2.46 | 0.45 |
| 14:5L:383:LEU:HD21 | 14:5L:403:ASP:HB3 | 1.99 | 0.45 |
| 14:5M:331:LYS:HE2 | 14:5M:331:LYS:HB2 | 1.76 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:383:LEU:HD21 | 14:5M:403:ASP:HB3 | 1.99 | 0.45 |
| 14:5N:383:LEU:HD21 | 14:5N:403:ASP:HB3 | 1.99 | 0.45 |
| 15:5O:168:ALA:O | 15:5O:171:LYS:HG3 | 2.16 | 0.45 |
| 16:5Q:91:ASP:OD2 | 16:5Q:94:ARG:NH1 | 2.49 | 0.45 |
| 18:6B:29:ILE:HD12 | 18:6B:87:LEU:HD21 | 1.99 | 0.45 |
| 20:6F:90:ALA:HB1 | 20:6F:98:THR:O | 2.16 | 0.45 |
| 22:6L:203:HIS:CD2 | 22:6L:204:PHE:H | 2.35 | 0.45 |
| 22:6L:240:TYR:O | 22:6L:244:VAL:HG22 | 2.17 | 0.45 |
| 24:6V:214:ARG:HG2 | 24:6V:219:MET:SD | 2.56 | 0.45 |
| 24:6W:472:SER:HB2 | 24:6W:481:LEU:CD2 | 2.46 | 0.45 |
| 24:6Y:505:LYS:HB3 | 24:6Y:506:PRO:HD2 | 1.98 | 0.45 |
| 28:7H:430:MET:HA | 28:7H:430:MET:CE | 2.47 | 0.45 |
| 29:7I:264:ARG:NH1 | 30:7K:362:GLN:HG3 | 2.31 | 0.45 |
| 30:7K:44:GLU:O | 30:7K:45:ARG:HG2 | 2.16 | 0.45 |
| 35:7U:183:LYS:HB2 | 35:7U:183:LYS:HE3 | 1.79 | 0.45 |
| 28:7X:430:MET:HA | 28:7X:430:MET:CE | 2.47 | 0.45 |
| 38:8C:92:GLU:OE2 | 38:8C:94:LYS:CE | 2.64 | 0.45 |
| 38:8D:63:VAL:HA | 38:8D:66:TYR:HD2 | 1.81 | 0.45 |
| 2:A4:40:LYS:HB3 | 24:6Z:187:PHE:HB2 | 1.97 | 0.45 |
| 1:B3:79:GLY:HA3 | 24:6W:221:ARG:HH22 | 1.81 | 0.45 |
| 1:B5:80:PRO:HD2 | 24:6X:221:ARG:HH12 | 1.82 | 0.45 |
| 2:B7:79:ARG:CZ | 18:6B:165:ASP:HB3 | 2.47 | 0.45 |
| 2:E3:364:PRO:HG2 | 22:6K:123:PRO:HB2 | 1.97 | 0.45 |
| 1:E8:32:PRO:HG3 | 24:6X:402:LYS:HG3 | 1.99 | 0.45 |
| 1:F2:276:ARG:HH12 | 22:6O:65:ARG:HH21 | 1.62 | 0.45 |
| 2:F7:278:ALA:HB3 | 22:6J:215:GLY:HA2 | 1.99 | 0.45 |
| 1:G2:8:GLN:OE1 | 1:G2:17:GLY:HA3 | 2.16 | 0.45 |
| 2:G3:14:ILE:HD11 | 2:G3:74:VAL:HG13 | 1.97 | 0.45 |
| 2:G3:205:ASP:HB3 | 2:G3:303:VAL:HA | 1.98 | 0.45 |
| 1:G4:175:VAL:O | 1:G4:175:VAL:HG13 | 2.17 | 0.45 |
| 1:G8:212:PHE:O | 1:G8:216:LYS:HA | 2.17 | 0.45 |
| 2:G9:119:LEU:HD11 | 2:G9:156:ARG:HB3 | 1.99 | 0.45 |
| 2:H1:254:GLU:O | 2:H1:258:ASN:ND2 | 2.50 | 0.45 |
| 1:H2:387:ALA:HA | 1:H2:390:ARG:NE | 2.32 | 0.45 |
| 1:H4:95:THR:OG1 | 1:H4:96:GLY:N | 2.49 | 0.45 |
| 2:H5:101:ASN:ND2 | 2:H5:143:GLY:HA2 | 2.31 | 0.45 |
| 1:H8:113:ILE:HA | 1:H8:116:VAL:HG12 | 1.98 | 0.45 |
| 2:I1:121:ARG:NH1 | 2:I1:121:ARG:CG | 2.60 | 0.45 |
| 1:I4:177:ASP:OD1 | 2:I5:248:LEU:HD21 | 2.17 | 0.45 |
| 1:I4:237:THR:HG23 | 1:I4:240:LEU:HD12 | 1.98 | 0.45 |
| 2:I5:266:HIS:ND1 | 2:I5:266:HIS:O | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I9:57:GLY:H | 2:K5:285:GLN:HB2 | 1.82 | 0.45 |
| 2:J5:21:TRP:CZ2 | 2:J5:65:CYS:HB2 | 2.51 | 0.45 |
| 2:J7:116:ASP:N | 2:J7:116:ASP:OD1 | 2.48 | 0.45 |
| 2:J7:174:SER:HB3 | 2:J7:177:VAL:O | 2.15 | 0.45 |
| 2:K7:72:PRO:HD2 | 1:K8:2:ARG:NH1 | 2.31 | 0.45 |
| 1:K8:236:ILE:HD12 | 1:K8:316:LEU:HD11 | 1.98 | 0.45 |
| 2:K9:217:LEU:HD23 | 2:K9:217:LEU:HA | 1.82 | 0.45 |
| 2:L1:215:ARG:HE | 29:7J:471:HIS:HE1 | 1.65 | 0.45 |
| 2:L3:344:VAL:HG13 | 2:L3:346:TRP:H | 1.82 | 0.45 |
| 2:L3:384:ILE:HA | 2:L3:387:ILE:HD12 | 1.97 | 0.45 |
| 1:M0:285:THR:OG1 | 1:M0:287:PRO:HD2 | 2.16 | 0.45 |
| 2:M3:384:ILE:HA | 2:M3:387:ILE:HD12 | 1.99 | 0.45 |
| 1:M6:5:VAL:HG12 | 1:M6:133:PHE:CD1 | 2.51 | 0.45 |
| 2:M7:11:GLN:NE2 | 1:M8:247:ASN:OD1 | 2.50 | 0.45 |
| 2:M7:30:ILE:HD12 | 2:M7:53:PHE:CE2 | 2.52 | 0.45 |
| 2:M9:431:ASP:O | 2:M9:435:VAL:HG23 | 2.17 | 0.45 |
| 1:N0:297:LYS:HA | 1:N0:297:LYS:HD3 | 1.80 | 0.45 |
| 1:N2:60:VAL:CG1 | 1:N2:86:ARG:HE | 2.29 | 0.45 |
| 1:N2:189:VAL:HA | 1:N2:192:LEU:HB2 | 1.99 | 0.45 |
| 2:N7:66:ILE:O | 2:N7:66:ILE:HG13 | 2.16 | 0.45 |
| 2:N7:114:ILE:HG21 | 2:N7:149:LEU:HD22 | 1.99 | 0.45 |
| 2:N9:119:LEU:CD2 | 2:N9:122:ILE:HD11 | 2.36 | 0.45 |
| 1:O0:174:LYS:HB3 | 1:O0:174:LYS:HE2 | 1.76 | 0.45 |
| 1:O0:250:LEU:HA | 1:O0:253:LEU:HD12 | 1.99 | 0.45 |
| 1:O2:203:ASP:N | 1:O2:203:ASP:OD1 | 2.50 | 0.45 |
| 1:O6:67:ASP:N | 1:O6:67:ASP:OD1 | 2.49 | 0.45 |
| 1:O6:233:MET:O | 1:O6:236:ILE:HG22 | 2.17 | 0.45 |
| 2:O7:70:LEU:HG | 2:O7:145:THR:HG23 | 1.98 | 0.45 |
| 2:O7:177:VAL:HG13 | 1:O8:327:ASP:HB3 | 1.99 | 0.45 |
| 2:O7:434:GLU:C | 2:O7:434:GLU:CD | 2.75 | 0.45 |
| 2:P3:417:GLU:HA | 2:P3:420:GLU:HG2 | 1.98 | 0.45 |
| 2:P5:174:SER:HA | 2:P5:205:ASP:OD2 | 2.17 | 0.45 |
| 2:Q3:279:GLU:OE2 | 2:Q3:280:LYS:HG3 | 2.17 | 0.45 |
| 1:Q4:217:LEU:CA | 20:6F:184:ARG:HH12 | 2.29 | 0.45 |
| 2:Q5:69:ASP:OD1 | 2:Q5:70:LEU:N | 2.49 | 0.45 |
| 2:Q5:320:ARG:HB3 | 2:Q5:358:GLN:O | 2.16 | 0.45 |
| 2:Q9:216:SER:OG | 2:Q9:217:LEU:N | 2.48 | 0.45 |
| 1:R0:301:CYS:SG | 1:R0:302:ALA:N | 2.90 | 0.45 |
| 1:R0:363:MET:O | 7:4Q:352:ASN:ND2 | 2.46 | 0.45 |
| 1:R0:391:ARG:O | 1:R0:392:LYS:C | 2.55 | 0.45 |
| 1:R2:311:LEU:HD23 | 1:R2:311:LEU:HA | 1.78 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R7:72:PRO:HD2 | 1:R8:2:ARG:HH12 | 1.82 | 0.45 |
| 2:R7:203:MET:HB2 | 2:R7:303:VAL:HG21 | 1.99 | 0.45 |
| 1:R8:425:TYR:OH | 17:5U:108:ASN:ND2 | 2.42 | 0.45 |
| 2:R9:57:GLY:H | 2:T5:285:GLN:CB | 2.29 | 0.45 |
| 2:R9:359:PRO:HD2 | 12:5F:118:ARG:NH2 | 2.32 | 0.45 |
| 1:S6:122:LYS:HA | 3:3X:65:SER:OG | 2.16 | 0.45 |
| 1:S8:68:LEU:HD12 | 1:S8:97:ALA:HB2 | 1.99 | 0.45 |
| 2:S9:306:ASP:HB3 | 2:S9:309:HIS:CD2 | 2.50 | 0.45 |
| 1:T0:4:ILE:HB | 1:T0:50:TYR:HE2 | 1.81 | 0.45 |
| 1:T0:65:LEU:HD12 | 1:T0:90:PHE:HE1 | 1.77 | 0.45 |
| 1:T0:418:LEU:O | 1:T0:421:GLU:HG2 | 2.17 | 0.45 |
| 2:T1:15:GLN:HB3 | 2:T1:228:ASN:ND2 | 2.32 | 0.45 |
| 1:T6:19:LYS:HG3 | 1:T6:227:HIS:CE1 | 2.52 | 0.45 |
| 2:T7:65:CYS:SG | 2:T7:87:PHE:HE1 | 2.39 | 0.45 |
| 2:U1:4:VAL:HG23 | 2:U1:134:GLY:O | 2.17 | 0.45 |
| 2:U1:280:LYS:HA | 2:U1:283:HIS:CD2 | 2.52 | 0.45 |
| 2:U7:301:MET:HE1 | 2:U7:307:PRO:HD3 | 1.99 | 0.45 |
| 2:V1:429:GLU:OE2 | 2:V1:429:GLU:HA | 2.16 | 0.45 |
| 1:V6:173:PRO:HD3 | 1:V6:380:ARG:HD3 | 1.97 | 0.45 |
| 1:V6:260:PHE:CD2 | 1:V6:263:LEU:HD23 | 2.52 | 0.45 |
| 1:V6:268:VAL:HG23 | 1:V6:368:ILE:HG13 | 1.99 | 0.45 |
| 2:V7:311:LYS:NZ | 2:V7:343:PHE:O | 2.39 | 0.45 |
| 1:V8:240:LEU:HD21 | 1:V8:249:ASP:HA | 1.98 | 0.45 |
| 2:V9:333:ALA:O | 2:V9:337:THR:HG23 | 2.17 | 0.45 |
| 2:W1:234:VAL:O | 2:W1:237:SER:OG | 2.31 | 0.45 |
| 1:W4:72:THR:O | 1:W4:76:VAL:HG23 | 2.17 | 0.45 |
| 1:W6:190:HIS:NE2 | 1:W6:414:ASN:OD1 | 2.49 | 0.45 |
| 2:W7:34:GLY:O | 2:W7:60:LYS:HA | 2.16 | 0.45 |
| 2:W7:47:ASP:OD1 | 2:W7:48:ALA:N | 2.50 | 0.45 |
| 1:W8:30:ILE:HG22 | 1:W8:36:TYR:HA | 1.98 | 0.45 |
| 2:W9:12:ALA:O | 2:W9:16:VAL:HG23 | 2.17 | 0.45 |
| 2:W9:16:VAL:HA | 2:W9:228:ASN:HB3 | 1.99 | 0.45 |
| 2:W9:298:PRO:HA | 2:W9:301:MET:HG3 | 1.98 | 0.45 |
| 1:X2:175:VAL:HG13 | 2:X3:329:ASN:ND2 | 2.32 | 0.45 |
| 1:X6:233:MET:O | 1:X6:237:THR:HG22 | 2.16 | 0.45 |
| 1:X8:396:HIS:HE1 | 1:X8:397:TRP:CE2 | 2.35 | 0.45 |
| 2:X9:333:ALA:O | 2:X9:337:THR:HG23 | 2.17 | 0.45 |
| 1:Y8:230:SER:HA | 1:Y8:233:MET:HG2 | 1.98 | 0.45 |
| 2:Z1:286:LEU:HG | 2:Z1:373:ARG:NH1 | 2.31 | 0.45 |
| 2:Z3:7:ILE:HD11 | 2:Z3:137:VAL:HG12 | 1.97 | 0.45 |
| 1:Z4:163:MET:HE2 | 1:Z4:251:ARG:HA | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z4:181:GLU:HG3 | 1:Z4:182:PRO:HD3 | 1.97 | 0.45 |
| 2:Z5:31:GLN:HB2 | 2:Z5:33:ASP:OD1 | 2.16 | 0.45 |
| 1:Z6:337:ASN:HB2 | 1:Z6:340:TYR:HD2 | 1.81 | 0.45 |
| 1:Z8:114:ASP:OD1 | 1:Z8:114:ASP:N | 2.48 | 0.45 |
| 1:Z8:177:ASP:OD2 | 2:Z9:248:LEU:HD21 | 2.17 | 0.45 |
| 1:0A:316:LEU:HD23 | 1:0A:317:PHE:N | 2.31 | 0.45 |
| 2:0F:383:ALA:O | 2:0F:387:ILE:HG12 | 2.16 | 0.45 |
| 1:0G:237:THR:HG23 | 1:0G:241:ARG:HE | 1.81 | 0.45 |
| 1:0I:101:TRP:CZ3 | 1:0I:187:LEU:HD23 | 2.52 | 0.45 |
| 1:0I:107:THR:OG1 | 1:0I:401:GLU:OE2 | 2.27 | 0.45 |
| 2:0J:109:THR:OG1 | 2:0J:411:GLU:OE2 | 2.25 | 0.45 |
| 1:0K:3:GLU:HG3 | 1:0K:127:CYS:SG | 2.56 | 0.45 |
| 1:0K:387:ALA:C | 1:0K:388:MET:HE1 | 2.36 | 0.45 |
| 2:0N:269:LEU:HD21 | 2:0N:301:MET:SD | 2.57 | 0.45 |
| 1:0O:52:ASN:OD1 | 1:0O:62:ARG:NH2 | 2.50 | 0.45 |
| 2:0P:403:ALA:HB2 | 1:0Q:344:TRP:HZ3 | 1.81 | 0.45 |
| 1:0Q:165:LEU:HD13 | 1:0Q:167:PHE:HZ | 1.81 | 0.45 |
| 2:0R:191:THR:HA | 2:0R:194:LEU:HB3 | 1.99 | 0.45 |
| 1:0U:198:GLU:HA | 1:0U:264:HIS:HB2 | 1.99 | 0.45 |
| 2:0Z:119:LEU:HD11 | 2:0Z:156:ARG:HD3 | 1.98 | 0.45 |
| 2:0Z:155:GLU:HB2 | 2:0Z:197:HIS:CE1 | 2.52 | 0.45 |
| 1:1A:8:GLN:OE1 | 1:1A:17:GLY:HA3 | 2.16 | 0.45 |
| 2:1B:227:LEU:O | 2:1B:231:ILE:HG13 | 2.17 | 0.45 |
| 1:1C:173:PRO:HB3 | 1:1C:384:GLN:HE22 | 1.82 | 0.45 |
| 2:1H:155:GLU:HG2 | 2:1H:197:HIS:NE2 | 2.31 | 0.45 |
| 2:1L:246:GLY:H | 2:1L:249:ASN:ND2 | 2.15 | 0.45 |
| 2:1X:50:ASN:O | 2:1X:64:ARG:NH2 | 2.50 | 0.45 |
| 2:1Z:2:ARG:HD2 | 2:1Z:242:LEU:HD22 | 1.99 | 0.45 |
| 1:2A:27:GLU:HA | 1:2A:359:LYS:HD3 | 1.98 | 0.45 |
| 2:2B:187:SER:O | 2:2B:191:THR:HG23 | 2.16 | 0.45 |
| 2:2B:244:PHE:HB2 | 2:2B:356:ASN:HD21 | 1.80 | 0.45 |
| 1:2C:86:ARG:HG2 | 1:2C:88:ASP:H | 1.80 | 0.45 |
| 2:2F:306:ASP:HB3 | 2:2F:309:HIS:HD2 | 1.81 | 0.45 |
| 1:2G:418:LEU:O | 1:2G:421:GLU:HG2 | 2.17 | 0.45 |
| 1:2I:203:ASP:OD1 | 1:2I:301:CYS:HA | 2.17 | 0.45 |
| 2:2J:68:LEU:HA | 2:2J:93:ILE:O | 2.17 | 0.45 |
| 2:2L:394:LYS:HB2 | 1:2M:346:PRO:HG3 | 1.98 | 0.45 |
| 1:2M:113:ILE:HA | 1:2M:116:VAL:HG22 | 1.98 | 0.45 |
| 1:2Q:320:ARG:CZ | 38:8A:201:LEU:HD12 | 2.46 | 0.45 |
| 1:2Q:340:TYR:CE2 | 38:8A:96:GLY:HA2 | 2.52 | 0.45 |
| 2:2R:56:THR:HA | 2:3H:285:GLN:HB3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2R:187:SER:O | 2:2R:191:THR:HG23 | 2.17 | 0.45 |
| 1:3A:212:PHE:CZ | 2:3B:326:LYS:HE3 | 2.52 | 0.45 |
| 1:3A:282:ARG:NH1 | 1:3A:292:GLN:OE1 | 2.44 | 0.45 |
| 1:3A:317:PHE:HE2 | 1:3A:326:VAL:HG13 | 1.81 | 0.45 |
| 2:3B:370:LYS:HD2 | 10:5D:162:ILE:HG21 | 1.97 | 0.45 |
| 1:3C:35:THR:HG21 | 38:8D:161:GLN:NE2 | 2.23 | 0.45 |
| 2:3D:139:ASN:OD1 | 2:3D:139:ASN:N | 2.50 | 0.45 |
| 2:3D:362:VAL:HG21 | 10:5D:220:GLN:NE2 | 2.32 | 0.45 |
| 1:3I:70:PRO:HB2 | 3:3Z:14:TYR:OH | 2.16 | 0.45 |
| 1:3I:199:CYS:SG | 1:3I:265:PHE:HD1 | 2.40 | 0.45 |
| 1:3I:317:PHE:HE2 | 1:3I:326:VAL:HG13 | 1.81 | 0.45 |
| 1:3I:386:THR:O | 1:3I:390:ARG:HG3 | 2.16 | 0.45 |
| 1:3M:246:LEU:O | 1:3M:352:SER:OG | 2.25 | 0.45 |
| 1:3O:3:GLU:HG3 | 1:3O:127:CYS:HB2 | 1.98 | 0.45 |
| 1:3O:170:VAL:HG22 | 1:3O:202:LEU:O | 2.17 | 0.45 |
| 1:3Q:273:LEU:H | 1:3Q:292:GLN:HE22 | 1.63 | 0.45 |
| 2:3R:7:ILE:HG12 | 2:3R:137:VAL:HG12 | 1.99 | 0.45 |
| 2:3R:66:ILE:HD12 | 2:3R:68:LEU:HD23 | 1.98 | 0.45 |
| 2:3R:188:VAL:HG21 | 2:3R:395:PHE:CE1 | 2.52 | 0.45 |
| 1:3S:49:VAL:O | 1:3S:62:ARG:NH1 | 2.50 | 0.45 |
| 1:3S:181:GLU:HB2 | 1:3S:182:PRO:CD | 2.46 | 0.45 |
| 1:3S:268:VAL:HG23 | 1:3S:300:MET:HB2 | 1.97 | 0.45 |
| 2:3T:90:GLU:HB3 | 2:3T:121:ARG:HH22 | 1.82 | 0.45 |
| 4:3Y:150:GLU:OE1 | 4:3Y:150:GLU:HA | 2.17 | 0.45 |
| 4:4A:150:GLU:OE1 | 4:4A:150:GLU:HA | 2.17 | 0.45 |
| 4:4C:150:GLU:OE1 | 4:4C:150:GLU:HA | 2.17 | 0.45 |
| 3:4F:173:ARG:O | 3:4F:177:VAL:HG23 | 2.16 | 0.45 |
| 5:4L:290:GLN:HB3 | 28:7H:306:LEU:CD2 | 2.46 | 0.45 |
| 5:4L:323:LEU:HA | 5:4L:326:GLU:OE1 | 2.17 | 0.45 |
| 5:4M:282:ARG:HE | 5:4M:282:ARG:HB2 | 1.46 | 0.45 |
| 7:4R:92:GLN:N | 7:4R:92:GLN:OE1 | 2.50 | 0.45 |
| 7:4U:57:ARG:HD2 | 12:5F:167:PRO:HB3 | 1.98 | 0.45 |
| 14:5M:18:GLU:OE2 | 14:5M:18:GLU:N | 2.50 | 0.45 |
| 14:5N:18:GLU:N | 14:5N:18:GLU:OE2 | 2.50 | 0.45 |
| 15:5O:23:LYS:HB2 | 15:5O:40:ILE:HD12 | 1.97 | 0.45 |
| 15:5P:268:GLY:HA2 | 15:5P:308:ALA:O | 2.17 | 0.45 |
| 15:5P:321:GLU:HB2 | 15:5P:322:PRO:HD3 | 1.97 | 0.45 |
| 18:5X:29:ILE:HD12 | 18:5X:87:LEU:HD21 | 1.99 | 0.45 |
| 18:5Y:29:ILE:HD12 | 18:5Y:87:LEU:HD21 | 1.99 | 0.45 |
| 18:6A:29:ILE:HD12 | 18:6A:87:LEU:HD21 | 1.99 | 0.45 |
| 18:6A:60:PRO:HA | 18:6A:63:LEU:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:6C:29:ILE:HD12 | 18:6C:87:LEU:HD21 | 1.99 | 0.45 |
| 18:6C:60:PRO:HA | 18:6C:63:LEU:HD12 | 1.98 | 0.45 |
| 18:6D:29:ILE:HD12 | 18:6D:87:LEU:HD21 | 1.99 | 0.45 |
| 20:6F:354:LEU:O | 20:6F:357:VAL:HG12 | 2.16 | 0.45 |
| 22:6K:132:SER:OG | 22:6K:212:GLU:OE1 | 2.28 | 0.45 |
| 22:6M:348:ALA:HA | 22:6M:351:ASN:ND2 | 2.32 | 0.45 |
| 24:6U:305:VAL:O | 24:6U:321:PHE:HB3 | 2.17 | 0.45 |
| 24:6U:613:LYS:HD2 | 24:6U:613:LYS:HA | 1.85 | 0.45 |
| 24:6V:171:THR:HG22 | 24:6V:180:TYR:HD1 | 1.81 | 0.45 |
| 24:6V:404:ARG:HD2 | 24:6V:404:ARG:HA | 1.86 | 0.45 |
| 24:6W:280:ASP:HA | 24:6W:289:ARG:HB2 | 1.98 | 0.45 |
| 24:6W:451:LYS:HD2 | 24:6W:468:ARG:CZ | 2.46 | 0.45 |
| 24:6X:282:ARG:NH1 | 24:6X:289:ARG:HD3 | 2.32 | 0.45 |
| 24:6Y:506:PRO:HB3 | 24:6Y:524:GLU:OE1 | 2.16 | 0.45 |
| 24:6Z:262:LEU:O | 24:6Z:266:LEU:HG | 2.17 | 0.45 |
| 24:6Z:606:ARG:O | 24:6Z:610:ILE:HG12 | 2.17 | 0.45 |
| 29:7I:254:MET:HE2 | 30:7K:341:ARG:NE | 2.31 | 0.45 |
| 38:8C:83:ARG:NH2 | 38:8C:85:ARG:CD | 2.67 | 0.45 |
| 2:4:280:LYS:NZ | 26:7D:64:PRO:CB | 2.80 | 0.45 |
| 1:7:141:GLY:HA3 | 39:7:502:GDP:O3A | 2.16 | 0.45 |
| 1:7:337:ASN:HD21 | 3:4B:69:TYR:N | 2.08 | 0.45 |
| 1:9:42:LEU:HD21 | 26:7E:121:LYS:CE | 2.32 | 0.45 |
| 1:9:436:PHE:CE1 | 3:4D:252:LYS:HB2 | 2.51 | 0.45 |
| 1:E6:37:HIS:CE1 | 22:6L:259:TYR:HE1 | 2.35 | 0.45 |
| 2:G1:414:GLU:HG2 | 2:G1:417:GLU:OE1 | 2.17 | 0.45 |
| 1:G2:388:MET:HE3 | 2:G3:348:PRO:HD2 | 1.98 | 0.45 |
| 2:G3:223:THR:OG1 | 2:G3:224:TYR:N | 2.50 | 0.45 |
| 2:G3:277:SER:O | 2:G3:281:ALA:HB2 | 2.16 | 0.45 |
| 1:G4:293:MET:HE1 | 1:G4:317:PHE:HE1 | 1.81 | 0.45 |
| 1:G6:49:VAL:HG11 | 1:G6:241:ARG:HG2 | 1.98 | 0.45 |
| 2:G7:259:LEU:HD11 | 2:G7:316:CYS:HB2 | 1.99 | 0.45 |
| 2:H3:47:ASP:OD1 | 2:H3:48:ALA:N | 2.50 | 0.45 |
| 2:H3:223:THR:OG1 | 2:H3:224:TYR:N | 2.50 | 0.45 |
| 1:I2:6:HIS:CE1 | 1:I2:8:GLN:HG2 | 2.52 | 0.45 |
| 1:I2:177:ASP:O | 2:I3:352:LYS:HA | 2.17 | 0.45 |
| 1:I4:180:VAL:HG23 | 1:I4:184:ASN:HD21 | 1.81 | 0.45 |
| 2:I5:50:ASN:O | 2:I5:64:ARG:NH2 | 2.50 | 0.45 |
| 2:I9:121:ARG:C | 2:I9:121:ARG:CD | 2.85 | 0.45 |
| 2:J1:143:GLY:O | 2:J1:147:SER:OG | 2.20 | 0.45 |
| 1:J4:395:LEU:O | 1:J4:399:THR:HG23 | 2.17 | 0.45 |
| 1:J6:233:MET:O | 1:J6:236:ILE:HG22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K1:387:ILE:O | 2:K1:391:LEU:HG | 2.17 | 0.45 |
| 2:K3:52:PHE:CE2 | 2:K3:243:ARG:HD3 | 2.51 | 0.45 |
| 2:K3:191:THR:HA | 2:K3:194:LEU:HB3 | 1.98 | 0.45 |
| 2:K5:430:LYS:O | 2:K5:434:GLU:HG2 | 2.17 | 0.45 |
| 2:L1:116:ASP:OD1 | 2:L1:156:ARG:NH1 | 2.50 | 0.45 |
| 1:L2:143:THR:O | 1:L2:147:MET:HB3 | 2.17 | 0.45 |
| 1:L4:161:ASP:HB3 | 1:L4:162:ARG:HH11 | 1.80 | 0.45 |
| 1:L4:174:LYS:HG3 | 1:L4:380:ARG:NH2 | 2.32 | 0.45 |
| 2:L7:325:PRO:HA | 2:L7:328:VAL:HG22 | 1.99 | 0.45 |
| 2:L9:9:ILE:HD13 | 2:L9:150:GLY:HA2 | 1.99 | 0.45 |
| 2:M1:22:GLU:O | 2:M1:26:LEU:HD23 | 2.17 | 0.45 |
| 2:M1:204:LEU:HD23 | 2:M1:302:MET:HB3 | 1.99 | 0.45 |
| 2:M3:27:GLU:HG2 | 2:M3:361:THR:OG1 | 2.16 | 0.45 |
| 2:M3:88:HIS:CE1 | 1:O0:280:GLN:HB2 | 2.51 | 0.45 |
| 2:M3:291:ILE:HA | 2:M3:294:ALA:HB3 | 1.99 | 0.45 |
| 2:M5:121:ARG:O | 2:M5:124:LYS:HG2 | 2.17 | 0.45 |
| 1:N0:100:ASN:HB3 | 1:N0:103:LYS:HB2 | 1.98 | 0.45 |
| 1:N0:321:MET:HG2 | 1:N0:363:MET:SD | 2.57 | 0.45 |
| 2:N1:231:ILE:O | 2:N1:235:ILE:HG12 | 2.17 | 0.45 |
| 2:N3:154:LEU:HG | 2:N3:197:HIS:HB3 | 1.98 | 0.45 |
| 1:N6:320:ARG:HH22 | 32:7O:67:ARG:HD3 | 1.81 | 0.45 |
| 1:O0:62:ARG:HG3 | 1:O0:123:GLU:CD | 2.36 | 0.45 |
| 1:O2:274:THR:HG21 | 1:O2:282:ARG:HD2 | 1.98 | 0.45 |
| 2:O3:52:PHE:CE2 | 2:O3:243:ARG:HD3 | 2.51 | 0.45 |
| 2:O3:163:LYS:N | 2:O3:163:LYS:HD2 | 2.31 | 0.45 |
| 1:O6:350:LYS:NZ | 1:O6:351:SER:O | 2.30 | 0.45 |
| 2:O7:167:LEU:HD13 | 2:O7:200:VAL:HB | 1.99 | 0.45 |
| 2:P5:90:GLU:HB2 | 2:P5:121:ARG:NH2 | 2.29 | 0.45 |
| 1:P6:354:CYS:SG | 1:P6:355:ASP:N | 2.90 | 0.45 |
| 1:P8:4:ILE:HB | 1:P8:50:TYR:CE1 | 2.51 | 0.45 |
| 1:P8:311:LEU:HA | 1:P8:311:LEU:HD12 | 1.81 | 0.45 |
| 1:Q6:361:LEU:HD23 | 1:Q6:361:LEU:HA | 1.83 | 0.45 |
| 1:R0:386:THR:O | 1:R0:390:ARG:HG3 | 2.17 | 0.45 |
| 1:R2:111:GLU:N | 1:R2:111:GLU:OE1 | 2.50 | 0.45 |
| 1:R4:263:LEU:HG | 1:R4:422:TYR:CZ | 2.52 | 0.45 |
| 2:R7:394:LYS:HB2 | 1:R8:346:PRO:HG3 | 1.99 | 0.45 |
| 1:R8:221:THR:HG21 | 7:4R:264:LYS:HG2 | 1.98 | 0.45 |
| 1:S4:392:LYS:HE2 | 13:5H:53:PHE:CD2 | 2.52 | 0.45 |
| 1:S4:404:ASP:HB3 | 1:S4:406:MET:SD | 2.57 | 0.45 |
| 1:S8:117:LEU:HA | 1:S8:117:LEU:HD23 | 1.81 | 0.45 |
| 2:S9:90:GLU:O | 2:S9:121:ARG:NH1 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T2:117:LEU:HD23 | 1:T2:117:LEU:HA | 1.78 | 0.45 |
| 2:T5:393:HIS:NE2 | 17:5U:30:LYS:HG2 | 2.31 | 0.45 |
| 1:T6:161:ASP:HB3 | 1:T6:162:ARG:HH11 | 1.82 | 0.45 |
| 1:T6:248:ALA:HA | 1:T6:252:LYS:HD2 | 1.98 | 0.45 |
| 1:T6:407:GLU:OE2 | 3:4H:81:PHE:HB3 | 2.16 | 0.45 |
| 2:U5:47:ASP:N | 2:U5:47:ASP:OD1 | 2.50 | 0.45 |
| 2:U5:363:VAL:HG23 | 2:U5:366:GLY:HA3 | 1.99 | 0.45 |
| 2:U9:91:GLN:N | 2:U9:121:ARG:HH22 | 2.14 | 0.45 |
| 2:V1:200:VAL:HG13 | 2:V1:268:MET:HE2 | 1.98 | 0.45 |
| 2:V1:417:GLU:OE1 | 2:V1:417:GLU:N | 2.36 | 0.45 |
| 2:V7:129:CYS:SG | 2:V7:130:THR:N | 2.89 | 0.45 |
| 2:W3:115:VAL:HG11 | 2:W3:152:LEU:HD23 | 1.98 | 0.45 |
| 1:W4:375:GLN:HB3 | 1:W4:422:TYR:HD2 | 1.82 | 0.45 |
| 2:W9:88:HIS:ND1 | 2:W9:89:PRO:HD2 | 2.32 | 0.45 |
| 1:X0:42:LEU:CD2 | 8:4X:97:PHE:CE2 | 2.92 | 0.45 |
| 1:X2:41:ASP:HA | 1:X2:44:LEU:HD13 | 1.98 | 0.45 |
| 1:X2:263:LEU:HD21 | 1:X2:421:GLU:OE1 | 2.17 | 0.45 |
| 1:X4:99:ASN:HD22 | 2:X5:258:ASN:HD21 | 1.63 | 0.45 |
| 1:X4:266:PHE:CE1 | 1:X4:370:ASN:HB2 | 2.51 | 0.45 |
| 1:X6:266:PHE:HE1 | 1:X6:370:ASN:HB2 | 1.81 | 0.45 |
| 1:Y2:395:LEU:O | 1:Y2:399:THR:HG23 | 2.16 | 0.45 |
| 2:Y3:298:PRO:HA | 2:Y3:301:MET:HG3 | 1.98 | 0.45 |
| 2:Y3:360:PRO:HD2 | 2:Y3:371:VAL:O | 2.17 | 0.45 |
| 1:Y4:237:THR:O | 1:Y4:241:ARG:NE | 2.42 | 0.45 |
| 1:Y4:257:LEU:HA | 1:Y4:312:THR:HG21 | 1.99 | 0.45 |
| 2:Y5:405:VAL:HG23 | 2:Y5:418:PHE:HE2 | 1.82 | 0.45 |
| 2:Y9:65:CYS:SG | 2:Y9:66:ILE:N | 2.90 | 0.45 |
| 2:Y9:90:GLU:HB2 | 2:0F:283:HIS:CE1 | 2.52 | 0.45 |
| 2:Y9:170:THR:O | 2:Y9:204:LEU:HB2 | 2.16 | 0.45 |
| 2:Z1:22:GLU:OE2 | 2:Z1:229:ARG:NH1 | 2.45 | 0.45 |
| 2:Z3:331:SER:O | 2:Z3:335:ILE:HG12 | 2.16 | 0.45 |
| 1:Z6:11:GLN:HG2 | 1:Z6:12:CYS:N | 2.32 | 0.45 |
| 2:Z7:15:GLN:HB3 | 2:Z7:228:ASN:ND2 | 2.32 | 0.45 |
| 2:Z7:246:GLY:HA3 | 2:Z7:356:ASN:HA | 1.98 | 0.45 |
| 1:Z8:21:TRP:CH2 | 1:Z8:61:PRO:HB3 | 2.51 | 0.45 |
| 2:0B:259:LEU:HB3 | 2:0B:268:MET:CE | 2.47 | 0.45 |
| 1:0C:86:ARG:HG2 | 1:0C:88:ASP:H | 1.80 | 0.45 |
| 1:0I:12:CYS:HB2 | 39:0I:502:GDP:C8 | 2.51 | 0.45 |
| 1:0K:126:SER:HB3 | 1:1A:291:GLN:HE22 | 1.81 | 0.45 |
| 2:0L:383:ALA:O | 2:0L:387:ILE:HG12 | 2.17 | 0.45 |
| 2:0N:246:GLY:HA3 | 2:0N:356:ASN:HA | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0O:270:PHE:HD2 | 1:0O:273:LEU:HD21 | 1.81 | 0.45 |
| 2:0P:336:LYS:O | 2:0P:339:ARG:NH2 | 2.46 | 0.45 |
| 2:0R:175:PRO:HB3 | 2:0R:390:ARG:HE | 1.81 | 0.45 |
| 2:0R:177:VAL:HG13 | 1:0S:327:ASP:OD2 | 2.17 | 0.45 |
| 1:0S:293:MET:SD | 1:0S:367:PHE:HB2 | 2.57 | 0.45 |
| 1:1A:163:MET:HG2 | 1:1A:250:LEU:HD22 | 1.98 | 0.45 |
| 1:1C:242:PHE:CD1 | 1:1C:356:ILE:HG13 | 2.52 | 0.45 |
| 2:1F:274:PRO:HB2 | 2:1F:276:ILE:CG1 | 2.47 | 0.45 |
| 1:1G:186:THR:HG22 | 1:1G:411:ALA:HB1 | 1.98 | 0.45 |
| 1:1G:193:VAL:HG12 | 1:1G:265:PHE:HZ | 1.82 | 0.45 |
| 1:1G:268:VAL:HB | 1:1G:300:MET:HB2 | 1.98 | 0.45 |
| 1:1G:385:PHE:HZ | 1:1G:408:PHE:HD1 | 1.64 | 0.45 |
| 1:1G:404:ASP:HB3 | 1:1G:406:MET:SD | 2.57 | 0.45 |
| 1:1G:418:LEU:O | 1:1G:421:GLU:HG2 | 2.17 | 0.45 |
| 2:1H:75:VAL:HG21 | 2:1H:94:SER:OG | 2.17 | 0.45 |
| 1:1M:174:LYS:HG3 | 1:1M:380:ARG:NH2 | 2.32 | 0.45 |
| 2:1N:279:GLU:HB3 | 9:4Z:118:LYS:NZ | 2.32 | 0.45 |
| 2:1P:98:ASP:OD2 | 2:1P:99:ALA:N | 2.50 | 0.45 |
| 1:1S:144:GLY:N | 39:1S:502:GDP:O1B | 2.49 | 0.45 |
| 2:1T:290:GLU:HA | 2:1T:293:ASN:HD22 | 1.81 | 0.45 |
| 1:1U:77:ARG:HH21 | 1:1U:90:PHE:HD2 | 1.64 | 0.45 |
| 2:1V:69:ASP:OD2 | 2:1V:70:LEU:N | 2.47 | 0.45 |
| 1:1W:135:VAL:O | 1:1W:166:THR:HA | 2.17 | 0.45 |
| 1:1W:286:VAL:O | 1:1W:289:LEU:HG | 2.16 | 0.45 |
| 2:1X:424:ASP:O | 2:1X:428:LEU:HG | 2.17 | 0.45 |
| 2:2B:250:VAL:HG23 | 2:2B:254:GLU:HG3 | 1.98 | 0.45 |
| 2:2F:312:TYR:HB2 | 2:2F:343:PHE:CD1 | 2.52 | 0.45 |
| 2:2J:394:LYS:HB2 | 1:2K:346:PRO:HG3 | 1.98 | 0.45 |
| 2:2L:56:THR:HG21 | 2:3B:283:HIS:O | 2.17 | 0.45 |
| 1:2M:48:ASN:N | 1:2M:48:ASN:OD1 | 2.49 | 0.45 |
| 1:2Q:10:GLY:HA2 | 1:2Q:143:THR:HG23 | 1.99 | 0.45 |
| 1:2S:178:THR:HG23 | 1:2S:181:GLU:HG3 | 1.99 | 0.45 |
| 2:2V:187:SER:O | 2:2V:191:THR:HG23 | 2.16 | 0.45 |
| 2:2V:297:GLU:CD | 38:8B:74:ILE:HG12 | 2.37 | 0.45 |
| 1:2W:183:TYR:O | 1:2W:187:LEU:HD13 | 2.16 | 0.45 |
| 2:2X:42:ILE:HD12 | 2:2X:42:ILE:HA | 1.68 | 0.45 |
| 1:2Y:72:THR:O | 1:2Y:76:VAL:HG23 | 2.16 | 0.45 |
| 1:2Y:317:PHE:HB3 | 1:2Y:321:MET:HE1 | 1.97 | 0.45 |
| 1:3A:170:VAL:HG21 | 1:3A:377:MET:SD | 2.57 | 0.45 |
| 2:3F:111:GLY:HA2 | 2:3F:114:ILE:HG22 | 1.99 | 0.45 |
| 1:3I:377:MET:O | 1:3I:380:ARG:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3J:192:HIS:HD2 | 2:3J:421:ALA:HA | 1.82 | 0.45 |
| 2:3L:88:HIS:N | 2:3L:91:GLN:OE1 | 2.47 | 0.45 |
| 2:3L:177:VAL:HG13 | 1:3M:327:ASP:HB2 | 1.98 | 0.45 |
| 1:3M:97:ALA:HB3 | 1:3M:143:THR:HG22 | 1.99 | 0.45 |
| 2:3N:5:ILE:HD11 | 2:3N:135:PHE:CE1 | 2.52 | 0.45 |
| 2:3P:21:TRP:CZ3 | 2:3P:63:PRO:HB3 | 2.52 | 0.45 |
| 2:3P:183:GLU:CD | 2:3P:184:PRO:HD3 | 2.37 | 0.45 |
| 1:3Q:265:PHE:HD2 | 1:3Q:422:TYR:HH | 1.65 | 0.45 |
| 2:3R:425:LEU:HD23 | 2:3R:429:GLU:HG2 | 1.98 | 0.45 |
| 1:3S:66:MET:SD | 1:3S:147:MET:HG2 | 2.57 | 0.45 |
| 2:3T:3:GLU:HB2 | 2:3T:129:CYS:SG | 2.57 | 0.45 |
| 2:3T:203:MET:C | 2:3T:204:LEU:HD12 | 2.37 | 0.45 |
| 4:4E:150:GLU:HA | 4:4E:150:GLU:OE1 | 2.17 | 0.45 |
| 4:4G:150:GLU:HA | 4:4G:150:GLU:OE1 | 2.17 | 0.45 |
| 4:4I:150:GLU:OE1 | 4:4I:150:GLU:HA | 2.17 | 0.45 |
| 7:4R:117:GLY:HA3 | 21:6G:37:ILE:HD11 | 1.98 | 0.45 |
| 9:4Z:80:ARG:NH1 | 9:4Z:84:ILE:HD11 | 2.31 | 0.45 |
| 10:5B:215:ALA:O | 10:5B:219:GLU:HG2 | 2.17 | 0.45 |
| 14:5L:18:GLU:OE2 | 14:5L:18:GLU:N | 2.50 | 0.45 |
| 14:5L:354:GLU:HB2 | 14:5L:368:HIS:HD2 | 1.81 | 0.45 |
| 14:5N:354:GLU:HB2 | 14:5N:368:HIS:HD2 | 1.81 | 0.45 |
| 15:5O:8:CYS:SG | 15:5O:80:ASP:HB2 | 2.57 | 0.45 |
| 15:5O:176:ILE:HG13 | 15:5O:177:GLY:N | 2.32 | 0.45 |
| 18:5Y:60:PRO:HA | 18:5Y:63:LEU:HD12 | 1.98 | 0.45 |
| 18:5Z:29:ILE:HD12 | 18:5Z:87:LEU:HD21 | 1.99 | 0.45 |
| 18:5Z:60:PRO:HA | 18:5Z:63:LEU:HD12 | 1.98 | 0.45 |
| 18:6B:60:PRO:HA | 18:6B:63:LEU:HD12 | 1.98 | 0.45 |
| 18:6D:60:PRO:HA | 18:6D:63:LEU:HD12 | 1.98 | 0.45 |
| 19:6E:74:VAL:HA | 19:6E:77:GLN:NE2 | 2.31 | 0.45 |
| 20:6F:49:ALA:O | 20:6F:53:SER:OG | 2.34 | 0.45 |
| 20:6F:344:LEU:CD1 | 20:6F:375:PRO:HB3 | 2.47 | 0.45 |
| 22:6I:294:LEU:HD12 | 22:6I:295:LYS:N | 2.31 | 0.45 |
| 22:6L:151:LYS:HE3 | 22:6L:151:LYS:HB3 | 1.79 | 0.45 |
| 24:6T:512:TYR:CZ | 24:6T:523:ILE:HG23 | 2.52 | 0.45 |
| 24:6V:507:ARG:HA | 24:6V:507:ARG:NH2 | 2.32 | 0.45 |
| 24:6V:593:LEU:CD1 | 24:6V:613:LYS:HD3 | 2.47 | 0.45 |
| 24:6X:617:ASP:OD2 | 24:6X:620:LYS:N | 2.43 | 0.45 |
| 24:6Y:184:ALA:HB1 | 24:6Y:188:THR:OG1 | 2.17 | 0.45 |
| 24:6Y:577:VAL:HG21 | 24:6Y:630:LEU:HD21 | 1.99 | 0.45 |
| 27:7G:105:LEU:HD23 | 27:7G:105:LEU:HA | 1.86 | 0.45 |
| 30:7L:375:SER:OG | 30:7L:377:GLU:OE2 | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:7S:240:HIS:O | 34:7S:244:MET:HG2 | 2.17 | 0.45 |
| 38:7Z:10:ALA:HA | 38:7Z:17:GLY:HA2 | 1.98 | 0.45 |
| 38:8A:73:TRP:CE3 | 38:8A:73:TRP:N | 2.85 | 0.45 |
| 38:8C:177:HIS:O | 38:8C:177:HIS:CG | 2.70 | 0.45 |
| 38:8C:182:ASN:HB3 | 38:8C:185:MET:HB2 | 1.97 | 0.45 |
| 2:4:11:GLN:HB3 | 41:4:501:GTP:PA | 2.57 | 0.45 |
| 1:A3:281:TYR:HD2 | 1:T6:87:PRO:HD2 | 1.80 | 0.45 |
| 1:A3:413:SER:HA | 3:4H:203:LYS:NZ | 2.32 | 0.45 |
| 2:D1:279:GLU:OE2 | 18:6A:167:SER:HA | 2.17 | 0.45 |
| 2:G1:226:ASN:O | 2:G1:230:LEU:HG | 2.17 | 0.45 |
| 1:G2:58:ARG:HD3 | 1:H8:280:GLN:HE22 | 1.82 | 0.45 |
| 1:G2:175:VAL:HG12 | 2:G3:329:ASN:CG | 2.38 | 0.45 |
| 1:G2:218:THR:N | 24:6W:418:ASP:OD2 | 2.46 | 0.45 |
| 1:G4:361:LEU:HD23 | 1:G4:361:LEU:HA | 1.74 | 0.45 |
| 1:G6:232:VAL:HG12 | 1:G6:236:ILE:HD11 | 1.99 | 0.45 |
| 1:G6:361:LEU:HD23 | 1:G6:361:LEU:HA | 1.79 | 0.45 |
| 1:G8:315:ALA:HB1 | 1:G8:317:PHE:CE1 | 2.52 | 0.45 |
| 2:H1:167:LEU:HB3 | 2:H1:169:PHE:CE2 | 2.52 | 0.45 |
| 1:H2:134:GLN:HE21 | 1:H2:167:PHE:HE2 | 1.64 | 0.45 |
| 1:H4:4:ILE:HB | 1:H4:50:TYR:HE1 | 1.82 | 0.45 |
| 1:H4:19:LYS:HD2 | 1:H4:22:GLU:OE1 | 2.17 | 0.45 |
| 2:H5:88:HIS:HB3 | 2:J1:283:HIS:CE1 | 2.52 | 0.45 |
| 1:H6:334:GLN:NE2 | 1:H6:348:ASN:H | 2.12 | 0.45 |
| 2:H7:47:ASP:N | 2:H7:47:ASP:OD1 | 2.49 | 0.45 |
| 1:H8:334:GLN:HE22 | 1:H8:348:ASN:H | 1.65 | 0.45 |
| 2:H9:313:MET:HB2 | 2:H9:380:ASN:HB3 | 1.99 | 0.45 |
| 1:I0:174:LYS:HG2 | 1:I0:380:ARG:NH2 | 2.32 | 0.45 |
| 1:I2:48:ASN:N | 1:I2:48:ASN:OD1 | 2.49 | 0.45 |
| 1:I2:186:THR:HG22 | 1:I2:411:ALA:HB1 | 1.99 | 0.45 |
| 1:I2:190:HIS:HD2 | 1:I2:411:ALA:HA | 1.82 | 0.45 |
| 1:I2:253:LEU:HD23 | 1:I2:253:LEU:HA | 1.92 | 0.45 |
| 2:I3:127:ASP:OD2 | 2:J9:293:ASN:ND2 | 2.50 | 0.45 |
| 1:I8:2:ARG:HE | 1:I8:240:LEU:HD22 | 1.81 | 0.45 |
| 1:I8:303:ALA:HA | 1:I8:376:GLU:OE2 | 2.17 | 0.45 |
| 2:I9:201:ALA:O | 2:I9:268:MET:HE2 | 2.17 | 0.45 |
| 2:J1:9:ILE:HD13 | 2:J1:150:GLY:HA2 | 1.97 | 0.45 |
| 1:J4:95:THR:OG1 | 1:J4:96:GLY:N | 2.49 | 0.45 |
| 2:J5:240:ALA:HB1 | 2:J5:356:ASN:HD22 | 1.82 | 0.45 |
| 1:J8:50:TYR:CE2 | 1:J8:241:ARG:HD3 | 2.52 | 0.45 |
| 1:J8:173:PRO:HD2 | 1:J8:380:ARG:NH1 | 2.32 | 0.45 |
| 2:J9:96:LYS:HE3 | 28:7X:463:ASN:HA | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K0:406:MET:SD | 1:K0:410:GLU:HG2 | 2.57 | 0.45 |
| 2:K1:377:MET:O | 2:K1:378:ILE:HD13 | 2.15 | 0.45 |
| 2:K5:12:ALA:HB2 | 41:K6:501:GTP:C8 | 2.52 | 0.45 |
| 2:K5:239:THR:HG23 | 2:K5:243:ARG:HE | 1.81 | 0.45 |
| 1:K6:139:LEU:HD22 | 1:K6:188:SER:OG | 2.17 | 0.45 |
| 1:K6:175:VAL:HG22 | 2:K7:329:ASN:ND2 | 2.32 | 0.45 |
| 1:K6:203:ASP:OD2 | 1:K6:302:ALA:N | 2.50 | 0.45 |
| 2:K9:9:ILE:HG22 | 2:K9:146:GLY:HA2 | 1.98 | 0.45 |
| 2:K9:428:LEU:HG | 2:K9:432:PHE:HE2 | 1.81 | 0.45 |
| 2:L5:88:HIS:HB2 | 2:N1:283:HIS:ND1 | 2.32 | 0.45 |
| 2:L7:11:GLN:O | 2:L7:14:ILE:HG12 | 2.16 | 0.45 |
| 2:L9:155:GLU:HG3 | 2:L9:156:ARG:N | 2.32 | 0.45 |
| 1:M0:246:LEU:HD22 | 1:M0:352:SER:HA | 1.99 | 0.45 |
| 1:M6:100:ASN:HB3 | 1:M6:103:LYS:HB2 | 1.99 | 0.45 |
| 2:M7:100:ALA:HB1 | 1:M8:252:LYS:HB3 | 1.99 | 0.45 |
| 2:N1:139:ASN:N | 2:N1:139:ASN:OD1 | 2.50 | 0.45 |
| 2:N1:221:ARG:NE | 30:7L:309:ASP:O | 2.50 | 0.45 |
| 1:N2:185:ALA:O | 1:N2:189:VAL:HG12 | 2.16 | 0.45 |
| 2:N3:116:ASP:OD2 | 2:N3:116:ASP:N | 2.50 | 0.45 |
| 2:N5:14:ILE:HD11 | 2:N5:74:VAL:HG13 | 1.98 | 0.45 |
| 2:N7:181:VAL:H | 1:N8:256:ASN:ND2 | 2.15 | 0.45 |
| 2:N9:279:GLU:HB2 | 2:N9:280:LYS:HZ2 | 1.82 | 0.45 |
| 2:O1:175:PRO:HB3 | 2:O1:390:ARG:NE | 2.32 | 0.45 |
| 2:O3:105:ARG:O | 2:O3:109:THR:OG1 | 2.35 | 0.45 |
| 1:O4:179:VAL:H | 2:O5:258:ASN:ND2 | 2.14 | 0.45 |
| 1:O4:417:ASP:O | 1:O4:421:GLU:HG2 | 2.17 | 0.45 |
| 1:O8:183:TYR:O | 1:O8:187:LEU:HD13 | 2.17 | 0.45 |
| 2:O9:91:GLN:HG3 | 2:O9:121:ARG:HH22 | 1.82 | 0.45 |
| 2:O9:156:ARG:HA | 2:O9:159:VAL:HG12 | 1.99 | 0.45 |
| 1:P4:313:ALA:HA | 1:P4:369:GLY:HA2 | 1.98 | 0.45 |
| 1:Q2:2:ARG:HB3 | 1:Q2:131:GLN:HB2 | 1.99 | 0.45 |
| 1:Q2:3:GLU:HB2 | 1:Q2:130:LEU:HD13 | 1.98 | 0.45 |
| 2:Q3:274:PRO:HB2 | 2:Q3:276:ILE:HG12 | 1.99 | 0.45 |
| 1:Q4:42:LEU:HA | 1:Q4:45:GLU:OE1 | 2.17 | 0.45 |
| 1:Q6:128:ASP:OD1 | 1:Q6:128:ASP:N | 2.50 | 0.45 |
| 1:Q8:77:ARG:HH21 | 24:6T:33:LEU:HD11 | 1.81 | 0.45 |
| 1:Q8:291:GLN:HG3 | 1:Q8:292:GLN:H | 1.82 | 0.45 |
| 2:Q9:66:ILE:O | 2:Q9:66:ILE:HG13 | 2.16 | 0.45 |
| 1:R0:69:GLU:C | 1:R0:92:PHE:HZ | 2.20 | 0.45 |
| 2:R3:69:ASP:OD1 | 2:R3:70:LEU:N | 2.50 | 0.45 |
| 1:R4:117:LEU:HA | 1:R4:117:LEU:HD23 | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:391:ARG:HG3 | 2:R7:346:TRP:CD2 | 2.52 | 0.45 |
| 2:R9:237:SER:HA | 2:R9:320:ARG:HD2 | 1.98 | 0.45 |
| 1:S0:177:ASP:N | 1:S0:181:GLU:OE2 | 2.50 | 0.45 |
| 2:S5:88:HIS:CG | 2:S5:89:PRO:HD2 | 2.52 | 0.45 |
| 2:S5:90:GLU:CD | 2:S5:121:ARG:HD3 | 2.38 | 0.45 |
| 2:S5:287:SER:H | 2:S5:290:GLU:CD | 2.19 | 0.45 |
| 1:S8:157:GLU:OE2 | 1:S8:157:GLU:HA | 2.17 | 0.45 |
| 2:S9:346:TRP:O | 2:S9:348:PRO:HD3 | 2.17 | 0.45 |
| 1:T2:405:GLU:HA | 1:T2:408:PHE:HD2 | 1.82 | 0.45 |
| 2:T3:5:ILE:HG22 | 2:T3:64:ARG:HB3 | 1.99 | 0.45 |
| 1:T4:175:VAL:HG22 | 2:T5:329:ASN:ND2 | 2.32 | 0.45 |
| 1:T4:384:GLN:HG2 | 2:T5:348:PRO:HB2 | 1.98 | 0.45 |
| 2:T5:145:THR:OG1 | 41:T6:501:GTP:O1B | 2.30 | 0.45 |
| 2:T5:417:GLU:HA | 2:T5:420:GLU:HG2 | 1.99 | 0.45 |
| 1:T6:376:GLU:HA | 1:T6:376:GLU:OE1 | 2.16 | 0.45 |
| 1:T6:376:GLU:OE1 | 1:T6:379:LYS:HD2 | 2.15 | 0.45 |
| 1:T8:114:ASP:N | 1:T8:114:ASP:OD1 | 2.50 | 0.45 |
| 1:U2:190:HIS:HD2 | 1:U2:414:ASN:OD1 | 2.00 | 0.45 |
| 2:U5:72:PRO:HD2 | 1:U6:2:ARG:HH12 | 1.82 | 0.45 |
| 2:U5:119:LEU:HD11 | 2:U5:156:ARG:CB | 2.47 | 0.45 |
| 2:U5:175:PRO:HG2 | 2:U5:176:GLN:OE1 | 2.17 | 0.45 |
| 1:V0:53:GLU:OE1 | 1:V0:57:GLY:HA2 | 2.17 | 0.45 |
| 1:V2:70:PRO:N | 1:V2:92:PHE:HZ | 2.15 | 0.45 |
| 2:V3:63:PRO:HB2 | 2:V3:65:CYS:SG | 2.56 | 0.45 |
| 1:V4:128:ASP:OD1 | 1:V4:129:CYS:N | 2.45 | 0.45 |
| 1:V4:273:LEU:HD23 | 1:V4:273:LEU:HA | 1.83 | 0.45 |
| 1:V6:137:HIS:ND1 | 1:V6:138:SER:O | 2.45 | 0.45 |
| 1:V6:172:SER:HB2 | 1:V6:205:GLU:OE2 | 2.17 | 0.45 |
| 2:W1:88:HIS:HB3 | 2:W1:91:GLN:CD | 2.38 | 0.45 |
| 2:W1:88:HIS:HD2 | 2:W1:121:ARG:HH22 | 1.63 | 0.45 |
| 2:W3:90:GLU:OE2 | 2:W3:90:GLU:CA | 2.64 | 0.45 |
| 2:W3:276:ILE:CD1 | 2:W3:284:GLU:HG2 | 2.47 | 0.45 |
| 2:W7:222:PRO:CD | 1:W8:324:LYS:HE3 | 2.47 | 0.45 |
| 1:X0:309:ARG:H | 1:X0:372:THR:CG2 | 2.30 | 0.45 |
| 1:X2:317:PHE:HB3 | 1:X2:321:MET:CE | 2.46 | 0.45 |
| 2:X5:217:LEU:HD11 | 2:X5:367:ASP:O | 2.17 | 0.45 |
| 1:X8:112:LEU:O | 1:X8:115:SER:OG | 2.30 | 0.45 |
| 1:Y0:21:TRP:HA | 1:Y0:24:VAL:HG12 | 1.99 | 0.45 |
| 1:Y0:183:TYR:HB3 | 1:Y0:398:TYR:HE2 | 1.81 | 0.45 |
| 1:Y2:47:ILE:HD12 | 1:Y2:59:TYR:CE1 | 2.52 | 0.45 |
| 1:Y4:101:TRP:CE3 | 1:Y4:403:MET:HE1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y6:30:ILE:HG13 | 1:Y6:35:THR:O | 2.17 | 0.45 |
| 1:Y8:173:PRO:HB3 | 1:Y8:384:GLN:HE22 | 1.82 | 0.45 |
| 1:Y8:395:LEU:HD23 | 1:Y8:395:LEU:HA | 1.79 | 0.45 |
| 2:Y9:187:SER:O | 2:Y9:191:THR:HG23 | 2.15 | 0.45 |
| 2:Y9:238:LEU:HD11 | 2:Y9:378:ILE:HD11 | 1.98 | 0.45 |
| 1:Z0:131:GLN:HE21 | 1:Z0:250:LEU:HB3 | 1.82 | 0.45 |
| 1:Z2:86:ARG:HD3 | 1:Z2:88:ASP:HB2 | 1.99 | 0.45 |
| 2:Z3:319:TYR:HD2 | 2:Z3:323:VAL:HG21 | 1.82 | 0.45 |
| 1:Z6:87:PRO:HA | 1:Z6:90:PHE:CD2 | 2.51 | 0.45 |
| 1:Z8:132:GLY:HA2 | 1:Z8:162:ARG:HB3 | 1.98 | 0.45 |
| 2:0B:12:ALA:O | 2:0B:16:VAL:HG23 | 2.17 | 0.45 |
| 2:0B:187:SER:O | 2:0B:191:THR:HG23 | 2.17 | 0.45 |
| 1:0C:45:GLU:HG3 | 1:0C:46:ARG:HG2 | 1.99 | 0.45 |
| 1:0E:318:ARG:HB3 | 1:0E:357:PRO:HA | 1.99 | 0.45 |
| 1:0G:5:VAL:HG23 | 1:0G:62:ARG:HG2 | 1.99 | 0.45 |
| 1:0G:397:TRP:HE1 | 2:0H:260:VAL:HB | 1.81 | 0.45 |
| 2:0J:66:ILE:HG13 | 2:0J:122:ILE:CD1 | 2.47 | 0.45 |
| 2:0J:336:LYS:O | 2:0J:339:ARG:NH2 | 2.50 | 0.45 |
| 1:0K:58:ARG:HH11 | 1:1A:281:TYR:HE1 | 1.65 | 0.45 |
| 1:0O:4:ILE:HD11 | 1:0O:134:GLN:HB2 | 1.99 | 0.45 |
| 1:0O:136:CYS:HG | 1:0O:167:PHE:HD2 | 1.65 | 0.45 |
| 1:0Q:175:VAL:O | 1:0Q:175:VAL:HG13 | 2.17 | 0.45 |
| 1:0Q:193:VAL:HG21 | 1:0Q:418:LEU:HD11 | 1.97 | 0.45 |
| 1:0Q:211:CYS:O | 1:0Q:216:LYS:N | 2.50 | 0.45 |
| 1:0S:320:ARG:HG2 | 1:0S:355:ASP:HB2 | 1.98 | 0.45 |
| 1:0S:372:THR:O | 1:0S:375:GLN:HG2 | 2.17 | 0.45 |
| 2:0V:105:ARG:HA | 2:0V:109:THR:OG1 | 2.17 | 0.45 |
| 2:0V:415:GLU:HA | 2:0V:418:PHE:HD2 | 1.82 | 0.45 |
| 1:0Y:221:THR:HG23 | 1:0Y:223:GLY:H | 1.81 | 0.45 |
| 2:1F:47:ASP:N | 2:1F:47:ASP:OD1 | 2.49 | 0.45 |
| 2:1H:223:THR:OG1 | 2:1H:224:TYR:N | 2.50 | 0.45 |
| 1:1K:200:MET:HE1 | 1:1K:368:ILE:CD1 | 2.47 | 0.45 |
| 1:1M:403:MET:HE3 | 1:1M:403:MET:HB2 | 1.86 | 0.45 |
| 2:1T:35:GLN:HB3 | 2:1T:59:GLY:O | 2.16 | 0.45 |
| 1:1U:232:VAL:HG21 | 1:1U:300:MET:HE2 | 1.99 | 0.45 |
| 2:1V:235:ILE:HD13 | 2:1V:238:LEU:HD21 | 1.99 | 0.45 |
| 2:1V:424:ASP:O | 2:1V:428:LEU:HD23 | 2.17 | 0.45 |
| 1:1W:414:ASN:HA | 1:1W:417:ASP:OD2 | 2.17 | 0.45 |
| 2:1X:305:CYS:HB3 | 2:1X:387:ILE:HD11 | 1.98 | 0.45 |
| 2:2B:21:TRP:CZ2 | 2:2B:65:CYS:HB2 | 2.51 | 0.45 |
| 1:2G:141:GLY:HA3 | 39:2G:502:GDP:O3A | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2G:262:ARG:NH2 | 1:2G:417:ASP:OD1 | 2.49 | 0.45 |
| 2:2J:79:ARG:O | 2:2J:84:ARG:HG2 | 2.16 | 0.45 |
| 1:2M:31:ASP:OD1 | 1:2M:34:GLY:N | 2.50 | 0.45 |
| 1:2Q:334:GLN:HA | 1:2Q:341:PHE:CE2 | 2.51 | 0.45 |
| 2:2T:27:GLU:CD | 2:2T:243:ARG:HH12 | 2.19 | 0.45 |
| 2:2T:245:ASP:HB3 | 38:8B:216:ARG:HG2 | 1.98 | 0.45 |
| 1:2U:49:VAL:HG11 | 1:2U:241:ARG:HG2 | 1.97 | 0.45 |
| 2:2X:406:HIS:HA | 2:2X:409:VAL:HG22 | 1.99 | 0.45 |
| 1:2Y:178:THR:CG2 | 1:2Y:181:GLU:HG3 | 2.47 | 0.45 |
| 1:3A:100:ASN:HB3 | 1:3A:103:LYS:HB2 | 1.98 | 0.45 |
| 2:3B:119:LEU:HD11 | 2:3B:156:ARG:CB | 2.47 | 0.45 |
| 1:3C:150:LEU:HD12 | 1:3C:153:SER:OG | 2.17 | 0.45 |
| 2:3F:267:PHE:HB2 | 2:3F:384:ILE:HD12 | 1.99 | 0.45 |
| 1:3G:100:ASN:HB3 | 1:3G:103:LYS:HB2 | 1.98 | 0.45 |
| 1:3G:117:LEU:HA | 1:3G:120:VAL:HG12 | 1.98 | 0.45 |
| 2:3H:9:ILE:HG22 | 2:3H:146:GLY:HA2 | 1.99 | 0.45 |
| 2:3J:133:GLN:HB3 | 2:3J:252:ILE:CG2 | 2.46 | 0.45 |
| 1:3M:77:ARG:NH1 | 3:4D:18:LYS:O | 2.50 | 0.45 |
| 2:3N:264:ARG:NH2 | 2:3N:431:ASP:OD1 | 2.49 | 0.45 |
| 1:3Q:135:VAL:HG11 | 1:3Q:152:ILE:HD11 | 1.99 | 0.45 |
| 2:3R:290:GLU:OE1 | 2:3R:290:GLU:N | 2.42 | 0.45 |
| 2:3R:397:LEU:HA | 2:3R:397:LEU:HD23 | 1.71 | 0.45 |
| 1:3S:286:VAL:HG12 | 1:3S:329:GLN:HG3 | 1.99 | 0.45 |
| 2:3T:141:VAL:HG13 | 2:3T:170:THR:HG21 | 1.99 | 0.45 |
| 2:3T:325:PRO:O | 2:3T:328:VAL:HG12 | 2.16 | 0.45 |
| 4:3W:150:GLU:OE1 | 4:3W:150:GLU:HA | 2.17 | 0.45 |
| 6:4P:96:ILE:O | 6:4P:100:GLU:HG2 | 2.17 | 0.45 |
| 10:5C:383:GLN:O | 10:5C:387:LYS:HG2 | 2.17 | 0.45 |
| 14:5L:136:SER:O | 14:5L:138:ASN:N | 2.46 | 0.45 |
| 14:5M:354:GLU:HB2 | 14:5M:368:HIS:HD2 | 1.81 | 0.45 |
| 14:5M:531:ASP:OD1 | 14:5M:531:ASP:N | 2.44 | 0.45 |
| 14:5N:136:SER:O | 14:5N:138:ASN:N | 2.46 | 0.45 |
| 15:5O:205:CYS:SG | 15:5O:205:CYS:O | 2.75 | 0.45 |
| 15:5O:333:GLU:HB3 | 30:7K:241:LYS:HZ3 | 1.76 | 0.45 |
| 15:5P:21:LEU:CD2 | 15:5P:21:LEU:C | 2.86 | 0.45 |
| 15:5P:145:PHE:CZ | 15:5P:149:LEU:HD11 | 2.52 | 0.45 |
| 17:5T:227:ARG:O | 17:5T:231:ARG:HG2 | 2.17 | 0.45 |
| 17:5U:188:LYS:HB3 | 17:5U:222:ILE:HD11 | 1.99 | 0.45 |
| 18:6B:70:TYR:HE1 | 18:6B:85:THR:HG22 | 1.81 | 0.45 |
| 20:6F:259:LEU:HD22 | 20:6F:281:LYS:HB2 | 1.99 | 0.45 |
| 20:6F:331:LEU:HD12 | 20:6F:357:VAL:HG11 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:6H:106:ARG:HB2 | 24:6X:81:THR:N | 2.32 | 0.45 |
| 22:6J:188:ARG:NH2 | 22:6J:256:TYR:O | 2.50 | 0.45 |
| 22:6N:64:VAL:HG12 | 24:6Y:399:ILE:HD13 | 1.98 | 0.45 |
| 22:6N:162:LEU:HD11 | 22:6N:225:ALA:HB1 | 1.99 | 0.45 |
| 24:6U:474:PHE:HE2 | 24:6U:500:ARG:HE | 1.64 | 0.45 |
| 24:6X:451:LYS:HB3 | 24:6X:468:ARG:NH1 | 2.32 | 0.45 |
| 24:6Z:23:SER:O | 24:6Z:25:LYS:N | 2.49 | 0.45 |
| 24:6Z:473:TYR:CD1 | 24:6Z:517:LEU:HD11 | 2.52 | 0.45 |
| 26:7D:49:PRO:HA | 26:7D:55:THR:OG1 | 2.17 | 0.45 |
| 29:7I:23:ILE:CG1 | 29:7I:24:PRO:HD2 | 2.46 | 0.45 |
| 30:7L:359:ASP:O | 30:7L:363:VAL:HG13 | 2.17 | 0.45 |
| 31:7M:60:ILE:HG13 | 31:7M:61:THR:N | 2.32 | 0.45 |
| 34:7R:97:ASN:O | 34:7R:100:GLN:HG3 | 2.17 | 0.45 |
| 38:8C:213:GLU:HG3 | 38:8C:214:HIS:N | 2.31 | 0.45 |
| 1:A3:41:ASP:H | 26:7F:122:VAL:HG23 | 1.80 | 0.45 |
| 1:C8:77:ARG:HG2 | 24:6V:318:PHE:CD2 | 2.52 | 0.45 |
| 2:G5:292:THR:HG21 | 2:G5:331:SER:HB3 | 1.99 | 0.45 |
| 1:G6:324:LYS:HG2 | 1:G6:328:GLU:OE1 | 2.16 | 0.45 |
| 2:G7:147:SER:HB2 | 2:G7:190:SER:HB3 | 1.98 | 0.45 |
| 2:G9:66:ILE:HD13 | 2:G9:91:GLN:HB3 | 1.99 | 0.45 |
| 2:H1:88:HIS:HB3 | 2:I7:283:HIS:CE1 | 2.51 | 0.45 |
| 2:H1:161:TYR:O | 2:H1:163:LYS:NZ | 2.35 | 0.45 |
| 2:H1:209:ILE:HG21 | 2:H1:227:LEU:HG | 1.98 | 0.45 |
| 2:H1:217:LEU:HB3 | 2:H1:219:ILE:CD1 | 2.46 | 0.45 |
| 2:H1:336:LYS:HA | 2:H1:336:LYS:HD3 | 1.82 | 0.45 |
| 1:H2:154:LYS:HA | 1:H2:154:LYS:HD3 | 1.86 | 0.45 |
| 2:H3:101:ASN:ND2 | 2:H3:143:GLY:HA2 | 2.32 | 0.45 |
| 2:H3:157:LEU:HD23 | 2:H3:157:LEU:HA | 1.79 | 0.45 |
| 1:H4:3:GLU:O | 1:H4:131:GLN:HB3 | 2.17 | 0.45 |
| 2:H5:47:ASP:OD1 | 2:H5:48:ALA:N | 2.50 | 0.45 |
| 1:H6:276:ARG:HH12 | 24:6V:489:ASN:C | 2.20 | 0.45 |
| 1:H8:175:VAL:HG22 | 1:H8:205:GLU:HB2 | 1.97 | 0.45 |
| 2:I1:76:ASP:O | 2:I1:80:THR:HG23 | 2.17 | 0.45 |
| 2:I3:88:HIS:ND1 | 2:J9:283:HIS:HB3 | 2.32 | 0.45 |
| 2:I5:105:ARG:O | 2:I5:110:ILE:HG12 | 2.17 | 0.45 |
| 2:I5:288:VAL:HG21 | 2:I5:328:VAL:HG12 | 1.99 | 0.45 |
| 2:I7:175:PRO:HB3 | 2:I7:390:ARG:HE | 1.82 | 0.45 |
| 1:I8:152:ILE:HD12 | 1:I8:164:MET:SD | 2.56 | 0.45 |
| 2:I9:102:ASN:HB3 | 2:I9:105:ARG:HB3 | 1.98 | 0.45 |
| 2:J1:172:TYR:HB2 | 2:J1:205:ASP:OD1 | 2.17 | 0.45 |
| 2:J5:45:GLY:O | 2:J5:46:ASP:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J5:66:ILE:O | 2:J5:66:ILE:HG13 | 2.16 | 0.45 |
| 1:K0:1:MET:HB3 | 1:K0:2:ARG:H | 1.68 | 0.45 |
| 1:K0:135:VAL:O | 1:K0:166:THR:HA | 2.17 | 0.45 |
| 2:K7:121:ARG:HD2 | 2:K7:125:LEU:HG | 1.99 | 0.45 |
| 1:L2:337:ASN:HD21 | 29:7J:462:LYS:HB2 | 1.82 | 0.45 |
| 1:L4:320:ARG:NH2 | 29:7J:350:LYS:HA | 2.25 | 0.45 |
| 2:L5:326:LYS:HE3 | 2:L5:327:ASP:CG | 2.37 | 0.45 |
| 2:L7:180:ALA:HB3 | 2:L7:183:GLU:HB3 | 1.98 | 0.45 |
| 2:L9:7:ILE:HG22 | 2:L9:66:ILE:HG12 | 1.99 | 0.45 |
| 2:L9:72:PRO:HD2 | 1:M0:2:ARG:NH1 | 2.32 | 0.45 |
| 1:M0:179:VAL:HG22 | 2:M1:258:ASN:HD22 | 1.82 | 0.45 |
| 2:M3:248:LEU:HD22 | 2:M3:354:GLY:HA2 | 1.98 | 0.45 |
| 2:M3:405:VAL:HG13 | 2:M3:418:PHE:HE2 | 1.82 | 0.45 |
| 1:M6:251:ARG:O | 1:M6:255:VAL:HG23 | 2.17 | 0.45 |
| 1:N2:404:ASP:HB3 | 1:N2:406:MET:SD | 2.57 | 0.45 |
| 2:N3:11:GLN:HE22 | 2:N3:74:VAL:HG11 | 1.82 | 0.45 |
| 1:N8:95:THR:OG1 | 1:N8:96:GLY:N | 2.50 | 0.45 |
| 2:N9:156:ARG:HA | 2:N9:159:VAL:HG22 | 1.99 | 0.45 |
| 1:O2:371:SER:OG | 1:O2:372:THR:N | 2.50 | 0.45 |
| 2:O3:278:ALA:HA | 2:O3:369:ALA:HB2 | 2.00 | 0.45 |
| 1:O6:248:ALA:HA | 1:O6:252:LYS:HD2 | 1.99 | 0.45 |
| 2:P3:124:LYS:HA | 2:P3:127:ASP:HB2 | 1.98 | 0.45 |
| 1:P4:28:HIS:NE2 | 1:P4:241:ARG:HD2 | 2.32 | 0.45 |
| 2:P5:26:LEU:HD23 | 2:P5:363:VAL:HG12 | 1.99 | 0.45 |
| 1:P6:199:CYS:HB2 | 1:P6:265:PHE:CD1 | 2.52 | 0.45 |
| 1:Q2:350:LYS:HZ3 | 1:Q2:351:SER:C | 2.20 | 0.45 |
| 1:Q6:167:PHE:CE2 | 1:Q6:233:MET:HG2 | 2.52 | 0.45 |
| 1:Q8:8:GLN:CD | 1:Q8:17:GLY:HA3 | 2.37 | 0.45 |
| 1:R6:138:SER:OG | 1:R6:139:LEU:N | 2.50 | 0.45 |
| 1:R8:6:HIS:CE1 | 1:R8:8:GLN:HG2 | 2.52 | 0.45 |
| 1:S4:185:ALA:O | 1:S4:189:VAL:HG13 | 2.16 | 0.45 |
| 1:S6:227:HIS:CG | 7:4T:241:PHE:CZ | 3.01 | 0.45 |
| 1:S8:390:ARG:HB3 | 13:5I:54:ILE:HD12 | 1.97 | 0.45 |
| 1:T0:390:ARG:HE | 1:T0:391:ARG:HE | 1.65 | 0.45 |
| 2:T1:285:GLN:O | 2:T1:285:GLN:HG3 | 2.16 | 0.45 |
| 1:T2:190:HIS:NE2 | 1:T2:414:ASN:OD1 | 2.50 | 0.45 |
| 1:T4:40:SER:OG | 21:6H:93:HIS:NE2 | 2.50 | 0.45 |
| 1:T4:231:ALA:HB2 | 7:4U:128:LEU:HD11 | 1.98 | 0.45 |
| 2:T5:306:ASP:HB3 | 2:T5:309:HIS:CD2 | 2.52 | 0.45 |
| 1:T8:385:PHE:HZ | 1:T8:408:PHE:HD1 | 1.64 | 0.45 |
| 1:U2:31:ASP:HB2 | 1:U2:32:PRO:HD2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U2:375:GLN:HB2 | 1:U2:419:VAL:HG13 | 1.99 | 0.45 |
| 1:U6:95:THR:OG1 | 1:U6:96:GLY:N | 2.50 | 0.45 |
| 1:U8:5:VAL:HG23 | 1:U8:62:ARG:HG2 | 1.99 | 0.45 |
| 2:U9:325:PRO:HA | 2:U9:328:VAL:HG12 | 1.99 | 0.45 |
| 2:V1:208:ALA:O | 2:V1:212:ILE:HG12 | 2.17 | 0.45 |
| 1:V4:117:LEU:HA | 1:V4:120:VAL:HG12 | 1.98 | 0.45 |
| 1:W0:246:LEU:HD22 | 1:W0:352:SER:HA | 1.99 | 0.45 |
| 2:W7:237:SER:HG | 2:W7:376:CYS:HG | 1.65 | 0.45 |
| 2:W9:33:ASP:HA | 2:W9:85:GLN:CB | 2.46 | 0.45 |
| 1:X0:63:ALA:O | 1:X0:64:ILE:HD13 | 2.17 | 0.45 |
| 2:X3:11:GLN:OE1 | 41:X4:501:GTP:C8 | 2.70 | 0.45 |
| 2:X3:429:GLU:O | 2:X3:432:PHE:N | 2.50 | 0.45 |
| 2:X5:88:HIS:HB3 | 2:Z1:283:HIS:CE1 | 2.52 | 0.45 |
| 2:X7:7:ILE:HG22 | 2:X7:66:ILE:HG12 | 1.99 | 0.45 |
| 2:X7:70:LEU:HA | 2:X7:95:GLY:HA3 | 1.98 | 0.45 |
| 1:Y0:203:ASP:N | 1:Y0:203:ASP:OD1 | 2.49 | 0.45 |
| 1:Y0:204:ASN:ND2 | 39:Y0:502:GDP:HN22 | 2.14 | 0.45 |
| 1:Y4:2:ARG:HH21 | 1:Y4:240:LEU:HA | 1.81 | 0.45 |
| 1:Y4:86:ARG:HG2 | 1:Y4:88:ASP:H | 1.81 | 0.45 |
| 2:Y5:121:ARG:HD2 | 2:Y5:121:ARG:HA | 1.84 | 0.45 |
| 1:Y6:60:VAL:HG21 | 1:Y6:86:ARG:NH2 | 2.31 | 0.45 |
| 1:Y8:267:MET:HE2 | 1:Y8:301:CYS:HB2 | 1.97 | 0.45 |
| 1:Y8:330:MET:HA | 1:Y8:333:VAL:HG12 | 1.99 | 0.45 |
| 1:Z0:418:LEU:O | 1:Z0:421:GLU:HG2 | 2.17 | 0.45 |
| 2:Z1:107:HIS:HD2 | 2:Z1:151:SER:OG | 2.00 | 0.45 |
| 1:Z2:66:MET:CE | 1:Z2:116:VAL:HG21 | 2.47 | 0.45 |
| 2:Z3:241:SER:HB3 | 2:Z3:250:VAL:H | 1.81 | 0.45 |
| 1:Z6:167:PHE:CE1 | 1:Z6:200:MET:HG3 | 2.52 | 0.45 |
| 1:Z6:244:GLY:HA3 | 1:Z6:354:CYS:HA | 1.99 | 0.45 |
| 1:Z8:233:MET:O | 1:Z8:237:THR:HG22 | 2.17 | 0.45 |
| 2:Z9:338:LYS:HA | 2:Z9:338:LYS:HD2 | 1.74 | 0.45 |
| 1:0E:344:TRP:HH2 | 1:0E:425:TYR:O | 2.00 | 0.45 |
| 2:0F:175:PRO:HG2 | 2:0F:176:GLN:OE1 | 2.17 | 0.45 |
| 1:0I:62:ARG:HG3 | 1:0I:123:GLU:OE2 | 2.17 | 0.45 |
| 2:0J:25:CYS:SG | 2:0J:86:LEU:HD11 | 2.57 | 0.45 |
| 2:0L:343:PHE:CZ | 2:0L:350:GLY:HA3 | 2.52 | 0.45 |
| 2:0L:407:TRP:NE1 | 1:0M:258:ILE:O | 2.44 | 0.45 |
| 1:0O:21:TRP:CZ3 | 1:0O:61:PRO:HB3 | 2.52 | 0.45 |
| 1:0O:317:PHE:HD2 | 1:0O:353:VAL:HG22 | 1.81 | 0.45 |
| 1:0Q:183:TYR:O | 1:0Q:187:LEU:HD13 | 2.17 | 0.45 |
| 2:0R:325:PRO:HA | 2:0R:328:VAL:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0R:326:LYS:HE3 | 2:0R:327:ASP:OD2 | 2.17 | 0.45 |
| 1:0Y:283:ALA:O | 1:0Y:284:LEU:HD23 | 2.16 | 0.45 |
| 1:0Y:389:PHE:HE1 | 1:0Y:395:LEU:HD11 | 1.82 | 0.45 |
| 2:0Z:57:GLY:CA | 9:4Z:165:ARG:HH22 | 2.30 | 0.45 |
| 2:1B:178:SER:HB3 | 2:1B:183:GLU:OE2 | 2.16 | 0.45 |
| 1:1C:117:LEU:HD23 | 1:1C:117:LEU:HA | 1.80 | 0.45 |
| 1:1C:391:ARG:NH2 | 2:1D:435:VAL:HA | 2.31 | 0.45 |
| 1:1M:21:TRP:CZ3 | 1:1M:61:PRO:HB3 | 2.52 | 0.45 |
| 1:1M:117:LEU:HD23 | 1:1M:117:LEU:HA | 1.82 | 0.45 |
| 2:1N:179:THR:HG21 | 1:1O:246:LEU:HD21 | 1.98 | 0.45 |
| 2:1P:317:LEU:HB3 | 2:1P:319:TYR:HE1 | 1.82 | 0.45 |
| 1:1Q:41:ASP:N | 1:1Q:41:ASP:OD2 | 2.50 | 0.45 |
| 1:1U:244:GLY:HA2 | 1:1U:355:ASP:OD2 | 2.17 | 0.45 |
| 2:1V:55:GLU:HG2 | 2:1V:61:HIS:CE1 | 2.52 | 0.45 |
| 2:1V:230:LEU:HD23 | 2:1V:230:LEU:HA | 1.77 | 0.45 |
| 1:1W:204:ASN:OD1 | 39:1W:502:GDP:O2' | 2.35 | 0.45 |
| 1:1W:391:ARG:HH22 | 2:1X:435:VAL:HG12 | 1.82 | 0.45 |
| 1:1W:415:MET:O | 1:1W:419:VAL:HG23 | 2.17 | 0.45 |
| 2:1X:12:ALA:O | 2:1X:16:VAL:HG23 | 2.17 | 0.45 |
| 2:1Z:384:ILE:HA | 2:1Z:387:ILE:HD12 | 1.98 | 0.45 |
| 1:2C:189:VAL:O | 1:2C:193:VAL:HG22 | 2.17 | 0.45 |
| 2:2D:7:ILE:HG12 | 2:2D:137:VAL:HG12 | 1.98 | 0.45 |
| 2:2D:178:SER:OG | 1:2E:347:ASN:HB3 | 2.17 | 0.45 |
| 2:2F:123:ARG:NH2 | 2:2F:160:ASP:OD1 | 2.50 | 0.45 |
| 1:2G:117:LEU:HD11 | 1:2G:154:LYS:HB3 | 1.98 | 0.45 |
| 2:2L:238:LEU:HD12 | 2:2L:238:LEU:HA | 1.84 | 0.45 |
| 1:2M:12:CYS:HB3 | 1:2M:138:SER:OG | 2.17 | 0.45 |
| 1:2M:172:SER:HB2 | 1:2M:380:ARG:NH2 | 2.32 | 0.45 |
| 1:2M:174:LYS:HE2 | 1:2M:174:LYS:HB3 | 1.76 | 0.45 |
| 1:2M:200:MET:HE1 | 1:2M:236:ILE:HD13 | 1.99 | 0.45 |
| 1:2Q:395:LEU:O | 1:2Q:399:THR:HG23 | 2.16 | 0.45 |
| 2:2X:214:ARG:CZ | 38:8B:18:VAL:HG22 | 2.46 | 0.45 |
| 2:3D:8:HIS:CD2 | 2:3D:138:PHE:HD2 | 2.34 | 0.45 |
| 2:3D:26:LEU:HD21 | 2:3D:364:PRO:HD2 | 1.99 | 0.45 |
| 2:3F:165:SER:HA | 2:3F:199:ASP:OD2 | 2.17 | 0.45 |
| 1:3G:53:GLU:OE1 | 1:3G:57:GLY:HA2 | 2.17 | 0.45 |
| 2:3H:56:THR:HG21 | 3:3X:34:SER:HA | 1.99 | 0.45 |
| 1:3M:2:ARG:HE | 1:3M:240:LEU:HD22 | 1.81 | 0.45 |
| 2:3N:278:ALA:HA | 2:3N:369:ALA:HB2 | 1.99 | 0.45 |
| 1:3Q:139:LEU:HD12 | 1:3Q:170:VAL:HG12 | 1.99 | 0.45 |
| 1:3S:322:SER:O | 1:3S:326:VAL:HG23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3S:355:ASP:O | 1:3S:356:ILE:HD13 | 2.16 | 0.45 |
| 4:4C:121:MET:HE1 | 4:4C:134:PHE:CE1 | 2.52 | 0.45 |
| 5:4L:326:GLU:HB2 | 5:4L:327:LYS:NZ | 2.32 | 0.45 |
| 6:4O:452:ARG:O | 6:4O:455:VAL:HG12 | 2.17 | 0.45 |
| 9:4Z:344:ALA:O | 9:4Z:348:GLU:HG3 | 2.17 | 0.45 |
| 10:5A:262:ILE:HG12 | 10:5A:265:LYS:HE3 | 1.98 | 0.45 |
| 12:5F:385:ASP:OD1 | 12:5F:386:ILE:N | 2.49 | 0.45 |
| 13:5I:99:ASN:HD22 | 13:5I:99:ASN:N | 2.15 | 0.45 |
| 13:5J:99:ASN:HD22 | 13:5J:99:ASN:N | 2.15 | 0.45 |
| 14:5L:354:GLU:OE1 | 14:5L:354:GLU:N | 2.47 | 0.45 |
| 14:5M:136:SER:O | 14:5M:138:ASN:N | 2.46 | 0.45 |
| 14:5M:354:GLU:OE1 | 14:5M:354:GLU:N | 2.48 | 0.45 |
| 14:5N:218:VAL:O | 14:5N:232:GLY:N | 2.50 | 0.45 |
| 15:5P:14:LEU:HD23 | 15:5P:14:LEU:N | 2.26 | 0.45 |
| 15:5P:62:LEU:HD22 | 15:5P:78:TYR:CE2 | 2.52 | 0.45 |
| 18:5X:60:PRO:HA | 18:5X:63:LEU:HD12 | 1.98 | 0.45 |
| 18:5X:70:TYR:HE1 | 18:5X:85:THR:HG22 | 1.81 | 0.45 |
| 18:5X:180:ARG:O | 18:5X:184:THR:HG23 | 2.17 | 0.45 |
| 18:6A:70:TYR:HE1 | 18:6A:85:THR:HG22 | 1.81 | 0.45 |
| 18:6C:70:TYR:HE1 | 18:6C:85:THR:HG22 | 1.82 | 0.45 |
| 22:6I:265:ASP:OD2 | 22:6I:266:LYS:N | 2.50 | 0.45 |
| 22:6M:83:TRP:HB2 | 22:6M:86:LEU:HB2 | 1.98 | 0.45 |
| 22:6O:193:MET:HG2 | 22:6O:194:TYR:CD1 | 2.52 | 0.45 |
| 22:6P:271:ARG:O | 22:6P:275:LEU:HG | 2.17 | 0.45 |
| 24:6T:460:HIS:HB2 | 24:6T:465:LEU:HD22 | 1.99 | 0.45 |
| 24:6V:500:ARG:HE | 24:6V:500:ARG:HB2 | 1.62 | 0.45 |
| 24:6X:255:HIS:HA | 24:6X:258:ASP:OD1 | 2.17 | 0.45 |
| 24:6Y:482:ILE:HB | 24:6Y:498:LEU:HB3 | 1.99 | 0.45 |
| 24:6Z:472:SER:HB2 | 24:6Z:481:LEU:CD2 | 2.46 | 0.45 |
| 26:7F:30:PHE:HA | 26:7F:98:LEU:HD11 | 1.99 | 0.45 |
| 26:7F:116:GLN:O | 26:7F:117:ARG:C | 2.55 | 0.45 |
| 26:7F:119:MET:HE3 | 26:7F:119:MET:CA | 2.44 | 0.45 |
| 34:7S:220:VAL:HG21 | 35:7U:170:PHE:HD1 | 1.82 | 0.45 |
| 37:7Y:188:LEU:HD23 | 37:7Y:188:LEU:C | 2.37 | 0.45 |
| 38:8B:186:LEU:O | 38:8B:188:ARG:NH2 | 2.50 | 0.45 |
| 1:A1:55:THR:HG21 | 24:6Y:107:VAL:HG21 | 1.98 | 0.44 |
| 1:F2:54:ALA:O | 1:G8:283:ALA:HA | 2.17 | 0.44 |
| 2:G9:211:ASP:OD1 | 2:G9:215:ARG:NH1 | 2.51 | 0.44 |
| 2:G9:322:ASP:O | 2:G9:373:ARG:NE | 2.41 | 0.44 |
| 1:H2:26:ASP:O | 1:H2:359:LYS:NZ | 2.34 | 0.44 |
| 2:H3:278:ALA:HA | 2:H3:369:ALA:CB | 2.43 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I1:9:ILE:HG13 | 2:I1:9:ILE:O | 2.18 | 0.44 |
| 2:I1:137:VAL:HG22 | 2:I1:168:GLY:HA2 | 1.99 | 0.44 |
| 1:I4:173:PRO:HD2 | 1:I4:380:ARG:NH1 | 2.32 | 0.44 |
| 2:I7:9:ILE:HG22 | 2:I7:146:GLY:HA2 | 1.99 | 0.44 |
| 1:I8:17:GLY:HA2 | 1:I8:20:PHE:HB3 | 1.98 | 0.44 |
| 1:J0:122:LYS:HA | 1:J0:125:GLU:OE2 | 2.16 | 0.44 |
| 2:J3:3:GLU:HB2 | 2:J3:129:CYS:SG | 2.57 | 0.44 |
| 2:J3:274:PRO:HG3 | 2:J3:286:LEU:HD11 | 1.97 | 0.44 |
| 2:J5:344:VAL:HG11 | 2:J5:346:TRP:CE2 | 2.52 | 0.44 |
| 1:J6:421:GLU:HA | 1:J6:424:GLN:HB3 | 1.99 | 0.44 |
| 2:J9:133:GLN:NE2 | 2:J9:251:ASP:HB3 | 2.32 | 0.44 |
| 2:J9:370:LYS:HD2 | 5:4M:266:PHE:CE2 | 2.51 | 0.44 |
| 1:K0:203:ASP:OD2 | 1:K0:302:ALA:N | 2.50 | 0.44 |
| 2:K1:84:ARG:HH12 | 28:7X:407:LYS:CG | 2.28 | 0.44 |
| 2:K1:235:ILE:HD13 | 2:K1:238:LEU:HD21 | 1.99 | 0.44 |
| 2:K1:333:ALA:O | 2:K1:337:THR:HG23 | 2.18 | 0.44 |
| 2:K7:344:VAL:HG13 | 2:K7:346:TRP:H | 1.81 | 0.44 |
| 2:K9:52:PHE:HZ | 2:K9:239:THR:HG21 | 1.82 | 0.44 |
| 2:K9:53:PHE:HB3 | 2:K9:61:HIS:HB3 | 1.99 | 0.44 |
| 2:L3:266:HIS:ND1 | 2:L3:266:HIS:O | 2.49 | 0.44 |
| 2:L3:333:ALA:O | 2:L3:337:THR:HG23 | 2.17 | 0.44 |
| 1:L4:54:ALA:O | 1:L4:55:THR:OG1 | 2.28 | 0.44 |
| 1:L6:267:MET:HB2 | 1:L6:301:CYS:SG | 2.57 | 0.44 |
| 1:L6:404:ASP:HB3 | 1:L6:406:MET:SD | 2.57 | 0.44 |
| 2:L9:265:ILE:HD11 | 2:L9:435:VAL:HG21 | 2.00 | 0.44 |
| 2:M3:139:ASN:OD1 | 2:M3:170:THR:HG22 | 2.17 | 0.44 |
| 2:M5:84:ARG:NH1 | 37:7Y:136:GLU:OE2 | 2.50 | 0.44 |
| 1:M6:73:MET:HA | 1:M6:76:VAL:CG2 | 2.46 | 0.44 |
| 2:M7:88:HIS:HB3 | 2:M7:89:PRO:HD3 | 1.98 | 0.44 |
| 1:N2:233:MET:O | 1:N2:236:ILE:HG22 | 2.17 | 0.44 |
| 1:N2:289:LEU:HD23 | 1:N2:365:ALA:HB2 | 1.98 | 0.44 |
| 1:N2:356:ILE:HD12 | 29:7J:105:PHE:HZ | 1.81 | 0.44 |
| 2:N7:414:GLU:HG2 | 2:N7:416:GLY:H | 1.81 | 0.44 |
| 2:O1:9:ILE:HG22 | 2:O1:146:GLY:HA2 | 1.99 | 0.44 |
| 2:O1:12:ALA:O | 2:O1:16:VAL:HG23 | 2.17 | 0.44 |
| 2:O3:90:GLU:HB3 | 2:O3:121:ARG:HH12 | 1.82 | 0.44 |
| 1:O4:361:LEU:CD2 | 19:6E:73:HIS:HD2 | 2.30 | 0.44 |
| 1:O4:395:LEU:O | 1:O4:399:THR:HG23 | 2.17 | 0.44 |
| 1:O6:405:GLU:OE2 | 1:O6:405:GLU:N | 2.50 | 0.44 |
| 2:O9:9:ILE:HG22 | 2:O9:146:GLY:HA2 | 1.99 | 0.44 |
| 2:O9:90:GLU:C | 2:O9:121:ARG:HH12 | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:7:ILE:HD11 | 2:P3:137:VAL:HG12 | 1.98 | 0.44 |
| 2:P5:336:LYS:O | 2:P5:339:ARG:NH2 | 2.50 | 0.44 |
| 1:P8:28:HIS:NE2 | 1:P8:241:ARG:HD2 | 2.31 | 0.44 |
| 1:Q0:391:ARG:HE | 2:Q1:346:TRP:HH2 | 1.66 | 0.44 |
| 1:Q2:3:GLU:HB2 | 1:Q2:130:LEU:HA | 1.98 | 0.44 |
| 1:Q4:58:ARG:NH1 | 1:Q4:83:GLN:O | 2.50 | 0.44 |
| 1:Q6:67:ASP:CG | 1:Q6:68:LEU:H | 2.21 | 0.44 |
| 1:Q8:207:LEU:HB3 | 1:Q8:225:LEU:HD22 | 1.99 | 0.44 |
| 2:R3:27:GLU:OE1 | 2:R3:243:ARG:NH1 | 2.50 | 0.44 |
| 2:R3:47:ASP:OD2 | 2:R3:50:ASN:HB2 | 2.18 | 0.44 |
| 2:R3:88:HIS:ND1 | 2:S9:283:HIS:HB3 | 2.32 | 0.44 |
| 2:R3:121:ARG:HA | 2:R3:121:ARG:HD2 | 1.69 | 0.44 |
| 1:R4:359:LYS:HA | 21:6G:55:TRP:CZ2 | 2.52 | 0.44 |
| 1:R4:371:SER:OG | 1:R4:372:THR:N | 2.49 | 0.44 |
| 2:R5:31:GLN:HG3 | 11:5E:8:ARG:NH1 | 2.32 | 0.44 |
| 2:R5:317:LEU:HB3 | 2:R5:319:TYR:HE1 | 1.82 | 0.44 |
| 2:R7:9:ILE:HG22 | 2:R7:146:GLY:HA2 | 1.99 | 0.44 |
| 1:R8:125:GLU:OE2 | 1:T4:336:LYS:HE2 | 2.17 | 0.44 |
| 1:S2:329:GLN:HA | 1:S2:332:ASN:ND2 | 2.32 | 0.44 |
| 1:S4:385:PHE:HZ | 1:S4:408:PHE:HB3 | 1.81 | 0.44 |
| 2:S7:414:GLU:HG2 | 2:S7:417:GLU:HG2 | 1.99 | 0.44 |
| 1:S8:148:GLY:O | 1:S8:152:ILE:HG12 | 2.17 | 0.44 |
| 2:S9:392:ASP:OD2 | 2:S9:422:ARG:NH1 | 2.50 | 0.44 |
| 1:T0:403:MET:HE3 | 1:T0:403:MET:HB2 | 1.78 | 0.44 |
| 2:T1:297:GLU:HG2 | 2:T1:299:ALA:H | 1.82 | 0.44 |
| 1:T2:135:VAL:HG12 | 1:T2:137:HIS:HD2 | 1.82 | 0.44 |
| 1:T2:309:ARG:H | 1:T2:372:THR:CG2 | 2.30 | 0.44 |
| 1:T4:135:VAL:HG21 | 1:T4:152:ILE:HD11 | 1.99 | 0.44 |
| 1:T6:337:ASN:HD21 | 17:5U:48:THR:N | 2.13 | 0.44 |
| 1:T6:337:ASN:ND2 | 17:5U:48:THR:H | 2.15 | 0.44 |
| 2:T7:211:ASP:OD1 | 2:T7:214:ARG:NH2 | 2.50 | 0.44 |
| 2:U5:122:ILE:HA | 2:U5:125:LEU:HD12 | 1.98 | 0.44 |
| 1:V2:282:ARG:HD3 | 1:V2:282:ARG:H | 1.82 | 0.44 |
| 2:V3:9:ILE:HG22 | 2:V3:146:GLY:HA2 | 1.98 | 0.44 |
| 1:V6:258:ILE:HD11 | 1:V6:266:PHE:HZ | 1.82 | 0.44 |
| 1:V6:273:LEU:H | 1:V6:292:GLN:NE2 | 2.14 | 0.44 |
| 1:V8:186:THR:HG22 | 1:V8:411:ALA:HB1 | 1.99 | 0.44 |
| 2:W3:35:GLN:N | 2:W3:35:GLN:OE1 | 2.50 | 0.44 |
| 2:W3:177:VAL:HG13 | 1:W4:327:ASP:HB3 | 1.99 | 0.44 |
| 1:W4:45:GLU:N | 1:W4:45:GLU:OE1 | 2.49 | 0.44 |
| 2:W7:4:VAL:HG23 | 2:W7:134:GLY:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X0:3:GLU:HB2 | 1:X0:130:LEU:HA | 1.99 | 0.44 |
| 1:X0:86:ARG:HG2 | 1:X0:88:ASP:H | 1.83 | 0.44 |
| 1:X4:237:THR:O | 1:X4:241:ARG:NE | 2.49 | 0.44 |
| 2:X5:50:ASN:O | 2:X5:64:ARG:NH2 | 2.50 | 0.44 |
| 2:X7:182:VAL:HG12 | 2:X7:182:VAL:O | 2.16 | 0.44 |
| 2:X7:210:TYR:CE1 | 2:X7:227:LEU:HD11 | 2.52 | 0.44 |
| 1:Y0:2:ARG:HB3 | 1:Y0:131:GLN:HE21 | 1.82 | 0.44 |
| 1:Y4:49:VAL:HG13 | 1:Y4:50:TYR:CD2 | 2.52 | 0.44 |
| 1:Y6:317:PHE:HE2 | 1:Y6:326:VAL:HG13 | 1.83 | 0.44 |
| 1:Y8:395:LEU:O | 1:Y8:399:THR:HG23 | 2.17 | 0.44 |
| 2:Y9:221:ARG:HB3 | 1:Z0:322:SER:HB2 | 1.97 | 0.44 |
| 2:Y9:305:CYS:SG | 2:Y9:383:ALA:HB1 | 2.57 | 0.44 |
| 2:Y9:312:TYR:HB2 | 2:Y9:343:PHE:CD1 | 2.53 | 0.44 |
| 1:Z0:20:PHE:CE1 | 1:Z0:233:MET:HG2 | 2.51 | 0.44 |
| 1:Z0:150:LEU:HD12 | 1:Z0:150:LEU:HA | 1.80 | 0.44 |
| 2:Z1:287:SER:N | 2:Z1:290:GLU:OE2 | 2.50 | 0.44 |
| 1:Z4:294:TRP:CG | 1:Z4:333:VAL:HG21 | 2.52 | 0.44 |
| 1:Z6:116:VAL:O | 1:Z6:120:VAL:HG22 | 2.17 | 0.44 |
| 1:Z6:164:MET:O | 1:Z6:197:ASP:HB2 | 2.17 | 0.44 |
| 2:Z7:31:GLN:HB2 | 2:Z7:33:ASP:OD1 | 2.16 | 0.44 |
| 2:Z9:296:PHE:HE2 | 2:Z9:335:ILE:HG21 | 1.82 | 0.44 |
| 1:0A:405:GLU:HA | 1:0A:408:PHE:HD2 | 1.81 | 0.44 |
| 1:0C:262:ARG:NH2 | 1:0C:418:LEU:HD13 | 2.32 | 0.44 |
| 2:0F:83:TYR:HD1 | 2:0F:86:LEU:HD13 | 1.82 | 0.44 |
| 2:0F:176:GLN:HE22 | 2:0F:304:LYS:HE2 | 1.82 | 0.44 |
| 2:0H:21:TRP:CH2 | 2:0H:63:PRO:HB3 | 2.52 | 0.44 |
| 2:0J:116:ASP:N | 2:0J:116:ASP:OD1 | 2.48 | 0.44 |
| 2:0J:210:TYR:HH | 1:0K:323:THR:HG1 | 1.64 | 0.44 |
| 1:0K:130:LEU:HB2 | 1:0K:162:ARG:HD2 | 1.98 | 0.44 |
| 1:0K:395:LEU:HG | 1:0K:399:THR:OG1 | 2.17 | 0.44 |
| 2:0L:69:ASP:O | 2:0L:94:SER:HA | 2.17 | 0.44 |
| 2:0L:307:PRO:HB2 | 2:0L:312:TYR:CE1 | 2.52 | 0.44 |
| 1:0O:117:LEU:O | 1:0O:121:ARG:HB2 | 2.17 | 0.44 |
| 1:0S:21:TRP:CZ3 | 1:0S:61:PRO:HB3 | 2.53 | 0.44 |
| 1:0S:374:ILE:HG12 | 1:0S:378:PHE:CE2 | 2.52 | 0.44 |
| 2:0X:209:ILE:HG21 | 2:0X:227:LEU:HG | 1.99 | 0.44 |
| 2:0Z:177:VAL:HG13 | 1:1A:327:ASP:HB3 | 1.99 | 0.44 |
| 2:1B:405:VAL:O | 2:1B:409:VAL:HG23 | 2.17 | 0.44 |
| 1:1C:382:SER:HB2 | 1:1C:415:MET:HG2 | 1.99 | 0.44 |
| 1:1E:52:ASN:OD1 | 1:1E:62:ARG:NH2 | 2.41 | 0.44 |
| 2:1F:88:HIS:CD2 | 2:1F:90:GLU:H | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1F:313:MET:HE2 | 2:1F:380:ASN:HD22 | 1.82 | 0.44 |
| 2:1H:210:TYR:HA | 2:1H:213:CYS:SG | 2.57 | 0.44 |
| 2:1H:288:VAL:O | 2:1H:292:THR:OG1 | 2.19 | 0.44 |
| 1:1Q:364:SER:OG | 1:1Q:365:ALA:N | 2.50 | 0.44 |
| 2:1R:250:VAL:HG23 | 2:1R:254:GLU:HG3 | 1.99 | 0.44 |
| 2:1T:330:ALA:O | 2:1T:334:THR:HG23 | 2.16 | 0.44 |
| 2:1V:417:GLU:HA | 2:1V:420:GLU:HG2 | 1.99 | 0.44 |
| 1:1W:244:GLY:HA2 | 1:1W:355:ASP:CG | 2.38 | 0.44 |
| 1:2E:1:MET:O | 1:2E:129:CYS:HB2 | 2.16 | 0.44 |
| 1:2E:137:HIS:ND1 | 1:2E:138:SER:O | 2.48 | 0.44 |
| 2:2F:133:GLN:HB3 | 2:2F:252:ILE:HG21 | 1.98 | 0.44 |
| 1:2G:204:ASN:HD21 | 39:2G:502:GDP:N2 | 2.15 | 0.44 |
| 2:2H:123:ARG:NH2 | 38:8B:37:TYR:HB2 | 2.32 | 0.44 |
| 2:2H:185:TYR:CE1 | 2:2H:398:MET:HE3 | 2.53 | 0.44 |
| 1:2I:418:LEU:O | 1:2I:422:TYR:HD2 | 2.00 | 0.44 |
| 2:2L:88:HIS:CE1 | 2:3B:280:LYS:HD2 | 2.52 | 0.44 |
| 2:2L:222:PRO:CD | 1:2M:324:LYS:HE3 | 2.45 | 0.44 |
| 2:2N:123:ARG:NH2 | 38:8D:78:ASP:OD1 | 2.51 | 0.44 |
| 2:2R:116:ASP:OD1 | 2:2R:117:LEU:N | 2.50 | 0.44 |
| 2:2R:271:SER:HB2 | 2:2R:377:MET:HB3 | 1.99 | 0.44 |
| 1:2S:324:LYS:NZ | 38:8A:57:LEU:HD21 | 2.31 | 0.44 |
| 2:2V:137:VAL:HG22 | 2:2V:168:GLY:HA2 | 1.98 | 0.44 |
| 1:3C:275:SER:O | 1:3C:279:GLN:HG3 | 2.17 | 0.44 |
| 2:3D:237:SER:HA | 2:3D:320:ARG:HD2 | 1.99 | 0.44 |
| 1:3G:113:ILE:HD11 | 1:3G:151:LEU:HA | 1.99 | 0.44 |
| 1:3K:34:GLY:HA3 | 1:3K:58:ARG:CD | 2.46 | 0.44 |
| 1:3K:138:SER:HA | 1:3K:169:VAL:HG22 | 1.99 | 0.44 |
| 1:3M:403:MET:HB2 | 1:3M:403:MET:HE2 | 1.76 | 0.44 |
| 2:3N:83:TYR:HB3 | 2:3N:86:LEU:HB3 | 1.98 | 0.44 |
| 2:3N:391:LEU:HD23 | 2:3N:391:LEU:HA | 1.82 | 0.44 |
| 2:3P:3:GLU:HB2 | 2:3P:129:CYS:SG | 2.58 | 0.44 |
| 2:3P:394:LYS:HB2 | 1:3Q:346:PRO:HG3 | 1.98 | 0.44 |
| 1:3Q:91:VAL:HG11 | 1:3Q:116:VAL:HG23 | 1.98 | 0.44 |
| 2:3R:75:VAL:HG21 | 2:3R:94:SER:CB | 2.47 | 0.44 |
| 1:3S:389:PHE:O | 1:3S:392:LYS:NZ | 2.40 | 0.44 |
| 2:3T:195:LEU:HD21 | 2:3T:264:ARG:HD2 | 1.99 | 0.44 |
| 13:5H:99:ASN:HD22 | 13:5H:99:ASN:N | 2.15 | 0.44 |
| 13:5I:70:LYS:HE2 | 13:5I:70:LYS:HB3 | 1.43 | 0.44 |
| 13:5K:99:ASN:HD22 | 13:5K:99:ASN:N | 2.15 | 0.44 |
| 14:5L:319:TYR:CE2 | 14:5L:334:LEU:HB3 | 2.52 | 0.44 |
| 14:5L:399:SER:HG | 14:5L:401:TRP:HE1 | 1.63 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5L:531:ASP:OD1 | 14:5L:531:ASP:N | 2.44 | 0.44 |
| 14:5M:218:VAL:O | 14:5M:232:GLY:N | 2.50 | 0.44 |
| 14:5M:399:SER:HG | 14:5M:401:TRP:HE1 | 1.63 | 0.44 |
| 14:5N:319:TYR:CE2 | 14:5N:334:LEU:HB3 | 2.52 | 0.44 |
| 15:5P:264:GLU:OE2 | 15:5P:314:ARG:HA | 2.16 | 0.44 |
| 15:5P:334:LEU:C | 15:5P:334:LEU:CD2 | 2.85 | 0.44 |
| 16:5Q:94:ARG:HH11 | 16:5Q:166:PRO:HD2 | 1.82 | 0.44 |
| 17:5S:221:GLU:OE2 | 17:5S:222:ILE:N | 2.50 | 0.44 |
| 17:5T:221:GLU:OE2 | 17:5T:222:ILE:N | 2.50 | 0.44 |
| 17:5U:221:GLU:OE2 | 17:5U:222:ILE:N | 2.50 | 0.44 |
| 18:5Y:70:TYR:HE1 | 18:5Y:85:THR:HG22 | 1.82 | 0.44 |
| 18:5Z:70:TYR:HE1 | 18:5Z:85:THR:HG22 | 1.82 | 0.44 |
| 18:6C:101:LYS:O | 24:6Z:178:ASN:ND2 | 2.34 | 0.44 |
| 18:6D:70:TYR:HE1 | 18:6D:85:THR:HG22 | 1.82 | 0.44 |
| 22:6K:54:ARG:HG3 | 22:6K:55:THR:HG23 | 2.00 | 0.44 |
| 22:6K:162:LEU:HD11 | 22:6K:225:ALA:HB1 | 1.99 | 0.44 |
| 22:6K:342:ASP:O | 22:6K:346:PHE:HB2 | 2.17 | 0.44 |
| 22:6N:188:ARG:HD3 | 22:6N:192:LYS:HB2 | 1.99 | 0.44 |
| 24:6T:454:ASP:OD2 | 24:6T:454:ASP:N | 2.50 | 0.44 |
| 24:6U:40:GLN:HG3 | 24:6U:41:ARG:HG2 | 1.98 | 0.44 |
| 24:6U:536:ASP:OD1 | 24:6U:537:GLU:N | 2.51 | 0.44 |
| 24:6V:124:TYR:N | 24:6V:124:TYR:CD2 | 2.84 | 0.44 |
| 24:6W:11:LEU:HB3 | 24:6W:12:PRO:HD2 | 1.99 | 0.44 |
| 24:6W:512:TYR:CZ | 24:6W:523:ILE:HG23 | 2.52 | 0.44 |
| 24:6X:253:PRO:HB2 | 24:6X:256:LEU:HB2 | 1.98 | 0.44 |
| 24:6X:562:LEU:O | 24:6X:566:VAL:HG22 | 2.17 | 0.44 |
| 24:6Y:561:SER:O | 24:6Y:565:GLN:HG3 | 2.17 | 0.44 |
| 26:7F:79:GLN:OE1 | 26:7F:87:HIS:HD2 | 2.00 | 0.44 |
| 28:7H:404:HIS:O | 28:7H:405:ASN:C | 2.55 | 0.44 |
| 34:7S:227:LYS:HB2 | 35:7U:181:LEU:HD21 | 1.98 | 0.44 |
| 37:7Y:94:ARG:NH1 | 37:7Y:117:GLN:NE2 | 2.65 | 0.44 |
| 38:8A:196:MET:CE | 38:8A:201:LEU:CD2 | 2.94 | 0.44 |
| 1:7:280:GLN:HE22 | 1:T0:58:ARG:NH2 | 2.13 | 0.44 |
| 1:A3:262:ARG:HH12 | 3:4H:240:ARG:HH11 | 1.64 | 0.44 |
| 1:D4:320:ARG:HG3 | 18:6B:152:GLN:HG2 | 1.99 | 0.44 |
| 1:F6:216:LYS:C | 24:6T:422:ASN:HD21 | 2.20 | 0.44 |
| 2:G3:250:VAL:HG23 | 2:G3:254:GLU:HG3 | 2.00 | 0.44 |
| 2:G3:320:ARG:O | 2:G3:373:ARG:HA | 2.17 | 0.44 |
| 1:G4:185:ALA:O | 1:G4:189:VAL:HG23 | 2.17 | 0.44 |
| 1:G6:228:LEU:HD23 | 1:G6:228:LEU:HA | 1.85 | 0.44 |
| 1:G8:26:ASP:O | 1:G8:359:LYS:NZ | 2.34 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G8:116:VAL:HG23 | 1:G8:151:LEU:HD11 | 1.98 | 0.44 |
| 2:G9:362:VAL:HG22 | 2:G9:363:VAL:O | 2.18 | 0.44 |
| 1:H8:232:VAL:O | 1:H8:236:ILE:HG12 | 2.17 | 0.44 |
| 1:H8:382:SER:HB3 | 1:H8:415:MET:HG2 | 1.99 | 0.44 |
| 2:I1:91:GLN:O | 2:I1:93:ILE:HG12 | 2.17 | 0.44 |
| 1:I2:2:ARG:HB3 | 1:I2:131:GLN:HB2 | 1.99 | 0.44 |
| 2:I7:222:PRO:O | 1:I8:322:SER:OG | 2.28 | 0.44 |
| 2:I9:403:ALA:HB2 | 1:J0:344:TRP:HZ3 | 1.82 | 0.44 |
| 1:J0:386:THR:O | 1:J0:390:ARG:HG3 | 2.16 | 0.44 |
| 2:J1:4:VAL:HG22 | 2:J1:133:GLN:HB2 | 1.99 | 0.44 |
| 2:J1:69:ASP:OD1 | 2:J1:70:LEU:N | 2.47 | 0.44 |
| 2:J1:212:ILE:O | 2:J1:216:SER:OG | 2.34 | 0.44 |
| 1:J2:74:ASP:OD2 | 16:5Q:181:THR:CG2 | 2.64 | 0.44 |
| 1:J4:83:GLN:O | 1:L0:281:TYR:OH | 2.25 | 0.44 |
| 1:J4:131:GLN:HE21 | 1:J4:250:LEU:HB3 | 1.83 | 0.44 |
| 2:J5:151:SER:HB2 | 2:J5:193:SER:OG | 2.17 | 0.44 |
| 2:J7:223:THR:HG23 | 2:J7:225:THR:H | 1.82 | 0.44 |
| 1:J8:117:LEU:HD23 | 1:J8:117:LEU:HA | 1.84 | 0.44 |
| 1:J8:359:LYS:HA | 1:J8:359:LYS:HD2 | 1.73 | 0.44 |
| 2:J9:28:HIS:CE1 | 2:J9:49:PHE:HA | 2.51 | 0.44 |
| 2:K1:221:ARG:NH1 | 2:K1:223:THR:OG1 | 2.50 | 0.44 |
| 2:K3:21:TRP:CZ2 | 2:K3:65:CYS:HB2 | 2.53 | 0.44 |
| 1:K6:138:SER:O | 1:K6:139:LEU:HD23 | 2.17 | 0.44 |
| 2:K9:407:TRP:O | 2:K9:411:GLU:HG2 | 2.17 | 0.44 |
| 1:L2:272:PRO:HB2 | 1:L2:282:ARG:HH12 | 1.82 | 0.44 |
| 1:L2:396:HIS:H | 1:L2:396:HIS:CD2 | 2.33 | 0.44 |
| 1:L4:317:PHE:HE2 | 1:L4:326:VAL:HG13 | 1.81 | 0.44 |
| 1:L6:177:ASP:O | 2:L7:352:LYS:HA | 2.17 | 0.44 |
| 1:M0:396:HIS:HA | 1:M0:399:THR:OG1 | 2.17 | 0.44 |
| 2:M3:69:ASP:OD1 | 2:M3:70:LEU:N | 2.49 | 0.44 |
| 2:M3:76:ASP:HA | 2:M3:79:ARG:HB2 | 1.98 | 0.44 |
| 2:M5:254:GLU:HB3 | 2:M5:352:LYS:HE2 | 1.99 | 0.44 |
| 2:M5:409:VAL:HA | 2:M5:413:MET:O | 2.16 | 0.44 |
| 1:M6:395:LEU:O | 1:M6:399:THR:HG23 | 2.17 | 0.44 |
| 2:M7:201:ALA:O | 2:M7:268:MET:HE2 | 2.16 | 0.44 |
| 2:M7:287:SER:H | 2:M7:290:GLU:CD | 2.20 | 0.44 |
| 2:N1:220:GLU:OE1 | 2:N1:220:GLU:N | 2.50 | 0.44 |
| 2:N5:34:GLY:HA3 | 2:N5:60:LYS:NZ | 2.33 | 0.44 |
| 1:N8:66:MET:HE1 | 1:N8:151:LEU:HD22 | 1.99 | 0.44 |
| 1:N8:101:TRP:HB2 | 1:N8:184:ASN:OD1 | 2.16 | 0.44 |
| 2:N9:80:THR:O | 2:N9:80:THR:HG22 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O1:18:ASN:HD21 | 37:7Y:242:LEU:HD11 | 1.82 | 0.44 |
| 1:O2:132:GLY:HA2 | 1:O2:162:ARG:HB3 | 2.00 | 0.44 |
| 1:O4:4:ILE:HB | 1:O4:50:TYR:HE2 | 1.81 | 0.44 |
| 1:O4:218:THR:HG23 | 19:6E:9:THR:HG21 | 1.97 | 0.44 |
| 2:O7:3:GLU:HB2 | 2:O7:129:CYS:SG | 2.57 | 0.44 |
| 2:O9:217:LEU:HD22 | 2:O9:367:ASP:OD1 | 2.17 | 0.44 |
| 2:O9:384:ILE:HD12 | 2:O9:384:ILE:H | 1.82 | 0.44 |
| 1:P4:131:GLN:HE21 | 1:P4:250:LEU:HB2 | 1.82 | 0.44 |
| 1:P4:198:GLU:HA | 1:P4:264:HIS:HB2 | 1.98 | 0.44 |
| 1:P6:177:ASP:N | 1:P6:181:GLU:OE2 | 2.50 | 0.44 |
| 2:P7:326:LYS:HE3 | 2:P7:326:LYS:HB3 | 1.82 | 0.44 |
| 1:P8:220:PRO:HD2 | 2:P9:326:LYS:HD3 | 1.98 | 0.44 |
| 2:Q1:27:GLU:OE2 | 2:Q1:243:ARG:NH2 | 2.49 | 0.44 |
| 1:Q2:51:PHE:O | 1:Q2:62:ARG:NH2 | 2.50 | 0.44 |
| 1:Q4:68:LEU:HD12 | 1:Q4:97:ALA:HB2 | 2.00 | 0.44 |
| 2:Q5:33:ASP:O | 2:Q5:60:LYS:NZ | 2.49 | 0.44 |
| 1:Q6:26:ASP:O | 1:Q6:359:LYS:NZ | 2.29 | 0.44 |
| 1:Q6:101:TRP:HB2 | 1:Q6:184:ASN:OD1 | 2.17 | 0.44 |
| 1:Q6:193:VAL:HG13 | 1:Q6:194:GLU:HG3 | 1.99 | 0.44 |
| 2:R1:239:THR:HG23 | 2:R1:243:ARG:HE | 1.83 | 0.44 |
| 2:R1:377:MET:SD | 2:R1:379:SER:HB2 | 2.58 | 0.44 |
| 1:R2:92:PHE:CZ | 24:6V:35:TYR:CE1 | 2.85 | 0.44 |
| 2:R7:238:LEU:HD22 | 2:R7:378:ILE:HD11 | 1.98 | 0.44 |
| 1:S0:309:ARG:O | 1:S0:372:THR:HG22 | 2.17 | 0.44 |
| 2:S1:6:SER:O | 2:S1:65:CYS:HA | 2.16 | 0.44 |
| 2:S1:116:ASP:OD1 | 2:S1:156:ARG:NH2 | 2.51 | 0.44 |
| 1:S4:86:ARG:HG2 | 1:S4:88:ASP:H | 1.82 | 0.44 |
| 1:S4:193:VAL:HG13 | 1:S4:194:GLU:OE1 | 2.18 | 0.44 |
| 1:S6:275:SER:O | 1:S6:279:GLN:HG3 | 2.18 | 0.44 |
| 2:S9:102:ASN:ND2 | 2:S9:411:GLU:HG2 | 2.32 | 0.44 |
| 2:S9:223:THR:HG22 | 1:T0:322:SER:HA | 2.00 | 0.44 |
| 2:S9:328:VAL:HG11 | 2:S9:355:ILE:HD11 | 1.99 | 0.44 |
| 1:T6:309:ARG:H | 1:T6:372:THR:CG2 | 2.30 | 0.44 |
| 2:T7:242:LEU:HD11 | 2:T7:252:ILE:HB | 1.99 | 0.44 |
| 1:T8:245:GLN:HG2 | 31:7N:29:GLU:OE2 | 2.17 | 0.44 |
| 2:U5:76:ASP:OD2 | 1:U6:46:ARG:NH2 | 2.50 | 0.44 |
| 2:U5:259:LEU:HD11 | 2:U5:316:CYS:HB2 | 2.00 | 0.44 |
| 1:V0:7:ILE:O | 1:V0:135:VAL:HA | 2.18 | 0.44 |
| 2:V1:32:PRO:HB3 | 2:V1:83:TYR:CE1 | 2.52 | 0.44 |
| 1:V6:177:ASP:O | 2:V7:352:LYS:HA | 2.17 | 0.44 |
| 1:V8:178:THR:OG1 | 1:V8:181:GLU:OE1 | 2.34 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W2:31:ASP:HB2 | 1:W2:32:PRO:HD2 | 1.99 | 0.44 |
| 2:W3:11:GLN:OE1 | 2:W3:15:GLN:NE2 | 2.50 | 0.44 |
| 2:W5:279:GLU:OE2 | 2:W5:280:LYS:HG3 | 2.17 | 0.44 |
| 1:W6:190:HIS:HD2 | 1:W6:411:ALA:HA | 1.76 | 0.44 |
| 1:W8:286:VAL:CG2 | 1:W8:287:PRO:HD3 | 2.46 | 0.44 |
| 2:W9:205:ASP:OD1 | 2:W9:303:VAL:HG13 | 2.17 | 0.44 |
| 2:W9:306:ASP:HB3 | 2:W9:309:HIS:HD2 | 1.81 | 0.44 |
| 2:W9:377:MET:HE3 | 2:W9:379:SER:HB3 | 1.98 | 0.44 |
| 1:X0:382:SER:HB3 | 1:X0:415:MET:HG2 | 2.00 | 0.44 |
| 1:X2:260:PHE:HB2 | 1:X2:263:LEU:HD23 | 1.99 | 0.44 |
| 1:X4:272:PRO:HA | 1:X4:292:GLN:OE1 | 2.17 | 0.44 |
| 1:X6:14:ASN:OD1 | 1:X6:65:LEU:HD22 | 2.17 | 0.44 |
| 1:X6:284:LEU:HD23 | 1:X6:284:LEU:HA | 1.84 | 0.44 |
| 1:Y2:263:LEU:HD22 | 1:Y2:422:TYR:CE1 | 2.52 | 0.44 |
| 1:Y8:206:ALA:HA | 1:Y8:209:ASP:OD1 | 2.17 | 0.44 |
| 1:Y8:391:ARG:HG3 | 2:Y9:346:TRP:CG | 2.52 | 0.44 |
| 1:Z2:8:GLN:HG3 | 1:Z2:65:LEU:HD23 | 1.98 | 0.44 |
| 1:Z2:65:LEU:HD11 | 1:Z2:76:VAL:HG11 | 1.99 | 0.44 |
| 1:Z4:272:PRO:HB2 | 1:Z4:282:ARG:HH12 | 1.82 | 0.44 |
| 1:Z6:321:MET:HE2 | 1:Z6:321:MET:HB3 | 1.82 | 0.44 |
| 2:Z7:101:ASN:ND2 | 1:Z8:256:ASN:OD1 | 2.49 | 0.44 |
| 2:Z7:398:MET:HE1 | 1:Z8:345:ILE:HG23 | 1.98 | 0.44 |
| 1:0C:306:ARG:HH22 | 1:0C:310:TYR:HE2 | 1.64 | 0.44 |
| 2:0J:12:ALA:HB2 | 41:0K:501:GTP:C8 | 2.51 | 0.44 |
| 1:0K:180:VAL:HG23 | 1:0K:184:ASN:ND2 | 2.33 | 0.44 |
| 1:0O:211:CYS:SG | 1:0O:217:LEU:HB2 | 2.57 | 0.44 |
| 2:0P:5:ILE:HG22 | 2:0P:64:ARG:HB3 | 1.99 | 0.44 |
| 2:0R:193:SER:HA | 2:0R:196:GLU:OE2 | 2.17 | 0.44 |
| 2:0R:398:MET:SD | 1:0S:345:ILE:HG23 | 2.57 | 0.44 |
| 1:0S:152:ILE:HG23 | 1:0S:164:MET:SD | 2.58 | 0.44 |
| 1:0U:244:GLY:N | 1:0U:247:ASN:HD21 | 2.15 | 0.44 |
| 1:0U:274:THR:OG1 | 1:0U:282:ARG:NH1 | 2.50 | 0.44 |
| 2:0V:3:GLU:OE2 | 2:0V:131:GLY:N | 2.50 | 0.44 |
| 1:0W:113:ILE:HD13 | 1:0W:150:LEU:HD22 | 1.99 | 0.44 |
| 1:0W:165:LEU:CD2 | 1:0W:250:LEU:HD11 | 2.46 | 0.44 |
| 2:0X:175:PRO:HB3 | 2:0X:390:ARG:HE | 1.82 | 0.44 |
| 2:0Z:50:ASN:O | 2:0Z:64:ARG:NH2 | 2.50 | 0.44 |
| 2:0Z:56:THR:HG23 | 2:0Z:60:LYS:CB | 2.34 | 0.44 |
| 2:1B:413:MET:HB3 | 2:1B:417:GLU:OE2 | 2.17 | 0.44 |
| 2:1D:388:PHE:HD1 | 2:1D:391:LEU:HD21 | 1.82 | 0.44 |
| 1:1E:192:LEU:HD22 | 1:1E:265:PHE:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1G:334:GLN:HE22 | 1:1G:348:ASN:N | 2.10 | 0.44 |
| 2:1H:398:MET:HA | 2:1H:401:LYS:HE2 | 2.00 | 0.44 |
| 2:1L:201:ALA:O | 2:1L:268:MET:HE2 | 2.18 | 0.44 |
| 2:1R:56:THR:O | 2:1R:60:LYS:HB3 | 2.17 | 0.44 |
| 2:1T:109:THR:OG1 | 2:1T:411:GLU:OE2 | 2.31 | 0.44 |
| 1:1W:385:PHE:HZ | 1:1W:408:PHE:HD1 | 1.64 | 0.44 |
| 2:1X:9:ILE:HG12 | 2:1X:68:LEU:HD11 | 1.99 | 0.44 |
| 2:1Z:428:LEU:HA | 2:1Z:431:ASP:OD1 | 2.17 | 0.44 |
| 2:2D:223:THR:HG23 | 2:2D:225:THR:H | 1.82 | 0.44 |
| 2:2F:21:TRP:CZ3 | 2:2F:63:PRO:HB3 | 2.52 | 0.44 |
| 2:2H:14:ILE:HD11 | 2:2H:74:VAL:HG13 | 1.99 | 0.44 |
| 2:2J:211:ASP:OD1 | 2:2J:214:ARG:NH2 | 2.42 | 0.44 |
| 2:2L:98:ASP:OD1 | 2:2L:99:ALA:N | 2.50 | 0.44 |
| 1:2M:395:LEU:O | 1:2M:399:THR:HG23 | 2.17 | 0.44 |
| 2:2N:288:VAL:O | 2:2N:292:THR:OG1 | 2.28 | 0.44 |
| 1:2Q:209:ASP:OD2 | 38:8A:105:ARG:HA | 2.17 | 0.44 |
| 2:2R:90:GLU:HB3 | 2:3H:283:HIS:CE1 | 2.52 | 0.44 |
| 2:2R:238:LEU:HD11 | 2:2R:255:PHE:CZ | 2.52 | 0.44 |
| 1:2U:86:ARG:HG2 | 1:2U:88:ASP:H | 1.82 | 0.44 |
| 1:2U:172:SER:OG | 1:2U:205:GLU:OE1 | 2.18 | 0.44 |
| 1:2U:299:MET:N | 38:8B:105:ARG:HH22 | 2.14 | 0.44 |
| 2:2V:109:THR:HA | 2:2V:112:LYS:NZ | 2.31 | 0.44 |
| 2:2V:183:GLU:HG3 | 2:2V:184:PRO:HD3 | 1.99 | 0.44 |
| 1:2Y:3:GLU:HB2 | 1:2Y:130:LEU:HA | 1.98 | 0.44 |
| 2:2Z:341:ILE:HG23 | 38:8C:74:ILE:HD11 | 1.99 | 0.44 |
| 1:3A:178:THR:CG2 | 1:3A:181:GLU:HG3 | 2.47 | 0.44 |
| 1:3A:297:LYS:HB3 | 1:3A:297:LYS:HE3 | 1.79 | 0.44 |
| 1:3C:167:PHE:CZ | 1:3C:233:MET:HG2 | 2.52 | 0.44 |
| 1:3C:173:PRO:HD2 | 1:3C:380:ARG:NE | 2.31 | 0.44 |
| 1:3C:177:ASP:O | 2:3D:352:LYS:HA | 2.17 | 0.44 |
| 2:3J:278:ALA:HA | 2:3J:369:ALA:HB2 | 1.99 | 0.44 |
| 1:3K:130:LEU:HB2 | 1:3K:162:ARG:HE | 1.82 | 0.44 |
| 1:3K:170:VAL:HG21 | 1:3K:377:MET:SD | 2.58 | 0.44 |
| 1:3K:203:ASP:N | 1:3K:203:ASP:OD1 | 2.49 | 0.44 |
| 1:3K:317:PHE:HB3 | 1:3K:321:MET:SD | 2.57 | 0.44 |
| 2:3L:76:ASP:HA | 2:3L:79:ARG:HB2 | 1.98 | 0.44 |
| 1:3M:244:GLY:H | 1:3M:247:ASN:HD21 | 1.65 | 0.44 |
| 2:3N:265:ILE:CD1 | 2:3N:435:VAL:HG21 | 2.47 | 0.44 |
| 2:3R:3:GLU:HB2 | 2:3R:129:CYS:SG | 2.57 | 0.44 |
| 2:3R:246:GLY:HA3 | 2:3R:356:ASN:HA | 2.00 | 0.44 |
| 2:3R:402:ARG:HA | 2:3R:402:ARG:HD3 | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3S:415:MET:O | 1:3S:418:LEU:HG | 2.17 | 0.44 |
| 2:3T:288:VAL:CG2 | 2:3T:327:ASP:HB2 | 2.43 | 0.44 |
| 3:4J:101:LYS:HA | 3:4J:102:PRO:HD3 | 1.84 | 0.44 |
| 3:4J:178:LYS:HA | 3:4J:178:LYS:HD2 | 1.80 | 0.44 |
| 3:4J:191:ILE:HD11 | 3:4J:228:ALA:CB | 2.47 | 0.44 |
| 7:4R:83:ASP:OD1 | 7:4R:84:THR:N | 2.50 | 0.44 |
| 10:5B:314:LYS:HD2 | 10:5B:317:ILE:HD11 | 1.98 | 0.44 |
| 14:5L:24:HIS:CG | 14:5L:25:PRO:HD2 | 2.51 | 0.44 |
| 14:5M:319:TYR:CE2 | 14:5M:334:LEU:HB3 | 2.52 | 0.44 |
| 14:5N:190:LEU:HD11 | 14:5N:228:PHE:HB3 | 1.99 | 0.44 |
| 14:5N:531:ASP:N | 14:5N:531:ASP:OD1 | 2.44 | 0.44 |
| 15:5O:331:ASP:CG | 30:7K:241:LYS:HE2 | 2.38 | 0.44 |
| 17:5T:82:LYS:HA | 17:5T:82:LYS:HD3 | 1.77 | 0.44 |
| 17:5U:82:LYS:HA | 17:5U:82:LYS:HD3 | 1.77 | 0.44 |
| 17:5U:174:SER:OG | 17:5U:175:PRO:CD | 2.65 | 0.44 |
| 18:5X:125:ARG:NH1 | 18:5X:201:ALA:O | 2.50 | 0.44 |
| 18:5X:216:ALA:O | 18:5X:220:THR:HG22 | 2.18 | 0.44 |
| 18:6A:216:ALA:O | 18:6A:220:THR:HG22 | 2.18 | 0.44 |
| 18:6D:216:ALA:O | 18:6D:220:THR:HG22 | 2.18 | 0.44 |
| 20:6F:237:CYS:SG | 20:6F:238:LEU:N | 2.90 | 0.44 |
| 20:6F:394:ARG:HH12 | 33:7Q:185:ARG:CZ | 2.30 | 0.44 |
| 22:6P:145:SER:HB2 | 22:6P:148:ASN:CG | 2.37 | 0.44 |
| 23:6R:52:LEU:HD23 | 23:6R:52:LEU:C | 2.38 | 0.44 |
| 23:6S:65:LEU:HD12 | 23:6S:65:LEU:HA | 1.80 | 0.44 |
| 24:6T:481:LEU:HD23 | 24:6T:481:LEU:H | 1.83 | 0.44 |
| 24:6U:88:TRP:HA | 24:6U:126:GLU:HG3 | 1.99 | 0.44 |
| 24:6U:481:LEU:HB2 | 24:6U:500:ARG:HB3 | 1.99 | 0.44 |
| 24:6X:315:ARG:CG | 24:6X:315:ARG:NH1 | 2.72 | 0.44 |
| 24:6Y:106:VAL:HG22 | 24:6Y:107:VAL:H | 1.81 | 0.44 |
| 24:6Z:11:LEU:HD12 | 24:6Z:14:TYR:CE2 | 2.52 | 0.44 |
| 26:7D:30:PHE:HA | 26:7D:98:LEU:HD11 | 1.99 | 0.44 |
| 26:7D:79:GLN:OE1 | 26:7D:87:HIS:HD2 | 2.00 | 0.44 |
| 30:7L:316:GLU:HG2 | 30:7L:319:ARG:HH12 | 1.82 | 0.44 |
| 35:7T:173:ILE:HA | 35:7T:176:ASN:HD22 | 1.82 | 0.44 |
| 37:7Y:139:ARG:O | 37:7Y:140:SER:HB3 | 2.16 | 0.44 |
| 38:8D:64:ASP:OD2 | 38:8D:65:VAL:N | 2.50 | 0.44 |
| 1:9:219:THR:OG1 | 26:7E:142:PHE:CE2 | 2.60 | 0.44 |
| 2:A2:279:GLU:CG | 26:7F:82:PRO:HG2 | 2.47 | 0.44 |
| 2:C9:12:ALA:HB2 | 41:C9:501:GTP:C8 | 2.53 | 0.44 |
| 2:G3:223:THR:HG23 | 2:G3:225:THR:H | 1.82 | 0.44 |
| 1:G4:272:PRO:HD3 | 1:G4:364:SER:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:292:GLN:HG2 | 1:G4:298:ASN:HD22 | 1.83 | 0.44 |
| 2:G5:280:LYS:HB3 | 2:G5:284:GLU:OE1 | 2.17 | 0.44 |
| 1:G6:237:THR:HG23 | 1:G6:241:ARG:HH21 | 1.82 | 0.44 |
| 2:G7:53:PHE:HB3 | 2:G7:61:HIS:HB3 | 2.00 | 0.44 |
| 1:G8:407:GLU:O | 1:G8:410:GLU:HG2 | 2.17 | 0.44 |
| 1:H2:180:VAL:HG23 | 1:H2:184:ASN:ND2 | 2.32 | 0.44 |
| 2:H5:317:LEU:HB3 | 2:H5:319:TYR:HE1 | 1.81 | 0.44 |
| 1:H6:4:ILE:HB | 1:H6:50:TYR:HE1 | 1.83 | 0.44 |
| 2:H7:9:ILE:HG22 | 2:H7:146:GLY:HA2 | 2.00 | 0.44 |
| 2:H7:223:THR:OG1 | 2:H7:224:TYR:N | 2.50 | 0.44 |
| 2:H7:430:LYS:O | 2:H7:434:GLU:HG2 | 2.17 | 0.44 |
| 1:H8:221:THR:HG23 | 1:H8:223:GLY:H | 1.82 | 0.44 |
| 2:I5:65:CYS:SG | 2:I5:66:ILE:N | 2.90 | 0.44 |
| 2:I5:90:GLU:O | 2:I5:121:ARG:NH1 | 2.32 | 0.44 |
| 2:J1:204:LEU:HD13 | 2:J1:302:MET:HB3 | 1.98 | 0.44 |
| 1:J2:46:ARG:HD3 | 1:J2:46:ARG:HA | 1.81 | 0.44 |
| 1:J2:167:PHE:HE1 | 1:J2:200:MET:SD | 2.41 | 0.44 |
| 2:J3:65:CYS:SG | 2:J3:66:ILE:N | 2.90 | 0.44 |
| 1:J6:189:VAL:O | 1:J6:193:VAL:HG23 | 2.18 | 0.44 |
| 1:J6:309:ARG:NH1 | 1:J6:343:GLU:OE2 | 2.50 | 0.44 |
| 2:K1:70:LEU:HD22 | 2:K1:110:ILE:HD12 | 1.99 | 0.44 |
| 1:K4:167:PHE:CE2 | 1:K4:233:MET:HG2 | 2.53 | 0.44 |
| 1:K6:21:TRP:CZ3 | 1:K6:61:PRO:HB3 | 2.52 | 0.44 |
| 1:K6:68:LEU:HD21 | 1:K6:112:LEU:HD22 | 1.99 | 0.44 |
| 2:K7:259:LEU:HD11 | 2:K7:316:CYS:HB2 | 2.00 | 0.44 |
| 1:K8:21:TRP:O | 1:K8:25:SER:OG | 2.27 | 0.44 |
| 1:K8:345:ILE:O | 1:K8:348:ASN:ND2 | 2.48 | 0.44 |
| 2:L5:66:ILE:O | 2:L5:66:ILE:HG13 | 2.17 | 0.44 |
| 1:L6:167:PHE:HE1 | 1:L6:200:MET:SD | 2.40 | 0.44 |
| 2:L7:17:GLY:HA2 | 2:L7:20:CYS:HB3 | 2.00 | 0.44 |
| 1:M6:1:MET:HE1 | 37:7Y:116:MET:CB | 2.36 | 0.44 |
| 1:M6:183:TYR:HE2 | 1:M6:394:PHE:HB2 | 1.82 | 0.44 |
| 1:N2:225:LEU:HD12 | 1:N2:225:LEU:H | 1.82 | 0.44 |
| 2:N3:137:VAL:HG22 | 2:N3:168:GLY:HA2 | 1.98 | 0.44 |
| 2:N3:313:MET:CE | 2:N3:382:THR:HG23 | 2.47 | 0.44 |
| 2:N3:414:GLU:HG2 | 2:N3:415:GLU:N | 2.32 | 0.44 |
| 2:N5:172:TYR:CE2 | 2:N5:203:MET:SD | 3.10 | 0.44 |
| 2:O1:9:ILE:HD13 | 2:O1:150:GLY:HA2 | 1.98 | 0.44 |
| 2:O1:177:VAL:HG13 | 1:O2:327:ASP:HB3 | 1.99 | 0.44 |
| 2:O5:324:VAL:HG13 | 2:O5:326:LYS:H | 1.82 | 0.44 |
| 2:O9:143:GLY:O | 2:O9:147:SER:OG | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P3:102:ASN:ND2 | 2:P3:105:ARG:HB2 | 2.32 | 0.44 |
| 2:P3:210:TYR:OH | 2:P3:224:TYR:HE1 | 2.00 | 0.44 |
| 2:P3:338:LYS:HA | 2:P3:338:LYS:HD2 | 1.67 | 0.44 |
| 1:P4:343:GLU:HG3 | 1:P4:344:TRP:N | 2.33 | 0.44 |
| 2:P7:9:ILE:CG1 | 2:P7:139:ASN:HB3 | 2.46 | 0.44 |
| 2:Q1:174:SER:HB3 | 2:Q1:177:VAL:O | 2.16 | 0.44 |
| 2:Q1:259:LEU:HD11 | 2:Q1:316:CYS:HB2 | 1.99 | 0.44 |
| 2:Q3:15:GLN:HB3 | 2:Q3:228:ASN:HD21 | 1.81 | 0.44 |
| 2:Q3:191:THR:HA | 2:Q3:194:LEU:HB3 | 1.98 | 0.44 |
| 2:Q9:79:ARG:O | 2:Q9:84:ARG:HG2 | 2.17 | 0.44 |
| 2:Q9:165:SER:HB3 | 2:Q9:256:GLN:NE2 | 2.31 | 0.44 |
| 1:R0:212:PHE:CE1 | 1:R0:220:PRO:HG3 | 2.53 | 0.44 |
| 1:R2:117:LEU:HD23 | 1:R2:117:LEU:HA | 1.73 | 0.44 |
| 2:R3:335:ILE:HG23 | 2:R3:341:ILE:HD11 | 1.99 | 0.44 |
| 1:R8:95:THR:HG23 | 1:R8:96:GLY:N | 2.32 | 0.44 |
| 1:R8:117:LEU:HA | 1:R8:117:LEU:HD23 | 1.80 | 0.44 |
| 1:S0:210:ILE:O | 1:S0:214:THR:OG1 | 2.31 | 0.44 |
| 1:S6:198:GLU:HB3 | 1:S6:258:ILE:HD11 | 1.99 | 0.44 |
| 2:S7:384:ILE:HG22 | 2:S7:388:PHE:CE2 | 2.52 | 0.44 |
| 2:S9:105:ARG:HA | 2:S9:411:GLU:HG3 | 2.00 | 0.44 |
| 2:T1:118:ALA:O | 2:T1:122:ILE:HG13 | 2.17 | 0.44 |
| 1:T2:44:LEU:O | 1:T2:47:ILE:HG12 | 2.18 | 0.44 |
| 1:T2:100:ASN:HB3 | 1:T2:103:LYS:HB2 | 2.00 | 0.44 |
| 2:T3:175:PRO:HB3 | 2:T3:390:ARG:NE | 2.32 | 0.44 |
| 1:T6:1:MET:CE | 26:7F:67:GLN:NE2 | 2.80 | 0.44 |
| 1:T6:68:LEU:HD13 | 1:T6:108:GLU:HG2 | 2.00 | 0.44 |
| 2:T7:343:PHE:HE2 | 2:T7:350:GLY:HA3 | 1.83 | 0.44 |
| 2:U1:286:LEU:HD12 | 2:U1:290:GLU:OE2 | 2.17 | 0.44 |
| 1:U2:273:LEU:HD23 | 1:U2:273:LEU:HA | 1.82 | 0.44 |
| 2:U3:222:PRO:CD | 1:U4:324:LYS:HE3 | 2.48 | 0.44 |
| 1:U6:189:VAL:O | 1:U6:193:VAL:HG13 | 2.17 | 0.44 |
| 1:U8:6:HIS:CE1 | 1:U8:8:GLN:HE21 | 2.35 | 0.44 |
| 2:U9:167:LEU:HD22 | 2:U9:200:VAL:HB | 1.99 | 0.44 |
| 2:U9:183:GLU:HG3 | 2:U9:184:PRO:HD3 | 2.00 | 0.44 |
| 2:V1:154:LEU:HD23 | 2:V1:154:LEU:HA | 1.77 | 0.44 |
| 1:V6:208:TYR:CE1 | 1:V6:225:LEU:HD11 | 2.53 | 0.44 |
| 1:V8:221:THR:OG1 | 1:V8:222:PHE:N | 2.50 | 0.44 |
| 2:V9:129:CYS:SG | 2:V9:130:THR:N | 2.90 | 0.44 |
| 1:W2:199:CYS:HG | 1:W2:265:PHE:HD1 | 1.66 | 0.44 |
| 1:W4:273:LEU:H | 1:W4:292:GLN:HE22 | 1.65 | 0.44 |
| 2:W5:108:TYR:O | 2:W5:112:LYS:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W5:271:SER:OG | 2:W5:377:MET:HB3 | 2.18 | 0.44 |
| 1:W6:21:TRP:CZ3 | 1:W6:61:PRO:HB3 | 2.53 | 0.44 |
| 1:W6:133:PHE:HB2 | 1:W6:164:MET:SD | 2.58 | 0.44 |
| 2:W9:139:ASN:N | 2:W9:139:ASN:OD1 | 2.50 | 0.44 |
| 1:X2:320:ARG:HH22 | 1:X2:357:PRO:CG | 2.30 | 0.44 |
| 2:X3:21:TRP:CZ3 | 2:X3:63:PRO:HB3 | 2.52 | 0.44 |
| 2:X3:32:PRO:HB3 | 2:X3:83:TYR:CE1 | 2.53 | 0.44 |
| 2:X5:239:THR:O | 2:X5:239:THR:HG22 | 2.17 | 0.44 |
| 1:X6:190:HIS:HD2 | 1:X6:414:ASN:ND2 | 2.16 | 0.44 |
| 2:X7:5:ILE:HD11 | 2:X7:135:PHE:CE1 | 2.52 | 0.44 |
| 2:X7:83:TYR:HB3 | 2:X7:86:LEU:HB3 | 1.99 | 0.44 |
| 2:X7:413:MET:HB3 | 2:X7:417:GLU:OE2 | 2.17 | 0.44 |
| 1:X8:183:TYR:O | 1:X8:187:LEU:HD13 | 2.18 | 0.44 |
| 2:X9:23:LEU:HD11 | 2:X9:233:GLN:NE2 | 2.32 | 0.44 |
| 2:Y1:322:ASP:OD2 | 2:Y1:373:ARG:NH2 | 2.50 | 0.44 |
| 1:Y4:105:HIS:NE2 | 1:Y4:150:LEU:HD13 | 2.32 | 0.44 |
| 1:Y4:266:PHE:CE1 | 1:Y4:370:ASN:HB2 | 2.52 | 0.44 |
| 1:Y4:317:PHE:HB3 | 1:Y4:321:MET:CE | 2.47 | 0.44 |
| 1:Y8:286:VAL:HG22 | 1:Y8:287:PRO:HD3 | 1.99 | 0.44 |
| 2:Y9:305:CYS:SG | 2:Y9:306:ASP:N | 2.88 | 0.44 |
| 2:Z1:326:LYS:NZ | 2:Z1:327:ASP:OD1 | 2.45 | 0.44 |
| 1:Z2:211:CYS:SG | 1:Z2:220:PRO:HB3 | 2.58 | 0.44 |
| 2:Z5:254:GLU:HB3 | 2:Z5:352:LYS:HE2 | 1.99 | 0.44 |
| 2:Z5:280:LYS:O | 2:Z5:283:HIS:HB3 | 2.17 | 0.44 |
| 1:Z8:182:PRO:HB2 | 1:Z8:385:PHE:HD1 | 1.81 | 0.44 |
| 1:0E:66:MET:CE | 1:0E:112:LEU:HD21 | 2.46 | 0.44 |
| 2:0F:80:THR:HG22 | 2:0F:80:THR:O | 2.18 | 0.44 |
| 1:0G:304:ASP:OD2 | 1:0G:306:ARG:NH2 | 2.50 | 0.44 |
| 2:0H:297:GLU:HG2 | 2:0H:298:PRO:HD2 | 1.98 | 0.44 |
| 2:0H:398:MET:HG2 | 1:0I:345:ILE:HA | 2.00 | 0.44 |
| 1:0I:117:LEU:O | 1:0I:121:ARG:HB2 | 2.17 | 0.44 |
| 1:0M:259:PRO:HG3 | 1:0M:311:LEU:HD21 | 1.98 | 0.44 |
| 2:0N:234:VAL:HG22 | 2:0N:272:TYR:CD2 | 2.53 | 0.44 |
| 2:0N:297:GLU:HG2 | 2:0N:298:PRO:HD2 | 1.98 | 0.44 |
| 2:0N:398:MET:SD | 1:0O:345:ILE:HG23 | 2.58 | 0.44 |
| 1:0O:55:THR:HG23 | 1:1E:282:ARG:O | 2.17 | 0.44 |
| 1:0O:61:PRO:HG2 | 1:0O:85:PHE:CE1 | 2.52 | 0.44 |
| 2:0P:56:THR:HG23 | 2:1F:285:GLN:HB2 | 1.99 | 0.44 |
| 2:0P:286:LEU:HG | 2:0P:373:ARG:NH1 | 2.32 | 0.44 |
| 2:0P:405:VAL:O | 2:0P:409:VAL:HG23 | 2.17 | 0.44 |
| 2:0R:177:VAL:HG21 | 2:0R:207:GLU:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0R:280:LYS:HA | 2:0R:283:HIS:HB3 | 1.99 | 0.44 |
| 1:0S:103:LYS:C | 1:0S:103:LYS:HD3 | 2.38 | 0.44 |
| 2:0X:227:LEU:O | 2:0X:231:ILE:HG12 | 2.17 | 0.44 |
| 1:1A:256:ASN:HD22 | 1:1A:350:LYS:HB2 | 1.81 | 0.44 |
| 1:1C:173:PRO:HG2 | 1:1C:380:ARG:HE | 1.82 | 0.44 |
| 1:1C:324:LYS:HA | 1:1C:327:ASP:OD1 | 2.17 | 0.44 |
| 1:1C:396:HIS:CD2 | 1:1C:396:HIS:N | 2.85 | 0.44 |
| 1:1K:304:ASP:OD2 | 1:1K:306:ARG:NH2 | 2.50 | 0.44 |
| 1:1K:415:MET:O | 1:1K:419:VAL:HG22 | 2.17 | 0.44 |
| 2:1L:298:PRO:HA | 2:1L:301:MET:HG3 | 1.99 | 0.44 |
| 1:1M:246:LEU:HD22 | 1:1M:352:SER:HA | 1.98 | 0.44 |
| 2:1N:223:THR:HG22 | 2:1N:224:TYR:N | 2.31 | 0.44 |
| 2:1P:100:ALA:HA | 1:1Q:252:LYS:HE3 | 1.99 | 0.44 |
| 2:1V:141:VAL:O | 2:1V:147:SER:OG | 2.35 | 0.44 |
| 2:1Z:108:TYR:HA | 2:1Z:112:LYS:NZ | 2.32 | 0.44 |
| 1:2C:4:ILE:HB | 1:2C:50:TYR:HE1 | 1.83 | 0.44 |
| 2:2D:352:LYS:NZ | 2:2D:353:CYS:O | 2.50 | 0.44 |
| 2:2F:328:VAL:O | 2:2F:332:VAL:HG22 | 2.17 | 0.44 |
| 2:2F:425:LEU:HD23 | 2:2F:425:LEU:HA | 1.82 | 0.44 |
| 2:2H:9:ILE:HG22 | 2:2H:146:GLY:HA2 | 1.98 | 0.44 |
| 1:2K:5:VAL:HG12 | 1:2K:133:PHE:HD1 | 1.83 | 0.44 |
| 1:2K:176:SER:OG | 2:2L:349:THR:OG1 | 2.23 | 0.44 |
| 1:2W:77:ARG:HD2 | 1:2W:77:ARG:HA | 1.76 | 0.44 |
| 1:2Y:404:ASP:HB3 | 1:2Y:406:MET:SD | 2.57 | 0.44 |
| 2:2Z:214:ARG:NH2 | 38:8C:61:LYS:HA | 2.30 | 0.44 |
| 1:3A:54:ALA:HB3 | 1:3A:58:ARG:O | 2.17 | 0.44 |
| 1:3A:67:ASP:CG | 1:3A:68:LEU:H | 2.21 | 0.44 |
| 2:3B:282:TYR:CD2 | 2:3B:282:TYR:N | 2.85 | 0.44 |
| 2:3B:358:GLN:NE2 | 38:8D:212:PRO:CB | 2.81 | 0.44 |
| 2:3B:425:LEU:HD23 | 2:3B:425:LEU:HA | 1.78 | 0.44 |
| 1:3C:161:ASP:OD2 | 1:3C:162:ARG:NH1 | 2.51 | 0.44 |
| 2:3D:2:ARG:HD2 | 2:3D:242:LEU:HD22 | 1.98 | 0.44 |
| 2:3J:283:HIS:CD2 | 2:3J:284:GLU:HB2 | 2.51 | 0.44 |
| 2:3J:417:GLU:HA | 2:3J:420:GLU:HG2 | 1.99 | 0.44 |
| 1:3K:167:PHE:CE2 | 1:3K:233:MET:HG2 | 2.51 | 0.44 |
| 1:3K:354:CYS:SG | 1:3K:355:ASP:N | 2.90 | 0.44 |
| 1:3Q:263:LEU:HD21 | 1:3Q:311:LEU:HD22 | 1.98 | 0.44 |
| 1:3Q:273:LEU:H | 1:3Q:292:GLN:NE2 | 2.16 | 0.44 |
| 1:3Q:395:LEU:O | 1:3Q:399:THR:HG23 | 2.16 | 0.44 |
| 2:3R:287:SER:OG | 2:3R:290:GLU:OE1 | 2.33 | 0.44 |
| 1:3S:183:TYR:HB3 | 1:3S:398:TYR:HE2 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3T:390:ARG:HG2 | 2:3T:394:LYS:HZ1 | 1.81 | 0.44 |
| 3:4B:44:ALA:HB3 | 3:4B:116:PRO:HG3 | 1.99 | 0.44 |
| 3:4J:132:ILE:HD11 | 3:4J:161:PHE:CZ | 2.52 | 0.44 |
| 5:4L:327:LYS:HA | 5:4L:330:GLU:OE1 | 2.17 | 0.44 |
| 5:4L:340:LEU:HG | 5:4L:344:LEU:HD23 | 1.99 | 0.44 |
| 5:4M:300:GLU:O | 5:4M:303:GLU:HG3 | 2.17 | 0.44 |
| 6:4P:67:LYS:HG3 | 20:6F:244:PRO:O | 2.17 | 0.44 |
| 7:4R:104:ARG:HE | 7:4R:110:LEU:HD12 | 1.82 | 0.44 |
| 7:4U:13:PRO:HG2 | 7:4U:14:GLU:OE2 | 2.17 | 0.44 |
| 8:4V:460:ALA:O | 8:4V:463:THR:OG1 | 2.33 | 0.44 |
| 10:5A:458:ARG:HB3 | 10:5A:458:ARG:HH11 | 1.82 | 0.44 |
| 12:5F:295:ARG:NH2 | 12:5F:325:ASP:OD2 | 2.50 | 0.44 |
| 14:5L:512:PHE:N | 14:5L:512:PHE:HD2 | 2.14 | 0.44 |
| 14:5M:24:HIS:CG | 14:5M:25:PRO:HD2 | 2.51 | 0.44 |
| 14:5N:24:HIS:CG | 14:5N:25:PRO:HD2 | 2.51 | 0.44 |
| 14:5N:354:GLU:OE1 | 14:5N:354:GLU:N | 2.48 | 0.44 |
| 14:5N:514:LYS:HD2 | 14:5N:530:THR:HG22 | 1.98 | 0.44 |
| 15:5P:52:TYR:CE2 | 15:5P:55:LEU:HD21 | 2.52 | 0.44 |
| 15:5P:333:GLU:HA | 15:5P:336:ARG:NH1 | 2.32 | 0.44 |
| 18:5Y:125:ARG:NH1 | 18:5Y:201:ALA:O | 2.50 | 0.44 |
| 18:5Y:216:ALA:O | 18:5Y:220:THR:HG22 | 2.18 | 0.44 |
| 18:5Z:125:ARG:NH1 | 18:5Z:201:ALA:O | 2.50 | 0.44 |
| 18:5Z:216:ALA:O | 18:5Z:220:THR:HG22 | 2.18 | 0.44 |
| 18:6A:125:ARG:NH1 | 18:6A:201:ALA:O | 2.50 | 0.44 |
| 18:6B:125:ARG:NH1 | 18:6B:201:ALA:O | 2.50 | 0.44 |
| 18:6B:216:ALA:O | 18:6B:220:THR:HG22 | 2.18 | 0.44 |
| 18:6C:125:ARG:NH1 | 18:6C:201:ALA:O | 2.50 | 0.44 |
| 18:6C:216:ALA:O | 18:6C:220:THR:HG22 | 2.18 | 0.44 |
| 18:6D:125:ARG:NH1 | 18:6D:201:ALA:O | 2.50 | 0.44 |
| 22:6I:10:PHE:HB3 | 22:6I:15:TRP:CD1 | 2.52 | 0.44 |
| 22:6I:275:LEU:HD13 | 22:6I:328:THR:HG21 | 1.99 | 0.44 |
| 22:6J:16:LYS:HD3 | 22:6J:20:TYR:CD2 | 2.53 | 0.44 |
| 22:6L:62:SER:O | 22:6L:62:SER:OG | 2.29 | 0.44 |
| 22:6N:130:LEU:O | 22:6N:209:ASN:ND2 | 2.51 | 0.44 |
| 22:6O:308:HIS:CD2 | 24:6Z:560:ARG:HH12 | 2.35 | 0.44 |
| 24:6U:558:LEU:HD11 | 24:6U:612:LEU:HD13 | 2.00 | 0.44 |
| 24:6U:573:VAL:HG12 | 24:6U:600:ALA:HB1 | 1.98 | 0.44 |
| 24:7A:218:GLY:O | 24:7A:221:ARG:NE | 2.49 | 0.44 |
| 25:7C:20:ARG:C | 25:7C:20:ARG:HD2 | 2.38 | 0.44 |
| 26:7E:30:PHE:HA | 26:7E:98:LEU:HD11 | 1.99 | 0.44 |
| 26:7E:79:GLN:OE1 | 26:7E:87:HIS:HD2 | 2.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:7J:140:GLU:HA | 29:7J:143:ARG:HG3 | 1.99 | 0.44 |
| 30:7K:111:LEU:HD23 | 30:7K:111:LEU:HA | 1.82 | 0.44 |
| 37:7Y:50:LEU:HB3 | 37:7Y:61:VAL:HG22 | 1.99 | 0.44 |
| 37:7Y:54:ARG:HB3 | 37:7Y:57:GLN:HB2 | 1.98 | 0.44 |
| 38:8A:170:PHE:HE1 | 38:8A:174:SER:HB3 | 1.82 | 0.44 |
| 38:8D:76:ASP:OD2 | 38:8D:77:LYS:N | 2.49 | 0.44 |
| 1:5:33:THR:OG1 | 18:5Y:100:GLU:OE1 | 2.36 | 0.44 |
| 2:A4:396:ASP:OD2 | 4:4I:53:ASN:ND2 | 2.49 | 0.44 |
| 2:E7:282:TYR:HH | 22:6L:81:ASN:CA | 2.19 | 0.44 |
| 1:F0:177:ASP:OD2 | 39:F0:502:GDP:H3' | 2.17 | 0.44 |
| 2:G3:221:ARG:HB3 | 1:G4:322:SER:OG | 2.18 | 0.44 |
| 1:G4:95:THR:OG1 | 1:G4:96:GLY:N | 2.50 | 0.44 |
| 2:G5:9:ILE:HG13 | 2:G5:9:ILE:O | 2.17 | 0.44 |
| 1:G6:48:ASN:OD1 | 1:G6:48:ASN:N | 2.51 | 0.44 |
| 1:G8:202:LEU:HD13 | 1:G8:300:MET:HB3 | 2.00 | 0.44 |
| 2:G9:305:CYS:HB2 | 2:G9:387:ILE:HD11 | 1.99 | 0.44 |
| 2:H5:155:GLU:HB2 | 2:H5:197:HIS:CE1 | 2.52 | 0.44 |
| 2:H5:188:VAL:O | 2:H5:191:THR:HG22 | 2.17 | 0.44 |
| 1:H8:91:VAL:HG11 | 1:H8:116:VAL:HG23 | 2.00 | 0.44 |
| 1:I2:26:ASP:O | 1:I2:359:LYS:NZ | 2.33 | 0.44 |
| 1:I2:95:THR:HG23 | 1:I2:96:GLY:N | 2.33 | 0.44 |
| 1:I2:172:SER:HB3 | 1:I2:175:VAL:HG22 | 1.99 | 0.44 |
| 1:I2:208:TYR:HA | 1:I2:211:CYS:SG | 2.57 | 0.44 |
| 2:I7:58:ALA:HB1 | 6:4N:474:PRO:HB3 | 1.98 | 0.44 |
| 2:I7:88:HIS:CE1 | 2:K3:283:HIS:HA | 2.52 | 0.44 |
| 2:I7:198:THR:HG21 | 2:I7:201:ALA:HB2 | 2.00 | 0.44 |
| 2:I7:271:SER:OG | 2:I7:301:MET:HA | 2.17 | 0.44 |
| 2:I9:21:TRP:CZ2 | 2:I9:65:CYS:HB3 | 2.53 | 0.44 |
| 2:I9:217:LEU:HB3 | 2:I9:219:ILE:CD1 | 2.48 | 0.44 |
| 1:J0:152:ILE:HD12 | 1:J0:164:MET:SD | 2.58 | 0.44 |
| 2:J1:326:LYS:HG3 | 2:J1:327:ASP:N | 2.32 | 0.44 |
| 2:J5:187:SER:HB2 | 2:J5:391:LEU:HD21 | 1.98 | 0.44 |
| 2:J7:83:TYR:HB3 | 2:J7:86:LEU:HB3 | 1.99 | 0.44 |
| 1:J8:176:SER:HB3 | 2:J9:349:THR:OG1 | 2.17 | 0.44 |
| 1:J8:373:ALA:O | 1:J8:376:GLU:HG3 | 2.17 | 0.44 |
| 2:J9:39:ASP:N | 2:J9:39:ASP:OD2 | 2.51 | 0.44 |
| 2:J9:74:VAL:O | 2:J9:77:GLU:HG3 | 2.18 | 0.44 |
| 1:K4:316:LEU:HB2 | 1:K4:366:THR:OG1 | 2.17 | 0.44 |
| 2:K5:155:GLU:HB2 | 2:K5:197:HIS:CE1 | 2.53 | 0.44 |
| 2:K5:367:ASP:OD2 | 2:K5:367:ASP:N | 2.49 | 0.44 |
| 2:K9:90:GLU:CB | 2:K9:121:ARG:HH12 | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K9:96:LYS:HG2 | 1:L0:1:MET:HE2 | 1.98 | 0.44 |
| 2:K9:397:LEU:HD23 | 2:K9:397:LEU:HA | 1.80 | 0.44 |
| 2:L1:66:ILE:HD11 | 2:L1:122:ILE:HD11 | 2.00 | 0.44 |
| 2:L3:276:ILE:HD13 | 2:L3:281:ALA:HA | 1.95 | 0.44 |
| 1:L4:31:ASP:OD2 | 1:L4:35:THR:OG1 | 2.36 | 0.44 |
| 2:L5:417:GLU:HA | 2:L5:420:GLU:HG2 | 1.99 | 0.44 |
| 1:L6:307:HIS:NE2 | 34:7S:129:ARG:HD3 | 2.33 | 0.44 |
| 1:L6:391:ARG:HH22 | 2:L7:435:VAL:HA | 1.82 | 0.44 |
| 2:L9:72:PRO:HD2 | 1:M0:2:ARG:HH12 | 1.83 | 0.44 |
| 1:M0:87:PRO:HD2 | 2:N7:283:HIS:HB2 | 1.99 | 0.44 |
| 1:M0:320:ARG:HD3 | 30:7K:306:PRO:HG3 | 1.99 | 0.44 |
| 2:M3:39:ASP:N | 2:M3:39:ASP:OD1 | 2.49 | 0.44 |
| 2:M7:88:HIS:C | 1:O4:281:TYR:OH | 2.55 | 0.44 |
| 2:N3:271:SER:N | 2:N3:377:MET:O | 2.48 | 0.44 |
| 2:N5:114:ILE:HG21 | 2:N5:149:LEU:HD22 | 1.99 | 0.44 |
| 2:N5:116:ASP:OD2 | 2:N5:117:LEU:N | 2.48 | 0.44 |
| 2:N5:244:PHE:HB3 | 32:7O:87:ASP:OD1 | 2.17 | 0.44 |
| 1:N6:244:GLY:HA2 | 1:N6:355:ASP:CG | 2.38 | 0.44 |
| 2:N9:12:ALA:HB2 | 41:O0:501:GTP:C8 | 2.52 | 0.44 |
| 2:N9:108:TYR:O | 2:N9:112:LYS:HG2 | 2.18 | 0.44 |
| 1:O0:361:LEU:HD23 | 1:O0:361:LEU:HA | 1.82 | 0.44 |
| 1:O0:403:MET:HE3 | 1:O0:403:MET:HB2 | 1.80 | 0.44 |
| 2:O5:167:LEU:HD13 | 2:O5:200:VAL:HB | 2.00 | 0.44 |
| 2:P3:286:LEU:CD2 | 2:P3:371:VAL:HG13 | 2.46 | 0.44 |
| 1:P4:135:VAL:HG12 | 1:P4:137:HIS:HD2 | 1.83 | 0.44 |
| 1:P6:317:PHE:HB3 | 1:P6:321:MET:SD | 2.58 | 0.44 |
| 1:Q0:178:THR:HG22 | 2:Q1:258:ASN:HD21 | 1.82 | 0.44 |
| 1:Q2:117:LEU:HA | 1:Q2:117:LEU:HD23 | 1.77 | 0.44 |
| 1:Q2:176:SER:HB3 | 2:Q3:349:THR:HG21 | 1.97 | 0.44 |
| 1:Q4:86:ARG:HG3 | 1:S0:281:TYR:HB3 | 1.99 | 0.44 |
| 1:Q4:149:THR:HB | 1:Q4:191:GLN:HG2 | 1.99 | 0.44 |
| 1:Q8:107:THR:OG1 | 1:Q8:401:GLU:OE2 | 2.21 | 0.44 |
| 1:Q8:154:LYS:HD3 | 1:Q8:154:LYS:HA | 1.82 | 0.44 |
| 2:Q9:405:VAL:HG21 | 17:5S:112:VAL:HG11 | 1.98 | 0.44 |
| 1:R2:327:ASP:OD1 | 1:R2:328:GLU:N | 2.51 | 0.44 |
| 2:R3:14:ILE:HD11 | 2:R3:74:VAL:HG13 | 2.00 | 0.44 |
| 2:R9:246:GLY:O | 7:4R:260:LYS:NZ | 2.44 | 0.44 |
| 1:S2:190:HIS:NE2 | 1:S2:410:GLU:OE2 | 2.50 | 0.44 |
| 1:S2:232:VAL:O | 1:S2:236:ILE:HG12 | 2.17 | 0.44 |
| 2:S7:271:SER:HB3 | 2:S7:377:MET:HB3 | 1.98 | 0.44 |
| 1:S8:128:ASP:OD1 | 1:S8:129:CYS:N | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S8:178:THR:OG1 | 1:S8:181:GLU:HG3 | 2.17 | 0.44 |
| 1:S8:290:THR:HG21 | 1:S8:329:GLN:HE21 | 1.82 | 0.44 |
| 2:S9:3:GLU:HB2 | 2:S9:129:CYS:SG | 2.58 | 0.44 |
| 2:S9:143:GLY:HA3 | 41:S9:501:GTP:PB | 2.57 | 0.44 |
| 1:T0:128:ASP:N | 1:T0:128:ASP:OD1 | 2.50 | 0.44 |
| 2:T1:198:THR:HG23 | 2:T1:266:HIS:HE1 | 1.82 | 0.44 |
| 1:T2:307:HIS:CE1 | 13:5J:8:GLU:HB3 | 2.53 | 0.44 |
| 1:T4:253:LEU:HD23 | 1:T4:253:LEU:HA | 1.78 | 0.44 |
| 2:T5:217:LEU:HB3 | 2:T5:219:ILE:HD12 | 1.99 | 0.44 |
| 2:T7:56:THR:HG23 | 2:T7:60:LYS:HB3 | 1.98 | 0.44 |
| 2:T7:121:ARG:HA | 2:T7:121:ARG:HD2 | 1.70 | 0.44 |
| 1:T8:418:LEU:O | 1:T8:421:GLU:HG2 | 2.18 | 0.44 |
| 1:U2:244:GLY:H | 1:U2:247:ASN:HD21 | 1.63 | 0.44 |
| 2:U3:222:PRO:HD2 | 1:U4:324:LYS:HE3 | 1.99 | 0.44 |
| 2:U5:267:PHE:HB2 | 2:U5:384:ILE:HD12 | 1.98 | 0.44 |
| 2:U7:203:MET:C | 2:U7:204:LEU:HD12 | 2.38 | 0.44 |
| 1:U8:21:TRP:CZ3 | 1:U8:61:PRO:HB3 | 2.53 | 0.44 |
| 2:V1:216:SER:O | 2:V1:280:LYS:NZ | 2.49 | 0.44 |
| 1:V2:6:HIS:CE1 | 1:V2:8:GLN:HG2 | 2.53 | 0.44 |
| 1:V2:183:TYR:HB3 | 1:V2:398:TYR:HE2 | 1.81 | 0.44 |
| 1:V2:270:PHE:HD2 | 1:V2:273:LEU:HD21 | 1.83 | 0.44 |
| 2:V3:68:LEU:HA | 2:V3:93:ILE:O | 2.18 | 0.44 |
| 1:V4:417:ASP:HA | 1:V4:420:SER:HB2 | 1.98 | 0.44 |
| 1:V6:51:PHE:HB3 | 1:V6:59:TYR:HB3 | 2.00 | 0.44 |
| 1:V6:198:GLU:HG3 | 1:V6:266:PHE:HE2 | 1.83 | 0.44 |
| 2:V7:135:PHE:HB2 | 2:V7:166:LYS:HG2 | 1.99 | 0.44 |
| 1:V8:27:GLU:O | 1:V8:43:GLN:NE2 | 2.50 | 0.44 |
| 1:V8:86:ARG:HB3 | 1:V8:89:ASN:OD1 | 2.17 | 0.44 |
| 1:V8:233:MET:O | 1:V8:237:THR:HG22 | 2.17 | 0.44 |
| 1:W0:387:ALA:HA | 1:W0:390:ARG:HH21 | 1.83 | 0.44 |
| 1:W4:418:LEU:O | 1:W4:421:GLU:HG2 | 2.18 | 0.44 |
| 2:W5:325:PRO:HA | 2:W5:328:VAL:HG12 | 1.99 | 0.44 |
| 1:W8:95:THR:OG1 | 1:W8:96:GLY:N | 2.51 | 0.44 |
| 2:W9:88:HIS:CG | 2:Y5:283:HIS:NE2 | 2.86 | 0.44 |
| 1:X2:260:PHE:HB2 | 1:X2:263:LEU:HB2 | 2.00 | 0.44 |
| 1:X2:396:HIS:CD2 | 2:X3:263:PRO:HD3 | 2.53 | 0.44 |
| 2:X5:269:LEU:HD13 | 2:X5:301:MET:SD | 2.57 | 0.44 |
| 1:X6:156:ARG:HD2 | 1:X6:156:ARG:HA | 1.85 | 0.44 |
| 2:X9:178:SER:HB2 | 1:Y0:347:ASN:ND2 | 2.33 | 0.44 |
| 2:X9:205:ASP:HB2 | 2:X9:303:VAL:HA | 1.98 | 0.44 |
| 2:X9:267:PHE:HB3 | 2:X9:384:ILE:HG21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y1:203:MET:HB3 | 2:Y1:203:MET:HE2 | 1.61 | 0.44 |
| 2:Y3:252:ILE:HA | 2:Y3:255:PHE:HE2 | 1.82 | 0.44 |
| 2:Y5:333:ALA:O | 2:Y5:337:THR:HG23 | 2.18 | 0.44 |
| 1:Y6:100:ASN:HB3 | 1:Y6:103:LYS:HB2 | 1.98 | 0.44 |
| 1:Y6:382:SER:HB3 | 1:Y6:415:MET:HG2 | 1.99 | 0.44 |
| 1:Y8:116:VAL:HA | 1:Y8:119:VAL:HG22 | 1.98 | 0.44 |
| 1:Y8:182:PRO:HB2 | 1:Y8:385:PHE:HD1 | 1.83 | 0.44 |
| 1:Z4:405:GLU:O | 1:Z4:409:THR:HG23 | 2.17 | 0.44 |
| 2:Z5:20:CYS:SG | 2:Z5:235:ILE:HG21 | 2.57 | 0.44 |
| 2:Z5:203:MET:HB2 | 2:Z5:303:VAL:HG21 | 1.99 | 0.44 |
| 2:Z7:278:ALA:HA | 2:Z7:369:ALA:HB2 | 2.00 | 0.44 |
| 1:Z8:211:CYS:HA | 1:Z8:215:LEU:HB2 | 1.98 | 0.44 |
| 1:0A:10:GLY:O | 1:0A:14:ASN:HB2 | 2.18 | 0.44 |
| 1:0A:14:ASN:OD1 | 1:0A:65:LEU:HD22 | 2.17 | 0.44 |
| 1:0A:345:ILE:O | 1:0A:348:ASN:ND2 | 2.50 | 0.44 |
| 2:0B:90:GLU:O | 2:0B:121:ARG:NH1 | 2.49 | 0.44 |
| 1:0E:313:ALA:HB1 | 1:0E:367:PHE:HE1 | 1.81 | 0.44 |
| 1:0I:371:SER:OG | 1:0I:372:THR:N | 2.50 | 0.44 |
| 2:0J:292:THR:HG1 | 2:0J:319:TYR:HH | 1.62 | 0.44 |
| 2:0J:329:ASN:HA | 2:0J:332:VAL:HG12 | 1.99 | 0.44 |
| 2:0J:338:LYS:HG3 | 2:0J:340:THR:HG22 | 1.99 | 0.44 |
| 1:0K:249:ASP:OD2 | 1:0K:250:LEU:N | 2.48 | 0.44 |
| 2:0L:28:HIS:ND1 | 2:0L:49:PHE:HA | 2.32 | 0.44 |
| 1:0M:378:PHE:HB3 | 1:0M:415:MET:HE3 | 2.00 | 0.44 |
| 1:0M:396:HIS:H | 1:0M:396:HIS:CD2 | 2.34 | 0.44 |
| 2:0P:257:THR:OG1 | 2:0P:258:ASN:N | 2.50 | 0.44 |
| 1:0S:180:VAL:HG22 | 1:0S:183:TYR:HB2 | 1.98 | 0.44 |
| 2:0Z:73:THR:HG23 | 2:0Z:74:VAL:N | 2.33 | 0.44 |
| 2:0Z:329:ASN:HA | 2:0Z:332:VAL:HG12 | 2.00 | 0.44 |
| 1:1A:35:THR:OG1 | 1:1A:37:HIS:NE2 | 2.48 | 0.44 |
| 2:1D:283:HIS:HD2 | 2:1D:284:GLU:HB2 | 1.82 | 0.44 |
| 1:1E:344:TRP:O | 1:1E:345:ILE:HD13 | 2.18 | 0.44 |
| 1:1E:396:HIS:H | 1:1E:396:HIS:CD2 | 2.36 | 0.44 |
| 1:1G:337:ASN:HB3 | 1:1G:340:TYR:CD2 | 2.52 | 0.44 |
| 2:1H:417:GLU:HA | 2:1H:420:GLU:HG2 | 1.99 | 0.44 |
| 2:1L:222:PRO:HD2 | 1:1M:324:LYS:HE3 | 1.99 | 0.44 |
| 2:1N:27:GLU:OE1 | 2:1N:243:ARG:NH1 | 2.51 | 0.44 |
| 2:1N:319:TYR:HB2 | 2:1N:355:ILE:HA | 1.98 | 0.44 |
| 1:1O:21:TRP:CZ2 | 1:1O:63:ALA:HB2 | 2.52 | 0.44 |
| 2:1P:174:SER:HB2 | 2:1P:177:VAL:O | 2.16 | 0.44 |
| 1:1S:26:ASP:O | 1:1S:359:LYS:NZ | 2.29 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1V:223:THR:OG1 | 2:1V:224:TYR:N | 2.51 | 0.44 |
| 2:2B:161:TYR:CE1 | 38:8A:80:TYR:CB | 3.01 | 0.44 |
| 1:2C:86:ARG:HB3 | 1:2C:89:ASN:OD1 | 2.17 | 0.44 |
| 1:2E:220:PRO:HD2 | 2:2F:326:LYS:HZ3 | 1.83 | 0.44 |
| 1:2E:233:MET:HA | 1:2E:236:ILE:HG22 | 2.00 | 0.44 |
| 2:2F:185:TYR:CE1 | 2:2F:398:MET:HE3 | 2.53 | 0.44 |
| 1:2G:95:THR:OG1 | 1:2G:96:GLY:N | 2.51 | 0.44 |
| 1:2G:163:MET:HB3 | 1:2G:250:LEU:HD22 | 1.98 | 0.44 |
| 1:2M:204:ASN:OD1 | 39:2M:501:GDP:O2' | 2.35 | 0.44 |
| 2:2R:195:LEU:HD11 | 2:2R:264:ARG:HD2 | 1.99 | 0.44 |
| 1:2U:52:ASN:ND2 | 1:2U:123:GLU:OE1 | 2.51 | 0.44 |
| 1:2U:121:ARG:NH2 | 1:2U:158:GLU:OE2 | 2.47 | 0.44 |
| 1:2U:221:THR:OG1 | 1:2U:222:PHE:N | 2.50 | 0.44 |
| 2:2X:141:VAL:HG13 | 2:2X:170:THR:CG2 | 2.47 | 0.44 |
| 1:3C:141:GLY:HA3 | 39:3C:502:GDP:O3A | 2.17 | 0.44 |
| 1:3C:185:ALA:O | 1:3C:189:VAL:HG12 | 2.18 | 0.44 |
| 1:3G:83:GLN:N | 1:3G:83:GLN:OE1 | 2.50 | 0.44 |
| 1:3G:253:LEU:HD11 | 1:3G:316:LEU:HD21 | 2.00 | 0.44 |
| 1:3I:135:VAL:HG12 | 1:3I:137:HIS:HD2 | 1.83 | 0.44 |
| 2:3J:397:LEU:HD23 | 2:3J:397:LEU:HA | 1.80 | 0.44 |
| 2:3L:296:PHE:HE2 | 2:3L:335:ILE:HD13 | 1.80 | 0.44 |
| 1:3M:52:ASN:ND2 | 1:3M:52:ASN:N | 2.59 | 0.44 |
| 1:3M:170:VAL:HG22 | 1:3M:202:LEU:O | 2.17 | 0.44 |
| 2:3T:176:GLN:HG2 | 2:3T:177:VAL:HG13 | 1.99 | 0.44 |
| 2:3T:185:TYR:CD2 | 2:3T:395:PHE:HE1 | 2.35 | 0.44 |
| 3:3X:44:ALA:HB3 | 3:3X:116:PRO:HG3 | 1.99 | 0.44 |
| 3:4F:44:ALA:HB3 | 3:4F:116:PRO:HG3 | 1.99 | 0.44 |
| 4:4I:35:LYS:NZ | 3:4J:253:ASN:OD1 | 2.29 | 0.44 |
| 5:4M:61:LEU:HD13 | 19:6E:124:GLU:HG3 | 2.00 | 0.44 |
| 5:4M:287:LYS:O | 5:4M:290:GLN:HB3 | 2.17 | 0.44 |
| 8:4W:268:GLU:O | 8:4W:272:VAL:HG22 | 2.17 | 0.44 |
| 10:5B:141:LEU:HD23 | 10:5B:141:LEU:HA | 1.84 | 0.44 |
| 14:5L:218:VAL:CG1 | 14:5L:281:LYS:HZ2 | 2.30 | 0.44 |
| 15:5P:330:LEU:C | 15:5P:330:LEU:CD2 | 2.85 | 0.44 |
| 19:6E:157:ASP:N | 19:6E:157:ASP:OD1 | 2.49 | 0.44 |
| 22:6L:220:ASP:OD2 | 24:6V:440:ASN:HB3 | 2.17 | 0.44 |
| 22:6O:240:TYR:O | 22:6O:244:VAL:HG12 | 2.18 | 0.44 |
| 24:6V:85:LEU:H | 24:6V:85:LEU:HD23 | 1.83 | 0.44 |
| 24:6V:556:ASP:O | 24:6V:560:ARG:HG3 | 2.18 | 0.44 |
| 24:6Z:103:LYS:HG2 | 24:6Z:116:ILE:HG12 | 1.99 | 0.44 |
| 24:6Z:252:LYS:HG2 | 24:6Z:253:PRO:HD2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:7G:194:PRO:HA | 27:7G:210:TYR:CE2 | 2.53 | 0.44 |
| 31:7M:23:LEU:CD2 | 31:7M:25:THR:HG23 | 2.48 | 0.44 |
| 34:7R:265:THR:HA | 34:7R:268:ASP:OD2 | 2.18 | 0.44 |
| 38:8B:18:VAL:HG12 | 38:8B:20:SER:H | 1.82 | 0.44 |
| 1:5:262:ARG:HH12 | 3:3Z:240:ARG:HH11 | 1.63 | 0.44 |
| 1:C0:320:ARG:HH12 | 18:6C:53:GLY:HA3 | 1.83 | 0.44 |
| 1:C6:142:GLY:N | 39:C6:501:GDP:O1B | 2.51 | 0.44 |
| 1:D2:212:PHE:HB3 | 24:6X:249:ARG:NH2 | 2.31 | 0.44 |
| 1:F0:357:PRO:HD2 | 22:6N:111:PRO:HB2 | 2.00 | 0.44 |
| 2:G9:384:ILE:HA | 2:G9:387:ILE:HD12 | 2.00 | 0.44 |
| 2:H1:165:SER:HB3 | 2:H1:256:GLN:HE22 | 1.81 | 0.44 |
| 2:H3:217:LEU:HB3 | 2:H3:219:ILE:HG13 | 1.98 | 0.44 |
| 2:H5:100:ALA:HA | 1:H6:252:LYS:HE2 | 2.00 | 0.44 |
| 1:H6:229:ILE:HG22 | 1:H6:233:MET:SD | 2.57 | 0.44 |
| 1:I0:5:VAL:HB | 1:I0:133:PHE:HD1 | 1.82 | 0.44 |
| 1:I0:218:THR:H | 24:6X:489:ASN:HB2 | 1.80 | 0.44 |
| 1:I2:176:SER:HB2 | 2:I3:349:THR:OG1 | 2.18 | 0.44 |
| 2:I7:155:GLU:HB2 | 2:I7:197:HIS:CE1 | 2.53 | 0.44 |
| 1:J0:211:CYS:HA | 1:J0:215:LEU:HB2 | 2.00 | 0.44 |
| 2:J1:88:HIS:HB3 | 2:K7:283:HIS:CG | 2.53 | 0.44 |
| 2:J1:266:HIS:O | 2:J1:266:HIS:ND1 | 2.49 | 0.44 |
| 1:J6:222:PHE:HD2 | 2:J7:247:ALA:HB1 | 1.81 | 0.44 |
| 2:J9:278:ALA:HB2 | 5:4M:270:LYS:HD2 | 1.99 | 0.44 |
| 2:K1:217:LEU:HB3 | 2:K1:219:ILE:HD12 | 1.99 | 0.44 |
| 1:K6:114:ASP:OD2 | 1:K6:115:SER:N | 2.51 | 0.44 |
| 1:K6:211:CYS:HB3 | 1:K6:217:LEU:HD12 | 1.99 | 0.44 |
| 2:K9:170:THR:HG21 | 2:K9:194:LEU:HD11 | 1.98 | 0.44 |
| 1:L0:273:LEU:H | 1:L0:292:GLN:NE2 | 2.15 | 0.44 |
| 1:L2:317:PHE:HB3 | 1:L2:321:MET:SD | 2.57 | 0.44 |
| 2:L5:222:PRO:O | 1:L6:322:SER:OG | 2.28 | 0.44 |
| 2:L7:4:VAL:CG1 | 2:L7:133:GLN:HB2 | 2.47 | 0.44 |
| 1:M4:31:ASP:HB2 | 1:M4:32:PRO:HD2 | 2.00 | 0.44 |
| 1:M4:105:HIS:CD2 | 1:M4:150:LEU:HD12 | 2.53 | 0.44 |
| 1:M6:80:PRO:HB2 | 15:5P:69:PHE:CE1 | 2.52 | 0.44 |
| 2:M7:119:LEU:HD21 | 2:M7:156:ARG:HB3 | 1.99 | 0.44 |
| 2:M7:145:THR:OG1 | 41:M7:501:GTP:O1B | 2.36 | 0.44 |
| 1:M8:125:GLU:OE2 | 1:M8:159:TYR:OH | 2.34 | 0.44 |
| 1:M8:325:GLU:O | 1:M8:329:GLN:HG2 | 2.18 | 0.44 |
| 1:N0:105:HIS:CD2 | 1:N0:150:LEU:HB2 | 2.53 | 0.44 |
| 1:N0:220:PRO:HD2 | 2:N1:326:LYS:HD3 | 1.99 | 0.44 |
| 1:N6:218:THR:OG1 | 1:N6:219:THR:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O0:166:THR:HG23 | 1:O0:199:CYS:HA | 2.00 | 0.44 |
| 1:O0:173:PRO:HD2 | 1:O0:380:ARG:CZ | 2.47 | 0.44 |
| 2:O3:181:VAL:HB | 1:O4:256:ASN:HD22 | 1.82 | 0.44 |
| 2:O3:346:TRP:CD1 | 2:O3:346:TRP:O | 2.71 | 0.44 |
| 2:O3:362:VAL:HG21 | 19:6E:104:TYR:CD2 | 2.53 | 0.44 |
| 1:O4:232:VAL:HG11 | 1:O4:268:VAL:HG11 | 2.00 | 0.44 |
| 2:P5:145:THR:OG1 | 41:P6:501:GTP:O1B | 2.35 | 0.44 |
| 2:P5:425:LEU:HD12 | 2:P5:425:LEU:HA | 1.84 | 0.44 |
| 1:P6:107:THR:OG1 | 1:P6:108:GLU:OE1 | 2.15 | 0.44 |
| 1:P8:3:GLU:HG3 | 1:P8:127:CYS:SG | 2.58 | 0.44 |
| 2:Q1:151:SER:O | 2:Q1:155:GLU:HG3 | 2.17 | 0.44 |
| 2:Q5:286:LEU:HD23 | 2:Q5:286:LEU:HA | 1.80 | 0.44 |
| 1:Q6:249:ASP:OD1 | 1:Q6:252:LYS:N | 2.48 | 0.44 |
| 1:R0:95:THR:HG23 | 1:R0:96:GLY:N | 2.32 | 0.44 |
| 1:R0:167:PHE:CZ | 1:R0:233:MET:HG2 | 2.52 | 0.44 |
| 1:R2:65:LEU:HD13 | 1:R2:90:PHE:HE1 | 1.83 | 0.44 |
| 1:R2:404:ASP:N | 1:R2:407:GLU:OE2 | 2.39 | 0.44 |
| 2:R3:260:VAL:HG23 | 2:R3:260:VAL:O | 2.17 | 0.44 |
| 2:R9:364:PRO:O | 12:5F:113:LYS:NZ | 2.37 | 0.44 |
| 1:S2:175:VAL:HG23 | 1:S2:175:VAL:O | 2.18 | 0.44 |
| 1:S2:253:LEU:HD21 | 1:S2:316:LEU:HD11 | 1.99 | 0.44 |
| 1:S8:49:VAL:HG11 | 1:S8:241:ARG:HG2 | 1.98 | 0.44 |
| 1:T0:114:ASP:OD1 | 1:T0:115:SER:N | 2.51 | 0.44 |
| 2:T3:327:ASP:N | 2:T3:327:ASP:OD1 | 2.44 | 0.44 |
| 2:T7:220:GLU:H | 2:T7:220:GLU:CD | 2.19 | 0.44 |
| 1:U2:285:THR:OG1 | 1:U2:287:PRO:HD2 | 2.17 | 0.44 |
| 2:U3:276:ILE:HA | 2:U3:280:LYS:HD2 | 1.99 | 0.44 |
| 2:U5:69:ASP:OD2 | 2:U5:71:GLU:N | 2.46 | 0.44 |
| 1:U6:177:ASP:OD2 | 2:U7:248:LEU:HD11 | 2.18 | 0.44 |
| 1:U8:100:ASN:HB3 | 1:U8:103:LYS:HB2 | 1.99 | 0.44 |
| 2:U9:87:PHE:CB | 2:U9:92:LEU:HD21 | 2.48 | 0.44 |
| 2:U9:88:HIS:HB2 | 2:W5:283:HIS:HB3 | 1.99 | 0.44 |
| 2:U9:279:GLU:HB2 | 2:U9:280:LYS:NZ | 2.33 | 0.44 |
| 1:V0:178:THR:HG23 | 1:V0:181:GLU:HG3 | 2.00 | 0.44 |
| 1:V0:282:ARG:HE | 1:V0:288:GLU:HG2 | 1.82 | 0.44 |
| 1:V2:162:ARG:HD3 | 1:V2:162:ARG:HA | 1.83 | 0.44 |
| 2:W7:14:ILE:HD11 | 2:W7:74:VAL:HG22 | 1.98 | 0.44 |
| 2:W7:344:VAL:HG11 | 2:W7:346:TRP:CE2 | 2.53 | 0.44 |
| 1:W8:3:GLU:HB2 | 1:W8:130:LEU:HA | 2.00 | 0.44 |
| 2:W9:3:GLU:HG2 | 2:W9:64:ARG:NH1 | 2.32 | 0.44 |
| 2:X3:21:TRP:CZ2 | 2:X3:65:CYS:HB2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X4:12:CYS:SG | 1:X4:16:ILE:HD11 | 2.57 | 0.44 |
| 1:X4:109:GLY:HA2 | 1:X4:113:ILE:HG13 | 2.00 | 0.44 |
| 1:X4:396:HIS:CE1 | 1:X4:397:TRP:CE2 | 3.05 | 0.44 |
| 1:X6:205:GLU:HG2 | 1:X6:206:ALA:N | 2.33 | 0.44 |
| 2:Y1:69:ASP:OD1 | 2:Y1:70:LEU:N | 2.50 | 0.44 |
| 2:Y1:292:THR:OG1 | 2:Y1:319:TYR:OH | 2.31 | 0.44 |
| 1:Z0:234:SER:HA | 1:Z0:237:THR:HG22 | 1.99 | 0.44 |
| 1:Z2:107:THR:OG1 | 1:Z2:108:GLU:OE1 | 2.33 | 0.44 |
| 1:Z4:24:VAL:HA | 1:Z4:27:GLU:HG2 | 2.00 | 0.44 |
| 1:Z4:68:LEU:HD21 | 1:Z4:112:LEU:HD22 | 1.99 | 0.44 |
| 1:Z6:3:GLU:O | 1:Z6:131:GLN:N | 2.43 | 0.44 |
| 1:Z6:23:VAL:HG21 | 1:Z6:230:SER:HB3 | 1.98 | 0.44 |
| 1:Z8:103:LYS:NZ | 1:Z8:108:GLU:OE2 | 2.43 | 0.44 |
| 1:Z8:205:GLU:HG2 | 1:Z8:206:ALA:N | 2.33 | 0.44 |
| 1:Z8:379:LYS:HA | 1:Z8:379:LYS:HD2 | 1.65 | 0.44 |
| 2:Z9:15:GLN:HB3 | 2:Z9:228:ASN:HD21 | 1.82 | 0.44 |
| 1:0A:101:TRP:CE3 | 1:0A:187:LEU:HD23 | 2.52 | 0.44 |
| 1:0A:317:PHE:HE2 | 1:0A:326:VAL:HG13 | 1.83 | 0.44 |
| 1:0A:418:LEU:O | 1:0A:421:GLU:HG2 | 2.18 | 0.44 |
| 2:0B:414:GLU:HG2 | 2:0B:416:GLY:H | 1.81 | 0.44 |
| 1:0C:386:THR:O | 1:0C:390:ARG:HG3 | 2.17 | 0.44 |
| 1:0E:309:ARG:H | 1:0E:372:THR:HG22 | 1.83 | 0.44 |
| 1:0G:167:PHE:HD1 | 1:0G:200:MET:HB3 | 1.83 | 0.44 |
| 1:0G:233:MET:HE3 | 1:0G:236:ILE:HG21 | 1.98 | 0.44 |
| 2:0H:102:ASN:ND2 | 2:0H:411:GLU:HG3 | 2.22 | 0.44 |
| 2:0L:127:ASP:OD1 | 2:1B:293:ASN:ND2 | 2.51 | 0.44 |
| 1:0O:67:ASP:HB3 | 1:0O:92:PHE:HE1 | 1.83 | 0.44 |
| 2:0P:88:HIS:HB3 | 2:1F:283:HIS:CE1 | 2.52 | 0.44 |
| 1:0S:87:PRO:HA | 1:0S:90:PHE:CD2 | 2.53 | 0.44 |
| 2:0X:90:GLU:HB3 | 2:0X:121:ARG:HH22 | 1.82 | 0.44 |
| 1:1A:135:VAL:HG12 | 1:1A:137:HIS:HD2 | 1.82 | 0.44 |
| 1:1A:358:PRO:HG2 | 1:1A:361:LEU:HD23 | 1.99 | 0.44 |
| 1:1E:156:ARG:HD2 | 1:1E:156:ARG:HA | 1.86 | 0.44 |
| 2:1L:75:VAL:HG11 | 2:1L:94:SER:HB3 | 1.99 | 0.44 |
| 1:1W:212:PHE:O | 1:1W:216:LYS:HD2 | 2.17 | 0.44 |
| 2:1Z:152:LEU:O | 2:1Z:156:ARG:HG2 | 2.17 | 0.44 |
| 1:2C:391:ARG:O | 2:2D:262:TYR:OH | 2.32 | 0.44 |
| 2:2D:417:GLU:HA | 2:2D:420:GLU:HG2 | 2.00 | 0.44 |
| 1:2E:193:VAL:HG12 | 1:2E:265:PHE:CZ | 2.49 | 0.44 |
| 2:2J:76:ASP:O | 2:2J:80:THR:HG22 | 2.17 | 0.44 |
| 1:2K:21:TRP:CZ3 | 1:2K:61:PRO:HB3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2L:49:PHE:HB2 | 2:2L:53:PHE:HD2 | 1.83 | 0.44 |
| 2:2L:195:LEU:HD12 | 2:2L:428:LEU:HD12 | 1.99 | 0.44 |
| 2:2N:217:LEU:HD11 | 2:2N:367:ASP:CB | 2.47 | 0.44 |
| 2:2R:90:GLU:HG3 | 2:2R:121:ARG:CZ | 2.47 | 0.44 |
| 1:2S:64:ILE:HD13 | 1:2S:120:VAL:HG12 | 2.00 | 0.44 |
| 2:2T:69:ASP:OD2 | 2:2T:70:LEU:N | 2.51 | 0.44 |
| 2:2T:110:ILE:O | 2:2T:113:GLU:HG3 | 2.18 | 0.44 |
| 1:2U:290:THR:HG21 | 1:2U:329:GLN:CG | 2.47 | 0.44 |
| 2:2V:170:THR:HG21 | 2:2V:194:LEU:HD21 | 1.99 | 0.44 |
| 2:2Z:312:TYR:HB2 | 2:2Z:343:PHE:HD1 | 1.83 | 0.44 |
| 2:2Z:429:GLU:O | 2:2Z:433:GLU:HG3 | 2.17 | 0.44 |
| 1:3A:83:GLN:NE2 | 14:5N:80:GLY:HA3 | 2.33 | 0.44 |
| 2:3B:269:LEU:HG | 2:3B:384:ILE:HD11 | 1.99 | 0.44 |
| 1:3C:245:GLN:HG2 | 38:8D:198:THR:HG21 | 1.98 | 0.44 |
| 2:3D:76:ASP:O | 2:3D:80:THR:HG23 | 2.17 | 0.44 |
| 2:3D:109:THR:O | 2:3D:112:LYS:HG2 | 2.17 | 0.44 |
| 2:3F:3:GLU:HB2 | 2:3F:129:CYS:SG | 2.57 | 0.44 |
| 1:3G:134:GLN:HE21 | 1:3G:167:PHE:HE2 | 1.65 | 0.44 |
| 1:3I:309:ARG:NH1 | 1:3I:341:PHE:O | 2.50 | 0.44 |
| 1:3I:364:SER:OG | 1:3I:365:ALA:N | 2.49 | 0.44 |
| 1:3K:3:GLU:HB2 | 1:3K:130:LEU:HA | 1.99 | 0.44 |
| 1:3K:95:THR:HG21 | 3:4B:138:GLY:CA | 2.48 | 0.44 |
| 2:3L:356:ASN:OD1 | 2:3L:357:TYR:N | 2.51 | 0.44 |
| 1:3M:391:ARG:NH2 | 2:3N:435:VAL:HG13 | 2.25 | 0.44 |
| 1:3Q:67:ASP:OD2 | 1:3Q:68:LEU:N | 2.46 | 0.44 |
| 1:3Q:215:LEU:HB3 | 1:3Q:217:LEU:HG | 1.99 | 0.44 |
| 2:3R:27:GLU:OE1 | 2:3R:243:ARG:NH1 | 2.51 | 0.44 |
| 1:3S:177:ASP:HA | 2:3T:353:CYS:SG | 2.58 | 0.44 |
| 2:3T:156:ARG:O | 2:3T:159:VAL:HG22 | 2.16 | 0.44 |
| 2:3T:195:LEU:O | 2:3T:266:HIS:NE2 | 2.45 | 0.44 |
| 3:3Z:44:ALA:HB3 | 3:3Z:116:PRO:HG3 | 1.99 | 0.44 |
| 3:4D:44:ALA:HB3 | 3:4D:116:PRO:HG3 | 1.99 | 0.44 |
| 3:4J:225:VAL:O | 3:4J:284:LYS:NZ | 2.46 | 0.44 |
| 5:4M:219:ARG:O | 5:4M:222:GLU:HG3 | 2.16 | 0.44 |
| 5:4M:319:GLU:OE2 | 5:4M:320:GLN:HG3 | 2.16 | 0.44 |
| 6:4P:130:ASP:OD1 | 6:4P:131:GLU:N | 2.51 | 0.44 |
| 7:4R:301:ARG:HG3 | 20:6F:130:LEU:HD13 | 1.99 | 0.44 |
| 7:4T:209:ARG:HH12 | 31:7M:53:ILE:CG1 | 2.29 | 0.44 |
| 8:4W:348:ALA:O | 8:4W:351:GLU:HG3 | 2.17 | 0.44 |
| 9:4Y:365:ALA:HA | 9:4Y:368:ASP:OD2 | 2.17 | 0.44 |
| 10:5A:264:ALA:O | 10:5A:267:LEU:HG | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:5C:488:GLY:HA2 | 10:5C:491:ARG:HG2 | 2.00 | 0.44 |
| 12:5G:256:PRO:HA | 12:5G:257:PRO:HD3 | 1.86 | 0.44 |
| 12:5G:290:PHE:HD2 | 12:5G:292:LEU:HD22 | 1.81 | 0.44 |
| 13:5H:70:LYS:HE2 | 13:5H:70:LYS:HB3 | 1.43 | 0.44 |
| 13:5J:70:LYS:HE2 | 13:5J:70:LYS:HB3 | 1.43 | 0.44 |
| 14:5L:218:VAL:HG12 | 14:5L:281:LYS:NZ | 2.32 | 0.44 |
| 14:5M:415:LYS:HZ3 | 23:6R:22:MET:HG3 | 1.80 | 0.44 |
| 15:5P:37:MET:HG3 | 15:5P:46:PHE:HB3 | 1.99 | 0.44 |
| 17:5U:177:ASP:O | 17:5U:181:LEU:N | 2.46 | 0.44 |
| 19:6E:17:VAL:CG1 | 19:6E:28:ARG:HG2 | 2.46 | 0.44 |
| 21:6H:125:GLU:O | 21:6H:129:VAL:HG22 | 2.17 | 0.44 |
| 22:6J:108:ARG:HH22 | 24:6U:283:THR:C | 2.21 | 0.44 |
| 22:6L:114:THR:HG23 | 22:6L:117:GLY:H | 1.82 | 0.44 |
| 23:6Q:13:THR:O | 23:6Q:17:THR:HG23 | 2.18 | 0.44 |
| 24:6T:505:LYS:N | 24:6T:510:GLU:O | 2.48 | 0.44 |
| 24:6U:119:VAL:HG11 | 24:6U:179:PHE:HD1 | 1.82 | 0.44 |
| 24:6V:268:ASN:O | 24:6V:299:GLU:HB3 | 2.18 | 0.44 |
| 24:6X:592:ASP:N | 24:6X:592:ASP:OD1 | 2.49 | 0.44 |
| 24:6Y:507:ARG:HA | 24:6Y:507:ARG:HH21 | 1.83 | 0.44 |
| 24:6Z:255:HIS:CE1 | 24:6Z:256:LEU:HG | 2.52 | 0.44 |
| 24:6Z:285:MET:O | 24:6Z:285:MET:HG3 | 2.18 | 0.44 |
| 29:7I:149:ARG:HH21 | 29:7I:172:VAL:HB | 1.82 | 0.44 |
| 29:7I:171:THR:O | 29:7I:171:THR:OG1 | 2.34 | 0.44 |
| 30:7L:371:ASP:OD2 | 30:7L:372:LEU:N | 2.51 | 0.44 |
| 34:7R:226:LEU:HG | 35:7T:181:LEU:HD22 | 1.99 | 0.44 |
| 38:8B:80:TYR:O | 38:8B:80:TYR:CD2 | 2.70 | 0.44 |
| 38:8B:219:LEU:HD23 | 38:8B:219:LEU:HA | 1.81 | 0.44 |
| 1:A7:360:GLY:O | 24:6T:109:SER:N | 2.50 | 0.44 |
| 1:D0:226:ASN:OD1 | 39:D0:501:GDP:N1 | 2.35 | 0.44 |
| 1:E8:204:ASN:ND2 | 39:E8:502:GDP:HN22 | 2.15 | 0.44 |
| 1:G2:175:VAL:O | 1:G2:175:VAL:HG23 | 2.18 | 0.44 |
| 2:G3:156:ARG:HA | 2:G3:159:VAL:HG12 | 1.99 | 0.44 |
| 1:G4:33:THR:O | 1:G4:58:ARG:NH2 | 2.51 | 0.44 |
| 2:G5:80:THR:O | 2:G5:80:THR:HG22 | 2.18 | 0.44 |
| 2:G5:367:ASP:OD1 | 2:G5:367:ASP:N | 2.50 | 0.44 |
| 1:G8:190:HIS:NE2 | 1:G8:414:ASN:OD1 | 2.50 | 0.44 |
| 2:G9:177:VAL:HG21 | 2:G9:207:GLU:OE1 | 2.17 | 0.44 |
| 2:G9:287:SER:OG | 2:G9:290:GLU:OE1 | 2.32 | 0.44 |
| 2:H1:113:GLU:OE1 | 2:H1:113:GLU:N | 2.50 | 0.44 |
| 2:H3:92:LEU:N | 2:H3:92:LEU:HD23 | 2.32 | 0.44 |
| 1:H6:48:ASN:OD1 | 1:H6:49:VAL:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H7:11:GLN:OE1 | 2:H7:15:GLN:NE2 | 2.49 | 0.44 |
| 2:I1:63:PRO:HB2 | 2:I1:65:CYS:SG | 2.57 | 0.44 |
| 2:I1:431:ASP:O | 2:I1:435:VAL:HG23 | 2.17 | 0.44 |
| 2:I3:266:HIS:O | 2:I3:266:HIS:ND1 | 2.46 | 0.44 |
| 1:I4:57:GLY:O | 28:7X:312:LEU:HD21 | 2.18 | 0.44 |
| 2:I5:9:ILE:CG1 | 2:I5:139:ASN:HB3 | 2.47 | 0.44 |
| 2:I5:217:LEU:HB3 | 2:I5:219:ILE:HD12 | 1.99 | 0.44 |
| 2:I9:352:LYS:NZ | 2:I9:353:CYS:O | 2.51 | 0.44 |
| 2:J1:65:CYS:SG | 2:J1:87:PHE:HE1 | 2.41 | 0.44 |
| 2:J1:165:SER:HB3 | 2:J1:256:GLN:NE2 | 2.31 | 0.44 |
| 1:J4:35:THR:HA | 1:J4:57:GLY:O | 2.18 | 0.44 |
| 1:J4:73:MET:HA | 1:J4:76:VAL:HG22 | 2.00 | 0.44 |
| 2:J5:91:GLN:NE2 | 2:J5:121:ARG:HH22 | 2.12 | 0.44 |
| 2:J5:205:ASP:OD1 | 2:J5:206:ASN:N | 2.51 | 0.44 |
| 1:K4:141:GLY:HA3 | 39:K4:502:GDP:O3A | 2.18 | 0.44 |
| 2:K9:255:PHE:HA | 2:K9:259:LEU:HD13 | 1.99 | 0.44 |
| 2:K9:282:TYR:N | 2:K9:282:TYR:CD2 | 2.86 | 0.44 |
| 1:L2:272:PRO:HB2 | 1:L2:282:ARG:NH1 | 2.33 | 0.44 |
| 1:L2:334:GLN:HE22 | 1:L2:347:ASN:H | 1.66 | 0.44 |
| 2:L3:330:ALA:O | 2:L3:334:THR:HG23 | 2.17 | 0.44 |
| 1:L4:56:GLY:H | 29:7J:329:SER:HB2 | 1.81 | 0.44 |
| 1:L6:11:GLN:HE22 | 2:L7:248:LEU:HA | 1.80 | 0.44 |
| 1:L6:70:PRO:N | 1:L6:92:PHE:HZ | 2.15 | 0.44 |
| 2:L9:81:GLY:O | 2:L9:84:ARG:NH1 | 2.50 | 0.44 |
| 2:L9:387:ILE:HG12 | 2:L9:390:ARG:HH22 | 1.83 | 0.44 |
| 1:M0:2:ARG:HB3 | 1:M0:131:GLN:HB2 | 1.98 | 0.44 |
| 2:M3:167:LEU:HD13 | 2:M3:200:VAL:HB | 1.99 | 0.44 |
| 1:M4:167:PHE:CE2 | 1:M4:233:MET:HG2 | 2.52 | 0.44 |
| 1:M4:174:LYS:HE2 | 1:M4:174:LYS:HA | 2.00 | 0.44 |
| 2:M5:9:ILE:HD11 | 2:M5:153:LEU:HD23 | 1.99 | 0.44 |
| 2:M9:194:LEU:O | 2:M9:198:THR:OG1 | 2.29 | 0.44 |
| 2:N3:104:ALA:HB1 | 2:N3:411:GLU:CD | 2.38 | 0.44 |
| 2:N3:242:LEU:HD11 | 2:N3:252:ILE:HG12 | 1.99 | 0.44 |
| 2:N3:386:GLU:HB2 | 2:N3:390:ARG:NH2 | 2.17 | 0.44 |
| 2:N3:390:ARG:O | 2:N3:394:LYS:HE2 | 2.18 | 0.44 |
| 1:N6:203:ASP:N | 1:N6:203:ASP:OD1 | 2.51 | 0.44 |
| 1:N8:177:ASP:OD2 | 39:N8:502:GDP:H3' | 2.17 | 0.44 |
| 1:O0:217:LEU:HD13 | 27:7G:51:ARG:NH1 | 2.33 | 0.44 |
| 2:O1:110:ILE:O | 2:O1:114:ILE:HG12 | 2.17 | 0.44 |
| 1:O2:99:ASN:ND2 | 2:O3:254:GLU:OE1 | 2.50 | 0.44 |
| 2:O3:47:ASP:N | 2:O3:47:ASP:OD1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O5:76:ASP:OD1 | 1:O6:46:ARG:NH2 | 2.50 | 0.44 |
| 1:O6:410:GLU:OE1 | 1:V2:340:TYR:OH | 2.36 | 0.44 |
| 2:O7:9:ILE:HG22 | 2:O7:146:GLY:HA2 | 1.98 | 0.44 |
| 2:P3:12:ALA:HB2 | 41:P4:501:GTP:C8 | 2.53 | 0.44 |
| 1:P4:212:PHE:HA | 27:7G:171:LYS:NZ | 2.33 | 0.44 |
| 1:P4:371:SER:OG | 1:P4:372:THR:N | 2.51 | 0.44 |
| 2:P5:139:ASN:OD1 | 2:P5:170:THR:HG22 | 2.18 | 0.44 |
| 2:P5:249:ASN:OD1 | 27:7G:183:GLY:HA3 | 2.17 | 0.44 |
| 2:P7:213:CYS:HA | 2:P7:217:LEU:HB2 | 2.00 | 0.44 |
| 2:P9:40:LYS:HB3 | 19:6E:158:LEU:O | 2.17 | 0.44 |
| 2:P9:217:LEU:HD13 | 2:P9:367:ASP:OD2 | 2.18 | 0.44 |
| 1:Q0:345:ILE:O | 1:Q0:348:ASN:ND2 | 2.50 | 0.44 |
| 1:Q2:272:PRO:HD3 | 1:Q2:364:SER:HA | 1.99 | 0.44 |
| 2:Q3:212:ILE:O | 2:Q3:216:SER:OG | 2.32 | 0.44 |
| 2:Q3:313:MET:HE2 | 2:Q3:346:TRP:CZ2 | 2.53 | 0.44 |
| 1:Q4:237:THR:O | 1:Q4:237:THR:HG22 | 2.17 | 0.44 |
| 2:Q5:399:TYR:O | 2:Q5:402:ARG:NH1 | 2.50 | 0.44 |
| 1:Q6:404:ASP:HB2 | 1:Q6:406:MET:SD | 2.58 | 0.44 |
| 1:Q8:418:LEU:O | 1:Q8:422:TYR:HD2 | 2.01 | 0.44 |
| 1:R0:371:SER:OG | 1:R0:372:THR:N | 2.50 | 0.44 |
| 2:R1:4:VAL:HG23 | 2:R1:134:GLY:O | 2.18 | 0.44 |
| 2:R5:9:ILE:HD13 | 2:R5:150:GLY:HA2 | 1.99 | 0.44 |
| 2:R7:258:ASN:O | 2:R7:259:LEU:HD12 | 2.17 | 0.44 |
| 1:S0:113:ILE:HA | 1:S0:116:VAL:HG22 | 1.98 | 0.44 |
| 1:S4:116:VAL:O | 1:S4:120:VAL:HG23 | 2.18 | 0.44 |
| 1:S4:245:GLN:HE21 | 1:S4:246:LEU:HD21 | 1.81 | 0.44 |
| 1:S4:314:SER:HA | 1:S4:350:LYS:O | 2.18 | 0.44 |
| 1:S4:325:GLU:HA | 1:S4:328:GLU:HG3 | 2.00 | 0.44 |
| 2:T1:8:HIS:CD2 | 2:T1:17:GLY:HA3 | 2.53 | 0.44 |
| 2:T1:306:ASP:HB3 | 2:T1:309:HIS:HD2 | 1.82 | 0.44 |
| 1:T2:385:PHE:HZ | 1:T2:408:PHE:HB3 | 1.82 | 0.44 |
| 2:T3:102:ASN:HB3 | 2:T3:105:ARG:HB3 | 1.99 | 0.44 |
| 2:T3:335:ILE:CG2 | 2:T3:341:ILE:HD11 | 2.47 | 0.44 |
| 2:T5:121:ARG:HA | 2:T5:121:ARG:HD2 | 1.85 | 0.44 |
| 2:T5:334:THR:HG21 | 13:5J:135:ASN:ND2 | 2.32 | 0.44 |
| 2:T7:434:GLU:OE1 | 13:5K:67:LYS:NZ | 2.50 | 0.44 |
| 1:U2:325:GLU:O | 1:U2:329:GLN:HB2 | 2.18 | 0.44 |
| 1:U4:166:THR:OG1 | 1:U4:199:CYS:SG | 2.73 | 0.44 |
| 2:U5:4:VAL:HG23 | 2:U5:134:GLY:O | 2.17 | 0.44 |
| 2:U5:312:TYR:HB2 | 2:U5:343:PHE:HD1 | 1.82 | 0.44 |
| 1:U8:207:LEU:HB3 | 1:U8:225:LEU:HD22 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U8:309:ARG:O | 1:U8:372:THR:HG22 | 2.18 | 0.44 |
| 1:U8:415:MET:O | 1:U8:419:VAL:HG13 | 2.18 | 0.44 |
| 1:V2:417:ASP:OD1 | 1:V2:418:LEU:N | 2.51 | 0.44 |
| 2:V3:300:SER:O | 2:V3:300:SER:OG | 2.32 | 0.44 |
| 1:V4:276:ARG:HH11 | 1:V4:279:GLN:HB3 | 1.83 | 0.44 |
| 1:V6:404:ASP:HB3 | 1:V6:406:MET:SD | 2.58 | 0.44 |
| 1:W0:3:GLU:HB2 | 1:W0:130:LEU:HA | 2.00 | 0.44 |
| 1:W4:190:HIS:HD2 | 1:W4:414:ASN:HB2 | 1.83 | 0.44 |
| 1:W6:36:TYR:CZ | 1:W6:44:LEU:HD21 | 2.53 | 0.44 |
| 1:W6:392:LYS:HD2 | 1:W6:395:LEU:HD22 | 2.00 | 0.44 |
| 2:W7:119:LEU:HA | 2:W7:122:ILE:HG22 | 1.98 | 0.44 |
| 1:X0:40:SER:CB | 8:4X:99:PRO:HG3 | 2.48 | 0.44 |
| 2:X3:119:LEU:HA | 2:X3:122:ILE:HG22 | 1.99 | 0.44 |
| 2:X3:236:SER:OG | 2:X3:243:ARG:NH2 | 2.51 | 0.44 |
| 2:X5:62:VAL:HG21 | 2:X5:91:GLN:HE22 | 1.81 | 0.44 |
| 2:X5:111:GLY:HA2 | 2:X5:114:ILE:HG22 | 1.99 | 0.44 |
| 1:X6:232:VAL:HG11 | 1:X6:268:VAL:HG11 | 2.00 | 0.44 |
| 2:Y1:34:GLY:HA3 | 2:Y1:60:LYS:NZ | 2.32 | 0.44 |
| 1:Y4:2:ARG:NE | 1:Y4:240:LEU:HD22 | 2.32 | 0.44 |
| 1:Y4:418:LEU:O | 1:Y4:421:GLU:HG2 | 2.17 | 0.44 |
| 2:Y9:7:ILE:HD12 | 2:Y9:66:ILE:HG12 | 1.98 | 0.44 |
| 1:Z2:177:ASP:OD2 | 1:Z2:178:THR:HG23 | 2.17 | 0.44 |
| 2:Z3:101:ASN:C | 2:Z3:186:ASN:HD21 | 2.21 | 0.44 |
| 2:Z5:23:LEU:HD22 | 2:Z5:236:SER:OG | 2.17 | 0.44 |
| 2:Z5:30:ILE:HG12 | 2:Z5:36:MET:HG3 | 2.00 | 0.44 |
| 2:Z5:111:GLY:HA2 | 2:Z5:114:ILE:HG22 | 2.00 | 0.44 |
| 2:0B:70:LEU:HB3 | 2:0B:97:GLU:O | 2.18 | 0.44 |
| 2:0F:73:THR:HG23 | 1:0G:2:ARG:HH12 | 1.83 | 0.44 |
| 1:0G:207:LEU:HB3 | 1:0G:225:LEU:HD22 | 1.99 | 0.44 |
| 2:0H:83:TYR:HD1 | 2:0H:86:LEU:HD13 | 1.82 | 0.44 |
| 1:0K:21:TRP:CZ3 | 1:0K:61:PRO:HB3 | 2.53 | 0.44 |
| 1:0K:286:VAL:CG2 | 1:0K:287:PRO:HD3 | 2.48 | 0.44 |
| 1:0M:3:GLU:HB2 | 1:0M:130:LEU:HA | 1.99 | 0.44 |
| 1:0M:372:THR:O | 1:0M:375:GLN:HG3 | 2.18 | 0.44 |
| 2:0P:407:TRP:CE2 | 1:0Q:255:VAL:HA | 2.53 | 0.44 |
| 2:0R:149:LEU:HA | 2:0R:152:LEU:HD12 | 2.00 | 0.44 |
| 2:0V:156:ARG:HA | 2:0V:159:VAL:HG12 | 2.00 | 0.44 |
| 1:0W:112:LEU:O | 1:0W:116:VAL:HG23 | 2.18 | 0.44 |
| 1:0W:180:VAL:HG23 | 1:0W:184:ASN:ND2 | 2.32 | 0.44 |
| 1:0Y:116:VAL:O | 1:0Y:120:VAL:HG22 | 2.18 | 0.44 |
| 1:1G:345:ILE:HB | 1:1G:348:ASN:HD21 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1H:420:GLU:O | 2:1H:424:ASP:HB2 | 2.17 | 0.44 |
| 2:1L:156:ARG:HA | 2:1L:159:VAL:HG22 | 2.00 | 0.44 |
| 2:1N:205:ASP:OD2 | 2:1N:206:ASN:N | 2.49 | 0.44 |
| 2:1N:227:LEU:O | 2:1N:231:ILE:HG12 | 2.17 | 0.44 |
| 1:1O:257:LEU:HD21 | 1:1O:314:SER:HB3 | 2.00 | 0.44 |
| 1:1Q:393:ALA:O | 1:1Q:394:PHE:HB2 | 2.17 | 0.44 |
| 2:1R:69:ASP:OD1 | 2:1R:70:LEU:N | 2.47 | 0.44 |
| 2:1R:198:THR:HG21 | 2:1R:201:ALA:HB2 | 2.00 | 0.44 |
| 2:1T:205:ASP:OD2 | 2:1T:303:VAL:HG13 | 2.17 | 0.44 |
| 1:1U:220:PRO:HD2 | 2:1V:326:LYS:HD3 | 1.99 | 0.44 |
| 1:1W:153:SER:OG | 1:1W:191:GLN:NE2 | 2.47 | 0.44 |
| 1:1W:161:ASP:N | 1:1W:161:ASP:OD1 | 2.42 | 0.44 |
| 2:2B:12:ALA:HB2 | 41:2C:501:GTP:C8 | 2.53 | 0.44 |
| 2:2D:384:ILE:HG13 | 2:2D:385:GLY:N | 2.33 | 0.44 |
| 1:2E:220:PRO:HD2 | 2:2F:326:LYS:NZ | 2.33 | 0.44 |
| 1:2G:301:CYS:SG | 1:2G:302:ALA:N | 2.91 | 0.44 |
| 2:2L:96:LYS:HE3 | 38:8C:6:LEU:HD23 | 2.00 | 0.44 |
| 1:2M:421:GLU:HA | 1:2M:424:GLN:HB3 | 2.00 | 0.44 |
| 2:2P:122:ILE:HG13 | 2:2P:123:ARG:N | 2.33 | 0.44 |
| 1:2Q:139:LEU:HD12 | 1:2Q:170:VAL:HG12 | 1.98 | 0.44 |
| 1:2Q:278:SER:O | 1:2Q:278:SER:OG | 2.36 | 0.44 |
| 1:2Q:332:ASN:ND2 | 38:7Z:1:MET:HA | 2.31 | 0.44 |
| 2:2R:304:LYS:HA | 2:2R:304:LYS:HD2 | 1.74 | 0.44 |
| 1:2S:117:LEU:HD11 | 1:2S:154:LYS:HB3 | 2.00 | 0.44 |
| 1:2S:295:ASP:OD2 | 1:2S:297:LYS:HB2 | 2.17 | 0.44 |
| 2:2T:387:ILE:HG12 | 2:2T:390:ARG:HH22 | 1.83 | 0.44 |
| 2:2V:7:ILE:HG12 | 2:2V:137:VAL:HG12 | 1.99 | 0.44 |
| 1:2W:133:PHE:HZ | 1:2W:159:TYR:HD2 | 1.66 | 0.44 |
| 2:2X:157:LEU:HD23 | 2:2X:157:LEU:HA | 1.82 | 0.44 |
| 2:2Z:137:VAL:HG11 | 2:2Z:154:LEU:HD21 | 2.00 | 0.44 |
| 2:2Z:214:ARG:HG3 | 38:8C:66:TYR:CE1 | 2.53 | 0.44 |
| 2:2Z:286:LEU:HD12 | 2:2Z:286:LEU:HA | 1.76 | 0.44 |
| 2:2Z:426:ALA:O | 2:2Z:430:LYS:HG2 | 2.18 | 0.44 |
| 1:3C:359:LYS:HD3 | 1:3C:360:GLY:N | 2.33 | 0.44 |
| 1:3G:198:GLU:HA | 1:3G:264:HIS:HB2 | 1.98 | 0.44 |
| 2:3H:182:VAL:HG12 | 2:3H:182:VAL:O | 2.17 | 0.44 |
| 2:3L:339:ARG:HA | 2:3L:339:ARG:NE | 2.27 | 0.44 |
| 2:3P:84:ARG:HE | 23:6S:15:ARG:NH2 | 2.07 | 0.44 |
| 2:3R:66:ILE:HG12 | 2:3R:122:ILE:HD11 | 2.00 | 0.44 |
| 1:3S:4:ILE:CG2 | 1:3S:50:TYR:HE1 | 2.30 | 0.44 |
| 4:4I:50:MET:HE3 | 4:4I:50:MET:HB2 | 1.94 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:4N:487:ILE:HD13 | 6:4N:487:ILE:HA | 1.84 | 0.44 |
| 6:4O:323:ARG:O | 6:4O:326:GLU:HG3 | 2.17 | 0.44 |
| 7:4R:33:THR:O | 7:4R:37:GLN:HG3 | 2.17 | 0.44 |
| 7:4T:276:ASP:OD2 | 7:4T:277:ALA:N | 2.50 | 0.44 |
| 8:4W:133:TYR:CD2 | 8:4W:134:LEU:HD23 | 2.52 | 0.44 |
| 9:4Y:364:LYS:HA | 9:4Y:367:GLU:HG2 | 1.98 | 0.44 |
| 10:5B:133:ARG:O | 10:5B:137:THR:HG23 | 2.18 | 0.44 |
| 12:5F:298:ASP:CB | 12:7B:13:PRO:CG | 2.95 | 0.44 |
| 12:5F:347:PRO:HG2 | 12:5F:350:VAL:HG21 | 2.00 | 0.44 |
| 17:5S:114:LEU:N | 17:5S:114:LEU:HD22 | 2.32 | 0.44 |
| 22:6I:275:LEU:O | 22:6I:279:LEU:HG | 2.17 | 0.44 |
| 22:6J:138:ASP:N | 22:6J:138:ASP:OD1 | 2.48 | 0.44 |
| 22:6J:209:ASN:O | 22:6J:213:THR:HG23 | 2.18 | 0.44 |
| 22:6O:177:LEU:HD12 | 22:6O:183:ASN:HB2 | 1.98 | 0.44 |
| 23:6S:13:THR:O | 23:6S:17:THR:HG23 | 2.18 | 0.44 |
| 24:6T:435:LEU:HA | 24:6T:438:LEU:HB2 | 1.99 | 0.44 |
| 24:6V:452:MET:HE1 | 24:6V:528:ARG:HH11 | 1.82 | 0.44 |
| 24:6Z:84:LYS:HE3 | 24:6Z:84:LYS:HB3 | 1.83 | 0.44 |
| 24:6Z:469:PHE:CD2 | 24:6Z:482:ILE:HG23 | 2.53 | 0.44 |
| 29:7I:128:ARG:NH1 | 29:7I:143:ARG:HD2 | 2.33 | 0.44 |
| 29:7J:269:GLY:H | 30:7L:368:ARG:HH12 | 1.65 | 0.44 |
| 29:7J:469:LEU:HB3 | 29:7J:473:GLY:HA2 | 1.98 | 0.44 |
| 34:7R:269:TRP:HB3 | 35:7T:223:PHE:HE2 | 1.80 | 0.44 |
| 35:7T:137:ASN:O | 35:7T:141:LYS:HG2 | 2.18 | 0.44 |
| 37:7Y:128:TYR:CD2 | 37:7Y:128:TYR:O | 2.71 | 0.44 |
| 38:8B:170:PHE:O | 38:8B:170:PHE:CG | 2.68 | 0.44 |
| 1:9:306:ARG:NH1 | 3:4D:60:PRO:O | 2.50 | 0.44 |
| 2:A2:218:ASP:OD1 | 26:7F:81:LYS:HD3 | 2.17 | 0.44 |
| 2:B9:145:THR:OG1 | 41:C0:501:GTP:O1B | 2.36 | 0.44 |
| 2:C5:220:GLU:HB3 | 18:5X:160:ASP:OD1 | 2.17 | 0.44 |
| 1:E0:204:ASN:ND2 | 39:E0:501:GDP:HN22 | 2.15 | 0.44 |
| 2:E3:360:PRO:O | 22:6J:92:GLN:NE2 | 2.50 | 0.44 |
| 2:E5:12:ALA:HB2 | 41:E6:501:GTP:C8 | 2.53 | 0.44 |
| 1:G2:7:ILE:O | 1:G2:135:VAL:HA | 2.18 | 0.44 |
| 1:G2:222:PHE:CD1 | 1:G2:225:LEU:HD12 | 2.52 | 0.44 |
| 1:G2:289:LEU:HD23 | 1:G2:365:ALA:HB2 | 2.00 | 0.44 |
| 1:G4:8:GLN:O | 1:G4:66:MET:HG2 | 2.17 | 0.44 |
| 1:G4:272:PRO:O | 1:G4:273:LEU:HD23 | 2.18 | 0.44 |
| 1:G4:309:ARG:H | 1:G4:372:THR:HG22 | 1.82 | 0.44 |
| 1:G4:317:PHE:HB3 | 1:G4:321:MET:SD | 2.58 | 0.44 |
| 2:G5:4:VAL:HG23 | 2:G5:134:GLY:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G6:23:VAL:HG11 | 1:G6:230:SER:HB3 | 1.99 | 0.44 |
| 2:G9:110:ILE:O | 2:G9:114:ILE:HG12 | 2.18 | 0.44 |
| 2:H1:90:GLU:OE1 | 2:I7:283:HIS:ND1 | 2.50 | 0.44 |
| 2:H1:403:ALA:HB2 | 1:H2:344:TRP:HZ3 | 1.82 | 0.44 |
| 2:H3:317:LEU:HB3 | 2:H3:319:TYR:CE1 | 2.46 | 0.44 |
| 1:H4:350:LYS:NZ | 1:H4:352:SER:OG | 2.50 | 0.44 |
| 1:I0:309:ARG:H | 1:I0:372:THR:CG2 | 2.29 | 0.44 |
| 2:I1:139:ASN:N | 2:I1:139:ASN:OD1 | 2.50 | 0.44 |
| 1:I2:3:GLU:HB2 | 1:I2:130:LEU:HD13 | 1.99 | 0.44 |
| 1:I2:192:LEU:HD13 | 1:I2:199:CYS:SG | 2.57 | 0.44 |
| 2:I3:56:THR:O | 2:I3:60:LYS:HB3 | 2.18 | 0.44 |
| 1:I4:262:ARG:NH2 | 1:I4:417:ASP:OD1 | 2.51 | 0.44 |
| 1:I4:270:PHE:HD2 | 1:I4:273:LEU:HG | 1.82 | 0.44 |
| 2:I5:110:ILE:O | 2:I5:113:GLU:HG3 | 2.18 | 0.44 |
| 2:I5:399:TYR:HE2 | 2:I5:415:GLU:OE1 | 2.00 | 0.44 |
| 1:I8:91:VAL:CG2 | 1:I8:119:VAL:HG21 | 2.47 | 0.44 |
| 1:I8:91:VAL:HG21 | 1:I8:119:VAL:HG21 | 1.99 | 0.44 |
| 2:I9:121:ARG:HD2 | 2:I9:121:ARG:C | 2.38 | 0.44 |
| 1:J0:271:THR:OG1 | 1:J0:365:ALA:HB3 | 2.18 | 0.44 |
| 2:J1:306:ASP:HB3 | 2:J1:309:HIS:HD2 | 1.82 | 0.44 |
| 1:J2:130:LEU:HB2 | 1:J2:162:ARG:HE | 1.83 | 0.44 |
| 1:J2:176:SER:O | 1:J2:176:SER:OG | 2.31 | 0.44 |
| 2:J3:9:ILE:HD13 | 2:J3:150:GLY:HA2 | 1.99 | 0.44 |
| 2:J3:76:ASP:O | 2:J3:80:THR:HG23 | 2.17 | 0.44 |
| 1:J4:237:THR:CG2 | 1:J4:240:LEU:HD12 | 2.48 | 0.44 |
| 2:J5:245:ASP:OD1 | 5:4L:475:HIS:O | 2.35 | 0.44 |
| 2:J9:223:THR:OG1 | 2:J9:224:TYR:N | 2.50 | 0.44 |
| 1:K0:203:ASP:N | 1:K0:203:ASP:OD1 | 2.50 | 0.44 |
| 2:K1:107:HIS:CD2 | 2:K1:152:LEU:HD13 | 2.52 | 0.44 |
| 2:K3:90:GLU:H | 2:K3:90:GLU:CD | 2.21 | 0.44 |
| 2:K3:156:ARG:HA | 2:K3:159:VAL:HG12 | 1.99 | 0.44 |
| 2:K5:207:GLU:OE1 | 2:K5:304:LYS:HD2 | 2.17 | 0.44 |
| 2:K5:279:GLU:HG3 | 2:K5:280:LYS:N | 2.33 | 0.44 |
| 2:K7:205:ASP:OD2 | 2:K7:206:ASN:N | 2.49 | 0.44 |
| 1:K8:95:THR:HG23 | 1:K8:96:GLY:N | 2.33 | 0.44 |
| 1:K8:125:GLU:OE2 | 1:M4:336:LYS:NZ | 2.46 | 0.44 |
| 1:L0:173:PRO:HD2 | 1:L0:380:ARG:CZ | 2.48 | 0.44 |
| 2:L1:75:VAL:HG11 | 2:L1:94:SER:HB3 | 2.00 | 0.44 |
| 2:L3:89:PRO:HB3 | 29:7J:320:PRO:CD | 2.43 | 0.44 |
| 1:L4:3:GLU:HB2 | 1:L4:130:LEU:HA | 1.99 | 0.44 |
| 2:L5:90:GLU:N | 2:L5:90:GLU:OE2 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L5:114:ILE:HG21 | 2:L5:149:LEU:HD22 | 1.99 | 0.44 |
| 2:L5:261:PRO:HB2 | 2:L5:262:TYR:CD2 | 2.52 | 0.44 |
| 2:L7:291:ILE:HA | 2:L7:294:ALA:HB3 | 2.00 | 0.44 |
| 1:M0:5:VAL:HB | 1:M0:133:PHE:CD1 | 2.52 | 0.44 |
| 1:M0:49:VAL:HG11 | 1:M0:241:ARG:HG2 | 1.99 | 0.44 |
| 1:M0:186:THR:HG22 | 1:M0:411:ALA:HB1 | 2.00 | 0.44 |
| 1:M2:139:LEU:HD12 | 1:M2:170:VAL:HG22 | 1.98 | 0.44 |
| 2:M3:90:GLU:HG3 | 2:M3:121:ARG:CZ | 2.47 | 0.44 |
| 2:M3:205:ASP:OD1 | 2:M3:207:GLU:HG2 | 2.18 | 0.44 |
| 1:M4:244:GLY:H | 1:M4:247:ASN:HD21 | 1.64 | 0.44 |
| 1:M6:31:ASP:HB2 | 1:M6:32:PRO:HD2 | 2.00 | 0.44 |
| 1:M6:278:SER:O | 1:M6:278:SER:OG | 2.29 | 0.44 |
| 2:N1:90:GLU:CB | 1:O8:281:TYR:CE2 | 2.90 | 0.44 |
| 2:N1:288:VAL:HG13 | 2:N1:319:TYR:HE2 | 1.83 | 0.44 |
| 1:N2:52:ASN:O | 1:N2:60:VAL:HG12 | 2.18 | 0.44 |
| 2:N5:70:LEU:HB3 | 2:N5:97:GLU:O | 2.18 | 0.44 |
| 1:N6:191:GLN:HE21 | 1:N6:195:ASN:HD21 | 1.64 | 0.44 |
| 2:N9:21:TRP:CZ2 | 2:N9:65:CYS:HB2 | 2.53 | 0.44 |
| 2:O1:89:PRO:HB2 | 2:O1:90:GLU:OE1 | 2.18 | 0.44 |
| 2:O1:121:ARG:HA | 2:O1:121:ARG:HD2 | 1.78 | 0.44 |
| 2:O1:225:THR:HG21 | 37:7Y:241:THR:CB | 2.48 | 0.44 |
| 1:O4:183:TYR:O | 1:O4:187:LEU:HD13 | 2.17 | 0.44 |
| 1:O4:244:GLY:HA2 | 1:O4:355:ASP:OD1 | 2.18 | 0.44 |
| 2:O5:394:LYS:HB2 | 1:O6:346:PRO:HG3 | 2.00 | 0.44 |
| 2:P5:111:GLY:HA2 | 2:P5:114:ILE:HG22 | 1.99 | 0.44 |
| 2:Q1:66:ILE:HD12 | 2:Q1:68:LEU:HD23 | 1.99 | 0.44 |
| 2:Q1:320:ARG:O | 2:Q1:373:ARG:HA | 2.17 | 0.44 |
| 1:Q2:111:GLU:N | 1:Q2:111:GLU:OE1 | 2.49 | 0.44 |
| 2:Q3:65:CYS:SG | 2:Q3:66:ILE:N | 2.91 | 0.44 |
| 1:Q4:379:LYS:HG3 | 1:Q4:419:VAL:HG11 | 1.98 | 0.44 |
| 1:Q8:137:HIS:O | 1:Q8:168:SER:HA | 2.17 | 0.44 |
| 1:R0:237:THR:O | 1:R0:237:THR:HG22 | 2.18 | 0.44 |
| 2:R1:91:GLN:O | 2:R1:93:ILE:HG12 | 2.17 | 0.44 |
| 2:R1:387:ILE:HG12 | 2:R1:390:ARG:HH22 | 1.82 | 0.44 |
| 1:R2:7:ILE:HD13 | 1:R2:151:LEU:HD21 | 2.00 | 0.44 |
| 1:R4:77:ARG:HH22 | 1:R4:87:PRO:HG3 | 1.81 | 0.44 |
| 2:R5:377:MET:HG2 | 2:R5:378:ILE:N | 2.33 | 0.44 |
| 1:R6:114:ASP:OD1 | 1:R6:115:SER:N | 2.51 | 0.44 |
| 1:R6:257:LEU:O | 1:R6:259:PRO:HD3 | 2.18 | 0.44 |
| 2:R7:100:ALA:HA | 1:R8:252:LYS:HE2 | 1.99 | 0.44 |
| 2:R9:279:GLU:N | 2:R9:279:GLU:OE1 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R9:288:VAL:HG13 | 2:R9:319:TYR:HE2 | 1.81 | 0.44 |
| 1:S0:58:ARG:HB2 | 1:T6:280:GLN:HE22 | 1.83 | 0.44 |
| 2:S7:14:ILE:HD11 | 2:S7:74:VAL:CG1 | 2.48 | 0.44 |
| 2:S7:105:ARG:HA | 2:S7:411:GLU:HG2 | 1.99 | 0.44 |
| 1:S8:170:VAL:HG22 | 1:S8:202:LEU:O | 2.18 | 0.44 |
| 1:T0:189:VAL:O | 1:T0:193:VAL:HG13 | 2.17 | 0.44 |
| 2:T1:76:ASP:OD2 | 1:T2:46:ARG:NH2 | 2.51 | 0.44 |
| 1:T6:287:PRO:HA | 1:T6:290:THR:HG22 | 1.99 | 0.44 |
| 2:U1:88:HIS:ND1 | 2:V7:283:HIS:HA | 2.32 | 0.44 |
| 2:U1:201:ALA:O | 2:U1:268:MET:HE1 | 2.17 | 0.44 |
| 2:U5:174:SER:HB3 | 2:U5:207:GLU:HB2 | 1.99 | 0.44 |
| 2:U7:90:GLU:HB3 | 2:U7:121:ARG:HH22 | 1.83 | 0.44 |
| 1:U8:31:ASP:OD1 | 1:U8:35:THR:N | 2.49 | 0.44 |
| 1:U8:246:LEU:HD22 | 1:U8:352:SER:HA | 1.99 | 0.44 |
| 2:U9:72:PRO:HD2 | 1:V0:2:ARG:NH1 | 2.32 | 0.44 |
| 2:U9:93:ILE:HD12 | 2:U9:117:LEU:HD21 | 2.00 | 0.44 |
| 1:V0:371:SER:OG | 1:V0:372:THR:N | 2.50 | 0.44 |
| 1:V2:78:SER:HB2 | 6:4P:23:ARG:HE | 1.83 | 0.44 |
| 1:V2:175:VAL:HG13 | 2:V3:329:ASN:ND2 | 2.32 | 0.44 |
| 1:V6:414:ASN:HA | 1:V6:417:ASP:OD2 | 2.18 | 0.44 |
| 2:V7:363:VAL:HG23 | 2:V7:366:GLY:HA3 | 1.99 | 0.44 |
| 1:V8:322:SER:OG | 1:V8:325:GLU:HB3 | 2.18 | 0.44 |
| 1:W0:91:VAL:HG21 | 1:W0:119:VAL:HG21 | 2.00 | 0.44 |
| 1:W4:285:THR:HB | 1:W4:287:PRO:HD2 | 1.98 | 0.44 |
| 1:W4:304:ASP:HB3 | 1:W4:307:HIS:ND1 | 2.32 | 0.44 |
| 2:W5:327:ASP:OD1 | 2:W5:328:VAL:N | 2.50 | 0.44 |
| 1:W8:33:THR:HG23 | 1:W8:35:THR:HG23 | 1.99 | 0.44 |
| 2:W9:157:LEU:HD23 | 2:W9:157:LEU:HA | 1.84 | 0.44 |
| 1:X2:58:ARG:NH1 | 1:X2:84:ILE:HA | 2.33 | 0.44 |
| 1:X2:192:LEU:HD22 | 1:X2:196:ALA:HB2 | 2.00 | 0.44 |
| 1:X4:114:ASP:N | 1:X4:114:ASP:OD1 | 2.49 | 0.44 |
| 2:X5:65:CYS:SG | 2:X5:66:ILE:N | 2.91 | 0.44 |
| 1:X6:184:ASN:OD1 | 1:X6:398:TYR:OH | 2.28 | 0.44 |
| 1:Y0:268:VAL:HG12 | 1:Y0:269:GLY:N | 2.33 | 0.44 |
| 1:Y0:418:LEU:O | 1:Y0:421:GLU:HG2 | 2.17 | 0.44 |
| 1:Y2:232:VAL:HG22 | 1:Y2:270:PHE:HB2 | 2.00 | 0.44 |
| 2:Y3:301:MET:HE1 | 2:Y3:307:PRO:HD3 | 1.99 | 0.44 |
| 1:Y6:275:SER:OG | 1:Y6:278:SER:OG | 2.19 | 0.44 |
| 2:Y9:129:CYS:SG | 2:Y9:130:THR:N | 2.91 | 0.44 |
| 2:Z1:286:LEU:H | 2:Z1:286:LEU:HD23 | 1.81 | 0.44 |
| 2:Z3:73:THR:OG1 | 2:Z3:74:VAL:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z4:132:GLY:HA2 | 1:Z4:162:ARG:HB3 | 1.98 | 0.44 |
| 2:Z5:167:LEU:HD13 | 2:Z5:200:VAL:HB | 1.98 | 0.44 |
| 2:Z7:167:LEU:HD13 | 2:Z7:200:VAL:HB | 1.98 | 0.44 |
| 2:Z7:232:ALA:HA | 2:Z7:235:ILE:HG22 | 1.99 | 0.44 |
| 1:0A:3:GLU:HG3 | 1:0A:127:CYS:HB2 | 1.99 | 0.44 |
| 1:0C:332:ASN:OD1 | 1:0C:336:LYS:HE3 | 2.18 | 0.44 |
| 1:0E:43:GLN:O | 1:0E:47:ILE:HG23 | 2.18 | 0.44 |
| 1:0E:286:VAL:HG21 | 1:0E:325:GLU:HB3 | 1.99 | 0.44 |
| 1:0E:334:GLN:HA | 1:0E:341:PHE:CE2 | 2.53 | 0.44 |
| 2:0F:353:CYS:SG | 2:0F:354:GLY:N | 2.90 | 0.44 |
| 1:0G:394:PHE:HE2 | 2:0H:347:CYS:SG | 2.40 | 0.44 |
| 2:0H:191:THR:HA | 2:0H:194:LEU:HB3 | 2.00 | 0.44 |
| 2:0J:2:ARG:NE | 2:0J:242:LEU:O | 2.45 | 0.44 |
| 1:0K:406:MET:SD | 1:0K:406:MET:N | 2.88 | 0.44 |
| 1:0O:374:ILE:HD12 | 1:0O:374:ILE:H | 1.83 | 0.44 |
| 1:0Q:314:SER:HA | 1:0Q:350:LYS:O | 2.18 | 0.44 |
| 1:0Q:379:LYS:HD3 | 1:0Q:419:VAL:HG21 | 2.00 | 0.44 |
| 2:0R:28:HIS:CE1 | 2:0R:49:PHE:HA | 2.53 | 0.44 |
| 2:0R:396:ASP:HA | 2:0R:399:TYR:HB3 | 1.99 | 0.44 |
| 1:0S:314:SER:HB2 | 1:0S:368:ILE:HG23 | 1.99 | 0.44 |
| 1:0U:135:VAL:HG12 | 1:0U:137:HIS:HD2 | 1.83 | 0.44 |
| 1:0U:185:ALA:O | 1:0U:189:VAL:HG22 | 2.17 | 0.44 |
| 2:0V:167:LEU:HD13 | 2:0V:200:VAL:HB | 2.00 | 0.44 |
| 1:0W:392:LYS:HD2 | 1:0W:395:LEU:HD22 | 1.99 | 0.44 |
| 2:1D:53:PHE:HB3 | 2:1D:61:HIS:HB3 | 2.00 | 0.44 |
| 2:1D:377:MET:O | 2:1D:378:ILE:HD13 | 2.17 | 0.44 |
| 1:1G:145:SER:OG | 1:1G:146:GLY:N | 2.51 | 0.44 |
| 1:1K:180:VAL:HG23 | 1:1K:184:ASN:ND2 | 2.32 | 0.44 |
| 2:1L:222:PRO:CD | 1:1M:324:LYS:HE3 | 2.47 | 0.44 |
| 2:1N:407:TRP:CG | 1:1O:255:VAL:HG23 | 2.52 | 0.44 |
| 1:1O:2:ARG:HH21 | 1:1O:240:LEU:HA | 1.83 | 0.44 |
| 1:1O:213:ARG:HE | 1:1O:297:LYS:NZ | 2.13 | 0.44 |
| 1:1Q:174:LYS:HD2 | 1:1Q:174:LYS:H | 1.82 | 0.44 |
| 1:1Q:309:ARG:H | 1:1Q:372:THR:CG2 | 2.29 | 0.44 |
| 2:1R:266:HIS:O | 2:1R:266:HIS:ND1 | 2.49 | 0.44 |
| 1:2E:396:HIS:H | 1:2E:396:HIS:CD2 | 2.35 | 0.44 |
| 2:2F:21:TRP:CZ2 | 2:2F:65:CYS:HB3 | 2.52 | 0.44 |
| 2:2F:251:ASP:OD1 | 2:2F:253:THR:HG22 | 2.17 | 0.44 |
| 2:2H:245:ASP:OD1 | 2:2H:245:ASP:N | 2.49 | 0.44 |
| 2:2H:279:GLU:CD | 10:5B:167:ILE:HD13 | 2.37 | 0.44 |
| 2:2H:282:TYR:OH | 10:5B:163:ARG:HB3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2K:201:VAL:HG22 | 1:2K:266:PHE:O | 2.18 | 0.44 |
| 2:2L:213:CYS:HA | 2:2L:217:LEU:HB2 | 1.98 | 0.44 |
| 1:2M:262:ARG:HH22 | 1:2M:414:ASN:HD22 | 1.66 | 0.44 |
| 1:2S:248:ALA:HA | 1:2S:252:LYS:HD2 | 2.00 | 0.44 |
| 1:2U:77:ARG:NH1 | 17:5T:201:LEU:HG | 2.33 | 0.44 |
| 1:2W:39:ASP:OD1 | 1:2W:40:SER:N | 2.50 | 0.44 |
| 2:2X:137:VAL:HG22 | 2:2X:168:GLY:HA2 | 2.00 | 0.44 |
| 2:2X:156:ARG:HA | 2:2X:159:VAL:HG12 | 2.00 | 0.44 |
| 2:2X:313:MET:HB2 | 2:2X:380:ASN:HB3 | 1.99 | 0.44 |
| 2:3D:7:ILE:HG12 | 2:3D:137:VAL:HG12 | 1.99 | 0.44 |
| 2:3F:164:LYS:HZ1 | 3:3V:136:HIS:HB2 | 1.82 | 0.44 |
| 2:3F:187:SER:OG | 2:3F:391:LEU:HD21 | 2.18 | 0.44 |
| 2:3H:21:TRP:CZ3 | 2:3H:63:PRO:HB3 | 2.53 | 0.44 |
| 1:3I:218:THR:OG1 | 1:3I:219:THR:HG23 | 2.17 | 0.44 |
| 1:3K:170:VAL:HG22 | 1:3K:202:LEU:O | 2.17 | 0.44 |
| 1:3M:327:ASP:OD1 | 1:3M:328:GLU:N | 2.50 | 0.44 |
| 2:3N:163:LYS:HE3 | 3:4D:137:ARG:HG2 | 1.98 | 0.44 |
| 1:3Q:165:LEU:HD23 | 1:3Q:165:LEU:HA | 1.87 | 0.44 |
| 1:3Q:256:ASN:O | 1:3Q:312:THR:HG21 | 2.18 | 0.44 |
| 2:3R:276:ILE:HD11 | 2:3R:281:ALA:HA | 1.99 | 0.44 |
| 1:3S:167:PHE:CZ | 1:3S:233:MET:HG2 | 2.52 | 0.44 |
| 3:4H:44:ALA:HB3 | 3:4H:116:PRO:HG3 | 1.99 | 0.44 |
| 6:4O:114:GLU:OE2 | 6:4O:115:LYS:HG3 | 2.18 | 0.44 |
| 6:4O:147:GLU:HA | 6:4O:150:ASP:OD1 | 2.18 | 0.44 |
| 6:4O:474:PRO:HG3 | 6:4P:138:LYS:HB3 | 2.00 | 0.44 |
| 7:4Q:367:ARG:HD2 | 7:4Q:367:ARG:HA | 1.87 | 0.44 |
| 7:4S:3:ARG:H | 7:4S:3:ARG:HG3 | 1.51 | 0.44 |
| 7:4U:137:THR:HG23 | 31:7N:120:TRP:CH2 | 2.53 | 0.44 |
| 8:4W:468:MET:CE | 8:4W:470:TYR:CE1 | 3.00 | 0.44 |
| 9:4Z:39:TRP:HE1 | 14:5L:583:ASP:HB3 | 1.82 | 0.44 |
| 9:4Z:400:ARG:HE | 9:4Z:400:ARG:HB2 | 1.60 | 0.44 |
| 11:5E:103:VAL:N | 11:5E:104:PRO:CD | 2.80 | 0.44 |
| 14:5N:228:PHE:CD1 | 14:5N:228:PHE:O | 2.70 | 0.44 |
| 15:5P:155:SER:OG | 15:5P:156:GLY:N | 2.50 | 0.44 |
| 15:5P:279:ALA:CA | 15:5P:298:VAL:HG21 | 2.46 | 0.44 |
| 21:6H:109:THR:C | 24:6X:82:ALA:HB3 | 2.38 | 0.44 |
| 22:6N:50:PHE:O | 22:6N:53:THR:OG1 | 2.29 | 0.44 |
| 24:6T:185:ASP:O | 24:6T:188:THR:OG1 | 2.32 | 0.44 |
| 24:6T:558:LEU:HD23 | 24:6T:612:LEU:CD2 | 2.48 | 0.44 |
| 24:6U:574:ARG:O | 24:6U:578:ILE:HG12 | 2.18 | 0.44 |
| 24:6X:111:MET:HG2 | 24:6X:213:TYR:CE2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:7H:300:GLY:O | 28:7H:304:LYS:HG3 | 2.18 | 0.44 |
| 28:7H:361:TRP:HA | 28:7H:361:TRP:HE3 | 1.82 | 0.44 |
| 36:7V:23:PHE:CE2 | 36:7V:72:LEU:HD13 | 2.53 | 0.44 |
| 28:7X:301:GLU:H | 28:7X:301:GLU:HG3 | 1.60 | 0.44 |
| 28:7X:306:LEU:HD23 | 28:7X:306:LEU:HA | 1.86 | 0.44 |
| 2:4:364:PRO:HB2 | 26:7D:53:TYR:HD1 | 1.75 | 0.44 |
| 2:A4:44:GLY:N | 24:6Z:124:TYR:OH | 2.49 | 0.44 |
| 2:A4:357:TYR:CB | 26:7F:146:ASN:HA | 2.44 | 0.44 |
| 1:D4:47:ILE:HD11 | 22:6N:23:TYR:CE2 | 2.53 | 0.44 |
| 1:G2:51:PHE:HB3 | 1:G2:59:TYR:HB3 | 1.98 | 0.44 |
| 1:G2:190:HIS:NE2 | 1:G2:410:GLU:OE1 | 2.50 | 0.44 |
| 2:G5:5:ILE:HG22 | 2:G5:64:ARG:HB3 | 2.00 | 0.44 |
| 2:G5:56:THR:OG1 | 2:I1:284:GLU:O | 2.35 | 0.44 |
| 2:G5:60:LYS:NZ | 2:I1:282:TYR:HA | 2.33 | 0.44 |
| 1:G6:40:SER:OG | 1:G6:42:LEU:HG | 2.17 | 0.44 |
| 1:G6:406:MET:SD | 1:G6:406:MET:N | 2.91 | 0.44 |
| 2:G7:69:ASP:OD1 | 2:G7:70:LEU:N | 2.51 | 0.44 |
| 2:G9:79:ARG:NH1 | 2:G9:92:LEU:O | 2.48 | 0.44 |
| 1:H2:53:GLU:CD | 1:H2:53:GLU:H | 2.21 | 0.44 |
| 1:H2:309:ARG:H | 1:H2:372:THR:CG2 | 2.30 | 0.44 |
| 1:H4:7:ILE:HB | 1:H4:135:VAL:HG22 | 2.00 | 0.44 |
| 1:H4:45:GLU:OE1 | 1:H4:46:ARG:HG2 | 2.17 | 0.44 |
| 1:H4:91:VAL:CG1 | 1:H4:116:VAL:HG12 | 2.48 | 0.44 |
| 2:H5:91:GLN:NE2 | 2:H5:121:ARG:HH21 | 2.16 | 0.44 |
| 2:H5:223:THR:HG23 | 2:H5:225:THR:H | 1.83 | 0.44 |
| 1:H8:107:THR:OG1 | 1:H8:401:GLU:OE2 | 2.22 | 0.44 |
| 2:H9:83:TYR:HB3 | 2:H9:86:LEU:HB3 | 2.00 | 0.44 |
| 1:I2:252:LYS:HA | 1:I2:255:VAL:CG1 | 2.36 | 0.44 |
| 1:J0:58:ARG:HB2 | 6:4O:224:ARG:HH12 | 1.83 | 0.44 |
| 2:J1:7:ILE:HG12 | 2:J1:137:VAL:HG12 | 1.99 | 0.44 |
| 2:J3:325:PRO:O | 2:J3:328:VAL:HG12 | 2.17 | 0.44 |
| 1:J4:48:ASN:HB3 | 16:5Q:126:PHE:CZ | 2.53 | 0.44 |
| 2:J9:52:PHE:CE2 | 2:J9:243:ARG:HD3 | 2.53 | 0.44 |
| 2:J9:255:PHE:HA | 2:J9:259:LEU:HD13 | 2.00 | 0.44 |
| 2:K1:84:ARG:NH1 | 28:7X:407:LYS:HG3 | 2.32 | 0.44 |
| 2:K3:69:ASP:OD1 | 2:K3:71:GLU:N | 2.49 | 0.44 |
| 2:K3:220:GLU:OE1 | 2:K3:220:GLU:N | 2.50 | 0.44 |
| 2:K3:294:ALA:O | 2:K3:300:SER:OG | 2.31 | 0.44 |
| 1:K4:114:ASP:OD2 | 1:K4:115:SER:N | 2.51 | 0.44 |
| 2:K5:76:ASP:O | 2:K5:80:THR:HG23 | 2.17 | 0.44 |
| 2:K5:187:SER:O | 2:K5:191:THR:HG23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K6:273:LEU:O | 1:K6:292:GLN:NE2 | 2.49 | 0.44 |
| 2:K7:227:LEU:O | 2:K7:231:ILE:HG12 | 2.17 | 0.44 |
| 2:K9:274:PRO:HB2 | 2:K9:276:ILE:HG12 | 1.99 | 0.44 |
| 1:L0:5:VAL:HG22 | 1:L0:62:ARG:HD3 | 2.00 | 0.44 |
| 1:L2:233:MET:O | 1:L2:236:ILE:HG22 | 2.16 | 0.44 |
| 2:L3:73:THR:HG21 | 1:L4:2:ARG:HH22 | 1.83 | 0.44 |
| 1:L6:274:THR:OG1 | 1:L6:279:GLN:OE1 | 2.35 | 0.44 |
| 2:L7:53:PHE:HB3 | 2:L7:61:HIS:HB3 | 1.99 | 0.44 |
| 2:L7:259:LEU:HD23 | 2:L7:268:MET:HG2 | 2.00 | 0.44 |
| 1:M0:22:GLU:HG2 | 1:M0:81:TYR:HB2 | 2.00 | 0.44 |
| 1:M0:179:VAL:HG12 | 2:M1:349:THR:O | 2.18 | 0.44 |
| 2:M3:221:ARG:NH2 | 30:7K:189:PHE:O | 2.50 | 0.44 |
| 1:M8:175:VAL:HG13 | 1:M8:205:GLU:OE1 | 2.18 | 0.44 |
| 1:N0:97:ALA:HA | 1:N0:103:LYS:HE3 | 1.98 | 0.44 |
| 1:N0:317:PHE:HE2 | 1:N0:326:VAL:HG13 | 1.82 | 0.44 |
| 2:N3:233:GLN:O | 2:N3:237:SER:OG | 2.23 | 0.44 |
| 1:N6:139:LEU:HD12 | 1:N6:170:VAL:HG12 | 2.00 | 0.44 |
| 2:N9:133:GLN:HB3 | 2:N9:252:ILE:HG21 | 2.00 | 0.44 |
| 2:O1:417:GLU:HA | 2:O1:420:GLU:HG2 | 1.99 | 0.44 |
| 1:O2:161:ASP:OD1 | 1:O2:162:ARG:NH1 | 2.50 | 0.44 |
| 1:O2:408:PHE:O | 1:O2:412:GLU:HG3 | 2.17 | 0.44 |
| 1:O4:178:THR:HG23 | 1:O4:181:GLU:HG3 | 2.00 | 0.44 |
| 2:O5:9:ILE:HD13 | 2:O5:150:GLY:HA2 | 1.99 | 0.44 |
| 2:O5:31:GLN:HE21 | 2:O5:37:PRO:HG3 | 1.81 | 0.44 |
| 2:O5:157:LEU:HD23 | 2:O5:157:LEU:HA | 1.83 | 0.44 |
| 1:O8:320:ARG:HG3 | 32:7P:67:ARG:NH1 | 2.33 | 0.44 |
| 2:O9:12:ALA:HB2 | 41:O9:501:GTP:C8 | 2.52 | 0.44 |
| 1:P4:272:PRO:HB2 | 1:P4:282:ARG:HH12 | 1.83 | 0.44 |
| 2:P5:66:ILE:HD12 | 2:P5:68:LEU:HD23 | 1.99 | 0.44 |
| 2:P5:327:ASP:N | 2:P5:327:ASP:OD1 | 2.51 | 0.44 |
| 1:Q0:51:PHE:HB3 | 1:Q0:59:TYR:HB3 | 2.00 | 0.44 |
| 1:Q2:53:GLU:OE2 | 1:Q2:54:ALA:N | 2.51 | 0.44 |
| 2:Q3:260:VAL:HG23 | 2:Q3:260:VAL:O | 2.18 | 0.44 |
| 2:Q5:27:GLU:OE1 | 2:Q5:243:ARG:NH1 | 2.46 | 0.44 |
| 1:Q8:70:PRO:HG2 | 2:Q9:2:ARG:HE | 1.83 | 0.44 |
| 1:Q8:167:PHE:CE2 | 1:Q8:233:MET:HG2 | 2.52 | 0.44 |
| 1:Q8:263:LEU:HG | 1:Q8:422:TYR:CE1 | 2.53 | 0.44 |
| 1:R0:31:ASP:HB2 | 1:R0:32:PRO:HD2 | 1.99 | 0.44 |
| 2:R1:55:GLU:HG2 | 2:R1:61:HIS:CE1 | 2.53 | 0.44 |
| 2:R1:66:ILE:HG13 | 2:R1:66:ILE:O | 2.17 | 0.44 |
| 1:R6:67:ASP:OD2 | 1:R6:72:THR:OG1 | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R8:343:GLU:OE2 | 1:R8:430:ALA:N | 2.51 | 0.44 |
| 2:S5:9:ILE:HG22 | 2:S5:146:GLY:HA2 | 1.99 | 0.44 |
| 1:S6:149:THR:HG22 | 1:S6:191:GLN:HG2 | 1.99 | 0.44 |
| 2:S7:188:VAL:HG12 | 2:S7:421:ALA:HB1 | 1.98 | 0.44 |
| 2:S7:274:PRO:HD3 | 2:S7:374:ALA:HA | 2.00 | 0.44 |
| 1:S8:337:ASN:HD21 | 17:5S:48:THR:N | 2.16 | 0.44 |
| 2:S9:431:ASP:OD1 | 13:5I:60:HIS:NE2 | 2.51 | 0.44 |
| 2:T1:2:ARG:NH2 | 2:T1:47:ASP:OD2 | 2.51 | 0.44 |
| 1:T2:391:ARG:NE | 2:T3:346:TRP:HE1 | 2.16 | 0.44 |
| 2:T3:8:HIS:CD2 | 2:T3:138:PHE:HD2 | 2.35 | 0.44 |
| 2:T3:384:ILE:HD12 | 2:T3:384:ILE:H | 1.82 | 0.44 |
| 2:T5:349:THR:HG23 | 2:T5:349:THR:O | 2.16 | 0.44 |
| 1:T6:177:ASP:N | 1:T6:181:GLU:OE2 | 2.51 | 0.44 |
| 1:T8:175:VAL:HG13 | 1:T8:175:VAL:O | 2.18 | 0.44 |
| 1:T8:389:PHE:O | 1:T8:392:LYS:NZ | 2.48 | 0.44 |
| 2:U1:399:TYR:O | 2:U1:402:ARG:NH1 | 2.50 | 0.44 |
| 1:U2:135:VAL:HG11 | 1:U2:152:ILE:HD11 | 1.99 | 0.44 |
| 1:U2:282:ARG:HD3 | 1:U2:282:ARG:H | 1.82 | 0.44 |
| 1:U4:386:THR:O | 1:U4:390:ARG:HG3 | 2.18 | 0.44 |
| 1:U8:190:HIS:HD2 | 1:U8:414:ASN:HB2 | 1.83 | 0.44 |
| 1:U8:263:LEU:HD22 | 1:U8:422:TYR:HE1 | 1.83 | 0.44 |
| 2:V3:165:SER:HA | 2:V3:199:ASP:OD2 | 2.18 | 0.44 |
| 1:V6:253:LEU:HA | 1:V6:350:LYS:HZ2 | 1.83 | 0.44 |
| 2:V7:175:PRO:HB3 | 2:V7:390:ARG:NE | 2.32 | 0.44 |
| 1:W0:418:LEU:HG | 1:W0:422:TYR:HE2 | 1.82 | 0.44 |
| 2:W1:305:CYS:HB2 | 2:W1:383:ALA:HB1 | 2.00 | 0.44 |
| 1:W2:111:GLU:N | 1:W2:111:GLU:OE2 | 2.50 | 0.44 |
| 2:W3:5:ILE:HD11 | 2:W3:135:PHE:CE1 | 2.51 | 0.44 |
| 1:W4:51:PHE:HB3 | 1:W4:59:TYR:HB3 | 1.99 | 0.44 |
| 2:W7:284:GLU:HG2 | 2:W7:285:GLN:H | 1.83 | 0.44 |
| 1:X2:207:LEU:HB3 | 1:X2:225:LEU:HD22 | 1.99 | 0.44 |
| 2:X3:186:ASN:OD1 | 2:X3:408:TYR:OH | 2.36 | 0.44 |
| 2:X3:233:GLN:NE2 | 2:X3:272:TYR:OH | 2.51 | 0.44 |
| 2:X5:11:GLN:HB3 | 41:X6:501:GTP:O2A | 2.18 | 0.44 |
| 1:X8:58:ARG:HH11 | 1:X8:84:ILE:HA | 1.82 | 0.44 |
| 1:Y0:167:PHE:CZ | 1:Y0:233:MET:HG2 | 2.53 | 0.44 |
| 2:Y3:145:THR:HG23 | 2:Y3:149:LEU:HD21 | 2.00 | 0.44 |
| 2:Y3:318:MET:N | 2:Y3:318:MET:SD | 2.91 | 0.44 |
| 2:Y3:345:ASP:OD1 | 2:Y3:346:TRP:N | 2.51 | 0.44 |
| 2:Y5:150:GLY:O | 2:Y5:154:LEU:HB2 | 2.18 | 0.44 |
| 1:Y8:199:CYS:SG | 1:Y8:200:MET:N | 2.91 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y9:103:PHE:CD2 | 2:Y9:189:LEU:HD23 | 2.53 | 0.44 |
| 2:Y9:209:ILE:HD13 | 2:Y9:227:LEU:HG | 1.99 | 0.44 |
| 2:Y9:269:LEU:HD21 | 2:Y9:301:MET:SD | 2.58 | 0.44 |
| 2:Y9:280:LYS:HA | 2:Y9:283:HIS:HB3 | 1.99 | 0.44 |
| 2:Z3:66:ILE:O | 2:Z3:66:ILE:HG13 | 2.17 | 0.44 |
| 1:Z4:153:SER:HB3 | 1:Z4:195:ASN:HD22 | 1.83 | 0.44 |
| 1:Z6:27:GLU:OE1 | 1:Z6:318:ARG:NH2 | 2.46 | 0.44 |
| 1:Z6:49:VAL:HG21 | 1:Z6:240:LEU:HD22 | 2.00 | 0.44 |
| 1:Z6:177:ASP:O | 2:Z7:352:LYS:HA | 2.18 | 0.44 |
| 1:Z6:294:TRP:CD1 | 1:Z6:333:VAL:HG21 | 2.52 | 0.44 |
| 1:Z8:65:LEU:HD13 | 1:Z8:90:PHE:CD1 | 2.52 | 0.44 |
| 1:Z8:173:PRO:O | 1:Z8:176:SER:OG | 2.34 | 0.44 |
| 1:Z8:212:PHE:HE1 | 1:Z8:220:PRO:HG3 | 1.82 | 0.44 |
| 2:Z9:34:GLY:HA3 | 2:Z9:60:LYS:HZ2 | 1.83 | 0.44 |
| 1:0A:42:LEU:HA | 1:0A:45:GLU:OE1 | 2.17 | 0.44 |
| 2:0B:28:HIS:CE1 | 2:0B:49:PHE:HA | 2.53 | 0.44 |
| 2:0B:119:LEU:HA | 2:0B:122:ILE:HG22 | 2.00 | 0.44 |
| 2:0B:188:VAL:HG23 | 2:0B:189:LEU:HD12 | 2.00 | 0.44 |
| 2:0B:296:PHE:HE2 | 2:0B:335:ILE:HG12 | 1.83 | 0.44 |
| 1:0C:61:PRO:HG2 | 1:0C:85:PHE:CE1 | 2.52 | 0.44 |
| 1:0C:186:THR:HG21 | 1:0C:385:PHE:CG | 2.53 | 0.44 |
| 1:0E:8:GLN:OE1 | 1:0E:65:LEU:HD12 | 2.18 | 0.44 |
| 2:0F:32:PRO:HA | 2:0F:86:LEU:HD12 | 2.00 | 0.44 |
| 1:0G:91:VAL:HG11 | 1:0G:116:VAL:HG12 | 1.98 | 0.44 |
| 1:0K:111:GLU:N | 1:0K:111:GLU:OE1 | 2.50 | 0.44 |
| 2:0L:217:LEU:HD13 | 2:0L:367:ASP:OD2 | 2.18 | 0.44 |
| 2:0L:330:ALA:O | 2:0L:334:THR:HG23 | 2.18 | 0.44 |
| 2:0L:344:VAL:HG21 | 2:0L:346:TRP:HE1 | 1.82 | 0.44 |
| 2:0N:73:THR:OG1 | 2:0N:74:VAL:N | 2.51 | 0.44 |
| 1:0O:3:GLU:HB2 | 1:0O:130:LEU:HD13 | 1.99 | 0.44 |
| 2:0P:8:HIS:CD2 | 2:0P:138:PHE:HD2 | 2.35 | 0.44 |
| 1:0Q:297:LYS:HA | 1:0Q:297:LYS:HD3 | 1.74 | 0.44 |
| 2:0R:377:MET:O | 2:0R:378:ILE:HD13 | 2.18 | 0.44 |
| 2:0V:223:THR:OG1 | 2:0V:224:TYR:N | 2.51 | 0.44 |
| 1:0Y:186:THR:HG22 | 1:0Y:411:ALA:HB1 | 2.00 | 0.44 |
| 1:0Y:404:ASP:HB3 | 1:0Y:406:MET:SD | 2.58 | 0.44 |
| 2:0Z:254:GLU:O | 2:0Z:257:THR:OG1 | 2.29 | 0.44 |
| 2:1D:111:GLY:HA2 | 2:1D:114:ILE:HG22 | 1.99 | 0.44 |
| 1:1G:67:ASP:OD2 | 1:1G:72:THR:HG21 | 2.18 | 0.44 |
| 1:1K:162:ARG:HD3 | 1:1K:162:ARG:HA | 1.79 | 0.44 |
| 2:1N:174:SER:HB2 | 2:1N:205:ASP:OD2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1N:346:TRP:N | 2:1N:346:TRP:CD1 | 2.80 | 0.44 |
| 2:1N:368:LEU:HD23 | 2:1N:368:LEU:HA | 1.91 | 0.44 |
| 2:1P:21:TRP:HZ2 | 2:1P:65:CYS:HB2 | 1.82 | 0.44 |
| 1:1Q:325:GLU:O | 1:1Q:329:GLN:HB2 | 2.17 | 0.44 |
| 2:1V:3:GLU:HB2 | 2:1V:129:CYS:SG | 2.58 | 0.44 |
| 1:1W:34:GLY:O | 1:1W:58:ARG:HA | 2.18 | 0.44 |
| 2:1X:109:THR:OG1 | 2:1X:411:GLU:OE2 | 2.31 | 0.44 |
| 2:1X:290:GLU:OE1 | 2:1X:290:GLU:N | 2.43 | 0.44 |
| 1:2A:167:PHE:HE1 | 1:2A:200:MET:HG3 | 1.83 | 0.44 |
| 2:2B:261:PRO:HG3 | 2:2B:313:MET:HE2 | 2.00 | 0.44 |
| 2:2B:288:VAL:HG13 | 2:2B:319:TYR:HE2 | 1.82 | 0.44 |
| 2:2D:3:GLU:HG3 | 2:2D:51:THR:HA | 1.99 | 0.44 |
| 2:2D:72:PRO:HD2 | 1:2E:2:ARG:NH1 | 2.33 | 0.44 |
| 1:2E:3:GLU:HB2 | 1:2E:130:LEU:HA | 2.00 | 0.44 |
| 1:2E:276:ARG:HE | 1:2E:276:ARG:HB2 | 1.65 | 0.44 |
| 2:2F:143:GLY:HA3 | 41:2G:501:GTP:O2B | 2.18 | 0.44 |
| 2:2H:88:HIS:HE1 | 2:2H:90:GLU:CB | 2.25 | 0.44 |
| 2:2L:246:GLY:HA2 | 2:2L:357:TYR:CD2 | 2.53 | 0.44 |
| 2:2N:235:ILE:HA | 2:2N:238:LEU:HG | 1.99 | 0.44 |
| 2:2R:214:ARG:HE | 38:8A:65:VAL:CG1 | 2.31 | 0.44 |
| 1:2S:220:PRO:HD2 | 2:2T:326:LYS:HD3 | 1.99 | 0.44 |
| 2:2T:116:ASP:N | 2:2T:116:ASP:OD1 | 2.49 | 0.44 |
| 1:2U:12:CYS:HB3 | 1:2U:138:SER:OG | 2.17 | 0.44 |
| 2:2V:156:ARG:HA | 2:2V:159:VAL:HG12 | 2.00 | 0.44 |
| 1:2W:11:GLN:HE21 | 1:2W:15:GLN:HE22 | 1.65 | 0.44 |
| 1:2W:49:VAL:HG11 | 1:2W:241:ARG:HG2 | 1.98 | 0.44 |
| 1:2W:297:LYS:HD3 | 1:2W:297:LYS:HA | 1.48 | 0.44 |
| 1:3A:213:ARG:HD2 | 38:8C:47:PHE:CE1 | 2.53 | 0.44 |
| 2:3B:224:TYR:CD1 | 1:3C:323:THR:HG21 | 2.53 | 0.44 |
| 1:3C:183:TYR:O | 1:3C:187:LEU:HD13 | 2.18 | 0.44 |
| 1:3C:244:GLY:HA2 | 1:3C:355:ASP:OD2 | 2.18 | 0.44 |
| 1:3C:391:ARG:HD3 | 2:3D:346:TRP:CZ2 | 2.52 | 0.44 |
| 2:3F:312:TYR:HB2 | 2:3F:343:PHE:CD1 | 2.53 | 0.44 |
| 1:3G:140:GLY:O | 1:3G:184:ASN:ND2 | 2.35 | 0.44 |
| 2:3H:14:ILE:HD11 | 2:3H:74:VAL:HG13 | 1.99 | 0.44 |
| 2:3H:349:THR:O | 2:3H:349:THR:OG1 | 2.34 | 0.44 |
| 2:3J:317:LEU:HB3 | 2:3J:319:TYR:HE1 | 1.82 | 0.44 |
| 1:3K:391:ARG:HB2 | 2:3L:346:TRP:CZ3 | 2.53 | 0.44 |
| 1:3M:52:ASN:ND2 | 1:3M:62:ARG:HB2 | 2.32 | 0.44 |
| 2:3P:157:LEU:HA | 2:3P:157:LEU:HD23 | 1.76 | 0.44 |
| 2:3P:402:ARG:HD3 | 2:3P:402:ARG:HA | 1.87 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3Q:137:HIS:ND1 | 1:3Q:138:SER:O | 2.51 | 0.44 |
| 1:3Q:276:ARG:HB2 | 38:8D:232:PHE:CE2 | 2.52 | 0.44 |
| 2:3R:394:LYS:HB2 | 1:3S:346:PRO:HG3 | 2.00 | 0.44 |
| 4:3W:17:ILE:HD11 | 4:3W:163:ARG:HH12 | 1.82 | 0.44 |
| 4:4G:2:PHE:HZ | 23:6S:3:LEU:HD12 | 1.83 | 0.44 |
| 4:4I:17:ILE:HD11 | 4:4I:163:ARG:HH12 | 1.82 | 0.44 |
| 3:4J:260:ILE:HD11 | 3:4J:262:TYR:CZ | 2.53 | 0.44 |
| 5:4L:320:GLN:CD | 28:7H:428:LEU:HD12 | 2.38 | 0.44 |
| 10:5A:338:LYS:HA | 10:5A:341:GLU:CD | 2.38 | 0.44 |
| 10:5C:187:MET:O | 10:5C:190:ILE:HG13 | 2.18 | 0.44 |
| 10:5C:338:LYS:HA | 10:5C:341:GLU:OE1 | 2.18 | 0.44 |
| 12:5F:310:VAL:HG13 | 12:5F:311:HIS:CD2 | 2.53 | 0.44 |
| 12:5G:359:LEU:HD21 | 12:5G:363:MET:HA | 2.00 | 0.44 |
| 13:5H:124:VAL:HG21 | 13:5H:131:GLU:OE2 | 2.17 | 0.44 |
| 13:5K:124:VAL:HG21 | 13:5K:131:GLU:OE2 | 2.17 | 0.44 |
| 14:5M:590:VAL:HG21 | 14:5M:622:TRP:CZ3 | 2.53 | 0.44 |
| 14:5N:590:VAL:HG21 | 14:5N:622:TRP:CZ3 | 2.53 | 0.44 |
| 15:5O:5:LEU:HD11 | 15:5O:82:PHE:CZ | 2.49 | 0.44 |
| 15:5P:21:LEU:HD23 | 15:5P:22:TRP:N | 2.33 | 0.44 |
| 16:5Q:79:ARG:HD2 | 16:5Q:81:HIS:HE1 | 1.82 | 0.44 |
| 18:5Y:173:HIS:HA | 18:5Y:212:ILE:O | 2.17 | 0.44 |
| 20:6F:215:GLU:OE1 | 20:6F:216:GLY:N | 2.51 | 0.44 |
| 22:6K:49:SER:OG | 22:6K:51:ILE:HG22 | 2.18 | 0.44 |
| 22:6N:264:GLN:HA | 24:6Y:406:ALA:HB2 | 1.98 | 0.44 |
| 22:6O:295:LYS:HD3 | 22:6O:295:LYS:HA | 1.82 | 0.44 |
| 24:6T:525:VAL:HB | 24:6T:530:PHE:CE2 | 2.48 | 0.44 |
| 24:6V:34:THR:HG22 | 24:6V:35:TYR:N | 2.33 | 0.44 |
| 24:6V:117:ARG:NH1 | 24:6V:134:GLU:OE2 | 2.50 | 0.44 |
| 24:6V:378:TRP:O | 24:6V:382:ASN:ND2 | 2.48 | 0.44 |
| 24:6V:525:VAL:HB | 24:6V:530:PHE:CE2 | 2.50 | 0.44 |
| 24:6X:42:GLU:OE1 | 24:6X:42:GLU:N | 2.50 | 0.44 |
| 24:6Y:472:SER:HB3 | 24:6Y:481:LEU:CD2 | 2.48 | 0.44 |
| 24:6Z:315:ARG:HG3 | 24:6Z:315:ARG:HH11 | 1.82 | 0.44 |
| 24:6Z:327:LEU:HD23 | 24:6Z:348:TYR:CD2 | 2.53 | 0.44 |
| 26:7E:49:PRO:C | 26:7E:56:LEU:HD21 | 2.38 | 0.44 |
| 29:7J:129:SER:O | 29:7J:129:SER:OG | 2.28 | 0.44 |
| 30:7L:380:VAL:HA | 30:7L:436:CYS:SG | 2.57 | 0.44 |
| 38:7Z:8:GLU:OE1 | 38:7Z:8:GLU:N | 2.39 | 0.44 |
| 2:6:372:GLN:NE2 | 24:6V:88:TRP:CD2 | 2.86 | 0.44 |
| 2:G1:165:SER:OG | 2:G1:256:GLN:OE1 | 2.33 | 0.44 |
| 2:G1:424:ASP:O | 2:G1:428:LEU:HD23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G2:175:VAL:CG2 | 1:G2:205:GLU:HB2 | 2.47 | 0.44 |
| 1:G2:238:CYS:SG | 1:G2:318:ARG:NH2 | 2.91 | 0.44 |
| 2:G7:317:LEU:HB3 | 2:G7:319:TYR:CE1 | 2.49 | 0.44 |
| 2:G7:394:LYS:NZ | 1:G8:347:ASN:HD21 | 2.15 | 0.44 |
| 1:G8:156:ARG:HA | 1:G8:156:ARG:HD2 | 1.84 | 0.44 |
| 2:G9:251:ASP:OD2 | 2:G9:253:THR:N | 2.50 | 0.44 |
| 2:H5:69:ASP:OD1 | 2:H5:71:GLU:N | 2.48 | 0.44 |
| 2:H7:88:HIS:O | 2:H7:90:GLU:N | 2.51 | 0.44 |
| 2:H9:102:ASN:HB3 | 2:H9:105:ARG:HB3 | 2.00 | 0.44 |
| 2:I1:217:LEU:HB3 | 2:I1:219:ILE:CD1 | 2.47 | 0.44 |
| 2:I1:266:HIS:O | 2:I1:266:HIS:ND1 | 2.46 | 0.44 |
| 2:I3:271:SER:HB2 | 2:I3:301:MET:HA | 2.00 | 0.44 |
| 2:I5:259:LEU:HD23 | 2:I5:268:MET:HG2 | 1.99 | 0.44 |
| 2:I5:271:SER:HA | 2:I5:302:MET:HG2 | 2.00 | 0.44 |
| 2:I5:312:TYR:CD1 | 2:I5:381:SER:HB2 | 2.53 | 0.44 |
| 1:J0:21:TRP:CZ2 | 1:J0:63:ALA:HB2 | 2.53 | 0.44 |
| 2:J1:14:ILE:HD11 | 2:J1:74:VAL:HG13 | 1.99 | 0.44 |
| 2:J3:370:LYS:HD2 | 5:4L:425:GLU:HB3 | 1.99 | 0.44 |
| 2:J5:27:GLU:OE1 | 2:J5:243:ARG:NH1 | 2.50 | 0.44 |
| 2:J7:80:THR:CB | 29:7J:390:LEU:HD11 | 2.48 | 0.44 |
| 1:J8:152:ILE:HD12 | 1:J8:164:MET:SD | 2.57 | 0.44 |
| 1:K0:186:THR:OG1 | 1:K0:411:ALA:HB1 | 2.18 | 0.44 |
| 2:K1:70:LEU:HB2 | 2:K1:98:ASP:OD2 | 2.18 | 0.44 |
| 2:K1:190:SER:O | 2:K1:194:LEU:HG | 2.18 | 0.44 |
| 2:K1:339:ARG:HE | 2:K1:342:GLN:NE2 | 2.16 | 0.44 |
| 2:K3:319:TYR:HB3 | 2:K3:323:VAL:HG21 | 2.00 | 0.44 |
| 1:K4:116:VAL:HA | 1:K4:119:VAL:HG22 | 1.99 | 0.44 |
| 1:K6:282:ARG:HE | 1:K6:282:ARG:HB2 | 1.65 | 0.44 |
| 2:K7:317:LEU:HB3 | 2:K7:319:TYR:HE1 | 1.83 | 0.44 |
| 1:K8:183:TYR:HB3 | 1:K8:398:TYR:HE2 | 1.83 | 0.44 |
| 1:K8:186:THR:HG22 | 1:K8:411:ALA:HB1 | 1.99 | 0.44 |
| 1:L2:35:THR:HG1 | 1:L2:37:HIS:HE2 | 1.63 | 0.44 |
| 2:L3:413:MET:HB3 | 2:L3:417:GLU:OE2 | 2.18 | 0.44 |
| 2:L5:287:SER:N | 2:L5:290:GLU:OE2 | 2.48 | 0.44 |
| 2:L9:103:PHE:CE1 | 2:L9:148:GLY:HA2 | 2.53 | 0.44 |
| 1:M0:95:THR:OG1 | 1:M0:96:GLY:N | 2.51 | 0.44 |
| 2:M3:281:ALA:HB1 | 30:7K:213:PHE:CB | 2.47 | 0.44 |
| 1:M4:105:HIS:CG | 1:M4:150:LEU:HD12 | 2.53 | 0.44 |
| 1:M6:359:LYS:HD3 | 37:7Y:142:ARG:HH21 | 1.83 | 0.44 |
| 2:M7:63:PRO:HB2 | 2:M7:65:CYS:SG | 2.58 | 0.44 |
| 1:M8:5:VAL:HG12 | 1:M8:133:PHE:HD1 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M9:72:PRO:HD2 | 1:N0:2:ARG:NH1 | 2.33 | 0.44 |
| 1:N0:270:PHE:O | 1:N0:298:ASN:ND2 | 2.44 | 0.44 |
| 2:N3:287:SER:OG | 2:N3:288:VAL:N | 2.50 | 0.44 |
| 1:N6:135:VAL:HG11 | 1:N6:152:ILE:HD11 | 2.00 | 0.44 |
| 2:N7:176:GLN:HG2 | 2:N7:177:VAL:N | 2.33 | 0.44 |
| 2:O1:387:ILE:HD13 | 2:O1:390:ARG:HH12 | 1.82 | 0.44 |
| 1:O2:42:LEU:HD23 | 1:O2:45:GLU:OE2 | 2.18 | 0.44 |
| 1:O2:65:LEU:HD13 | 1:O2:90:PHE:CE1 | 2.48 | 0.44 |
| 1:O6:246:LEU:HD22 | 1:O6:352:SER:HA | 2.00 | 0.44 |
| 1:O6:393:ALA:C | 1:O6:395:LEU:N | 2.71 | 0.44 |
| 2:P3:75:VAL:HG11 | 2:P3:94:SER:HB2 | 2.00 | 0.44 |
| 2:P3:274:PRO:HG3 | 2:P3:286:LEU:HD11 | 2.00 | 0.44 |
| 1:P8:54:ALA:O | 1:P8:55:THR:HG23 | 2.18 | 0.44 |
| 2:P9:50:ASN:O | 2:P9:64:ARG:NH2 | 2.50 | 0.44 |
| 2:P9:182:VAL:HG22 | 1:Q0:256:ASN:HD21 | 1.81 | 0.44 |
| 2:P9:387:ILE:HD12 | 2:P9:390:ARG:NH2 | 2.31 | 0.44 |
| 2:Q3:116:ASP:OD1 | 2:Q3:156:ARG:NH1 | 2.39 | 0.44 |
| 2:Q3:261:PRO:CG | 2:Q3:346:TRP:HH2 | 2.31 | 0.44 |
| 1:Q4:218:THR:H | 20:6F:184:ARG:NH1 | 2.15 | 0.44 |
| 2:Q5:175:PRO:HB3 | 2:Q5:390:ARG:HE | 1.83 | 0.44 |
| 2:Q5:234:VAL:HG13 | 2:Q5:376:CYS:SG | 2.58 | 0.44 |
| 1:Q8:46:ARG:NH2 | 1:Q8:240:LEU:HD12 | 2.33 | 0.44 |
| 1:Q8:208:TYR:CE1 | 1:Q8:225:LEU:HD11 | 2.53 | 0.44 |
| 1:Q8:406:MET:O | 1:Q8:409:THR:HG22 | 2.18 | 0.44 |
| 2:R1:155:GLU:OE2 | 2:R1:197:HIS:HE1 | 2.01 | 0.44 |
| 2:R3:209:ILE:HG23 | 2:R3:230:LEU:HD21 | 2.00 | 0.44 |
| 1:R4:309:ARG:O | 1:R4:372:THR:HG22 | 2.17 | 0.44 |
| 1:R4:391:ARG:NH1 | 1:R4:391:ARG:CG | 2.54 | 0.44 |
| 2:R5:263:PRO:HB2 | 17:5T:84:ARG:HG2 | 1.99 | 0.44 |
| 1:R6:391:ARG:O | 2:R7:262:TYR:OH | 2.33 | 0.44 |
| 1:R8:49:VAL:HG11 | 1:R8:241:ARG:HG2 | 2.00 | 0.44 |
| 2:R9:97:GLU:OE1 | 1:S0:251:ARG:NH2 | 2.47 | 0.44 |
| 1:S0:92:PHE:CE2 | 24:6Z:40:GLN:CG | 2.99 | 0.44 |
| 1:S2:233:MET:O | 1:S2:237:THR:HG22 | 2.18 | 0.44 |
| 1:S2:309:ARG:H | 1:S2:372:THR:HG22 | 1.83 | 0.44 |
| 1:S8:94:GLN:CD | 24:6W:42:GLU:OE1 | 2.56 | 0.44 |
| 2:T1:188:VAL:O | 2:T1:191:THR:HG22 | 2.18 | 0.44 |
| 1:T2:238:CYS:SG | 1:T2:239:CYS:N | 2.91 | 0.44 |
| 2:T3:223:THR:OG1 | 1:T4:245:GLN:NE2 | 2.51 | 0.44 |
| 1:T4:404:ASP:OD2 | 1:T4:406:MET:HG2 | 2.18 | 0.44 |
| 2:T5:133:GLN:HB3 | 2:T5:252:ILE:HG21 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U1:328:VAL:O | 2:U1:332:VAL:HG22 | 2.18 | 0.44 |
| 1:U2:309:ARG:H | 1:U2:372:THR:CG2 | 2.30 | 0.44 |
| 1:U4:166:THR:HG1 | 1:U4:199:CYS:HG | 1.64 | 0.44 |
| 2:U7:73:THR:O | 2:U7:77:GLU:HG2 | 2.18 | 0.44 |
| 2:U9:311:LYS:HG2 | 2:U9:342:GLN:HG3 | 2.00 | 0.44 |
| 1:V0:174:LYS:HA | 1:V0:174:LYS:HD3 | 1.91 | 0.44 |
| 1:V2:6:HIS:CE1 | 1:V2:136:CYS:HG | 2.35 | 0.44 |
| 1:V6:252:LYS:HA | 1:V6:255:VAL:HG12 | 2.00 | 0.44 |
| 1:V6:266:PHE:HE1 | 1:V6:370:ASN:HD22 | 1.64 | 0.44 |
| 1:W4:3:GLU:HG3 | 1:W4:127:CYS:SG | 2.58 | 0.44 |
| 2:W7:3:GLU:N | 2:W7:3:GLU:OE1 | 2.50 | 0.44 |
| 2:W9:20:CYS:HA | 2:W9:232:ALA:HB1 | 2.00 | 0.44 |
| 2:W9:172:TYR:CZ | 2:W9:203:MET:SD | 3.11 | 0.44 |
| 2:W9:328:VAL:O | 2:W9:332:VAL:HG22 | 2.18 | 0.44 |
| 1:X0:3:GLU:HG3 | 1:X0:127:CYS:SG | 2.57 | 0.44 |
| 1:X2:200:MET:N | 1:X2:200:MET:SD | 2.91 | 0.44 |
| 2:X3:89:PRO:HD2 | 2:Y9:283:HIS:ND1 | 2.32 | 0.44 |
| 1:X4:135:VAL:HG22 | 1:X4:137:HIS:HD2 | 1.83 | 0.44 |
| 1:X6:204:ASN:OD1 | 39:X6:502:GDP:O2' | 2.35 | 0.44 |
| 2:X9:405:VAL:HG11 | 2:X9:415:GLU:OE2 | 2.18 | 0.44 |
| 1:Y0:19:LYS:NZ | 1:Y0:227:HIS:HD2 | 2.16 | 0.44 |
| 2:Y1:31:GLN:HE21 | 2:Y1:37:PRO:HG3 | 1.83 | 0.44 |
| 2:Y1:179:THR:O | 1:Y2:350:LYS:HD2 | 2.18 | 0.44 |
| 2:Y1:182:VAL:HG22 | 2:Y1:185:TYR:HB2 | 1.99 | 0.44 |
| 2:Y1:318:MET:HE2 | 2:Y1:318:MET:HB3 | 1.83 | 0.44 |
| 2:Y3:62:VAL:HG12 | 2:Y3:88:HIS:CD2 | 2.52 | 0.44 |
| 2:Y3:147:SER:OG | 2:Y3:190:SER:HB2 | 2.17 | 0.44 |
| 1:Y4:50:TYR:OH | 1:Y4:237:THR:HB | 2.18 | 0.44 |
| 1:Y8:11:GLN:NE2 | 39:Y8:501:GDP:O3B | 2.51 | 0.44 |
| 1:Z0:58:ARG:HD3 | 1:0G:280:GLN:NE2 | 2.31 | 0.44 |
| 1:Z2:260:PHE:HB2 | 1:Z2:263:LEU:HG | 2.00 | 0.44 |
| 2:Z3:111:GLY:HA2 | 2:Z3:114:ILE:HG22 | 2.00 | 0.44 |
| 2:Z7:91:GLN:NE2 | 2:0N:283:HIS:HE1 | 2.11 | 0.44 |
| 1:0C:6:HIS:CE1 | 1:0C:8:GLN:HG2 | 2.53 | 0.44 |
| 1:0C:236:ILE:HG13 | 1:0C:237:THR:HG23 | 2.00 | 0.44 |
| 1:0E:270:PHE:CD1 | 1:0E:366:THR:HG22 | 2.53 | 0.44 |
| 2:0F:167:LEU:HG | 2:0F:252:ILE:HD11 | 2.00 | 0.44 |
| 2:0F:407:TRP:HZ2 | 1:0G:258:ILE:HB | 1.82 | 0.44 |
| 1:0G:114:ASP:N | 1:0G:114:ASP:OD1 | 2.50 | 0.44 |
| 2:0J:198:THR:HG21 | 2:0J:201:ALA:HB2 | 1.99 | 0.44 |
| 1:0K:69:GLU:N | 1:0K:69:GLU:OE2 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0L:26:LEU:HD23 | 2:0L:363:VAL:HG12 | 1.99 | 0.44 |
| 1:0M:392:LYS:HB3 | 1:0M:395:LEU:HD22 | 2.00 | 0.44 |
| 2:0N:353:CYS:SG | 2:0N:354:GLY:N | 2.90 | 0.44 |
| 1:0O:54:ALA:HA | 1:1E:283:ALA:HB2 | 1.99 | 0.44 |
| 1:0O:270:PHE:CD2 | 1:0O:273:LEU:HD21 | 2.52 | 0.44 |
| 1:0Q:27:GLU:CD | 1:0Q:241:ARG:HH12 | 2.22 | 0.44 |
| 1:0S:180:VAL:HG23 | 1:0S:183:TYR:HD1 | 1.83 | 0.44 |
| 1:0S:312:THR:OG1 | 1:0S:313:ALA:N | 2.51 | 0.44 |
| 2:0V:8:HIS:CD2 | 2:0V:17:GLY:HA3 | 2.53 | 0.44 |
| 2:0V:384:ILE:HG13 | 2:0V:432:PHE:CE1 | 2.53 | 0.44 |
| 1:0W:20:PHE:O | 1:0W:24:VAL:HG23 | 2.18 | 0.44 |
| 2:0Z:271:SER:OG | 2:0Z:377:MET:HB3 | 2.18 | 0.44 |
| 2:1D:101:ASN:ND2 | 2:1D:143:GLY:HA2 | 2.33 | 0.44 |
| 1:1G:113:ILE:HG13 | 1:1G:114:ASP:N | 2.33 | 0.44 |
| 2:1H:9:ILE:HD13 | 2:1H:150:GLY:HA2 | 2.00 | 0.44 |
| 1:1K:375:GLN:HG3 | 1:1K:376:GLU:OE2 | 2.18 | 0.44 |
| 1:1O:6:HIS:CE1 | 1:1O:8:GLN:HG2 | 2.53 | 0.44 |
| 1:1O:135:VAL:O | 1:1O:166:THR:HA | 2.18 | 0.44 |
| 1:1Q:282:ARG:NH2 | 1:1Q:288:GLU:HG3 | 2.32 | 0.44 |
| 1:1S:178:THR:OG1 | 1:1S:179:VAL:N | 2.51 | 0.44 |
| 2:1T:414:GLU:OE1 | 2:1T:414:GLU:N | 2.51 | 0.44 |
| 1:1U:83:GLN:O | 1:2K:281:TYR:OH | 2.25 | 0.44 |
| 2:1X:370:LYS:HD2 | 9:4Z:387:ARG:HB3 | 2.00 | 0.44 |
| 2:1Z:123:ARG:NH2 | 38:7Z:37:TYR:HA | 2.32 | 0.44 |
| 2:2D:66:ILE:O | 2:2D:66:ILE:HG13 | 2.18 | 0.44 |
| 1:2E:51:PHE:HB3 | 1:2E:59:TYR:HB3 | 2.00 | 0.44 |
| 1:2E:173:PRO:HG2 | 1:2E:380:ARG:HH21 | 1.83 | 0.44 |
| 2:2H:5:ILE:HG22 | 2:2H:64:ARG:HB3 | 2.00 | 0.44 |
| 2:2J:88:HIS:CD2 | 2:2J:90:GLU:HB3 | 2.53 | 0.44 |
| 1:2M:1:MET:O | 1:2M:129:CYS:HB3 | 2.18 | 0.44 |
| 2:2N:116:ASP:HB2 | 38:8D:73:TRP:HZ3 | 1.76 | 0.44 |
| 2:2N:123:ARG:CD | 38:8D:75:SER:HB3 | 2.44 | 0.44 |
| 2:2P:282:TYR:CZ | 10:5C:164:ASP:OD2 | 2.67 | 0.44 |
| 1:2Q:95:THR:HG23 | 1:2Q:96:GLY:N | 2.32 | 0.44 |
| 1:2Q:297:LYS:HB2 | 1:2Q:297:LYS:HE3 | 1.78 | 0.44 |
| 2:2T:271:SER:OG | 2:2T:301:MET:SD | 2.76 | 0.44 |
| 2:2T:312:TYR:HD1 | 2:2T:381:SER:HG | 1.64 | 0.44 |
| 2:2V:116:ASP:OD2 | 2:2V:156:ARG:NH1 | 2.51 | 0.44 |
| 1:2W:309:ARG:NH1 | 1:2W:339:SER:O | 2.50 | 0.44 |
| 2:2X:304:LYS:HA | 2:2X:304:LYS:HD2 | 1.81 | 0.44 |
| 2:2Z:66:ILE:O | 2:2Z:66:ILE:HG13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3B:139:ASN:N | 2:3B:139:ASN:OD1 | 2.51 | 0.44 |
| 1:3C:183:TYR:OH | 1:3C:388:MET:HB3 | 2.18 | 0.44 |
| 1:3G:86:ARG:HB3 | 1:3G:89:ASN:OD1 | 2.18 | 0.44 |
| 1:3G:175:VAL:O | 1:3G:175:VAL:HG23 | 2.18 | 0.44 |
| 2:3H:167:LEU:HD13 | 2:3H:200:VAL:HB | 1.99 | 0.44 |
| 2:3J:246:GLY:HA2 | 2:3J:357:TYR:CD2 | 2.53 | 0.44 |
| 2:3N:70:LEU:HB2 | 2:3N:98:ASP:HA | 1.98 | 0.44 |
| 1:3O:134:GLN:HE21 | 1:3O:167:PHE:HE2 | 1.66 | 0.44 |
| 1:3O:165:LEU:HD23 | 1:3O:165:LEU:HA | 1.73 | 0.44 |
| 1:3S:52:ASN:OD1 | 1:3S:62:ARG:NH2 | 2.51 | 0.44 |
| 2:3T:90:GLU:C | 2:3T:121:ARG:HH12 | 2.20 | 0.44 |
| 2:3T:390:ARG:C | 2:3T:394:LYS:HZ2 | 2.22 | 0.44 |
| 4:3Y:35:LYS:NZ | 3:3Z:254:LYS:O | 2.34 | 0.44 |
| 5:4M:127:LEU:HA | 5:4M:127:LEU:HD23 | 1.73 | 0.44 |
| 7:4R:226:LEU:HD23 | 7:4R:226:LEU:HA | 1.85 | 0.44 |
| 7:4R:328:ALA:O | 7:4R:331:ILE:HG22 | 2.18 | 0.44 |
| 10:5A:375:GLU:HA | 10:5A:378:ASN:ND2 | 2.33 | 0.44 |
| 11:5E:143:ILE:HG21 | 11:5E:148:LEU:HD13 | 2.00 | 0.44 |
| 12:5F:90:PRO:HB3 | 24:6Z:25:LYS:HB2 | 1.99 | 0.44 |
| 13:5I:124:VAL:HG21 | 13:5I:131:GLU:OE2 | 2.17 | 0.44 |
| 13:5J:124:VAL:HG21 | 13:5J:131:GLU:OE2 | 2.17 | 0.44 |
| 14:5L:590:VAL:HG21 | 14:5L:622:TRP:CZ3 | 2.53 | 0.44 |
| 14:5N:165:THR:CG2 | 14:5N:171:MET:SD | 3.06 | 0.44 |
| 14:5N:399:SER:HG | 14:5N:401:TRP:HE1 | 1.57 | 0.44 |
| 15:5O:36:GLU:OE2 | 15:5O:49:ARG:CG | 2.60 | 0.44 |
| 15:5O:227:TYR:C | 15:5O:227:TYR:HD1 | 2.22 | 0.44 |
| 18:5Z:104:LEU:HD13 | 24:6W:180:TYR:CE1 | 2.53 | 0.44 |
| 22:6P:188:ARG:CD | 22:6P:192:LYS:HB2 | 2.47 | 0.44 |
| 24:6X:305:VAL:O | 24:6X:321:PHE:HB3 | 2.18 | 0.44 |
| 24:6Y:90:GLU:HG2 | 24:6Y:91:ASN:ND2 | 2.33 | 0.44 |
| 24:6Y:295:HIS:HD2 | 24:6Y:304:GLU:OE2 | 1.99 | 0.44 |
| 24:6Y:469:PHE:CD2 | 24:6Y:482:ILE:HG23 | 2.53 | 0.44 |
| 24:6Z:371:ALA:HB1 | 24:6Z:375:THR:OG1 | 2.17 | 0.44 |
| 31:7M:46:GLN:O | 31:7M:50:MET:HG3 | 2.18 | 0.44 |
| 38:8A:122:LYS:O | 38:8A:126:THR:HG23 | 2.18 | 0.44 |
| 2:4:226:ASN:ND2 | 26:7D:78:ALA:HB1 | 2.33 | 0.43 |
| 2:A2:279:GLU:CD | 26:7F:82:PRO:HG2 | 2.36 | 0.43 |
| 2:D5:279:GLU:OE2 | 18:6C:178:GLN:CG | 2.65 | 0.43 |
| 1:G2:55:THR:H | 1:G2:58:ARG:HB3 | 1.82 | 0.43 |
| 1:G2:109:GLY:HA2 | 1:G2:147:MET:CE | 2.48 | 0.43 |
| 2:G3:420:GLU:HA | 2:G3:423:GLU:HG3 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:107:THR:OG1 | 1:G4:401:GLU:OE2 | 2.27 | 0.43 |
| 1:G4:391:ARG:HH22 | 2:G5:435:VAL:HA | 1.82 | 0.43 |
| 1:G6:14:ASN:HD21 | 1:G6:65:LEU:HB3 | 1.83 | 0.43 |
| 1:G6:107:THR:OG1 | 1:G6:401:GLU:OE2 | 2.23 | 0.43 |
| 1:G8:3:GLU:HG2 | 1:G8:127:CYS:SG | 2.58 | 0.43 |
| 2:G9:420:GLU:HA | 2:G9:423:GLU:CG | 2.48 | 0.43 |
| 1:H4:8:GLN:CD | 1:H4:17:GLY:HA3 | 2.38 | 0.43 |
| 2:H9:223:THR:OG1 | 2:H9:224:TYR:N | 2.51 | 0.43 |
| 2:I1:88:HIS:HE1 | 2:I1:90:GLU:HB3 | 1.83 | 0.43 |
| 2:I3:415:GLU:OE1 | 2:I3:415:GLU:N | 2.51 | 0.43 |
| 2:I5:9:ILE:HG21 | 2:I5:153:LEU:HD21 | 1.98 | 0.43 |
| 2:I7:55:GLU:HG2 | 2:I7:61:HIS:CE1 | 2.53 | 0.43 |
| 1:I8:260:PHE:HB2 | 1:I8:263:LEU:HD23 | 1.99 | 0.43 |
| 1:I8:359:LYS:HD2 | 1:I8:360:GLY:N | 2.32 | 0.43 |
| 1:J0:69:GLU:C | 1:J0:92:PHE:HZ | 2.21 | 0.43 |
| 1:J2:68:LEU:HD12 | 1:J2:97:ALA:HB2 | 2.00 | 0.43 |
| 2:J7:368:LEU:HD23 | 2:J7:368:LEU:HA | 1.88 | 0.43 |
| 1:J8:25:SER:OG | 1:J8:30:ILE:O | 2.36 | 0.43 |
| 2:J9:72:PRO:HD2 | 1:K0:2:ARG:NH1 | 2.32 | 0.43 |
| 2:J9:121:ARG:HE | 2:J9:124:LYS:NZ | 2.16 | 0.43 |
| 2:J9:200:VAL:HG13 | 2:J9:268:MET:HE3 | 2.00 | 0.43 |
| 2:K1:8:HIS:HD2 | 2:K1:13:GLY:O | 2.00 | 0.43 |
| 2:K1:184:PRO:HG2 | 2:K1:394:LYS:HG2 | 2.00 | 0.43 |
| 2:K3:66:ILE:O | 2:K3:66:ILE:HG13 | 2.18 | 0.43 |
| 2:K3:328:VAL:O | 2:K3:332:VAL:HG22 | 2.17 | 0.43 |
| 1:K6:165:LEU:HD23 | 1:K6:165:LEU:HA | 1.89 | 0.43 |
| 1:K8:50:TYR:OH | 1:K8:237:THR:HB | 2.17 | 0.43 |
| 1:K8:211:CYS:HA | 1:K8:215:LEU:HB2 | 1.99 | 0.43 |
| 2:L1:325:PRO:HA | 2:L1:328:VAL:HG12 | 2.00 | 0.43 |
| 1:L2:70:PRO:N | 1:L2:92:PHE:HZ | 2.16 | 0.43 |
| 1:L2:192:LEU:HD23 | 1:L2:192:LEU:HA | 1.84 | 0.43 |
| 2:L3:149:LEU:HA | 2:L3:152:LEU:HB3 | 2.00 | 0.43 |
| 1:L6:86:ARG:HG2 | 1:L6:88:ASP:H | 1.83 | 0.43 |
| 1:L6:309:ARG:H | 1:L6:372:THR:HG22 | 1.83 | 0.43 |
| 2:L7:333:ALA:O | 2:L7:337:THR:HG23 | 2.18 | 0.43 |
| 2:M1:271:SER:OG | 2:M1:377:MET:HB3 | 2.18 | 0.43 |
| 2:M3:46:ASP:HB2 | 2:M3:49:PHE:HD2 | 1.80 | 0.43 |
| 1:M4:317:PHE:HB3 | 1:M4:321:MET:SD | 2.57 | 0.43 |
| 1:M6:208:TYR:CE1 | 1:M6:225:LEU:HD11 | 2.53 | 0.43 |
| 2:M7:315:CYS:SG | 2:M7:316:CYS:N | 2.91 | 0.43 |
| 1:N2:199:CYS:SG | 1:N2:265:PHE:HD1 | 2.40 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N3:60:LYS:NZ | 2:N3:85:GLN:HG2 | 2.33 | 0.43 |
| 1:N6:204:ASN:HD21 | 39:N6:503:GDP:N2 | 2.16 | 0.43 |
| 2:N7:289:ALA:HB3 | 32:7O:20:THR:HG22 | 1.99 | 0.43 |
| 1:O2:107:THR:OG1 | 1:O2:108:GLU:OE1 | 2.26 | 0.43 |
| 2:O3:344:VAL:HG11 | 2:O3:346:TRP:CE3 | 2.53 | 0.43 |
| 1:O4:344:TRP:CE3 | 1:O4:345:ILE:HG13 | 2.53 | 0.43 |
| 2:O7:56:THR:HG22 | 2:Q5:285:GLN:HB2 | 2.00 | 0.43 |
| 2:O9:28:HIS:CE1 | 2:O9:49:PHE:HA | 2.53 | 0.43 |
| 2:O9:189:LEU:HD11 | 2:O9:418:PHE:HE1 | 1.82 | 0.43 |
| 1:P4:199:CYS:HB2 | 1:P4:265:PHE:HD1 | 1.82 | 0.43 |
| 1:Q0:238:CYS:SG | 1:Q0:239:CYS:N | 2.90 | 0.43 |
| 1:Q2:371:SER:OG | 1:Q2:372:THR:N | 2.51 | 0.43 |
| 2:Q5:9:ILE:HG22 | 2:Q5:146:GLY:HA2 | 2.00 | 0.43 |
| 2:Q5:163:LYS:HD3 | 2:Q5:163:LYS:HA | 1.84 | 0.43 |
| 1:Q8:7:ILE:HB | 1:Q8:135:VAL:HG22 | 1.99 | 0.43 |
| 1:R0:311:LEU:HA | 1:R0:311:LEU:HD23 | 1.73 | 0.43 |
| 2:R1:72:PRO:HD2 | 1:R2:2:ARG:HH12 | 1.83 | 0.43 |
| 2:R1:301:MET:HE1 | 2:R1:307:PRO:HD3 | 2.00 | 0.43 |
| 1:R4:293:MET:HG3 | 1:R4:367:PHE:HB2 | 1.99 | 0.43 |
| 1:R6:217:LEU:HD23 | 1:R6:217:LEU:HA | 1.87 | 0.43 |
| 2:R9:76:ASP:OD2 | 1:S0:46:ARG:NH2 | 2.43 | 0.43 |
| 2:R9:259:LEU:HD21 | 2:R9:316:CYS:HB2 | 1.99 | 0.43 |
| 2:S1:237:SER:HA | 2:S1:320:ARG:HD2 | 1.99 | 0.43 |
| 1:S2:405:GLU:O | 1:S2:409:THR:HG23 | 2.17 | 0.43 |
| 1:S4:178:THR:O | 1:S4:181:GLU:HG3 | 2.18 | 0.43 |
| 1:S4:219:THR:HB | 2:S5:324:VAL:HG11 | 2.00 | 0.43 |
| 1:S4:392:LYS:HZ1 | 13:5H:53:PHE:HA | 1.82 | 0.43 |
| 2:S5:187:SER:OG | 2:S5:391:LEU:HD21 | 2.17 | 0.43 |
| 2:S7:76:ASP:O | 2:S7:80:THR:HG23 | 2.18 | 0.43 |
| 1:S8:65:LEU:HD12 | 1:S8:90:PHE:CE1 | 2.53 | 0.43 |
| 1:S8:271:THR:CG2 | 1:S8:365:ALA:HB3 | 2.48 | 0.43 |
| 1:S8:362:LYS:NZ | 7:4T:299:TYR:HB3 | 2.33 | 0.43 |
| 2:T1:11:GLN:HB3 | 41:T2:501:GTP:O2A | 2.18 | 0.43 |
| 2:T3:66:ILE:HG13 | 2:T3:66:ILE:O | 2.18 | 0.43 |
| 1:T6:125:GLU:HB2 | 3:4H:65:SER:OG | 2.17 | 0.43 |
| 1:T6:345:ILE:HB | 1:T6:348:ASN:HD21 | 1.82 | 0.43 |
| 2:T7:88:HIS:CD2 | 2:T7:89:PRO:HD3 | 2.41 | 0.43 |
| 1:U2:170:VAL:HG12 | 1:U2:202:LEU:O | 2.17 | 0.43 |
| 1:U2:178:THR:HG23 | 1:U2:181:GLU:HG3 | 1.99 | 0.43 |
| 1:U2:314:SER:HA | 1:U2:350:LYS:O | 2.19 | 0.43 |
| 1:U6:42:LEU:HD23 | 1:U6:356:ILE:HD11 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U6:117:LEU:HA | 1:U6:120:VAL:HG12 | 1.99 | 0.43 |
| 1:U6:271:THR:HG22 | 1:U6:289:LEU:HD23 | 1.99 | 0.43 |
| 1:U8:31:ASP:OD2 | 1:U8:33:THR:OG1 | 2.31 | 0.43 |
| 1:V0:309:ARG:H | 1:V0:372:THR:CG2 | 2.31 | 0.43 |
| 1:V4:111:GLU:N | 1:V4:111:GLU:OE1 | 2.51 | 0.43 |
| 1:V4:285:THR:H | 1:V4:288:GLU:HG3 | 1.83 | 0.43 |
| 1:V6:163:MET:CE | 1:V6:164:MET:H | 2.30 | 0.43 |
| 2:V7:288:VAL:HG21 | 2:V7:327:ASP:HB2 | 2.01 | 0.43 |
| 1:V8:167:PHE:CZ | 1:V8:233:MET:HG2 | 2.53 | 0.43 |
| 1:W0:334:GLN:NE2 | 1:W0:348:ASN:H | 2.13 | 0.43 |
| 2:W1:222:PRO:CD | 1:W2:324:LYS:HE3 | 2.48 | 0.43 |
| 1:W2:330:MET:HA | 1:W2:333:VAL:HG12 | 1.99 | 0.43 |
| 2:W3:88:HIS:HB3 | 2:W3:91:GLN:HB2 | 1.99 | 0.43 |
| 2:W5:155:GLU:HG3 | 2:W5:197:HIS:CE1 | 2.53 | 0.43 |
| 1:W8:274:THR:OG1 | 1:W8:282:ARG:NH1 | 2.50 | 0.43 |
| 2:X3:334:THR:HA | 2:X3:337:THR:HG22 | 1.99 | 0.43 |
| 2:X3:409:VAL:HA | 2:X3:413:MET:O | 2.18 | 0.43 |
| 1:X4:22:GLU:HG3 | 1:X4:81:TYR:CD1 | 2.52 | 0.43 |
| 1:X4:138:SER:OG | 1:X4:139:LEU:N | 2.51 | 0.43 |
| 1:X4:379:LYS:HZ2 | 1:X4:419:VAL:HB | 1.82 | 0.43 |
| 2:X5:222:PRO:HD2 | 1:X6:324:LYS:HE3 | 2.00 | 0.43 |
| 2:X7:174:SER:OG | 2:X7:207:GLU:HB2 | 2.18 | 0.43 |
| 1:X8:239:CYS:SG | 1:X8:248:ALA:N | 2.83 | 0.43 |
| 2:X9:216:SER:OG | 2:X9:217:LEU:N | 2.50 | 0.43 |
| 2:X9:286:LEU:O | 2:X9:286:LEU:CD1 | 2.66 | 0.43 |
| 1:Y2:128:ASP:OD1 | 1:Y2:129:CYS:N | 2.48 | 0.43 |
| 2:Y3:88:HIS:HB3 | 2:Z9:283:HIS:ND1 | 2.32 | 0.43 |
| 2:Y3:240:ALA:HB1 | 2:Y3:356:ASN:HD22 | 1.83 | 0.43 |
| 1:Y4:219:THR:O | 1:Y4:219:THR:OG1 | 2.32 | 0.43 |
| 1:Y4:309:ARG:O | 1:Y4:371:SER:OG | 2.31 | 0.43 |
| 1:Y8:183:TYR:CZ | 1:Y8:388:MET:HG2 | 2.52 | 0.43 |
| 1:Y8:326:VAL:HG12 | 1:Y8:330:MET:HE3 | 1.99 | 0.43 |
| 2:Y9:118:ALA:O | 2:Y9:122:ILE:HG12 | 2.18 | 0.43 |
| 2:Y9:155:GLU:O | 2:Y9:158:SER:OG | 2.35 | 0.43 |
| 2:Y9:183:GLU:HG3 | 2:Y9:184:PRO:HD3 | 2.00 | 0.43 |
| 2:Z5:73:THR:HG23 | 1:Z6:2:ARG:HH12 | 1.83 | 0.43 |
| 2:Z7:76:ASP:OD2 | 2:Z7:79:ARG:HD2 | 2.18 | 0.43 |
| 2:0B:129:CYS:SG | 2:0B:130:THR:N | 2.90 | 0.43 |
| 1:0C:378:PHE:HA | 1:0C:381:VAL:HG12 | 2.00 | 0.43 |
| 1:0E:367:PHE:O | 1:0E:368:ILE:HD13 | 2.18 | 0.43 |
| 2:0F:74:VAL:O | 2:0F:78:VAL:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0G:343:GLU:OE1 | 1:0G:344:TRP:HD1 | 2.01 | 0.43 |
| 1:0G:377:MET:SD | 1:0G:380:ARG:NH1 | 2.91 | 0.43 |
| 1:0I:114:ASP:N | 1:0I:114:ASP:OD1 | 2.48 | 0.43 |
| 1:0I:246:LEU:HD23 | 1:0I:246:LEU:HA | 1.83 | 0.43 |
| 1:0I:301:CYS:SG | 1:0I:302:ALA:N | 2.91 | 0.43 |
| 2:0J:288:VAL:HG13 | 2:0J:319:TYR:HE2 | 1.83 | 0.43 |
| 1:0K:62:ARG:HG3 | 1:0K:123:GLU:OE2 | 2.18 | 0.43 |
| 2:0L:234:VAL:HG22 | 2:0L:272:TYR:CD2 | 2.53 | 0.43 |
| 1:0O:31:ASP:OD2 | 1:0O:33:THR:OG1 | 2.21 | 0.43 |
| 1:0O:257:LEU:HD12 | 1:0O:312:THR:OG1 | 2.18 | 0.43 |
| 2:0R:9:ILE:HG22 | 2:0R:146:GLY:HA2 | 1.99 | 0.43 |
| 2:0R:398:MET:CG | 1:0S:346:PRO:HD2 | 2.48 | 0.43 |
| 1:0Y:272:PRO:HB2 | 1:0Y:282:ARG:HH12 | 1.83 | 0.43 |
| 2:1B:387:ILE:HG12 | 2:1B:390:ARG:NH2 | 2.32 | 0.43 |
| 1:1C:175:VAL:HG22 | 1:1C:205:GLU:HB2 | 1.99 | 0.43 |
| 2:1D:257:THR:OG1 | 2:1D:258:ASN:ND2 | 2.51 | 0.43 |
| 1:1E:219:THR:O | 1:1E:219:THR:OG1 | 2.35 | 0.43 |
| 1:1E:233:MET:O | 1:1E:237:THR:HG22 | 2.18 | 0.43 |
| 2:1F:9:ILE:HG13 | 2:1F:9:ILE:O | 2.18 | 0.43 |
| 1:1K:321:MET:HG2 | 1:1K:363:MET:SD | 2.58 | 0.43 |
| 2:1P:300:SER:O | 2:1P:300:SER:OG | 2.32 | 0.43 |
| 2:1R:56:THR:HG23 | 2:1R:60:LYS:CB | 2.48 | 0.43 |
| 1:1S:4:ILE:HB | 1:1S:50:TYR:HE1 | 1.83 | 0.43 |
| 1:1S:5:VAL:HG22 | 1:1S:133:PHE:CD1 | 2.52 | 0.43 |
| 2:1V:305:CYS:HB3 | 2:1V:387:ILE:HD11 | 2.00 | 0.43 |
| 2:1X:379:SER:OG | 2:1X:380:ASN:N | 2.51 | 0.43 |
| 2:1Z:326:LYS:HD2 | 2:1Z:327:ASP:N | 2.33 | 0.43 |
| 1:2A:86:ARG:HD3 | 1:2A:88:ASP:HB2 | 2.00 | 0.43 |
| 1:2A:418:LEU:O | 1:2A:422:TYR:HD2 | 1.99 | 0.43 |
| 1:2A:418:LEU:O | 1:2A:421:GLU:HG2 | 2.18 | 0.43 |
| 1:2C:311:LEU:HD23 | 1:2C:311:LEU:HA | 1.73 | 0.43 |
| 1:2E:86:ARG:HB3 | 1:2E:89:ASN:OD1 | 2.18 | 0.43 |
| 2:2F:221:ARG:HB3 | 1:2G:322:SER:OG | 2.18 | 0.43 |
| 1:2I:324:LYS:HA | 1:2I:327:ASP:OD1 | 2.18 | 0.43 |
| 2:2L:317:LEU:HB3 | 2:2L:319:TYR:CE1 | 2.53 | 0.43 |
| 2:2L:425:LEU:HD23 | 2:2L:425:LEU:HA | 1.85 | 0.43 |
| 1:2M:178:THR:HG23 | 1:2M:181:GLU:HG3 | 1.99 | 0.43 |
| 2:2R:156:ARG:HA | 2:2R:159:VAL:HG12 | 2.00 | 0.43 |
| 1:2S:373:ALA:O | 1:2S:376:GLU:HG3 | 2.18 | 0.43 |
| 2:2T:166:LYS:N | 2:2T:199:ASP:OD2 | 2.51 | 0.43 |
| 2:2T:304:LYS:HD2 | 2:2T:304:LYS:HA | 1.78 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2U:183:TYR:O | 1:2U:187:LEU:HD13 | 2.18 | 0.43 |
| 2:2V:280:LYS:HA | 2:2V:283:HIS:HB3 | 2.01 | 0.43 |
| 1:2W:260:PHE:HB2 | 1:2W:263:LEU:HD13 | 2.00 | 0.43 |
| 2:2X:179:THR:O | 1:2Y:350:LYS:HG2 | 2.17 | 0.43 |
| 2:2X:305:CYS:HB3 | 2:2X:387:ILE:HD11 | 2.00 | 0.43 |
| 1:2Y:95:THR:HG23 | 1:2Y:96:GLY:N | 2.32 | 0.43 |
| 1:2Y:203:ASP:OD1 | 1:2Y:203:ASP:N | 2.49 | 0.43 |
| 2:2Z:76:ASP:HA | 2:2Z:79:ARG:HB2 | 1.99 | 0.43 |
| 2:2Z:85:GLN:HG3 | 14:5N:503:ARG:HH22 | 1.83 | 0.43 |
| 2:2Z:90:GLU:HG3 | 2:2Z:121:ARG:CZ | 2.48 | 0.43 |
| 1:3C:86:ARG:HD3 | 1:3C:88:ASP:HB3 | 2.00 | 0.43 |
| 2:3D:121:ARG:HA | 2:3D:121:ARG:HD2 | 1.84 | 0.43 |
| 2:3H:147:SER:HB2 | 2:3H:190:SER:HB3 | 2.00 | 0.43 |
| 1:3K:334:GLN:HE22 | 1:3K:348:ASN:H | 1.65 | 0.43 |
| 2:3L:420:GLU:HA | 2:3L:423:GLU:HG3 | 2.00 | 0.43 |
| 1:3O:354:CYS:SG | 1:3O:355:ASP:N | 2.91 | 0.43 |
| 2:3R:60:LYS:NZ | 2:3R:85:GLN:O | 2.51 | 0.43 |
| 2:3R:90:GLU:OE2 | 2:3R:121:ARG:NH1 | 2.51 | 0.43 |
| 2:3R:176:GLN:NE2 | 2:3R:207:GLU:OE2 | 2.52 | 0.43 |
| 1:3S:263:LEU:HD13 | 1:3S:422:TYR:CE1 | 2.53 | 0.43 |
| 4:3Y:17:ILE:HD11 | 4:3Y:163:ARG:HH12 | 1.82 | 0.43 |
| 3:4B:45:ARG:HD2 | 3:4B:48:ALA:HB2 | 1.99 | 0.43 |
| 4:4E:17:ILE:HD11 | 4:4E:163:ARG:HH12 | 1.82 | 0.43 |
| 4:4G:17:ILE:HD11 | 4:4G:163:ARG:HH12 | 1.82 | 0.43 |
| 3:4H:93:LYS:HA | 3:4H:93:LYS:HD3 | 1.47 | 0.43 |
| 9:4Z:387:ARG:O | 9:4Z:391:ILE:HG13 | 2.18 | 0.43 |
| 15:5P:40:ILE:HD13 | 37:7Y:56:MET:CB | 2.47 | 0.43 |
| 15:5P:241:LEU:HD23 | 15:5P:241:LEU:HA | 1.82 | 0.43 |
| 18:5X:73:GLN:HB3 | 18:5X:75:ASP:O | 2.18 | 0.43 |
| 18:5Z:73:GLN:HB3 | 18:5Z:75:ASP:O | 2.18 | 0.43 |
| 18:6A:173:HIS:HA | 18:6A:212:ILE:O | 2.17 | 0.43 |
| 18:6B:173:HIS:HA | 18:6B:212:ILE:O | 2.17 | 0.43 |
| 18:6C:173:HIS:HA | 18:6C:212:ILE:O | 2.17 | 0.43 |
| 18:6D:73:GLN:HB3 | 18:6D:75:ASP:O | 2.17 | 0.43 |
| 20:6F:161:GLY:O | 20:6F:166:PRO:HB3 | 2.17 | 0.43 |
| 21:6H:65:LEU:HD23 | 21:6H:68:ALA:HB2 | 2.00 | 0.43 |
| 22:6I:307:ARG:O | 22:6I:311:VAL:HG23 | 2.18 | 0.43 |
| 22:6P:190:LEU:HA | 22:6P:214:PHE:CE2 | 2.53 | 0.43 |
| 23:6Q:30:GLU:HA | 23:6Q:30:GLU:OE1 | 2.18 | 0.43 |
| 24:6T:252:LYS:HD2 | 24:6T:253:PRO:HD2 | 2.00 | 0.43 |
| 24:6T:443:LYS:HD2 | 24:6T:443:LYS:N | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:415:THR:HG23 | 24:6U:418:ASP:H | 1.83 | 0.43 |
| 24:6W:282:ARG:NH1 | 24:6W:289:ARG:HD3 | 2.33 | 0.43 |
| 24:6X:19:PRO:HD2 | 24:6X:22:LEU:HD21 | 2.00 | 0.43 |
| 24:6X:103:LYS:HG2 | 24:6X:116:ILE:HG12 | 2.00 | 0.43 |
| 24:6Y:456:ASP:OD1 | 24:6Y:457:THR:HG23 | 2.18 | 0.43 |
| 25:7C:69:ILE:HD11 | 27:7G:116:ASN:C | 2.38 | 0.43 |
| 29:7I:8:GLN:O | 29:7I:12:LYS:HE2 | 2.18 | 0.43 |
| 29:7I:233:LYS:O | 29:7I:237:MET:HG2 | 2.18 | 0.43 |
| 35:7U:101:LEU:HD23 | 35:7U:101:LEU:HA | 1.88 | 0.43 |
| 36:7W:23:PHE:CE2 | 36:7W:72:LEU:HD13 | 2.53 | 0.43 |
| 36:7W:95:PHE:O | 36:7W:99:GLU:HG2 | 2.18 | 0.43 |
| 37:7Y:123:ARG:HD2 | 37:7Y:128:TYR:OH | 2.18 | 0.43 |
| 38:8C:92:GLU:CG | 38:8C:94:LYS:HE3 | 2.48 | 0.43 |
| 1:A3:308:GLY:O | 3:4H:104:PRO:HB3 | 2.19 | 0.43 |
| 1:D4:226:ASN:ND2 | 39:D4:501:GDP:O6 | 2.34 | 0.43 |
| 1:F2:360:GLY:C | 22:6O:109:ILE:HD11 | 2.38 | 0.43 |
| 2:G3:250:VAL:HG21 | 2:G3:352:LYS:HE3 | 2.00 | 0.43 |
| 2:G3:282:TYR:HH | 22:6M:134:ASN:ND2 | 2.13 | 0.43 |
| 2:G9:203:MET:SD | 2:G9:267:PHE:HD1 | 2.41 | 0.43 |
| 2:G9:364:PRO:HG3 | 22:6P:164:LYS:NZ | 2.33 | 0.43 |
| 1:H2:117:LEU:HA | 1:H2:120:VAL:HG12 | 2.00 | 0.43 |
| 2:H3:4:VAL:HG23 | 2:H3:134:GLY:O | 2.18 | 0.43 |
| 1:H4:191:GLN:HG3 | 1:H4:195:ASN:OD1 | 2.18 | 0.43 |
| 2:H7:55:GLU:HG2 | 2:H7:61:HIS:CE1 | 2.53 | 0.43 |
| 2:I3:71:GLU:CD | 2:I3:98:ASP:HB2 | 2.39 | 0.43 |
| 1:I4:387:ALA:HA | 1:I4:390:ARG:HH21 | 1.83 | 0.43 |
| 2:I5:324:VAL:HG21 | 2:I5:326:LYS:NZ | 2.27 | 0.43 |
| 2:I7:172:TYR:CZ | 2:I7:203:MET:SD | 3.11 | 0.43 |
| 1:I8:117:LEU:HA | 1:I8:120:VAL:HG12 | 2.00 | 0.43 |
| 1:J0:191:GLN:HA | 1:J0:194:GLU:OE1 | 2.18 | 0.43 |
| 1:J6:274:THR:HG21 | 1:J6:279:GLN:OE1 | 2.18 | 0.43 |
| 2:J7:431:ASP:O | 2:J7:435:VAL:HG22 | 2.17 | 0.43 |
| 1:J8:317:PHE:HB3 | 1:J8:321:MET:SD | 2.58 | 0.43 |
| 2:J9:315:CYS:SG | 2:J9:379:SER:HB3 | 2.58 | 0.43 |
| 2:K3:106:GLY:O | 2:K3:149:LEU:N | 2.51 | 0.43 |
| 1:K4:3:GLU:HB2 | 1:K4:130:LEU:HD23 | 2.00 | 0.43 |
| 1:K4:387:ALA:HA | 1:K4:390:ARG:NE | 2.32 | 0.43 |
| 2:K7:180:ALA:HB3 | 2:K7:183:GLU:HG3 | 2.00 | 0.43 |
| 2:K7:278:ALA:HA | 2:K7:369:ALA:HB2 | 2.00 | 0.43 |
| 1:L0:396:HIS:H | 1:L0:396:HIS:CD2 | 2.34 | 0.43 |
| 1:L4:114:ASP:OD1 | 1:L4:115:SER:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L5:175:PRO:HB3 | 2:L5:390:ARG:NE | 2.33 | 0.43 |
| 2:L7:278:ALA:HB3 | 6:4P:209:LYS:HZ2 | 1.83 | 0.43 |
| 2:L9:397:LEU:HD23 | 2:L9:397:LEU:HA | 1.85 | 0.43 |
| 1:M0:2:ARG:HE | 1:M0:240:LEU:HD22 | 1.83 | 0.43 |
| 1:M2:246:LEU:HD22 | 1:M2:352:SER:HA | 1.99 | 0.43 |
| 2:M5:327:ASP:N | 2:M5:327:ASP:OD1 | 2.50 | 0.43 |
| 1:M6:37:HIS:HE1 | 15:5P:295:ASN:ND2 | 2.10 | 0.43 |
| 1:M8:228:LEU:HD23 | 1:M8:228:LEU:HA | 1.89 | 0.43 |
| 2:N1:21:TRP:CZ2 | 2:N1:65:CYS:HB2 | 2.53 | 0.43 |
| 2:N1:425:LEU:HA | 2:N1:425:LEU:HD23 | 1.71 | 0.43 |
| 2:N5:322:ASP:N | 2:N5:322:ASP:OD1 | 2.52 | 0.43 |
| 1:N8:344:TRP:CE3 | 1:N8:345:ILE:HG13 | 2.53 | 0.43 |
| 2:N9:167:LEU:HD13 | 2:N9:200:VAL:HB | 1.99 | 0.43 |
| 2:N9:216:SER:OG | 2:N9:217:LEU:N | 2.51 | 0.43 |
| 2:O3:407:TRP:O | 2:O3:411:GLU:HG2 | 2.18 | 0.43 |
| 2:O5:285:GLN:HG3 | 19:6E:13:LYS:CE | 2.48 | 0.43 |
| 2:O7:101:ASN:OD1 | 1:O8:252:LYS:HG3 | 2.18 | 0.43 |
| 2:O7:244:PHE:HB2 | 2:O7:356:ASN:HD21 | 1.82 | 0.43 |
| 2:O7:287:SER:HB3 | 2:O7:290:GLU:OE1 | 2.18 | 0.43 |
| 1:O8:211:CYS:HB3 | 1:O8:217:LEU:HD12 | 2.00 | 0.43 |
| 2:P3:72:PRO:HD2 | 1:P4:2:ARG:NH1 | 2.34 | 0.43 |
| 1:P4:122:LYS:NZ | 1:R0:291:GLN:HB3 | 2.33 | 0.43 |
| 2:P5:334:THR:HA | 2:P5:337:THR:HG22 | 2.00 | 0.43 |
| 1:P6:174:LYS:HE2 | 1:P6:174:LYS:HB3 | 1.74 | 0.43 |
| 2:P7:10:GLY:O | 2:P7:14:ILE:HD12 | 2.18 | 0.43 |
| 2:P7:47:ASP:N | 2:P7:47:ASP:OD1 | 2.50 | 0.43 |
| 1:P8:3:GLU:HG3 | 1:P8:127:CYS:HB2 | 1.99 | 0.43 |
| 1:P8:334:GLN:NE2 | 1:P8:348:ASN:H | 2.15 | 0.43 |
| 2:P9:211:ASP:OD2 | 2:P9:215:ARG:NH1 | 2.51 | 0.43 |
| 2:P9:246:GLY:HA2 | 2:P9:357:TYR:CD2 | 2.53 | 0.43 |
| 2:Q1:47:ASP:N | 2:Q1:47:ASP:OD1 | 2.51 | 0.43 |
| 1:Q2:180:VAL:HG23 | 1:Q2:184:ASN:HD21 | 1.83 | 0.43 |
| 2:Q3:123:ARG:C | 2:Q3:125:LEU:N | 2.72 | 0.43 |
| 1:Q4:220:PRO:HD2 | 2:Q5:326:LYS:HD3 | 2.01 | 0.43 |
| 1:R0:117:LEU:HA | 1:R0:117:LEU:HD23 | 1.83 | 0.43 |
| 1:R2:317:PHE:HB3 | 1:R2:321:MET:SD | 2.58 | 0.43 |
| 2:R3:155:GLU:HG2 | 2:R3:197:HIS:ND1 | 2.33 | 0.43 |
| 2:R9:306:ASP:HB3 | 2:R9:309:HIS:CD2 | 2.52 | 0.43 |
| 1:S0:380:ARG:O | 1:S0:383:GLU:HG3 | 2.19 | 0.43 |
| 1:S2:121:ARG:HG2 | 1:S2:125:GLU:OE1 | 2.18 | 0.43 |
| 1:S6:20:PHE:HA | 1:S6:230:SER:HB2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S9:88:HIS:CG | 2:S9:89:PRO:HD2 | 2.52 | 0.43 |
| 1:T0:15:GLN:CD | 7:4T:367:ARG:HH12 | 2.22 | 0.43 |
| 1:T0:292:GLN:HG2 | 1:T0:298:ASN:ND2 | 2.34 | 0.43 |
| 1:T0:405:GLU:N | 1:T0:405:GLU:OE2 | 2.51 | 0.43 |
| 2:T1:335:ILE:HG23 | 2:T1:341:ILE:HD11 | 2.00 | 0.43 |
| 1:T2:51:PHE:HB3 | 1:T2:59:TYR:HB3 | 2.00 | 0.43 |
| 1:T4:418:LEU:HG | 1:T4:422:TYR:CE2 | 2.52 | 0.43 |
| 1:T8:227:HIS:CE1 | 31:7N:3:ILE:HA | 2.53 | 0.43 |
| 1:T8:233:MET:O | 1:T8:236:ILE:HG22 | 2.17 | 0.43 |
| 2:U1:224:TYR:CD2 | 1:U2:245:GLN:HG2 | 2.53 | 0.43 |
| 2:U5:266:HIS:O | 2:U5:266:HIS:ND1 | 2.51 | 0.43 |
| 2:U7:68:LEU:HA | 2:U7:93:ILE:O | 2.18 | 0.43 |
| 2:U7:425:LEU:HD23 | 2:U7:425:LEU:HA | 1.76 | 0.43 |
| 1:V0:10:GLY:O | 1:V0:14:ASN:HB2 | 2.17 | 0.43 |
| 1:V6:4:ILE:CG2 | 1:V6:50:TYR:HE1 | 2.30 | 0.43 |
| 2:V7:147:SER:OG | 2:V7:190:SER:HB2 | 2.19 | 0.43 |
| 2:V7:224:TYR:HB2 | 1:V8:245:GLN:OE1 | 2.18 | 0.43 |
| 2:W1:224:TYR:CZ | 1:W2:323:THR:HG21 | 2.53 | 0.43 |
| 1:W2:20:PHE:HA | 1:W2:230:SER:HB3 | 2.00 | 0.43 |
| 1:W4:186:THR:HG22 | 1:W4:411:ALA:HB1 | 2.00 | 0.43 |
| 1:X0:43:GLN:O | 1:X0:47:ILE:N | 2.51 | 0.43 |
| 1:X2:249:ASP:HB2 | 1:X2:252:LYS:CD | 2.49 | 0.43 |
| 2:X3:70:LEU:HA | 2:X3:95:GLY:HA3 | 1.99 | 0.43 |
| 2:X5:5:ILE:HD11 | 2:X5:135:PHE:HE1 | 1.82 | 0.43 |
| 1:X6:418:LEU:O | 1:X6:421:GLU:HG3 | 2.18 | 0.43 |
| 1:Y2:6:HIS:HA | 1:Y2:134:GLN:O | 2.18 | 0.43 |
| 1:Y4:46:ARG:HA | 1:Y4:46:ARG:HD3 | 1.82 | 0.43 |
| 1:Y8:178:THR:HG22 | 1:Y8:179:VAL:H | 1.83 | 0.43 |
| 2:Y9:73:THR:CG2 | 1:Z0:2:ARG:HH22 | 2.30 | 0.43 |
| 2:Y9:252:ILE:HA | 2:Y9:255:PHE:CE2 | 2.53 | 0.43 |
| 1:Z0:101:TRP:HB2 | 1:Z0:184:ASN:OD1 | 2.18 | 0.43 |
| 1:Z2:330:MET:HA | 1:Z2:333:VAL:HG12 | 2.00 | 0.43 |
| 2:Z5:306:ASP:HB3 | 2:Z5:309:HIS:HD2 | 1.82 | 0.43 |
| 1:Z6:239:CYS:SG | 1:Z6:316:LEU:HD23 | 2.58 | 0.43 |
| 2:Z7:17:GLY:HA2 | 2:Z7:20:CYS:SG | 2.58 | 0.43 |
| 2:Z7:238:LEU:HD11 | 2:Z7:255:PHE:CE1 | 2.53 | 0.43 |
| 2:Z9:139:ASN:O | 2:Z9:171:VAL:HG23 | 2.18 | 0.43 |
| 1:0A:58:ARG:HD3 | 1:0Q:280:GLN:NE2 | 2.31 | 0.43 |
| 1:0C:178:THR:HG22 | 1:0C:179:VAL:N | 2.33 | 0.43 |
| 1:0E:314:SER:OG | 1:0E:368:ILE:HB | 2.17 | 0.43 |
| 2:0F:248:LEU:HA | 2:0F:248:LEU:HD23 | 1.78 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0F:286:LEU:H | 2:0F:286:LEU:HD23 | 1.83 | 0.43 |
| 1:0G:371:SER:OG | 1:0G:372:THR:N | 2.50 | 0.43 |
| 2:0H:8:HIS:O | 2:0H:68:LEU:HD23 | 2.18 | 0.43 |
| 1:0I:69:GLU:O | 1:0I:72:THR:OG1 | 2.36 | 0.43 |
| 2:0J:153:LEU:HD23 | 2:0J:153:LEU:HA | 1.88 | 0.43 |
| 2:0L:5:ILE:HD11 | 2:0L:135:PHE:CD1 | 2.54 | 0.43 |
| 2:0L:138:PHE:HZ | 2:0L:235:ILE:HG13 | 1.83 | 0.43 |
| 2:0L:370:LYS:HD2 | 2:0L:370:LYS:HA | 1.85 | 0.43 |
| 1:0M:207:LEU:HB3 | 1:0M:225:LEU:HD22 | 2.00 | 0.43 |
| 2:0N:344:VAL:HG21 | 2:0N:346:TRP:CE3 | 2.50 | 0.43 |
| 1:0O:50:TYR:OH | 1:0O:237:THR:HG21 | 2.18 | 0.43 |
| 1:0U:77:ARG:HE | 1:0U:90:PHE:HE2 | 1.64 | 0.43 |
| 1:0U:183:TYR:HA | 1:0U:385:PHE:HE1 | 1.83 | 0.43 |
| 1:0Y:389:PHE:CD1 | 1:0Y:395:LEU:HD11 | 2.52 | 0.43 |
| 2:0Z:9:ILE:HG22 | 2:0Z:146:GLY:HA2 | 1.99 | 0.43 |
| 1:1C:178:THR:OG1 | 1:1C:181:GLU:HG3 | 2.18 | 0.43 |
| 1:1C:207:LEU:HB3 | 1:1C:225:LEU:HD22 | 1.99 | 0.43 |
| 1:1C:214:THR:O | 1:1C:275:SER:OG | 2.27 | 0.43 |
| 2:1D:100:ALA:HB1 | 1:1E:252:LYS:HA | 1.99 | 0.43 |
| 1:1E:314:SER:HA | 1:1E:350:LYS:O | 2.19 | 0.43 |
| 1:1G:95:THR:OG1 | 1:1G:96:GLY:N | 2.51 | 0.43 |
| 1:1K:3:GLU:HG3 | 1:1K:127:CYS:SG | 2.58 | 0.43 |
| 1:1M:334:GLN:HE22 | 1:1M:348:ASN:H | 1.64 | 0.43 |
| 1:1O:128:ASP:OD1 | 1:1O:128:ASP:N | 2.47 | 0.43 |
| 2:1P:267:PHE:HB2 | 2:1P:384:ILE:HD12 | 1.99 | 0.43 |
| 1:1Q:167:PHE:HE1 | 1:1Q:200:MET:SD | 2.41 | 0.43 |
| 1:1Q:203:ASP:OD1 | 1:1Q:204:ASN:N | 2.51 | 0.43 |
| 2:1R:120:ASP:OD1 | 2:1R:121:ARG:N | 2.50 | 0.43 |
| 2:1T:367:ASP:OD1 | 2:1T:367:ASP:N | 2.48 | 0.43 |
| 1:1U:173:PRO:HD3 | 1:1U:380:ARG:NH1 | 2.33 | 0.43 |
| 2:1V:195:LEU:CD1 | 2:1V:428:LEU:HD21 | 2.48 | 0.43 |
| 2:1Z:56:THR:OG1 | 2:1Z:60:LYS:HB3 | 2.18 | 0.43 |
| 2:1Z:156:ARG:NH2 | 38:7Z:29:GLY:HA2 | 2.28 | 0.43 |
| 1:2A:414:ASN:HA | 1:2A:417:ASP:OD2 | 2.19 | 0.43 |
| 1:2G:246:LEU:HD22 | 1:2G:352:SER:HA | 2.00 | 0.43 |
| 2:2H:137:VAL:HG22 | 2:2H:168:GLY:HA2 | 1.98 | 0.43 |
| 1:2M:66:MET:HG3 | 1:2M:116:VAL:HG11 | 2.00 | 0.43 |
| 1:2M:178:THR:HA | 2:2N:352:LYS:HD2 | 2.00 | 0.43 |
| 2:2N:203:MET:O | 2:2N:204:LEU:HD12 | 2.18 | 0.43 |
| 1:2Q:334:GLN:NE2 | 1:2Q:348:ASN:H | 2.07 | 0.43 |
| 2:2T:2:ARG:O | 2:2T:2:ARG:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2U:58:ARG:HG3 | 1:3K:280:GLN:HE22 | 1.82 | 0.43 |
| 1:2Y:334:GLN:NE2 | 1:2Y:348:ASN:H | 2.15 | 0.43 |
| 2:3B:327:ASP:N | 2:3B:327:ASP:OD1 | 2.51 | 0.43 |
| 2:3B:339:ARG:NE | 38:8C:39:LYS:HZ3 | 1.77 | 0.43 |
| 2:3F:430:LYS:O | 2:3F:434:GLU:HG3 | 2.18 | 0.43 |
| 2:3J:344:VAL:HG13 | 2:3J:346:TRP:H | 1.83 | 0.43 |
| 1:3M:179:VAL:HG13 | 2:3N:349:THR:O | 2.18 | 0.43 |
| 1:3Q:90:PHE:HB2 | 3:4H:19:LEU:HD13 | 1.98 | 0.43 |
| 1:3Q:382:SER:HB3 | 1:3Q:415:MET:HG2 | 2.00 | 0.43 |
| 2:3R:267:PHE:HB3 | 2:3R:384:ILE:HG21 | 2.00 | 0.43 |
| 1:3S:185:ALA:O | 1:3S:189:VAL:HG12 | 2.18 | 0.43 |
| 3:3X:45:ARG:HD2 | 3:3X:48:ALA:HB2 | 1.99 | 0.43 |
| 4:3Y:1:MET:HG3 | 4:3Y:2:PHE:HD1 | 1.83 | 0.43 |
| 3:4B:93:LYS:HA | 3:4B:93:LYS:HD3 | 1.47 | 0.43 |
| 4:4C:17:ILE:HD11 | 4:4C:163:ARG:HH12 | 1.82 | 0.43 |
| 3:4D:38:THR:HG21 | 4:4E:3:LYS:HB2 | 1.99 | 0.43 |
| 3:4D:93:LYS:HD3 | 3:4D:93:LYS:HA | 1.47 | 0.43 |
| 3:4F:45:ARG:HD2 | 3:4F:48:ALA:HB2 | 1.99 | 0.43 |
| 3:4J:253:ASN:OD1 | 3:4J:254:LYS:N | 2.51 | 0.43 |
| 9:4Y:419:ASP:OD2 | 9:4Y:423:ARG:NH1 | 2.50 | 0.43 |
| 10:5A:264:ALA:O | 10:5A:268:MET:HG2 | 2.18 | 0.43 |
| 10:5C:499:ILE:C | 10:5C:499:ILE:CD1 | 2.87 | 0.43 |
| 11:5E:143:ILE:HG22 | 11:5E:144:PRO:O | 2.18 | 0.43 |
| 14:5L:385:CYS:HB2 | 14:5L:401:TRP:CZ3 | 2.53 | 0.43 |
| 14:5M:150:THR:HG22 | 14:5M:166:ALA:HA | 1.99 | 0.43 |
| 15:5O:130:LYS:HE3 | 15:5O:130:LYS:HB2 | 1.79 | 0.43 |
| 15:5P:6:ARG:HD3 | 15:5P:27:PHE:CD2 | 2.53 | 0.43 |
| 15:5P:52:TYR:CE1 | 15:5P:68:VAL:HG23 | 2.52 | 0.43 |
| 15:5P:172:TRP:O | 15:5P:176:ILE:HG13 | 2.18 | 0.43 |
| 15:5P:216:GLU:HG2 | 15:5P:217:GLU:N | 2.33 | 0.43 |
| 15:5P:338:LEU:C | 15:5P:338:LEU:CD1 | 2.85 | 0.43 |
| 17:5S:224:ARG:O | 17:5S:228:THR:HG23 | 2.17 | 0.43 |
| 17:5U:224:ARG:O | 17:5U:228:THR:HG23 | 2.17 | 0.43 |
| 18:5Y:73:GLN:HB3 | 18:5Y:75:ASP:O | 2.17 | 0.43 |
| 18:5Z:173:HIS:HA | 18:5Z:212:ILE:O | 2.17 | 0.43 |
| 18:6A:16:GLN:HG2 | 18:6A:114:LEU:HB3 | 2.01 | 0.43 |
| 18:6B:16:GLN:HG2 | 18:6B:114:LEU:HB3 | 2.00 | 0.43 |
| 18:6C:73:GLN:HB3 | 18:6C:75:ASP:O | 2.17 | 0.43 |
| 20:6F:51:ALA:O | 20:6F:112:PRO:HG2 | 2.18 | 0.43 |
| 20:6F:79:THR:HG23 | 20:6F:81:CYS:SG | 2.58 | 0.43 |
| 20:6F:372:ARG:O | 20:6F:372:ARG:HD2 | 2.16 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6J:122:ALA:HB3 | 22:6J:128:GLU:HG3 | 2.00 | 0.43 |
| 22:6M:137:GLU:HB3 | 22:6M:141:LYS:CE | 2.48 | 0.43 |
| 22:6N:68:CYS:HB2 | 24:6Y:289:ARG:HH21 | 1.82 | 0.43 |
| 23:6R:34:PHE:CD2 | 23:6R:34:PHE:C | 2.91 | 0.43 |
| 24:6U:451:LYS:HD2 | 24:6U:468:ARG:CZ | 2.47 | 0.43 |
| 24:6U:615:ARG:HG2 | 24:6U:616:LEU:HD23 | 1.98 | 0.43 |
| 24:6V:210:VAL:HG12 | 24:6V:214:ARG:HD2 | 2.00 | 0.43 |
| 24:6V:252:LYS:HG2 | 24:6V:257:LEU:HD21 | 1.99 | 0.43 |
| 24:6Y:469:PHE:CE2 | 24:6Y:482:ILE:HG23 | 2.52 | 0.43 |
| 24:6Z:554:ASP:OD2 | 24:6Z:557:VAL:HG23 | 2.18 | 0.43 |
| 29:7J:445:ASN:HA | 29:7J:448:VAL:HG12 | 2.00 | 0.43 |
| 38:8B:167:ASP:OD1 | 38:8B:168:PRO:CD | 2.65 | 0.43 |
| 38:8C:201:LEU:CD1 | 38:8C:201:LEU:C | 2.85 | 0.43 |
| 38:8D:163:PHE:N | 38:8D:163:PHE:CD1 | 2.87 | 0.43 |
| 1:A1:337:ASN:HD21 | 3:4F:69:TYR:H | 1.66 | 0.43 |
| 2:F1:364:PRO:HG2 | 22:6O:123:PRO:HB2 | 2.00 | 0.43 |
| 1:G2:114:ASP:N | 1:G2:114:ASP:OD2 | 2.52 | 0.43 |
| 2:G7:175:PRO:HG2 | 2:G7:176:GLN:OE1 | 2.19 | 0.43 |
| 1:G8:396:HIS:CE1 | 1:G8:397:TRP:CE2 | 3.06 | 0.43 |
| 2:G9:390:ARG:O | 2:G9:394:LYS:HG2 | 2.18 | 0.43 |
| 1:H2:186:THR:HG22 | 1:H2:411:ALA:HB1 | 2.01 | 0.43 |
| 2:H5:194:LEU:O | 2:H5:198:THR:HG22 | 2.18 | 0.43 |
| 1:H8:383:GLU:HA | 1:H8:386:THR:HG22 | 2.00 | 0.43 |
| 1:I0:418:LEU:HG | 1:I0:422:TYR:CE2 | 2.50 | 0.43 |
| 1:I2:219:THR:O | 1:I2:219:THR:OG1 | 2.33 | 0.43 |
| 2:I3:79:ARG:NH1 | 2:I3:92:LEU:O | 2.52 | 0.43 |
| 2:I7:52:PHE:CE2 | 2:I7:243:ARG:HD3 | 2.54 | 0.43 |
| 2:I7:72:PRO:HD2 | 1:I8:2:ARG:NH1 | 2.33 | 0.43 |
| 1:I8:207:LEU:HB3 | 1:I8:225:LEU:HD22 | 2.01 | 0.43 |
| 2:I9:294:ALA:HA | 2:I9:297:GLU:OE1 | 2.18 | 0.43 |
| 2:J3:276:ILE:HG23 | 2:J3:280:LYS:HB2 | 1.99 | 0.43 |
| 2:J5:21:TRP:CZ3 | 2:J5:63:PRO:HB3 | 2.53 | 0.43 |
| 2:J7:8:HIS:CD2 | 2:J7:138:PHE:HD2 | 2.36 | 0.43 |
| 1:K0:152:ILE:HD12 | 1:K0:164:MET:SD | 2.58 | 0.43 |
| 2:K1:339:ARG:HA | 2:K1:342:GLN:HE22 | 1.84 | 0.43 |
| 1:K6:180:VAL:HG23 | 1:K6:184:ASN:HD21 | 1.83 | 0.43 |
| 2:K7:34:GLY:HA3 | 2:K7:60:LYS:NZ | 2.33 | 0.43 |
| 2:K7:88:HIS:CG | 2:K7:89:PRO:CD | 3.02 | 0.43 |
| 2:L1:85:GLN:NE2 | 30:7K:75:ASP:OD2 | 2.51 | 0.43 |
| 1:L2:317:PHE:HE2 | 1:L2:326:VAL:HG13 | 1.83 | 0.43 |
| 2:L3:102:ASN:HB3 | 2:L3:105:ARG:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L3:288:VAL:O | 2:L3:292:THR:OG1 | 2.26 | 0.43 |
| 2:L5:286:LEU:O | 2:L5:373:ARG:NH1 | 2.51 | 0.43 |
| 2:L9:116:ASP:OD1 | 2:L9:117:LEU:N | 2.51 | 0.43 |
| 1:M0:174:LYS:HE2 | 1:M0:174:LYS:HB3 | 1.74 | 0.43 |
| 2:M1:156:ARG:HA | 2:M1:159:VAL:HG12 | 1.99 | 0.43 |
| 1:M4:178:THR:CG2 | 1:M4:181:GLU:HG3 | 2.48 | 0.43 |
| 1:M4:178:THR:HG23 | 1:M4:181:GLU:HG3 | 2.00 | 0.43 |
| 2:M5:2:ARG:HA | 2:M5:133:GLN:HE21 | 1.83 | 0.43 |
| 2:M5:286:LEU:HD13 | 2:M5:286:LEU:HA | 1.89 | 0.43 |
| 2:M7:76:ASP:O | 2:M7:80:THR:HG23 | 2.18 | 0.43 |
| 2:M7:373:ARG:HH12 | 30:7K:84:VAL:HG22 | 1.84 | 0.43 |
| 1:M8:39:ASP:OD1 | 1:M8:40:SER:N | 2.51 | 0.43 |
| 1:M8:360:GLY:O | 1:M8:361:LEU:HG | 2.18 | 0.43 |
| 1:M8:382:SER:HB2 | 1:M8:415:MET:HG2 | 2.00 | 0.43 |
| 2:N1:156:ARG:O | 2:N1:159:VAL:HG12 | 2.19 | 0.43 |
| 2:N1:176:GLN:HE22 | 2:N1:304:LYS:HE2 | 1.83 | 0.43 |
| 1:N2:49:VAL:HG11 | 1:N2:241:ARG:HG2 | 1.99 | 0.43 |
| 2:N3:180:ALA:HB3 | 2:N3:183:GLU:HB2 | 1.99 | 0.43 |
| 1:N6:77:ARG:HD3 | 1:N6:90:PHE:HE2 | 1.83 | 0.43 |
| 1:N6:294:TRP:CD1 | 1:N6:333:VAL:HG21 | 2.53 | 0.43 |
| 2:N7:72:PRO:HD2 | 1:N8:2:ARG:NH1 | 2.33 | 0.43 |
| 1:N8:111:GLU:HG3 | 25:7C:30:ARG:HH22 | 1.84 | 0.43 |
| 1:O0:350:LYS:NZ | 1:O0:351:SER:O | 2.33 | 0.43 |
| 1:O6:383:GLU:OE2 | 1:O6:384:GLN:HG3 | 2.18 | 0.43 |
| 2:O7:125:LEU:HD23 | 2:O7:125:LEU:HA | 1.74 | 0.43 |
| 2:O9:90:GLU:O | 2:O9:121:ARG:NH1 | 2.52 | 0.43 |
| 1:P4:172:SER:HB3 | 1:P4:175:VAL:CG2 | 2.49 | 0.43 |
| 2:P5:174:SER:HB3 | 2:P5:177:VAL:O | 2.18 | 0.43 |
| 2:P9:178:SER:OG | 1:Q0:347:ASN:ND2 | 2.52 | 0.43 |
| 2:Q3:123:ARG:C | 2:Q3:125:LEU:H | 2.22 | 0.43 |
| 2:Q5:90:GLU:HB2 | 2:Q5:121:ARG:HH22 | 1.83 | 0.43 |
| 1:Q8:174:LYS:HE2 | 1:Q8:174:LYS:HB3 | 1.77 | 0.43 |
| 1:R0:405:GLU:N | 1:R0:405:GLU:OE1 | 2.52 | 0.43 |
| 2:R1:119:LEU:O | 2:R1:122:ILE:HG22 | 2.18 | 0.43 |
| 2:R1:221:ARG:HB3 | 1:R2:322:SER:OG | 2.18 | 0.43 |
| 2:R3:178:SER:HB2 | 1:R4:347:ASN:OD1 | 2.18 | 0.43 |
| 2:R3:227:LEU:O | 2:R3:231:ILE:HG12 | 2.18 | 0.43 |
| 2:R5:420:GLU:HA | 2:R5:423:GLU:OE2 | 2.19 | 0.43 |
| 1:R6:379:LYS:HG3 | 1:R6:419:VAL:HG11 | 2.00 | 0.43 |
| 1:R8:75:SER:O | 1:R8:78:SER:OG | 2.36 | 0.43 |
| 1:R8:113:ILE:HD11 | 1:R8:151:LEU:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S2:424:GLN:HE22 | 17:5V:104:PHE:H | 1.66 | 0.43 |
| 2:S9:298:PRO:HB3 | 2:S9:307:PRO:HD2 | 2.01 | 0.43 |
| 1:T2:173:PRO:HD2 | 1:T2:380:ARG:NH2 | 2.32 | 0.43 |
| 2:T3:163:LYS:HA | 2:T3:163:LYS:HD3 | 1.82 | 0.43 |
| 1:T4:274:THR:HG21 | 1:T4:282:ARG:HD2 | 2.00 | 0.43 |
| 1:T4:393:ALA:O | 1:T4:395:LEU:N | 2.51 | 0.43 |
| 1:T6:100:ASN:HB3 | 1:T6:103:LYS:HB2 | 1.99 | 0.43 |
| 1:T6:111:GLU:OE1 | 1:T6:111:GLU:N | 2.50 | 0.43 |
| 2:T7:21:TRP:CD1 | 2:T7:87:PHE:HZ | 2.36 | 0.43 |
| 2:T7:287:SER:HB3 | 2:T7:290:GLU:OE2 | 2.18 | 0.43 |
| 2:U1:65:CYS:SG | 2:U1:66:ILE:N | 2.91 | 0.43 |
| 1:U2:145:SER:OG | 1:U2:146:GLY:N | 2.51 | 0.43 |
| 1:U2:162:ARG:HA | 1:U2:162:ARG:HD3 | 1.81 | 0.43 |
| 2:U5:35:GLN:HB3 | 2:U5:59:GLY:O | 2.18 | 0.43 |
| 2:U5:79:ARG:O | 2:U5:84:ARG:HG2 | 2.18 | 0.43 |
| 2:U7:129:CYS:SG | 2:U7:130:THR:N | 2.90 | 0.43 |
| 1:U8:289:LEU:HD11 | 1:U8:363:MET:HG2 | 2.00 | 0.43 |
| 2:V1:419:SER:O | 2:V1:423:GLU:HG2 | 2.18 | 0.43 |
| 2:V3:200:VAL:HG13 | 2:V3:268:MET:HE2 | 1.99 | 0.43 |
| 1:V4:325:GLU:O | 1:V4:329:GLN:HG2 | 2.18 | 0.43 |
| 1:V6:123:GLU:O | 1:V6:126:SER:OG | 2.34 | 0.43 |
| 1:V6:378:PHE:HA | 1:V6:381:VAL:HG22 | 1.99 | 0.43 |
| 2:V7:53:PHE:HB3 | 2:V7:61:HIS:HB3 | 1.99 | 0.43 |
| 2:W3:88:HIS:CD2 | 2:W3:89:PRO:CD | 2.98 | 0.43 |
| 1:W4:7:ILE:O | 1:W4:135:VAL:HA | 2.18 | 0.43 |
| 2:W9:90:GLU:OE2 | 2:W9:90:GLU:HA | 2.18 | 0.43 |
| 1:X8:409:THR:HA | 1:X8:412:GLU:OE2 | 2.18 | 0.43 |
| 1:Y0:344:TRP:CE3 | 1:Y0:345:ILE:HG13 | 2.53 | 0.43 |
| 1:Y2:3:GLU:HG3 | 1:Y2:127:CYS:SG | 2.58 | 0.43 |
| 1:Y2:233:MET:O | 1:Y2:237:THR:HG22 | 2.18 | 0.43 |
| 2:Y3:31:GLN:HE21 | 2:Y3:37:PRO:HG3 | 1.83 | 0.43 |
| 2:Y3:115:VAL:HG13 | 2:Y3:153:LEU:HD13 | 2.00 | 0.43 |
| 2:Y3:331:SER:O | 2:Y3:334:THR:OG1 | 2.27 | 0.43 |
| 1:Y8:185:ALA:O | 1:Y8:189:VAL:HG22 | 2.18 | 0.43 |
| 1:Y8:267:MET:CE | 1:Y8:301:CYS:HB2 | 2.48 | 0.43 |
| 2:Y9:11:GLN:NE2 | 2:Y9:71:GLU:OE2 | 2.51 | 0.43 |
| 1:Z0:189:VAL:HA | 1:Z0:192:LEU:HB3 | 2.00 | 0.43 |
| 1:Z2:248:ALA:HA | 1:Z2:252:LYS:HD2 | 2.00 | 0.43 |
| 1:Z4:237:THR:HG23 | 1:Z4:241:ARG:HE | 1.83 | 0.43 |
| 2:Z5:181:VAL:CG2 | 1:Z6:256:ASN:HD22 | 2.32 | 0.43 |
| 2:Z5:256:GLN:O | 2:Z5:260:VAL:HB | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:19:ALA:O | 2:Z7:22:GLU:HG3 | 2.18 | 0.43 |
| 2:Z7:195:LEU:HD23 | 2:Z7:195:LEU:HA | 1.86 | 0.43 |
| 2:Z7:220:GLU:OE2 | 2:Z7:221:ARG:HG3 | 2.17 | 0.43 |
| 1:Z8:33:THR:O | 1:Z8:58:ARG:NH2 | 2.51 | 0.43 |
| 1:Z8:46:ARG:HA | 1:Z8:46:ARG:HD3 | 1.85 | 0.43 |
| 1:Z8:205:GLU:HG2 | 1:Z8:206:ALA:H | 1.82 | 0.43 |
| 1:Z8:219:THR:O | 1:Z8:219:THR:OG1 | 2.31 | 0.43 |
| 1:Z8:274:THR:OG1 | 1:Z8:278:SER:OG | 2.31 | 0.43 |
| 2:Z9:268:MET:HE3 | 2:Z9:378:ILE:HG22 | 1.99 | 0.43 |
| 1:0A:3:GLU:O | 1:0A:131:GLN:N | 2.47 | 0.43 |
| 1:0E:317:PHE:HE2 | 1:0E:326:VAL:HG13 | 1.82 | 0.43 |
| 2:0F:261:PRO:HG2 | 2:0F:262:TYR:CD2 | 2.53 | 0.43 |
| 1:0G:19:LYS:HG3 | 1:0G:226:ASN:HB2 | 2.01 | 0.43 |
| 2:0H:102:ASN:ND2 | 2:0H:105:ARG:HB2 | 2.33 | 0.43 |
| 2:0J:269:LEU:HD21 | 2:0J:301:MET:SD | 2.58 | 0.43 |
| 1:0K:418:LEU:HD23 | 1:0K:418:LEU:HA | 1.81 | 0.43 |
| 1:0O:109:GLY:O | 1:0O:113:ILE:HG22 | 2.18 | 0.43 |
| 1:0O:207:LEU:HD11 | 1:0O:229:ILE:HD11 | 2.00 | 0.43 |
| 2:0P:83:TYR:HB3 | 2:0P:86:LEU:HB3 | 2.00 | 0.43 |
| 2:0R:107:HIS:CD2 | 2:0R:152:LEU:HG | 2.53 | 0.43 |
| 1:0S:274:THR:OG1 | 1:0S:282:ARG:NH1 | 2.51 | 0.43 |
| 2:0V:117:LEU:HA | 2:0V:120:ASP:OD1 | 2.18 | 0.43 |
| 2:0V:402:ARG:HA | 2:0V:402:ARG:HD3 | 1.80 | 0.43 |
| 2:0X:56:THR:HG23 | 2:1N:285:GLN:HA | 2.00 | 0.43 |
| 2:0X:124:LYS:HZ3 | 2:1N:293:ASN:HB2 | 1.83 | 0.43 |
| 2:0Z:211:ASP:OD1 | 2:0Z:215:ARG:NH1 | 2.50 | 0.43 |
| 2:0Z:246:GLY:HA2 | 2:0Z:357:TYR:CD2 | 2.54 | 0.43 |
| 1:1C:11:GLN:HB3 | 39:1C:502:GDP:O1A | 2.18 | 0.43 |
| 2:1F:164:LYS:HE2 | 2:1F:164:LYS:HA | 2.01 | 0.43 |
| 2:1F:170:THR:OG1 | 2:1F:203:MET:SD | 2.76 | 0.43 |
| 2:1F:417:GLU:HA | 2:1F:420:GLU:HG2 | 2.00 | 0.43 |
| 1:1K:274:THR:HG21 | 1:1K:282:ARG:HH11 | 1.83 | 0.43 |
| 2:1L:174:SER:OG | 2:1L:205:ASP:HB3 | 2.18 | 0.43 |
| 2:1P:155:GLU:HB2 | 2:1P:197:HIS:CE1 | 2.53 | 0.43 |
| 2:1P:282:TYR:CD2 | 2:1P:282:TYR:C | 2.92 | 0.43 |
| 2:1P:318:MET:HB2 | 2:1P:376:CYS:HB3 | 2.00 | 0.43 |
| 1:1Q:4:ILE:HB | 1:1Q:50:TYR:HE1 | 1.83 | 0.43 |
| 1:1Q:102:ALA:HB2 | 1:1Q:403:MET:HE3 | 1.99 | 0.43 |
| 1:1U:172:SER:HB3 | 1:1U:175:VAL:CG2 | 2.48 | 0.43 |
| 1:1W:116:VAL:O | 1:1W:120:VAL:HG22 | 2.19 | 0.43 |
| 1:2A:292:GLN:HG2 | 1:2A:298:ASN:ND2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2B:110:ILE:O | 2:2B:113:GLU:HG3 | 2.19 | 0.43 |
| 1:2E:233:MET:O | 1:2E:237:THR:HG22 | 2.17 | 0.43 |
| 2:2F:96:LYS:NZ | 38:8B:64:ASP:OD1 | 2.48 | 0.43 |
| 2:2F:413:MET:HB3 | 2:2F:417:GLU:OE2 | 2.18 | 0.43 |
| 2:2H:90:GLU:HB3 | 2:2H:121:ARG:HH12 | 1.82 | 0.43 |
| 1:2I:1:MET:O | 1:2I:129:CYS:HB3 | 2.18 | 0.43 |
| 1:2I:202:LEU:HD13 | 1:2I:300:MET:HB3 | 2.00 | 0.43 |
| 1:2K:128:ASP:OD1 | 1:2K:128:ASP:N | 2.49 | 0.43 |
| 1:2K:167:PHE:CE1 | 1:2K:200:MET:HG3 | 2.53 | 0.43 |
| 1:2K:167:PHE:CE2 | 1:2K:233:MET:HG2 | 2.54 | 0.43 |
| 2:2P:251:ASP:OD2 | 2:2P:253:THR:N | 2.51 | 0.43 |
| 1:2Q:167:PHE:CZ | 1:2Q:233:MET:HG2 | 2.54 | 0.43 |
| 2:2R:308:ARG:HH22 | 38:8A:72:ASP:CB | 2.26 | 0.43 |
| 2:2T:133:GLN:HB3 | 2:2T:252:ILE:CG2 | 2.47 | 0.43 |
| 1:2U:324:LYS:HE2 | 38:8A:19:PHE:CE2 | 2.53 | 0.43 |
| 1:2U:362:LYS:HE2 | 1:2U:362:LYS:HB2 | 1.81 | 0.43 |
| 2:2X:90:GLU:H | 2:3N:283:HIS:CE1 | 2.36 | 0.43 |
| 2:2X:108:TYR:HA | 2:2X:112:LYS:NZ | 2.34 | 0.43 |
| 1:2Y:43:GLN:O | 1:2Y:47:ILE:HG23 | 2.18 | 0.43 |
| 1:3A:167:PHE:CE2 | 1:3A:233:MET:HG2 | 2.52 | 0.43 |
| 2:3B:28:HIS:CE1 | 2:3B:49:PHE:HA | 2.52 | 0.43 |
| 2:3B:79:ARG:O | 2:3B:84:ARG:HG2 | 2.18 | 0.43 |
| 2:3B:251:ASP:OD1 | 2:3B:253:THR:N | 2.51 | 0.43 |
| 1:3G:53:GLU:OE2 | 1:3G:53:GLU:HA | 2.18 | 0.43 |
| 1:3I:52:ASN:ND2 | 1:3I:52:ASN:N | 2.65 | 0.43 |
| 1:3I:77:ARG:NH1 | 3:3Z:18:LYS:O | 2.51 | 0.43 |
| 1:3I:183:TYR:O | 1:3I:187:LEU:HD13 | 2.19 | 0.43 |
| 1:3K:77:ARG:CZ | 3:4B:19:LEU:HA | 2.48 | 0.43 |
| 2:3L:220:GLU:H | 2:3L:220:GLU:CD | 2.20 | 0.43 |
| 1:3O:86:ARG:HB3 | 1:3O:89:ASN:OD1 | 2.18 | 0.43 |
| 2:3T:251:ASP:OD1 | 2:3T:254:GLU:HG2 | 2.18 | 0.43 |
| 3:3Z:45:ARG:HD2 | 3:3Z:48:ALA:HB2 | 1.99 | 0.43 |
| 4:4A:17:ILE:HD11 | 4:4A:163:ARG:HH12 | 1.82 | 0.43 |
| 3:4B:38:THR:HG22 | 4:4C:4:ASN:OD1 | 2.17 | 0.43 |
| 4:4G:1:MET:HG3 | 4:4G:2:PHE:HD1 | 1.83 | 0.43 |
| 6:4O:295:GLU:HA | 6:4O:298:ARG:HD2 | 2.00 | 0.43 |
| 6:4O:303:LYS:HD2 | 6:4O:303:LYS:HA | 1.79 | 0.43 |
| 6:4P:72:LYS:NZ | 32:7P:88:LEU:HD13 | 2.34 | 0.43 |
| 7:4U:96:THR:O | 7:4U:96:THR:OG1 | 2.29 | 0.43 |
| 7:4U:216:LEU:HD23 | 7:4U:216:LEU:HA | 1.79 | 0.43 |
| 9:4Y:357:SER:O | 9:4Y:360:THR:OG1 | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:4Z:294:GLU:HA | 9:4Z:297:ARG:CD | 2.48 | 0.43 |
| 10:5A:331:MET:HE3 | 10:5A:331:MET:O | 2.17 | 0.43 |
| 10:5A:481:LEU:HG | 10:5B:154:MET:SD | 2.58 | 0.43 |
| 14:5L:356:PHE:CZ | 14:5L:369:LEU:HD13 | 2.53 | 0.43 |
| 14:5M:356:PHE:CZ | 14:5M:369:LEU:HD13 | 2.53 | 0.43 |
| 14:5M:385:CYS:HB2 | 14:5M:401:TRP:CZ3 | 2.53 | 0.43 |
| 14:5N:150:THR:HG22 | 14:5N:166:ALA:HA | 1.99 | 0.43 |
| 14:5N:220:GLN:HB2 | 14:5N:281:LYS:NZ | 2.32 | 0.43 |
| 17:5T:185:LEU:HD22 | 17:5T:185:LEU:HA | 1.77 | 0.43 |
| 18:5X:173:HIS:HA | 18:5X:212:ILE:O | 2.17 | 0.43 |
| 18:5Y:16:GLN:HG2 | 18:5Y:114:LEU:HB3 | 2.01 | 0.43 |
| 18:5Z:16:GLN:HG2 | 18:5Z:114:LEU:HB3 | 2.01 | 0.43 |
| 18:6A:73:GLN:HB3 | 18:6A:75:ASP:O | 2.18 | 0.43 |
| 18:6B:73:GLN:HB3 | 18:6B:75:ASP:O | 2.18 | 0.43 |
| 18:6C:16:GLN:HG2 | 18:6C:114:LEU:HB3 | 2.01 | 0.43 |
| 18:6D:16:GLN:HG2 | 18:6D:114:LEU:HB3 | 2.00 | 0.43 |
| 18:6D:173:HIS:HA | 18:6D:212:ILE:O | 2.17 | 0.43 |
| 21:6G:119:ASP:OD2 | 21:6G:120:ASP:N | 2.52 | 0.43 |
| 21:6H:155:TRP:HB3 | 21:6H:191:ARG:HD3 | 2.00 | 0.43 |
| 21:6H:178:LEU:HD23 | 21:6H:178:LEU:HA | 1.85 | 0.43 |
| 24:6T:417:GLU:OE2 | 24:6T:417:GLU:N | 2.40 | 0.43 |
| 24:6T:569:LYS:O | 24:6T:573:VAL:HG13 | 2.18 | 0.43 |
| 24:6T:591:ASP:N | 24:6T:591:ASP:OD2 | 2.51 | 0.43 |
| 24:6U:106:VAL:HG22 | 24:6U:107:VAL:H | 1.83 | 0.43 |
| 24:6X:130:MET:HE2 | 24:6X:130:MET:HB2 | 1.90 | 0.43 |
| 26:7E:53:TYR:HB2 | 26:7E:55:THR:HG23 | 2.00 | 0.43 |
| 29:7J:137:VAL:O | 29:7J:143:ARG:NH1 | 2.52 | 0.43 |
| 34:7R:92:LEU:HD13 | 35:7T:36:GLN:NE2 | 2.33 | 0.43 |
| 38:8A:197:THR:HG23 | 38:8A:200:ALA:HB3 | 1.99 | 0.43 |
| 2:2:415:GLU:CD | 4:3W:86:TYR:CZ | 2.90 | 0.43 |
| 1:G4:5:VAL:HB | 1:G4:133:PHE:HD1 | 1.82 | 0.43 |
| 1:G4:49:VAL:HG11 | 1:G4:241:ARG:HG2 | 2.01 | 0.43 |
| 1:G4:101:TRP:HB2 | 1:G4:184:ASN:OD1 | 2.19 | 0.43 |
| 2:G5:223:THR:OG1 | 2:G5:224:TYR:N | 2.51 | 0.43 |
| 2:G5:322:ASP:HB3 | 2:G5:373:ARG:HH21 | 1.83 | 0.43 |
| 1:G6:68:LEU:HB3 | 1:G6:96:GLY:HA2 | 2.01 | 0.43 |
| 2:G9:88:HIS:HB3 | 2:I5:283:HIS:HD1 | 1.82 | 0.43 |
| 2:G9:323:VAL:HG23 | 2:G9:355:ILE:HG23 | 2.00 | 0.43 |
| 2:H1:393:HIS:CE1 | 2:H1:397:LEU:HD21 | 2.53 | 0.43 |
| 1:H2:192:LEU:HD23 | 1:H2:192:LEU:HA | 1.86 | 0.43 |
| 2:H3:331:SER:O | 2:H3:334:THR:OG1 | 2.24 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H4:335:ASN:O | 1:H4:338:SER:OG | 2.37 | 0.43 |
| 1:H6:327:ASP:OD1 | 1:H6:328:GLU:N | 2.52 | 0.43 |
| 1:H8:135:VAL:HG12 | 1:H8:137:HIS:HD2 | 1.84 | 0.43 |
| 2:H9:66:ILE:HG13 | 2:H9:66:ILE:O | 2.18 | 0.43 |
| 2:I3:344:VAL:HG22 | 2:I3:346:TRP:CE3 | 2.52 | 0.43 |
| 1:I4:180:VAL:HG23 | 1:I4:184:ASN:ND2 | 2.34 | 0.43 |
| 1:J0:21:TRP:CZ3 | 1:J0:61:PRO:HB3 | 2.53 | 0.43 |
| 2:J1:245:ASP:OD1 | 2:J1:245:ASP:N | 2.48 | 0.43 |
| 1:J2:135:VAL:HG12 | 1:J2:137:HIS:HD2 | 1.83 | 0.43 |
| 2:J5:327:ASP:OD2 | 2:J5:327:ASP:N | 2.50 | 0.43 |
| 2:J9:27:GLU:HG2 | 2:J9:361:THR:HG21 | 2.01 | 0.43 |
| 2:K1:211:ASP:OD1 | 2:K1:214:ARG:NH2 | 2.51 | 0.43 |
| 2:K7:413:MET:HB3 | 2:K7:417:GLU:OE2 | 2.19 | 0.43 |
| 1:L0:117:LEU:HA | 1:L0:120:VAL:HG12 | 1.99 | 0.43 |
| 1:L0:148:GLY:O | 1:L0:152:ILE:HG12 | 2.18 | 0.43 |
| 2:L1:370:LYS:HE2 | 6:4O:363:ARG:HB2 | 2.00 | 0.43 |
| 1:L2:128:ASP:OD1 | 1:L2:128:ASP:N | 2.43 | 0.43 |
| 2:L3:346:TRP:CZ3 | 2:L3:435:VAL:HG13 | 2.53 | 0.43 |
| 2:L5:200:VAL:HG21 | 2:L5:256:GLN:HE21 | 1.83 | 0.43 |
| 2:L7:306:ASP:HB3 | 2:L7:309:HIS:CD2 | 2.53 | 0.43 |
| 1:M0:192:LEU:HD23 | 1:M0:192:LEU:HA | 1.86 | 0.43 |
| 1:M2:58:ARG:CZ | 2:N9:282:TYR:HE1 | 2.32 | 0.43 |
| 1:M4:95:THR:OG1 | 1:M4:96:GLY:N | 2.51 | 0.43 |
| 2:M5:76:ASP:OD1 | 2:M5:77:GLU:N | 2.52 | 0.43 |
| 1:M6:68:LEU:HD21 | 1:M6:112:LEU:HD22 | 2.01 | 0.43 |
| 2:N7:88:HIS:ND1 | 2:P5:283:HIS:HB3 | 2.33 | 0.43 |
| 2:N7:109:THR:OG1 | 2:N7:110:ILE:HD12 | 2.19 | 0.43 |
| 1:N8:68:LEU:HA | 1:N8:93:GLY:H | 1.84 | 0.43 |
| 2:N9:123:ARG:HG3 | 2:N9:123:ARG:HH11 | 1.83 | 0.43 |
| 2:N9:178:SER:OG | 1:O0:347:ASN:HB3 | 2.17 | 0.43 |
| 2:N9:278:ALA:HA | 2:N9:369:ALA:HB2 | 2.00 | 0.43 |
| 1:O0:123:GLU:O | 1:O0:126:SER:OG | 2.36 | 0.43 |
| 2:O1:221:ARG:NH2 | 37:7Y:224:PHE:CD2 | 2.86 | 0.43 |
| 2:O3:294:ALA:HA | 2:O3:297:GLU:OE1 | 2.19 | 0.43 |
| 1:O4:220:PRO:HG2 | 2:O5:326:LYS:HE3 | 2.00 | 0.43 |
| 1:O4:379:LYS:HA | 1:O4:382:SER:OG | 2.18 | 0.43 |
| 1:O6:355:ASP:OD2 | 32:7P:115:THR:HG22 | 2.19 | 0.43 |
| 2:P5:407:TRP:O | 2:P5:411:GLU:HG2 | 2.18 | 0.43 |
| 1:P6:139:LEU:HD22 | 1:P6:188:SER:OG | 2.17 | 0.43 |
| 1:P6:268:VAL:O | 1:P6:300:MET:N | 2.41 | 0.43 |
| 1:P8:344:TRP:CE3 | 1:P8:345:ILE:HG12 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:252:LYS:HE3 | 1:Q0:350:LYS:CE | 2.47 | 0.43 |
| 2:Q3:47:ASP:N | 2:Q3:47:ASP:OD1 | 2.52 | 0.43 |
| 1:Q6:8:GLN:OE1 | 1:Q6:17:GLY:HA3 | 2.18 | 0.43 |
| 1:Q8:220:PRO:HD2 | 2:Q9:326:LYS:HD3 | 2.00 | 0.43 |
| 1:Q8:237:THR:O | 1:Q8:241:ARG:HG3 | 2.18 | 0.43 |
| 2:Q9:137:VAL:HG22 | 2:Q9:168:GLY:HA2 | 2.00 | 0.43 |
| 2:R1:137:VAL:HG22 | 2:R1:168:GLY:HA2 | 2.00 | 0.43 |
| 1:R2:173:PRO:HD2 | 1:R2:380:ARG:NH2 | 2.33 | 0.43 |
| 1:R4:334:GLN:HE22 | 1:R4:347:ASN:CA | 2.31 | 0.43 |
| 1:R6:117:LEU:HD23 | 1:R6:117:LEU:HA | 1.77 | 0.43 |
| 1:R6:309:ARG:H | 1:R6:372:THR:HG22 | 1.84 | 0.43 |
| 1:R8:112:LEU:HD23 | 1:R8:147:MET:SD | 2.58 | 0.43 |
| 1:R8:278:SER:O | 1:R8:278:SER:OG | 2.34 | 0.43 |
| 1:S0:167:PHE:CZ | 1:S0:233:MET:HG2 | 2.54 | 0.43 |
| 1:S0:389:PHE:O | 1:S0:392:LYS:NZ | 2.32 | 0.43 |
| 2:S1:21:TRP:HZ2 | 2:S1:65:CYS:HB3 | 1.81 | 0.43 |
| 2:S1:279:GLU:HG2 | 2:S1:280:LYS:N | 2.33 | 0.43 |
| 1:S2:31:ASP:OD2 | 1:S2:37:HIS:HD2 | 2.02 | 0.43 |
| 1:S2:121:ARG:NH2 | 1:S2:158:GLU:OE2 | 2.45 | 0.43 |
| 1:S4:7:ILE:O | 1:S4:135:VAL:HA | 2.18 | 0.43 |
| 1:S4:213:ARG:HH21 | 1:S4:297:LYS:NZ | 2.17 | 0.43 |
| 2:S5:194:LEU:O | 2:S5:198:THR:OG1 | 2.32 | 0.43 |
| 2:S7:88:HIS:CG | 2:S7:89:PRO:HD2 | 2.53 | 0.43 |
| 1:S8:292:GLN:HG2 | 1:S8:298:ASN:HD22 | 1.82 | 0.43 |
| 2:S9:434:GLU:OE1 | 13:5I:67:LYS:NZ | 2.48 | 0.43 |
| 1:T0:145:SER:OG | 1:T0:188:SER:OG | 2.27 | 0.43 |
| 1:T0:278:SER:O | 1:T0:278:SER:OG | 2.32 | 0.43 |
| 1:T0:397:TRP:HZ2 | 2:T1:256:GLN:HB2 | 1.82 | 0.43 |
| 2:T1:33:ASP:HA | 2:T1:85:GLN:HB2 | 2.00 | 0.43 |
| 2:T1:423:GLU:OE1 | 17:5T:19:ARG:NH1 | 2.51 | 0.43 |
| 2:T3:121:ARG:HD2 | 2:T3:121:ARG:HA | 1.87 | 0.43 |
| 2:T3:167:LEU:HD21 | 2:T3:256:GLN:HE22 | 1.82 | 0.43 |
| 2:T5:174:SER:OG | 2:T5:207:GLU:HB2 | 2.18 | 0.43 |
| 1:T6:70:PRO:HG2 | 2:T7:2:ARG:NH1 | 2.32 | 0.43 |
| 2:T7:5:ILE:HG22 | 2:T7:64:ARG:HB3 | 2.01 | 0.43 |
| 2:T7:72:PRO:HD2 | 1:T8:2:ARG:HH12 | 1.84 | 0.43 |
| 2:T7:266:HIS:O | 2:T7:266:HIS:ND1 | 2.47 | 0.43 |
| 1:T8:109:GLY:HA2 | 1:T8:147:MET:SD | 2.58 | 0.43 |
| 1:U6:183:TYR:HB3 | 1:U6:398:TYR:HE2 | 1.83 | 0.43 |
| 1:U6:292:GLN:HA | 1:U6:295:ASP:OD2 | 2.17 | 0.43 |
| 2:U7:21:TRP:CZ3 | 2:U7:63:PRO:HB3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V1:236:SER:O | 2:V1:243:ARG:NH2 | 2.52 | 0.43 |
| 1:V4:21:TRP:CZ3 | 1:V4:61:PRO:HB3 | 2.53 | 0.43 |
| 1:V4:31:ASP:OD2 | 1:V4:33:THR:OG1 | 2.34 | 0.43 |
| 1:V4:232:VAL:CG1 | 1:V4:268:VAL:HG11 | 2.48 | 0.43 |
| 2:V7:275:ILE:HG13 | 2:V7:275:ILE:O | 2.18 | 0.43 |
| 2:V9:98:ASP:OD1 | 2:V9:100:ALA:N | 2.32 | 0.43 |
| 1:W4:197:ASP:HB3 | 1:W4:198:GLU:OE1 | 2.19 | 0.43 |
| 1:W4:203:ASP:N | 1:W4:203:ASP:OD1 | 2.50 | 0.43 |
| 1:W4:283:ALA:O | 1:W4:284:LEU:HD23 | 2.19 | 0.43 |
| 2:W5:56:THR:HG21 | 2:Y1:283:HIS:O | 2.18 | 0.43 |
| 2:W7:325:PRO:HA | 2:W7:328:VAL:HG12 | 2.01 | 0.43 |
| 2:W9:135:PHE:HB2 | 2:W9:166:LYS:HG2 | 2.00 | 0.43 |
| 1:X0:10:GLY:HA2 | 1:X0:143:THR:HG23 | 2.00 | 0.43 |
| 1:X2:121:ARG:NH2 | 1:X2:158:GLU:OE2 | 2.51 | 0.43 |
| 1:X2:267:MET:N | 1:X2:267:MET:SD | 2.92 | 0.43 |
| 2:X3:305:CYS:SG | 2:X3:306:ASP:N | 2.86 | 0.43 |
| 2:X3:392:ASP:OD2 | 2:X3:422:ARG:NH1 | 2.51 | 0.43 |
| 1:X6:282:ARG:HG2 | 1:X6:283:ALA:O | 2.18 | 0.43 |
| 1:X6:417:ASP:HA | 1:X6:420:SER:OG | 2.18 | 0.43 |
| 2:Y1:5:ILE:HD11 | 2:Y1:135:PHE:HE1 | 1.82 | 0.43 |
| 2:Y1:33:ASP:O | 2:Y1:60:LYS:NZ | 2.50 | 0.43 |
| 2:Y3:174:SER:HB2 | 2:Y3:177:VAL:O | 2.19 | 0.43 |
| 2:Y3:246:GLY:HA3 | 2:Y3:356:ASN:HA | 2.01 | 0.43 |
| 1:Y4:123:GLU:O | 1:Y4:126:SER:OG | 2.27 | 0.43 |
| 1:Y6:211:CYS:HB2 | 1:Y6:217:LEU:HD12 | 1.99 | 0.43 |
| 1:Y8:122:LYS:O | 1:Y8:126:SER:OG | 2.20 | 0.43 |
| 1:Y8:267:MET:HE1 | 1:Y8:303:ALA:O | 2.18 | 0.43 |
| 2:Z1:290:GLU:HA | 2:Z1:293:ASN:ND2 | 2.34 | 0.43 |
| 1:Z2:122:LYS:HD2 | 1:0I:292:GLN:HE22 | 1.84 | 0.43 |
| 2:Z3:151:SER:HB3 | 2:Z3:193:SER:OG | 2.18 | 0.43 |
| 2:Z5:166:LYS:HB2 | 2:Z5:199:ASP:OD2 | 2.18 | 0.43 |
| 1:Z6:8:GLN:HG3 | 1:Z6:136:CYS:SG | 2.58 | 0.43 |
| 1:Z6:183:TYR:HD2 | 1:Z6:398:TYR:HE2 | 1.66 | 0.43 |
| 1:Z6:403:MET:HE3 | 1:Z6:403:MET:HB2 | 1.75 | 0.43 |
| 2:Z7:12:ALA:O | 2:Z7:16:VAL:HG23 | 2.18 | 0.43 |
| 2:Z7:70:LEU:HB3 | 2:Z7:97:GLU:O | 2.18 | 0.43 |
| 2:Z7:73:THR:OG1 | 2:Z7:74:VAL:N | 2.51 | 0.43 |
| 2:Z9:88:HIS:HB3 | 2:0P:283:HIS:CE1 | 2.54 | 0.43 |
| 2:0B:305:CYS:HB3 | 2:0B:387:ILE:HD11 | 2.00 | 0.43 |
| 1:0C:240:LEU:HD11 | 1:0C:250:LEU:HD11 | 2.00 | 0.43 |
| 1:0C:297:LYS:HA | 1:0C:297:LYS:HD3 | 1.63 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0E:3:GLU:HB2 | 1:0E:130:LEU:HD13 | 2.00 | 0.43 |
| 1:0E:272:PRO:C | 1:0E:273:LEU:HD12 | 2.39 | 0.43 |
| 2:0F:338:LYS:HA | 2:0F:338:LYS:HD2 | 1.75 | 0.43 |
| 1:0G:314:SER:HA | 1:0G:350:LYS:O | 2.18 | 0.43 |
| 1:0I:268:VAL:O | 1:0I:300:MET:N | 2.41 | 0.43 |
| 2:0L:203:MET:HE3 | 2:0L:267:PHE:HB3 | 2.00 | 0.43 |
| 1:0M:233:MET:O | 1:0M:237:THR:HG22 | 2.18 | 0.43 |
| 2:0N:320:ARG:HD3 | 2:0N:360:PRO:HG3 | 1.99 | 0.43 |
| 1:0O:297:LYS:HD3 | 1:0O:297:LYS:HA | 1.78 | 0.43 |
| 2:0R:83:TYR:HB3 | 2:0R:86:LEU:HB3 | 2.01 | 0.43 |
| 2:0V:306:ASP:HB3 | 2:0V:309:HIS:HD2 | 1.82 | 0.43 |
| 2:0Z:54:SER:HB2 | 2:0Z:128:ASN:HD21 | 1.82 | 0.43 |
| 2:0Z:60:LYS:HD2 | 2:0Z:60:LYS:HA | 1.77 | 0.43 |
| 2:0Z:317:LEU:HB3 | 2:0Z:319:TYR:CE1 | 2.50 | 0.43 |
| 2:1B:172:TYR:CE2 | 2:1B:203:MET:HG2 | 2.53 | 0.43 |
| 1:1C:91:VAL:HG21 | 1:1C:116:VAL:HG22 | 2.00 | 0.43 |
| 2:1D:312:TYR:HB2 | 2:1D:343:PHE:HD1 | 1.84 | 0.43 |
| 1:1E:418:LEU:O | 1:1E:421:GLU:HG2 | 2.19 | 0.43 |
| 1:1G:203:ASP:OD1 | 1:1G:204:ASN:N | 2.52 | 0.43 |
| 1:1M:167:PHE:CE2 | 1:1M:233:MET:HG2 | 2.54 | 0.43 |
| 1:1O:123:GLU:O | 1:1O:126:SER:OG | 2.36 | 0.43 |
| 1:1Q:391:ARG:O | 1:1Q:391:ARG:CG | 2.66 | 0.43 |
| 2:1R:202:VAL:HG22 | 2:1R:268:MET:HB2 | 2.00 | 0.43 |
| 1:1S:198:GLU:HA | 1:1S:264:HIS:HB2 | 2.01 | 0.43 |
| 1:1U:359:LYS:NZ | 9:4Z:304:ALA:HB1 | 2.33 | 0.43 |
| 2:1X:65:CYS:SG | 2:1X:87:PHE:HE1 | 2.42 | 0.43 |
| 2:1Z:187:SER:OG | 2:1Z:391:LEU:HD21 | 2.18 | 0.43 |
| 2:2B:28:HIS:CE1 | 2:2B:49:PHE:HA | 2.53 | 0.43 |
| 1:2E:60:VAL:HG23 | 1:2E:84:ILE:O | 2.19 | 0.43 |
| 2:2F:185:TYR:HD2 | 2:2F:418:PHE:HE1 | 1.65 | 0.43 |
| 1:2G:156:ARG:NH1 | 1:2G:197:ASP:OD2 | 2.51 | 0.43 |
| 2:2H:212:ILE:O | 2:2H:216:SER:OG | 2.28 | 0.43 |
| 1:2I:145:SER:OG | 1:2I:146:GLY:N | 2.50 | 0.43 |
| 1:2K:273:LEU:H | 1:2K:292:GLN:HE22 | 1.66 | 0.43 |
| 2:2L:204:LEU:HD23 | 2:2L:204:LEU:HA | 1.81 | 0.43 |
| 1:2M:35:THR:OG1 | 1:2M:37:HIS:NE2 | 2.51 | 0.43 |
| 2:2N:203:MET:HE3 | 2:2N:267:PHE:CD1 | 2.50 | 0.43 |
| 2:2N:377:MET:O | 2:2N:378:ILE:HD13 | 2.18 | 0.43 |
| 2:2P:398:MET:HG3 | 1:2Q:346:PRO:HD2 | 2.00 | 0.43 |
| 1:2U:248:ALA:HA | 1:2U:252:LYS:HD2 | 2.00 | 0.43 |
| 1:2W:6:HIS:CE1 | 1:2W:8:GLN:HG2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2X:265:ILE:HD11 | 2:2X:435:VAL:HG21 | 1.99 | 0.43 |
| 2:2X:394:LYS:HB2 | 1:2Y:346:PRO:HG3 | 2.01 | 0.43 |
| 1:2Y:86:ARG:HB3 | 1:2Y:89:ASN:OD1 | 2.18 | 0.43 |
| 1:3A:198:GLU:HB3 | 1:3A:258:ILE:HD11 | 2.01 | 0.43 |
| 2:3B:237:SER:HA | 2:3B:320:ARG:HD2 | 2.01 | 0.43 |
| 1:3C:178:THR:OG1 | 1:3C:179:VAL:N | 2.51 | 0.43 |
| 1:3C:239:CYS:SG | 1:3C:248:ALA:N | 2.78 | 0.43 |
| 2:3F:266:HIS:O | 2:3F:266:HIS:ND1 | 2.51 | 0.43 |
| 2:3H:201:ALA:O | 2:3H:268:MET:HE1 | 2.18 | 0.43 |
| 1:3I:6:HIS:CE1 | 1:3I:8:GLN:HG2 | 2.53 | 0.43 |
| 1:3I:209:ASP:N | 1:3I:209:ASP:OD2 | 2.51 | 0.43 |
| 1:3K:86:ARG:HB3 | 1:3K:89:ASN:OD1 | 2.18 | 0.43 |
| 2:3N:205:ASP:OD1 | 2:3N:206:ASN:N | 2.45 | 0.43 |
| 1:3Q:4:ILE:HD11 | 1:3Q:134:GLN:HB2 | 1.99 | 0.43 |
| 1:3Q:31:ASP:OD2 | 1:3Q:33:THR:OG1 | 2.28 | 0.43 |
| 1:3S:334:GLN:NE2 | 1:3S:348:ASN:H | 2.15 | 0.43 |
| 3:3V:45:ARG:HB2 | 3:3V:45:ARG:CZ | 2.48 | 0.43 |
| 3:3V:93:LYS:HA | 3:3V:93:LYS:HD3 | 1.47 | 0.43 |
| 3:3Z:93:LYS:HD3 | 3:3Z:93:LYS:HA | 1.47 | 0.43 |
| 4:4A:94:LEU:HB2 | 4:4A:152:LEU:HD11 | 1.99 | 0.43 |
| 4:4C:1:MET:HG3 | 4:4C:2:PHE:HD1 | 1.83 | 0.43 |
| 3:4D:45:ARG:HD2 | 3:4D:48:ALA:HB2 | 1.99 | 0.43 |
| 3:4F:93:LYS:HD3 | 3:4F:93:LYS:HA | 1.47 | 0.43 |
| 6:4O:457:GLU:O | 6:4O:461:LYS:HG2 | 2.18 | 0.43 |
| 7:4R:106:ASP:OD1 | 7:4R:106:ASP:N | 2.51 | 0.43 |
| 7:4T:239:SER:HA | 31:7M:8:ASP:OD2 | 2.18 | 0.43 |
| 7:4U:155:GLU:OE2 | 33:7Q:155:ARG:NH2 | 2.51 | 0.43 |
| 8:4W:288:THR:O | 8:4W:292:MET:HG2 | 2.19 | 0.43 |
| 8:4W:400:GLN:O | 8:4W:403:LEU:HG | 2.17 | 0.43 |
| 10:5B:258:ILE:HG13 | 10:5B:259:GLU:N | 2.33 | 0.43 |
| 12:5F:274:ARG:HA | 12:5F:295:ARG:HD3 | 2.00 | 0.43 |
| 12:5F:340:ILE:HD11 | 12:5F:369:ALA:HB1 | 2.01 | 0.43 |
| 14:5L:150:THR:HG22 | 14:5L:166:ALA:HA | 2.00 | 0.43 |
| 14:5L:291:GLU:OE2 | 14:5L:317:ASN:ND2 | 2.51 | 0.43 |
| 14:5N:356:PHE:CZ | 14:5N:369:LEU:HD13 | 2.53 | 0.43 |
| 15:5O:334:LEU:HG | 30:7K:241:LYS:NZ | 2.33 | 0.43 |
| 18:5X:16:GLN:HG2 | 18:5X:114:LEU:HB3 | 2.01 | 0.43 |
| 21:6G:189:MET:HE2 | 21:6G:191:ARG:HD2 | 2.00 | 0.43 |
| 22:6J:204:PHE:HA | 22:6J:227:TYR:OH | 2.17 | 0.43 |
| 22:6M:138:ASP:HA | 22:6M:141:LYS:HG2 | 2.01 | 0.43 |
| 24:6T:96:LEU:HD11 | 24:6T:191:PHE:CE2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6T:481:LEU:C | 24:6T:482:ILE:HD12 | 2.39 | 0.43 |
| 24:6U:123:TYR:HE2 | 24:6U:163:PRO:HG3 | 1.84 | 0.43 |
| 24:6U:343:ARG:HB2 | 24:6U:345:ASP:OD2 | 2.17 | 0.43 |
| 24:6U:482:ILE:CG2 | 24:6U:497:PHE:HB3 | 2.47 | 0.43 |
| 24:6W:332:VAL:HG21 | 24:6W:342:PHE:HE1 | 1.83 | 0.43 |
| 24:6W:417:GLU:OE2 | 24:6W:417:GLU:N | 2.42 | 0.43 |
| 24:6X:280:ASP:HA | 24:6X:289:ARG:HB2 | 2.00 | 0.43 |
| 24:6Z:274:ARG:NE | 24:6Z:372:ASP:OD2 | 2.43 | 0.43 |
| 24:6Z:480:ASN:HD21 | 24:6Z:503:ILE:HD12 | 1.83 | 0.43 |
| 24:7A:45:LEU:HD23 | 24:7A:45:LEU:HA | 1.83 | 0.43 |
| 26:7D:58:ILE:H | 26:7D:58:ILE:CD1 | 2.06 | 0.43 |
| 27:7G:196:GLU:HB2 | 27:7G:199:ASN:OD1 | 2.18 | 0.43 |
| 30:7K:138:GLU:HG2 | 30:7K:138:GLU:O | 2.17 | 0.43 |
| 38:8B:197:THR:HG22 | 38:8B:199:THR:HG22 | 2.00 | 0.43 |
| 38:8D:220:VAL:HG13 | 38:8D:221:ARG:HG2 | 2.00 | 0.43 |
| 1:3:306:ARG:HH21 | 3:3X:60:PRO:HD2 | 1.81 | 0.43 |
| 1:B3:39:ASP:O | 18:5Z:119:ARG:NH1 | 2.52 | 0.43 |
| 2:G5:108:TYR:O | 2:G5:112:LYS:NZ | 2.30 | 0.43 |
| 1:G6:128:ASP:OD1 | 1:G6:128:ASP:N | 2.42 | 0.43 |
| 1:G6:285:THR:HB | 1:G6:287:PRO:HD2 | 2.00 | 0.43 |
| 2:G7:191:THR:HA | 2:G7:194:LEU:HB3 | 2.01 | 0.43 |
| 1:G8:272:PRO:HD3 | 1:G8:364:SER:HA | 2.00 | 0.43 |
| 2:G9:156:ARG:O | 2:G9:160:ASP:HB2 | 2.18 | 0.43 |
| 2:G9:409:VAL:HA | 2:G9:413:MET:O | 2.19 | 0.43 |
| 2:H1:327:ASP:OD1 | 2:H1:328:VAL:N | 2.51 | 0.43 |
| 1:H4:174:LYS:HB3 | 1:H4:174:LYS:HE2 | 1.76 | 0.43 |
| 1:H4:253:LEU:HD23 | 1:H4:253:LEU:HA | 1.93 | 0.43 |
| 1:H4:289:LEU:HD23 | 1:H4:365:ALA:HB2 | 2.00 | 0.43 |
| 1:H4:297:LYS:HA | 1:H4:297:LYS:HD3 | 1.81 | 0.43 |
| 2:H5:156:ARG:HA | 2:H5:159:VAL:HG12 | 2.00 | 0.43 |
| 2:H5:191:THR:HG21 | 2:H5:425:LEU:HD21 | 1.99 | 0.43 |
| 1:H6:219:THR:O | 1:H6:219:THR:HG23 | 2.18 | 0.43 |
| 2:H7:53:PHE:O | 2:H7:64:ARG:NH2 | 2.51 | 0.43 |
| 1:I2:66:MET:HE3 | 1:I2:66:MET:HB3 | 1.97 | 0.43 |
| 1:I4:415:MET:O | 1:I4:419:VAL:HG22 | 2.18 | 0.43 |
| 1:J0:260:PHE:HB2 | 1:J0:263:LEU:HD23 | 1.99 | 0.43 |
| 2:J1:235:ILE:O | 2:J1:239:THR:HG23 | 2.18 | 0.43 |
| 2:J3:320:ARG:HE | 2:J3:320:ARG:HB3 | 1.61 | 0.43 |
| 2:J5:335:ILE:HG23 | 2:J5:341:ILE:HD11 | 2.00 | 0.43 |
| 1:J8:221:THR:HG22 | 2:J9:324:VAL:HG12 | 1.99 | 0.43 |
| 1:J8:395:LEU:O | 1:J8:399:THR:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J9:42:ILE:HG22 | 2:J9:43:GLY:N | 2.30 | 0.43 |
| 2:J9:200:VAL:HG13 | 2:J9:268:MET:CE | 2.49 | 0.43 |
| 1:K0:48:ASN:N | 1:K0:48:ASN:OD1 | 2.52 | 0.43 |
| 2:K3:53:PHE:HB3 | 2:K3:61:HIS:HB3 | 2.00 | 0.43 |
| 2:K3:76:ASP:OD2 | 1:K4:46:ARG:NH2 | 2.51 | 0.43 |
| 2:K3:221:ARG:HB3 | 1:K4:322:SER:HB2 | 1.98 | 0.43 |
| 1:K6:173:PRO:HB3 | 1:K6:384:GLN:HE22 | 1.83 | 0.43 |
| 2:L3:116:ASP:OD2 | 2:L3:116:ASP:N | 2.51 | 0.43 |
| 1:L4:337:ASN:HB3 | 1:L4:340:TYR:HD2 | 1.83 | 0.43 |
| 2:L5:33:ASP:OD2 | 2:L5:35:GLN:NE2 | 2.51 | 0.43 |
| 2:L5:341:ILE:O | 2:L5:341:ILE:HG13 | 2.18 | 0.43 |
| 1:L6:304:ASP:OD2 | 1:L6:306:ARG:HG2 | 2.18 | 0.43 |
| 2:L7:8:HIS:CD2 | 2:L7:138:PHE:HD2 | 2.36 | 0.43 |
| 1:M4:229:ILE:HG22 | 1:M4:233:MET:SD | 2.58 | 0.43 |
| 2:N1:223:THR:HG1 | 1:N2:245:GLN:HE22 | 1.61 | 0.43 |
| 2:N3:173:PRO:HB3 | 2:N3:183:GLU:OE2 | 2.18 | 0.43 |
| 2:N7:344:VAL:HG22 | 2:N7:346:TRP:H | 1.82 | 0.43 |
| 1:N8:150:LEU:O | 1:N8:154:LYS:HG2 | 2.18 | 0.43 |
| 1:O0:202:LEU:CD2 | 1:O0:229:ILE:HG12 | 2.48 | 0.43 |
| 2:O1:21:TRP:CZ3 | 2:O1:63:PRO:HB3 | 2.52 | 0.43 |
| 1:O6:4:ILE:HB | 1:O6:50:TYR:HE1 | 1.83 | 0.43 |
| 1:O6:138:SER:OG | 1:O6:139:LEU:N | 2.51 | 0.43 |
| 1:O8:350:LYS:NZ | 1:O8:352:SER:HB2 | 2.33 | 0.43 |
| 1:P4:126:SER:HA | 1:R0:291:GLN:HE22 | 1.84 | 0.43 |
| 2:P5:151:SER:O | 2:P5:155:GLU:HG2 | 2.18 | 0.43 |
| 1:P6:69:GLU:C | 1:P6:92:PHE:HZ | 2.22 | 0.43 |
| 2:P7:75:VAL:HG12 | 2:P7:79:ARG:HE | 1.82 | 0.43 |
| 2:P9:90:GLU:HB3 | 2:P9:121:ARG:NH1 | 2.26 | 0.43 |
| 1:Q0:122:LYS:NZ | 1:R6:291:GLN:O | 2.51 | 0.43 |
| 1:Q0:325:GLU:O | 1:Q0:329:GLN:HG2 | 2.19 | 0.43 |
| 1:Q2:83:GLN:O | 1:R8:281:TYR:OH | 2.22 | 0.43 |
| 1:Q2:384:GLN:HG2 | 2:Q3:348:PRO:HB3 | 2.00 | 0.43 |
| 2:Q5:223:THR:HG22 | 2:Q5:224:TYR:N | 2.34 | 0.43 |
| 1:Q8:11:GLN:HE22 | 2:Q9:249:ASN:H | 1.65 | 0.43 |
| 2:R1:305:CYS:HB3 | 2:R1:387:ILE:HD11 | 2.00 | 0.43 |
| 1:R2:42:LEU:HD12 | 1:R2:42:LEU:HA | 1.83 | 0.43 |
| 2:R3:325:PRO:HA | 2:R3:328:VAL:HG22 | 2.01 | 0.43 |
| 2:R5:288:VAL:HG11 | 2:R5:328:VAL:HG12 | 2.00 | 0.43 |
| 1:S0:92:PHE:CE2 | 24:6Z:40:GLN:CD | 2.80 | 0.43 |
| 1:S2:89:ASN:ND2 | 1:S2:123:GLU:OE2 | 2.51 | 0.43 |
| 1:S2:424:GLN:NE2 | 17:5V:104:PHE:HB2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S5:306:ASP:HB3 | 2:S5:309:HIS:CD2 | 2.54 | 0.43 |
| 1:S6:132:GLY:HA2 | 1:S6:162:ARG:HB3 | 2.00 | 0.43 |
| 1:S6:295:ASP:OD1 | 13:5H:105:GLY:HA3 | 2.19 | 0.43 |
| 2:S9:62:VAL:HG23 | 2:S9:62:VAL:O | 2.18 | 0.43 |
| 2:T3:305:CYS:SG | 2:T3:306:ASP:N | 2.91 | 0.43 |
| 1:T6:286:VAL:HG23 | 1:T6:287:PRO:HD3 | 2.01 | 0.43 |
| 2:T7:403:ALA:HB2 | 1:T8:344:TRP:HZ3 | 1.84 | 0.43 |
| 1:U8:6:HIS:CE1 | 1:U8:136:CYS:HG | 2.37 | 0.43 |
| 1:V0:117:LEU:HA | 1:V0:120:VAL:HG12 | 2.00 | 0.43 |
| 2:V1:119:LEU:HD23 | 2:V1:119:LEU:HA | 1.75 | 0.43 |
| 2:V9:246:GLY:HA3 | 2:V9:356:ASN:HA | 2.00 | 0.43 |
| 1:W0:208:TYR:CE1 | 1:W0:225:LEU:HD11 | 2.53 | 0.43 |
| 2:W5:72:PRO:HG3 | 1:W6:1:MET:HG2 | 2.00 | 0.43 |
| 2:W5:238:LEU:HD13 | 2:W5:318:MET:HE1 | 1.99 | 0.43 |
| 2:W5:417:GLU:HA | 2:W5:420:GLU:HG2 | 2.01 | 0.43 |
| 1:W6:3:GLU:HB2 | 1:W6:130:LEU:HA | 2.00 | 0.43 |
| 2:W9:113:GLU:OE1 | 2:W9:113:GLU:N | 2.50 | 0.43 |
| 1:X0:163:MET:HB3 | 1:X0:250:LEU:HD22 | 1.99 | 0.43 |
| 1:X0:174:LYS:HD2 | 1:X0:174:LYS:H | 1.84 | 0.43 |
| 1:X2:24:VAL:HG11 | 1:X2:50:TYR:HD2 | 1.83 | 0.43 |
| 1:X2:234:SER:HA | 1:X2:237:THR:HG22 | 2.01 | 0.43 |
| 1:X8:21:TRP:CZ3 | 1:X8:61:PRO:HB3 | 2.53 | 0.43 |
| 1:Y2:22:GLU:HG2 | 1:Y2:81:TYR:CD1 | 2.54 | 0.43 |
| 1:Y4:50:TYR:HE2 | 1:Y4:241:ARG:HD3 | 1.80 | 0.43 |
| 1:Y4:406:MET:N | 1:Y4:406:MET:SD | 2.92 | 0.43 |
| 2:Y9:232:ALA:HA | 2:Y9:235:ILE:HG22 | 2.01 | 0.43 |
| 2:Z1:68:LEU:HA | 2:Z1:93:ILE:O | 2.18 | 0.43 |
| 1:Z4:67:ASP:N | 1:Z4:67:ASP:OD1 | 2.52 | 0.43 |
| 2:Z5:121:ARG:HA | 2:Z5:121:ARG:HE | 1.82 | 0.43 |
| 2:Z5:223:THR:HG23 | 2:Z5:225:THR:N | 2.32 | 0.43 |
| 2:Z7:187:SER:O | 2:Z7:191:THR:HG23 | 2.19 | 0.43 |
| 1:0A:50:TYR:CD2 | 1:0A:241:ARG:HD3 | 2.54 | 0.43 |
| 2:0B:417:GLU:HA | 2:0B:420:GLU:HG2 | 2.01 | 0.43 |
| 1:0C:120:VAL:HA | 1:0C:123:GLU:HG3 | 2.00 | 0.43 |
| 2:0H:239:THR:O | 2:0H:242:LEU:HG | 2.19 | 0.43 |
| 2:0H:337:THR:O | 2:0H:339:ARG:NH1 | 2.52 | 0.43 |
| 1:0K:272:PRO:HB2 | 1:0K:282:ARG:NH1 | 2.34 | 0.43 |
| 2:0L:349:THR:HG23 | 2:0L:349:THR:O | 2.19 | 0.43 |
| 1:0M:156:ARG:HA | 1:0M:156:ARG:HD2 | 1.83 | 0.43 |
| 2:0N:102:ASN:ND2 | 2:0N:105:ARG:HB2 | 2.33 | 0.43 |
| 2:0N:207:GLU:HG3 | 2:0N:304:LYS:HD2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Q:286:VAL:CG2 | 1:0Q:287:PRO:HD3 | 2.48 | 0.43 |
| 1:0Q:317:PHE:HE2 | 1:0Q:326:VAL:HG13 | 1.83 | 0.43 |
| 1:0S:62:ARG:HG3 | 1:0S:123:GLU:OE2 | 2.19 | 0.43 |
| 1:0U:17:GLY:HA2 | 1:0U:20:PHE:HB3 | 2.00 | 0.43 |
| 1:0U:415:MET:O | 1:0U:419:VAL:HG22 | 2.17 | 0.43 |
| 1:0W:396:HIS:H | 1:0W:396:HIS:CD2 | 2.36 | 0.43 |
| 2:0Z:253:THR:HA | 2:0Z:256:GLN:HE22 | 1.83 | 0.43 |
| 2:0Z:333:ALA:O | 2:0Z:337:THR:HG23 | 2.18 | 0.43 |
| 1:1A:414:ASN:HA | 1:1A:417:ASP:OD2 | 2.19 | 0.43 |
| 1:1C:7:ILE:HB | 1:1C:135:VAL:HG22 | 2.01 | 0.43 |
| 1:1C:330:MET:SD | 1:1C:331:LEU:N | 2.92 | 0.43 |
| 1:1E:49:VAL:HG11 | 1:1E:241:ARG:HG2 | 2.01 | 0.43 |
| 1:1E:318:ARG:HG2 | 1:1E:354:CYS:SG | 2.58 | 0.43 |
| 2:1F:196:GLU:OE2 | 2:1F:197:HIS:NE2 | 2.51 | 0.43 |
| 2:1H:238:LEU:HD12 | 2:1H:239:THR:HG23 | 2.00 | 0.43 |
| 1:1M:117:LEU:HA | 1:1M:120:VAL:HG12 | 2.00 | 0.43 |
| 2:1P:191:THR:HG21 | 2:1P:425:LEU:HD21 | 2.00 | 0.43 |
| 1:1S:200:MET:HE1 | 1:1S:368:ILE:HG12 | 2.01 | 0.43 |
| 2:1T:167:LEU:HD13 | 2:1T:200:VAL:HB | 2.01 | 0.43 |
| 2:1X:204:LEU:HD23 | 2:1X:231:ILE:HD12 | 2.01 | 0.43 |
| 2:2F:72:PRO:HD2 | 1:2G:2:ARG:NH1 | 2.33 | 0.43 |
| 2:2F:212:ILE:O | 2:2F:216:SER:OG | 2.31 | 0.43 |
| 2:2H:76:ASP:OD2 | 1:2I:46:ARG:NH2 | 2.51 | 0.43 |
| 2:2H:204:LEU:HD12 | 2:2H:204:LEU:HA | 1.91 | 0.43 |
| 1:2I:99:ASN:ND2 | 2:2J:254:GLU:OE1 | 2.52 | 0.43 |
| 1:2I:177:ASP:N | 1:2I:181:GLU:OE2 | 2.51 | 0.43 |
| 2:2P:220:GLU:H | 2:2P:220:GLU:CD | 2.21 | 0.43 |
| 2:2P:282:TYR:OH | 10:5C:163:ARG:HB3 | 2.19 | 0.43 |
| 2:2R:280:LYS:HA | 2:2R:283:HIS:HB3 | 2.01 | 0.43 |
| 1:2S:68:LEU:HD21 | 1:2S:112:LEU:HD22 | 2.01 | 0.43 |
| 2:2T:298:PRO:HA | 2:2T:301:MET:CG | 2.49 | 0.43 |
| 2:2V:88:HIS:HB3 | 2:3L:283:HIS:HB2 | 2.01 | 0.43 |
| 1:2W:21:TRP:CZ3 | 1:2W:61:PRO:HB3 | 2.53 | 0.43 |
| 1:2Y:317:PHE:HB3 | 1:2Y:321:MET:HE3 | 2.01 | 0.43 |
| 1:3A:77:ARG:CZ | 38:8D:220:VAL:HA | 2.49 | 0.43 |
| 1:3C:170:VAL:N | 1:3C:202:LEU:O | 2.47 | 0.43 |
| 1:3C:250:LEU:HD12 | 1:3C:250:LEU:HA | 1.84 | 0.43 |
| 1:3G:52:ASN:HD21 | 1:3G:62:ARG:HG3 | 1.84 | 0.43 |
| 1:3G:170:VAL:HG22 | 1:3G:202:LEU:O | 2.18 | 0.43 |
| 1:3G:202:LEU:CD2 | 1:3G:229:ILE:HG12 | 2.48 | 0.43 |
| 2:3H:175:PRO:HG2 | 2:3H:176:GLN:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3I:90:PHE:HB2 | 3:3Z:19:LEU:HD13 | 2.01 | 0.43 |
| 1:3M:88:ASP:OD2 | 3:4D:262:TYR:HB3 | 2.17 | 0.43 |
| 1:3M:268:VAL:HG23 | 1:3M:300:MET:HB2 | 2.01 | 0.43 |
| 1:3M:391:ARG:HH11 | 2:3N:346:TRP:HE3 | 1.66 | 0.43 |
| 2:3N:130:THR:HG23 | 2:3N:131:GLY:N | 2.33 | 0.43 |
| 1:3O:391:ARG:HB2 | 2:3P:346:TRP:CH2 | 2.54 | 0.43 |
| 2:3R:195:LEU:HD21 | 2:3R:264:ARG:HH11 | 1.83 | 0.43 |
| 1:3S:246:LEU:HD22 | 1:3S:352:SER:HA | 2.00 | 0.43 |
| 4:3W:1:MET:HG3 | 4:3W:2:PHE:HD1 | 1.83 | 0.43 |
| 4:4A:1:MET:HG3 | 4:4A:2:PHE:HD1 | 1.83 | 0.43 |
| 4:4E:94:LEU:HB2 | 4:4E:152:LEU:HD11 | 1.99 | 0.43 |
| 3:4H:45:ARG:HD2 | 3:4H:48:ALA:HB2 | 1.99 | 0.43 |
| 3:4J:282:GLU:HB3 | 3:4J:283:GLN:HE21 | 1.82 | 0.43 |
| 6:4O:103:ARG:HD2 | 6:4O:103:ARG:HA | 1.70 | 0.43 |
| 6:4O:146:LYS:HB3 | 6:4O:146:LYS:HE2 | 1.77 | 0.43 |
| 6:4O:351:LYS:HE3 | 6:4O:351:LYS:HB3 | 1.93 | 0.43 |
| 7:4R:63:ASP:O | 7:4R:67:THR:HG23 | 2.19 | 0.43 |
| 7:4R:116:VAL:HG12 | 21:6G:37:ILE:HG12 | 2.01 | 0.43 |
| 8:4V:400:GLN:O | 8:4V:403:LEU:HG | 2.19 | 0.43 |
| 8:4W:229:GLU:O | 8:4W:233:LYS:HG3 | 2.18 | 0.43 |
| 10:5C:243:LEU:O | 10:5C:246:ILE:HG12 | 2.19 | 0.43 |
| 12:5F:44:ILE:HG23 | 12:5F:44:ILE:O | 2.17 | 0.43 |
| 14:5L:415:LYS:HE3 | 14:5L:415:LYS:HB3 | 1.49 | 0.43 |
| 14:5M:509:ALA:HB2 | 14:5M:513:PHE:CZ | 2.54 | 0.43 |
| 14:5N:190:LEU:CD1 | 14:5N:228:PHE:HB3 | 2.48 | 0.43 |
| 14:5N:509:ALA:HB3 | 14:5N:513:PHE:CZ | 2.54 | 0.43 |
| 15:5P:52:TYR:C | 15:5P:54:GLU:H | 2.21 | 0.43 |
| 19:6E:67:HIS:HE1 | 19:6E:72:GLU:HG3 | 1.84 | 0.43 |
| 22:6J:134:ASN:HD21 | 24:6T:440:ASN:HD21 | 1.66 | 0.43 |
| 22:6M:216:MET:N | 22:6M:216:MET:SD | 2.89 | 0.43 |
| 24:6T:257:LEU:HD12 | 24:6T:257:LEU:HA | 1.76 | 0.43 |
| 24:6T:469:PHE:CB | 24:6T:484:GLU:HA | 2.48 | 0.43 |
| 24:6U:121:LEU:HD11 | 24:6U:130:MET:HE1 | 2.00 | 0.43 |
| 24:6U:490:THR:HG22 | 24:6U:492:ILE:HG12 | 2.01 | 0.43 |
| 24:6V:106:VAL:HG12 | 24:6V:113:ASN:C | 2.39 | 0.43 |
| 24:6W:152:ARG:HD3 | 24:6W:160:PHE:CG | 2.53 | 0.43 |
| 24:6W:473:TYR:OH | 24:6W:478:ASP:OD1 | 2.33 | 0.43 |
| 24:6Y:436:HIS:O | 24:6Y:440:ASN:ND2 | 2.52 | 0.43 |
| 27:7G:130:THR:O | 27:7G:130:THR:OG1 | 2.37 | 0.43 |
| 29:7J:134:SER:O | 29:7J:137:VAL:HG12 | 2.19 | 0.43 |
| 29:7J:232:ASP:OD1 | 29:7J:233:LYS:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:7K:201:TRP:CD2 | 30:7K:208:PRO:HG3 | 2.53 | 0.43 |
| 35:7U:107:THR:HA | 35:7U:110:THR:HG22 | 1.99 | 0.43 |
| 37:7Y:59:PRO:O | 37:7Y:60:LYS:C | 2.54 | 0.43 |
| 37:7Y:74:LEU:O | 37:7Y:78:VAL:HG23 | 2.18 | 0.43 |
| 38:8C:61:LYS:HB2 | 38:8C:61:LYS:HE2 | 1.59 | 0.43 |
| 1:1:306:ARG:HH21 | 3:3V:60:PRO:HD2 | 1.81 | 0.43 |
| 1:3:306:ARG:HD3 | 3:3X:69:TYR:CE1 | 2.53 | 0.43 |
| 2:4:280:LYS:NZ | 26:7D:64:PRO:CG | 2.79 | 0.43 |
| 2:8:372:GLN:NE2 | 24:6W:88:TRP:CD2 | 2.87 | 0.43 |
| 2:A2:18:ASN:O | 26:7F:114:PRO:CB | 2.65 | 0.43 |
| 1:A3:78:SER:O | 24:6Z:148:ILE:HA | 2.19 | 0.43 |
| 2:E9:88:HIS:CE1 | 2:G5:280:LYS:HA | 2.52 | 0.43 |
| 1:G2:31:ASP:OD1 | 1:G2:34:GLY:N | 2.52 | 0.43 |
| 1:G6:198:GLU:HA | 1:G6:264:HIS:HB2 | 2.01 | 0.43 |
| 1:G6:313:ALA:HA | 1:G6:369:GLY:HA2 | 2.00 | 0.43 |
| 1:G6:314:SER:OG | 1:G6:368:ILE:O | 2.30 | 0.43 |
| 2:G7:155:GLU:HB2 | 2:G7:197:HIS:CE1 | 2.53 | 0.43 |
| 1:G8:91:VAL:CG2 | 1:G8:116:VAL:HG12 | 2.47 | 0.43 |
| 2:G9:198:THR:HG21 | 2:G9:201:ALA:HB2 | 2.00 | 0.43 |
| 2:G9:223:THR:OG1 | 2:G9:224:TYR:N | 2.52 | 0.43 |
| 2:H1:74:VAL:O | 2:H1:78:VAL:HG23 | 2.19 | 0.43 |
| 1:H2:228:LEU:HD23 | 1:H2:228:LEU:HA | 1.82 | 0.43 |
| 1:H2:289:LEU:HD21 | 1:H2:365:ALA:HB2 | 2.00 | 0.43 |
| 2:H3:66:ILE:O | 2:H3:66:ILE:HG13 | 2.19 | 0.43 |
| 1:H6:20:PHE:HA | 1:H6:230:SER:HB2 | 2.01 | 0.43 |
| 1:I0:167:PHE:CE2 | 1:I0:233:MET:HG2 | 2.53 | 0.43 |
| 2:I1:178:SER:OG | 1:I2:347:ASN:HB3 | 2.19 | 0.43 |
| 2:I1:218:ASP:OD2 | 2:I1:280:LYS:NZ | 2.52 | 0.43 |
| 1:I2:135:VAL:HG12 | 1:I2:137:HIS:HD2 | 1.84 | 0.43 |
| 2:I7:213:CYS:HA | 2:I7:217:LEU:HB2 | 1.99 | 0.43 |
| 1:J4:3:GLU:HG3 | 1:J4:127:CYS:HB2 | 1.99 | 0.43 |
| 2:J9:109:THR:OG1 | 2:J9:411:GLU:OE2 | 2.31 | 0.43 |
| 2:K3:90:GLU:HG2 | 2:K3:121:ARG:HH22 | 1.84 | 0.43 |
| 1:K6:77:ARG:HH21 | 1:K6:90:PHE:HD2 | 1.66 | 0.43 |
| 2:K9:31:GLN:HB2 | 2:K9:33:ASP:OD1 | 2.18 | 0.43 |
| 1:L0:49:VAL:HG11 | 1:L0:241:ARG:HG2 | 2.00 | 0.43 |
| 1:L0:220:PRO:HD2 | 2:L1:326:LYS:HD2 | 1.99 | 0.43 |
| 2:L5:329:ASN:HA | 2:L5:332:VAL:HG12 | 2.00 | 0.43 |
| 2:M3:229:ARG:NH1 | 2:M3:363:VAL:HG21 | 2.34 | 0.43 |
| 1:M4:304:ASP:HB3 | 1:M4:307:HIS:CG | 2.53 | 0.43 |
| 1:M6:75:SER:CB | 15:5P:48:LYS:NZ | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M8:5:VAL:HG23 | 1:M8:62:ARG:HG2 | 1.98 | 0.43 |
| 1:M8:285:THR:HG23 | 1:M8:288:GLU:H | 1.84 | 0.43 |
| 1:N0:393:ALA:C | 1:N0:395:LEU:N | 2.70 | 0.43 |
| 2:N1:102:ASN:HB3 | 2:N1:105:ARG:HB3 | 2.01 | 0.43 |
| 2:N3:27:GLU:OE1 | 2:N3:243:ARG:NH1 | 2.50 | 0.43 |
| 2:N3:377:MET:SD | 2:N3:379:SER:HB3 | 2.59 | 0.43 |
| 2:N5:73:THR:HG21 | 1:N6:2:ARG:HH22 | 1.84 | 0.43 |
| 2:N5:362:VAL:O | 32:7O:78:TYR:OH | 2.20 | 0.43 |
| 2:N5:407:TRP:O | 2:N5:411:GLU:HG2 | 2.18 | 0.43 |
| 1:N6:77:ARG:HD2 | 27:7G:165:PHE:HZ | 1.81 | 0.43 |
| 2:N7:12:ALA:O | 2:N7:16:VAL:HG23 | 2.18 | 0.43 |
| 2:N9:111:GLY:O | 2:N9:115:VAL:HG22 | 2.18 | 0.43 |
| 2:N9:306:ASP:HB3 | 2:N9:309:HIS:CD2 | 2.53 | 0.43 |
| 2:O1:229:ARG:NH2 | 37:7Y:241:THR:O | 2.51 | 0.43 |
| 1:O2:51:PHE:HB3 | 1:O2:59:TYR:HB3 | 2.00 | 0.43 |
| 2:O3:90:GLU:HB3 | 2:O3:121:ARG:NH1 | 2.34 | 0.43 |
| 2:O5:123:ARG:HH11 | 2:O5:123:ARG:CG | 2.30 | 0.43 |
| 1:O6:359:LYS:HD2 | 32:7P:110:GLN:HG2 | 2.00 | 0.43 |
| 2:O7:280:LYS:HA | 2:O7:283:HIS:HB3 | 2.01 | 0.43 |
| 2:O7:345:ASP:N | 2:O7:345:ASP:OD1 | 2.51 | 0.43 |
| 2:P3:210:TYR:HH | 2:P3:224:TYR:HE1 | 1.67 | 0.43 |
| 2:P7:56:THR:HG23 | 2:P7:60:LYS:HB3 | 2.01 | 0.43 |
| 2:P7:240:ALA:HB1 | 2:P7:356:ASN:HD22 | 1.83 | 0.43 |
| 1:Q0:55:THR:HG21 | 7:4R:178:VAL:HG21 | 2.00 | 0.43 |
| 1:Q2:334:GLN:NE2 | 1:Q2:348:ASN:H | 2.17 | 0.43 |
| 1:Q2:350:LYS:HZ1 | 1:Q2:352:SER:HB2 | 1.84 | 0.43 |
| 2:Q5:79:ARG:O | 2:Q5:84:ARG:HG2 | 2.18 | 0.43 |
| 1:Q8:310:TYR:O | 1:Q8:342:VAL:HG23 | 2.19 | 0.43 |
| 2:Q9:174:SER:HG | 2:Q9:207:GLU:H | 1.64 | 0.43 |
| 2:R5:164:LYS:HA | 2:R5:164:LYS:HD3 | 1.89 | 0.43 |
| 1:R6:27:GLU:OE1 | 1:R6:241:ARG:NH1 | 2.49 | 0.43 |
| 1:R6:173:PRO:HG3 | 1:R6:380:ARG:HD2 | 2.01 | 0.43 |
| 1:R6:211:CYS:HA | 1:R6:215:LEU:HB2 | 2.00 | 0.43 |
| 1:R6:309:ARG:H | 1:R6:372:THR:CG2 | 2.32 | 0.43 |
| 2:R7:313:MET:N | 2:R7:380:ASN:O | 2.45 | 0.43 |
| 2:R9:88:HIS:ND1 | 2:R9:90:GLU:OE2 | 2.52 | 0.43 |
| 1:S4:375:GLN:HB3 | 1:S4:422:TYR:CD2 | 2.54 | 0.43 |
| 2:S7:117:LEU:HA | 2:S7:120:ASP:OD1 | 2.18 | 0.43 |
| 2:T1:288:VAL:HG13 | 2:T1:319:TYR:HE2 | 1.82 | 0.43 |
| 1:T2:391:ARG:HG2 | 13:5J:55:VAL:HB | 2.01 | 0.43 |
| 2:T3:364:PRO:HG3 | 21:6H:66:PRO:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T5:296:PHE:HD2 | 2:T5:335:ILE:HD13 | 1.83 | 0.43 |
| 1:U4:5:VAL:HG22 | 1:U4:133:PHE:CD1 | 2.53 | 0.43 |
| 1:U4:331:LEU:O | 1:U4:335:ASN:ND2 | 2.52 | 0.43 |
| 1:U6:108:GLU:HA | 1:U6:111:GLU:OE2 | 2.18 | 0.43 |
| 2:U9:5:ILE:HG22 | 2:U9:64:ARG:HD3 | 2.01 | 0.43 |
| 2:U9:129:CYS:SG | 2:U9:130:THR:N | 2.92 | 0.43 |
| 1:V2:117:LEU:HD11 | 1:V2:154:LYS:HB3 | 1.99 | 0.43 |
| 1:V2:123:GLU:O | 1:V2:126:SER:OG | 2.36 | 0.43 |
| 2:V3:102:ASN:HB3 | 2:V3:105:ARG:HB3 | 2.00 | 0.43 |
| 1:V4:175:VAL:O | 1:V4:175:VAL:HG13 | 2.19 | 0.43 |
| 1:V4:324:LYS:O | 1:V4:328:GLU:HG3 | 2.18 | 0.43 |
| 1:V6:418:LEU:HB2 | 1:V6:422:TYR:HE2 | 1.83 | 0.43 |
| 2:W1:5:ILE:O | 2:W1:136:LEU:HD23 | 2.18 | 0.43 |
| 2:W1:422:ARG:NH1 | 2:W1:426:ALA:HB2 | 2.34 | 0.43 |
| 2:W3:236:SER:O | 2:W3:243:ARG:NH2 | 2.50 | 0.43 |
| 1:W4:83:GLN:N | 1:W4:83:GLN:OE1 | 2.51 | 0.43 |
| 2:W7:398:MET:CG | 1:W8:346:PRO:HD2 | 2.48 | 0.43 |
| 1:W8:173:PRO:HG2 | 1:W8:174:LYS:NZ | 2.33 | 0.43 |
| 2:W9:119:LEU:O | 2:W9:122:ILE:HG22 | 2.19 | 0.43 |
| 2:X3:184:PRO:HB2 | 2:X3:398:MET:HE1 | 2.00 | 0.43 |
| 1:X4:58:ARG:NH1 | 1:X4:84:ILE:HA | 2.34 | 0.43 |
| 1:X4:113:ILE:HD12 | 1:X4:150:LEU:HD13 | 2.01 | 0.43 |
| 1:X4:237:THR:HG23 | 1:X4:241:ARG:NH2 | 2.34 | 0.43 |
| 1:X4:406:MET:O | 1:X4:410:GLU:HG2 | 2.18 | 0.43 |
| 2:X5:70:LEU:HD11 | 2:X5:149:LEU:HD21 | 2.01 | 0.43 |
| 2:X5:107:HIS:CD2 | 2:X5:152:LEU:HB2 | 2.54 | 0.43 |
| 2:X7:420:GLU:HA | 2:X7:423:GLU:HG3 | 2.01 | 0.43 |
| 1:X8:111:GLU:OE1 | 1:X8:111:GLU:N | 2.52 | 0.43 |
| 1:X8:244:GLY:HA2 | 1:X8:355:ASP:CG | 2.39 | 0.43 |
| 1:X8:396:HIS:CE1 | 1:X8:397:TRP:CE2 | 3.06 | 0.43 |
| 2:Y1:290:GLU:OE1 | 2:Y1:290:GLU:N | 2.38 | 0.43 |
| 1:Y2:50:TYR:CE2 | 1:Y2:241:ARG:HD3 | 2.54 | 0.43 |
| 1:Y2:214:THR:OG1 | 1:Y2:215:LEU:N | 2.52 | 0.43 |
| 1:Y4:297:LYS:HA | 1:Y4:297:LYS:HD3 | 1.74 | 0.43 |
| 2:Y5:70:LEU:HB3 | 2:Y5:97:GLU:O | 2.19 | 0.43 |
| 2:Y9:90:GLU:OE1 | 2:0F:283:HIS:ND1 | 2.52 | 0.43 |
| 1:Z2:379:LYS:HA | 1:Z2:379:LYS:HD2 | 1.71 | 0.43 |
| 2:Z3:233:GLN:HG3 | 2:Z3:272:TYR:CZ | 2.53 | 0.43 |
| 2:Z3:252:ILE:HA | 2:Z3:255:PHE:CE2 | 2.53 | 0.43 |
| 2:Z3:271:SER:HB2 | 2:Z3:301:MET:HG2 | 2.01 | 0.43 |
| 2:Z3:275:ILE:O | 2:Z3:275:ILE:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z6:121:ARG:NH2 | 1:Z6:158:GLU:OE2 | 2.26 | 0.43 |
| 1:Z6:250:LEU:HA | 1:Z6:253:LEU:HD12 | 2.00 | 0.43 |
| 2:Z7:33:ASP:OD2 | 2:Z7:35:GLN:NE2 | 2.51 | 0.43 |
| 2:Z7:252:ILE:HA | 2:Z7:255:PHE:HE2 | 1.82 | 0.43 |
| 2:Z9:31:GLN:HB2 | 2:Z9:33:ASP:OD1 | 2.18 | 0.43 |
| 1:0C:48:ASN:OD1 | 1:0C:48:ASN:N | 2.52 | 0.43 |
| 1:0C:58:ARG:HA | 1:0C:58:ARG:HD2 | 1.84 | 0.43 |
| 1:0E:39:ASP:OD1 | 1:0E:39:ASP:N | 2.45 | 0.43 |
| 1:0E:135:VAL:HG21 | 1:0E:152:ILE:HD11 | 2.01 | 0.43 |
| 1:0E:267:MET:SD | 1:0E:299:MET:HB3 | 2.59 | 0.43 |
| 2:0H:403:ALA:HB2 | 1:0I:344:TRP:HZ3 | 1.83 | 0.43 |
| 1:0I:165:LEU:HB3 | 1:0I:167:PHE:CZ | 2.54 | 0.43 |
| 1:0M:150:LEU:HD12 | 1:0M:150:LEU:HA | 1.89 | 0.43 |
| 1:0M:350:LYS:NZ | 1:0M:352:SER:HB3 | 2.32 | 0.43 |
| 1:0O:378:PHE:HB3 | 1:0O:415:MET:SD | 2.58 | 0.43 |
| 2:0R:147:SER:OG | 2:0R:148:GLY:N | 2.52 | 0.43 |
| 2:0R:156:ARG:HA | 2:0R:159:VAL:HG22 | 1.99 | 0.43 |
| 2:0V:204:LEU:HD23 | 2:0V:231:ILE:HD12 | 2.00 | 0.43 |
| 2:0V:420:GLU:O | 2:0V:424:ASP:HB2 | 2.17 | 0.43 |
| 1:0W:162:ARG:HA | 1:0W:162:ARG:HD3 | 1.85 | 0.43 |
| 2:0X:402:ARG:HA | 2:0X:402:ARG:HD3 | 1.77 | 0.43 |
| 2:0Z:405:VAL:O | 2:0Z:409:VAL:HG22 | 2.17 | 0.43 |
| 2:1B:289:ALA:O | 2:1B:293:ASN:ND2 | 2.52 | 0.43 |
| 2:1D:266:HIS:ND1 | 2:1D:266:HIS:O | 2.51 | 0.43 |
| 1:1E:374:ILE:HD11 | 1:1E:422:TYR:CZ | 2.54 | 0.43 |
| 1:1G:313:ALA:HB1 | 1:1G:367:PHE:HE1 | 1.83 | 0.43 |
| 1:1K:5:VAL:HG12 | 1:1K:133:PHE:HD1 | 1.83 | 0.43 |
| 2:1L:69:ASP:OD1 | 2:1L:70:LEU:N | 2.51 | 0.43 |
| 2:1N:305:CYS:SG | 2:1N:306:ASP:N | 2.90 | 0.43 |
| 2:1N:387:ILE:HG23 | 2:1N:390:ARG:NH2 | 2.34 | 0.43 |
| 1:1O:170:VAL:N | 1:1O:202:LEU:O | 2.41 | 0.43 |
| 1:1Q:212:PHE:HZ | 2:1R:326:LYS:HG3 | 1.83 | 0.43 |
| 2:1R:402:ARG:HA | 2:1R:402:ARG:HD3 | 1.80 | 0.43 |
| 2:1T:361:THR:HA | 2:1T:370:LYS:NZ | 2.33 | 0.43 |
| 1:1W:244:GLY:N | 1:1W:247:ASN:HD21 | 2.16 | 0.43 |
| 2:1Z:237:SER:HA | 2:1Z:320:ARG:HD2 | 1.99 | 0.43 |
| 1:2C:125:GLU:O | 38:8A:56:PRO:HD3 | 2.18 | 0.43 |
| 2:2D:88:HIS:CD2 | 2:2T:283:HIS:CD2 | 3.07 | 0.43 |
| 1:2M:68:LEU:HD23 | 1:2M:68:LEU:HA | 1.74 | 0.43 |
| 1:2Q:49:VAL:HG11 | 1:2Q:241:ARG:HG2 | 2.00 | 0.43 |
| 1:2S:163:MET:HB3 | 1:2S:250:LEU:HD22 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2V:414:GLU:OE1 | 2:2V:414:GLU:N | 2.51 | 0.43 |
| 1:2W:95:THR:HG23 | 1:2W:96:GLY:N | 2.33 | 0.43 |
| 1:2Y:105:HIS:CD2 | 1:2Y:150:LEU:HB2 | 2.53 | 0.43 |
| 1:2Y:391:ARG:HG3 | 2:2Z:262:TYR:OH | 2.19 | 0.43 |
| 2:2Z:312:TYR:HB2 | 2:2Z:343:PHE:CD1 | 2.54 | 0.43 |
| 1:3A:22:GLU:HG2 | 1:3A:81:TYR:CD1 | 2.53 | 0.43 |
| 2:3B:50:ASN:O | 2:3B:64:ARG:NH2 | 2.52 | 0.43 |
| 2:3F:88:HIS:HB3 | 2:3F:90:GLU:CD | 2.39 | 0.43 |
| 2:3F:205:ASP:OD2 | 2:3F:206:ASN:N | 2.51 | 0.43 |
| 1:3G:172:SER:HB2 | 1:3G:205:GLU:OE2 | 2.19 | 0.43 |
| 2:3H:27:GLU:OE1 | 2:3H:243:ARG:NH1 | 2.51 | 0.43 |
| 1:3I:170:VAL:HG22 | 1:3I:202:LEU:O | 2.18 | 0.43 |
| 1:3I:173:PRO:HG2 | 1:3I:380:ARG:HH21 | 1.84 | 0.43 |
| 2:3J:194:LEU:O | 2:3J:198:THR:OG1 | 2.37 | 0.43 |
| 2:3J:253:THR:O | 2:3J:257:THR:HG23 | 2.19 | 0.43 |
| 2:3J:280:LYS:O | 2:3J:283:HIS:HB3 | 2.19 | 0.43 |
| 2:3L:251:ASP:OD2 | 2:3L:254:GLU:HG2 | 2.19 | 0.43 |
| 1:3O:180:VAL:HB | 1:3O:183:TYR:HB2 | 2.01 | 0.43 |
| 1:3O:220:PRO:HG2 | 2:3P:326:LYS:HB2 | 2.01 | 0.43 |
| 1:3S:213:ARG:HH21 | 1:3S:297:LYS:HE3 | 1.82 | 0.43 |
| 4:4C:94:LEU:HB2 | 4:4C:152:LEU:HD11 | 1.99 | 0.43 |
| 4:4E:1:MET:HG3 | 4:4E:2:PHE:HD1 | 1.83 | 0.43 |
| 4:4I:1:MET:HG3 | 4:4I:2:PHE:HD1 | 1.83 | 0.43 |
| 5:4L:292:ALA:O | 5:4L:296:GLU:HG3 | 2.19 | 0.43 |
| 5:4M:286:LEU:HD13 | 28:7X:313:ALA:HA | 2.01 | 0.43 |
| 7:4Q:320:PHE:CG | 12:7B:91:LEU:HD12 | 2.53 | 0.43 |
| 7:4R:281:GLN:HA | 33:7Q:186:VAL:HG11 | 1.99 | 0.43 |
| 7:4T:332:LEU:HD23 | 7:4T:332:LEU:HA | 1.85 | 0.43 |
| 10:5C:256:ALA:O | 10:5C:259:GLU:HG3 | 2.18 | 0.43 |
| 11:5E:23:ARG:HH11 | 11:5E:23:ARG:HG2 | 1.83 | 0.43 |
| 12:5F:291:VAL:O | 12:5F:291:VAL:HG23 | 2.19 | 0.43 |
| 12:5F:356:THR:HG23 | 12:5F:368:GLU:OE2 | 2.18 | 0.43 |
| 14:5M:415:LYS:HE3 | 23:6R:23:ILE:HG13 | 2.00 | 0.43 |
| 14:5M:514:LYS:HG2 | 14:5M:557:ASN:HB3 | 2.00 | 0.43 |
| 15:5O:175:LEU:HD12 | 15:5O:175:LEU:HA | 1.88 | 0.43 |
| 15:5P:143:LYS:O | 15:5P:147:ASP:N | 2.48 | 0.43 |
| 17:5T:185:LEU:HD13 | 17:5T:222:ILE:CG1 | 2.49 | 0.43 |
| 19:6E:12:ASN:ND2 | 19:6E:17:VAL:HG23 | 2.33 | 0.43 |
| 20:6F:156:ASP:OD2 | 20:6F:156:ASP:N | 2.50 | 0.43 |
| 22:6I:96:LYS:HE3 | 22:6I:97:PRO:O | 2.18 | 0.43 |
| 22:6K:138:ASP:N | 22:6K:138:ASP:OD2 | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6L:271:ARG:O | 22:6L:275:LEU:HG | 2.18 | 0.43 |
| 22:6M:197:ASP:O | 22:6M:199:SER:N | 2.52 | 0.43 |
| 22:6O:279:LEU:O | 22:6O:283:ILE:HG13 | 2.18 | 0.43 |
| 24:6T:11:LEU:HD21 | 24:6T:14:TYR:CE2 | 2.53 | 0.43 |
| 24:6T:274:ARG:NE | 24:6T:372:ASP:OD2 | 2.38 | 0.43 |
| 24:6T:388:GLU:OE1 | 24:6T:389:GLU:HG3 | 2.18 | 0.43 |
| 24:6T:488:ARG:N | 24:6T:488:ARG:CD | 2.73 | 0.43 |
| 24:6U:91:ASN:O | 24:6U:126:GLU:HB2 | 2.18 | 0.43 |
| 24:6U:270:LYS:C | 24:6U:271:LYS:HD2 | 2.39 | 0.43 |
| 24:6W:574:ARG:O | 24:6W:578:ILE:HG12 | 2.19 | 0.43 |
| 24:6Y:185:ASP:O | 24:6Y:189:ARG:HG3 | 2.19 | 0.43 |
| 24:6Y:592:ASP:N | 24:6Y:592:ASP:OD1 | 2.52 | 0.43 |
| 12:7B:8:LYS:HE2 | 12:7B:8:LYS:HB3 | 1.83 | 0.43 |
| 29:7J:87:LYS:HA | 29:7J:92:TYR:CE2 | 2.53 | 0.43 |
| 29:7J:316:VAL:HG21 | 29:7J:326:ILE:CG2 | 2.47 | 0.43 |
| 29:7J:346:ARG:HG3 | 29:7J:347:PRO:HD2 | 2.00 | 0.43 |
| 34:7R:157:ARG:O | 34:7R:161:THR:HG23 | 2.18 | 0.43 |
| 35:7T:37:ARG:O | 35:7T:40:ILE:HG22 | 2.18 | 0.43 |
| 28:7X:451:LYS:HA | 28:7X:451:LYS:HD3 | 1.66 | 0.43 |
| 38:8A:26:THR:HG23 | 38:8A:27:HIS:CD2 | 2.53 | 0.43 |
| 38:8C:197:THR:HG23 | 38:8C:200:ALA:CB | 2.49 | 0.43 |
| 1:9:40:SER:C | 26:7E:25:TYR:HE2 | 2.22 | 0.43 |
| 1:G2:219:THR:N | 24:6W:418:ASP:OD1 | 2.48 | 0.43 |
| 1:G4:173:PRO:HD2 | 1:G4:380:ARG:HH21 | 1.83 | 0.43 |
| 2:G5:68:LEU:HD13 | 2:G5:93:ILE:HB | 2.01 | 0.43 |
| 2:G5:172:TYR:OH | 2:G5:191:THR:HG22 | 2.19 | 0.43 |
| 2:G7:127:ASP:OD2 | 2:I3:293:ASN:ND2 | 2.52 | 0.43 |
| 1:G8:177:ASP:OD1 | 39:G8:501:GDP:H3' | 2.17 | 0.43 |
| 1:G8:286:VAL:CG2 | 1:G8:287:PRO:HD3 | 2.49 | 0.43 |
| 2:G9:76:ASP:O | 2:G9:80:THR:HG22 | 2.18 | 0.43 |
| 2:G9:316:CYS:O | 2:G9:377:MET:HA | 2.19 | 0.43 |
| 2:H3:50:ASN:O | 2:H3:64:ARG:NH2 | 2.52 | 0.43 |
| 1:H4:117:LEU:HA | 1:H4:120:VAL:HG12 | 2.00 | 0.43 |
| 1:H6:86:ARG:HG2 | 1:H6:88:ASP:H | 1.82 | 0.43 |
| 1:H6:276:ARG:HD2 | 24:6V:490:THR:O | 2.15 | 0.43 |
| 1:H8:208:TYR:HA | 1:H8:211:CYS:SG | 2.59 | 0.43 |
| 2:I3:199:ASP:OD2 | 2:I3:256:GLN:NE2 | 2.51 | 0.43 |
| 1:I4:69:GLU:O | 1:I4:72:THR:OG1 | 2.37 | 0.43 |
| 2:I5:230:LEU:O | 2:I5:234:VAL:HG23 | 2.18 | 0.43 |
| 2:I7:266:HIS:O | 2:I7:266:HIS:ND1 | 2.47 | 0.43 |
| 1:I8:355:ASP:O | 1:I8:356:ILE:HD13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I9:73:THR:CG2 | 1:J0:2:ARG:HH22 | 2.32 | 0.43 |
| 1:J2:139:LEU:HG | 1:J2:168:SER:HB3 | 2.01 | 0.43 |
| 2:J3:178:SER:HB3 | 2:J3:183:GLU:OE2 | 2.19 | 0.43 |
| 1:J4:8:GLN:CD | 1:J4:17:GLY:HA3 | 2.38 | 0.43 |
| 2:J7:21:TRP:CZ3 | 2:J7:63:PRO:HB3 | 2.53 | 0.43 |
| 2:J7:282:TYR:HD1 | 5:4M:209:LEU:CD2 | 1.89 | 0.43 |
| 2:J9:141:VAL:O | 2:J9:147:SER:OG | 2.37 | 0.43 |
| 2:J9:397:LEU:HD23 | 2:J9:397:LEU:HA | 1.88 | 0.43 |
| 1:K0:287:PRO:HD3 | 1:K0:325:GLU:OE1 | 2.18 | 0.43 |
| 2:K1:136:LEU:HA | 2:K1:167:LEU:O | 2.19 | 0.43 |
| 1:K4:99:ASN:ND2 | 2:K5:254:GLU:OE1 | 2.51 | 0.43 |
| 1:K4:101:TRP:HD1 | 1:K4:145:SER:HG | 1.62 | 0.43 |
| 2:K7:7:ILE:HG12 | 2:K7:137:VAL:HG12 | 2.00 | 0.43 |
| 2:K7:151:SER:HB2 | 2:K7:193:SER:OG | 2.19 | 0.43 |
| 1:K8:4:ILE:HB | 1:K8:50:TYR:HE1 | 1.84 | 0.43 |
| 1:K8:39:ASP:OD1 | 1:K8:40:SER:N | 2.50 | 0.43 |
| 1:K8:139:LEU:HD22 | 1:K8:188:SER:OG | 2.17 | 0.43 |
| 2:K9:72:PRO:HD2 | 1:L0:2:ARG:NH1 | 2.33 | 0.43 |
| 2:K9:102:ASN:HB3 | 2:K9:105:ARG:HB3 | 2.00 | 0.43 |
| 1:L4:392:LYS:HD2 | 1:L4:395:LEU:HD22 | 2.00 | 0.43 |
| 1:L6:172:SER:HB3 | 1:L6:205:GLU:OE2 | 2.19 | 0.43 |
| 1:L6:175:VAL:HG13 | 2:L7:329:ASN:ND2 | 2.34 | 0.43 |
| 2:L7:233:GLN:HE22 | 2:L7:360:PRO:HB3 | 1.84 | 0.43 |
| 2:L9:205:ASP:OD1 | 2:L9:206:ASN:N | 2.48 | 0.43 |
| 2:M1:69:ASP:OD1 | 2:M1:71:GLU:HG2 | 2.18 | 0.43 |
| 2:M1:88:HIS:CE1 | 1:N8:280:GLN:HB2 | 2.53 | 0.43 |
| 2:M1:331:SER:O | 2:M1:334:THR:OG1 | 2.25 | 0.43 |
| 1:M2:117:LEU:HA | 1:M2:120:VAL:HG12 | 2.01 | 0.43 |
| 1:M2:183:TYR:HB3 | 1:M2:398:TYR:HE2 | 1.83 | 0.43 |
| 1:M2:406:MET:N | 1:M2:406:MET:SD | 2.91 | 0.43 |
| 2:M3:91:GLN:HG3 | 2:M3:121:ARG:NH2 | 2.33 | 0.43 |
| 2:M3:283:HIS:CD2 | 30:7K:199:TYR:HH | 2.29 | 0.43 |
| 1:M6:61:PRO:HD3 | 1:M6:84:ILE:HG12 | 2.00 | 0.43 |
| 1:M8:33:THR:O | 1:M8:58:ARG:NE | 2.50 | 0.43 |
| 1:M8:130:LEU:HB2 | 1:M8:162:ARG:HE | 1.83 | 0.43 |
| 2:M9:167:LEU:HD13 | 2:M9:200:VAL:HB | 2.00 | 0.43 |
| 2:M9:266:HIS:ND1 | 2:M9:266:HIS:O | 2.52 | 0.43 |
| 2:M9:397:LEU:HD23 | 2:M9:397:LEU:HA | 1.89 | 0.43 |
| 2:N1:279:GLU:HA | 2:N1:282:TYR:HB3 | 2.00 | 0.43 |
| 2:N7:380:ASN:OD1 | 2:N7:381:SER:N | 2.51 | 0.43 |
| 2:O5:358:GLN:NE2 | 19:6E:58:SER:HB2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O7:113:GLU:N | 2:O7:113:GLU:OE2 | 2.52 | 0.43 |
| 2:P3:91:GLN:NE2 | 2:P3:121:ARG:HH21 | 2.17 | 0.43 |
| 2:P3:287:SER:OG | 2:P3:288:VAL:N | 2.51 | 0.43 |
| 2:P3:317:LEU:HB3 | 2:P3:319:TYR:CE1 | 2.52 | 0.43 |
| 1:P4:220:PRO:HD2 | 2:P5:326:LYS:HD3 | 2.01 | 0.43 |
| 2:P7:223:THR:HG23 | 2:P7:225:THR:H | 1.84 | 0.43 |
| 1:P8:36:TYR:CD2 | 21:6G:163:THR:HG21 | 2.54 | 0.43 |
| 2:P9:5:ILE:HG22 | 2:P9:64:ARG:HB3 | 2.01 | 0.43 |
| 2:P9:274:PRO:HB2 | 2:P9:276:ILE:HG12 | 1.99 | 0.43 |
| 1:Q0:167:PHE:HE1 | 1:Q0:200:MET:SD | 2.42 | 0.43 |
| 2:Q1:312:TYR:HB2 | 2:Q1:343:PHE:HD1 | 1.83 | 0.43 |
| 1:Q2:54:ALA:HB3 | 1:Q2:58:ARG:HB2 | 2.00 | 0.43 |
| 1:Q2:344:TRP:CE3 | 1:Q2:345:ILE:HG13 | 2.53 | 0.43 |
| 1:Q4:30:ILE:CD1 | 1:Q4:59:TYR:HB2 | 2.48 | 0.43 |
| 1:Q4:39:ASP:OD1 | 1:Q4:39:ASP:N | 2.51 | 0.43 |
| 1:Q4:267:MET:HB2 | 1:Q4:301:CYS:SG | 2.58 | 0.43 |
| 2:Q5:305:CYS:HB3 | 2:Q5:387:ILE:HD11 | 1.99 | 0.43 |
| 1:Q6:371:SER:OG | 1:Q6:372:THR:N | 2.52 | 0.43 |
| 1:Q8:117:LEU:HD23 | 1:Q8:117:LEU:HA | 1.79 | 0.43 |
| 1:Q8:389:PHE:O | 1:Q8:392:LYS:NZ | 2.33 | 0.43 |
| 2:Q9:283:HIS:CE1 | 2:Q9:284:GLU:HB2 | 2.53 | 0.43 |
| 2:R1:53:PHE:O | 2:R1:64:ARG:NH2 | 2.50 | 0.43 |
| 2:R1:212:ILE:O | 2:R1:216:SER:OG | 2.33 | 0.43 |
| 2:R1:306:ASP:HB3 | 2:R1:309:HIS:CD2 | 2.54 | 0.43 |
| 1:R6:70:PRO:HD3 | 1:R6:92:PHE:HZ | 1.83 | 0.43 |
| 1:R8:54:ALA:HB3 | 1:R8:58:ARG:HB3 | 2.01 | 0.43 |
| 1:S0:320:ARG:HH12 | 12:5F:105:THR:HA | 1.84 | 0.43 |
| 1:S0:371:SER:OG | 1:S0:372:THR:N | 2.51 | 0.43 |
| 2:S1:175:PRO:HG2 | 2:S1:176:GLN:OE1 | 2.19 | 0.43 |
| 2:S5:175:PRO:HB3 | 2:S5:390:ARG:NE | 2.33 | 0.43 |
| 2:S7:42:ILE:HD11 | 12:5F:254:GLN:HG3 | 2.00 | 0.43 |
| 2:S9:5:ILE:HD11 | 2:S9:135:PHE:CE1 | 2.54 | 0.43 |
| 2:S9:90:GLU:HB3 | 2:S9:121:ARG:HH12 | 1.84 | 0.43 |
| 2:S9:123:ARG:NH2 | 2:S9:160:ASP:OD2 | 2.51 | 0.43 |
| 2:S9:206:ASN:OD1 | 41:S9:501:GTP:N2 | 2.52 | 0.43 |
| 2:S9:293:ASN:OD1 | 2:S9:338:LYS:NZ | 2.52 | 0.43 |
| 1:T2:391:ARG:HE | 2:T3:346:TRP:HZ2 | 1.66 | 0.43 |
| 2:T5:15:GLN:HB3 | 2:T5:228:ASN:HD21 | 1.84 | 0.43 |
| 2:T5:62:VAL:HG23 | 2:T5:62:VAL:O | 2.19 | 0.43 |
| 1:T6:396:HIS:CD2 | 1:T6:396:HIS:H | 2.36 | 0.43 |
| 2:T7:357:TYR:CD1 | 24:7A:20:GLN:HB3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T8:15:GLN:HB3 | 1:T8:226:ASN:ND2 | 2.34 | 0.43 |
| 2:U1:276:ILE:HG13 | 2:U1:280:LYS:HB2 | 2.00 | 0.43 |
| 2:U1:305:CYS:SG | 2:U1:383:ALA:HB1 | 2.59 | 0.43 |
| 1:U2:128:ASP:OD1 | 1:U2:128:ASP:N | 2.51 | 0.43 |
| 1:U4:61:PRO:HG2 | 1:U4:85:PHE:CE1 | 2.53 | 0.43 |
| 1:U4:69:GLU:C | 1:U4:92:PHE:HZ | 2.22 | 0.43 |
| 2:U7:88:HIS:HE1 | 2:W3:280:LYS:HB3 | 1.84 | 0.43 |
| 1:U8:4:ILE:HA | 1:U8:132:GLY:O | 2.19 | 0.43 |
| 2:V3:8:HIS:CD2 | 2:V3:138:PHE:HD2 | 2.36 | 0.43 |
| 1:V4:139:LEU:HD12 | 1:V4:170:VAL:HG12 | 2.00 | 0.43 |
| 1:V4:276:ARG:NH1 | 1:V4:279:GLN:HB3 | 2.34 | 0.43 |
| 2:V7:60:LYS:NZ | 2:V7:85:GLN:O | 2.46 | 0.43 |
| 1:V8:101:TRP:CE3 | 1:V8:403:MET:HE1 | 2.54 | 0.43 |
| 2:V9:90:GLU:OE1 | 2:V9:90:GLU:N | 2.48 | 0.43 |
| 1:W0:250:LEU:HD23 | 1:W0:250:LEU:HA | 1.74 | 0.43 |
| 1:W0:414:ASN:HA | 1:W0:417:ASP:OD2 | 2.19 | 0.43 |
| 2:W1:397:LEU:HD23 | 2:W1:397:LEU:HA | 1.84 | 0.43 |
| 1:W2:170:VAL:N | 1:W2:202:LEU:O | 2.44 | 0.43 |
| 1:W6:72:THR:O | 1:W6:76:VAL:HG23 | 2.19 | 0.43 |
| 1:W6:117:LEU:HD23 | 1:W6:117:LEU:HA | 1.85 | 0.43 |
| 2:W7:276:ILE:HD11 | 2:W7:281:ALA:CA | 2.42 | 0.43 |
| 1:X2:314:SER:HB2 | 1:X2:350:LYS:HB3 | 2.00 | 0.43 |
| 2:X3:267:PHE:HB3 | 2:X3:384:ILE:HG21 | 2.00 | 0.43 |
| 1:X4:199:CYS:SG | 1:X4:265:PHE:HD1 | 2.41 | 0.43 |
| 1:X6:131:GLN:HE21 | 1:X6:250:LEU:HD13 | 1.83 | 0.43 |
| 1:X6:198:GLU:HB3 | 1:X6:258:ILE:HD11 | 1.99 | 0.43 |
| 2:X7:406:HIS:HA | 2:X7:409:VAL:CG1 | 2.45 | 0.43 |
| 1:X8:46:ARG:HA | 1:X8:46:ARG:HD3 | 1.83 | 0.43 |
| 2:X9:286:LEU:O | 2:X9:286:LEU:HD13 | 2.18 | 0.43 |
| 1:Y0:208:TYR:CE1 | 1:Y0:225:LEU:HD11 | 2.53 | 0.43 |
| 1:Y0:358:PRO:HG3 | 1:Y0:364:SER:HB3 | 1.99 | 0.43 |
| 2:Y5:427:ALA:HA | 2:Y5:430:LYS:CD | 2.49 | 0.43 |
| 1:Y6:5:VAL:HG23 | 1:Y6:62:ARG:HG2 | 2.01 | 0.43 |
| 1:Y6:204:ASN:HD21 | 39:Y6:502:GDP:HN22 | 1.67 | 0.43 |
| 1:Z0:55:THR:H | 1:Z0:58:ARG:HB3 | 1.84 | 0.43 |
| 1:Z0:166:THR:OG1 | 1:Z0:199:CYS:HB3 | 2.19 | 0.43 |
| 1:Z0:379:LYS:HD3 | 1:Z0:419:VAL:CG2 | 2.39 | 0.43 |
| 1:Z2:91:VAL:HG21 | 1:Z2:116:VAL:HG22 | 2.00 | 0.43 |
| 1:Z2:180:VAL:HG23 | 1:Z2:184:ASN:ND2 | 2.34 | 0.43 |
| 2:Z3:183:GLU:CD | 2:Z3:184:PRO:HD3 | 2.39 | 0.43 |
| 2:Z3:272:TYR:O | 2:Z3:300:SER:OG | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z4:87:PRO:HA | 1:Z4:90:PHE:CD2 | 2.53 | 0.43 |
| 1:Z6:150:LEU:HD12 | 1:Z6:150:LEU:HA | 1.80 | 0.43 |
| 1:Z8:95:THR:OG1 | 1:Z8:96:GLY:N | 2.52 | 0.43 |
| 1:0A:8:GLN:OE1 | 1:0A:65:LEU:HD23 | 2.18 | 0.43 |
| 2:0B:99:ALA:HA | 2:0B:105:ARG:HD3 | 2.00 | 0.43 |
| 1:0C:116:VAL:O | 1:0C:120:VAL:HG22 | 2.18 | 0.43 |
| 1:0C:135:VAL:O | 1:0C:166:THR:HA | 2.19 | 0.43 |
| 1:0E:20:PHE:HA | 1:0E:230:SER:OG | 2.19 | 0.43 |
| 1:0E:297:LYS:HA | 1:0E:297:LYS:HD3 | 1.84 | 0.43 |
| 2:0F:21:TRP:CH2 | 2:0F:63:PRO:HB3 | 2.54 | 0.43 |
| 2:0F:286:LEU:HD13 | 2:0F:371:VAL:HG13 | 2.01 | 0.43 |
| 1:0G:270:PHE:HD2 | 1:0G:273:LEU:HD21 | 1.84 | 0.43 |
| 1:0I:237:THR:O | 1:0I:240:LEU:HG | 2.18 | 0.43 |
| 1:0I:372:THR:O | 1:0I:375:GLN:HG3 | 2.19 | 0.43 |
| 2:0J:221:ARG:HB3 | 1:0K:322:SER:OG | 2.18 | 0.43 |
| 2:0J:274:PRO:HB2 | 2:0J:276:ILE:HG12 | 2.01 | 0.43 |
| 2:0J:320:ARG:O | 2:0J:373:ARG:HA | 2.19 | 0.43 |
| 2:0L:175:PRO:HB3 | 2:0L:390:ARG:NE | 2.33 | 0.43 |
| 2:0N:9:ILE:HB | 2:0N:139:ASN:HB3 | 2.01 | 0.43 |
| 1:0O:95:THR:OG1 | 1:0O:96:GLY:N | 2.52 | 0.43 |
| 2:0P:341:ILE:HD13 | 2:0P:341:ILE:HA | 1.86 | 0.43 |
| 1:0Q:169:VAL:HG12 | 1:0Q:202:LEU:HB3 | 2.00 | 0.43 |
| 2:0R:175:PRO:O | 2:0R:394:LYS:NZ | 2.52 | 0.43 |
| 1:0U:156:ARG:HD2 | 1:0U:156:ARG:HA | 1.79 | 0.43 |
| 2:0V:170:THR:HG21 | 2:0V:194:LEU:HD11 | 2.00 | 0.43 |
| 1:0W:180:VAL:HG23 | 1:0W:184:ASN:HD21 | 1.84 | 0.43 |
| 1:0W:314:SER:HA | 1:0W:350:LYS:O | 2.18 | 0.43 |
| 2:0X:125:LEU:HD23 | 2:0X:125:LEU:HA | 1.79 | 0.43 |
| 2:0X:305:CYS:SG | 2:0X:306:ASP:N | 2.92 | 0.43 |
| 1:1A:270:PHE:CD1 | 1:1A:366:THR:HG22 | 2.53 | 0.43 |
| 2:1B:205:ASP:OD2 | 2:1B:206:ASN:N | 2.47 | 0.43 |
| 1:1C:3:GLU:O | 1:1C:4:ILE:HD13 | 2.18 | 0.43 |
| 1:1C:309:ARG:H | 1:1C:372:THR:HG22 | 1.84 | 0.43 |
| 1:1E:272:PRO:HA | 1:1E:292:GLN:OE1 | 2.19 | 0.43 |
| 1:1E:414:ASN:HA | 1:1E:417:ASP:OD2 | 2.19 | 0.43 |
| 1:1E:420:SER:O | 1:1E:423:GLN:HG3 | 2.19 | 0.43 |
| 2:1F:56:THR:HG21 | 2:1V:283:HIS:O | 2.19 | 0.43 |
| 1:1G:51:PHE:HB3 | 1:1G:59:TYR:HB3 | 2.01 | 0.43 |
| 1:1G:167:PHE:CE2 | 1:1G:233:MET:HG2 | 2.54 | 0.43 |
| 1:1G:315:ALA:HB1 | 1:1G:317:PHE:CE1 | 2.54 | 0.43 |
| 2:1L:21:TRP:CZ3 | 2:1L:63:PRO:HB3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1N:115:VAL:HG11 | 2:1N:152:LEU:HD23 | 2.01 | 0.43 |
| 1:1Q:309:ARG:NH1 | 1:1Q:339:SER:O | 2.51 | 0.43 |
| 1:1S:3:GLU:HB2 | 1:1S:130:LEU:HD13 | 2.00 | 0.43 |
| 1:1S:152:ILE:HD12 | 1:1S:164:MET:SD | 2.59 | 0.43 |
| 1:1S:173:PRO:HD2 | 1:1S:380:ARG:CZ | 2.49 | 0.43 |
| 1:1S:174:LYS:HB3 | 1:1S:174:LYS:HE2 | 1.79 | 0.43 |
| 1:1S:207:LEU:HB3 | 1:1S:225:LEU:HD22 | 2.00 | 0.43 |
| 2:1T:9:ILE:HG22 | 2:1T:146:GLY:HA2 | 2.00 | 0.43 |
| 2:1T:281:ALA:C | 2:1T:283:HIS:H | 2.22 | 0.43 |
| 1:1U:154:LYS:HA | 1:1U:154:LYS:HD3 | 1.86 | 0.43 |
| 2:1V:266:HIS:O | 2:1V:266:HIS:ND1 | 2.48 | 0.43 |
| 2:1X:34:GLY:HA3 | 2:1X:60:LYS:NZ | 2.32 | 0.43 |
| 2:1X:108:TYR:HA | 2:1X:112:LYS:NZ | 2.32 | 0.43 |
| 2:1X:111:GLY:O | 2:1X:115:VAL:HG12 | 2.18 | 0.43 |
| 2:1X:393:HIS:CE1 | 2:1X:397:LEU:HD21 | 2.53 | 0.43 |
| 1:2A:72:THR:O | 1:2A:75:SER:OG | 2.29 | 0.43 |
| 1:2A:113:ILE:HD12 | 1:2A:113:ILE:HA | 1.85 | 0.43 |
| 1:2A:313:ALA:HB1 | 1:2A:367:PHE:HE1 | 1.83 | 0.43 |
| 1:2C:297:LYS:HE3 | 1:2C:297:LYS:HB2 | 1.82 | 0.43 |
| 2:2D:325:PRO:HA | 2:2D:328:VAL:HG22 | 2.00 | 0.43 |
| 1:2E:314:SER:HA | 1:2E:350:LYS:O | 2.18 | 0.43 |
| 1:2K:72:THR:O | 1:2K:75:SER:OG | 2.28 | 0.43 |
| 1:2K:317:PHE:HB3 | 1:2K:321:MET:SD | 2.58 | 0.43 |
| 2:2L:21:TRP:CZ3 | 2:2L:63:PRO:HB3 | 2.54 | 0.43 |
| 2:2L:92:LEU:N | 2:2L:92:LEU:HD23 | 2.34 | 0.43 |
| 2:2L:204:LEU:CD2 | 2:2L:302:MET:HB3 | 2.49 | 0.43 |
| 1:2M:31:ASP:OD1 | 1:2M:35:THR:N | 2.45 | 0.43 |
| 1:2M:39:ASP:OD1 | 1:2M:39:ASP:N | 2.51 | 0.43 |
| 2:2N:7:ILE:HD11 | 2:2N:137:VAL:HG12 | 2.01 | 0.43 |
| 2:2N:11:GLN:OE1 | 2:2N:15:GLN:NE2 | 2.51 | 0.43 |
| 2:2N:246:GLY:HA2 | 2:2N:357:TYR:CD2 | 2.53 | 0.43 |
| 1:2Q:273:LEU:HD23 | 1:2Q:273:LEU:HA | 1.80 | 0.43 |
| 1:2S:173:PRO:HD2 | 1:2S:380:ARG:NH1 | 2.34 | 0.43 |
| 2:2X:40:LYS:HE3 | 2:2X:40:LYS:HB3 | 1.70 | 0.43 |
| 2:2Z:238:LEU:HD12 | 2:2Z:378:ILE:HD11 | 2.01 | 0.43 |
| 2:2Z:331:SER:O | 2:2Z:334:THR:OG1 | 2.28 | 0.43 |
| 1:3A:22:GLU:HG2 | 1:3A:81:TYR:HB2 | 2.00 | 0.43 |
| 1:3C:42:LEU:HG | 38:8D:192:ASN:OD1 | 2.19 | 0.43 |
| 2:3F:220:GLU:O | 1:3G:324:LYS:NZ | 2.44 | 0.43 |
| 2:3F:331:SER:O | 2:3F:334:THR:OG1 | 2.30 | 0.43 |
| 2:3H:66:ILE:O | 2:3H:66:ILE:HG13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3J:179:THR:O | 1:3K:350:LYS:HD2 | 2.19 | 0.43 |
| 1:3K:174:LYS:HE2 | 1:3K:174:LYS:HB3 | 1.81 | 0.43 |
| 2:3L:5:ILE:HD11 | 2:3L:135:PHE:HE1 | 1.83 | 0.43 |
| 1:3M:292:GLN:HG2 | 1:3M:298:ASN:ND2 | 2.34 | 0.43 |
| 2:3N:17:GLY:HA2 | 2:3N:20:CYS:HB2 | 2.01 | 0.43 |
| 2:3N:153:LEU:HA | 2:3N:153:LEU:HD12 | 1.85 | 0.43 |
| 1:3O:90:PHE:HB2 | 3:4F:19:LEU:HD13 | 2.00 | 0.43 |
| 1:3O:100:ASN:HB3 | 1:3O:103:LYS:HB2 | 1.99 | 0.43 |
| 2:3P:53:PHE:HB3 | 2:3P:61:HIS:HB3 | 2.00 | 0.43 |
| 2:3P:312:TYR:HB2 | 2:3P:343:PHE:CD1 | 2.54 | 0.43 |
| 2:3R:36:MET:HG3 | 2:3R:41:THR:HG22 | 2.01 | 0.43 |
| 1:3S:203:ASP:N | 1:3S:203:ASP:OD1 | 2.52 | 0.43 |
| 2:3T:235:ILE:HD13 | 2:3T:238:LEU:HD21 | 1.99 | 0.43 |
| 4:3W:94:LEU:HB2 | 4:3W:152:LEU:HD11 | 1.99 | 0.43 |
| 4:4I:94:LEU:HB2 | 4:4I:152:LEU:HD11 | 1.99 | 0.43 |
| 5:4M:55:GLN:NE2 | 5:4M:59:ASP:OD2 | 2.51 | 0.43 |
| 9:4Z:343:ALA:O | 9:4Z:346:LYS:HG2 | 2.18 | 0.43 |
| 10:5A:478:LEU:HD23 | 10:5A:481:LEU:HD12 | 2.01 | 0.43 |
| 10:5B:110:GLU:O | 10:5B:114:LYS:HD3 | 2.18 | 0.43 |
| 10:5B:246:ILE:HD12 | 10:5B:246:ILE:HA | 1.92 | 0.43 |
| 10:5C:173:MET:O | 10:5C:177:GLU:HG2 | 2.18 | 0.43 |
| 12:5F:25:ASP:O | 12:5G:262:ARG:NH1 | 2.51 | 0.43 |
| 12:5F:271:LEU:CD2 | 12:7B:23:MET:CG | 2.86 | 0.43 |
| 12:5G:339:ASP:OD1 | 12:5G:339:ASP:N | 2.51 | 0.43 |
| 14:5L:416:ILE:O | 23:6Q:22:MET:HE2 | 2.18 | 0.43 |
| 14:5L:485:VAL:HG21 | 14:5L:516:VAL:HG11 | 2.00 | 0.43 |
| 14:5N:334:LEU:HD23 | 14:5N:334:LEU:H | 1.84 | 0.43 |
| 14:5N:485:VAL:HG21 | 14:5N:516:VAL:HG11 | 2.00 | 0.43 |
| 15:5O:270:LEU:HD12 | 15:5O:307:ILE:CD1 | 2.47 | 0.43 |
| 15:5P:20:ILE:HG13 | 19:6E:104:TYR:CE1 | 2.53 | 0.43 |
| 18:6C:204:LEU:HD11 | 18:6C:209:PRO:O | 2.19 | 0.43 |
| 18:6D:204:LEU:HD11 | 18:6D:209:PRO:O | 2.19 | 0.43 |
| 19:6E:31:LYS:HB2 | 19:6E:37:THR:HG22 | 2.01 | 0.43 |
| 21:6H:20:ARG:HD2 | 21:6H:124:ASP:OD2 | 2.18 | 0.43 |
| 22:6I:192:LYS:HA | 22:6I:195:ASP:OD1 | 2.19 | 0.43 |
| 22:6J:81:ASN:OD1 | 22:6J:82:LEU:N | 2.52 | 0.43 |
| 22:6L:206:ASP:HA | 22:6L:209:ASN:HD21 | 1.83 | 0.43 |
| 22:6L:308:HIS:CD2 | 24:6W:560:ARG:HH12 | 2.37 | 0.43 |
| 22:6P:150:TYR:HB3 | 22:6P:228:PHE:HD1 | 1.83 | 0.43 |
| 24:6T:124:TYR:CE2 | 24:6T:150:ARG:HG3 | 2.53 | 0.43 |
| 24:6T:213:TYR:HA | 24:6T:216:THR:HG22 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:38:GLY:HA3 | 24:6U:42:GLU:HG2 | 2.00 | 0.43 |
| 24:6U:151:HIS:CE1 | 24:6U:153:VAL:HG12 | 2.54 | 0.43 |
| 24:6V:279:TRP:CZ2 | 24:6V:364:ARG:HG3 | 2.53 | 0.43 |
| 24:6X:130:MET:HE3 | 24:6X:153:VAL:CG2 | 2.48 | 0.43 |
| 12:7B:32:GLN:OE1 | 12:7B:32:GLN:N | 2.51 | 0.43 |
| 25:7C:13:GLU:O | 25:7C:16:GLU:HG3 | 2.19 | 0.43 |
| 26:7E:50:SER:HA | 26:7E:56:LEU:CD2 | 2.48 | 0.43 |
| 27:7G:187:ARG:HD3 | 27:7G:187:ARG:H | 1.84 | 0.43 |
| 34:7S:130:ARG:HH22 | 34:7S:134:LEU:HD12 | 1.84 | 0.43 |
| 34:7S:226:LEU:HA | 34:7S:229:ASP:OD2 | 2.19 | 0.43 |
| 38:8B:95:LYS:HA | 38:8B:100:SER:CB | 2.47 | 0.43 |
| 38:8B:120:GLN:O | 38:8B:124:GLU:HG3 | 2.18 | 0.43 |
| 1:7:142:GLY:N | 39:7:502:GDP:O2B | 2.51 | 0.43 |
| 1:7:204:ASN:HD21 | 39:7:502:GDP:HN22 | 1.65 | 0.43 |
| 1:9:83:GLN:HE21 | 24:6X:177:ARG:HH12 | 1.67 | 0.43 |
| 1:A3:281:TYR:CE2 | 1:T6:87:PRO:HD3 | 2.54 | 0.43 |
| 2:E9:18:ASN:ND2 | 22:6N:116:TYR:HE1 | 2.16 | 0.43 |
| 1:G2:371:SER:OG | 1:G2:372:THR:N | 2.52 | 0.43 |
| 2:G5:198:THR:HG21 | 2:G5:201:ALA:HB2 | 1.99 | 0.43 |
| 1:G8:7:ILE:HB | 1:G8:135:VAL:HG22 | 2.01 | 0.43 |
| 1:G8:157:GLU:OE1 | 1:G8:158:GLU:HG3 | 2.19 | 0.43 |
| 2:G9:33:ASP:OD1 | 2:G9:34:GLY:N | 2.52 | 0.43 |
| 2:G9:417:GLU:HA | 2:G9:420:GLU:HG2 | 2.00 | 0.43 |
| 2:H1:57:GLY:H | 2:I7:285:GLN:CB | 2.31 | 0.43 |
| 2:H1:237:SER:HA | 2:H1:320:ARG:HH11 | 1.84 | 0.43 |
| 1:H2:379:LYS:HA | 1:H2:382:SER:HG | 1.84 | 0.43 |
| 2:H5:196:GLU:OE2 | 2:H5:197:HIS:NE2 | 2.52 | 0.43 |
| 1:H6:218:THR:HG21 | 24:6V:488:ARG:HB3 | 1.99 | 0.43 |
| 1:I0:68:LEU:HD23 | 1:I0:68:LEU:HA | 1.88 | 0.43 |
| 2:I3:296:PHE:CE1 | 2:I3:377:MET:HG3 | 2.53 | 0.43 |
| 1:I4:273:LEU:HD23 | 1:I4:273:LEU:HA | 1.86 | 0.43 |
| 2:I5:238:LEU:HD12 | 2:I5:238:LEU:HA | 1.80 | 0.43 |
| 2:I7:96:LYS:HE2 | 28:7H:463:ASN:HA | 1.99 | 0.43 |
| 1:J0:111:GLU:OE1 | 1:J0:111:GLU:N | 2.51 | 0.43 |
| 1:J0:265:PHE:HE2 | 1:J0:418:LEU:HD11 | 1.82 | 0.43 |
| 1:J6:152:ILE:HD12 | 1:J6:164:MET:SD | 2.59 | 0.43 |
| 2:J9:211:ASP:OD1 | 2:J9:214:ARG:NH2 | 2.51 | 0.43 |
| 2:K1:88:HIS:ND1 | 2:L7:283:HIS:HA | 2.33 | 0.43 |
| 2:K1:133:GLN:HE22 | 2:K1:252:ILE:H | 1.67 | 0.43 |
| 2:K3:11:GLN:OE1 | 2:K3:15:GLN:NE2 | 2.52 | 0.43 |
| 2:K3:60:LYS:HE2 | 2:K3:88:HIS:HE1 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K4:145:SER:OG | 1:K4:146:GLY:N | 2.52 | 0.43 |
| 1:K8:177:ASP:N | 1:K8:181:GLU:OE2 | 2.52 | 0.43 |
| 1:K8:310:TYR:CD1 | 1:K8:371:SER:HB2 | 2.54 | 0.43 |
| 1:L2:183:TYR:O | 1:L2:187:LEU:HD13 | 2.19 | 0.43 |
| 1:L2:215:LEU:HD23 | 1:L2:215:LEU:HA | 1.78 | 0.43 |
| 2:L3:11:GLN:HB3 | 41:L4:501:GTP:PA | 2.59 | 0.43 |
| 2:L5:320:ARG:O | 2:L5:373:ARG:HA | 2.19 | 0.43 |
| 1:L6:43:GLN:O | 1:L6:47:ILE:HG23 | 2.19 | 0.43 |
| 2:L7:90:GLU:HB3 | 2:N3:283:HIS:CE1 | 2.54 | 0.43 |
| 2:L7:392:ASP:OD1 | 2:L7:425:LEU:HB3 | 2.19 | 0.43 |
| 2:M3:4:VAL:HG22 | 2:M3:133:GLN:HB2 | 2.00 | 0.43 |
| 2:M5:76:ASP:HA | 2:M5:79:ARG:HB2 | 2.00 | 0.43 |
| 2:M5:297:GLU:HG3 | 2:M5:299:ALA:HB3 | 1.99 | 0.43 |
| 1:M6:183:TYR:OH | 1:M6:388:MET:HB3 | 2.17 | 0.43 |
| 1:M6:192:LEU:HD23 | 1:M6:192:LEU:HA | 1.86 | 0.43 |
| 1:N0:309:ARG:H | 1:N0:372:THR:CG2 | 2.32 | 0.43 |
| 2:N1:91:GLN:HG3 | 2:N1:121:ARG:NH2 | 2.34 | 0.43 |
| 2:N3:312:TYR:HB2 | 2:N3:343:PHE:CD1 | 2.54 | 0.43 |
| 2:N5:11:GLN:HB3 | 41:N6:501:GTP:O2A | 2.19 | 0.43 |
| 2:N7:14:ILE:HD11 | 2:N7:74:VAL:HG22 | 2.00 | 0.43 |
| 2:N7:268:MET:HE2 | 2:N7:268:MET:HB2 | 1.86 | 0.43 |
| 1:N8:3:GLU:HG3 | 1:N8:127:CYS:HB2 | 2.00 | 0.43 |
| 2:N9:34:GLY:HA3 | 2:N9:60:LYS:NZ | 2.34 | 0.43 |
| 1:O0:217:LEU:HD11 | 27:7G:52:VAL:HG12 | 2.01 | 0.43 |
| 1:O2:276:ARG:HA | 1:O2:279:GLN:NE2 | 2.33 | 0.43 |
| 1:O4:320:ARG:HH12 | 19:6E:86:THR:HA | 1.83 | 0.43 |
| 1:O4:358:PRO:HG2 | 1:O4:361:LEU:HD12 | 2.01 | 0.43 |
| 2:O5:109:THR:HB | 2:O5:110:ILE:HD12 | 2.01 | 0.43 |
| 1:O8:221:THR:OG1 | 1:O8:222:PHE:N | 2.52 | 0.43 |
| 2:O9:244:PHE:HB2 | 2:O9:356:ASN:HD21 | 1.83 | 0.43 |
| 2:O9:301:MET:HE1 | 2:O9:307:PRO:HD3 | 2.01 | 0.43 |
| 2:P3:206:ASN:OD1 | 41:P4:501:GTP:N2 | 2.52 | 0.43 |
| 1:P4:54:ALA:HB3 | 1:P4:58:ARG:HB3 | 2.01 | 0.43 |
| 1:P6:68:LEU:HD21 | 1:P6:112:LEU:HD22 | 2.01 | 0.43 |
| 1:P6:186:THR:HG22 | 1:P6:411:ALA:HB1 | 2.00 | 0.43 |
| 2:P7:109:THR:HG23 | 2:P7:411:GLU:OE2 | 2.18 | 0.43 |
| 2:P9:76:ASP:O | 2:P9:80:THR:HG23 | 2.19 | 0.43 |
| 2:Q3:53:PHE:HB3 | 2:Q3:61:HIS:HB3 | 2.01 | 0.43 |
| 1:Q8:47:ILE:HG22 | 1:Q8:51:PHE:HB2 | 2.00 | 0.43 |
| 1:Q8:232:VAL:HG11 | 1:Q8:268:VAL:HG11 | 2.01 | 0.43 |
| 2:Q9:4:VAL:HG23 | 2:Q9:134:GLY:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q9:320:ARG:HE | 2:Q9:320:ARG:HB3 | 1.63 | 0.43 |
| 1:R2:48:ASN:OD1 | 1:R2:48:ASN:N | 2.49 | 0.43 |
| 1:R2:221:THR:HG23 | 1:R2:223:GLY:H | 1.84 | 0.43 |
| 1:R2:317:PHE:HE2 | 1:R2:326:VAL:HG13 | 1.83 | 0.43 |
| 2:R3:65:CYS:SG | 2:R3:66:ILE:N | 2.91 | 0.43 |
| 2:R5:192:HIS:HD2 | 2:R5:421:ALA:HA | 1.82 | 0.43 |
| 1:R6:86:ARG:HD3 | 1:R6:88:ASP:OD1 | 2.19 | 0.43 |
| 1:R6:140:GLY:O | 1:R6:184:ASN:ND2 | 2.51 | 0.43 |
| 1:S0:138:SER:OG | 1:S0:139:LEU:N | 2.52 | 0.43 |
| 2:S1:288:VAL:HG13 | 2:S1:319:TYR:HE2 | 1.83 | 0.43 |
| 2:S7:5:ILE:HD11 | 2:S7:135:PHE:CD1 | 2.54 | 0.43 |
| 1:S8:379:LYS:HG3 | 1:S8:419:VAL:HG21 | 2.00 | 0.43 |
| 1:T0:117:LEU:HA | 1:T0:120:VAL:HG12 | 2.01 | 0.43 |
| 2:T3:279:GLU:N | 2:T3:279:GLU:OE1 | 2.51 | 0.43 |
| 1:T4:42:LEU:HD22 | 21:6H:97:ARG:HD3 | 2.00 | 0.43 |
| 1:T4:72:THR:O | 1:T4:76:VAL:HG23 | 2.19 | 0.43 |
| 1:T6:272:PRO:HD3 | 1:T6:364:SER:HA | 2.00 | 0.43 |
| 2:T7:116:ASP:OD1 | 2:T7:117:LEU:N | 2.52 | 0.43 |
| 2:U1:271:SER:HB3 | 2:U1:377:MET:HB3 | 1.99 | 0.43 |
| 1:U4:293:MET:HE3 | 1:U4:367:PHE:HB2 | 2.00 | 0.43 |
| 1:U4:297:LYS:HZ2 | 1:U4:306:ARG:HH22 | 1.66 | 0.43 |
| 2:V3:22:GLU:HG2 | 2:V3:83:TYR:CE2 | 2.54 | 0.43 |
| 2:V3:66:ILE:O | 2:V3:66:ILE:HG13 | 2.19 | 0.43 |
| 2:V3:211:ASP:OD2 | 2:V3:215:ARG:NH1 | 2.51 | 0.43 |
| 1:V8:297:LYS:HD2 | 1:V8:297:LYS:H | 1.84 | 0.43 |
| 2:V9:157:LEU:HD23 | 2:V9:157:LEU:HA | 1.83 | 0.43 |
| 2:V9:224:TYR:HB2 | 1:W0:245:GLN:NE2 | 2.34 | 0.43 |
| 1:W0:6:HIS:HA | 1:W0:134:GLN:O | 2.18 | 0.43 |
| 1:W0:226:ASN:OD1 | 39:W0:502:GDP:N2 | 2.47 | 0.43 |
| 1:W4:150:LEU:HD12 | 1:W4:153:SER:OG | 2.19 | 0.43 |
| 1:W6:5:VAL:HG23 | 1:W6:62:ARG:HG2 | 1.99 | 0.43 |
| 2:W7:399:TYR:OH | 2:W7:415:GLU:OE2 | 2.36 | 0.43 |
| 1:W8:387:ALA:HA | 1:W8:390:ARG:HH21 | 1.83 | 0.43 |
| 2:W9:175:PRO:HB3 | 2:W9:390:ARG:NE | 2.34 | 0.43 |
| 1:X0:170:VAL:N | 1:X0:202:LEU:O | 2.45 | 0.43 |
| 2:X5:27:GLU:HG3 | 2:X5:28:HIS:HD2 | 1.83 | 0.43 |
| 2:X5:271:SER:HB2 | 2:X5:377:MET:HE2 | 2.00 | 0.43 |
| 2:X7:34:GLY:HA3 | 2:X7:60:LYS:HZ2 | 1.84 | 0.43 |
| 1:X8:19:LYS:HE3 | 1:X8:19:LYS:HB3 | 1.90 | 0.43 |
| 2:Y3:276:ILE:HG23 | 2:Y3:280:LYS:HB2 | 2.01 | 0.43 |
| 2:Y5:149:LEU:HA | 2:Y5:152:LEU:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y5:201:ALA:O | 2:Y5:268:MET:HE2 | 2.19 | 0.43 |
| 2:Y9:406:HIS:HA | 2:Y9:409:VAL:HG22 | 2.01 | 0.43 |
| 1:Z0:237:THR:HG23 | 1:Z0:241:ARG:HH21 | 1.82 | 0.43 |
| 1:Z0:268:VAL:O | 1:Z0:300:MET:N | 2.45 | 0.43 |
| 1:Z0:382:SER:HB2 | 1:Z0:415:MET:HE3 | 2.00 | 0.43 |
| 2:Z1:3:GLU:HG3 | 2:Z1:51:THR:HA | 2.00 | 0.43 |
| 2:Z3:320:ARG:O | 2:Z3:373:ARG:HA | 2.18 | 0.43 |
| 1:Z4:50:TYR:HD2 | 1:Z4:241:ARG:HD3 | 1.84 | 0.43 |
| 2:Z5:175:PRO:HG2 | 2:Z5:176:GLN:OE1 | 2.19 | 0.43 |
| 2:Z5:399:TYR:OH | 2:Z5:415:GLU:OE2 | 2.24 | 0.43 |
| 2:Z9:191:THR:HA | 2:Z9:194:LEU:HB3 | 1.99 | 0.43 |
| 2:0B:167:LEU:HD13 | 2:0B:200:VAL:HB | 2.01 | 0.43 |
| 1:0C:250:LEU:HA | 1:0C:253:LEU:HD12 | 2.00 | 0.43 |
| 1:0E:258:ILE:HG23 | 1:0E:258:ILE:O | 2.18 | 0.43 |
| 2:0F:312:TYR:HD1 | 2:0F:381:SER:HB2 | 1.84 | 0.43 |
| 1:0G:170:VAL:HG22 | 1:0G:202:LEU:O | 2.18 | 0.43 |
| 1:0I:21:TRP:CH2 | 1:0I:61:PRO:HB3 | 2.54 | 0.43 |
| 2:0J:64:ARG:HB3 | 2:0J:125:LEU:HD21 | 2.01 | 0.43 |
| 2:0J:174:SER:HB3 | 2:0J:177:VAL:O | 2.18 | 0.43 |
| 2:0J:176:GLN:NE2 | 2:0J:207:GLU:OE1 | 2.51 | 0.43 |
| 2:0J:318:MET:HB2 | 2:0J:376:CYS:HB3 | 2.01 | 0.43 |
| 1:0K:344:TRP:CE3 | 1:0K:345:ILE:HG13 | 2.54 | 0.43 |
| 1:0M:8:GLN:O | 1:0M:66:MET:HB2 | 2.19 | 0.43 |
| 2:0N:431:ASP:O | 2:0N:434:GLU:HG2 | 2.19 | 0.43 |
| 1:0O:67:ASP:OD2 | 1:0O:72:THR:HG21 | 2.19 | 0.43 |
| 1:0O:388:MET:HE2 | 1:0O:388:MET:CA | 2.49 | 0.43 |
| 1:0S:8:GLN:CD | 1:0S:17:GLY:HA3 | 2.39 | 0.43 |
| 1:0W:153:SER:O | 1:0W:157:GLU:HG2 | 2.19 | 0.43 |
| 1:0W:404:ASP:HB3 | 1:0W:406:MET:SD | 2.58 | 0.43 |
| 1:0Y:417:ASP:HA | 1:0Y:420:SER:HG | 1.84 | 0.43 |
| 2:0Z:312:TYR:CE2 | 2:0Z:341:ILE:HG12 | 2.54 | 0.43 |
| 2:1B:51:THR:HG21 | 2:1B:243:ARG:HG2 | 2.00 | 0.43 |
| 2:1B:204:LEU:HD22 | 2:1B:302:MET:CB | 2.49 | 0.43 |
| 1:1C:314:SER:HA | 1:1C:350:LYS:O | 2.19 | 0.43 |
| 2:1D:240:ALA:HB1 | 2:1D:356:ASN:HD22 | 1.83 | 0.43 |
| 1:1E:53:GLU:HB2 | 1:1E:59:TYR:CE1 | 2.54 | 0.43 |
| 1:1G:364:SER:OG | 1:1G:365:ALA:N | 2.52 | 0.43 |
| 1:1G:396:HIS:CD2 | 2:1H:263:PRO:HD3 | 2.54 | 0.43 |
| 2:1H:266:HIS:O | 2:1H:266:HIS:ND1 | 2.47 | 0.43 |
| 1:1K:72:THR:O | 1:1K:75:SER:OG | 2.17 | 0.43 |
| 2:1L:149:LEU:HA | 2:1L:152:LEU:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1N:172:TYR:CZ | 2:1N:203:MET:SD | 3.12 | 0.43 |
| 2:1N:176:GLN:HG2 | 2:1N:177:VAL:N | 2.33 | 0.43 |
| 2:1P:403:ALA:HB2 | 1:1Q:344:TRP:HZ3 | 1.84 | 0.43 |
| 2:1R:403:ALA:HB2 | 1:1S:344:TRP:HZ3 | 1.83 | 0.43 |
| 1:1S:345:ILE:HB | 1:1S:348:ASN:HD21 | 1.83 | 0.43 |
| 2:1V:91:GLN:HG2 | 2:1V:121:ARG:NH2 | 2.30 | 0.43 |
| 2:1X:3:GLU:HG3 | 2:1X:51:THR:HA | 2.00 | 0.43 |
| 2:1X:102:ASN:ND2 | 2:1X:105:ARG:H | 2.16 | 0.43 |
| 1:2C:203:ASP:OD1 | 1:2C:301:CYS:HA | 2.18 | 0.43 |
| 1:2C:207:LEU:HD23 | 1:2C:207:LEU:HA | 1.90 | 0.43 |
| 2:2F:246:GLY:HA2 | 2:2F:357:TYR:CD2 | 2.54 | 0.43 |
| 1:2G:77:ARG:HE | 1:2G:90:PHE:HE2 | 1.64 | 0.43 |
| 2:2H:8:HIS:CD2 | 2:2H:138:PHE:HD2 | 2.37 | 0.43 |
| 1:2K:151:LEU:HD12 | 1:2K:151:LEU:HA | 1.84 | 0.43 |
| 1:2S:165:LEU:HG | 1:2S:250:LEU:HD11 | 2.01 | 0.43 |
| 1:2U:220:PRO:HD2 | 2:2V:326:LYS:HG2 | 2.01 | 0.43 |
| 2:2X:205:ASP:OD2 | 2:2X:206:ASN:N | 2.46 | 0.43 |
| 1:2Y:114:ASP:OD1 | 1:2Y:115:SER:N | 2.51 | 0.43 |
| 1:3A:414:ASN:HA | 1:3A:417:ASP:OD2 | 2.19 | 0.43 |
| 2:3B:121:ARG:HA | 2:3B:121:ARG:HD3 | 1.88 | 0.43 |
| 1:3C:382:SER:HB2 | 1:3C:415:MET:HG2 | 2.01 | 0.43 |
| 1:3C:386:THR:O | 1:3C:390:ARG:HG3 | 2.19 | 0.43 |
| 1:3C:396:HIS:CD2 | 2:3D:263:PRO:HD3 | 2.54 | 0.43 |
| 2:3D:280:LYS:HA | 2:3D:283:HIS:HB3 | 2.00 | 0.43 |
| 2:3F:402:ARG:HD2 | 2:3F:405:VAL:HG21 | 2.01 | 0.43 |
| 1:3I:161:ASP:OD2 | 1:3I:161:ASP:N | 2.51 | 0.43 |
| 1:3I:218:THR:O | 2:3J:326:LYS:HE2 | 2.19 | 0.43 |
| 1:3K:101:TRP:CE3 | 1:3K:403:MET:HE1 | 2.53 | 0.43 |
| 1:3K:183:TYR:O | 1:3K:187:LEU:HD13 | 2.19 | 0.43 |
| 1:3K:404:ASP:HB3 | 1:3K:406:MET:SD | 2.59 | 0.43 |
| 1:3M:309:ARG:NH1 | 1:3M:341:PHE:O | 2.51 | 0.43 |
| 1:3M:354:CYS:SG | 1:3M:355:ASP:N | 2.92 | 0.43 |
| 1:3O:49:VAL:O | 1:3O:62:ARG:NH1 | 2.52 | 0.43 |
| 1:3Q:173:PRO:HG2 | 1:3Q:174:LYS:NZ | 2.34 | 0.43 |
| 2:3R:231:ILE:O | 2:3R:235:ILE:HG12 | 2.18 | 0.43 |
| 2:3R:345:ASP:OD1 | 2:3R:346:TRP:N | 2.51 | 0.43 |
| 1:3S:6:HIS:CD2 | 1:3S:134:GLN:HG3 | 2.47 | 0.43 |
| 1:3S:406:MET:SD | 1:3S:406:MET:N | 2.92 | 0.43 |
| 2:3T:251:ASP:OD1 | 2:3T:253:THR:OG1 | 2.29 | 0.43 |
| 2:3T:417:GLU:HA | 2:3T:420:GLU:CD | 2.39 | 0.43 |
| 3:3V:216:ILE:HD13 | 3:3V:216:ILE:HA | 1.89 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4G:36:ARG:O | 3:4H:260:ILE:HG13 | 2.19 | 0.43 |
| 4:4G:94:LEU:HB2 | 4:4G:152:LEU:HD11 | 1.99 | 0.43 |
| 3:4H:216:ILE:HD13 | 3:4H:216:ILE:HA | 1.89 | 0.43 |
| 6:4O:277:GLU:HA | 6:4O:280:LYS:HD2 | 2.01 | 0.43 |
| 8:4W:225:SER:O | 8:4W:228:ARG:HG2 | 2.19 | 0.43 |
| 8:4W:457:LEU:HD23 | 8:4W:457:LEU:HA | 1.79 | 0.43 |
| 10:5C:481:LEU:HD11 | 10:5C:494:LEU:CD2 | 2.47 | 0.43 |
| 13:5H:93:ASN:HB2 | 13:5H:96:TRP:CZ2 | 2.54 | 0.43 |
| 14:5L:159:SER:O | 14:5L:159:SER:OG | 2.35 | 0.43 |
| 14:5L:189:THR:OG1 | 14:5L:189:THR:O | 2.33 | 0.43 |
| 14:5L:334:LEU:H | 14:5L:334:LEU:HD23 | 1.84 | 0.43 |
| 14:5M:189:THR:O | 14:5M:189:THR:OG1 | 2.33 | 0.43 |
| 14:5M:211:CYS:SG | 14:5M:219:LEU:HB3 | 2.59 | 0.43 |
| 14:5N:415:LYS:HB3 | 14:5N:415:LYS:HE3 | 1.49 | 0.43 |
| 15:5O:35:VAL:CG2 | 15:5O:52:TYR:HB2 | 2.49 | 0.43 |
| 15:5P:5:LEU:HD23 | 15:5P:5:LEU:HA | 1.88 | 0.43 |
| 15:5P:361:LEU:HB2 | 15:5P:364:ASP:OD2 | 2.18 | 0.43 |
| 18:5X:182:VAL:HG12 | 18:5X:182:VAL:O | 2.18 | 0.43 |
| 18:5X:204:LEU:HD11 | 18:5X:209:PRO:O | 2.19 | 0.43 |
| 18:6B:204:LEU:HD11 | 18:6B:209:PRO:O | 2.19 | 0.43 |
| 20:6F:159:ASP:HB3 | 20:6F:302:PRO:HA | 2.00 | 0.43 |
| 22:6L:96:LYS:HD3 | 22:6L:97:PRO:O | 2.18 | 0.43 |
| 22:6L:201:ARG:HG2 | 22:6L:239:GLU:OE2 | 2.18 | 0.43 |
| 24:6U:315:ARG:HG3 | 24:6U:315:ARG:HH11 | 1.84 | 0.43 |
| 24:6V:274:ARG:HB3 | 24:6V:372:ASP:OD1 | 2.18 | 0.43 |
| 24:6W:469:PHE:HB3 | 24:6W:484:GLU:HB3 | 2.01 | 0.43 |
| 24:6W:483:PHE:CE1 | 24:6W:496:LYS:HB2 | 2.53 | 0.43 |
| 24:6X:435:LEU:HD12 | 24:6X:435:LEU:H | 1.84 | 0.43 |
| 24:6Y:274:ARG:H | 24:6Y:375:THR:HG21 | 1.84 | 0.43 |
| 24:6Y:274:ARG:NE | 24:6Y:372:ASP:OD2 | 2.46 | 0.43 |
| 24:6Z:602:LEU:HG | 24:6Z:604:PHE:HD1 | 1.83 | 0.43 |
| 28:7H:410:HIS:O | 28:7H:414:GLN:HG3 | 2.19 | 0.43 |
| 31:7N:102:ILE:CD1 | 31:7N:108:SER:HB3 | 2.49 | 0.43 |
| 32:7P:96:GLU:OE1 | 32:7P:100:ARG:HB2 | 2.18 | 0.43 |
| 34:7R:208:ARG:HA | 34:7R:211:ARG:HH21 | 1.82 | 0.43 |
| 28:7X:410:HIS:O | 28:7X:414:GLN:HG3 | 2.19 | 0.43 |
| 38:8B:122:LYS:O | 38:8B:126:THR:HG22 | 2.19 | 0.43 |
| 1:B5:280:GLN:NE2 | 24:6X:105:SER:O | 2.51 | 0.43 |
| 1:B8:279:GLN:NE2 | 24:6Y:109:SER:HB2 | 2.34 | 0.43 |
| 1:C4:47:ILE:HD11 | 22:6I:23:TYR:CE2 | 2.54 | 0.43 |
| 1:D4:39:ASP:OD1 | 18:6B:149:LYS:HG2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D5:179:THR:OG1 | 41:D5:501:GTP:O3' | 2.36 | 0.43 |
| 1:E0:32:PRO:HG2 | 24:6T:403:PRO:HD2 | 2.01 | 0.43 |
| 1:G2:180:VAL:HG23 | 1:G2:184:ASN:ND2 | 2.34 | 0.43 |
| 2:G7:56:THR:HG23 | 2:G7:60:LYS:HB3 | 2.00 | 0.43 |
| 2:H1:167:LEU:HD23 | 2:H1:167:LEU:HA | 1.86 | 0.43 |
| 1:H2:35:THR:OG1 | 1:H2:37:HIS:NE2 | 2.51 | 0.43 |
| 2:H5:176:GLN:HG2 | 2:H5:177:VAL:HG23 | 2.01 | 0.43 |
| 2:H9:205:ASP:OD2 | 2:H9:303:VAL:HG13 | 2.19 | 0.43 |
| 2:I1:76:ASP:OD2 | 1:I2:46:ARG:NH2 | 2.49 | 0.43 |
| 2:I1:204:LEU:HD13 | 2:I1:231:ILE:HD12 | 2.00 | 0.43 |
| 1:I2:218:THR:HG21 | 24:6Y:488:ARG:CA | 2.48 | 0.43 |
| 1:I4:250:LEU:HD23 | 1:I4:250:LEU:HA | 1.86 | 0.43 |
| 2:I5:272:TYR:HD2 | 2:I5:275:ILE:HD11 | 1.84 | 0.43 |
| 2:I9:291:ILE:HA | 2:I9:294:ALA:HB3 | 2.00 | 0.43 |
| 1:J0:417:ASP:HA | 1:J0:420:SER:OG | 2.19 | 0.43 |
| 1:J2:295:ASP:OD2 | 1:J2:297:LYS:N | 2.46 | 0.43 |
| 1:J4:170:VAL:HG22 | 1:J4:202:LEU:O | 2.19 | 0.43 |
| 2:J7:22:GLU:O | 2:J7:26:LEU:HD23 | 2.19 | 0.43 |
| 2:J9:151:SER:HB2 | 2:J9:193:SER:OG | 2.19 | 0.43 |
| 2:K3:213:CYS:SG | 2:K3:219:ILE:HB | 2.59 | 0.43 |
| 1:K6:390:ARG:HG3 | 1:K6:391:ARG:HG3 | 2.00 | 0.43 |
| 2:K7:318:MET:HB2 | 2:K7:376:CYS:HB3 | 2.00 | 0.43 |
| 1:K8:145:SER:OG | 1:K8:146:GLY:N | 2.52 | 0.43 |
| 2:K9:9:ILE:HG12 | 2:K9:68:LEU:HD11 | 2.01 | 0.43 |
| 2:L3:35:GLN:HB3 | 2:L3:59:GLY:O | 2.19 | 0.43 |
| 1:L4:192:LEU:HD23 | 1:L4:192:LEU:HA | 1.82 | 0.43 |
| 1:L6:304:ASP:HB3 | 1:L6:307:HIS:ND1 | 2.34 | 0.43 |
| 2:L7:5:ILE:HB | 2:L7:64:ARG:O | 2.19 | 0.43 |
| 1:M6:186:THR:HG22 | 1:M6:411:ALA:HB1 | 2.01 | 0.43 |
| 1:M8:60:VAL:HG21 | 1:M8:86:ARG:HE | 1.84 | 0.43 |
| 2:M9:205:ASP:OD1 | 2:M9:303:VAL:HG13 | 2.19 | 0.43 |
| 1:N0:163:MET:HG3 | 1:N0:250:LEU:HD22 | 2.01 | 0.43 |
| 1:N0:246:LEU:HD22 | 1:N0:352:SER:HA | 2.00 | 0.43 |
| 2:N1:300:SER:O | 2:N1:300:SER:OG | 2.30 | 0.43 |
| 2:N3:209:ILE:HD13 | 2:N3:227:LEU:HD13 | 2.00 | 0.43 |
| 2:N3:290:GLU:HA | 2:N3:293:ASN:HD22 | 1.82 | 0.43 |
| 2:O1:405:VAL:HG13 | 2:O1:418:PHE:HE2 | 1.84 | 0.43 |
| 1:O2:281:TYR:CD2 | 1:O2:281:TYR:N | 2.86 | 0.43 |
| 2:O7:189:LEU:HD11 | 2:O7:418:PHE:CE1 | 2.52 | 0.43 |
| 1:O8:404:ASP:OD1 | 1:O8:405:GLU:N | 2.52 | 0.43 |
| 2:P5:88:HIS:HD2 | 2:P5:121:ARG:NH2 | 2.15 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P5:175:PRO:HG2 | 2:P5:176:GLN:OE1 | 2.19 | 0.43 |
| 2:P5:241:SER:OG | 2:P5:250:VAL:O | 2.34 | 0.43 |
| 1:P6:68:LEU:HB3 | 1:P6:96:GLY:HA2 | 2.01 | 0.43 |
| 1:P6:344:TRP:CE3 | 1:P6:345:ILE:HG13 | 2.53 | 0.43 |
| 2:P7:70:LEU:HD13 | 2:P7:110:ILE:HG21 | 2.01 | 0.43 |
| 1:P8:268:VAL:O | 1:P8:300:MET:N | 2.39 | 0.43 |
| 1:Q0:108:GLU:OE1 | 1:Q0:108:GLU:N | 2.52 | 0.43 |
| 2:Q3:56:THR:O | 2:Q3:57:GLY:C | 2.56 | 0.43 |
| 2:Q3:349:THR:HG22 | 2:Q3:349:THR:O | 2.19 | 0.43 |
| 1:Q4:237:THR:CG2 | 1:Q4:240:LEU:HD12 | 2.49 | 0.43 |
| 1:Q8:122:LYS:HA | 1:Q8:125:GLU:OE1 | 2.18 | 0.43 |
| 2:R1:69:ASP:OD2 | 2:R1:70:LEU:N | 2.51 | 0.43 |
| 2:R1:199:ASP:HA | 17:5S:84:ARG:HH22 | 1.83 | 0.43 |
| 2:R5:322:ASP:HB2 | 19:6E:221:THR:HG22 | 2.01 | 0.43 |
| 2:R7:90:GLU:HB3 | 2:R7:121:ARG:NH1 | 2.26 | 0.43 |
| 2:R9:21:TRP:CZ3 | 2:R9:63:PRO:HB3 | 2.54 | 0.43 |
| 2:R9:269:LEU:HD21 | 2:R9:384:ILE:HG13 | 2.00 | 0.43 |
| 1:S0:69:GLU:OE1 | 1:S0:69:GLU:HA | 2.19 | 0.43 |
| 1:S4:71:GLY:HA2 | 24:6U:29:LYS:HZ1 | 1.84 | 0.43 |
| 1:S4:271:THR:OG1 | 1:S4:365:ALA:HB3 | 2.19 | 0.43 |
| 1:S4:303:ALA:C | 13:5H:9:GLN:HE21 | 2.22 | 0.43 |
| 2:S5:49:PHE:HE2 | 2:S5:55:GLU:HB2 | 1.83 | 0.43 |
| 1:S8:216:LYS:HB2 | 1:S8:275:SER:HG | 1.83 | 0.43 |
| 1:S8:228:LEU:HD23 | 1:S8:228:LEU:HA | 1.84 | 0.43 |
| 1:T0:6:HIS:CE1 | 1:T0:8:GLN:HE21 | 2.37 | 0.43 |
| 1:T2:138:SER:O | 1:T2:139:LEU:HD23 | 2.19 | 0.43 |
| 1:T6:275:SER:OG | 1:T6:278:SER:HB3 | 2.18 | 0.43 |
| 2:T7:137:VAL:HG11 | 2:T7:154:LEU:HD11 | 2.00 | 0.43 |
| 1:T8:50:TYR:OH | 1:T8:237:THR:OG1 | 2.31 | 0.43 |
| 2:U7:72:PRO:HD2 | 1:U8:2:ARG:NH1 | 2.34 | 0.43 |
| 2:U7:335:ILE:HG23 | 2:U7:341:ILE:HD11 | 2.01 | 0.43 |
| 1:U8:6:HIS:HD2 | 1:U8:134:GLN:OE1 | 2.01 | 0.43 |
| 1:V0:242:PHE:CD1 | 1:V0:356:ILE:HG13 | 2.54 | 0.43 |
| 1:V0:250:LEU:HD12 | 1:V0:250:LEU:HA | 1.87 | 0.43 |
| 1:V0:396:HIS:CE1 | 1:V0:397:TRP:CE2 | 3.06 | 0.43 |
| 1:V6:161:ASP:OD2 | 1:V6:161:ASP:N | 2.45 | 0.43 |
| 1:V6:394:PHE:CE2 | 2:V7:261:PRO:HB3 | 2.54 | 0.43 |
| 1:W0:135:VAL:O | 1:W0:166:THR:HA | 2.18 | 0.43 |
| 1:W2:173:PRO:HD3 | 1:W2:380:ARG:HD3 | 2.00 | 0.43 |
| 2:W7:88:HIS:CD2 | 2:W7:89:PRO:CD | 3.00 | 0.43 |
| 2:W9:7:ILE:O | 2:W9:7:ILE:CG2 | 2.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X5:116:ASP:N | 2:X5:116:ASP:OD1 | 2.51 | 0.43 |
| 1:X6:128:ASP:OD1 | 1:X6:128:ASP:N | 2.52 | 0.43 |
| 2:X7:384:ILE:HA | 2:X7:387:ILE:HD12 | 2.01 | 0.43 |
| 1:X8:412:GLU:HA | 1:X8:415:MET:HE2 | 2.01 | 0.43 |
| 2:X9:121:ARG:HA | 2:X9:121:ARG:HD2 | 1.79 | 0.43 |
| 2:Y3:3:GLU:HB2 | 2:Y3:129:CYS:SG | 2.59 | 0.43 |
| 2:Y3:181:VAL:H | 1:Y4:256:ASN:ND2 | 2.17 | 0.43 |
| 2:Z5:181:VAL:HG12 | 1:Z6:347:ASN:O | 2.19 | 0.43 |
| 1:Z6:165:LEU:HB2 | 1:Z6:250:LEU:HD11 | 2.01 | 0.43 |
| 2:Z7:28:HIS:CD2 | 2:Z7:244:PHE:HZ | 2.36 | 0.43 |
| 1:Z8:148:GLY:O | 1:Z8:152:ILE:HG12 | 2.19 | 0.43 |
| 2:0F:99:ALA:HA | 2:0F:105:ARG:HD3 | 2.01 | 0.43 |
| 2:0J:98:ASP:OD1 | 2:0J:99:ALA:N | 2.51 | 0.43 |
| 2:0J:304:LYS:HA | 2:0J:304:LYS:HD3 | 1.79 | 0.43 |
| 2:0N:90:GLU:HB3 | 2:0N:121:ARG:HH12 | 1.82 | 0.43 |
| 2:0N:345:ASP:N | 2:0N:345:ASP:OD1 | 2.52 | 0.43 |
| 1:0O:19:LYS:HE3 | 1:0O:19:LYS:HB3 | 1.81 | 0.43 |
| 1:0O:211:CYS:SG | 1:0O:220:PRO:HB3 | 2.59 | 0.43 |
| 1:0O:286:VAL:HG23 | 1:0O:287:PRO:HD3 | 2.00 | 0.43 |
| 2:0P:175:PRO:HB3 | 2:0P:390:ARG:HE | 1.84 | 0.43 |
| 1:0Q:405:GLU:HA | 1:0Q:408:PHE:HD2 | 1.84 | 0.43 |
| 2:0X:66:ILE:CD1 | 2:0X:122:ILE:HD11 | 2.49 | 0.43 |
| 1:0Y:207:LEU:HD11 | 1:0Y:229:ILE:CD1 | 2.33 | 0.43 |
| 2:0Z:320:ARG:O | 2:0Z:373:ARG:HA | 2.18 | 0.43 |
| 2:1B:53:PHE:HA | 2:1B:62:VAL:O | 2.19 | 0.43 |
| 2:1F:182:VAL:HG23 | 2:1F:186:ASN:ND2 | 2.33 | 0.43 |
| 1:1G:118:ASP:O | 1:1G:122:LYS:HG2 | 2.18 | 0.43 |
| 1:1G:165:LEU:HD13 | 1:1G:167:PHE:HE1 | 1.84 | 0.43 |
| 2:1H:101:ASN:HD22 | 2:1H:143:GLY:HA2 | 1.84 | 0.43 |
| 1:1K:113:ILE:HD12 | 1:1K:150:LEU:HD22 | 2.01 | 0.43 |
| 1:1K:215:LEU:HD11 | 1:1K:273:LEU:HD22 | 2.00 | 0.43 |
| 1:1K:415:MET:O | 1:1K:418:LEU:HG | 2.19 | 0.43 |
| 1:1Q:173:PRO:HD2 | 1:1Q:380:ARG:NH1 | 2.34 | 0.43 |
| 1:1S:334:GLN:NE2 | 1:1S:348:ASN:H | 2.07 | 0.43 |
| 2:1V:88:HIS:CG | 2:1V:89:PRO:HD2 | 2.45 | 0.43 |
| 2:1V:176:GLN:HG2 | 2:1V:177:VAL:N | 2.34 | 0.43 |
| 1:1W:55:THR:CG2 | 1:2M:284:LEU:HD23 | 2.39 | 0.43 |
| 2:1X:189:LEU:HD11 | 2:1X:418:PHE:CE1 | 2.53 | 0.43 |
| 2:1Z:179:THR:O | 1:2A:350:LYS:HD2 | 2.19 | 0.43 |
| 1:2C:117:LEU:HA | 1:2C:120:VAL:HG12 | 2.00 | 0.43 |
| 1:2E:20:PHE:HA | 1:2E:230:SER:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2E:335:ASN:O | 1:2E:338:SER:OG | 2.36 | 0.43 |
| 1:2I:391:ARG:HH22 | 2:2J:435:VAL:HA | 1.83 | 0.43 |
| 2:2L:57:GLY:HA3 | 10:5D:156:TYR:OH | 2.18 | 0.43 |
| 1:2M:210:ILE:O | 1:2M:214:THR:OG1 | 2.28 | 0.43 |
| 1:2M:317:PHE:HE2 | 1:2M:326:VAL:HG13 | 1.84 | 0.43 |
| 2:2N:277:SER:H | 2:2N:280:LYS:HD3 | 1.84 | 0.43 |
| 1:2Q:77:ARG:HD2 | 1:2Q:90:PHE:CE2 | 2.54 | 0.43 |
| 1:2Y:2:ARG:HB3 | 1:2Y:131:GLN:HB2 | 2.00 | 0.43 |
| 2:2Z:156:ARG:HA | 2:2Z:159:VAL:HG12 | 2.01 | 0.43 |
| 2:3B:287:SER:H | 2:3B:290:GLU:CD | 2.21 | 0.43 |
| 1:3C:355:ASP:CG | 38:8D:198:THR:HG22 | 2.31 | 0.43 |
| 1:3G:192:LEU:HA | 1:3G:192:LEU:HD23 | 1.79 | 0.43 |
| 2:3H:65:CYS:SG | 2:3H:66:ILE:N | 2.92 | 0.43 |
| 1:3I:5:VAL:HG22 | 1:3I:62:ARG:HD3 | 2.00 | 0.43 |
| 1:3M:309:ARG:NH1 | 1:3M:339:SER:O | 2.51 | 0.43 |
| 1:3M:371:SER:OG | 1:3M:372:THR:N | 2.52 | 0.43 |
| 2:3N:174:SER:HA | 2:3N:205:ASP:OD2 | 2.19 | 0.43 |
| 1:3S:197:ASP:N | 1:3S:197:ASP:OD1 | 2.49 | 0.43 |
| 2:3T:204:LEU:HD23 | 2:3T:231:ILE:HD12 | 2.01 | 0.43 |
| 2:3T:209:ILE:HD12 | 2:3T:209:ILE:H | 1.83 | 0.43 |
| 2:3T:280:LYS:HA | 2:3T:283:HIS:HB3 | 2.00 | 0.43 |
| 2:3T:391:LEU:HA | 2:3T:394:LYS:HG2 | 2.00 | 0.43 |
| 3:3X:93:LYS:HA | 3:3X:93:LYS:HD3 | 1.47 | 0.43 |
| 3:3X:216:ILE:HD13 | 3:3X:216:ILE:HA | 1.89 | 0.43 |
| 4:4E:22:LEU:N | 3:4F:258:ASP:OD2 | 2.48 | 0.43 |
| 7:4R:192:GLU:OE1 | 7:4R:196:ARG:NH1 | 2.51 | 0.43 |
| 9:4Z:39:TRP:NE1 | 14:5L:583:ASP:HB3 | 2.34 | 0.43 |
| 10:5B:120:GLU:CG | 10:5C:359:ARG:HH12 | 2.29 | 0.43 |
| 13:5I:93:ASN:HB2 | 13:5I:96:TRP:CZ2 | 2.54 | 0.43 |
| 13:5J:93:ASN:HB2 | 13:5J:96:TRP:CZ2 | 2.54 | 0.43 |
| 13:5K:93:ASN:HB2 | 13:5K:96:TRP:CZ2 | 2.54 | 0.43 |
| 14:5L:55:HIS:HE2 | 14:5L:88:TRP:HH2 | 1.67 | 0.43 |
| 14:5L:248:VAL:HB | 14:5L:252:ASP:HB2 | 1.99 | 0.43 |
| 14:5L:425:GLN:OE1 | 14:5L:425:GLN:N | 2.44 | 0.43 |
| 14:5M:20:GLY:N | 14:5M:296:SER:OG | 2.52 | 0.43 |
| 14:5M:113:CYS:SG | 14:5M:159:SER:HB3 | 2.59 | 0.43 |
| 14:5M:248:VAL:HB | 14:5M:252:ASP:HB2 | 1.99 | 0.43 |
| 14:5M:334:LEU:H | 14:5M:334:LEU:HD23 | 1.84 | 0.43 |
| 14:5M:425:GLN:OE1 | 14:5M:425:GLN:N | 2.44 | 0.43 |
| 14:5M:485:VAL:HG21 | 14:5M:516:VAL:HG11 | 2.00 | 0.43 |
| 14:5N:20:GLY:N | 14:5N:296:SER:OG | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5N:291:GLU:OE2 | 14:5N:317:ASN:ND2 | 2.51 | 0.43 |
| 15:5O:16:PRO:HB3 | 15:5O:276:ASN:ND2 | 2.33 | 0.43 |
| 15:5P:139:VAL:HG23 | 15:5P:140:HIS:CE1 | 2.53 | 0.43 |
| 15:5P:169:ILE:HD12 | 15:5P:169:ILE:H | 1.84 | 0.43 |
| 18:5Y:204:LEU:HD11 | 18:5Y:209:PRO:O | 2.19 | 0.43 |
| 18:5Z:204:LEU:HD11 | 18:5Z:209:PRO:O | 2.19 | 0.43 |
| 18:6A:204:LEU:HD11 | 18:6A:209:PRO:O | 2.19 | 0.43 |
| 22:6I:324:LYS:HA | 22:6I:327:GLU:OE1 | 2.19 | 0.43 |
| 22:6J:104:LEU:HD23 | 22:6J:104:LEU:HA | 1.90 | 0.43 |
| 22:6L:305:VAL:HG12 | 22:6L:343:TYR:HD2 | 1.84 | 0.43 |
| 22:6M:27:LEU:HD12 | 22:6M:27:LEU:HA | 1.78 | 0.43 |
| 22:6N:122:ALA:HB1 | 22:6N:127:THR:OG1 | 2.18 | 0.43 |
| 24:6T:565:GLN:NE2 | 24:6T:602:LEU:HB2 | 2.33 | 0.43 |
| 24:6U:560:ARG:HA | 24:6U:563:LYS:HE3 | 2.01 | 0.43 |
| 24:6V:505:LYS:HD2 | 24:6V:510:GLU:HB3 | 2.01 | 0.43 |
| 24:6X:258:ASP:OD2 | 24:6X:259:GLY:N | 2.52 | 0.43 |
| 24:6Y:95:VAL:O | 24:6Y:187:PHE:HD2 | 2.01 | 0.43 |
| 24:6Y:182:VAL:HG13 | 24:6Y:203:LEU:HB2 | 1.99 | 0.43 |
| 24:6Y:273:LEU:HD11 | 24:6Y:298:LEU:HD21 | 2.01 | 0.43 |
| 24:6Y:332:VAL:HG21 | 24:6Y:342:PHE:CE1 | 2.54 | 0.43 |
| 24:6Y:434:ASP:O | 24:6Y:438:LEU:HD23 | 2.19 | 0.43 |
| 24:6Z:274:ARG:HD3 | 24:6Z:295:HIS:CE1 | 2.54 | 0.43 |
| 24:6Z:437:LYS:HE2 | 24:6Z:475:MET:O | 2.18 | 0.43 |
| 28:7H:399:VAL:HG13 | 28:7H:402:ARG:HD2 | 2.01 | 0.43 |
| 29:7I:117:ASN:C | 29:7I:120:PRO:HD2 | 2.38 | 0.43 |
| 36:7W:20:GLU:O | 36:7W:24:ASN:OD1 | 2.37 | 0.43 |
| 2:2:415:GLU:CD | 4:3W:86:TYR:OH | 2.57 | 0.43 |
| 2:C7:89:PRO:HB3 | 22:6K:18:PRO:HG2 | 2.00 | 0.43 |
| 2:F9:282:TYR:CE1 | 22:6K:133:PRO:HG3 | 2.54 | 0.43 |
| 1:G2:212:PHE:HZ | 2:G3:326:LYS:HG3 | 1.84 | 0.43 |
| 2:G3:46:ASP:O | 2:G3:47:ASP:C | 2.57 | 0.43 |
| 1:G4:237:THR:HG22 | 1:G4:237:THR:O | 2.18 | 0.43 |
| 2:G5:266:HIS:O | 2:G5:266:HIS:ND1 | 2.52 | 0.43 |
| 2:G5:313:MET:HB2 | 2:G5:380:ASN:HB3 | 2.01 | 0.43 |
| 1:G6:51:PHE:HB3 | 1:G6:59:TYR:HB3 | 2.01 | 0.43 |
| 1:G6:117:LEU:HD23 | 1:G6:117:LEU:HA | 1.85 | 0.43 |
| 1:G6:314:SER:HA | 1:G6:350:LYS:O | 2.19 | 0.43 |
| 1:G8:293:MET:HE2 | 1:G8:367:PHE:HB2 | 2.00 | 0.43 |
| 2:G9:184:PRO:HG2 | 2:G9:398:MET:CE | 2.49 | 0.43 |
| 2:G9:404:PHE:CG | 2:G9:404:PHE:O | 2.72 | 0.43 |
| 2:H1:90:GLU:HB3 | 2:H1:121:ARG:HH12 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H4:317:PHE:HB3 | 1:H4:321:MET:SD | 2.59 | 0.43 |
| 1:H6:31:ASP:OD2 | 1:H6:33:THR:OG1 | 2.29 | 0.43 |
| 1:H6:36:TYR:CZ | 1:H6:44:LEU:HD21 | 2.54 | 0.43 |
| 2:I1:312:TYR:HB2 | 2:I1:343:PHE:HD1 | 1.84 | 0.43 |
| 1:I2:289:LEU:HD23 | 1:I2:365:ALA:HB2 | 2.01 | 0.43 |
| 2:I3:90:GLU:HG2 | 2:I3:121:ARG:HH12 | 1.84 | 0.43 |
| 2:I5:90:GLU:OE1 | 2:I5:90:GLU:N | 2.52 | 0.43 |
| 2:I5:150:GLY:HA2 | 2:I5:153:LEU:HG | 2.01 | 0.43 |
| 2:I5:184:PRO:HG3 | 2:I5:394:LYS:HD2 | 2.00 | 0.43 |
| 2:I9:227:LEU:O | 2:I9:231:ILE:HG12 | 2.18 | 0.43 |
| 2:J1:246:GLY:HA2 | 2:J1:357:TYR:CD2 | 2.54 | 0.43 |
| 1:J2:114:ASP:OD2 | 1:J2:115:SER:N | 2.52 | 0.43 |
| 2:J3:121:ARG:HA | 2:J3:121:ARG:HD2 | 1.70 | 0.43 |
| 1:J4:77:ARG:HE | 1:J4:90:PHE:HE2 | 1.66 | 0.43 |
| 2:J9:398:MET:HG3 | 1:K0:346:PRO:HD2 | 2.01 | 0.43 |
| 1:K0:2:ARG:HE | 1:K0:240:LEU:HD22 | 1.84 | 0.43 |
| 2:K3:33:ASP:HA | 2:K3:85:GLN:HB2 | 2.01 | 0.43 |
| 2:K3:176:GLN:NE2 | 2:K3:207:GLU:OE1 | 2.51 | 0.43 |
| 1:K4:218:THR:OG1 | 1:K4:219:THR:N | 2.51 | 0.43 |
| 1:K4:235:GLY:HA3 | 1:K4:366:THR:HG21 | 2.00 | 0.43 |
| 1:K4:404:ASP:OD1 | 1:K4:405:GLU:N | 2.49 | 0.43 |
| 1:K6:50:TYR:OH | 1:K6:237:THR:OG1 | 2.26 | 0.43 |
| 1:K6:145:SER:OG | 1:K6:146:GLY:N | 2.52 | 0.43 |
| 2:K7:60:LYS:HD2 | 2:K7:60:LYS:HA | 1.85 | 0.43 |
| 2:K7:223:THR:OG1 | 2:K7:224:TYR:N | 2.52 | 0.43 |
| 2:K7:288:VAL:HG13 | 2:K7:319:TYR:HE2 | 1.83 | 0.43 |
| 2:K7:405:VAL:HG13 | 2:K7:418:PHE:HE2 | 1.84 | 0.43 |
| 2:K9:122:ILE:HD11 | 2:K9:135:PHE:CE1 | 2.54 | 0.43 |
| 2:K9:311:LYS:HG2 | 2:K9:342:GLN:HE21 | 1.83 | 0.43 |
| 1:L4:138:SER:O | 1:L4:139:LEU:HD23 | 2.18 | 0.43 |
| 1:L6:138:SER:O | 1:L6:139:LEU:HD23 | 2.19 | 0.43 |
| 1:M0:31:ASP:HB2 | 1:M0:32:PRO:HD2 | 2.01 | 0.43 |
| 2:M1:35:GLN:OE1 | 2:M1:35:GLN:N | 2.52 | 0.43 |
| 2:M3:286:LEU:HD12 | 2:M3:286:LEU:HA | 1.82 | 0.43 |
| 2:M7:346:TRP:CE3 | 2:M7:347:CYS:HB3 | 2.54 | 0.43 |
| 1:N0:248:ALA:HA | 1:N0:252:LYS:HD2 | 2.00 | 0.43 |
| 2:N1:8:HIS:CD2 | 2:N1:17:GLY:HA3 | 2.54 | 0.43 |
| 1:N2:48:ASN:OD1 | 1:N2:48:ASN:N | 2.51 | 0.43 |
| 1:N2:67:ASP:N | 1:N2:67:ASP:OD1 | 2.52 | 0.43 |
| 1:N2:70:PRO:N | 1:N2:92:PHE:HZ | 2.15 | 0.43 |
| 2:N3:102:ASN:HD22 | 2:N3:105:ARG:CD | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N5:175:PRO:HB3 | 2:N5:390:ARG:HE | 1.83 | 0.43 |
| 2:N5:413:MET:HB3 | 2:N5:417:GLU:OE2 | 2.18 | 0.43 |
| 1:N8:36:TYR:CE2 | 1:N8:44:LEU:HD21 | 2.53 | 0.43 |
| 1:N8:210:ILE:O | 1:N8:214:THR:OG1 | 2.31 | 0.43 |
| 2:O3:28:HIS:CE1 | 2:O3:49:PHE:HA | 2.54 | 0.43 |
| 2:O5:88:HIS:ND1 | 2:O5:89:PRO:CD | 2.80 | 0.43 |
| 2:O5:328:VAL:O | 2:O5:332:VAL:HG23 | 2.19 | 0.43 |
| 1:O6:309:ARG:H | 1:O6:372:THR:CG2 | 2.32 | 0.43 |
| 2:O7:51:THR:HG23 | 2:O7:52:PHE:CD2 | 2.54 | 0.43 |
| 1:O8:155:ILE:HD12 | 1:O8:155:ILE:HA | 1.86 | 0.43 |
| 2:P3:203:MET:HE3 | 2:P3:267:PHE:HB3 | 2.00 | 0.43 |
| 1:P8:271:THR:HG21 | 1:P8:289:LEU:O | 2.19 | 0.43 |
| 2:P9:65:CYS:SG | 2:P9:66:ILE:N | 2.92 | 0.43 |
| 1:Q2:382:SER:HB2 | 1:Q2:415:MET:HG2 | 2.01 | 0.43 |
| 1:Q4:219:THR:HG23 | 1:Q4:219:THR:O | 2.19 | 0.43 |
| 1:Q6:55:THR:H | 1:Q6:58:ARG:HB3 | 1.84 | 0.43 |
| 1:Q8:16:ILE:CD1 | 1:Q8:229:ILE:HD13 | 2.49 | 0.43 |
| 1:Q8:193:VAL:HG11 | 1:Q8:418:LEU:HD22 | 2.01 | 0.43 |
| 2:Q9:16:VAL:HA | 2:Q9:228:ASN:HB3 | 1.99 | 0.43 |
| 1:R8:199:CYS:HB2 | 1:R8:265:PHE:HD1 | 1.83 | 0.43 |
| 1:S0:272:PRO:HD3 | 1:S0:364:SER:HA | 2.01 | 0.43 |
| 1:S4:167:PHE:CE2 | 1:S4:233:MET:HG2 | 2.54 | 0.43 |
| 1:S4:177:ASP:O | 2:S5:352:LYS:HD2 | 2.19 | 0.43 |
| 2:S5:49:PHE:CE2 | 2:S5:55:GLU:HB2 | 2.53 | 0.43 |
| 1:S6:114:ASP:OD1 | 1:S6:115:SER:N | 2.52 | 0.43 |
| 2:S9:72:PRO:HD2 | 1:T0:2:ARG:NH1 | 2.34 | 0.43 |
| 1:T0:3:GLU:HB2 | 1:T0:130:LEU:HA | 2.01 | 0.43 |
| 1:T0:249:ASP:OD1 | 1:T0:252:LYS:HE3 | 2.19 | 0.43 |
| 1:T0:329:GLN:O | 1:T0:333:VAL:HG23 | 2.19 | 0.43 |
| 2:T1:251:ASP:OD1 | 2:T1:254:GLU:HG2 | 2.19 | 0.43 |
| 1:T2:386:THR:HG22 | 1:T2:412:GLU:OE1 | 2.19 | 0.43 |
| 2:T3:11:GLN:HB3 | 41:T4:501:GTP:O2A | 2.19 | 0.43 |
| 1:T4:406:MET:O | 1:T4:410:GLU:HG2 | 2.18 | 0.43 |
| 2:T5:76:ASP:HA | 2:T5:79:ARG:HD2 | 1.99 | 0.43 |
| 1:T6:92:PHE:N | 1:T6:92:PHE:CD2 | 2.87 | 0.43 |
| 2:T7:62:VAL:HG23 | 2:T7:62:VAL:O | 2.19 | 0.43 |
| 2:T7:72:PRO:HG3 | 1:T8:1:MET:HG2 | 2.01 | 0.43 |
| 2:T7:431:ASP:OD2 | 13:5K:60:HIS:NE2 | 2.52 | 0.43 |
| 1:T8:8:GLN:CD | 1:T8:17:GLY:HA3 | 2.39 | 0.43 |
| 2:U1:141:VAL:HG13 | 2:U1:170:THR:CG2 | 2.49 | 0.43 |
| 1:U6:173:PRO:HD2 | 1:U6:380:ARG:NH1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U6:190:HIS:CD2 | 1:U6:414:ASN:HB2 | 2.53 | 0.43 |
| 2:U9:125:LEU:HD23 | 2:U9:125:LEU:HA | 1.80 | 0.43 |
| 1:V0:20:PHE:HA | 1:V0:230:SER:HB3 | 2.01 | 0.43 |
| 2:V1:9:ILE:HD11 | 2:V1:153:LEU:HD22 | 2.01 | 0.43 |
| 2:V3:278:ALA:HB3 | 2:V3:279:GLU:OE1 | 2.19 | 0.43 |
| 1:V8:138:SER:HA | 1:V8:169:VAL:HG22 | 2.01 | 0.43 |
| 2:V9:237:SER:HA | 2:V9:320:ARG:HD2 | 2.00 | 0.43 |
| 1:W0:150:LEU:HD12 | 1:W0:153:SER:OG | 2.19 | 0.43 |
| 2:W1:369:ALA:O | 2:W1:371:VAL:HG23 | 2.19 | 0.43 |
| 2:W3:414:GLU:HG2 | 2:W3:416:GLY:H | 1.84 | 0.43 |
| 1:W6:113:ILE:HD13 | 1:W6:150:LEU:HD22 | 2.00 | 0.43 |
| 2:W9:11:GLN:HA | 2:W9:14:ILE:HD11 | 2.01 | 0.43 |
| 2:W9:417:GLU:HA | 2:W9:420:GLU:HG2 | 2.01 | 0.43 |
| 1:X0:334:GLN:NE2 | 1:X0:348:ASN:OD1 | 2.51 | 0.43 |
| 1:X0:389:PHE:O | 1:X0:392:LYS:NZ | 2.34 | 0.43 |
| 1:X2:251:ARG:O | 1:X2:255:VAL:HG22 | 2.19 | 0.43 |
| 2:X3:253:THR:O | 2:X3:257:THR:HG23 | 2.19 | 0.43 |
| 2:X3:301:MET:HE1 | 2:X3:307:PRO:HD3 | 2.01 | 0.43 |
| 2:X3:365:GLY:O | 8:4V:437:ARG:NH1 | 2.51 | 0.43 |
| 2:X3:387:ILE:HD12 | 2:X3:390:ARG:NH2 | 2.32 | 0.43 |
| 1:X4:156:ARG:HA | 1:X4:156:ARG:HD2 | 1.76 | 0.43 |
| 1:X6:52:ASN:OD1 | 1:X6:62:ARG:NH2 | 2.48 | 0.43 |
| 2:X7:183:GLU:OE2 | 2:X7:184:PRO:HD3 | 2.18 | 0.43 |
| 1:Y2:204:ASN:OD1 | 39:Y2:501:GDP:O2' | 2.36 | 0.43 |
| 2:Y3:90:GLU:H | 2:Z9:283:HIS:CE1 | 2.36 | 0.43 |
| 2:Y3:246:GLY:H | 2:Y3:249:ASN:HD21 | 1.66 | 0.43 |
| 1:Y4:95:THR:OG1 | 1:Y4:96:GLY:N | 2.52 | 0.43 |
| 1:Y4:190:HIS:NE2 | 1:Y4:410:GLU:HG3 | 2.33 | 0.43 |
| 1:Y8:139:LEU:HD12 | 1:Y8:170:VAL:HG22 | 2.01 | 0.43 |
| 2:Z1:65:CYS:SG | 2:Z1:66:ILE:N | 2.92 | 0.43 |
| 1:Z2:175:VAL:HG13 | 2:Z3:329:ASN:ND2 | 2.34 | 0.43 |
| 2:Z3:407:TRP:O | 2:Z3:411:GLU:HG2 | 2.19 | 0.43 |
| 1:Z8:83:GLN:O | 1:0O:281:TYR:OH | 2.20 | 0.43 |
| 1:Z8:190:HIS:HD2 | 1:Z8:414:ASN:HB2 | 1.83 | 0.43 |
| 1:Z8:285:THR:OG1 | 1:Z8:288:GLU:HG2 | 2.19 | 0.43 |
| 1:0A:67:ASP:N | 1:0A:67:ASP:OD1 | 2.51 | 0.43 |
| 2:0B:115:VAL:HG21 | 2:0B:152:LEU:HG | 1.99 | 0.43 |
| 1:0C:206:ALA:HA | 1:0C:209:ASP:OD1 | 2.19 | 0.43 |
| 1:0C:268:VAL:HG23 | 1:0C:300:MET:SD | 2.58 | 0.43 |
| 1:0C:273:LEU:N | 1:0C:292:GLN:HE22 | 2.12 | 0.43 |
| 1:0E:42:LEU:HD12 | 1:0E:42:LEU:H | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0E:219:THR:O | 1:0E:219:THR:OG1 | 2.34 | 0.43 |
| 1:0E:285:THR:HG23 | 1:0E:287:PRO:HD2 | 2.01 | 0.43 |
| 1:0G:51:PHE:HB3 | 1:0G:59:TYR:HB3 | 2.01 | 0.43 |
| 2:0H:55:GLU:O | 2:0X:285:GLN:NE2 | 2.52 | 0.43 |
| 2:0H:234:VAL:HG22 | 2:0H:272:TYR:CD1 | 2.53 | 0.43 |
| 2:0H:397:LEU:HD23 | 2:0H:397:LEU:HA | 1.87 | 0.43 |
| 1:0K:58:ARG:HH11 | 1:0K:84:ILE:HA | 1.84 | 0.43 |
| 1:0K:385:PHE:CD1 | 1:0K:385:PHE:C | 2.92 | 0.43 |
| 2:0L:69:ASP:OD1 | 2:0L:70:LEU:N | 2.51 | 0.43 |
| 2:0L:429:GLU:O | 2:0L:433:GLU:HG2 | 2.19 | 0.43 |
| 1:0M:220:PRO:HG2 | 2:0N:326:LYS:HB2 | 1.99 | 0.43 |
| 1:0M:297:LYS:HA | 1:0M:297:LYS:HD3 | 1.79 | 0.43 |
| 1:0M:379:LYS:HA | 1:0M:382:SER:OG | 2.19 | 0.43 |
| 2:0N:377:MET:SD | 2:0N:378:ILE:N | 2.92 | 0.43 |
| 2:0N:405:VAL:O | 2:0N:409:VAL:HG23 | 2.19 | 0.43 |
| 2:0P:330:ALA:O | 2:0P:334:THR:HG23 | 2.18 | 0.43 |
| 1:0Q:69:GLU:O | 1:0Q:72:THR:OG1 | 2.37 | 0.43 |
| 1:0Q:207:LEU:HD11 | 1:0Q:229:ILE:HD11 | 1.99 | 0.43 |
| 1:0S:178:THR:OG1 | 1:0S:179:VAL:N | 2.52 | 0.43 |
| 2:0V:101:ASN:ND2 | 2:0V:143:GLY:HA2 | 2.33 | 0.43 |
| 2:0X:139:ASN:O | 2:0X:170:THR:HA | 2.19 | 0.43 |
| 1:0Y:83:GLN:O | 1:1O:281:TYR:OH | 2.28 | 0.43 |
| 2:1B:269:LEU:HD12 | 2:1B:269:LEU:H | 1.83 | 0.43 |
| 1:1C:155:ILE:HD12 | 1:1C:155:ILE:HA | 1.89 | 0.43 |
| 2:1D:90:GLU:HB3 | 2:1D:121:ARG:HH12 | 1.84 | 0.43 |
| 2:1F:217:LEU:HB3 | 2:1F:219:ILE:CD1 | 2.49 | 0.43 |
| 1:1G:212:PHE:HZ | 2:1H:326:LYS:HB2 | 1.84 | 0.43 |
| 1:1K:123:GLU:O | 1:1K:126:SER:OG | 2.23 | 0.43 |
| 2:1L:305:CYS:HB3 | 2:1L:387:ILE:HD11 | 2.01 | 0.43 |
| 1:1M:414:ASN:HA | 1:1M:417:ASP:OD2 | 2.19 | 0.43 |
| 1:1Q:135:VAL:O | 1:1Q:166:THR:HA | 2.18 | 0.43 |
| 1:1S:355:ASP:O | 1:1S:356:ILE:HD13 | 2.19 | 0.43 |
| 1:1S:414:ASN:O | 1:1S:418:LEU:HB2 | 2.19 | 0.43 |
| 2:1T:149:LEU:HA | 2:1T:152:LEU:HD12 | 2.00 | 0.43 |
| 2:1V:203:MET:C | 2:1V:204:LEU:HD12 | 2.40 | 0.43 |
| 2:1V:407:TRP:CD2 | 1:1W:255:VAL:HG23 | 2.54 | 0.43 |
| 2:1Z:329:ASN:HA | 2:1Z:332:VAL:HG22 | 2.00 | 0.43 |
| 1:2A:301:CYS:SG | 1:2A:302:ALA:N | 2.92 | 0.43 |
| 2:2B:120:ASP:OD2 | 38:8A:73:TRP:CD2 | 2.71 | 0.43 |
| 2:2D:372:GLN:HE21 | 10:5A:376:LEU:HD11 | 1.84 | 0.43 |
| 2:2F:185:TYR:HE1 | 2:2F:398:MET:HE3 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2I:397:TRP:HE1 | 2:2J:260:VAL:HG13 | 1.84 | 0.43 |
| 2:2J:47:ASP:OD1 | 2:2J:47:ASP:N | 2.51 | 0.43 |
| 2:2J:301:MET:HE1 | 2:2J:307:PRO:HD3 | 2.00 | 0.43 |
| 2:2J:417:GLU:OE2 | 2:2J:417:GLU:N | 2.34 | 0.43 |
| 2:2L:4:VAL:HG23 | 2:2L:134:GLY:O | 2.18 | 0.43 |
| 1:2M:177:ASP:OD1 | 2:2N:248:LEU:HD11 | 2.19 | 0.43 |
| 1:2M:194:GLU:OE1 | 1:2M:194:GLU:N | 2.50 | 0.43 |
| 2:2P:406:HIS:HA | 2:2P:409:VAL:HG22 | 2.01 | 0.43 |
| 1:2Q:114:ASP:OD1 | 1:2Q:115:SER:N | 2.51 | 0.43 |
| 1:2Q:156:ARG:NH1 | 1:2Q:197:ASP:OD2 | 2.51 | 0.43 |
| 2:2R:214:ARG:NH1 | 38:8A:61:LYS:HZ3 | 2.17 | 0.43 |
| 2:2T:76:ASP:HA | 2:2T:79:ARG:HD2 | 2.00 | 0.43 |
| 2:2T:119:LEU:HA | 2:2T:122:ILE:HG12 | 2.01 | 0.43 |
| 2:2T:174:SER:OG | 2:2T:207:GLU:OE1 | 2.29 | 0.43 |
| 1:2U:172:SER:OG | 1:2U:173:PRO:HD2 | 2.18 | 0.43 |
| 2:2X:417:GLU:O | 2:2X:420:GLU:HG2 | 2.19 | 0.43 |
| 1:2Y:42:LEU:HD12 | 38:8C:195:MET:HB3 | 2.00 | 0.43 |
| 1:3A:95:THR:HG23 | 1:3A:96:GLY:N | 2.34 | 0.43 |
| 1:3A:167:PHE:CZ | 1:3A:233:MET:HG2 | 2.53 | 0.43 |
| 1:3A:173:PRO:HG2 | 1:3A:174:LYS:NZ | 2.34 | 0.43 |
| 1:3A:183:TYR:O | 1:3A:187:LEU:HD13 | 2.18 | 0.43 |
| 2:3B:9:ILE:HD11 | 2:3B:153:LEU:HD23 | 2.01 | 0.43 |
| 2:3B:71:GLU:HB3 | 2:3B:98:ASP:OD1 | 2.19 | 0.43 |
| 2:3B:77:GLU:OE2 | 38:8D:199:THR:CG2 | 2.67 | 0.43 |
| 2:3B:231:ILE:HA | 2:3B:234:VAL:HG12 | 2.00 | 0.43 |
| 2:3D:66:ILE:O | 2:3D:66:ILE:HG13 | 2.19 | 0.43 |
| 1:3G:152:ILE:HG22 | 1:3G:195:ASN:HB3 | 2.00 | 0.43 |
| 1:3G:273:LEU:HD23 | 1:3G:273:LEU:HA | 1.88 | 0.43 |
| 2:3J:398:MET:HG3 | 1:3K:346:PRO:HD2 | 2.01 | 0.43 |
| 2:3L:33:ASP:OD1 | 2:3L:33:ASP:N | 2.51 | 0.43 |
| 1:3O:91:VAL:HG11 | 1:3O:116:VAL:HG23 | 2.00 | 0.43 |
| 1:3O:183:TYR:OH | 1:3O:388:MET:HB3 | 2.18 | 0.43 |
| 2:3P:72:PRO:HG2 | 1:3Q:46:ARG:HH22 | 1.84 | 0.43 |
| 2:3P:391:LEU:HD23 | 2:3P:391:LEU:HA | 1.89 | 0.43 |
| 2:3R:179:THR:O | 1:3S:350:LYS:HD2 | 2.19 | 0.43 |
| 3:3Z:216:ILE:HD13 | 3:3Z:216:ILE:HA | 1.89 | 0.43 |
| 3:4D:216:ILE:HD13 | 3:4D:216:ILE:HA | 1.89 | 0.43 |
| 3:4F:86:ASP:O | 3:4F:90:ILE:HG12 | 2.19 | 0.43 |
| 3:4J:184:LEU:HD12 | 3:4J:184:LEU:C | 2.38 | 0.43 |
| 6:4O:22:ALA:O | 6:4O:26:GLU:HG2 | 2.18 | 0.43 |
| 7:4U:77:ARG:NE | 24:6Y:19:PRO:HG3 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:4X:127:THR:HA | 8:4X:130:VAL:HG22 | 2.01 | 0.43 |
| 10:5B:264:ALA:O | 10:5B:268:MET:HG3 | 2.19 | 0.43 |
| 10:5C:376:LEU:HD23 | 10:5C:376:LEU:HA | 1.91 | 0.43 |
| 10:5D:233:GLU:OE1 | 10:5D:234:LEU:HD22 | 2.18 | 0.43 |
| 11:5E:2:LEU:HG | 11:5E:93:TYR:HB2 | 2.00 | 0.43 |
| 11:5E:110:GLN:CB | 11:5E:111:PRO:HD2 | 2.49 | 0.43 |
| 14:5L:20:GLY:N | 14:5L:296:SER:OG | 2.52 | 0.43 |
| 14:5L:96:ILE:HG22 | 14:5L:97:HIS:CD2 | 2.54 | 0.43 |
| 14:5L:339:HIS:NE2 | 14:5L:365:ARG:HD2 | 2.34 | 0.43 |
| 14:5L:417:ILE:HG13 | 14:5L:418:PHE:N | 2.34 | 0.43 |
| 14:5M:55:HIS:HE2 | 14:5M:88:TRP:HH2 | 1.67 | 0.43 |
| 14:5N:248:VAL:HB | 14:5N:252:ASP:HB2 | 1.99 | 0.43 |
| 14:5N:417:ILE:HG13 | 14:5N:418:PHE:N | 2.34 | 0.43 |
| 15:5O:172:TRP:HE1 | 15:5O:207:GLY:HA3 | 1.84 | 0.43 |
| 15:5O:176:ILE:HG13 | 15:5O:177:GLY:H | 1.83 | 0.43 |
| 15:5P:20:ILE:CG1 | 19:6E:104:TYR:CE1 | 3.02 | 0.43 |
| 15:5P:47:LEU:HD12 | 15:5P:47:LEU:HA | 1.73 | 0.43 |
| 17:5V:219:LEU:HA | 17:5V:222:ILE:HD12 | 2.01 | 0.43 |
| 18:6B:104:LEU:HD13 | 24:6Y:180:TYR:CE1 | 2.53 | 0.43 |
| 20:6F:107:VAL:HG12 | 20:6F:114:ASN:HD21 | 1.84 | 0.43 |
| 22:6N:60:LYS:HE3 | 22:6N:60:LYS:HB3 | 1.79 | 0.43 |
| 24:6U:36:VAL:CG2 | 24:6U:45:LEU:HD11 | 2.49 | 0.43 |
| 24:6U:349:ASN:HB2 | 24:6U:352:ASP:OD1 | 2.19 | 0.43 |
| 24:6W:119:VAL:HG21 | 24:6W:179:PHE:HD1 | 1.84 | 0.43 |
| 24:6W:279:TRP:CZ2 | 24:6W:364:ARG:HG3 | 2.53 | 0.43 |
| 24:6Y:562:LEU:HD23 | 24:6Y:562:LEU:HA | 1.72 | 0.43 |
| 24:6Z:156:ASP:OD1 | 24:6Z:157:ASP:N | 2.52 | 0.43 |
| 28:7H:451:LYS:CG | 28:7H:452:ASN:H | 2.32 | 0.43 |
| 29:7J:140:GLU:HG3 | 29:7J:144:GLN:NE2 | 2.33 | 0.43 |
| 36:7V:20:GLU:O | 36:7V:24:ASN:OD1 | 2.37 | 0.43 |
| 38:8C:218:PRO:HD2 | 38:8C:222:GLU:OE1 | 2.19 | 0.43 |
| 2:4:26:LEU:HD22 | 26:7D:48:LEU:HD11 | 2.00 | 0.42 |
| 2:6:324:VAL:HG11 | 26:7D:142:PHE:CZ | 2.52 | 0.42 |
| 1:A5:78:SER:O | 24:7A:148:ILE:HA | 2.19 | 0.42 |
| 2:B0:145:THR:OG1 | 41:B0:501:GTP:O1B | 2.37 | 0.42 |
| 2:B9:206:ASN:ND2 | 41:C0:501:GTP:O2' | 2.51 | 0.42 |
| 2:D7:145:THR:HG22 | 41:D7:501:GTP:O3B | 2.19 | 0.42 |
| 2:E3:370:LYS:HG2 | 22:6J:82:LEU:HB2 | 2.01 | 0.42 |
| 1:E8:357:PRO:HD2 | 22:6M:111:PRO:HB2 | 2.00 | 0.42 |
| 1:G2:228:LEU:HD23 | 1:G2:228:LEU:HA | 1.82 | 0.42 |
| 1:G2:272:PRO:HB2 | 1:G2:282:ARG:NH1 | 2.24 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G4:31:ASP:OD2 | 1:G4:33:THR:OG1 | 2.37 | 0.42 |
| 2:G7:221:ARG:NH1 | 22:6O:178:GLY:O | 2.52 | 0.42 |
| 2:G9:98:ASP:OD2 | 2:G9:99:ALA:N | 2.52 | 0.42 |
| 2:G9:101:ASN:HD22 | 2:G9:143:GLY:HA2 | 1.83 | 0.42 |
| 1:H2:68:LEU:HG | 1:H2:147:MET:HE1 | 2.00 | 0.42 |
| 1:H4:2:ARG:HB3 | 1:H4:131:GLN:HB2 | 2.01 | 0.42 |
| 1:H6:193:VAL:HG11 | 1:H6:418:LEU:CD1 | 2.49 | 0.42 |
| 2:H7:200:VAL:HG13 | 2:H7:268:MET:CE | 2.49 | 0.42 |
| 1:I0:3:GLU:HG3 | 1:I0:127:CYS:HB2 | 2.00 | 0.42 |
| 1:I0:246:LEU:HD22 | 1:I0:352:SER:HA | 2.00 | 0.42 |
| 2:I1:83:TYR:HB3 | 2:I1:86:LEU:HB3 | 2.00 | 0.42 |
| 1:I2:286:VAL:O | 1:I2:290:THR:HG23 | 2.18 | 0.42 |
| 2:I7:294:ALA:O | 2:I7:300:SER:OG | 2.25 | 0.42 |
| 1:I8:273:LEU:H | 1:I8:292:GLN:NE2 | 2.16 | 0.42 |
| 2:I9:346:TRP:CH2 | 2:I9:435:VAL:HG23 | 2.54 | 0.42 |
| 1:J0:77:ARG:HE | 1:J0:90:PHE:HE2 | 1.67 | 0.42 |
| 1:J2:69:GLU:OE1 | 1:J2:70:PRO:HD2 | 2.19 | 0.42 |
| 2:J3:286:LEU:O | 2:J3:373:ARG:NH1 | 2.51 | 0.42 |
| 2:J3:362:VAL:HG11 | 2:J3:370:LYS:HB3 | 2.01 | 0.42 |
| 2:J5:9:ILE:HD13 | 2:J5:150:GLY:HA2 | 2.01 | 0.42 |
| 1:J6:173:PRO:HD2 | 1:J6:380:ARG:CZ | 2.48 | 0.42 |
| 2:J9:145:THR:OG1 | 41:K0:501:GTP:O1B | 2.36 | 0.42 |
| 2:K3:290:GLU:OE1 | 2:K3:290:GLU:N | 2.42 | 0.42 |
| 1:K4:167:PHE:HD1 | 1:K4:200:MET:HB2 | 1.85 | 0.42 |
| 2:K5:401:LYS:HB3 | 2:K5:401:LYS:HE3 | 1.88 | 0.42 |
| 1:K6:404:ASP:HB3 | 1:K6:406:MET:SD | 2.59 | 0.42 |
| 2:L1:76:ASP:O | 2:L1:80:THR:HG23 | 2.19 | 0.42 |
| 1:L2:3:GLU:HB2 | 1:L2:130:LEU:HA | 2.01 | 0.42 |
| 1:L2:53:GLU:HG3 | 1:L2:59:TYR:CE1 | 2.54 | 0.42 |
| 2:L3:205:ASP:OD2 | 2:L3:206:ASN:N | 2.52 | 0.42 |
| 2:L5:111:GLY:O | 2:L5:115:VAL:HG12 | 2.18 | 0.42 |
| 1:L6:304:ASP:HB3 | 1:L6:307:HIS:HD1 | 1.84 | 0.42 |
| 2:L7:201:ALA:O | 2:L7:268:MET:HE2 | 2.19 | 0.42 |
| 2:L9:384:ILE:HG13 | 2:L9:385:GLY:N | 2.34 | 0.42 |
| 1:M0:355:ASP:HB3 | 29:7I:109:THR:HA | 2.00 | 0.42 |
| 2:M1:217:LEU:HB3 | 2:M1:219:ILE:HD12 | 2.01 | 0.42 |
| 2:M1:274:PRO:HD3 | 2:M1:374:ALA:HA | 2.00 | 0.42 |
| 2:M1:334:THR:HA | 2:M1:337:THR:HG22 | 2.01 | 0.42 |
| 1:M2:58:ARG:CZ | 2:N9:282:TYR:CE1 | 3.02 | 0.42 |
| 1:M2:123:GLU:O | 1:M2:126:SER:OG | 2.37 | 0.42 |
| 1:M4:178:THR:OG1 | 1:M4:179:VAL:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:M7:89:PRO:HB3 | 19:6E:25:VAL:HG11 | 1.95 | 0.42 |
| 1:M8:45:GLU:OE2 | 19:6E:20:LEU:HG | 2.19 | 0.42 |
| 1:M8:175:VAL:CG2 | 1:M8:205:GLU:HG2 | 2.45 | 0.42 |
| 1:M8:314:SER:OG | 1:M8:368:ILE:HB | 2.19 | 0.42 |
| 2:M9:242:LEU:HD11 | 2:M9:252:ILE:HG12 | 2.00 | 0.42 |
| 1:N0:418:LEU:O | 1:N0:421:GLU:HG2 | 2.19 | 0.42 |
| 2:N3:156:ARG:HA | 2:N3:159:VAL:HG22 | 2.01 | 0.42 |
| 2:N5:51:THR:HG21 | 2:N5:243:ARG:HG2 | 2.01 | 0.42 |
| 1:N6:67:ASP:N | 1:N6:67:ASP:OD1 | 2.53 | 0.42 |
| 2:N9:62:VAL:HG21 | 2:N9:88:HIS:HB2 | 2.01 | 0.42 |
| 2:O3:297:GLU:OE1 | 2:O3:297:GLU:N | 2.47 | 0.42 |
| 1:O4:211:CYS:HA | 1:O4:215:LEU:HB2 | 2.00 | 0.42 |
| 1:O8:11:GLN:HA | 1:O8:72:THR:HG21 | 2.01 | 0.42 |
| 2:P3:203:MET:SD | 2:P3:267:PHE:HD1 | 2.42 | 0.42 |
| 1:P4:31:ASP:HB2 | 1:P4:32:PRO:HD2 | 2.01 | 0.42 |
| 1:P6:178:THR:OG1 | 1:P6:181:GLU:HG3 | 2.19 | 0.42 |
| 1:P8:190:HIS:HD2 | 1:P8:411:ALA:HA | 1.83 | 0.42 |
| 2:P9:21:TRP:CH2 | 2:P9:63:PRO:HB3 | 2.53 | 0.42 |
| 1:Q6:108:GLU:HA | 1:Q6:111:GLU:OE2 | 2.19 | 0.42 |
| 1:Q6:174:LYS:HE2 | 1:Q6:174:LYS:HB2 | 1.82 | 0.42 |
| 1:Q6:186:THR:HG22 | 1:Q6:411:ALA:HB1 | 2.00 | 0.42 |
| 1:Q8:83:GLN:N | 1:Q8:83:GLN:OE1 | 2.51 | 0.42 |
| 2:Q9:147:SER:OG | 2:Q9:190:SER:HB3 | 2.19 | 0.42 |
| 2:R1:276:ILE:HD12 | 2:R1:276:ILE:HA | 1.78 | 0.42 |
| 1:R4:128:ASP:OD1 | 1:R4:129:CYS:N | 2.51 | 0.42 |
| 1:R4:397:TRP:CZ2 | 2:R5:256:GLN:HB3 | 2.54 | 0.42 |
| 1:R6:178:THR:OG1 | 1:R6:181:GLU:HG3 | 2.18 | 0.42 |
| 2:R7:330:ALA:O | 2:R7:334:THR:HG23 | 2.19 | 0.42 |
| 1:R8:10:GLY:HA2 | 1:R8:143:THR:HG23 | 1.99 | 0.42 |
| 1:R8:237:THR:HG22 | 1:R8:237:THR:O | 2.19 | 0.42 |
| 1:S0:219:THR:HB | 2:S1:324:VAL:HG11 | 2.00 | 0.42 |
| 1:S0:317:PHE:HB3 | 1:S0:321:MET:SD | 2.59 | 0.42 |
| 2:S1:176:GLN:HG2 | 2:S1:177:VAL:N | 2.34 | 0.42 |
| 1:S4:174:LYS:HB3 | 13:5H:14:PHE:CE2 | 2.54 | 0.42 |
| 1:S4:192:LEU:HD22 | 1:S4:196:ALA:HB2 | 2.01 | 0.42 |
| 1:S8:222:PHE:CZ | 2:S9:325:PRO:HB3 | 2.54 | 0.42 |
| 1:T0:95:THR:HG23 | 1:T0:96:GLY:H | 1.84 | 0.42 |
| 1:T2:414:ASN:HD21 | 3:4D:84:LYS:HD2 | 1.83 | 0.42 |
| 2:T3:70:LEU:HD12 | 2:T3:145:THR:HG22 | 2.01 | 0.42 |
| 2:T5:274:PRO:HD3 | 2:T5:374:ALA:HA | 2.01 | 0.42 |
| 1:T6:246:LEU:HD22 | 1:T6:352:SER:HA | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T7:209:ILE:HG23 | 2:T7:230:LEU:HD11 | 2.01 | 0.42 |
| 2:U1:223:THR:OG1 | 2:U1:224:TYR:N | 2.52 | 0.42 |
| 2:U3:32:PRO:HB3 | 2:U3:83:TYR:CE1 | 2.54 | 0.42 |
| 2:U5:101:ASN:ND2 | 2:U5:143:GLY:HA2 | 2.34 | 0.42 |
| 1:U8:161:ASP:OD2 | 1:U8:162:ARG:NH1 | 2.52 | 0.42 |
| 1:U8:208:TYR:CE1 | 1:U8:225:LEU:HD11 | 2.54 | 0.42 |
| 2:U9:14:ILE:HD11 | 2:U9:74:VAL:HG13 | 2.00 | 0.42 |
| 2:U9:280:LYS:HA | 2:U9:280:LYS:HD3 | 1.84 | 0.42 |
| 1:V0:249:ASP:H | 1:V0:252:LYS:HD3 | 1.84 | 0.42 |
| 2:V1:139:ASN:O | 2:V1:170:THR:HA | 2.19 | 0.42 |
| 1:V4:53:GLU:OE1 | 1:V4:57:GLY:HA2 | 2.19 | 0.42 |
| 1:V4:285:THR:O | 1:V4:288:GLU:HG3 | 2.18 | 0.42 |
| 2:V7:212:ILE:HG23 | 2:V7:275:ILE:HD12 | 2.01 | 0.42 |
| 2:V7:426:ALA:O | 2:V7:430:LYS:HG2 | 2.19 | 0.42 |
| 1:V8:86:ARG:HG2 | 1:V8:88:ASP:H | 1.84 | 0.42 |
| 1:W4:101:TRP:CE3 | 1:W4:403:MET:HE1 | 2.54 | 0.42 |
| 1:W4:289:LEU:HD23 | 1:W4:365:ALA:HB2 | 2.01 | 0.42 |
| 1:W6:130:LEU:HB2 | 1:W6:162:ARG:HE | 1.84 | 0.42 |
| 1:W6:209:ASP:OD1 | 1:W6:213:ARG:HD3 | 2.19 | 0.42 |
| 1:W6:260:PHE:HB2 | 1:W6:263:LEU:HD13 | 2.01 | 0.42 |
| 1:W6:325:GLU:O | 1:W6:329:GLN:HB2 | 2.19 | 0.42 |
| 1:X2:167:PHE:HZ | 1:X2:236:ILE:HD11 | 1.83 | 0.42 |
| 1:X2:177:ASP:OD1 | 2:X3:248:LEU:HD11 | 2.18 | 0.42 |
| 2:X3:27:GLU:HG3 | 2:X3:28:HIS:HD2 | 1.84 | 0.42 |
| 2:X3:224:TYR:CD1 | 2:X3:227:LEU:HD12 | 2.52 | 0.42 |
| 1:X4:309:ARG:H | 1:X4:372:THR:HG22 | 1.84 | 0.42 |
| 2:X5:180:ALA:HB1 | 1:X6:256:ASN:HD21 | 1.83 | 0.42 |
| 1:X6:8:GLN:HB3 | 1:X6:13:GLY:O | 2.19 | 0.42 |
| 1:X6:171:PRO:HG3 | 1:X6:181:GLU:HB3 | 2.01 | 0.42 |
| 1:Y0:2:ARG:HE | 1:Y0:240:LEU:HD22 | 1.84 | 0.42 |
| 2:Y3:318:MET:HE1 | 2:Y3:376:CYS:O | 2.20 | 0.42 |
| 1:Y8:337:ASN:ND2 | 1:Y8:337:ASN:O | 2.51 | 0.42 |
| 2:Y9:149:LEU:HA | 2:Y9:152:LEU:HB3 | 2.01 | 0.42 |
| 2:Z1:71:GLU:N | 2:Z1:98:ASP:OD2 | 2.52 | 0.42 |
| 1:Z2:156:ARG:HD2 | 1:Z2:156:ARG:HA | 1.94 | 0.42 |
| 1:Z2:204:ASN:ND2 | 39:Z2:503:GDP:HN22 | 2.17 | 0.42 |
| 1:Z2:204:ASN:HD21 | 39:Z2:503:GDP:HN22 | 1.66 | 0.42 |
| 1:Z2:409:THR:HA | 1:Z2:412:GLU:OE2 | 2.19 | 0.42 |
| 2:Z5:338:LYS:NZ | 2:Z5:340:THR:HG23 | 2.34 | 0.42 |
| 2:Z7:157:LEU:HD13 | 2:Z7:166:LYS:HD3 | 2.01 | 0.42 |
| 1:Z8:67:ASP:N | 1:Z8:67:ASP:OD1 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z8:179:VAL:HG12 | 2:Z9:349:THR:O | 2.19 | 0.42 |
| 1:Z8:294:TRP:CG | 1:Z8:333:VAL:HG21 | 2.54 | 0.42 |
| 2:Z9:85:GLN:O | 2:Z9:88:HIS:NE2 | 2.52 | 0.42 |
| 1:0A:21:TRP:CH2 | 1:0A:61:PRO:HB3 | 2.54 | 0.42 |
| 2:0B:9:ILE:O | 2:0B:9:ILE:HG13 | 2.18 | 0.42 |
| 2:0B:139:ASN:O | 2:0B:171:VAL:HG23 | 2.18 | 0.42 |
| 2:0H:288:VAL:O | 2:0H:292:THR:OG1 | 2.24 | 0.42 |
| 1:0M:116:VAL:O | 1:0M:120:VAL:HG12 | 2.19 | 0.42 |
| 1:0Q:170:VAL:HG22 | 1:0Q:202:LEU:O | 2.19 | 0.42 |
| 1:0S:43:GLN:O | 1:0S:47:ILE:HG23 | 2.19 | 0.42 |
| 2:0V:267:PHE:HB2 | 2:0V:384:ILE:HD12 | 2.00 | 0.42 |
| 2:0V:298:PRO:HA | 2:0V:301:MET:HG3 | 2.01 | 0.42 |
| 2:0X:223:THR:OG1 | 2:0X:224:TYR:N | 2.51 | 0.42 |
| 2:0Z:337:THR:O | 2:0Z:339:ARG:NH1 | 2.52 | 0.42 |
| 1:1C:98:GLY:HA2 | 2:1D:254:GLU:OE1 | 2.18 | 0.42 |
| 2:1D:88:HIS:HE2 | 2:1D:90:GLU:HB2 | 1.84 | 0.42 |
| 1:1M:418:LEU:O | 1:1M:421:GLU:HG2 | 2.19 | 0.42 |
| 2:1N:202:VAL:HG22 | 2:1N:268:MET:HB2 | 1.99 | 0.42 |
| 1:1O:221:THR:OG1 | 1:1O:222:PHE:N | 2.52 | 0.42 |
| 2:1P:269:LEU:HD21 | 2:1P:384:ILE:HG23 | 2.01 | 0.42 |
| 1:1Q:201:VAL:HG21 | 1:1Q:374:ILE:HD11 | 2.01 | 0.42 |
| 2:1R:287:SER:OG | 2:1R:288:VAL:N | 2.52 | 0.42 |
| 2:1R:305:CYS:HB3 | 2:1R:387:ILE:HD11 | 2.00 | 0.42 |
| 1:1S:257:LEU:HD21 | 1:1S:314:SER:OG | 2.19 | 0.42 |
| 1:1S:309:ARG:H | 1:1S:372:THR:HG22 | 1.84 | 0.42 |
| 1:1S:396:HIS:H | 1:1S:396:HIS:CD2 | 2.37 | 0.42 |
| 2:1T:242:LEU:HD11 | 2:1T:252:ILE:HG12 | 2.01 | 0.42 |
| 1:1U:263:LEU:HD13 | 1:1U:422:TYR:CE1 | 2.54 | 0.42 |
| 1:1W:53:GLU:OE1 | 1:1W:57:GLY:HA2 | 2.19 | 0.42 |
| 2:1Z:175:PRO:HB3 | 2:1Z:390:ARG:NE | 2.33 | 0.42 |
| 1:2A:20:PHE:CD1 | 1:2A:233:MET:HE2 | 2.54 | 0.42 |
| 1:2A:200:MET:HE1 | 1:2A:236:ILE:HG21 | 2.01 | 0.42 |
| 2:2B:47:ASP:N | 2:2B:47:ASP:OD1 | 2.50 | 0.42 |
| 2:2B:88:HIS:ND1 | 2:2R:283:HIS:HA | 2.34 | 0.42 |
| 1:2C:141:GLY:HA3 | 39:2C:502:GDP:PB | 2.59 | 0.42 |
| 2:2D:115:VAL:HG11 | 2:2D:152:LEU:HG | 2.00 | 0.42 |
| 2:2D:317:LEU:HB3 | 2:2D:319:TYR:HE1 | 1.84 | 0.42 |
| 1:2E:152:ILE:HG22 | 1:2E:195:ASN:HB3 | 1.99 | 0.42 |
| 2:2F:325:PRO:HA | 2:2F:328:VAL:HG22 | 2.00 | 0.42 |
| 1:2I:118:ASP:CB | 38:8C:99:THR:HG21 | 2.27 | 0.42 |
| 1:2Q:257:LEU:HA | 1:2Q:312:THR:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2R:21:TRP:CZ3 | 2:2R:63:PRO:HB3 | 2.54 | 0.42 |
| 2:2R:72:PRO:HD2 | 1:2S:2:ARG:NH1 | 2.34 | 0.42 |
| 1:2S:253:LEU:HD23 | 1:2S:253:LEU:HA | 1.89 | 0.42 |
| 2:2T:287:SER:H | 2:2T:290:GLU:CD | 2.21 | 0.42 |
| 1:2U:43:GLN:O | 1:2U:47:ILE:HG23 | 2.19 | 0.42 |
| 2:2X:27:GLU:OE1 | 2:2X:243:ARG:NH1 | 2.52 | 0.42 |
| 1:2Y:331:LEU:HG | 1:2Y:335:ASN:OD1 | 2.19 | 0.42 |
| 2:2Z:8:HIS:CD2 | 2:2Z:17:GLY:HA3 | 2.54 | 0.42 |
| 2:2Z:279:GLU:N | 2:2Z:279:GLU:CD | 2.72 | 0.42 |
| 2:2Z:339:ARG:CZ | 38:8C:78:ASP:HA | 2.49 | 0.42 |
| 1:3A:34:GLY:HA3 | 1:3A:58:ARG:HD3 | 1.99 | 0.42 |
| 1:3A:306:ARG:H | 1:3A:306:ARG:HG2 | 1.68 | 0.42 |
| 1:3C:50:TYR:CE2 | 1:3C:241:ARG:HD3 | 2.53 | 0.42 |
| 1:3C:100:ASN:HB3 | 1:3C:103:LYS:HB2 | 2.00 | 0.42 |
| 1:3C:395:LEU:O | 1:3C:399:THR:HG23 | 2.18 | 0.42 |
| 2:3D:217:LEU:O | 2:3D:219:ILE:HG12 | 2.19 | 0.42 |
| 2:3H:90:GLU:OE1 | 2:3H:90:GLU:N | 2.52 | 0.42 |
| 2:3H:121:ARG:NH2 | 3:3X:36:PHE:CG | 2.86 | 0.42 |
| 2:3H:164:LYS:HE3 | 3:3X:136:HIS:HB2 | 1.99 | 0.42 |
| 2:3H:269:LEU:HD23 | 2:3H:269:LEU:HA | 1.85 | 0.42 |
| 2:3J:14:ILE:HD11 | 2:3J:74:VAL:HG13 | 2.00 | 0.42 |
| 1:3K:220:PRO:HG2 | 2:3L:326:LYS:HB2 | 2.00 | 0.42 |
| 1:3M:273:LEU:H | 1:3M:292:GLN:HE22 | 1.66 | 0.42 |
| 2:3P:203:MET:HB2 | 2:3P:303:VAL:HG21 | 2.01 | 0.42 |
| 1:3Q:68:LEU:HD21 | 1:3Q:112:LEU:HD22 | 2.00 | 0.42 |
| 1:3Q:167:PHE:CE2 | 1:3Q:233:MET:HG2 | 2.54 | 0.42 |
| 2:3R:37:PRO:HB2 | 2:3R:39:ASP:OD2 | 2.19 | 0.42 |
| 2:3T:139:ASN:OD1 | 2:3T:139:ASN:N | 2.51 | 0.42 |
| 3:3V:86:ASP:O | 3:3V:90:ILE:HG12 | 2.19 | 0.42 |
| 3:3V:119:THR:OG1 | 3:3V:163:ASP:OD1 | 2.37 | 0.42 |
| 3:3X:86:ASP:O | 3:3X:90:ILE:HG12 | 2.19 | 0.42 |
| 3:3X:119:THR:OG1 | 3:3X:163:ASP:OD1 | 2.37 | 0.42 |
| 3:4B:9:LEU:HD22 | 3:4B:173:ARG:HH11 | 1.84 | 0.42 |
| 3:4B:86:ASP:O | 3:4B:90:ILE:HG12 | 2.19 | 0.42 |
| 3:4B:216:ILE:HD13 | 3:4B:216:ILE:HA | 1.89 | 0.42 |
| 3:4H:119:THR:OG1 | 3:4H:163:ASP:OD1 | 2.37 | 0.42 |
| 5:4L:452:LYS:HA | 5:4L:452:LYS:HD3 | 1.75 | 0.42 |
| 5:4M:265:GLU:OE2 | 5:4M:268:ARG:NH2 | 2.52 | 0.42 |
| 5:4M:286:LEU:HD23 | 5:4M:286:LEU:HA | 1.79 | 0.42 |
| 6:4O:287:SER:HB2 | 6:4O:291:ARG:CZ | 2.49 | 0.42 |
| 7:4R:349:LEU:HD23 | 7:4R:349:LEU:HA | 1.91 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:4U:137:THR:OG1 | 7:4U:140:ASP:HB2 | 2.19 | 0.42 |
| 8:4W:370:VAL:O | 8:4W:374:GLU:HG2 | 2.18 | 0.42 |
| 8:4X:138:ASP:OD1 | 8:4X:139:ALA:N | 2.52 | 0.42 |
| 10:5C:247:GLU:O | 10:5C:251:GLU:HG2 | 2.19 | 0.42 |
| 10:5C:295:ARG:CZ | 38:8B:194:GLU:HB2 | 2.49 | 0.42 |
| 10:5D:226:ARG:HH21 | 10:5D:230:ARG:CZ | 2.32 | 0.42 |
| 13:5I:136:PHE:CD2 | 19:6E:259:SER:HB2 | 2.43 | 0.42 |
| 14:5L:164:ILE:HG23 | 14:5L:174:TRP:CD1 | 2.53 | 0.42 |
| 14:5L:241:GLY:O | 14:5L:243:THR:HG23 | 2.18 | 0.42 |
| 14:5M:96:ILE:HG22 | 14:5M:97:HIS:CD2 | 2.54 | 0.42 |
| 14:5M:339:HIS:NE2 | 14:5M:365:ARG:HD2 | 2.34 | 0.42 |
| 14:5M:387:CYS:HB2 | 14:5M:429:THR:O | 2.18 | 0.42 |
| 14:5N:113:CYS:SG | 14:5N:159:SER:HB3 | 2.59 | 0.42 |
| 14:5N:241:GLY:O | 14:5N:243:THR:HG23 | 2.18 | 0.42 |
| 14:5N:339:HIS:NE2 | 14:5N:365:ARG:HD2 | 2.34 | 0.42 |
| 15:5O:214:ALA:HA | 15:5O:217:GLU:HG3 | 2.01 | 0.42 |
| 15:5P:100:PRO:HB3 | 15:5P:156:GLY:HA3 | 2.00 | 0.42 |
| 17:5S:87:VAL:HG13 | 17:5S:88:PRO:HD2 | 2.01 | 0.42 |
| 17:5U:87:VAL:HG13 | 17:5U:88:PRO:HD2 | 2.01 | 0.42 |
| 18:5X:180:ARG:HH21 | 18:5X:180:ARG:HG3 | 1.83 | 0.42 |
| 21:6H:12:ASN:OD1 | 21:6H:13:GLY:N | 2.43 | 0.42 |
| 22:6K:157:VAL:HG21 | 22:6K:225:ALA:CB | 2.49 | 0.42 |
| 22:6L:207:PHE:HB3 | 22:6L:227:TYR:OH | 2.19 | 0.42 |
| 22:6M:83:TRP:CZ3 | 22:6N:36:VAL:HG11 | 2.54 | 0.42 |
| 22:6N:240:TYR:O | 22:6N:244:VAL:HG12 | 2.19 | 0.42 |
| 22:6N:277:SER:O | 22:6N:281:LYS:HG2 | 2.19 | 0.42 |
| 22:6O:288:GLY:O | 22:6O:291:GLU:HG3 | 2.19 | 0.42 |
| 24:6V:345:ASP:N | 24:6V:345:ASP:OD2 | 2.49 | 0.42 |
| 24:6Z:505:LYS:HZ2 | 24:6Z:506:PRO:HD2 | 1.84 | 0.42 |
| 24:7A:152:ARG:HD3 | 24:7A:160:PHE:CG | 2.54 | 0.42 |
| 26:7F:103:PRO:HG3 | 26:7F:128:GLY:HA2 | 2.01 | 0.42 |
| 36:7V:75:PHE:HZ | 36:7V:98:VAL:HG21 | 1.84 | 0.42 |
| 36:7W:75:PHE:HZ | 36:7W:98:VAL:HG21 | 1.84 | 0.42 |
| 38:8C:93:LYS:HE3 | 38:8C:102:PHE:CZ | 2.54 | 0.42 |
| 2:A4:33:ASP:HB3 | 18:6D:77:THR:HG21 | 2.00 | 0.42 |
| 2:D1:76:ASP:OD2 | 22:6M:21:THR:OG1 | 2.37 | 0.42 |
| 1:E8:41:ASP:OD1 | 22:6M:188:ARG:HD3 | 2.18 | 0.42 |
| 2:E9:222:PRO:HA | 22:6N:32:LYS:HA | 2.00 | 0.42 |
| 2:F5:218:ASP:O | 22:6I:176:LYS:NZ | 2.50 | 0.42 |
| 2:G1:230:LEU:HD22 | 2:G1:368:LEU:HD11 | 2.01 | 0.42 |
| 2:G3:114:ILE:HG21 | 2:G3:149:LEU:HD22 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G3:267:PHE:HB2 | 2:G3:384:ILE:HG21 | 2.01 | 0.42 |
| 1:G6:372:THR:O | 1:G6:375:GLN:HG3 | 2.20 | 0.42 |
| 2:G7:230:LEU:O | 2:G7:234:VAL:HG23 | 2.19 | 0.42 |
| 2:G9:121:ARG:HD2 | 2:G9:124:LYS:HE3 | 2.00 | 0.42 |
| 2:G9:316:CYS:O | 2:G9:317:LEU:HD23 | 2.18 | 0.42 |
| 2:H1:70:LEU:HB3 | 2:H1:97:GLU:O | 2.19 | 0.42 |
| 1:H4:173:PRO:HB3 | 1:H4:384:GLN:HE22 | 1.84 | 0.42 |
| 1:H4:253:LEU:HD11 | 1:H4:316:LEU:HD11 | 2.00 | 0.42 |
| 1:H6:3:GLU:HG3 | 1:H6:127:CYS:SG | 2.59 | 0.42 |
| 1:H6:232:VAL:O | 1:H6:236:ILE:HG12 | 2.18 | 0.42 |
| 2:H7:65:CYS:SG | 2:H7:66:ILE:N | 2.91 | 0.42 |
| 2:H7:69:ASP:OD1 | 2:H7:70:LEU:N | 2.48 | 0.42 |
| 2:H7:72:PRO:HD2 | 1:H8:2:ARG:NH1 | 2.34 | 0.42 |
| 1:I2:49:VAL:C | 1:I2:62:ARG:HH12 | 2.22 | 0.42 |
| 2:I5:4:VAL:HG13 | 2:I5:134:GLY:O | 2.19 | 0.42 |
| 1:I8:3:GLU:HB2 | 1:I8:130:LEU:HD13 | 2.00 | 0.42 |
| 1:I8:275:SER:O | 1:I8:279:GLN:HG3 | 2.19 | 0.42 |
| 2:I9:172:TYR:CZ | 2:I9:203:MET:SD | 3.12 | 0.42 |
| 2:J3:334:THR:HA | 2:J3:337:THR:HG22 | 2.01 | 0.42 |
| 2:J5:155:GLU:HB2 | 2:J5:197:HIS:CE1 | 2.54 | 0.42 |
| 1:J6:279:GLN:HB3 | 5:4M:184:ARG:HG3 | 2.01 | 0.42 |
| 2:J7:223:THR:OG1 | 2:J7:224:TYR:N | 2.52 | 0.42 |
| 2:J7:244:PHE:HE1 | 29:7J:417:TYR:CG | 2.37 | 0.42 |
| 2:J7:317:LEU:HB3 | 2:J7:319:TYR:HE1 | 1.85 | 0.42 |
| 1:J8:39:ASP:OD1 | 1:J8:40:SER:N | 2.52 | 0.42 |
| 2:J9:123:ARG:NH2 | 2:J9:160:ASP:OD2 | 2.46 | 0.42 |
| 1:K0:175:VAL:HG22 | 2:K1:329:ASN:ND2 | 2.34 | 0.42 |
| 2:K3:75:VAL:HG11 | 2:K3:94:SER:HB2 | 2.01 | 0.42 |
| 2:K3:90:GLU:CG | 2:K3:121:ARG:HH22 | 2.31 | 0.42 |
| 1:K8:175:VAL:HG13 | 2:K9:329:ASN:ND2 | 2.34 | 0.42 |
| 2:L5:381:SER:OG | 2:L5:382:THR:N | 2.52 | 0.42 |
| 2:L7:60:LYS:HE3 | 2:L7:88:HIS:NE2 | 2.34 | 0.42 |
| 2:L7:238:LEU:HD12 | 2:L7:239:THR:HG23 | 2.01 | 0.42 |
| 2:L7:241:SER:OG | 2:L7:250:VAL:O | 2.30 | 0.42 |
| 2:M3:172:TYR:CZ | 2:M3:203:MET:SD | 3.12 | 0.42 |
| 2:M3:224:TYR:CD1 | 1:M4:323:THR:HG21 | 2.54 | 0.42 |
| 2:M7:89:PRO:HB2 | 19:6E:25:VAL:HG11 | 1.93 | 0.42 |
| 2:M9:49:PHE:HB2 | 2:M9:53:PHE:HD2 | 1.83 | 0.42 |
| 1:N2:31:ASP:HB2 | 1:N2:32:PRO:HD2 | 2.00 | 0.42 |
| 1:N2:178:THR:HG22 | 2:N3:352:LYS:HE2 | 2.00 | 0.42 |
| 2:N3:4:VAL:HG12 | 2:N3:134:GLY:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N6:320:ARG:NH2 | 32:7O:67:ARG:HD3 | 2.32 | 0.42 |
| 1:N8:51:PHE:HB3 | 1:N8:59:TYR:HB3 | 2.01 | 0.42 |
| 1:O0:131:GLN:HE21 | 1:O0:250:LEU:HG | 1.84 | 0.42 |
| 1:O0:272:PRO:HG2 | 27:7G:54:HIS:CD2 | 2.54 | 0.42 |
| 1:O2:204:ASN:ND2 | 39:O2:502:GDP:HN22 | 2.16 | 0.42 |
| 2:O5:319:TYR:HB3 | 2:O5:323:VAL:HG21 | 2.01 | 0.42 |
| 1:O6:344:TRP:CE3 | 1:O6:345:ILE:HG13 | 2.54 | 0.42 |
| 2:O9:326:LYS:HG3 | 2:O9:327:ASP:N | 2.34 | 0.42 |
| 2:P3:338:LYS:HZ2 | 2:P3:339:ARG:N | 2.17 | 0.42 |
| 1:P6:67:ASP:OD1 | 1:P6:68:LEU:N | 2.47 | 0.42 |
| 2:P9:319:TYR:HD2 | 2:P9:323:VAL:HG21 | 1.84 | 0.42 |
| 2:Q1:167:LEU:HD13 | 2:Q1:200:VAL:HB | 2.01 | 0.42 |
| 1:Q2:108:GLU:HA | 1:Q2:111:GLU:OE2 | 2.19 | 0.42 |
| 1:Q2:219:THR:O | 1:Q2:219:THR:OG1 | 2.33 | 0.42 |
| 1:Q8:113:ILE:HD12 | 1:Q8:116:VAL:CG1 | 2.48 | 0.42 |
| 2:Q9:164:LYS:HB3 | 2:Q9:164:LYS:HE3 | 1.58 | 0.42 |
| 2:Q9:417:GLU:HA | 2:Q9:420:GLU:HG2 | 2.01 | 0.42 |
| 1:R0:317:PHE:HB3 | 1:R0:321:MET:SD | 2.59 | 0.42 |
| 1:R4:177:ASP:OD2 | 2:R5:248:LEU:HD11 | 2.19 | 0.42 |
| 1:R6:1:MET:N | 1:R6:48:ASN:OD1 | 2.53 | 0.42 |
| 2:S1:51:THR:HG21 | 2:S1:243:ARG:HG2 | 2.01 | 0.42 |
| 1:S4:189:VAL:O | 1:S4:193:VAL:HG12 | 2.18 | 0.42 |
| 1:S4:312:THR:HB | 1:S4:350:LYS:HZ2 | 1.84 | 0.42 |
| 2:S5:266:HIS:O | 2:S5:266:HIS:ND1 | 2.49 | 0.42 |
| 1:S6:128:ASP:OD1 | 1:S6:128:ASP:N | 2.44 | 0.42 |
| 1:S6:359:LYS:HB3 | 31:7M:9:ARG:CZ | 2.48 | 0.42 |
| 2:S7:145:THR:OG1 | 41:S8:501:GTP:O1B | 2.37 | 0.42 |
| 2:S7:288:VAL:HG21 | 2:S7:327:ASP:OD1 | 2.19 | 0.42 |
| 2:S7:315:CYS:SG | 2:S7:316:CYS:N | 2.92 | 0.42 |
| 2:S9:9:ILE:HD13 | 2:S9:150:GLY:HA2 | 2.01 | 0.42 |
| 2:S9:167:LEU:HD21 | 2:S9:256:GLN:HE22 | 1.84 | 0.42 |
| 2:S9:174:SER:OG | 2:S9:207:GLU:OE1 | 2.37 | 0.42 |
| 1:T2:170:VAL:HG22 | 1:T2:202:LEU:O | 2.19 | 0.42 |
| 2:T5:327:ASP:OD1 | 2:T5:327:ASP:N | 2.50 | 0.42 |
| 1:T6:307:HIS:CD2 | 17:5U:52:PRO:HB3 | 2.54 | 0.42 |
| 1:T8:173:PRO:HB3 | 1:T8:384:GLN:HE22 | 1.84 | 0.42 |
| 1:U2:3:GLU:HG3 | 1:U2:127:CYS:SG | 2.60 | 0.42 |
| 1:U4:295:ASP:HB2 | 1:U4:298:ASN:HB2 | 2.02 | 0.42 |
| 2:U5:53:PHE:HA | 2:U5:62:VAL:O | 2.19 | 0.42 |
| 2:U7:336:LYS:HZ2 | 2:U7:350:GLY:H | 1.66 | 0.42 |
| 2:U9:88:HIS:HA | 2:W5:283:HIS:CG | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U9:97:GLU:OE2 | 2:U9:105:ARG:NH2 | 2.52 | 0.42 |
| 2:U9:246:GLY:N | 2:U9:249:ASN:HD21 | 2.15 | 0.42 |
| 2:U9:286:LEU:HD12 | 2:U9:290:GLU:OE2 | 2.18 | 0.42 |
| 2:V3:394:LYS:HB2 | 1:V4:346:PRO:HG3 | 2.01 | 0.42 |
| 1:V4:41:ASP:OD1 | 1:V4:41:ASP:N | 2.52 | 0.42 |
| 1:V4:122:LYS:HA | 1:V4:122:LYS:HD3 | 1.81 | 0.42 |
| 1:V4:272:PRO:HD3 | 1:V4:364:SER:HA | 2.01 | 0.42 |
| 1:V6:95:THR:HG23 | 1:V6:96:GLY:N | 2.34 | 0.42 |
| 2:V7:101:ASN:OD1 | 2:V7:186:ASN:ND2 | 2.49 | 0.42 |
| 2:V7:331:SER:O | 2:V7:334:THR:OG1 | 2.24 | 0.42 |
| 1:W0:165:LEU:HD23 | 1:W0:165:LEU:HA | 1.83 | 0.42 |
| 2:W1:223:THR:OG1 | 1:W2:245:GLN:NE2 | 2.41 | 0.42 |
| 1:W2:128:ASP:N | 1:W2:128:ASP:OD1 | 2.50 | 0.42 |
| 1:W2:156:ARG:HD2 | 1:W2:156:ARG:HA | 1.72 | 0.42 |
| 1:W2:274:THR:HG21 | 1:W2:282:ARG:HD2 | 2.00 | 0.42 |
| 2:W5:175:PRO:HG2 | 2:W5:176:GLN:OE1 | 2.19 | 0.42 |
| 1:W6:208:TYR:CE1 | 1:W6:225:LEU:HD11 | 2.54 | 0.42 |
| 2:W7:172:TYR:CZ | 2:W7:203:MET:SD | 3.12 | 0.42 |
| 2:W9:430:LYS:HA | 2:W9:433:GLU:OE2 | 2.19 | 0.42 |
| 1:X0:70:PRO:N | 1:X0:92:PHE:HZ | 2.16 | 0.42 |
| 1:X2:39:ASP:OD1 | 1:X2:40:SER:N | 2.51 | 0.42 |
| 2:X3:70:LEU:HB3 | 2:X3:97:GLU:O | 2.18 | 0.42 |
| 2:X3:209:ILE:HG12 | 2:X3:227:LEU:HD22 | 2.01 | 0.42 |
| 2:X3:352:LYS:HD2 | 2:X3:352:LYS:HA | 1.83 | 0.42 |
| 1:X6:30:ILE:HG13 | 1:X6:35:THR:O | 2.19 | 0.42 |
| 2:X7:69:ASP:OD1 | 2:X7:70:LEU:N | 2.52 | 0.42 |
| 2:Y3:124:LYS:HA | 2:Y3:127:ASP:OD1 | 2.19 | 0.42 |
| 2:Y3:264:ARG:HH22 | 2:Y3:431:ASP:CG | 2.23 | 0.42 |
| 2:Y3:428:LEU:HA | 2:Y3:431:ASP:OD1 | 2.19 | 0.42 |
| 1:Y6:273:LEU:H | 1:Y6:292:GLN:NE2 | 2.10 | 0.42 |
| 1:Y8:189:VAL:O | 1:Y8:193:VAL:HG13 | 2.19 | 0.42 |
| 2:Y9:12:ALA:HA | 2:Y9:15:GLN:OE1 | 2.19 | 0.42 |
| 2:Y9:73:THR:OG1 | 2:Y9:74:VAL:N | 2.52 | 0.42 |
| 2:Y9:407:TRP:O | 2:Y9:411:GLU:HG2 | 2.19 | 0.42 |
| 1:Z0:251:ARG:O | 1:Z0:255:VAL:HG13 | 2.19 | 0.42 |
| 1:Z0:272:PRO:HA | 1:Z0:292:GLN:OE1 | 2.20 | 0.42 |
| 1:Z0:316:LEU:HB3 | 1:Z0:366:THR:OG1 | 2.19 | 0.42 |
| 1:Z2:167:PHE:CE2 | 1:Z2:233:MET:SD | 3.13 | 0.42 |
| 1:Z2:181:GLU:HG2 | 1:Z2:182:PRO:HD3 | 2.00 | 0.42 |
| 2:Z3:21:TRP:CZ2 | 2:Z3:65:CYS:HB2 | 2.54 | 0.42 |
| 2:Z5:176:GLN:HG2 | 2:Z5:177:VAL:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z5:268:MET:HB3 | 2:Z5:378:ILE:HG23 | 2.01 | 0.42 |
| 1:Z6:202:LEU:CD2 | 1:Z6:229:ILE:HD13 | 2.48 | 0.42 |
| 2:Z7:27:GLU:OE1 | 2:Z7:28:HIS:HD2 | 2.02 | 0.42 |
| 2:0B:21:TRP:CZ3 | 2:0B:63:PRO:HB3 | 2.54 | 0.42 |
| 1:0C:335:ASN:O | 1:0C:338:SER:OG | 2.37 | 0.42 |
| 1:0E:293:MET:SD | 1:0E:367:PHE:HB2 | 2.60 | 0.42 |
| 1:0E:313:ALA:HB1 | 1:0E:367:PHE:CE1 | 2.55 | 0.42 |
| 1:0G:183:TYR:O | 1:0G:187:LEU:HD13 | 2.19 | 0.42 |
| 2:0J:75:VAL:HG21 | 2:0J:94:SER:HB2 | 2.02 | 0.42 |
| 1:0M:2:ARG:HH21 | 1:0M:240:LEU:HD13 | 1.83 | 0.42 |
| 1:0O:219:THR:O | 1:0O:219:THR:OG1 | 2.31 | 0.42 |
| 1:0O:379:LYS:HA | 1:0O:379:LYS:HD2 | 1.72 | 0.42 |
| 1:0O:383:GLU:OE2 | 1:0O:384:GLN:HG3 | 2.19 | 0.42 |
| 1:0U:415:MET:O | 1:0U:418:LEU:HG | 2.19 | 0.42 |
| 2:0X:33:ASP:OD1 | 2:0X:34:GLY:N | 2.53 | 0.42 |
| 2:1B:157:LEU:HD23 | 2:1B:157:LEU:HA | 1.79 | 0.42 |
| 2:1D:196:GLU:OE2 | 2:1D:197:HIS:NE2 | 2.52 | 0.42 |
| 1:1E:77:ARG:HE | 1:1E:90:PHE:HE2 | 1.67 | 0.42 |
| 1:1E:273:LEU:N | 1:1E:292:GLN:HE22 | 2.12 | 0.42 |
| 1:1E:391:ARG:O | 2:1F:262:TYR:OH | 2.37 | 0.42 |
| 1:1G:156:ARG:HD2 | 1:1G:156:ARG:HA | 1.86 | 0.42 |
| 1:1G:213:ARG:NH2 | 1:1G:297:LYS:HG3 | 2.34 | 0.42 |
| 2:1L:431:ASP:O | 2:1L:435:VAL:HG22 | 2.20 | 0.42 |
| 1:1O:285:THR:HG23 | 1:1O:288:GLU:H | 1.84 | 0.42 |
| 2:1R:176:GLN:HG2 | 2:1R:177:VAL:N | 2.34 | 0.42 |
| 1:1U:382:SER:HB3 | 1:1U:415:MET:HG2 | 2.00 | 0.42 |
| 1:1W:144:GLY:N | 39:1W:502:GDP:O1B | 2.52 | 0.42 |
| 2:2B:119:LEU:HD12 | 2:2B:120:ASP:OD1 | 2.19 | 0.42 |
| 1:2C:219:THR:O | 1:2C:219:THR:OG1 | 2.31 | 0.42 |
| 1:2C:418:LEU:O | 1:2C:421:GLU:HG2 | 2.18 | 0.42 |
| 2:2D:14:ILE:HD11 | 2:2D:74:VAL:HG22 | 2.01 | 0.42 |
| 2:2D:278:ALA:HA | 2:2D:369:ALA:HB2 | 2.00 | 0.42 |
| 2:2L:51:THR:HG21 | 2:2L:243:ARG:HG2 | 2.00 | 0.42 |
| 2:2L:417:GLU:H | 2:2L:417:GLU:CD | 2.23 | 0.42 |
| 2:2N:90:GLU:H | 2:3D:283:HIS:CE1 | 2.37 | 0.42 |
| 2:2N:145:THR:OG1 | 41:2N:501:GTP:O1B | 2.37 | 0.42 |
| 2:2N:409:VAL:HA | 2:2N:413:MET:O | 2.19 | 0.42 |
| 2:2P:65:CYS:SG | 2:2P:87:PHE:HE1 | 2.42 | 0.42 |
| 1:2U:233:MET:O | 1:2U:237:THR:HG22 | 2.19 | 0.42 |
| 2:2V:251:ASP:OD1 | 2:2V:253:THR:HG22 | 2.19 | 0.42 |
| 2:2X:223:THR:OG1 | 2:2X:224:TYR:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2Z:333:ALA:O | 2:2Z:337:THR:HG23 | 2.18 | 0.42 |
| 1:3A:192:LEU:HD23 | 1:3A:192:LEU:HA | 1.83 | 0.42 |
| 1:3C:105:HIS:CE1 | 1:3C:150:LEU:HD13 | 2.53 | 0.42 |
| 2:3D:90:GLU:HG3 | 2:3D:121:ARG:NH1 | 2.34 | 0.42 |
| 2:3F:124:LYS:NZ | 3:3V:35:CYS:SG | 2.93 | 0.42 |
| 2:3F:420:GLU:HA | 2:3F:423:GLU:HG3 | 2.01 | 0.42 |
| 1:3I:418:LEU:O | 1:3I:421:GLU:HG2 | 2.18 | 0.42 |
| 1:3K:128:ASP:OD1 | 1:3K:128:ASP:N | 2.48 | 0.42 |
| 1:3K:139:LEU:HA | 1:3K:145:SER:OG | 2.19 | 0.42 |
| 1:3M:330:MET:HA | 1:3M:333:VAL:HG12 | 2.01 | 0.42 |
| 1:3O:154:LYS:HA | 1:3O:154:LYS:HD3 | 1.90 | 0.42 |
| 2:3P:84:ARG:NE | 23:6S:15:ARG:HH22 | 2.12 | 0.42 |
| 2:3P:191:THR:HA | 2:3P:194:LEU:HB3 | 2.01 | 0.42 |
| 2:3R:72:PRO:HD2 | 1:3S:2:ARG:NH1 | 2.34 | 0.42 |
| 2:3R:297:GLU:OE1 | 2:3R:297:GLU:N | 2.36 | 0.42 |
| 1:3S:113:ILE:O | 1:3S:116:VAL:HG12 | 2.19 | 0.42 |
| 2:3T:119:LEU:O | 2:3T:122:ILE:HG22 | 2.19 | 0.42 |
| 4:3Y:94:LEU:HB2 | 4:3Y:152:LEU:HD11 | 1.99 | 0.42 |
| 3:3Z:86:ASP:O | 3:3Z:90:ILE:HG12 | 2.19 | 0.42 |
| 3:4D:86:ASP:O | 3:4D:90:ILE:HG12 | 2.19 | 0.42 |
| 3:4F:216:ILE:HD13 | 3:4F:216:ILE:HA | 1.89 | 0.42 |
| 3:4H:86:ASP:O | 3:4H:90:ILE:HG12 | 2.19 | 0.42 |
| 5:4M:324:MET:HG3 | 5:4M:325:MET:SD | 2.59 | 0.42 |
| 7:4S:18:ARG:CZ | 7:4S:18:ARG:HB2 | 2.49 | 0.42 |
| 9:4Z:197:ALA:HA | 9:4Z:200:GLU:OE2 | 2.19 | 0.42 |
| 9:4Z:395:LYS:HE3 | 9:4Z:395:LYS:HB2 | 1.85 | 0.42 |
| 10:5A:335:ALA:O | 10:5A:338:LYS:HG3 | 2.19 | 0.42 |
| 10:5B:291:GLU:O | 10:5B:294:LEU:HG | 2.19 | 0.42 |
| 10:5C:138:HIS:O | 10:5C:142:GLU:HG2 | 2.18 | 0.42 |
| 10:5C:206:ARG:HA | 10:5C:209:GLU:OE1 | 2.19 | 0.42 |
| 14:5L:387:CYS:HB2 | 14:5L:429:THR:O | 2.19 | 0.42 |
| 14:5L:506:SER:HB2 | 14:5L:508:PHE:CE2 | 2.55 | 0.42 |
| 14:5M:164:ILE:HG23 | 14:5M:174:TRP:CD1 | 2.54 | 0.42 |
| 14:5M:210:TYR:CE1 | 14:5M:220:GLN:HB2 | 2.54 | 0.42 |
| 14:5M:241:GLY:O | 14:5M:243:THR:HG23 | 2.18 | 0.42 |
| 14:5M:492:SER:HB3 | 14:5M:508:PHE:CE1 | 2.55 | 0.42 |
| 14:5N:55:HIS:HE2 | 14:5N:88:TRP:HH2 | 1.67 | 0.42 |
| 14:5N:96:ILE:HG22 | 14:5N:97:HIS:CD2 | 2.54 | 0.42 |
| 14:5N:164:ILE:HG23 | 14:5N:174:TRP:CD1 | 2.54 | 0.42 |
| 14:5N:425:GLN:OE1 | 14:5N:425:GLN:N | 2.44 | 0.42 |
| 15:5O:350:ASP:OD1 | 15:5O:353:ARG:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5P:93:ARG:HD3 | 15:5P:162:GLU:OE2 | 2.19 | 0.42 |
| 15:5P:263:PHE:HE2 | 15:5P:326:LEU:HD23 | 1.83 | 0.42 |
| 17:5T:87:VAL:HG13 | 17:5T:88:PRO:HD2 | 2.01 | 0.42 |
| 17:5T:228:THR:HA | 17:5T:231:ARG:NE | 2.34 | 0.42 |
| 21:6H:159:ALA:O | 21:6H:163:THR:HG23 | 2.18 | 0.42 |
| 22:6J:141:LYS:HE3 | 22:6J:141:LYS:HB3 | 1.86 | 0.42 |
| 22:6J:201:ARG:HB3 | 22:6J:237:TYR:HB3 | 2.00 | 0.42 |
| 22:6M:146:LEU:HD12 | 22:6M:149:ILE:HD12 | 2.00 | 0.42 |
| 22:6N:264:GLN:NE2 | 24:6Y:406:ALA:HA | 2.34 | 0.42 |
| 22:6O:171:GLU:HA | 22:6O:174:GLU:OE1 | 2.20 | 0.42 |
| 22:6P:274:GLU:O | 22:6P:278:GLN:NE2 | 2.52 | 0.42 |
| 24:6T:103:LYS:HG2 | 24:6T:116:ILE:HG12 | 2.01 | 0.42 |
| 24:6U:36:VAL:O | 24:6U:42:GLU:HB3 | 2.18 | 0.42 |
| 24:6U:97:ARG:NH2 | 24:6U:99:TYR:OH | 2.48 | 0.42 |
| 24:6U:473:TYR:CD1 | 24:6U:517:LEU:HD11 | 2.54 | 0.42 |
| 24:6V:130:MET:HE3 | 24:6V:130:MET:HB2 | 1.86 | 0.42 |
| 24:6X:505:LYS:HZ2 | 24:6X:510:GLU:HG3 | 1.84 | 0.42 |
| 24:6Z:256:LEU:HD23 | 24:6Z:256:LEU:HA | 1.86 | 0.42 |
| 24:6Z:472:SER:HB2 | 24:6Z:481:LEU:HD21 | 2.01 | 0.42 |
| 24:7A:123:TYR:HD1 | 24:7A:130:MET:SD | 2.42 | 0.42 |
| 24:7A:142:ILE:HG13 | 24:7A:144:GLN:HG3 | 2.00 | 0.42 |
| 26:7D:136:PHE:HB3 | 26:7D:137:PRO:CD | 2.44 | 0.42 |
| 29:7I:136:LEU:HD12 | 29:7I:136:LEU:HA | 1.80 | 0.42 |
| 30:7K:268:ASP:N | 30:7K:268:ASP:OD1 | 2.51 | 0.42 |
| 31:7N:60:ILE:H | 31:7N:60:ILE:HG12 | 1.69 | 0.42 |
| 34:7R:95:ILE:O | 34:7R:98:GLU:HG3 | 2.19 | 0.42 |
| 34:7R:141:GLU:O | 34:7R:144:GLU:HG3 | 2.19 | 0.42 |
| 38:8B:207:ASP:OD1 | 38:8B:208:GLU:N | 2.50 | 0.42 |
| 38:8B:229:ASN:HB2 | 38:8B:232:PHE:CZ | 2.54 | 0.42 |
| 2:A2:29:GLY:O | 26:7F:45:MET:CE | 1.87 | 0.42 |
| 2:F5:88:HIS:HB3 | 2:H1:283:HIS:CE1 | 2.54 | 0.42 |
| 2:F5:365:GLY:H | 22:6I:165:MET:HE3 | 1.83 | 0.42 |
| 1:G2:101:TRP:HB2 | 1:G2:184:ASN:OD1 | 2.19 | 0.42 |
| 1:G2:208:TYR:CE1 | 1:G2:225:LEU:HD11 | 2.54 | 0.42 |
| 1:G4:217:LEU:HD23 | 1:G4:217:LEU:HA | 1.85 | 0.42 |
| 2:G5:332:VAL:HA | 2:G5:335:ILE:HG22 | 2.02 | 0.42 |
| 1:G6:149:THR:HG23 | 1:G6:191:GLN:HG2 | 2.01 | 0.42 |
| 1:G6:177:ASP:N | 1:G6:181:GLU:OE2 | 2.52 | 0.42 |
| 1:G8:137:HIS:CE1 | 1:G8:168:SER:HB3 | 2.54 | 0.42 |
| 2:H3:4:VAL:HG13 | 2:H3:52:PHE:HE1 | 1.84 | 0.42 |
| 2:H3:220:GLU:H | 2:H3:220:GLU:CD | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H4:179:VAL:HG22 | 2:H5:258:ASN:HD22 | 1.84 | 0.42 |
| 1:H4:251:ARG:O | 1:H4:255:VAL:HG23 | 2.19 | 0.42 |
| 1:H4:309:ARG:H | 1:H4:372:THR:CG2 | 2.31 | 0.42 |
| 1:H8:48:ASN:O | 1:H8:62:ARG:NH2 | 2.52 | 0.42 |
| 2:H9:35:GLN:OE1 | 2:H9:35:GLN:N | 2.53 | 0.42 |
| 1:I0:414:ASN:HA | 1:I0:417:ASP:OD2 | 2.20 | 0.42 |
| 1:I2:22:GLU:HG2 | 1:I2:81:TYR:HB2 | 2.00 | 0.42 |
| 1:I4:214:THR:O | 1:I4:275:SER:OG | 2.32 | 0.42 |
| 1:I4:395:LEU:HD23 | 1:I4:395:LEU:HA | 1.88 | 0.42 |
| 1:I8:396:HIS:HA | 1:I8:399:THR:OG1 | 2.19 | 0.42 |
| 2:I9:114:ILE:HD12 | 2:I9:114:ILE:HA | 1.89 | 0.42 |
| 2:I9:141:VAL:O | 2:I9:147:SER:OG | 2.37 | 0.42 |
| 2:I9:266:HIS:O | 2:I9:266:HIS:ND1 | 2.50 | 0.42 |
| 2:J3:165:SER:HA | 2:J3:199:ASP:OD2 | 2.19 | 0.42 |
| 1:J4:163:MET:HB3 | 1:J4:250:LEU:HD22 | 2.01 | 0.42 |
| 1:J4:360:GLY:N | 16:5Q:12:GLN:O | 2.49 | 0.42 |
| 1:J6:52:ASN:OD1 | 1:J6:62:ARG:NH2 | 2.52 | 0.42 |
| 1:J6:185:ALA:O | 1:J6:189:VAL:HG12 | 2.19 | 0.42 |
| 2:J7:406:HIS:HA | 2:J7:409:VAL:HG22 | 2.00 | 0.42 |
| 1:K0:135:VAL:HG12 | 1:K0:137:HIS:HD2 | 1.84 | 0.42 |
| 1:K0:182:PRO:O | 1:K0:186:THR:HG22 | 2.19 | 0.42 |
| 2:K1:266:HIS:O | 2:K1:266:HIS:ND1 | 2.52 | 0.42 |
| 2:K3:414:GLU:N | 2:K3:414:GLU:OE1 | 2.52 | 0.42 |
| 1:K6:3:GLU:HB2 | 1:K6:130:LEU:HA | 2.00 | 0.42 |
| 2:K7:108:TYR:HA | 2:K7:112:LYS:NZ | 2.33 | 0.42 |
| 1:K8:137:HIS:NE2 | 1:K8:168:SER:OG | 2.52 | 0.42 |
| 1:K8:222:PHE:HD1 | 1:K8:225:LEU:HD12 | 1.84 | 0.42 |
| 1:K8:391:ARG:HB3 | 2:K9:346:TRP:CZ3 | 2.54 | 0.42 |
| 1:L0:186:THR:HG22 | 1:L0:411:ALA:HB1 | 2.00 | 0.42 |
| 2:L1:330:ALA:O | 2:L1:334:THR:HG23 | 2.20 | 0.42 |
| 2:L7:155:GLU:OE1 | 2:L7:156:ARG:HG2 | 2.20 | 0.42 |
| 2:L7:172:TYR:CD2 | 2:L7:203:MET:HG2 | 2.53 | 0.42 |
| 2:M1:84:ARG:HH21 | 27:7G:114:GLY:HA2 | 1.83 | 0.42 |
| 1:M2:240:LEU:HD11 | 1:M2:250:LEU:HD13 | 2.02 | 0.42 |
| 2:M3:125:LEU:HA | 2:M3:125:LEU:HD23 | 1.81 | 0.42 |
| 1:M8:65:LEU:HD12 | 1:M8:90:PHE:CE1 | 2.54 | 0.42 |
| 1:M8:98:GLY:HA2 | 2:M9:254:GLU:OE2 | 2.19 | 0.42 |
| 2:M9:189:LEU:HD11 | 2:M9:418:PHE:CE1 | 2.55 | 0.42 |
| 2:N1:430:LYS:O | 2:N1:433:GLU:HG2 | 2.19 | 0.42 |
| 1:N2:117:LEU:HD11 | 1:N2:154:LYS:HB3 | 2.02 | 0.42 |
| 1:N2:219:THR:O | 1:N2:219:THR:OG1 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N8:414:ASN:HA | 1:N8:417:ASP:OD1 | 2.20 | 0.42 |
| 2:O1:76:ASP:OD1 | 1:O2:46:ARG:NH2 | 2.51 | 0.42 |
| 2:O3:326:LYS:HG3 | 2:O3:327:ASP:N | 2.35 | 0.42 |
| 2:O5:3:GLU:HG3 | 2:O5:51:THR:HA | 2.01 | 0.42 |
| 1:O6:138:SER:HA | 1:O6:169:VAL:HG22 | 2.01 | 0.42 |
| 1:O6:179:VAL:H | 2:O7:258:ASN:ND2 | 2.17 | 0.42 |
| 1:O6:279:GLN:NE2 | 32:7P:100:ARG:O | 2.52 | 0.42 |
| 2:O7:384:ILE:HG13 | 2:O7:385:GLY:N | 2.33 | 0.42 |
| 1:O8:49:VAL:HG11 | 1:O8:241:ARG:HG2 | 2.00 | 0.42 |
| 1:O8:337:ASN:HB2 | 1:O8:340:TYR:HD2 | 1.84 | 0.42 |
| 2:O9:280:LYS:O | 2:O9:283:HIS:HB3 | 2.20 | 0.42 |
| 2:P3:205:ASP:OD1 | 2:P3:206:ASN:N | 2.49 | 0.42 |
| 2:P3:306:ASP:HB3 | 2:P3:309:HIS:HD2 | 1.84 | 0.42 |
| 2:P3:312:TYR:HB2 | 2:P3:343:PHE:CD1 | 2.54 | 0.42 |
| 1:P8:3:GLU:HB2 | 1:P8:130:LEU:HA | 2.01 | 0.42 |
| 1:P8:40:SER:OG | 1:P8:43:GLN:HG3 | 2.19 | 0.42 |
| 1:Q0:117:LEU:HA | 1:Q0:117:LEU:HD23 | 1.80 | 0.42 |
| 2:Q1:414:GLU:OE1 | 2:Q1:414:GLU:N | 2.52 | 0.42 |
| 1:Q2:114:ASP:OD1 | 1:Q2:115:SER:N | 2.52 | 0.42 |
| 1:Q4:302:ALA:N | 1:Q4:377:MET:HE2 | 2.34 | 0.42 |
| 2:R1:116:ASP:OD1 | 2:R1:117:LEU:N | 2.53 | 0.42 |
| 2:R1:155:GLU:HG2 | 2:R1:197:HIS:ND1 | 2.34 | 0.42 |
| 2:R1:176:GLN:HG2 | 2:R1:177:VAL:N | 2.33 | 0.42 |
| 2:R1:360:PRO:O | 2:R1:370:LYS:NZ | 2.50 | 0.42 |
| 1:R6:8:GLN:CD | 1:R6:17:GLY:HA3 | 2.40 | 0.42 |
| 1:R6:272:PRO:HD3 | 1:R6:364:SER:HA | 2.00 | 0.42 |
| 1:R6:375:GLN:HB2 | 1:R6:419:VAL:HG13 | 2.01 | 0.42 |
| 1:S0:4:ILE:HB | 1:S0:50:TYR:HE1 | 1.83 | 0.42 |
| 2:S5:235:ILE:O | 2:S5:239:THR:HG23 | 2.19 | 0.42 |
| 2:S9:189:LEU:HD13 | 2:S9:413:MET:SD | 2.60 | 0.42 |
| 2:T1:165:SER:OG | 2:T1:256:GLN:NE2 | 2.52 | 0.42 |
| 2:T1:259:LEU:HD21 | 2:T1:316:CYS:HB2 | 2.00 | 0.42 |
| 2:T3:326:LYS:HD2 | 2:T3:327:ASP:N | 2.33 | 0.42 |
| 1:T4:325:GLU:O | 1:T4:329:GLN:HG2 | 2.20 | 0.42 |
| 2:T5:88:HIS:ND1 | 2:T5:89:PRO:HD2 | 2.34 | 0.42 |
| 2:T7:241:SER:OG | 2:T7:250:VAL:O | 2.24 | 0.42 |
| 2:U5:119:LEU:HD11 | 2:U5:156:ARG:HB3 | 2.01 | 0.42 |
| 2:U5:217:LEU:O | 2:U5:219:ILE:HD12 | 2.19 | 0.42 |
| 1:U6:286:VAL:HG21 | 1:U6:325:GLU:HB3 | 2.01 | 0.42 |
| 1:U6:309:ARG:O | 1:U6:372:THR:HG22 | 2.19 | 0.42 |
| 2:V1:255:PHE:HA | 2:V1:259:LEU:HD13 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V6:203:ASP:HB2 | 1:V6:205:GLU:CD | 2.40 | 0.42 |
| 1:V8:138:SER:O | 1:V8:139:LEU:HD23 | 2.19 | 0.42 |
| 1:W0:417:ASP:HA | 1:W0:420:SER:OG | 2.19 | 0.42 |
| 1:W2:249:ASP:O | 1:W2:253:LEU:HG | 2.19 | 0.42 |
| 1:W2:273:LEU:H | 1:W2:292:GLN:HE22 | 1.67 | 0.42 |
| 1:W2:325:GLU:O | 1:W2:329:GLN:HB2 | 2.19 | 0.42 |
| 1:W4:86:ARG:HB3 | 1:W4:89:ASN:OD1 | 2.19 | 0.42 |
| 1:W4:260:PHE:HB2 | 1:W4:263:LEU:HD23 | 2.00 | 0.42 |
| 2:W7:69:ASP:OD1 | 2:W7:70:LEU:N | 2.46 | 0.42 |
| 2:W7:254:GLU:N | 2:W7:254:GLU:OE1 | 2.52 | 0.42 |
| 1:W8:273:LEU:HD23 | 1:W8:273:LEU:HA | 1.89 | 0.42 |
| 2:W9:33:ASP:N | 2:W9:33:ASP:OD1 | 2.51 | 0.42 |
| 1:X2:164:MET:HB3 | 1:X2:197:ASP:HB2 | 2.02 | 0.42 |
| 1:X2:239:CYS:SG | 1:X2:240:LEU:N | 2.92 | 0.42 |
| 2:X3:331:SER:O | 2:X3:334:THR:HG22 | 2.19 | 0.42 |
| 1:X4:165:LEU:HD12 | 1:X4:165:LEU:HA | 1.68 | 0.42 |
| 1:X4:165:LEU:HD11 | 1:X4:200:MET:HG2 | 2.00 | 0.42 |
| 2:X5:33:ASP:O | 2:X5:60:LYS:NZ | 2.52 | 0.42 |
| 2:X7:344:VAL:HG13 | 2:X7:346:TRP:HB3 | 2.02 | 0.42 |
| 2:X9:121:ARG:HE | 2:X9:124:LYS:NZ | 2.17 | 0.42 |
| 1:Y2:418:LEU:O | 1:Y2:421:GLU:HG2 | 2.19 | 0.42 |
| 2:Y5:34:GLY:HA3 | 2:Y5:60:LYS:NZ | 2.34 | 0.42 |
| 1:Z0:11:GLN:HG2 | 1:Z0:12:CYS:H | 1.84 | 0.42 |
| 2:Z3:11:GLN:HE22 | 2:Z3:15:GLN:NE2 | 2.17 | 0.42 |
| 1:Z6:30:ILE:HG13 | 1:Z6:35:THR:O | 2.20 | 0.42 |
| 2:Z7:17:GLY:HA3 | 2:Z7:67:PHE:CZ | 2.53 | 0.42 |
| 1:Z8:116:VAL:HG21 | 1:Z8:151:LEU:HD21 | 2.01 | 0.42 |
| 1:Z8:175:VAL:HA | 2:Z9:329:ASN:OD1 | 2.19 | 0.42 |
| 1:Z8:247:ASN:O | 1:Z8:252:LYS:NZ | 2.50 | 0.42 |
| 1:Z8:293:MET:SD | 1:Z8:367:PHE:HB2 | 2.59 | 0.42 |
| 2:Z9:33:ASP:O | 2:Z9:60:LYS:NZ | 2.51 | 0.42 |
| 1:0A:113:ILE:HD13 | 1:0A:150:LEU:CD2 | 2.50 | 0.42 |
| 1:0C:304:ASP:HB3 | 1:0C:307:HIS:CG | 2.54 | 0.42 |
| 1:0E:270:PHE:HD1 | 1:0E:366:THR:HG22 | 1.84 | 0.42 |
| 2:0F:425:LEU:HD23 | 2:0F:429:GLU:HG2 | 2.00 | 0.42 |
| 1:0G:13:GLY:HA2 | 1:0G:16:ILE:HG12 | 2.01 | 0.42 |
| 1:0I:148:GLY:O | 1:0I:152:ILE:HG12 | 2.19 | 0.42 |
| 1:0I:314:SER:HA | 1:0I:350:LYS:O | 2.19 | 0.42 |
| 2:0L:147:SER:OG | 2:0L:148:GLY:N | 2.51 | 0.42 |
| 1:0M:21:TRP:CZ3 | 1:0M:61:PRO:HB3 | 2.54 | 0.42 |
| 1:0M:46:ARG:HA | 1:0M:46:ARG:HD3 | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0M:222:PHE:CD1 | 1:0M:225:LEU:HD12 | 2.54 | 0.42 |
| 2:0N:407:TRP:O | 2:0N:411:GLU:HG2 | 2.20 | 0.42 |
| 1:0Q:21:TRP:CZ3 | 1:0Q:61:PRO:HB3 | 2.55 | 0.42 |
| 2:0R:27:GLU:HG3 | 2:0R:28:HIS:CD2 | 2.55 | 0.42 |
| 1:0U:322:SER:O | 1:0U:326:VAL:HG23 | 2.19 | 0.42 |
| 2:0V:271:SER:HB3 | 2:0V:377:MET:HB3 | 2.02 | 0.42 |
| 2:0V:286:LEU:CD2 | 2:0V:371:VAL:HG13 | 2.48 | 0.42 |
| 1:0W:69:GLU:C | 1:0W:92:PHE:HZ | 2.22 | 0.42 |
| 2:0X:88:HIS:ND1 | 2:1N:283:HIS:HB2 | 2.34 | 0.42 |
| 2:0X:229:ARG:HD3 | 2:0X:363:VAL:HG11 | 2.02 | 0.42 |
| 2:0X:370:LYS:HD3 | 2:0X:370:LYS:HA | 1.81 | 0.42 |
| 1:0Y:344:TRP:O | 1:0Y:345:ILE:HD13 | 2.17 | 0.42 |
| 2:0Z:298:PRO:HA | 2:0Z:301:MET:HG3 | 2.01 | 0.42 |
| 1:1A:415:MET:O | 1:1A:419:VAL:HG23 | 2.18 | 0.42 |
| 1:1A:418:LEU:O | 1:1A:421:GLU:HG2 | 2.19 | 0.42 |
| 1:1C:4:ILE:HA | 1:1C:132:GLY:O | 2.19 | 0.42 |
| 1:1C:418:LEU:O | 1:1C:421:GLU:HG2 | 2.19 | 0.42 |
| 2:1D:420:GLU:O | 2:1D:424:ASP:HB2 | 2.19 | 0.42 |
| 1:1E:169:VAL:HG21 | 1:1E:204:ASN:OD1 | 2.19 | 0.42 |
| 2:1F:35:GLN:HA | 2:1F:35:GLN:OE1 | 2.19 | 0.42 |
| 2:1H:170:THR:OG1 | 2:1H:203:MET:SD | 2.77 | 0.42 |
| 2:1H:213:CYS:HA | 2:1H:217:LEU:CD1 | 2.50 | 0.42 |
| 1:1K:112:LEU:O | 1:1K:115:SER:OG | 2.33 | 0.42 |
| 1:1K:190:HIS:CD2 | 1:1K:411:ALA:HA | 2.54 | 0.42 |
| 1:1M:220:PRO:HA | 1:1M:224:ASP:OD2 | 2.18 | 0.42 |
| 2:1N:156:ARG:HA | 2:1N:159:VAL:HG12 | 2.02 | 0.42 |
| 1:1Q:21:TRP:CZ3 | 1:1Q:61:PRO:HB3 | 2.54 | 0.42 |
| 1:1Q:67:ASP:CG | 1:1Q:68:LEU:H | 2.22 | 0.42 |
| 1:1Q:175:VAL:HG12 | 2:1R:329:ASN:ND2 | 2.33 | 0.42 |
| 2:1R:231:ILE:HD13 | 2:1R:231:ILE:HA | 1.84 | 0.42 |
| 1:1S:212:PHE:CZ | 2:1T:326:LYS:HD3 | 2.54 | 0.42 |
| 1:1U:414:ASN:HA | 1:1U:417:ASP:OD2 | 2.20 | 0.42 |
| 1:1W:53:GLU:HA | 1:1W:53:GLU:OE2 | 2.19 | 0.42 |
| 1:1W:123:GLU:O | 1:1W:126:SER:OG | 2.37 | 0.42 |
| 1:1W:403:MET:HE3 | 1:1W:403:MET:HB2 | 1.91 | 0.42 |
| 2:1X:73:THR:OG1 | 2:1X:74:VAL:N | 2.52 | 0.42 |
| 2:1Z:217:LEU:HD12 | 2:1Z:277:SER:OG | 2.20 | 0.42 |
| 1:2A:327:ASP:N | 1:2A:327:ASP:OD2 | 2.47 | 0.42 |
| 2:2B:175:PRO:HG2 | 2:2B:176:GLN:OE1 | 2.20 | 0.42 |
| 1:2E:68:LEU:HD12 | 1:2E:143:THR:HG22 | 2.00 | 0.42 |
| 2:2F:205:ASP:OD1 | 2:2F:206:ASN:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2G:86:ARG:HG2 | 1:2G:88:ASP:H | 1.83 | 0.42 |
| 2:2H:11:GLN:HB3 | 41:2I:501:GTP:PA | 2.60 | 0.42 |
| 1:2I:60:VAL:O | 1:2I:60:VAL:HG23 | 2.19 | 0.42 |
| 1:2K:167:PHE:HE1 | 1:2K:200:MET:HG3 | 1.84 | 0.42 |
| 1:2M:94:GLN:NE2 | 38:8D:116:GLN:HB3 | 2.33 | 0.42 |
| 1:2M:173:PRO:HA | 1:2M:176:SER:OG | 2.20 | 0.42 |
| 2:2N:68:LEU:HD22 | 2:2N:149:LEU:HD11 | 2.01 | 0.42 |
| 2:2N:121:ARG:HD2 | 2:2N:121:ARG:HA | 1.68 | 0.42 |
| 2:2P:187:SER:O | 2:2P:191:THR:HG23 | 2.20 | 0.42 |
| 2:2T:221:ARG:HB3 | 1:2U:322:SER:HB2 | 2.01 | 0.42 |
| 2:2V:154:LEU:HA | 2:2V:154:LEU:HD23 | 1.74 | 0.42 |
| 1:2W:167:PHE:CZ | 1:2W:233:MET:HG2 | 2.53 | 0.42 |
| 1:2Y:67:ASP:OD2 | 1:2Y:72:THR:OG1 | 2.37 | 0.42 |
| 1:2Y:193:VAL:HG12 | 1:2Y:265:PHE:CZ | 2.54 | 0.42 |
| 2:2Z:325:PRO:HA | 2:2Z:328:VAL:HG12 | 2.00 | 0.42 |
| 2:2Z:398:MET:HG3 | 1:3A:346:PRO:HD2 | 2.00 | 0.42 |
| 1:3C:137:HIS:ND1 | 1:3C:138:SER:O | 2.42 | 0.42 |
| 2:3H:240:ALA:HB1 | 2:3H:356:ASN:HD22 | 1.84 | 0.42 |
| 1:3K:209:ASP:OD1 | 1:3K:210:ILE:N | 2.52 | 0.42 |
| 1:3M:390:ARG:HE | 1:3M:390:ARG:HB2 | 1.70 | 0.42 |
| 1:3O:285:THR:HG22 | 1:3O:288:GLU:HB2 | 2.01 | 0.42 |
| 1:3O:414:ASN:HA | 1:3O:417:ASP:OD2 | 2.20 | 0.42 |
| 2:3T:107:HIS:O | 2:3T:152:LEU:HD22 | 2.19 | 0.42 |
| 2:3T:236:SER:O | 2:3T:243:ARG:NH2 | 2.49 | 0.42 |
| 3:3X:9:LEU:HD22 | 3:3X:173:ARG:HH11 | 1.84 | 0.42 |
| 3:4F:9:LEU:HD22 | 3:4F:173:ARG:HH11 | 1.84 | 0.42 |
| 3:4J:225:VAL:HG11 | 3:4J:281:PHE:CE1 | 2.55 | 0.42 |
| 6:4O:302:ARG:NH1 | 6:4O:305:ILE:HD13 | 2.34 | 0.42 |
| 6:4P:72:LYS:HD2 | 32:7P:88:LEU:HD22 | 2.01 | 0.42 |
| 9:4Z:339:ALA:O | 9:4Z:342:LYS:HG2 | 2.20 | 0.42 |
| 11:5E:161:ARG:HA | 11:5E:161:ARG:HD2 | 1.80 | 0.42 |
| 12:5G:274:ARG:HB2 | 12:5G:323:TYR:CZ | 2.55 | 0.42 |
| 14:5N:492:SER:HB3 | 14:5N:508:PHE:CD1 | 2.54 | 0.42 |
| 15:5P:20:ILE:HG13 | 19:6E:104:TYR:CD1 | 2.54 | 0.42 |
| 20:6F:56:GLU:CG | 20:6F:296:LYS:HD3 | 2.49 | 0.42 |
| 24:6T:613:LYS:O | 24:6T:617:ASP:CB | 2.64 | 0.42 |
| 24:6X:514:TYR:C | 24:6X:517:LEU:HD13 | 2.32 | 0.42 |
| 24:6Y:24:ASP:N | 24:6Y:24:ASP:OD1 | 2.52 | 0.42 |
| 25:7C:106:LEU:HD23 | 25:7C:106:LEU:HA | 1.90 | 0.42 |
| 26:7D:116:GLN:HG2 | 26:7D:123:TYR:CZ | 2.54 | 0.42 |
| 26:7E:116:GLN:HG2 | 26:7E:123:TYR:CZ | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:7H:415:THR:O | 28:7H:418:SER:OG | 2.36 | 0.42 |
| 37:7Y:94:ARG:NH2 | 37:7Y:108:PRO:O | 2.53 | 0.42 |
| 37:7Y:158:TYR:CZ | 37:7Y:162:LEU:HD12 | 2.54 | 0.42 |
| 1:3:423:GLN:HE22 | 3:3X:107:ALA:C | 2.22 | 0.42 |
| 2:6:434:GLU:OE2 | 4:4A:100:ARG:NE | 2.48 | 0.42 |
| 2:8:364:PRO:HB2 | 26:7E:53:TYR:HD1 | 1.83 | 0.42 |
| 1:9:42:LEU:HD21 | 26:7E:121:LYS:NZ | 2.34 | 0.42 |
| 1:C6:276:ARG:HD3 | 24:6U:341:LYS:HE3 | 2.00 | 0.42 |
| 2:F1:81:GLY:HA3 | 22:6O:116:TYR:HE2 | 1.85 | 0.42 |
| 1:G2:219:THR:OG1 | 1:G2:219:THR:O | 2.38 | 0.42 |
| 1:G2:262:ARG:NH2 | 1:G2:417:ASP:OD1 | 2.53 | 0.42 |
| 1:G4:198:GLU:HA | 1:G4:264:HIS:HB2 | 2.02 | 0.42 |
| 1:G4:344:TRP:CE3 | 1:G4:345:ILE:HG13 | 2.55 | 0.42 |
| 1:G4:379:LYS:HA | 1:G4:382:SER:OG | 2.18 | 0.42 |
| 1:G6:55:THR:H | 1:G6:58:ARG:HB3 | 1.84 | 0.42 |
| 2:G7:12:ALA:HB2 | 41:G7:501:GTP:C8 | 2.54 | 0.42 |
| 1:G8:80:PRO:HB2 | 1:G8:81:TYR:CD1 | 2.54 | 0.42 |
| 2:G9:24:TYR:HA | 2:G9:27:GLU:OE1 | 2.19 | 0.42 |
| 2:G9:178:SER:OG | 2:G9:183:GLU:OE2 | 2.22 | 0.42 |
| 2:G9:279:GLU:HG2 | 2:G9:280:LYS:N | 2.34 | 0.42 |
| 2:H1:76:ASP:O | 2:H1:80:THR:HG23 | 2.19 | 0.42 |
| 2:H3:74:VAL:O | 2:H3:78:VAL:HG23 | 2.19 | 0.42 |
| 1:H4:26:ASP:O | 1:H4:359:LYS:NZ | 2.24 | 0.42 |
| 1:H4:207:LEU:HB3 | 1:H4:225:LEU:HD22 | 2.02 | 0.42 |
| 1:H4:418:LEU:O | 1:H4:421:GLU:HG2 | 2.19 | 0.42 |
| 2:H5:388:PHE:HD1 | 2:H5:391:LEU:HD21 | 1.85 | 0.42 |
| 1:H6:391:ARG:O | 2:H7:262:TYR:OH | 2.37 | 0.42 |
| 1:H8:139:LEU:HG | 1:H8:168:SER:HB3 | 2.01 | 0.42 |
| 2:H9:108:TYR:HB2 | 2:H9:411:GLU:OE2 | 2.18 | 0.42 |
| 1:I0:128:ASP:OD1 | 1:I0:128:ASP:N | 2.52 | 0.42 |
| 2:I1:55:GLU:HG2 | 2:I1:61:HIS:CE1 | 2.54 | 0.42 |
| 2:I1:88:HIS:HB3 | 2:I1:91:GLN:CD | 2.40 | 0.42 |
| 2:I3:74:VAL:O | 2:I3:78:VAL:HG23 | 2.19 | 0.42 |
| 1:I4:240:LEU:HD21 | 1:I4:249:ASP:HB2 | 2.01 | 0.42 |
| 2:I7:8:HIS:CD2 | 2:I7:138:PHE:HD2 | 2.37 | 0.42 |
| 2:I9:317:LEU:HB3 | 2:I9:319:TYR:HE1 | 1.84 | 0.42 |
| 2:J1:119:LEU:O | 2:J1:122:ILE:HG22 | 2.20 | 0.42 |
| 1:J2:87:PRO:HB2 | 16:5Q:184:GLU:HB3 | 2.01 | 0.42 |
| 1:J2:289:LEU:HD21 | 1:J2:363:MET:HG2 | 2.01 | 0.42 |
| 2:J3:217:LEU:HB3 | 2:J3:219:ILE:HD12 | 2.02 | 0.42 |
| 2:J7:286:LEU:HD23 | 2:J7:286:LEU:HA | 1.91 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J8:2:ARG:HB3 | 1:J8:131:GLN:HB2 | 2.01 | 0.42 |
| 1:K0:415:MET:O | 1:K0:418:LEU:HG | 2.19 | 0.42 |
| 2:K1:404:PHE:CE1 | 2:K1:408:TYR:HE2 | 2.37 | 0.42 |
| 2:K5:90:GLU:O | 2:K5:121:ARG:NH1 | 2.50 | 0.42 |
| 2:K7:101:ASN:CG | 1:K8:252:LYS:HZ2 | 2.22 | 0.42 |
| 1:K8:167:PHE:CE2 | 1:K8:233:MET:HG2 | 2.55 | 0.42 |
| 2:K9:428:LEU:HG | 2:K9:432:PHE:CE2 | 2.54 | 0.42 |
| 1:L0:135:VAL:HG21 | 1:L0:152:ILE:HD11 | 2.02 | 0.42 |
| 2:L1:280:LYS:HA | 2:L1:283:HIS:HB3 | 2.01 | 0.42 |
| 2:L9:267:PHE:HB2 | 2:L9:384:ILE:HD12 | 2.01 | 0.42 |
| 2:L9:405:VAL:HG13 | 2:L9:418:PHE:HE2 | 1.84 | 0.42 |
| 1:M2:174:LYS:HE2 | 1:M2:174:LYS:HB3 | 1.82 | 0.42 |
| 2:M3:88:HIS:O | 1:O0:281:TYR:OH | 2.27 | 0.42 |
| 2:N3:205:ASP:O | 2:N3:209:ILE:HD12 | 2.18 | 0.42 |
| 2:N3:208:ALA:CA | 2:N3:304:LYS:HE3 | 2.49 | 0.42 |
| 2:N5:3:GLU:HG3 | 2:N5:51:THR:HA | 2.01 | 0.42 |
| 2:N5:88:HIS:CE1 | 2:N5:121:ARG:HH22 | 2.38 | 0.42 |
| 1:N8:179:VAL:HB | 2:N9:258:ASN:HD22 | 1.84 | 0.42 |
| 2:N9:70:LEU:HB3 | 2:N9:97:GLU:O | 2.19 | 0.42 |
| 2:N9:176:GLN:HG2 | 2:N9:207:GLU:OE1 | 2.19 | 0.42 |
| 2:O1:322:ASP:OD1 | 2:O1:322:ASP:N | 2.49 | 0.42 |
| 2:O3:5:ILE:HD11 | 2:O3:135:PHE:CE1 | 2.54 | 0.42 |
| 2:O3:119:LEU:HA | 2:O3:122:ILE:HG22 | 2.01 | 0.42 |
| 1:O4:35:THR:HG1 | 1:O4:37:HIS:HE2 | 1.63 | 0.42 |
| 1:O4:208:TYR:HB3 | 2:O5:326:LYS:NZ | 2.34 | 0.42 |
| 2:O7:26:LEU:HD12 | 2:O7:363:VAL:HG22 | 2.01 | 0.42 |
| 2:O7:364:PRO:HD3 | 32:7P:78:TYR:CE2 | 2.54 | 0.42 |
| 2:P3:255:PHE:O | 2:P3:259:LEU:N | 2.47 | 0.42 |
| 1:P4:40:SER:OG | 1:P4:43:GLN:HG3 | 2.19 | 0.42 |
| 1:P4:114:ASP:OD2 | 1:P4:115:SER:N | 2.52 | 0.42 |
| 1:P6:238:CYS:SG | 1:P6:239:CYS:N | 2.93 | 0.42 |
| 2:P7:129:CYS:SG | 2:P7:130:THR:N | 2.91 | 0.42 |
| 2:P9:39:ASP:OD1 | 2:P9:40:LYS:N | 2.52 | 0.42 |
| 1:Q2:8:GLN:CD | 1:Q2:17:GLY:HA3 | 2.39 | 0.42 |
| 2:Q5:346:TRP:CD1 | 2:Q5:346:TRP:N | 2.86 | 0.42 |
| 2:Q9:72:PRO:HD2 | 1:R0:2:ARG:HH12 | 1.85 | 0.42 |
| 2:Q9:286:LEU:HD22 | 2:Q9:371:VAL:HG13 | 2.01 | 0.42 |
| 1:R0:289:LEU:HD13 | 1:R0:363:MET:HE2 | 2.00 | 0.42 |
| 1:R0:320:ARG:NH1 | 12:7B:72:ALA:O | 2.46 | 0.42 |
| 2:R1:72:PRO:HD2 | 1:R2:2:ARG:NH1 | 2.34 | 0.42 |
| 2:R1:345:ASP:OD1 | 2:R1:345:ASP:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:311:LEU:HA | 1:R4:311:LEU:HD23 | 1.77 | 0.42 |
| 2:R5:42:ILE:HG13 | 2:R5:43:GLY:N | 2.34 | 0.42 |
| 2:R7:21:TRP:CZ3 | 2:R7:63:PRO:HB3 | 2.55 | 0.42 |
| 2:R7:102:ASN:HB3 | 2:R7:105:ARG:HB3 | 2.00 | 0.42 |
| 2:S1:27:GLU:HG3 | 2:S1:361:THR:HG21 | 2.01 | 0.42 |
| 2:S1:125:LEU:HD23 | 2:S1:125:LEU:HA | 1.90 | 0.42 |
| 1:S4:285:THR:OG1 | 1:S4:287:PRO:HD2 | 2.18 | 0.42 |
| 1:T2:253:LEU:HA | 1:T2:253:LEU:HD23 | 1.79 | 0.42 |
| 2:T3:21:TRP:CZ2 | 2:T3:65:CYS:HB3 | 2.55 | 0.42 |
| 2:T7:109:THR:HG23 | 2:T7:411:GLU:OE2 | 2.18 | 0.42 |
| 2:T7:279:GLU:OE1 | 2:T7:279:GLU:CA | 2.62 | 0.42 |
| 2:U1:369:ALA:O | 2:U1:371:VAL:HG23 | 2.19 | 0.42 |
| 2:U3:326:LYS:HG3 | 2:U3:327:ASP:N | 2.34 | 0.42 |
| 1:U6:397:TRP:CH2 | 2:U7:256:GLN:HB3 | 2.55 | 0.42 |
| 1:V2:77:ARG:HE | 1:V2:90:PHE:HE2 | 1.68 | 0.42 |
| 1:V4:39:ASP:OD1 | 1:V4:39:ASP:N | 2.48 | 0.42 |
| 1:V4:123:GLU:O | 1:V4:126:SER:OG | 2.37 | 0.42 |
| 1:V4:212:PHE:CE1 | 1:V4:220:PRO:HG3 | 2.54 | 0.42 |
| 1:V8:21:TRP:CZ3 | 1:V8:61:PRO:HB3 | 2.55 | 0.42 |
| 2:V9:30:ILE:HD12 | 2:V9:53:PHE:CD2 | 2.53 | 0.42 |
| 2:V9:222:PRO:HD2 | 1:W0:324:LYS:HE3 | 2.01 | 0.42 |
| 2:V9:402:ARG:HD3 | 2:V9:402:ARG:HA | 1.90 | 0.42 |
| 2:W1:212:ILE:HG23 | 2:W1:275:ILE:HD12 | 2.00 | 0.42 |
| 1:W2:380:ARG:O | 1:W2:383:GLU:HG3 | 2.18 | 0.42 |
| 2:W5:169:PHE:HZ | 2:W5:238:LEU:HD23 | 1.84 | 0.42 |
| 1:W6:192:LEU:HD23 | 1:W6:192:LEU:HA | 1.83 | 0.42 |
| 2:W7:91:GLN:HE21 | 2:W7:125:LEU:HD21 | 1.83 | 0.42 |
| 1:W8:246:LEU:HD22 | 1:W8:352:SER:HA | 2.01 | 0.42 |
| 2:W9:301:MET:HE1 | 2:W9:307:PRO:HD3 | 2.00 | 0.42 |
| 1:X2:183:TYR:O | 1:X2:187:LEU:HD13 | 2.19 | 0.42 |
| 2:X3:34:GLY:HA3 | 2:X3:60:LYS:NZ | 2.34 | 0.42 |
| 1:X4:68:LEU:HD23 | 1:X4:68:LEU:HA | 1.82 | 0.42 |
| 2:X5:322:ASP:OD1 | 2:X5:322:ASP:N | 2.52 | 0.42 |
| 1:X6:276:ARG:HB3 | 8:4W:187:HIS:CE1 | 2.54 | 0.42 |
| 1:X8:178:THR:OG1 | 2:X9:258:ASN:OD1 | 2.37 | 0.42 |
| 2:X9:9:ILE:HD13 | 2:X9:150:GLY:HA2 | 2.00 | 0.42 |
| 1:Y0:361:LEU:HA | 8:4W:292:MET:HE2 | 2.01 | 0.42 |
| 2:Y3:98:ASP:OD2 | 2:Y3:99:ALA:N | 2.52 | 0.42 |
| 1:Y6:275:SER:O | 1:Y6:279:GLN:HG3 | 2.19 | 0.42 |
| 1:Y8:172:SER:HB3 | 1:Y8:203:ASP:OD2 | 2.20 | 0.42 |
| 1:Y8:179:VAL:HB | 2:Y9:258:ASN:HD22 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z0:164:MET:HE3 | 1:Z0:164:MET:HB3 | 1.81 | 0.42 |
| 1:Z0:235:GLY:HA3 | 1:Z0:366:THR:HG21 | 2.00 | 0.42 |
| 1:Z0:287:PRO:HA | 1:Z0:290:THR:HG22 | 2.00 | 0.42 |
| 2:Z1:280:LYS:HA | 2:Z1:283:HIS:HB3 | 2.00 | 0.42 |
| 2:Z1:338:LYS:HA | 2:Z1:338:LYS:HD2 | 1.77 | 0.42 |
| 2:Z3:268:MET:SD | 2:Z3:380:ASN:HB2 | 2.59 | 0.42 |
| 2:Z5:7:ILE:HD11 | 2:Z5:137:VAL:HG12 | 2.01 | 0.42 |
| 1:Z6:350:LYS:NZ | 1:Z6:352:SER:HB3 | 2.35 | 0.42 |
| 2:Z9:24:TYR:O | 2:Z9:27:GLU:HG2 | 2.18 | 0.42 |
| 1:0A:117:LEU:HD23 | 1:0A:117:LEU:HA | 1.86 | 0.42 |
| 2:0B:252:ILE:HD12 | 2:0B:252:ILE:H | 1.85 | 0.42 |
| 1:0E:237:THR:HG23 | 1:0E:241:ARG:HH21 | 1.85 | 0.42 |
| 1:0G:52:ASN:OD1 | 1:0G:62:ARG:NH2 | 2.51 | 0.42 |
| 1:0G:391:ARG:HD3 | 2:0H:346:TRP:NE1 | 2.34 | 0.42 |
| 2:0H:332:VAL:HA | 2:0H:335:ILE:HG22 | 2.01 | 0.42 |
| 2:0H:338:LYS:HA | 2:0H:338:LYS:HD2 | 1.78 | 0.42 |
| 1:0I:121:ARG:NH2 | 1:0I:158:GLU:OE2 | 2.52 | 0.42 |
| 1:0M:116:VAL:HG23 | 1:0M:151:LEU:HD11 | 2.02 | 0.42 |
| 1:0O:156:ARG:HD2 | 1:0O:156:ARG:HA | 1.83 | 0.42 |
| 2:0P:31:GLN:HB2 | 2:0P:33:ASP:OD1 | 2.19 | 0.42 |
| 2:0P:65:CYS:SG | 2:0P:66:ILE:N | 2.92 | 0.42 |
| 2:0P:397:LEU:HD23 | 2:0P:397:LEU:HA | 1.93 | 0.42 |
| 1:0U:104:GLY:HA2 | 1:0U:147:MET:CE | 2.49 | 0.42 |
| 1:0U:125:GLU:OE1 | 1:1K:291:GLN:NE2 | 2.52 | 0.42 |
| 2:0V:88:HIS:CG | 2:1L:283:HIS:HB3 | 2.54 | 0.42 |
| 2:0V:104:ALA:HB1 | 2:0V:411:GLU:CD | 2.39 | 0.42 |
| 1:0W:140:GLY:O | 1:0W:184:ASN:ND2 | 2.52 | 0.42 |
| 1:0Y:315:ALA:HB1 | 1:0Y:317:PHE:CE1 | 2.54 | 0.42 |
| 2:0Z:307:PRO:HB2 | 2:0Z:312:TYR:HE1 | 1.85 | 0.42 |
| 2:1D:14:ILE:HD11 | 2:1D:74:VAL:HG13 | 2.01 | 0.42 |
| 1:1E:31:ASP:OD2 | 1:1E:33:THR:OG1 | 2.22 | 0.42 |
| 1:1E:69:GLU:C | 1:1E:92:PHE:HZ | 2.23 | 0.42 |
| 1:1K:58:ARG:HA | 1:1K:58:ARG:HD2 | 1.84 | 0.42 |
| 2:1L:227:LEU:O | 2:1L:231:ILE:HG12 | 2.20 | 0.42 |
| 1:1M:39:ASP:OD1 | 1:1M:40:SER:N | 2.53 | 0.42 |
| 1:1M:295:ASP:HB3 | 1:1M:297:LYS:HG3 | 2.02 | 0.42 |
| 1:1Q:69:GLU:OE2 | 1:1Q:70:PRO:HD2 | 2.19 | 0.42 |
| 2:1R:21:TRP:CZ2 | 2:1R:65:CYS:HB3 | 2.53 | 0.42 |
| 2:1R:36:MET:HG3 | 2:1R:61:HIS:NE2 | 2.33 | 0.42 |
| 2:1T:179:THR:O | 1:1U:350:LYS:HD2 | 2.19 | 0.42 |
| 2:1V:79:ARG:NE | 2:1V:92:LEU:HD12 | 2.26 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1V:329:ASN:HA | 2:1V:332:VAL:HG12 | 2.01 | 0.42 |
| 2:1Z:70:LEU:HB3 | 2:1Z:97:GLU:O | 2.18 | 0.42 |
| 2:1Z:195:LEU:HD21 | 2:1Z:264:ARG:CD | 2.47 | 0.42 |
| 2:2B:161:TYR:HE1 | 38:8A:80:TYR:CB | 2.32 | 0.42 |
| 1:2C:396:HIS:HE1 | 1:2C:397:TRP:CZ2 | 2.36 | 0.42 |
| 2:2D:96:LYS:HG2 | 1:2E:1:MET:HE1 | 2.00 | 0.42 |
| 2:2D:365:GLY:HA2 | 10:5A:390:GLN:HE22 | 1.84 | 0.42 |
| 2:2H:282:TYR:CE2 | 10:5B:164:ASP:OD1 | 2.72 | 0.42 |
| 2:2H:326:LYS:HG3 | 2:2H:327:ASP:N | 2.35 | 0.42 |
| 1:2I:86:ARG:HG2 | 1:2I:88:ASP:H | 1.85 | 0.42 |
| 1:2I:337:ASN:HB3 | 1:2I:340:TYR:CD2 | 2.55 | 0.42 |
| 2:2J:8:HIS:CD2 | 2:2J:138:PHE:HD2 | 2.38 | 0.42 |
| 1:2K:114:ASP:OD1 | 1:2K:115:SER:N | 2.53 | 0.42 |
| 1:2K:404:ASP:HB3 | 1:2K:406:MET:SD | 2.60 | 0.42 |
| 2:2L:205:ASP:OD1 | 2:2L:303:VAL:HG13 | 2.20 | 0.42 |
| 1:2M:314:SER:HA | 1:2M:350:LYS:O | 2.20 | 0.42 |
| 1:2Q:320:ARG:NH2 | 38:8A:198:THR:CA | 2.74 | 0.42 |
| 2:2V:215:ARG:HB2 | 38:8B:66:TYR:CE1 | 2.52 | 0.42 |
| 1:2W:418:LEU:O | 1:2W:421:GLU:HG2 | 2.19 | 0.42 |
| 2:2X:170:THR:HG22 | 2:2X:171:VAL:N | 2.35 | 0.42 |
| 1:2Y:170:VAL:N | 1:2Y:202:LEU:O | 2.48 | 0.42 |
| 2:2Z:21:TRP:CZ3 | 2:2Z:63:PRO:HB3 | 2.55 | 0.42 |
| 2:2Z:86:LEU:HD23 | 2:2Z:86:LEU:C | 2.39 | 0.42 |
| 1:3A:165:LEU:HD23 | 1:3A:165:LEU:HA | 1.83 | 0.42 |
| 1:3A:274:THR:HG23 | 1:3A:282:ARG:NH1 | 2.35 | 0.42 |
| 1:3C:117:LEU:HA | 1:3C:120:VAL:HG12 | 2.00 | 0.42 |
| 1:3G:160:PRO:HG2 | 1:3G:161:ASP:OD1 | 2.19 | 0.42 |
| 1:3O:67:ASP:N | 1:3O:67:ASP:OD1 | 2.52 | 0.42 |
| 2:3P:415:GLU:OE1 | 2:3P:415:GLU:N | 2.51 | 0.42 |
| 2:3R:392:ASP:HB2 | 2:3R:425:LEU:HD22 | 2.00 | 0.42 |
| 1:3S:6:HIS:CD2 | 1:3S:134:GLN:HE21 | 2.38 | 0.42 |
| 3:3Z:9:LEU:HD22 | 3:3Z:173:ARG:HH11 | 1.84 | 0.42 |
| 3:3Z:34:SER:OG | 3:3Z:35:CYS:N | 2.53 | 0.42 |
| 4:4A:27:LYS:HE3 | 4:4A:27:LYS:HB3 | 1.94 | 0.42 |
| 3:4D:34:SER:OG | 3:4D:35:CYS:N | 2.53 | 0.42 |
| 3:4H:34:SER:OG | 3:4H:35:CYS:N | 2.53 | 0.42 |
| 5:4L:342:ALA:O | 5:4L:345:GLU:HG3 | 2.18 | 0.42 |
| 5:4M:22:LEU:HD12 | 5:4M:22:LEU:HA | 1.79 | 0.42 |
| 7:4R:331:ILE:HD11 | 12:5F:85:LEU:HD13 | 2.01 | 0.42 |
| 8:4W:130:VAL:O | 8:4W:134:LEU:HG | 2.20 | 0.42 |
| 10:5B:303:LYS:HD3 | 10:5B:303:LYS:HA | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:5F:200:ASP:OD1 | 12:5F:200:ASP:N | 2.52 | 0.42 |
| 14:5L:174:TRP:CD2 | 14:5L:185:PRO:HB3 | 2.53 | 0.42 |
| 14:5L:187:ASP:OD1 | 14:5L:187:ASP:N | 2.46 | 0.42 |
| 14:5L:339:HIS:CE1 | 14:5L:365:ARG:HD2 | 2.54 | 0.42 |
| 14:5M:110:ASP:OD1 | 14:5M:154:LYS:HD3 | 2.18 | 0.42 |
| 14:5M:155:PHE:HE1 | 14:5M:162:LYS:HE2 | 1.84 | 0.42 |
| 14:5M:174:TRP:CD2 | 14:5M:185:PRO:HB3 | 2.53 | 0.42 |
| 14:5M:187:ASP:OD1 | 14:5M:187:ASP:N | 2.46 | 0.42 |
| 14:5N:155:PHE:HE1 | 14:5N:162:LYS:HE2 | 1.84 | 0.42 |
| 15:5O:34:GLU:CG | 15:5O:49:ARG:CD | 2.84 | 0.42 |
| 15:5O:172:TRP:O | 15:5O:176:ILE:HG12 | 2.20 | 0.42 |
| 15:5O:327:ALA:O | 15:5O:342:SER:OG | 2.35 | 0.42 |
| 16:5Q:43:THR:HA | 16:5Q:61:ILE:HG22 | 2.00 | 0.42 |
| 16:5Q:101:ASP:OD1 | 16:5Q:102:GLU:N | 2.51 | 0.42 |
| 17:5V:225:ASP:O | 17:5V:229:LEU:HG | 2.18 | 0.42 |
| 20:6F:361:LEU:CG | 20:6F:362:PRO:HD2 | 2.49 | 0.42 |
| 23:6R:30:GLU:HA | 23:6R:53:ARG:NH1 | 2.34 | 0.42 |
| 24:6U:103:LYS:HG2 | 24:6U:116:ILE:HG12 | 2.02 | 0.42 |
| 24:6U:152:ARG:HD3 | 24:6U:160:PHE:CG | 2.54 | 0.42 |
| 24:6Y:299:GLU:HG3 | 24:6Y:300:ASP:CG | 2.40 | 0.42 |
| 30:7K:63:PRO:HG2 | 30:7K:65:LYS:NZ | 2.34 | 0.42 |
| 30:7K:296:THR:O | 30:7K:296:THR:OG1 | 2.37 | 0.42 |
| 34:7R:273:LEU:HD23 | 35:7T:227:TRP:HD1 | 1.84 | 0.42 |
| 28:7X:415:THR:O | 28:7X:418:SER:OG | 2.36 | 0.42 |
| 37:7Y:134:PRO:HG2 | 37:7Y:137:LEU:HD12 | 2.01 | 0.42 |
| 38:8C:43:HIS:HD2 | 38:8C:47:PHE:HB2 | 1.85 | 0.42 |
| 38:8C:229:ASN:HB3 | 38:8C:232:PHE:CE2 | 2.54 | 0.42 |
| 38:8D:223:THR:HG23 | 38:8D:224:PHE:HD2 | 1.84 | 0.42 |
| 1:5:55:THR:HG22 | 24:6V:107:VAL:HG21 | 2.01 | 0.42 |
| 1:A3:41:ASP:H | 26:7F:122:VAL:HB | 1.85 | 0.42 |
| 1:B1:362:LYS:HE2 | 18:5Y:94:PHE:CZ | 2.54 | 0.42 |
| 1:B8:276:ARG:NH2 | 24:6Y:210:VAL:HG21 | 2.34 | 0.42 |
| 2:E3:18:ASN:ND2 | 22:6K:116:TYR:HE1 | 2.17 | 0.42 |
| 1:E6:33:THR:CG2 | 22:6L:262:TYR:HB2 | 2.45 | 0.42 |
| 1:G2:152:ILE:HG22 | 1:G2:195:ASN:HB3 | 2.01 | 0.42 |
| 2:G3:175:PRO:HG2 | 2:G3:176:GLN:OE1 | 2.19 | 0.42 |
| 1:G6:253:LEU:HD21 | 1:G6:316:LEU:HD11 | 2.02 | 0.42 |
| 1:G8:8:GLN:NE2 | 1:G8:17:GLY:HA3 | 2.34 | 0.42 |
| 1:G8:213:ARG:O | 1:G8:216:LYS:HG3 | 2.20 | 0.42 |
| 2:H1:291:ILE:HA | 2:H1:294:ALA:HB3 | 2.02 | 0.42 |
| 1:H4:199:CYS:HB2 | 1:H4:265:PHE:CD1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H6:46:ARG:HA | 1:H6:46:ARG:HD3 | 1.87 | 0.42 |
| 2:H7:139:ASN:OD1 | 2:H7:170:THR:HG22 | 2.19 | 0.42 |
| 1:H8:289:LEU:HD21 | 1:H8:363:MET:HG2 | 2.00 | 0.42 |
| 2:H9:88:HIS:HA | 2:H9:89:PRO:HD3 | 1.87 | 0.42 |
| 1:I0:257:LEU:HD21 | 1:I0:314:SER:HB2 | 1.99 | 0.42 |
| 1:I0:289:LEU:O | 1:I0:293:MET:HG3 | 2.19 | 0.42 |
| 2:I1:8:HIS:HB2 | 2:I1:14:ILE:HG22 | 2.02 | 0.42 |
| 2:I1:66:ILE:O | 2:I1:66:ILE:HG13 | 2.20 | 0.42 |
| 2:J1:415:GLU:N | 2:J1:415:GLU:OE2 | 2.52 | 0.42 |
| 1:J2:69:GLU:C | 1:J2:92:PHE:HZ | 2.23 | 0.42 |
| 1:J4:113:ILE:HA | 1:J4:116:VAL:HG12 | 2.02 | 0.42 |
| 1:J6:194:GLU:N | 1:J6:194:GLU:OE1 | 2.53 | 0.42 |
| 2:J7:179:THR:O | 1:J8:350:LYS:HD2 | 2.19 | 0.42 |
| 2:J7:398:MET:HG3 | 1:J8:346:PRO:HD2 | 2.01 | 0.42 |
| 2:J9:149:LEU:HA | 2:J9:152:LEU:HB3 | 2.02 | 0.42 |
| 2:J9:252:ILE:HD12 | 2:J9:252:ILE:HA | 1.92 | 0.42 |
| 1:K0:17:GLY:HA2 | 1:K0:20:PHE:HB3 | 2.00 | 0.42 |
| 1:K0:208:TYR:OH | 2:K1:325:PRO:HB2 | 2.20 | 0.42 |
| 1:K0:233:MET:O | 1:K0:237:THR:HG22 | 2.19 | 0.42 |
| 1:K8:309:ARG:H | 1:K8:372:THR:HG22 | 1.84 | 0.42 |
| 2:L3:14:ILE:HD11 | 2:L3:74:VAL:CG1 | 2.49 | 0.42 |
| 2:L3:392:ASP:OD2 | 2:L3:422:ARG:NH1 | 2.52 | 0.42 |
| 2:L5:213:CYS:HA | 2:L5:217:LEU:HB2 | 2.01 | 0.42 |
| 1:L6:379:LYS:HA | 1:L6:382:SER:OG | 2.19 | 0.42 |
| 2:L7:66:ILE:HD12 | 2:L7:68:LEU:HD23 | 2.00 | 0.42 |
| 1:M0:414:ASN:HA | 1:M0:417:ASP:OD2 | 2.19 | 0.42 |
| 2:M1:391:LEU:HD23 | 2:M1:391:LEU:HA | 1.88 | 0.42 |
| 1:M2:314:SER:HA | 1:M2:350:LYS:O | 2.20 | 0.42 |
| 2:M3:223:THR:OG1 | 2:M3:224:TYR:N | 2.52 | 0.42 |
| 2:M3:241:SER:OG | 2:M3:250:VAL:O | 2.36 | 0.42 |
| 2:M3:271:SER:OG | 2:M3:377:MET:HB3 | 2.20 | 0.42 |
| 1:M6:271:THR:OG1 | 1:M6:272:PRO:HA | 2.20 | 0.42 |
| 2:M7:90:GLU:HB3 | 1:O4:281:TYR:HE2 | 1.81 | 0.42 |
| 2:M7:90:GLU:CB | 1:O4:281:TYR:HE2 | 2.33 | 0.42 |
| 1:M8:56:GLY:H | 19:6E:14:GLN:HE21 | 1.67 | 0.42 |
| 1:M8:327:ASP:OD2 | 1:M8:328:GLU:N | 2.52 | 0.42 |
| 2:N1:9:ILE:HD13 | 2:N1:150:GLY:HA2 | 2.01 | 0.42 |
| 2:N7:346:TRP:CZ3 | 2:N7:435:VAL:HG13 | 2.54 | 0.42 |
| 2:N9:109:THR:OG1 | 2:N9:110:ILE:HD12 | 2.19 | 0.42 |
| 2:O3:108:TYR:O | 2:O3:112:LYS:HG2 | 2.19 | 0.42 |
| 2:O3:138:PHE:HE1 | 2:O3:169:PHE:CD2 | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O3:296:PHE:HE1 | 2:O3:377:MET:HG3 | 1.85 | 0.42 |
| 1:O4:403:MET:HE3 | 1:O4:403:MET:HB2 | 1.87 | 0.42 |
| 2:O5:12:ALA:HB2 | 41:O6:501:GTP:C8 | 2.55 | 0.42 |
| 2:O5:79:ARG:O | 2:O5:84:ARG:HG2 | 2.19 | 0.42 |
| 2:O5:171:VAL:HA | 2:O5:204:LEU:O | 2.19 | 0.42 |
| 2:O5:387:ILE:HG12 | 2:O5:390:ARG:HH22 | 1.85 | 0.42 |
| 1:P4:74:ASP:OD2 | 27:7G:188:GLY:N | 2.50 | 0.42 |
| 1:P4:397:TRP:CZ2 | 2:P5:256:GLN:HB3 | 2.55 | 0.42 |
| 2:P5:68:LEU:HA | 2:P5:93:ILE:O | 2.18 | 0.42 |
| 1:P8:95:THR:HG23 | 1:P8:96:GLY:N | 2.34 | 0.42 |
| 1:P8:175:VAL:HG22 | 2:P9:329:ASN:ND2 | 2.34 | 0.42 |
| 2:P9:114:ILE:HG21 | 2:P9:149:LEU:HD22 | 2.02 | 0.42 |
| 2:P9:174:SER:HA | 2:P9:205:ASP:OD1 | 2.20 | 0.42 |
| 2:P9:276:ILE:HG23 | 2:P9:280:LYS:HB2 | 2.01 | 0.42 |
| 2:Q1:153:LEU:HD12 | 2:Q1:153:LEU:HA | 1.82 | 0.42 |
| 1:Q2:117:LEU:HA | 1:Q2:120:VAL:HG12 | 2.02 | 0.42 |
| 1:Q2:249:ASP:OD1 | 1:Q2:252:LYS:N | 2.48 | 0.42 |
| 2:Q3:265:ILE:CD1 | 2:Q3:435:VAL:HG21 | 2.49 | 0.42 |
| 2:Q5:11:GLN:O | 2:Q5:15:GLN:HG3 | 2.18 | 0.42 |
| 1:Q8:345:ILE:HD12 | 1:Q8:346:PRO:HD2 | 2.02 | 0.42 |
| 2:Q9:145:THR:OG1 | 41:R0:501:GTP:O1B | 2.36 | 0.42 |
| 1:R2:65:LEU:HB2 | 1:R2:90:PHE:HD1 | 1.84 | 0.42 |
| 2:S1:405:VAL:O | 2:S1:409:VAL:HG23 | 2.20 | 0.42 |
| 1:S2:54:ALA:N | 1:S2:58:ARG:O | 2.43 | 0.42 |
| 1:S4:167:PHE:CZ | 1:S4:233:MET:HG2 | 2.55 | 0.42 |
| 1:S6:101:TRP:CE3 | 1:S6:187:LEU:HD23 | 2.55 | 0.42 |
| 1:S6:309:ARG:H | 1:S6:372:THR:CG2 | 2.32 | 0.42 |
| 2:S7:294:ALA:O | 2:S7:297:GLU:HG2 | 2.19 | 0.42 |
| 1:S8:239:CYS:SG | 1:S8:247:ASN:HA | 2.59 | 0.42 |
| 2:S9:407:TRP:HZ2 | 1:T0:258:ILE:HB | 1.84 | 0.42 |
| 2:T1:71:GLU:HG3 | 2:T1:73:THR:HG22 | 2.00 | 0.42 |
| 2:T1:216:SER:HB3 | 2:T1:275:ILE:O | 2.19 | 0.42 |
| 1:T2:292:GLN:HG2 | 1:T2:298:ASN:ND2 | 2.32 | 0.42 |
| 1:T6:192:LEU:HD23 | 1:T6:192:LEU:HA | 1.85 | 0.42 |
| 1:T6:207:LEU:HB3 | 1:T6:225:LEU:HD22 | 2.01 | 0.42 |
| 2:U1:53:PHE:HD1 | 2:U1:63:PRO:HA | 1.84 | 0.42 |
| 2:U1:325:PRO:HA | 2:U1:328:VAL:HG12 | 2.01 | 0.42 |
| 1:U2:178:THR:CG2 | 1:U2:181:GLU:HG3 | 2.49 | 0.42 |
| 1:U2:271:THR:HG22 | 1:U2:289:LEU:HD22 | 2.00 | 0.42 |
| 2:V3:250:VAL:HG13 | 2:V3:254:GLU:HB2 | 2.02 | 0.42 |
| 2:V7:344:VAL:HG11 | 2:V7:346:TRP:CE2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V8:273:LEU:H | 1:V8:292:GLN:NE2 | 2.14 | 0.42 |
| 2:V9:36:MET:HA | 2:V9:37:PRO:HD3 | 1.91 | 0.42 |
| 2:V9:274:PRO:HG2 | 2:V9:371:VAL:HG11 | 2.01 | 0.42 |
| 2:W1:60:LYS:HB2 | 2:X7:282:TYR:CE1 | 2.54 | 0.42 |
| 1:W4:3:GLU:HB2 | 1:W4:130:LEU:HA | 2.00 | 0.42 |
| 2:W9:47:ASP:N | 2:W9:47:ASP:OD1 | 2.52 | 0.42 |
| 2:W9:234:VAL:HG13 | 2:W9:376:CYS:SG | 2.59 | 0.42 |
| 1:X0:95:THR:HG23 | 1:X0:96:GLY:N | 2.35 | 0.42 |
| 1:X4:203:ASP:OD2 | 1:X4:302:ALA:N | 2.53 | 0.42 |
| 2:X5:132:LEU:HD22 | 2:X5:164:LYS:HD3 | 2.00 | 0.42 |
| 2:X7:216:SER:OG | 2:X7:217:LEU:N | 2.51 | 0.42 |
| 2:X9:52:PHE:CE2 | 2:X9:243:ARG:HD3 | 2.55 | 0.42 |
| 2:X9:133:GLN:HB3 | 2:X9:252:ILE:HG21 | 2.01 | 0.42 |
| 1:Y0:3:GLU:HG3 | 1:Y0:127:CYS:SG | 2.60 | 0.42 |
| 1:Y0:396:HIS:HE1 | 1:Y0:397:TRP:CE2 | 2.38 | 0.42 |
| 1:Y4:276:ARG:HD3 | 8:4W:405:GLU:CD | 2.39 | 0.42 |
| 2:Y9:147:SER:OG | 2:Y9:148:GLY:N | 2.52 | 0.42 |
| 1:Z0:257:LEU:HD13 | 1:Z0:312:THR:HB | 2.01 | 0.42 |
| 1:Z4:147:MET:HB2 | 1:Z4:147:MET:HE2 | 1.89 | 0.42 |
| 2:Z5:90:GLU:OE2 | 2:Z5:124:LYS:NZ | 2.52 | 0.42 |
| 2:Z5:209:ILE:HG22 | 2:Z5:227:LEU:HD22 | 2.02 | 0.42 |
| 2:Z7:34:GLY:HA3 | 2:Z7:60:LYS:NZ | 2.31 | 0.42 |
| 1:Z8:11:GLN:HG2 | 1:Z8:12:CYS:N | 2.34 | 0.42 |
| 1:Z8:174:LYS:HE2 | 1:Z8:174:LYS:HB3 | 1.76 | 0.42 |
| 1:Z8:385:PHE:HZ | 1:Z8:408:PHE:HD1 | 1.67 | 0.42 |
| 2:Z9:52:PHE:CE2 | 2:Z9:243:ARG:HD3 | 2.55 | 0.42 |
| 1:0A:100:ASN:HB3 | 1:0A:103:LYS:HB2 | 2.01 | 0.42 |
| 1:0A:384:GLN:HB3 | 2:0B:348:PRO:HG3 | 2.01 | 0.42 |
| 1:0A:412:GLU:O | 1:0A:415:MET:HE3 | 2.20 | 0.42 |
| 1:0C:204:ASN:HD22 | 39:0C:502:GDP:HN22 | 1.68 | 0.42 |
| 2:0H:81:GLY:O | 2:0H:84:ARG:NH1 | 2.49 | 0.42 |
| 1:0I:116:VAL:O | 1:0I:120:VAL:HG12 | 2.20 | 0.42 |
| 1:0K:217:LEU:HD23 | 1:0K:217:LEU:HA | 1.90 | 0.42 |
| 2:0L:155:GLU:HB2 | 2:0L:197:HIS:CE1 | 2.54 | 0.42 |
| 2:0L:205:ASP:OD2 | 2:0L:206:ASN:N | 2.53 | 0.42 |
| 1:0M:154:LYS:HA | 1:0M:154:LYS:HD3 | 1.87 | 0.42 |
| 2:0N:205:ASP:OD1 | 2:0N:206:ASN:N | 2.53 | 0.42 |
| 2:0P:287:SER:N | 2:0P:290:GLU:OE2 | 2.52 | 0.42 |
| 1:0S:135:VAL:HG22 | 1:0S:137:HIS:HD2 | 1.85 | 0.42 |
| 1:0S:327:ASP:O | 1:0S:330:MET:HG3 | 2.20 | 0.42 |
| 1:0U:211:CYS:SG | 1:0U:217:LEU:HB3 | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0W:208:TYR:HA | 1:0W:211:CYS:SG | 2.59 | 0.42 |
| 2:0X:74:VAL:O | 2:0X:78:VAL:HG23 | 2.20 | 0.42 |
| 1:0Y:314:SER:HA | 1:0Y:350:LYS:O | 2.20 | 0.42 |
| 2:1B:9:ILE:HD11 | 2:1B:153:LEU:HD23 | 2.01 | 0.42 |
| 1:1E:180:VAL:HG23 | 1:1E:184:ASN:ND2 | 2.34 | 0.42 |
| 1:1K:58:ARG:HH11 | 1:1K:84:ILE:HA | 1.84 | 0.42 |
| 1:1K:396:HIS:CD2 | 2:1L:263:PRO:HD3 | 2.55 | 0.42 |
| 2:1L:425:LEU:HD23 | 2:1L:425:LEU:HA | 1.93 | 0.42 |
| 1:1O:4:ILE:CD1 | 1:1O:131:GLN:HB3 | 2.50 | 0.42 |
| 2:1T:246:GLY:HA2 | 2:1T:357:TYR:CD2 | 2.54 | 0.42 |
| 2:1T:420:GLU:O | 2:1T:424:ASP:HB2 | 2.20 | 0.42 |
| 1:1U:248:ALA:CB | 1:1U:252:LYS:HD3 | 2.49 | 0.42 |
| 1:1U:273:LEU:N | 1:1U:292:GLN:HE22 | 2.16 | 0.42 |
| 1:1U:404:ASP:HB3 | 1:1U:406:MET:SD | 2.60 | 0.42 |
| 2:1V:268:MET:HB3 | 2:1V:378:ILE:HG23 | 2.00 | 0.42 |
| 2:1X:396:ASP:CG | 2:1X:422:ARG:HH21 | 2.23 | 0.42 |
| 2:1Z:11:GLN:NE2 | 1:2A:247:ASN:OD1 | 2.53 | 0.42 |
| 1:2A:165:LEU:CD1 | 1:2A:250:LEU:HD13 | 2.49 | 0.42 |
| 2:2B:401:LYS:HE3 | 2:2B:401:LYS:HB3 | 1.89 | 0.42 |
| 1:2C:389:PHE:O | 1:2C:392:LYS:NZ | 2.38 | 0.42 |
| 2:2D:362:VAL:HG21 | 10:5A:383:GLN:NE2 | 2.35 | 0.42 |
| 2:2D:413:MET:HB3 | 2:2D:417:GLU:OE2 | 2.20 | 0.42 |
| 2:2F:334:THR:HA | 2:2F:337:THR:HG22 | 2.01 | 0.42 |
| 1:2G:263:LEU:HA | 1:2G:422:TYR:OH | 2.18 | 0.42 |
| 2:2H:101:ASN:ND2 | 2:2H:143:GLY:HA2 | 2.34 | 0.42 |
| 1:2K:208:TYR:HA | 1:2K:211:CYS:SG | 2.59 | 0.42 |
| 2:2N:119:LEU:HD11 | 2:2N:156:ARG:HD3 | 2.00 | 0.42 |
| 2:2N:186:ASN:OD1 | 2:2N:408:TYR:OH | 2.38 | 0.42 |
| 1:2Q:320:ARG:CZ | 38:8A:198:THR:HG23 | 2.24 | 0.42 |
| 1:2S:1:MET:HB3 | 1:2S:2:ARG:H | 1.62 | 0.42 |
| 1:2S:391:ARG:NH2 | 2:2T:434:GLU:O | 2.53 | 0.42 |
| 2:2V:90:GLU:O | 2:2V:121:ARG:NH1 | 2.40 | 0.42 |
| 2:2X:115:VAL:HG11 | 2:2X:152:LEU:HD23 | 2.02 | 0.42 |
| 2:2X:279:GLU:N | 2:2X:279:GLU:CD | 2.72 | 0.42 |
| 2:2Z:107:HIS:CD2 | 2:2Z:152:LEU:HB2 | 2.55 | 0.42 |
| 2:3D:11:GLN:HB3 | 41:3D:501:GTP:PA | 2.60 | 0.42 |
| 2:3F:56:THR:HG1 | 3:3V:34:SER:HA | 1.83 | 0.42 |
| 1:3G:66:MET:SD | 1:3G:147:MET:HG2 | 2.59 | 0.42 |
| 1:3I:135:VAL:O | 1:3I:166:THR:HA | 2.19 | 0.42 |
| 1:3I:337:ASN:HB3 | 1:3I:340:TYR:HD2 | 1.85 | 0.42 |
| 2:3L:271:SER:OG | 2:3L:377:MET:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3L:391:LEU:HD23 | 2:3L:391:LEU:HA | 1.84 | 0.42 |
| 1:3O:317:PHE:CE2 | 1:3O:326:VAL:HG13 | 2.55 | 0.42 |
| 2:3P:127:ASP:OD2 | 3:4F:134:VAL:HG23 | 2.19 | 0.42 |
| 2:3P:313:MET:HB2 | 2:3P:380:ASN:HB3 | 2.00 | 0.42 |
| 1:3Q:192:LEU:HD23 | 1:3Q:192:LEU:HA | 1.88 | 0.42 |
| 1:3Q:284:LEU:HD23 | 1:3Q:284:LEU:HA | 1.80 | 0.42 |
| 2:3R:53:PHE:HB3 | 2:3R:61:HIS:HB3 | 2.01 | 0.42 |
| 3:3V:9:LEU:HD22 | 3:3V:173:ARG:HH11 | 1.84 | 0.42 |
| 3:3V:34:SER:OG | 3:3V:35:CYS:N | 2.53 | 0.42 |
| 3:3X:34:SER:OG | 3:3X:35:CYS:N | 2.53 | 0.42 |
| 3:4B:34:SER:OG | 3:4B:35:CYS:N | 2.53 | 0.42 |
| 5:4L:348:ALA:HA | 5:4L:351:ASP:OD2 | 2.20 | 0.42 |
| 6:4O:165:TYR:OH | 29:7I:221:PRO:O | 2.19 | 0.42 |
| 7:4T:180:TYR:CE1 | 31:7M:80:PRO:HD3 | 2.54 | 0.42 |
| 7:4T:199:VAL:O | 7:4T:203:THR:HG23 | 2.19 | 0.42 |
| 10:5A:472:GLN:CB | 10:5A:476:ARG:HH21 | 2.31 | 0.42 |
| 10:5C:257:GLN:O | 10:5C:261:LYS:HG2 | 2.18 | 0.42 |
| 10:5C:292:GLU:HG2 | 10:5C:295:ARG:NH1 | 2.35 | 0.42 |
| 10:5C:470:LEU:HD23 | 10:5C:470:LEU:HA | 1.84 | 0.42 |
| 13:5I:61:LEU:HD12 | 13:5I:67:LYS:HD3 | 2.00 | 0.42 |
| 13:5J:61:LEU:HD12 | 13:5J:67:LYS:HD3 | 2.00 | 0.42 |
| 14:5L:155:PHE:HE1 | 14:5L:162:LYS:HE2 | 1.84 | 0.42 |
| 14:5M:253:ILE:HG23 | 14:5M:265:LEU:HB2 | 2.01 | 0.42 |
| 14:5N:110:ASP:OD1 | 14:5N:154:LYS:HD3 | 2.18 | 0.42 |
| 14:5N:174:TRP:CD2 | 14:5N:185:PRO:HB3 | 2.53 | 0.42 |
| 14:5N:339:HIS:CE1 | 14:5N:365:ARG:HD2 | 2.54 | 0.42 |
| 15:5O:226:ARG:HH11 | 15:5O:226:ARG:CB | 2.28 | 0.42 |
| 15:5P:9:PHE:CG | 15:5P:75:LEU:HD23 | 2.55 | 0.42 |
| 17:5T:224:ARG:O | 17:5T:228:THR:HG23 | 2.19 | 0.42 |
| 17:5V:199:LEU:HD11 | 17:5V:211:ARG:HD3 | 2.01 | 0.42 |
| 20:6F:84:ALA:HB2 | 20:6F:114:ASN:HA | 2.00 | 0.42 |
| 22:6I:307:ARG:HG3 | 22:6I:326:PHE:CZ | 2.54 | 0.42 |
| 22:6J:114:THR:O | 22:6J:118:VAL:HG23 | 2.20 | 0.42 |
| 22:6L:96:LYS:HZ2 | 22:6L:99:THR:HG23 | 1.83 | 0.42 |
| 22:6L:150:TYR:HB3 | 22:6L:228:PHE:HB2 | 2.00 | 0.42 |
| 22:6M:240:TYR:O | 22:6M:244:VAL:HG12 | 2.19 | 0.42 |
| 22:6O:270:ALA:O | 22:6O:273:VAL:HG12 | 2.20 | 0.42 |
| 24:6U:273:LEU:HA | 24:6U:375:THR:HG22 | 2.00 | 0.42 |
| 24:6V:253:PRO:HB3 | 24:6V:255:HIS:CE1 | 2.54 | 0.42 |
| 24:6V:257:LEU:HA | 24:6V:257:LEU:HD23 | 1.78 | 0.42 |
| 24:6W:472:SER:HB2 | 24:6W:481:LEU:HD21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6X:119:VAL:HG11 | 24:6X:179:PHE:HD1 | 1.84 | 0.42 |
| 24:6X:293:VAL:CG2 | 24:6X:306:LEU:HB2 | 2.50 | 0.42 |
| 24:6X:304:GLU:OE2 | 24:6X:306:LEU:HG | 2.19 | 0.42 |
| 24:6Z:106:VAL:HG12 | 24:6Z:113:ASN:C | 2.40 | 0.42 |
| 24:6Z:124:TYR:HD1 | 24:6Z:124:TYR:H | 1.67 | 0.42 |
| 24:6Z:435:LEU:HA | 24:6Z:438:LEU:HB3 | 2.01 | 0.42 |
| 29:7I:5:GLY:H | 29:7I:12:LYS:NZ | 2.17 | 0.42 |
| 29:7I:216:LYS:HG3 | 29:7I:217:TYR:H | 1.84 | 0.42 |
| 30:7K:42:ASN:HB3 | 30:7K:45:ARG:CZ | 2.49 | 0.42 |
| 38:8A:86:TYR:CD2 | 38:8A:104:LYS:HG2 | 2.49 | 0.42 |
| 38:8B:176:THR:O | 38:8B:177:HIS:CD2 | 2.72 | 0.42 |
| 2:4:30:ILE:N | 26:7D:45:MET:CE | 2.82 | 0.42 |
| 1:7:55:THR:CG2 | 24:6W:107:VAL:HG21 | 2.48 | 0.42 |
| 2:C1:145:THR:OG1 | 41:C1:501:GTP:O3B | 2.36 | 0.42 |
| 1:D0:219:THR:HG22 | 24:6W:254:SER:HB2 | 2.02 | 0.42 |
| 2:G1:312:TYR:O | 2:G1:344:VAL:HB | 2.18 | 0.42 |
| 1:G2:272:PRO:HD3 | 1:G2:364:SER:HA | 2.00 | 0.42 |
| 1:G2:317:PHE:HB3 | 1:G2:321:MET:SD | 2.60 | 0.42 |
| 2:G3:289:ALA:HA | 2:G3:331:SER:OG | 2.20 | 0.42 |
| 1:G4:37:HIS:CE1 | 24:6X:458:HIS:CE1 | 3.07 | 0.42 |
| 2:G5:157:LEU:HD23 | 2:G5:157:LEU:HA | 1.75 | 0.42 |
| 2:G7:181:VAL:HB | 1:G8:256:ASN:HD22 | 1.85 | 0.42 |
| 1:G8:152:ILE:HD13 | 1:G8:152:ILE:HA | 1.90 | 0.42 |
| 1:G8:367:PHE:CZ | 1:G8:369:GLY:HA3 | 2.54 | 0.42 |
| 1:H2:207:LEU:HD23 | 1:H2:210:ILE:HD11 | 2.01 | 0.42 |
| 2:H5:35:GLN:HB3 | 2:H5:59:GLY:O | 2.20 | 0.42 |
| 2:H5:137:VAL:HG22 | 2:H5:168:GLY:HA2 | 2.02 | 0.42 |
| 2:H7:407:TRP:CD2 | 1:H8:255:VAL:HG23 | 2.54 | 0.42 |
| 1:I4:244:GLY:H | 1:I4:247:ASN:HD21 | 1.68 | 0.42 |
| 2:I7:3:GLU:HG3 | 2:I7:51:THR:HA | 2.02 | 0.42 |
| 2:I7:332:VAL:HA | 2:I7:335:ILE:HG22 | 2.01 | 0.42 |
| 1:J0:40:SER:HB3 | 28:7H:413:TYR:CD1 | 2.54 | 0.42 |
| 1:J0:152:ILE:HD13 | 1:J0:152:ILE:HA | 1.87 | 0.42 |
| 1:J0:153:SER:O | 1:J0:157:GLU:HG2 | 2.19 | 0.42 |
| 1:J0:192:LEU:HD23 | 1:J0:192:LEU:HA | 1.84 | 0.42 |
| 2:J1:33:ASP:OD2 | 2:J1:35:GLN:NE2 | 2.45 | 0.42 |
| 2:J5:116:ASP:OD1 | 2:J5:117:LEU:N | 2.51 | 0.42 |
| 2:J5:370:LYS:HE2 | 2:J5:370:LYS:HB3 | 1.93 | 0.42 |
| 2:J7:12:ALA:HB2 | 41:J8:501:GTP:C8 | 2.55 | 0.42 |
| 1:J8:95:THR:HG23 | 1:J8:96:GLY:N | 2.33 | 0.42 |
| 1:J8:101:TRP:CE3 | 1:J8:403:MET:HE1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J9:29:GLY:HA3 | 2:J9:40:LYS:NZ | 2.34 | 0.42 |
| 1:K0:334:GLN:NE2 | 1:K0:348:ASN:H | 2.17 | 0.42 |
| 2:K1:21:TRP:CZ3 | 2:K1:63:PRO:HB3 | 2.55 | 0.42 |
| 2:K1:133:GLN:HE21 | 2:K1:252:ILE:HG22 | 1.82 | 0.42 |
| 2:K1:286:LEU:HA | 2:K1:286:LEU:HD23 | 1.79 | 0.42 |
| 2:K3:236:SER:OG | 2:K3:243:ARG:NH2 | 2.53 | 0.42 |
| 1:K6:66:MET:HG3 | 1:K6:116:VAL:HG11 | 2.01 | 0.42 |
| 1:K6:219:THR:O | 1:K6:219:THR:OG1 | 2.34 | 0.42 |
| 1:K8:173:PRO:HD2 | 1:K8:380:ARG:CZ | 2.50 | 0.42 |
| 1:K8:334:GLN:HE22 | 1:K8:348:ASN:H | 1.68 | 0.42 |
| 2:L1:125:LEU:HA | 2:L1:125:LEU:HD23 | 1.82 | 0.42 |
| 2:L3:226:ASN:ND2 | 29:7J:360:GLN:HE22 | 2.17 | 0.42 |
| 2:L5:31:GLN:HB2 | 2:L5:33:ASP:OD1 | 2.20 | 0.42 |
| 2:L5:392:ASP:OD2 | 2:L5:422:ARG:NH1 | 2.53 | 0.42 |
| 1:L6:173:PRO:HD2 | 1:L6:380:ARG:NH2 | 2.35 | 0.42 |
| 2:L7:3:GLU:HA | 2:L7:51:THR:HG23 | 2.00 | 0.42 |
| 2:L7:90:GLU:OE1 | 2:L7:121:ARG:NH2 | 2.53 | 0.42 |
| 2:L7:203:MET:CE | 2:L7:267:PHE:HB3 | 2.50 | 0.42 |
| 1:M0:21:TRP:CZ3 | 1:M0:61:PRO:HB3 | 2.54 | 0.42 |
| 1:M4:19:LYS:HZ3 | 30:7K:159:ARG:HD3 | 1.84 | 0.42 |
| 1:M4:186:THR:HG22 | 1:M4:411:ALA:HB1 | 2.01 | 0.42 |
| 1:M4:324:LYS:O | 1:M4:328:GLU:HG3 | 2.20 | 0.42 |
| 1:M6:95:THR:HG23 | 1:M6:96:GLY:N | 2.34 | 0.42 |
| 1:M8:22:GLU:HG2 | 1:M8:81:TYR:HB2 | 2.01 | 0.42 |
| 1:M8:404:ASP:OD1 | 1:M8:405:GLU:N | 2.49 | 0.42 |
| 1:N0:334:GLN:NE2 | 1:N0:348:ASN:H | 2.15 | 0.42 |
| 2:N1:224:TYR:O | 2:N1:228:ASN:ND2 | 2.52 | 0.42 |
| 2:N1:370:LYS:HD3 | 30:7L:329:ARG:N | 2.35 | 0.42 |
| 1:N2:237:THR:O | 1:N2:237:THR:HG22 | 2.19 | 0.42 |
| 2:N3:276:ILE:O | 2:N3:368:LEU:HD23 | 2.19 | 0.42 |
| 2:N9:276:ILE:HD12 | 2:N9:276:ILE:HA | 1.93 | 0.42 |
| 1:O0:203:ASP:O | 1:O0:207:LEU:HD23 | 2.20 | 0.42 |
| 2:O1:189:LEU:HD11 | 2:O1:418:PHE:HE1 | 1.85 | 0.42 |
| 1:O2:391:ARG:HH21 | 1:O2:391:ARG:CB | 2.31 | 0.42 |
| 1:O4:190:HIS:HD2 | 1:O4:414:ASN:HB3 | 1.84 | 0.42 |
| 1:P8:51:PHE:HB3 | 1:P8:59:TYR:HB3 | 2.02 | 0.42 |
| 1:Q2:2:ARG:HE | 1:Q2:240:LEU:HD22 | 1.83 | 0.42 |
| 1:Q2:406:MET:SD | 1:Q2:406:MET:N | 2.93 | 0.42 |
| 2:Q3:85:GLN:OE1 | 2:Q3:85:GLN:HA | 2.20 | 0.42 |
| 1:Q4:24:VAL:HG11 | 1:Q4:50:TYR:CD2 | 2.54 | 0.42 |
| 1:Q4:161:ASP:O | 1:Q4:251:ARG:NH2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q8:117:LEU:HA | 1:Q8:120:VAL:HG12 | 2.01 | 0.42 |
| 1:Q8:165:LEU:HD13 | 1:Q8:167:PHE:CZ | 2.55 | 0.42 |
| 1:Q8:326:VAL:O | 1:Q8:330:MET:HG3 | 2.19 | 0.42 |
| 1:R8:228:LEU:O | 1:R8:232:VAL:HG23 | 2.19 | 0.42 |
| 1:R8:301:CYS:SG | 1:R8:302:ALA:N | 2.93 | 0.42 |
| 1:S0:11:GLN:NE2 | 2:S1:249:ASN:OD1 | 2.53 | 0.42 |
| 1:S2:273:LEU:H | 1:S2:292:GLN:HE22 | 1.68 | 0.42 |
| 2:S5:274:PRO:HD3 | 2:S5:374:ALA:HA | 2.01 | 0.42 |
| 1:S6:68:LEU:HB3 | 1:S6:96:GLY:HA2 | 2.00 | 0.42 |
| 1:S6:334:GLN:HE22 | 1:S6:348:ASN:H | 1.66 | 0.42 |
| 2:S7:425:LEU:HD12 | 2:S7:425:LEU:HA | 1.83 | 0.42 |
| 2:S9:21:TRP:CZ3 | 2:S9:63:PRO:HB3 | 2.54 | 0.42 |
| 1:T4:67:ASP:N | 1:T4:67:ASP:OD1 | 2.52 | 0.42 |
| 1:T4:287:PRO:HA | 1:T4:290:THR:HG22 | 2.01 | 0.42 |
| 1:T4:309:ARG:H | 1:T4:372:THR:CG2 | 2.32 | 0.42 |
| 2:T5:165:SER:HB2 | 2:T5:256:GLN:NE2 | 2.35 | 0.42 |
| 2:T5:207:GLU:OE2 | 17:5U:38:PHE:HB3 | 2.19 | 0.42 |
| 1:T6:392:LYS:HD3 | 1:T6:392:LYS:HA | 1.63 | 0.42 |
| 1:T8:68:LEU:HB3 | 1:T8:96:GLY:HA2 | 2.02 | 0.42 |
| 1:T8:210:ILE:O | 1:T8:214:THR:OG1 | 2.32 | 0.42 |
| 1:U2:192:LEU:HD23 | 1:U2:192:LEU:HA | 1.88 | 0.42 |
| 1:U4:3:GLU:HG3 | 1:U4:127:CYS:SG | 2.60 | 0.42 |
| 1:U6:22:GLU:O | 1:U6:25:SER:OG | 2.37 | 0.42 |
| 2:U7:286:LEU:HD12 | 2:U7:286:LEU:HA | 1.75 | 0.42 |
| 2:U7:328:VAL:HG11 | 2:U7:355:ILE:HD11 | 2.02 | 0.42 |
| 2:U7:396:ASP:OD2 | 2:U7:422:ARG:NH2 | 2.52 | 0.42 |
| 2:V1:4:VAL:HG23 | 2:V1:134:GLY:O | 2.18 | 0.42 |
| 1:V2:6:HIS:HD2 | 1:V2:134:GLN:OE1 | 2.02 | 0.42 |
| 1:V2:86:ARG:HG2 | 1:V2:88:ASP:H | 1.85 | 0.42 |
| 1:V2:135:VAL:HG21 | 1:V2:152:ILE:HD11 | 2.00 | 0.42 |
| 2:V3:88:HIS:HD2 | 2:V3:90:GLU:H | 1.67 | 0.42 |
| 2:V9:8:HIS:HB2 | 2:V9:67:PHE:HD1 | 1.84 | 0.42 |
| 2:V9:21:TRP:CH2 | 2:V9:63:PRO:HB3 | 2.55 | 0.42 |
| 1:W2:170:VAL:HG22 | 1:W2:202:LEU:O | 2.19 | 0.42 |
| 1:W2:257:LEU:HA | 1:W2:312:THR:HG21 | 2.02 | 0.42 |
| 2:W3:76:ASP:O | 2:W3:80:THR:HG23 | 2.20 | 0.42 |
| 2:W3:147:SER:OG | 2:W3:190:SER:HB2 | 2.19 | 0.42 |
| 2:W5:21:TRP:CZ3 | 2:W5:63:PRO:HB3 | 2.55 | 0.42 |
| 2:W5:102:ASN:HB3 | 2:W5:105:ARG:HB3 | 2.00 | 0.42 |
| 2:W7:136:LEU:HA | 2:W7:167:LEU:O | 2.19 | 0.42 |
| 1:W8:356:ILE:HD13 | 1:W8:356:ILE:HA | 1.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X0:145:SER:OG | 1:X0:188:SER:OG | 2.24 | 0.42 |
| 1:X4:95:THR:OG1 | 1:X4:96:GLY:N | 2.53 | 0.42 |
| 2:X7:195:LEU:HA | 2:X7:195:LEU:HD23 | 1.74 | 0.42 |
| 1:X8:3:GLU:HG3 | 1:X8:127:CYS:SG | 2.59 | 0.42 |
| 2:X9:214:ARG:HD2 | 2:X9:215:ARG:HE | 1.85 | 0.42 |
| 2:X9:253:THR:O | 2:X9:257:THR:HG23 | 2.20 | 0.42 |
| 2:Y1:274:PRO:HB2 | 2:Y1:276:ILE:HG12 | 2.02 | 0.42 |
| 1:Y2:379:LYS:HG3 | 1:Y2:419:VAL:HG21 | 2.01 | 0.42 |
| 2:Y5:31:GLN:HE21 | 2:Y5:37:PRO:HG3 | 1.83 | 0.42 |
| 1:Y8:87:PRO:HA | 1:Y8:90:PHE:CD2 | 2.55 | 0.42 |
| 2:Y9:32:PRO:HB3 | 2:Y9:83:TYR:CE1 | 2.54 | 0.42 |
| 1:Z0:123:GLU:O | 1:Z0:126:SER:OG | 2.36 | 0.42 |
| 1:Z0:350:LYS:HZ1 | 1:Z0:352:SER:HB2 | 1.83 | 0.42 |
| 1:Z2:130:LEU:HD12 | 1:Z2:130:LEU:H | 1.84 | 0.42 |
| 1:Z4:100:ASN:ND2 | 1:Z4:103:LYS:HG3 | 2.34 | 0.42 |
| 1:Z6:232:VAL:HG11 | 1:Z6:268:VAL:HG11 | 2.01 | 0.42 |
| 2:Z7:108:TYR:O | 2:Z7:112:LYS:NZ | 2.29 | 0.42 |
| 2:Z7:334:THR:HA | 2:Z7:337:THR:HG22 | 2.02 | 0.42 |
| 2:Z7:345:ASP:OD2 | 2:Z7:346:TRP:N | 2.53 | 0.42 |
| 1:0A:101:TRP:CZ3 | 1:0A:187:LEU:HD23 | 2.55 | 0.42 |
| 2:0B:50:ASN:O | 2:0B:64:ARG:NH2 | 2.51 | 0.42 |
| 2:0B:312:TYR:HD2 | 2:0B:343:PHE:HE1 | 1.68 | 0.42 |
| 1:0C:95:THR:OG1 | 1:0C:96:GLY:N | 2.53 | 0.42 |
| 1:0C:128:ASP:OD1 | 1:0C:128:ASP:N | 2.49 | 0.42 |
| 1:0C:285:THR:OG1 | 1:0C:287:PRO:HD2 | 2.20 | 0.42 |
| 1:0E:371:SER:OG | 1:0E:372:THR:N | 2.53 | 0.42 |
| 2:0F:326:LYS:HG3 | 2:0F:327:ASP:N | 2.34 | 0.42 |
| 1:0G:156:ARG:HD2 | 1:0G:156:ARG:HA | 1.79 | 0.42 |
| 1:0G:334:GLN:HA | 1:0G:341:PHE:CE2 | 2.55 | 0.42 |
| 1:0I:26:ASP:O | 1:0I:359:LYS:NZ | 2.30 | 0.42 |
| 2:0J:73:THR:OG1 | 2:0J:74:VAL:N | 2.53 | 0.42 |
| 2:0J:349:THR:O | 2:0J:349:THR:OG1 | 2.38 | 0.42 |
| 1:0K:253:LEU:HD11 | 1:0K:316:LEU:HD11 | 2.02 | 0.42 |
| 1:0K:321:MET:SD | 1:0K:363:MET:HG3 | 2.60 | 0.42 |
| 2:0L:183:GLU:HG2 | 2:0L:184:PRO:HD3 | 2.01 | 0.42 |
| 1:0M:60:VAL:HG11 | 1:1C:281:TYR:HB3 | 2.02 | 0.42 |
| 2:0N:176:GLN:HE22 | 2:0N:304:LYS:HE2 | 1.85 | 0.42 |
| 2:0P:200:VAL:HG13 | 2:0P:268:MET:CE | 2.50 | 0.42 |
| 1:0S:182:PRO:CG | 1:0S:384:GLN:HE21 | 2.32 | 0.42 |
| 1:0W:382:SER:HB3 | 1:0W:415:MET:HG2 | 2.01 | 0.42 |
| 1:0Y:70:PRO:N | 1:0Y:92:PHE:HZ | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0Y:203:ASP:OD1 | 1:0Y:204:ASN:N | 2.52 | 0.42 |
| 1:0Y:414:ASN:HA | 1:0Y:417:ASP:OD2 | 2.20 | 0.42 |
| 2:0Z:21:TRP:CD1 | 2:0Z:87:PHE:HZ | 2.38 | 0.42 |
| 2:0Z:58:ALA:C | 9:4Z:165:ARG:NH2 | 2.73 | 0.42 |
| 2:0Z:301:MET:HE1 | 2:0Z:307:PRO:HD3 | 2.01 | 0.42 |
| 2:1B:257:THR:HG23 | 2:1B:258:ASN:ND2 | 2.35 | 0.42 |
| 1:1C:8:GLN:NE2 | 1:1C:17:GLY:HA3 | 2.35 | 0.42 |
| 1:1C:384:GLN:HB3 | 2:1D:348:PRO:HG3 | 2.01 | 0.42 |
| 2:1F:312:TYR:CE2 | 2:1F:341:ILE:HG12 | 2.55 | 0.42 |
| 1:1G:31:ASP:OD1 | 1:1G:34:GLY:N | 2.52 | 0.42 |
| 2:1H:259:LEU:HD21 | 2:1H:316:CYS:HB2 | 2.01 | 0.42 |
| 1:1K:175:VAL:HG23 | 1:1K:175:VAL:O | 2.18 | 0.42 |
| 2:1L:66:ILE:HG13 | 2:1L:66:ILE:O | 2.19 | 0.42 |
| 2:1L:331:SER:O | 2:1L:334:THR:N | 2.52 | 0.42 |
| 2:1N:334:THR:HA | 2:1N:337:THR:HG22 | 2.01 | 0.42 |
| 2:1P:175:PRO:HB3 | 2:1P:390:ARG:HD2 | 2.01 | 0.42 |
| 1:1Q:170:VAL:HG22 | 1:1Q:202:LEU:O | 2.19 | 0.42 |
| 2:1R:14:ILE:HD11 | 2:1R:74:VAL:HG13 | 2.02 | 0.42 |
| 2:1R:401:LYS:HB2 | 1:1S:344:TRP:CZ3 | 2.54 | 0.42 |
| 1:1S:39:ASP:OD1 | 1:1S:40:SER:N | 2.52 | 0.42 |
| 2:1T:236:SER:O | 2:1T:243:ARG:NH2 | 2.53 | 0.42 |
| 2:1V:93:ILE:HD12 | 2:1V:117:LEU:HG | 2.02 | 0.42 |
| 2:1V:203:MET:O | 2:1V:204:LEU:HD12 | 2.20 | 0.42 |
| 1:1W:6:HIS:CE1 | 1:1W:8:GLN:HG2 | 2.54 | 0.42 |
| 2:2B:120:ASP:CG | 38:8A:73:TRP:CE2 | 2.93 | 0.42 |
| 2:2B:223:THR:HG23 | 2:2B:225:THR:H | 1.85 | 0.42 |
| 2:2D:12:ALA:HB2 | 41:2E:501:GTP:C8 | 2.54 | 0.42 |
| 1:2E:5:VAL:HG12 | 1:2E:133:PHE:HD1 | 1.85 | 0.42 |
| 1:2E:114:ASP:OD1 | 38:8B:93:LYS:HE2 | 2.20 | 0.42 |
| 2:2H:242:LEU:HD23 | 2:2H:242:LEU:HA | 1.89 | 0.42 |
| 2:2H:282:TYR:CE1 | 10:5B:163:ARG:CD | 3.03 | 0.42 |
| 2:2J:387:ILE:HG12 | 2:2J:390:ARG:HH22 | 1.85 | 0.42 |
| 2:2L:217:LEU:HD23 | 2:2L:217:LEU:HA | 1.90 | 0.42 |
| 2:2N:174:SER:OG | 2:2N:207:GLU:HB2 | 2.20 | 0.42 |
| 2:2N:430:LYS:O | 2:2N:433:GLU:HG3 | 2.18 | 0.42 |
| 2:2P:72:PRO:HD2 | 1:2Q:2:ARG:NH1 | 2.35 | 0.42 |
| 1:2Q:2:ARG:HE | 1:2Q:240:LEU:HD22 | 1.84 | 0.42 |
| 2:2R:216:SER:HB3 | 2:2R:275:ILE:O | 2.19 | 0.42 |
| 2:2T:4:VAL:HG23 | 2:2T:134:GLY:O | 2.19 | 0.42 |
| 2:2T:66:ILE:O | 2:2T:66:ILE:HG13 | 2.20 | 0.42 |
| 2:2T:189:LEU:HD11 | 2:2T:418:PHE:HE1 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2U:178:THR:CG2 | 1:2U:181:GLU:HG3 | 2.49 | 0.42 |
| 1:2U:263:LEU:HD22 | 1:2U:422:TYR:CE1 | 2.52 | 0.42 |
| 1:2Y:156:ARG:HA | 1:2Y:156:ARG:HD2 | 1.80 | 0.42 |
| 1:2Y:212:PHE:CZ | 38:8C:117:TRP:HB3 | 2.54 | 0.42 |
| 1:3A:77:ARG:NH2 | 38:8D:220:VAL:HG23 | 2.35 | 0.42 |
| 2:3B:26:LEU:HD22 | 2:3B:363:VAL:HG12 | 2.00 | 0.42 |
| 2:3B:40:LYS:HE3 | 2:3B:40:LYS:HB3 | 1.84 | 0.42 |
| 1:3C:130:LEU:HA | 1:3C:130:LEU:HD23 | 1.92 | 0.42 |
| 1:3C:392:LYS:HD2 | 1:3C:395:LEU:HD22 | 2.02 | 0.42 |
| 2:3D:35:GLN:N | 2:3D:35:GLN:OE1 | 2.53 | 0.42 |
| 1:3G:77:ARG:NH1 | 1:3G:83:GLN:HA | 2.35 | 0.42 |
| 1:3K:271:THR:HG21 | 1:3K:293:MET:HG3 | 2.00 | 0.42 |
| 2:3L:128:ASN:HA | 3:4B:171:PRO:HB3 | 2.00 | 0.42 |
| 1:3O:99:ASN:ND2 | 2:3P:254:GLU:OE1 | 2.52 | 0.42 |
| 2:3R:325:PRO:HA | 2:3R:328:VAL:HG12 | 2.02 | 0.42 |
| 1:3S:179:VAL:HG13 | 2:3T:349:THR:O | 2.20 | 0.42 |
| 4:3W:21:PRO:HD2 | 3:3X:258:ASP:OD1 | 2.19 | 0.42 |
| 3:4F:34:SER:OG | 3:4F:35:CYS:N | 2.53 | 0.42 |
| 3:4H:9:LEU:HD22 | 3:4H:173:ARG:HH11 | 1.84 | 0.42 |
| 7:4Q:324:GLN:HG2 | 24:6T:22:LEU:H | 1.84 | 0.42 |
| 9:4Z:62:GLU:O | 9:4Z:66:VAL:HG23 | 2.19 | 0.42 |
| 9:4Z:204:LEU:O | 9:4Z:207:LYS:HG2 | 2.20 | 0.42 |
| 9:4Z:343:ALA:HA | 9:4Z:346:LYS:HE3 | 2.02 | 0.42 |
| 10:5A:354:LYS:HA | 10:5A:357:GLU:OE1 | 2.19 | 0.42 |
| 13:5H:69:GLU:OE1 | 13:5H:69:GLU:HA | 2.19 | 0.42 |
| 13:5I:69:GLU:OE1 | 13:5I:69:GLU:HA | 2.19 | 0.42 |
| 13:5J:69:GLU:OE1 | 13:5J:69:GLU:HA | 2.19 | 0.42 |
| 14:5L:7:LEU:HB2 | 14:5L:622:TRP:CZ3 | 2.55 | 0.42 |
| 14:5L:253:ILE:HG23 | 14:5L:265:LEU:HB2 | 2.01 | 0.42 |
| 14:5M:7:LEU:HB2 | 14:5M:622:TRP:CZ3 | 2.55 | 0.42 |
| 14:5M:339:HIS:CE1 | 14:5M:365:ARG:HD2 | 2.54 | 0.42 |
| 14:5M:507:LEU:HD22 | 14:5M:537:TRP:CE3 | 2.55 | 0.42 |
| 14:5N:7:LEU:HB2 | 14:5N:622:TRP:CZ3 | 2.55 | 0.42 |
| 14:5N:253:ILE:HG23 | 14:5N:265:LEU:HB2 | 2.01 | 0.42 |
| 15:5O:7:TYR:CE2 | 15:5O:30:PRO:CG | 3.02 | 0.42 |
| 15:5P:6:ARG:HG2 | 15:5P:29:TYR:HE1 | 1.85 | 0.42 |
| 17:5T:205:SER:O | 17:5T:209:LYS:HE2 | 2.19 | 0.42 |
| 17:5U:188:LYS:O | 17:5U:191:SER:OG | 2.32 | 0.42 |
| 20:6F:284:GLN:HA | 20:6F:284:GLN:OE1 | 2.20 | 0.42 |
| 21:6H:11:LEU:HD11 | 21:6H:204:VAL:HG13 | 2.01 | 0.42 |
| 22:6J:16:LYS:HB2 | 22:6J:39:GLN:NE2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6L:261:ASP:O | 22:6L:266:LYS:NZ | 2.43 | 0.42 |
| 22:6N:106:ASP:OD1 | 22:6N:107:GLU:N | 2.52 | 0.42 |
| 24:6T:592:ASP:OD1 | 24:6T:592:ASP:N | 2.51 | 0.42 |
| 24:6Z:569:LYS:O | 24:6Z:573:VAL:HG13 | 2.19 | 0.42 |
| 29:7I:127:ASP:HB2 | 29:7I:150:ARG:HH22 | 1.83 | 0.42 |
| 29:7J:305:THR:HG23 | 29:7J:308:LEU:HD12 | 2.00 | 0.42 |
| 29:7J:438:VAL:CG2 | 29:7J:443:LEU:HD21 | 2.49 | 0.42 |
| 37:7Y:94:ARG:HH12 | 37:7Y:117:GLN:NE2 | 2.17 | 0.42 |
| 37:7Y:214:ASP:OD2 | 37:7Y:229:ALA:CB | 2.68 | 0.42 |
| 38:8C:8:GLU:HG2 | 38:8C:9:ALA:N | 2.34 | 0.42 |
| 38:8C:71:HIS:ND1 | 38:8C:71:HIS:C | 2.73 | 0.42 |
| 38:8C:83:ARG:HD3 | 38:8C:83:ARG:C | 2.38 | 0.42 |
| 1:5:44:LEU:HG | 18:5Y:84:ARG:HH22 | 1.84 | 0.42 |
| 1:9:83:GLN:HG3 | 24:6X:177:ARG:NH2 | 2.33 | 0.42 |
| 1:A1:337:ASN:HD21 | 3:4F:69:TYR:N | 2.17 | 0.42 |
| 2:B2:278:ALA:HB3 | 18:5Z:43:ASN:ND2 | 2.28 | 0.42 |
| 1:C4:53:GLU:OE1 | 22:6I:23:TYR:OH | 2.30 | 0.42 |
| 1:E6:320:ARG:HH12 | 22:6L:115:SER:HA | 1.85 | 0.42 |
| 1:E8:35:THR:HG21 | 22:6M:260:VAL:H | 1.84 | 0.42 |
| 1:G6:8:GLN:CD | 1:G6:17:GLY:HA3 | 2.40 | 0.42 |
| 1:G6:28:HIS:CD2 | 1:G6:47:ILE:HG22 | 2.54 | 0.42 |
| 1:G6:173:PRO:HB3 | 1:G6:384:GLN:HE22 | 1.85 | 0.42 |
| 1:G8:212:PHE:HE1 | 1:G8:220:PRO:HG3 | 1.85 | 0.42 |
| 1:G8:396:HIS:H | 1:G8:396:HIS:CD2 | 2.38 | 0.42 |
| 2:G9:155:GLU:CD | 2:G9:197:HIS:HE2 | 2.23 | 0.42 |
| 2:G9:170:THR:HG21 | 2:G9:194:LEU:HD11 | 2.00 | 0.42 |
| 2:H1:262:TYR:CE2 | 2:H1:435:VAL:HG21 | 2.55 | 0.42 |
| 1:H2:135:VAL:O | 1:H2:166:THR:HA | 2.19 | 0.42 |
| 1:H2:240:LEU:HD12 | 1:H2:240:LEU:H | 1.85 | 0.42 |
| 2:H3:165:SER:OG | 2:H3:252:ILE:HD12 | 2.19 | 0.42 |
| 1:H4:242:PHE:CD1 | 1:H4:356:ILE:HG13 | 2.54 | 0.42 |
| 2:H5:50:ASN:O | 2:H5:64:ARG:NH2 | 2.52 | 0.42 |
| 2:H5:98:ASP:OD1 | 2:H5:99:ALA:N | 2.53 | 0.42 |
| 2:H7:205:ASP:OD1 | 2:H7:303:VAL:HG13 | 2.18 | 0.42 |
| 1:H8:170:VAL:HG22 | 1:H8:202:LEU:O | 2.19 | 0.42 |
| 2:H9:137:VAL:HG22 | 2:H9:168:GLY:HA2 | 2.02 | 0.42 |
| 2:H9:331:SER:O | 2:H9:334:THR:N | 2.53 | 0.42 |
| 1:I0:152:ILE:HD12 | 1:I0:164:MET:SD | 2.60 | 0.42 |
| 2:I1:165:SER:HA | 2:I1:199:ASP:OD1 | 2.19 | 0.42 |
| 1:I2:97:ALA:HA | 1:I2:103:LYS:HE3 | 2.02 | 0.42 |
| 2:I3:154:LEU:HD23 | 2:I3:154:LEU:HA | 1.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I4:154:LYS:HA | 1:I4:154:LYS:HD3 | 1.91 | 0.42 |
| 2:I7:139:ASN:O | 2:I7:170:THR:HA | 2.19 | 0.42 |
| 1:I8:97:ALA:HA | 1:I8:103:LYS:HE3 | 2.01 | 0.42 |
| 1:J0:4:ILE:HB | 1:J0:50:TYR:HE1 | 1.84 | 0.42 |
| 1:J0:165:LEU:HD23 | 1:J0:165:LEU:HA | 1.87 | 0.42 |
| 2:J1:18:ASN:HD21 | 2:J1:78:VAL:HG22 | 1.85 | 0.42 |
| 2:J1:73:THR:HG21 | 1:J2:2:ARG:HH22 | 1.85 | 0.42 |
| 2:J1:413:MET:HB3 | 2:J1:417:GLU:OE2 | 2.20 | 0.42 |
| 1:J2:173:PRO:HD2 | 1:J2:380:ARG:NH1 | 2.34 | 0.42 |
| 1:J2:287:PRO:HD3 | 1:J2:325:GLU:OE2 | 2.20 | 0.42 |
| 1:J4:113:ILE:HA | 1:J4:113:ILE:HD13 | 1.84 | 0.42 |
| 1:J6:117:LEU:HD23 | 1:J6:117:LEU:HA | 1.91 | 0.42 |
| 1:J8:5:VAL:HB | 1:J8:133:PHE:HD1 | 1.85 | 0.42 |
| 1:J8:53:GLU:HB2 | 29:7J:372:PHE:HZ | 1.84 | 0.42 |
| 2:K1:36:MET:HA | 2:K1:37:PRO:HD3 | 1.92 | 0.42 |
| 2:K1:392:ASP:CG | 2:K1:425:LEU:HD13 | 2.40 | 0.42 |
| 2:K5:183:GLU:HG3 | 2:K5:184:PRO:HD3 | 2.01 | 0.42 |
| 1:K8:2:ARG:HB3 | 1:K8:131:GLN:HB2 | 2.01 | 0.42 |
| 1:L4:173:PRO:HD2 | 1:L4:380:ARG:CZ | 2.50 | 0.42 |
| 1:L4:294:TRP:CD1 | 1:L4:333:VAL:HG21 | 2.55 | 0.42 |
| 2:L5:26:LEU:HD23 | 2:L5:363:VAL:HG12 | 2.02 | 0.42 |
| 1:L6:189:VAL:HA | 1:L6:192:LEU:HB2 | 2.02 | 0.42 |
| 1:L6:233:MET:O | 1:L6:236:ILE:HG22 | 2.19 | 0.42 |
| 1:L6:272:PRO:O | 1:L6:273:LEU:HD23 | 2.19 | 0.42 |
| 2:L7:70:LEU:HD12 | 2:L7:145:THR:OG1 | 2.20 | 0.42 |
| 2:L9:213:CYS:O | 2:L9:219:ILE:N | 2.52 | 0.42 |
| 1:M0:198:GLU:HB3 | 1:M0:258:ILE:HD11 | 2.02 | 0.42 |
| 2:M1:8:HIS:CD2 | 2:M1:138:PHE:HD2 | 2.37 | 0.42 |
| 2:M1:317:LEU:HB3 | 2:M1:319:TYR:HE1 | 1.85 | 0.42 |
| 1:M2:309:ARG:NH1 | 1:M2:339:SER:O | 2.52 | 0.42 |
| 2:M5:73:THR:HG23 | 1:M6:2:ARG:HH22 | 1.85 | 0.42 |
| 2:M5:93:ILE:HD12 | 2:M5:117:LEU:HD21 | 2.01 | 0.42 |
| 1:M6:77:ARG:HG2 | 1:M6:90:PHE:CE2 | 2.55 | 0.42 |
| 1:M6:165:LEU:HD11 | 1:M6:250:LEU:HD11 | 2.01 | 0.42 |
| 1:M6:396:HIS:CE1 | 1:M6:397:TRP:CE2 | 3.07 | 0.42 |
| 2:M7:66:ILE:O | 2:M7:66:ILE:HG13 | 2.19 | 0.42 |
| 1:M8:273:LEU:H | 1:M8:292:GLN:HE22 | 1.66 | 0.42 |
| 1:N0:95:THR:HG23 | 1:N0:96:GLY:N | 2.35 | 0.42 |
| 1:N2:314:SER:HA | 1:N2:350:LYS:O | 2.20 | 0.42 |
| 2:N5:21:TRP:CZ3 | 2:N5:63:PRO:HB3 | 2.55 | 0.42 |
| 2:N5:274:PRO:HG3 | 2:N5:286:LEU:HD11 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N7:125:LEU:HD23 | 2:N7:125:LEU:HA | 1.84 | 0.42 |
| 1:O0:179:VAL:HB | 2:O1:258:ASN:HD22 | 1.83 | 0.42 |
| 2:O1:217:LEU:HG | 2:O1:275:ILE:HG22 | 2.00 | 0.42 |
| 2:O1:407:TRP:CD1 | 1:O2:255:VAL:HG23 | 2.54 | 0.42 |
| 2:O3:21:TRP:CZ2 | 2:O3:65:CYS:HB2 | 2.54 | 0.42 |
| 2:O3:90:GLU:HB3 | 2:O3:121:ARG:CZ | 2.49 | 0.42 |
| 1:O4:165:LEU:HD11 | 1:O4:250:LEU:HD23 | 2.02 | 0.42 |
| 1:O4:360:GLY:HA2 | 19:6E:77:GLN:HG2 | 2.01 | 0.42 |
| 1:O4:361:LEU:HD22 | 19:6E:73:HIS:HD2 | 1.84 | 0.42 |
| 1:O6:403:MET:HE3 | 1:O6:403:MET:HB2 | 1.69 | 0.42 |
| 2:O7:331:SER:O | 2:O7:334:THR:OG1 | 2.30 | 0.42 |
| 1:O8:138:SER:HA | 1:O8:169:VAL:HG22 | 2.02 | 0.42 |
| 1:O8:344:TRP:CE3 | 1:O8:345:ILE:HG13 | 2.54 | 0.42 |
| 2:O9:66:ILE:O | 2:O9:66:ILE:HG13 | 2.19 | 0.42 |
| 2:O9:188:VAL:HG21 | 2:O9:395:PHE:CE1 | 2.54 | 0.42 |
| 2:P3:274:PRO:CB | 2:P3:286:LEU:HD11 | 2.50 | 0.42 |
| 1:P4:121:ARG:O | 1:P4:125:GLU:HG2 | 2.20 | 0.42 |
| 2:P5:27:GLU:CD | 2:P5:243:ARG:HH12 | 2.23 | 0.42 |
| 2:P5:88:HIS:CG | 2:P5:89:PRO:CD | 3.01 | 0.42 |
| 2:P5:155:GLU:CD | 2:P5:197:HIS:HE1 | 2.23 | 0.42 |
| 2:P5:205:ASP:O | 2:P5:209:ILE:HG13 | 2.19 | 0.42 |
| 1:P6:213:ARG:HE | 1:P6:297:LYS:HZ2 | 1.67 | 0.42 |
| 1:P8:141:GLY:HA3 | 39:P8:502:GDP:PB | 2.60 | 0.42 |
| 1:P8:198:GLU:HA | 1:P8:264:HIS:HB2 | 2.02 | 0.42 |
| 1:Q0:5:VAL:CG2 | 1:Q0:133:PHE:HD1 | 2.32 | 0.42 |
| 1:Q2:183:TYR:O | 1:Q2:187:LEU:HD13 | 2.19 | 0.42 |
| 1:Q6:183:TYR:O | 1:Q6:187:LEU:HD13 | 2.20 | 0.42 |
| 1:Q8:21:TRP:O | 1:Q8:25:SER:OG | 2.34 | 0.42 |
| 2:Q9:279:GLU:HA | 7:4Q:336:GLN:NE2 | 2.35 | 0.42 |
| 1:R0:5:VAL:CG1 | 1:R0:133:PHE:HD1 | 2.32 | 0.42 |
| 2:R1:217:LEU:HD21 | 2:R1:368:LEU:HD23 | 2.02 | 0.42 |
| 1:R2:70:PRO:HG2 | 2:R3:2:ARG:NH1 | 2.35 | 0.42 |
| 1:R4:325:GLU:O | 1:R4:329:GLN:HG2 | 2.20 | 0.42 |
| 1:R4:362:LYS:HE3 | 1:R4:362:LYS:HB3 | 1.83 | 0.42 |
| 2:R5:116:ASP:OD1 | 2:R5:117:LEU:N | 2.53 | 0.42 |
| 2:R5:118:ALA:O | 2:R5:122:ILE:HG13 | 2.20 | 0.42 |
| 2:R5:156:ARG:HA | 2:R5:159:VAL:HG12 | 2.00 | 0.42 |
| 1:R6:172:SER:OG | 1:R6:173:PRO:HD2 | 2.20 | 0.42 |
| 1:S0:417:ASP:OD1 | 1:S0:418:LEU:N | 2.52 | 0.42 |
| 1:S2:377:MET:HG3 | 1:S2:378:PHE:N | 2.34 | 0.42 |
| 1:S4:228:LEU:O | 1:S4:232:VAL:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S4:251:ARG:O | 1:S4:255:VAL:HG22 | 2.19 | 0.42 |
| 1:S6:240:LEU:HD11 | 1:S6:250:LEU:HD13 | 2.02 | 0.42 |
| 1:T0:211:CYS:HB3 | 1:T0:220:PRO:HB3 | 2.01 | 0.42 |
| 1:T0:237:THR:HG23 | 1:T0:241:ARG:HE | 1.84 | 0.42 |
| 1:T2:28:HIS:CG | 1:T2:47:ILE:HG22 | 2.54 | 0.42 |
| 1:T2:192:LEU:HD23 | 1:T2:192:LEU:HA | 1.80 | 0.42 |
| 2:T3:271:SER:HB3 | 2:T3:301:MET:HA | 2.02 | 0.42 |
| 1:T4:174:LYS:HG3 | 1:T4:380:ARG:NH2 | 2.34 | 0.42 |
| 2:T5:9:ILE:HD13 | 2:T5:150:GLY:HA2 | 2.01 | 0.42 |
| 2:T5:260:VAL:HG23 | 2:T5:260:VAL:O | 2.20 | 0.42 |
| 1:T6:135:VAL:HG12 | 1:T6:165:LEU:O | 2.19 | 0.42 |
| 1:T6:204:ASN:ND2 | 39:T6:502:GDP:HN22 | 2.17 | 0.42 |
| 1:T6:233:MET:O | 1:T6:237:THR:HG22 | 2.20 | 0.42 |
| 2:T7:14:ILE:HD11 | 2:T7:74:VAL:HG22 | 2.02 | 0.42 |
| 1:T8:86:ARG:NH2 | 1:T8:88:ASP:OD2 | 2.52 | 0.42 |
| 1:T8:301:CYS:SG | 1:T8:302:ALA:N | 2.92 | 0.42 |
| 2:U5:222:PRO:CD | 1:U6:324:LYS:HE3 | 2.49 | 0.42 |
| 2:U5:236:SER:O | 2:U5:243:ARG:NH2 | 2.53 | 0.42 |
| 1:U8:179:VAL:HG23 | 2:U9:349:THR:O | 2.19 | 0.42 |
| 1:U8:220:PRO:HD2 | 2:U9:326:LYS:HD3 | 2.00 | 0.42 |
| 1:V0:6:HIS:CE1 | 1:V0:8:GLN:HG2 | 2.54 | 0.42 |
| 1:V0:285:THR:OG1 | 1:V0:287:PRO:HD2 | 2.19 | 0.42 |
| 2:V1:6:SER:OG | 2:V1:8:HIS:HE1 | 2.03 | 0.42 |
| 2:V1:75:VAL:HG11 | 2:V1:94:SER:HB2 | 2.01 | 0.42 |
| 1:V4:379:LYS:O | 1:V4:383:GLU:HG2 | 2.19 | 0.42 |
| 1:V6:134:GLN:HE22 | 1:V6:237:THR:HG21 | 1.85 | 0.42 |
| 2:V7:139:ASN:N | 2:V7:139:ASN:OD1 | 2.52 | 0.42 |
| 1:V8:173:PRO:HG2 | 1:V8:174:LYS:NZ | 2.34 | 0.42 |
| 1:V8:287:PRO:HD3 | 1:V8:325:GLU:OE1 | 2.20 | 0.42 |
| 2:V9:112:LYS:HD3 | 2:V9:112:LYS:HA | 1.77 | 0.42 |
| 2:V9:211:ASP:CG | 2:V9:215:ARG:HH12 | 2.23 | 0.42 |
| 2:W1:102:ASN:HB3 | 2:W1:105:ARG:HB3 | 2.01 | 0.42 |
| 1:W2:221:THR:OG1 | 1:W2:222:PHE:N | 2.53 | 0.42 |
| 2:W3:73:THR:HA | 1:W4:46:ARG:HH21 | 1.84 | 0.42 |
| 1:X2:49:VAL:HG23 | 1:X2:50:TYR:CD1 | 2.55 | 0.42 |
| 1:X4:181:GLU:OE1 | 1:X4:181:GLU:HA | 2.20 | 0.42 |
| 1:X4:244:GLY:HA2 | 1:X4:355:ASP:CG | 2.39 | 0.42 |
| 2:X7:167:LEU:HG | 2:X7:252:ILE:HD11 | 2.02 | 0.42 |
| 2:X9:195:LEU:HD23 | 2:X9:195:LEU:HA | 1.76 | 0.42 |
| 1:Y0:30:ILE:HG13 | 1:Y0:35:THR:O | 2.20 | 0.42 |
| 2:Y1:90:GLU:HB3 | 2:Y1:121:ARG:HH22 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y1:121:ARG:HD2 | 2:Y1:124:LYS:HE3 | 2.01 | 0.42 |
| 1:Y2:208:TYR:CE1 | 1:Y2:225:LEU:HD11 | 2.55 | 0.42 |
| 1:Y4:221:THR:OG1 | 1:Y4:222:PHE:N | 2.53 | 0.42 |
| 1:Y4:284:LEU:HD23 | 1:Y4:284:LEU:HA | 1.89 | 0.42 |
| 1:Y4:322:SER:OG | 1:Y4:325:GLU:OE1 | 2.36 | 0.42 |
| 1:Y8:237:THR:HG23 | 1:Y8:241:ARG:HE | 1.85 | 0.42 |
| 1:Z2:70:PRO:HG2 | 2:Z3:2:ARG:NH1 | 2.34 | 0.42 |
| 1:Z2:91:VAL:HG11 | 1:Z2:116:VAL:HG22 | 2.02 | 0.42 |
| 2:Z3:188:VAL:HG23 | 2:Z3:189:LEU:HD12 | 2.01 | 0.42 |
| 1:Z6:58:ARG:HH11 | 1:Z6:84:ILE:HA | 1.84 | 0.42 |
| 1:Z8:130:LEU:HD23 | 1:Z8:162:ARG:HG3 | 2.02 | 0.42 |
| 2:Z9:325:PRO:HA | 2:Z9:328:VAL:HG12 | 2.02 | 0.42 |
| 2:0B:90:GLU:H | 2:0R:283:HIS:CE1 | 2.37 | 0.42 |
| 2:0F:280:LYS:HA | 2:0F:283:HIS:HB3 | 2.02 | 0.42 |
| 2:0F:332:VAL:HA | 2:0F:335:ILE:HG22 | 2.00 | 0.42 |
| 2:0H:209:ILE:HG21 | 2:0H:227:LEU:HG | 2.02 | 0.42 |
| 1:0I:3:GLU:HA | 1:0I:49:VAL:HG23 | 2.00 | 0.42 |
| 1:0I:162:ARG:HA | 1:0I:162:ARG:HD3 | 1.87 | 0.42 |
| 2:0J:54:SER:O | 2:0J:61:HIS:HA | 2.20 | 0.42 |
| 1:0K:317:PHE:HE2 | 1:0K:326:VAL:HG13 | 1.84 | 0.42 |
| 2:0L:103:PHE:N | 2:0L:186:ASN:OD1 | 2.53 | 0.42 |
| 2:0L:261:PRO:HG3 | 2:0L:346:TRP:HH2 | 1.84 | 0.42 |
| 2:0L:288:VAL:O | 2:0L:292:THR:OG1 | 2.29 | 0.42 |
| 2:0N:166:LYS:HE2 | 2:0N:166:LYS:HB2 | 1.92 | 0.42 |
| 2:0N:280:LYS:HA | 2:0N:283:HIS:HB3 | 2.02 | 0.42 |
| 2:0N:330:ALA:O | 2:0N:334:THR:HG23 | 2.20 | 0.42 |
| 1:0O:207:LEU:HD13 | 1:0O:225:LEU:HB3 | 2.01 | 0.42 |
| 1:0Q:179:VAL:HB | 2:0R:258:ASN:HD22 | 1.84 | 0.42 |
| 2:0R:154:LEU:HD12 | 2:0R:154:LEU:HA | 1.87 | 0.42 |
| 1:0S:374:ILE:HG13 | 1:0S:377:MET:CE | 2.49 | 0.42 |
| 1:0U:393:ALA:O | 1:0U:395:LEU:N | 2.53 | 0.42 |
| 2:0V:231:ILE:O | 2:0V:235:ILE:HG12 | 2.19 | 0.42 |
| 1:1A:389:PHE:O | 1:1A:392:LYS:NZ | 2.32 | 0.42 |
| 2:1D:237:SER:HA | 2:1D:320:ARG:HD2 | 2.01 | 0.42 |
| 1:1E:12:CYS:SG | 1:1E:13:GLY:N | 2.93 | 0.42 |
| 1:1E:138:SER:OG | 1:1E:139:LEU:N | 2.52 | 0.42 |
| 1:1K:152:ILE:HD13 | 1:1K:152:ILE:HA | 1.88 | 0.42 |
| 1:1K:173:PRO:HA | 1:1K:176:SER:HB3 | 2.01 | 0.42 |
| 1:1K:208:TYR:HE1 | 1:1K:225:LEU:HD21 | 1.85 | 0.42 |
| 2:1L:165:SER:HB2 | 2:1L:199:ASP:OD2 | 2.19 | 0.42 |
| 2:1L:287:SER:H | 2:1L:290:GLU:CD | 2.17 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1L:317:LEU:HB3 | 2:1L:319:TYR:CE1 | 2.54 | 0.42 |
| 2:1L:331:SER:O | 2:1L:334:THR:OG1 | 2.25 | 0.42 |
| 1:1M:390:ARG:HE | 1:1M:390:ARG:HB2 | 1.60 | 0.42 |
| 1:1M:421:GLU:HA | 1:1M:424:GLN:HB3 | 2.00 | 0.42 |
| 2:1N:88:HIS:HB3 | 2:1N:91:GLN:CG | 2.48 | 0.42 |
| 1:1Q:280:GLN:HE21 | 9:4Z:193:LEU:HD23 | 1.84 | 0.42 |
| 1:1S:314:SER:HA | 1:1S:350:LYS:O | 2.20 | 0.42 |
| 2:1V:109:THR:OG1 | 2:1V:411:GLU:OE2 | 2.35 | 0.42 |
| 1:1W:39:ASP:OD1 | 1:1W:39:ASP:N | 2.46 | 0.42 |
| 2:1X:417:GLU:OE1 | 2:1X:417:GLU:N | 2.44 | 0.42 |
| 2:1Z:156:ARG:NH2 | 38:7Z:29:GLY:O | 2.52 | 0.42 |
| 2:1Z:238:LEU:HD12 | 2:1Z:238:LEU:HA | 1.84 | 0.42 |
| 2:1Z:335:ILE:HA | 2:1Z:338:LYS:HG2 | 2.00 | 0.42 |
| 1:2A:14:ASN:HD22 | 1:2A:65:LEU:HD22 | 1.84 | 0.42 |
| 1:2A:27:GLU:HA | 1:2A:359:LYS:CD | 2.49 | 0.42 |
| 2:2B:72:PRO:HD2 | 1:2C:2:ARG:NH1 | 2.35 | 0.42 |
| 1:2C:116:VAL:HA | 1:2C:119:VAL:HG12 | 2.01 | 0.42 |
| 1:2C:174:LYS:HE2 | 1:2C:174:LYS:HB3 | 1.74 | 0.42 |
| 1:2C:233:MET:O | 1:2C:237:THR:HG22 | 2.19 | 0.42 |
| 2:2L:50:ASN:O | 2:2L:64:ARG:NH2 | 2.52 | 0.42 |
| 1:2M:114:ASP:OD2 | 38:8D:101:ASP:HA | 2.20 | 0.42 |
| 1:2M:203:ASP:O | 1:2M:207:LEU:HD23 | 2.20 | 0.42 |
| 1:2M:256:ASN:O | 1:2M:312:THR:HG21 | 2.19 | 0.42 |
| 2:2N:88:HIS:CG | 2:3D:283:HIS:HA | 2.54 | 0.42 |
| 2:2P:239:THR:HG23 | 2:2P:243:ARG:HH21 | 1.85 | 0.42 |
| 2:2R:181:VAL:HG23 | 2:2R:182:VAL:HG13 | 2.00 | 0.42 |
| 2:2R:246:GLY:HA3 | 2:2R:356:ASN:HA | 2.02 | 0.42 |
| 1:2S:311:LEU:HD23 | 1:2S:311:LEU:HA | 1.74 | 0.42 |
| 1:2U:31:ASP:OD2 | 1:2U:35:THR:OG1 | 2.38 | 0.42 |
| 1:2U:98:GLY:HA2 | 2:2V:254:GLU:OE1 | 2.20 | 0.42 |
| 1:2U:337:ASN:CG | 38:8B:97:PHE:HA | 2.39 | 0.42 |
| 2:2V:391:LEU:HD23 | 2:2V:391:LEU:HA | 1.82 | 0.42 |
| 1:3A:107:THR:OG1 | 1:3A:108:GLU:OE1 | 2.21 | 0.42 |
| 2:3B:47:ASP:HB2 | 38:8D:218:PRO:HD3 | 2.01 | 0.42 |
| 2:3B:76:ASP:O | 2:3B:80:THR:HG22 | 2.20 | 0.42 |
| 1:3C:213:ARG:HH12 | 38:8D:104:LYS:HE2 | 1.83 | 0.42 |
| 1:3G:152:ILE:HD12 | 1:3G:164:MET:SD | 2.60 | 0.42 |
| 2:3J:220:GLU:CG | 38:8B:177:HIS:HB3 | 2.49 | 0.42 |
| 1:3K:309:ARG:H | 1:3K:372:THR:HG22 | 1.85 | 0.42 |
| 2:3L:133:GLN:HB3 | 2:3L:252:ILE:HG21 | 2.01 | 0.42 |
| 1:3M:2:ARG:HB3 | 1:3M:131:GLN:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3Q:77:ARG:NH1 | 3:4H:18:LYS:C | 2.73 | 0.42 |
| 2:3R:28:HIS:CE1 | 2:3R:49:PHE:HA | 2.54 | 0.42 |
| 2:3R:111:GLY:HA2 | 2:3R:114:ILE:HG22 | 2.02 | 0.42 |
| 2:3R:209:ILE:HG23 | 2:3R:230:LEU:HD11 | 2.02 | 0.42 |
| 1:3S:309:ARG:H | 1:3S:372:THR:HG22 | 1.84 | 0.42 |
| 1:3S:418:LEU:O | 1:3S:421:GLU:HG2 | 2.20 | 0.42 |
| 2:3T:173:PRO:HB3 | 2:3T:183:GLU:HG2 | 2.02 | 0.42 |
| 3:4D:9:LEU:HD22 | 3:4D:173:ARG:HH11 | 1.84 | 0.42 |
| 5:4L:367:GLN:O | 5:4L:371:ILE:HG13 | 2.20 | 0.42 |
| 10:5C:250:LYS:O | 10:5C:254:MET:HG2 | 2.19 | 0.42 |
| 12:5F:43:HIS:NE2 | 12:5F:53:HIS:HB2 | 2.34 | 0.42 |
| 12:5F:288:ARG:HD3 | 12:5F:288:ARG:HA | 1.67 | 0.42 |
| 13:5H:61:LEU:HD12 | 13:5H:67:LYS:HD3 | 2.00 | 0.42 |
| 13:5K:61:LEU:HD12 | 13:5K:67:LYS:HD3 | 2.00 | 0.42 |
| 14:5L:12:GLY:HA2 | 14:5L:338:ALA:CB | 2.49 | 0.42 |
| 14:5L:111:PHE:C | 14:5L:155:PHE:HD2 | 2.22 | 0.42 |
| 14:5M:12:GLY:HA2 | 14:5M:338:ALA:CB | 2.49 | 0.42 |
| 14:5M:416:ILE:O | 14:5M:416:ILE:HG23 | 2.19 | 0.42 |
| 14:5N:127:ASN:HB2 | 38:8D:227:LYS:HZ1 | 1.83 | 0.42 |
| 14:5N:384:GLU:OE2 | 14:5N:385:CYS:N | 2.53 | 0.42 |
| 15:5P:23:LYS:HB2 | 15:5P:40:ILE:HD12 | 2.00 | 0.42 |
| 15:5P:178:PRO:HG2 | 15:5P:183:GLN:HE22 | 1.85 | 0.42 |
| 16:5Q:56:ASP:OD2 | 16:5Q:56:ASP:C | 2.57 | 0.42 |
| 17:5T:179:GLN:HE21 | 17:5T:179:GLN:HB3 | 1.49 | 0.42 |
| 20:6F:13:ILE:HD12 | 20:6F:13:ILE:HA | 1.86 | 0.42 |
| 20:6F:56:GLU:HG2 | 20:6F:296:LYS:HD3 | 2.01 | 0.42 |
| 22:6K:168:THR:HA | 22:6K:171:GLU:CD | 2.39 | 0.42 |
| 22:6N:16:LYS:HD3 | 22:6N:20:TYR:CE2 | 2.55 | 0.42 |
| 22:6N:171:GLU:HA | 22:6N:174:GLU:OE1 | 2.19 | 0.42 |
| 22:6O:276:LEU:HD12 | 22:6O:276:LEU:HA | 1.81 | 0.42 |
| 22:6P:266:LYS:O | 22:6P:269:GLU:HG3 | 2.20 | 0.42 |
| 24:6T:400:LEU:HD23 | 24:6T:400:LEU:H | 1.83 | 0.42 |
| 24:6U:469:PHE:CD2 | 24:6U:482:ILE:HG23 | 2.53 | 0.42 |
| 24:6V:460:HIS:HB2 | 24:6V:465:LEU:HD22 | 2.02 | 0.42 |
| 24:6V:629:PHE:CZ | 24:6V:633:LEU:HD11 | 2.55 | 0.42 |
| 24:6W:8:ILE:HA | 24:6W:9:PRO:HD3 | 1.92 | 0.42 |
| 24:6W:273:LEU:HA | 24:6W:375:THR:HG22 | 2.01 | 0.42 |
| 24:6W:345:ASP:OD1 | 24:6W:346:GLN:N | 2.53 | 0.42 |
| 24:6Y:93:ARG:HD2 | 26:7F:48:LEU:HB2 | 2.01 | 0.42 |
| 24:6Y:198:GLU:HG2 | 24:6Y:198:GLU:O | 2.19 | 0.42 |
| 24:6Y:460:HIS:HB2 | 24:6Y:465:LEU:HD22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Z:138:ASP:OD1 | 24:6Z:139:ASN:N | 2.51 | 0.42 |
| 29:7J:333:THR:O | 29:7J:337:ARG:HG2 | 2.20 | 0.42 |
| 30:7K:243:LEU:HD23 | 30:7K:243:LEU:HA | 1.90 | 0.42 |
| 30:7L:399:LEU:HB2 | 30:7L:403:ASP:OD2 | 2.19 | 0.42 |
| 37:7Y:126:LYS:HB3 | 37:7Y:212:TRP:NE1 | 2.35 | 0.42 |
| 1:C6:320:ARG:NH2 | 18:5X:186:LYS:O | 2.52 | 0.42 |
| 2:E1:282:TYR:HE2 | 22:6I:83:TRP:HE1 | 1.66 | 0.42 |
| 1:G0:212:PHE:CZ | 2:G1:326:LYS:HG3 | 2.54 | 0.42 |
| 2:G1:317:LEU:HA | 2:G1:317:LEU:HD23 | 1.85 | 0.42 |
| 1:G2:318:ARG:HD3 | 1:G2:358:PRO:HD3 | 2.02 | 0.42 |
| 2:G5:203:MET:HE3 | 2:G5:267:PHE:HB3 | 2.01 | 0.42 |
| 2:G7:14:ILE:HD11 | 2:G7:69:ASP:HB2 | 2.02 | 0.42 |
| 2:G7:296:PHE:HE1 | 2:G7:377:MET:HG3 | 1.84 | 0.42 |
| 2:G9:181:VAL:HG23 | 2:G9:182:VAL:HG13 | 2.02 | 0.42 |
| 2:G9:189:LEU:HD11 | 2:G9:418:PHE:CZ | 2.55 | 0.42 |
| 2:G9:290:GLU:HA | 2:G9:293:ASN:HD22 | 1.85 | 0.42 |
| 1:H2:91:VAL:CG1 | 1:H2:116:VAL:HG12 | 2.49 | 0.42 |
| 1:H4:122:LYS:NZ | 1:J0:291:GLN:HB3 | 2.35 | 0.42 |
| 2:H7:223:THR:HG23 | 2:H7:225:THR:H | 1.84 | 0.42 |
| 1:I4:117:LEU:HA | 1:I4:120:VAL:HG12 | 2.02 | 0.42 |
| 2:I5:99:ALA:HB2 | 2:I5:110:ILE:HD11 | 2.01 | 0.42 |
| 2:I5:193:SER:HB2 | 2:I5:197:HIS:ND1 | 2.35 | 0.42 |
| 2:I7:237:SER:HA | 2:I7:320:ARG:HD2 | 2.02 | 0.42 |
| 2:I9:178:SER:HB3 | 2:I9:183:GLU:OE2 | 2.19 | 0.42 |
| 1:J0:175:VAL:HB | 2:J1:329:ASN:HD21 | 1.85 | 0.42 |
| 2:J1:33:ASP:HA | 2:J1:85:GLN:HB2 | 2.01 | 0.42 |
| 1:J4:135:VAL:O | 1:J4:166:THR:HA | 2.19 | 0.42 |
| 1:J4:357:PRO:HG2 | 16:5Q:14:PRO:HB3 | 2.02 | 0.42 |
| 2:J5:271:SER:OG | 2:J5:377:MET:HB3 | 2.19 | 0.42 |
| 2:J5:420:GLU:O | 2:J5:423:GLU:HG3 | 2.19 | 0.42 |
| 2:J7:218:ASP:OD2 | 2:J7:280:LYS:HE2 | 2.14 | 0.42 |
| 2:J7:274:PRO:HG3 | 2:J7:286:LEU:HD21 | 2.00 | 0.42 |
| 1:K0:169:VAL:HG23 | 1:K0:203:ASP:HA | 2.02 | 0.42 |
| 2:K1:388:PHE:HD2 | 2:K1:432:PHE:HE2 | 1.66 | 0.42 |
| 2:K3:100:ALA:HA | 1:K4:252:LYS:HE3 | 2.01 | 0.42 |
| 1:K4:201:VAL:HG12 | 1:K4:266:PHE:O | 2.20 | 0.42 |
| 1:K4:272:PRO:HB2 | 1:K4:282:ARG:HH12 | 1.84 | 0.42 |
| 1:K4:354:CYS:SG | 1:K4:355:ASP:N | 2.92 | 0.42 |
| 1:K8:116:VAL:O | 1:K8:120:VAL:HG12 | 2.19 | 0.42 |
| 1:L0:117:LEU:HA | 1:L0:117:LEU:HD23 | 1.79 | 0.42 |
| 1:L0:237:THR:O | 1:L0:237:THR:HG22 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L3:238:LEU:HD12 | 2:L3:239:THR:HG23 | 2.02 | 0.42 |
| 1:L4:339:SER:H | 35:7U:147:ASN:HD21 | 1.66 | 0.42 |
| 1:L4:397:TRP:CZ2 | 2:L5:256:GLN:HB3 | 2.55 | 0.42 |
| 2:L5:63:PRO:HG2 | 2:L5:87:PHE:CE1 | 2.55 | 0.42 |
| 1:L6:68:LEU:HB3 | 1:L6:96:GLY:HA2 | 2.01 | 0.42 |
| 1:L6:165:LEU:HD13 | 1:L6:250:LEU:HD11 | 2.02 | 0.42 |
| 2:L7:105:ARG:O | 2:L7:110:ILE:HG12 | 2.20 | 0.42 |
| 1:M0:232:VAL:HG11 | 1:M0:268:VAL:HG11 | 2.02 | 0.42 |
| 1:M0:274:THR:HG21 | 1:M0:282:ARG:HD2 | 2.02 | 0.42 |
| 1:M0:403:MET:HE2 | 1:M0:403:MET:HB2 | 1.84 | 0.42 |
| 2:M3:326:LYS:HG3 | 2:M3:327:ASP:N | 2.35 | 0.42 |
| 1:M4:114:ASP:N | 1:M4:114:ASP:OD1 | 2.53 | 0.42 |
| 1:M4:120:VAL:HG11 | 1:M4:155:ILE:HD11 | 2.02 | 0.42 |
| 2:M5:209:ILE:HD13 | 2:M5:231:ILE:HD11 | 2.01 | 0.42 |
| 2:M9:345:ASP:OD1 | 2:M9:346:TRP:N | 2.53 | 0.42 |
| 1:N0:145:SER:OG | 1:N0:146:GLY:N | 2.53 | 0.42 |
| 2:N1:74:VAL:O | 2:N1:78:VAL:HG23 | 2.19 | 0.42 |
| 2:N3:105:ARG:HG2 | 2:N3:105:ARG:HH11 | 1.83 | 0.42 |
| 2:N3:245:ASP:N | 2:N3:245:ASP:OD1 | 2.47 | 0.42 |
| 2:N5:245:ASP:N | 32:7O:87:ASP:OD1 | 2.53 | 0.42 |
| 2:N7:157:LEU:HD23 | 2:N7:157:LEU:HA | 1.85 | 0.42 |
| 2:N7:191:THR:HA | 2:N7:194:LEU:HB3 | 2.01 | 0.42 |
| 2:N9:266:HIS:ND1 | 2:N9:266:HIS:O | 2.52 | 0.42 |
| 2:N9:306:ASP:OD2 | 2:N9:308:ARG:HB2 | 2.20 | 0.42 |
| 2:O1:119:LEU:HA | 2:O1:122:ILE:HG12 | 2.01 | 0.42 |
| 2:O5:120:ASP:OD1 | 2:O5:121:ARG:N | 2.53 | 0.42 |
| 2:O5:396:ASP:CG | 2:O5:422:ARG:HE | 2.22 | 0.42 |
| 2:O9:88:HIS:O | 2:O9:90:GLU:N | 2.53 | 0.42 |
| 1:P4:48:ASN:O | 1:P4:62:ARG:NH1 | 2.48 | 0.42 |
| 2:P9:258:ASN:C | 2:P9:259:LEU:HD12 | 2.40 | 0.42 |
| 2:Q3:47:ASP:HB2 | 32:7P:216:LYS:HB3 | 2.02 | 0.42 |
| 2:Q3:320:ARG:HE | 2:Q3:320:ARG:HB3 | 1.64 | 0.42 |
| 1:Q4:8:GLN:CD | 1:Q4:17:GLY:HA3 | 2.40 | 0.42 |
| 1:Q4:217:LEU:HD22 | 20:6F:184:ARG:NH1 | 2.34 | 0.42 |
| 1:Q4:344:TRP:CE3 | 1:Q4:345:ILE:HG13 | 2.55 | 0.42 |
| 1:Q6:39:ASP:OD1 | 1:Q6:39:ASP:N | 2.45 | 0.42 |
| 1:Q8:318:ARG:HB3 | 1:Q8:357:PRO:HA | 2.02 | 0.42 |
| 2:Q9:132:LEU:O | 2:Q9:164:LYS:NZ | 2.45 | 0.42 |
| 1:R0:309:ARG:O | 1:R0:372:THR:HG22 | 2.20 | 0.42 |
| 1:R0:391:ARG:HD2 | 2:R1:346:TRP:CG | 2.55 | 0.42 |
| 1:R2:172:SER:HB3 | 1:R2:175:VAL:CG2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R2:178:THR:HG22 | 1:R2:180:VAL:H | 1.84 | 0.42 |
| 1:R2:396:HIS:CD2 | 1:R2:396:HIS:H | 2.37 | 0.42 |
| 2:R3:223:THR:OG1 | 2:R3:224:TYR:N | 2.53 | 0.42 |
| 2:R5:245:ASP:OD1 | 2:R5:245:ASP:N | 2.51 | 0.42 |
| 2:R7:137:VAL:HG22 | 2:R7:168:GLY:HA2 | 2.02 | 0.42 |
| 2:R7:170:THR:HG21 | 2:R7:194:LEU:HD11 | 2.01 | 0.42 |
| 2:S1:183:GLU:HG3 | 2:S1:184:PRO:HD3 | 2.02 | 0.42 |
| 1:S6:178:THR:HG22 | 2:S7:352:LYS:HE2 | 2.01 | 0.42 |
| 1:S6:252:LYS:HE3 | 1:S6:350:LYS:HE2 | 2.02 | 0.42 |
| 1:S8:176:SER:O | 1:S8:176:SER:OG | 2.33 | 0.42 |
| 1:T2:138:SER:OG | 1:T2:139:LEU:N | 2.53 | 0.42 |
| 2:T5:176:GLN:NE2 | 2:T5:207:GLU:OE2 | 2.52 | 0.42 |
| 2:T5:320:ARG:HE | 2:T5:320:ARG:HB3 | 1.64 | 0.42 |
| 1:T6:207:LEU:HD23 | 1:T6:207:LEU:HA | 1.84 | 0.42 |
| 2:T7:139:ASN:N | 2:T7:139:ASN:OD1 | 2.53 | 0.42 |
| 2:T7:157:LEU:HA | 2:T7:157:LEU:HD23 | 1.74 | 0.42 |
| 2:U5:76:ASP:O | 2:U5:80:THR:HG22 | 2.19 | 0.42 |
| 1:U6:50:TYR:HD1 | 1:U6:50:TYR:HA | 1.62 | 0.42 |
| 1:U6:138:SER:OG | 1:U6:139:LEU:N | 2.52 | 0.42 |
| 1:U6:220:PRO:HD2 | 2:U7:326:LYS:HD3 | 2.02 | 0.42 |
| 2:U7:9:ILE:HG22 | 2:U7:146:GLY:HA2 | 2.01 | 0.42 |
| 1:U8:8:GLN:NE2 | 1:U8:17:GLY:HA3 | 2.35 | 0.42 |
| 1:U8:273:LEU:H | 1:U8:292:GLN:HE22 | 1.67 | 0.42 |
| 1:V0:173:PRO:HG2 | 1:V0:174:LYS:HE2 | 2.01 | 0.42 |
| 1:V0:362:LYS:HB3 | 1:V0:362:LYS:HE3 | 1.80 | 0.42 |
| 2:V1:222:PRO:CD | 1:V2:324:LYS:HE3 | 2.49 | 0.42 |
| 1:V6:2:ARG:NH2 | 1:V6:131:GLN:HG3 | 2.33 | 0.42 |
| 1:V6:167:PHE:CZ | 1:V6:236:ILE:HD11 | 2.54 | 0.42 |
| 1:V6:186:THR:HG22 | 1:V6:411:ALA:HB1 | 2.01 | 0.42 |
| 2:V9:35:GLN:N | 2:V9:35:GLN:OE1 | 2.53 | 0.42 |
| 2:V9:213:CYS:HA | 2:V9:217:LEU:HB2 | 2.01 | 0.42 |
| 2:V9:413:MET:HB3 | 2:V9:417:GLU:OE2 | 2.19 | 0.42 |
| 2:W1:186:ASN:OD1 | 2:W1:408:TYR:OH | 2.36 | 0.42 |
| 2:W3:55:GLU:HG2 | 2:W3:61:HIS:CE1 | 2.55 | 0.42 |
| 2:W3:103:PHE:CE1 | 2:W3:148:GLY:HA2 | 2.55 | 0.42 |
| 2:W3:286:LEU:O | 2:W3:373:ARG:NH1 | 2.53 | 0.42 |
| 2:W5:154:LEU:HG | 2:W5:197:HIS:HB3 | 2.01 | 0.42 |
| 1:W6:271:THR:HG22 | 1:W6:289:LEU:HG | 2.01 | 0.42 |
| 2:W7:35:GLN:OE1 | 2:W7:35:GLN:N | 2.53 | 0.42 |
| 2:W7:237:SER:OG | 2:W7:376:CYS:SG | 2.75 | 0.42 |
| 1:W8:22:GLU:HG2 | 1:W8:81:TYR:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W8:86:ARG:HB3 | 1:W8:89:ASN:OD1 | 2.19 | 0.42 |
| 2:W9:84:ARG:CG | 2:W9:84:ARG:NH1 | 2.82 | 0.42 |
| 1:X0:144:GLY:N | 39:X0:502:GDP:O1B | 2.51 | 0.42 |
| 1:X2:141:GLY:HA3 | 39:X2:501:GDP:O3A | 2.20 | 0.42 |
| 1:X2:322:SER:O | 1:X2:326:VAL:HG23 | 2.19 | 0.42 |
| 1:X4:208:TYR:CE1 | 1:X4:225:LEU:HD11 | 2.55 | 0.42 |
| 1:X4:359:LYS:HE2 | 8:4V:452:LEU:HB3 | 2.00 | 0.42 |
| 1:X6:210:ILE:HD13 | 1:X6:210:ILE:HA | 1.91 | 0.42 |
| 2:Y3:180:ALA:HB3 | 2:Y3:183:GLU:HG3 | 2.02 | 0.42 |
| 2:Y3:290:GLU:OE1 | 2:Y3:290:GLU:N | 2.39 | 0.42 |
| 2:Y5:70:LEU:HD11 | 2:Y5:110:ILE:HG12 | 2.02 | 0.42 |
| 2:Y5:225:THR:HG22 | 2:Y5:229:ARG:HE | 1.85 | 0.42 |
| 1:Y6:156:ARG:HA | 1:Y6:156:ARG:HD2 | 1.90 | 0.42 |
| 1:Y8:304:ASP:HB3 | 1:Y8:307:HIS:CG | 2.53 | 0.42 |
| 1:Y8:392:LYS:HD2 | 1:Y8:395:LEU:HD12 | 2.01 | 0.42 |
| 1:Z0:12:CYS:O | 1:Z0:16:ILE:HG22 | 2.20 | 0.42 |
| 2:Z1:73:THR:OG1 | 2:Z1:74:VAL:N | 2.53 | 0.42 |
| 2:Z1:362:VAL:HB | 2:Z1:370:LYS:HE3 | 2.00 | 0.42 |
| 1:Z2:152:ILE:HG22 | 1:Z2:195:ASN:HB3 | 2.02 | 0.42 |
| 1:Z2:284:LEU:HG | 1:Z2:362:LYS:NZ | 2.34 | 0.42 |
| 2:Z3:203:MET:SD | 2:Z3:203:MET:N | 2.93 | 0.42 |
| 1:Z4:7:ILE:HG12 | 1:Z4:64:ILE:HD13 | 2.01 | 0.42 |
| 1:Z4:69:GLU:OE2 | 1:Z4:69:GLU:N | 2.52 | 0.42 |
| 1:Z4:136:CYS:SG | 1:Z4:167:PHE:HB2 | 2.60 | 0.42 |
| 1:Z4:248:ALA:CB | 1:Z4:252:LYS:HD3 | 2.49 | 0.42 |
| 1:Z4:270:PHE:O | 1:Z4:298:ASN:ND2 | 2.32 | 0.42 |
| 2:Z5:268:MET:SD | 2:Z5:380:ASN:HB2 | 2.59 | 0.42 |
| 2:Z7:377:MET:SD | 2:Z7:379:SER:HB2 | 2.60 | 0.42 |
| 1:Z8:394:PHE:HA | 2:Z9:261:PRO:HA | 2.02 | 0.42 |
| 2:Z9:262:TYR:HD2 | 2:Z9:265:ILE:HD12 | 1.84 | 0.42 |
| 1:0C:11:GLN:N | 39:0C:502:GDP:O2B | 2.44 | 0.42 |
| 1:0C:235:GLY:O | 1:0C:316:LEU:HD22 | 2.19 | 0.42 |
| 1:0E:374:ILE:HD11 | 1:0E:422:TYR:CZ | 2.55 | 0.42 |
| 2:0F:377:MET:O | 2:0F:378:ILE:HD13 | 2.20 | 0.42 |
| 1:0G:5:VAL:HG12 | 1:0G:133:PHE:HD1 | 1.84 | 0.42 |
| 1:0G:11:GLN:NE2 | 39:0G:501:GDP:C8 | 2.84 | 0.42 |
| 1:0G:138:SER:O | 1:0G:145:SER:OG | 2.32 | 0.42 |
| 2:0J:111:GLY:HA2 | 2:0J:114:ILE:HG22 | 2.02 | 0.42 |
| 2:0J:407:TRP:NE1 | 1:0K:258:ILE:O | 2.44 | 0.42 |
| 2:0L:107:HIS:O | 2:0L:152:LEU:HD12 | 2.20 | 0.42 |
| 1:0M:393:ALA:O | 1:0M:395:LEU:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0P:28:HIS:CE1 | 2:0P:49:PHE:HA | 2.55 | 0.42 |
| 2:0P:252:ILE:HD12 | 2:0P:255:PHE:CE2 | 2.54 | 0.42 |
| 1:0Q:136:CYS:SG | 1:0Q:167:PHE:HD2 | 2.43 | 0.42 |
| 1:0S:207:LEU:HB2 | 1:0S:225:LEU:HD23 | 2.02 | 0.42 |
| 1:0U:21:TRP:HA | 1:0U:24:VAL:HG12 | 2.01 | 0.42 |
| 1:0U:95:THR:HG23 | 1:0U:96:GLY:N | 2.35 | 0.42 |
| 2:0V:3:GLU:N | 2:0V:3:GLU:OE1 | 2.53 | 0.42 |
| 2:0V:21:TRP:CZ3 | 2:0V:63:PRO:HB3 | 2.55 | 0.42 |
| 2:0V:99:ALA:HA | 2:0V:105:ARG:HD3 | 2.01 | 0.42 |
| 1:0W:152:ILE:HG23 | 1:0W:164:MET:SD | 2.60 | 0.42 |
| 1:0W:178:THR:HA | 2:0X:352:LYS:HD2 | 2.00 | 0.42 |
| 1:0W:414:ASN:O | 1:0W:418:LEU:HB2 | 2.19 | 0.42 |
| 2:0X:318:MET:HB2 | 2:0X:376:CYS:HB3 | 2.01 | 0.42 |
| 1:1A:112:LEU:O | 1:1A:116:VAL:HG23 | 2.20 | 0.42 |
| 2:1B:320:ARG:O | 2:1B:373:ARG:HA | 2.19 | 0.42 |
| 1:1C:344:TRP:O | 1:1C:345:ILE:HD13 | 2.19 | 0.42 |
| 2:1D:125:LEU:HD23 | 2:1D:125:LEU:HA | 1.90 | 0.42 |
| 2:1D:221:ARG:HB3 | 1:1E:322:SER:OG | 2.20 | 0.42 |
| 2:1D:387:ILE:HG12 | 2:1D:390:ARG:NH2 | 2.33 | 0.42 |
| 1:1E:337:ASN:HB3 | 1:1E:340:TYR:CD2 | 2.55 | 0.42 |
| 2:1F:176:GLN:HG2 | 2:1F:177:VAL:N | 2.33 | 0.42 |
| 1:1G:190:HIS:CD2 | 1:1G:411:ALA:HA | 2.55 | 0.42 |
| 1:1G:222:PHE:CE1 | 2:1H:325:PRO:HG2 | 2.55 | 0.42 |
| 1:1K:49:VAL:HG13 | 1:1K:50:TYR:CD1 | 2.55 | 0.42 |
| 1:1K:244:GLY:H | 1:1K:247:ASN:HD21 | 1.66 | 0.42 |
| 2:1L:200:VAL:HG13 | 2:1L:268:MET:HE1 | 2.01 | 0.42 |
| 2:1L:217:LEU:HB3 | 2:1L:219:ILE:CD1 | 2.50 | 0.42 |
| 2:1N:326:LYS:HG3 | 2:1N:327:ASP:N | 2.34 | 0.42 |
| 2:1P:14:ILE:HD11 | 2:1P:74:VAL:HG13 | 2.00 | 0.42 |
| 2:1P:370:LYS:O | 9:4Z:164:GLN:NE2 | 2.53 | 0.42 |
| 1:1Q:97:ALA:O | 1:1Q:103:LYS:HD3 | 2.20 | 0.42 |
| 1:1Q:178:THR:OG1 | 1:1Q:181:GLU:HG3 | 2.19 | 0.42 |
| 1:1U:229:ILE:HG22 | 1:1U:233:MET:CE | 2.50 | 0.42 |
| 2:1V:284:GLU:OE1 | 2:1V:286:LEU:HD22 | 2.19 | 0.42 |
| 2:1V:301:MET:HE1 | 2:1V:307:PRO:HD3 | 2.00 | 0.42 |
| 1:1W:167:PHE:CE2 | 1:1W:233:MET:HG2 | 2.54 | 0.42 |
| 2:2B:177:VAL:HG13 | 1:2C:327:ASP:CG | 2.40 | 0.42 |
| 1:2E:41:ASP:HA | 1:2E:44:LEU:HD13 | 2.02 | 0.42 |
| 2:2F:394:LYS:HB2 | 1:2G:346:PRO:HG3 | 2.01 | 0.42 |
| 2:2H:414:GLU:N | 2:2H:414:GLU:OE1 | 2.53 | 0.42 |
| 2:2J:121:ARG:HH11 | 2:2J:121:ARG:CG | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2K:130:LEU:HB2 | 1:2K:162:ARG:HE | 1.84 | 0.42 |
| 1:2M:122:LYS:NZ | 1:3C:291:GLN:HB3 | 2.35 | 0.42 |
| 2:2N:4:VAL:HG23 | 2:2N:134:GLY:O | 2.19 | 0.42 |
| 2:2N:102:ASN:HD22 | 2:2N:105:ARG:HB2 | 1.85 | 0.42 |
| 2:2N:212:ILE:HD13 | 2:2N:212:ILE:HA | 1.89 | 0.42 |
| 2:2P:69:ASP:OD1 | 2:2P:70:LEU:N | 2.53 | 0.42 |
| 1:2Q:332:ASN:HD21 | 38:7Z:1:MET:CA | 2.31 | 0.42 |
| 1:2S:166:THR:OG1 | 1:2S:199:CYS:SG | 2.74 | 0.42 |
| 1:2U:117:LEU:HA | 1:2U:120:VAL:HG12 | 2.01 | 0.42 |
| 2:2V:102:ASN:HB3 | 2:2V:105:ARG:HB3 | 2.01 | 0.42 |
| 2:2Z:121:ARG:HA | 2:2Z:121:ARG:HD2 | 1.77 | 0.42 |
| 2:2Z:244:PHE:HB2 | 2:2Z:356:ASN:HD21 | 1.84 | 0.42 |
| 1:3A:58:ARG:HB2 | 1:3A:58:ARG:HH21 | 1.85 | 0.42 |
| 1:3A:105:HIS:CD2 | 1:3A:150:LEU:HB2 | 2.55 | 0.42 |
| 2:3D:9:ILE:HD11 | 2:3D:153:LEU:HD23 | 2.01 | 0.42 |
| 2:3D:274:PRO:HB2 | 2:3D:276:ILE:HG12 | 2.02 | 0.42 |
| 2:3F:164:LYS:NZ | 3:3V:136:HIS:HB2 | 2.35 | 0.42 |
| 2:3F:402:ARG:HA | 2:3F:402:ARG:HD3 | 1.77 | 0.42 |
| 1:3G:203:ASP:OD2 | 1:3G:302:ALA:N | 2.53 | 0.42 |
| 1:3G:391:ARG:HD2 | 2:3H:346:TRP:CE2 | 2.54 | 0.42 |
| 2:3H:91:GLN:HE21 | 3:3X:36:PHE:HE2 | 1.65 | 0.42 |
| 1:3I:317:PHE:HB3 | 1:3I:321:MET:CE | 2.50 | 0.42 |
| 2:3L:72:PRO:HD2 | 1:3M:2:ARG:NH1 | 2.33 | 0.42 |
| 1:3M:122:LYS:HZ1 | 3:4D:262:TYR:HA | 1.85 | 0.42 |
| 1:3M:391:ARG:HG3 | 2:3N:346:TRP:CE3 | 2.55 | 0.42 |
| 2:3N:66:ILE:HD12 | 2:3N:68:LEU:HD23 | 2.01 | 0.42 |
| 1:3S:45:GLU:OE2 | 1:3S:46:ARG:HG2 | 2.19 | 0.42 |
| 2:3T:105:ARG:HB2 | 2:3T:411:GLU:OE1 | 2.20 | 0.42 |
| 3:3X:282:GLU:OE2 | 3:3X:290:PHE:HB2 | 2.20 | 0.42 |
| 7:4S:18:ARG:CZ | 7:4S:18:ARG:CB | 2.97 | 0.42 |
| 7:4T:267:THR:HG22 | 7:4T:269:THR:H | 1.85 | 0.42 |
| 7:4T:292:GLU:O | 7:4T:295:GLU:HG3 | 2.20 | 0.42 |
| 7:4U:66:LEU:HA | 7:4U:69:MET:HE2 | 2.02 | 0.42 |
| 8:4W:277:ALA:O | 8:4W:281:GLN:HG2 | 2.19 | 0.42 |
| 9:4Z:345:GLU:HA | 9:4Z:348:GLU:OE1 | 2.20 | 0.42 |
| 10:5A:277:GLU:HA | 10:5A:280:LYS:HD2 | 2.01 | 0.42 |
| 13:5K:69:GLU:OE1 | 13:5K:69:GLU:HA | 2.19 | 0.42 |
| 14:5L:511:THR:HB | 14:5L:531:ASP:CB | 2.48 | 0.42 |
| 14:5N:12:GLY:HA2 | 14:5N:338:ALA:CB | 2.49 | 0.42 |
| 14:5N:484:CYS:SG | 14:5N:496:TRP:HB2 | 2.59 | 0.42 |
| 15:5O:321:GLU:O | 15:5O:325:GLN:NE2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5P:148:ARG:HH21 | 15:5P:151:ASP:HB2 | 1.84 | 0.42 |
| 17:5S:220:ALA:O | 17:5S:223:GLU:HB2 | 2.19 | 0.42 |
| 17:5T:220:ALA:O | 17:5T:223:GLU:HB2 | 2.19 | 0.42 |
| 17:5U:205:SER:O | 17:5U:209:LYS:HE2 | 2.19 | 0.42 |
| 17:5U:220:ALA:O | 17:5U:223:GLU:HB2 | 2.19 | 0.42 |
| 18:5Y:128:GLN:CD | 18:5Y:129:PRO:HD3 | 2.39 | 0.42 |
| 22:6I:220:ASP:HA | 22:6I:223:LEU:HB3 | 2.02 | 0.42 |
| 22:6M:164:LYS:O | 22:6M:168:THR:HG23 | 2.19 | 0.42 |
| 22:6O:220:ASP:OD1 | 22:6O:220:ASP:N | 2.52 | 0.42 |
| 24:6U:271:LYS:HB3 | 24:6U:298:LEU:HD12 | 2.00 | 0.42 |
| 24:6W:185:ASP:HB3 | 24:6W:188:THR:HG23 | 2.00 | 0.42 |
| 24:6Z:274:ARG:HB3 | 24:6Z:372:ASP:OD2 | 2.20 | 0.42 |
| 25:7C:10:GLU:O | 25:7C:14:ARG:HD3 | 2.20 | 0.42 |
| 25:7C:17:MET:HE1 | 25:7C:21:LEU:HD21 | 2.00 | 0.42 |
| 27:7G:21:VAL:HG12 | 27:7G:23:VAL:HG13 | 2.02 | 0.42 |
| 30:7L:388:LEU:HD23 | 30:7L:388:LEU:HA | 1.81 | 0.42 |
| 31:7N:91:PRO:HB2 | 31:7N:96:THR:HG22 | 2.02 | 0.42 |
| 34:7R:215:ALA:O | 34:7R:219:LYS:HG2 | 2.20 | 0.42 |
| 34:7R:245:ARG:O | 34:7R:248:LYS:HG3 | 2.20 | 0.42 |
| 35:7T:164:ARG:NH2 | 36:7V:63:ASP:O | 2.52 | 0.42 |
| 2:A0:47:ASP:OD2 | 24:6X:136:ARG:NH2 | 2.38 | 0.42 |
| 1:A3:80:PRO:HB3 | 24:6Z:175:TYR:CE2 | 2.54 | 0.42 |
| 2:E9:32:PRO:HD2 | 22:6N:127:THR:HB | 2.01 | 0.42 |
| 1:G2:32:PRO:HD2 | 24:6W:527:ASN:ND2 | 2.31 | 0.42 |
| 2:G3:65:CYS:SG | 2:G3:66:ILE:N | 2.92 | 0.42 |
| 1:G4:207:LEU:HB3 | 1:G4:225:LEU:HD22 | 2.02 | 0.42 |
| 2:G5:111:GLY:HA2 | 2:G5:114:ILE:HG22 | 2.01 | 0.42 |
| 2:G5:150:GLY:O | 2:G5:153:LEU:HG | 2.20 | 0.42 |
| 2:G7:90:GLU:OE1 | 2:G7:90:GLU:N | 2.53 | 0.42 |
| 2:G7:288:VAL:HG13 | 2:G7:373:ARG:HD3 | 2.01 | 0.42 |
| 2:G9:195:LEU:HD11 | 2:G9:264:ARG:NH1 | 2.34 | 0.42 |
| 2:G9:422:ARG:HD2 | 2:G9:422:ARG:HA | 1.81 | 0.42 |
| 2:H1:35:GLN:N | 2:H1:35:GLN:OE1 | 2.52 | 0.42 |
| 2:H1:50:ASN:O | 2:H1:64:ARG:NH2 | 2.53 | 0.42 |
| 2:H1:71:GLU:CG | 2:H1:98:ASP:HB2 | 2.50 | 0.42 |
| 1:H2:272:PRO:HD3 | 1:H2:364:SER:HA | 2.02 | 0.42 |
| 2:H3:223:THR:HG23 | 2:H3:225:THR:H | 1.85 | 0.42 |
| 1:H4:67:ASP:OD2 | 1:H4:72:THR:OG1 | 2.28 | 0.42 |
| 1:H4:414:ASN:HA | 1:H4:417:ASP:OD2 | 2.20 | 0.42 |
| 2:H5:317:LEU:HD11 | 2:H5:351:PHE:CD1 | 2.46 | 0.42 |
| 1:H6:140:GLY:O | 1:H6:184:ASN:ND2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H7:53:PHE:HD1 | 2:H7:63:PRO:HA | 1.85 | 0.42 |
| 2:H7:241:SER:OG | 2:H7:250:VAL:O | 2.29 | 0.42 |
| 2:H9:139:ASN:O | 2:H9:170:THR:HA | 2.19 | 0.42 |
| 2:H9:387:ILE:HG12 | 2:H9:390:ARG:NH2 | 2.32 | 0.42 |
| 2:I1:100:ALA:HA | 1:I2:252:LYS:HE2 | 2.02 | 0.42 |
| 2:I3:253:THR:O | 2:I3:256:GLN:HB2 | 2.20 | 0.42 |
| 1:I4:356:ILE:HD13 | 1:I4:356:ILE:HA | 1.83 | 0.42 |
| 1:I4:407:GLU:O | 1:I4:410:GLU:HG2 | 2.20 | 0.42 |
| 2:I5:9:ILE:HD12 | 2:I5:150:GLY:HA3 | 2.02 | 0.42 |
| 2:I5:88:HIS:HA | 2:I5:89:PRO:HD3 | 1.84 | 0.42 |
| 2:I5:235:ILE:O | 2:I5:239:THR:HG23 | 2.19 | 0.42 |
| 1:I8:414:ASN:HA | 1:I8:417:ASP:OD2 | 2.20 | 0.42 |
| 2:I9:88:HIS:HD2 | 2:I9:91:GLN:HG3 | 1.85 | 0.42 |
| 2:J1:384:ILE:HA | 2:J1:387:ILE:HD12 | 2.02 | 0.42 |
| 1:J4:86:ARG:HG2 | 1:J4:88:ASP:H | 1.85 | 0.42 |
| 2:J7:198:THR:HG21 | 2:J7:201:ALA:HB2 | 2.01 | 0.42 |
| 1:K4:273:LEU:H | 1:K4:292:GLN:NE2 | 2.18 | 0.42 |
| 2:K5:66:ILE:O | 2:K5:66:ILE:HG13 | 2.19 | 0.42 |
| 2:K9:14:ILE:HD11 | 2:K9:74:VAL:CG1 | 2.50 | 0.42 |
| 1:L0:350:LYS:HZ3 | 1:L0:351:SER:C | 2.22 | 0.42 |
| 2:L7:217:LEU:HD12 | 2:L7:277:SER:OG | 2.20 | 0.42 |
| 1:M4:156:ARG:HD2 | 1:M4:156:ARG:HA | 1.82 | 0.42 |
| 2:M5:58:ALA:CB | 37:7Y:215:HIS:N | 2.81 | 0.42 |
| 2:N1:225:THR:HG21 | 29:7J:114:GLU:OE1 | 2.20 | 0.42 |
| 2:N1:306:ASP:HB3 | 2:N1:309:HIS:HD2 | 1.85 | 0.42 |
| 2:N5:192:HIS:CD2 | 2:N5:421:ALA:HA | 2.53 | 0.42 |
| 2:N5:384:ILE:HA | 2:N5:387:ILE:HD12 | 2.02 | 0.42 |
| 1:N6:417:ASP:OD1 | 1:N6:418:LEU:N | 2.53 | 0.42 |
| 1:O2:3:GLU:HG3 | 1:O2:127:CYS:HB2 | 2.02 | 0.42 |
| 2:O3:14:ILE:HD11 | 2:O3:74:VAL:CG1 | 2.49 | 0.42 |
| 2:O3:21:TRP:CZ3 | 2:O3:63:PRO:HB3 | 2.54 | 0.42 |
| 2:O3:306:ASP:HB3 | 2:O3:309:HIS:CD2 | 2.55 | 0.42 |
| 1:O6:173:PRO:HG3 | 1:O6:380:ARG:HD2 | 2.01 | 0.42 |
| 2:O9:175:PRO:HB3 | 2:O9:390:ARG:NE | 2.35 | 0.42 |
| 2:P5:123:ARG:NH2 | 2:P5:160:ASP:OD2 | 2.53 | 0.42 |
| 1:P6:117:LEU:HD23 | 1:P6:117:LEU:HA | 1.83 | 0.42 |
| 2:P7:116:ASP:OD1 | 2:P7:117:LEU:N | 2.51 | 0.42 |
| 1:P8:321:MET:HG2 | 1:P8:363:MET:SD | 2.60 | 0.42 |
| 1:P8:405:GLU:HA | 1:P8:408:PHE:HD2 | 1.84 | 0.42 |
| 2:Q1:31:GLN:NE2 | 2:Q1:37:PRO:HG3 | 2.35 | 0.42 |
| 2:Q1:337:THR:O | 5:4M:22:LEU:HD11 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q1:429:GLU:O | 2:Q1:433:GLU:HG2 | 2.20 | 0.42 |
| 2:Q3:241:SER:OG | 2:Q3:250:VAL:O | 2.30 | 0.42 |
| 2:Q3:345:ASP:N | 2:Q3:345:ASP:OD1 | 2.52 | 0.42 |
| 1:Q4:95:THR:HG23 | 1:Q4:96:GLY:N | 2.35 | 0.42 |
| 2:Q9:279:GLU:HA | 7:4Q:336:GLN:HE21 | 1.85 | 0.42 |
| 2:R5:284:GLU:HA | 2:R5:284:GLU:OE2 | 2.20 | 0.42 |
| 2:R5:387:ILE:HG12 | 2:R5:390:ARG:HH22 | 1.85 | 0.42 |
| 2:R9:137:VAL:HG22 | 2:R9:168:GLY:HA2 | 2.02 | 0.42 |
| 2:R9:170:THR:HG21 | 2:R9:194:LEU:HD11 | 2.02 | 0.42 |
| 2:R9:430:LYS:HB3 | 2:R9:430:LYS:HE3 | 1.81 | 0.42 |
| 1:S0:113:ILE:HA | 1:S0:113:ILE:HD12 | 1.92 | 0.42 |
| 1:S0:128:ASP:OD1 | 1:S0:128:ASP:N | 2.53 | 0.42 |
| 1:S0:150:LEU:HA | 1:S0:150:LEU:HD12 | 1.69 | 0.42 |
| 2:S1:306:ASP:HB3 | 2:S1:309:HIS:HD2 | 1.85 | 0.42 |
| 2:S1:405:VAL:HB | 17:5V:112:VAL:HG11 | 2.02 | 0.42 |
| 1:S2:194:GLU:OE2 | 1:S2:414:ASN:ND2 | 2.48 | 0.42 |
| 1:S4:135:VAL:HG11 | 1:S4:152:ILE:HD11 | 2.01 | 0.42 |
| 1:S4:216:LYS:HG3 | 1:S4:275:SER:OG | 2.20 | 0.42 |
| 1:S4:286:VAL:HB | 1:S4:325:GLU:OE1 | 2.20 | 0.42 |
| 1:S4:330:MET:SD | 1:S4:349:VAL:HG11 | 2.60 | 0.42 |
| 1:S6:2:ARG:HB3 | 1:S6:131:GLN:HB2 | 2.02 | 0.42 |
| 1:S6:246:LEU:HD22 | 1:S6:352:SER:HA | 2.01 | 0.42 |
| 1:S6:359:LYS:O | 31:7M:9:ARG:NH2 | 2.52 | 0.42 |
| 2:T1:90:GLU:O | 2:T1:90:GLU:HG2 | 2.20 | 0.42 |
| 2:T1:217:LEU:HD21 | 2:T1:368:LEU:HD23 | 2.02 | 0.42 |
| 1:T2:307:HIS:CD2 | 17:5T:52:PRO:HB3 | 2.55 | 0.42 |
| 1:T4:164:MET:HE3 | 1:T4:164:MET:HB2 | 1.96 | 0.42 |
| 1:T4:174:LYS:HD2 | 1:T4:380:ARG:HH22 | 1.83 | 0.42 |
| 2:T5:17:GLY:HA2 | 2:T5:20:CYS:HB2 | 2.02 | 0.42 |
| 2:T5:102:ASN:HB3 | 2:T5:105:ARG:HB3 | 2.02 | 0.42 |
| 2:T5:265:ILE:HD11 | 2:T5:435:VAL:HG21 | 2.02 | 0.42 |
| 2:T5:414:GLU:HG2 | 2:T5:417:GLU:OE2 | 2.19 | 0.42 |
| 2:T7:286:LEU:HD13 | 2:T7:286:LEU:HA | 1.87 | 0.42 |
| 1:T8:112:LEU:O | 1:T8:116:VAL:HG23 | 2.20 | 0.42 |
| 2:U1:115:VAL:HG22 | 2:U1:119:LEU:HD13 | 2.02 | 0.42 |
| 2:U1:267:PHE:HB2 | 2:U1:384:ILE:HD12 | 2.02 | 0.42 |
| 2:U3:51:THR:HG21 | 2:U3:243:ARG:HG2 | 2.01 | 0.42 |
| 2:U3:203:MET:HE1 | 2:U3:267:PHE:HD1 | 1.85 | 0.42 |
| 1:U4:234:SER:O | 1:U4:241:ARG:NH2 | 2.53 | 0.42 |
| 1:U6:130:LEU:HB2 | 1:U6:162:ARG:HE | 1.83 | 0.42 |
| 2:U9:52:PHE:HZ | 2:U9:239:THR:HG21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U9:108:TYR:HA | 2:U9:112:LYS:HE3 | 2.02 | 0.42 |
| 1:V0:77:ARG:O | 1:V0:83:GLN:NE2 | 2.52 | 0.42 |
| 1:V0:117:LEU:O | 1:V0:121:ARG:HB2 | 2.19 | 0.42 |
| 1:V0:311:LEU:HD23 | 1:V0:311:LEU:HA | 1.88 | 0.42 |
| 2:V1:217:LEU:HA | 2:V1:217:LEU:HD23 | 1.82 | 0.42 |
| 2:V1:284:GLU:O | 2:V1:285:GLN:NE2 | 2.53 | 0.42 |
| 1:V2:174:LYS:HA | 1:V2:174:LYS:HD2 | 1.78 | 0.42 |
| 1:V4:61:PRO:HG2 | 1:V4:85:PHE:CE1 | 2.55 | 0.42 |
| 1:V6:122:LYS:NZ | 1:V6:123:GLU:OE1 | 2.52 | 0.42 |
| 2:V7:11:GLN:OE1 | 2:V7:15:GLN:NE2 | 2.53 | 0.42 |
| 2:V7:101:ASN:HD21 | 2:V7:180:ALA:HB1 | 1.85 | 0.42 |
| 2:V7:244:PHE:HB2 | 2:V7:356:ASN:HD21 | 1.85 | 0.42 |
| 2:V7:406:HIS:CD2 | 1:V8:261:PRO:HD3 | 2.55 | 0.42 |
| 1:V8:309:ARG:O | 1:V8:371:SER:OG | 2.23 | 0.42 |
| 2:W1:331:SER:O | 2:W1:334:THR:OG1 | 2.23 | 0.42 |
| 2:W1:358:GLN:OE1 | 2:W1:359:PRO:HD2 | 2.20 | 0.42 |
| 1:W6:67:ASP:OD2 | 1:W6:72:THR:OG1 | 2.23 | 0.42 |
| 2:W7:177:VAL:HG13 | 1:W8:327:ASP:HB3 | 2.02 | 0.42 |
| 1:W8:100:ASN:HB3 | 1:W8:103:LYS:HB2 | 2.01 | 0.42 |
| 1:W8:167:PHE:CE2 | 1:W8:233:MET:HG2 | 2.55 | 0.42 |
| 1:W8:167:PHE:CZ | 1:W8:233:MET:HG2 | 2.54 | 0.42 |
| 1:X0:165:LEU:HD23 | 1:X0:165:LEU:HA | 1.81 | 0.42 |
| 1:X2:21:TRP:CZ3 | 1:X2:61:PRO:HB3 | 2.55 | 0.42 |
| 1:X4:395:LEU:HD21 | 1:X4:405:GLU:CD | 2.40 | 0.42 |
| 2:X5:89:PRO:HD2 | 2:Z1:283:HIS:ND1 | 2.35 | 0.42 |
| 2:X7:406:HIS:CD2 | 1:X8:261:PRO:HD3 | 2.55 | 0.42 |
| 1:X8:120:VAL:O | 1:X8:123:GLU:HG3 | 2.19 | 0.42 |
| 1:X8:232:VAL:HG22 | 1:X8:270:PHE:HB2 | 2.02 | 0.42 |
| 1:X8:250:LEU:H | 1:X8:250:LEU:CD1 | 2.31 | 0.42 |
| 1:Y0:24:VAL:HG21 | 1:Y0:50:TYR:CE2 | 2.54 | 0.42 |
| 1:Y0:175:VAL:HG13 | 2:Y1:329:ASN:ND2 | 2.34 | 0.42 |
| 2:Y1:231:ILE:O | 2:Y1:234:VAL:HG12 | 2.20 | 0.42 |
| 2:Y1:286:LEU:HD11 | 2:Y1:372:GLN:H | 1.84 | 0.42 |
| 1:Y2:203:ASP:O | 1:Y2:207:LEU:HG | 2.20 | 0.42 |
| 1:Y2:317:PHE:HE2 | 1:Y2:326:VAL:HG13 | 1.84 | 0.42 |
| 1:Y6:396:HIS:HA | 1:Y6:399:THR:OG1 | 2.20 | 0.42 |
| 2:Y9:70:LEU:HG | 2:Y9:145:THR:HG23 | 2.02 | 0.42 |
| 2:Y9:80:THR:HG22 | 2:Y9:80:THR:O | 2.20 | 0.42 |
| 1:Z0:163:MET:HE3 | 1:Z0:251:ARG:HA | 2.00 | 0.42 |
| 2:Z1:174:SER:HB3 | 2:Z1:177:VAL:O | 2.19 | 0.42 |
| 1:Z6:411:ALA:O | 1:Z6:415:MET:HG2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:176:GLN:NE2 | 2:Z7:207:GLU:OE2 | 2.53 | 0.42 |
| 2:Z9:258:ASN:C | 2:Z9:259:LEU:HD22 | 2.40 | 0.42 |
| 2:Z9:320:ARG:O | 2:Z9:373:ARG:HA | 2.20 | 0.42 |
| 1:0A:413:SER:HA | 1:0A:416:ASN:ND2 | 2.33 | 0.42 |
| 1:0C:33:THR:O | 1:0C:58:ARG:NH2 | 2.53 | 0.42 |
| 1:0E:386:THR:O | 1:0E:390:ARG:HG3 | 2.19 | 0.42 |
| 2:0F:236:SER:HA | 2:0F:239:THR:HG22 | 2.01 | 0.42 |
| 1:0I:131:GLN:HE21 | 1:0I:250:LEU:HB3 | 1.85 | 0.42 |
| 1:0I:210:ILE:HD11 | 1:0I:273:LEU:HD12 | 2.00 | 0.42 |
| 1:0I:385:PHE:HZ | 1:0I:408:PHE:HD1 | 1.66 | 0.42 |
| 1:0K:240:LEU:HD12 | 1:0K:240:LEU:H | 1.85 | 0.42 |
| 2:0L:31:GLN:HB2 | 2:0L:33:ASP:OD1 | 2.20 | 0.42 |
| 2:0L:305:CYS:CB | 2:0L:387:ILE:HD11 | 2.50 | 0.42 |
| 1:0M:83:GLN:O | 1:1C:281:TYR:OH | 2.30 | 0.42 |
| 1:0M:257:LEU:HD23 | 1:0M:312:THR:HB | 2.02 | 0.42 |
| 1:0M:290:THR:HA | 1:0M:293:MET:HB2 | 2.02 | 0.42 |
| 1:0M:418:LEU:HD23 | 1:0M:418:LEU:HA | 1.86 | 0.42 |
| 2:0N:5:ILE:HD11 | 2:0N:135:PHE:CD1 | 2.55 | 0.42 |
| 1:0O:85:PHE:HB2 | 1:0O:90:PHE:CZ | 2.55 | 0.42 |
| 1:0O:194:GLU:OE1 | 1:0O:194:GLU:N | 2.53 | 0.42 |
| 1:0O:244:GLY:HA3 | 1:0O:354:CYS:HA | 2.02 | 0.42 |
| 1:0O:344:TRP:CE3 | 1:0O:345:ILE:HG13 | 2.54 | 0.42 |
| 1:0O:388:MET:CA | 1:0O:388:MET:CE | 2.96 | 0.42 |
| 1:0O:388:MET:HE3 | 1:0O:388:MET:HB2 | 1.84 | 0.42 |
| 2:0P:280:LYS:O | 2:0P:283:HIS:HB3 | 2.20 | 0.42 |
| 2:0R:57:GLY:H | 2:1H:285:GLN:NE2 | 2.18 | 0.42 |
| 1:0S:73:MET:SD | 1:0S:92:PHE:CZ | 3.13 | 0.42 |
| 1:0S:260:PHE:HB3 | 1:0S:262:ARG:NH2 | 2.34 | 0.42 |
| 1:0S:285:THR:O | 1:0S:288:GLU:HB3 | 2.20 | 0.42 |
| 1:0U:316:LEU:HB2 | 1:0U:366:THR:OG1 | 2.20 | 0.42 |
| 1:0W:113:ILE:HD13 | 1:0W:150:LEU:CD2 | 2.50 | 0.42 |
| 1:0W:268:VAL:O | 1:0W:300:MET:N | 2.49 | 0.42 |
| 2:0X:90:GLU:HG3 | 2:0X:121:ARG:HH12 | 1.85 | 0.42 |
| 2:1B:196:GLU:OE2 | 2:1B:197:HIS:NE2 | 2.53 | 0.42 |
| 1:1C:103:LYS:HA | 1:1C:107:THR:OG1 | 2.20 | 0.42 |
| 2:1D:203:MET:O | 2:1D:204:LEU:HD12 | 2.19 | 0.42 |
| 2:1D:301:MET:HE1 | 2:1D:307:PRO:HD3 | 2.02 | 0.42 |
| 1:1E:112:LEU:O | 1:1E:116:VAL:HG23 | 2.20 | 0.42 |
| 1:1E:269:GLY:HA2 | 1:1E:300:MET:SD | 2.60 | 0.42 |
| 1:1E:309:ARG:H | 1:1E:372:THR:HG22 | 1.85 | 0.42 |
| 1:1G:153:SER:O | 1:1G:157:GLU:HG2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1H:396:ASP:HB2 | 2:1H:422:ARG:HH12 | 1.84 | 0.42 |
| 1:1K:86:ARG:HG2 | 1:1K:88:ASP:H | 1.84 | 0.42 |
| 2:1P:379:SER:OG | 2:1P:380:ASN:N | 2.53 | 0.42 |
| 1:1Q:95:THR:OG1 | 1:1Q:96:GLY:N | 2.52 | 0.42 |
| 1:1Q:274:THR:HG21 | 1:1Q:282:ARG:HH11 | 1.85 | 0.42 |
| 2:1R:182:VAL:HG22 | 2:1R:185:TYR:HB2 | 2.02 | 0.42 |
| 2:1R:312:TYR:HD2 | 2:1R:343:PHE:HE1 | 1.67 | 0.42 |
| 2:1T:312:TYR:HB2 | 2:1T:343:PHE:HD1 | 1.84 | 0.42 |
| 1:1U:244:GLY:H | 1:1U:247:ASN:HD21 | 1.68 | 0.42 |
| 2:1X:76:ASP:O | 2:1X:80:THR:HG22 | 2.19 | 0.42 |
| 2:1X:108:TYR:O | 2:1X:112:LYS:HD3 | 2.20 | 0.42 |
| 2:1X:175:PRO:HB2 | 2:1X:176:GLN:NE2 | 2.34 | 0.42 |
| 2:2B:88:HIS:HB3 | 2:2R:283:HIS:CG | 2.54 | 0.42 |
| 1:2C:239:CYS:SG | 1:2C:248:ALA:N | 2.89 | 0.42 |
| 2:2D:156:ARG:HA | 2:2D:159:VAL:HG12 | 2.02 | 0.42 |
| 2:2D:181:VAL:HB | 1:2E:256:ASN:HD22 | 1.84 | 0.42 |
| 1:2G:86:ARG:HB3 | 1:2G:89:ASN:OD1 | 2.20 | 0.42 |
| 1:2G:273:LEU:H | 1:2G:292:GLN:HE22 | 1.67 | 0.42 |
| 2:2H:129:CYS:SG | 2:2H:130:THR:N | 2.92 | 0.42 |
| 2:2J:123:ARG:CZ | 38:8C:75:SER:HB3 | 2.49 | 0.42 |
| 1:2K:141:GLY:HA3 | 39:2K:502:GDP:PB | 2.60 | 0.42 |
| 2:2L:52:PHE:CE2 | 2:2L:243:ARG:HD3 | 2.55 | 0.42 |
| 1:2M:164:MET:HE3 | 1:2M:164:MET:HB2 | 1.95 | 0.42 |
| 1:2M:367:PHE:O | 1:2M:368:ILE:HD13 | 2.20 | 0.42 |
| 2:2P:179:THR:O | 1:2Q:350:LYS:HD2 | 2.19 | 0.42 |
| 1:2Q:154:LYS:HD3 | 1:2Q:154:LYS:HA | 1.87 | 0.42 |
| 1:2S:62:ARG:HG3 | 1:2S:123:GLU:OE2 | 2.19 | 0.42 |
| 1:2S:145:SER:OG | 1:2S:146:GLY:N | 2.53 | 0.42 |
| 2:2T:372:GLN:NE2 | 10:5C:267:LEU:HD11 | 2.34 | 0.42 |
| 1:2W:128:ASP:OD1 | 1:2W:128:ASP:N | 2.46 | 0.42 |
| 2:2X:271:SER:OG | 2:2X:272:TYR:N | 2.53 | 0.42 |
| 1:3M:177:ASP:OD1 | 2:3N:353:CYS:HB2 | 2.20 | 0.42 |
| 2:3N:156:ARG:HA | 2:3N:159:VAL:HG12 | 2.02 | 0.42 |
| 2:3N:406:HIS:HA | 2:3N:409:VAL:HG12 | 2.01 | 0.42 |
| 1:3O:292:GLN:HG2 | 1:3O:298:ASN:HD22 | 1.83 | 0.42 |
| 2:3R:76:ASP:HA | 2:3R:79:ARG:HB2 | 2.02 | 0.42 |
| 1:3S:46:ARG:HD3 | 1:3S:46:ARG:HA | 1.84 | 0.42 |
| 2:3T:53:PHE:HB3 | 2:3T:61:HIS:HB3 | 2.02 | 0.42 |
| 3:3V:282:GLU:OE2 | 3:3V:290:PHE:HB2 | 2.20 | 0.42 |
| 4:3Y:30:SER:H | 4:3Y:57:THR:HG22 | 1.83 | 0.42 |
| 4:4G:27:LYS:HE3 | 4:4G:27:LYS:HB3 | 1.94 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4G:30:SER:H | 4:4G:57:THR:HG22 | 1.83 | 0.42 |
| 3:4H:282:GLU:OE2 | 3:4H:290:PHE:HB2 | 2.20 | 0.42 |
| 4:4I:30:SER:H | 4:4I:57:THR:HG22 | 1.83 | 0.42 |
| 3:4J:145:TRP:CD1 | 3:4J:149:ILE:HD11 | 2.55 | 0.42 |
| 6:4N:467:ALA:HA | 6:4N:470:LYS:NZ | 2.34 | 0.42 |
| 7:4U:164:ARG:O | 7:4U:167:GLU:HG3 | 2.19 | 0.42 |
| 9:4Y:440:VAL:N | 9:4Y:441:PRO:HD2 | 2.35 | 0.42 |
| 10:5B:321:LYS:HA | 10:5B:321:LYS:HD2 | 1.88 | 0.42 |
| 12:5F:46:ASP:HB3 | 12:5F:48:PRO:HD2 | 2.02 | 0.42 |
| 12:5F:273:ARG:O | 12:5F:273:ARG:HG3 | 2.19 | 0.42 |
| 14:5L:576:LEU:HD11 | 14:5L:578:LYS:HE3 | 2.02 | 0.42 |
| 14:5M:24:HIS:CB | 14:5M:29:THR:HB | 2.50 | 0.42 |
| 14:5M:470:GLY:N | 14:5M:490:ASP:OD1 | 2.52 | 0.42 |
| 14:5M:500:THR:O | 14:5M:502:LYS:N | 2.53 | 0.42 |
| 14:5M:576:LEU:HD11 | 14:5M:578:LYS:HE3 | 2.02 | 0.42 |
| 14:5N:470:GLY:N | 14:5N:490:ASP:OD1 | 2.52 | 0.42 |
| 18:5Z:128:GLN:CD | 18:5Z:129:PRO:HD3 | 2.39 | 0.42 |
| 18:6B:128:GLN:CD | 18:6B:129:PRO:HD3 | 2.39 | 0.42 |
| 20:6F:131:GLU:CD | 20:6F:131:GLU:N | 2.73 | 0.42 |
| 22:6K:157:VAL:HG21 | 22:6K:225:ALA:HB2 | 2.02 | 0.42 |
| 22:6L:165:MET:HE2 | 22:6L:218:LEU:HD23 | 2.01 | 0.42 |
| 22:6P:10:PHE:HB3 | 22:6P:15:TRP:CD1 | 2.55 | 0.42 |
| 22:6P:157:VAL:HG11 | 22:6P:225:ALA:HB2 | 2.00 | 0.42 |
| 24:6W:592:ASP:OD1 | 24:6W:592:ASP:N | 2.52 | 0.42 |
| 24:6X:438:LEU:HD22 | 24:6X:476:MET:HG2 | 2.00 | 0.42 |
| 24:6X:574:ARG:HG2 | 24:6X:630:LEU:HD21 | 2.01 | 0.42 |
| 24:6Y:274:ARG:HB3 | 24:6Y:372:ASP:OD2 | 2.20 | 0.42 |
| 24:6Z:474:PHE:CZ | 24:6Z:481:LEU:HD22 | 2.55 | 0.42 |
| 24:7A:112:GLU:HB2 | 24:7A:209:PRO:HG2 | 2.01 | 0.42 |
| 26:7F:56:LEU:HD13 | 26:7F:56:LEU:HA | 1.88 | 0.42 |
| 29:7J:167:ILE:CD1 | 29:7J:167:ILE:O | 2.68 | 0.42 |
| 30:7K:173:GLU:HG2 | 30:7K:173:GLU:O | 2.19 | 0.42 |
| 30:7K:379:PHE:O | 30:7K:437:VAL:HG12 | 2.19 | 0.42 |
| 38:8A:117:TRP:O | 38:8A:121:LEU:HG | 2.20 | 0.42 |
| 2:2:44:GLY:HA3 | 24:6T:124:TYR:OH | 2.19 | 0.42 |
| 1:3:11:GLN:HB3 | 39:3:502:GDP:O1A | 2.19 | 0.42 |
| 1:9:436:PHE:CZ | 3:4D:252:LYS:HB2 | 2.55 | 0.42 |
| 2:B4:357:TYR:HE1 | 24:6W:221:ARG:O | 2.02 | 0.42 |
| 1:E0:276:ARG:HB3 | 24:6T:314:GLY:HA3 | 2.02 | 0.42 |
| 1:E4:33:THR:CG2 | 24:6V:403:PRO:HB2 | 2.50 | 0.42 |
| 2:F9:12:ALA:HB2 | 41:G0:501:GTP:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G0:219:THR:HB | 2:G1:324:VAL:HG11 | 2.02 | 0.42 |
| 1:G2:70:PRO:N | 1:G2:92:PHE:HZ | 2.18 | 0.42 |
| 1:G2:403:MET:HE3 | 1:G2:403:MET:HB2 | 1.77 | 0.42 |
| 2:G3:219:ILE:HG23 | 22:6M:175:ALA:HB1 | 2.02 | 0.42 |
| 2:G3:312:TYR:HB2 | 2:G3:343:PHE:HD1 | 1.84 | 0.42 |
| 2:G7:47:ASP:N | 2:G7:47:ASP:OD1 | 2.52 | 0.42 |
| 2:G9:176:GLN:NE2 | 2:G9:207:GLU:HG2 | 2.35 | 0.42 |
| 2:G9:291:ILE:HD12 | 2:G9:375:VAL:HG23 | 2.02 | 0.42 |
| 2:H3:119:LEU:O | 2:H3:122:ILE:HG22 | 2.20 | 0.42 |
| 2:H7:157:LEU:HD23 | 2:H7:157:LEU:HA | 1.80 | 0.42 |
| 2:H7:271:SER:HA | 2:H7:302:MET:HG2 | 2.02 | 0.42 |
| 2:H9:276:ILE:HD13 | 2:H9:276:ILE:HA | 1.89 | 0.42 |
| 1:I0:113:ILE:HG21 | 1:I0:150:LEU:HD22 | 2.02 | 0.42 |
| 1:I4:396:HIS:HE1 | 1:I4:397:TRP:CZ2 | 2.38 | 0.42 |
| 2:I5:9:ILE:HG22 | 2:I5:68:LEU:HD11 | 2.02 | 0.42 |
| 2:I5:312:TYR:HB2 | 2:I5:343:PHE:HD1 | 1.85 | 0.42 |
| 2:I7:33:ASP:OD1 | 2:I7:35:GLN:NE2 | 2.49 | 0.42 |
| 2:I7:109:THR:OG1 | 2:I7:411:GLU:OE2 | 2.37 | 0.42 |
| 2:I7:138:PHE:CD1 | 2:I7:169:PHE:HB2 | 2.54 | 0.42 |
| 1:I8:364:SER:OG | 1:I8:365:ALA:N | 2.53 | 0.42 |
| 2:I9:96:LYS:HD2 | 1:J0:129:CYS:SG | 2.60 | 0.42 |
| 2:J1:31:GLN:HE21 | 2:J1:37:PRO:HG3 | 1.84 | 0.42 |
| 2:J1:79:ARG:O | 2:J1:84:ARG:HG2 | 2.20 | 0.42 |
| 2:J3:266:HIS:ND1 | 2:J3:266:HIS:O | 2.51 | 0.42 |
| 1:J8:39:ASP:O | 29:7J:386:HIS:ND1 | 2.44 | 0.42 |
| 1:J8:414:ASN:HA | 1:J8:417:ASP:OD2 | 2.20 | 0.42 |
| 2:J9:165:SER:OG | 2:J9:256:GLN:NE2 | 2.53 | 0.42 |
| 2:K1:79:ARG:O | 2:K1:84:ARG:HG2 | 2.19 | 0.42 |
| 1:K6:250:LEU:HD23 | 1:K6:250:LEU:HA | 1.87 | 0.42 |
| 1:K6:260:PHE:HB2 | 1:K6:263:LEU:HD23 | 2.01 | 0.42 |
| 1:K8:212:PHE:HZ | 2:K9:326:LYS:HD3 | 1.84 | 0.42 |
| 2:K9:21:TRP:CZ3 | 2:K9:63:PRO:HB3 | 2.55 | 0.42 |
| 1:L0:91:VAL:HG11 | 1:L0:116:VAL:HG12 | 2.02 | 0.42 |
| 1:L0:121:ARG:NH2 | 1:L0:158:GLU:OE2 | 2.46 | 0.42 |
| 2:L1:8:HIS:CD2 | 2:L1:138:PHE:HD2 | 2.38 | 0.42 |
| 2:L3:123:ARG:NH2 | 2:L3:160:ASP:OD2 | 2.52 | 0.42 |
| 2:L5:155:GLU:O | 2:L5:158:SER:OG | 2.30 | 0.42 |
| 2:L5:399:TYR:O | 2:L5:402:ARG:NH1 | 2.51 | 0.42 |
| 1:L6:108:GLU:HA | 1:L6:111:GLU:OE2 | 2.20 | 0.42 |
| 1:L6:204:ASN:OD1 | 39:L6:502:GDP:O2' | 2.38 | 0.42 |
| 2:L7:115:VAL:HG21 | 2:L7:152:LEU:HG | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L9:88:HIS:HB2 | 1:N6:281:TYR:CZ | 2.54 | 0.42 |
| 2:M1:5:ILE:HD11 | 2:M1:135:PHE:CE1 | 2.54 | 0.42 |
| 2:M1:122:ILE:HD13 | 2:M1:157:LEU:HD11 | 2.02 | 0.42 |
| 1:M2:362:LYS:HA | 1:M2:362:LYS:HD2 | 1.60 | 0.42 |
| 2:M3:201:ALA:O | 2:M3:268:MET:HE2 | 2.20 | 0.42 |
| 1:M4:362:LYS:HE3 | 1:M4:363:MET:HE2 | 2.02 | 0.42 |
| 2:M5:174:SER:HB3 | 2:M5:177:VAL:O | 2.20 | 0.42 |
| 1:M6:46:ARG:HH12 | 37:7Y:115:CYS:HG | 1.68 | 0.42 |
| 2:M9:137:VAL:HG22 | 2:M9:168:GLY:HA2 | 2.02 | 0.42 |
| 2:M9:217:LEU:HD21 | 2:M9:368:LEU:HD23 | 2.02 | 0.42 |
| 2:M9:422:ARG:O | 2:M9:422:ARG:HD2 | 2.20 | 0.42 |
| 1:N0:138:SER:O | 1:N0:139:LEU:HD23 | 2.20 | 0.42 |
| 2:N3:7:ILE:HD11 | 2:N3:137:VAL:HG12 | 2.01 | 0.42 |
| 2:N3:320:ARG:HB3 | 2:N3:358:GLN:O | 2.20 | 0.42 |
| 1:N8:273:LEU:H | 1:N8:292:GLN:HE22 | 1.68 | 0.42 |
| 2:N9:188:VAL:HG23 | 2:N9:189:LEU:HD12 | 2.01 | 0.42 |
| 2:N9:305:CYS:HB3 | 2:N9:387:ILE:HD11 | 2.02 | 0.42 |
| 1:O0:203:ASP:OD2 | 1:O0:301:CYS:HA | 2.20 | 0.42 |
| 2:O1:132:LEU:HD11 | 2:O1:134:GLY:O | 2.20 | 0.42 |
| 2:O7:54:SER:O | 2:O7:61:HIS:HA | 2.20 | 0.42 |
| 1:O8:12:CYS:SG | 1:O8:138:SER:HB2 | 2.60 | 0.42 |
| 1:P6:173:PRO:HB3 | 1:P6:384:GLN:HE22 | 1.84 | 0.42 |
| 2:P7:113:GLU:N | 2:P7:113:GLU:OE2 | 2.53 | 0.42 |
| 2:P9:313:MET:N | 2:P9:380:ASN:O | 2.43 | 0.42 |
| 2:Q3:176:GLN:HG2 | 2:Q3:207:GLU:OE1 | 2.19 | 0.42 |
| 1:Q4:334:GLN:HE22 | 1:Q4:347:ASN:HA | 1.85 | 0.42 |
| 1:Q6:108:GLU:OE1 | 1:Q6:108:GLU:N | 2.53 | 0.42 |
| 1:Q8:260:PHE:HE2 | 1:Q8:262:ARG:HD3 | 1.84 | 0.42 |
| 1:Q8:285:THR:HB | 1:Q8:287:PRO:HD2 | 2.02 | 0.42 |
| 1:R2:321:MET:HG2 | 1:R2:363:MET:SD | 2.59 | 0.42 |
| 1:R4:275:SER:OG | 19:6E:185:GLU:OE1 | 2.33 | 0.42 |
| 1:R4:356:ILE:HD13 | 1:R4:356:ILE:HA | 1.92 | 0.42 |
| 1:S0:114:ASP:OD1 | 1:S0:115:SER:N | 2.53 | 0.42 |
| 1:S2:192:LEU:HD23 | 1:S2:192:LEU:HA | 1.91 | 0.42 |
| 1:S4:287:PRO:CA | 1:S4:329:GLN:HE22 | 2.30 | 0.42 |
| 1:S8:8:GLN:CD | 1:S8:17:GLY:HA3 | 2.39 | 0.42 |
| 2:T1:245:ASP:HB3 | 7:4U:5:VAL:HG13 | 2.01 | 0.42 |
| 1:T2:54:ALA:HB3 | 1:T2:58:ARG:HB3 | 2.01 | 0.42 |
| 1:T2:102:ALA:HB2 | 1:T2:403:MET:HE3 | 2.01 | 0.42 |
| 1:T2:325:GLU:HA | 1:T2:328:GLU:HG2 | 2.02 | 0.42 |
| 1:T2:344:TRP:CE3 | 1:T2:345:ILE:HG13 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T3:62:VAL:HA | 2:T3:63:PRO:HD3 | 1.93 | 0.42 |
| 1:T4:2:ARG:HE | 1:T4:240:LEU:HD22 | 1.85 | 0.42 |
| 1:T4:232:VAL:O | 1:T4:236:ILE:HG12 | 2.20 | 0.42 |
| 1:T6:117:LEU:HA | 1:T6:117:LEU:HD23 | 1.83 | 0.42 |
| 1:T8:382:SER:HB2 | 1:T8:415:MET:SD | 2.60 | 0.42 |
| 2:U1:111:GLY:HA2 | 2:U1:114:ILE:HG22 | 2.02 | 0.42 |
| 2:U3:33:ASP:OD2 | 2:U3:34:GLY:N | 2.53 | 0.42 |
| 1:U4:77:ARG:HH21 | 1:U4:90:PHE:HD2 | 1.68 | 0.42 |
| 1:U4:289:LEU:HD11 | 1:U4:363:MET:HB3 | 2.02 | 0.42 |
| 2:U9:87:PHE:HB3 | 2:U9:92:LEU:HD21 | 2.02 | 0.42 |
| 2:U9:88:HIS:HB3 | 2:U9:91:GLN:HG2 | 2.02 | 0.42 |
| 2:U9:102:ASN:HB3 | 2:U9:105:ARG:CB | 2.50 | 0.42 |
| 2:U9:334:THR:HA | 2:U9:337:THR:HG22 | 2.02 | 0.42 |
| 1:V0:309:ARG:H | 1:V0:372:THR:HG22 | 1.84 | 0.42 |
| 1:V2:22:GLU:HG2 | 1:V2:81:TYR:HD2 | 1.85 | 0.42 |
| 1:V2:289:LEU:HD11 | 1:V2:363:MET:HG2 | 2.02 | 0.42 |
| 2:V3:205:ASP:OD2 | 2:V3:303:VAL:HG13 | 2.19 | 0.42 |
| 1:V4:117:LEU:HA | 1:V4:117:LEU:HD23 | 1.88 | 0.42 |
| 1:V6:97:ALA:HB3 | 1:V6:143:THR:HG22 | 2.02 | 0.42 |
| 2:W1:35:GLN:N | 2:W1:35:GLN:OE1 | 2.53 | 0.42 |
| 2:W1:288:VAL:HG11 | 2:W1:323:VAL:HG13 | 2.01 | 0.42 |
| 2:W3:89:PRO:HD3 | 2:X9:283:HIS:CG | 2.55 | 0.42 |
| 2:W3:116:ASP:OD1 | 2:W3:156:ARG:NH1 | 2.52 | 0.42 |
| 2:W3:139:ASN:OD1 | 2:W3:139:ASN:N | 2.52 | 0.42 |
| 2:W3:286:LEU:HD12 | 2:W3:286:LEU:HA | 1.89 | 0.42 |
| 1:W6:379:LYS:HG3 | 1:W6:419:VAL:HG11 | 2.02 | 0.42 |
| 2:W7:79:ARG:O | 2:W7:84:ARG:HG2 | 2.19 | 0.42 |
| 2:W7:312:TYR:HB2 | 2:W7:343:PHE:CD1 | 2.55 | 0.42 |
| 2:W7:401:LYS:HE3 | 2:W7:401:LYS:HB3 | 1.82 | 0.42 |
| 1:W8:4:ILE:HB | 1:W8:50:TYR:HE1 | 1.83 | 0.42 |
| 2:W9:88:HIS:HE2 | 2:W9:121:ARG:NH2 | 2.13 | 0.42 |
| 1:X0:387:ALA:HA | 1:X0:390:ARG:HH21 | 1.85 | 0.42 |
| 1:X4:249:ASP:OD2 | 1:X4:252:LYS:HB2 | 2.20 | 0.42 |
| 1:X8:292:GLN:HG2 | 1:X8:298:ASN:HD22 | 1.84 | 0.42 |
| 1:Y0:244:GLY:HA3 | 1:Y0:354:CYS:HA | 2.01 | 0.42 |
| 1:Y2:86:ARG:HG2 | 1:Y2:88:ASP:H | 1.84 | 0.42 |
| 2:Y5:395:PHE:CE2 | 2:Y5:422:ARG:HD3 | 2.55 | 0.42 |
| 1:Y8:11:GLN:HG2 | 1:Y8:12:CYS:N | 2.35 | 0.42 |
| 2:Y9:186:ASN:O | 2:Y9:190:SER:OG | 2.31 | 0.42 |
| 1:Z0:21:TRP:CZ3 | 1:Z0:61:PRO:HB3 | 2.55 | 0.42 |
| 1:Z0:58:ARG:HH11 | 1:Z0:84:ILE:HA | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z0:156:ARG:HD3 | 1:Z0:164:MET:CE | 2.49 | 0.42 |
| 1:Z0:198:GLU:HA | 1:Z0:264:HIS:HB2 | 2.02 | 0.42 |
| 1:Z0:254:ALA:HB1 | 1:Z0:258:ILE:HD12 | 2.02 | 0.42 |
| 2:Z1:265:ILE:HG23 | 2:Z1:432:PHE:CZ | 2.55 | 0.42 |
| 1:Z2:66:MET:HE2 | 1:Z2:147:MET:HG3 | 2.02 | 0.42 |
| 1:Z4:114:ASP:N | 1:Z4:114:ASP:OD1 | 2.53 | 0.42 |
| 1:Z6:272:PRO:O | 1:Z6:273:LEU:HD23 | 2.20 | 0.42 |
| 1:Z8:232:VAL:HG22 | 1:Z8:270:PHE:HB2 | 2.02 | 0.42 |
| 2:0B:11:GLN:HB3 | 41:0C:501:GTP:PA | 2.60 | 0.42 |
| 1:0C:67:ASP:OD2 | 1:0C:72:THR:OG1 | 2.37 | 0.42 |
| 1:0C:249:ASP:OD1 | 1:0C:252:LYS:N | 2.45 | 0.42 |
| 1:0G:61:PRO:HG2 | 1:0G:85:PHE:CE1 | 2.54 | 0.42 |
| 1:0I:95:THR:OG1 | 1:0I:96:GLY:N | 2.53 | 0.42 |
| 1:0I:297:LYS:HD3 | 1:0I:297:LYS:HA | 1.83 | 0.42 |
| 2:0J:68:LEU:HA | 2:0J:93:ILE:O | 2.19 | 0.42 |
| 2:0J:147:SER:OG | 2:0J:190:SER:HB3 | 2.20 | 0.42 |
| 1:0K:15:GLN:HB3 | 1:0K:226:ASN:ND2 | 2.35 | 0.42 |
| 1:0K:148:GLY:O | 1:0K:151:LEU:HG | 2.20 | 0.42 |
| 1:0K:313:ALA:HA | 1:0K:369:GLY:HA2 | 2.02 | 0.42 |
| 1:0M:214:THR:OG1 | 1:0M:215:LEU:N | 2.53 | 0.42 |
| 1:0M:388:MET:N | 1:0M:388:MET:HE2 | 2.35 | 0.42 |
| 2:0N:147:SER:OG | 2:0N:148:GLY:N | 2.53 | 0.42 |
| 1:0Q:60:VAL:HG12 | 1:1G:281:TYR:HD1 | 1.85 | 0.42 |
| 2:0R:320:ARG:O | 2:0R:373:ARG:HA | 2.20 | 0.42 |
| 1:0S:103:LYS:NZ | 1:0S:108:GLU:HG2 | 2.34 | 0.42 |
| 1:0S:156:ARG:HA | 1:0S:156:ARG:HD2 | 1.87 | 0.42 |
| 1:0S:314:SER:HB2 | 1:0S:368:ILE:CG2 | 2.49 | 0.42 |
| 1:0U:200:MET:HG2 | 1:0U:202:LEU:CD2 | 2.49 | 0.42 |
| 1:0U:337:ASN:HB3 | 1:0U:340:TYR:HD2 | 1.85 | 0.42 |
| 2:0V:205:ASP:OD2 | 2:0V:303:VAL:HG13 | 2.20 | 0.42 |
| 2:0V:253:THR:HA | 2:0V:256:GLN:NE2 | 2.35 | 0.42 |
| 2:0V:313:MET:HB3 | 2:0V:380:ASN:HB3 | 2.01 | 0.42 |
| 2:0X:2:ARG:HB2 | 2:0X:242:LEU:HD11 | 2.02 | 0.42 |
| 2:0X:178:SER:HB3 | 2:0X:183:GLU:OE2 | 2.20 | 0.42 |
| 1:0Y:267:MET:SD | 1:0Y:303:ALA:HB3 | 2.60 | 0.42 |
| 2:1B:403:ALA:HB2 | 1:1C:344:TRP:HZ3 | 1.85 | 0.42 |
| 2:1D:271:SER:OG | 2:1D:300:SER:O | 2.24 | 0.42 |
| 2:1F:93:ILE:O | 2:1F:93:ILE:HG22 | 2.19 | 0.42 |
| 2:1H:434:GLU:O | 2:1H:437:ALA:HB3 | 2.20 | 0.42 |
| 1:1K:8:GLN:CD | 1:1K:17:GLY:HA3 | 2.40 | 0.42 |
| 2:1L:121:ARG:NH1 | 2:1L:121:ARG:CG | 2.63 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1M:257:LEU:HD21 | 1:1M:314:SER:HB2 | 2.01 | 0.42 |
| 2:1P:21:TRP:CZ3 | 2:1P:63:PRO:HB3 | 2.55 | 0.42 |
| 2:1R:58:ALA:N | 10:5B:156:TYR:CE2 | 2.88 | 0.42 |
| 2:1R:121:ARG:HD2 | 2:1R:125:LEU:HG | 2.01 | 0.42 |
| 1:1U:374:ILE:O | 1:1U:377:MET:HG3 | 2.20 | 0.42 |
| 1:1W:72:THR:O | 1:1W:75:SER:OG | 2.26 | 0.42 |
| 1:1W:405:GLU:HA | 1:1W:408:PHE:HD2 | 1.84 | 0.42 |
| 2:1X:35:GLN:HB3 | 2:1X:59:GLY:O | 2.19 | 0.42 |
| 1:2A:68:LEU:HD23 | 1:2A:68:LEU:HA | 1.83 | 0.42 |
| 1:2A:205:GLU:HG2 | 1:2A:206:ALA:N | 2.34 | 0.42 |
| 2:2B:56:THR:HG23 | 2:2B:60:LYS:HB3 | 2.02 | 0.42 |
| 2:2B:120:ASP:OD1 | 38:8A:73:TRP:NE1 | 2.52 | 0.42 |
| 1:2C:391:ARG:HG3 | 2:2D:346:TRP:CG | 2.55 | 0.42 |
| 2:2H:88:HIS:HE1 | 2:2H:90:GLU:HB3 | 1.83 | 0.42 |
| 1:2I:86:ARG:HD3 | 1:2I:88:ASP:OD1 | 2.19 | 0.42 |
| 2:2J:174:SER:HB3 | 2:2J:177:VAL:O | 2.18 | 0.42 |
| 2:2J:276:ILE:HG23 | 2:2J:280:LYS:HB2 | 2.01 | 0.42 |
| 1:2K:274:THR:OG1 | 1:2K:282:ARG:NH1 | 2.52 | 0.42 |
| 1:2M:6:HIS:CE1 | 1:2M:8:GLN:HG2 | 2.55 | 0.42 |
| 1:2M:224:ASP:OD2 | 1:2M:225:LEU:N | 2.53 | 0.42 |
| 2:2P:175:PRO:HG2 | 2:2P:176:GLN:OE1 | 2.20 | 0.42 |
| 2:2P:370:LYS:HE3 | 2:2P:370:LYS:HB3 | 1.88 | 0.42 |
| 1:2Q:253:LEU:HD21 | 1:2Q:316:LEU:HD21 | 2.01 | 0.42 |
| 2:2R:125:LEU:HD12 | 2:2R:125:LEU:HA | 1.84 | 0.42 |
| 2:2R:304:LYS:HE2 | 38:8A:68:THR:HG21 | 2.01 | 0.42 |
| 2:2T:145:THR:OG1 | 41:2U:501:GTP:O1B | 2.37 | 0.42 |
| 2:2T:298:PRO:HD3 | 38:8A:25:ILE:HG13 | 2.02 | 0.42 |
| 2:2V:313:MET:SD | 2:2V:344:VAL:HG11 | 2.60 | 0.42 |
| 2:2V:397:LEU:HD23 | 2:2V:397:LEU:HA | 1.88 | 0.42 |
| 1:2W:356:ILE:HD13 | 1:2W:356:ILE:HA | 1.93 | 0.42 |
| 1:2Y:22:GLU:HG2 | 1:2Y:81:TYR:HB2 | 2.02 | 0.42 |
| 1:2Y:170:VAL:HG21 | 1:2Y:201:VAL:HG13 | 2.02 | 0.42 |
| 2:2Z:224:TYR:O | 2:2Z:228:ASN:ND2 | 2.53 | 0.42 |
| 2:2Z:272:TYR:HB3 | 2:2Z:275:ILE:HD11 | 2.02 | 0.42 |
| 2:2Z:397:LEU:HD23 | 2:2Z:397:LEU:HA | 1.89 | 0.42 |
| 1:3A:80:PRO:HD3 | 10:5D:139:MET:SD | 2.60 | 0.42 |
| 2:3B:262:TYR:CB | 2:3B:265:ILE:HD12 | 2.50 | 0.42 |
| 1:3G:177:ASP:O | 2:3H:352:LYS:HD2 | 2.20 | 0.42 |
| 2:3H:203:MET:O | 2:3H:204:LEU:HD12 | 2.20 | 0.42 |
| 1:3I:11:GLN:N | 39:3I:502:GDP:O2B | 2.38 | 0.42 |
| 1:3I:208:TYR:CE1 | 1:3I:225:LEU:HD11 | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3J:9:ILE:HG22 | 2:3J:146:GLY:HA2 | 2.02 | 0.42 |
| 2:3J:79:ARG:NH1 | 2:3J:94:SER:OG | 2.53 | 0.42 |
| 1:3M:67:ASP:OD2 | 1:3M:68:LEU:N | 2.49 | 0.42 |
| 1:3O:113:ILE:HG12 | 1:3O:150:LEU:HD22 | 2.02 | 0.42 |
| 1:3Q:70:PRO:N | 1:3Q:92:PHE:HZ | 2.16 | 0.42 |
| 1:3S:166:THR:HG1 | 1:3S:199:CYS:HB2 | 1.85 | 0.42 |
| 1:3S:186:THR:HG21 | 1:3S:385:PHE:CG | 2.54 | 0.42 |
| 3:3V:15:ARG:HB2 | 3:3V:19:LEU:HD12 | 2.01 | 0.42 |
| 3:3Z:282:GLU:OE2 | 3:3Z:290:PHE:HB2 | 2.20 | 0.42 |
| 4:4A:30:SER:H | 4:4A:57:THR:HG22 | 1.83 | 0.42 |
| 3:4B:282:GLU:OE2 | 3:4B:290:PHE:HB2 | 2.20 | 0.42 |
| 3:4D:282:GLU:OE2 | 3:4D:290:PHE:HB2 | 2.20 | 0.42 |
| 4:4E:30:SER:H | 4:4E:57:THR:HG22 | 1.83 | 0.42 |
| 3:4F:282:GLU:OE2 | 3:4F:290:PHE:HB2 | 2.20 | 0.42 |
| 6:4O:268:ARG:HA | 6:4O:271:ARG:HD2 | 2.01 | 0.42 |
| 6:4P:138:LYS:HA | 6:4P:141:VAL:HG22 | 2.01 | 0.42 |
| 7:4R:100:TRP:O | 7:4R:104:ARG:HB2 | 2.20 | 0.42 |
| 8:4W:463:THR:HG22 | 8:4W:464:VAL:N | 2.35 | 0.42 |
| 9:4Z:67:GLU:OE1 | 9:4Z:70:ARG:NH1 | 2.53 | 0.42 |
| 10:5C:193:VAL:O | 10:5C:197:GLU:HG2 | 2.19 | 0.42 |
| 10:5C:348:ARG:O | 10:5C:352:GLU:HG2 | 2.19 | 0.42 |
| 12:5F:304:ARG:HD3 | 12:7B:7:MET:HE3 | 2.02 | 0.42 |
| 14:5L:470:GLY:N | 14:5L:490:ASP:OD1 | 2.52 | 0.42 |
| 14:5L:484:CYS:SG | 14:5L:496:TRP:HB2 | 2.59 | 0.42 |
| 14:5L:500:THR:O | 14:5L:502:LYS:N | 2.53 | 0.42 |
| 14:5M:484:CYS:SG | 14:5M:496:TRP:HB2 | 2.59 | 0.42 |
| 14:5N:24:HIS:CB | 14:5N:29:THR:HB | 2.50 | 0.42 |
| 14:5N:500:THR:O | 14:5N:502:LYS:N | 2.53 | 0.42 |
| 14:5N:576:LEU:HD11 | 14:5N:578:LYS:HE3 | 2.02 | 0.42 |
| 17:5S:205:SER:O | 17:5S:209:LYS:HE2 | 2.19 | 0.42 |
| 17:5V:207:VAL:HG22 | 17:5V:211:ARG:NH1 | 2.34 | 0.42 |
| 18:6A:128:GLN:CD | 18:6A:129:PRO:HD3 | 2.39 | 0.42 |
| 18:6C:128:GLN:CD | 18:6C:129:PRO:HD3 | 2.39 | 0.42 |
| 19:6E:59:LEU:HD12 | 19:6E:60:GLY:H | 1.85 | 0.42 |
| 20:6F:181:ARG:NH1 | 20:6F:243:TYR:OH | 2.53 | 0.42 |
| 22:6O:17:ILE:HD13 | 22:6O:17:ILE:HA | 1.93 | 0.42 |
| 22:6P:101:ASN:N | 22:6P:101:ASN:OD1 | 2.50 | 0.42 |
| 24:6V:536:ASP:HB3 | 24:6V:539:THR:HG23 | 2.02 | 0.42 |
| 24:6X:112:GLU:CD | 24:6X:210:VAL:HG23 | 2.41 | 0.42 |
| 24:6X:514:TYR:C | 24:6X:517:LEU:HD12 | 2.35 | 0.42 |
| 24:6Y:152:ARG:HD3 | 24:6Y:160:PHE:CG | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Y:435:LEU:O | 24:6Y:439:MET:HG2 | 2.20 | 0.42 |
| 24:6Y:536:ASP:OD1 | 24:6Y:537:GLU:N | 2.52 | 0.42 |
| 24:6Y:606:ARG:O | 24:6Y:610:ILE:HG13 | 2.20 | 0.42 |
| 24:6Z:415:THR:HG23 | 24:6Z:418:ASP:H | 1.85 | 0.42 |
| 24:6Z:484:GLU:HG3 | 24:6Z:484:GLU:O | 2.19 | 0.42 |
| 24:7A:6:PRO:HD3 | 31:7N:84:TYR:CD1 | 2.49 | 0.42 |
| 24:7A:140:SER:HB2 | 24:7A:142:ILE:HG12 | 2.01 | 0.42 |
| 27:7G:32:GLN:HG2 | 27:7G:32:GLN:H | 1.72 | 0.42 |
| 27:7G:49:HIS:CD2 | 27:7G:50:GLU:HG3 | 2.55 | 0.42 |
| 29:7I:106:THR:O | 29:7I:106:THR:HG23 | 2.20 | 0.42 |
| 29:7J:274:TYR:CD1 | 29:7J:279:ALA:HB2 | 2.55 | 0.42 |
| 30:7K:69:HIS:CG | 30:7K:70:PRO:HD2 | 2.55 | 0.42 |
| 33:7Q:157:LEU:HD23 | 33:7Q:157:LEU:HA | 1.85 | 0.42 |
| 28:7X:314:GLN:O | 28:7X:317:GLU:HG3 | 2.20 | 0.42 |
| 38:8B:166:GLU:N | 38:8B:166:GLU:CD | 2.73 | 0.42 |
| 38:8B:171:ASP:O | 38:8B:173:ALA:N | 2.53 | 0.42 |
| 38:8D:62:THR:OG1 | 38:8D:63:VAL:N | 2.51 | 0.42 |
| 1:A3:44:LEU:CD2 | 18:6C:84:ARG:HH22 | 2.30 | 0.41 |
| 1:B8:279:GLN:NE2 | 24:6Y:108:GLU:O | 2.52 | 0.41 |
| 2:C5:280:LYS:HZ1 | 18:5X:166:HIS:HB3 | 1.85 | 0.41 |
| 1:C6:359:LYS:O | 24:6U:336:THR:HG23 | 2.19 | 0.41 |
| 1:E2:276:ARG:HB3 | 24:6U:314:GLY:HA3 | 2.02 | 0.41 |
| 1:E6:53:GLU:HB2 | 22:6L:255:PHE:CZ | 2.54 | 0.41 |
| 1:F6:37:HIS:NE2 | 24:6T:458:HIS:HE1 | 2.17 | 0.41 |
| 1:G2:108:GLU:HA | 1:G2:111:GLU:OE2 | 2.19 | 0.41 |
| 1:G2:175:VAL:HG12 | 2:G3:329:ASN:OD1 | 2.20 | 0.41 |
| 1:G6:95:THR:HG23 | 1:G6:96:GLY:H | 1.85 | 0.41 |
| 1:G6:156:ARG:NH1 | 1:G6:197:ASP:OD1 | 2.53 | 0.41 |
| 2:G7:15:GLN:HB3 | 2:G7:228:ASN:HD21 | 1.85 | 0.41 |
| 2:G7:212:ILE:O | 2:G7:216:SER:OG | 2.30 | 0.41 |
| 2:G7:221:ARG:NH1 | 22:6O:177:LEU:O | 2.53 | 0.41 |
| 2:G7:242:LEU:HD12 | 2:G7:252:ILE:HG12 | 2.02 | 0.41 |
| 2:G7:289:ALA:HA | 2:G7:331:SER:OG | 2.20 | 0.41 |
| 1:G8:55:THR:HG23 | 1:I4:282:ARG:O | 2.19 | 0.41 |
| 1:G8:311:LEU:HD21 | 1:G8:372:THR:HB | 2.01 | 0.41 |
| 1:H2:77:ARG:HH21 | 1:H2:90:PHE:HD2 | 1.68 | 0.41 |
| 1:H2:286:VAL:CG2 | 1:H2:287:PRO:HD3 | 2.50 | 0.41 |
| 2:H7:170:THR:HG21 | 2:H7:194:LEU:HD11 | 2.02 | 0.41 |
| 1:H8:172:SER:HB3 | 1:H8:175:VAL:CG2 | 2.49 | 0.41 |
| 1:I4:289:LEU:HD23 | 1:I4:365:ALA:HB2 | 2.00 | 0.41 |
| 2:I5:35:GLN:HB3 | 2:I5:59:GLY:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I8:249:ASP:OD2 | 1:I8:252:LYS:N | 2.41 | 0.41 |
| 2:I9:139:ASN:O | 2:I9:170:THR:HA | 2.20 | 0.41 |
| 2:I9:271:SER:OG | 2:I9:377:MET:HB3 | 2.20 | 0.41 |
| 2:J1:317:LEU:HB3 | 2:J1:319:TYR:HE1 | 1.85 | 0.41 |
| 2:J5:88:HIS:HB3 | 2:L1:283:HIS:CG | 2.55 | 0.41 |
| 2:J5:167:LEU:HD13 | 2:J5:200:VAL:HB | 2.01 | 0.41 |
| 1:J8:163:MET:HB3 | 1:J8:250:LEU:HD22 | 2.03 | 0.41 |
| 1:J8:190:HIS:CD2 | 1:J8:411:ALA:HA | 2.54 | 0.41 |
| 1:J8:207:LEU:HB3 | 1:J8:225:LEU:HD22 | 2.02 | 0.41 |
| 2:J9:21:TRP:HZ2 | 2:J9:65:CYS:HB3 | 1.85 | 0.41 |
| 2:J9:256:GLN:N | 2:J9:256:GLN:OE1 | 2.53 | 0.41 |
| 1:K0:19:LYS:HE3 | 1:K0:19:LYS:HB3 | 1.90 | 0.41 |
| 2:K1:320:ARG:O | 2:K1:373:ARG:HA | 2.19 | 0.41 |
| 1:K6:67:ASP:N | 1:K6:67:ASP:OD1 | 2.52 | 0.41 |
| 2:K7:3:GLU:HB2 | 2:K7:129:CYS:SG | 2.60 | 0.41 |
| 1:K8:5:VAL:HG12 | 1:K8:133:PHE:CD1 | 2.55 | 0.41 |
| 1:K8:86:ARG:HG2 | 1:K8:88:ASP:H | 1.85 | 0.41 |
| 2:K9:205:ASP:O | 2:K9:209:ILE:HG13 | 2.19 | 0.41 |
| 2:K9:282:TYR:N | 2:K9:282:TYR:HD2 | 2.18 | 0.41 |
| 1:L0:2:ARG:HB3 | 1:L0:131:GLN:HB2 | 2.02 | 0.41 |
| 2:L1:328:VAL:HG11 | 2:L1:355:ILE:HD11 | 2.02 | 0.41 |
| 2:L3:62:VAL:HA | 2:L3:63:PRO:HD3 | 1.85 | 0.41 |
| 2:L7:165:SER:HB2 | 2:L7:256:GLN:NE2 | 2.35 | 0.41 |
| 1:M0:52:ASN:HD22 | 1:M0:86:ARG:HH21 | 1.67 | 0.41 |
| 1:M2:190:HIS:NE2 | 1:M2:414:ASN:OD1 | 2.53 | 0.41 |
| 1:M4:221:THR:HG21 | 30:7K:156:ASP:HB3 | 2.02 | 0.41 |
| 2:M5:224:TYR:OH | 1:M6:323:THR:HG21 | 2.20 | 0.41 |
| 1:M6:396:HIS:CD2 | 2:M7:263:PRO:HD3 | 2.55 | 0.41 |
| 2:M7:9:ILE:HD13 | 2:M7:150:GLY:HA2 | 2.02 | 0.41 |
| 2:M7:26:LEU:HD21 | 2:M7:363:VAL:HG12 | 2.02 | 0.41 |
| 2:M7:115:VAL:HG22 | 2:M7:119:LEU:HD13 | 2.01 | 0.41 |
| 2:N1:72:PRO:HD2 | 1:N2:2:ARG:NH1 | 2.34 | 0.41 |
| 2:N1:247:ALA:HB2 | 2:N1:357:TYR:CZ | 2.55 | 0.41 |
| 2:N5:88:HIS:CE1 | 2:N5:90:GLU:H | 2.38 | 0.41 |
| 2:N5:269:LEU:HD11 | 2:N5:384:ILE:HG13 | 2.02 | 0.41 |
| 1:N6:278:SER:HB2 | 1:N6:281:TYR:CD2 | 2.55 | 0.41 |
| 2:N7:88:HIS:ND1 | 2:N7:89:PRO:HD2 | 2.35 | 0.41 |
| 1:N8:390:ARG:HB3 | 2:N9:346:TRP:CZ3 | 2.44 | 0.41 |
| 1:O2:20:PHE:HA | 1:O2:230:SER:OG | 2.19 | 0.41 |
| 1:O2:344:TRP:CE3 | 1:O2:345:ILE:HG13 | 2.54 | 0.41 |
| 2:O3:155:GLU:HG2 | 2:O3:197:HIS:NE2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O3:219:ILE:O | 2:O3:219:ILE:HG13 | 2.20 | 0.41 |
| 1:O4:125:GLU:OE2 | 1:O4:159:TYR:OH | 2.38 | 0.41 |
| 2:O5:53:PHE:HB3 | 2:O5:61:HIS:HB3 | 2.01 | 0.41 |
| 2:O7:121:ARG:HA | 2:O7:121:ARG:HD2 | 1.85 | 0.41 |
| 1:O8:22:GLU:HG2 | 1:O8:81:TYR:CD2 | 2.55 | 0.41 |
| 1:P4:100:ASN:HB3 | 1:P4:103:LYS:HB2 | 2.02 | 0.41 |
| 1:P6:165:LEU:HD23 | 1:P6:250:LEU:HD13 | 2.02 | 0.41 |
| 2:P7:266:HIS:O | 2:P7:266:HIS:ND1 | 2.52 | 0.41 |
| 1:P8:375:GLN:HB2 | 1:P8:419:VAL:HG13 | 2.02 | 0.41 |
| 2:Q1:289:ALA:HA | 2:Q1:331:SER:OG | 2.20 | 0.41 |
| 2:Q1:290:GLU:OE1 | 2:Q1:290:GLU:N | 2.44 | 0.41 |
| 1:Q2:73:MET:CE | 1:Q2:90:PHE:HB3 | 2.50 | 0.41 |
| 2:Q3:320:ARG:O | 2:Q3:373:ARG:HA | 2.19 | 0.41 |
| 1:Q4:311:LEU:HA | 1:Q4:311:LEU:HD23 | 1.71 | 0.41 |
| 1:Q6:42:LEU:HD23 | 1:Q6:42:LEU:HA | 1.81 | 0.41 |
| 1:Q6:387:ALA:HA | 1:Q6:390:ARG:HH21 | 1.85 | 0.41 |
| 1:Q8:46:ARG:HG3 | 1:Q8:46:ARG:O | 2.20 | 0.41 |
| 1:Q8:193:VAL:HG23 | 1:Q8:194:GLU:OE1 | 2.20 | 0.41 |
| 2:Q9:163:LYS:HA | 2:Q9:163:LYS:HD3 | 1.77 | 0.41 |
| 2:Q9:325:PRO:HA | 2:Q9:328:VAL:HG12 | 2.01 | 0.41 |
| 1:R0:95:THR:HG23 | 1:R0:96:GLY:H | 1.85 | 0.41 |
| 2:R1:361:THR:OG1 | 2:R1:362:VAL:N | 2.53 | 0.41 |
| 2:R7:320:ARG:O | 2:R7:373:ARG:HA | 2.21 | 0.41 |
| 2:R9:431:ASP:OD1 | 17:5U:87:VAL:HG21 | 2.20 | 0.41 |
| 1:S0:320:ARG:CZ | 12:5F:108:ASN:HD22 | 2.33 | 0.41 |
| 2:S1:397:LEU:HD23 | 2:S1:397:LEU:HA | 1.86 | 0.41 |
| 1:S2:405:GLU:HA | 1:S2:408:PHE:HD2 | 1.84 | 0.41 |
| 1:S4:174:LYS:HB3 | 13:5H:14:PHE:HE2 | 1.84 | 0.41 |
| 2:S5:14:ILE:HD11 | 2:S5:74:VAL:CG1 | 2.48 | 0.41 |
| 1:S6:107:THR:OG1 | 1:S6:108:GLU:OE1 | 2.26 | 0.41 |
| 1:S6:190:HIS:HE2 | 1:S6:410:GLU:HG2 | 1.84 | 0.41 |
| 1:T0:249:ASP:H | 1:T0:252:LYS:HE3 | 1.85 | 0.41 |
| 1:T0:335:ASN:O | 1:T0:338:SER:OG | 2.35 | 0.41 |
| 2:T5:14:ILE:HD11 | 2:T5:74:VAL:HG13 | 2.01 | 0.41 |
| 1:T6:178:THR:HG22 | 1:T6:180:VAL:H | 1.85 | 0.41 |
| 2:T7:207:GLU:OE1 | 2:T7:207:GLU:HA | 2.20 | 0.41 |
| 2:U1:33:ASP:OD2 | 2:U1:34:GLY:N | 2.53 | 0.41 |
| 2:U1:286:LEU:HD11 | 2:U1:291:ILE:CG2 | 2.49 | 0.41 |
| 1:U2:163:MET:HB3 | 1:U2:250:LEU:HD22 | 2.00 | 0.41 |
| 2:U5:60:LYS:HD3 | 2:W1:282:TYR:CE2 | 2.54 | 0.41 |
| 1:U6:86:ARG:HB3 | 1:U6:89:ASN:OD1 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U7:217:LEU:HD23 | 2:U7:217:LEU:HA | 1.88 | 0.41 |
| 1:U8:387:ALA:HA | 1:U8:390:ARG:HH21 | 1.85 | 0.41 |
| 2:V1:216:SER:OG | 2:V1:217:LEU:N | 2.53 | 0.41 |
| 2:V7:253:THR:HG23 | 2:V7:254:GLU:OE2 | 2.20 | 0.41 |
| 2:V7:401:LYS:HE3 | 2:V7:401:LYS:HB3 | 1.79 | 0.41 |
| 1:W0:273:LEU:H | 1:W0:292:GLN:NE2 | 2.18 | 0.41 |
| 1:W0:286:VAL:HB | 1:W0:287:PRO:HD3 | 2.02 | 0.41 |
| 2:W7:5:ILE:HD11 | 2:W7:135:PHE:HE1 | 1.84 | 0.41 |
| 2:W9:286:LEU:HD11 | 2:W9:291:ILE:CG2 | 2.51 | 0.41 |
| 1:X0:273:LEU:H | 1:X0:292:GLN:HE22 | 1.68 | 0.41 |
| 1:X0:417:ASP:HA | 1:X0:420:SER:OG | 2.20 | 0.41 |
| 2:X5:301:MET:C | 2:X5:303:VAL:H | 2.23 | 0.41 |
| 1:X6:396:HIS:CE1 | 1:X6:397:TRP:CE2 | 3.08 | 0.41 |
| 2:X7:73:THR:HG23 | 2:X7:74:VAL:N | 2.35 | 0.41 |
| 2:X7:89:PRO:HD2 | 2:Z3:283:HIS:ND1 | 2.34 | 0.41 |
| 2:X7:409:VAL:HA | 2:X7:413:MET:O | 2.20 | 0.41 |
| 1:X8:190:HIS:HD2 | 1:X8:414:ASN:ND2 | 2.18 | 0.41 |
| 1:X8:403:MET:HE2 | 1:X8:403:MET:HB2 | 1.73 | 0.41 |
| 2:X9:21:TRP:CZ3 | 2:X9:63:PRO:HB3 | 2.55 | 0.41 |
| 1:Y0:101:TRP:CE3 | 1:Y0:403:MET:HE1 | 2.54 | 0.41 |
| 2:Y1:236:SER:HA | 2:Y1:239:THR:HG22 | 2.02 | 0.41 |
| 1:Y2:266:PHE:CE1 | 1:Y2:370:ASN:HB2 | 2.55 | 0.41 |
| 2:Y5:190:SER:O | 2:Y5:194:LEU:HG | 2.19 | 0.41 |
| 2:Y5:401:LYS:HE3 | 2:Y5:401:LYS:HB3 | 1.89 | 0.41 |
| 1:Y6:257:LEU:HD23 | 1:Y6:312:THR:HG23 | 2.02 | 0.41 |
| 1:Y8:267:MET:HE3 | 1:Y8:303:ALA:HB3 | 2.02 | 0.41 |
| 1:Z0:50:TYR:HD2 | 1:Z0:241:ARG:HD3 | 1.85 | 0.41 |
| 1:Z0:181:GLU:OE2 | 2:Z1:349:THR:HG21 | 2.20 | 0.41 |
| 1:Z0:396:HIS:CE1 | 1:Z0:397:TRP:CE2 | 3.08 | 0.41 |
| 2:Z1:34:GLY:HA3 | 2:Z1:60:LYS:NZ | 2.35 | 0.41 |
| 2:Z5:81:GLY:O | 2:Z5:84:ARG:NH1 | 2.52 | 0.41 |
| 2:Z5:407:TRP:O | 2:Z5:411:GLU:HG2 | 2.20 | 0.41 |
| 1:Z8:43:GLN:O | 1:Z8:47:ILE:HG23 | 2.20 | 0.41 |
| 1:Z8:233:MET:O | 1:Z8:236:ILE:HG22 | 2.20 | 0.41 |
| 1:Z8:294:TRP:CD1 | 1:Z8:333:VAL:HG21 | 2.55 | 0.41 |
| 1:Z8:310:TYR:HB2 | 1:Z8:341:PHE:CD1 | 2.55 | 0.41 |
| 2:Z9:287:SER:HB3 | 2:Z9:290:GLU:CD | 2.40 | 0.41 |
| 2:0B:208:ALA:HA | 2:0B:211:ASP:OD2 | 2.20 | 0.41 |
| 2:0B:320:ARG:HE | 2:0B:320:ARG:HB3 | 1.54 | 0.41 |
| 2:0F:83:TYR:CD1 | 2:0F:86:LEU:HD13 | 2.55 | 0.41 |
| 1:0G:49:VAL:HG13 | 1:0G:50:TYR:CD2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0G:379:LYS:HD3 | 1:0G:419:VAL:HG21 | 2.02 | 0.41 |
| 1:0I:156:ARG:NH1 | 1:0I:160:PRO:O | 2.53 | 0.41 |
| 2:0J:209:ILE:HA | 2:0J:212:ILE:HG12 | 2.02 | 0.41 |
| 2:0J:297:GLU:OE1 | 2:0J:298:PRO:HD2 | 2.20 | 0.41 |
| 2:0J:392:ASP:OD1 | 2:0J:422:ARG:NH1 | 2.53 | 0.41 |
| 1:0M:140:GLY:O | 1:0M:184:ASN:ND2 | 2.52 | 0.41 |
| 2:0N:30:ILE:HG12 | 2:0N:36:MET:HG2 | 2.02 | 0.41 |
| 2:0N:141:VAL:HG22 | 2:0N:171:VAL:O | 2.20 | 0.41 |
| 2:0N:224:TYR:CD2 | 1:0O:245:GLN:HB3 | 2.54 | 0.41 |
| 1:0O:327:ASP:N | 1:0O:327:ASP:OD2 | 2.52 | 0.41 |
| 1:0O:358:PRO:HG2 | 1:0O:361:LEU:HD13 | 2.01 | 0.41 |
| 1:0O:396:HIS:HE1 | 1:0O:397:TRP:CZ2 | 2.37 | 0.41 |
| 2:0P:33:ASP:OD2 | 2:0P:35:GLN:NE2 | 2.53 | 0.41 |
| 2:0P:222:PRO:HD2 | 1:0Q:324:LYS:HE3 | 2.02 | 0.41 |
| 1:0Q:250:LEU:HD13 | 1:0Q:250:LEU:HA | 1.92 | 0.41 |
| 1:0Q:276:ARG:HA | 1:0Q:279:GLN:HG3 | 2.01 | 0.41 |
| 1:0S:374:ILE:HG12 | 1:0S:378:PHE:CZ | 2.54 | 0.41 |
| 1:0U:190:HIS:CD2 | 1:0U:411:ALA:HA | 2.55 | 0.41 |
| 1:0W:344:TRP:O | 1:0W:345:ILE:HD13 | 2.19 | 0.41 |
| 1:0W:375:GLN:NE2 | 1:0W:423:GLN:HE21 | 2.18 | 0.41 |
| 2:0X:427:ALA:HA | 2:0X:430:LYS:HE2 | 2.01 | 0.41 |
| 2:0Z:7:ILE:HD11 | 2:0Z:137:VAL:HG12 | 2.02 | 0.41 |
| 2:0Z:21:TRP:CZ2 | 2:0Z:65:CYS:HB2 | 2.55 | 0.41 |
| 2:0Z:75:VAL:HG11 | 2:0Z:94:SER:HB2 | 2.02 | 0.41 |
| 2:0Z:367:ASP:OD2 | 2:0Z:368:LEU:HD12 | 2.20 | 0.41 |
| 1:1A:256:ASN:HD22 | 1:1A:350:LYS:HD3 | 1.85 | 0.41 |
| 2:1F:2:ARG:HB2 | 2:1F:242:LEU:HD11 | 2.01 | 0.41 |
| 2:1F:420:GLU:O | 2:1F:424:ASP:HB2 | 2.19 | 0.41 |
| 1:1G:169:VAL:HG22 | 1:1G:202:LEU:HB2 | 2.01 | 0.41 |
| 2:1H:252:ILE:O | 2:1H:256:GLN:NE2 | 2.51 | 0.41 |
| 2:1L:53:PHE:HB3 | 2:1L:61:HIS:HB3 | 2.01 | 0.41 |
| 2:1P:377:MET:HE3 | 2:1P:379:SER:HB3 | 2.01 | 0.41 |
| 1:1Q:384:GLN:HB3 | 2:1R:348:PRO:HG3 | 2.01 | 0.41 |
| 2:1R:58:ALA:N | 10:5B:156:TYR:HE2 | 2.18 | 0.41 |
| 2:1V:320:ARG:NH2 | 2:1V:359:PRO:O | 2.53 | 0.41 |
| 2:1X:227:LEU:O | 2:1X:230:LEU:HG | 2.20 | 0.41 |
| 2:1X:330:ALA:O | 2:1X:334:THR:HG23 | 2.20 | 0.41 |
| 1:2A:286:VAL:CG2 | 1:2A:287:PRO:HD3 | 2.48 | 0.41 |
| 1:2A:417:ASP:OD1 | 1:2A:418:LEU:N | 2.53 | 0.41 |
| 2:2B:145:THR:OG1 | 41:2C:501:GTP:O1B | 2.38 | 0.41 |
| 1:2C:192:LEU:HD23 | 1:2C:192:LEU:HA | 1.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2C:201:VAL:HG21 | 1:2C:374:ILE:HD11 | 2.01 | 0.41 |
| 1:2E:216:LYS:HB2 | 1:2E:275:SER:OG | 2.20 | 0.41 |
| 1:2E:418:LEU:O | 1:2E:421:GLU:HG2 | 2.20 | 0.41 |
| 2:2F:335:ILE:HG23 | 2:2F:341:ILE:HD11 | 2.02 | 0.41 |
| 1:2I:395:LEU:O | 1:2I:399:THR:HG23 | 2.20 | 0.41 |
| 2:2L:195:LEU:O | 2:2L:266:HIS:NE2 | 2.54 | 0.41 |
| 1:2Q:183:TYR:HB3 | 1:2Q:398:TYR:HE2 | 1.84 | 0.41 |
| 1:2Q:309:ARG:NH1 | 1:2Q:339:SER:O | 2.53 | 0.41 |
| 1:2S:48:ASN:OD1 | 1:2S:48:ASN:N | 2.52 | 0.41 |
| 1:2U:320:ARG:HH12 | 38:8B:197:THR:C | 2.23 | 0.41 |
| 2:2V:308:ARG:NH2 | 38:8B:73:TRP:N | 2.68 | 0.41 |
| 2:2V:312:TYR:HB2 | 2:2V:343:PHE:CD1 | 2.54 | 0.41 |
| 2:2V:384:ILE:HA | 2:2V:387:ILE:HD12 | 2.02 | 0.41 |
| 1:3A:161:ASP:OD1 | 1:3A:161:ASP:N | 2.41 | 0.41 |
| 2:3B:62:VAL:HA | 2:3B:63:PRO:HD3 | 1.91 | 0.41 |
| 2:3B:203:MET:O | 2:3B:204:LEU:HD22 | 2.20 | 0.41 |
| 1:3C:44:LEU:HA | 1:3C:47:ILE:CD1 | 2.50 | 0.41 |
| 1:3C:95:THR:HG23 | 1:3C:96:GLY:N | 2.35 | 0.41 |
| 1:3C:203:ASP:OD1 | 1:3C:302:ALA:N | 2.51 | 0.41 |
| 2:3D:154:LEU:HD11 | 2:3D:166:LYS:HD2 | 2.01 | 0.41 |
| 2:3D:173:PRO:HB3 | 2:3D:183:GLU:OE2 | 2.20 | 0.41 |
| 2:3F:179:THR:O | 1:3G:350:LYS:HD2 | 2.20 | 0.41 |
| 1:3G:50:TYR:OH | 1:3G:237:THR:HG21 | 2.20 | 0.41 |
| 1:3I:317:PHE:CD2 | 1:3I:321:MET:HE1 | 2.55 | 0.41 |
| 2:3L:109:THR:OG1 | 2:3L:411:GLU:OE2 | 2.31 | 0.41 |
| 2:3L:184:PRO:O | 2:3L:188:VAL:HG22 | 2.20 | 0.41 |
| 2:3L:217:LEU:HD22 | 2:3L:367:ASP:HB3 | 2.02 | 0.41 |
| 2:3P:22:GLU:OE2 | 2:3P:363:VAL:HG11 | 2.20 | 0.41 |
| 1:3Q:272:PRO:HB2 | 1:3Q:282:ARG:NH1 | 2.32 | 0.41 |
| 2:3R:52:PHE:CE2 | 2:3R:243:ARG:HD3 | 2.55 | 0.41 |
| 2:3R:157:LEU:HD23 | 2:3R:157:LEU:HA | 1.79 | 0.41 |
| 1:3S:165:LEU:HD23 | 1:3S:165:LEU:HA | 1.93 | 0.41 |
| 4:3W:30:SER:H | 4:3W:57:THR:HG22 | 1.83 | 0.41 |
| 3:4D:15:ARG:HB2 | 3:4D:19:LEU:HD12 | 2.02 | 0.41 |
| 3:4H:15:ARG:HB2 | 3:4H:19:LEU:HD12 | 2.01 | 0.41 |
| 6:4N:488:SER:HA | 6:4N:491:LEU:HD12 | 2.01 | 0.41 |
| 9:4Y:420:ILE:HD13 | 9:4Y:420:ILE:HA | 1.91 | 0.41 |
| 10:5A:364:ALA:O | 10:5A:367:GLU:HG3 | 2.20 | 0.41 |
| 10:5B:314:LYS:HA | 10:5B:317:ILE:HG12 | 2.02 | 0.41 |
| 11:5E:110:GLN:HB3 | 11:5E:111:PRO:HD2 | 2.02 | 0.41 |
| 11:5E:238:THR:HA | 11:5E:239:PRO:HD3 | 1.91 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:5H:6:PRO:HB3 | 13:5H:40:ARG:O | 2.20 | 0.41 |
| 14:5L:24:HIS:CB | 14:5L:29:THR:HB | 2.50 | 0.41 |
| 14:5L:319:TYR:HA | 14:5L:334:LEU:HA | 2.01 | 0.41 |
| 14:5L:587:CYS:HB3 | 14:5L:589:PHE:CD1 | 2.51 | 0.41 |
| 14:5M:587:CYS:HB3 | 14:5M:589:PHE:CD1 | 2.51 | 0.41 |
| 14:5N:587:CYS:HB3 | 14:5N:589:PHE:CD1 | 2.51 | 0.41 |
| 15:5O:268:GLY:HA2 | 15:5O:308:ALA:O | 2.20 | 0.41 |
| 15:5P:11:SER:HB3 | 15:5P:75:LEU:HA | 2.02 | 0.41 |
| 15:5P:12:GLU:OE1 | 15:5P:12:GLU:N | 2.48 | 0.41 |
| 17:5U:205:SER:OG | 17:5U:208:LYS:HG3 | 2.20 | 0.41 |
| 18:5X:128:GLN:CD | 18:5X:129:PRO:HD3 | 2.39 | 0.41 |
| 18:6D:128:GLN:CD | 18:6D:129:PRO:HD3 | 2.39 | 0.41 |
| 21:6H:14:LEU:HG | 21:6H:131:TYR:CE2 | 2.50 | 0.41 |
| 22:6I:102:ILE:O | 22:6I:102:ILE:HG13 | 2.19 | 0.41 |
| 22:6I:186:ARG:O | 22:6I:189:LYS:HB2 | 2.20 | 0.41 |
| 22:6L:330:ALA:N | 22:6L:331:PRO:HD2 | 2.35 | 0.41 |
| 22:6P:170:ARG:HH12 | 22:6P:249:SER:HA | 1.84 | 0.41 |
| 22:6P:273:VAL:O | 22:6P:276:LEU:HG | 2.20 | 0.41 |
| 23:6R:28:LYS:H | 23:6R:28:LYS:HE3 | 1.84 | 0.41 |
| 24:6U:40:GLN:HA | 24:6U:40:GLN:OE1 | 2.20 | 0.41 |
| 24:6U:480:ASN:ND2 | 24:6U:503:ILE:HD12 | 2.34 | 0.41 |
| 24:6U:480:ASN:OD1 | 24:6U:480:ASN:N | 2.53 | 0.41 |
| 24:6U:505:LYS:HG3 | 24:6U:510:GLU:O | 2.19 | 0.41 |
| 24:6V:565:GLN:NE2 | 24:6V:602:LEU:HB2 | 2.34 | 0.41 |
| 24:6W:274:ARG:HD3 | 24:6W:295:HIS:HE1 | 1.85 | 0.41 |
| 24:6W:577:VAL:HG21 | 24:6W:630:LEU:HD21 | 2.02 | 0.41 |
| 24:6X:420:LEU:HD12 | 24:6X:423:CYS:SG | 2.60 | 0.41 |
| 24:6Y:42:GLU:N | 24:6Y:42:GLU:CD | 2.73 | 0.41 |
| 24:6Y:445:ILE:HG22 | 24:6Y:474:PHE:CD1 | 2.55 | 0.41 |
| 24:6Z:153:VAL:HG23 | 24:6Z:175:TYR:CZ | 2.55 | 0.41 |
| 24:6Z:560:ARG:HA | 24:6Z:563:LYS:HE3 | 2.01 | 0.41 |
| 26:7E:50:SER:N | 26:7E:56:LEU:HD21 | 2.35 | 0.41 |
| 29:7I:253:ASN:HB3 | 30:7K:341:ARG:HH22 | 1.83 | 0.41 |
| 29:7J:117:ASN:HB3 | 29:7J:120:PRO:HG2 | 2.01 | 0.41 |
| 29:7J:233:LYS:HD2 | 29:7J:233:LYS:HA | 1.89 | 0.41 |
| 29:7J:424:LEU:HD23 | 29:7J:424:LEU:HA | 1.85 | 0.41 |
| 30:7K:340:VAL:HG11 | 30:7K:354:TYR:HE1 | 1.85 | 0.41 |
| 30:7K:399:LEU:HB2 | 30:7K:403:ASP:OD1 | 2.20 | 0.41 |
| 34:7R:167:THR:HG23 | 35:7T:115:MET:HA | 2.02 | 0.41 |
| 28:7X:301:GLU:OE1 | 28:7X:302:ALA:N | 2.53 | 0.41 |
| 38:7Z:12:LEU:HB3 | 38:7Z:18:VAL:CG2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8C:206:PRO:CG | 38:8C:209:HIS:CE1 | 3.03 | 0.41 |
| 38:8C:229:ASN:HB3 | 38:8C:232:PHE:CZ | 2.54 | 0.41 |
| 1:A3:40:SER:HA | 26:7F:122:VAL:CB | 2.49 | 0.41 |
| 1:F0:53:GLU:HB2 | 22:6N:255:PHE:CE1 | 2.54 | 0.41 |
| 1:F8:218:THR:N | 24:6U:418:ASP:OD2 | 2.49 | 0.41 |
| 1:G0:388:MET:HE3 | 2:G1:348:PRO:HD3 | 2.01 | 0.41 |
| 2:G1:259:LEU:HD11 | 2:G1:316:CYS:HB2 | 2.01 | 0.41 |
| 1:G2:344:TRP:CE3 | 1:G2:345:ILE:HG13 | 2.55 | 0.41 |
| 2:G3:117:LEU:HD12 | 2:G3:117:LEU:HA | 1.89 | 0.41 |
| 2:G3:238:LEU:HD11 | 2:G3:255:PHE:CZ | 2.56 | 0.41 |
| 1:G4:3:GLU:HB2 | 1:G4:130:LEU:HA | 2.01 | 0.41 |
| 1:G4:421:GLU:HA | 1:G4:424:GLN:HB3 | 2.03 | 0.41 |
| 1:G8:100:ASN:HB3 | 1:G8:103:LYS:HB2 | 2.02 | 0.41 |
| 2:G9:188:VAL:HG21 | 2:G9:395:PHE:CG | 2.55 | 0.41 |
| 2:H1:261:PRO:HG2 | 2:H1:262:TYR:CD2 | 2.55 | 0.41 |
| 1:H2:286:VAL:HG21 | 1:H2:325:GLU:HB3 | 2.02 | 0.41 |
| 1:H2:317:PHE:HB3 | 1:H2:321:MET:SD | 2.60 | 0.41 |
| 2:H3:7:ILE:HD11 | 2:H3:137:VAL:HG12 | 2.01 | 0.41 |
| 2:H3:344:VAL:HG13 | 2:H3:347:CYS:H | 1.84 | 0.41 |
| 1:H4:154:LYS:HD3 | 1:H4:154:LYS:HA | 1.87 | 0.41 |
| 1:H4:213:ARG:NH2 | 1:H4:297:LYS:HG3 | 2.35 | 0.41 |
| 2:H5:72:PRO:HD2 | 1:H6:2:ARG:NH1 | 2.35 | 0.41 |
| 2:H7:195:LEU:HD21 | 2:H7:264:ARG:CD | 2.49 | 0.41 |
| 2:H9:33:ASP:OD1 | 2:H9:33:ASP:N | 2.51 | 0.41 |
| 1:I0:273:LEU:H | 1:I0:292:GLN:HE22 | 1.67 | 0.41 |
| 1:I0:297:LYS:HA | 1:I0:297:LYS:HD3 | 1.89 | 0.41 |
| 1:I2:164:MET:HE3 | 1:I2:164:MET:HB2 | 1.88 | 0.41 |
| 1:I2:236:ILE:HG23 | 1:I2:237:THR:HG23 | 2.01 | 0.41 |
| 1:I4:116:VAL:HA | 1:I4:119:VAL:HG12 | 2.03 | 0.41 |
| 2:I5:79:ARG:HH11 | 2:I5:92:LEU:HB2 | 1.85 | 0.41 |
| 2:I7:145:THR:OG1 | 41:I8:501:GTP:O1B | 2.38 | 0.41 |
| 2:I7:368:LEU:HD13 | 2:I7:368:LEU:HA | 1.96 | 0.41 |
| 1:I8:185:ALA:O | 1:I8:189:VAL:HG12 | 2.20 | 0.41 |
| 2:I9:14:ILE:HD11 | 2:I9:74:VAL:HG13 | 2.01 | 0.41 |
| 2:I9:278:ALA:HA | 2:I9:369:ALA:HB2 | 2.02 | 0.41 |
| 2:J1:237:SER:HA | 2:J1:320:ARG:HD2 | 2.01 | 0.41 |
| 2:J1:262:TYR:HE2 | 2:J1:346:TRP:CZ3 | 2.38 | 0.41 |
| 2:J3:62:VAL:HA | 2:J3:63:PRO:HD3 | 1.93 | 0.41 |
| 1:J4:68:LEU:HD21 | 1:J4:112:LEU:HD22 | 2.02 | 0.41 |
| 2:J5:264:ARG:NH2 | 2:J5:431:ASP:OD2 | 2.53 | 0.41 |
| 1:J6:21:TRP:CZ3 | 1:J6:61:PRO:HB3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J6:91:VAL:HG11 | 1:J6:116:VAL:HG22 | 2.02 | 0.41 |
| 2:J7:9:ILE:HD13 | 2:J7:150:GLY:HA2 | 2.01 | 0.41 |
| 1:K0:5:VAL:HG23 | 1:K0:62:ARG:HG2 | 2.02 | 0.41 |
| 1:K0:212:PHE:HZ | 2:K1:326:LYS:HB2 | 1.85 | 0.41 |
| 2:K1:103:PHE:CE1 | 2:K1:148:GLY:HA2 | 2.55 | 0.41 |
| 2:K1:210:TYR:HE1 | 2:K1:227:LEU:CD1 | 2.32 | 0.41 |
| 1:K4:178:THR:HG22 | 1:K4:181:GLU:HG3 | 2.02 | 0.41 |
| 1:K4:309:ARG:NH1 | 1:K4:341:PHE:O | 2.53 | 0.41 |
| 2:L1:288:VAL:HG13 | 2:L1:319:TYR:HE2 | 1.84 | 0.41 |
| 1:L2:263:LEU:HD13 | 1:L2:422:TYR:CE2 | 2.55 | 0.41 |
| 2:L5:206:ASN:OD1 | 41:L6:501:GTP:N2 | 2.53 | 0.41 |
| 2:L5:213:CYS:SG | 2:L5:219:ILE:HB | 2.60 | 0.41 |
| 2:L7:217:LEU:HG | 2:L7:219:ILE:HG12 | 2.02 | 0.41 |
| 2:L9:125:LEU:HD23 | 2:L9:125:LEU:HA | 1.82 | 0.41 |
| 1:M0:48:ASN:OD1 | 1:M0:48:ASN:N | 2.53 | 0.41 |
| 1:M6:7:ILE:O | 1:M6:135:VAL:HA | 2.20 | 0.41 |
| 1:M8:175:VAL:HG23 | 1:M8:175:VAL:O | 2.20 | 0.41 |
| 1:N2:167:PHE:CE2 | 1:N2:233:MET:HG2 | 2.54 | 0.41 |
| 1:N2:320:ARG:NH1 | 29:7J:110:THR:HA | 2.28 | 0.41 |
| 2:N5:98:ASP:OD1 | 2:N5:99:ALA:N | 2.52 | 0.41 |
| 1:N6:396:HIS:H | 1:N6:396:HIS:CD2 | 2.38 | 0.41 |
| 2:N7:32:PRO:HB3 | 2:N7:83:TYR:CE1 | 2.56 | 0.41 |
| 2:N7:52:PHE:CZ | 2:N7:239:THR:HG21 | 2.55 | 0.41 |
| 1:N8:320:ARG:HH22 | 27:7G:132:THR:HA | 1.85 | 0.41 |
| 1:O0:67:ASP:OD2 | 1:O0:72:THR:OG1 | 2.32 | 0.41 |
| 2:O1:65:CYS:SG | 2:O1:66:ILE:N | 2.94 | 0.41 |
| 1:O4:130:LEU:HB2 | 1:O4:162:ARG:HE | 1.85 | 0.41 |
| 1:O6:282:ARG:NH1 | 1:O6:288:GLU:OE2 | 2.54 | 0.41 |
| 1:P4:180:VAL:HG23 | 1:P4:184:ASN:HD21 | 1.85 | 0.41 |
| 2:P7:4:VAL:HG23 | 2:P7:134:GLY:O | 2.20 | 0.41 |
| 2:P7:66:ILE:HD11 | 2:P7:122:ILE:HD11 | 2.03 | 0.41 |
| 2:P9:306:ASP:OD2 | 2:U7:282:TYR:OH | 2.28 | 0.41 |
| 1:Q0:338:SER:O | 1:Q0:338:SER:OG | 2.38 | 0.41 |
| 2:Q5:88:HIS:HB3 | 2:Q5:91:GLN:HG3 | 2.01 | 0.41 |
| 1:Q8:219:THR:HB | 2:Q9:324:VAL:HG11 | 2.02 | 0.41 |
| 1:Q8:311:LEU:HA | 1:Q8:342:VAL:CG2 | 2.50 | 0.41 |
| 2:Q9:298:PRO:HB3 | 2:Q9:307:PRO:HD2 | 2.01 | 0.41 |
| 2:Q9:428:LEU:HG | 2:Q9:432:PHE:HE2 | 1.85 | 0.41 |
| 1:R2:114:ASP:OD2 | 1:R2:114:ASP:N | 2.51 | 0.41 |
| 2:R3:49:PHE:HB2 | 2:R3:53:PHE:HD2 | 1.85 | 0.41 |
| 1:R4:42:LEU:HD23 | 21:6G:94:THR:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:395:LEU:HD21 | 1:R4:405:GLU:OE1 | 2.20 | 0.41 |
| 2:R5:113:GLU:OE2 | 2:R5:113:GLU:N | 2.52 | 0.41 |
| 2:R5:176:GLN:HG2 | 2:R5:177:VAL:H | 1.85 | 0.41 |
| 1:S0:117:LEU:HD23 | 1:S0:117:LEU:HA | 1.76 | 0.41 |
| 1:S0:154:LYS:HA | 1:S0:154:LYS:HD3 | 1.93 | 0.41 |
| 1:S0:344:TRP:CE3 | 1:S0:345:ILE:HG13 | 2.56 | 0.41 |
| 1:S0:361:LEU:HD23 | 1:S0:361:LEU:HA | 1.94 | 0.41 |
| 1:S2:83:GLN:O | 1:T8:281:TYR:OH | 2.29 | 0.41 |
| 1:S2:424:GLN:NE2 | 17:5V:104:PHE:HD2 | 2.18 | 0.41 |
| 1:S4:178:THR:HG22 | 2:S5:352:LYS:HE2 | 2.02 | 0.41 |
| 2:S5:116:ASP:OD1 | 2:S5:117:LEU:N | 2.53 | 0.41 |
| 1:S6:138:SER:OG | 1:S6:139:LEU:N | 2.53 | 0.41 |
| 2:S7:288:VAL:HG13 | 2:S7:319:TYR:HE2 | 1.85 | 0.41 |
| 1:S8:156:ARG:NH1 | 1:S8:197:ASP:OD1 | 2.53 | 0.41 |
| 1:S8:216:LYS:HB2 | 1:S8:275:SER:OG | 2.20 | 0.41 |
| 1:S8:317:PHE:HB3 | 1:S8:321:MET:SD | 2.60 | 0.41 |
| 2:S9:326:LYS:HD2 | 2:S9:327:ASP:N | 2.35 | 0.41 |
| 1:T0:285:THR:CB | 1:T0:287:PRO:HD2 | 2.49 | 0.41 |
| 2:T1:98:ASP:OD1 | 2:T1:100:ALA:HB2 | 2.20 | 0.41 |
| 2:T1:324:VAL:HG23 | 2:T1:326:LYS:HG2 | 2.01 | 0.41 |
| 1:T2:44:LEU:HD23 | 1:T2:44:LEU:HA | 1.78 | 0.41 |
| 1:T2:189:VAL:O | 1:T2:193:VAL:HG13 | 2.19 | 0.41 |
| 2:T3:265:ILE:HD11 | 2:T3:435:VAL:HG21 | 2.03 | 0.41 |
| 1:T4:157:GLU:OE2 | 3:4F:90:ILE:HD12 | 2.20 | 0.41 |
| 2:T5:335:ILE:HG23 | 2:T5:341:ILE:HD11 | 2.03 | 0.41 |
| 1:T8:218:THR:HG23 | 1:T8:219:THR:H | 1.85 | 0.41 |
| 2:U1:62:VAL:HG22 | 2:U1:88:HIS:HD2 | 1.85 | 0.41 |
| 1:U2:396:HIS:CE1 | 1:U2:397:TRP:CE2 | 3.07 | 0.41 |
| 2:U3:53:PHE:HD1 | 2:U3:63:PRO:HA | 1.85 | 0.41 |
| 1:U4:31:ASP:OD1 | 1:U4:35:THR:N | 2.51 | 0.41 |
| 2:U7:177:VAL:HG13 | 1:U8:327:ASP:HB3 | 2.02 | 0.41 |
| 2:V1:91:GLN:HG2 | 2:V1:121:ARG:NH2 | 2.35 | 0.41 |
| 2:V3:90:GLU:HB3 | 2:V3:121:ARG:HH12 | 1.84 | 0.41 |
| 1:V6:21:TRP:CZ3 | 1:V6:61:PRO:HB3 | 2.55 | 0.41 |
| 2:W1:425:LEU:O | 2:W1:429:GLU:HG2 | 2.20 | 0.41 |
| 2:W5:136:LEU:HA | 2:W5:167:LEU:O | 2.20 | 0.41 |
| 2:W5:358:GLN:OE1 | 2:W5:359:PRO:HD2 | 2.21 | 0.41 |
| 2:W7:8:HIS:HB2 | 2:W7:67:PHE:HD1 | 1.86 | 0.41 |
| 1:W8:286:VAL:HG23 | 1:W8:287:PRO:HD3 | 2.01 | 0.41 |
| 1:W8:414:ASN:HA | 1:W8:417:ASP:OD2 | 2.20 | 0.41 |
| 2:W9:84:ARG:HB2 | 2:W9:84:ARG:NH1 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:326:LYS:HG3 | 2:W9:327:ASP:N | 2.35 | 0.41 |
| 1:X0:41:ASP:OD1 | 8:4X:114:ARG:NH1 | 2.53 | 0.41 |
| 2:X3:175:PRO:HB3 | 2:X3:390:ARG:NE | 2.36 | 0.41 |
| 2:X3:216:SER:OG | 2:X3:217:LEU:N | 2.53 | 0.41 |
| 1:X4:232:VAL:HG11 | 1:X4:268:VAL:HG11 | 2.02 | 0.41 |
| 2:X5:246:GLY:HA2 | 2:X5:357:TYR:CD2 | 2.55 | 0.41 |
| 2:X5:336:LYS:O | 2:X5:339:ARG:NH2 | 2.53 | 0.41 |
| 1:X6:21:TRP:CZ3 | 1:X6:61:PRO:HB3 | 2.54 | 0.41 |
| 1:X6:170:VAL:HG22 | 1:X6:202:LEU:O | 2.20 | 0.41 |
| 1:X6:199:CYS:SG | 1:X6:265:PHE:HD1 | 2.44 | 0.41 |
| 2:X7:322:ASP:OD1 | 2:X7:322:ASP:N | 2.48 | 0.41 |
| 1:X8:214:THR:OG1 | 1:X8:215:LEU:N | 2.53 | 0.41 |
| 1:X8:406:MET:O | 1:X8:410:GLU:HG2 | 2.20 | 0.41 |
| 1:Y0:6:HIS:HA | 1:Y0:134:GLN:O | 2.19 | 0.41 |
| 1:Y0:138:SER:O | 1:Y0:139:LEU:HD23 | 2.20 | 0.41 |
| 2:Y1:191:THR:HG21 | 2:Y1:425:LEU:HD21 | 2.02 | 0.41 |
| 2:Y1:413:MET:HB3 | 2:Y1:417:GLU:OE2 | 2.19 | 0.41 |
| 2:Y3:89:PRO:HD2 | 2:Z9:283:HIS:ND1 | 2.35 | 0.41 |
| 1:Y4:68:LEU:HD21 | 1:Y4:112:LEU:HD22 | 2.01 | 0.41 |
| 1:Y6:328:GLU:O | 1:Y6:332:ASN:ND2 | 2.52 | 0.41 |
| 1:Y8:11:GLN:HG2 | 1:Y8:12:CYS:H | 1.84 | 0.41 |
| 1:Y8:406:MET:SD | 1:Y8:406:MET:N | 2.93 | 0.41 |
| 1:Y8:417:ASP:HA | 1:Y8:420:SER:OG | 2.20 | 0.41 |
| 1:Z0:31:ASP:OD2 | 1:Z0:33:THR:HB | 2.20 | 0.41 |
| 1:Z2:183:TYR:O | 1:Z2:187:LEU:HD13 | 2.20 | 0.41 |
| 1:Z2:395:LEU:HD23 | 1:Z2:395:LEU:HA | 1.76 | 0.41 |
| 1:Z8:138:SER:HA | 1:Z8:169:VAL:HG12 | 2.03 | 0.41 |
| 1:Z8:183:TYR:O | 1:Z8:187:LEU:HD13 | 2.20 | 0.41 |
| 2:Z9:212:ILE:O | 2:Z9:216:SER:OG | 2.33 | 0.41 |
| 1:0A:8:GLN:HB3 | 1:0A:13:GLY:O | 2.18 | 0.41 |
| 1:0A:325:GLU:HA | 1:0A:328:GLU:HG3 | 2.02 | 0.41 |
| 1:0C:12:CYS:O | 1:0C:16:ILE:HG12 | 2.19 | 0.41 |
| 1:0E:48:ASN:OD1 | 1:0E:49:VAL:N | 2.53 | 0.41 |
| 2:0F:3:GLU:HG3 | 2:0F:51:THR:HA | 2.01 | 0.41 |
| 2:0F:91:GLN:HG3 | 2:0F:121:ARG:NH2 | 2.35 | 0.41 |
| 2:0F:240:ALA:HB1 | 2:0F:356:ASN:HD22 | 1.83 | 0.41 |
| 1:0K:67:ASP:OD1 | 1:0K:67:ASP:N | 2.53 | 0.41 |
| 1:0M:284:LEU:HG | 1:0M:362:LYS:HD3 | 2.02 | 0.41 |
| 1:0O:62:ARG:HH21 | 1:0O:127:CYS:HB3 | 1.85 | 0.41 |
| 1:0O:116:VAL:O | 1:0O:120:VAL:HG12 | 2.20 | 0.41 |
| 1:0O:388:MET:O | 1:0O:391:ARG:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0P:102:ASN:ND2 | 2:0P:105:ARG:HB2 | 2.35 | 0.41 |
| 2:0R:49:PHE:HD2 | 2:0R:53:PHE:HB2 | 1.85 | 0.41 |
| 2:0R:174:SER:HB3 | 2:0R:207:GLU:CD | 2.40 | 0.41 |
| 2:0R:285:GLN:NE2 | 2:0R:286:LEU:O | 2.52 | 0.41 |
| 1:1A:7:ILE:HD13 | 1:1A:151:LEU:HD21 | 2.02 | 0.41 |
| 1:1A:175:VAL:HG22 | 2:1B:329:ASN:HD21 | 1.84 | 0.41 |
| 1:1A:286:VAL:HG12 | 1:1A:329:GLN:HG2 | 2.01 | 0.41 |
| 2:1B:170:THR:HG21 | 2:1B:194:LEU:HD11 | 2.02 | 0.41 |
| 1:1C:31:ASP:HB2 | 1:1C:32:PRO:HD2 | 2.02 | 0.41 |
| 2:1D:27:GLU:OE2 | 2:1D:243:ARG:NH1 | 2.53 | 0.41 |
| 1:1E:270:PHE:O | 1:1E:273:LEU:HD23 | 2.20 | 0.41 |
| 1:1E:379:LYS:HD2 | 1:1E:379:LYS:HA | 1.93 | 0.41 |
| 2:1F:287:SER:N | 2:1F:290:GLU:OE2 | 2.53 | 0.41 |
| 1:1G:12:CYS:SG | 1:1G:138:SER:HB3 | 2.60 | 0.41 |
| 2:1H:182:VAL:HG23 | 2:1H:186:ASN:ND2 | 2.34 | 0.41 |
| 2:1H:213:CYS:HA | 2:1H:217:LEU:HD13 | 2.01 | 0.41 |
| 2:1H:404:PHE:HB3 | 2:1H:407:TRP:HD1 | 1.85 | 0.41 |
| 1:1K:318:ARG:HB2 | 1:1K:364:SER:OG | 2.20 | 0.41 |
| 1:1M:372:THR:O | 1:1M:375:GLN:HG3 | 2.20 | 0.41 |
| 2:1P:205:ASP:OD2 | 2:1P:303:VAL:HG13 | 2.19 | 0.41 |
| 1:1S:117:LEU:HA | 1:1S:120:VAL:HG12 | 2.01 | 0.41 |
| 2:1V:176:GLN:HG2 | 2:1V:177:VAL:HG13 | 2.02 | 0.41 |
| 1:1W:69:GLU:C | 1:1W:92:PHE:HZ | 2.23 | 0.41 |
| 1:1W:392:LYS:HD2 | 1:1W:395:LEU:HD22 | 2.02 | 0.41 |
| 2:1X:203:MET:O | 2:1X:204:LEU:HD12 | 2.20 | 0.41 |
| 2:1Z:22:GLU:HG2 | 2:1Z:83:TYR:OH | 2.19 | 0.41 |
| 2:1Z:258:ASN:HD22 | 2:1Z:352:LYS:HZ2 | 1.68 | 0.41 |
| 1:2A:130:LEU:HD23 | 1:2A:130:LEU:HA | 1.81 | 0.41 |
| 1:2C:263:LEU:HA | 1:2C:422:TYR:OH | 2.20 | 0.41 |
| 1:2E:246:LEU:HD22 | 1:2E:352:SER:HA | 2.02 | 0.41 |
| 2:2F:179:THR:O | 1:2G:350:LYS:HD2 | 2.20 | 0.41 |
| 2:2F:205:ASP:OD1 | 2:2F:207:GLU:N | 2.53 | 0.41 |
| 1:2G:68:LEU:HB3 | 1:2G:96:GLY:HA2 | 2.02 | 0.41 |
| 1:2G:273:LEU:H | 1:2G:292:GLN:NE2 | 2.18 | 0.41 |
| 2:2H:325:PRO:HA | 2:2H:328:VAL:HG22 | 2.02 | 0.41 |
| 1:2M:117:LEU:HA | 1:2M:120:VAL:HG12 | 2.02 | 0.41 |
| 2:2N:274:PRO:HB2 | 2:2N:276:ILE:HG12 | 2.01 | 0.41 |
| 1:2Q:3:GLU:HG3 | 1:2Q:127:CYS:SG | 2.59 | 0.41 |
| 2:2R:9:ILE:HD13 | 2:2R:150:GLY:HA2 | 2.01 | 0.41 |
| 1:2S:208:TYR:CE1 | 1:2S:225:LEU:HD11 | 2.55 | 0.41 |
| 2:2T:122:ILE:HD11 | 2:2T:157:LEU:HD21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2V:231:ILE:HD13 | 2:2V:231:ILE:HA | 1.83 | 0.41 |
| 1:2W:297:LYS:CE | 38:8B:47:PHE:HA | 2.50 | 0.41 |
| 1:2Y:232:VAL:O | 1:2Y:236:ILE:HG12 | 2.20 | 0.41 |
| 2:3B:42:ILE:HD12 | 2:3B:42:ILE:HA | 1.64 | 0.41 |
| 1:3C:140:GLY:HA3 | 1:3C:181:GLU:OE1 | 2.20 | 0.41 |
| 1:3C:244:GLY:H | 1:3C:247:ASN:HD21 | 1.68 | 0.41 |
| 2:3H:5:ILE:HD11 | 2:3H:135:PHE:CE1 | 2.55 | 0.41 |
| 2:3H:9:ILE:HD11 | 2:3H:153:LEU:HD23 | 2.03 | 0.41 |
| 2:3J:122:ILE:O | 2:3J:125:LEU:HB2 | 2.20 | 0.41 |
| 2:3L:122:ILE:HA | 2:3L:125:LEU:HB2 | 2.02 | 0.41 |
| 2:3P:114:ILE:HD12 | 2:3P:114:ILE:HA | 1.91 | 0.41 |
| 1:3Q:78:SER:OG | 14:5N:192:THR:O | 2.31 | 0.41 |
| 1:3Q:246:LEU:HD12 | 1:3Q:246:LEU:HA | 1.84 | 0.41 |
| 1:3Q:282:ARG:HH21 | 1:3Q:288:GLU:CD | 2.24 | 0.41 |
| 1:3S:30:ILE:HG13 | 1:3S:35:THR:O | 2.20 | 0.41 |
| 1:3S:190:HIS:HD2 | 1:3S:414:ASN:HB2 | 1.84 | 0.41 |
| 1:3S:237:THR:HG23 | 1:3S:241:ARG:HE | 1.85 | 0.41 |
| 2:3T:264:ARG:NH1 | 2:3T:428:LEU:HD13 | 2.35 | 0.41 |
| 2:3T:288:VAL:HG21 | 2:3T:327:ASP:CB | 2.44 | 0.41 |
| 3:3X:15:ARG:HB2 | 3:3X:19:LEU:HD12 | 2.01 | 0.41 |
| 3:3Z:15:ARG:HB2 | 3:3Z:19:LEU:HD12 | 2.02 | 0.41 |
| 4:4C:30:SER:H | 4:4C:57:THR:HG22 | 1.83 | 0.41 |
| 3:4F:15:ARG:HB2 | 3:4F:19:LEU:HD12 | 2.01 | 0.41 |
| 7:4U:46:GLN:CD | 11:5E:15:ARG:HH22 | 2.23 | 0.41 |
| 8:4W:210:GLU:HA | 8:4W:213:LEU:HD12 | 2.02 | 0.41 |
| 8:4W:255:GLU:HA | 8:4W:258:GLU:HG3 | 2.01 | 0.41 |
| 9:4Z:362:GLN:O | 9:4Z:366:GLU:HG2 | 2.20 | 0.41 |
| 13:5I:6:PRO:HB3 | 13:5I:40:ARG:O | 2.20 | 0.41 |
| 13:5K:6:PRO:HB3 | 13:5K:40:ARG:O | 2.20 | 0.41 |
| 14:5M:319:TYR:HA | 14:5M:334:LEU:HA | 2.01 | 0.41 |
| 14:5M:363:PHE:HD1 | 14:5M:377:ARG:CD | 2.30 | 0.41 |
| 14:5N:319:TYR:HA | 14:5N:334:LEU:HA | 2.01 | 0.41 |
| 15:5P:24:TYR:OH | 15:5P:46:PHE:CE1 | 2.73 | 0.41 |
| 15:5P:263:PHE:HB3 | 15:5P:312:ALA:O | 2.20 | 0.41 |
| 15:5P:285:TYR:HB3 | 15:5P:289:LEU:HD12 | 2.02 | 0.41 |
| 15:5P:313:ASP:OD2 | 15:5P:318:ASP:N | 2.53 | 0.41 |
| 16:5Q:104:ILE:O | 16:5Q:108:GLU:HG2 | 2.20 | 0.41 |
| 16:5Q:192:TYR:HE2 | 35:7T:130:LYS:HE3 | 1.85 | 0.41 |
| 17:5S:69:LYS:HA | 17:5S:69:LYS:HD3 | 1.73 | 0.41 |
| 17:5T:205:SER:OG | 17:5T:208:LYS:HG3 | 2.20 | 0.41 |
| 18:5X:39:TYR:CE1 | 18:5X:82:ASP:HB3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:5Z:39:TYR:CE1 | 18:5Z:82:ASP:HB3 | 2.55 | 0.41 |
| 18:6D:39:TYR:CE1 | 18:6D:82:ASP:HB3 | 2.55 | 0.41 |
| 20:6F:218:GLU:H | 20:6F:218:GLU:CD | 2.22 | 0.41 |
| 21:6H:27:THR:HG22 | 21:6H:27:THR:O | 2.20 | 0.41 |
| 22:6J:162:LEU:HD11 | 22:6J:225:ALA:HB1 | 2.01 | 0.41 |
| 22:6J:186:ARG:O | 22:6J:189:LYS:HB2 | 2.20 | 0.41 |
| 22:6J:321:LEU:HD12 | 22:6J:321:LEU:HA | 1.95 | 0.41 |
| 22:6K:307:ARG:O | 22:6K:311:VAL:HG23 | 2.20 | 0.41 |
| 22:6M:106:ASP:OD2 | 24:6X:286:TYR:HA | 2.19 | 0.41 |
| 22:6O:201:ARG:HB3 | 22:6O:237:TYR:HB3 | 2.03 | 0.41 |
| 22:6O:294:LEU:HD23 | 22:6O:297:PHE:HD2 | 1.85 | 0.41 |
| 24:6T:280:ASP:HA | 24:6T:289:ARG:HB2 | 2.01 | 0.41 |
| 24:6T:285:MET:HG3 | 24:6T:285:MET:O | 2.20 | 0.41 |
| 24:6V:290:ARG:HG3 | 24:6V:291:PRO:HD2 | 2.01 | 0.41 |
| 24:6V:469:PHE:CE2 | 24:6V:482:ILE:HG23 | 2.55 | 0.41 |
| 24:6Y:197:LYS:HE2 | 24:6Y:197:LYS:HB3 | 1.59 | 0.41 |
| 24:6Y:288:ASP:OD1 | 24:6Y:288:ASP:N | 2.53 | 0.41 |
| 24:6Y:502:LYS:HB3 | 24:6Y:511:ILE:HD12 | 2.01 | 0.41 |
| 25:7C:8:VAL:O | 25:7C:11:THR:HG22 | 2.20 | 0.41 |
| 25:7C:110:ARG:NH2 | 30:7K:251:LYS:HD3 | 2.35 | 0.41 |
| 38:8B:180:THR:C | 38:8B:181:LYS:HD2 | 2.40 | 0.41 |
| 1:3:10:GLY:HA3 | 39:3:502:GDP:O1B | 2.20 | 0.41 |
| 1:B1:276:ARG:HH12 | 24:6V:210:VAL:HG21 | 1.85 | 0.41 |
| 1:E0:143:THR:OG1 | 39:E0:501:GDP:O1B | 2.38 | 0.41 |
| 2:G1:240:ALA:O | 2:G1:356:ASN:ND2 | 2.53 | 0.41 |
| 1:G2:228:LEU:O | 1:G2:232:VAL:HG23 | 2.20 | 0.41 |
| 2:G3:276:ILE:HG22 | 2:G3:281:ALA:HB2 | 2.02 | 0.41 |
| 2:G5:322:ASP:OD2 | 24:6X:433:ARG:NH1 | 2.52 | 0.41 |
| 1:G6:86:ARG:NH1 | 1:G6:89:ASN:OD1 | 2.53 | 0.41 |
| 1:G8:316:LEU:HD22 | 1:G8:352:SER:OG | 2.20 | 0.41 |
| 2:G9:76:ASP:HA | 2:G9:79:ARG:HD2 | 2.02 | 0.41 |
| 2:G9:370:LYS:HG2 | 24:6Z:439:MET:SD | 2.60 | 0.41 |
| 2:H1:21:TRP:CD1 | 2:H1:87:PHE:HZ | 2.38 | 0.41 |
| 2:H1:154:LEU:HA | 2:H1:154:LEU:HD23 | 1.87 | 0.41 |
| 2:H3:203:MET:C | 2:H3:204:LEU:HD12 | 2.40 | 0.41 |
| 2:H5:191:THR:HA | 2:H5:194:LEU:HB3 | 2.01 | 0.41 |
| 1:H6:53:GLU:OE2 | 1:H6:57:GLY:N | 2.53 | 0.41 |
| 1:H6:192:LEU:HD23 | 1:H6:192:LEU:HA | 1.85 | 0.41 |
| 2:H9:125:LEU:HD23 | 2:H9:125:LEU:HA | 1.80 | 0.41 |
| 2:H9:255:PHE:HD1 | 2:H9:259:LEU:HD22 | 1.85 | 0.41 |
| 2:I5:361:THR:OG1 | 2:I5:362:VAL:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J2:152:ILE:HD13 | 1:J2:152:ILE:HA | 1.90 | 0.41 |
| 2:J3:397:LEU:HD23 | 2:J3:397:LEU:HA | 1.90 | 0.41 |
| 1:J4:396:HIS:HA | 1:J4:399:THR:OG1 | 2.21 | 0.41 |
| 2:J5:183:GLU:HG3 | 2:J5:184:PRO:HD3 | 2.02 | 0.41 |
| 1:J6:5:VAL:HG12 | 1:J6:62:ARG:HD3 | 2.03 | 0.41 |
| 1:J6:391:ARG:HD3 | 2:J7:346:TRP:CD2 | 2.55 | 0.41 |
| 2:J7:425:LEU:HD23 | 2:J7:425:LEU:HA | 1.91 | 0.41 |
| 2:K3:12:ALA:HB2 | 41:K4:501:GTP:C8 | 2.56 | 0.41 |
| 2:K3:35:GLN:HG3 | 2:K3:59:GLY:O | 2.21 | 0.41 |
| 2:K5:265:ILE:HD11 | 2:K5:435:VAL:HG21 | 2.01 | 0.41 |
| 2:K7:129:CYS:SG | 2:K7:130:THR:N | 2.93 | 0.41 |
| 2:K9:334:THR:HA | 2:K9:337:THR:HG22 | 2.03 | 0.41 |
| 1:L2:22:GLU:HG2 | 1:L2:81:TYR:CD2 | 2.55 | 0.41 |
| 2:L7:132:LEU:HD22 | 2:L7:164:LYS:HD3 | 2.02 | 0.41 |
| 2:L7:316:CYS:O | 2:L7:377:MET:HA | 2.20 | 0.41 |
| 1:M0:148:GLY:O | 1:M0:152:ILE:HG12 | 2.19 | 0.41 |
| 2:M1:9:ILE:HD11 | 2:M1:153:LEU:HD23 | 2.03 | 0.41 |
| 1:M2:201:VAL:HG12 | 1:M2:301:CYS:SG | 2.61 | 0.41 |
| 1:M4:297:LYS:HD3 | 1:M4:297:LYS:HA | 1.87 | 0.41 |
| 1:M8:69:GLU:HG2 | 1:M8:71:GLY:H | 1.85 | 0.41 |
| 1:M8:364:SER:OG | 1:M8:365:ALA:N | 2.54 | 0.41 |
| 2:M9:4:VAL:HG23 | 2:M9:134:GLY:O | 2.20 | 0.41 |
| 2:M9:21:TRP:CZ3 | 2:M9:63:PRO:HB3 | 2.55 | 0.41 |
| 1:N2:238:CYS:SG | 1:N2:318:ARG:NE | 2.93 | 0.41 |
| 2:N3:112:LYS:HA | 2:N3:112:LYS:HD3 | 1.93 | 0.41 |
| 2:N3:274:PRO:HB2 | 2:N3:276:ILE:HG12 | 2.02 | 0.41 |
| 2:N3:275:ILE:O | 2:N3:275:ILE:HG23 | 2.20 | 0.41 |
| 2:N3:317:LEU:HB3 | 2:N3:319:TYR:CE1 | 2.48 | 0.41 |
| 2:N5:72:PRO:HD2 | 1:N6:2:ARG:NH1 | 2.35 | 0.41 |
| 1:N8:321:MET:HE2 | 1:N8:363:MET:HG3 | 2.03 | 0.41 |
| 2:N9:157:LEU:HD23 | 2:N9:157:LEU:HA | 1.88 | 0.41 |
| 1:O0:14:ASN:HD22 | 1:O0:65:LEU:HD22 | 1.84 | 0.41 |
| 2:O1:76:ASP:HA | 2:O1:79:ARG:HD2 | 2.02 | 0.41 |
| 2:O1:217:LEU:HD23 | 2:O1:217:LEU:HA | 1.83 | 0.41 |
| 1:O2:3:GLU:HB2 | 1:O2:130:LEU:HD13 | 2.02 | 0.41 |
| 1:O4:77:ARG:HH12 | 37:7Y:22:GLU:HG3 | 1.84 | 0.41 |
| 2:O7:294:ALA:HA | 2:O7:297:GLU:OE1 | 2.21 | 0.41 |
| 2:P5:42:ILE:CG2 | 27:7G:217:ILE:HG21 | 2.50 | 0.41 |
| 1:P6:180:VAL:HG23 | 1:P6:184:ASN:ND2 | 2.35 | 0.41 |
| 2:P7:304:LYS:HD2 | 2:P7:304:LYS:HA | 1.74 | 0.41 |
| 1:Q0:66:MET:HE3 | 1:Q0:116:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q3:188:VAL:O | 2:Q3:191:THR:HG22 | 2.20 | 0.41 |
| 2:Q3:200:VAL:HG13 | 2:Q3:268:MET:CE | 2.50 | 0.41 |
| 1:Q6:418:LEU:HD12 | 1:Q6:418:LEU:HA | 1.87 | 0.41 |
| 2:Q9:405:VAL:H | 2:Q9:405:VAL:HG22 | 1.68 | 0.41 |
| 2:R1:290:GLU:OE1 | 2:R1:290:GLU:N | 2.44 | 0.41 |
| 1:R2:154:LYS:HD3 | 1:R2:154:LYS:HA | 1.88 | 0.41 |
| 1:R2:228:LEU:HD23 | 1:R2:228:LEU:HA | 1.83 | 0.41 |
| 1:R4:32:PRO:HG3 | 11:5E:176:VAL:HG21 | 2.01 | 0.41 |
| 1:R4:193:VAL:HG23 | 1:R4:194:GLU:HG2 | 2.02 | 0.41 |
| 2:R5:397:LEU:HD23 | 2:R5:397:LEU:HA | 1.89 | 0.41 |
| 1:R6:91:VAL:HG11 | 1:R6:116:VAL:HG22 | 2.01 | 0.41 |
| 1:R8:86:ARG:HD3 | 1:R8:88:ASP:OD1 | 2.20 | 0.41 |
| 1:S0:31:ASP:HB2 | 1:S0:32:PRO:HD2 | 2.03 | 0.41 |
| 2:S1:14:ILE:HD11 | 2:S1:74:VAL:CG1 | 2.50 | 0.41 |
| 1:S2:19:LYS:HA | 1:S2:19:LYS:HD2 | 1.88 | 0.41 |
| 1:S4:125:GLU:CD | 3:3V:66:THR:HG23 | 2.39 | 0.41 |
| 1:S4:226:ASN:OD1 | 39:S4:501:GDP:N1 | 2.53 | 0.41 |
| 1:S4:310:TYR:O | 1:S4:342:VAL:HG23 | 2.20 | 0.41 |
| 2:S5:246:GLY:HA3 | 2:S5:356:ASN:HA | 2.02 | 0.41 |
| 1:S6:244:GLY:H | 1:S6:247:ASN:HD21 | 1.67 | 0.41 |
| 1:S8:113:ILE:HD11 | 1:S8:151:LEU:HD13 | 2.03 | 0.41 |
| 1:T2:55:THR:H | 1:T2:58:ARG:HB3 | 1.85 | 0.41 |
| 2:T5:4:VAL:HG23 | 2:T5:134:GLY:O | 2.19 | 0.41 |
| 2:T5:317:LEU:HB3 | 2:T5:319:TYR:HE1 | 1.84 | 0.41 |
| 1:T6:101:TRP:HB2 | 1:T6:184:ASN:OD1 | 2.19 | 0.41 |
| 1:T6:390:ARG:HE | 1:T6:390:ARG:HB2 | 1.68 | 0.41 |
| 1:T8:44:LEU:O | 1:T8:47:ILE:HG12 | 2.19 | 0.41 |
| 1:U2:107:THR:OG1 | 1:U2:401:GLU:OE2 | 2.23 | 0.41 |
| 1:U4:192:LEU:HD23 | 1:U4:192:LEU:HA | 1.86 | 0.41 |
| 1:U6:53:GLU:HG3 | 1:U6:59:TYR:CE1 | 2.56 | 0.41 |
| 2:U9:9:ILE:CG1 | 2:U9:139:ASN:HB3 | 2.50 | 0.41 |
| 1:V0:282:ARG:HH12 | 1:V0:284:LEU:HG | 1.85 | 0.41 |
| 2:V1:10:GLY:O | 2:V1:14:ILE:HG13 | 2.20 | 0.41 |
| 1:V2:139:LEU:HD23 | 1:V2:139:LEU:HA | 1.89 | 0.41 |
| 1:W0:170:VAL:HG22 | 1:W0:202:LEU:O | 2.21 | 0.41 |
| 2:W1:90:GLU:HA | 2:W1:90:GLU:OE2 | 2.19 | 0.41 |
| 1:W2:95:THR:HG23 | 1:W2:96:GLY:N | 2.35 | 0.41 |
| 2:W5:306:ASP:HB3 | 2:W5:309:HIS:HD2 | 1.83 | 0.41 |
| 1:W6:50:TYR:OH | 1:W6:237:THR:HG21 | 2.20 | 0.41 |
| 2:W7:336:LYS:HZ3 | 2:W7:350:GLY:H | 1.68 | 0.41 |
| 2:X3:8:HIS:HE1 | 2:X3:21:TRP:HE1 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X3:14:ILE:O | 2:X3:18:ASN:ND2 | 2.52 | 0.41 |
| 1:X8:183:TYR:OH | 1:X8:388:MET:HB3 | 2.20 | 0.41 |
| 2:Y1:340:THR:HG23 | 2:Y1:341:ILE:HG23 | 2.02 | 0.41 |
| 2:Y1:428:LEU:HA | 2:Y1:431:ASP:OD1 | 2.21 | 0.41 |
| 1:Y2:156:ARG:HD2 | 1:Y2:156:ARG:HA | 1.86 | 0.41 |
| 2:Y3:282:TYR:OH | 8:4W:370:VAL:CB | 2.68 | 0.41 |
| 2:Y3:413:MET:HB3 | 2:Y3:417:GLU:OE2 | 2.21 | 0.41 |
| 1:Y4:3:GLU:HG3 | 1:Y4:127:CYS:SG | 2.60 | 0.41 |
| 1:Y4:143:THR:N | 39:Y4:502:GDP:O2B | 2.53 | 0.41 |
| 2:Y5:151:SER:HB2 | 2:Y5:193:SER:OG | 2.20 | 0.41 |
| 2:Y9:246:GLY:HA3 | 2:Y9:356:ASN:HA | 2.01 | 0.41 |
| 2:Y9:333:ALA:O | 2:Y9:337:THR:HG23 | 2.19 | 0.41 |
| 1:Z0:46:ARG:HA | 1:Z0:46:ARG:HD3 | 1.81 | 0.41 |
| 1:Z0:177:ASP:OD1 | 2:Z1:248:LEU:HD21 | 2.20 | 0.41 |
| 2:Z1:30:ILE:HG12 | 2:Z1:36:MET:HG2 | 2.01 | 0.41 |
| 1:Z2:8:GLN:HG2 | 1:Z2:65:LEU:HA | 2.02 | 0.41 |
| 2:Z3:127:ASP:OD1 | 2:0J:293:ASN:ND2 | 2.53 | 0.41 |
| 1:Z4:19:LYS:NZ | 1:Z4:227:HIS:HD2 | 2.18 | 0.41 |
| 1:Z4:172:SER:O | 1:Z4:176:SER:OG | 2.32 | 0.41 |
| 1:Z4:183:TYR:O | 1:Z4:187:LEU:HD13 | 2.20 | 0.41 |
| 1:Z4:385:PHE:HZ | 1:Z4:408:PHE:HD1 | 1.68 | 0.41 |
| 2:Z5:359:PRO:HA | 2:Z5:360:PRO:HD3 | 1.92 | 0.41 |
| 1:Z6:5:VAL:HB | 1:Z6:133:PHE:CD1 | 2.55 | 0.41 |
| 1:Z6:65:LEU:HD22 | 1:Z6:90:PHE:CE1 | 2.55 | 0.41 |
| 2:Z7:286:LEU:HG | 2:Z7:373:ARG:NH1 | 2.35 | 0.41 |
| 2:Z9:322:ASP:OD1 | 2:Z9:322:ASP:N | 2.43 | 0.41 |
| 2:0B:275:ILE:O | 2:0B:275:ILE:HG23 | 2.19 | 0.41 |
| 1:0E:150:LEU:HA | 1:0E:150:LEU:HD12 | 1.83 | 0.41 |
| 1:0E:183:TYR:HB3 | 1:0E:398:TYR:HE2 | 1.84 | 0.41 |
| 2:0F:305:CYS:SG | 2:0F:383:ALA:HB1 | 2.59 | 0.41 |
| 1:0G:165:LEU:HD23 | 1:0G:165:LEU:HA | 1.93 | 0.41 |
| 1:0K:297:LYS:HA | 1:0K:297:LYS:HD3 | 1.73 | 0.41 |
| 2:0L:73:THR:OG1 | 2:0L:74:VAL:N | 2.54 | 0.41 |
| 2:0N:258:ASN:O | 2:0N:259:LEU:HD23 | 2.20 | 0.41 |
| 1:0O:68:LEU:HD21 | 1:0O:112:LEU:HD22 | 2.03 | 0.41 |
| 1:0O:367:PHE:O | 1:0O:368:ILE:HD13 | 2.21 | 0.41 |
| 2:0P:9:ILE:HB | 2:0P:139:ASN:HB3 | 2.02 | 0.41 |
| 1:0S:55:THR:H | 1:0S:58:ARG:HB3 | 1.85 | 0.41 |
| 1:0U:385:PHE:HZ | 1:0U:408:PHE:HD1 | 1.69 | 0.41 |
| 2:0V:119:LEU:HD21 | 2:0V:156:ARG:HB3 | 2.03 | 0.41 |
| 2:0V:241:SER:HB2 | 2:0V:250:VAL:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0V:250:VAL:HG23 | 2:0V:254:GLU:HG3 | 2.01 | 0.41 |
| 1:0W:5:VAL:HB | 1:0W:133:PHE:HD1 | 1.85 | 0.41 |
| 1:0W:117:LEU:HA | 1:0W:117:LEU:HD23 | 1.81 | 0.41 |
| 1:0W:311:LEU:HB3 | 1:0W:370:ASN:O | 2.20 | 0.41 |
| 1:0Y:4:ILE:HB | 1:0Y:50:TYR:CE1 | 2.46 | 0.41 |
| 2:1B:73:THR:HG23 | 2:1B:74:VAL:N | 2.35 | 0.41 |
| 1:1E:70:PRO:N | 1:1E:92:PHE:HZ | 2.18 | 0.41 |
| 1:1E:153:SER:O | 1:1E:157:GLU:HG2 | 2.20 | 0.41 |
| 1:1E:178:THR:OG1 | 1:1E:181:GLU:HG3 | 2.20 | 0.41 |
| 2:1F:137:VAL:HG22 | 2:1F:168:GLY:HA2 | 2.02 | 0.41 |
| 1:1G:415:MET:O | 1:1G:419:VAL:HG23 | 2.19 | 0.41 |
| 1:1K:219:THR:O | 1:1K:219:THR:OG1 | 2.35 | 0.41 |
| 2:1L:31:GLN:HE21 | 2:1L:37:PRO:HG3 | 1.84 | 0.41 |
| 2:1L:403:ALA:HB2 | 1:1M:344:TRP:HZ3 | 1.84 | 0.41 |
| 1:1M:74:ASP:O | 1:1M:78:SER:OG | 2.29 | 0.41 |
| 1:1O:101:TRP:HE3 | 1:1O:403:MET:HE1 | 1.84 | 0.41 |
| 1:1O:232:VAL:HG11 | 1:1O:268:VAL:HG11 | 2.02 | 0.41 |
| 1:1O:315:ALA:HB1 | 1:1O:317:PHE:CE1 | 2.55 | 0.41 |
| 2:1P:251:ASP:OD2 | 2:1P:253:THR:N | 2.54 | 0.41 |
| 2:1P:297:GLU:H | 2:1P:297:GLU:HG2 | 1.71 | 0.41 |
| 1:1Q:102:ALA:HB1 | 1:1Q:401:GLU:CB | 2.50 | 0.41 |
| 1:1Q:387:ALA:HA | 1:1Q:390:ARG:NH2 | 2.32 | 0.41 |
| 1:1U:21:TRP:CZ2 | 1:1U:63:ALA:HB2 | 2.56 | 0.41 |
| 1:1U:395:LEU:O | 1:1U:399:THR:HG23 | 2.20 | 0.41 |
| 2:1V:362:VAL:HG12 | 2:1V:370:LYS:HE2 | 2.02 | 0.41 |
| 2:1Z:322:ASP:HB3 | 2:1Z:373:ARG:HH21 | 1.85 | 0.41 |
| 1:2A:5:VAL:HG22 | 1:2A:133:PHE:CD1 | 2.56 | 0.41 |
| 1:2G:385:PHE:HZ | 1:2G:408:PHE:HD1 | 1.68 | 0.41 |
| 1:2I:91:VAL:CG1 | 1:2I:116:VAL:HG12 | 2.49 | 0.41 |
| 1:2I:113:ILE:HG12 | 1:2I:150:LEU:HG | 2.01 | 0.41 |
| 2:2J:101:ASN:ND2 | 2:2J:143:GLY:HA2 | 2.35 | 0.41 |
| 1:2K:4:ILE:HB | 1:2K:50:TYR:HE1 | 1.85 | 0.41 |
| 1:2K:235:GLY:HA3 | 1:2K:366:THR:HG21 | 2.01 | 0.41 |
| 1:2K:314:SER:HA | 1:2K:350:LYS:O | 2.19 | 0.41 |
| 2:2L:120:ASP:OD2 | 38:8C:24:TYR:HD1 | 2.04 | 0.41 |
| 1:2M:122:LYS:CE | 1:3C:291:GLN:HB3 | 2.50 | 0.41 |
| 2:2N:36:MET:HA | 2:2N:37:PRO:HD3 | 1.91 | 0.41 |
| 2:2N:417:GLU:HA | 2:2N:420:GLU:HG2 | 2.02 | 0.41 |
| 2:2P:56:THR:HA | 2:3F:285:GLN:HB2 | 2.03 | 0.41 |
| 1:2Q:39:ASP:OD1 | 1:2Q:40:SER:N | 2.53 | 0.41 |
| 2:2R:76:ASP:O | 2:2R:80:THR:HG23 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2S:2:ARG:HE | 1:2S:240:LEU:HD22 | 1.85 | 0.41 |
| 1:2S:396:HIS:HE1 | 1:2S:397:TRP:CZ2 | 2.38 | 0.41 |
| 1:2U:39:ASP:OD2 | 1:2U:40:SER:N | 2.53 | 0.41 |
| 1:2U:290:THR:HG21 | 1:2U:329:GLN:HG3 | 2.02 | 0.41 |
| 2:2V:356:ASN:OD1 | 2:2V:357:TYR:N | 2.52 | 0.41 |
| 1:2W:31:ASP:OD1 | 1:2W:34:GLY:N | 2.53 | 0.41 |
| 1:2W:203:ASP:N | 1:2W:203:ASP:OD1 | 2.51 | 0.41 |
| 1:2Y:273:LEU:H | 1:2Y:292:GLN:HE22 | 1.68 | 0.41 |
| 1:3A:304:ASP:HB2 | 38:8C:45:SER:OG | 2.19 | 0.41 |
| 2:3B:294:ALA:HA | 2:3B:297:GLU:OE1 | 2.21 | 0.41 |
| 1:3C:257:LEU:HA | 1:3C:312:THR:HG21 | 2.02 | 0.41 |
| 1:3C:376:GLU:OE2 | 1:3C:379:LYS:HD3 | 2.20 | 0.41 |
| 2:3D:8:HIS:CD2 | 2:3D:17:GLY:HA3 | 2.55 | 0.41 |
| 2:3D:47:ASP:HA | 2:3D:50:ASN:HD21 | 1.84 | 0.41 |
| 2:3D:340:THR:HG21 | 38:8D:74:ILE:O | 2.21 | 0.41 |
| 1:3G:60:VAL:O | 1:3G:60:VAL:HG23 | 2.21 | 0.41 |
| 2:3H:124:LYS:NZ | 3:3X:36:PHE:HA | 2.35 | 0.41 |
| 1:3I:39:ASP:OD1 | 1:3I:39:ASP:N | 2.53 | 0.41 |
| 2:3J:177:VAL:HG13 | 1:3K:327:ASP:HB3 | 2.01 | 0.41 |
| 2:3J:339:ARG:NH2 | 2:3J:342:GLN:HB3 | 2.32 | 0.41 |
| 1:3M:178:THR:OG1 | 1:3M:179:VAL:N | 2.54 | 0.41 |
| 2:3N:116:ASP:OD1 | 2:3N:116:ASP:N | 2.51 | 0.41 |
| 2:3N:194:LEU:HD12 | 2:3N:194:LEU:HA | 1.83 | 0.41 |
| 2:3R:21:TRP:CZ3 | 2:3R:63:PRO:HB3 | 2.55 | 0.41 |
| 1:3S:190:HIS:HD2 | 1:3S:411:ALA:HA | 1.81 | 0.41 |
| 1:3S:266:PHE:CE1 | 1:3S:370:ASN:HB2 | 2.55 | 0.41 |
| 4:4C:27:LYS:HE3 | 4:4C:27:LYS:HB3 | 1.94 | 0.41 |
| 5:4L:466:LEU:CD2 | 5:4M:139:LEU:HD22 | 2.50 | 0.41 |
| 7:4Q:320:PHE:CD1 | 12:7B:91:LEU:HD12 | 2.54 | 0.41 |
| 7:4U:180:TYR:OH | 31:7N:79:PRO:HA | 2.19 | 0.41 |
| 9:4Z:237:VAL:O | 9:4Z:240:SER:OG | 2.29 | 0.41 |
| 9:4Z:331:ARG:HD2 | 9:4Z:332:GLN:N | 2.34 | 0.41 |
| 9:4Z:396:MET:HE2 | 9:4Z:400:ARG:HD3 | 2.02 | 0.41 |
| 10:5A:307:GLU:O | 10:5A:310:LEU:HG | 2.20 | 0.41 |
| 10:5C:284:GLY:HA2 | 10:5C:287:VAL:HG12 | 2.02 | 0.41 |
| 10:5C:314:LYS:O | 10:5C:317:ILE:HG22 | 2.20 | 0.41 |
| 11:5E:185:ASP:OD2 | 11:5E:187:PRO:HD2 | 2.20 | 0.41 |
| 13:5I:18:ARG:HB3 | 24:6V:38:GLY:HA2 | 2.02 | 0.41 |
| 13:5J:6:PRO:HB3 | 13:5J:40:ARG:O | 2.20 | 0.41 |
| 14:5L:92:SER:O | 14:5L:94:GLN:N | 2.53 | 0.41 |
| 14:5M:92:SER:O | 14:5M:94:GLN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5N:92:SER:O | 14:5N:94:GLN:N | 2.53 | 0.41 |
| 14:5N:415:LYS:HZ1 | 23:6S:22:MET:HB2 | 1.83 | 0.41 |
| 14:5N:511:THR:HG21 | 14:5N:531:ASP:OD1 | 2.19 | 0.41 |
| 15:5P:179:THR:HA | 15:5P:193:ARG:NH1 | 2.35 | 0.41 |
| 16:5Q:20:LYS:HG3 | 16:5Q:113:PHE:CZ | 2.55 | 0.41 |
| 16:5Q:60:HIS:N | 16:5Q:60:HIS:CD2 | 2.87 | 0.41 |
| 17:5T:69:LYS:HA | 17:5T:69:LYS:HD3 | 1.72 | 0.41 |
| 18:5Y:39:TYR:CE1 | 18:5Y:82:ASP:HB3 | 2.55 | 0.41 |
| 18:6A:39:TYR:CE1 | 18:6A:82:ASP:HB3 | 2.55 | 0.41 |
| 18:6C:39:TYR:CZ | 26:7F:24:GLN:OE1 | 2.73 | 0.41 |
| 20:6F:263:LEU:HA | 20:6F:263:LEU:HD23 | 1.81 | 0.41 |
| 21:6H:137:LEU:N | 21:6H:138:PRO:HD2 | 2.36 | 0.41 |
| 22:6J:274:GLU:O | 22:6J:278:GLN:HG2 | 2.19 | 0.41 |
| 22:6K:264:GLN:HA | 24:6V:406:ALA:HB2 | 2.02 | 0.41 |
| 22:6P:196:ASN:OD1 | 22:6P:196:ASN:N | 2.54 | 0.41 |
| 24:6T:396:LYS:HE3 | 24:6T:396:LYS:HB2 | 1.84 | 0.41 |
| 24:6W:93:ARG:HD3 | 26:7E:45:MET:O | 2.19 | 0.41 |
| 24:6W:487:VAL:O | 24:6W:488:ARG:C | 2.58 | 0.41 |
| 24:6X:185:ASP:O | 24:6X:188:THR:OG1 | 2.32 | 0.41 |
| 24:6X:517:LEU:CD1 | 24:6X:517:LEU:N | 2.72 | 0.41 |
| 24:7A:92:ASP:OD1 | 24:7A:93:ARG:N | 2.52 | 0.41 |
| 29:7J:295:ASN:OD1 | 29:7J:298:THR:HG23 | 2.19 | 0.41 |
| 38:8C:59:GLU:OE1 | 38:8C:60:GLY:N | 2.53 | 0.41 |
| 2:8:225:THR:HG21 | 26:7E:113:ARG:HG2 | 2.02 | 0.41 |
| 2:G1:204:LEU:HD23 | 2:G1:302:MET:HB3 | 2.02 | 0.41 |
| 1:G2:314:SER:HA | 1:G2:350:LYS:O | 2.19 | 0.41 |
| 2:G5:5:ILE:HG22 | 2:G5:64:ARG:HD3 | 2.02 | 0.41 |
| 1:G6:216:LYS:HB2 | 1:G6:275:SER:OG | 2.20 | 0.41 |
| 1:G6:271:THR:CG2 | 1:G6:365:ALA:HB3 | 2.49 | 0.41 |
| 1:G8:384:GLN:O | 1:G8:388:MET:HG2 | 2.20 | 0.41 |
| 2:H1:90:GLU:HB2 | 2:H1:121:ARG:HH22 | 1.85 | 0.41 |
| 1:H2:7:ILE:HD13 | 1:H2:151:LEU:HD21 | 2.02 | 0.41 |
| 1:H4:99:ASN:ND2 | 2:H5:254:GLU:OE1 | 2.53 | 0.41 |
| 1:H6:414:ASN:HA | 1:H6:417:ASP:OD2 | 2.19 | 0.41 |
| 2:H7:114:ILE:HD12 | 2:H7:114:ILE:HA | 1.83 | 0.41 |
| 2:H7:182:VAL:HG23 | 2:H7:186:ASN:ND2 | 2.35 | 0.41 |
| 1:H8:215:LEU:HB3 | 1:H8:217:LEU:HG | 2.03 | 0.41 |
| 1:I0:235:GLY:HA3 | 1:I0:366:THR:HG21 | 2.01 | 0.41 |
| 2:I1:415:GLU:OE2 | 2:I1:415:GLU:N | 2.53 | 0.41 |
| 1:I2:198:GLU:HA | 1:I2:264:HIS:HB2 | 2.01 | 0.41 |
| 2:I3:318:MET:HB2 | 2:I3:376:CYS:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I4:385:PHE:HZ | 1:I4:408:PHE:HD1 | 1.67 | 0.41 |
| 1:I4:421:GLU:HA | 1:I4:424:GLN:HB3 | 2.01 | 0.41 |
| 2:I5:118:ALA:O | 2:I5:122:ILE:HG23 | 2.20 | 0.41 |
| 2:I5:328:VAL:O | 2:I5:332:VAL:HG23 | 2.20 | 0.41 |
| 2:I9:304:LYS:HA | 2:I9:304:LYS:HD3 | 1.89 | 0.41 |
| 2:J1:149:LEU:HA | 2:J1:152:LEU:HB3 | 2.03 | 0.41 |
| 2:J1:203:MET:O | 2:J1:204:LEU:HD22 | 2.21 | 0.41 |
| 2:J3:261:PRO:HG3 | 2:J3:313:MET:HE2 | 2.01 | 0.41 |
| 1:J6:50:TYR:OH | 1:J6:237:THR:HG21 | 2.20 | 0.41 |
| 2:J9:279:GLU:OE2 | 5:4M:267:ASN:ND2 | 2.53 | 0.41 |
| 2:K3:205:ASP:CG | 2:K3:206:ASN:H | 2.24 | 0.41 |
| 1:K4:55:THR:HG23 | 1:M0:282:ARG:O | 2.20 | 0.41 |
| 1:K4:183:TYR:HE2 | 1:K4:394:PHE:HB2 | 1.85 | 0.41 |
| 2:K5:397:LEU:HD23 | 2:K5:397:LEU:HA | 1.84 | 0.41 |
| 1:K6:203:ASP:OD1 | 1:K6:203:ASP:N | 2.51 | 0.41 |
| 2:K9:209:ILE:HG23 | 2:K9:230:LEU:HD11 | 2.02 | 0.41 |
| 2:K9:271:SER:OG | 2:K9:377:MET:HB3 | 2.19 | 0.41 |
| 1:L0:180:VAL:HG23 | 1:L0:184:ASN:HD21 | 1.85 | 0.41 |
| 2:L1:211:ASP:OD1 | 2:L1:214:ARG:NH2 | 2.53 | 0.41 |
| 1:L4:161:ASP:HB3 | 1:L4:162:ARG:NH1 | 2.35 | 0.41 |
| 1:L6:171:PRO:HG3 | 1:L6:181:GLU:HB3 | 2.03 | 0.41 |
| 2:M1:370:LYS:NZ | 30:7K:275:ASP:OD1 | 2.53 | 0.41 |
| 1:M2:273:LEU:H | 1:M2:292:GLN:HE22 | 1.68 | 0.41 |
| 2:M3:77:GLU:OE1 | 1:M4:243:PRO:HB3 | 2.20 | 0.41 |
| 2:M5:399:TYR:OH | 2:M5:415:GLU:OE1 | 2.19 | 0.41 |
| 1:M8:183:TYR:HB3 | 1:M8:398:TYR:HE2 | 1.86 | 0.41 |
| 1:N0:273:LEU:H | 1:N0:292:GLN:HE22 | 1.67 | 0.41 |
| 2:N1:290:GLU:HA | 2:N1:293:ASN:HD22 | 1.85 | 0.41 |
| 1:N2:117:LEU:HA | 1:N2:117:LEU:HD23 | 1.80 | 0.41 |
| 1:N2:152:ILE:HD13 | 1:N2:152:ILE:HA | 1.94 | 0.41 |
| 1:N2:229:ILE:HG22 | 1:N2:233:MET:SD | 2.60 | 0.41 |
| 2:N7:212:ILE:HG23 | 2:N7:275:ILE:HD12 | 2.02 | 0.41 |
| 2:N7:305:CYS:HB3 | 2:N7:387:ILE:HD11 | 2.01 | 0.41 |
| 1:N8:40:SER:HB3 | 27:7G:129:LEU:HD13 | 2.02 | 0.41 |
| 1:N8:170:VAL:HG21 | 1:N8:377:MET:SD | 2.60 | 0.41 |
| 1:N8:350:LYS:NZ | 1:N8:351:SER:O | 2.43 | 0.41 |
| 2:O1:364:PRO:O | 37:7Y:244:SER:HB2 | 2.20 | 0.41 |
| 1:O2:74:ASP:O | 1:O2:78:SER:OG | 2.32 | 0.41 |
| 1:O8:95:THR:OG1 | 1:O8:96:GLY:N | 2.53 | 0.41 |
| 2:O9:194:LEU:O | 2:O9:198:THR:OG1 | 2.36 | 0.41 |
| 2:P3:175:PRO:HB3 | 2:P3:390:ARG:HE | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P7:199:ASP:HB3 | 2:P7:256:GLN:OE1 | 2.20 | 0.41 |
| 1:Q0:39:ASP:OD1 | 1:Q0:39:ASP:N | 2.47 | 0.41 |
| 2:Q1:175:PRO:HB3 | 2:Q1:390:ARG:CZ | 2.50 | 0.41 |
| 1:Q4:2:ARG:HE | 1:Q4:240:LEU:CD2 | 2.34 | 0.41 |
| 1:Q6:217:LEU:HD23 | 1:Q6:217:LEU:HA | 1.89 | 0.41 |
| 1:Q8:112:LEU:HD23 | 1:Q8:112:LEU:HA | 1.83 | 0.41 |
| 1:Q8:418:LEU:HG | 1:Q8:422:TYR:CE2 | 2.49 | 0.41 |
| 2:R1:157:LEU:HD12 | 2:R1:157:LEU:HA | 1.92 | 0.41 |
| 1:R2:417:ASP:HA | 1:R2:420:SER:HB3 | 2.02 | 0.41 |
| 1:R4:6:HIS:CE1 | 1:R4:8:GLN:HG2 | 2.56 | 0.41 |
| 2:R5:290:GLU:HA | 2:R5:293:ASN:HD22 | 1.86 | 0.41 |
| 2:R7:397:LEU:HD23 | 2:R7:397:LEU:HA | 1.92 | 0.41 |
| 1:R8:7:ILE:HD13 | 1:R8:151:LEU:HD21 | 2.02 | 0.41 |
| 1:R8:192:LEU:HD23 | 1:R8:192:LEU:HA | 1.85 | 0.41 |
| 1:S2:2:ARG:HB3 | 1:S2:131:GLN:HB2 | 2.02 | 0.41 |
| 1:S4:170:VAL:HG11 | 1:S4:201:VAL:HG13 | 2.02 | 0.41 |
| 2:S7:334:THR:O | 2:S7:337:THR:HG22 | 2.20 | 0.41 |
| 1:S8:175:VAL:HG13 | 1:S8:175:VAL:O | 2.20 | 0.41 |
| 1:S8:377:MET:HG3 | 1:S8:380:ARG:NH2 | 2.36 | 0.41 |
| 2:S9:105:ARG:HB2 | 2:S9:411:GLU:HG2 | 2.02 | 0.41 |
| 2:S9:274:PRO:HD3 | 2:S9:374:ALA:HA | 2.02 | 0.41 |
| 1:T0:244:GLY:N | 1:T0:247:ASN:HD21 | 2.17 | 0.41 |
| 2:T1:195:LEU:HD21 | 2:T1:264:ARG:HH21 | 1.85 | 0.41 |
| 1:T6:194:GLU:HB3 | 3:4H:87:GLY:HA3 | 2.03 | 0.41 |
| 2:T7:156:ARG:HA | 2:T7:159:VAL:HG22 | 2.02 | 0.41 |
| 1:T8:128:ASP:OD1 | 1:T8:128:ASP:N | 2.45 | 0.41 |
| 2:U3:312:TYR:HB2 | 2:U3:343:PHE:CD1 | 2.56 | 0.41 |
| 2:U5:286:LEU:HD23 | 2:U5:286:LEU:HA | 1.84 | 0.41 |
| 2:U9:220:GLU:H | 2:U9:220:GLU:CD | 2.21 | 0.41 |
| 2:U9:270:SER:OG | 2:U9:271:SER:N | 2.54 | 0.41 |
| 1:V2:91:VAL:HG21 | 1:V2:116:VAL:HG12 | 2.01 | 0.41 |
| 1:V2:309:ARG:H | 1:V2:372:THR:CG2 | 2.33 | 0.41 |
| 2:V7:301:MET:HE1 | 2:V7:307:PRO:HD3 | 2.02 | 0.41 |
| 1:W2:178:THR:OG1 | 1:W2:179:VAL:N | 2.52 | 0.41 |
| 1:W2:263:LEU:HD23 | 1:W2:422:TYR:CE1 | 2.55 | 0.41 |
| 2:W3:195:LEU:HD23 | 2:W3:195:LEU:HA | 1.84 | 0.41 |
| 1:W4:137:HIS:ND1 | 1:W4:138:SER:O | 2.42 | 0.41 |
| 1:W8:86:ARG:HG2 | 1:W8:88:ASP:H | 1.85 | 0.41 |
| 1:W8:403:MET:HE2 | 1:W8:403:MET:HB2 | 1.87 | 0.41 |
| 1:X6:87:PRO:HA | 1:X6:90:PHE:CD2 | 2.55 | 0.41 |
| 1:X6:203:ASP:OD2 | 1:X6:302:ALA:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:X8:83:GLN:O | 1:Z4:281:TYR:OH | 2.33 | 0.41 |
| 1:Y6:148:GLY:O | 1:Y6:152:ILE:HG12 | 2.19 | 0.41 |
| 1:Y6:284:LEU:HA | 1:Y6:288:GLU:OE1 | 2.21 | 0.41 |
| 1:Y8:48:ASN:OD1 | 1:Y8:49:VAL:N | 2.53 | 0.41 |
| 1:Z0:293:MET:HA | 1:Z0:293:MET:HE3 | 2.01 | 0.41 |
| 1:Z0:327:ASP:OD2 | 1:Z0:327:ASP:N | 2.53 | 0.41 |
| 1:Z4:24:VAL:HA | 1:Z4:27:GLU:OE2 | 2.19 | 0.41 |
| 1:Z4:332:ASN:ND2 | 1:Z4:336:LYS:HE3 | 2.35 | 0.41 |
| 1:0A:423:GLN:NE2 | 1:0A:426:GLN:OE1 | 2.51 | 0.41 |
| 2:0B:11:GLN:NE2 | 2:0B:71:GLU:OE2 | 2.53 | 0.41 |
| 2:0B:245:ASP:N | 2:0B:245:ASP:OD1 | 2.39 | 0.41 |
| 2:0B:415:GLU:OE1 | 2:0B:418:PHE:HD2 | 2.03 | 0.41 |
| 1:0E:172:SER:OG | 1:0E:380:ARG:NH1 | 2.54 | 0.41 |
| 1:0E:226:ASN:O | 1:0E:230:SER:HB2 | 2.20 | 0.41 |
| 1:0G:334:GLN:HE22 | 1:0G:347:ASN:N | 2.18 | 0.41 |
| 1:0G:372:THR:O | 1:0G:375:GLN:HG3 | 2.21 | 0.41 |
| 1:0I:253:LEU:HD23 | 1:0I:253:LEU:HA | 1.90 | 0.41 |
| 2:0J:15:GLN:HB3 | 2:0J:228:ASN:ND2 | 2.35 | 0.41 |
| 2:0L:100:ALA:HB1 | 1:0M:252:LYS:HA | 2.01 | 0.41 |
| 2:0N:394:LYS:HB2 | 1:0O:346:PRO:HG3 | 2.03 | 0.41 |
| 1:0S:337:ASN:HB3 | 1:0S:340:TYR:HD2 | 1.86 | 0.41 |
| 1:0U:58:ARG:HG2 | 1:1K:280:GLN:HE22 | 1.86 | 0.41 |
| 2:0V:76:ASP:O | 2:0V:80:THR:HG22 | 2.19 | 0.41 |
| 2:0V:111:GLY:HA2 | 2:0V:114:ILE:HG22 | 2.02 | 0.41 |
| 2:0V:319:TYR:HB3 | 2:0V:323:VAL:HG21 | 2.02 | 0.41 |
| 2:0X:211:ASP:OD1 | 2:0X:214:ARG:NH2 | 2.48 | 0.41 |
| 2:0Z:36:MET:HG3 | 2:0Z:61:HIS:NE2 | 2.36 | 0.41 |
| 2:0Z:70:LEU:HD23 | 2:0Z:70:LEU:HA | 1.83 | 0.41 |
| 2:0Z:430:LYS:HA | 2:0Z:433:GLU:HG3 | 2.02 | 0.41 |
| 1:1A:116:VAL:O | 1:1A:120:VAL:HG12 | 2.19 | 0.41 |
| 2:1B:76:ASP:O | 2:1B:80:THR:HG22 | 2.20 | 0.41 |
| 2:1B:336:LYS:NZ | 2:1B:350:GLY:H | 2.18 | 0.41 |
| 1:1C:152:ILE:HA | 1:1C:155:ILE:HG22 | 2.02 | 0.41 |
| 1:1C:177:ASP:N | 1:1C:181:GLU:OE2 | 2.53 | 0.41 |
| 1:1E:69:GLU:OE2 | 1:1E:72:THR:HG23 | 2.21 | 0.41 |
| 2:1F:250:VAL:HG11 | 2:1F:318:MET:SD | 2.61 | 0.41 |
| 1:1G:257:LEU:HD21 | 1:1G:314:SER:OG | 2.21 | 0.41 |
| 1:1O:379:LYS:HG3 | 1:1O:419:VAL:HG21 | 2.03 | 0.41 |
| 2:1R:176:GLN:HG2 | 2:1R:177:VAL:HG23 | 2.02 | 0.41 |
| 1:1S:137:HIS:O | 1:1S:168:SER:HA | 2.20 | 0.41 |
| 1:1S:396:HIS:CE1 | 1:1S:397:TRP:CE2 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1T:312:TYR:CD1 | 2:1T:381:SER:HB2 | 2.56 | 0.41 |
| 1:1U:203:ASP:OD1 | 1:1U:204:ASN:N | 2.54 | 0.41 |
| 2:1V:66:ILE:HG13 | 2:1V:66:ILE:O | 2.20 | 0.41 |
| 2:1X:252:ILE:HD12 | 2:1X:252:ILE:HA | 1.87 | 0.41 |
| 2:1X:289:ALA:O | 2:1X:292:THR:OG1 | 2.34 | 0.41 |
| 1:2A:308:GLY:HA2 | 1:2A:426:GLN:NE2 | 2.36 | 0.41 |
| 1:2C:165:LEU:HG | 1:2C:250:LEU:HD11 | 2.02 | 0.41 |
| 1:2C:332:ASN:HB3 | 1:2C:336:LYS:NZ | 2.35 | 0.41 |
| 1:2C:379:LYS:HA | 1:2C:382:SER:OG | 2.20 | 0.41 |
| 2:2F:119:LEU:HD11 | 38:8B:73:TRP:HZ2 | 1.85 | 0.41 |
| 2:2H:21:TRP:CZ3 | 2:2H:63:PRO:HB3 | 2.56 | 0.41 |
| 2:2H:113:GLU:N | 2:2H:113:GLU:OE1 | 2.53 | 0.41 |
| 2:2H:405:VAL:O | 2:2H:409:VAL:HG23 | 2.20 | 0.41 |
| 1:2I:70:PRO:HG2 | 2:2J:2:ARG:HH11 | 1.85 | 0.41 |
| 2:2J:4:VAL:HG23 | 2:2J:134:GLY:O | 2.19 | 0.41 |
| 1:2K:170:VAL:HG22 | 1:2K:202:LEU:O | 2.21 | 0.41 |
| 1:2K:174:LYS:HB3 | 1:2K:174:LYS:HE2 | 1.80 | 0.41 |
| 2:2L:132:LEU:HB3 | 2:2L:164:LYS:HE3 | 2.02 | 0.41 |
| 1:2M:327:ASP:OD2 | 1:2M:328:GLU:N | 2.54 | 0.41 |
| 2:2N:102:ASN:HB2 | 2:2N:407:TRP:CZ2 | 2.55 | 0.41 |
| 2:2N:227:LEU:O | 2:2N:230:LEU:HG | 2.21 | 0.41 |
| 2:2P:73:THR:HA | 1:2Q:46:ARG:HH21 | 1.86 | 0.41 |
| 1:2Q:294:TRP:CE2 | 1:2Q:333:VAL:HG11 | 2.55 | 0.41 |
| 2:2R:8:HIS:NE2 | 2:2R:138:PHE:HD2 | 2.19 | 0.41 |
| 1:2S:36:TYR:CZ | 1:2S:44:LEU:HD21 | 2.56 | 0.41 |
| 1:2S:391:ARG:HH21 | 2:2T:435:VAL:HA | 1.85 | 0.41 |
| 1:2U:257:LEU:HD23 | 1:2U:312:THR:HG22 | 2.02 | 0.41 |
| 2:2V:8:HIS:HB2 | 2:2V:67:PHE:HD1 | 1.85 | 0.41 |
| 2:2V:370:LYS:HE2 | 2:2V:370:LYS:HB3 | 1.92 | 0.41 |
| 1:2W:101:TRP:HE3 | 1:2W:403:MET:HE1 | 1.85 | 0.41 |
| 2:2X:60:LYS:HB2 | 2:2X:60:LYS:HE2 | 1.83 | 0.41 |
| 2:2X:251:ASP:OD1 | 2:2X:254:GLU:HG2 | 2.20 | 0.41 |
| 2:2Z:121:ARG:NH1 | 2:2Z:121:ARG:HG3 | 2.35 | 0.41 |
| 1:3A:282:ARG:NH2 | 1:3A:292:GLN:OE1 | 2.50 | 0.41 |
| 2:3B:286:LEU:HD12 | 2:3B:286:LEU:HA | 1.77 | 0.41 |
| 2:3B:305:CYS:HB3 | 2:3B:387:ILE:HD11 | 2.02 | 0.41 |
| 2:3D:109:THR:HA | 2:3D:112:LYS:HE2 | 2.02 | 0.41 |
| 1:3I:246:LEU:HD23 | 1:3I:352:SER:HA | 2.02 | 0.41 |
| 2:3J:246:GLY:H | 2:3J:249:ASN:ND2 | 2.14 | 0.41 |
| 1:3K:175:VAL:O | 1:3K:175:VAL:HG13 | 2.20 | 0.41 |
| 2:3N:306:ASP:HB3 | 2:3N:309:HIS:HD2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3O:48:ASN:N | 1:3O:48:ASN:OD1 | 2.53 | 0.41 |
| 1:3O:52:ASN:OD1 | 1:3O:62:ARG:HB2 | 2.21 | 0.41 |
| 2:3P:113:GLU:OE2 | 2:3P:113:GLU:N | 2.54 | 0.41 |
| 1:3S:362:LYS:NZ | 38:8D:166:GLU:HA | 2.36 | 0.41 |
| 2:3T:175:PRO:HB3 | 2:3T:390:ARG:NE | 2.36 | 0.41 |
| 4:3Y:23:GLU:HG3 | 4:3Y:24:ILE:HG23 | 2.01 | 0.41 |
| 3:4B:15:ARG:HB2 | 3:4B:19:LEU:HD12 | 2.02 | 0.41 |
| 4:4I:36:ARG:CZ | 3:4J:260:ILE:HG22 | 2.50 | 0.41 |
| 7:4Q:322:LYS:HB3 | 7:4Q:322:LYS:HE2 | 1.74 | 0.41 |
| 8:4W:399:GLU:HA | 8:4W:402:VAL:HG12 | 2.02 | 0.41 |
| 10:5B:120:GLU:HA | 10:5B:123:ILE:HD12 | 2.02 | 0.41 |
| 13:5I:65:VAL:HA | 13:5I:66:PRO:HD3 | 1.94 | 0.41 |
| 14:5L:434:THR:CG2 | 14:5L:439:ARG:HB2 | 2.49 | 0.41 |
| 14:5L:482:ASP:OD1 | 14:5L:482:ASP:N | 2.53 | 0.41 |
| 14:5M:434:THR:CG2 | 14:5M:439:ARG:HB2 | 2.49 | 0.41 |
| 14:5M:482:ASP:OD1 | 14:5M:482:ASP:N | 2.52 | 0.41 |
| 14:5N:434:THR:CG2 | 14:5N:439:ARG:HB2 | 2.49 | 0.41 |
| 17:5S:178:ARG:CZ | 17:5S:232:GLY:O | 2.67 | 0.41 |
| 17:5S:205:SER:OG | 17:5S:208:LYS:HG3 | 2.20 | 0.41 |
| 17:5V:179:GLN:HE21 | 17:5V:179:GLN:CA | 2.31 | 0.41 |
| 18:5X:89:GLU:OE2 | 18:5X:89:GLU:HA | 2.19 | 0.41 |
| 18:6A:17:HIS:CE1 | 18:6A:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6A:99:LEU:HD11 | 18:6A:107:VAL:HG11 | 2.02 | 0.41 |
| 18:6B:17:HIS:CE1 | 18:6B:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6B:39:TYR:CE1 | 18:6B:82:ASP:HB3 | 2.55 | 0.41 |
| 18:6B:99:LEU:HD11 | 18:6B:107:VAL:HG11 | 2.02 | 0.41 |
| 18:6C:17:HIS:CE1 | 18:6C:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6C:39:TYR:CE1 | 18:6C:82:ASP:HB3 | 2.55 | 0.41 |
| 18:6C:99:LEU:HD11 | 18:6C:107:VAL:HG11 | 2.02 | 0.41 |
| 18:6D:99:LEU:HD11 | 18:6D:107:VAL:HG11 | 2.02 | 0.41 |
| 20:6F:13:ILE:H | 20:6F:16:TRP:HB3 | 1.85 | 0.41 |
| 22:6I:275:LEU:HD23 | 22:6I:275:LEU:HA | 1.89 | 0.41 |
| 22:6K:190:LEU:HG | 22:6K:191:PHE:CD2 | 2.55 | 0.41 |
| 24:6V:218:GLY:O | 24:6V:221:ARG:NE | 2.53 | 0.41 |
| 24:6V:316:ASP:OD1 | 24:6V:317:PRO:HD2 | 2.20 | 0.41 |
| 24:6Y:372:ASP:HB2 | 24:6Y:375:THR:HG23 | 2.03 | 0.41 |
| 24:6Y:437:LYS:HE2 | 24:6Y:475:MET:O | 2.20 | 0.41 |
| 24:7A:103:LYS:HG2 | 24:7A:116:ILE:HG12 | 2.01 | 0.41 |
| 29:7I:220:LEU:HD23 | 29:7I:223:TYR:HD2 | 1.85 | 0.41 |
| 29:7J:358:LEU:HD23 | 29:7J:358:LEU:HA | 1.83 | 0.41 |
| 36:7V:94:LEU:O | 36:7V:97:VAL:HG12 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:7W:94:LEU:O | 36:7W:97:VAL:HG12 | 2.20 | 0.41 |
| 28:7X:410:HIS:HA | 28:7X:411:PRO:HD2 | 1.92 | 0.41 |
| 28:7X:410:HIS:ND1 | 28:7X:411:PRO:HD2 | 2.34 | 0.41 |
| 37:7Y:92:TYR:CZ | 37:7Y:108:PRO:HD2 | 2.55 | 0.41 |
| 37:7Y:169:THR:OG1 | 37:7Y:170:SER:N | 2.53 | 0.41 |
| 38:8A:72:ASP:HA | 38:8A:73:TRP:CE3 | 2.56 | 0.41 |
| 2:8:364:PRO:HB2 | 26:7E:53:TYR:CD1 | 2.56 | 0.41 |
| 2:A0:44:GLY:CA | 24:6X:124:TYR:OH | 2.60 | 0.41 |
| 1:A7:276:ARG:O | 24:6T:115:ARG:NH2 | 2.48 | 0.41 |
| 1:C8:90:PHE:HD2 | 24:6V:318:PHE:HZ | 1.68 | 0.41 |
| 2:G1:251:ASP:OD2 | 2:G1:254:GLU:HG2 | 2.20 | 0.41 |
| 2:G3:364:PRO:HB2 | 22:6M:165:MET:SD | 2.60 | 0.41 |
| 1:G6:117:LEU:HA | 1:G6:120:VAL:HG12 | 2.03 | 0.41 |
| 1:G6:148:GLY:O | 1:G6:152:ILE:HG12 | 2.21 | 0.41 |
| 1:G6:292:GLN:HG2 | 1:G6:298:ASN:ND2 | 2.35 | 0.41 |
| 1:G8:61:PRO:HG2 | 1:G8:85:PHE:CE1 | 2.55 | 0.41 |
| 1:G8:177:ASP:O | 2:G9:352:LYS:HA | 2.20 | 0.41 |
| 1:G8:314:SER:HA | 1:G8:350:LYS:O | 2.21 | 0.41 |
| 2:G9:248:LEU:HD12 | 2:G9:248:LEU:HA | 1.82 | 0.41 |
| 1:H2:134:GLN:NE2 | 1:H2:167:PHE:HE2 | 2.18 | 0.41 |
| 2:H3:333:ALA:O | 2:H3:337:THR:HG23 | 2.20 | 0.41 |
| 1:H4:6:HIS:CE1 | 1:H4:8:GLN:HG2 | 2.55 | 0.41 |
| 1:H8:117:LEU:HA | 1:H8:117:LEU:HD23 | 1.80 | 0.41 |
| 2:H9:124:LYS:HA | 2:H9:124:LYS:HD3 | 1.86 | 0.41 |
| 1:I2:273:LEU:H | 1:I2:292:GLN:HE22 | 1.66 | 0.41 |
| 2:I3:425:LEU:HD23 | 2:I3:425:LEU:HA | 1.87 | 0.41 |
| 2:I7:335:ILE:HD12 | 2:I7:335:ILE:HA | 1.89 | 0.41 |
| 2:I7:384:ILE:HA | 2:I7:387:ILE:HD12 | 2.03 | 0.41 |
| 2:J5:287:SER:HB3 | 2:J5:290:GLU:OE1 | 2.20 | 0.41 |
| 1:K4:334:GLN:HA | 1:K4:341:PHE:CE2 | 2.56 | 0.41 |
| 2:K7:175:PRO:HG2 | 2:K7:176:GLN:OE1 | 2.19 | 0.41 |
| 1:K8:77:ARG:HH21 | 1:K8:90:PHE:HD2 | 1.68 | 0.41 |
| 1:K8:128:ASP:OD1 | 1:K8:128:ASP:N | 2.45 | 0.41 |
| 1:K8:178:THR:OG1 | 2:K9:258:ASN:ND2 | 2.54 | 0.41 |
| 1:L0:174:LYS:HE2 | 1:L0:174:LYS:HB3 | 1.92 | 0.41 |
| 1:L0:217:LEU:HD23 | 1:L0:217:LEU:HA | 1.95 | 0.41 |
| 1:L2:314:SER:HA | 1:L2:350:LYS:O | 2.20 | 0.41 |
| 2:L3:9:ILE:HD13 | 2:L3:150:GLY:HA2 | 2.01 | 0.41 |
| 1:L4:203:ASP:OD2 | 1:L4:302:ALA:N | 2.54 | 0.41 |
| 2:L5:223:THR:HG23 | 2:L5:225:THR:H | 1.84 | 0.41 |
| 2:L7:234:VAL:HG13 | 2:L7:376:CYS:SG | 2.60 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L7:432:PHE:HA | 2:L7:435:VAL:HG12 | 2.02 | 0.41 |
| 2:L9:391:LEU:HD23 | 2:L9:391:LEU:HA | 1.90 | 0.41 |
| 1:M0:237:THR:O | 1:M0:237:THR:HG22 | 2.21 | 0.41 |
| 2:M1:213:CYS:HA | 2:M1:217:LEU:HB2 | 2.02 | 0.41 |
| 1:M4:48:ASN:N | 1:M4:48:ASN:OD1 | 2.54 | 0.41 |
| 2:M7:238:LEU:HD11 | 2:M7:255:PHE:CZ | 2.56 | 0.41 |
| 2:M7:274:PRO:HD3 | 2:M7:374:ALA:HA | 2.03 | 0.41 |
| 1:M8:154:LYS:HD3 | 1:M8:154:LYS:HA | 1.93 | 0.41 |
| 2:M9:223:THR:OG1 | 2:M9:224:TYR:N | 2.54 | 0.41 |
| 2:M9:325:PRO:HA | 2:M9:328:VAL:HG12 | 2.01 | 0.41 |
| 1:N0:379:LYS:HA | 1:N0:382:SER:HG | 1.86 | 0.41 |
| 2:N1:88:HIS:HB2 | 1:O8:281:TYR:CZ | 2.55 | 0.41 |
| 1:N2:246:LEU:HD22 | 1:N2:352:SER:HA | 2.03 | 0.41 |
| 1:N2:309:ARG:H | 1:N2:372:THR:CG2 | 2.33 | 0.41 |
| 2:N3:203:MET:O | 2:N3:204:LEU:HD22 | 2.21 | 0.41 |
| 1:N6:167:PHE:HD1 | 1:N6:200:MET:HB2 | 1.85 | 0.41 |
| 1:N8:101:TRP:HE3 | 1:N8:403:MET:HE1 | 1.85 | 0.41 |
| 2:N9:14:ILE:HG12 | 2:N9:67:PHE:HB3 | 2.01 | 0.41 |
| 1:O0:154:LYS:HB2 | 1:O0:154:LYS:HE2 | 1.86 | 0.41 |
| 1:O0:309:ARG:NH1 | 1:O0:341:PHE:O | 2.54 | 0.41 |
| 1:O2:95:THR:OG1 | 1:O2:96:GLY:N | 2.52 | 0.41 |
| 2:O3:111:GLY:HA2 | 2:O3:114:ILE:HG22 | 2.02 | 0.41 |
| 2:O3:356:ASN:OD1 | 2:O3:357:TYR:N | 2.52 | 0.41 |
| 2:O5:367:ASP:OD2 | 32:7P:129:ARG:NH1 | 2.44 | 0.41 |
| 1:O6:273:LEU:H | 1:O6:292:GLN:NE2 | 2.17 | 0.41 |
| 2:O7:70:LEU:HB3 | 2:O7:97:GLU:O | 2.21 | 0.41 |
| 2:O7:102:ASN:HB3 | 2:O7:105:ARG:HB3 | 2.02 | 0.41 |
| 2:O9:139:ASN:N | 2:O9:139:ASN:OD1 | 2.54 | 0.41 |
| 2:O9:280:LYS:HA | 2:O9:283:HIS:HB3 | 2.03 | 0.41 |
| 1:P4:3:GLU:O | 1:P4:131:GLN:HB3 | 2.20 | 0.41 |
| 2:P5:249:ASN:HD21 | 27:7G:184:LYS:H | 1.69 | 0.41 |
| 2:P5:326:LYS:HE3 | 2:P5:326:LYS:HB3 | 1.75 | 0.41 |
| 1:P8:48:ASN:OD1 | 1:P8:49:VAL:N | 2.53 | 0.41 |
| 1:P8:103:LYS:HA | 1:P8:107:THR:OG1 | 2.20 | 0.41 |
| 2:P9:327:ASP:N | 2:P9:327:ASP:OD1 | 2.54 | 0.41 |
| 2:P9:383:ALA:O | 2:P9:386:GLU:HB3 | 2.21 | 0.41 |
| 2:P9:399:TYR:OH | 2:P9:415:GLU:OE1 | 2.25 | 0.41 |
| 2:Q1:191:THR:HA | 2:Q1:194:LEU:HB3 | 2.02 | 0.41 |
| 1:Q2:68:LEU:HD23 | 1:Q2:68:LEU:HA | 1.85 | 0.41 |
| 2:Q3:54:SER:O | 2:Q3:61:HIS:HA | 2.20 | 0.41 |
| 1:Q8:135:VAL:HG21 | 1:Q8:152:ILE:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R1:22:GLU:HG2 | 2:R1:83:TYR:OH | 2.21 | 0.41 |
| 1:R2:174:LYS:HB3 | 1:R2:174:LYS:HE2 | 1.93 | 0.41 |
| 2:R3:9:ILE:HG23 | 2:R3:68:LEU:HD11 | 2.01 | 0.41 |
| 2:R5:275:ILE:HG13 | 2:R5:275:ILE:O | 2.21 | 0.41 |
| 1:R6:284:LEU:HD13 | 1:R6:284:LEU:HA | 1.93 | 0.41 |
| 1:S0:192:LEU:HD23 | 1:S0:192:LEU:HA | 1.87 | 0.41 |
| 2:S1:370:LYS:HE3 | 2:S1:370:LYS:HB2 | 1.85 | 0.41 |
| 1:S2:28:HIS:NE2 | 1:S2:241:ARG:HD2 | 2.34 | 0.41 |
| 1:S4:49:VAL:O | 1:S4:62:ARG:NH1 | 2.53 | 0.41 |
| 1:S4:212:PHE:HZ | 2:S5:326:LYS:HD3 | 1.84 | 0.41 |
| 1:S8:337:ASN:HD21 | 17:5S:48:THR:H | 1.69 | 0.41 |
| 2:S9:15:GLN:HB3 | 2:S9:228:ASN:HD21 | 1.86 | 0.41 |
| 2:T1:21:TRP:CZ3 | 2:T1:63:PRO:HB3 | 2.56 | 0.41 |
| 1:T2:306:ARG:HE | 17:5T:52:PRO:HA | 1.85 | 0.41 |
| 2:T3:358:GLN:OE1 | 2:T3:359:PRO:HD2 | 2.20 | 0.41 |
| 1:T6:135:VAL:HG22 | 1:T6:137:HIS:HD2 | 1.85 | 0.41 |
| 1:T6:173:PRO:HD3 | 1:T6:380:ARG:CZ | 2.51 | 0.41 |
| 1:T6:391:ARG:NH1 | 13:5K:61:LEU:HD21 | 2.35 | 0.41 |
| 2:T7:236:SER:HA | 2:T7:239:THR:HG22 | 2.02 | 0.41 |
| 2:U1:121:ARG:HD2 | 2:U1:121:ARG:HA | 1.86 | 0.41 |
| 1:U4:145:SER:OG | 1:U4:188:SER:OG | 2.24 | 0.41 |
| 1:U4:173:PRO:HD2 | 1:U4:380:ARG:HE | 1.85 | 0.41 |
| 1:U6:4:ILE:HB | 1:U6:50:TYR:HE1 | 1.86 | 0.41 |
| 1:U6:20:PHE:HA | 1:U6:230:SER:HB3 | 2.03 | 0.41 |
| 2:U9:69:ASP:OD2 | 2:U9:70:LEU:N | 2.52 | 0.41 |
| 1:V0:42:LEU:HD12 | 1:V0:42:LEU:HA | 1.91 | 0.41 |
| 2:V3:286:LEU:HD12 | 2:V3:286:LEU:HA | 1.78 | 0.41 |
| 1:V4:61:PRO:HG2 | 1:V4:85:PHE:HE1 | 1.86 | 0.41 |
| 1:V6:7:ILE:O | 1:V6:135:VAL:HA | 2.20 | 0.41 |
| 1:V6:58:ARG:HG2 | 1:X2:280:GLN:NE2 | 2.33 | 0.41 |
| 1:V8:31:ASP:HB2 | 1:V8:32:PRO:HD2 | 2.02 | 0.41 |
| 1:V8:100:ASN:HB3 | 1:V8:103:LYS:HB2 | 2.01 | 0.41 |
| 1:V8:173:PRO:HD2 | 1:V8:380:ARG:CZ | 2.50 | 0.41 |
| 1:V8:290:THR:HG21 | 1:V8:329:GLN:HG3 | 2.02 | 0.41 |
| 1:W0:318:ARG:HB3 | 1:W0:357:PRO:HA | 2.02 | 0.41 |
| 2:W1:65:CYS:SG | 2:W1:66:ILE:N | 2.94 | 0.41 |
| 2:W1:301:MET:HE1 | 2:W1:307:PRO:HD3 | 2.02 | 0.41 |
| 1:W2:324:LYS:O | 1:W2:328:GLU:HG2 | 2.20 | 0.41 |
| 1:W4:65:LEU:HD12 | 1:W4:90:PHE:CE1 | 2.55 | 0.41 |
| 1:W6:45:GLU:HG3 | 1:W6:46:ARG:HG2 | 2.03 | 0.41 |
| 2:W7:9:ILE:HD13 | 2:W7:150:GLY:HA2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W7:170:THR:OG1 | 2:W7:203:MET:SD | 2.78 | 0.41 |
| 1:X0:60:VAL:HG11 | 1:Y6:281:TYR:HB3 | 2.03 | 0.41 |
| 1:X0:173:PRO:HD2 | 1:X0:380:ARG:CZ | 2.51 | 0.41 |
| 1:X0:334:GLN:HE22 | 1:X0:348:ASN:H | 1.69 | 0.41 |
| 1:X2:266:PHE:CB | 1:X2:368:ILE:HD11 | 2.51 | 0.41 |
| 2:X3:75:VAL:HG11 | 2:X3:94:SER:HB3 | 2.03 | 0.41 |
| 2:X5:9:ILE:HD13 | 2:X5:150:GLY:HA2 | 2.02 | 0.41 |
| 1:Y0:46:ARG:HA | 1:Y0:46:ARG:HD3 | 1.86 | 0.41 |
| 2:Y1:141:VAL:O | 2:Y1:147:SER:OG | 2.37 | 0.41 |
| 1:Y2:46:ARG:HD3 | 1:Y2:46:ARG:HA | 1.82 | 0.41 |
| 1:Y2:49:VAL:O | 1:Y2:62:ARG:NH1 | 2.53 | 0.41 |
| 2:Y3:25:CYS:HB3 | 2:Y3:30:ILE:HB | 2.01 | 0.41 |
| 2:Y3:121:ARG:HD2 | 2:Y3:121:ARG:HA | 1.84 | 0.41 |
| 2:Y5:203:MET:HE3 | 2:Y5:384:ILE:HG23 | 2.02 | 0.41 |
| 1:Y8:306:ARG:HH22 | 1:Y8:310:TYR:HE2 | 1.67 | 0.41 |
| 2:Y9:99:ALA:HA | 2:Y9:105:ARG:HD3 | 2.02 | 0.41 |
| 1:Z2:192:LEU:HD11 | 1:Z2:199:CYS:SG | 2.61 | 0.41 |
| 1:Z4:206:ALA:O | 1:Z4:210:ILE:HG23 | 2.20 | 0.41 |
| 2:Z5:76:ASP:HA | 2:Z5:79:ARG:HG3 | 2.02 | 0.41 |
| 2:Z5:209:ILE:O | 2:Z5:212:ILE:HB | 2.19 | 0.41 |
| 2:Z5:383:ALA:O | 2:Z5:387:ILE:HG12 | 2.20 | 0.41 |
| 1:Z6:45:GLU:HG2 | 1:Z6:46:ARG:HG2 | 2.01 | 0.41 |
| 2:0B:9:ILE:HD12 | 2:0B:146:GLY:HA2 | 2.03 | 0.41 |
| 2:0B:132:LEU:HD21 | 2:0B:135:PHE:CZ | 2.56 | 0.41 |
| 1:0C:24:VAL:HA | 1:0C:27:GLU:HG3 | 2.01 | 0.41 |
| 1:0C:317:PHE:HB2 | 1:0C:353:VAL:HG12 | 2.03 | 0.41 |
| 1:0E:137:HIS:O | 1:0E:168:SER:HA | 2.20 | 0.41 |
| 1:0E:228:LEU:O | 1:0E:232:VAL:HG23 | 2.20 | 0.41 |
| 1:0I:151:LEU:HA | 1:0I:151:LEU:HD23 | 1.75 | 0.41 |
| 2:0J:79:ARG:O | 2:0J:84:ARG:HG2 | 2.20 | 0.41 |
| 2:0J:210:TYR:OH | 1:0K:323:THR:OG1 | 2.35 | 0.41 |
| 1:0O:388:MET:CE | 2:0P:348:PRO:HD3 | 2.50 | 0.41 |
| 2:0P:223:THR:OG1 | 2:0P:224:TYR:N | 2.52 | 0.41 |
| 1:0Q:379:LYS:HA | 1:0Q:379:LYS:HD2 | 1.85 | 0.41 |
| 2:0V:270:SER:OG | 2:0V:302:MET:SD | 2.78 | 0.41 |
| 2:0V:344:VAL:HG23 | 2:0V:347:CYS:HB3 | 2.02 | 0.41 |
| 1:0W:144:GLY:N | 39:0W:502:GDP:O1B | 2.51 | 0.41 |
| 1:0W:374:ILE:HD11 | 1:0W:422:TYR:CE1 | 2.55 | 0.41 |
| 1:0Y:59:TYR:CD2 | 1:0Y:59:TYR:N | 2.88 | 0.41 |
| 2:0Z:139:ASN:N | 2:0Z:139:ASN:OD1 | 2.53 | 0.41 |
| 2:1B:167:LEU:HD11 | 2:1B:252:ILE:HG23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1B:205:ASP:O | 2:1B:209:ILE:HG13 | 2.19 | 0.41 |
| 2:1B:274:PRO:HB2 | 2:1B:276:ILE:HG12 | 2.02 | 0.41 |
| 2:1B:286:LEU:HG | 2:1B:371:VAL:HG23 | 2.02 | 0.41 |
| 2:1D:305:CYS:HB3 | 2:1D:387:ILE:HD11 | 2.01 | 0.41 |
| 2:1F:379:SER:OG | 2:1F:380:ASN:N | 2.54 | 0.41 |
| 1:1G:388:MET:HE1 | 2:1H:346:TRP:O | 2.19 | 0.41 |
| 1:1K:67:ASP:CG | 1:1K:68:LEU:H | 2.23 | 0.41 |
| 1:1M:24:VAL:HG21 | 1:1M:50:TYR:HD2 | 1.85 | 0.41 |
| 1:1M:53:GLU:HB2 | 1:1M:59:TYR:CE1 | 2.56 | 0.41 |
| 1:1M:119:VAL:O | 1:1M:123:GLU:HG2 | 2.21 | 0.41 |
| 1:1M:174:LYS:HE2 | 1:1M:174:LYS:HB3 | 1.83 | 0.41 |
| 1:1O:12:CYS:O | 1:1O:16:ILE:HG23 | 2.20 | 0.41 |
| 1:1O:208:TYR:HA | 1:1O:211:CYS:SG | 2.60 | 0.41 |
| 1:1Q:100:ASN:ND2 | 1:1Q:103:LYS:HB2 | 2.34 | 0.41 |
| 1:1Q:386:THR:O | 1:1Q:390:ARG:HG3 | 2.20 | 0.41 |
| 2:1R:83:TYR:HB3 | 2:1R:86:LEU:HB3 | 2.03 | 0.41 |
| 1:1S:162:ARG:HA | 1:1S:162:ARG:HD3 | 1.79 | 0.41 |
| 1:1U:121:ARG:O | 1:1U:125:GLU:HG3 | 2.20 | 0.41 |
| 2:1V:246:GLY:HA2 | 2:1V:357:TYR:CD2 | 2.55 | 0.41 |
| 1:1W:77:ARG:HH21 | 1:1W:90:PHE:HD2 | 1.68 | 0.41 |
| 1:1W:148:GLY:O | 1:1W:152:ILE:HG12 | 2.21 | 0.41 |
| 2:1X:90:GLU:HB3 | 2:2N:283:HIS:CE1 | 2.56 | 0.41 |
| 2:1Z:62:VAL:CG2 | 2:1Z:88:HIS:HB2 | 2.49 | 0.41 |
| 2:2B:246:GLY:HA2 | 2:2B:357:TYR:CD2 | 2.55 | 0.41 |
| 2:2B:276:ILE:HD13 | 2:2B:276:ILE:HA | 1.91 | 0.41 |
| 1:2C:167:PHE:CZ | 1:2C:233:MET:HG2 | 2.56 | 0.41 |
| 1:2E:414:ASN:HA | 1:2E:417:ASP:OD2 | 2.21 | 0.41 |
| 2:2F:4:VAL:HG23 | 2:2F:134:GLY:O | 2.20 | 0.41 |
| 2:2F:98:ASP:OD1 | 2:2F:99:ALA:N | 2.53 | 0.41 |
| 2:2F:116:ASP:HB2 | 38:8B:73:TRP:CZ3 | 2.56 | 0.41 |
| 2:2F:274:PRO:HB2 | 2:2F:276:ILE:CG1 | 2.50 | 0.41 |
| 2:2H:363:VAL:HG23 | 2:2H:366:GLY:HA3 | 2.01 | 0.41 |
| 1:2I:116:VAL:O | 1:2I:120:VAL:HG12 | 2.21 | 0.41 |
| 1:2I:165:LEU:HD23 | 1:2I:165:LEU:HA | 1.83 | 0.41 |
| 1:2K:95:THR:HG23 | 1:2K:96:GLY:N | 2.35 | 0.41 |
| 2:2L:137:VAL:HG22 | 2:2L:168:GLY:HA2 | 2.01 | 0.41 |
| 2:2P:271:SER:HB2 | 2:2P:377:MET:HB3 | 2.00 | 0.41 |
| 1:2Q:101:TRP:HB2 | 1:2Q:184:ASN:OD1 | 2.20 | 0.41 |
| 2:2R:88:HIS:CG | 2:3H:283:HIS:HA | 2.56 | 0.41 |
| 2:2T:213:CYS:HA | 2:2T:217:LEU:HB2 | 2.01 | 0.41 |
| 1:2U:396:HIS:HE1 | 1:2U:397:TRP:CZ2 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2V:69:ASP:OD1 | 2:2V:70:LEU:N | 2.53 | 0.41 |
| 1:2W:50:TYR:CE2 | 1:2W:241:ARG:HD3 | 2.55 | 0.41 |
| 1:2W:174:LYS:HE2 | 1:2W:174:LYS:HB3 | 1.86 | 0.41 |
| 2:2Z:62:VAL:HG23 | 2:2Z:62:VAL:O | 2.20 | 0.41 |
| 1:3C:394:PHE:CE2 | 2:3D:261:PRO:HB3 | 2.55 | 0.41 |
| 2:3D:119:LEU:HD23 | 2:3D:119:LEU:HA | 1.80 | 0.41 |
| 2:3F:258:ASN:HB2 | 2:3F:259:LEU:HD12 | 2.03 | 0.41 |
| 1:3M:70:PRO:N | 1:3M:92:PHE:HZ | 2.18 | 0.41 |
| 1:3O:69:GLU:O | 1:3O:72:THR:OG1 | 2.39 | 0.41 |
| 1:3Q:178:THR:HG22 | 2:3R:352:LYS:CE | 2.50 | 0.41 |
| 2:3R:184:PRO:O | 2:3R:188:VAL:HG13 | 2.21 | 0.41 |
| 3:3V:8:SER:O | 3:3V:12:SER:HB3 | 2.21 | 0.41 |
| 3:3V:218:LEU:HA | 3:3V:218:LEU:HD23 | 1.84 | 0.41 |
| 4:4C:23:GLU:HG3 | 4:4C:24:ILE:HG23 | 2.02 | 0.41 |
| 4:4C:177:LEU:HD12 | 4:4C:178:PRO:HD2 | 2.03 | 0.41 |
| 3:4F:8:SER:O | 3:4F:12:SER:HB3 | 2.21 | 0.41 |
| 3:4H:218:LEU:HA | 3:4H:218:LEU:HD23 | 1.84 | 0.41 |
| 5:4M:272:MET:HE3 | 5:4M:273:GLU:HG3 | 2.02 | 0.41 |
| 5:4M:305:ALA:O | 5:4M:308:GLU:HG3 | 2.19 | 0.41 |
| 6:4O:352:ARG:HE | 6:4O:356:GLU:HG2 | 1.86 | 0.41 |
| 7:4T:239:SER:O | 7:4T:243:THR:HG22 | 2.21 | 0.41 |
| 8:4W:332:ARG:O | 8:4W:336:GLU:HG2 | 2.20 | 0.41 |
| 8:4W:379:ALA:O | 8:4W:382:GLU:HG2 | 2.20 | 0.41 |
| 9:4Y:349:GLU:O | 9:4Y:353:LEU:HD23 | 2.20 | 0.41 |
| 9:4Z:349:GLU:HA | 9:4Z:352:TYR:CD2 | 2.55 | 0.41 |
| 11:5E:75:LEU:O | 11:5E:78:ILE:HG22 | 2.20 | 0.41 |
| 14:5L:112:SER:HB3 | 14:5L:155:PHE:CD2 | 2.55 | 0.41 |
| 14:5L:125:ASP:OD1 | 14:5L:125:ASP:N | 2.48 | 0.41 |
| 14:5M:58:LYS:HB3 | 14:5M:58:LYS:HE3 | 1.90 | 0.41 |
| 14:5N:482:ASP:OD1 | 14:5N:482:ASP:N | 2.53 | 0.41 |
| 15:5O:206:HIS:ND1 | 15:5O:206:HIS:C | 2.73 | 0.41 |
| 15:5P:179:THR:HA | 15:5P:193:ARG:HH11 | 1.85 | 0.41 |
| 15:5P:338:LEU:HD12 | 15:5P:339:ARG:N | 2.35 | 0.41 |
| 18:5X:99:LEU:HD11 | 18:5X:107:VAL:HG11 | 2.02 | 0.41 |
| 18:5Y:17:HIS:CE1 | 18:5Y:21:GLN:HG3 | 2.55 | 0.41 |
| 18:5Z:89:GLU:HA | 18:5Z:89:GLU:OE2 | 2.19 | 0.41 |
| 18:5Z:99:LEU:HD11 | 18:5Z:107:VAL:HG11 | 2.02 | 0.41 |
| 18:6B:89:GLU:OE2 | 18:6B:89:GLU:HA | 2.19 | 0.41 |
| 21:6H:48:LYS:HA | 21:6H:48:LYS:HD3 | 1.73 | 0.41 |
| 22:6I:135:ARG:HB2 | 22:6I:205:GLU:OE1 | 2.20 | 0.41 |
| 22:6J:96:LYS:HA | 22:6J:96:LYS:HD2 | 1.81 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:6K:96:LYS:HD3 | 22:6K:97:PRO:HG2 | 2.02 | 0.41 |
| 22:6L:291:GLU:OE1 | 22:6L:292:ARG:HG3 | 2.21 | 0.41 |
| 22:6M:16:LYS:HG2 | 22:6M:20:TYR:CD2 | 2.55 | 0.41 |
| 22:6M:177:LEU:HB3 | 22:6M:187:MET:CE | 2.50 | 0.41 |
| 22:6M:244:VAL:HG11 | 22:6M:256:TYR:CE2 | 2.56 | 0.41 |
| 24:6T:156:ASP:N | 24:6T:156:ASP:OD2 | 2.53 | 0.41 |
| 24:6W:107:VAL:HG22 | 24:6W:108:GLU:N | 2.29 | 0.41 |
| 24:6W:218:GLY:O | 24:6W:221:ARG:NE | 2.50 | 0.41 |
| 24:6W:482:ILE:N | 24:6W:482:ILE:CD1 | 2.83 | 0.41 |
| 24:6X:83:THR:OG1 | 24:6X:84:LYS:N | 2.54 | 0.41 |
| 24:6Y:281:GLU:O | 24:6Y:281:GLU:HG2 | 2.20 | 0.41 |
| 24:6Z:577:VAL:HG21 | 24:6Z:630:LEU:HD21 | 2.03 | 0.41 |
| 24:7A:106:VAL:HG12 | 24:7A:113:ASN:C | 2.41 | 0.41 |
| 24:7A:132:VAL:HG12 | 24:7A:147:PHE:HB3 | 2.02 | 0.41 |
| 27:7G:184:LYS:HB3 | 27:7G:184:LYS:HE3 | 1.81 | 0.41 |
| 27:7G:212:LYS:HG3 | 27:7G:235:PRO:HG2 | 2.03 | 0.41 |
| 28:7H:410:HIS:HA | 28:7H:411:PRO:HD2 | 1.92 | 0.41 |
| 30:7K:190:GLN:HG2 | 30:7K:191:PRO:HD2 | 2.02 | 0.41 |
| 30:7K:245:LYS:HG2 | 30:7K:249:ASP:OD1 | 2.20 | 0.41 |
| 30:7L:272:LEU:HD22 | 30:7L:276:HIS:CD2 | 2.56 | 0.41 |
| 32:7P:30:ILE:HG23 | 32:7P:32:ASN:H | 1.85 | 0.41 |
| 32:7P:112:LEU:HD23 | 32:7P:112:LEU:HA | 1.81 | 0.41 |
| 33:7Q:137:LEU:HD13 | 33:7Q:142:ASP:OD1 | 2.20 | 0.41 |
| 35:7T:115:MET:HG3 | 35:7T:117:GLY:H | 1.85 | 0.41 |
| 38:8D:166:GLU:N | 38:8D:166:GLU:CD | 2.73 | 0.41 |
| 1:B3:360:GLY:O | 24:6W:108:GLU:HB3 | 2.21 | 0.41 |
| 2:C1:278:ALA:HB3 | 18:6D:43:ASN:ND2 | 2.21 | 0.41 |
| 1:D4:56:GLY:N | 22:6N:54:ARG:HD2 | 2.35 | 0.41 |
| 1:E6:217:LEU:HB3 | 24:6W:312:ASN:OD1 | 2.20 | 0.41 |
| 2:E7:12:ALA:HB2 | 41:E8:501:GTP:C8 | 2.56 | 0.41 |
| 2:F7:127:ASP:OD2 | 2:H3:293:ASN:ND2 | 2.53 | 0.41 |
| 2:G3:237:SER:HA | 2:G3:320:ARG:HD2 | 2.02 | 0.41 |
| 1:G4:154:LYS:O | 1:G4:157:GLU:HG3 | 2.20 | 0.41 |
| 1:G4:404:ASP:OD1 | 1:G4:405:GLU:N | 2.49 | 0.41 |
| 2:G9:155:GLU:O | 2:G9:158:SER:OG | 2.29 | 0.41 |
| 2:G9:170:THR:OG1 | 2:G9:203:MET:HG3 | 2.19 | 0.41 |
| 2:H1:4:VAL:HG23 | 2:H1:134:GLY:O | 2.21 | 0.41 |
| 2:H1:88:HIS:CE1 | 2:I7:283:HIS:HA | 2.56 | 0.41 |
| 2:H1:391:LEU:HA | 2:H1:394:LYS:HG2 | 2.01 | 0.41 |
| 1:H2:244:GLY:H | 1:H2:247:ASN:HD21 | 1.68 | 0.41 |
| 1:H4:317:PHE:CE2 | 1:H4:326:VAL:HG13 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H4:322:SER:O | 1:H4:326:VAL:HG23 | 2.20 | 0.41 |
| 2:H5:125:LEU:HA | 2:H5:125:LEU:HD23 | 1.81 | 0.41 |
| 2:H5:157:LEU:HD23 | 2:H5:157:LEU:HA | 1.80 | 0.41 |
| 1:H6:2:ARG:HE | 1:H6:240:LEU:HD23 | 1.84 | 0.41 |
| 2:H7:425:LEU:HD23 | 2:H7:425:LEU:HA | 1.88 | 0.41 |
| 1:H8:167:PHE:CE2 | 1:H8:233:MET:HG2 | 2.55 | 0.41 |
| 2:H9:26:LEU:HD21 | 2:H9:364:PRO:HD2 | 2.02 | 0.41 |
| 1:I0:156:ARG:HA | 1:I0:156:ARG:HD2 | 1.88 | 0.41 |
| 1:I0:208:TYR:OH | 2:I1:325:PRO:HB2 | 2.21 | 0.41 |
| 1:I4:207:LEU:HB3 | 1:I4:225:LEU:HD22 | 2.02 | 0.41 |
| 2:I5:319:TYR:HE1 | 2:I5:375:VAL:HG13 | 1.86 | 0.41 |
| 2:I9:66:ILE:HG13 | 2:I9:66:ILE:O | 2.19 | 0.41 |
| 2:J3:2:ARG:NH2 | 16:5Q:175:LEU:HD23 | 2.35 | 0.41 |
| 2:J3:8:HIS:NE2 | 2:J3:138:PHE:HD2 | 2.18 | 0.41 |
| 2:J9:88:HIS:HB3 | 2:L5:283:HIS:CG | 2.55 | 0.41 |
| 1:K0:183:TYR:O | 1:K0:187:LEU:HD13 | 2.20 | 0.41 |
| 1:K0:192:LEU:HD23 | 1:K0:192:LEU:HA | 1.89 | 0.41 |
| 1:K6:152:ILE:HD13 | 1:K6:152:ILE:HA | 1.90 | 0.41 |
| 2:K7:21:TRP:CZ2 | 2:K7:65:CYS:HB3 | 2.56 | 0.41 |
| 2:L1:276:ILE:HG23 | 2:L1:280:LYS:HB2 | 2.02 | 0.41 |
| 1:L2:8:GLN:CD | 1:L2:17:GLY:HA3 | 2.41 | 0.41 |
| 2:L3:305:CYS:HB3 | 2:L3:387:ILE:HD11 | 2.02 | 0.41 |
| 2:L3:372:GLN:HE22 | 6:4O:415:HIS:CE1 | 2.39 | 0.41 |
| 1:L4:174:LYS:HB3 | 1:L4:174:LYS:HE2 | 1.82 | 0.41 |
| 1:L4:283:ALA:O | 1:L4:284:LEU:HD22 | 2.20 | 0.41 |
| 1:L6:173:PRO:HD2 | 1:L6:380:ARG:NE | 2.35 | 0.41 |
| 2:L7:138:PHE:CE1 | 2:L7:169:PHE:HB2 | 2.56 | 0.41 |
| 2:L7:288:VAL:O | 2:L7:292:THR:OG1 | 2.30 | 0.41 |
| 2:M1:133:GLN:HB3 | 2:M1:252:ILE:HG21 | 2.03 | 0.41 |
| 1:M2:389:PHE:O | 1:M2:392:LYS:NZ | 2.34 | 0.41 |
| 1:M4:19:LYS:HB3 | 1:M4:19:LYS:HE3 | 1.91 | 0.41 |
| 2:M5:114:ILE:HA | 2:M5:114:ILE:HD12 | 1.84 | 0.41 |
| 2:M5:178:SER:OG | 2:M5:183:GLU:OE2 | 2.25 | 0.41 |
| 2:M5:333:ALA:O | 2:M5:337:THR:HG23 | 2.21 | 0.41 |
| 1:M6:156:ARG:HA | 1:M6:156:ARG:HD2 | 1.89 | 0.41 |
| 2:M9:298:PRO:HA | 2:M9:301:MET:HG2 | 2.03 | 0.41 |
| 1:N0:113:ILE:HD11 | 1:N0:151:LEU:HA | 2.02 | 0.41 |
| 2:N3:397:LEU:HD23 | 2:N3:397:LEU:HA | 1.86 | 0.41 |
| 2:N7:102:ASN:HB3 | 2:N7:105:ARG:HB3 | 2.02 | 0.41 |
| 2:N7:174:SER:OG | 2:N7:207:GLU:HB2 | 2.21 | 0.41 |
| 1:N8:175:VAL:O | 1:N8:175:VAL:HG13 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N9:345:ASP:OD2 | 2:N9:345:ASP:N | 2.50 | 0.41 |
| 2:N9:407:TRP:O | 2:N9:411:GLU:HG2 | 2.21 | 0.41 |
| 1:O0:3:GLU:HB2 | 1:O0:130:LEU:HA | 2.01 | 0.41 |
| 1:O0:7:ILE:HD13 | 1:O0:151:LEU:HD21 | 2.02 | 0.41 |
| 1:O0:8:GLN:CD | 1:O0:17:GLY:HA3 | 2.41 | 0.41 |
| 2:O5:119:LEU:O | 2:O5:122:ILE:HG22 | 2.21 | 0.41 |
| 2:O5:210:TYR:OH | 1:O6:323:THR:OG1 | 2.30 | 0.41 |
| 2:O7:124:LYS:HB3 | 2:O7:124:LYS:HE2 | 1.84 | 0.41 |
| 2:O7:217:LEU:HD23 | 2:O7:217:LEU:HA | 1.89 | 0.41 |
| 2:O9:133:GLN:HB3 | 2:O9:252:ILE:HG21 | 2.03 | 0.41 |
| 2:O9:334:THR:HA | 2:O9:337:THR:HG22 | 2.02 | 0.41 |
| 2:O9:346:TRP:CD1 | 2:O9:346:TRP:N | 2.88 | 0.41 |
| 2:P3:27:GLU:OE1 | 2:P3:243:ARG:NH2 | 2.52 | 0.41 |
| 2:P3:387:ILE:HD12 | 2:P3:390:ARG:HH22 | 1.85 | 0.41 |
| 2:P3:425:LEU:HD12 | 2:P3:425:LEU:HA | 1.87 | 0.41 |
| 1:P4:213:ARG:HE | 1:P4:297:LYS:HE2 | 1.83 | 0.41 |
| 1:P4:218:THR:HG23 | 27:7G:172:GLY:HA2 | 2.03 | 0.41 |
| 1:P4:314:SER:HA | 1:P4:350:LYS:O | 2.21 | 0.41 |
| 2:P7:72:PRO:HD2 | 1:P8:2:ARG:HH12 | 1.86 | 0.41 |
| 1:P8:309:ARG:H | 1:P8:372:THR:HG22 | 1.86 | 0.41 |
| 2:P9:208:ALA:O | 2:P9:212:ILE:HG12 | 2.19 | 0.41 |
| 2:P9:326:LYS:HE2 | 2:P9:326:LYS:HB3 | 1.78 | 0.41 |
| 2:P9:358:GLN:OE1 | 19:6E:164:GLY:HA3 | 2.20 | 0.41 |
| 2:P9:417:GLU:HA | 2:P9:420:GLU:CG | 2.47 | 0.41 |
| 2:Q1:90:GLU:HG3 | 2:Q1:121:ARG:HH22 | 1.85 | 0.41 |
| 2:Q3:178:SER:HB3 | 1:Q4:347:ASN:CG | 2.40 | 0.41 |
| 2:Q3:217:LEU:HB3 | 2:Q3:219:ILE:CD1 | 2.51 | 0.41 |
| 2:Q3:313:MET:HE3 | 2:Q3:313:MET:HA | 2.02 | 0.41 |
| 1:Q6:87:PRO:HD3 | 1:S2:281:TYR:CD2 | 2.54 | 0.41 |
| 1:Q6:140:GLY:O | 1:Q6:184:ASN:ND2 | 2.53 | 0.41 |
| 1:Q8:404:ASP:HB3 | 1:Q8:406:MET:SD | 2.60 | 0.41 |
| 2:Q9:125:LEU:HD23 | 2:Q9:125:LEU:HA | 1.88 | 0.41 |
| 2:Q9:220:GLU:HG2 | 2:Q9:221:ARG:HG3 | 2.03 | 0.41 |
| 2:Q9:370:LYS:HB2 | 2:Q9:370:LYS:HE3 | 1.83 | 0.41 |
| 2:R1:297:GLU:H | 2:R1:297:GLU:HG2 | 1.74 | 0.41 |
| 2:R3:11:GLN:OE1 | 2:R3:15:GLN:NE2 | 2.54 | 0.41 |
| 2:R5:2:ARG:HB2 | 2:R5:242:LEU:HD22 | 2.03 | 0.41 |
| 2:R5:35:GLN:N | 2:R5:35:GLN:OE1 | 2.53 | 0.41 |
| 2:R5:155:GLU:HG2 | 2:R5:197:HIS:HE1 | 1.86 | 0.41 |
| 2:R5:344:VAL:HG11 | 2:R5:346:TRP:CE2 | 2.56 | 0.41 |
| 2:R5:359:PRO:HG3 | 19:6E:219:PRO:HG3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:8:GLN:OE1 | 1:R6:17:GLY:HA3 | 2.20 | 0.41 |
| 1:R6:311:LEU:HD23 | 1:R6:311:LEU:HA | 1.88 | 0.41 |
| 1:S0:121:ARG:HD3 | 17:5U:48:THR:O | 2.20 | 0.41 |
| 1:S2:274:THR:HG21 | 1:S2:282:ARG:NE | 2.36 | 0.41 |
| 1:S4:11:GLN:NE2 | 2:S5:249:ASN:OD1 | 2.54 | 0.41 |
| 1:S4:221:THR:OG1 | 1:S4:222:PHE:N | 2.53 | 0.41 |
| 2:S5:137:VAL:HG11 | 2:S5:154:LEU:HD11 | 2.02 | 0.41 |
| 1:S6:167:PHE:CE2 | 1:S6:233:MET:HG2 | 2.56 | 0.41 |
| 1:S6:391:ARG:HG2 | 2:S7:346:TRP:CE3 | 2.56 | 0.41 |
| 2:S7:62:VAL:HA | 2:S7:63:PRO:HD3 | 1.91 | 0.41 |
| 2:S7:194:LEU:O | 2:S7:198:THR:OG1 | 2.39 | 0.41 |
| 2:T5:21:TRP:CZ3 | 2:T5:63:PRO:HB3 | 2.56 | 0.41 |
| 1:T6:14:ASN:ND2 | 1:T6:65:LEU:HD23 | 2.33 | 0.41 |
| 1:T6:403:MET:HE3 | 1:T6:403:MET:HB2 | 1.95 | 0.41 |
| 2:T7:12:ALA:HB2 | 41:T8:501:GTP:C8 | 2.56 | 0.41 |
| 2:U1:122:ILE:HD13 | 2:U1:157:LEU:HD21 | 2.02 | 0.41 |
| 1:U2:286:VAL:HG12 | 1:U2:329:GLN:HG2 | 2.01 | 0.41 |
| 2:U3:119:LEU:O | 2:U3:122:ILE:HG22 | 2.21 | 0.41 |
| 2:U5:191:THR:HA | 2:U5:194:LEU:HB2 | 2.02 | 0.41 |
| 1:U6:211:CYS:HB2 | 1:U6:217:LEU:HD12 | 2.02 | 0.41 |
| 1:U6:272:PRO:HD3 | 1:U6:364:SER:HA | 2.02 | 0.41 |
| 2:U7:5:ILE:HG22 | 2:U7:64:ARG:HD3 | 2.03 | 0.41 |
| 1:U8:117:LEU:HD11 | 1:U8:154:LYS:HB3 | 2.03 | 0.41 |
| 2:U9:336:LYS:HE3 | 2:U9:351:PHE:CD2 | 2.55 | 0.41 |
| 1:V0:141:GLY:O | 1:V0:145:SER:OG | 2.22 | 0.41 |
| 2:V1:72:PRO:HG3 | 1:V2:1:MET:HG3 | 2.02 | 0.41 |
| 2:V1:312:TYR:HB2 | 2:V1:343:PHE:CD1 | 2.56 | 0.41 |
| 2:V1:370:LYS:HD2 | 2:V1:370:LYS:HA | 1.92 | 0.41 |
| 1:V2:101:TRP:HB2 | 1:V2:184:ASN:OD1 | 2.20 | 0.41 |
| 2:V3:6:SER:O | 2:V3:65:CYS:HA | 2.20 | 0.41 |
| 2:V3:145:THR:O | 2:V3:149:LEU:HG | 2.21 | 0.41 |
| 2:V3:405:VAL:HG23 | 2:V3:418:PHE:HE2 | 1.85 | 0.41 |
| 1:V6:24:VAL:HG12 | 1:V6:28:HIS:HD2 | 1.86 | 0.41 |
| 1:V6:289:LEU:HD23 | 1:V6:289:LEU:HA | 1.91 | 0.41 |
| 1:V6:317:PHE:HB2 | 1:V6:353:VAL:HG12 | 2.03 | 0.41 |
| 1:V6:421:GLU:HA | 1:V6:424:GLN:HB3 | 2.03 | 0.41 |
| 2:V7:21:TRP:CZ2 | 2:V7:65:CYS:HB2 | 2.55 | 0.41 |
| 2:V7:53:PHE:HA | 2:V7:62:VAL:O | 2.21 | 0.41 |
| 2:V7:65:CYS:SG | 2:V7:66:ILE:N | 2.93 | 0.41 |
| 1:V8:251:ARG:O | 1:V8:255:VAL:HG22 | 2.19 | 0.41 |
| 2:V9:248:LEU:HD22 | 2:V9:354:GLY:HA2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V9:298:PRO:HA | 2:V9:301:MET:HG3 | 2.01 | 0.41 |
| 2:V9:318:MET:HE2 | 2:V9:376:CYS:O | 2.21 | 0.41 |
| 1:W0:123:GLU:OE1 | 1:W0:123:GLU:HA | 2.21 | 0.41 |
| 2:W1:89:PRO:CG | 2:X7:280:LYS:NZ | 2.84 | 0.41 |
| 2:W1:406:HIS:CD2 | 1:W2:261:PRO:HD3 | 2.56 | 0.41 |
| 1:W2:186:THR:HG22 | 1:W2:411:ALA:HB1 | 2.03 | 0.41 |
| 2:W3:5:ILE:HD11 | 2:W3:135:PHE:HE1 | 1.85 | 0.41 |
| 2:W5:121:ARG:HA | 2:W5:121:ARG:HD2 | 1.81 | 0.41 |
| 1:W6:7:ILE:O | 1:W6:135:VAL:HA | 2.20 | 0.41 |
| 1:W6:22:GLU:HG2 | 1:W6:81:TYR:CD1 | 2.55 | 0.41 |
| 2:W7:191:THR:HA | 2:W7:194:LEU:HB2 | 2.02 | 0.41 |
| 2:W9:56:THR:HG22 | 2:Y5:285:GLN:N | 2.35 | 0.41 |
| 1:X0:21:TRP:CZ2 | 1:X0:63:ALA:HB2 | 2.55 | 0.41 |
| 1:X2:10:GLY:O | 1:X2:14:ASN:HB2 | 2.20 | 0.41 |
| 1:X2:203:ASP:OD2 | 1:X2:302:ALA:N | 2.54 | 0.41 |
| 1:X2:222:PHE:HD1 | 1:X2:225:LEU:HD12 | 1.85 | 0.41 |
| 2:X5:103:PHE:HD1 | 2:X5:147:SER:HB3 | 1.85 | 0.41 |
| 2:X5:401:LYS:HE3 | 2:X5:401:LYS:HB3 | 1.81 | 0.41 |
| 2:X7:70:LEU:HB2 | 2:X7:98:ASP:HA | 2.03 | 0.41 |
| 2:X7:147:SER:OG | 2:X7:190:SER:HB2 | 2.20 | 0.41 |
| 2:X7:311:LYS:HE3 | 2:X7:344:VAL:HB | 2.02 | 0.41 |
| 1:X8:297:LYS:HA | 1:X8:297:LYS:HD3 | 1.92 | 0.41 |
| 2:X9:286:LEU:HD12 | 2:X9:286:LEU:N | 2.35 | 0.41 |
| 2:X9:360:PRO:HD2 | 2:X9:371:VAL:O | 2.20 | 0.41 |
| 1:Y0:336:LYS:HD2 | 1:Y0:336:LYS:HA | 1.75 | 0.41 |
| 1:Y2:224:ASP:N | 1:Y2:224:ASP:OD1 | 2.49 | 0.41 |
| 2:Y3:246:GLY:HA2 | 2:Y3:357:TYR:CD2 | 2.55 | 0.41 |
| 1:Y4:207:LEU:HD23 | 1:Y4:225:LEU:HB3 | 2.02 | 0.41 |
| 2:Y5:79:ARG:NH1 | 2:Y5:94:SER:OG | 2.53 | 0.41 |
| 1:Z2:5:VAL:HG22 | 1:Z2:62:ARG:HD3 | 2.02 | 0.41 |
| 2:Z5:62:VAL:HA | 2:Z5:63:PRO:HD3 | 1.95 | 0.41 |
| 2:Z5:117:LEU:HD12 | 2:Z5:117:LEU:HA | 1.86 | 0.41 |
| 2:Z5:183:GLU:OE1 | 2:Z5:184:PRO:HD3 | 2.19 | 0.41 |
| 1:Z6:105:HIS:NE2 | 1:Z6:150:LEU:HD13 | 2.35 | 0.41 |
| 1:0A:179:VAL:HG13 | 2:0B:349:THR:O | 2.20 | 0.41 |
| 1:0A:310:TYR:HB2 | 1:0A:341:PHE:CD1 | 2.55 | 0.41 |
| 2:0F:115:VAL:HG23 | 2:0F:153:LEU:HD13 | 2.02 | 0.41 |
| 2:0F:398:MET:HE1 | 1:0G:345:ILE:HA | 2.03 | 0.41 |
| 1:0G:19:LYS:HE3 | 1:0G:19:LYS:HB3 | 1.79 | 0.41 |
| 1:0G:113:ILE:HD13 | 1:0G:150:LEU:CD2 | 2.42 | 0.41 |
| 2:0H:166:LYS:HE2 | 2:0H:166:LYS:HB2 | 1.95 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0I:219:THR:O | 1:0I:219:THR:OG1 | 2.34 | 0.41 |
| 1:0I:286:VAL:CG2 | 1:0I:287:PRO:HD3 | 2.50 | 0.41 |
| 2:0J:325:PRO:HA | 2:0J:328:VAL:HG12 | 2.03 | 0.41 |
| 1:0K:91:VAL:HG11 | 1:0K:116:VAL:HG12 | 2.02 | 0.41 |
| 1:0K:199:CYS:SG | 1:0K:200:MET:N | 2.93 | 0.41 |
| 1:0K:233:MET:HA | 1:0K:236:ILE:HG22 | 2.02 | 0.41 |
| 2:0N:53:PHE:HB3 | 2:0N:61:HIS:HB3 | 2.02 | 0.41 |
| 2:0P:288:VAL:O | 2:0P:292:THR:OG1 | 2.25 | 0.41 |
| 2:0R:207:GLU:OE2 | 2:0R:304:LYS:HG2 | 2.20 | 0.41 |
| 1:0S:19:LYS:HE3 | 1:0S:19:LYS:HB3 | 1.89 | 0.41 |
| 1:0S:117:LEU:HD13 | 1:0S:154:LYS:HD3 | 2.01 | 0.41 |
| 1:0W:414:ASN:HA | 1:0W:417:ASP:OD2 | 2.21 | 0.41 |
| 2:0X:56:THR:OG1 | 2:1N:285:GLN:HB2 | 2.20 | 0.41 |
| 1:1A:117:LEU:HA | 1:1A:117:LEU:HD23 | 1.75 | 0.41 |
| 2:1B:217:LEU:HD13 | 2:1B:367:ASP:OD1 | 2.20 | 0.41 |
| 1:1C:5:VAL:HG12 | 1:1C:133:PHE:HD1 | 1.85 | 0.41 |
| 1:1C:270:PHE:CD2 | 1:1C:273:LEU:HD21 | 2.45 | 0.41 |
| 2:1F:289:ALA:O | 2:1F:293:ASN:ND2 | 2.53 | 0.41 |
| 1:1G:414:ASN:HA | 1:1G:417:ASP:OD2 | 2.20 | 0.41 |
| 2:1H:264:ARG:NH1 | 2:1H:431:ASP:OD2 | 2.45 | 0.41 |
| 2:1L:195:LEU:HD21 | 2:1L:264:ARG:HD2 | 2.02 | 0.41 |
| 2:1N:101:ASN:ND2 | 2:1N:143:GLY:HA2 | 2.36 | 0.41 |
| 2:1N:221:ARG:HB3 | 1:1O:322:SER:HB2 | 2.02 | 0.41 |
| 2:1N:403:ALA:HB2 | 1:1O:344:TRP:HZ3 | 1.85 | 0.41 |
| 1:1O:135:VAL:HG12 | 1:1O:137:HIS:HD2 | 1.85 | 0.41 |
| 2:1P:139:ASN:OD1 | 2:1P:170:THR:HG22 | 2.21 | 0.41 |
| 2:1X:119:LEU:HA | 2:1X:122:ILE:HG22 | 2.03 | 0.41 |
| 2:1X:223:THR:OG1 | 2:1X:224:TYR:N | 2.54 | 0.41 |
| 1:2A:65:LEU:HD12 | 1:2A:90:PHE:CE1 | 2.55 | 0.41 |
| 2:2D:155:GLU:HG3 | 2:2D:197:HIS:NE2 | 2.35 | 0.41 |
| 2:2H:425:LEU:HD23 | 2:2H:425:LEU:HA | 1.87 | 0.41 |
| 1:2I:314:SER:HA | 1:2I:350:LYS:O | 2.21 | 0.41 |
| 1:2I:359:LYS:HD2 | 1:2I:359:LYS:HA | 1.84 | 0.41 |
| 2:2J:179:THR:O | 1:2K:350:LYS:HD2 | 2.20 | 0.41 |
| 1:2K:10:GLY:HA2 | 1:2K:143:THR:HG23 | 2.02 | 0.41 |
| 1:2K:286:VAL:CG2 | 1:2K:287:PRO:HD3 | 2.49 | 0.41 |
| 2:2L:224:TYR:CD1 | 1:2M:323:THR:HG21 | 2.56 | 0.41 |
| 2:2P:76:ASP:O | 2:2P:80:THR:HG22 | 2.20 | 0.41 |
| 2:2P:181:VAL:HG23 | 2:2P:182:VAL:HG13 | 2.01 | 0.41 |
| 2:2P:262:TYR:HB2 | 2:2P:265:ILE:CG1 | 2.42 | 0.41 |
| 1:2S:22:GLU:HG2 | 1:2S:81:TYR:CD2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2V:199:ASP:OD2 | 2:2V:256:GLN:HG2 | 2.21 | 0.41 |
| 2:2X:143:GLY:O | 2:2X:147:SER:OG | 2.31 | 0.41 |
| 1:2Y:213:ARG:HD2 | 38:8C:108:PHE:CE2 | 2.55 | 0.41 |
| 2:2Z:121:ARG:HH11 | 2:2Z:121:ARG:HG3 | 1.81 | 0.41 |
| 1:3A:244:GLY:H | 1:3A:247:ASN:HD21 | 1.68 | 0.41 |
| 2:3B:121:ARG:C | 2:3B:121:ARG:CD | 2.88 | 0.41 |
| 2:3B:395:PHE:CE2 | 2:3B:422:ARG:HD3 | 2.56 | 0.41 |
| 1:3C:145:SER:OG | 1:3C:146:GLY:N | 2.53 | 0.41 |
| 2:3F:271:SER:OG | 2:3F:272:TYR:N | 2.53 | 0.41 |
| 1:3G:6:HIS:CE1 | 1:3G:8:GLN:HG2 | 2.56 | 0.41 |
| 1:3I:4:ILE:HB | 1:3I:50:TYR:HE1 | 1.84 | 0.41 |
| 2:3J:271:SER:OG | 2:3J:272:TYR:N | 2.54 | 0.41 |
| 1:3M:19:LYS:HE3 | 1:3M:19:LYS:HB3 | 1.89 | 0.41 |
| 2:3N:3:GLU:HG3 | 2:3N:51:THR:HA | 2.02 | 0.41 |
| 2:3P:55:GLU:OE2 | 2:3P:59:GLY:N | 2.53 | 0.41 |
| 2:3R:33:ASP:N | 2:3R:33:ASP:OD1 | 2.53 | 0.41 |
| 4:3W:177:LEU:HD12 | 4:3W:178:PRO:HD2 | 2.03 | 0.41 |
| 3:3X:8:SER:O | 3:3X:12:SER:HB3 | 2.21 | 0.41 |
| 4:3Y:27:LYS:HE3 | 4:3Y:27:LYS:HB3 | 1.94 | 0.41 |
| 4:3Y:95:ASP:OD1 | 4:3Y:99:VAL:HG22 | 2.20 | 0.41 |
| 4:3Y:177:LEU:HD12 | 4:3Y:178:PRO:HD2 | 2.03 | 0.41 |
| 3:3Z:8:SER:O | 3:3Z:12:SER:HB3 | 2.21 | 0.41 |
| 3:3Z:130:LEU:HA | 3:3Z:131:PRO:HD3 | 1.95 | 0.41 |
| 4:4A:95:ASP:OD1 | 4:4A:99:VAL:HG22 | 2.20 | 0.41 |
| 4:4A:177:LEU:HD12 | 4:4A:178:PRO:HD2 | 2.03 | 0.41 |
| 4:4C:95:ASP:OD1 | 4:4C:99:VAL:HG22 | 2.20 | 0.41 |
| 4:4E:95:ASP:OD1 | 4:4E:99:VAL:HG22 | 2.20 | 0.41 |
| 4:4E:177:LEU:HD12 | 4:4E:178:PRO:HD2 | 2.03 | 0.41 |
| 4:4G:177:LEU:HD12 | 4:4G:178:PRO:HD2 | 2.03 | 0.41 |
| 4:4I:177:LEU:HD12 | 4:4I:178:PRO:HD2 | 2.03 | 0.41 |
| 3:4J:189:SER:O | 3:4J:189:SER:OG | 2.32 | 0.41 |
| 6:4P:116:ASP:OD2 | 6:4P:117:ARG:N | 2.53 | 0.41 |
| 7:4R:4:LEU:HD12 | 7:4R:4:LEU:HA | 1.84 | 0.41 |
| 7:4R:245:ASP:OD1 | 7:4R:245:ASP:N | 2.53 | 0.41 |
| 7:4S:13:PRO:HG2 | 7:4S:14:GLU:OE2 | 2.21 | 0.41 |
| 9:4Z:327:ILE:HG13 | 9:4Z:328:ASP:N | 2.34 | 0.41 |
| 10:5C:328:LEU:HD23 | 10:5C:328:LEU:HA | 1.90 | 0.41 |
| 10:5C:497:MET:O | 10:5C:497:MET:HG3 | 2.17 | 0.41 |
| 15:5O:227:TYR:CD1 | 15:5O:227:TYR:O | 2.73 | 0.41 |
| 16:5Q:173:ARG:HH11 | 16:5Q:173:ARG:CG | 2.09 | 0.41 |
| 17:5S:126:GLN:HB3 | 17:5S:129:GLN:NE2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5T:126:GLN:HB3 | 17:5T:129:GLN:NE2 | 2.36 | 0.41 |
| 17:5U:69:LYS:HA | 17:5U:69:LYS:HD3 | 1.72 | 0.41 |
| 17:5U:126:GLN:HB3 | 17:5U:129:GLN:NE2 | 2.36 | 0.41 |
| 18:5Y:89:GLU:HA | 18:5Y:89:GLU:OE2 | 2.19 | 0.41 |
| 18:5Y:99:LEU:HD11 | 18:5Y:107:VAL:HG11 | 2.02 | 0.41 |
| 18:5Z:17:HIS:CE1 | 18:5Z:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6C:89:GLU:OE2 | 18:6C:89:GLU:HA | 2.19 | 0.41 |
| 18:6D:17:HIS:CE1 | 18:6D:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6D:89:GLU:HA | 18:6D:89:GLU:OE2 | 2.19 | 0.41 |
| 19:6E:92:ARG:HG3 | 19:6E:99:ARG:CD | 2.50 | 0.41 |
| 21:6H:111:VAL:HG23 | 24:6X:81:THR:HG22 | 2.03 | 0.41 |
| 21:6H:111:VAL:HG12 | 24:6X:82:ALA:O | 2.21 | 0.41 |
| 22:6N:65:ARG:HH11 | 22:6N:101:ASN:HB2 | 1.85 | 0.41 |
| 22:6O:321:LEU:HD12 | 22:6O:321:LEU:HA | 1.78 | 0.41 |
| 24:6T:119:VAL:HG21 | 24:6T:179:PHE:CD1 | 2.55 | 0.41 |
| 24:6U:130:MET:HG3 | 24:6U:153:VAL:HG22 | 2.02 | 0.41 |
| 24:6U:190:GLU:HG3 | 24:6U:191:PHE:N | 2.36 | 0.41 |
| 24:6U:612:LEU:HD12 | 24:6U:612:LEU:HA | 1.84 | 0.41 |
| 24:6V:343:ARG:HB2 | 24:6V:345:ASP:OD2 | 2.21 | 0.41 |
| 24:6V:435:LEU:HA | 24:6V:438:LEU:HB2 | 2.01 | 0.41 |
| 24:6V:485:PRO:HA | 24:6V:486:PRO:HD3 | 1.90 | 0.41 |
| 24:6W:263:ARG:HG2 | 24:6W:263:ARG:HH21 | 1.85 | 0.41 |
| 24:6W:615:ARG:HG2 | 24:6W:616:LEU:HD23 | 2.02 | 0.41 |
| 24:6X:451:LYS:CE | 24:6X:468:ARG:NH1 | 2.71 | 0.41 |
| 24:6Y:9:PRO:HB2 | 24:6Y:11:LEU:HD23 | 2.01 | 0.41 |
| 24:6Y:138:ASP:OD1 | 24:6Y:139:ASN:N | 2.52 | 0.41 |
| 24:6Y:273:LEU:HA | 24:6Y:375:THR:HG22 | 2.01 | 0.41 |
| 24:6Y:376:LYS:HA | 24:6Y:390:MET:HE2 | 2.03 | 0.41 |
| 28:7H:404:HIS:CE1 | 28:7H:406:PRO:HB3 | 2.55 | 0.41 |
| 35:7T:147:ASN:O | 35:7T:150:ILE:HG22 | 2.20 | 0.41 |
| 35:7U:125:SER:O | 35:7U:128:VAL:HG22 | 2.20 | 0.41 |
| 35:7U:221:GLN:O | 35:7U:224:GLU:HG3 | 2.21 | 0.41 |
| 36:7W:102:MET:O | 36:7W:102:MET:SD | 2.78 | 0.41 |
| 38:8A:122:LYS:HA | 38:8A:125:ASN:ND2 | 2.34 | 0.41 |
| 38:8A:194:GLU:O | 38:8A:196:MET:HG2 | 2.21 | 0.41 |
| 38:8D:112:ILE:O | 38:8D:116:GLN:HG2 | 2.20 | 0.41 |
| 2:2:42:ILE:HD12 | 24:6T:93:ARG:HB3 | 2.02 | 0.41 |
| 1:9:217:LEU:HD11 | 26:7E:136:PHE:HB3 | 2.02 | 0.41 |
| 2:B4:143:GLY:HA3 | 41:B5:501:GTP:O2B | 2.20 | 0.41 |
| 2:D7:285:GLN:HG3 | 24:6Z:256:LEU:HD11 | 2.02 | 0.41 |
| 2:E5:357:TYR:CE2 | 22:6K:97:PRO:HD3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F5:11:GLN:HB3 | 41:F5:501:GTP:PA | 2.60 | 0.41 |
| 1:G2:2:ARG:O | 1:G2:49:VAL:HG23 | 2.20 | 0.41 |
| 2:G3:53:PHE:HB3 | 2:G3:61:HIS:HB3 | 2.03 | 0.41 |
| 2:G3:176:GLN:HG2 | 2:G3:177:VAL:N | 2.35 | 0.41 |
| 2:G9:119:LEU:HD23 | 2:G9:119:LEU:HA | 1.93 | 0.41 |
| 2:G9:338:LYS:HD2 | 2:G9:338:LYS:HA | 1.90 | 0.41 |
| 2:H3:9:ILE:HD13 | 2:H3:150:GLY:HA2 | 2.02 | 0.41 |
| 1:H6:240:LEU:HD11 | 1:H6:250:LEU:HD13 | 2.03 | 0.41 |
| 1:I0:49:VAL:HG11 | 1:I0:241:ARG:HG2 | 2.02 | 0.41 |
| 2:I1:100:ALA:CB | 1:I2:252:LYS:HB3 | 2.49 | 0.41 |
| 2:I1:191:THR:HA | 2:I1:194:LEU:HB3 | 2.03 | 0.41 |
| 1:I4:198:GLU:HA | 1:I4:264:HIS:HB2 | 2.02 | 0.41 |
| 2:I5:286:LEU:HD12 | 2:I5:286:LEU:HA | 1.80 | 0.41 |
| 2:I5:387:ILE:HA | 2:I5:390:ARG:NH1 | 2.36 | 0.41 |
| 2:I7:287:SER:H | 2:I7:290:GLU:CD | 2.19 | 0.41 |
| 2:I7:395:PHE:CE2 | 2:I7:422:ARG:HD3 | 2.56 | 0.41 |
| 1:I8:389:PHE:O | 1:I8:392:LYS:NZ | 2.33 | 0.41 |
| 1:I8:404:ASP:OD1 | 1:I8:405:GLU:N | 2.49 | 0.41 |
| 2:J1:186:ASN:O | 2:J1:190:SER:OG | 2.29 | 0.41 |
| 1:J4:101:TRP:HE3 | 1:J4:403:MET:HE1 | 1.86 | 0.41 |
| 2:J5:27:GLU:HG2 | 2:J5:361:THR:HG21 | 2.02 | 0.41 |
| 2:J5:55:GLU:OE2 | 2:J5:59:GLY:N | 2.54 | 0.41 |
| 2:J7:85:GLN:O | 2:L3:283:HIS:NE2 | 2.23 | 0.41 |
| 2:K1:29:GLY:HA2 | 28:7X:402:ARG:HH22 | 1.84 | 0.41 |
| 2:K1:404:PHE:CZ | 2:K1:408:TYR:HE2 | 2.39 | 0.41 |
| 2:K3:172:TYR:CZ | 2:K3:203:MET:SD | 3.13 | 0.41 |
| 1:K4:250:LEU:HD23 | 1:K4:250:LEU:HA | 1.77 | 0.41 |
| 1:K6:273:LEU:H | 1:K6:292:GLN:NE2 | 2.19 | 0.41 |
| 1:K8:173:PRO:HB3 | 1:K8:384:GLN:HE22 | 1.86 | 0.41 |
| 1:K8:178:THR:CG2 | 1:K8:181:GLU:HG3 | 2.51 | 0.41 |
| 2:K9:125:LEU:HD23 | 2:K9:125:LEU:HA | 1.89 | 0.41 |
| 1:L0:140:GLY:O | 1:L0:184:ASN:ND2 | 2.52 | 0.41 |
| 2:L1:88:HIS:ND1 | 2:L1:89:PRO:HD2 | 2.35 | 0.41 |
| 2:L1:227:LEU:O | 2:L1:231:ILE:HG12 | 2.20 | 0.41 |
| 2:L3:76:ASP:O | 2:L3:80:THR:HG23 | 2.20 | 0.41 |
| 2:L3:201:ALA:O | 2:L3:268:MET:HE2 | 2.20 | 0.41 |
| 1:L4:212:PHE:HZ | 2:L5:326:LYS:HG3 | 1.86 | 0.41 |
| 1:L4:273:LEU:H | 1:L4:292:GLN:NE2 | 2.17 | 0.41 |
| 1:L4:338:SER:H | 35:7U:147:ASN:HD22 | 1.69 | 0.41 |
| 2:L5:152:LEU:HA | 2:L5:155:GLU:OE2 | 2.21 | 0.41 |
| 1:L6:165:LEU:HD23 | 1:L6:167:PHE:CZ | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L9:69:ASP:OD1 | 2:L9:70:LEU:N | 2.53 | 0.41 |
| 2:M1:204:LEU:HD22 | 2:M1:231:ILE:HD12 | 2.03 | 0.41 |
| 2:M1:216:SER:OG | 2:M1:217:LEU:N | 2.54 | 0.41 |
| 2:M1:245:ASP:OD1 | 2:M1:245:ASP:N | 2.46 | 0.41 |
| 1:M2:3:GLU:HG3 | 1:M2:127:CYS:SG | 2.61 | 0.41 |
| 1:M2:39:ASP:OD1 | 1:M2:39:ASP:N | 2.50 | 0.41 |
| 1:M2:183:TYR:O | 1:M2:187:LEU:HD13 | 2.21 | 0.41 |
| 2:M3:362:VAL:HG12 | 2:M3:363:VAL:N | 2.35 | 0.41 |
| 2:M3:395:PHE:CE2 | 2:M3:422:ARG:HD3 | 2.55 | 0.41 |
| 1:M4:165:LEU:CD2 | 1:M4:250:LEU:HD21 | 2.49 | 0.41 |
| 2:M5:326:LYS:HE2 | 2:M5:326:LYS:HB3 | 1.90 | 0.41 |
| 1:M6:309:ARG:NH1 | 1:M6:339:SER:O | 2.54 | 0.41 |
| 2:M7:42:ILE:H | 2:M7:42:ILE:HG13 | 1.64 | 0.41 |
| 1:M8:220:PRO:HG2 | 2:M9:326:LYS:HB2 | 2.03 | 0.41 |
| 2:M9:79:ARG:HH12 | 2:M9:94:SER:HB3 | 1.85 | 0.41 |
| 2:M9:274:PRO:HB2 | 2:M9:276:ILE:CG1 | 2.50 | 0.41 |
| 1:N0:91:VAL:CG1 | 1:N0:116:VAL:HG12 | 2.50 | 0.41 |
| 1:N0:382:SER:HB3 | 1:N0:415:MET:HG2 | 2.03 | 0.41 |
| 2:N1:175:PRO:HB3 | 2:N1:390:ARG:HD2 | 2.02 | 0.41 |
| 1:N2:19:LYS:HB3 | 1:N2:19:LYS:HE3 | 1.84 | 0.41 |
| 2:N3:60:LYS:HA | 2:N3:60:LYS:HD2 | 1.86 | 0.41 |
| 2:N3:111:GLY:O | 2:N3:115:VAL:HG12 | 2.20 | 0.41 |
| 2:N3:217:LEU:HD13 | 2:N3:367:ASP:OD1 | 2.21 | 0.41 |
| 2:N7:247:ALA:HB2 | 2:N7:357:TYR:CZ | 2.56 | 0.41 |
| 1:N8:69:GLU:OE2 | 1:N8:69:GLU:N | 2.54 | 0.41 |
| 2:N9:90:GLU:OE1 | 2:N9:90:GLU:CA | 2.67 | 0.41 |
| 1:O4:62:ARG:HG3 | 1:O4:123:GLU:HG3 | 2.03 | 0.41 |
| 1:O4:396:HIS:CD2 | 1:O4:396:HIS:H | 2.39 | 0.41 |
| 1:O8:135:VAL:HG12 | 1:O8:137:HIS:HD2 | 1.86 | 0.41 |
| 2:P3:14:ILE:HD11 | 2:P3:74:VAL:CG1 | 2.50 | 0.41 |
| 1:P4:232:VAL:O | 1:P4:236:ILE:HG12 | 2.19 | 0.41 |
| 2:P5:239:THR:HG23 | 2:P5:243:ARG:HE | 1.86 | 0.41 |
| 2:P5:434:GLU:OE2 | 2:P5:435:VAL:HG23 | 2.21 | 0.41 |
| 1:P6:28:HIS:NE2 | 1:P6:241:ARG:HD2 | 2.36 | 0.41 |
| 1:P6:292:GLN:HG2 | 1:P6:298:ASN:ND2 | 2.36 | 0.41 |
| 2:P7:320:ARG:O | 2:P7:373:ARG:HA | 2.20 | 0.41 |
| 2:P7:342:GLN:HE21 | 2:P7:342:GLN:HB2 | 1.67 | 0.41 |
| 1:P8:284:LEU:HA | 1:P8:284:LEU:HD23 | 1.75 | 0.41 |
| 1:P8:313:ALA:HA | 1:P8:369:GLY:HA2 | 2.02 | 0.41 |
| 2:P9:195:LEU:HD12 | 2:P9:195:LEU:HA | 1.82 | 0.41 |
| 2:P9:377:MET:HG2 | 2:P9:378:ILE:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q0:174:LYS:HD3 | 1:Q0:205:GLU:OE1 | 2.20 | 0.41 |
| 2:Q1:217:LEU:HD13 | 2:Q1:367:ASP:OD2 | 2.19 | 0.41 |
| 2:Q1:312:TYR:HB2 | 2:Q1:343:PHE:CD1 | 2.55 | 0.41 |
| 1:Q2:12:CYS:HB3 | 1:Q2:138:SER:HB2 | 2.02 | 0.41 |
| 1:Q2:383:GLU:OE2 | 1:Q2:384:GLN:HG3 | 2.21 | 0.41 |
| 2:Q5:179:THR:O | 1:Q6:350:LYS:HG2 | 2.20 | 0.41 |
| 1:Q8:152:ILE:HD13 | 1:Q8:152:ILE:HA | 1.90 | 0.41 |
| 2:Q9:261:PRO:HG3 | 2:Q9:313:MET:HE2 | 2.02 | 0.41 |
| 2:R1:322:ASP:HA | 7:4R:15:ARG:HH22 | 1.85 | 0.41 |
| 1:R6:228:LEU:HD23 | 1:R6:228:LEU:HA | 1.82 | 0.41 |
| 1:R8:287:PRO:HA | 1:R8:290:THR:HG22 | 2.01 | 0.41 |
| 1:S0:289:LEU:HD22 | 1:S0:363:MET:HG2 | 2.03 | 0.41 |
| 2:S1:137:VAL:HG13 | 2:S1:168:GLY:HA2 | 2.02 | 0.41 |
| 1:S4:27:GLU:OE1 | 1:S4:241:ARG:NH1 | 2.48 | 0.41 |
| 1:S6:287:PRO:HB3 | 13:5H:100:MET:SD | 2.61 | 0.41 |
| 1:S8:309:ARG:H | 1:S8:372:THR:CG2 | 2.31 | 0.41 |
| 1:S8:414:ASN:ND2 | 3:3Z:84:LYS:HD2 | 2.35 | 0.41 |
| 2:T1:79:ARG:O | 2:T1:84:ARG:HG2 | 2.21 | 0.41 |
| 2:T1:282:TYR:HE1 | 7:4U:31:LYS:HG3 | 1.86 | 0.41 |
| 1:T2:337:ASN:ND2 | 17:5T:48:THR:H | 2.19 | 0.41 |
| 2:T5:8:HIS:CD2 | 2:T5:138:PHE:HD2 | 2.39 | 0.41 |
| 2:T5:305:CYS:HB3 | 2:T5:387:ILE:HD11 | 2.03 | 0.41 |
| 2:T7:305:CYS:HB3 | 2:T7:387:ILE:HD11 | 2.02 | 0.41 |
| 2:T7:342:GLN:NE2 | 13:5K:74:ASN:HD21 | 2.18 | 0.41 |
| 1:T8:3:GLU:OE1 | 1:T8:62:ARG:NH1 | 2.54 | 0.41 |
| 1:T8:101:TRP:HB2 | 1:T8:184:ASN:OD1 | 2.20 | 0.41 |
| 1:T8:121:ARG:NH2 | 1:T8:158:GLU:OE2 | 2.44 | 0.41 |
| 1:T8:309:ARG:H | 1:T8:372:THR:HG22 | 1.84 | 0.41 |
| 1:U2:310:TYR:N | 1:U2:340:TYR:O | 2.47 | 0.41 |
| 2:U3:205:ASP:OD2 | 2:U3:303:VAL:HG13 | 2.20 | 0.41 |
| 1:U6:273:LEU:H | 1:U6:292:GLN:NE2 | 2.14 | 0.41 |
| 2:U7:242:LEU:HD11 | 2:U7:251:ASP:HA | 2.03 | 0.41 |
| 1:U8:218:THR:HG23 | 1:U8:219:THR:H | 1.84 | 0.41 |
| 1:V2:272:PRO:HD3 | 1:V2:364:SER:HA | 2.03 | 0.41 |
| 2:V3:75:VAL:HG11 | 2:V3:94:SER:HB2 | 2.03 | 0.41 |
| 2:V3:177:VAL:HG13 | 1:V4:327:ASP:HB3 | 2.03 | 0.41 |
| 1:V6:163:MET:HE3 | 1:V6:164:MET:H | 1.85 | 0.41 |
| 1:V8:140:GLY:HA3 | 1:V8:181:GLU:OE2 | 2.20 | 0.41 |
| 2:W1:3:GLU:HG3 | 2:W1:51:THR:HA | 2.02 | 0.41 |
| 1:W2:161:ASP:OD1 | 1:W2:162:ARG:NH1 | 2.54 | 0.41 |
| 2:W5:88:HIS:HB3 | 2:W5:91:GLN:CG | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W6:145:SER:OG | 1:W6:188:SER:OG | 2.31 | 0.41 |
| 1:W6:219:THR:O | 1:W6:219:THR:OG1 | 2.35 | 0.41 |
| 1:W8:6:HIS:O | 1:W8:63:ALA:HA | 2.20 | 0.41 |
| 1:W8:68:LEU:HD23 | 1:W8:93:GLY:HA3 | 2.02 | 0.41 |
| 2:W9:31:GLN:HE21 | 2:W9:37:PRO:HG3 | 1.85 | 0.41 |
| 1:X2:105:HIS:NE2 | 1:X2:150:LEU:HD13 | 2.36 | 0.41 |
| 1:X2:128:ASP:OD1 | 1:X2:128:ASP:N | 2.46 | 0.41 |
| 1:X2:252:LYS:HD2 | 1:X2:252:LYS:N | 2.34 | 0.41 |
| 2:X3:143:GLY:HA3 | 41:X4:501:GTP:O2B | 2.21 | 0.41 |
| 2:X3:149:LEU:HA | 2:X3:152:LEU:HB3 | 2.01 | 0.41 |
| 1:X4:312:THR:OG1 | 1:X4:313:ALA:N | 2.54 | 0.41 |
| 2:X5:21:TRP:CZ3 | 2:X5:63:PRO:HB3 | 2.55 | 0.41 |
| 2:X7:89:PRO:HD2 | 2:Z3:280:LYS:HZ1 | 1.85 | 0.41 |
| 1:Y0:295:ASP:HB3 | 1:Y0:298:ASN:HB2 | 2.03 | 0.41 |
| 2:Y1:26:LEU:HD21 | 2:Y1:363:VAL:HG12 | 2.02 | 0.41 |
| 2:Y1:203:MET:HE1 | 2:Y1:303:VAL:HG11 | 2.02 | 0.41 |
| 2:Y1:209:ILE:HD13 | 2:Y1:231:ILE:HD11 | 2.02 | 0.41 |
| 1:Y2:170:VAL:HG22 | 1:Y2:202:LEU:O | 2.20 | 0.41 |
| 1:Y2:183:TYR:O | 1:Y2:187:LEU:HD13 | 2.21 | 0.41 |
| 1:Y8:133:PHE:HD2 | 1:Y8:164:MET:HE2 | 1.86 | 0.41 |
| 2:Y9:312:TYR:HD2 | 2:Y9:343:PHE:HE1 | 1.66 | 0.41 |
| 1:Z0:101:TRP:CZ3 | 1:Z0:187:LEU:HD23 | 2.56 | 0.41 |
| 1:Z0:179:VAL:HG12 | 2:Z1:349:THR:O | 2.21 | 0.41 |
| 2:Z1:187:SER:O | 2:Z1:191:THR:HG23 | 2.20 | 0.41 |
| 1:Z2:246:LEU:O | 1:Z2:352:SER:OG | 2.30 | 0.41 |
| 2:Z3:209:ILE:HD11 | 2:Z3:231:ILE:HD11 | 2.03 | 0.41 |
| 1:Z6:21:TRP:CH2 | 1:Z6:61:PRO:HB3 | 2.56 | 0.41 |
| 1:Z6:69:GLU:HG2 | 1:Z6:72:THR:HG23 | 2.03 | 0.41 |
| 2:Z7:407:TRP:O | 2:Z7:411:GLU:HG2 | 2.20 | 0.41 |
| 1:Z8:25:SER:OG | 1:Z8:30:ILE:HG23 | 2.20 | 0.41 |
| 1:Z8:65:LEU:HD13 | 1:Z8:90:PHE:HD1 | 1.86 | 0.41 |
| 1:Z8:140:GLY:O | 1:Z8:184:ASN:ND2 | 2.54 | 0.41 |
| 1:Z8:156:ARG:HD2 | 1:Z8:156:ARG:HA | 1.84 | 0.41 |
| 1:Z8:383:GLU:OE2 | 1:Z8:384:GLN:HG3 | 2.20 | 0.41 |
| 2:0B:269:LEU:N | 2:0B:379:SER:O | 2.54 | 0.41 |
| 2:0B:391:LEU:HD23 | 2:0B:391:LEU:HA | 1.93 | 0.41 |
| 1:0C:39:ASP:N | 1:0C:39:ASP:OD1 | 2.53 | 0.41 |
| 1:0E:199:CYS:HG | 1:0E:265:PHE:HD1 | 1.66 | 0.41 |
| 1:0E:318:ARG:HG2 | 1:0E:354:CYS:SG | 2.61 | 0.41 |
| 1:0G:167:PHE:CE1 | 1:0G:233:MET:HE1 | 2.55 | 0.41 |
| 1:0G:174:LYS:HG3 | 1:0G:380:ARG:NH2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0I:177:ASP:N | 1:0I:181:GLU:OE2 | 2.54 | 0.41 |
| 1:0K:151:LEU:HD12 | 1:0K:152:ILE:N | 2.36 | 0.41 |
| 1:0K:198:GLU:HA | 1:0K:264:HIS:HB2 | 2.02 | 0.41 |
| 2:0N:111:GLY:HA2 | 2:0N:114:ILE:HG22 | 2.03 | 0.41 |
| 2:0N:223:THR:OG1 | 2:0N:224:TYR:N | 2.53 | 0.41 |
| 1:0O:3:GLU:O | 1:0O:131:GLN:N | 2.47 | 0.41 |
| 2:0P:90:GLU:HB2 | 2:1F:283:HIS:CE1 | 2.55 | 0.41 |
| 1:0Q:40:SER:OG | 1:0Q:43:GLN:HG3 | 2.20 | 0.41 |
| 1:0Q:397:TRP:HE1 | 2:0R:260:VAL:HB | 1.86 | 0.41 |
| 2:0R:306:ASP:HB3 | 2:0R:309:HIS:HD2 | 1.85 | 0.41 |
| 1:0S:19:LYS:O | 1:0S:23:VAL:HG22 | 2.21 | 0.41 |
| 1:0U:12:CYS:HB2 | 39:0U:501:GDP:C8 | 2.56 | 0.41 |
| 1:0U:137:HIS:O | 1:0U:168:SER:HA | 2.21 | 0.41 |
| 1:0U:382:SER:HB3 | 1:0U:415:MET:HG2 | 2.02 | 0.41 |
| 2:0V:336:LYS:HZ3 | 2:0V:349:THR:HA | 1.86 | 0.41 |
| 2:0V:413:MET:HB3 | 2:0V:417:GLU:OE2 | 2.21 | 0.41 |
| 1:0W:40:SER:OG | 1:0W:43:GLN:HG3 | 2.21 | 0.41 |
| 1:0W:207:LEU:HD23 | 1:0W:207:LEU:HA | 1.92 | 0.41 |
| 2:0Z:125:LEU:HD23 | 2:0Z:125:LEU:HA | 1.85 | 0.41 |
| 2:0Z:168:GLY:O | 2:0Z:201:ALA:HA | 2.20 | 0.41 |
| 1:1A:392:LYS:HB3 | 1:1A:395:LEU:HD22 | 2.02 | 0.41 |
| 2:1B:19:ALA:HB2 | 2:1B:228:ASN:HB3 | 2.01 | 0.41 |
| 1:1C:166:THR:OG1 | 1:1C:198:GLU:O | 2.37 | 0.41 |
| 2:1F:399:TYR:OH | 2:1F:415:GLU:OE1 | 2.24 | 0.41 |
| 1:1G:7:ILE:HB | 1:1G:135:VAL:HG22 | 2.03 | 0.41 |
| 2:1H:325:PRO:HA | 2:1H:328:VAL:HG22 | 2.02 | 0.41 |
| 1:1Q:391:ARG:O | 1:1Q:391:ARG:HG3 | 2.21 | 0.41 |
| 1:1S:210:ILE:O | 1:1S:214:THR:OG1 | 2.28 | 0.41 |
| 2:1T:83:TYR:HB3 | 2:1T:86:LEU:HB3 | 2.03 | 0.41 |
| 2:1T:88:HIS:CG | 2:2J:283:HIS:HA | 2.54 | 0.41 |
| 1:1U:113:ILE:HD13 | 1:1U:150:LEU:CD2 | 2.47 | 0.41 |
| 2:1X:4:VAL:HG23 | 2:1X:134:GLY:O | 2.19 | 0.41 |
| 2:1X:235:ILE:HD13 | 2:1X:238:LEU:HD21 | 2.03 | 0.41 |
| 2:2B:9:ILE:HG22 | 2:2B:146:GLY:HA2 | 2.03 | 0.41 |
| 1:2C:70:PRO:N | 1:2C:92:PHE:HZ | 2.18 | 0.41 |
| 2:2D:282:TYR:OH | 10:5A:380:ARG:HB2 | 2.15 | 0.41 |
| 2:2F:26:LEU:HD23 | 2:2F:363:VAL:HG22 | 2.02 | 0.41 |
| 2:2F:56:THR:HA | 2:2V:285:GLN:HB2 | 2.03 | 0.41 |
| 1:2G:309:ARG:H | 1:2G:372:THR:HG22 | 1.86 | 0.41 |
| 1:2I:313:ALA:HB1 | 1:2I:367:PHE:HE1 | 1.86 | 0.41 |
| 2:2J:171:VAL:HA | 2:2J:204:LEU:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2M:31:ASP:HB2 | 1:2M:32:PRO:HD2 | 2.03 | 0.41 |
| 2:2N:246:GLY:HA3 | 2:2N:356:ASN:HA | 2.02 | 0.41 |
| 2:2P:268:MET:N | 2:2P:268:MET:SD | 2.94 | 0.41 |
| 1:2Q:86:ARG:HB3 | 1:2Q:89:ASN:OD1 | 2.20 | 0.41 |
| 1:2Q:113:ILE:HA | 1:2Q:116:VAL:CG2 | 2.50 | 0.41 |
| 1:2Q:228:LEU:HD23 | 1:2Q:228:LEU:HA | 1.90 | 0.41 |
| 2:2R:402:ARG:HD3 | 2:2R:402:ARG:HA | 1.92 | 0.41 |
| 2:2T:139:ASN:OD1 | 2:2T:139:ASN:N | 2.53 | 0.41 |
| 2:2T:271:SER:HB2 | 2:2T:377:MET:HE2 | 2.01 | 0.41 |
| 2:2T:305:CYS:O | 2:2T:305:CYS:SG | 2.79 | 0.41 |
| 2:2T:306:ASP:HB3 | 2:2T:309:HIS:ND1 | 2.35 | 0.41 |
| 2:2V:305:CYS:HB3 | 2:2V:387:ILE:HD11 | 2.02 | 0.41 |
| 1:2W:395:LEU:O | 1:2W:399:THR:HG23 | 2.20 | 0.41 |
| 1:2Y:36:TYR:CZ | 1:2Y:44:LEU:HD21 | 2.56 | 0.41 |
| 2:2Z:237:SER:HA | 2:2Z:320:ARG:HH11 | 1.84 | 0.41 |
| 1:3A:208:TYR:CE1 | 1:3A:225:LEU:HD11 | 2.55 | 0.41 |
| 2:3B:30:ILE:HG13 | 2:3B:53:PHE:CZ | 2.56 | 0.41 |
| 1:3C:208:TYR:HB3 | 2:3D:326:LYS:NZ | 2.36 | 0.41 |
| 2:3D:139:ASN:O | 2:3D:170:THR:HA | 2.21 | 0.41 |
| 2:3D:172:TYR:CD2 | 2:3D:203:MET:HG2 | 2.55 | 0.41 |
| 2:3F:172:TYR:CZ | 2:3F:203:MET:SD | 3.14 | 0.41 |
| 2:3F:251:ASP:OD1 | 2:3F:253:THR:N | 2.53 | 0.41 |
| 1:3G:39:ASP:OD1 | 1:3G:40:SER:N | 2.51 | 0.41 |
| 2:3H:72:PRO:HD2 | 1:3I:2:ARG:NH1 | 2.36 | 0.41 |
| 2:3H:175:PRO:HB3 | 2:3H:390:ARG:NE | 2.36 | 0.41 |
| 2:3H:236:SER:OG | 2:3H:243:ARG:NH2 | 2.54 | 0.41 |
| 1:3I:21:TRP:CZ3 | 1:3I:61:PRO:HB3 | 2.55 | 0.41 |
| 1:3I:320:ARG:HG3 | 23:6Q:65:LEU:CD2 | 2.51 | 0.41 |
| 2:3J:264:ARG:NH2 | 2:3J:431:ASP:OD2 | 2.54 | 0.41 |
| 1:3M:94:GLN:HG3 | 1:3M:95:THR:HG23 | 2.02 | 0.41 |
| 1:3M:122:LYS:HG3 | 3:4D:260:ILE:HD11 | 2.02 | 0.41 |
| 2:3N:167:LEU:HD13 | 2:3N:200:VAL:HB | 2.02 | 0.41 |
| 4:3W:95:ASP:OD1 | 4:3W:99:VAL:HG22 | 2.20 | 0.41 |
| 3:3Z:218:LEU:HA | 3:3Z:218:LEU:HD23 | 1.84 | 0.41 |
| 3:4B:88:GLU:O | 3:4B:92:THR:HG23 | 2.21 | 0.41 |
| 3:4D:8:SER:O | 3:4D:12:SER:HB3 | 2.21 | 0.41 |
| 4:4G:23:GLU:HG3 | 4:4G:24:ILE:HG23 | 2.02 | 0.41 |
| 4:4G:95:ASP:OD1 | 4:4G:99:VAL:HG22 | 2.20 | 0.41 |
| 3:4H:8:SER:O | 3:4H:12:SER:HB3 | 2.21 | 0.41 |
| 4:4I:95:ASP:OD1 | 4:4I:99:VAL:HG22 | 2.20 | 0.41 |
| 5:4L:428:THR:HG21 | 16:5Q:63:ARG:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:4L:431:VAL:HG21 | 16:5Q:64:ALA:HB1 | 2.03 | 0.41 |
| 6:4O:131:GLU:O | 6:4O:135:LEU:HD23 | 2.20 | 0.41 |
| 9:4Z:68:LEU:HB3 | 10:5A:356:ARG:NH2 | 2.35 | 0.41 |
| 10:5B:113:LYS:HB2 | 10:5B:113:LYS:HE2 | 1.85 | 0.41 |
| 10:5C:389:LYS:O | 10:5C:393:GLU:HG2 | 2.20 | 0.41 |
| 10:5C:405:VAL:O | 10:5C:408:VAL:HG22 | 2.21 | 0.41 |
| 14:5L:58:LYS:HB3 | 14:5L:58:LYS:HE3 | 1.90 | 0.41 |
| 14:5M:125:ASP:OD1 | 14:5M:125:ASP:N | 2.48 | 0.41 |
| 14:5N:125:ASP:OD1 | 14:5N:125:ASP:N | 2.48 | 0.41 |
| 14:5N:354:GLU:HB2 | 14:5N:368:HIS:CD2 | 2.55 | 0.41 |
| 15:5O:109:ILE:O | 15:5O:113:ILE:HG12 | 2.21 | 0.41 |
| 15:5O:244:PRO:HD2 | 15:5O:300:GLN:HE22 | 1.86 | 0.41 |
| 15:5O:334:LEU:HG | 30:7K:241:LYS:HZ2 | 1.86 | 0.41 |
| 17:5V:208:LYS:HA | 17:5V:211:ARG:HG2 | 2.02 | 0.41 |
| 18:5X:17:HIS:CE1 | 18:5X:21:GLN:HG3 | 2.55 | 0.41 |
| 18:6A:89:GLU:OE2 | 18:6A:89:GLU:HA | 2.19 | 0.41 |
| 22:6M:204:PHE:HB3 | 22:6M:227:TYR:CE2 | 2.55 | 0.41 |
| 22:6M:264:GLN:HE22 | 24:6X:407:VAL:HG13 | 1.86 | 0.41 |
| 22:6N:208:ARG:O | 22:6N:212:GLU:HG3 | 2.21 | 0.41 |
| 24:6T:130:MET:HB2 | 24:6T:130:MET:HE2 | 1.78 | 0.41 |
| 24:6T:518:TYR:O | 24:6T:532:LEU:HD12 | 2.20 | 0.41 |
| 24:6U:482:ILE:HD12 | 24:6U:482:ILE:N | 2.35 | 0.41 |
| 24:6V:411:ASN:ND2 | 24:6V:413:TYR:HD2 | 2.19 | 0.41 |
| 24:6V:480:ASN:OD1 | 24:6V:480:ASN:N | 2.53 | 0.41 |
| 24:6V:613:LYS:O | 24:6V:617:ASP:CB | 2.68 | 0.41 |
| 24:6X:113:ASN:OD1 | 24:6X:114:HIS:ND1 | 2.46 | 0.41 |
| 24:6X:274:ARG:HB3 | 24:6X:372:ASP:OD2 | 2.21 | 0.41 |
| 24:6X:556:ASP:O | 24:6X:560:ARG:HG3 | 2.21 | 0.41 |
| 24:6Z:185:ASP:O | 24:6Z:189:ARG:HG3 | 2.20 | 0.41 |
| 24:6Z:386:THR:N | 24:6Z:389:GLU:OE1 | 2.46 | 0.41 |
| 12:7B:80:PRO:HD2 | 12:7B:82:LYS:HE3 | 2.01 | 0.41 |
| 28:7H:410:HIS:ND1 | 28:7H:411:PRO:HD2 | 2.34 | 0.41 |
| 29:7J:87:LYS:HA | 29:7J:92:TYR:HE2 | 1.84 | 0.41 |
| 30:7K:17:MET:O | 30:7K:18:THR:OG1 | 2.38 | 0.41 |
| 32:7O:35:GLU:OE1 | 32:7O:35:GLU:HA | 2.21 | 0.41 |
| 34:7S:258:MET:O | 34:7S:261:MET:HG3 | 2.20 | 0.41 |
| 36:7V:41:GLU:O | 36:7V:45:ARG:HG2 | 2.20 | 0.41 |
| 38:7Z:1:MET:HB3 | 38:7Z:2:ASN:H | 1.70 | 0.41 |
| 38:7Z:38:GLU:HG2 | 38:7Z:38:GLU:O | 2.21 | 0.41 |
| 38:8A:85:ARG:HE | 38:8A:85:ARG:HB3 | 1.63 | 0.41 |
| 38:8A:196:MET:HE3 | 38:8A:201:LEU:CD2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8D:201:LEU:HD23 | 38:8D:201:LEU:O | 2.21 | 0.41 |
| 1:9:228:LEU:HD21 | 26:7E:136:PHE:CE1 | 2.56 | 0.41 |
| 1:A1:55:THR:CG2 | 24:6Y:107:VAL:HG21 | 2.51 | 0.41 |
| 2:A2:15:GLN:OE1 | 26:7F:113:ARG:NH2 | 2.50 | 0.41 |
| 2:B9:221:ARG:HH22 | 18:6C:30:MET:HG3 | 1.84 | 0.41 |
| 2:D3:100:ALA:N | 41:D3:501:GTP:O3G | 2.53 | 0.41 |
| 1:E6:53:GLU:HB2 | 22:6L:255:PHE:CE1 | 2.55 | 0.41 |
| 2:G1:379:SER:OG | 2:G1:380:ASN:N | 2.54 | 0.41 |
| 1:G2:91:VAL:HG11 | 1:G2:116:VAL:HG22 | 2.02 | 0.41 |
| 1:G2:232:VAL:CG1 | 1:G2:268:VAL:HG11 | 2.50 | 0.41 |
| 2:G7:8:HIS:CD2 | 2:G7:138:PHE:HD2 | 2.38 | 0.41 |
| 2:G7:15:GLN:HB3 | 2:G7:228:ASN:ND2 | 2.36 | 0.41 |
| 2:H1:53:PHE:HA | 2:H1:62:VAL:O | 2.20 | 0.41 |
| 2:H3:127:ASP:OD1 | 2:I9:293:ASN:ND2 | 2.54 | 0.41 |
| 1:H4:72:THR:O | 1:H4:75:SER:OG | 2.27 | 0.41 |
| 2:H5:119:LEU:O | 2:H5:122:ILE:HG22 | 2.21 | 0.41 |
| 2:H5:172:TYR:CZ | 2:H5:203:MET:SD | 3.13 | 0.41 |
| 1:H6:77:ARG:O | 1:H6:83:GLN:NE2 | 2.54 | 0.41 |
| 2:H9:175:PRO:HB3 | 2:H9:390:ARG:NE | 2.36 | 0.41 |
| 2:H9:175:PRO:HG2 | 2:H9:176:GLN:OE1 | 2.21 | 0.41 |
| 2:I1:91:GLN:HA | 2:I1:121:ARG:HH12 | 1.86 | 0.41 |
| 2:I1:156:ARG:HA | 2:I1:159:VAL:HG22 | 2.02 | 0.41 |
| 1:I2:177:ASP:OD1 | 2:I3:248:LEU:HD11 | 2.20 | 0.41 |
| 1:I2:215:LEU:HB3 | 1:I2:217:LEU:HG | 2.03 | 0.41 |
| 1:I4:9:GLY:HA2 | 1:I4:66:MET:HE3 | 2.02 | 0.41 |
| 1:I4:183:TYR:HE2 | 1:I4:394:PHE:HB2 | 1.85 | 0.41 |
| 1:I4:186:THR:HG21 | 1:I4:412:GLU:OE2 | 2.21 | 0.41 |
| 1:I4:401:GLU:OE1 | 1:I4:403:MET:HB2 | 2.21 | 0.41 |
| 2:I5:238:LEU:HD11 | 2:I5:255:PHE:CZ | 2.56 | 0.41 |
| 2:I7:179:THR:O | 1:I8:350:LYS:HD2 | 2.20 | 0.41 |
| 2:I7:227:LEU:O | 2:I7:230:LEU:HG | 2.21 | 0.41 |
| 2:I9:245:ASP:OD1 | 2:I9:245:ASP:N | 2.53 | 0.41 |
| 1:J2:190:HIS:NE2 | 1:J2:414:ASN:OD1 | 2.53 | 0.41 |
| 2:J3:77:GLU:OE1 | 16:5Q:154:ALA:HB3 | 2.21 | 0.41 |
| 2:J3:119:LEU:O | 2:J3:122:ILE:HG22 | 2.21 | 0.41 |
| 2:J3:142:GLY:O | 2:J3:186:ASN:ND2 | 2.46 | 0.41 |
| 1:J8:54:ALA:O | 1:J8:55:THR:OG1 | 2.35 | 0.41 |
| 2:J9:27:GLU:OE1 | 2:J9:243:ARG:NH1 | 2.53 | 0.41 |
| 2:J9:183:GLU:O | 2:J9:187:SER:OG | 2.33 | 0.41 |
| 2:K1:90:GLU:HB3 | 2:L7:283:HIS:CE1 | 2.56 | 0.41 |
| 2:K1:114:ILE:HD12 | 2:K1:114:ILE:HA | 1.93 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K5:246:GLY:HA2 | 2:K5:357:TYR:CD2 | 2.55 | 0.41 |
| 2:K5:335:ILE:HD13 | 2:K5:335:ILE:HA | 1.87 | 0.41 |
| 1:K6:283:ALA:HB1 | 29:7I:9:ALA:HB2 | 2.03 | 0.41 |
| 2:K7:278:ALA:HB2 | 6:4O:263:GLN:HE22 | 1.86 | 0.41 |
| 1:K8:68:LEU:HB3 | 1:K8:96:GLY:HA2 | 2.02 | 0.41 |
| 2:K9:9:ILE:HD13 | 2:K9:150:GLY:HA2 | 2.01 | 0.41 |
| 1:L0:95:THR:HG23 | 1:L0:96:GLY:N | 2.36 | 0.41 |
| 1:L0:192:LEU:HD23 | 1:L0:192:LEU:HA | 1.87 | 0.41 |
| 2:L3:213:CYS:HA | 2:L3:217:LEU:HB2 | 2.02 | 0.41 |
| 2:L5:56:THR:HG23 | 2:N1:285:GLN:HA | 2.02 | 0.41 |
| 2:L5:157:LEU:HA | 2:L5:157:LEU:HD23 | 1.76 | 0.41 |
| 1:M0:208:TYR:CE1 | 1:M0:225:LEU:HD11 | 2.55 | 0.41 |
| 2:M3:139:ASN:O | 2:M3:170:THR:HA | 2.20 | 0.41 |
| 2:M3:250:VAL:HB | 2:M3:254:GLU:HG3 | 2.02 | 0.41 |
| 1:M4:151:LEU:O | 1:M4:155:ILE:HG12 | 2.21 | 0.41 |
| 2:M5:176:GLN:HG2 | 2:M5:177:VAL:N | 2.35 | 0.41 |
| 1:M6:75:SER:C | 15:5P:48:LYS:HE3 | 2.34 | 0.41 |
| 2:M7:157:LEU:HD23 | 2:M7:157:LEU:HA | 1.82 | 0.41 |
| 2:M7:196:GLU:OE2 | 2:M7:197:HIS:NE2 | 2.53 | 0.41 |
| 1:N0:417:ASP:OD1 | 1:N0:418:LEU:N | 2.54 | 0.41 |
| 2:N3:80:THR:HG22 | 2:N3:80:THR:O | 2.20 | 0.41 |
| 2:N5:183:GLU:CD | 2:N5:184:PRO:HD3 | 2.41 | 0.41 |
| 2:N5:191:THR:O | 2:N5:194:LEU:N | 2.54 | 0.41 |
| 1:N6:405:GLU:HA | 1:N6:408:PHE:HD2 | 1.85 | 0.41 |
| 1:N8:274:THR:HG23 | 1:N8:282:ARG:NH1 | 2.36 | 0.41 |
| 1:O2:155:ILE:HD12 | 1:O2:155:ILE:HA | 1.93 | 0.41 |
| 2:O5:318:MET:O | 2:O5:375:VAL:HA | 2.21 | 0.41 |
| 2:O7:90:GLU:OE2 | 2:O7:90:GLU:CA | 2.69 | 0.41 |
| 2:O7:322:ASP:N | 2:O7:322:ASP:OD1 | 2.54 | 0.41 |
| 1:P6:46:ARG:HD3 | 1:P6:46:ARG:HA | 1.85 | 0.41 |
| 1:P6:311:LEU:HA | 1:P6:311:LEU:HD23 | 1.72 | 0.41 |
| 2:P7:71:GLU:HB3 | 2:P7:98:ASP:OD1 | 2.20 | 0.41 |
| 2:P9:4:VAL:HG23 | 2:P9:134:GLY:O | 2.20 | 0.41 |
| 2:Q5:331:SER:O | 2:Q5:334:THR:HG22 | 2.20 | 0.41 |
| 1:Q6:153:SER:HB2 | 1:Q6:191:GLN:HE21 | 1.86 | 0.41 |
| 1:R2:39:ASP:OD1 | 1:R2:39:ASP:N | 2.51 | 0.41 |
| 1:R4:113:ILE:HD12 | 1:R4:113:ILE:HA | 1.86 | 0.41 |
| 1:R4:320:ARG:HE | 7:4R:102:ILE:HD11 | 1.86 | 0.41 |
| 1:R4:424:GLN:NE2 | 17:5T:104:PHE:HB2 | 2.35 | 0.41 |
| 2:R5:179:THR:HG21 | 41:R6:501:GTP:H3' | 2.03 | 0.41 |
| 2:R7:327:ASP:N | 2:R7:327:ASP:OD1 | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R8:279:GLN:HE22 | 7:4R:236:THR:HG21 | 1.85 | 0.41 |
| 2:S1:88:HIS:CD2 | 2:T7:283:HIS:HB3 | 2.56 | 0.41 |
| 2:S1:90:GLU:HG2 | 2:S1:121:ARG:HH12 | 1.86 | 0.41 |
| 1:S2:286:VAL:HG22 | 1:S2:363:MET:HE1 | 2.03 | 0.41 |
| 1:S4:205:GLU:OE1 | 1:S4:205:GLU:HA | 2.20 | 0.41 |
| 1:S6:117:LEU:HD11 | 1:S6:154:LYS:HB3 | 2.03 | 0.41 |
| 2:S9:51:THR:HG21 | 2:S9:243:ARG:HG2 | 2.03 | 0.41 |
| 1:T0:15:GLN:OE1 | 7:4T:367:ARG:NH2 | 2.40 | 0.41 |
| 2:T5:254:GLU:HB3 | 2:T5:352:LYS:HE2 | 2.03 | 0.41 |
| 2:T7:324:VAL:HG23 | 2:T7:326:LYS:HG3 | 2.02 | 0.41 |
| 1:T8:186:THR:HG22 | 1:T8:411:ALA:HB1 | 2.03 | 0.41 |
| 1:U6:178:THR:HG23 | 1:U6:181:GLU:HG3 | 2.03 | 0.41 |
| 2:U9:81:GLY:O | 2:U9:84:ARG:HG3 | 2.21 | 0.41 |
| 2:V1:417:GLU:HA | 2:V1:420:GLU:CG | 2.50 | 0.41 |
| 1:V8:43:GLN:HG2 | 1:V8:242:PHE:CZ | 2.55 | 0.41 |
| 2:V9:280:LYS:HA | 2:V9:283:HIS:HB3 | 2.03 | 0.41 |
| 1:W0:1:MET:O | 1:W0:129:CYS:HB3 | 2.21 | 0.41 |
| 1:W0:21:TRP:CZ3 | 1:W0:61:PRO:HB3 | 2.56 | 0.41 |
| 2:W1:344:VAL:HG11 | 2:W1:346:TRP:CE2 | 2.56 | 0.41 |
| 2:W1:406:HIS:HA | 2:W1:409:VAL:CG2 | 2.48 | 0.41 |
| 2:W5:103:PHE:CE1 | 2:W5:148:GLY:HA2 | 2.55 | 0.41 |
| 2:W7:35:GLN:HB3 | 2:W7:59:GLY:O | 2.21 | 0.41 |
| 2:W7:156:ARG:HA | 2:W7:159:VAL:HG22 | 2.03 | 0.41 |
| 2:W7:189:LEU:HD11 | 2:W7:418:PHE:HE1 | 1.84 | 0.41 |
| 1:X0:293:MET:HE3 | 1:X0:367:PHE:HB2 | 2.02 | 0.41 |
| 1:X2:175:VAL:HG13 | 2:X3:329:ASN:HD21 | 1.86 | 0.41 |
| 2:X3:328:VAL:O | 2:X3:332:VAL:HG13 | 2.21 | 0.41 |
| 1:X4:265:PHE:HE2 | 1:X4:418:LEU:HD11 | 1.86 | 0.41 |
| 2:X5:203:MET:HE1 | 2:X5:387:ILE:HD13 | 2.03 | 0.41 |
| 2:X5:217:LEU:HA | 2:X5:217:LEU:HD12 | 1.79 | 0.41 |
| 1:X6:58:ARG:NH1 | 1:X6:83:GLN:O | 2.54 | 0.41 |
| 2:X7:56:THR:HA | 2:Z3:285:GLN:HB3 | 2.01 | 0.41 |
| 1:X8:167:PHE:CE2 | 1:X8:233:MET:HG2 | 2.56 | 0.41 |
| 1:X8:409:THR:HA | 1:X8:412:GLU:CD | 2.41 | 0.41 |
| 1:Y2:22:GLU:OE2 | 1:Y2:80:PRO:HG2 | 2.20 | 0.41 |
| 1:Y2:273:LEU:HD23 | 1:Y2:273:LEU:HA | 1.94 | 0.41 |
| 1:Y4:142:GLY:N | 39:Y4:502:GDP:O2B | 2.53 | 0.41 |
| 1:Y4:397:TRP:HE1 | 2:Y5:260:VAL:HB | 1.85 | 0.41 |
| 2:Y5:189:LEU:HD23 | 2:Y5:189:LEU:HA | 1.93 | 0.41 |
| 1:Y6:4:ILE:HD11 | 1:Y6:134:GLN:HB2 | 2.03 | 0.41 |
| 1:Z4:45:GLU:H | 1:Z4:45:GLU:HG2 | 1.71 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z7:72:PRO:HD2 | 1:Z8:2:ARG:NH1 | 2.36 | 0.41 |
| 1:Z8:30:ILE:HG13 | 1:Z8:35:THR:C | 2.41 | 0.41 |
| 2:Z9:221:ARG:HB3 | 1:0A:322:SER:HB2 | 2.01 | 0.41 |
| 1:0C:64:ILE:HG13 | 1:0C:89:ASN:OD1 | 2.20 | 0.41 |
| 1:0C:182:PRO:O | 1:0C:186:THR:HG23 | 2.21 | 0.41 |
| 1:0E:414:ASN:HA | 1:0E:417:ASP:OD2 | 2.20 | 0.41 |
| 2:0F:166:LYS:HE2 | 2:0F:166:LYS:HB2 | 1.87 | 0.41 |
| 2:0F:335:ILE:HD12 | 2:0F:335:ILE:HA | 1.94 | 0.41 |
| 1:0G:68:LEU:HD21 | 1:0G:112:LEU:HD22 | 2.03 | 0.41 |
| 1:0K:272:PRO:O | 1:0K:273:LEU:HD23 | 2.20 | 0.41 |
| 1:0K:415:MET:O | 1:0K:419:VAL:HG22 | 2.21 | 0.41 |
| 1:0M:68:LEU:HD23 | 1:0M:68:LEU:HA | 1.84 | 0.41 |
| 2:0N:286:LEU:HD12 | 2:0N:286:LEU:HA | 1.85 | 0.41 |
| 1:0Q:311:LEU:O | 1:0Q:348:ASN:ND2 | 2.53 | 0.41 |
| 1:0S:69:GLU:OE2 | 1:0S:69:GLU:N | 2.53 | 0.41 |
| 1:0S:375:GLN:HA | 1:0S:378:PHE:CD2 | 2.56 | 0.41 |
| 1:0U:176:SER:O | 1:0U:176:SER:OG | 2.36 | 0.41 |
| 1:0U:249:ASP:O | 1:0U:253:LEU:HG | 2.21 | 0.41 |
| 2:0V:88:HIS:HA | 2:0V:89:PRO:HD3 | 1.88 | 0.41 |
| 1:0W:415:MET:O | 1:0W:419:VAL:HG22 | 2.21 | 0.41 |
| 2:0X:137:VAL:HG22 | 2:0X:168:GLY:HA2 | 2.03 | 0.41 |
| 2:0X:218:ASP:OD1 | 2:0X:280:LYS:NZ | 2.54 | 0.41 |
| 2:0X:274:PRO:HB2 | 2:0X:276:ILE:CG1 | 2.51 | 0.41 |
| 1:0Y:112:LEU:O | 1:0Y:116:VAL:HG23 | 2.20 | 0.41 |
| 1:0Y:383:GLU:OE2 | 1:0Y:384:GLN:HG3 | 2.21 | 0.41 |
| 2:0Z:69:ASP:OD2 | 2:0Z:71:GLU:N | 2.53 | 0.41 |
| 1:1A:297:LYS:HA | 1:1A:297:LYS:HD3 | 1.80 | 0.41 |
| 2:1D:104:ALA:HB1 | 2:1D:411:GLU:CD | 2.41 | 0.41 |
| 2:1D:137:VAL:HG22 | 2:1D:168:GLY:HA2 | 2.03 | 0.41 |
| 2:1D:156:ARG:HA | 2:1D:159:VAL:HG12 | 2.03 | 0.41 |
| 2:1D:217:LEU:HD13 | 2:1D:367:ASP:OD2 | 2.21 | 0.41 |
| 1:1E:117:LEU:HB3 | 1:1E:121:ARG:HH22 | 1.86 | 0.41 |
| 1:1E:371:SER:OG | 1:1E:372:THR:N | 2.53 | 0.41 |
| 2:1F:101:ASN:ND2 | 2:1F:143:GLY:HA2 | 2.36 | 0.41 |
| 2:1F:315:CYS:SG | 2:1F:316:CYS:N | 2.94 | 0.41 |
| 2:1F:326:LYS:HE3 | 2:1F:326:LYS:HB3 | 1.94 | 0.41 |
| 2:1H:305:CYS:SG | 2:1H:306:ASP:N | 2.93 | 0.41 |
| 1:1K:105:HIS:HB3 | 1:1K:106:TYR:CD2 | 2.56 | 0.41 |
| 1:1K:116:VAL:O | 1:1K:120:VAL:HG12 | 2.21 | 0.41 |
| 1:1K:396:HIS:CE1 | 1:1K:397:TRP:CE2 | 3.09 | 0.41 |
| 2:1L:246:GLY:HA2 | 2:1L:357:TYR:CD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1N:9:ILE:HG23 | 2:1N:68:LEU:HD11 | 2.01 | 0.41 |
| 1:1O:116:VAL:O | 1:1O:120:VAL:HG12 | 2.20 | 0.41 |
| 2:1P:4:VAL:HG23 | 2:1P:134:GLY:O | 2.21 | 0.41 |
| 1:1Q:289:LEU:HD11 | 1:1Q:363:MET:HG2 | 2.03 | 0.41 |
| 2:1T:53:PHE:HB3 | 2:1T:61:HIS:HB3 | 2.03 | 0.41 |
| 2:1V:35:GLN:HB3 | 2:1V:59:GLY:O | 2.20 | 0.41 |
| 2:1X:370:LYS:HG3 | 9:4Z:391:ILE:HD11 | 2.03 | 0.41 |
| 2:1Z:175:PRO:HG2 | 2:1Z:176:GLN:OE1 | 2.21 | 0.41 |
| 2:1Z:262:TYR:HD1 | 2:1Z:264:ARG:H | 1.69 | 0.41 |
| 1:2A:48:ASN:N | 1:2A:48:ASN:OD1 | 2.54 | 0.41 |
| 1:2A:263:LEU:HD13 | 1:2A:422:TYR:CE1 | 2.55 | 0.41 |
| 1:2C:152:ILE:HD13 | 1:2C:152:ILE:HA | 1.88 | 0.41 |
| 1:2C:178:THR:HG23 | 1:2C:181:GLU:HG3 | 2.03 | 0.41 |
| 2:2D:33:ASP:O | 2:2D:60:LYS:NZ | 2.44 | 0.41 |
| 1:2E:417:ASP:OD1 | 1:2E:418:LEU:N | 2.53 | 0.41 |
| 2:2F:133:GLN:HB3 | 2:2F:252:ILE:CG2 | 2.51 | 0.41 |
| 1:2I:239:CYS:SG | 1:2I:248:ALA:N | 2.86 | 0.41 |
| 2:2J:242:LEU:HD23 | 2:2J:242:LEU:HA | 1.87 | 0.41 |
| 2:2J:259:LEU:HD11 | 2:2J:316:CYS:HB2 | 2.03 | 0.41 |
| 2:2L:132:LEU:HD12 | 2:2L:132:LEU:HA | 1.89 | 0.41 |
| 2:2L:163:LYS:HA | 2:2L:163:LYS:HD3 | 1.85 | 0.41 |
| 1:2M:382:SER:HB3 | 1:2M:415:MET:HG2 | 2.01 | 0.41 |
| 2:2P:5:ILE:HD11 | 2:2P:135:PHE:CE1 | 2.56 | 0.41 |
| 2:2R:184:PRO:O | 2:2R:188:VAL:HG22 | 2.21 | 0.41 |
| 2:2R:285:GLN:NE2 | 2:2R:286:LEU:O | 2.53 | 0.41 |
| 2:2R:335:ILE:HG23 | 2:2R:341:ILE:HD11 | 2.03 | 0.41 |
| 2:2T:188:VAL:HG21 | 2:2T:395:PHE:CE1 | 2.56 | 0.41 |
| 1:2W:150:LEU:HD12 | 1:2W:150:LEU:HA | 1.85 | 0.41 |
| 1:2W:290:THR:HA | 1:2W:293:MET:HB2 | 2.02 | 0.41 |
| 1:2Y:355:ASP:O | 1:2Y:356:ILE:HD13 | 2.21 | 0.41 |
| 2:2Z:90:GLU:O | 2:2Z:91:GLN:C | 2.59 | 0.41 |
| 2:2Z:420:GLU:O | 2:2Z:423:GLU:HG3 | 2.21 | 0.41 |
| 1:3A:141:GLY:HA3 | 39:3A:502:GDP:O3A | 2.21 | 0.41 |
| 1:3A:178:THR:HA | 2:3B:352:LYS:HD2 | 2.02 | 0.41 |
| 1:3A:284:LEU:HD13 | 1:3A:284:LEU:HA | 1.96 | 0.41 |
| 2:3D:55:GLU:OE1 | 2:3D:59:GLY:N | 2.54 | 0.41 |
| 1:3I:292:GLN:HG2 | 1:3I:298:ASN:ND2 | 2.35 | 0.41 |
| 2:3J:276:ILE:HG23 | 2:3J:280:LYS:HB2 | 2.02 | 0.41 |
| 2:3J:280:LYS:HA | 2:3J:283:HIS:HB3 | 2.03 | 0.41 |
| 1:3K:328:GLU:OE2 | 1:3K:332:ASN:ND2 | 2.53 | 0.41 |
| 2:3N:236:SER:OG | 2:3N:243:ARG:NH2 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3P:290:GLU:HG2 | 2:3P:291:ILE:N | 2.36 | 0.41 |
| 2:3R:235:ILE:O | 2:3R:239:THR:HG23 | 2.20 | 0.41 |
| 1:3S:53:GLU:OE2 | 1:3S:58:ARG:N | 2.51 | 0.41 |
| 2:3T:172:TYR:CZ | 2:3T:203:MET:SD | 3.14 | 0.41 |
| 3:3X:88:GLU:O | 3:3X:92:THR:HG23 | 2.21 | 0.41 |
| 3:3Z:88:GLU:O | 3:3Z:92:THR:HG23 | 2.21 | 0.41 |
| 4:4A:23:GLU:HG3 | 4:4A:24:ILE:HG23 | 2.01 | 0.41 |
| 3:4B:8:SER:O | 3:4B:12:SER:HB3 | 2.21 | 0.41 |
| 3:4F:88:GLU:O | 3:4F:92:THR:HG23 | 2.21 | 0.41 |
| 5:4L:303:GLU:OE1 | 5:4L:307:ARG:HG3 | 2.20 | 0.41 |
| 7:4R:148:GLN:NE2 | 19:6E:216:PRO:O | 2.50 | 0.41 |
| 7:4S:34:LEU:HD23 | 7:4S:34:LEU:HA | 1.91 | 0.41 |
| 7:4U:64:ASP:OD1 | 12:5F:161:ARG:NH2 | 2.41 | 0.41 |
| 8:4W:407:GLU:OE2 | 8:4W:411:ARG:HG3 | 2.21 | 0.41 |
| 8:4W:424:LYS:HA | 8:4W:427:VAL:HG12 | 2.03 | 0.41 |
| 9:4Y:335:LEU:HD12 | 9:4Y:336:ARG:HD2 | 2.03 | 0.41 |
| 10:5A:296:ILE:O | 10:5A:300:ILE:HG23 | 2.21 | 0.41 |
| 10:5C:338:LYS:NZ | 14:5M:544:ALA:HB3 | 2.36 | 0.41 |
| 10:5D:205:GLN:O | 10:5D:208:GLU:HG3 | 2.20 | 0.41 |
| 14:5L:165:THR:HG22 | 14:5L:171:MET:HG3 | 2.03 | 0.41 |
| 14:5M:165:THR:HG22 | 14:5M:171:MET:HG3 | 2.03 | 0.41 |
| 14:5M:576:LEU:HB3 | 14:5M:591:GLY:HA2 | 2.02 | 0.41 |
| 14:5N:58:LYS:HB3 | 14:5N:58:LYS:HE3 | 1.90 | 0.41 |
| 15:5O:61:PHE:CD1 | 15:5O:64:SER:HB3 | 2.55 | 0.41 |
| 15:5O:192:LEU:HA | 15:5O:192:LEU:HD12 | 1.81 | 0.41 |
| 15:5P:295:ASN:O | 15:5P:298:VAL:HG12 | 2.21 | 0.41 |
| 18:5X:65:VAL:O | 18:5X:69:THR:HG22 | 2.21 | 0.41 |
| 18:5Z:73:GLN:HG2 | 18:5Z:79:VAL:HG12 | 2.03 | 0.41 |
| 18:6A:5:VAL:HG11 | 18:6A:62:GLU:CG | 2.48 | 0.41 |
| 18:6A:73:GLN:HG2 | 18:6A:79:VAL:HG12 | 2.03 | 0.41 |
| 18:6C:73:GLN:HG2 | 18:6C:79:VAL:HG12 | 2.03 | 0.41 |
| 20:6F:86:ASP:N | 20:6F:86:ASP:OD1 | 2.52 | 0.41 |
| 20:6F:367:ALA:O | 20:6F:371:THR:HG23 | 2.20 | 0.41 |
| 21:6H:11:LEU:HB3 | 21:6H:12:ASN:H | 1.50 | 0.41 |
| 22:6N:16:LYS:HD3 | 22:6N:20:TYR:CD2 | 2.55 | 0.41 |
| 22:6N:55:THR:OG1 | 22:6N:56:GLN:HG3 | 2.20 | 0.41 |
| 22:6O:294:LEU:HA | 22:6O:297:PHE:HD2 | 1.86 | 0.41 |
| 22:6P:291:GLU:HB3 | 22:6P:347:CYS:SG | 2.61 | 0.41 |
| 24:6T:24:ASP:OD1 | 24:6T:24:ASP:N | 2.49 | 0.41 |
| 24:6T:470:ILE:HD11 | 24:6T:485:PRO:HG2 | 2.01 | 0.41 |
| 24:6X:106:VAL:HG12 | 24:6X:113:ASN:C | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6Z:167:SER:CB | 24:6Z:197:LYS:HZ2 | 2.34 | 0.41 |
| 27:7G:23:VAL:HG23 | 27:7G:24:LYS:N | 2.32 | 0.41 |
| 29:7I:145:ALA:HB3 | 29:7I:171:THR:HB | 2.03 | 0.41 |
| 30:7K:180:ALA:O | 30:7K:183:THR:OG1 | 2.34 | 0.41 |
| 31:7N:35:SER:OG | 31:7N:36:ASP:N | 2.53 | 0.41 |
| 32:7O:30:ILE:HD12 | 32:7O:30:ILE:HA | 1.94 | 0.41 |
| 34:7S:267:VAL:O | 34:7S:271:LYS:HG2 | 2.21 | 0.41 |
| 36:7W:41:GLU:O | 36:7W:45:ARG:HG2 | 2.20 | 0.41 |
| 28:7X:392:LEU:HD21 | 28:7X:433:SER:HA | 2.03 | 0.41 |
| 38:8C:2:ASN:HB3 | 38:8C:5:LYS:HB2 | 2.02 | 0.41 |
| 1:3:337:ASN:HD21 | 3:3X:69:TYR:H | 1.68 | 0.41 |
| 1:9:83:GLN:CG | 24:6X:177:ARG:HH22 | 2.34 | 0.41 |
| 1:9:309:ARG:HG2 | 3:4D:104:PRO:HG3 | 2.03 | 0.41 |
| 2:A0:44:GLY:CA | 24:6X:124:TYR:HH | 2.33 | 0.41 |
| 2:A2:365:GLY:HA3 | 26:7F:38:ASN:OD1 | 2.20 | 0.41 |
| 2:A4:42:ILE:HG21 | 24:6Z:93:ARG:NH1 | 2.36 | 0.41 |
| 2:A8:223:THR:HG23 | 18:5X:51:MET:CE | 2.45 | 0.41 |
| 1:B5:357:PRO:HG2 | 18:6A:22:ARG:NH2 | 2.35 | 0.41 |
| 1:B8:70:PRO:HB2 | 24:6Y:243:LYS:HE2 | 2.02 | 0.41 |
| 1:D6:74:ASP:OD1 | 24:6Z:319:PRO:HD2 | 2.20 | 0.41 |
| 2:G1:51:THR:HG21 | 2:G1:243:ARG:HG2 | 2.01 | 0.41 |
| 2:G1:239:THR:HG23 | 2:G1:243:ARG:HE | 1.86 | 0.41 |
| 1:G2:5:VAL:HG12 | 1:G2:133:PHE:CD1 | 2.56 | 0.41 |
| 1:G2:240:LEU:HD21 | 1:G2:249:ASP:HB3 | 2.02 | 0.41 |
| 1:G2:319:GLY:O | 1:G2:321:MET:HG3 | 2.21 | 0.41 |
| 2:G3:39:ASP:O | 24:6W:537:GLU:HB2 | 2.21 | 0.41 |
| 2:G3:125:LEU:HD23 | 2:G3:125:LEU:HA | 1.86 | 0.41 |
| 2:G5:28:HIS:CE1 | 2:G5:49:PHE:HA | 2.56 | 0.41 |
| 2:G5:288:VAL:O | 2:G5:292:THR:OG1 | 2.23 | 0.41 |
| 1:G6:219:THR:HG22 | 24:6Y:418:ASP:CG | 2.41 | 0.41 |
| 2:G7:274:PRO:HD3 | 2:G7:374:ALA:HA | 2.02 | 0.41 |
| 1:G8:117:LEU:HA | 1:G8:117:LEU:HD23 | 1.86 | 0.41 |
| 1:G8:371:SER:OG | 1:G8:372:THR:N | 2.54 | 0.41 |
| 2:H1:203:MET:SD | 2:H1:267:PHE:HB3 | 2.60 | 0.41 |
| 2:H1:415:GLU:OE1 | 2:H1:415:GLU:N | 2.54 | 0.41 |
| 1:H2:41:ASP:HA | 1:H2:44:LEU:HG | 2.03 | 0.41 |
| 1:H2:173:PRO:HG2 | 1:H2:380:ARG:HH21 | 1.85 | 0.41 |
| 1:H2:218:THR:CB | 24:6T:488:ARG:O | 2.66 | 0.41 |
| 1:H2:248:ALA:HA | 1:H2:252:LYS:HD2 | 2.02 | 0.41 |
| 1:H2:415:MET:O | 1:H2:419:VAL:HG22 | 2.21 | 0.41 |
| 2:H3:250:VAL:HG23 | 2:H3:254:GLU:HG3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H4:127:CYS:SG | 1:H4:128:ASP:N | 2.94 | 0.41 |
| 1:H4:152:ILE:HD13 | 1:H4:152:ILE:HA | 1.92 | 0.41 |
| 2:H5:223:THR:OG1 | 2:H5:224:TYR:N | 2.53 | 0.41 |
| 2:H5:388:PHE:O | 2:H5:391:LEU:HG | 2.21 | 0.41 |
| 1:H6:9:GLY:HA2 | 1:H6:66:MET:HE3 | 2.03 | 0.41 |
| 1:H8:128:ASP:OD1 | 1:H8:129:CYS:N | 2.51 | 0.41 |
| 1:H8:137:HIS:O | 1:H8:168:SER:HA | 2.21 | 0.41 |
| 1:H8:213:ARG:O | 1:H8:216:LYS:HG3 | 2.20 | 0.41 |
| 1:H8:272:PRO:HB2 | 1:H8:282:ARG:HH12 | 1.86 | 0.41 |
| 1:H8:371:SER:OG | 1:H8:372:THR:N | 2.53 | 0.41 |
| 2:H9:74:VAL:O | 2:H9:78:VAL:HG23 | 2.21 | 0.41 |
| 2:H9:238:LEU:HD11 | 2:H9:255:PHE:CE2 | 2.56 | 0.41 |
| 1:I0:164:MET:N | 1:I0:197:ASP:OD2 | 2.53 | 0.41 |
| 1:I0:385:PHE:HD2 | 1:I0:412:GLU:OE2 | 2.04 | 0.41 |
| 2:I1:88:HIS:CE1 | 2:I1:90:GLU:HB3 | 2.55 | 0.41 |
| 1:I2:7:ILE:HB | 1:I2:135:VAL:HG22 | 2.03 | 0.41 |
| 1:I2:134:GLN:HE22 | 1:I2:237:THR:HG21 | 1.85 | 0.41 |
| 2:I3:216:SER:OG | 2:I3:217:LEU:N | 2.54 | 0.41 |
| 2:I3:223:THR:HG23 | 2:I3:225:THR:H | 1.85 | 0.41 |
| 1:I4:95:THR:HG23 | 1:I4:96:GLY:H | 1.85 | 0.41 |
| 1:I4:113:ILE:HA | 1:I4:116:VAL:CG1 | 2.48 | 0.41 |
| 1:I4:218:THR:HG21 | 24:6Z:488:ARG:HA | 2.02 | 0.41 |
| 1:I4:235:GLY:HA3 | 1:I4:366:THR:HG21 | 2.02 | 0.41 |
| 1:I4:268:VAL:O | 1:I4:300:MET:N | 2.41 | 0.41 |
| 2:I5:113:GLU:OE2 | 2:I5:114:ILE:HB | 2.21 | 0.41 |
| 2:I5:389:SER:N | 2:I5:429:GLU:OE2 | 2.54 | 0.41 |
| 2:I7:290:GLU:HA | 2:I7:293:ASN:HD22 | 1.86 | 0.41 |
| 2:I7:395:PHE:HE2 | 2:I7:422:ARG:HD3 | 1.86 | 0.41 |
| 1:I8:192:LEU:HD23 | 1:I8:192:LEU:HA | 1.86 | 0.41 |
| 2:I9:11:GLN:OE1 | 2:I9:15:GLN:NE2 | 2.53 | 0.41 |
| 2:I9:119:LEU:HD11 | 2:I9:156:ARG:CB | 2.51 | 0.41 |
| 2:I9:371:VAL:HG12 | 2:I9:373:ARG:H | 1.86 | 0.41 |
| 1:J0:56:GLY:O | 6:4O:224:ARG:HD3 | 2.21 | 0.41 |
| 2:J1:34:GLY:HA3 | 2:J1:60:LYS:NZ | 2.36 | 0.41 |
| 2:J1:125:LEU:HD23 | 2:J1:125:LEU:HA | 1.82 | 0.41 |
| 2:J1:176:GLN:HG2 | 2:J1:177:VAL:N | 2.36 | 0.41 |
| 1:J4:354:CYS:SG | 1:J4:355:ASP:N | 2.94 | 0.41 |
| 2:J5:298:PRO:HB3 | 2:J5:307:PRO:HD2 | 2.01 | 0.41 |
| 2:J5:401:LYS:HB3 | 2:J5:401:LYS:HE3 | 1.86 | 0.41 |
| 1:J6:56:GLY:HA2 | 6:4O:386:PHE:CD2 | 2.56 | 0.41 |
| 1:J6:356:ILE:HD13 | 1:J6:356:ILE:HA | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J6:403:MET:HE3 | 1:J6:403:MET:HB2 | 1.93 | 0.41 |
| 2:J7:60:LYS:HA | 2:J7:60:LYS:HD2 | 1.68 | 0.41 |
| 2:J7:119:LEU:O | 2:J7:122:ILE:HG22 | 2.21 | 0.41 |
| 2:J7:141:VAL:O | 2:J7:147:SER:OG | 2.36 | 0.41 |
| 2:J7:244:PHE:HB2 | 2:J7:356:ASN:HD21 | 1.85 | 0.41 |
| 2:J7:298:PRO:HA | 2:J7:301:MET:HG3 | 2.03 | 0.41 |
| 2:J7:305:CYS:HB3 | 2:J7:387:ILE:HD11 | 2.03 | 0.41 |
| 1:J8:297:LYS:HA | 1:J8:297:LYS:HD3 | 1.75 | 0.41 |
| 2:J9:23:LEU:HD11 | 2:J9:233:GLN:OE1 | 2.20 | 0.41 |
| 2:J9:266:HIS:O | 2:J9:266:HIS:ND1 | 2.49 | 0.41 |
| 1:K0:137:HIS:NE2 | 1:K0:166:THR:OG1 | 2.54 | 0.41 |
| 2:K1:8:HIS:CD2 | 2:K1:138:PHE:HD2 | 2.38 | 0.41 |
| 2:K1:76:ASP:OD1 | 2:K1:79:ARG:HD2 | 2.21 | 0.41 |
| 2:K3:9:ILE:CG1 | 2:K3:139:ASN:HB3 | 2.50 | 0.41 |
| 2:K3:86:LEU:HD12 | 2:K3:86:LEU:HA | 1.94 | 0.41 |
| 1:K4:233:MET:O | 1:K4:237:THR:HG22 | 2.20 | 0.41 |
| 2:K5:21:TRP:CZ3 | 2:K5:63:PRO:HB3 | 2.56 | 0.41 |
| 2:K5:122:ILE:HA | 2:K5:125:LEU:HD12 | 2.02 | 0.41 |
| 2:K5:178:SER:OG | 2:K5:183:GLU:OE2 | 2.34 | 0.41 |
| 1:K6:273:LEU:H | 1:K6:292:GLN:HE22 | 1.68 | 0.41 |
| 2:K7:60:LYS:HD3 | 2:M3:282:TYR:CZ | 2.55 | 0.41 |
| 1:K8:69:GLU:OE2 | 1:K8:72:THR:HG23 | 2.20 | 0.41 |
| 1:K8:273:LEU:H | 1:K8:292:GLN:NE2 | 2.18 | 0.41 |
| 1:K8:310:TYR:HA | 1:K8:371:SER:HA | 2.02 | 0.41 |
| 2:K9:163:LYS:HA | 2:K9:163:LYS:HD3 | 1.73 | 0.41 |
| 1:L0:284:LEU:HD13 | 1:L0:284:LEU:HA | 1.94 | 0.41 |
| 1:L0:350:LYS:NZ | 1:L0:351:SER:O | 2.48 | 0.41 |
| 2:L1:175:PRO:HB3 | 2:L1:390:ARG:NE | 2.36 | 0.41 |
| 1:L2:107:THR:OG1 | 1:L2:108:GLU:OE1 | 2.27 | 0.41 |
| 1:L2:374:ILE:HD12 | 1:L2:374:ILE:HA | 1.96 | 0.41 |
| 2:L3:27:GLU:OE1 | 2:L3:243:ARG:NH1 | 2.54 | 0.41 |
| 2:L3:327:ASP:OD1 | 2:L3:327:ASP:N | 2.51 | 0.41 |
| 1:L4:3:GLU:HB2 | 1:L4:130:LEU:HD13 | 2.01 | 0.41 |
| 1:L4:215:LEU:HB3 | 1:L4:217:LEU:HG | 2.01 | 0.41 |
| 1:L4:273:LEU:O | 1:L4:292:GLN:NE2 | 2.53 | 0.41 |
| 1:L4:309:ARG:H | 1:L4:372:THR:HG22 | 1.86 | 0.41 |
| 1:L4:406:MET:N | 1:L4:406:MET:SD | 2.94 | 0.41 |
| 2:L5:76:ASP:HA | 2:L5:79:ARG:HB2 | 2.03 | 0.41 |
| 1:L6:6:HIS:CE1 | 1:L6:8:GLN:HG2 | 2.55 | 0.41 |
| 1:L6:49:VAL:HG11 | 1:L6:241:ARG:HG2 | 2.03 | 0.41 |
| 1:L6:238:CYS:SG | 1:L6:318:ARG:NE | 2.93 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L6:362:LYS:HE2 | 6:4P:169:PHE:CE2 | 2.55 | 0.41 |
| 2:L7:5:ILE:HG22 | 2:L7:64:ARG:HB3 | 2.03 | 0.41 |
| 2:L7:210:TYR:CE1 | 2:L7:227:LEU:HD11 | 2.56 | 0.41 |
| 2:L7:235:ILE:O | 2:L7:238:LEU:HG | 2.21 | 0.41 |
| 2:L7:276:ILE:HD13 | 2:L7:276:ILE:HA | 1.92 | 0.41 |
| 2:L9:33:ASP:HA | 2:L9:85:GLN:HB2 | 2.03 | 0.41 |
| 2:L9:137:VAL:HG22 | 2:L9:168:GLY:HA2 | 2.02 | 0.41 |
| 2:L9:183:GLU:HG3 | 2:L9:184:PRO:HD3 | 2.02 | 0.41 |
| 1:M0:139:LEU:HD12 | 1:M0:170:VAL:HG12 | 2.02 | 0.41 |
| 1:M0:257:LEU:HD21 | 1:M0:314:SER:HB3 | 2.02 | 0.41 |
| 1:M0:382:SER:HB2 | 1:M0:415:MET:HG2 | 2.02 | 0.41 |
| 2:M1:153:LEU:HD12 | 2:M1:153:LEU:HA | 1.89 | 0.41 |
| 2:M1:325:PRO:HA | 2:M1:328:VAL:HG12 | 2.03 | 0.41 |
| 2:M3:115:VAL:O | 2:M3:119:LEU:HG | 2.21 | 0.41 |
| 2:M3:137:VAL:HG22 | 2:M3:168:GLY:HA2 | 2.02 | 0.41 |
| 1:M4:113:ILE:HA | 1:M4:116:VAL:HG22 | 2.03 | 0.41 |
| 1:M6:76:VAL:HG23 | 1:M6:77:ARG:N | 2.36 | 0.41 |
| 1:M6:271:THR:HG22 | 1:M6:365:ALA:HB3 | 2.02 | 0.41 |
| 2:M7:39:ASP:OD2 | 2:M7:40:LYS:N | 2.49 | 0.41 |
| 2:M9:287:SER:H | 2:M9:290:GLU:CD | 2.25 | 0.41 |
| 2:N1:8:HIS:CD2 | 2:N1:138:PHE:HD2 | 2.39 | 0.41 |
| 2:N1:147:SER:HB2 | 2:N1:190:SER:OG | 2.21 | 0.41 |
| 2:N1:430:LYS:HA | 2:N1:430:LYS:HD2 | 1.85 | 0.41 |
| 1:N2:178:THR:HA | 2:N3:352:LYS:HD2 | 2.03 | 0.41 |
| 1:N2:362:LYS:HE3 | 30:7L:305:GLN:O | 2.20 | 0.41 |
| 2:N3:33:ASP:OD1 | 2:N3:34:GLY:N | 2.53 | 0.41 |
| 2:N3:216:SER:OG | 2:N3:217:LEU:N | 2.54 | 0.41 |
| 2:N5:90:GLU:HB2 | 2:N5:121:ARG:NH2 | 2.35 | 0.41 |
| 2:N5:125:LEU:HD23 | 2:N5:125:LEU:HA | 1.78 | 0.41 |
| 1:N6:155:ILE:HD12 | 1:N6:155:ILE:HA | 1.84 | 0.41 |
| 1:N6:276:ARG:HA | 1:N6:279:GLN:HB2 | 2.02 | 0.41 |
| 2:N7:70:LEU:HD13 | 2:N7:110:ILE:HG21 | 2.02 | 0.41 |
| 2:N7:72:PRO:HD2 | 1:N8:2:ARG:HH12 | 1.85 | 0.41 |
| 2:N7:286:LEU:HA | 2:N7:286:LEU:HD23 | 1.79 | 0.41 |
| 1:N8:45:GLU:HG3 | 1:N8:46:ARG:HG2 | 2.02 | 0.41 |
| 1:N8:405:GLU:HA | 1:N8:408:PHE:HD2 | 1.86 | 0.41 |
| 2:N9:70:LEU:HD11 | 2:N9:149:LEU:HD21 | 2.03 | 0.41 |
| 1:O0:274:THR:OG1 | 27:7G:54:HIS:HE1 | 2.04 | 0.41 |
| 2:O1:320:ARG:HE | 2:O1:320:ARG:HB3 | 1.59 | 0.41 |
| 2:O1:396:ASP:OD2 | 2:O1:422:ARG:NH2 | 2.49 | 0.41 |
| 1:O4:190:HIS:CD2 | 1:O4:414:ASN:HB3 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O5:19:ALA:HB2 | 32:7P:120:TYR:OH | 2.21 | 0.41 |
| 2:O5:272:TYR:HD2 | 2:O5:275:ILE:HD11 | 1.86 | 0.41 |
| 1:O6:132:GLY:HA2 | 1:O6:162:ARG:HB3 | 2.02 | 0.41 |
| 2:O7:26:LEU:HD23 | 2:O7:26:LEU:HA | 1.89 | 0.41 |
| 2:O7:79:ARG:O | 2:O7:84:ARG:HG2 | 2.21 | 0.41 |
| 1:O8:86:ARG:HD3 | 1:O8:88:ASP:HB3 | 2.02 | 0.41 |
| 2:O9:174:SER:OG | 2:O9:207:GLU:HB2 | 2.21 | 0.41 |
| 2:P3:15:GLN:HB3 | 2:P3:228:ASN:ND2 | 2.36 | 0.41 |
| 2:P3:175:PRO:HG2 | 2:P3:176:GLN:OE1 | 2.21 | 0.41 |
| 2:P5:200:VAL:HG23 | 2:P5:256:GLN:HG3 | 2.03 | 0.41 |
| 2:P5:306:ASP:HB3 | 2:P5:309:HIS:CD2 | 2.56 | 0.41 |
| 1:P6:309:ARG:H | 1:P6:372:THR:HG22 | 1.85 | 0.41 |
| 2:P9:306:ASP:HB3 | 2:P9:309:HIS:CD2 | 2.56 | 0.41 |
| 1:Q0:213:ARG:NH2 | 1:Q0:297:LYS:HG3 | 2.36 | 0.41 |
| 2:Q1:402:ARG:O | 2:Q1:405:VAL:HG12 | 2.21 | 0.41 |
| 1:Q2:69:GLU:OE2 | 1:Q2:69:GLU:N | 2.54 | 0.41 |
| 2:Q3:100:ALA:HA | 1:Q4:252:LYS:HE2 | 2.03 | 0.41 |
| 2:Q3:119:LEU:HA | 2:Q3:122:ILE:HG22 | 2.03 | 0.41 |
| 1:Q4:11:GLN:N | 39:Q4:502:GDP:O2B | 2.36 | 0.41 |
| 2:Q5:8:HIS:CD2 | 2:Q5:138:PHE:HD2 | 2.39 | 0.41 |
| 2:Q5:10:GLY:O | 2:Q5:13:GLY:N | 2.54 | 0.41 |
| 2:Q5:86:LEU:O | 2:Q5:86:LEU:HG | 2.19 | 0.41 |
| 2:Q5:222:PRO:HD2 | 1:Q6:324:LYS:HE3 | 2.03 | 0.41 |
| 1:Q6:53:GLU:OE2 | 7:4R:351:ARG:NH1 | 2.54 | 0.41 |
| 1:Q6:286:VAL:HB | 1:Q6:287:PRO:HD3 | 2.03 | 0.41 |
| 1:Q8:71:GLY:HA2 | 24:6T:29:LYS:HD3 | 2.02 | 0.41 |
| 1:Q8:228:LEU:HD23 | 1:Q8:228:LEU:HA | 1.81 | 0.41 |
| 1:Q8:295:ASP:OD1 | 1:Q8:297:LYS:N | 2.54 | 0.41 |
| 2:Q9:274:PRO:HB2 | 2:Q9:276:ILE:CG1 | 2.51 | 0.41 |
| 2:Q9:290:GLU:OE1 | 2:Q9:290:GLU:N | 2.37 | 0.41 |
| 1:R0:167:PHE:CE2 | 1:R0:233:MET:HG2 | 2.56 | 0.41 |
| 1:R0:207:LEU:HD23 | 1:R0:207:LEU:HA | 1.85 | 0.41 |
| 2:R1:207:GLU:OE2 | 2:R1:207:GLU:HA | 2.21 | 0.41 |
| 1:R2:94:GLN:HB3 | 24:6V:35:TYR:CE2 | 2.56 | 0.41 |
| 2:R3:221:ARG:HB3 | 1:R4:322:SER:OG | 2.21 | 0.41 |
| 1:R4:245:GLN:NE2 | 21:6G:58:GLU:HG3 | 2.36 | 0.41 |
| 2:R5:59:GLY:HA3 | 11:5E:245:PRO:HG3 | 2.02 | 0.41 |
| 2:R5:322:ASP:HB2 | 19:6E:221:THR:CG2 | 2.50 | 0.41 |
| 2:R5:344:VAL:HG12 | 2:R5:347:CYS:H | 1.85 | 0.41 |
| 1:R6:282:ARG:NH2 | 1:R6:292:GLN:OE1 | 2.53 | 0.41 |
| 1:R6:309:ARG:O | 1:R6:372:THR:HG22 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R7:70:LEU:HD23 | 2:R7:70:LEU:HA | 1.89 | 0.41 |
| 2:R7:175:PRO:HG2 | 2:R7:176:GLN:OE1 | 2.20 | 0.41 |
| 2:R7:195:LEU:HD23 | 2:R7:195:LEU:HA | 1.84 | 0.41 |
| 2:R7:205:ASP:OD1 | 2:R7:303:VAL:HG13 | 2.20 | 0.41 |
| 1:R8:111:GLU:HG3 | 13:5J:119:VAL:CG1 | 2.35 | 0.41 |
| 2:R9:377:MET:SD | 2:R9:379:SER:HB3 | 2.60 | 0.41 |
| 1:S0:30:ILE:HG13 | 1:S0:35:THR:O | 2.20 | 0.41 |
| 1:S0:135:VAL:HG12 | 1:S0:137:HIS:HD2 | 1.86 | 0.41 |
| 1:S0:174:LYS:HE2 | 1:S0:174:LYS:HB3 | 1.72 | 0.41 |
| 1:S0:396:HIS:H | 1:S0:396:HIS:CD2 | 2.37 | 0.41 |
| 2:S1:279:GLU:OE1 | 2:S1:279:GLU:N | 2.53 | 0.41 |
| 1:S2:284:LEU:HB3 | 7:4R:352:ASN:OD1 | 2.21 | 0.41 |
| 1:S2:395:LEU:HD12 | 1:S2:395:LEU:HA | 1.92 | 0.41 |
| 1:S4:175:VAL:HG12 | 1:S4:205:GLU:HG2 | 2.02 | 0.41 |
| 2:S5:196:GLU:OE2 | 2:S5:197:HIS:NE2 | 2.53 | 0.41 |
| 2:S7:73:THR:HG23 | 2:S7:74:VAL:N | 2.36 | 0.41 |
| 2:S7:76:ASP:HA | 2:S7:79:ARG:HB2 | 2.03 | 0.41 |
| 2:S7:247:ALA:HB2 | 2:S7:357:TYR:OH | 2.21 | 0.41 |
| 2:S9:81:GLY:HA2 | 12:5F:212:ARG:HH21 | 1.86 | 0.41 |
| 2:S9:90:GLU:CB | 2:S9:121:ARG:HH12 | 2.34 | 0.41 |
| 2:S9:175:PRO:HB3 | 2:S9:390:ARG:NE | 2.35 | 0.41 |
| 1:T0:26:ASP:OD2 | 1:T0:359:LYS:HD2 | 2.21 | 0.41 |
| 1:T0:183:TYR:OH | 1:T0:388:MET:HB3 | 2.20 | 0.41 |
| 1:T0:253:LEU:HD23 | 1:T0:253:LEU:HA | 1.83 | 0.41 |
| 2:T1:71:GLU:O | 2:T1:71:GLU:HG2 | 2.21 | 0.41 |
| 2:T1:116:ASP:OD2 | 2:T1:156:ARG:NH1 | 2.54 | 0.41 |
| 1:T2:237:THR:O | 1:T2:237:THR:HG22 | 2.20 | 0.41 |
| 1:T2:271:THR:CG2 | 1:T2:365:ALA:HB3 | 2.51 | 0.41 |
| 1:T4:112:LEU:O | 1:T4:116:VAL:HG23 | 2.21 | 0.41 |
| 1:T4:333:VAL:HG23 | 13:5J:102:ALA:O | 2.20 | 0.41 |
| 2:T5:79:ARG:O | 2:T5:84:ARG:HG2 | 2.20 | 0.41 |
| 2:T5:288:VAL:HG13 | 2:T5:319:TYR:HE2 | 1.85 | 0.41 |
| 2:T5:371:VAL:HG22 | 2:T5:373:ARG:H | 1.85 | 0.41 |
| 2:T5:392:ASP:OD2 | 2:T5:422:ARG:NH1 | 2.54 | 0.41 |
| 1:T6:77:ARG:HH21 | 24:7A:46:ALA:HB1 | 1.84 | 0.41 |
| 1:T6:204:ASN:HD21 | 39:T6:502:GDP:N2 | 2.18 | 0.41 |
| 1:T6:290:THR:HG21 | 1:T6:329:GLN:CG | 2.50 | 0.41 |
| 2:T7:7:ILE:HD11 | 2:T7:137:VAL:HG12 | 2.02 | 0.41 |
| 2:T7:237:SER:HA | 2:T7:320:ARG:HD2 | 2.01 | 0.41 |
| 1:T8:192:LEU:HD23 | 1:T8:192:LEU:HA | 1.83 | 0.41 |
| 1:T8:309:ARG:NH1 | 1:T8:339:SER:O | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T8:345:ILE:HB | 1:T8:348:ASN:HD21 | 1.85 | 0.41 |
| 2:U1:125:LEU:HD23 | 2:U1:125:LEU:HA | 1.92 | 0.41 |
| 2:U1:259:LEU:HD21 | 2:U1:316:CYS:SG | 2.60 | 0.41 |
| 2:U1:312:TYR:HD1 | 2:U1:381:SER:HB3 | 1.86 | 0.41 |
| 1:U2:148:GLY:O | 1:U2:151:LEU:HG | 2.20 | 0.41 |
| 1:U2:173:PRO:HA | 1:U2:176:SER:HB3 | 2.02 | 0.41 |
| 1:U2:417:ASP:HA | 1:U2:420:SER:OG | 2.21 | 0.41 |
| 1:U4:297:LYS:NZ | 1:U4:306:ARG:HH22 | 2.19 | 0.41 |
| 2:U5:70:LEU:HB3 | 2:U5:97:GLU:O | 2.21 | 0.41 |
| 2:U5:290:GLU:HG2 | 2:U5:291:ILE:N | 2.36 | 0.41 |
| 2:U5:305:CYS:HB3 | 2:U5:387:ILE:HD11 | 2.02 | 0.41 |
| 2:U5:406:HIS:HA | 2:U5:409:VAL:HG22 | 2.02 | 0.41 |
| 2:U7:222:PRO:CD | 1:U8:324:LYS:HE3 | 2.50 | 0.41 |
| 2:U7:320:ARG:NH2 | 2:U7:359:PRO:O | 2.54 | 0.41 |
| 1:U8:95:THR:HG23 | 1:U8:96:GLY:N | 2.35 | 0.41 |
| 1:U8:190:HIS:CD2 | 1:U8:414:ASN:HB2 | 2.55 | 0.41 |
| 1:U8:329:GLN:HA | 1:U8:332:ASN:ND2 | 2.35 | 0.41 |
| 2:U9:116:ASP:OD1 | 2:U9:117:LEU:N | 2.54 | 0.41 |
| 2:U9:397:LEU:HD12 | 2:U9:397:LEU:HA | 1.86 | 0.41 |
| 1:V0:282:ARG:NH2 | 1:V0:284:LEU:HA | 2.35 | 0.41 |
| 2:V1:72:PRO:HD2 | 1:V2:2:ARG:NH1 | 2.35 | 0.41 |
| 2:V1:88:HIS:HA | 2:W7:283:HIS:CD2 | 2.56 | 0.41 |
| 2:V1:266:HIS:O | 2:V1:266:HIS:ND1 | 2.54 | 0.41 |
| 2:V3:122:ILE:CD1 | 2:V3:157:LEU:HD21 | 2.50 | 0.41 |
| 2:V3:328:VAL:HG11 | 2:V3:355:ILE:HD11 | 2.02 | 0.41 |
| 1:V4:22:GLU:HG2 | 1:V4:81:TYR:HB2 | 2.02 | 0.41 |
| 1:V4:317:PHE:HB3 | 1:V4:321:MET:SD | 2.61 | 0.41 |
| 2:V7:327:ASP:OD1 | 2:V7:328:VAL:N | 2.54 | 0.41 |
| 1:V8:21:TRP:CZ2 | 1:V8:63:ALA:HB2 | 2.56 | 0.41 |
| 1:V8:396:HIS:CE1 | 1:V8:397:TRP:CE2 | 3.08 | 0.41 |
| 2:V9:58:ALA:HB1 | 8:4W:148:GLN:O | 2.21 | 0.41 |
| 2:V9:255:PHE:O | 2:V9:259:LEU:HB2 | 2.20 | 0.41 |
| 1:W0:285:THR:HG23 | 1:W0:288:GLU:H | 1.85 | 0.41 |
| 1:W2:183:TYR:HB3 | 1:W2:398:TYR:HE2 | 1.86 | 0.41 |
| 1:W2:183:TYR:O | 1:W2:187:LEU:HD13 | 2.20 | 0.41 |
| 2:W3:72:PRO:HG3 | 1:W4:1:MET:HG3 | 2.02 | 0.41 |
| 1:W4:131:GLN:NE2 | 1:W4:249:ASP:OD1 | 2.54 | 0.41 |
| 2:W5:255:PHE:O | 2:W5:259:LEU:HB2 | 2.21 | 0.41 |
| 2:W7:239:THR:O | 2:W7:239:THR:HG22 | 2.21 | 0.41 |
| 2:W7:391:LEU:HD23 | 2:W7:391:LEU:HA | 1.91 | 0.41 |
| 1:W8:364:SER:OG | 1:W8:365:ALA:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W9:79:ARG:CG | 2:W9:92:LEU:HD23 | 2.51 | 0.41 |
| 2:W9:178:SER:OG | 1:X0:347:ASN:HB3 | 2.21 | 0.41 |
| 2:W9:327:ASP:OD1 | 2:W9:328:VAL:N | 2.54 | 0.41 |
| 1:X0:40:SER:HB3 | 8:4X:99:PRO:HD3 | 2.01 | 0.41 |
| 1:X0:263:LEU:HG | 1:X0:422:TYR:HE1 | 1.83 | 0.41 |
| 1:X2:5:VAL:HB | 1:X2:133:PHE:HD1 | 1.85 | 0.41 |
| 1:X2:62:ARG:HG2 | 1:X2:123:GLU:OE2 | 2.21 | 0.41 |
| 2:X3:246:GLY:HA2 | 2:X3:357:TYR:CD2 | 2.56 | 0.41 |
| 1:X4:10:GLY:HA2 | 1:X4:143:THR:HG23 | 2.01 | 0.41 |
| 1:X4:234:SER:HA | 1:X4:237:THR:HG22 | 2.03 | 0.41 |
| 2:X5:167:LEU:HD21 | 2:X5:252:ILE:HG13 | 2.02 | 0.41 |
| 2:X5:181:VAL:H | 1:X6:256:ASN:ND2 | 2.19 | 0.41 |
| 2:X5:255:PHE:CE1 | 2:X5:378:ILE:HD12 | 2.55 | 0.41 |
| 2:X5:255:PHE:HD1 | 2:X5:259:LEU:HD12 | 1.86 | 0.41 |
| 2:X7:282:TYR:HE2 | 2:X7:283:HIS:CE1 | 2.39 | 0.41 |
| 2:X7:328:VAL:O | 2:X7:332:VAL:HG13 | 2.21 | 0.41 |
| 1:X8:60:VAL:HA | 1:X8:61:PRO:HD3 | 1.91 | 0.41 |
| 1:X8:67:ASP:OD1 | 1:X8:67:ASP:N | 2.53 | 0.41 |
| 1:X8:95:THR:OG1 | 1:X8:96:GLY:N | 2.54 | 0.41 |
| 2:X9:11:GLN:HB3 | 41:Y0:501:GTP:O2A | 2.21 | 0.41 |
| 2:X9:239:THR:HG22 | 2:X9:239:THR:O | 2.20 | 0.41 |
| 1:Y0:105:HIS:CD2 | 1:Y0:150:LEU:HB2 | 2.56 | 0.41 |
| 1:Y0:150:LEU:O | 1:Y0:154:LYS:HG2 | 2.20 | 0.41 |
| 1:Y0:396:HIS:CE1 | 1:Y0:397:TRP:CE2 | 3.08 | 0.41 |
| 2:Y1:387:ILE:HG12 | 2:Y1:390:ARG:HH12 | 1.86 | 0.41 |
| 2:Y3:21:TRP:CZ2 | 2:Y3:65:CYS:HB2 | 2.56 | 0.41 |
| 2:Y3:211:ASP:OD2 | 2:Y3:214:ARG:NH2 | 2.48 | 0.41 |
| 1:Y4:251:ARG:O | 1:Y4:255:VAL:HG22 | 2.21 | 0.41 |
| 1:Y4:321:MET:HE2 | 1:Y4:363:MET:HG3 | 2.03 | 0.41 |
| 2:Y5:11:GLN:HB3 | 41:Y6:501:GTP:O2A | 2.20 | 0.41 |
| 2:Y5:251:ASP:OD1 | 2:Y5:252:ILE:N | 2.54 | 0.41 |
| 1:Y6:154:LYS:HD3 | 1:Y6:154:LYS:HA | 1.85 | 0.41 |
| 1:Y6:280:GLN:HG2 | 8:4X:126:ASP:OD2 | 2.21 | 0.41 |
| 1:Y8:91:VAL:HG21 | 1:Y8:116:VAL:HG12 | 2.03 | 0.41 |
| 2:Y9:5:ILE:HG22 | 2:Y9:64:ARG:HD3 | 2.03 | 0.41 |
| 2:Y9:56:THR:N | 2:Y9:60:LYS:O | 2.54 | 0.41 |
| 2:Y9:317:LEU:HD21 | 2:Y9:377:MET:HG2 | 2.03 | 0.41 |
| 1:Z0:336:LYS:HA | 1:Z0:336:LYS:HD2 | 1.78 | 0.41 |
| 2:Z1:21:TRP:CH2 | 2:Z1:63:PRO:HB3 | 2.55 | 0.41 |
| 2:Z1:324:VAL:HG22 | 2:Z1:326:LYS:HG2 | 2.02 | 0.41 |
| 1:Z2:172:SER:HB3 | 1:Z2:205:GLU:OE1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Z2:274:THR:OG1 | 1:Z2:282:ARG:NH1 | 2.51 | 0.41 |
| 1:Z2:328:GLU:O | 1:Z2:332:ASN:ND2 | 2.54 | 0.41 |
| 2:Z3:65:CYS:SG | 2:Z3:66:ILE:N | 2.94 | 0.41 |
| 2:Z5:84:ARG:HH11 | 2:Z5:84:ARG:HG3 | 1.83 | 0.41 |
| 1:Z6:101:TRP:CZ3 | 1:Z6:187:LEU:HD23 | 2.56 | 0.41 |
| 1:Z6:128:ASP:N | 1:Z6:128:ASP:OD1 | 2.48 | 0.41 |
| 1:Z6:165:LEU:HD12 | 1:Z6:166:THR:N | 2.36 | 0.41 |
| 2:Z7:192:HIS:HD2 | 2:Z7:421:ALA:HA | 1.86 | 0.41 |
| 2:Z7:296:PHE:HE1 | 2:Z7:377:MET:HG3 | 1.86 | 0.41 |
| 2:Z7:306:ASP:HB3 | 2:Z7:309:HIS:HD2 | 1.85 | 0.41 |
| 2:Z7:393:HIS:HD2 | 2:Z7:394:LYS:NZ | 2.19 | 0.41 |
| 1:Z8:164:MET:HB3 | 1:Z8:197:ASP:CG | 2.41 | 0.41 |
| 2:Z9:175:PRO:HG2 | 2:Z9:176:GLN:OE1 | 2.20 | 0.41 |
| 2:Z9:259:LEU:HD12 | 2:Z9:268:MET:HE1 | 2.02 | 0.41 |
| 1:0A:375:GLN:O | 1:0A:379:LYS:HG2 | 2.21 | 0.41 |
| 2:0B:319:TYR:HD2 | 2:0B:323:VAL:HG11 | 1.86 | 0.41 |
| 2:0B:380:ASN:OD1 | 2:0B:381:SER:N | 2.54 | 0.41 |
| 1:0C:41:ASP:HA | 1:0C:44:LEU:HD23 | 2.03 | 0.41 |
| 1:0C:260:PHE:HB2 | 1:0C:263:LEU:HD23 | 2.03 | 0.41 |
| 1:0E:118:ASP:O | 1:0E:122:LYS:HG2 | 2.21 | 0.41 |
| 2:0F:33:ASP:O | 2:0F:60:LYS:NZ | 2.49 | 0.41 |
| 2:0F:124:LYS:HA | 2:0F:127:ASP:OD2 | 2.21 | 0.41 |
| 2:0F:289:ALA:O | 2:0F:293:ASN:ND2 | 2.52 | 0.41 |
| 1:0G:161:ASP:HB2 | 1:0G:162:ARG:NH1 | 2.36 | 0.41 |
| 1:0I:58:ARG:HH11 | 1:0Y:281:TYR:HE1 | 1.68 | 0.41 |
| 1:0I:325:GLU:HA | 1:0I:328:GLU:HG3 | 2.03 | 0.41 |
| 1:0I:344:TRP:CE3 | 1:0I:345:ILE:HG13 | 2.56 | 0.41 |
| 1:0I:389:PHE:O | 1:0I:392:LYS:NZ | 2.24 | 0.41 |
| 1:0I:397:TRP:HE1 | 2:0J:260:VAL:HB | 1.86 | 0.41 |
| 2:0J:3:GLU:HG3 | 2:0J:51:THR:HA | 2.02 | 0.41 |
| 1:0K:86:ARG:NH1 | 1:0K:89:ASN:OD1 | 2.54 | 0.41 |
| 1:0K:193:VAL:HG11 | 1:0K:418:LEU:CD1 | 2.50 | 0.41 |
| 1:0K:289:LEU:HD23 | 1:0K:365:ALA:HB2 | 2.02 | 0.41 |
| 2:0L:88:HIS:HB3 | 2:1B:283:HIS:CG | 2.56 | 0.41 |
| 2:0L:209:ILE:HD13 | 2:0L:231:ILE:HD11 | 2.03 | 0.41 |
| 2:0L:212:ILE:O | 2:0L:216:SER:OG | 2.35 | 0.41 |
| 1:0M:62:ARG:HG3 | 1:0M:123:GLU:OE2 | 2.20 | 0.41 |
| 1:0M:193:VAL:HG21 | 1:0M:418:LEU:HD11 | 2.03 | 0.41 |
| 1:0M:271:THR:OG1 | 1:0M:365:ALA:HB3 | 2.21 | 0.41 |
| 1:0M:334:GLN:NE2 | 1:0M:348:ASN:H | 2.16 | 0.41 |
| 2:0N:115:VAL:HG23 | 2:0N:153:LEU:HD13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:0N:195:LEU:CD1 | 2:0N:428:LEU:HD21 | 2.51 | 0.41 |
| 1:0O:100:ASN:ND2 | 1:0O:103:LYS:HG3 | 2.36 | 0.41 |
| 1:0O:103:LYS:HA | 1:0O:107:THR:HB | 2.02 | 0.41 |
| 1:0O:379:LYS:HD3 | 1:0O:419:VAL:HG11 | 2.02 | 0.41 |
| 2:0P:88:HIS:ND1 | 2:1F:283:HIS:HA | 2.36 | 0.41 |
| 2:0P:312:TYR:HB2 | 2:0P:343:PHE:CD1 | 2.56 | 0.41 |
| 1:0Q:95:THR:OG1 | 1:0Q:96:GLY:N | 2.54 | 0.41 |
| 2:0R:7:ILE:HG22 | 2:0R:66:ILE:HB | 2.03 | 0.41 |
| 2:0R:17:GLY:HA2 | 2:0R:20:CYS:SG | 2.61 | 0.41 |
| 2:0R:47:ASP:OD1 | 2:0R:50:ASN:ND2 | 2.54 | 0.41 |
| 2:0R:52:PHE:HZ | 2:0R:239:THR:HG21 | 1.86 | 0.41 |
| 2:0R:71:GLU:HB3 | 2:0R:98:ASP:OD1 | 2.20 | 0.41 |
| 2:0R:154:LEU:HG | 2:0R:197:HIS:HB3 | 2.02 | 0.41 |
| 1:0S:363:MET:HB3 | 1:0S:363:MET:HE2 | 1.91 | 0.41 |
| 1:0U:55:THR:H | 1:0U:58:ARG:HB3 | 1.86 | 0.41 |
| 1:0U:113:ILE:HG22 | 1:0U:117:LEU:HD22 | 2.03 | 0.41 |
| 1:0U:252:LYS:HE3 | 1:0U:252:LYS:HB2 | 1.92 | 0.41 |
| 1:0U:350:LYS:HZ1 | 1:0U:352:SER:HB3 | 1.85 | 0.41 |
| 1:0U:397:TRP:O | 1:0U:401:GLU:HG2 | 2.21 | 0.41 |
| 2:0V:195:LEU:HD23 | 2:0V:196:GLU:HB3 | 2.03 | 0.41 |
| 2:0V:334:THR:HA | 2:0V:337:THR:HG22 | 2.02 | 0.41 |
| 1:0W:286:VAL:CG2 | 1:0W:287:PRO:HD3 | 2.51 | 0.41 |
| 2:0X:237:SER:HA | 2:0X:320:ARG:HD2 | 2.03 | 0.41 |
| 1:0Y:100:ASN:HB3 | 1:0Y:103:LYS:HB2 | 2.02 | 0.41 |
| 1:0Y:274:THR:OG1 | 1:0Y:282:ARG:NH1 | 2.54 | 0.41 |
| 1:0Y:289:LEU:O | 1:0Y:293:MET:HG3 | 2.19 | 0.41 |
| 2:0Z:176:GLN:HE22 | 2:0Z:304:LYS:HE2 | 1.86 | 0.41 |
| 1:1A:91:VAL:HG11 | 1:1A:116:VAL:HG13 | 2.03 | 0.41 |
| 2:1B:203:MET:CE | 2:1B:267:PHE:HB3 | 2.51 | 0.41 |
| 1:1C:393:ALA:O | 1:1C:394:PHE:HB2 | 2.20 | 0.41 |
| 2:1D:346:TRP:CE3 | 2:1D:346:TRP:C | 2.94 | 0.41 |
| 2:1D:363:VAL:HG13 | 2:1D:366:GLY:HA3 | 2.01 | 0.41 |
| 1:1E:66:MET:HE1 | 1:1E:147:MET:CG | 2.51 | 0.41 |
| 1:1E:297:LYS:HA | 1:1E:297:LYS:HD3 | 1.74 | 0.41 |
| 2:1F:90:GLU:HB3 | 2:1F:121:ARG:NH1 | 2.24 | 0.41 |
| 2:1F:139:ASN:N | 2:1F:139:ASN:OD1 | 2.53 | 0.41 |
| 2:1F:235:ILE:HD13 | 2:1F:235:ILE:HA | 1.79 | 0.41 |
| 2:1F:329:ASN:HA | 2:1F:332:VAL:HG12 | 2.02 | 0.41 |
| 2:1H:269:LEU:HD21 | 2:1H:301:MET:SD | 2.61 | 0.41 |
| 2:1H:431:ASP:HA | 2:1H:434:GLU:HG3 | 2.03 | 0.41 |
| 1:1K:185:ALA:O | 1:1K:189:VAL:HG12 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1L:63:PRO:O | 2:1L:91:GLN:NE2 | 2.54 | 0.41 |
| 1:1M:113:ILE:HD13 | 1:1M:150:LEU:CD2 | 2.50 | 0.41 |
| 1:1M:331:LEU:HD12 | 1:1M:331:LEU:HA | 1.82 | 0.41 |
| 2:1N:93:ILE:HD12 | 2:1N:117:LEU:HD21 | 2.02 | 0.41 |
| 2:1N:121:ARG:HD2 | 2:1N:121:ARG:HA | 1.84 | 0.41 |
| 2:1N:165:SER:HA | 2:1N:199:ASP:OD2 | 2.21 | 0.41 |
| 2:1N:401:LYS:HB3 | 2:1N:401:LYS:HE3 | 1.90 | 0.41 |
| 1:1O:95:THR:HG23 | 1:1O:96:GLY:H | 1.86 | 0.41 |
| 1:1O:204:ASN:OD1 | 39:1O:501:GDP:O2' | 2.39 | 0.41 |
| 2:1P:28:HIS:CE1 | 2:1P:49:PHE:HA | 2.56 | 0.41 |
| 2:1P:56:THR:HA | 2:2F:285:GLN:HB2 | 2.03 | 0.41 |
| 2:1P:402:ARG:HD3 | 2:1P:402:ARG:HA | 1.87 | 0.41 |
| 1:1Q:102:ALA:HB1 | 1:1Q:401:GLU:CG | 2.50 | 0.41 |
| 1:1Q:192:LEU:HD23 | 1:1Q:192:LEU:HA | 1.87 | 0.41 |
| 2:1R:312:TYR:CE2 | 2:1R:341:ILE:HG12 | 2.56 | 0.41 |
| 2:1T:176:GLN:HG2 | 2:1T:177:VAL:N | 2.36 | 0.41 |
| 1:1U:51:PHE:O | 1:1U:62:ARG:NH2 | 2.54 | 0.41 |
| 1:1U:56:GLY:HA3 | 10:5B:239:ARG:HB2 | 2.03 | 0.41 |
| 2:1V:227:LEU:O | 2:1V:231:ILE:HG12 | 2.21 | 0.41 |
| 2:1V:231:ILE:O | 2:1V:234:VAL:HG12 | 2.20 | 0.41 |
| 1:1W:51:PHE:HB3 | 1:1W:59:TYR:HB3 | 2.03 | 0.41 |
| 1:1W:379:LYS:O | 1:1W:383:GLU:HG2 | 2.21 | 0.41 |
| 2:1X:363:VAL:HG13 | 2:1X:366:GLY:HA3 | 2.03 | 0.41 |
| 2:1Z:319:TYR:HB2 | 2:1Z:355:ILE:HD13 | 2.02 | 0.41 |
| 1:2A:210:ILE:O | 1:2A:214:THR:OG1 | 2.26 | 0.41 |
| 1:2A:314:SER:HA | 1:2A:350:LYS:O | 2.20 | 0.41 |
| 2:2B:5:ILE:HD11 | 2:2B:135:PHE:CE1 | 2.55 | 0.41 |
| 2:2B:318:MET:HE2 | 2:2B:376:CYS:O | 2.20 | 0.41 |
| 1:2C:128:ASP:OD1 | 1:2C:128:ASP:N | 2.42 | 0.41 |
| 1:2C:198:GLU:HA | 1:2C:264:HIS:HB2 | 2.03 | 0.41 |
| 1:2C:237:THR:HG23 | 1:2C:241:ARG:HH21 | 1.85 | 0.41 |
| 1:2C:260:PHE:HB2 | 1:2C:263:LEU:HD13 | 2.02 | 0.41 |
| 1:2C:417:ASP:OD1 | 1:2C:418:LEU:N | 2.53 | 0.41 |
| 2:2D:90:GLU:HB3 | 2:2D:121:ARG:HH12 | 1.86 | 0.41 |
| 2:2D:123:ARG:HG2 | 2:2D:123:ARG:NH1 | 2.36 | 0.41 |
| 2:2D:269:LEU:HD23 | 2:2D:269:LEU:HA | 1.94 | 0.41 |
| 1:2E:43:GLN:O | 1:2E:47:ILE:HG23 | 2.20 | 0.41 |
| 1:2E:48:ASN:N | 1:2E:48:ASN:OD1 | 2.52 | 0.41 |
| 1:2E:70:PRO:N | 1:2E:92:PHE:HZ | 2.19 | 0.41 |
| 2:2F:121:ARG:HD2 | 2:2F:121:ARG:HA | 1.74 | 0.41 |
| 2:2F:125:LEU:HD12 | 2:2F:125:LEU:HA | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2F:155:GLU:HB2 | 2:2F:197:HIS:CE1 | 2.56 | 0.41 |
| 1:2G:8:GLN:CD | 1:2G:17:GLY:HA3 | 2.41 | 0.41 |
| 1:2G:117:LEU:HD23 | 1:2G:117:LEU:HA | 1.78 | 0.41 |
| 1:2G:286:VAL:HG22 | 1:2G:321:MET:HE3 | 2.02 | 0.41 |
| 1:2G:317:PHE:HB3 | 1:2G:321:MET:SD | 2.60 | 0.41 |
| 2:2H:179:THR:O | 1:2I:350:LYS:HD2 | 2.21 | 0.41 |
| 2:2H:387:ILE:HG12 | 2:2H:390:ARG:NH2 | 2.35 | 0.41 |
| 1:2I:67:ASP:CG | 1:2I:68:LEU:H | 2.24 | 0.41 |
| 1:2I:309:ARG:NH1 | 1:2I:341:PHE:O | 2.53 | 0.41 |
| 1:2I:385:PHE:HZ | 1:2I:408:PHE:HD1 | 1.68 | 0.41 |
| 2:2J:62:VAL:HA | 2:2J:63:PRO:HD3 | 1.96 | 0.41 |
| 2:2J:185:TYR:CE1 | 2:2J:398:MET:HE3 | 2.55 | 0.41 |
| 1:2K:173:PRO:HD2 | 1:2K:380:ARG:CZ | 2.51 | 0.41 |
| 1:2M:17:GLY:HA2 | 1:2M:20:PHE:HB3 | 2.03 | 0.41 |
| 1:2M:167:PHE:CE1 | 1:2M:200:MET:HG3 | 2.56 | 0.41 |
| 2:2N:183:GLU:CG | 2:2N:184:PRO:HD3 | 2.51 | 0.41 |
| 2:2N:301:MET:HE1 | 2:2N:307:PRO:HD3 | 2.03 | 0.41 |
| 2:2P:227:LEU:O | 2:2P:231:ILE:HG12 | 2.21 | 0.41 |
| 1:2Q:77:ARG:HH11 | 17:5S:201:LEU:HG | 1.86 | 0.41 |
| 1:2Q:209:ASP:OD2 | 38:8A:105:ARG:CA | 2.68 | 0.41 |
| 1:2Q:213:ARG:HH11 | 38:8A:108:PHE:HE2 | 1.67 | 0.41 |
| 1:2Q:271:THR:CG2 | 1:2Q:365:ALA:HB3 | 2.49 | 0.41 |
| 1:2Q:406:MET:O | 1:2Q:410:GLU:HG2 | 2.21 | 0.41 |
| 2:2R:306:ASP:HB3 | 2:2R:309:HIS:HD2 | 1.84 | 0.41 |
| 1:2S:273:LEU:H | 1:2S:292:GLN:NE2 | 2.19 | 0.41 |
| 2:2T:312:TYR:HB2 | 2:2T:343:PHE:CD1 | 2.56 | 0.41 |
| 1:2U:154:LYS:HA | 1:2U:157:GLU:HG2 | 2.03 | 0.41 |
| 2:2V:60:LYS:HE2 | 2:2V:88:HIS:HE1 | 1.86 | 0.41 |
| 1:2W:148:GLY:O | 1:2W:152:ILE:HG12 | 2.21 | 0.41 |
| 2:2X:8:HIS:NE2 | 2:2X:138:PHE:HD2 | 2.19 | 0.41 |
| 2:2X:9:ILE:HD13 | 2:2X:150:GLY:HA2 | 2.01 | 0.41 |
| 2:2X:287:SER:N | 2:2X:290:GLU:OE2 | 2.28 | 0.41 |
| 1:2Y:43:GLN:HE21 | 38:8C:195:MET:CE | 2.34 | 0.41 |
| 2:2Z:125:LEU:HD23 | 2:2Z:125:LEU:HA | 1.88 | 0.41 |
| 2:2Z:216:SER:HB3 | 2:2Z:275:ILE:O | 2.21 | 0.41 |
| 2:2Z:278:ALA:HA | 2:2Z:369:ALA:HB2 | 2.02 | 0.41 |
| 1:3A:282:ARG:NH2 | 1:3A:288:GLU:HG3 | 2.32 | 0.41 |
| 2:3B:171:VAL:HA | 2:3B:204:LEU:O | 2.21 | 0.41 |
| 2:3B:179:THR:O | 1:3C:350:LYS:HD2 | 2.21 | 0.41 |
| 2:3B:298:PRO:HD2 | 38:8C:25:ILE:HG23 | 2.02 | 0.41 |
| 2:3D:287:SER:H | 2:3D:290:GLU:CD | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3F:81:GLY:O | 2:3F:84:ARG:NH1 | 2.50 | 0.41 |
| 2:3F:288:VAL:HG21 | 2:3F:327:ASP:HB2 | 2.03 | 0.41 |
| 1:3G:90:PHE:CD2 | 3:3X:19:LEU:HD22 | 2.56 | 0.41 |
| 2:3H:3:GLU:HB2 | 2:3H:129:CYS:SG | 2.61 | 0.41 |
| 1:3I:182:PRO:O | 1:3I:186:THR:HG23 | 2.21 | 0.41 |
| 2:3J:246:GLY:HA3 | 2:3J:356:ASN:HA | 2.03 | 0.41 |
| 2:3J:394:LYS:HB2 | 1:3K:346:PRO:HG3 | 2.03 | 0.41 |
| 2:3L:11:GLN:HB3 | 41:3M:501:GTP:O2A | 2.20 | 0.41 |
| 1:3M:86:ARG:HB3 | 1:3M:89:ASN:OD1 | 2.21 | 0.41 |
| 1:3M:152:ILE:HD12 | 1:3M:164:MET:SD | 2.61 | 0.41 |
| 1:3O:391:ARG:HB2 | 2:3P:346:TRP:CZ3 | 2.56 | 0.41 |
| 1:3Q:35:THR:HG21 | 14:5N:239:GLN:HE22 | 1.86 | 0.41 |
| 1:3Q:65:LEU:HD13 | 1:3Q:90:PHE:HD1 | 1.83 | 0.41 |
| 1:3Q:137:HIS:O | 1:3Q:168:SER:HA | 2.21 | 0.41 |
| 1:3Q:206:ALA:HA | 1:3Q:209:ASP:OD2 | 2.21 | 0.41 |
| 1:3Q:253:LEU:HD21 | 1:3Q:316:LEU:HD21 | 2.03 | 0.41 |
| 2:3R:172:TYR:CE2 | 2:3R:203:MET:SD | 3.13 | 0.41 |
| 2:3R:358:GLN:HG3 | 2:3R:359:PRO:HD2 | 2.01 | 0.41 |
| 1:3S:12:CYS:HB2 | 39:3S:502:GDP:C8 | 2.56 | 0.41 |
| 1:3S:260:PHE:HB2 | 1:3S:263:LEU:HD23 | 2.03 | 0.41 |
| 1:3S:284:LEU:HB3 | 1:3S:363:MET:HE2 | 2.03 | 0.41 |
| 1:3S:284:LEU:HD13 | 1:3S:284:LEU:HA | 1.98 | 0.41 |
| 1:3S:344:TRP:CE3 | 1:3S:345:ILE:HG13 | 2.56 | 0.41 |
| 2:3T:112:LYS:HA | 2:3T:112:LYS:HE3 | 2.03 | 0.41 |
| 2:3T:138:PHE:CE1 | 2:3T:169:PHE:HB2 | 2.56 | 0.41 |
| 2:3T:210:TYR:OH | 2:3T:224:TYR:HE1 | 2.04 | 0.41 |
| 2:3T:316:CYS:HB3 | 2:3T:378:ILE:CG2 | 2.51 | 0.41 |
| 3:3V:9:LEU:HD23 | 3:3V:9:LEU:HA | 1.88 | 0.41 |
| 3:3V:88:GLU:O | 3:3V:92:THR:HG23 | 2.21 | 0.41 |
| 3:3V:111:LYS:HE2 | 3:3V:111:LYS:HB2 | 1.81 | 0.41 |
| 3:3V:236:VAL:N | 3:3V:237:PRO:HD2 | 2.36 | 0.41 |
| 4:3W:14:LEU:HB2 | 4:3W:25:TRP:NE1 | 2.36 | 0.41 |
| 4:3W:69:LEU:HD21 | 4:3W:153:ARG:HA | 2.02 | 0.41 |
| 3:3X:9:LEU:HD23 | 3:3X:9:LEU:HA | 1.89 | 0.41 |
| 3:3X:236:VAL:N | 3:3X:237:PRO:HD2 | 2.36 | 0.41 |
| 4:3Y:2:PHE:HZ | 23:6Q:3:LEU:CD1 | 2.34 | 0.41 |
| 4:3Y:69:LEU:HD21 | 4:3Y:153:ARG:HA | 2.02 | 0.41 |
| 3:3Z:236:VAL:N | 3:3Z:237:PRO:HD2 | 2.36 | 0.41 |
| 4:4A:69:LEU:HD21 | 4:4A:153:ARG:HA | 2.02 | 0.41 |
| 3:4D:88:GLU:O | 3:4D:92:THR:HG23 | 2.21 | 0.41 |
| 3:4D:218:LEU:HA | 3:4D:218:LEU:HD23 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4D:236:VAL:N | 3:4D:237:PRO:HD2 | 2.36 | 0.41 |
| 4:4E:23:GLU:HG3 | 4:4E:24:ILE:HG23 | 2.02 | 0.41 |
| 4:4E:69:LEU:HD21 | 4:4E:153:ARG:HA | 2.02 | 0.41 |
| 3:4F:236:VAL:N | 3:4F:237:PRO:HD2 | 2.36 | 0.41 |
| 3:4H:88:GLU:O | 3:4H:92:THR:HG23 | 2.21 | 0.41 |
| 4:4I:14:LEU:HB2 | 4:4I:25:TRP:NE1 | 2.36 | 0.41 |
| 4:4I:69:LEU:HD21 | 4:4I:153:ARG:HA | 2.02 | 0.41 |
| 5:4L:323:LEU:HD13 | 5:4L:326:GLU:OE1 | 2.20 | 0.41 |
| 5:4L:464:GLN:O | 5:4L:468:SER:N | 2.41 | 0.41 |
| 5:4M:265:GLU:HG2 | 5:4M:268:ARG:HH21 | 1.85 | 0.41 |
| 6:4O:103:ARG:CZ | 30:7K:395:ALA:HA | 2.51 | 0.41 |
| 6:4O:487:ILE:HA | 6:4O:490:VAL:HG12 | 2.03 | 0.41 |
| 7:4R:169:GLU:O | 7:4R:172:THR:HG22 | 2.20 | 0.41 |
| 7:4R:183:LEU:HD23 | 7:4R:183:LEU:HA | 1.88 | 0.41 |
| 7:4R:332:LEU:HD23 | 7:4R:332:LEU:HA | 1.83 | 0.41 |
| 7:4U:147:GLU:HA | 7:4U:150:VAL:HG12 | 2.03 | 0.41 |
| 7:4U:261:ASP:OD2 | 7:4U:262:HIS:N | 2.53 | 0.41 |
| 8:4V:424:LYS:HA | 8:4V:427:VAL:HG12 | 2.03 | 0.41 |
| 8:4W:468:MET:O | 8:4X:127:THR:CG2 | 2.69 | 0.41 |
| 9:4Z:89:LYS:HA | 9:4Z:89:LYS:HD2 | 1.84 | 0.41 |
| 9:4Z:291:HIS:HA | 9:4Z:294:GLU:HG3 | 2.01 | 0.41 |
| 9:4Z:329:GLN:HE21 | 9:4Z:332:GLN:NE2 | 2.19 | 0.41 |
| 10:5A:265:LYS:HA | 10:5A:268:MET:HG2 | 2.03 | 0.41 |
| 10:5C:430:TYR:O | 10:5C:433:GLU:HG2 | 2.21 | 0.41 |
| 12:5F:280:PHE:CE1 | 12:5F:290:PHE:HB2 | 2.56 | 0.41 |
| 14:5L:354:GLU:HB2 | 14:5L:368:HIS:CD2 | 2.55 | 0.41 |
| 14:5L:561:VAL:HG13 | 14:5L:562:ASP:O | 2.21 | 0.41 |
| 14:5L:576:LEU:HB3 | 14:5L:591:GLY:HA2 | 2.02 | 0.41 |
| 14:5L:580:TRP:HA | 14:5L:586:HIS:O | 2.21 | 0.41 |
| 14:5M:354:GLU:HB2 | 14:5M:368:HIS:CD2 | 2.55 | 0.41 |
| 14:5M:492:SER:HA | 14:5M:507:LEU:O | 2.21 | 0.41 |
| 14:5N:553:LEU:H | 14:5N:553:LEU:HD23 | 1.86 | 0.41 |
| 14:5N:561:VAL:HG13 | 14:5N:562:ASP:O | 2.21 | 0.41 |
| 15:5P:12:GLU:OE2 | 15:5P:74:LYS:HE3 | 2.21 | 0.41 |
| 15:5P:119:LEU:HD23 | 15:5P:119:LEU:HA | 1.92 | 0.41 |
| 16:5Q:20:LYS:HG2 | 16:5Q:25:TYR:HE2 | 1.86 | 0.41 |
| 17:5S:31:THR:HB | 17:5S:36:PHE:CZ | 2.56 | 0.41 |
| 17:5T:31:THR:HB | 17:5T:36:PHE:CZ | 2.56 | 0.41 |
| 17:5T:185:LEU:HD13 | 17:5T:222:ILE:HG12 | 2.03 | 0.41 |
| 17:5U:31:THR:HB | 17:5U:36:PHE:CZ | 2.56 | 0.41 |
| 18:5X:73:GLN:HG2 | 18:5X:79:VAL:HG12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:5Y:73:GLN:HG2 | 18:5Y:79:VAL:HG12 | 2.03 | 0.41 |
| 18:6B:73:GLN:HG2 | 18:6B:79:VAL:HG12 | 2.03 | 0.41 |
| 18:6D:73:GLN:HG2 | 18:6D:79:VAL:HG12 | 2.03 | 0.41 |
| 18:6D:103:PRO:HD3 | 24:7A:178:ASN:HB3 | 2.02 | 0.41 |
| 19:6E:221:THR:O | 19:6E:225:GLU:HG2 | 2.21 | 0.41 |
| 20:6F:86:ASP:HB3 | 20:6F:247:TYR:HE1 | 1.86 | 0.41 |
| 21:6G:15:ASP:HB2 | 21:6G:19:ARG:HH21 | 1.85 | 0.41 |
| 21:6H:136:GLN:HE22 | 21:6H:170:LEU:HB3 | 1.85 | 0.41 |
| 22:6J:88:GLU:N | 22:6J:88:GLU:OE2 | 2.53 | 0.41 |
| 22:6K:193:MET:HG2 | 22:6K:194:TYR:CD1 | 2.56 | 0.41 |
| 22:6O:114:THR:HG23 | 22:6O:117:GLY:N | 2.24 | 0.41 |
| 22:6P:294:LEU:O | 22:6P:294:LEU:HD23 | 2.20 | 0.41 |
| 24:6T:18:LEU:HD23 | 24:6T:18:LEU:HA | 1.92 | 0.41 |
| 24:6T:344:LYS:H | 24:6T:344:LYS:HG2 | 1.66 | 0.41 |
| 24:6T:376:LYS:O | 24:6T:380:LYS:HG3 | 2.20 | 0.41 |
| 24:6T:629:PHE:O | 24:6T:633:LEU:HD23 | 2.21 | 0.41 |
| 24:6U:432:LYS:HE3 | 24:6U:432:LYS:HB2 | 1.96 | 0.41 |
| 24:6U:474:PHE:HD2 | 24:6U:500:ARG:HH21 | 1.68 | 0.41 |
| 24:6V:24:ASP:OD1 | 24:6V:25:LYS:N | 2.54 | 0.41 |
| 24:6V:123:TYR:HE2 | 24:6V:163:PRO:HG3 | 1.86 | 0.41 |
| 24:6V:552:MET:HB2 | 24:6V:607:HIS:CD2 | 2.56 | 0.41 |
| 24:6X:299:GLU:HG3 | 24:6X:300:ASP:N | 2.36 | 0.41 |
| 24:6Y:156:ASP:OD1 | 24:6Y:157:ASP:N | 2.54 | 0.41 |
| 24:6Z:451:LYS:HB3 | 24:6Z:468:ARG:HG3 | 2.02 | 0.41 |
| 24:6Z:482:ILE:HD13 | 24:6Z:498:LEU:HD23 | 2.03 | 0.41 |
| 24:7A:6:PRO:CD | 31:7N:83:THR:HG23 | 2.50 | 0.41 |
| 25:7C:105:SER:HB3 | 30:7K:248:GLU:HG2 | 2.02 | 0.41 |
| 26:7F:138:THR:HG23 | 26:7F:139:PRO:HD2 | 1.97 | 0.41 |
| 28:7H:392:LEU:HD21 | 28:7H:433:SER:HA | 2.03 | 0.41 |
| 29:7J:383:GLY:HA2 | 29:7J:386:HIS:CD2 | 2.56 | 0.41 |
| 30:7K:33:GLU:N | 30:7K:33:GLU:OE1 | 2.54 | 0.41 |
| 31:7N:28:THR:HG23 | 31:7N:31:LEU:H | 1.85 | 0.41 |
| 34:7S:257:ARG:NH1 | 34:7S:261:MET:HG2 | 2.35 | 0.41 |
| 35:7U:130:LYS:HE3 | 35:7U:130:LYS:HB3 | 1.82 | 0.41 |
| 38:8B:113:ARG:HD2 | 38:8B:113:ARG:HA | 1.92 | 0.41 |
| 38:8D:70:LYS:HD3 | 38:8D:71:HIS:H | 1.86 | 0.41 |
| 38:8D:228:THR:HG23 | 38:8D:228:THR:O | 2.21 | 0.41 |
| 1:3:83:GLN:HB2 | 24:6U:177:ARG:NH2 | 2.34 | 0.41 |
| 1:3:306:ARG:NH2 | 3:3X:60:PRO:HB2 | 2.36 | 0.41 |
| 2:8:29:GLY:CA | 26:7E:45:MET:HE1 | 2.48 | 0.41 |
| 1:A3:40:SER:CB | 26:7F:125:TYR:CD1 | 3.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C8:142:GLY:N | 39:C8:502:GDP:O2B | 2.54 | 0.41 |
| 2:E7:11:GLN:HB3 | 41:E8:501:GTP:O2A | 2.20 | 0.41 |
| 2:G3:3:GLU:O | 2:G3:133:GLN:N | 2.36 | 0.41 |
| 1:G4:122:LYS:CE | 1:I0:291:GLN:HB3 | 2.51 | 0.41 |
| 2:G5:183:GLU:CG | 2:G5:184:PRO:HD3 | 2.52 | 0.41 |
| 1:G6:203:ASP:OD2 | 1:G6:204:ASN:N | 2.54 | 0.41 |
| 2:G7:274:PRO:HB2 | 2:G7:276:ILE:CG1 | 2.51 | 0.41 |
| 1:G8:190:HIS:HD2 | 1:G8:411:ALA:HA | 1.80 | 0.41 |
| 1:G8:227:HIS:O | 1:G8:230:SER:OG | 2.36 | 0.41 |
| 1:G8:232:VAL:CG1 | 1:G8:268:VAL:HG11 | 2.51 | 0.41 |
| 2:G9:57:GLY:H | 2:I5:285:GLN:HG2 | 1.85 | 0.41 |
| 2:G9:259:LEU:HD21 | 2:G9:316:CYS:HB2 | 2.03 | 0.41 |
| 2:G9:312:TYR:HA | 2:G9:381:SER:HB2 | 2.03 | 0.41 |
| 2:H1:96:LYS:HA | 1:H2:1:MET:SD | 2.61 | 0.41 |
| 2:H3:403:ALA:HB2 | 1:H4:344:TRP:HZ3 | 1.86 | 0.41 |
| 1:H4:387:ALA:HA | 1:H4:390:ARG:HH21 | 1.85 | 0.41 |
| 2:H7:155:GLU:HB2 | 2:H7:197:HIS:CE1 | 2.56 | 0.41 |
| 2:H7:266:HIS:O | 2:H7:266:HIS:ND1 | 2.52 | 0.41 |
| 1:H8:386:THR:O | 1:H8:390:ARG:HB2 | 2.20 | 0.41 |
| 2:H9:178:SER:HB2 | 2:H9:183:GLU:OE2 | 2.21 | 0.41 |
| 1:I2:334:GLN:NE2 | 1:I2:348:ASN:H | 2.12 | 0.41 |
| 1:I2:395:LEU:HD12 | 1:I2:395:LEU:HA | 1.84 | 0.41 |
| 2:I3:11:GLN:HB3 | 41:I4:501:GTP:PA | 2.61 | 0.41 |
| 1:I4:137:HIS:O | 1:I4:168:SER:HA | 2.21 | 0.41 |
| 2:I7:276:ILE:HD13 | 2:I7:276:ILE:HA | 1.85 | 0.41 |
| 1:I8:21:TRP:HA | 1:I8:24:VAL:HG22 | 2.02 | 0.41 |
| 1:I8:203:ASP:OD2 | 1:I8:302:ALA:N | 2.54 | 0.41 |
| 1:J0:135:VAL:O | 1:J0:166:THR:HA | 2.21 | 0.41 |
| 2:J1:101:ASN:ND2 | 2:J1:143:GLY:HA2 | 2.36 | 0.41 |
| 1:J2:164:MET:HB3 | 1:J2:197:ASP:OD2 | 2.21 | 0.41 |
| 2:J5:121:ARG:HD2 | 2:J5:121:ARG:HA | 1.98 | 0.41 |
| 1:J8:295:ASP:OD1 | 1:J8:296:ALA:N | 2.54 | 0.41 |
| 1:K0:178:THR:OG1 | 2:K1:258:ASN:ND2 | 2.52 | 0.41 |
| 1:K0:399:THR:HA | 1:K0:403:MET:O | 2.21 | 0.41 |
| 2:K3:56:THR:HG21 | 2:L9:283:HIS:O | 2.21 | 0.41 |
| 1:K6:272:PRO:HD3 | 1:K6:364:SER:HA | 2.03 | 0.41 |
| 2:K7:287:SER:H | 2:K7:290:GLU:CD | 2.24 | 0.41 |
| 2:K9:241:SER:OG | 2:K9:250:VAL:O | 2.24 | 0.41 |
| 2:L1:286:LEU:HD13 | 2:L1:286:LEU:HA | 1.94 | 0.41 |
| 1:L2:99:ASN:ND2 | 2:L3:254:GLU:OE1 | 2.54 | 0.41 |
| 2:L3:79:ARG:O | 2:L3:84:ARG:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L4:173:PRO:HB3 | 1:L4:384:GLN:HE22 | 1.86 | 0.41 |
| 1:L6:318:ARG:HD3 | 1:L6:358:PRO:HD3 | 2.03 | 0.41 |
| 2:L7:22:GLU:O | 2:L7:26:LEU:HG | 2.21 | 0.41 |
| 2:L7:112:LYS:HD3 | 2:L7:112:LYS:O | 2.21 | 0.41 |
| 1:M0:257:LEU:HA | 1:M0:312:THR:HG21 | 2.02 | 0.41 |
| 2:M5:125:LEU:HA | 2:M5:125:LEU:HD23 | 1.81 | 0.41 |
| 2:M5:306:ASP:HB3 | 2:M5:309:HIS:HD2 | 1.86 | 0.41 |
| 1:M6:403:MET:HE3 | 1:M6:403:MET:HB2 | 1.82 | 0.41 |
| 2:M7:154:LEU:HD23 | 2:M7:154:LEU:HA | 1.90 | 0.41 |
| 2:M7:166:LYS:O | 2:M7:198:THR:OG1 | 2.38 | 0.41 |
| 1:N0:192:LEU:HD23 | 1:N0:192:LEU:HA | 1.81 | 0.41 |
| 2:N1:283:HIS:CD2 | 2:N1:284:GLU:HG2 | 2.55 | 0.41 |
| 1:N2:192:LEU:HD23 | 1:N2:192:LEU:HA | 1.93 | 0.41 |
| 2:N5:305:CYS:HB3 | 2:N5:387:ILE:HD11 | 2.02 | 0.41 |
| 2:N7:271:SER:HB3 | 2:N7:377:MET:HE2 | 2.02 | 0.41 |
| 2:N9:3:GLU:HB2 | 2:N9:129:CYS:SG | 2.61 | 0.41 |
| 2:N9:246:GLY:HA3 | 2:N9:356:ASN:HA | 2.03 | 0.41 |
| 2:N9:279:GLU:HB2 | 2:N9:280:LYS:NZ | 2.36 | 0.41 |
| 2:O1:14:ILE:HD11 | 2:O1:74:VAL:CG1 | 2.51 | 0.41 |
| 2:O1:216:SER:OG | 2:O1:217:LEU:N | 2.53 | 0.41 |
| 1:O2:356:ILE:CD1 | 37:7Y:234:HIS:HA | 2.50 | 0.41 |
| 1:O4:203:ASP:O | 1:O4:207:LEU:HD23 | 2.22 | 0.41 |
| 1:O6:65:LEU:HD13 | 1:O6:90:PHE:HE1 | 1.84 | 0.41 |
| 1:O6:83:GLN:O | 1:Q4:281:TYR:OH | 2.23 | 0.41 |
| 1:O6:276:ARG:HH12 | 32:7P:97:LEU:HB3 | 1.86 | 0.41 |
| 2:O7:389:SER:N | 2:O7:429:GLU:OE2 | 2.54 | 0.41 |
| 1:O8:177:ASP:OD2 | 2:O9:248:LEU:HD11 | 2.21 | 0.41 |
| 2:O9:406:HIS:HA | 2:O9:409:VAL:CG1 | 2.46 | 0.41 |
| 2:P3:9:ILE:HG22 | 2:P3:146:GLY:HA2 | 2.02 | 0.41 |
| 2:P5:387:ILE:HG13 | 2:P5:390:ARG:HH21 | 1.86 | 0.41 |
| 1:P8:219:THR:O | 1:P8:219:THR:OG1 | 2.30 | 0.41 |
| 2:Q1:286:LEU:HA | 2:Q1:286:LEU:HD12 | 1.73 | 0.41 |
| 1:Q2:189:VAL:O | 1:Q2:193:VAL:HG13 | 2.20 | 0.41 |
| 1:Q2:271:THR:OG1 | 1:Q2:272:PRO:HA | 2.21 | 0.41 |
| 2:Q5:88:HIS:HE2 | 2:S1:284:GLU:HB2 | 1.86 | 0.41 |
| 2:Q5:306:ASP:HB3 | 2:Q5:309:HIS:HD2 | 1.85 | 0.41 |
| 1:Q6:385:PHE:HZ | 1:Q6:408:PHE:HD1 | 1.68 | 0.41 |
| 2:Q9:21:TRP:CZ2 | 2:Q9:65:CYS:HB3 | 2.56 | 0.41 |
| 2:R3:259:LEU:HD23 | 2:R3:268:MET:HG2 | 2.03 | 0.41 |
| 2:R3:420:GLU:HA | 2:R3:423:GLU:HG3 | 2.03 | 0.41 |
| 1:R4:85:PHE:HB2 | 1:R4:90:PHE:CZ | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R4:232:VAL:O | 1:R4:236:ILE:HG12 | 2.21 | 0.41 |
| 2:R5:84:ARG:NH2 | 11:5E:10:PRO:HB2 | 2.36 | 0.41 |
| 2:R9:15:GLN:HB3 | 2:R9:228:ASN:HD21 | 1.86 | 0.41 |
| 2:R9:161:TYR:HD1 | 13:5J:124:VAL:HG13 | 1.85 | 0.41 |
| 2:R9:394:LYS:HB2 | 1:S0:346:PRO:HG3 | 2.03 | 0.41 |
| 2:S1:145:THR:O | 2:S1:149:LEU:HD23 | 2.21 | 0.41 |
| 1:S2:100:ASN:HB3 | 1:S2:103:LYS:HB2 | 2.02 | 0.41 |
| 1:S4:215:LEU:HD22 | 24:6U:12:PRO:HG2 | 2.02 | 0.41 |
| 1:S4:375:GLN:HB3 | 1:S4:422:TYR:HD2 | 1.86 | 0.41 |
| 1:S4:392:LYS:HD3 | 13:5H:55:VAL:CG1 | 2.51 | 0.41 |
| 1:S8:189:VAL:O | 1:S8:193:VAL:HG13 | 2.21 | 0.41 |
| 1:S8:192:LEU:HD22 | 1:S8:196:ALA:HB2 | 2.03 | 0.41 |
| 2:S9:79:ARG:O | 2:S9:84:ARG:HG2 | 2.20 | 0.41 |
| 2:S9:337:THR:OG1 | 13:5I:21:ASN:ND2 | 2.52 | 0.41 |
| 2:T3:70:LEU:HB3 | 2:T3:97:GLU:O | 2.21 | 0.41 |
| 1:T8:65:LEU:HD13 | 1:T8:90:PHE:CE1 | 2.55 | 0.41 |
| 1:T8:165:LEU:HD23 | 1:T8:165:LEU:HA | 1.85 | 0.41 |
| 2:U1:289:ALA:O | 2:U1:293:ASN:ND2 | 2.54 | 0.41 |
| 1:U2:203:ASP:N | 1:U2:203:ASP:OD1 | 2.54 | 0.41 |
| 2:U3:298:PRO:HA | 2:U3:301:MET:HE2 | 2.02 | 0.41 |
| 1:U4:273:LEU:H | 1:U4:292:GLN:NE2 | 2.19 | 0.41 |
| 2:U9:89:PRO:HD3 | 2:W5:283:HIS:ND1 | 2.37 | 0.41 |
| 1:V0:162:ARG:HD3 | 1:V0:162:ARG:HA | 1.84 | 0.41 |
| 1:V6:19:LYS:HB3 | 1:V6:19:LYS:HE3 | 1.86 | 0.41 |
| 1:V6:293:MET:HG3 | 1:V6:367:PHE:HB2 | 2.03 | 0.41 |
| 1:V6:350:LYS:HB3 | 1:V6:350:LYS:HE2 | 1.63 | 0.41 |
| 2:V7:96:LYS:HD2 | 1:V8:129:CYS:SG | 2.61 | 0.41 |
| 1:V8:58:ARG:HH12 | 1:V8:84:ILE:HA | 1.86 | 0.41 |
| 1:V8:167:PHE:CE2 | 1:V8:233:MET:HG2 | 2.56 | 0.41 |
| 1:W0:19:LYS:NZ | 1:W0:227:HIS:HD2 | 2.19 | 0.41 |
| 2:W1:50:ASN:O | 2:W1:64:ARG:NH2 | 2.54 | 0.41 |
| 2:W1:53:PHE:HB3 | 2:W1:61:HIS:HB3 | 2.02 | 0.41 |
| 2:W1:74:VAL:O | 2:W1:77:GLU:HG3 | 2.21 | 0.41 |
| 1:W2:203:ASP:N | 1:W2:203:ASP:OD1 | 2.50 | 0.41 |
| 2:W7:205:ASP:OD2 | 2:W7:303:VAL:HG22 | 2.21 | 0.41 |
| 2:W7:399:TYR:O | 2:W7:402:ARG:NH1 | 2.52 | 0.41 |
| 2:W9:11:GLN:HE22 | 2:W9:74:VAL:CG1 | 2.33 | 0.41 |
| 2:W9:90:GLU:CB | 2:W9:121:ARG:NH1 | 2.84 | 0.41 |
| 1:X0:152:ILE:HD13 | 1:X0:152:ILE:HA | 1.85 | 0.41 |
| 2:X3:107:HIS:CD2 | 2:X3:152:LEU:HB2 | 2.56 | 0.41 |
| 2:X3:252:ILE:HD12 | 2:X3:255:PHE:CE2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X5:319:TYR:HB2 | 2:X5:355:ILE:HG12 | 2.02 | 0.41 |
| 2:X9:320:ARG:HE | 2:X9:320:ARG:HB3 | 1.72 | 0.41 |
| 1:Y0:292:GLN:HG2 | 1:Y0:298:ASN:ND2 | 2.36 | 0.41 |
| 2:Y1:23:LEU:HD12 | 2:Y1:26:LEU:HD11 | 2.03 | 0.41 |
| 2:Y1:132:LEU:HD23 | 2:Y1:164:LYS:HE3 | 2.03 | 0.41 |
| 2:Y3:216:SER:OG | 2:Y3:217:LEU:N | 2.53 | 0.41 |
| 1:Y4:192:LEU:HD22 | 1:Y4:196:ALA:HB2 | 2.02 | 0.41 |
| 2:Y5:21:TRP:CZ3 | 2:Y5:63:PRO:HB3 | 2.56 | 0.41 |
| 1:Y6:41:ASP:N | 1:Y6:41:ASP:OD1 | 2.53 | 0.41 |
| 1:Y8:68:LEU:HD23 | 1:Y8:93:GLY:HA3 | 2.03 | 0.41 |
| 1:Y8:380:ARG:NH1 | 1:Y8:383:GLU:OE2 | 2.53 | 0.41 |
| 2:Y9:136:LEU:HD21 | 2:Y9:138:PHE:CE1 | 2.56 | 0.41 |
| 1:Z0:19:LYS:HE3 | 1:Z0:19:LYS:HB3 | 1.90 | 0.41 |
| 1:Z0:100:ASN:HB3 | 1:Z0:103:LYS:HB2 | 2.02 | 0.41 |
| 1:Z0:114:ASP:OD1 | 1:Z0:115:SER:N | 2.52 | 0.41 |
| 2:Z1:181:VAL:HG22 | 1:Z2:347:ASN:O | 2.21 | 0.41 |
| 2:Z3:397:LEU:HD23 | 2:Z3:397:LEU:HA | 1.90 | 0.41 |
| 2:Z5:66:ILE:HG13 | 2:Z5:66:ILE:O | 2.21 | 0.41 |
| 2:Z7:429:GLU:O | 2:Z7:433:GLU:HG2 | 2.21 | 0.41 |
| 1:Z8:19:LYS:HE3 | 1:Z8:19:LYS:HB3 | 1.84 | 0.41 |
| 1:Z8:203:ASP:O | 1:Z8:207:LEU:HD13 | 2.21 | 0.41 |
| 1:Z8:317:PHE:HB2 | 1:Z8:353:VAL:HG22 | 2.03 | 0.41 |
| 2:Z9:397:LEU:HD23 | 2:Z9:397:LEU:HA | 1.87 | 0.41 |
| 1:0A:109:GLY:O | 1:0A:113:ILE:HG22 | 2.21 | 0.41 |
| 1:0A:237:THR:HG23 | 1:0A:241:ARG:HE | 1.86 | 0.41 |
| 1:0E:152:ILE:HD13 | 1:0E:155:ILE:HD11 | 2.04 | 0.41 |
| 2:0F:239:THR:O | 2:0F:242:LEU:HG | 2.21 | 0.41 |
| 1:0G:21:TRP:CH2 | 1:0G:61:PRO:HB3 | 2.56 | 0.41 |
| 1:0G:136:CYS:SG | 1:0G:167:PHE:HD2 | 2.44 | 0.41 |
| 1:0G:242:PHE:CD1 | 1:0G:356:ILE:HG13 | 2.56 | 0.41 |
| 1:0I:379:LYS:HA | 1:0I:382:SER:OG | 2.21 | 0.41 |
| 2:0J:203:MET:CE | 2:0J:267:PHE:HB3 | 2.51 | 0.41 |
| 2:0L:359:PRO:HA | 2:0L:360:PRO:HD3 | 1.97 | 0.41 |
| 2:0P:325:PRO:HA | 2:0P:328:VAL:HG12 | 2.03 | 0.41 |
| 1:0Q:344:TRP:CE3 | 1:0Q:345:ILE:HG13 | 2.56 | 0.41 |
| 2:0R:312:TYR:CE2 | 2:0R:341:ILE:HG12 | 2.55 | 0.41 |
| 2:0R:352:LYS:HD2 | 2:0R:352:LYS:HA | 1.88 | 0.41 |
| 1:0S:396:HIS:HA | 1:0S:399:THR:HG22 | 2.03 | 0.41 |
| 1:0U:107:THR:HB | 1:0U:108:GLU:OE1 | 2.21 | 0.41 |
| 1:0U:174:LYS:HD3 | 1:0U:174:LYS:C | 2.40 | 0.41 |
| 2:0V:246:GLY:HA2 | 2:0V:357:TYR:CD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0W:103:LYS:HA | 1:0W:107:THR:HG23 | 2.02 | 0.41 |
| 1:0W:116:VAL:O | 1:0W:120:VAL:HG12 | 2.21 | 0.41 |
| 2:1B:175:PRO:HG2 | 2:1B:176:GLN:OE1 | 2.21 | 0.41 |
| 2:1F:76:ASP:OD1 | 2:1F:79:ARG:NH2 | 2.54 | 0.41 |
| 2:1H:207:GLU:OE2 | 2:1H:210:TYR:HB2 | 2.21 | 0.41 |
| 1:1K:137:HIS:O | 1:1K:168:SER:HA | 2.21 | 0.41 |
| 1:1M:58:ARG:HD2 | 1:1M:58:ARG:HA | 1.88 | 0.41 |
| 1:1O:314:SER:OG | 1:1O:368:ILE:HB | 2.21 | 0.41 |
| 1:1Q:68:LEU:HD21 | 1:1Q:112:LEU:HD22 | 2.03 | 0.41 |
| 1:1Q:293:MET:HE2 | 1:1Q:367:PHE:HB2 | 2.03 | 0.41 |
| 2:1R:327:ASP:OD1 | 2:1R:327:ASP:N | 2.51 | 0.41 |
| 2:1R:353:CYS:SG | 2:1R:354:GLY:N | 2.94 | 0.41 |
| 1:1S:172:SER:HG | 1:1S:380:ARG:HH22 | 1.66 | 0.41 |
| 1:1S:356:ILE:HD13 | 1:1S:356:ILE:HA | 1.83 | 0.41 |
| 1:1W:165:LEU:HD21 | 1:1W:250:LEU:HD11 | 2.03 | 0.41 |
| 2:1Z:147:SER:OG | 2:1Z:148:GLY:N | 2.54 | 0.41 |
| 1:2A:285:THR:HB | 1:2A:287:PRO:HD2 | 2.02 | 0.41 |
| 2:2B:32:PRO:HB3 | 2:2B:83:TYR:CE1 | 2.55 | 0.41 |
| 1:2C:25:SER:OG | 1:2C:30:ILE:O | 2.38 | 0.41 |
| 1:2C:279:GLN:NE2 | 1:2C:282:ARG:HD3 | 2.36 | 0.41 |
| 2:2F:76:ASP:O | 2:2F:80:THR:HG23 | 2.21 | 0.41 |
| 2:2F:288:VAL:HG11 | 2:2F:328:VAL:HG12 | 2.02 | 0.41 |
| 1:2G:125:GLU:OE1 | 38:8B:53:ALA:HB1 | 2.21 | 0.41 |
| 2:2H:72:PRO:HD2 | 1:2I:2:ARG:NH1 | 2.36 | 0.41 |
| 2:2L:3:GLU:HB2 | 2:2L:129:CYS:SG | 2.61 | 0.41 |
| 1:2M:43:GLN:O | 1:2M:47:ILE:HG23 | 2.20 | 0.41 |
| 1:2M:172:SER:HB2 | 1:2M:380:ARG:HH21 | 1.85 | 0.41 |
| 2:2N:119:LEU:O | 2:2N:122:ILE:HG12 | 2.20 | 0.41 |
| 2:2P:69:ASP:OD1 | 2:2P:71:GLU:N | 2.53 | 0.41 |
| 1:2Q:58:ARG:HG2 | 1:3G:280:GLN:HE22 | 1.86 | 0.41 |
| 1:2Q:233:MET:HA | 1:2Q:236:ILE:HG22 | 2.02 | 0.41 |
| 1:2Q:295:ASP:OD2 | 1:2Q:297:LYS:HB2 | 2.20 | 0.41 |
| 1:2S:395:LEU:O | 1:2S:399:THR:HG23 | 2.20 | 0.41 |
| 1:2U:95:THR:HG23 | 1:2U:96:GLY:N | 2.35 | 0.41 |
| 1:2U:107:THR:OG1 | 1:2U:108:GLU:OE1 | 2.25 | 0.41 |
| 1:2U:325:GLU:O | 1:2U:329:GLN:HB2 | 2.21 | 0.41 |
| 2:2V:90:GLU:HG3 | 2:2V:121:ARG:NH1 | 2.36 | 0.41 |
| 1:2W:10:GLY:HA2 | 1:2W:143:THR:HG23 | 2.02 | 0.41 |
| 1:2W:117:LEU:HA | 1:2W:117:LEU:HD23 | 1.84 | 0.41 |
| 1:3A:67:ASP:OD1 | 1:3A:143:THR:HG21 | 2.20 | 0.41 |
| 2:3B:224:TYR:O | 2:3B:228:ASN:ND2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3B:317:LEU:HB3 | 2:3B:319:TYR:HE1 | 1.86 | 0.41 |
| 2:3B:398:MET:CG | 1:3C:346:PRO:HD2 | 2.51 | 0.41 |
| 1:3C:306:ARG:NE | 38:8D:97:PHE:H | 2.19 | 0.41 |
| 2:3D:405:VAL:O | 2:3D:409:VAL:HG23 | 2.21 | 0.41 |
| 2:3F:298:PRO:HG3 | 2:3F:308:ARG:HH12 | 1.86 | 0.41 |
| 2:3F:428:LEU:HA | 2:3F:431:ASP:OD1 | 2.21 | 0.41 |
| 1:3I:30:ILE:CD1 | 1:3I:59:TYR:HB2 | 2.51 | 0.41 |
| 1:3I:192:LEU:HA | 1:3I:192:LEU:HD23 | 1.80 | 0.41 |
| 1:3I:273:LEU:H | 1:3I:292:GLN:HE22 | 1.67 | 0.41 |
| 1:3I:317:PHE:CB | 1:3I:321:MET:HE1 | 2.50 | 0.41 |
| 2:3J:122:ILE:HD13 | 2:3J:125:LEU:CD1 | 2.51 | 0.41 |
| 2:3J:326:LYS:HE3 | 2:3J:326:LYS:HB3 | 1.88 | 0.41 |
| 2:3L:269:LEU:HD21 | 2:3L:301:MET:SD | 2.61 | 0.41 |
| 1:3M:165:LEU:HD11 | 1:3M:250:LEU:HD11 | 2.03 | 0.41 |
| 2:3N:221:ARG:HB2 | 38:8C:174:SER:OG | 2.21 | 0.41 |
| 1:3Q:152:ILE:HD12 | 1:3Q:164:MET:SD | 2.61 | 0.41 |
| 2:3R:420:GLU:HA | 2:3R:423:GLU:HG3 | 2.03 | 0.41 |
| 4:3W:23:GLU:HG3 | 4:3W:24:ILE:HG23 | 2.01 | 0.41 |
| 3:3Z:10:PHE:HB3 | 3:3Z:140:LYS:HZ2 | 1.85 | 0.41 |
| 3:3Z:111:LYS:HE2 | 3:3Z:111:LYS:HB2 | 1.81 | 0.41 |
| 4:4A:14:LEU:HB2 | 4:4A:25:TRP:NE1 | 2.36 | 0.41 |
| 3:4B:236:VAL:N | 3:4B:237:PRO:HD2 | 2.36 | 0.41 |
| 4:4C:69:LEU:HD21 | 4:4C:153:ARG:HA | 2.02 | 0.41 |
| 3:4D:10:PHE:HB3 | 3:4D:140:LYS:HZ2 | 1.85 | 0.41 |
| 4:4E:14:LEU:HB2 | 4:4E:25:TRP:NE1 | 2.36 | 0.41 |
| 4:4G:14:LEU:HB2 | 4:4G:25:TRP:NE1 | 2.36 | 0.41 |
| 3:4H:9:LEU:HD23 | 3:4H:9:LEU:HA | 1.88 | 0.41 |
| 3:4H:10:PHE:HB3 | 3:4H:140:LYS:HZ2 | 1.85 | 0.41 |
| 3:4H:236:VAL:N | 3:4H:237:PRO:HD2 | 2.36 | 0.41 |
| 4:4I:21:PRO:HD2 | 3:4J:258:ASP:OD1 | 2.21 | 0.41 |
| 6:4P:152:LEU:HA | 6:4P:152:LEU:HD23 | 1.86 | 0.41 |
| 7:4Q:324:GLN:CA | 24:6T:22:LEU:HD23 | 2.51 | 0.41 |
| 7:4S:14:GLU:HB2 | 7:4S:18:ARG:HH12 | 1.86 | 0.41 |
| 9:4Z:402:ALA:HA | 9:4Z:405:GLN:NE2 | 2.36 | 0.41 |
| 10:5C:180:GLU:OE2 | 10:5C:183:ARG:NH2 | 2.54 | 0.41 |
| 10:5C:421:VAL:HG22 | 10:5C:424:MET:HE3 | 2.03 | 0.41 |
| 11:5E:165:LEU:HD23 | 11:5E:165:LEU:HA | 1.86 | 0.41 |
| 12:5F:332:ASN:O | 12:7B:47:GLN:NE2 | 2.54 | 0.41 |
| 14:5L:111:PHE:C | 14:5L:155:PHE:CD2 | 2.94 | 0.41 |
| 14:5L:553:LEU:H | 14:5L:553:LEU:HD23 | 1.86 | 0.41 |
| 14:5L:562:ASP:OD1 | 14:5L:607:LYS:HG3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:277:LYS:HE2 | 14:5M:277:LYS:HB2 | 1.90 | 0.41 |
| 14:5M:553:LEU:H | 14:5M:553:LEU:HD23 | 1.86 | 0.41 |
| 14:5M:561:VAL:HG13 | 14:5M:562:ASP:O | 2.21 | 0.41 |
| 14:5M:580:TRP:HA | 14:5M:586:HIS:O | 2.21 | 0.41 |
| 14:5N:562:ASP:OD1 | 14:5N:607:LYS:HG3 | 2.21 | 0.41 |
| 14:5N:576:LEU:HB3 | 14:5N:591:GLY:HA2 | 2.02 | 0.41 |
| 15:5O:289:LEU:C | 15:5O:289:LEU:CD2 | 2.85 | 0.41 |
| 15:5P:52:TYR:CD2 | 15:5P:55:LEU:CD2 | 3.03 | 0.41 |
| 16:5Q:39:PHE:CE2 | 16:5Q:61:ILE:HD13 | 2.56 | 0.41 |
| 17:5T:181:LEU:C | 17:5T:181:LEU:CD2 | 2.85 | 0.41 |
| 18:5Y:65:VAL:O | 18:5Y:69:THR:HG22 | 2.21 | 0.41 |
| 18:5Y:192:SER:O | 18:5Y:196:VAL:HG23 | 2.21 | 0.41 |
| 18:6B:5:VAL:HG13 | 18:6B:62:GLU:HG2 | 2.03 | 0.41 |
| 18:6B:192:SER:O | 18:6B:196:VAL:HG23 | 2.21 | 0.41 |
| 18:6C:192:SER:O | 18:6C:196:VAL:HG23 | 2.21 | 0.41 |
| 18:6D:65:VAL:O | 18:6D:69:THR:HG22 | 2.21 | 0.41 |
| 18:6D:192:SER:O | 18:6D:196:VAL:HG23 | 2.21 | 0.41 |
| 20:6F:51:ALA:O | 20:6F:52:LEU:HD23 | 2.21 | 0.41 |
| 20:6F:193:ARG:O | 20:6F:193:ARG:HG3 | 2.20 | 0.41 |
| 22:6L:345:ALA:O | 22:6L:349:VAL:HG22 | 2.20 | 0.41 |
| 24:6V:344:LYS:H | 24:6V:344:LYS:HG2 | 1.66 | 0.41 |
| 24:6Z:280:ASP:HA | 24:6Z:289:ARG:HB2 | 2.02 | 0.41 |
| 24:6Z:469:PHE:CB | 24:6Z:484:GLU:HA | 2.51 | 0.41 |
| 29:7I:167:ILE:HD12 | 29:7I:167:ILE:HA | 1.92 | 0.41 |
| 29:7I:253:ASN:CB | 30:7K:341:ARG:NH2 | 2.84 | 0.41 |
| 33:7Q:148:LEU:HD13 | 33:7Q:148:LEU:HA | 1.89 | 0.41 |
| 34:7R:185:MET:O | 34:7R:188:ILE:HG22 | 2.20 | 0.41 |
| 38:8B:84:ILE:H | 38:8B:84:ILE:HG12 | 1.66 | 0.41 |
| 1:A3:423:GLN:HB3 | 3:4H:109:ALA:HB2 | 2.02 | 0.40 |
| 1:F6:276:ARG:HD3 | 24:6T:419:SER:HB2 | 2.03 | 0.40 |
| 1:G2:22:GLU:HG2 | 1:G2:81:TYR:CE1 | 2.56 | 0.40 |
| 2:G7:62:VAL:HA | 2:G7:63:PRO:HD3 | 1.97 | 0.40 |
| 1:G8:145:SER:OG | 1:G8:146:GLY:N | 2.54 | 0.40 |
| 2:G9:430:LYS:O | 2:G9:433:GLU:HG3 | 2.22 | 0.40 |
| 2:H1:217:LEU:HD23 | 2:H1:217:LEU:HA | 1.84 | 0.40 |
| 1:H2:49:VAL:HG13 | 1:H2:50:TYR:CD2 | 2.57 | 0.40 |
| 2:H3:102:ASN:ND2 | 2:H3:105:ARG:HB2 | 2.36 | 0.40 |
| 2:H3:194:LEU:O | 2:H3:198:THR:HG22 | 2.21 | 0.40 |
| 2:H5:200:VAL:HG13 | 2:H5:268:MET:CE | 2.51 | 0.40 |
| 1:I0:330:MET:SD | 1:I0:349:VAL:HG11 | 2.60 | 0.40 |
| 2:I1:403:ALA:HB2 | 1:I2:344:TRP:HZ3 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I4:48:ASN:OD1 | 1:I4:48:ASN:N | 2.54 | 0.40 |
| 1:I4:125:GLU:OE1 | 1:K0:336:LYS:NZ | 2.48 | 0.40 |
| 1:I4:218:THR:OG1 | 24:6Z:488:ARG:CA | 2.67 | 0.40 |
| 1:I4:325:GLU:O | 1:I4:329:GLN:HB2 | 2.22 | 0.40 |
| 2:I5:90:GLU:H | 2:K1:283:HIS:HE1 | 1.67 | 0.40 |
| 2:I5:139:ASN:O | 2:I5:170:THR:HA | 2.20 | 0.40 |
| 2:I5:387:ILE:HG12 | 2:I5:390:ARG:HH22 | 1.86 | 0.40 |
| 2:I9:389:SER:N | 2:I9:429:GLU:OE2 | 2.54 | 0.40 |
| 2:I9:402:ARG:HA | 2:I9:402:ARG:HD3 | 1.83 | 0.40 |
| 1:J0:52:ASN:O | 1:J0:60:VAL:HG12 | 2.20 | 0.40 |
| 1:J0:58:ARG:HB2 | 6:4O:224:ARG:NH1 | 2.36 | 0.40 |
| 1:J0:176:SER:HB2 | 2:J1:349:THR:OG1 | 2.21 | 0.40 |
| 2:J1:280:LYS:O | 2:J1:283:HIS:HB3 | 2.21 | 0.40 |
| 2:J5:101:ASN:ND2 | 2:J5:143:GLY:HA2 | 2.36 | 0.40 |
| 2:J9:428:LEU:HG | 2:J9:432:PHE:CE2 | 2.55 | 0.40 |
| 1:K0:99:ASN:ND2 | 2:K1:254:GLU:OE2 | 2.55 | 0.40 |
| 2:K1:75:VAL:HG11 | 2:K1:94:SER:HB3 | 2.02 | 0.40 |
| 2:K1:326:LYS:HG3 | 2:K1:327:ASP:N | 2.36 | 0.40 |
| 2:K1:344:VAL:HG22 | 2:K1:346:TRP:HD1 | 1.85 | 0.40 |
| 1:L2:68:LEU:HB3 | 1:L2:96:GLY:HA2 | 2.03 | 0.40 |
| 2:L3:11:GLN:NE2 | 2:L3:71:GLU:OE2 | 2.53 | 0.40 |
| 1:L4:371:SER:OG | 1:L4:372:THR:N | 2.53 | 0.40 |
| 2:L5:62:VAL:HA | 2:L5:63:PRO:HD3 | 1.87 | 0.40 |
| 1:L6:67:ASP:N | 1:L6:67:ASP:OD1 | 2.52 | 0.40 |
| 2:L7:9:ILE:HD13 | 2:L7:137:VAL:HG13 | 2.03 | 0.40 |
| 2:L7:278:ALA:HB3 | 6:4P:209:LYS:NZ | 2.36 | 0.40 |
| 2:L7:278:ALA:HA | 2:L7:369:ALA:HB2 | 2.03 | 0.40 |
| 2:M1:3:GLU:HB2 | 2:M1:129:CYS:SG | 2.60 | 0.40 |
| 1:M2:152:ILE:HD12 | 1:M2:164:MET:SD | 2.61 | 0.40 |
| 1:M4:49:VAL:HG11 | 1:M4:241:ARG:HG2 | 2.02 | 0.40 |
| 1:M4:218:THR:OG1 | 1:M4:219:THR:N | 2.54 | 0.40 |
| 2:M7:325:PRO:HA | 2:M7:328:VAL:HG12 | 2.02 | 0.40 |
| 1:M8:174:LYS:HE2 | 1:M8:174:LYS:HB3 | 1.92 | 0.40 |
| 2:M9:9:ILE:HG12 | 2:M9:68:LEU:HD11 | 2.03 | 0.40 |
| 1:N0:221:THR:HG22 | 1:N0:222:PHE:N | 2.36 | 0.40 |
| 2:N1:2:ARG:HA | 2:N1:133:GLN:HE21 | 1.86 | 0.40 |
| 2:N1:177:VAL:HG21 | 2:N1:207:GLU:OE1 | 2.21 | 0.40 |
| 1:N2:183:TYR:HB3 | 1:N2:398:TYR:HE2 | 1.86 | 0.40 |
| 2:N3:3:GLU:HB2 | 2:N3:129:CYS:SG | 2.61 | 0.40 |
| 1:N8:103:LYS:O | 1:N8:108:GLU:HB2 | 2.22 | 0.40 |
| 1:N8:208:TYR:CE1 | 1:N8:225:LEU:HD11 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N9:261:PRO:HG3 | 2:N9:313:MET:HE2 | 2.03 | 0.40 |
| 2:O1:70:LEU:HG | 2:O1:145:THR:HG23 | 2.01 | 0.40 |
| 2:O1:225:THR:HG21 | 37:7Y:241:THR:HB | 2.03 | 0.40 |
| 2:O1:401:LYS:HB3 | 2:O1:401:LYS:HE3 | 1.91 | 0.40 |
| 1:O2:3:GLU:HB2 | 1:O2:130:LEU:HA | 2.03 | 0.40 |
| 1:O2:183:TYR:O | 1:O2:187:LEU:HD13 | 2.21 | 0.40 |
| 2:O3:291:ILE:HG22 | 37:7Y:90:LEU:HD22 | 2.03 | 0.40 |
| 1:O4:317:PHE:HB3 | 1:O4:321:MET:SD | 2.62 | 0.40 |
| 2:O7:178:SER:OG | 1:O8:347:ASN:ND2 | 2.54 | 0.40 |
| 2:O7:287:SER:N | 2:O7:290:GLU:OE2 | 2.25 | 0.40 |
| 1:O8:403:MET:HE3 | 1:O8:403:MET:HB2 | 1.86 | 0.40 |
| 2:O9:428:LEU:HG | 2:O9:432:PHE:CE2 | 2.56 | 0.40 |
| 2:P3:117:LEU:HD12 | 2:P3:117:LEU:HA | 1.90 | 0.40 |
| 1:P4:31:ASP:OD2 | 1:P4:33:THR:OG1 | 2.36 | 0.40 |
| 2:P7:115:VAL:HG22 | 2:P7:119:LEU:HD23 | 2.01 | 0.40 |
| 2:P7:156:ARG:HA | 2:P7:159:VAL:HG12 | 2.03 | 0.40 |
| 2:P7:334:THR:O | 2:P7:338:LYS:HG3 | 2.21 | 0.40 |
| 1:Q0:313:ALA:HA | 1:Q0:369:GLY:HA2 | 2.02 | 0.40 |
| 2:Q1:430:LYS:O | 2:Q1:433:GLU:N | 2.53 | 0.40 |
| 1:Q2:167:PHE:HE1 | 1:Q2:200:MET:SD | 2.44 | 0.40 |
| 2:Q3:86:LEU:O | 2:Q3:86:LEU:CG | 2.68 | 0.40 |
| 2:Q3:315:CYS:SG | 2:Q3:379:SER:HB3 | 2.61 | 0.40 |
| 1:Q6:173:PRO:HB3 | 1:Q6:384:GLN:HE22 | 1.86 | 0.40 |
| 1:Q8:232:VAL:CG1 | 1:Q8:268:VAL:HG11 | 2.50 | 0.40 |
| 2:Q9:88:HIS:ND1 | 2:S5:283:HIS:HB3 | 2.36 | 0.40 |
| 2:Q9:176:GLN:HG2 | 2:Q9:177:VAL:N | 2.36 | 0.40 |
| 1:R0:190:HIS:CD2 | 1:R0:414:ASN:HB2 | 2.56 | 0.40 |
| 1:R0:405:GLU:HA | 1:R0:408:PHE:HD2 | 1.86 | 0.40 |
| 2:R1:112:LYS:HB2 | 2:R1:113:GLU:OE2 | 2.21 | 0.40 |
| 2:R1:401:LYS:HB3 | 2:R1:401:LYS:HE3 | 1.90 | 0.40 |
| 1:R2:5:VAL:CG1 | 1:R2:133:PHE:HD1 | 2.34 | 0.40 |
| 1:R4:163:MET:SD | 1:R4:251:ARG:HG3 | 2.61 | 0.40 |
| 2:R5:192:HIS:O | 2:R5:192:HIS:ND1 | 2.53 | 0.40 |
| 2:R5:325:PRO:HA | 2:R5:328:VAL:HG22 | 2.03 | 0.40 |
| 1:R6:156:ARG:NH1 | 1:R6:197:ASP:OD1 | 2.54 | 0.40 |
| 1:R6:227:HIS:O | 1:R6:230:SER:OG | 2.28 | 0.40 |
| 2:R7:320:ARG:HE | 2:R7:320:ARG:HB3 | 1.58 | 0.40 |
| 1:R8:313:ALA:HA | 1:R8:369:GLY:HA2 | 2.02 | 0.40 |
| 2:R9:346:TRP:CD1 | 2:R9:346:TRP:N | 2.88 | 0.40 |
| 1:S2:274:THR:HG21 | 1:S2:282:ARG:CD | 2.51 | 0.40 |
| 2:S5:384:ILE:H | 2:S5:384:ILE:HG12 | 1.72 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:S5:398:MET:HG3 | 1:S6:346:PRO:HD2 | 2.03 | 0.40 |
| 1:S6:164:MET:N | 1:S6:197:ASP:OD2 | 2.54 | 0.40 |
| 2:S9:72:PRO:HD2 | 1:T0:2:ARG:HH12 | 1.85 | 0.40 |
| 1:T0:374:ILE:HD12 | 1:T0:374:ILE:HA | 1.94 | 0.40 |
| 2:T1:198:THR:HG23 | 2:T1:266:HIS:CE1 | 2.56 | 0.40 |
| 2:T1:326:LYS:HE3 | 2:T1:326:LYS:HB2 | 1.98 | 0.40 |
| 1:T2:393:ALA:HB2 | 2:T3:346:TRP:CE3 | 2.56 | 0.40 |
| 1:T2:415:MET:O | 1:T2:419:VAL:HG13 | 2.22 | 0.40 |
| 1:T4:306:ARG:NH2 | 13:5J:104:MET:O | 2.54 | 0.40 |
| 2:T5:11:GLN:HB3 | 41:T6:501:GTP:PA | 2.61 | 0.40 |
| 2:T5:21:TRP:CZ2 | 2:T5:65:CYS:HB3 | 2.56 | 0.40 |
| 1:T6:214:THR:OG1 | 1:T6:215:LEU:N | 2.54 | 0.40 |
| 1:T6:245:GLN:HG2 | 33:7Q:139:GLU:CD | 2.41 | 0.40 |
| 1:T6:376:GLU:OE2 | 13:5K:43:THR:HG22 | 2.21 | 0.40 |
| 2:T7:176:GLN:CD | 2:T7:176:GLN:H | 2.25 | 0.40 |
| 2:U1:35:GLN:HB3 | 2:U1:59:GLY:O | 2.20 | 0.40 |
| 2:U1:177:VAL:HG13 | 1:U2:327:ASP:HB3 | 2.03 | 0.40 |
| 1:U2:391:ARG:HG3 | 2:U3:346:TRP:CE3 | 2.55 | 0.40 |
| 2:U3:6:SER:O | 2:U3:65:CYS:HA | 2.19 | 0.40 |
| 1:U4:396:HIS:CE1 | 1:U4:397:TRP:CE2 | 3.08 | 0.40 |
| 2:U5:76:ASP:HA | 2:U5:79:ARG:HE | 1.86 | 0.40 |
| 1:U6:286:VAL:CG2 | 1:U6:287:PRO:HD3 | 2.51 | 0.40 |
| 1:U6:390:ARG:HE | 1:U6:390:ARG:HB2 | 1.70 | 0.40 |
| 1:U8:20:PHE:O | 1:U8:23:VAL:HG12 | 2.21 | 0.40 |
| 2:U9:53:PHE:HB3 | 2:U9:61:HIS:HB3 | 2.03 | 0.40 |
| 2:U9:239:THR:HG22 | 2:U9:239:THR:O | 2.20 | 0.40 |
| 2:V1:369:ALA:O | 2:V1:371:VAL:HG23 | 2.21 | 0.40 |
| 1:V2:272:PRO:O | 1:V2:273:LEU:HD23 | 2.21 | 0.40 |
| 2:V3:35:GLN:HB3 | 2:V3:59:GLY:O | 2.20 | 0.40 |
| 2:V3:133:GLN:HB3 | 2:V3:252:ILE:HG21 | 2.02 | 0.40 |
| 2:V3:191:THR:HA | 2:V3:194:LEU:HB2 | 2.03 | 0.40 |
| 2:V3:222:PRO:CD | 1:V4:324:LYS:HE3 | 2.51 | 0.40 |
| 2:V3:265:ILE:HD11 | 2:V3:435:VAL:HG21 | 2.03 | 0.40 |
| 1:V6:208:TYR:HA | 1:V6:211:CYS:SG | 2.61 | 0.40 |
| 2:V7:76:ASP:O | 2:V7:80:THR:HG22 | 2.22 | 0.40 |
| 2:V7:298:PRO:HA | 2:V7:301:MET:HG3 | 2.03 | 0.40 |
| 2:V9:33:ASP:O | 2:V9:60:LYS:NZ | 2.42 | 0.40 |
| 2:V9:121:ARG:HA | 2:V9:121:ARG:HD2 | 1.81 | 0.40 |
| 2:W1:151:SER:HB2 | 2:W1:193:SER:OG | 2.21 | 0.40 |
| 1:W6:154:LYS:O | 1:W6:157:GLU:HG3 | 2.22 | 0.40 |
| 1:W6:387:ALA:HA | 1:W6:390:ARG:HH21 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W7:79:ARG:HG2 | 2:W7:92:LEU:HD13 | 2.03 | 0.40 |
| 2:W7:179:THR:O | 1:W8:350:LYS:HD2 | 2.21 | 0.40 |
| 2:W7:204:LEU:HD22 | 2:W7:231:ILE:HD12 | 2.03 | 0.40 |
| 1:W8:121:ARG:NH2 | 1:W8:158:GLU:OE2 | 2.47 | 0.40 |
| 2:W9:5:ILE:HG12 | 2:W9:135:PHE:HD1 | 1.86 | 0.40 |
| 1:X2:222:PHE:HA | 1:X2:225:LEU:HD12 | 2.03 | 0.40 |
| 2:X3:360:PRO:HD2 | 2:X3:371:VAL:HG23 | 2.02 | 0.40 |
| 1:X4:30:ILE:HG13 | 1:X4:35:THR:O | 2.21 | 0.40 |
| 1:X6:6:HIS:CE1 | 1:X6:8:GLN:HG2 | 2.55 | 0.40 |
| 2:X7:121:ARG:HD2 | 2:X7:121:ARG:HA | 1.72 | 0.40 |
| 1:X8:177:ASP:OD1 | 2:X9:248:LEU:HD11 | 2.21 | 0.40 |
| 2:X9:62:VAL:HB | 2:X9:88:HIS:ND1 | 2.36 | 0.40 |
| 2:X9:244:PHE:HB2 | 2:X9:356:ASN:HD21 | 1.87 | 0.40 |
| 2:Y1:327:ASP:OD1 | 2:Y1:328:VAL:N | 2.53 | 0.40 |
| 1:Y2:404:ASP:OD1 | 1:Y2:405:GLU:N | 2.54 | 0.40 |
| 1:Y4:134:GLN:HA | 1:Y4:165:LEU:O | 2.21 | 0.40 |
| 2:Y5:251:ASP:HB3 | 2:Y5:254:GLU:OE2 | 2.21 | 0.40 |
| 1:Y8:12:CYS:SG | 1:Y8:138:SER:HB3 | 2.62 | 0.40 |
| 1:Y8:95:THR:HG23 | 1:Y8:96:GLY:N | 2.36 | 0.40 |
| 1:Y8:314:SER:HA | 1:Y8:350:LYS:O | 2.21 | 0.40 |
| 1:Z0:190:HIS:CD2 | 1:Z0:414:ASN:HB2 | 2.55 | 0.40 |
| 1:Z0:322:SER:OG | 1:Z0:325:GLU:HG2 | 2.21 | 0.40 |
| 2:Z1:278:ALA:HA | 2:Z1:369:ALA:HB2 | 2.03 | 0.40 |
| 1:Z2:250:LEU:HA | 1:Z2:253:LEU:HD12 | 2.03 | 0.40 |
| 1:Z2:297:LYS:HD3 | 1:Z2:297:LYS:HA | 1.74 | 0.40 |
| 1:Z2:394:PHE:HA | 2:Z3:261:PRO:HA | 2.02 | 0.40 |
| 2:Z3:3:GLU:HB2 | 2:Z3:129:CYS:SG | 2.61 | 0.40 |
| 2:Z3:194:LEU:HG | 2:Z3:198:THR:HG21 | 2.03 | 0.40 |
| 2:Z3:236:SER:HA | 2:Z3:239:THR:HG22 | 2.02 | 0.40 |
| 1:Z4:156:ARG:HD2 | 1:Z4:156:ARG:HA | 1.91 | 0.40 |
| 2:Z5:9:ILE:HD13 | 2:Z5:150:GLY:HA2 | 2.03 | 0.40 |
| 2:Z5:296:PHE:CE2 | 2:Z5:335:ILE:HD13 | 2.56 | 0.40 |
| 1:Z8:54:ALA:HB3 | 1:Z8:58:ARG:HB3 | 2.03 | 0.40 |
| 1:0A:58:ARG:HH11 | 1:0A:84:ILE:HA | 1.86 | 0.40 |
| 1:0A:130:LEU:HG | 1:0A:132:GLY:N | 2.36 | 0.40 |
| 1:0E:152:ILE:HD13 | 1:0E:152:ILE:HA | 1.90 | 0.40 |
| 2:0F:9:ILE:HB | 2:0F:139:ASN:HB3 | 2.03 | 0.40 |
| 2:0F:223:THR:HG23 | 2:0F:225:THR:H | 1.86 | 0.40 |
| 2:0F:349:THR:O | 2:0F:349:THR:HG23 | 2.21 | 0.40 |
| 1:0G:121:ARG:NH2 | 1:0G:158:GLU:OE2 | 2.54 | 0.40 |
| 1:0G:311:LEU:HD23 | 1:0G:312:THR:HG23 | 2.01 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0I:8:GLN:O | 1:0I:66:MET:HB2 | 2.21 | 0.40 |
| 1:0I:378:PHE:HB3 | 1:0I:415:MET:SD | 2.61 | 0.40 |
| 2:0J:187:SER:O | 2:0J:190:SER:OG | 2.32 | 0.40 |
| 1:0M:414:ASN:HA | 1:0M:417:ASP:OD2 | 2.20 | 0.40 |
| 2:0N:12:ALA:HA | 2:0N:15:GLN:OE1 | 2.21 | 0.40 |
| 1:0O:286:VAL:CG2 | 1:0O:287:PRO:HD3 | 2.51 | 0.40 |
| 1:0Q:343:GLU:HG2 | 1:0Q:344:TRP:N | 2.35 | 0.40 |
| 1:0S:135:VAL:HG13 | 1:0S:166:THR:HA | 2.03 | 0.40 |
| 1:0W:3:GLU:OE2 | 1:0W:3:GLU:N | 2.54 | 0.40 |
| 2:0X:223:THR:HG23 | 2:0X:225:THR:H | 1.86 | 0.40 |
| 1:0Y:97:ALA:HA | 1:0Y:103:LYS:HE3 | 2.03 | 0.40 |
| 2:0Z:101:ASN:HD22 | 2:0Z:143:GLY:HA2 | 1.86 | 0.40 |
| 2:0Z:209:ILE:HG21 | 2:0Z:227:LEU:HG | 2.02 | 0.40 |
| 2:1B:88:HIS:HB3 | 2:1B:90:GLU:CD | 2.41 | 0.40 |
| 1:1C:162:ARG:HA | 1:1C:162:ARG:HD3 | 1.86 | 0.40 |
| 1:1C:172:SER:O | 1:1C:176:SER:OG | 2.31 | 0.40 |
| 1:1E:268:VAL:HG12 | 1:1E:368:ILE:HG13 | 2.03 | 0.40 |
| 2:1F:5:ILE:HD11 | 2:1F:135:PHE:HE1 | 1.85 | 0.40 |
| 2:1F:75:VAL:HG11 | 2:1F:94:SER:OG | 2.22 | 0.40 |
| 1:1G:174:LYS:HE2 | 1:1G:174:LYS:HB3 | 1.94 | 0.40 |
| 2:1H:384:ILE:HG23 | 2:1H:432:PHE:CE1 | 2.56 | 0.40 |
| 2:1L:328:VAL:O | 2:1L:332:VAL:HG12 | 2.20 | 0.40 |
| 2:1N:402:ARG:HD3 | 2:1N:402:ARG:HA | 1.81 | 0.40 |
| 1:1O:375:GLN:HB2 | 1:1O:419:VAL:HG23 | 2.02 | 0.40 |
| 2:1P:417:GLU:HA | 2:1P:420:GLU:HG2 | 2.03 | 0.40 |
| 2:1R:235:ILE:O | 2:1R:239:THR:HG23 | 2.21 | 0.40 |
| 2:1T:335:ILE:HD13 | 2:1T:335:ILE:HA | 1.94 | 0.40 |
| 2:1T:377:MET:SD | 2:1T:379:SER:HB2 | 2.61 | 0.40 |
| 2:1V:34:GLY:HA3 | 2:1V:60:LYS:NZ | 2.35 | 0.40 |
| 1:1W:273:LEU:H | 1:1W:292:GLN:NE2 | 2.19 | 0.40 |
| 2:1X:191:THR:HA | 2:1X:194:LEU:HD12 | 2.03 | 0.40 |
| 2:1X:425:LEU:HA | 2:1X:428:LEU:HG | 2.02 | 0.40 |
| 2:1Z:328:VAL:O | 2:1Z:332:VAL:HG13 | 2.20 | 0.40 |
| 1:2A:167:PHE:CE1 | 1:2A:200:MET:HG3 | 2.56 | 0.40 |
| 1:2A:396:HIS:CE1 | 1:2A:397:TRP:CE2 | 3.08 | 0.40 |
| 1:2E:392:LYS:HD2 | 1:2E:395:LEU:HD22 | 2.03 | 0.40 |
| 2:2H:87:PHE:O | 2:2H:89:PRO:HD3 | 2.22 | 0.40 |
| 2:2H:287:SER:HG | 2:2H:290:GLU:CD | 2.22 | 0.40 |
| 1:2I:101:TRP:HE3 | 1:2I:403:MET:HE1 | 1.86 | 0.40 |
| 1:2I:183:TYR:O | 1:2I:187:LEU:HD13 | 2.21 | 0.40 |
| 1:2I:210:ILE:O | 1:2I:214:THR:OG1 | 2.31 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2J:216:SER:O | 2:2J:280:LYS:NZ | 2.35 | 0.40 |
| 2:2L:21:TRP:CZ2 | 2:2L:65:CYS:HB2 | 2.57 | 0.40 |
| 1:2M:396:HIS:HA | 1:2M:399:THR:OG1 | 2.20 | 0.40 |
| 2:2N:33:ASP:OD1 | 2:2N:34:GLY:N | 2.54 | 0.40 |
| 2:2N:251:ASP:OD1 | 2:2N:254:GLU:HG2 | 2.20 | 0.40 |
| 2:2P:124:LYS:HA | 2:2P:127:ASP:OD2 | 2.21 | 0.40 |
| 2:2P:297:GLU:OE2 | 38:7Z:25:ILE:N | 2.54 | 0.40 |
| 1:2S:183:TYR:O | 1:2S:187:LEU:HD13 | 2.20 | 0.40 |
| 1:2S:328:GLU:HB3 | 38:8A:67:PHE:CZ | 2.56 | 0.40 |
| 1:2S:371:SER:OG | 1:2S:372:THR:N | 2.54 | 0.40 |
| 2:2T:242:LEU:HD23 | 2:2T:242:LEU:HA | 1.92 | 0.40 |
| 1:2W:5:VAL:HG22 | 1:2W:133:PHE:CD1 | 2.55 | 0.40 |
| 2:2X:276:ILE:HD11 | 2:2X:280:LYS:CD | 2.52 | 0.40 |
| 1:3A:306:ARG:NH1 | 38:8C:51:GLN:HA | 2.36 | 0.40 |
| 2:3B:141:VAL:O | 2:3B:147:SER:OG | 2.38 | 0.40 |
| 2:3F:56:THR:HG21 | 3:3V:34:SER:HA | 2.03 | 0.40 |
| 2:3H:274:PRO:HD3 | 2:3H:374:ALA:HA | 2.02 | 0.40 |
| 1:3I:67:ASP:OD1 | 1:3I:68:LEU:N | 2.49 | 0.40 |
| 1:3I:167:PHE:CZ | 1:3I:233:MET:HG2 | 2.57 | 0.40 |
| 1:3K:19:LYS:NZ | 1:3K:227:HIS:HD2 | 2.19 | 0.40 |
| 2:3N:356:ASN:OD1 | 2:3N:357:TYR:N | 2.54 | 0.40 |
| 1:3O:391:ARG:HD3 | 2:3P:346:TRP:CZ2 | 2.56 | 0.40 |
| 1:3Q:5:VAL:HB | 1:3Q:133:PHE:CD1 | 2.55 | 0.40 |
| 1:3S:190:HIS:CD2 | 1:3S:414:ASN:HB2 | 2.56 | 0.40 |
| 2:3T:339:ARG:HG3 | 2:3T:339:ARG:O | 2.21 | 0.40 |
| 4:4C:2:PHE:HZ | 23:6R:3:LEU:HD12 | 1.84 | 0.40 |
| 4:4C:14:LEU:HB2 | 4:4C:25:TRP:NE1 | 2.36 | 0.40 |
| 3:4F:9:LEU:HD23 | 3:4F:9:LEU:HA | 1.89 | 0.40 |
| 4:4G:69:LEU:HD21 | 4:4G:153:ARG:HA | 2.02 | 0.40 |
| 3:4H:111:LYS:HE2 | 3:4H:111:LYS:HB2 | 1.81 | 0.40 |
| 5:4L:464:GLN:O | 5:4L:468:SER:CB | 2.69 | 0.40 |
| 6:4P:118:SER:O | 6:4P:121:GLU:HG2 | 2.22 | 0.40 |
| 7:4U:122:ARG:H | 7:4U:122:ARG:HG2 | 1.77 | 0.40 |
| 9:4Z:72:GLU:O | 9:4Z:75:ILE:HG22 | 2.20 | 0.40 |
| 9:4Z:143:LEU:O | 9:4Z:147:GLU:HG2 | 2.21 | 0.40 |
| 9:4Z:183:ARG:HA | 9:4Z:186:ASP:OD1 | 2.21 | 0.40 |
| 9:4Z:345:GLU:HA | 9:4Z:348:GLU:CD | 2.41 | 0.40 |
| 9:4Z:377:VAL:O | 9:4Z:381:LEU:HD23 | 2.21 | 0.40 |
| 10:5C:453:LEU:HD23 | 10:5C:453:LEU:HA | 1.87 | 0.40 |
| 11:5E:175:ASP:OD1 | 11:5E:176:VAL:N | 2.54 | 0.40 |
| 12:5F:216:ALA:HB1 | 12:5F:217:PRO:HD2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5L:454:ILE:O | 14:5L:454:ILE:HG13 | 2.20 | 0.40 |
| 14:5M:57:ASP:HB3 | 14:5M:76:ILE:O | 2.20 | 0.40 |
| 14:5M:454:ILE:O | 14:5M:454:ILE:HG13 | 2.20 | 0.40 |
| 14:5M:562:ASP:OD1 | 14:5M:607:LYS:HG3 | 2.21 | 0.40 |
| 14:5M:604:THR:CG2 | 14:5M:609:ARG:H | 2.34 | 0.40 |
| 14:5N:366:LEU:HD13 | 14:5N:366:LEU:HA | 1.82 | 0.40 |
| 14:5N:580:TRP:HA | 14:5N:586:HIS:O | 2.21 | 0.40 |
| 14:5N:616:GLU:O | 14:5N:618:GLY:N | 2.54 | 0.40 |
| 15:5O:249:ASP:OD2 | 15:5O:251:ALA:N | 2.46 | 0.40 |
| 15:5P:145:PHE:CE1 | 15:5P:149:LEU:HD21 | 2.56 | 0.40 |
| 17:5S:18:GLN:H | 17:5S:18:GLN:HG3 | 1.68 | 0.40 |
| 17:5T:18:GLN:H | 17:5T:18:GLN:HG3 | 1.68 | 0.40 |
| 18:5X:103:PRO:HD3 | 24:6U:178:ASN:HB3 | 2.03 | 0.40 |
| 18:5X:192:SER:O | 18:5X:196:VAL:HG23 | 2.21 | 0.40 |
| 18:5Z:192:SER:O | 18:5Z:196:VAL:HG23 | 2.21 | 0.40 |
| 18:6A:65:VAL:O | 18:6A:69:THR:HG22 | 2.21 | 0.40 |
| 18:6A:192:SER:O | 18:6A:196:VAL:HG23 | 2.21 | 0.40 |
| 18:6B:65:VAL:O | 18:6B:69:THR:HG22 | 2.21 | 0.40 |
| 18:6C:65:VAL:O | 18:6C:69:THR:HG22 | 2.21 | 0.40 |
| 18:6C:128:GLN:CD | 18:6C:128:GLN:H | 2.17 | 0.40 |
| 22:6I:130:LEU:HD12 | 22:6I:130:LEU:HA | 1.89 | 0.40 |
| 22:6K:186:ARG:O | 22:6K:189:LYS:HB2 | 2.21 | 0.40 |
| 22:6L:294:LEU:HD23 | 22:6L:294:LEU:HA | 1.91 | 0.40 |
| 22:6N:224:MET:N | 22:6N:224:MET:SD | 2.94 | 0.40 |
| 22:6P:62:SER:O | 22:6P:62:SER:OG | 2.35 | 0.40 |
| 22:6P:145:SER:HB2 | 22:6P:148:ASN:OD1 | 2.21 | 0.40 |
| 22:6P:240:TYR:O | 22:6P:244:VAL:HG22 | 2.21 | 0.40 |
| 24:6T:92:ASP:OD2 | 24:6T:93:ARG:N | 2.54 | 0.40 |
| 24:6T:255:HIS:HA | 24:6T:258:ASP:OD1 | 2.21 | 0.40 |
| 24:6T:293:VAL:CG2 | 24:6T:306:LEU:HB2 | 2.51 | 0.40 |
| 24:6T:429:LYS:HG3 | 24:6T:430:PRO:O | 2.21 | 0.40 |
| 24:6T:506:PRO:HB3 | 24:6T:524:GLU:OE1 | 2.21 | 0.40 |
| 24:6U:119:VAL:CG2 | 24:6U:132:VAL:HG13 | 2.51 | 0.40 |
| 24:6X:288:ASP:OD1 | 24:6X:288:ASP:N | 2.54 | 0.40 |
| 24:6X:438:LEU:CD2 | 24:6X:476:MET:HG2 | 2.51 | 0.40 |
| 24:6X:450:VAL:HG23 | 24:6X:531:GLU:O | 2.21 | 0.40 |
| 24:6X:518:TYR:CE1 | 24:6X:521:ALA:HB2 | 2.56 | 0.40 |
| 25:7C:10:GLU:HB3 | 25:7C:14:ARG:NH2 | 2.36 | 0.40 |
| 28:7H:301:GLU:H | 28:7H:301:GLU:HG3 | 1.73 | 0.40 |
| 29:7J:330:GLU:O | 29:7J:330:GLU:HG3 | 2.21 | 0.40 |
| 28:7X:398:ASP:OD1 | 28:7X:400:THR:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:8A:62:THR:OG1 | 38:8A:63:VAL:N | 2.54 | 0.40 |
| 38:8B:228:THR:HG23 | 38:8B:228:THR:O | 2.21 | 0.40 |
| 1:9:420:SER:OG | 3:4D:209:ARG:NH1 | 2.53 | 0.40 |
| 2:B4:278:ALA:HB3 | 18:6A:43:ASN:ND2 | 2.32 | 0.40 |
| 2:B9:278:ALA:H | 18:6C:43:ASN:HD22 | 1.69 | 0.40 |
| 2:E1:11:GLN:HB3 | 41:E1:501:GTP:O2A | 2.22 | 0.40 |
| 1:E4:276:ARG:CZ | 24:6V:314:GLY:H | 2.34 | 0.40 |
| 2:E7:56:THR:HA | 2:G3:285:GLN:HB2 | 2.02 | 0.40 |
| 1:G0:388:MET:CE | 2:G1:348:PRO:HD3 | 2.51 | 0.40 |
| 1:G4:27:GLU:OE1 | 1:G4:241:ARG:NH1 | 2.48 | 0.40 |
| 1:G4:166:THR:OG1 | 1:G4:199:CYS:SG | 2.71 | 0.40 |
| 2:G5:182:VAL:HG23 | 2:G5:186:ASN:ND2 | 2.37 | 0.40 |
| 2:G5:305:CYS:HB3 | 2:G5:387:ILE:HD11 | 2.03 | 0.40 |
| 1:G6:212:PHE:O | 1:G6:216:LYS:HA | 2.21 | 0.40 |
| 1:G6:317:PHE:CE2 | 1:G6:326:VAL:HG13 | 2.56 | 0.40 |
| 1:G8:135:VAL:HG21 | 1:G8:152:ILE:HD11 | 2.04 | 0.40 |
| 1:G8:173:PRO:CG | 1:G8:380:ARG:HE | 2.34 | 0.40 |
| 2:H1:52:PHE:O | 2:H1:64:ARG:HG3 | 2.21 | 0.40 |
| 2:H1:167:LEU:HD13 | 2:H1:169:PHE:CZ | 2.56 | 0.40 |
| 1:H2:6:HIS:CE1 | 1:H2:8:GLN:HG2 | 2.56 | 0.40 |
| 1:H2:297:LYS:HA | 1:H2:297:LYS:HD3 | 1.87 | 0.40 |
| 1:H2:304:ASP:HB3 | 1:H2:307:HIS:CG | 2.56 | 0.40 |
| 2:H5:2:ARG:HA | 2:H5:133:GLN:HE21 | 1.86 | 0.40 |
| 2:H5:72:PRO:HD2 | 1:H6:2:ARG:HH12 | 1.86 | 0.40 |
| 2:H7:220:GLU:H | 2:H7:220:GLU:HG2 | 1.79 | 0.40 |
| 2:H9:69:ASP:OD1 | 2:H9:71:GLU:N | 2.55 | 0.40 |
| 1:I2:155:ILE:HG22 | 1:I2:164:MET:HE1 | 2.03 | 0.40 |
| 2:I3:76:ASP:O | 2:I3:80:THR:HG22 | 2.20 | 0.40 |
| 2:I3:431:ASP:O | 2:I3:435:VAL:HG22 | 2.21 | 0.40 |
| 1:I4:2:ARG:HB3 | 1:I4:131:GLN:HB2 | 2.03 | 0.40 |
| 2:I5:52:PHE:O | 2:I5:64:ARG:N | 2.51 | 0.40 |
| 2:I7:65:CYS:SG | 2:I7:66:ILE:N | 2.94 | 0.40 |
| 1:I8:268:VAL:HG13 | 1:I8:300:MET:HB2 | 2.03 | 0.40 |
| 1:J0:180:VAL:HG23 | 1:J0:184:ASN:HD21 | 1.86 | 0.40 |
| 2:J1:406:HIS:HA | 2:J1:409:VAL:HG22 | 2.02 | 0.40 |
| 1:J4:219:THR:O | 1:J4:219:THR:OG1 | 2.33 | 0.40 |
| 2:J5:172:TYR:CZ | 2:J5:203:MET:SD | 3.15 | 0.40 |
| 2:J5:313:MET:HE1 | 2:J5:435:VAL:HG11 | 2.02 | 0.40 |
| 1:J6:334:GLN:NE2 | 1:J6:348:ASN:H | 2.15 | 0.40 |
| 2:J9:327:ASP:N | 2:J9:327:ASP:OD1 | 2.51 | 0.40 |
| 2:J9:384:ILE:HA | 2:J9:387:ILE:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J9:425:LEU:HA | 2:J9:425:LEU:HD23 | 1.82 | 0.40 |
| 1:K0:101:TRP:HE3 | 1:K0:403:MET:HE1 | 1.85 | 0.40 |
| 2:K1:227:LEU:O | 2:K1:230:LEU:HG | 2.21 | 0.40 |
| 2:K3:217:LEU:CD1 | 2:K3:275:ILE:HG22 | 2.50 | 0.40 |
| 1:K4:152:ILE:HD12 | 1:K4:164:MET:SD | 2.62 | 0.40 |
| 1:K4:306:ARG:NH2 | 28:7H:451:LYS:NZ | 2.68 | 0.40 |
| 2:K5:195:LEU:HD23 | 2:K5:195:LEU:HA | 1.90 | 0.40 |
| 1:K6:5:VAL:CG2 | 1:K6:133:PHE:HD1 | 2.32 | 0.40 |
| 1:K6:50:TYR:CE2 | 1:K6:241:ARG:HD3 | 2.56 | 0.40 |
| 1:K6:212:PHE:HZ | 2:K7:326:LYS:HG3 | 1.86 | 0.40 |
| 2:K7:8:HIS:CD2 | 2:K7:138:PHE:HD2 | 2.39 | 0.40 |
| 1:K8:25:SER:HB3 | 1:K8:30:ILE:HG23 | 2.03 | 0.40 |
| 2:K9:387:ILE:HG12 | 2:K9:390:ARG:HH22 | 1.86 | 0.40 |
| 1:L0:350:LYS:HZ1 | 1:L0:352:SER:HB2 | 1.86 | 0.40 |
| 2:L1:111:GLY:O | 2:L1:115:VAL:HG12 | 2.21 | 0.40 |
| 1:L2:67:ASP:CG | 1:L2:68:LEU:H | 2.24 | 0.40 |
| 1:L2:215:LEU:HB3 | 1:L2:217:LEU:HG | 2.03 | 0.40 |
| 1:L2:304:ASP:OD2 | 1:L2:306:ARG:NH1 | 2.55 | 0.40 |
| 2:L3:306:ASP:HB3 | 2:L3:309:HIS:CD2 | 2.57 | 0.40 |
| 1:L4:14:ASN:HD22 | 1:L4:65:LEU:HD22 | 1.86 | 0.40 |
| 1:L6:178:THR:OG1 | 1:L6:179:VAL:N | 2.54 | 0.40 |
| 1:L6:337:ASN:OD1 | 28:7X:455:MET:HB3 | 2.20 | 0.40 |
| 2:L7:103:PHE:CD1 | 2:L7:189:LEU:HB3 | 2.56 | 0.40 |
| 2:L9:175:PRO:HB3 | 2:L9:390:ARG:HD2 | 2.03 | 0.40 |
| 1:M0:228:LEU:HD23 | 1:M0:228:LEU:HA | 1.92 | 0.40 |
| 1:M2:6:HIS:CE1 | 1:M2:136:CYS:HG | 2.38 | 0.40 |
| 1:M4:154:LYS:HA | 1:M4:154:LYS:HD3 | 1.91 | 0.40 |
| 1:M6:190:HIS:HD2 | 1:M6:411:ALA:HA | 1.87 | 0.40 |
| 1:M8:7:ILE:HB | 1:M8:135:VAL:HG22 | 2.02 | 0.40 |
| 2:M9:417:GLU:HA | 2:M9:420:GLU:HG2 | 2.03 | 0.40 |
| 1:N0:2:ARG:HB3 | 1:N0:131:GLN:HB2 | 2.03 | 0.40 |
| 2:N1:14:ILE:HD11 | 2:N1:74:VAL:HG22 | 2.04 | 0.40 |
| 2:N3:111:GLY:HA2 | 2:N3:149:LEU:HD13 | 2.03 | 0.40 |
| 2:N3:313:MET:HE3 | 2:N3:382:THR:HG23 | 2.02 | 0.40 |
| 1:N8:108:GLU:HA | 1:N8:111:GLU:OE1 | 2.20 | 0.40 |
| 2:O1:367:ASP:OD1 | 2:O1:367:ASP:N | 2.47 | 0.40 |
| 2:O3:101:ASN:HD22 | 2:O3:143:GLY:HA2 | 1.86 | 0.40 |
| 2:O3:313:MET:HG2 | 2:O3:346:TRP:HZ3 | 1.73 | 0.40 |
| 1:O4:113:ILE:HA | 1:O4:116:VAL:HG22 | 2.03 | 0.40 |
| 1:O4:361:LEU:HD23 | 1:O4:361:LEU:HA | 1.73 | 0.40 |
| 2:O5:75:VAL:HG12 | 2:O5:79:ARG:HE | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O7:62:VAL:HA | 2:O7:63:PRO:HD3 | 1.94 | 0.40 |
| 2:O9:116:ASP:OD1 | 2:O9:117:LEU:N | 2.54 | 0.40 |
| 2:P3:195:LEU:HD23 | 2:P3:195:LEU:HA | 1.87 | 0.40 |
| 1:P6:211:CYS:HA | 1:P6:215:LEU:HB2 | 2.03 | 0.40 |
| 2:P7:103:PHE:HD1 | 2:P7:147:SER:OG | 2.04 | 0.40 |
| 1:P8:167:PHE:HE1 | 1:P8:200:MET:SD | 2.44 | 0.40 |
| 1:P8:239:CYS:SG | 1:P8:247:ASN:HA | 2.61 | 0.40 |
| 2:P9:113:GLU:OE1 | 2:P9:113:GLU:N | 2.55 | 0.40 |
| 2:Q1:139:ASN:OD1 | 2:Q1:170:THR:HG22 | 2.20 | 0.40 |
| 1:Q8:135:VAL:O | 1:Q8:166:THR:HA | 2.21 | 0.40 |
| 1:Q8:172:SER:HB3 | 1:Q8:175:VAL:CG2 | 2.51 | 0.40 |
| 2:Q9:35:GLN:N | 2:Q9:35:GLN:OE1 | 2.54 | 0.40 |
| 1:R2:379:LYS:O | 1:R2:383:GLU:HG2 | 2.21 | 0.40 |
| 1:R4:69:GLU:CD | 1:R4:71:GLY:H | 2.25 | 0.40 |
| 2:R9:100:ALA:HA | 1:S0:252:LYS:HE2 | 2.02 | 0.40 |
| 1:S2:383:GLU:OE2 | 1:S2:384:GLN:HG3 | 2.22 | 0.40 |
| 2:S5:11:GLN:OE1 | 2:S5:15:GLN:NE2 | 2.54 | 0.40 |
| 2:S5:70:LEU:HB2 | 2:S5:98:ASP:HA | 2.03 | 0.40 |
| 1:T0:320:ARG:NH1 | 12:5F:210:THR:HA | 2.36 | 0.40 |
| 2:T1:156:ARG:HA | 2:T1:159:VAL:HG22 | 2.03 | 0.40 |
| 2:T1:319:TYR:CZ | 2:T1:328:VAL:HG23 | 2.56 | 0.40 |
| 1:T2:8:GLN:NE2 | 1:T2:17:GLY:HA3 | 2.36 | 0.40 |
| 1:T2:322:SER:OG | 1:T2:325:GLU:HG3 | 2.21 | 0.40 |
| 2:T3:2:ARG:HD3 | 2:T3:242:LEU:HD22 | 2.03 | 0.40 |
| 1:T4:95:THR:HG23 | 1:T4:96:GLY:N | 2.35 | 0.40 |
| 1:T8:117:LEU:HA | 1:T8:120:VAL:HG12 | 2.03 | 0.40 |
| 1:U2:28:HIS:NE2 | 1:U2:241:ARG:HD2 | 2.36 | 0.40 |
| 1:U2:77:ARG:O | 1:U2:83:GLN:NE2 | 2.54 | 0.40 |
| 1:U4:242:PHE:CD1 | 1:U4:356:ILE:HG13 | 2.56 | 0.40 |
| 2:U5:183:GLU:HG3 | 2:U5:184:PRO:HD3 | 2.03 | 0.40 |
| 2:U7:287:SER:N | 2:U7:290:GLU:OE2 | 2.52 | 0.40 |
| 2:U9:428:LEU:HG | 2:U9:432:PHE:HE2 | 1.85 | 0.40 |
| 1:V2:128:ASP:OD1 | 1:V2:129:CYS:N | 2.52 | 0.40 |
| 2:V3:9:ILE:HD11 | 2:V3:153:LEU:HD23 | 2.04 | 0.40 |
| 1:V6:304:ASP:HB3 | 1:V6:307:HIS:CG | 2.56 | 0.40 |
| 2:V7:31:GLN:HB2 | 2:V7:33:ASP:OD1 | 2.21 | 0.40 |
| 1:V8:101:TRP:HE3 | 1:V8:403:MET:HE1 | 1.87 | 0.40 |
| 1:W0:186:THR:HG22 | 1:W0:411:ALA:HB1 | 2.03 | 0.40 |
| 2:W1:34:GLY:O | 2:W1:60:LYS:HA | 2.21 | 0.40 |
| 2:W3:76:ASP:HA | 2:W3:79:ARG:HB2 | 2.03 | 0.40 |
| 1:W4:228:LEU:HD23 | 1:W4:228:LEU:HA | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:W5:4:VAL:HG23 | 2:W5:134:GLY:O | 2.21 | 0.40 |
| 1:W8:97:ALA:HA | 1:W8:103:LYS:HE3 | 2.03 | 0.40 |
| 1:X0:175:VAL:HG23 | 1:X0:175:VAL:O | 2.21 | 0.40 |
| 1:X2:61:PRO:HG2 | 1:X2:85:PHE:CE1 | 2.56 | 0.40 |
| 1:X2:100:ASN:HB3 | 1:X2:103:LYS:HB2 | 2.02 | 0.40 |
| 2:X3:195:LEU:HD12 | 2:X3:196:GLU:HB3 | 2.03 | 0.40 |
| 1:X4:50:TYR:CE2 | 1:X4:241:ARG:HD3 | 2.55 | 0.40 |
| 2:X5:116:ASP:O | 2:X5:119:LEU:HG | 2.22 | 0.40 |
| 2:X5:216:SER:OG | 2:X5:217:LEU:N | 2.55 | 0.40 |
| 1:X6:114:ASP:N | 1:X6:114:ASP:OD1 | 2.53 | 0.40 |
| 2:X7:119:LEU:HA | 2:X7:122:ILE:HG22 | 2.03 | 0.40 |
| 2:X7:246:GLY:HA2 | 2:X7:357:TYR:CD2 | 2.56 | 0.40 |
| 1:X8:8:GLN:CD | 1:X8:17:GLY:HA3 | 2.42 | 0.40 |
| 1:Y0:95:THR:OG1 | 1:Y0:96:GLY:N | 2.54 | 0.40 |
| 1:Y0:156:ARG:HA | 1:Y0:156:ARG:HD2 | 1.93 | 0.40 |
| 1:Y0:257:LEU:HD23 | 1:Y0:312:THR:HG23 | 2.03 | 0.40 |
| 1:Y0:266:PHE:CE1 | 1:Y0:370:ASN:HB2 | 2.56 | 0.40 |
| 2:Y3:17:GLY:HA2 | 2:Y3:20:CYS:HB3 | 2.03 | 0.40 |
| 2:Y3:312:TYR:HB2 | 2:Y3:343:PHE:CD1 | 2.55 | 0.40 |
| 2:Y5:3:GLU:O | 2:Y5:133:GLN:N | 2.39 | 0.40 |
| 2:Y5:406:HIS:HA | 2:Y5:409:VAL:CG1 | 2.49 | 0.40 |
| 1:Y8:100:ASN:HB3 | 1:Y8:103:LYS:HB2 | 2.03 | 0.40 |
| 1:Z2:174:LYS:HE2 | 1:Z2:174:LYS:HB3 | 1.81 | 0.40 |
| 1:Z2:396:HIS:HE1 | 1:Z2:397:TRP:CZ2 | 2.40 | 0.40 |
| 2:Z3:181:VAL:HG22 | 1:Z4:256:ASN:ND2 | 2.29 | 0.40 |
| 1:Z6:65:LEU:HD21 | 1:Z6:76:VAL:HG11 | 2.03 | 0.40 |
| 2:Z9:359:PRO:HA | 2:Z9:360:PRO:HD3 | 1.93 | 0.40 |
| 1:0A:177:ASP:O | 2:0B:352:LYS:HA | 2.20 | 0.40 |
| 1:0A:183:TYR:O | 1:0A:187:LEU:HD13 | 2.21 | 0.40 |
| 2:0H:30:ILE:HG12 | 2:0H:36:MET:HG2 | 2.03 | 0.40 |
| 2:0H:175:PRO:HB3 | 2:0H:390:ARG:HE | 1.84 | 0.40 |
| 2:0H:203:MET:HE1 | 2:0H:384:ILE:HD13 | 2.02 | 0.40 |
| 2:0J:117:LEU:HD13 | 2:0J:117:LEU:HA | 1.97 | 0.40 |
| 2:0J:181:VAL:CG2 | 1:0K:256:ASN:HD22 | 2.34 | 0.40 |
| 1:0K:209:ASP:OD1 | 1:0K:210:ILE:N | 2.54 | 0.40 |
| 2:0L:111:GLY:HA2 | 2:0L:114:ILE:HG22 | 2.04 | 0.40 |
| 2:0L:320:ARG:O | 2:0L:373:ARG:HA | 2.21 | 0.40 |
| 1:0M:16:ILE:HG21 | 1:0M:136:CYS:SG | 2.61 | 0.40 |
| 2:0N:65:CYS:SG | 2:0N:87:PHE:HE1 | 2.45 | 0.40 |
| 2:0R:188:VAL:HG21 | 2:0R:395:PHE:CE1 | 2.57 | 0.40 |
| 1:0S:217:LEU:HD23 | 1:0S:217:LEU:HA | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0S:285:THR:OG1 | 1:0S:287:PRO:HD2 | 2.20 | 0.40 |
| 1:0W:256:ASN:HD22 | 1:0W:350:LYS:HG2 | 1.85 | 0.40 |
| 1:0W:421:GLU:HA | 1:0W:424:GLN:HB3 | 2.03 | 0.40 |
| 2:0X:302:MET:N | 2:0X:302:MET:SD | 2.94 | 0.40 |
| 1:0Y:185:ALA:O | 1:0Y:189:VAL:HG23 | 2.21 | 0.40 |
| 1:0Y:361:LEU:HD23 | 1:0Y:362:LYS:H | 1.86 | 0.40 |
| 1:1A:190:HIS:O | 1:1A:193:VAL:HG22 | 2.21 | 0.40 |
| 1:1A:401:GLU:N | 1:1A:401:GLU:OE1 | 2.54 | 0.40 |
| 1:1A:418:LEU:O | 1:1A:422:TYR:HD2 | 2.04 | 0.40 |
| 1:1C:165:LEU:HD23 | 1:1C:165:LEU:HA | 1.92 | 0.40 |
| 2:1D:346:TRP:CE3 | 2:1D:347:CYS:HB2 | 2.57 | 0.40 |
| 1:1E:258:ILE:HD11 | 1:1E:266:PHE:CZ | 2.56 | 0.40 |
| 2:1F:36:MET:HA | 2:1F:37:PRO:HD3 | 1.89 | 0.40 |
| 2:1F:76:ASP:O | 2:1F:80:THR:HG22 | 2.20 | 0.40 |
| 2:1F:93:ILE:HD13 | 2:1F:93:ILE:HA | 1.88 | 0.40 |
| 2:1F:246:GLY:HA2 | 2:1F:357:TYR:CD2 | 2.56 | 0.40 |
| 2:1H:21:TRP:CZ2 | 2:1H:65:CYS:HB2 | 2.56 | 0.40 |
| 2:1H:125:LEU:HD23 | 2:1H:125:LEU:HA | 1.95 | 0.40 |
| 1:1K:60:VAL:HG23 | 1:1K:84:ILE:O | 2.21 | 0.40 |
| 2:1N:313:MET:HE2 | 2:1N:313:MET:HB3 | 1.72 | 0.40 |
| 1:1O:58:ARG:HD2 | 1:1O:58:ARG:HA | 1.89 | 0.40 |
| 1:1O:271:THR:OG1 | 1:1O:365:ALA:HB3 | 2.20 | 0.40 |
| 2:1P:133:GLN:HB3 | 2:1P:252:ILE:HG21 | 2.02 | 0.40 |
| 2:1R:278:ALA:CB | 9:4Z:229:LEU:HD21 | 2.51 | 0.40 |
| 1:1S:415:MET:O | 1:1S:419:VAL:HG23 | 2.21 | 0.40 |
| 2:1V:384:ILE:HG13 | 2:1V:385:GLY:N | 2.35 | 0.40 |
| 1:1W:2:ARG:HB3 | 1:1W:131:GLN:HB2 | 2.03 | 0.40 |
| 1:1W:154:LYS:HA | 1:1W:154:LYS:HD3 | 1.85 | 0.40 |
| 2:1X:182:VAL:HG11 | 2:1X:404:PHE:CD1 | 2.56 | 0.40 |
| 2:1X:318:MET:O | 2:1X:375:VAL:HA | 2.21 | 0.40 |
| 1:2A:46:ARG:HD3 | 1:2A:46:ARG:HA | 1.87 | 0.40 |
| 1:2A:283:ALA:O | 1:2A:284:LEU:HD23 | 2.20 | 0.40 |
| 1:2C:183:TYR:O | 1:2C:187:LEU:HD13 | 2.21 | 0.40 |
| 1:2C:272:PRO:HB3 | 1:2C:282:ARG:HH22 | 1.86 | 0.40 |
| 1:2C:385:PHE:HZ | 1:2C:408:PHE:HD1 | 1.69 | 0.40 |
| 1:2E:95:THR:HB | 38:8B:83:ARG:HH11 | 1.82 | 0.40 |
| 1:2E:356:ILE:HD13 | 1:2E:356:ILE:HA | 1.93 | 0.40 |
| 2:2F:402:ARG:HA | 2:2F:402:ARG:HD3 | 1.82 | 0.40 |
| 1:2G:5:VAL:CG2 | 1:2G:133:PHE:HD1 | 2.33 | 0.40 |
| 1:2K:48:ASN:OD1 | 1:2K:48:ASN:N | 2.53 | 0.40 |
| 1:2M:286:VAL:CG2 | 1:2M:287:PRO:HD3 | 2.48 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2N:271:SER:HB3 | 2:2N:301:MET:HG2 | 2.02 | 0.40 |
| 2:2P:181:VAL:HG22 | 1:2Q:256:ASN:HD22 | 1.86 | 0.40 |
| 1:2Q:211:CYS:SG | 1:2Q:217:LEU:HB2 | 2.60 | 0.40 |
| 1:2Q:354:CYS:SG | 1:2Q:355:ASP:N | 2.94 | 0.40 |
| 1:2S:198:GLU:HA | 1:2S:264:HIS:HB2 | 2.04 | 0.40 |
| 1:2S:257:LEU:HA | 1:2S:312:THR:HG21 | 2.02 | 0.40 |
| 2:2V:70:LEU:HD23 | 2:2V:70:LEU:HA | 1.83 | 0.40 |
| 2:2X:32:PRO:O | 2:2X:86:LEU:HB2 | 2.21 | 0.40 |
| 2:2X:90:GLU:HG3 | 2:2X:121:ARG:CZ | 2.51 | 0.40 |
| 1:3C:203:ASP:O | 1:3C:207:LEU:HG | 2.20 | 0.40 |
| 2:3F:290:GLU:HG2 | 2:3F:291:ILE:N | 2.36 | 0.40 |
| 2:3H:290:GLU:HG2 | 2:3H:291:ILE:N | 2.36 | 0.40 |
| 2:3J:254:GLU:HB3 | 2:3J:352:LYS:HE2 | 2.03 | 0.40 |
| 1:3K:249:ASP:O | 1:3K:253:LEU:HG | 2.21 | 0.40 |
| 1:3K:396:HIS:HE1 | 1:3K:397:TRP:CZ2 | 2.38 | 0.40 |
| 1:3M:192:LEU:HD23 | 1:3M:192:LEU:HA | 1.81 | 0.40 |
| 1:3M:211:CYS:HA | 1:3M:215:LEU:HB2 | 2.03 | 0.40 |
| 1:3M:324:LYS:HA | 1:3M:327:ASP:OD2 | 2.20 | 0.40 |
| 1:3O:174:LYS:HB3 | 1:3O:174:LYS:HE2 | 1.75 | 0.40 |
| 2:3P:79:ARG:NH1 | 2:3P:92:LEU:O | 2.54 | 0.40 |
| 1:3Q:77:ARG:NH1 | 3:4H:18:LYS:HB3 | 2.32 | 0.40 |
| 1:3Q:88:ASP:OD2 | 3:4H:262:TYR:HB3 | 2.21 | 0.40 |
| 1:3S:65:LEU:HD12 | 1:3S:90:PHE:CD1 | 2.57 | 0.40 |
| 4:3Y:57:THR:OG1 | 4:3Y:158:ALA:HB2 | 2.21 | 0.40 |
| 3:3Z:9:LEU:HD23 | 3:3Z:9:LEU:HA | 1.88 | 0.40 |
| 4:4G:69:LEU:HD23 | 4:4G:69:LEU:H | 1.87 | 0.40 |
| 6:4O:304:GLU:OE2 | 6:4O:305:ILE:HG13 | 2.21 | 0.40 |
| 6:4O:368:GLN:O | 6:4O:371:LEU:HG | 2.22 | 0.40 |
| 9:4Y:429:ILE:HD11 | 9:4Y:442:MET:HB2 | 2.03 | 0.40 |
| 9:4Z:352:TYR:HB3 | 9:4Z:356:TRP:CZ3 | 2.56 | 0.40 |
| 10:5B:285:MET:O | 10:5B:289:GLU:HG2 | 2.21 | 0.40 |
| 10:5C:133:ARG:HD3 | 10:5C:133:ARG:HA | 1.68 | 0.40 |
| 10:5C:230:ARG:O | 10:5C:233:GLU:HG3 | 2.20 | 0.40 |
| 12:5F:38:PRO:HG2 | 12:5G:380:TRP:NE1 | 2.37 | 0.40 |
| 14:5L:57:ASP:HB3 | 14:5L:76:ILE:O | 2.20 | 0.40 |
| 14:5L:604:THR:CG2 | 14:5L:609:ARG:H | 2.34 | 0.40 |
| 14:5L:616:GLU:O | 14:5L:618:GLY:N | 2.54 | 0.40 |
| 14:5M:230:ASN:OD1 | 14:5M:230:ASN:N | 2.54 | 0.40 |
| 14:5N:57:ASP:HB3 | 14:5N:76:ILE:O | 2.20 | 0.40 |
| 15:5O:12:GLU:OE1 | 15:5O:74:LYS:CG | 2.70 | 0.40 |
| 15:5O:313:ASP:OD1 | 15:5O:313:ASP:N | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5R:66:LYS:HB3 | 17:5R:66:LYS:HE2 | 1.98 | 0.40 |
| 17:5S:141:LYS:HE3 | 17:5S:141:LYS:HB3 | 1.92 | 0.40 |
| 17:5S:196:TYR:HA | 17:5S:199:LEU:HD12 | 2.03 | 0.40 |
| 18:5X:36:ASN:OD1 | 18:5X:84:ARG:NH2 | 2.46 | 0.40 |
| 18:5Y:128:GLN:CD | 18:5Y:128:GLN:H | 2.17 | 0.40 |
| 18:5Z:65:VAL:O | 18:5Z:69:THR:HG22 | 2.21 | 0.40 |
| 18:6A:7:LEU:CD1 | 18:6A:69:THR:HG21 | 2.51 | 0.40 |
| 18:6A:128:GLN:CD | 18:6A:128:GLN:H | 2.17 | 0.40 |
| 19:6E:117:LEU:O | 19:6E:121:LEU:HG | 2.21 | 0.40 |
| 21:6G:188:THR:O | 21:6G:189:MET:HG2 | 2.21 | 0.40 |
| 22:6I:187:MET:HE1 | 22:6I:255:PHE:HB2 | 2.03 | 0.40 |
| 22:6I:203:HIS:CD2 | 22:6I:204:PHE:H | 2.39 | 0.40 |
| 22:6I:314:CYS:SG | 22:6I:321:LEU:HB2 | 2.60 | 0.40 |
| 22:6M:279:LEU:HD23 | 22:6M:329:LEU:HD21 | 2.02 | 0.40 |
| 22:6P:206:ASP:HA | 22:6P:209:ASN:HD21 | 1.85 | 0.40 |
| 22:6P:280:LYS:HA | 22:6P:283:ILE:HG12 | 2.03 | 0.40 |
| 24:6T:480:ASN:ND2 | 24:6T:503:ILE:HD12 | 2.36 | 0.40 |
| 24:6U:24:ASP:N | 24:6U:24:ASP:OD1 | 2.54 | 0.40 |
| 24:6U:135:PRO:HG2 | 24:6U:137:GLN:HE22 | 1.86 | 0.40 |
| 24:6U:156:ASP:OD2 | 24:6U:157:ASP:N | 2.53 | 0.40 |
| 24:6U:288:ASP:OD1 | 24:6U:288:ASP:N | 2.55 | 0.40 |
| 24:6V:469:PHE:HB3 | 24:6V:484:GLU:HB3 | 2.04 | 0.40 |
| 24:6W:106:VAL:HG22 | 24:6W:107:VAL:H | 1.87 | 0.40 |
| 24:6W:496:LYS:HB3 | 24:6W:496:LYS:HE2 | 1.80 | 0.40 |
| 24:6X:329:LYS:HD3 | 24:6X:348:TYR:HA | 2.03 | 0.40 |
| 24:6Y:615:ARG:HG2 | 24:6Y:616:LEU:HD23 | 2.03 | 0.40 |
| 24:7A:25:LYS:O | 24:7A:25:LYS:HD3 | 2.22 | 0.40 |
| 24:7A:96:LEU:O | 24:7A:122:TYR:HA | 2.20 | 0.40 |
| 12:7B:53:HIS:CG | 12:7B:58:ARG:HH21 | 2.39 | 0.40 |
| 27:7G:69:LYS:O | 27:7G:73:GLU:HG3 | 2.21 | 0.40 |
| 29:7J:167:ILE:O | 29:7J:167:ILE:HG23 | 2.21 | 0.40 |
| 34:7R:218:MET:N | 34:7R:218:MET:SD | 2.94 | 0.40 |
| 34:7R:228:LYS:HB2 | 34:7R:228:LYS:HE2 | 1.82 | 0.40 |
| 37:7Y:38:ALA:O | 37:7Y:42:THR:HG23 | 2.21 | 0.40 |
| 37:7Y:142:ARG:O | 37:7Y:143:TYR:HB2 | 2.20 | 0.40 |
| 38:7Z:36:GLU:HG3 | 38:7Z:38:GLU:O | 2.22 | 0.40 |
| 38:8C:234:GLU:CD | 38:8C:234:GLU:H | 2.25 | 0.40 |
| 1:A3:215:LEU:HD11 | 26:7F:136:PHE:CD2 | 2.50 | 0.40 |
| 1:E2:48:ASN:HB2 | 22:6J:181:ASN:HB2 | 2.04 | 0.40 |
| 2:G3:73:THR:HA | 1:G4:46:ARG:HH21 | 1.85 | 0.40 |
| 2:G3:157:LEU:HA | 2:G3:157:LEU:HD23 | 1.83 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G3:205:ASP:OD2 | 2:G3:206:ASN:N | 2.54 | 0.40 |
| 2:G3:329:ASN:O | 2:G3:332:VAL:HG12 | 2.22 | 0.40 |
| 1:G4:8:GLN:CD | 1:G4:17:GLY:HA3 | 2.42 | 0.40 |
| 1:G4:173:PRO:HA | 1:G4:176:SER:HB3 | 2.03 | 0.40 |
| 1:G8:113:ILE:HA | 1:G8:116:VAL:HG22 | 2.02 | 0.40 |
| 2:G9:21:TRP:CD1 | 2:G9:87:PHE:HZ | 2.40 | 0.40 |
| 2:H1:69:ASP:OD2 | 2:H1:71:GLU:N | 2.51 | 0.40 |
| 2:H3:11:GLN:NE2 | 1:H4:247:ASN:OD1 | 2.54 | 0.40 |
| 2:H3:276:ILE:HG22 | 2:H3:281:ALA:HB2 | 2.03 | 0.40 |
| 1:H4:325:GLU:O | 1:H4:329:GLN:HB2 | 2.22 | 0.40 |
| 2:H7:125:LEU:HD23 | 2:H7:125:LEU:HA | 1.87 | 0.40 |
| 2:H9:177:VAL:HG13 | 1:I0:327:ASP:HB3 | 2.04 | 0.40 |
| 2:H9:203:MET:C | 2:H9:204:LEU:HD12 | 2.41 | 0.40 |
| 2:H9:209:ILE:HG21 | 2:H9:227:LEU:HG | 2.03 | 0.40 |
| 1:I0:107:THR:OG1 | 1:I0:401:GLU:OE2 | 2.18 | 0.40 |
| 2:I1:318:MET:O | 2:I1:375:VAL:HA | 2.21 | 0.40 |
| 1:I2:131:GLN:HE21 | 1:I2:250:LEU:HB3 | 1.87 | 0.40 |
| 2:I3:139:ASN:O | 2:I3:170:THR:HA | 2.21 | 0.40 |
| 2:I3:251:ASP:OD1 | 2:I3:252:ILE:N | 2.54 | 0.40 |
| 2:I5:287:SER:N | 2:I5:290:GLU:OE2 | 2.25 | 0.40 |
| 1:I8:48:ASN:N | 1:I8:48:ASN:OD1 | 2.55 | 0.40 |
| 1:I8:334:GLN:HA | 1:I8:341:PHE:CE2 | 2.56 | 0.40 |
| 1:I8:397:TRP:CD2 | 2:I9:256:GLN:NE2 | 2.90 | 0.40 |
| 1:J0:170:VAL:HG21 | 1:J0:377:MET:SD | 2.61 | 0.40 |
| 1:J0:221:THR:HG21 | 5:4L:357:ARG:NH2 | 2.36 | 0.40 |
| 1:J0:286:VAL:HG22 | 1:J0:321:MET:HE3 | 2.02 | 0.40 |
| 1:J2:113:ILE:HA | 1:J2:116:VAL:HG22 | 2.03 | 0.40 |
| 2:J5:8:HIS:NE2 | 2:J5:138:PHE:HD2 | 2.19 | 0.40 |
| 2:J5:384:ILE:HA | 2:J5:387:ILE:HD12 | 2.02 | 0.40 |
| 2:J5:397:LEU:HA | 2:J5:397:LEU:HD23 | 1.85 | 0.40 |
| 2:J5:425:LEU:HA | 2:J5:425:LEU:HD23 | 1.83 | 0.40 |
| 1:J6:178:THR:OG1 | 1:J6:181:GLU:HG3 | 2.20 | 0.40 |
| 2:J9:90:GLU:HG3 | 2:J9:121:ARG:HH12 | 1.86 | 0.40 |
| 2:J9:297:GLU:OE1 | 2:J9:297:GLU:N | 2.46 | 0.40 |
| 2:K1:76:ASP:HA | 2:K1:79:ARG:HB2 | 2.04 | 0.40 |
| 2:K3:170:THR:OG1 | 2:K3:203:MET:SD | 2.79 | 0.40 |
| 2:K3:178:SER:OG | 1:K4:347:ASN:HB3 | 2.21 | 0.40 |
| 2:K7:60:LYS:HD3 | 2:M3:282:TYR:OH | 2.21 | 0.40 |
| 1:L0:68:LEU:HD23 | 1:L0:68:LEU:HA | 1.93 | 0.40 |
| 1:L2:6:HIS:CE1 | 1:L2:8:GLN:HG2 | 2.56 | 0.40 |
| 1:L2:189:VAL:HA | 1:L2:192:LEU:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L4:350:LYS:HZ3 | 1:L4:351:SER:C | 2.23 | 0.40 |
| 1:L6:31:ASP:OD1 | 1:L6:35:THR:N | 2.38 | 0.40 |
| 2:M1:305:CYS:HB3 | 2:M1:387:ILE:HD11 | 2.03 | 0.40 |
| 2:M3:81:GLY:O | 2:M3:84:ARG:HG3 | 2.20 | 0.40 |
| 2:M5:96:LYS:NZ | 2:M5:96:LYS:HB2 | 2.36 | 0.40 |
| 1:M6:325:GLU:O | 1:M6:329:GLN:HB2 | 2.22 | 0.40 |
| 2:M7:101:ASN:ND2 | 2:M7:143:GLY:HA2 | 2.36 | 0.40 |
| 2:M7:285:GLN:NE2 | 30:7K:84:VAL:CG1 | 2.79 | 0.40 |
| 1:M8:203:ASP:OD1 | 1:M8:301:CYS:HA | 2.21 | 0.40 |
| 2:M9:6:SER:O | 2:M9:65:CYS:HA | 2.21 | 0.40 |
| 2:M9:8:HIS:CD2 | 2:M9:17:GLY:HA3 | 2.56 | 0.40 |
| 2:N1:51:THR:HG21 | 2:N1:243:ARG:HG2 | 2.03 | 0.40 |
| 2:N1:156:ARG:HA | 2:N1:159:VAL:HG12 | 2.03 | 0.40 |
| 1:N6:45:GLU:H | 1:N6:45:GLU:HG2 | 1.73 | 0.40 |
| 1:N6:250:LEU:H | 1:N6:250:LEU:HD12 | 1.86 | 0.40 |
| 2:O1:258:ASN:C | 2:O1:259:LEU:HD12 | 2.40 | 0.40 |
| 2:O1:371:VAL:HG22 | 2:O1:373:ARG:H | 1.86 | 0.40 |
| 1:O2:20:PHE:HB2 | 1:O2:233:MET:HE3 | 2.03 | 0.40 |
| 1:O4:362:LYS:HB2 | 19:6E:76:ALA:O | 2.21 | 0.40 |
| 2:O7:3:GLU:HG2 | 2:O7:64:ARG:NH1 | 2.36 | 0.40 |
| 2:P3:407:TRP:CD1 | 1:P4:255:VAL:HG23 | 2.56 | 0.40 |
| 1:P4:4:ILE:HB | 1:P4:50:TYR:CE1 | 2.55 | 0.40 |
| 2:P5:165:SER:HA | 2:P5:199:ASP:OD2 | 2.21 | 0.40 |
| 1:P6:272:PRO:O | 1:P6:273:LEU:HD23 | 2.21 | 0.40 |
| 2:P9:279:GLU:N | 2:P9:279:GLU:OE1 | 2.54 | 0.40 |
| 1:Q4:221:THR:OG1 | 1:Q4:222:PHE:N | 2.55 | 0.40 |
| 1:R0:406:MET:O | 1:R0:410:GLU:HG2 | 2.22 | 0.40 |
| 2:R1:9:ILE:HD13 | 2:R1:150:GLY:HA2 | 2.03 | 0.40 |
| 2:R1:66:ILE:HD12 | 2:R1:68:LEU:HD23 | 2.02 | 0.40 |
| 2:R1:249:ASN:O | 7:4R:3:ARG:NH1 | 2.55 | 0.40 |
| 1:R4:117:LEU:HD11 | 1:R4:154:LYS:HB3 | 2.02 | 0.40 |
| 1:S2:387:ALA:HA | 1:S2:390:ARG:HH21 | 1.87 | 0.40 |
| 1:S4:21:TRP:CZ3 | 1:S4:61:PRO:HB3 | 2.56 | 0.40 |
| 1:S6:45:GLU:H | 1:S6:45:GLU:HG2 | 1.70 | 0.40 |
| 1:T0:263:LEU:HA | 1:T0:422:TYR:OH | 2.22 | 0.40 |
| 2:T1:114:ILE:HD12 | 2:T1:114:ILE:HA | 1.89 | 0.40 |
| 1:T2:112:LEU:HD12 | 1:T2:112:LEU:HA | 1.84 | 0.40 |
| 1:T4:215:LEU:HD23 | 1:T4:217:LEU:HD11 | 2.03 | 0.40 |
| 1:T4:273:LEU:H | 1:T4:292:GLN:NE2 | 2.20 | 0.40 |
| 1:T6:67:ASP:N | 1:T6:67:ASP:OD1 | 2.53 | 0.40 |
| 2:T7:401:LYS:HB3 | 2:T7:401:LYS:HE3 | 1.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T8:49:VAL:HG11 | 1:T8:241:ARG:HG2 | 2.03 | 0.40 |
| 2:U1:96:LYS:HD2 | 1:U2:129:CYS:SG | 2.61 | 0.40 |
| 1:U4:23:VAL:HG21 | 1:U4:230:SER:OG | 2.21 | 0.40 |
| 2:U5:312:TYR:HB2 | 2:U5:343:PHE:CD1 | 2.56 | 0.40 |
| 1:U6:207:LEU:HD22 | 1:U6:228:LEU:HD23 | 2.03 | 0.40 |
| 1:U6:418:LEU:O | 1:U6:421:GLU:HG2 | 2.21 | 0.40 |
| 1:U8:293:MET:HE2 | 1:U8:293:MET:HB3 | 1.90 | 0.40 |
| 2:U9:32:PRO:HB3 | 2:U9:83:TYR:CE1 | 2.56 | 0.40 |
| 2:U9:108:TYR:O | 2:U9:112:LYS:HG2 | 2.22 | 0.40 |
| 2:V1:102:ASN:HB3 | 2:V1:105:ARG:HB3 | 2.04 | 0.40 |
| 1:V2:117:LEU:HA | 1:V2:117:LEU:HD23 | 1.83 | 0.40 |
| 1:V2:211:CYS:HA | 1:V2:215:LEU:HB2 | 2.03 | 0.40 |
| 1:V4:31:ASP:OD1 | 1:V4:35:THR:N | 2.45 | 0.40 |
| 1:V6:91:VAL:HG21 | 1:V6:119:VAL:HG21 | 2.03 | 0.40 |
| 1:V6:151:LEU:O | 1:V6:155:ILE:HG12 | 2.22 | 0.40 |
| 2:V7:51:THR:HG21 | 2:V7:243:ARG:HG2 | 2.02 | 0.40 |
| 2:V7:271:SER:OG | 2:V7:377:MET:HB3 | 2.21 | 0.40 |
| 2:W1:14:ILE:HD11 | 2:W1:74:VAL:HG13 | 2.02 | 0.40 |
| 2:W3:139:ASN:O | 2:W3:170:THR:HA | 2.22 | 0.40 |
| 2:W3:222:PRO:CD | 1:W4:324:LYS:HE3 | 2.51 | 0.40 |
| 2:W3:224:TYR:CE2 | 1:W4:323:THR:HG21 | 2.56 | 0.40 |
| 2:W3:248:LEU:HD22 | 2:W3:354:GLY:HA2 | 2.03 | 0.40 |
| 1:W6:203:ASP:OD2 | 1:W6:302:ALA:N | 2.55 | 0.40 |
| 1:W6:405:GLU:HA | 1:W6:408:PHE:HD2 | 1.85 | 0.40 |
| 2:W7:242:LEU:HD11 | 2:W7:252:ILE:HG12 | 2.02 | 0.40 |
| 1:X0:192:LEU:HD23 | 1:X0:192:LEU:HA | 1.85 | 0.40 |
| 1:X2:125:GLU:OE2 | 1:X2:159:TYR:OH | 2.28 | 0.40 |
| 1:X2:257:LEU:HG | 1:X2:370:ASN:HB2 | 2.04 | 0.40 |
| 1:X4:135:VAL:HG11 | 1:X4:152:ILE:HD11 | 2.03 | 0.40 |
| 1:X4:155:ILE:HD12 | 1:X4:155:ILE:HA | 1.84 | 0.40 |
| 1:X4:171:PRO:HG3 | 1:X4:181:GLU:HB3 | 2.02 | 0.40 |
| 2:X5:324:VAL:HG23 | 2:X5:327:ASP:OD2 | 2.21 | 0.40 |
| 1:X6:21:TRP:HA | 1:X6:24:VAL:HG22 | 2.03 | 0.40 |
| 1:X6:396:HIS:HA | 1:X6:399:THR:CG2 | 2.47 | 0.40 |
| 2:X7:5:ILE:HD11 | 2:X7:135:PHE:HE1 | 1.86 | 0.40 |
| 2:X7:417:GLU:HA | 2:X7:420:GLU:CG | 2.50 | 0.40 |
| 2:X9:319:TYR:HB3 | 2:X9:323:VAL:HG21 | 2.03 | 0.40 |
| 1:Y0:183:TYR:O | 1:Y0:187:LEU:HD13 | 2.21 | 0.40 |
| 2:Y1:107:HIS:NE2 | 2:Y1:152:LEU:HD13 | 2.36 | 0.40 |
| 2:Y1:201:ALA:O | 2:Y1:268:MET:HE2 | 2.22 | 0.40 |
| 2:Y1:315:CYS:HG | 2:Y1:379:SER:HG | 1.65 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Y3:26:LEU:HD21 | 2:Y3:363:VAL:HG22 | 2.03 | 0.40 |
| 2:Y3:72:PRO:HD2 | 1:Y4:2:ARG:HH12 | 1.87 | 0.40 |
| 2:Y3:189:LEU:HD11 | 2:Y3:418:PHE:HE1 | 1.86 | 0.40 |
| 1:Y4:152:ILE:HD12 | 1:Y4:164:MET:SD | 2.61 | 0.40 |
| 1:Y4:322:SER:OG | 1:Y4:322:SER:O | 2.39 | 0.40 |
| 1:Y6:170:VAL:HG22 | 1:Y6:202:LEU:O | 2.21 | 0.40 |
| 1:Y6:232:VAL:HG22 | 1:Y6:270:PHE:HB2 | 2.04 | 0.40 |
| 1:Y8:151:LEU:HD13 | 1:Y8:151:LEU:HA | 1.92 | 0.40 |
| 1:Y8:311:LEU:HD22 | 1:Y8:370:ASN:ND2 | 2.37 | 0.40 |
| 2:Y9:290:GLU:HA | 2:Y9:293:ASN:OD1 | 2.21 | 0.40 |
| 1:Z0:235:GLY:O | 1:Z0:316:LEU:HD23 | 2.21 | 0.40 |
| 1:Z2:19:LYS:HG3 | 1:Z2:226:ASN:HB3 | 2.01 | 0.40 |
| 1:Z2:46:ARG:HD3 | 1:Z2:46:ARG:HA | 1.76 | 0.40 |
| 1:Z2:128:ASP:N | 1:Z2:128:ASP:OD1 | 2.52 | 0.40 |
| 1:Z4:263:LEU:HD11 | 1:Z4:425:TYR:CE2 | 2.56 | 0.40 |
| 2:Z5:121:ARG:NE | 2:Z5:124:LYS:HE3 | 2.35 | 0.40 |
| 1:Z6:174:LYS:HB3 | 1:Z6:174:LYS:HE2 | 1.83 | 0.40 |
| 1:0A:2:ARG:NE | 1:0A:240:LEU:HD22 | 2.34 | 0.40 |
| 1:0A:248:ALA:HA | 1:0A:252:LYS:HD2 | 2.02 | 0.40 |
| 2:0B:248:LEU:HD23 | 2:0B:248:LEU:HA | 1.83 | 0.40 |
| 2:0H:221:ARG:HB3 | 1:0I:322:SER:OG | 2.21 | 0.40 |
| 1:0I:105:HIS:CD2 | 1:0I:150:LEU:HG | 2.56 | 0.40 |
| 1:0I:161:ASP:HB3 | 1:0I:162:ARG:NH1 | 2.37 | 0.40 |
| 1:0I:414:ASN:HA | 1:0I:417:ASP:OD2 | 2.21 | 0.40 |
| 2:0J:252:ILE:HD12 | 2:0J:252:ILE:HA | 1.91 | 0.40 |
| 2:0J:257:THR:OG1 | 2:0J:258:ASN:N | 2.55 | 0.40 |
| 1:0K:20:PHE:HA | 1:0K:230:SER:OG | 2.21 | 0.40 |
| 2:0L:9:ILE:HG13 | 2:0L:68:LEU:HD11 | 2.04 | 0.40 |
| 1:0M:14:ASN:HD22 | 1:0M:65:LEU:HD22 | 1.87 | 0.40 |
| 1:0M:170:VAL:HG22 | 1:0M:202:LEU:O | 2.20 | 0.40 |
| 2:0N:320:ARG:O | 2:0N:373:ARG:HA | 2.21 | 0.40 |
| 1:0O:58:ARG:HD2 | 1:0O:58:ARG:HA | 1.87 | 0.40 |
| 1:0Q:19:LYS:HG3 | 1:0Q:226:ASN:HB2 | 2.03 | 0.40 |
| 1:0Q:21:TRP:CH2 | 1:0Q:61:PRO:HB3 | 2.56 | 0.40 |
| 2:0R:72:PRO:HG3 | 1:0S:1:MET:HG2 | 2.04 | 0.40 |
| 2:0R:330:ALA:O | 2:0R:334:THR:HG23 | 2.22 | 0.40 |
| 1:0S:199:CYS:SG | 1:0S:265:PHE:HD1 | 2.44 | 0.40 |
| 2:0X:9:ILE:HG23 | 2:0X:68:LEU:HD11 | 2.03 | 0.40 |
| 2:0X:53:PHE:HA | 2:0X:62:VAL:O | 2.22 | 0.40 |
| 2:0Z:4:VAL:HG13 | 2:0Z:52:PHE:HE1 | 1.86 | 0.40 |
| 2:0Z:102:ASN:OD1 | 1:1A:255:VAL:HG21 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1E:329:GLN:O | 1:1E:333:VAL:HG22 | 2.22 | 0.40 |
| 2:1F:195:LEU:HD23 | 2:1F:196:GLU:HB3 | 2.03 | 0.40 |
| 2:1H:4:VAL:HG23 | 2:1H:134:GLY:O | 2.20 | 0.40 |
| 2:1H:362:VAL:HG12 | 2:1H:370:LYS:NZ | 2.37 | 0.40 |
| 2:1L:331:SER:O | 2:1L:335:ILE:HD12 | 2.21 | 0.40 |
| 1:1M:337:ASN:HB3 | 1:1M:340:TYR:HD2 | 1.85 | 0.40 |
| 2:1N:56:THR:HG23 | 2:1N:60:LYS:CB | 2.51 | 0.40 |
| 2:1N:171:VAL:HA | 2:1N:204:LEU:O | 2.20 | 0.40 |
| 2:1N:251:ASP:OD1 | 2:1N:252:ILE:N | 2.52 | 0.40 |
| 2:1N:313:MET:HB2 | 2:1N:380:ASN:HB3 | 2.04 | 0.40 |
| 2:1N:366:GLY:O | 9:4Z:121:LYS:NZ | 2.50 | 0.40 |
| 1:1O:213:ARG:HB3 | 1:1O:297:LYS:HZ2 | 1.85 | 0.40 |
| 2:1P:90:GLU:HB3 | 2:1P:121:ARG:HH22 | 1.86 | 0.40 |
| 2:1P:188:VAL:O | 2:1P:191:THR:HG22 | 2.21 | 0.40 |
| 2:1P:405:VAL:O | 2:1P:409:VAL:HG23 | 2.21 | 0.40 |
| 2:1R:119:LEU:O | 2:1R:122:ILE:HG12 | 2.22 | 0.40 |
| 2:1T:430:LYS:O | 2:1T:433:GLU:HG3 | 2.21 | 0.40 |
| 2:1V:322:ASP:HB3 | 2:1V:373:ARG:HH21 | 1.84 | 0.40 |
| 2:1X:138:PHE:CZ | 2:1X:235:ILE:HG13 | 2.56 | 0.40 |
| 2:1Z:262:TYR:CD1 | 2:1Z:265:ILE:HG13 | 2.56 | 0.40 |
| 1:2A:55:THR:HG23 | 1:2Q:282:ARG:O | 2.20 | 0.40 |
| 1:2A:174:LYS:HE2 | 1:2A:174:LYS:HB3 | 1.79 | 0.40 |
| 1:2C:165:LEU:HD23 | 1:2C:165:LEU:HA | 1.86 | 0.40 |
| 1:2C:283:ALA:HB3 | 1:2C:288:GLU:OE2 | 2.21 | 0.40 |
| 1:2E:77:ARG:HE | 1:2E:90:PHE:HE2 | 1.69 | 0.40 |
| 1:2E:152:ILE:HD13 | 1:2E:152:ILE:HA | 1.91 | 0.40 |
| 2:2F:240:ALA:HB1 | 2:2F:356:ASN:HD22 | 1.85 | 0.40 |
| 2:2H:75:VAL:HG11 | 2:2H:94:SER:HB3 | 2.04 | 0.40 |
| 2:2H:261:PRO:HG3 | 2:2H:313:MET:HE2 | 2.04 | 0.40 |
| 2:2J:21:TRP:CZ2 | 2:2J:65:CYS:HB3 | 2.57 | 0.40 |
| 2:2L:113:GLU:HG3 | 38:8C:8:GLU:OE1 | 2.20 | 0.40 |
| 2:2L:201:ALA:H | 2:2L:268:MET:HE1 | 1.85 | 0.40 |
| 2:2N:20:CYS:SG | 2:2N:235:ILE:HD11 | 2.61 | 0.40 |
| 2:2R:273:ALA:HA | 2:2R:274:PRO:HA | 1.84 | 0.40 |
| 1:2U:304:ASP:OD1 | 38:8B:103:SER:HB2 | 2.21 | 0.40 |
| 2:2X:4:VAL:HG23 | 2:2X:134:GLY:O | 2.22 | 0.40 |
| 2:2X:90:GLU:HB3 | 2:3N:283:HIS:CE1 | 2.55 | 0.40 |
| 1:2Y:138:SER:O | 1:2Y:139:LEU:HD23 | 2.21 | 0.40 |
| 2:2Z:3:GLU:HB2 | 2:2Z:129:CYS:SG | 2.61 | 0.40 |
| 2:2Z:399:TYR:OH | 2:2Z:415:GLU:OE2 | 2.38 | 0.40 |
| 1:3A:7:ILE:HB | 1:3A:135:VAL:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3C:7:ILE:O | 1:3C:135:VAL:HA | 2.21 | 0.40 |
| 2:3D:203:MET:HE1 | 2:3D:387:ILE:HG21 | 2.02 | 0.40 |
| 2:3F:246:GLY:H | 2:3F:249:ASN:HD21 | 1.69 | 0.40 |
| 2:3H:204:LEU:HD23 | 2:3H:231:ILE:HD12 | 2.03 | 0.40 |
| 1:3I:273:LEU:H | 1:3I:292:GLN:NE2 | 2.20 | 0.40 |
| 1:3K:179:VAL:HG13 | 2:3L:349:THR:O | 2.21 | 0.40 |
| 1:3M:265:PHE:HD2 | 1:3M:422:TYR:OH | 2.02 | 0.40 |
| 1:3O:198:GLU:HB3 | 1:3O:258:ILE:HD11 | 2.04 | 0.40 |
| 1:3O:404:ASP:HB3 | 1:3O:406:MET:SD | 2.61 | 0.40 |
| 2:3P:278:ALA:HA | 2:3P:369:ALA:HB2 | 2.04 | 0.40 |
| 2:3R:188:VAL:HA | 2:3R:191:THR:HG22 | 2.04 | 0.40 |
| 2:3R:195:LEU:HA | 2:3R:195:LEU:HD12 | 1.80 | 0.40 |
| 1:3S:262:ARG:NH2 | 1:3S:417:ASP:OD1 | 2.54 | 0.40 |
| 2:3T:311:LYS:NZ | 2:3T:343:PHE:O | 2.51 | 0.40 |
| 3:3X:218:LEU:HA | 3:3X:218:LEU:HD23 | 1.84 | 0.40 |
| 4:3Y:14:LEU:HB2 | 4:3Y:25:TRP:NE1 | 2.36 | 0.40 |
| 4:3Y:69:LEU:HD23 | 4:3Y:69:LEU:H | 1.87 | 0.40 |
| 4:3Y:86:TYR:HB3 | 4:3Y:108:TYR:CD2 | 2.56 | 0.40 |
| 4:4C:57:THR:OG1 | 4:4C:158:ALA:HB2 | 2.21 | 0.40 |
| 3:4D:111:LYS:HE2 | 3:4D:111:LYS:HB2 | 1.81 | 0.40 |
| 4:4I:23:GLU:HG3 | 4:4I:24:ILE:HG23 | 2.02 | 0.40 |
| 4:4I:69:LEU:HD23 | 4:4I:69:LEU:H | 1.87 | 0.40 |
| 5:4L:326:GLU:HB2 | 5:4L:327:LYS:HZ3 | 1.85 | 0.40 |
| 6:4O:333:MET:O | 6:4O:337:GLU:HG2 | 2.22 | 0.40 |
| 7:4R:112:MET:CG | 7:4R:113:PRO:CD | 2.89 | 0.40 |
| 8:4W:229:GLU:CG | 8:4W:233:LYS:HE2 | 2.51 | 0.40 |
| 8:4W:249:ALA:HA | 8:4W:252:LYS:CE | 2.50 | 0.40 |
| 8:4W:446:SER:N | 8:4W:449:GLU:OE1 | 2.48 | 0.40 |
| 8:4W:466:ARG:N | 8:4W:466:ARG:CD | 2.85 | 0.40 |
| 9:4Z:47:ARG:O | 9:4Z:51:GLU:HG2 | 2.21 | 0.40 |
| 10:5C:172:GLN:HE21 | 10:5C:176:GLU:HG3 | 1.81 | 0.40 |
| 11:5E:176:VAL:HA | 11:5E:181:TRP:CD1 | 2.57 | 0.40 |
| 11:5E:243:LYS:HD3 | 11:5E:243:LYS:HA | 1.74 | 0.40 |
| 12:5F:334:LEU:HB2 | 12:7B:47:GLN:HG3 | 2.02 | 0.40 |
| 12:5G:254:GLN:NE2 | 12:5G:255:LEU:O | 2.55 | 0.40 |
| 13:5J:91:LYS:HD3 | 17:5U:124:GLU:OE1 | 2.21 | 0.40 |
| 13:5K:76:THR:HA | 13:5K:79:THR:HG22 | 2.04 | 0.40 |
| 14:5L:165:THR:HG21 | 14:5L:200:VAL:HG11 | 2.02 | 0.40 |
| 14:5L:246:CYS:SG | 14:5L:247:GLU:N | 2.94 | 0.40 |
| 14:5L:277:LYS:HE2 | 14:5L:277:LYS:HB2 | 1.90 | 0.40 |
| 14:5L:459:GLN:OE1 | 14:5L:459:GLN:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:5M:246:CYS:SG | 14:5M:247:GLU:N | 2.94 | 0.40 |
| 14:5M:366:LEU:HD13 | 14:5M:366:LEU:HA | 1.82 | 0.40 |
| 14:5M:485:VAL:HA | 14:5M:494:ILE:O | 2.21 | 0.40 |
| 14:5M:616:GLU:O | 14:5M:618:GLY:N | 2.54 | 0.40 |
| 14:5N:165:THR:HG21 | 14:5N:200:VAL:HG11 | 2.02 | 0.40 |
| 14:5N:246:CYS:SG | 14:5N:247:GLU:N | 2.94 | 0.40 |
| 14:5N:454:ILE:O | 14:5N:454:ILE:HG13 | 2.21 | 0.40 |
| 14:5N:485:VAL:HA | 14:5N:494:ILE:O | 2.21 | 0.40 |
| 14:5N:604:THR:CG2 | 14:5N:609:ARG:H | 2.34 | 0.40 |
| 15:5O:123:LEU:O | 15:5O:269:GLY:HA2 | 2.21 | 0.40 |
| 15:5O:172:TRP:NE1 | 15:5O:207:GLY:HA3 | 2.36 | 0.40 |
| 15:5O:261:GLU:O | 15:5O:314:ARG:NH1 | 2.53 | 0.40 |
| 15:5P:241:LEU:HB2 | 15:5P:357:HIS:HB3 | 2.03 | 0.40 |
| 17:5T:141:LYS:HE3 | 17:5T:141:LYS:HB3 | 1.92 | 0.40 |
| 17:5U:18:GLN:H | 17:5U:18:GLN:HG3 | 1.68 | 0.40 |
| 17:5U:141:LYS:HE3 | 17:5U:141:LYS:HB3 | 1.92 | 0.40 |
| 17:5U:196:TYR:HA | 17:5U:199:LEU:HD12 | 2.03 | 0.40 |
| 18:5X:7:LEU:CD1 | 18:5X:69:THR:HG21 | 2.52 | 0.40 |
| 18:5Y:7:LEU:CD1 | 18:5Y:69:THR:HG21 | 2.51 | 0.40 |
| 18:5Z:7:LEU:CD1 | 18:5Z:69:THR:HG21 | 2.52 | 0.40 |
| 18:6B:7:LEU:CD1 | 18:6B:69:THR:HG21 | 2.51 | 0.40 |
| 18:6B:198:LEU:HD13 | 18:6B:198:LEU:HA | 1.79 | 0.40 |
| 21:6G:159:ALA:O | 21:6G:163:THR:HG23 | 2.21 | 0.40 |
| 21:6H:56:LYS:HZ2 | 21:6H:92:HIS:CE1 | 2.40 | 0.40 |
| 22:6M:177:LEU:HB3 | 22:6M:187:MET:HE1 | 2.02 | 0.40 |
| 22:6M:295:LYS:O | 22:6M:295:LYS:HD2 | 2.22 | 0.40 |
| 22:6N:70:ASN:HB2 | 22:6N:73:ASN:HD21 | 1.85 | 0.40 |
| 22:6N:78:GLN:OE1 | 22:6N:79:PRO:HD2 | 2.21 | 0.40 |
| 22:6O:45:PRO:HB3 | 22:6O:51:ILE:CG2 | 2.51 | 0.40 |
| 23:6Q:2:ASP:O | 23:6Q:6:GLN:HG3 | 2.21 | 0.40 |
| 23:6R:2:ASP:O | 23:6R:6:GLN:HG3 | 2.21 | 0.40 |
| 24:6T:110:ASN:ND2 | 24:6T:213:TYR:OH | 2.54 | 0.40 |
| 24:6U:243:LYS:HE3 | 24:6U:243:LYS:HB3 | 1.60 | 0.40 |
| 24:6U:554:ASP:OD2 | 24:6U:557:VAL:HG13 | 2.21 | 0.40 |
| 24:6W:125:LEU:HD23 | 24:6W:125:LEU:HA | 1.95 | 0.40 |
| 24:6W:512:TYR:CE1 | 24:6W:523:ILE:HG23 | 2.57 | 0.40 |
| 24:6X:256:LEU:HD23 | 24:6X:256:LEU:HA | 1.76 | 0.40 |
| 24:6X:378:TRP:O | 24:6X:382:ASN:ND2 | 2.49 | 0.40 |
| 24:6X:524:GLU:OE2 | 24:6X:527:ASN:N | 2.55 | 0.40 |
| 24:6Z:42:GLU:O | 24:6Z:42:GLU:HG2 | 2.20 | 0.40 |
| 24:6Z:402:LYS:HD2 | 24:6Z:402:LYS:HA | 1.82 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:7I:144:GLN:O | 29:7I:148:VAL:HG23 | 2.21 | 0.40 |
| 30:7K:175:ASP:HB3 | 30:7K:178:THR:OG1 | 2.21 | 0.40 |
| 31:7M:39:LEU:HB3 | 31:7M:43:VAL:HB | 2.02 | 0.40 |
| 34:7S:272:LYS:O | 34:7S:275:GLU:HG2 | 2.21 | 0.40 |
| 36:7V:90:GLU:CD | 36:7V:91:PRO:HD2 | 2.42 | 0.40 |
| 36:7W:90:GLU:CD | 36:7W:91:PRO:HD2 | 2.42 | 0.40 |
| 38:8C:113:ARG:HD2 | 38:8C:113:ARG:HA | 1.92 | 0.40 |
| 2:2:372:GLN:NE2 | 24:6T:88:TRP:CD1 | 2.90 | 0.40 |
| 1:A1:340:TYR:HD1 | 3:4F:104:PRO:HD3 | 1.84 | 0.40 |
| 1:D0:142:GLY:N | 39:D0:501:GDP:O1B | 2.53 | 0.40 |
| 1:D4:219:THR:HG22 | 24:6Y:254:SER:HB3 | 2.04 | 0.40 |
| 2:E5:31:GLN:OE1 | 22:6L:131:ARG:NH1 | 2.31 | 0.40 |
| 2:E5:282:TYR:HE1 | 22:6K:80:GLY:O | 2.01 | 0.40 |
| 2:E9:56:THR:HG23 | 2:G5:285:GLN:HA | 2.02 | 0.40 |
| 2:G1:259:LEU:HB3 | 2:G1:268:MET:HE3 | 2.03 | 0.40 |
| 2:G3:90:GLU:HB3 | 2:G3:121:ARG:NH1 | 2.26 | 0.40 |
| 2:G5:133:GLN:HB3 | 2:G5:252:ILE:HD11 | 2.03 | 0.40 |
| 2:G5:349:THR:O | 2:G5:349:THR:OG1 | 2.39 | 0.40 |
| 1:G6:344:TRP:CE3 | 1:G6:345:ILE:HG13 | 2.57 | 0.40 |
| 2:G7:397:LEU:HD23 | 2:G7:397:LEU:HA | 1.93 | 0.40 |
| 2:G7:402:ARG:HD3 | 2:G7:402:ARG:HA | 1.93 | 0.40 |
| 1:G8:262:ARG:NH2 | 1:G8:417:ASP:OD1 | 2.55 | 0.40 |
| 2:G9:74:VAL:O | 2:G9:78:VAL:HG23 | 2.21 | 0.40 |
| 2:G9:217:LEU:HD23 | 2:G9:217:LEU:HA | 1.80 | 0.40 |
| 2:G9:430:LYS:O | 2:G9:434:GLU:HG3 | 2.22 | 0.40 |
| 2:H1:325:PRO:HA | 2:H1:328:VAL:HG22 | 2.03 | 0.40 |
| 1:H2:414:ASN:HA | 1:H2:417:ASP:OD2 | 2.22 | 0.40 |
| 2:H3:36:MET:HA | 2:H3:37:PRO:HD3 | 1.96 | 0.40 |
| 2:H3:297:GLU:OE1 | 2:H3:297:GLU:N | 2.53 | 0.40 |
| 2:H3:389:SER:N | 2:H3:429:GLU:OE1 | 2.54 | 0.40 |
| 2:H9:79:ARG:O | 2:H9:84:ARG:HG2 | 2.21 | 0.40 |
| 2:I1:402:ARG:HD3 | 2:I1:402:ARG:HA | 1.89 | 0.40 |
| 1:I2:117:LEU:HA | 1:I2:117:LEU:HD23 | 1.83 | 0.40 |
| 2:I3:52:PHE:O | 2:I3:64:ARG:N | 2.46 | 0.40 |
| 2:I3:73:THR:HG23 | 1:I4:2:ARG:HH22 | 1.85 | 0.40 |
| 1:I4:19:LYS:O | 1:I4:23:VAL:HG23 | 2.20 | 0.40 |
| 1:I4:100:ASN:HB3 | 1:I4:103:LYS:HB2 | 2.03 | 0.40 |
| 2:I5:243:ARG:NH1 | 2:I5:244:PHE:HE2 | 2.19 | 0.40 |
| 2:I5:384:ILE:HG23 | 2:I5:432:PHE:CZ | 2.56 | 0.40 |
| 2:I7:402:ARG:HA | 2:I7:402:ARG:HD3 | 1.79 | 0.40 |
| 1:J0:232:VAL:HG22 | 1:J0:270:PHE:HB2 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J1:305:CYS:HB3 | 2:J1:387:ILE:HD11 | 2.03 | 0.40 |
| 2:J1:430:LYS:HA | 2:J1:433:GLU:OE2 | 2.22 | 0.40 |
| 2:J3:145:THR:OG1 | 41:J4:501:GTP:O1B | 2.40 | 0.40 |
| 1:J6:5:VAL:HG22 | 1:J6:133:PHE:CD1 | 2.54 | 0.40 |
| 1:J6:293:MET:HE2 | 1:J6:367:PHE:HD1 | 1.87 | 0.40 |
| 2:J7:7:ILE:HG12 | 2:J7:137:VAL:HG12 | 2.03 | 0.40 |
| 2:J7:90:GLU:CG | 2:J7:121:ARG:HH12 | 2.33 | 0.40 |
| 2:J9:12:ALA:HB2 | 41:K0:501:GTP:C8 | 2.56 | 0.40 |
| 2:J9:90:GLU:O | 2:J9:121:ARG:NH1 | 2.33 | 0.40 |
| 2:K3:327:ASP:OD1 | 2:K3:328:VAL:N | 2.55 | 0.40 |
| 1:K4:224:ASP:OD1 | 1:K4:225:LEU:N | 2.54 | 0.40 |
| 2:K5:213:CYS:HA | 2:K5:217:LEU:HB2 | 2.03 | 0.40 |
| 1:K8:165:LEU:HD23 | 1:K8:165:LEU:HA | 1.95 | 0.40 |
| 2:K9:178:SER:OG | 2:K9:183:GLU:OE2 | 2.30 | 0.40 |
| 1:L0:21:TRP:CZ3 | 1:L0:61:PRO:HB3 | 2.56 | 0.40 |
| 2:L1:176:GLN:OE1 | 2:L1:176:GLN:N | 2.44 | 0.40 |
| 1:L2:237:THR:HG23 | 1:L2:241:ARG:HH21 | 1.85 | 0.40 |
| 2:L5:88:HIS:O | 2:L5:90:GLU:N | 2.54 | 0.40 |
| 1:L6:48:ASN:OD1 | 1:L6:48:ASN:N | 2.55 | 0.40 |
| 1:L6:249:ASP:OD1 | 1:L6:252:LYS:N | 2.49 | 0.40 |
| 2:L9:113:GLU:OE1 | 2:L9:113:GLU:N | 2.54 | 0.40 |
| 1:M0:392:LYS:HD2 | 1:M0:395:LEU:HD22 | 2.03 | 0.40 |
| 1:M2:263:LEU:HD13 | 1:M2:422:TYR:CE1 | 2.56 | 0.40 |
| 2:M3:96:LYS:HG2 | 1:M4:1:MET:HE1 | 2.03 | 0.40 |
| 2:M3:103:PHE:CE1 | 2:M3:148:GLY:HA2 | 2.56 | 0.40 |
| 2:M5:62:VAL:HA | 2:M5:63:PRO:HD3 | 1.93 | 0.40 |
| 2:M5:137:VAL:HG22 | 2:M5:168:GLY:HA2 | 2.03 | 0.40 |
| 2:M5:230:LEU:HD12 | 2:M5:231:ILE:HD13 | 2.03 | 0.40 |
| 2:M5:417:GLU:HA | 2:M5:420:GLU:HG2 | 2.02 | 0.40 |
| 1:M6:199:CYS:HB2 | 1:M6:265:PHE:CD1 | 2.57 | 0.40 |
| 2:M7:279:GLU:O | 2:M7:280:LYS:C | 2.56 | 0.40 |
| 1:M8:77:ARG:HH21 | 1:M8:90:PHE:HD2 | 1.67 | 0.40 |
| 1:M8:345:ILE:HB | 1:M8:348:ASN:HD21 | 1.87 | 0.40 |
| 2:M9:14:ILE:HD11 | 2:M9:74:VAL:CG1 | 2.51 | 0.40 |
| 2:M9:65:CYS:SG | 2:M9:87:PHE:CE1 | 3.14 | 0.40 |
| 1:N0:1:MET:HB3 | 1:N0:2:ARG:H | 1.68 | 0.40 |
| 1:N0:318:ARG:HB3 | 1:N0:357:PRO:HA | 2.02 | 0.40 |
| 2:N1:306:ASP:HB3 | 2:N1:309:HIS:CD2 | 2.57 | 0.40 |
| 1:N2:126:SER:OG | 32:7P:22:ASN:OD1 | 2.38 | 0.40 |
| 1:N2:137:HIS:NE2 | 1:N2:166:THR:OG1 | 2.54 | 0.40 |
| 2:N5:12:ALA:HB2 | 41:N6:501:GTP:C8 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N5:79:ARG:O | 2:N5:84:ARG:HG2 | 2.21 | 0.40 |
| 2:N7:397:LEU:HA | 2:N7:397:LEU:HD23 | 1.85 | 0.40 |
| 1:N8:170:VAL:HG22 | 1:N8:202:LEU:O | 2.22 | 0.40 |
| 1:N8:317:PHE:HB3 | 1:N8:321:MET:HE3 | 2.03 | 0.40 |
| 2:O3:8:HIS:CD2 | 2:O3:138:PHE:HD2 | 2.39 | 0.40 |
| 2:O3:370:LYS:HE3 | 2:O3:370:LYS:HB2 | 1.77 | 0.40 |
| 2:O5:76:ASP:O | 2:O5:80:THR:HG23 | 2.21 | 0.40 |
| 2:O7:111:GLY:HA2 | 2:O7:114:ILE:HG22 | 2.04 | 0.40 |
| 2:O7:242:LEU:HD11 | 2:O7:252:ILE:HG12 | 2.04 | 0.40 |
| 2:O7:262:TYR:CE2 | 2:O7:346:TRP:CH2 | 3.09 | 0.40 |
| 2:P3:210:TYR:CE1 | 2:P3:227:LEU:HD21 | 2.56 | 0.40 |
| 1:P4:361:LEU:HD23 | 1:P4:361:LEU:HA | 1.89 | 0.40 |
| 2:P5:189:LEU:HD11 | 2:P5:418:PHE:CE1 | 2.53 | 0.40 |
| 2:P5:287:SER:N | 2:P5:290:GLU:OE2 | 2.55 | 0.40 |
| 2:P5:361:THR:OG1 | 2:P5:362:VAL:N | 2.55 | 0.40 |
| 1:P6:135:VAL:HG12 | 1:P6:137:HIS:HD2 | 1.87 | 0.40 |
| 1:P6:208:TYR:CE1 | 1:P6:225:LEU:HD11 | 2.56 | 0.40 |
| 2:P9:320:ARG:O | 2:P9:373:ARG:HA | 2.21 | 0.40 |
| 1:Q0:2:ARG:HB3 | 1:Q0:131:GLN:HB2 | 2.04 | 0.40 |
| 1:Q2:49:VAL:HG11 | 1:Q2:241:ARG:HG2 | 2.02 | 0.40 |
| 1:Q2:271:THR:CG2 | 1:Q2:365:ALA:HB3 | 2.52 | 0.40 |
| 2:Q3:206:ASN:OD1 | 41:Q4:501:GTP:N2 | 2.55 | 0.40 |
| 1:Q4:178:THR:OG1 | 1:Q4:181:GLU:HG3 | 2.22 | 0.40 |
| 2:Q5:10:GLY:O | 2:Q5:14:ILE:HD12 | 2.20 | 0.40 |
| 1:Q8:30:ILE:HG22 | 1:Q8:36:TYR:HA | 2.03 | 0.40 |
| 1:Q8:190:HIS:CD2 | 1:Q8:414:ASN:HB2 | 2.56 | 0.40 |
| 1:Q8:286:VAL:HA | 1:Q8:289:LEU:HG | 2.01 | 0.40 |
| 2:Q9:52:PHE:CZ | 2:Q9:239:THR:HG21 | 2.56 | 0.40 |
| 2:Q9:253:THR:O | 2:Q9:256:GLN:HB2 | 2.22 | 0.40 |
| 1:R0:20:PHE:O | 1:R0:23:VAL:HG22 | 2.22 | 0.40 |
| 2:R1:373:ARG:HH22 | 7:4R:28:GLY:HA3 | 1.86 | 0.40 |
| 1:R2:65:LEU:HD13 | 1:R2:90:PHE:CE1 | 2.56 | 0.40 |
| 1:R2:397:TRP:HZ2 | 2:R3:260:VAL:CG2 | 2.34 | 0.40 |
| 2:R3:4:VAL:HG23 | 2:R3:134:GLY:O | 2.21 | 0.40 |
| 1:R4:40:SER:HB3 | 21:6G:93:HIS:CE1 | 2.57 | 0.40 |
| 1:R4:135:VAL:HG22 | 1:R4:137:HIS:HD2 | 1.86 | 0.40 |
| 1:R4:192:LEU:HD23 | 1:R4:192:LEU:HA | 1.86 | 0.40 |
| 1:R4:257:LEU:HD21 | 1:R4:314:SER:HB2 | 2.04 | 0.40 |
| 1:R6:317:PHE:HB3 | 1:R6:321:MET:SD | 2.61 | 0.40 |
| 1:R8:69:GLU:N | 1:R8:69:GLU:OE2 | 2.54 | 0.40 |
| 1:R8:215:LEU:HB3 | 1:R8:217:LEU:HG | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S0:311:LEU:HA | 1:S0:311:LEU:HD23 | 1.76 | 0.40 |
| 2:S7:267:PHE:CB | 2:S7:384:ILE:HG21 | 2.51 | 0.40 |
| 2:S7:319:TYR:CZ | 2:S7:328:VAL:HG23 | 2.56 | 0.40 |
| 2:S9:4:VAL:HG23 | 2:S9:134:GLY:O | 2.21 | 0.40 |
| 2:S9:7:ILE:HG22 | 2:S9:66:ILE:HG12 | 2.03 | 0.40 |
| 2:T1:245:ASP:OD1 | 7:4U:7:GLN:HG2 | 2.21 | 0.40 |
| 1:T2:167:PHE:CZ | 1:T2:233:MET:HG2 | 2.57 | 0.40 |
| 2:T3:7:ILE:HG22 | 2:T3:66:ILE:HG12 | 2.03 | 0.40 |
| 1:T4:306:ARG:NH1 | 13:5J:106:TYR:HB2 | 2.34 | 0.40 |
| 1:T6:405:GLU:HG2 | 13:5K:53:PHE:HZ | 1.85 | 0.40 |
| 2:U3:312:TYR:O | 2:U3:344:VAL:HG13 | 2.21 | 0.40 |
| 1:U4:178:THR:CG2 | 1:U4:181:GLU:HG3 | 2.52 | 0.40 |
| 1:U4:257:LEU:HD21 | 1:U4:314:SER:HB2 | 2.03 | 0.40 |
| 2:U5:273:ALA:HA | 2:U5:274:PRO:HA | 1.89 | 0.40 |
| 1:U6:322:SER:HB3 | 1:U6:325:GLU:HG3 | 2.04 | 0.40 |
| 2:U7:250:VAL:HG23 | 2:U7:254:GLU:HG3 | 2.04 | 0.40 |
| 1:U8:61:PRO:HG2 | 1:U8:85:PHE:CE1 | 2.56 | 0.40 |
| 2:U9:193:SER:HB2 | 2:U9:197:HIS:CE1 | 2.56 | 0.40 |
| 2:U9:313:MET:HA | 2:U9:344:VAL:HG22 | 2.04 | 0.40 |
| 1:V0:116:VAL:O | 1:V0:120:VAL:HG12 | 2.21 | 0.40 |
| 2:V3:296:PHE:HE1 | 2:V3:312:TYR:HE2 | 1.69 | 0.40 |
| 2:V3:335:ILE:HD13 | 2:V3:335:ILE:HA | 1.89 | 0.40 |
| 1:V6:387:ALA:HA | 1:V6:390:ARG:HH21 | 1.85 | 0.40 |
| 2:V7:30:ILE:HD12 | 2:V7:53:PHE:CE2 | 2.56 | 0.40 |
| 2:V7:211:ASP:OD2 | 2:V7:215:ARG:NH1 | 2.54 | 0.40 |
| 2:V9:107:HIS:CD2 | 2:V9:152:LEU:HB2 | 2.56 | 0.40 |
| 2:V9:175:PRO:HG2 | 2:V9:176:GLN:OE1 | 2.21 | 0.40 |
| 1:W2:3:GLU:HB2 | 1:W2:130:LEU:HA | 2.03 | 0.40 |
| 2:W3:122:ILE:HD13 | 2:W3:157:LEU:HD11 | 2.02 | 0.40 |
| 1:W4:31:ASP:OD2 | 1:W4:37:HIS:NE2 | 2.55 | 0.40 |
| 1:W6:246:LEU:HD22 | 1:W6:352:SER:HA | 2.04 | 0.40 |
| 2:W7:224:TYR:CB | 1:W8:245:GLN:HE21 | 2.31 | 0.40 |
| 1:W8:192:LEU:HD23 | 1:W8:192:LEU:HA | 1.80 | 0.40 |
| 2:W9:142:GLY:O | 2:W9:186:ASN:ND2 | 2.55 | 0.40 |
| 2:W9:274:PRO:CB | 2:W9:286:LEU:HD11 | 2.49 | 0.40 |
| 2:W9:274:PRO:HG2 | 2:W9:371:VAL:HG11 | 2.03 | 0.40 |
| 1:X0:121:ARG:NH2 | 1:X0:158:GLU:OE2 | 2.52 | 0.40 |
| 1:X2:19:LYS:HD2 | 1:X2:22:GLU:OE2 | 2.22 | 0.40 |
| 1:X2:203:ASP:N | 1:X2:203:ASP:OD1 | 2.54 | 0.40 |
| 1:X2:396:HIS:CE1 | 1:X2:397:TRP:CE2 | 3.09 | 0.40 |
| 2:X5:237:SER:HA | 2:X5:320:ARG:HH11 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X5:255:PHE:HD1 | 2:X5:259:LEU:CD1 | 2.35 | 0.40 |
| 2:X7:335:ILE:HD12 | 2:X7:335:ILE:HA | 1.97 | 0.40 |
| 1:X8:101:TRP:HB2 | 1:X8:184:ASN:OD1 | 2.22 | 0.40 |
| 1:X8:154:LYS:HA | 1:X8:154:LYS:HD3 | 1.92 | 0.40 |
| 2:Y1:213:CYS:HA | 2:Y1:217:LEU:HB2 | 2.03 | 0.40 |
| 1:Y2:178:THR:HA | 2:Y3:352:LYS:HD2 | 2.04 | 0.40 |
| 2:Y3:335:ILE:HD13 | 2:Y3:335:ILE:HA | 1.90 | 0.40 |
| 2:Y5:271:SER:OG | 2:Y5:300:SER:O | 2.30 | 0.40 |
| 1:Y6:267:MET:H | 1:Y6:267:MET:HG2 | 1.71 | 0.40 |
| 1:Y8:270:PHE:CD2 | 1:Y8:273:LEU:HD21 | 2.56 | 0.40 |
| 2:Y9:338:LYS:HG3 | 2:Y9:340:THR:HG22 | 2.03 | 0.40 |
| 1:Z0:266:PHE:CD1 | 1:Z0:370:ASN:HB2 | 2.55 | 0.40 |
| 2:Z1:177:VAL:HG13 | 1:Z2:327:ASP:OD1 | 2.21 | 0.40 |
| 2:Z3:419:SER:O | 2:Z3:423:GLU:HG2 | 2.21 | 0.40 |
| 1:Z4:152:ILE:HD13 | 1:Z4:152:ILE:HA | 1.86 | 0.40 |
| 2:Z7:4:VAL:HG12 | 2:Z7:133:GLN:HB2 | 2.02 | 0.40 |
| 1:0A:21:TRP:CZ3 | 1:0A:61:PRO:HB3 | 2.57 | 0.40 |
| 1:0A:417:ASP:N | 1:0A:417:ASP:OD1 | 2.54 | 0.40 |
| 2:0B:286:LEU:HD23 | 2:0B:286:LEU:H | 1.85 | 0.40 |
| 2:0B:286:LEU:HG | 2:0B:373:ARG:NH1 | 2.37 | 0.40 |
| 1:0E:174:LYS:HZ1 | 1:0E:380:ARG:HH21 | 1.69 | 0.40 |
| 1:0E:314:SER:HA | 1:0E:350:LYS:O | 2.21 | 0.40 |
| 2:0H:66:ILE:O | 2:0H:66:ILE:HG13 | 2.20 | 0.40 |
| 2:0L:246:GLY:HA3 | 2:0L:356:ASN:HA | 2.03 | 0.40 |
| 1:0M:128:ASP:OD1 | 1:0M:129:CYS:N | 2.50 | 0.40 |
| 1:0M:175:VAL:HG22 | 1:0M:205:GLU:HB2 | 2.04 | 0.40 |
| 1:0M:317:PHE:HE2 | 1:0M:326:VAL:HG13 | 1.86 | 0.40 |
| 2:0P:88:HIS:CE1 | 2:1F:283:HIS:HA | 2.57 | 0.40 |
| 2:0P:174:SER:HB2 | 2:0P:205:ASP:OD1 | 2.22 | 0.40 |
| 2:0P:212:ILE:O | 2:0P:216:SER:OG | 2.26 | 0.40 |
| 1:0Q:203:ASP:OD1 | 1:0Q:301:CYS:HA | 2.21 | 0.40 |
| 2:0R:335:ILE:HD12 | 2:0R:335:ILE:HA | 1.85 | 0.40 |
| 1:0U:203:ASP:OD2 | 1:0U:302:ALA:N | 2.54 | 0.40 |
| 2:0V:93:ILE:HD12 | 2:0V:117:LEU:HD21 | 2.03 | 0.40 |
| 1:0W:99:ASN:ND2 | 2:0X:254:GLU:OE1 | 2.54 | 0.40 |
| 1:0Y:113:ILE:HD12 | 1:0Y:113:ILE:HA | 1.87 | 0.40 |
| 1:0Y:272:PRO:HD3 | 1:0Y:364:SER:HA | 2.02 | 0.40 |
| 2:0Z:286:LEU:HG | 2:0Z:371:VAL:HG23 | 2.02 | 0.40 |
| 1:1A:388:MET:CE | 2:1B:348:PRO:HD2 | 2.51 | 0.40 |
| 1:1C:334:GLN:NE2 | 1:1C:348:ASN:H | 2.14 | 0.40 |
| 2:1H:166:LYS:NZ | 2:1H:199:ASP:OD2 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1L:294:ALA:HA | 2:1L:297:GLU:OE1 | 2.22 | 0.40 |
| 2:1L:394:LYS:HB2 | 1:1M:346:PRO:HG3 | 2.03 | 0.40 |
| 1:1M:58:ARG:HG2 | 1:2C:280:GLN:HE22 | 1.86 | 0.40 |
| 1:1M:208:TYR:OH | 2:1N:325:PRO:HB2 | 2.20 | 0.40 |
| 1:1M:382:SER:HB3 | 1:1M:415:MET:HG2 | 2.03 | 0.40 |
| 1:1O:309:ARG:NH1 | 1:1O:339:SER:O | 2.54 | 0.40 |
| 1:1Q:121:ARG:NH2 | 1:1Q:158:GLU:OE2 | 2.55 | 0.40 |
| 2:1R:9:ILE:HG22 | 2:1R:146:GLY:HA2 | 2.03 | 0.40 |
| 2:1R:62:VAL:O | 2:1R:62:VAL:HG13 | 2.22 | 0.40 |
| 2:1R:331:SER:O | 2:1R:334:THR:N | 2.55 | 0.40 |
| 2:1V:36:MET:HA | 2:1V:37:PRO:HD3 | 1.97 | 0.40 |
| 2:1V:55:GLU:HG2 | 2:1V:61:HIS:ND1 | 2.36 | 0.40 |
| 2:1X:121:ARG:HA | 2:1X:121:ARG:HD2 | 1.82 | 0.40 |
| 1:2A:152:ILE:HG22 | 1:2A:195:ASN:HB3 | 2.02 | 0.40 |
| 1:2A:345:ILE:HB | 1:2A:348:ASN:HD21 | 1.86 | 0.40 |
| 1:2C:162:ARG:HA | 1:2C:162:ARG:HD3 | 1.90 | 0.40 |
| 2:2D:21:TRP:CZ2 | 2:2D:65:CYS:HB3 | 2.56 | 0.40 |
| 1:2E:144:GLY:N | 39:2E:502:GDP:O1B | 2.54 | 0.40 |
| 1:2G:178:THR:OG1 | 1:2G:181:GLU:HG3 | 2.22 | 0.40 |
| 1:2G:293:MET:HB3 | 1:2G:293:MET:HE2 | 1.98 | 0.40 |
| 2:2H:88:HIS:HE1 | 2:2H:121:ARG:NH2 | 2.17 | 0.40 |
| 1:2K:5:VAL:HG12 | 1:2K:133:PHE:CD1 | 2.57 | 0.40 |
| 1:2M:83:GLN:N | 1:2M:83:GLN:OE1 | 2.53 | 0.40 |
| 1:2Q:272:PRO:HD3 | 1:2Q:364:SER:HA | 2.03 | 0.40 |
| 1:2Q:405:GLU:HA | 1:2Q:408:PHE:HD2 | 1.86 | 0.40 |
| 2:2R:108:TYR:O | 2:2R:112:LYS:HG2 | 2.21 | 0.40 |
| 1:2S:414:ASN:HA | 1:2S:417:ASP:OD2 | 2.22 | 0.40 |
| 2:2T:298:PRO:HB3 | 2:2T:307:PRO:HD3 | 2.04 | 0.40 |
| 2:2T:420:GLU:HA | 2:2T:423:GLU:HG3 | 2.02 | 0.40 |
| 2:2V:387:ILE:HG12 | 2:2V:390:ARG:HH22 | 1.85 | 0.40 |
| 1:2W:290:THR:HG23 | 38:8B:54:THR:HG21 | 2.03 | 0.40 |
| 1:2W:317:PHE:HB3 | 1:2W:321:MET:SD | 2.61 | 0.40 |
| 2:2X:139:ASN:O | 2:2X:170:THR:HA | 2.22 | 0.40 |
| 1:2Y:54:ALA:N | 1:2Y:58:ARG:O | 2.49 | 0.40 |
| 1:2Y:203:ASP:OD2 | 1:2Y:302:ALA:N | 2.55 | 0.40 |
| 2:2Z:110:ILE:O | 2:2Z:113:GLU:HG3 | 2.21 | 0.40 |
| 2:2Z:188:VAL:HG21 | 2:2Z:395:PHE:CE1 | 2.57 | 0.40 |
| 2:2Z:235:ILE:O | 2:2Z:239:THR:HG22 | 2.21 | 0.40 |
| 1:3A:386:THR:O | 1:3A:390:ARG:HG3 | 2.21 | 0.40 |
| 2:3B:111:GLY:O | 2:3B:115:VAL:HG23 | 2.21 | 0.40 |
| 2:3B:120:ASP:OD2 | 2:3B:120:ASP:C | 2.59 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:3B:178:SER:OG | 1:3C:347:ASN:HB3 | 2.21 | 0.40 |
| 2:3H:205:ASP:OD1 | 2:3H:206:ASN:N | 2.47 | 0.40 |
| 2:3L:130:THR:HG23 | 2:3L:131:GLY:N | 2.37 | 0.40 |
| 2:3N:174:SER:HB3 | 2:3N:177:VAL:O | 2.20 | 0.40 |
| 2:3N:367:ASP:OD2 | 2:3N:367:ASP:N | 2.53 | 0.40 |
| 1:3Q:3:GLU:HB2 | 1:3Q:130:LEU:HA | 2.03 | 0.40 |
| 2:3R:268:MET:HA | 2:3R:379:SER:O | 2.21 | 0.40 |
| 2:3T:335:ILE:O | 2:3T:338:LYS:HB2 | 2.21 | 0.40 |
| 3:3V:77:ASN:ND2 | 3:3V:79:THR:HG23 | 2.37 | 0.40 |
| 4:3W:69:LEU:HD23 | 4:3W:69:LEU:H | 1.87 | 0.40 |
| 3:3X:77:ASN:ND2 | 3:3X:79:THR:HG23 | 2.37 | 0.40 |
| 3:3X:132:ILE:HG23 | 3:3X:143:ILE:CG2 | 2.51 | 0.40 |
| 3:3Z:77:ASN:ND2 | 3:3Z:79:THR:HG23 | 2.37 | 0.40 |
| 4:4A:57:THR:OG1 | 4:4A:158:ALA:HB2 | 2.22 | 0.40 |
| 3:4B:9:LEU:HD23 | 3:4B:9:LEU:HA | 1.89 | 0.40 |
| 3:4B:132:ILE:HG23 | 3:4B:143:ILE:CG2 | 2.52 | 0.40 |
| 4:4C:69:LEU:HD23 | 4:4C:69:LEU:H | 1.87 | 0.40 |
| 3:4D:9:LEU:HD23 | 3:4D:9:LEU:HA | 1.89 | 0.40 |
| 3:4D:77:ASN:ND2 | 3:4D:79:THR:HG23 | 2.37 | 0.40 |
| 3:4F:77:ASN:ND2 | 3:4F:79:THR:HG23 | 2.37 | 0.40 |
| 3:4H:77:ASN:ND2 | 3:4H:79:THR:HG23 | 2.37 | 0.40 |
| 3:4J:279:ALA:O | 3:4J:283:GLN:HG2 | 2.21 | 0.40 |
| 5:4L:252:GLU:O | 5:4L:256:MET:HG2 | 2.21 | 0.40 |
| 5:4M:40:GLU:OE1 | 5:4M:44:ARG:HD3 | 2.21 | 0.40 |
| 6:4O:150:ASP:OD1 | 6:4O:150:ASP:N | 2.54 | 0.40 |
| 6:4O:258:HIS:HA | 6:4O:261:GLU:OE1 | 2.22 | 0.40 |
| 7:4R:233:MET:HB3 | 7:4R:233:MET:HE3 | 1.83 | 0.40 |
| 7:4T:184:LEU:HD23 | 31:7M:78:HIS:CG | 2.53 | 0.40 |
| 7:4U:31:LYS:O | 7:4U:35:GLU:HG3 | 2.21 | 0.40 |
| 8:4W:473:LYS:HE3 | 8:4W:473:LYS:HB3 | 1.91 | 0.40 |
| 9:4Z:348:GLU:HB3 | 9:4Z:352:TYR:OH | 2.21 | 0.40 |
| 10:5B:101:ARG:O | 10:5B:105:MET:HG2 | 2.21 | 0.40 |
| 10:5C:331:MET:CE | 10:5C:334:ARG:HH21 | 2.32 | 0.40 |
| 12:5G:335:LEU:O | 12:5G:335:LEU:HD12 | 2.22 | 0.40 |
| 13:5J:76:THR:HA | 13:5J:79:THR:HG22 | 2.04 | 0.40 |
| 14:5L:366:LEU:HD13 | 14:5L:366:LEU:HA | 1.82 | 0.40 |
| 14:5M:165:THR:HG21 | 14:5M:200:VAL:HG11 | 2.02 | 0.40 |
| 14:5N:459:GLN:OE1 | 14:5N:459:GLN:N | 2.54 | 0.40 |
| 15:5P:140:HIS:CB | 15:5P:146:VAL:HG11 | 2.48 | 0.40 |
| 16:5Q:192:TYR:CE2 | 35:7T:130:LYS:HE3 | 2.56 | 0.40 |
| 17:5S:138:MET:H | 17:5S:138:MET:HG3 | 1.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:5T:196:TYR:HA | 17:5T:199:LEU:HD12 | 2.03 | 0.40 |
| 18:5Y:36:ASN:OD1 | 18:5Y:84:ARG:NH2 | 2.45 | 0.40 |
| 18:5Y:198:LEU:HD13 | 18:5Y:198:LEU:HA | 1.79 | 0.40 |
| 18:5Z:128:GLN:CD | 18:5Z:128:GLN:H | 2.17 | 0.40 |
| 18:6C:7:LEU:CD1 | 18:6C:69:THR:HG21 | 2.52 | 0.40 |
| 18:6D:7:LEU:CD1 | 18:6D:69:THR:HG21 | 2.52 | 0.40 |
| 22:6I:73:ASN:ND2 | 24:6T:310:GLU:OE1 | 2.54 | 0.40 |
| 22:6I:204:PHE:HB2 | 22:6I:227:TYR:CE2 | 2.56 | 0.40 |
| 22:6K:324:LYS:O | 22:6K:328:THR:HG23 | 2.21 | 0.40 |
| 22:6M:53:THR:HA | 22:6M:57:THR:HG21 | 2.03 | 0.40 |
| 22:6O:186:ARG:HA | 22:6O:189:LYS:HD2 | 2.03 | 0.40 |
| 22:6P:123:PRO:O | 22:6P:124:PHE:CG | 2.74 | 0.40 |
| 23:6S:2:ASP:O | 23:6S:6:GLN:HG3 | 2.21 | 0.40 |
| 24:6W:103:LYS:HG2 | 24:6W:116:ILE:HG12 | 2.03 | 0.40 |
| 24:6W:274:ARG:HB3 | 24:6W:372:ASP:OD2 | 2.21 | 0.40 |
| 24:6X:613:LYS:O | 24:6X:617:ASP:CB | 2.66 | 0.40 |
| 24:6Y:279:TRP:CZ2 | 24:6Y:364:ARG:HG3 | 2.56 | 0.40 |
| 28:7H:332:LEU:HD23 | 28:7H:332:LEU:HA | 1.78 | 0.40 |
| 29:7J:144:GLN:O | 29:7J:148:VAL:HG23 | 2.21 | 0.40 |
| 29:7J:461:ILE:HD13 | 29:7J:461:ILE:HA | 1.89 | 0.40 |
| 32:7O:62:THR:HG21 | 32:7O:67:ARG:HD2 | 2.02 | 0.40 |
| 35:7U:122:LYS:HA | 35:7U:122:LYS:HD3 | 1.94 | 0.40 |
| 37:7Y:137:LEU:HD21 | 37:7Y:162:LEU:HD22 | 2.03 | 0.40 |
| 38:8A:12:LEU:HD12 | 38:8A:12:LEU:HA | 1.88 | 0.40 |
| 2:G1:182:VAL:HG22 | 1:G2:256:ASN:ND2 | 2.36 | 0.40 |
| 1:G2:180:VAL:HG23 | 1:G2:184:ASN:HD21 | 1.86 | 0.40 |
| 1:G4:343:GLU:HG2 | 1:G4:344:TRP:N | 2.36 | 0.40 |
| 2:G5:90:GLU:HB2 | 2:I1:283:HIS:CE1 | 2.57 | 0.40 |
| 2:G5:319:TYR:HD2 | 2:G5:323:VAL:HG11 | 1.87 | 0.40 |
| 1:G6:135:VAL:HG11 | 1:G6:152:ILE:HD11 | 2.04 | 0.40 |
| 1:G6:317:PHE:HE2 | 1:G6:326:VAL:HG13 | 1.86 | 0.40 |
| 1:G8:252:LYS:HE2 | 1:G8:350:LYS:HE2 | 2.03 | 0.40 |
| 2:G9:47:ASP:OD1 | 2:G9:47:ASP:N | 2.54 | 0.40 |
| 2:G9:107:HIS:HB3 | 2:G9:108:TYR:CD2 | 2.56 | 0.40 |
| 2:G9:388:PHE:CD1 | 2:G9:391:LEU:HD12 | 2.56 | 0.40 |
| 2:H1:204:LEU:HD23 | 2:H1:231:ILE:HD12 | 2.04 | 0.40 |
| 2:H1:301:MET:HE1 | 2:H1:307:PRO:HD3 | 2.03 | 0.40 |
| 2:H3:177:VAL:HG13 | 1:H4:327:ASP:HB3 | 2.04 | 0.40 |
| 2:H3:327:ASP:N | 2:H3:327:ASP:OD1 | 2.52 | 0.40 |
| 1:H4:277:GLY:CA | 24:6U:492:ILE:CG2 | 2.99 | 0.40 |
| 2:H5:24:TYR:HD1 | 2:H5:24:TYR:HA | 1.77 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H5:102:ASN:HB3 | 2:H5:105:ARG:HB3 | 2.04 | 0.40 |
| 2:H5:346:TRP:CZ3 | 2:H5:435:VAL:HG13 | 2.57 | 0.40 |
| 1:H6:309:ARG:NH1 | 1:H6:339:SER:O | 2.55 | 0.40 |
| 2:H7:9:ILE:HD11 | 2:H7:153:LEU:HD22 | 2.02 | 0.40 |
| 2:H7:176:GLN:HG2 | 2:H7:177:VAL:N | 2.37 | 0.40 |
| 2:H9:90:GLU:O | 2:H9:121:ARG:NH1 | 2.53 | 0.40 |
| 2:H9:227:LEU:O | 2:H9:231:ILE:HG12 | 2.22 | 0.40 |
| 2:H9:318:MET:HB2 | 2:H9:376:CYS:HB3 | 2.04 | 0.40 |
| 2:I1:312:TYR:HB2 | 2:I1:343:PHE:CD1 | 2.56 | 0.40 |
| 1:I4:3:GLU:O | 1:I4:131:GLN:HB3 | 2.22 | 0.40 |
| 1:I4:273:LEU:O | 1:I4:292:GLN:NE2 | 2.51 | 0.40 |
| 2:I7:32:PRO:HB3 | 2:I7:83:TYR:CE1 | 2.56 | 0.40 |
| 2:I7:88:HIS:CG | 2:K3:283:HIS:HA | 2.56 | 0.40 |
| 1:I8:403:MET:HE3 | 1:I8:403:MET:HB2 | 1.67 | 0.40 |
| 2:I9:370:LYS:HD2 | 5:4L:317:TYR:CZ | 2.56 | 0.40 |
| 1:J2:98:GLY:HA2 | 2:J3:254:GLU:OE2 | 2.21 | 0.40 |
| 1:J2:100:ASN:HB3 | 1:J2:103:LYS:HB2 | 2.03 | 0.40 |
| 1:J4:50:TYR:CE2 | 1:J4:241:ARG:HD3 | 2.57 | 0.40 |
| 2:J5:301:MET:HE2 | 2:J5:301:MET:HB2 | 1.88 | 0.40 |
| 1:J8:58:ARG:HA | 1:J8:58:ARG:HD2 | 1.88 | 0.40 |
| 1:K0:22:GLU:HG2 | 1:K0:81:TYR:CD2 | 2.56 | 0.40 |
| 1:K4:244:GLY:HA2 | 1:K4:355:ASP:CG | 2.42 | 0.40 |
| 1:K4:314:SER:HA | 1:K4:350:LYS:O | 2.21 | 0.40 |
| 2:K7:252:ILE:HD12 | 2:K7:252:ILE:HA | 1.95 | 0.40 |
| 2:K7:252:ILE:HD12 | 2:K7:255:PHE:HE2 | 1.87 | 0.40 |
| 2:K9:4:VAL:HG23 | 2:K9:134:GLY:O | 2.21 | 0.40 |
| 2:K9:7:ILE:HG12 | 2:K9:137:VAL:HG12 | 2.02 | 0.40 |
| 2:K9:27:GLU:CD | 2:K9:243:ARG:HH12 | 2.24 | 0.40 |
| 2:L1:114:ILE:HG21 | 2:L1:149:LEU:HD22 | 2.04 | 0.40 |
| 2:L1:175:PRO:HG2 | 2:L1:176:GLN:OE1 | 2.21 | 0.40 |
| 2:L1:320:ARG:O | 2:L1:373:ARG:HA | 2.22 | 0.40 |
| 1:L2:301:CYS:SG | 1:L2:302:ALA:N | 2.95 | 0.40 |
| 2:L3:149:LEU:HD23 | 2:L3:149:LEU:H | 1.85 | 0.40 |
| 2:L5:21:TRP:CZ2 | 2:L5:65:CYS:HB3 | 2.57 | 0.40 |
| 1:L6:174:LYS:HE2 | 1:L6:174:LYS:HB3 | 1.82 | 0.40 |
| 1:L6:217:LEU:HD23 | 1:L6:217:LEU:HA | 1.93 | 0.40 |
| 1:L6:270:PHE:HD2 | 1:L6:273:LEU:HD21 | 1.86 | 0.40 |
| 2:L9:21:TRP:CZ3 | 2:L9:63:PRO:HB3 | 2.57 | 0.40 |
| 2:M1:191:THR:O | 2:M1:195:LEU:HG | 2.22 | 0.40 |
| 2:M3:72:PRO:HD2 | 1:M4:2:ARG:NH1 | 2.37 | 0.40 |
| 2:M3:244:PHE:HB2 | 2:M3:356:ASN:HD21 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M4:314:SER:HA | 1:M4:350:LYS:O | 2.21 | 0.40 |
| 2:M7:373:ARG:NH1 | 30:7K:84:VAL:HG22 | 2.36 | 0.40 |
| 1:M8:216:LYS:HB2 | 1:M8:275:SER:OG | 2.21 | 0.40 |
| 2:M9:282:TYR:HE2 | 29:7J:296:LYS:HB2 | 1.87 | 0.40 |
| 1:N0:5:VAL:HG12 | 1:N0:133:PHE:CD1 | 2.56 | 0.40 |
| 2:N3:182:VAL:HG12 | 2:N3:185:TYR:HB2 | 2.02 | 0.40 |
| 2:N5:236:SER:HA | 2:N5:239:THR:HG22 | 2.02 | 0.40 |
| 2:N5:420:GLU:HA | 2:N5:423:GLU:HG3 | 2.03 | 0.40 |
| 1:N6:49:VAL:HG11 | 1:N6:241:ARG:HG2 | 2.03 | 0.40 |
| 1:N6:101:TRP:HB2 | 1:N6:184:ASN:OD1 | 2.22 | 0.40 |
| 1:N8:175:VAL:HB | 2:N9:329:ASN:ND2 | 2.37 | 0.40 |
| 1:O0:117:LEU:HA | 1:O0:117:LEU:HD23 | 1.93 | 0.40 |
| 2:O1:75:VAL:HG11 | 2:O1:94:SER:HB3 | 2.03 | 0.40 |
| 1:O2:117:LEU:HD11 | 1:O2:154:LYS:HD3 | 2.04 | 0.40 |
| 2:O3:203:MET:HB2 | 2:O3:303:VAL:HG21 | 2.02 | 0.40 |
| 2:O3:335:ILE:HG23 | 2:O3:341:ILE:HD11 | 2.03 | 0.40 |
| 2:O3:402:ARG:HD3 | 2:O3:402:ARG:HA | 1.90 | 0.40 |
| 2:O5:21:TRP:CZ3 | 2:O5:63:PRO:HB3 | 2.56 | 0.40 |
| 2:O5:32:PRO:HB3 | 2:O5:83:TYR:CE1 | 2.56 | 0.40 |
| 2:O5:62:VAL:O | 2:O5:62:VAL:CG2 | 2.70 | 0.40 |
| 2:O5:151:SER:HB2 | 2:O5:193:SER:OG | 2.21 | 0.40 |
| 2:O5:320:ARG:HE | 2:O5:320:ARG:HB3 | 1.76 | 0.40 |
| 2:O7:327:ASP:OD1 | 2:O7:328:VAL:N | 2.55 | 0.40 |
| 2:O7:417:GLU:OE2 | 2:O7:417:GLU:N | 2.39 | 0.40 |
| 1:P4:69:GLU:OE2 | 1:P4:69:GLU:N | 2.54 | 0.40 |
| 1:P8:134:GLN:HE21 | 1:P8:167:PHE:HE2 | 1.69 | 0.40 |
| 2:P9:245:ASP:OD1 | 19:6E:166:LYS:HG3 | 2.21 | 0.40 |
| 1:Q0:344:TRP:CE3 | 1:Q0:345:ILE:HG12 | 2.57 | 0.40 |
| 2:Q1:349:THR:HG23 | 2:Q1:349:THR:O | 2.22 | 0.40 |
| 1:Q2:228:LEU:HD23 | 1:Q2:228:LEU:HA | 1.83 | 0.40 |
| 2:Q3:177:VAL:HG13 | 1:Q4:327:ASP:HB3 | 2.03 | 0.40 |
| 2:Q5:75:VAL:O | 2:Q5:79:ARG:HG3 | 2.22 | 0.40 |
| 1:Q6:23:VAL:HG11 | 1:Q6:230:SER:HB3 | 2.04 | 0.40 |
| 1:Q8:11:GLN:NE2 | 2:Q9:249:ASN:OD1 | 2.55 | 0.40 |
| 2:Q9:326:LYS:HG3 | 2:Q9:327:ASP:N | 2.37 | 0.40 |
| 2:R1:271:SER:OG | 2:R1:272:TYR:N | 2.54 | 0.40 |
| 1:R2:222:PHE:HD2 | 2:R3:247:ALA:HB1 | 1.85 | 0.40 |
| 2:R3:287:SER:N | 2:R3:290:GLU:OE2 | 2.54 | 0.40 |
| 1:R4:95:THR:HG23 | 1:R4:96:GLY:H | 1.87 | 0.40 |
| 1:R4:183:TYR:O | 1:R4:187:LEU:HD13 | 2.22 | 0.40 |
| 1:R6:145:SER:OG | 1:R6:146:GLY:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R6:229:ILE:O | 1:R6:233:MET:HG3 | 2.22 | 0.40 |
| 1:R8:58:ARG:NH2 | 1:T4:280:GLN:OE1 | 2.55 | 0.40 |
| 1:S0:390:ARG:O | 1:S0:392:LYS:NZ | 2.54 | 0.40 |
| 2:S1:174:SER:HB3 | 2:S1:177:VAL:O | 2.21 | 0.40 |
| 2:S5:287:SER:OG | 2:S5:288:VAL:N | 2.54 | 0.40 |
| 1:S6:5:VAL:HG22 | 1:S6:62:ARG:HD3 | 2.03 | 0.40 |
| 1:S6:8:GLN:CD | 1:S6:17:GLY:HA3 | 2.41 | 0.40 |
| 2:S7:203:MET:CE | 2:S7:267:PHE:HD1 | 2.35 | 0.40 |
| 1:S8:283:ALA:HB3 | 1:S8:288:GLU:OE1 | 2.22 | 0.40 |
| 1:T0:192:LEU:HD23 | 1:T0:192:LEU:HA | 1.86 | 0.40 |
| 2:T1:8:HIS:CD2 | 2:T1:138:PHE:HD2 | 2.39 | 0.40 |
| 2:T1:125:LEU:HD12 | 2:T1:125:LEU:HA | 1.83 | 0.40 |
| 2:T1:231:ILE:O | 2:T1:235:ILE:HD12 | 2.21 | 0.40 |
| 2:T5:90:GLU:CD | 2:T5:121:ARG:HD3 | 2.42 | 0.40 |
| 2:T5:125:LEU:HD23 | 2:T5:125:LEU:HA | 1.88 | 0.40 |
| 1:T6:16:ILE:HG21 | 1:T6:229:ILE:HG21 | 2.03 | 0.40 |
| 1:T6:267:MET:HE1 | 1:T6:303:ALA:O | 2.22 | 0.40 |
| 2:T7:327:ASP:OD2 | 2:T7:327:ASP:N | 2.49 | 0.40 |
| 1:T8:68:LEU:HD23 | 1:T8:68:LEU:HA | 1.92 | 0.40 |
| 2:U1:195:LEU:HD11 | 2:U1:264:ARG:NH1 | 2.36 | 0.40 |
| 1:U2:281:TYR:O | 1:U2:281:TYR:CG | 2.75 | 0.40 |
| 1:U4:162:ARG:HD3 | 1:U4:162:ARG:HA | 1.78 | 0.40 |
| 1:U4:283:ALA:O | 1:U4:288:GLU:HG2 | 2.21 | 0.40 |
| 1:U6:301:CYS:SG | 1:U6:302:ALA:N | 2.95 | 0.40 |
| 2:U7:247:ALA:HB2 | 2:U7:357:TYR:CZ | 2.57 | 0.40 |
| 2:U9:4:VAL:HG23 | 2:U9:134:GLY:O | 2.21 | 0.40 |
| 1:V0:117:LEU:HA | 1:V0:117:LEU:HD23 | 1.84 | 0.40 |
| 1:V0:217:LEU:HD23 | 1:V0:217:LEU:HA | 1.91 | 0.40 |
| 2:V1:26:LEU:HD23 | 2:V1:363:VAL:HG12 | 2.04 | 0.40 |
| 2:V1:280:LYS:HA | 2:V1:283:HIS:CD2 | 2.56 | 0.40 |
| 1:V2:48:ASN:OD1 | 1:V2:48:ASN:N | 2.53 | 0.40 |
| 1:V2:116:VAL:O | 1:V2:120:VAL:HG12 | 2.21 | 0.40 |
| 2:V3:100:ALA:HA | 1:V4:252:LYS:CG | 2.45 | 0.40 |
| 2:V3:203:MET:O | 2:V3:204:LEU:HD22 | 2.22 | 0.40 |
| 1:V4:268:VAL:HG12 | 1:V4:269:GLY:N | 2.36 | 0.40 |
| 1:V6:24:VAL:HG11 | 1:V6:50:TYR:CD2 | 2.57 | 0.40 |
| 1:V6:163:MET:SD | 1:V6:251:ARG:NH1 | 2.95 | 0.40 |
| 2:V7:276:ILE:HD13 | 2:V7:276:ILE:HA | 1.90 | 0.40 |
| 1:W2:113:ILE:HA | 1:W2:116:VAL:CG1 | 2.50 | 0.40 |
| 1:W4:39:ASP:OD1 | 1:W4:40:SER:N | 2.54 | 0.40 |
| 1:W4:138:SER:O | 1:W4:139:LEU:HD23 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W4:165:LEU:HD12 | 1:W4:165:LEU:HA | 1.82 | 0.40 |
| 2:W5:401:LYS:HE3 | 2:W5:401:LYS:HB3 | 1.93 | 0.40 |
| 1:W6:176:SER:O | 1:W6:176:SER:OG | 2.39 | 0.40 |
| 1:W6:203:ASP:N | 1:W6:203:ASP:OD1 | 2.54 | 0.40 |
| 2:W7:313:MET:HB2 | 2:W7:380:ASN:HB3 | 2.04 | 0.40 |
| 2:W9:147:SER:OG | 2:W9:190:SER:HB2 | 2.21 | 0.40 |
| 1:X2:297:LYS:HD3 | 1:X2:297:LYS:HA | 1.83 | 0.40 |
| 1:X2:382:SER:HB2 | 1:X2:415:MET:HE3 | 2.02 | 0.40 |
| 2:X3:73:THR:HG23 | 2:X3:74:VAL:N | 2.37 | 0.40 |
| 2:X3:401:LYS:HB3 | 2:X3:401:LYS:HE3 | 1.88 | 0.40 |
| 1:X8:257:LEU:HA | 1:X8:312:THR:HG21 | 2.02 | 0.40 |
| 1:X8:387:ALA:HA | 1:X8:390:ARG:HE | 1.86 | 0.40 |
| 2:X9:306:ASP:HB3 | 2:X9:309:HIS:HD2 | 1.86 | 0.40 |
| 1:Y0:359:LYS:HA | 1:Y0:359:LYS:HD3 | 1.85 | 0.40 |
| 2:Y1:286:LEU:O | 2:Y1:373:ARG:NH1 | 2.55 | 0.40 |
| 2:Y5:167:LEU:HD13 | 2:Y5:200:VAL:HB | 2.02 | 0.40 |
| 1:Y8:7:ILE:HB | 1:Y8:135:VAL:HG12 | 2.03 | 0.40 |
| 1:Z2:2:ARG:HH21 | 1:Z2:240:LEU:HG | 1.87 | 0.40 |
| 2:Z3:9:ILE:O | 2:Z3:139:ASN:HA | 2.21 | 0.40 |
| 2:Z3:54:SER:O | 2:Z3:61:HIS:HA | 2.21 | 0.40 |
| 2:Z3:223:THR:HG23 | 2:Z3:225:THR:H | 1.87 | 0.40 |
| 2:Z3:387:ILE:HD12 | 2:Z3:390:ARG:HH22 | 1.87 | 0.40 |
| 1:Z4:156:ARG:HG3 | 1:Z4:195:ASN:O | 2.21 | 0.40 |
| 1:Z4:414:ASN:O | 1:Z4:418:LEU:HB2 | 2.21 | 0.40 |
| 2:Z5:271:SER:OG | 2:Z5:272:TYR:N | 2.54 | 0.40 |
| 2:Z5:406:HIS:HA | 2:Z5:409:VAL:HG22 | 2.03 | 0.40 |
| 1:Z6:395:LEU:O | 1:Z6:399:THR:HG23 | 2.22 | 0.40 |
| 1:Z8:58:ARG:NH1 | 1:Z8:84:ILE:HA | 2.36 | 0.40 |
| 1:0A:130:LEU:HB3 | 1:0A:162:ARG:HD2 | 2.03 | 0.40 |
| 1:0C:68:LEU:HD13 | 1:0C:103:LYS:HZ2 | 1.86 | 0.40 |
| 1:0C:344:TRP:CE3 | 1:0C:345:ILE:HG13 | 2.57 | 0.40 |
| 1:0E:11:GLN:HE21 | 39:0E:501:GDP:PB | 2.45 | 0.40 |
| 1:0E:233:MET:HA | 1:0E:236:ILE:HG12 | 2.02 | 0.40 |
| 2:0F:25:CYS:SG | 2:0F:86:LEU:HD11 | 2.62 | 0.40 |
| 1:0G:95:THR:OG1 | 1:0G:96:GLY:N | 2.55 | 0.40 |
| 2:0H:89:PRO:HD2 | 2:0X:283:HIS:ND1 | 2.36 | 0.40 |
| 2:0H:407:TRP:HZ2 | 1:0I:258:ILE:HD12 | 1.86 | 0.40 |
| 1:0I:286:VAL:HG23 | 1:0I:287:PRO:HD3 | 2.03 | 0.40 |
| 1:0K:108:GLU:HA | 1:0K:111:GLU:OE2 | 2.21 | 0.40 |
| 1:0M:343:GLU:HG2 | 1:0M:344:TRP:N | 2.37 | 0.40 |
| 1:0O:39:ASP:OD1 | 1:0O:39:ASP:N | 2.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0O:271:THR:OG1 | 1:0O:272:PRO:HA | 2.22 | 0.40 |
| 1:0Q:285:THR:OG1 | 1:0Q:287:PRO:HD2 | 2.22 | 0.40 |
| 2:0R:207:GLU:HG3 | 2:0R:304:LYS:HB2 | 2.03 | 0.40 |
| 1:0S:166:THR:OG1 | 1:0S:199:CYS:HB3 | 2.22 | 0.40 |
| 1:0S:350:LYS:NZ | 1:0S:351:SER:O | 2.51 | 0.40 |
| 1:0U:203:ASP:OD1 | 1:0U:206:ALA:HB3 | 2.22 | 0.40 |
| 2:0V:346:TRP:CD1 | 2:0V:346:TRP:N | 2.78 | 0.40 |
| 1:0W:2:ARG:O | 1:0W:49:VAL:HG23 | 2.22 | 0.40 |
| 1:0W:19:LYS:O | 1:0W:23:VAL:HG13 | 2.22 | 0.40 |
| 2:0Z:392:ASP:HB2 | 2:0Z:425:LEU:HD22 | 2.04 | 0.40 |
| 1:1A:35:THR:HG1 | 1:1A:37:HIS:HE2 | 1.59 | 0.40 |
| 1:1E:198:GLU:HA | 1:1E:264:HIS:HB2 | 2.03 | 0.40 |
| 1:1E:208:TYR:HA | 1:1E:211:CYS:SG | 2.61 | 0.40 |
| 1:1E:215:LEU:HB3 | 1:1E:217:LEU:HG | 2.04 | 0.40 |
| 1:1E:272:PRO:HB3 | 1:1E:282:ARG:HH22 | 1.87 | 0.40 |
| 2:1F:217:LEU:HD23 | 2:1F:217:LEU:HA | 1.95 | 0.40 |
| 2:1H:47:ASP:HA | 2:1H:50:ASN:OD1 | 2.22 | 0.40 |
| 2:1H:317:LEU:HB3 | 2:1H:319:TYR:CE1 | 2.48 | 0.40 |
| 1:1K:152:ILE:HD12 | 1:1K:164:MET:SD | 2.62 | 0.40 |
| 1:1K:221:THR:OG1 | 1:1K:222:PHE:N | 2.55 | 0.40 |
| 2:1N:111:GLY:HA2 | 2:1N:114:ILE:HG22 | 2.03 | 0.40 |
| 1:1O:210:ILE:O | 1:1O:214:THR:OG1 | 2.31 | 0.40 |
| 2:1P:88:HIS:ND1 | 2:2F:283:HIS:O | 2.54 | 0.40 |
| 2:1P:274:PRO:HG3 | 2:1P:286:LEU:HD11 | 2.04 | 0.40 |
| 2:1T:4:VAL:HG23 | 2:1T:134:GLY:O | 2.22 | 0.40 |
| 1:1U:16:ILE:HG13 | 1:1U:17:GLY:N | 2.35 | 0.40 |
| 1:1W:193:VAL:HG13 | 1:1W:194:GLU:CD | 2.41 | 0.40 |
| 2:1Z:69:ASP:OD1 | 2:1Z:70:LEU:N | 2.54 | 0.40 |
| 1:2A:274:THR:HG21 | 1:2A:282:ARG:HD2 | 2.02 | 0.40 |
| 1:2A:359:LYS:HB3 | 1:2A:359:LYS:HE3 | 1.60 | 0.40 |
| 2:2D:73:THR:HG21 | 1:2E:2:ARG:HH22 | 1.86 | 0.40 |
| 2:2F:70:LEU:HD13 | 2:2F:110:ILE:HG21 | 2.03 | 0.40 |
| 1:2G:183:TYR:O | 1:2G:187:LEU:HD13 | 2.22 | 0.40 |
| 1:2K:396:HIS:HA | 1:2K:399:THR:CG2 | 2.51 | 0.40 |
| 2:2P:327:ASP:N | 2:2P:327:ASP:OD1 | 2.54 | 0.40 |
| 1:2Q:150:LEU:HD23 | 1:2Q:154:LYS:HG2 | 2.03 | 0.40 |
| 1:2Q:273:LEU:O | 1:2Q:292:GLN:NE2 | 2.53 | 0.40 |
| 1:2Q:316:LEU:O | 1:2Q:365:ALA:HA | 2.21 | 0.40 |
| 2:2R:157:LEU:HA | 2:2R:157:LEU:HD12 | 1.89 | 0.40 |
| 1:2S:153:SER:HB3 | 1:2S:195:ASN:HD21 | 1.86 | 0.40 |
| 1:2S:273:LEU:H | 1:2S:292:GLN:HE22 | 1.68 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2V:4:VAL:HG23 | 2:2V:134:GLY:O | 2.22 | 0.40 |
| 2:2V:179:THR:O | 1:2W:350:LYS:HG2 | 2.21 | 0.40 |
| 2:2V:308:ARG:HH21 | 38:8B:73:TRP:C | 2.25 | 0.40 |
| 1:2W:34:GLY:HA3 | 1:2W:58:ARG:HD3 | 2.03 | 0.40 |
| 1:2W:190:HIS:HD2 | 1:2W:414:ASN:HB2 | 1.86 | 0.40 |
| 2:2X:72:PRO:HD2 | 1:2Y:2:ARG:HH12 | 1.87 | 0.40 |
| 2:2X:187:SER:O | 2:2X:191:THR:HG23 | 2.22 | 0.40 |
| 2:2Z:9:ILE:HD13 | 2:2Z:150:GLY:HA2 | 2.02 | 0.40 |
| 2:2Z:101:ASN:ND2 | 2:2Z:143:GLY:HA2 | 2.36 | 0.40 |
| 1:3A:19:LYS:HB3 | 1:3A:19:LYS:HE3 | 1.91 | 0.40 |
| 2:3B:398:MET:HG3 | 1:3C:346:PRO:HD2 | 2.03 | 0.40 |
| 1:3C:167:PHE:CE2 | 1:3C:233:MET:HG2 | 2.56 | 0.40 |
| 1:3C:285:THR:HB | 1:3C:287:PRO:HD2 | 2.02 | 0.40 |
| 2:3H:121:ARG:HD2 | 2:3H:121:ARG:HA | 1.66 | 0.40 |
| 2:3H:219:ILE:HD13 | 2:3H:219:ILE:HA | 1.89 | 0.40 |
| 2:3H:397:LEU:HD23 | 2:3H:397:LEU:HA | 1.88 | 0.40 |
| 1:3I:32:PRO:HD3 | 1:3I:81:TYR:CZ | 2.56 | 0.40 |
| 1:3I:392:LYS:HD2 | 1:3I:395:LEU:HD22 | 2.03 | 0.40 |
| 2:3J:127:ASP:OD2 | 3:3Z:125:TYR:OH | 2.37 | 0.40 |
| 2:3N:9:ILE:HD13 | 2:3N:150:GLY:HA2 | 2.03 | 0.40 |
| 2:3N:56:THR:HG1 | 3:4D:34:SER:HA | 1.84 | 0.40 |
| 2:3N:413:MET:HB3 | 2:3N:417:GLU:OE2 | 2.21 | 0.40 |
| 1:3O:173:PRO:HD2 | 1:3O:380:ARG:NH2 | 2.36 | 0.40 |
| 1:3O:265:PHE:HD2 | 1:3O:422:TYR:OH | 2.05 | 0.40 |
| 1:3Q:213:ARG:HH21 | 1:3Q:297:LYS:HE3 | 1.86 | 0.40 |
| 1:3Q:250:LEU:HD12 | 1:3Q:250:LEU:H | 1.86 | 0.40 |
| 1:3S:3:GLU:HG3 | 1:3S:127:CYS:HB2 | 2.03 | 0.40 |
| 2:3T:14:ILE:HD13 | 2:3T:69:ASP:OD2 | 2.22 | 0.40 |
| 2:3T:81:GLY:O | 2:3T:84:ARG:HG3 | 2.22 | 0.40 |
| 2:3T:320:ARG:HE | 2:3T:320:ARG:HB3 | 1.68 | 0.40 |
| 2:3T:420:GLU:O | 2:3T:423:GLU:HG3 | 2.21 | 0.40 |
| 4:3W:57:THR:OG1 | 4:3W:158:ALA:HB2 | 2.21 | 0.40 |
| 4:3W:73:LEU:HD13 | 4:3W:73:LEU:HA | 1.94 | 0.40 |
| 3:3X:49:HIS:HB3 | 3:3X:113:ARG:NH1 | 2.36 | 0.40 |
| 4:4A:28:GLN:O | 4:4A:57:THR:HA | 2.21 | 0.40 |
| 4:4A:69:LEU:HD23 | 4:4A:69:LEU:H | 1.87 | 0.40 |
| 3:4B:49:HIS:HB3 | 3:4B:113:ARG:NH1 | 2.36 | 0.40 |
| 3:4B:77:ASN:ND2 | 3:4B:79:THR:HG23 | 2.37 | 0.40 |
| 3:4B:171:PRO:HG2 | 3:4B:172:TYR:CD2 | 2.56 | 0.40 |
| 3:4D:132:ILE:HG23 | 3:4D:143:ILE:CG2 | 2.51 | 0.40 |
| 3:4D:171:PRO:HG2 | 3:4D:172:TYR:CD2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4E:57:THR:OG1 | 4:4E:158:ALA:HB2 | 2.22 | 0.40 |
| 4:4E:69:LEU:HD23 | 4:4E:69:LEU:H | 1.87 | 0.40 |
| 3:4F:49:HIS:HB3 | 3:4F:113:ARG:NH1 | 2.36 | 0.40 |
| 3:4F:132:ILE:HG23 | 3:4F:143:ILE:CG2 | 2.52 | 0.40 |
| 3:4F:171:PRO:HG2 | 3:4F:172:TYR:CD2 | 2.56 | 0.40 |
| 3:4F:218:LEU:HA | 3:4F:218:LEU:HD23 | 1.84 | 0.40 |
| 4:4G:57:THR:OG1 | 4:4G:158:ALA:HB2 | 2.22 | 0.40 |
| 4:4G:86:TYR:HB3 | 4:4G:108:TYR:CD2 | 2.56 | 0.40 |
| 4:4I:73:LEU:HD13 | 4:4I:73:LEU:HA | 1.94 | 0.40 |
| 5:4L:470:ASP:OD2 | 5:4L:470:ASP:N | 2.52 | 0.40 |
| 5:4M:41:PHE:CE1 | 5:4M:45:THR:HG21 | 2.57 | 0.40 |
| 6:4O:72:LYS:NZ | 32:7O:88:LEU:HD22 | 2.37 | 0.40 |
| 10:5C:135:ARG:O | 10:5C:139:MET:HG3 | 2.21 | 0.40 |
| 10:5C:262:ILE:HG13 | 10:5C:263:GLN:N | 2.36 | 0.40 |
| 10:5C:354:LYS:HA | 10:5C:354:LYS:HD2 | 1.90 | 0.40 |
| 11:5E:76:SER:O | 11:5E:80:GLN:NE2 | 2.43 | 0.40 |
| 13:5H:76:THR:HA | 13:5H:79:THR:HG22 | 2.04 | 0.40 |
| 13:5I:76:THR:HA | 13:5I:79:THR:HG22 | 2.04 | 0.40 |
| 13:5K:61:LEU:HD23 | 13:5K:61:LEU:HA | 1.94 | 0.40 |
| 14:5L:25:PRO:HD3 | 14:5L:64:LEU:HD21 | 2.03 | 0.40 |
| 14:5M:386:PHE:O | 14:5M:387:CYS:C | 2.59 | 0.40 |
| 14:5M:459:GLN:OE1 | 14:5M:459:GLN:N | 2.54 | 0.40 |
| 14:5N:277:LYS:HE2 | 14:5N:277:LYS:HB2 | 1.90 | 0.40 |
| 14:5N:385:CYS:HB2 | 14:5N:401:TRP:CE3 | 2.56 | 0.40 |
| 15:5O:327:ALA:HA | 15:5O:343:LEU:CD2 | 2.52 | 0.40 |
| 15:5P:14:LEU:O | 15:5P:14:LEU:CG | 2.70 | 0.40 |
| 15:5P:84:ARG:HH11 | 15:5P:84:ARG:HG2 | 1.87 | 0.40 |
| 15:5P:206:HIS:CG | 15:5P:207:GLY:N | 2.90 | 0.40 |
| 18:5Z:36:ASN:OD1 | 18:5Z:84:ARG:NH2 | 2.45 | 0.40 |
| 18:6B:36:ASN:OD1 | 18:6B:84:ARG:NH2 | 2.45 | 0.40 |
| 18:6C:198:LEU:HD13 | 18:6C:198:LEU:HA | 1.79 | 0.40 |
| 18:6D:128:GLN:CD | 18:6D:128:GLN:H | 2.17 | 0.40 |
| 20:6F:59:LYS:O | 20:6F:297:VAL:HA | 2.22 | 0.40 |
| 20:6F:73:GLN:HE22 | 20:6F:114:ASN:CB | 2.34 | 0.40 |
| 20:6F:186:GLN:NE2 | 20:6F:234:LYS:HD3 | 2.37 | 0.40 |
| 22:6I:35:PRO:HA | 22:6I:38:ALA:HB3 | 2.02 | 0.40 |
| 22:6J:241:GLU:HG2 | 22:6J:242:ALA:N | 2.37 | 0.40 |
| 22:6L:321:LEU:HD12 | 22:6L:321:LEU:HA | 1.90 | 0.40 |
| 22:6P:122:ALA:HA | 22:6P:123:PRO:HD3 | 1.95 | 0.40 |
| 22:6P:168:THR:HA | 22:6P:171:GLU:OE1 | 2.22 | 0.40 |
| 24:6T:355:LEU:HD12 | 24:6T:355:LEU:HA | 1.82 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:6U:106:VAL:HG12 | 24:6U:113:ASN:C | 2.42 | 0.40 |
| 24:6V:288:ASP:OD1 | 24:6V:288:ASP:N | 2.55 | 0.40 |
| 24:6W:502:LYS:HB3 | 24:6W:511:ILE:HD12 | 2.03 | 0.40 |
| 24:6W:541:THR:HG22 | 24:6W:614:ARG:HH22 | 1.87 | 0.40 |
| 24:6W:613:LYS:HD2 | 24:6W:613:LYS:HA | 1.85 | 0.40 |
| 24:6Y:452:MET:HE1 | 24:6Y:528:ARG:HH11 | 1.86 | 0.40 |
| 24:6Z:92:ASP:N | 24:6Z:92:ASP:OD2 | 2.52 | 0.40 |
| 24:6Z:505:LYS:N | 24:6Z:510:GLU:O | 2.54 | 0.40 |
| 24:6Z:565:GLN:OE1 | 24:6Z:602:LEU:HB2 | 2.21 | 0.40 |
| 25:7C:13:GLU:OE2 | 25:7C:14:ARG:HD2 | 2.21 | 0.40 |
| 26:7D:91:HIS:CD2 | 26:7D:106:ASP:HB2 | 2.56 | 0.40 |
| 29:7I:5:GLY:H | 29:7I:12:LYS:HZ1 | 1.69 | 0.40 |
| 29:7J:413:ASP:OD1 | 29:7J:413:ASP:N | 2.52 | 0.40 |
| 30:7K:342:LEU:N | 30:7K:342:LEU:HD23 | 2.36 | 0.40 |
| 33:7Q:166:GLY:O | 33:7Q:170:THR:HG23 | 2.21 | 0.40 |
| 35:7T:157:ARG:HG3 | 36:7V:60:TRP:CH2 | 2.56 | 0.40 |
| 38:8A:72:ASP:N | 38:8A:72:ASP:OD2 | 2.54 | 0.40 |
| 38:8C:92:GLU:OE2 | 38:8C:94:LYS:NZ | 2.53 | 0.40 |
| 38:8C:228:THR:O | 38:8C:228:THR:HG23 | 2.21 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 0A | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 95 |
| 1 | 0C | 367/379 (97%) | 367 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | 0E | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 0G | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 0I | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 0K | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 0M | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 0O | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 0Q | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 0S | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 0U | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 0W | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 0Y | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 1 | 122/379 (32%) | 118 (97%) | 4 (3%) | 33 | 58 |
| 1 | 1A | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 1C | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 1E | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 1G | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 1K | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 1M | 367/379 (97%) | 364 (99%) | 3 (1%) | 79 | 87 |
| 1 | 1O | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 1Q | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 1S | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 1U | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 1W | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 2A | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 2C | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 2E | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 2G | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 2I | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 2K | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 2M | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 2Q | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | 2S | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 2U | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 2W | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 2Y | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 3 | 372/379 (98%) | 370 (100%) | 2 (0%) | 86 | 91 |
| 1 | 3A | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 3C | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 3G | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 3I | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 3K | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 3M | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | 3O | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | 3Q | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 3S | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | 5 | 374/379 (99%) | 372 (100%) | 2 (0%) | 86 | 91 |
| 1 | 7 | 375/379 (99%) | 373 (100%) | 2 (0%) | 86 | 91 |
| 1 | 9 | 374/379 (99%) | 373 (100%) | 1 (0%) | 91 | 95 |
| 1 | A1 | 371/379 (98%) | 370 (100%) | 1 (0%) | 91 | 95 |
| 1 | A3 | 373/379 (98%) | 372 (100%) | 1 (0%) | 91 | 95 |
| 1 | A5 | 369/379 (97%) | 369 (100%) | 0 | 100 | 100 |
| 1 | A7 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | A9 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | B1 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | B3 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | B5 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | B8 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | C0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | C2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | C4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | C6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | C8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | D0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | D2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | D4 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | D6 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | D8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | E0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | E2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | E4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | E6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | E8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | F0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | F2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | F6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | F8 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | G0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | G2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | G4 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | G6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | G8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | H2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | H4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | H6 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | H8 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | I0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | I2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | I4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | I8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | J0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | J2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | J4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | J6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | J8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | K0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | K4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | K6 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | K8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | L0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | L2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | L4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | L6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | M0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | M2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | M4 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | M6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | M8 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | N0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | N2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | N6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | N8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | O0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | O2 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | O4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | O6 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | O8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | P4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | P6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | P8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Q0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Q2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | Q4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Q6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Q8 | 361/379 (95%) | 359 (99%) | 2 (1%) | 84 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | R0 | 372/379 (98%) | 372 (100%) | 0 | 100 | 100 |
| 1 | R2 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | R4 | 369/379 (97%) | 368 (100%) | 1 (0%) | 91 | 95 |
| 1 | R6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | R8 | 370/379 (98%) | 370 (100%) | 0 | 100 | 100 |
| 1 | S0 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | S2 | 370/379 (98%) | 370 (100%) | 0 | 100 | 100 |
| 1 | S4 | 368/379 (97%) | 368 (100%) | 0 | 100 | 100 |
| 1 | S6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | S8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | T0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | T2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | T4 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | T6 | 367/379 (97%) | 364 (99%) | 3 (1%) | 79 | 87 |
| 1 | T8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | U2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | U4 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | U6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | U8 | 369/379 (97%) | 367 (100%) | 2 (0%) | 86 | 91 |
| 1 | V0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | V2 | 367/379 (97%) | 364 (99%) | 3 (1%) | 79 | 87 |
| 1 | V4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | V6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | V8 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | W0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | W2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | W4 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | W6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | W8 | 367/379 (97%) | 364 (99%) | 3 (1%) | 79 | 87 |
| 1 | X0 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | X2 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | X4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | X6 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | X8 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | Y0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Y2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Y4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Y6 | 367/379 (97%) | 365 (100%) | 2 (0%) | 86 | 91 |
| 1 | Y8 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | Z0 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Z2 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Z4 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 1 | Z6 | 367/379 (97%) | 366 (100%) | 1 (0%) | 91 | 95 |
| 1 | Z8 | 367/379 (97%) | 367 (100%) | 0 | 100 | 100 |
| 2 | 0B | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 0F | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 0H | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 0J | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 0L | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 0N | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | 0P | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 0R | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 0V | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | 0X | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 0Z | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | 1B | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | 1D | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 1F | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 1H | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | 1L | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | 1N | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | 1P | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | 1R | 359/374 (96%) | 351 (98%) | 8 (2%) | 47 | 68 |
| 2 | 1T | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 1V | 359/374 (96%) | 355 (99%) | 4 (1%) | 70 | 81 |
| 2 | 1X | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 1Z | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | 2 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | 2B | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2D | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2F | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2H | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2J | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 2L | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 2N | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2P | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | 2R | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 2T | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 2V | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 2X | 366/374 (98%) | 366 (100%) | 0 | 100 | 100 |
| 2 | 2Z | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | 3B | 365/374 (98%) | 362 (99%) | 3 (1%) | 79 | 87 |
| 2 | 3D | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3F | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 3H | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3J | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3L | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3N | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3P | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | 3R | 366/374 (98%) | 366 (100%) | 0 | 100 | 100 |
| 2 | 3T | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | 4 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | 6 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | 8 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | A0 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | A2 | 365/374 (98%) | 363 (100%) | 2 (0%) | 86 | 91 |
| 2 | A4 | 365/374 (98%) | 357 (98%) | 8 (2%) | 47 | 68 |
| 2 | A8 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | B0 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | B2 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | B4 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | B7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | B9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | C1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | C5 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | C7 | 365/374 (98%) | 363 (100%) | 2 (0%) | 86 | 91 |
| 2 | C9 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | D1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | D3 | 360/374 (96%) | 360 (100%) | 0 | 100 | 100 |
| 2 | D5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | D7 | 360/374 (96%) | 360 (100%) | 0 | 100 | 100 |
| 2 | E1 | 360/374 (96%) | 358 (99%) | 2 (1%) | 84 | 90 |
| 2 | E3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | E5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | E7 | 360/374 (96%) | 358 (99%) | 2 (1%) | 84 | 90 |
| 2 | E9 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | F1 | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | F3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | F5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | F7 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | F9 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | G1 | 365/374 (98%) | 362 (99%) | 3 (1%) | 79 | 87 |
| 2 | G3 | 365/374 (98%) | 362 (99%) | 3 (1%) | 79 | 87 |
| 2 | G5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | G7 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | G9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | H1 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | H3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | H5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | H7 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | H9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | I1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | I3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | I5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | I7 | 361/374 (96%) | 361 (100%) | 0 | 100 | 100 |
| 2 | I9 | 360/374 (96%) | 356 (99%) | 4 (1%) | 70 | 81 |
| 2 | J1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | J3 | 360/374 (96%) | 359 (100%) | 1 (0%) | 91 | 95 |
| 2 | J5 | 366/374 (98%) | 366 (100%) | 0 | 100 | 100 |
| 2 | J7 | 359/374 (96%) | 354 (99%) | 5 (1%) | 62 | 77 |
| 2 | J9 | 366/374 (98%) | 366 (100%) | 0 | 100 | 100 |
| 2 | K1 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | K3 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | K5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | K7 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | K9 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | L1 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | L3 | 359/374 (96%) | 355 (99%) | 4 (1%) | 70 | 81 |
| 2 | L5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | L7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | L9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | M1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | M3 | 365/374 (98%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 2 | M5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | M7 | 365/374 (98%) | 363 (100%) | 2 (0%) | 86 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | M9 | 366/374 (98%) | 365 (100%) | 1 (0%) | 91 | 95 |
| 2 | N1 | 360/374 (96%) | 360 (100%) | 0 | 100 | 100 |
| 2 | N3 | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | N5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | N7 | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | N9 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | O1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | O3 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | O5 | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | O7 | 361/374 (96%) | 360 (100%) | 1 (0%) | 91 | 95 |
| 2 | O9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | P3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | P5 | 365/374 (98%) | 362 (99%) | 3 (1%) | 79 | 87 |
| 2 | P7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | P9 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | Q1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Q3 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | Q5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Q9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | R1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | R3 | 360/374 (96%) | 360 (100%) | 0 | 100 | 100 |
| 2 | R5 | 365/374 (98%) | 363 (100%) | 2 (0%) | 86 | 91 |
| 2 | R7 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | R9 | 365/374 (98%) | 365 (100%) | 0 | 100 | 100 |
| 2 | S1 | 361/374 (96%) | 358 (99%) | 3 (1%) | 79 | 87 |
| 2 | S5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | S7 | 365/374 (98%) | 364 (100%) | 1 (0%) | 91 | 95 |
| 2 | S9 | 359/374 (96%) | 355 (99%) | 4 (1%) | 70 | 81 |
| 2 | T1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | T3 | 359/374 (96%) | 354 (99%) | 5 (1%) | 62 | 77 |
| 2 | T5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | T7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | U1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | U3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | U5 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | U7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | U9 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | V1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | V3 | 359/374 (96%) | 355 (99%) | 4 (1%) | 70 | 81 |
| 2 | V7 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | V9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | W1 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | W3 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | W5 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | W7 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | W9 | 359/374 (96%) | 350 (98%) | 9 (2%) | 42 | 65 |
| 2 | X3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | X5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | X7 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | X9 | 359/374 (96%) | 356 (99%) | 3 (1%) | 79 | 87 |
| 2 | Y1 | 359/374 (96%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 2 | Y3 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | Y5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | Y9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Z1 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Z3 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Z5 | 359/374 (96%) | 357 (99%) | 2 (1%) | 84 | 90 |
| 2 | Z7 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 2 | Z9 | 359/374 (96%) | 359 (100%) | 0 | 100 | 100 |
| 3 | 3V | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 3X | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 3Z | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | 4B | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 4D | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 4F | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 4H | 251/258 (97%) | 229 (91%) | 22 (9%) | 8 | 28 |
| 3 | 4J | 178/258 (69%) | 178 (100%) | 0 | 100 | 100 |
| 4 | 3W | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 3Y | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 4A | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 4C | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 4E | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 4G | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 4 | 4I | 170/176 (97%) | 159 (94%) | 11 (6%) | 14 | 39 |
| 5 | 4L | 191/399 (48%) | 190 (100%) | 1 (0%) | 86 | 91 |
| 5 | 4M | 267/399 (67%) | 266 (100%) | 1 (0%) | 89 | 93 |
| 6 | 4N | 46/422 (11%) | 45 (98%) | 1 (2%) | 47 | 68 |
| 6 | 4O | 403/422 (96%) | 402 (100%) | 1 (0%) | 92 | 96 |
| 6 | 4P | 159/422 (38%) | 159 (100%) | 0 | 100 | 100 |
| 7 | 4Q | 54/306 (18%) | 54 (100%) | 0 | 100 | 100 |
| 7 | 4R | 305/306 (100%) | 300 (98%) | 5 (2%) | 58 | 75 |
| 7 | 4S | 40/306 (13%) | 38 (95%) | 2 (5%) | 20 | 46 |
| 7 | 4T | 160/306 (52%) | 159 (99%) | 1 (1%) | 84 | 90 |
| 7 | 4U | 234/306 (76%) | 234 (100%) | 0 | 100 | 100 |
| 8 | 4V | 63/362 (17%) | 63 (100%) | 0 | 100 | 100 |
| 8 | 4W | 261/362 (72%) | 258 (99%) | 3 (1%) | 70 | 81 |
| 8 | 4X | 49/362 (14%) | 48 (98%) | 1 (2%) | 50 | 70 |
| 9 | 4Y | 98/374 (26%) | 98 (100%) | 0 | 100 | 100 |
| 9 | 4Z | 309/374 (83%) | 309 (100%) | 0 | 100 | 100 |
| 10 | 5A | 194/433 (45%) | 193 (100%) | 1 (0%) | 86 | 91 |
| 10 | 5B | 220/433 (51%) | 218 (99%) | 2 (1%) | 75 | 86 |
| 10 | 5C | 323/433 (75%) | 320 (99%) | 3 (1%) | 75 | 86 |
| 10 | 5D | 97/433 (22%) | 97 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 11 | 5E | 211/223 (95%) | 209 (99%) | 2 (1%) | 75 | 86 |
| 12 | 5F | 332/340 (98%) | 328 (99%) | 4 (1%) | 67 | 80 |
| 12 | 5G | 127/340 (37%) | 126 (99%) | 1 (1%) | 79 | 87 |
| 12 | 7B | 83/340 (24%) | 82 (99%) | 1 (1%) | 67 | 80 |
| 13 | 5H | 119/121 (98%) | 100 (84%) | 19 (16%) | 2 | 8 |
| 13 | 5I | 119/121 (98%) | 100 (84%) | 19 (16%) | 2 | 8 |
| 13 | 5J | 119/121 (98%) | 100 (84%) | 19 (16%) | 2 | 8 |
| 13 | 5K | 119/121 (98%) | 100 (84%) | 19 (16%) | 2 | 8 |
| 14 | 5L | 511/517 (99%) | 450 (88%) | 61 (12%) | 4 | 16 |
| 14 | 5M | 511/517 (99%) | 453 (89%) | 58 (11%) | 4 | 17 |
| 14 | 5N | 511/517 (99%) | 450 (88%) | 61 (12%) | 4 | 16 |
| 15 | 5O | 307/309 (99%) | 262 (85%) | 45 (15%) | 2 | 10 |
| 15 | 5P | 307/309 (99%) | 291 (95%) | 16 (5%) | 19 | 45 |
| 16 | 5Q | 162/167 (97%) | 160 (99%) | 2 (1%) | 67 | 80 |
| 17 | 5R | 15/206 (7%) | 15 (100%) | 0 | 100 | 100 |
| 17 | 5S | 169/206 (82%) | 141 (83%) | 28 (17%) | 2 | 7 |
| 17 | 5T | 168/206 (82%) | 137 (82%) | 31 (18%) | 1 | 4 |
| 17 | 5U | 169/206 (82%) | 139 (82%) | 30 (18%) | 1 | 5 |
| 17 | 5V | 94/206 (46%) | 92 (98%) | 2 (2%) | 48 | 69 |
| 18 | 5X | 202/210 (96%) | 169 (84%) | 33 (16%) | 2 | 7 |
| 18 | 5Y | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 18 | 5Z | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 18 | 6A | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 18 | 6B | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 18 | 6C | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 18 | 6D | 202/210 (96%) | 170 (84%) | 32 (16%) | 2 | 8 |
| 19 | 6E | 211/222 (95%) | 209 (99%) | 2 (1%) | 75 | 86 |
| 20 | 6F | 310/314 (99%) | 308 (99%) | 2 (1%) | 84 | 90 |
| 21 | 6G | 150/171 (88%) | 150 (100%) | 0 | 100 | 100 |
| 21 | 6H | 157/171 (92%) | 157 (100%) | 0 | 100 | 100 |
| 22 | 6I | 285/303 (94%) | 283 (99%) | 2 (1%) | 81 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 22 | 6J | 285/303 (94%) | 284 (100%) | 1 (0%) | 89 | 93 |
| 22 | 6K | 285/303 (94%) | 283 (99%) | 2 (1%) | 81 | 88 |
| 22 | 6L | 285/303 (94%) | 284 (100%) | 1 (0%) | 89 | 93 |
| 22 | 6M | 285/303 (94%) | 282 (99%) | 3 (1%) | 70 | 81 |
| 22 | 6N | 285/303 (94%) | 284 (100%) | 1 (0%) | 89 | 93 |
| 22 | 6O | 285/303 (94%) | 283 (99%) | 2 (1%) | 81 | 88 |
| 22 | 6P | 257/303 (85%) | 254 (99%) | 3 (1%) | 67 | 80 |
| 23 | 6Q | 76/78 (97%) | 68 (90%) | 8 (10%) | 5 | 21 |
| 23 | 6R | 76/78 (97%) | 69 (91%) | 7 (9%) | 7 | 26 |
| 23 | 6S | 76/78 (97%) | 71 (93%) | 5 (7%) | 14 | 39 |
| 24 | 6T | 500/549 (91%) | 495 (99%) | 5 (1%) | 73 | 83 |
| 24 | 6U | 503/549 (92%) | 496 (99%) | 7 (1%) | 62 | 77 |
| 24 | 6V | 498/549 (91%) | 493 (99%) | 5 (1%) | 73 | 83 |
| 24 | 6W | 502/549 (91%) | 494 (98%) | 8 (2%) | 58 | 75 |
| 24 | 6X | 505/549 (92%) | 495 (98%) | 10 (2%) | 50 | 70 |
| 24 | 6Y | 499/549 (91%) | 492 (99%) | 7 (1%) | 62 | 77 |
| 24 | 6Z | 500/549 (91%) | 495 (99%) | 5 (1%) | 73 | 83 |
| 24 | 7A | 162/549 (30%) | 161 (99%) | 1 (1%) | 84 | 90 |
| 25 | 7C | 84/95 (88%) | 84 (100%) | 0 | 100 | 100 |
| 26 | 7D | 112/122 (92%) | 97 (87%) | 15 (13%) | 3 | 12 |
| 26 | 7E | 112/122 (92%) | 96 (86%) | 16 (14%) | 2 | 10 |
| 26 | 7F | 112/122 (92%) | 96 (86%) | 16 (14%) | 2 | 10 |
| 27 | 7G | 179/186 (96%) | 179 (100%) | 0 | 100 | 100 |
| 28 | 7H | 110/347 (32%) | 99 (90%) | 11 (10%) | 6 | 22 |
| 28 | 7X | 110/347 (32%) | 97 (88%) | 13 (12%) | 4 | 16 |
| 29 | 7I | 177/371 (48%) | 176 (99%) | 1 (1%) | 84 | 90 |
| 29 | 7J | 280/371 (76%) | 278 (99%) | 2 (1%) | 81 | 88 |
| 30 | 7K | 332/350 (95%) | 329 (99%) | 3 (1%) | 75 | 86 |
| 30 | 7L | 132/350 (38%) | 132 (100%) | 0 | 100 | 100 |
| 31 | 7M | 71/115 (62%) | 70 (99%) | 1 (1%) | 62 | 77 |
| 31 | 7N | 104/115 (90%) | 104 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 32 | 7O | 47/191 (25%) | 47 (100%) | 0 | 100 | 100 |
| 32 | 7P | 148/191 (78%) | 148 (100%) | 0 | 100 | 100 |
| 33 | 7Q | 64/165 (39%) | 64 (100%) | 0 | 100 | 100 |
| 34 | 7R | 172/618 (28%) | 171 (99%) | 1 (1%) | 84 | 90 |
| 34 | 7S | 143/618 (23%) | 142 (99%) | 1 (1%) | 81 | 88 |
| 35 | 7T | 186/462 (40%) | 184 (99%) | 2 (1%) | 70 | 81 |
| 35 | 7U | 157/462 (34%) | 157 (100%) | 0 | 100 | 100 |
| 36 | 7V | 82/162 (51%) | 71 (87%) | 11 (13%) | 3 | 12 |
| 36 | 7W | 82/162 (51%) | 70 (85%) | 12 (15%) | 2 | 10 |
| 37 | 7Y | 209/267 (78%) | 205 (98%) | 4 (2%) | 52 | 71 |
| 38 | 7Z | 31/206 (15%) | 31 (100%) | 0 | 100 | 100 |
| 38 | 8A | 179/206 (87%) | 174 (97%) | 5 (3%) | 38 | 62 |
| 38 | 8B | 182/206 (88%) | 175 (96%) | 7 (4%) | 28 | 54 |
| 38 | 8C | 182/206 (88%) | 172 (94%) | 10 (6%) | 18 | 44 |
| 38 | 8D | 141/206 (68%) | 128 (91%) | 13 (9%) | 7 | 26 |
| All | All | 146455/160298 (91%) | 145005 (99%) | 1450 (1%) | 71 | 83 |

All (1450) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 291 | GLN |
| 1 | 1 | 292 | GLN |
| 1 | 1 | 293 | MET |
| 1 | 1 | 324 | LYS |
| 1 | 3 | 274 | THR |
| 1 | 3 | 297 | LYS |
| 1 | 5 | 2 | ARG |
| 1 | 5 | 221 | THR |
| 1 | 7 | 401 | GLU |
| 1 | 7 | 404 | ASP |
| 1 | 9 | 306 | ARG |
| 1 | A1 | 297 | LYS |
| 2 | A2 | 40 | LYS |
| 2 | A2 | 163 | LYS |
| 1 | A3 | 297 | LYS |
| 2 | A4 | 40 | LYS |
| 2 | A4 | 56 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A4 | 84 | ARG |
| 2 | A4 | 85 | GLN |
| 2 | A4 | 90 | GLU |
| 2 | A4 | 285 | GLN |
| 2 | A4 | 305 | CYS |
| 2 | A4 | 326 | LYS |
| 2 | A8 | 326 | LYS |
| 1 | A9 | 306 | ARG |
| 2 | B0 | 349 | THR |
| 1 | B1 | 406 | MET |
| 2 | B2 | 326 | LYS |
| 2 | B4 | 290 | GLU |
| 1 | B5 | 306 | ARG |
| 1 | B5 | 362 | LYS |
| 2 | B7 | 2 | ARG |
| 2 | B7 | 163 | LYS |
| 1 | B8 | 362 | LYS |
| 1 | C2 | 359 | LYS |
| 2 | C7 | 203 | MET |
| 2 | C7 | 349 | THR |
| 2 | C9 | 62 | VAL |
| 2 | D1 | 90 | GLU |
| 2 | D1 | 326 | LYS |
| 1 | D4 | 33 | THR |
| 1 | D4 | 67 | ASP |
| 2 | D5 | 276 | ILE |
| 1 | D6 | 379 | LYS |
| 1 | E0 | 199 | CYS |
| 2 | E1 | 170 | THR |
| 2 | E1 | 221 | ARG |
| 1 | E2 | 8 | GLN |
| 2 | E5 | 282 | TYR |
| 2 | E5 | 326 | LYS |
| 2 | E7 | 121 | ARG |
| 2 | E7 | 283 | HIS |
| 2 | E9 | 121 | ARG |
| 2 | F1 | 313 | MET |
| 2 | F1 | 326 | LYS |
| 2 | F1 | 346 | TRP |
| 2 | F5 | 2 | ARG |
| 2 | F7 | 36 | MET |
| 1 | F8 | 406 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F8 | 415 | MET |
| 1 | G0 | 391 | ARG |
| 2 | G1 | 344 | VAL |
| 2 | G1 | 345 | ASP |
| 2 | G1 | 347 | CYS |
| 1 | G2 | 391 | ARG |
| 2 | G3 | 39 | ASP |
| 2 | G3 | 46 | ASP |
| 2 | G3 | 85 | GLN |
| 1 | G4 | 406 | MET |
| 2 | G7 | 326 | LYS |
| 2 | H1 | 326 | LYS |
| 1 | H6 | 306 | ARG |
| 1 | H8 | 306 | ARG |
| 1 | H8 | 406 | MET |
| 2 | I1 | 56 | THR |
| 2 | I1 | 121 | ARG |
| 2 | I9 | 56 | THR |
| 2 | I9 | 121 | ARG |
| 2 | I9 | 282 | TYR |
| 2 | I9 | 326 | LYS |
| 2 | J3 | 56 | THR |
| 2 | J7 | 2 | ARG |
| 2 | J7 | 56 | THR |
| 2 | J7 | 121 | ARG |
| 2 | J7 | 282 | TYR |
| 2 | J7 | 284 | GLU |
| 1 | K0 | 1 | MET |
| 2 | K1 | 170 | THR |
| 2 | K3 | 217 | LEU |
| 2 | K5 | 285 | GLN |
| 1 | K6 | 406 | MET |
| 2 | K7 | 121 | ARG |
| 2 | K9 | 62 | VAL |
| 2 | K9 | 90 | GLU |
| 1 | L0 | 406 | MET |
| 2 | L1 | 90 | GLU |
| 2 | L3 | 90 | GLU |
| 2 | L3 | 91 | GLN |
| 2 | L3 | 121 | ARG |
| 2 | L3 | 339 | ARG |
| 2 | L7 | 221 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L7 | 430 | LYS |
| 2 | M3 | 42 | ILE |
| 2 | M3 | 46 | ASP |
| 2 | M3 | 49 | PHE |
| 2 | M3 | 221 | ARG |
| 1 | M4 | 324 | LYS |
| 2 | M5 | 121 | ARG |
| 2 | M7 | 221 | ARG |
| 2 | M7 | 285 | GLN |
| 1 | M8 | 406 | MET |
| 2 | M9 | 46 | ASP |
| 1 | N0 | 92 | PHE |
| 2 | N3 | 84 | ARG |
| 2 | N3 | 227 | LEU |
| 2 | N3 | 363 | VAL |
| 2 | N5 | 121 | ARG |
| 2 | N5 | 326 | LYS |
| 2 | N7 | 2 | ARG |
| 2 | N7 | 90 | GLU |
| 2 | N7 | 121 | ARG |
| 2 | N9 | 163 | LYS |
| 2 | O1 | 56 | THR |
| 2 | O1 | 85 | GLN |
| 1 | O2 | 282 | ARG |
| 1 | O2 | 391 | ARG |
| 2 | O3 | 90 | GLU |
| 2 | O3 | 346 | TRP |
| 2 | O5 | 121 | ARG |
| 2 | O5 | 123 | ARG |
| 2 | O5 | 163 | LYS |
| 1 | O6 | 281 | TYR |
| 1 | O6 | 406 | MET |
| 2 | O7 | 347 | CYS |
| 2 | P5 | 36 | MET |
| 2 | P5 | 42 | ILE |
| 2 | P5 | 62 | VAL |
| 2 | P7 | 279 | GLU |
| 2 | P7 | 341 | ILE |
| 1 | Q2 | 297 | LYS |
| 2 | Q3 | 56 | THR |
| 2 | Q3 | 62 | VAL |
| 1 | Q8 | 359 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q8 | 406 | MET |
| 2 | R1 | 62 | VAL |
| 2 | R1 | 90 | GLU |
| 1 | R2 | 396 | HIS |
| 1 | R2 | 401 | GLU |
| 1 | R4 | 391 | ARG |
| 2 | R5 | 2 | ARG |
| 2 | R5 | 56 | THR |
| 1 | S0 | 91 | VAL |
| 1 | S0 | 274 | THR |
| 2 | S1 | 56 | THR |
| 2 | S1 | 62 | VAL |
| 2 | S1 | 283 | HIS |
| 2 | S5 | 326 | LYS |
| 2 | S7 | 415 | GLU |
| 2 | S9 | 326 | LYS |
| 2 | S9 | 339 | ARG |
| 2 | S9 | 411 | GLU |
| 2 | S9 | 417 | GLU |
| 1 | T2 | 1 | MET |
| 2 | T3 | 56 | THR |
| 2 | T3 | 62 | VAL |
| 2 | T3 | 88 | HIS |
| 2 | T3 | 90 | GLU |
| 2 | T3 | 326 | LYS |
| 1 | T4 | 166 | THR |
| 2 | T5 | 56 | THR |
| 2 | T5 | 85 | GLN |
| 1 | T6 | 51 | PHE |
| 1 | T6 | 88 | ASP |
| 1 | T6 | 91 | VAL |
| 2 | T7 | 2 | ARG |
| 2 | T7 | 326 | LYS |
| 1 | U2 | 282 | ARG |
| 1 | U4 | 263 | LEU |
| 1 | U4 | 406 | MET |
| 2 | U7 | 56 | THR |
| 2 | U7 | 121 | ARG |
| 1 | U8 | 237 | THR |
| 1 | U8 | 282 | ARG |
| 2 | U9 | 90 | GLU |
| 2 | V1 | 56 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | V1 | 86 | LEU |
| 1 | V2 | 67 | ASP |
| 1 | V2 | 166 | THR |
| 1 | V2 | 282 | ARG |
| 2 | V3 | 56 | THR |
| 2 | V3 | 120 | ASP |
| 2 | V3 | 121 | ARG |
| 2 | V3 | 163 | LYS |
| 1 | V8 | 67 | ASP |
| 2 | W1 | 60 | LYS |
| 2 | W1 | 90 | GLU |
| 2 | W3 | 56 | THR |
| 1 | W4 | 53 | GLU |
| 2 | W5 | 339 | ARG |
| 1 | W8 | 58 | ARG |
| 1 | W8 | 342 | VAL |
| 1 | W8 | 344 | TRP |
| 2 | W9 | 5 | ILE |
| 2 | W9 | 14 | ILE |
| 2 | W9 | 69 | ASP |
| 2 | W9 | 70 | LEU |
| 2 | W9 | 74 | VAL |
| 2 | W9 | 76 | ASP |
| 2 | W9 | 83 | TYR |
| 2 | W9 | 105 | ARG |
| 2 | W9 | 284 | GLU |
| 1 | X0 | 67 | ASP |
| 1 | X2 | 67 | ASP |
| 2 | X5 | 297 | GLU |
| 2 | X5 | 430 | LYS |
| 2 | X7 | 282 | TYR |
| 2 | X7 | 326 | LYS |
| 1 | X8 | 406 | MET |
| 2 | X9 | 279 | GLU |
| 2 | X9 | 284 | GLU |
| 2 | X9 | 286 | LEU |
| 2 | Y1 | 339 | ARG |
| 2 | Y3 | 283 | HIS |
| 2 | Y3 | 327 | ASP |
| 2 | Y5 | 157 | LEU |
| 2 | Y5 | 159 | VAL |
| 1 | Y6 | 52 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y6 | 58 | ARG |
| 1 | Y8 | 324 | LYS |
| 2 | Z5 | 343 | PHE |
| 2 | Z5 | 346 | TRP |
| 1 | Z6 | 406 | MET |
| 1 | 0A | 406 | MET |
| 1 | 0E | 306 | ARG |
| 1 | 0E | 391 | ARG |
| 2 | 0F | 346 | TRP |
| 1 | 0G | 406 | MET |
| 1 | 0I | 406 | MET |
| 1 | 0K | 388 | MET |
| 1 | 0K | 415 | MET |
| 2 | 0L | 344 | VAL |
| 1 | 0M | 415 | MET |
| 2 | 0N | 2 | ARG |
| 2 | 0N | 346 | TRP |
| 2 | 0N | 347 | CYS |
| 2 | 0P | 344 | VAL |
| 2 | 0R | 5 | ILE |
| 1 | 0S | 154 | LYS |
| 1 | 0U | 306 | ARG |
| 2 | 0V | 346 | TRP |
| 2 | 0V | 347 | CYS |
| 2 | 0X | 326 | LYS |
| 1 | 0Y | 59 | TYR |
| 2 | 0Z | 56 | THR |
| 2 | 0Z | 326 | LYS |
| 2 | 1B | 326 | LYS |
| 2 | 1B | 347 | CYS |
| 1 | 1C | 396 | HIS |
| 2 | 1D | 326 | LYS |
| 2 | 1H | 326 | LYS |
| 2 | 1H | 344 | VAL |
| 2 | 1H | 347 | CYS |
| 2 | 1L | 56 | THR |
| 2 | 1L | 121 | ARG |
| 1 | 1M | 297 | LYS |
| 1 | 1M | 306 | ARG |
| 1 | 1M | 320 | ARG |
| 2 | 1N | 56 | THR |
| 2 | 1N | 85 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1N | 346 | TRP |
| 1 | 1O | 306 | ARG |
| 2 | 1P | 284 | GLU |
| 1 | 1Q | 396 | HIS |
| 2 | 1R | 55 | GLU |
| 2 | 1R | 56 | THR |
| 2 | 1R | 90 | GLU |
| 2 | 1R | 120 | ASP |
| 2 | 1R | 121 | ARG |
| 2 | 1R | 344 | VAL |
| 2 | 1R | 346 | TRP |
| 2 | 1R | 347 | CYS |
| 2 | 1T | 326 | LYS |
| 1 | 1U | 306 | ARG |
| 2 | 1V | 56 | THR |
| 2 | 1V | 121 | ARG |
| 2 | 1V | 282 | TYR |
| 2 | 1V | 283 | HIS |
| 1 | 1W | 306 | ARG |
| 2 | 1Z | 92 | LEU |
| 2 | 1Z | 326 | LYS |
| 1 | 2A | 406 | MET |
| 1 | 2C | 406 | MET |
| 2 | 2J | 56 | THR |
| 1 | 2K | 406 | MET |
| 2 | 2L | 282 | TYR |
| 2 | 2P | 2 | ARG |
| 2 | 2P | 279 | GLU |
| 2 | 2P | 283 | HIS |
| 1 | 2Q | 276 | ARG |
| 1 | 2Q | 406 | MET |
| 1 | 2S | 77 | ARG |
| 1 | 2S | 276 | ARG |
| 2 | 2T | 430 | LYS |
| 1 | 2U | 58 | ARG |
| 1 | 2U | 406 | MET |
| 2 | 2V | 326 | LYS |
| 1 | 2W | 58 | ARG |
| 1 | 2Y | 58 | ARG |
| 2 | 2Z | 56 | THR |
| 2 | 2Z | 121 | ARG |
| 2 | 2Z | 339 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 3A | 58 | ARG |
| 2 | 3B | 56 | THR |
| 2 | 3B | 121 | ARG |
| 2 | 3B | 276 | ILE |
| 1 | 3C | 47 | ILE |
| 1 | 3C | 53 | GLU |
| 2 | 3F | 316 | CYS |
| 1 | 3I | 52 | ASN |
| 1 | 3M | 52 | ASN |
| 1 | 3O | 52 | ASN |
| 1 | 3O | 406 | MET |
| 2 | 3T | 221 | ARG |
| 3 | 3V | 4 | ASP |
| 3 | 3V | 11 | THR |
| 3 | 3V | 12 | SER |
| 3 | 3V | 22 | LYS |
| 3 | 3V | 38 | THR |
| 3 | 3V | 53 | ASP |
| 3 | 3V | 56 | LYS |
| 3 | 3V | 79 | THR |
| 3 | 3V | 88 | GLU |
| 3 | 3V | 93 | LYS |
| 3 | 3V | 103 | SER |
| 3 | 3V | 111 | LYS |
| 3 | 3V | 143 | ILE |
| 3 | 3V | 152 | LEU |
| 3 | 3V | 168 | THR |
| 3 | 3V | 170 | GLU |
| 3 | 3V | 182 | ASP |
| 3 | 3V | 204 | THR |
| 3 | 3V | 208 | THR |
| 3 | 3V | 231 | VAL |
| 3 | 3V | 236 | VAL |
| 3 | 3V | 288 | ASP |
| 4 | 3W | 12 | SER |
| 4 | 3W | 30 | SER |
| 4 | 3W | 45 | SER |
| 4 | 3W | 55 | SER |
| 4 | 3W | 56 | THR |
| 4 | 3W | 99 | VAL |
| 4 | 3W | 140 | THR |
| 4 | 3W | 162 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 3W | 168 | SER |
| 4 | 3W | 171 | LEU |
| 4 | 3W | 173 | SER |
| 3 | 3X | 4 | ASP |
| 3 | 3X | 11 | THR |
| 3 | 3X | 12 | SER |
| 3 | 3X | 22 | LYS |
| 3 | 3X | 38 | THR |
| 3 | 3X | 53 | ASP |
| 3 | 3X | 56 | LYS |
| 3 | 3X | 79 | THR |
| 3 | 3X | 88 | GLU |
| 3 | 3X | 93 | LYS |
| 3 | 3X | 103 | SER |
| 3 | 3X | 111 | LYS |
| 3 | 3X | 143 | ILE |
| 3 | 3X | 152 | LEU |
| 3 | 3X | 168 | THR |
| 3 | 3X | 170 | GLU |
| 3 | 3X | 182 | ASP |
| 3 | 3X | 204 | THR |
| 3 | 3X | 208 | THR |
| 3 | 3X | 231 | VAL |
| 3 | 3X | 236 | VAL |
| 3 | 3X | 288 | ASP |
| 4 | 3Y | 12 | SER |
| 4 | 3Y | 30 | SER |
| 4 | 3Y | 45 | SER |
| 4 | 3Y | 55 | SER |
| 4 | 3Y | 56 | THR |
| 4 | 3Y | 99 | VAL |
| 4 | 3Y | 140 | THR |
| 4 | 3Y | 162 | ILE |
| 4 | 3Y | 168 | SER |
| 4 | 3Y | 171 | LEU |
| 4 | 3Y | 173 | SER |
| 3 | 3Z | 4 | ASP |
| 3 | 3Z | 11 | THR |
| 3 | 3Z | 12 | SER |
| 3 | 3Z | 22 | LYS |
| 3 | 3Z | 38 | THR |
| 3 | 3Z | 53 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 3Z | 56 | LYS |
| 3 | 3Z | 79 | THR |
| 3 | 3Z | 88 | GLU |
| 3 | 3Z | 93 | LYS |
| 3 | 3Z | 103 | SER |
| 3 | 3Z | 111 | LYS |
| 3 | 3Z | 143 | ILE |
| 3 | 3Z | 152 | LEU |
| 3 | 3Z | 168 | THR |
| 3 | 3Z | 170 | GLU |
| 3 | 3Z | 182 | ASP |
| 3 | 3Z | 204 | THR |
| 3 | 3Z | 208 | THR |
| 3 | 3Z | 231 | VAL |
| 3 | 3Z | 236 | VAL |
| 3 | 3Z | 288 | ASP |
| 4 | 4A | 12 | SER |
| 4 | 4A | 30 | SER |
| 4 | 4A | 45 | SER |
| 4 | 4A | 55 | SER |
| 4 | 4A | 56 | THR |
| 4 | 4A | 99 | VAL |
| 4 | 4A | 140 | THR |
| 4 | 4A | 162 | ILE |
| 4 | 4A | 168 | SER |
| 4 | 4A | 171 | LEU |
| 4 | 4A | 173 | SER |
| 3 | 4B | 4 | ASP |
| 3 | 4B | 11 | THR |
| 3 | 4B | 12 | SER |
| 3 | 4B | 22 | LYS |
| 3 | 4B | 38 | THR |
| 3 | 4B | 53 | ASP |
| 3 | 4B | 56 | LYS |
| 3 | 4B | 79 | THR |
| 3 | 4B | 88 | GLU |
| 3 | 4B | 93 | LYS |
| 3 | 4B | 103 | SER |
| 3 | 4B | 111 | LYS |
| 3 | 4B | 143 | ILE |
| 3 | 4B | 152 | LEU |
| 3 | 4B | 168 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 4B | 170 | GLU |
| 3 | 4B | 182 | ASP |
| 3 | 4B | 204 | THR |
| 3 | 4B | 208 | THR |
| 3 | 4B | 231 | VAL |
| 3 | 4B | 236 | VAL |
| 3 | 4B | 288 | ASP |
| 4 | 4C | 12 | SER |
| 4 | 4C | 30 | SER |
| 4 | 4C | 45 | SER |
| 4 | 4C | 55 | SER |
| 4 | 4C | 56 | THR |
| 4 | 4C | 99 | VAL |
| 4 | 4C | 140 | THR |
| 4 | 4C | 162 | ILE |
| 4 | 4C | 168 | SER |
| 4 | 4C | 171 | LEU |
| 4 | 4C | 173 | SER |
| 3 | 4D | 4 | ASP |
| 3 | 4D | 11 | THR |
| 3 | 4D | 12 | SER |
| 3 | 4D | 22 | LYS |
| 3 | 4D | 38 | THR |
| 3 | 4D | 53 | ASP |
| 3 | 4D | 56 | LYS |
| 3 | 4D | 79 | THR |
| 3 | 4D | 88 | GLU |
| 3 | 4D | 93 | LYS |
| 3 | 4D | 103 | SER |
| 3 | 4D | 111 | LYS |
| 3 | 4D | 143 | ILE |
| 3 | 4D | 152 | LEU |
| 3 | 4D | 168 | THR |
| 3 | 4D | 170 | GLU |
| 3 | 4D | 182 | ASP |
| 3 | 4D | 204 | THR |
| 3 | 4D | 208 | THR |
| 3 | 4D | 231 | VAL |
| 3 | 4D | 236 | VAL |
| 3 | 4D | 288 | ASP |
| 4 | 4E | 12 | SER |
| 4 | 4E | 30 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 4E | 45 | SER |
| 4 | 4E | 55 | SER |
| 4 | 4E | 56 | THR |
| 4 | 4E | 99 | VAL |
| 4 | 4E | 140 | THR |
| 4 | 4E | 162 | ILE |
| 4 | 4E | 168 | SER |
| 4 | 4E | 171 | LEU |
| 4 | 4E | 173 | SER |
| 3 | 4F | 4 | ASP |
| 3 | 4F | 11 | THR |
| 3 | 4F | 12 | SER |
| 3 | 4F | 22 | LYS |
| 3 | 4F | 38 | THR |
| 3 | 4F | 53 | ASP |
| 3 | 4F | 56 | LYS |
| 3 | 4F | 79 | THR |
| 3 | 4F | 88 | GLU |
| 3 | 4F | 93 | LYS |
| 3 | 4F | 103 | SER |
| 3 | 4F | 111 | LYS |
| 3 | 4F | 143 | ILE |
| 3 | 4F | 152 | LEU |
| 3 | 4F | 168 | THR |
| 3 | 4F | 170 | GLU |
| 3 | 4F | 182 | ASP |
| 3 | 4F | 204 | THR |
| 3 | 4F | 208 | THR |
| 3 | 4F | 231 | VAL |
| 3 | 4F | 236 | VAL |
| 3 | 4F | 288 | ASP |
| 4 | 4G | 12 | SER |
| 4 | 4G | 30 | SER |
| 4 | 4G | 45 | SER |
| 4 | 4G | 55 | SER |
| 4 | 4G | 56 | THR |
| 4 | 4G | 99 | VAL |
| 4 | 4G | 140 | THR |
| 4 | 4G | 162 | ILE |
| 4 | 4G | 168 | SER |
| 4 | 4G | 171 | LEU |
| 4 | 4G | 173 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 4H | 4 | ASP |
| 3 | 4H | 11 | THR |
| 3 | 4H | 12 | SER |
| 3 | 4H | 22 | LYS |
| 3 | 4H | 38 | THR |
| 3 | 4H | 53 | ASP |
| 3 | 4H | 56 | LYS |
| 3 | 4H | 79 | THR |
| 3 | 4H | 88 | GLU |
| 3 | 4H | 93 | LYS |
| 3 | 4H | 103 | SER |
| 3 | 4H | 111 | LYS |
| 3 | 4H | 143 | ILE |
| 3 | 4H | 152 | LEU |
| 3 | 4H | 168 | THR |
| 3 | 4H | 170 | GLU |
| 3 | 4H | 182 | ASP |
| 3 | 4H | 204 | THR |
| 3 | 4H | 208 | THR |
| 3 | 4H | 231 | VAL |
| 3 | 4H | 236 | VAL |
| 3 | 4H | 288 | ASP |
| 4 | 4I | 12 | SER |
| 4 | 4I | 30 | SER |
| 4 | 4I | 45 | SER |
| 4 | 4I | 55 | SER |
| 4 | 4I | 56 | THR |
| 4 | 4I | 99 | VAL |
| 4 | 4I | 140 | THR |
| 4 | 4I | 162 | ILE |
| 4 | 4I | 168 | SER |
| 4 | 4I | 171 | LEU |
| 4 | 4I | 173 | SER |
| 5 | 4L | 469 | THR |
| 5 | 4M | 146 | ARG |
| 6 | 4N | 475 | ARG |
| 6 | 4O | 358 | LYS |
| 7 | 4R | 12 | ASP |
| 7 | 4R | 14 | GLU |
| 7 | 4R | 58 | LEU |
| 7 | 4R | 98 | ARG |
| 7 | 4R | 301 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 4S | 3 | ARG |
| 7 | 4S | 11 | GLU |
| 7 | 4T | 209 | ARG |
| 8 | 4W | 461 | VAL |
| 8 | 4W | 463 | THR |
| 8 | 4W | 466 | ARG |
| 8 | 4X | 98 | MET |
| 10 | 5A | 338 | LYS |
| 10 | 5B | 90 | LYS |
| 10 | 5B | 260 | LYS |
| 10 | 5C | 230 | ARG |
| 10 | 5C | 429 | LYS |
| 10 | 5C | 493 | GLU |
| 11 | 5E | 110 | GLN |
| 11 | 5E | 112 | ARG |
| 12 | 5F | 43 | HIS |
| 12 | 5F | 44 | ILE |
| 12 | 5F | 58 | ARG |
| 12 | 5F | 199 | LYS |
| 12 | 5G | 283 | LYS |
| 13 | 5H | 3 | ARG |
| 13 | 5H | 28 | ASP |
| 13 | 5H | 31 | GLN |
| 13 | 5H | 33 | ILE |
| 13 | 5H | 37 | THR |
| 13 | 5H | 56 | ASP |
| 13 | 5H | 70 | LYS |
| 13 | 5H | 76 | THR |
| 13 | 5H | 78 | THR |
| 13 | 5H | 79 | THR |
| 13 | 5H | 84 | ASP |
| 13 | 5H | 85 | SER |
| 13 | 5H | 92 | GLU |
| 13 | 5H | 99 | ASN |
| 13 | 5H | 100 | MET |
| 13 | 5H | 103 | THR |
| 13 | 5H | 120 | THR |
| 13 | 5H | 124 | VAL |
| 13 | 5H | 126 | VAL |
| 13 | 5I | 3 | ARG |
| 13 | 5I | 28 | ASP |
| 13 | 5I | 31 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 5I | 33 | ILE |
| 13 | 5I | 37 | THR |
| 13 | 5I | 56 | ASP |
| 13 | 5I | 70 | LYS |
| 13 | 5I | 76 | THR |
| 13 | 5I | 78 | THR |
| 13 | 5I | 79 | THR |
| 13 | 5I | 84 | ASP |
| 13 | 5I | 85 | SER |
| 13 | 5I | 92 | GLU |
| 13 | 5I | 99 | ASN |
| 13 | 5I | 100 | MET |
| 13 | 5I | 103 | THR |
| 13 | 5I | 120 | THR |
| 13 | 5I | 124 | VAL |
| 13 | 5I | 126 | VAL |
| 13 | 5J | 3 | ARG |
| 13 | 5J | 28 | ASP |
| 13 | 5J | 31 | GLN |
| 13 | 5J | 33 | ILE |
| 13 | 5J | 37 | THR |
| 13 | 5J | 56 | ASP |
| 13 | 5J | 70 | LYS |
| 13 | 5J | 76 | THR |
| 13 | 5J | 78 | THR |
| 13 | 5J | 79 | THR |
| 13 | 5J | 84 | ASP |
| 13 | 5J | 85 | SER |
| 13 | 5J | 92 | GLU |
| 13 | 5J | 99 | ASN |
| 13 | 5J | 100 | MET |
| 13 | 5J | 103 | THR |
| 13 | 5J | 120 | THR |
| 13 | 5J | 124 | VAL |
| 13 | 5J | 126 | VAL |
| 13 | 5K | 3 | ARG |
| 13 | 5K | 28 | ASP |
| 13 | 5K | 31 | GLN |
| 13 | 5K | 33 | ILE |
| 13 | 5K | 37 | THR |
| 13 | 5K | 56 | ASP |
| 13 | 5K | 70 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 5K | 76 | THR |
| 13 | 5K | 78 | THR |
| 13 | 5K | 79 | THR |
| 13 | 5K | 84 | ASP |
| 13 | 5K | 85 | SER |
| 13 | 5K | 92 | GLU |
| 13 | 5K | 99 | ASN |
| 13 | 5K | 100 | MET |
| 13 | 5K | 103 | THR |
| 13 | 5K | 120 | THR |
| 13 | 5K | 124 | VAL |
| 13 | 5K | 126 | VAL |
| 14 | 5L | 9 | SER |
| 14 | 5L | 10 | VAL |
| 14 | 5L | 11 | ILE |
| 14 | 5L | 18 | GLU |
| 14 | 5L | 59 | VAL |
| 14 | 5L | 91 | GLU |
| 14 | 5L | 95 | LEU |
| 14 | 5L | 104 | VAL |
| 14 | 5L | 106 | VAL |
| 14 | 5L | 116 | ARG |
| 14 | 5L | 121 | LEU |
| 14 | 5L | 126 | ASP |
| 14 | 5L | 127 | ASN |
| 14 | 5L | 147 | THR |
| 14 | 5L | 153 | VAL |
| 14 | 5L | 158 | ASN |
| 14 | 5L | 164 | ILE |
| 14 | 5L | 180 | ASN |
| 14 | 5L | 186 | THR |
| 14 | 5L | 201 | VAL |
| 14 | 5L | 214 | THR |
| 14 | 5L | 227 | LEU |
| 14 | 5L | 228 | PHE |
| 14 | 5L | 245 | THR |
| 14 | 5L | 272 | SER |
| 14 | 5L | 282 | MET |
| 14 | 5L | 302 | MET |
| 14 | 5L | 322 | THR |
| 14 | 5L | 331 | LYS |
| 14 | 5L | 333 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5L | 337 | THR |
| 14 | 5L | 350 | ASN |
| 14 | 5L | 361 | THR |
| 14 | 5L | 366 | LEU |
| 14 | 5L | 370 | THR |
| 14 | 5L | 371 | THR |
| 14 | 5L | 383 | LEU |
| 14 | 5L | 415 | LYS |
| 14 | 5L | 421 | ASN |
| 14 | 5L | 429 | THR |
| 14 | 5L | 431 | ILE |
| 14 | 5L | 433 | SER |
| 14 | 5L | 434 | THR |
| 14 | 5L | 445 | GLU |
| 14 | 5L | 456 | ARG |
| 14 | 5L | 457 | THR |
| 14 | 5L | 458 | SER |
| 14 | 5L | 460 | THR |
| 14 | 5L | 464 | SER |
| 14 | 5L | 467 | ASP |
| 14 | 5L | 477 | ILE |
| 14 | 5L | 494 | ILE |
| 14 | 5L | 505 | THR |
| 14 | 5L | 526 | VAL |
| 14 | 5L | 530 | THR |
| 14 | 5L | 540 | TYR |
| 14 | 5L | 541 | ASP |
| 14 | 5L | 554 | ASP |
| 14 | 5L | 561 | VAL |
| 14 | 5L | 604 | THR |
| 14 | 5L | 619 | ILE |
| 14 | 5M | 9 | SER |
| 14 | 5M | 10 | VAL |
| 14 | 5M | 11 | ILE |
| 14 | 5M | 18 | GLU |
| 14 | 5M | 59 | VAL |
| 14 | 5M | 91 | GLU |
| 14 | 5M | 95 | LEU |
| 14 | 5M | 104 | VAL |
| 14 | 5M | 106 | VAL |
| 14 | 5M | 112 | SER |
| 14 | 5M | 121 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5M | 126 | ASP |
| 14 | 5M | 127 | ASN |
| 14 | 5M | 147 | THR |
| 14 | 5M | 153 | VAL |
| 14 | 5M | 158 | ASN |
| 14 | 5M | 164 | ILE |
| 14 | 5M | 180 | ASN |
| 14 | 5M | 186 | THR |
| 14 | 5M | 201 | VAL |
| 14 | 5M | 214 | THR |
| 14 | 5M | 224 | GLU |
| 14 | 5M | 228 | PHE |
| 14 | 5M | 245 | THR |
| 14 | 5M | 272 | SER |
| 14 | 5M | 282 | MET |
| 14 | 5M | 302 | MET |
| 14 | 5M | 322 | THR |
| 14 | 5M | 331 | LYS |
| 14 | 5M | 333 | GLU |
| 14 | 5M | 337 | THR |
| 14 | 5M | 350 | ASN |
| 14 | 5M | 361 | THR |
| 14 | 5M | 366 | LEU |
| 14 | 5M | 370 | THR |
| 14 | 5M | 371 | THR |
| 14 | 5M | 383 | LEU |
| 14 | 5M | 421 | ASN |
| 14 | 5M | 429 | THR |
| 14 | 5M | 431 | ILE |
| 14 | 5M | 433 | SER |
| 14 | 5M | 434 | THR |
| 14 | 5M | 445 | GLU |
| 14 | 5M | 456 | ARG |
| 14 | 5M | 457 | THR |
| 14 | 5M | 458 | SER |
| 14 | 5M | 460 | THR |
| 14 | 5M | 464 | SER |
| 14 | 5M | 467 | ASP |
| 14 | 5M | 477 | ILE |
| 14 | 5M | 505 | THR |
| 14 | 5M | 512 | PHE |
| 14 | 5M | 526 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5M | 530 | THR |
| 14 | 5M | 554 | ASP |
| 14 | 5M | 561 | VAL |
| 14 | 5M | 604 | THR |
| 14 | 5M | 619 | ILE |
| 14 | 5N | 9 | SER |
| 14 | 5N | 10 | VAL |
| 14 | 5N | 11 | ILE |
| 14 | 5N | 18 | GLU |
| 14 | 5N | 59 | VAL |
| 14 | 5N | 91 | GLU |
| 14 | 5N | 95 | LEU |
| 14 | 5N | 104 | VAL |
| 14 | 5N | 106 | VAL |
| 14 | 5N | 112 | SER |
| 14 | 5N | 121 | LEU |
| 14 | 5N | 126 | ASP |
| 14 | 5N | 127 | ASN |
| 14 | 5N | 147 | THR |
| 14 | 5N | 153 | VAL |
| 14 | 5N | 158 | ASN |
| 14 | 5N | 164 | ILE |
| 14 | 5N | 180 | ASN |
| 14 | 5N | 187 | ASP |
| 14 | 5N | 192 | THR |
| 14 | 5N | 201 | VAL |
| 14 | 5N | 214 | THR |
| 14 | 5N | 225 | ARG |
| 14 | 5N | 226 | VAL |
| 14 | 5N | 245 | THR |
| 14 | 5N | 272 | SER |
| 14 | 5N | 282 | MET |
| 14 | 5N | 302 | MET |
| 14 | 5N | 322 | THR |
| 14 | 5N | 333 | GLU |
| 14 | 5N | 337 | THR |
| 14 | 5N | 350 | ASN |
| 14 | 5N | 361 | THR |
| 14 | 5N | 366 | LEU |
| 14 | 5N | 370 | THR |
| 14 | 5N | 371 | THR |
| 14 | 5N | 383 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5N | 415 | LYS |
| 14 | 5N | 421 | ASN |
| 14 | 5N | 429 | THR |
| 14 | 5N | 431 | ILE |
| 14 | 5N | 433 | SER |
| 14 | 5N | 434 | THR |
| 14 | 5N | 445 | GLU |
| 14 | 5N | 456 | ARG |
| 14 | 5N | 457 | THR |
| 14 | 5N | 458 | SER |
| 14 | 5N | 460 | THR |
| 14 | 5N | 464 | SER |
| 14 | 5N | 467 | ASP |
| 14 | 5N | 477 | ILE |
| 14 | 5N | 505 | THR |
| 14 | 5N | 511 | THR |
| 14 | 5N | 512 | PHE |
| 14 | 5N | 526 | VAL |
| 14 | 5N | 530 | THR |
| 14 | 5N | 554 | ASP |
| 14 | 5N | 557 | ASN |
| 14 | 5N | 561 | VAL |
| 14 | 5N | 604 | THR |
| 14 | 5N | 619 | ILE |
| 15 | 5O | 4 | ASN |
| 15 | 5O | 14 | LEU |
| 15 | 5O | 15 | ASP |
| 15 | 5O | 23 | LYS |
| 15 | 5O | 29 | TYR |
| 15 | 5O | 34 | GLU |
| 15 | 5O | 35 | VAL |
| 15 | 5O | 39 | ASP |
| 15 | 5O | 43 | ARG |
| 15 | 5O | 49 | ARG |
| 15 | 5O | 55 | LEU |
| 15 | 5O | 56 | LYS |
| 15 | 5O | 59 | LEU |
| 15 | 5O | 60 | LEU |
| 15 | 5O | 62 | LEU |
| 15 | 5O | 68 | VAL |
| 15 | 5O | 73 | LEU |
| 15 | 5O | 77 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 5O | 101 | ASP |
| 15 | 5O | 119 | LEU |
| 15 | 5O | 120 | ILE |
| 15 | 5O | 135 | GLU |
| 15 | 5O | 154 | SER |
| 15 | 5O | 158 | VAL |
| 15 | 5O | 171 | LYS |
| 15 | 5O | 174 | GLU |
| 15 | 5O | 181 | SER |
| 15 | 5O | 203 | ASN |
| 15 | 5O | 206 | HIS |
| 15 | 5O | 217 | GLU |
| 15 | 5O | 226 | ARG |
| 15 | 5O | 227 | TYR |
| 15 | 5O | 233 | LEU |
| 15 | 5O | 259 | ILE |
| 15 | 5O | 262 | SER |
| 15 | 5O | 270 | LEU |
| 15 | 5O | 273 | LEU |
| 15 | 5O | 280 | GLU |
| 15 | 5O | 289 | LEU |
| 15 | 5O | 294 | PHE |
| 15 | 5O | 298 | VAL |
| 15 | 5O | 299 | GLU |
| 15 | 5O | 309 | LEU |
| 15 | 5O | 333 | GLU |
| 15 | 5O | 359 | THR |
| 15 | 5P | 14 | LEU |
| 15 | 5P | 15 | ASP |
| 15 | 5P | 18 | SER |
| 15 | 5P | 22 | TRP |
| 15 | 5P | 38 | VAL |
| 15 | 5P | 42 | ASN |
| 15 | 5P | 47 | LEU |
| 15 | 5P | 55 | LEU |
| 15 | 5P | 81 | GLU |
| 15 | 5P | 271 | TYR |
| 15 | 5P | 280 | GLU |
| 15 | 5P | 282 | LEU |
| 15 | 5P | 283 | GLU |
| 15 | 5P | 326 | LEU |
| 15 | 5P | 331 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 5P | 347 | PHE |
| 16 | 5Q | 56 | ASP |
| 16 | 5Q | 173 | ARG |
| 17 | 5S | 18 | GLN |
| 17 | 5S | 26 | LYS |
| 17 | 5S | 30 | LYS |
| 17 | 5S | 42 | LYS |
| 17 | 5S | 53 | ASP |
| 17 | 5S | 69 | LYS |
| 17 | 5S | 72 | SER |
| 17 | 5S | 78 | ASN |
| 17 | 5S | 82 | LYS |
| 17 | 5S | 83 | ILE |
| 17 | 5S | 92 | GLU |
| 17 | 5S | 106 | THR |
| 17 | 5S | 120 | VAL |
| 17 | 5S | 126 | GLN |
| 17 | 5S | 128 | THR |
| 17 | 5S | 136 | VAL |
| 17 | 5S | 138 | MET |
| 17 | 5S | 145 | ASP |
| 17 | 5S | 176 | GLU |
| 17 | 5S | 185 | LEU |
| 17 | 5S | 192 | VAL |
| 17 | 5S | 194 | THR |
| 17 | 5S | 216 | GLU |
| 17 | 5S | 217 | ARG |
| 17 | 5S | 225 | ASP |
| 17 | 5S | 227 | ARG |
| 17 | 5S | 230 | GLU |
| 17 | 5S | 233 | GLU |
| 17 | 5T | 18 | GLN |
| 17 | 5T | 26 | LYS |
| 17 | 5T | 30 | LYS |
| 17 | 5T | 42 | LYS |
| 17 | 5T | 53 | ASP |
| 17 | 5T | 69 | LYS |
| 17 | 5T | 72 | SER |
| 17 | 5T | 78 | ASN |
| 17 | 5T | 82 | LYS |
| 17 | 5T | 83 | ILE |
| 17 | 5T | 92 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 5T | 106 | THR |
| 17 | 5T | 120 | VAL |
| 17 | 5T | 126 | GLN |
| 17 | 5T | 128 | THR |
| 17 | 5T | 136 | VAL |
| 17 | 5T | 138 | MET |
| 17 | 5T | 145 | ASP |
| 17 | 5T | 176 | GLU |
| 17 | 5T | 177 | ASP |
| 17 | 5T | 179 | GLN |
| 17 | 5T | 180 | GLN |
| 17 | 5T | 185 | LEU |
| 17 | 5T | 192 | VAL |
| 17 | 5T | 194 | THR |
| 17 | 5T | 216 | GLU |
| 17 | 5T | 217 | ARG |
| 17 | 5T | 225 | ASP |
| 17 | 5T | 227 | ARG |
| 17 | 5T | 230 | GLU |
| 17 | 5T | 231 | ARG |
| 17 | 5U | 18 | GLN |
| 17 | 5U | 26 | LYS |
| 17 | 5U | 30 | LYS |
| 17 | 5U | 42 | LYS |
| 17 | 5U | 53 | ASP |
| 17 | 5U | 69 | LYS |
| 17 | 5U | 72 | SER |
| 17 | 5U | 78 | ASN |
| 17 | 5U | 82 | LYS |
| 17 | 5U | 83 | ILE |
| 17 | 5U | 92 | GLU |
| 17 | 5U | 106 | THR |
| 17 | 5U | 114 | LEU |
| 17 | 5U | 120 | VAL |
| 17 | 5U | 126 | GLN |
| 17 | 5U | 128 | THR |
| 17 | 5U | 136 | VAL |
| 17 | 5U | 138 | MET |
| 17 | 5U | 145 | ASP |
| 17 | 5U | 176 | GLU |
| 17 | 5U | 182 | VAL |
| 17 | 5U | 185 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 5U | 192 | VAL |
| 17 | 5U | 194 | THR |
| 17 | 5U | 216 | GLU |
| 17 | 5U | 217 | ARG |
| 17 | 5U | 225 | ASP |
| 17 | 5U | 227 | ARG |
| 17 | 5U | 230 | GLU |
| 17 | 5U | 233 | GLU |
| 17 | 5V | 176 | GLU |
| 17 | 5V | 177 | ASP |
| 18 | 5X | 27 | ASP |
| 18 | 5X | 31 | ASP |
| 18 | 5X | 35 | LEU |
| 18 | 5X | 47 | SER |
| 18 | 5X | 50 | SER |
| 18 | 5X | 55 | ASP |
| 18 | 5X | 56 | LYS |
| 18 | 5X | 58 | LEU |
| 18 | 5X | 65 | VAL |
| 18 | 5X | 77 | THR |
| 18 | 5X | 90 | LEU |
| 18 | 5X | 100 | GLU |
| 18 | 5X | 107 | VAL |
| 18 | 5X | 109 | THR |
| 18 | 5X | 110 | GLU |
| 18 | 5X | 116 | ASP |
| 18 | 5X | 121 | LEU |
| 18 | 5X | 123 | SER |
| 18 | 5X | 124 | SER |
| 18 | 5X | 131 | GLU |
| 18 | 5X | 136 | VAL |
| 18 | 5X | 174 | VAL |
| 18 | 5X | 175 | THR |
| 18 | 5X | 176 | LEU |
| 18 | 5X | 180 | ARG |
| 18 | 5X | 184 | THR |
| 18 | 5X | 193 | ASP |
| 18 | 5X | 195 | GLU |
| 18 | 5X | 197 | SER |
| 18 | 5X | 198 | LEU |
| 18 | 5X | 199 | LEU |
| 18 | 5X | 212 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 5X | 218 | SER |
| 18 | 5Y | 27 | ASP |
| 18 | 5Y | 31 | ASP |
| 18 | 5Y | 35 | LEU |
| 18 | 5Y | 47 | SER |
| 18 | 5Y | 50 | SER |
| 18 | 5Y | 55 | ASP |
| 18 | 5Y | 56 | LYS |
| 18 | 5Y | 58 | LEU |
| 18 | 5Y | 65 | VAL |
| 18 | 5Y | 77 | THR |
| 18 | 5Y | 90 | LEU |
| 18 | 5Y | 100 | GLU |
| 18 | 5Y | 107 | VAL |
| 18 | 5Y | 109 | THR |
| 18 | 5Y | 110 | GLU |
| 18 | 5Y | 116 | ASP |
| 18 | 5Y | 121 | LEU |
| 18 | 5Y | 123 | SER |
| 18 | 5Y | 124 | SER |
| 18 | 5Y | 131 | GLU |
| 18 | 5Y | 136 | VAL |
| 18 | 5Y | 174 | VAL |
| 18 | 5Y | 175 | THR |
| 18 | 5Y | 176 | LEU |
| 18 | 5Y | 184 | THR |
| 18 | 5Y | 193 | ASP |
| 18 | 5Y | 195 | GLU |
| 18 | 5Y | 197 | SER |
| 18 | 5Y | 198 | LEU |
| 18 | 5Y | 199 | LEU |
| 18 | 5Y | 212 | ILE |
| 18 | 5Y | 218 | SER |
| 18 | 5Z | 27 | ASP |
| 18 | 5Z | 31 | ASP |
| 18 | 5Z | 35 | LEU |
| 18 | 5Z | 47 | SER |
| 18 | 5Z | 50 | SER |
| 18 | 5Z | 55 | ASP |
| 18 | 5Z | 56 | LYS |
| 18 | 5Z | 58 | LEU |
| 18 | 5Z | 65 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 5Z | 77 | THR |
| 18 | 5Z | 90 | LEU |
| 18 | 5Z | 100 | GLU |
| 18 | 5Z | 107 | VAL |
| 18 | 5Z | 109 | THR |
| 18 | 5Z | 110 | GLU |
| 18 | 5Z | 116 | ASP |
| 18 | 5Z | 121 | LEU |
| 18 | 5Z | 123 | SER |
| 18 | 5Z | 124 | SER |
| 18 | 5Z | 131 | GLU |
| 18 | 5Z | 136 | VAL |
| 18 | 5Z | 174 | VAL |
| 18 | 5Z | 175 | THR |
| 18 | 5Z | 176 | LEU |
| 18 | 5Z | 184 | THR |
| 18 | 5Z | 193 | ASP |
| 18 | 5Z | 195 | GLU |
| 18 | 5Z | 197 | SER |
| 18 | 5Z | 198 | LEU |
| 18 | 5Z | 199 | LEU |
| 18 | 5Z | 212 | ILE |
| 18 | 5Z | 218 | SER |
| 18 | 6A | 27 | ASP |
| 18 | 6A | 31 | ASP |
| 18 | 6A | 35 | LEU |
| 18 | 6A | 47 | SER |
| 18 | 6A | 50 | SER |
| 18 | 6A | 55 | ASP |
| 18 | 6A | 56 | LYS |
| 18 | 6A | 58 | LEU |
| 18 | 6A | 65 | VAL |
| 18 | 6A | 77 | THR |
| 18 | 6A | 90 | LEU |
| 18 | 6A | 100 | GLU |
| 18 | 6A | 107 | VAL |
| 18 | 6A | 109 | THR |
| 18 | 6A | 110 | GLU |
| 18 | 6A | 116 | ASP |
| 18 | 6A | 121 | LEU |
| 18 | 6A | 123 | SER |
| 18 | 6A | 124 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 6A | 131 | GLU |
| 18 | 6A | 136 | VAL |
| 18 | 6A | 174 | VAL |
| 18 | 6A | 175 | THR |
| 18 | 6A | 176 | LEU |
| 18 | 6A | 184 | THR |
| 18 | 6A | 193 | ASP |
| 18 | 6A | 195 | GLU |
| 18 | 6A | 197 | SER |
| 18 | 6A | 198 | LEU |
| 18 | 6A | 199 | LEU |
| 18 | 6A | 212 | ILE |
| 18 | 6A | 218 | SER |
| 18 | 6B | 27 | ASP |
| 18 | 6B | 31 | ASP |
| 18 | 6B | 35 | LEU |
| 18 | 6B | 47 | SER |
| 18 | 6B | 50 | SER |
| 18 | 6B | 55 | ASP |
| 18 | 6B | 56 | LYS |
| 18 | 6B | 58 | LEU |
| 18 | 6B | 65 | VAL |
| 18 | 6B | 77 | THR |
| 18 | 6B | 90 | LEU |
| 18 | 6B | 100 | GLU |
| 18 | 6B | 107 | VAL |
| 18 | 6B | 109 | THR |
| 18 | 6B | 110 | GLU |
| 18 | 6B | 116 | ASP |
| 18 | 6B | 121 | LEU |
| 18 | 6B | 123 | SER |
| 18 | 6B | 124 | SER |
| 18 | 6B | 131 | GLU |
| 18 | 6B | 136 | VAL |
| 18 | 6B | 174 | VAL |
| 18 | 6B | 175 | THR |
| 18 | 6B | 176 | LEU |
| 18 | 6B | 184 | THR |
| 18 | 6B | 193 | ASP |
| 18 | 6B | 195 | GLU |
| 18 | 6B | 197 | SER |
| 18 | 6B | 198 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 6B | 199 | LEU |
| 18 | 6B | 212 | ILE |
| 18 | 6B | 218 | SER |
| 18 | 6C | 27 | ASP |
| 18 | 6C | 31 | ASP |
| 18 | 6C | 35 | LEU |
| 18 | 6C | 47 | SER |
| 18 | 6C | 50 | SER |
| 18 | 6C | 55 | ASP |
| 18 | 6C | 56 | LYS |
| 18 | 6C | 58 | LEU |
| 18 | 6C | 65 | VAL |
| 18 | 6C | 77 | THR |
| 18 | 6C | 90 | LEU |
| 18 | 6C | 100 | GLU |
| 18 | 6C | 107 | VAL |
| 18 | 6C | 109 | THR |
| 18 | 6C | 110 | GLU |
| 18 | 6C | 116 | ASP |
| 18 | 6C | 121 | LEU |
| 18 | 6C | 123 | SER |
| 18 | 6C | 124 | SER |
| 18 | 6C | 131 | GLU |
| 18 | 6C | 136 | VAL |
| 18 | 6C | 174 | VAL |
| 18 | 6C | 175 | THR |
| 18 | 6C | 176 | LEU |
| 18 | 6C | 184 | THR |
| 18 | 6C | 193 | ASP |
| 18 | 6C | 195 | GLU |
| 18 | 6C | 197 | SER |
| 18 | 6C | 198 | LEU |
| 18 | 6C | 199 | LEU |
| 18 | 6C | 212 | ILE |
| 18 | 6C | 218 | SER |
| 18 | 6D | 27 | ASP |
| 18 | 6D | 31 | ASP |
| 18 | 6D | 35 | LEU |
| 18 | 6D | 47 | SER |
| 18 | 6D | 50 | SER |
| 18 | 6D | 55 | ASP |
| 18 | 6D | 56 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 6D | 58 | LEU |
| 18 | 6D | 65 | VAL |
| 18 | 6D | 77 | THR |
| 18 | 6D | 90 | LEU |
| 18 | 6D | 100 | GLU |
| 18 | 6D | 107 | VAL |
| 18 | 6D | 109 | THR |
| 18 | 6D | 110 | GLU |
| 18 | 6D | 116 | ASP |
| 18 | 6D | 121 | LEU |
| 18 | 6D | 123 | SER |
| 18 | 6D | 124 | SER |
| 18 | 6D | 131 | GLU |
| 18 | 6D | 136 | VAL |
| 18 | 6D | 174 | VAL |
| 18 | 6D | 175 | THR |
| 18 | 6D | 176 | LEU |
| 18 | 6D | 184 | THR |
| 18 | 6D | 193 | ASP |
| 18 | 6D | 195 | GLU |
| 18 | 6D | 197 | SER |
| 18 | 6D | 198 | LEU |
| 18 | 6D | 199 | LEU |
| 18 | 6D | 212 | ILE |
| 18 | 6D | 218 | SER |
| 19 | 6E | 96 | ASP |
| 19 | 6E | 106 | ASN |
| 20 | 6F | 131 | GLU |
| 20 | 6F | 357 | VAL |
| 22 | 6I | 32 | LYS |
| 22 | 6I | 131 | ARG |
| 22 | 6J | 32 | LYS |
| 22 | 6K | 32 | LYS |
| 22 | 6K | 121 | LYS |
| 22 | 6L | 32 | LYS |
| 22 | 6M | 32 | LYS |
| 22 | 6M | 106 | ASP |
| 22 | 6M | 223 | LEU |
| 22 | 6N | 32 | LYS |
| 22 | 6O | 32 | LYS |
| 22 | 6O | 96 | LYS |
| 22 | 6P | 32 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 6P | 266 | LYS |
| 22 | 6P | 307 | ARG |
| 23 | 6Q | 4 | LYS |
| 23 | 6Q | 21 | THR |
| 23 | 6Q | 22 | MET |
| 23 | 6Q | 26 | GLN |
| 23 | 6Q | 45 | GLU |
| 23 | 6Q | 62 | GLN |
| 23 | 6Q | 65 | LEU |
| 23 | 6Q | 69 | GLN |
| 23 | 6R | 4 | LYS |
| 23 | 6R | 30 | GLU |
| 23 | 6R | 45 | GLU |
| 23 | 6R | 54 | ASN |
| 23 | 6R | 62 | GLN |
| 23 | 6R | 65 | LEU |
| 23 | 6R | 69 | GLN |
| 23 | 6S | 4 | LYS |
| 23 | 6S | 45 | GLU |
| 23 | 6S | 62 | GLN |
| 23 | 6S | 65 | LEU |
| 23 | 6S | 69 | GLN |
| 24 | 6T | 333 | LYS |
| 24 | 6T | 364 | ARG |
| 24 | 6T | 433 | ARG |
| 24 | 6T | 488 | ARG |
| 24 | 6T | 490 | THR |
| 24 | 6U | 14 | TYR |
| 24 | 6U | 33 | LEU |
| 24 | 6U | 35 | TYR |
| 24 | 6U | 41 | ARG |
| 24 | 6U | 364 | ARG |
| 24 | 6U | 433 | ARG |
| 24 | 6U | 492 | ILE |
| 24 | 6V | 6 | PRO |
| 24 | 6V | 11 | LEU |
| 24 | 6V | 16 | VAL |
| 24 | 6V | 150 | ARG |
| 24 | 6V | 364 | ARG |
| 24 | 6W | 10 | LYS |
| 24 | 6W | 37 | ASN |
| 24 | 6W | 39 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 6W | 40 | GLN |
| 24 | 6W | 91 | ASN |
| 24 | 6W | 364 | ARG |
| 24 | 6W | 433 | ARG |
| 24 | 6W | 469 | PHE |
| 24 | 6X | 150 | ARG |
| 24 | 6X | 223 | ARG |
| 24 | 6X | 315 | ARG |
| 24 | 6X | 364 | ARG |
| 24 | 6X | 433 | ARG |
| 24 | 6X | 469 | PHE |
| 24 | 6X | 473 | TYR |
| 24 | 6X | 478 | ASP |
| 24 | 6X | 489 | ASN |
| 24 | 6X | 517 | LEU |
| 24 | 6Y | 14 | TYR |
| 24 | 6Y | 15 | THR |
| 24 | 6Y | 35 | TYR |
| 24 | 6Y | 42 | GLU |
| 24 | 6Y | 43 | ASP |
| 24 | 6Y | 91 | ASN |
| 24 | 6Y | 364 | ARG |
| 24 | 6Z | 124 | TYR |
| 24 | 6Z | 150 | ARG |
| 24 | 6Z | 151 | HIS |
| 24 | 6Z | 364 | ARG |
| 24 | 6Z | 433 | ARG |
| 24 | 7A | 93 | ARG |
| 12 | 7B | 58 | ARG |
| 26 | 7D | 31 | VAL |
| 26 | 7D | 40 | THR |
| 26 | 7D | 58 | ILE |
| 26 | 7D | 59 | ARG |
| 26 | 7D | 70 | VAL |
| 26 | 7D | 74 | VAL |
| 26 | 7D | 88 | THR |
| 26 | 7D | 90 | THR |
| 26 | 7D | 92 | LEU |
| 26 | 7D | 94 | THR |
| 26 | 7D | 100 | LYS |
| 26 | 7D | 105 | THR |
| 26 | 7D | 108 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | 7D | 110 | VAL |
| 26 | 7D | 115 | GLU |
| 26 | 7E | 31 | VAL |
| 26 | 7E | 40 | THR |
| 26 | 7E | 56 | LEU |
| 26 | 7E | 70 | VAL |
| 26 | 7E | 74 | VAL |
| 26 | 7E | 88 | THR |
| 26 | 7E | 90 | THR |
| 26 | 7E | 92 | LEU |
| 26 | 7E | 94 | THR |
| 26 | 7E | 100 | LYS |
| 26 | 7E | 105 | THR |
| 26 | 7E | 108 | SER |
| 26 | 7E | 110 | VAL |
| 26 | 7E | 115 | GLU |
| 26 | 7E | 143 | ASP |
| 26 | 7E | 146 | ASN |
| 26 | 7F | 31 | VAL |
| 26 | 7F | 58 | ILE |
| 26 | 7F | 63 | LEU |
| 26 | 7F | 70 | VAL |
| 26 | 7F | 74 | VAL |
| 26 | 7F | 88 | THR |
| 26 | 7F | 90 | THR |
| 26 | 7F | 92 | LEU |
| 26 | 7F | 94 | THR |
| 26 | 7F | 100 | LYS |
| 26 | 7F | 105 | THR |
| 26 | 7F | 108 | SER |
| 26 | 7F | 110 | VAL |
| 26 | 7F | 119 | MET |
| 26 | 7F | 143 | ASP |
| 26 | 7F | 146 | ASN |
| 28 | 7H | 401 | THR |
| 28 | 7H | 410 | HIS |
| 28 | 7H | 415 | THR |
| 28 | 7H | 429 | ASP |
| 28 | 7H | 430 | MET |
| 28 | 7H | 432 | LEU |
| 28 | 7H | 437 | SER |
| 28 | 7H | 448 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 7H | 456 | VAL |
| 28 | 7H | 458 | SER |
| 28 | 7H | 459 | VAL |
| 29 | 7I | 4 | LYS |
| 29 | 7J | 167 | ILE |
| 29 | 7J | 330 | GLU |
| 30 | 7K | 3 | LEU |
| 30 | 7K | 7 | SER |
| 30 | 7K | 444 | ARG |
| 31 | 7M | 25 | THR |
| 34 | 7R | 248 | LYS |
| 34 | 7S | 228 | LYS |
| 35 | 7T | 179 | ARG |
| 35 | 7T | 185 | LYS |
| 36 | 7V | 24 | ASN |
| 36 | 7V | 32 | LYS |
| 36 | 7V | 39 | LEU |
| 36 | 7V | 54 | GLU |
| 36 | 7V | 73 | LEU |
| 36 | 7V | 76 | GLN |
| 36 | 7V | 80 | THR |
| 36 | 7V | 83 | ARG |
| 36 | 7V | 94 | LEU |
| 36 | 7V | 98 | VAL |
| 36 | 7V | 99 | GLU |
| 36 | 7W | 24 | ASN |
| 36 | 7W | 32 | LYS |
| 36 | 7W | 39 | LEU |
| 36 | 7W | 54 | GLU |
| 36 | 7W | 73 | LEU |
| 36 | 7W | 76 | GLN |
| 36 | 7W | 80 | THR |
| 36 | 7W | 83 | ARG |
| 36 | 7W | 94 | LEU |
| 36 | 7W | 98 | VAL |
| 36 | 7W | 102 | MET |
| 36 | 7W | 104 | ASP |
| 28 | 7X | 301 | GLU |
| 28 | 7X | 399 | VAL |
| 28 | 7X | 410 | HIS |
| 28 | 7X | 415 | THR |
| 28 | 7X | 429 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | 7X | 430 | MET |
| 28 | 7X | 432 | LEU |
| 28 | 7X | 437 | SER |
| 28 | 7X | 448 | THR |
| 28 | 7X | 451 | LYS |
| 28 | 7X | 456 | VAL |
| 28 | 7X | 458 | SER |
| 28 | 7X | 459 | VAL |
| 37 | 7Y | 55 | LEU |
| 37 | 7Y | 56 | MET |
| 37 | 7Y | 128 | TYR |
| 37 | 7Y | 129 | LYS |
| 38 | 8A | 91 | GLN |
| 38 | 8A | 93 | LYS |
| 38 | 8A | 100 | SER |
| 38 | 8A | 197 | THR |
| 38 | 8A | 204 | GLN |
| 38 | 8B | 25 | ILE |
| 38 | 8B | 80 | TYR |
| 38 | 8B | 158 | MET |
| 38 | 8B | 160 | ASP |
| 38 | 8B | 165 | LYS |
| 38 | 8B | 199 | THR |
| 38 | 8B | 201 | LEU |
| 38 | 8C | 72 | ASP |
| 38 | 8C | 73 | TRP |
| 38 | 8C | 74 | ILE |
| 38 | 8C | 80 | TYR |
| 38 | 8C | 83 | ARG |
| 38 | 8C | 197 | THR |
| 38 | 8C | 199 | THR |
| 38 | 8C | 201 | LEU |
| 38 | 8C | 204 | GLN |
| 38 | 8C | 208 | GLU |
| 38 | 8D | 80 | TYR |
| 38 | 8D | 83 | ARG |
| 38 | 8D | 84 | ILE |
| 38 | 8D | 85 | ARG |
| 38 | 8D | 91 | GLN |
| 38 | 8D | 93 | LYS |
| 38 | 8D | 160 | ASP |
| 38 | 8D | 163 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | 8D | 175 | ARG |
| 38 | 8D | 209 | HIS |
| 38 | 8D | 210 | HIS |
| 38 | 8D | 213 | GLU |
| 38 | 8D | 214 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2787) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 334 | GLN |
| 1 | 1 | 335 | ASN |
| 1 | 1 | 337 | ASN |
| 1 | 1 | 348 | ASN |
| 1 | 1 | 423 | GLN |
| 2 | 2 | 11 | GLN |
| 2 | 2 | 101 | ASN |
| 2 | 2 | 226 | ASN |
| 2 | 2 | 293 | ASN |
| 2 | 2 | 309 | HIS |
| 2 | 2 | 356 | ASN |
| 1 | 3 | 14 | ASN |
| 1 | 3 | 204 | ASN |
| 1 | 3 | 247 | ASN |
| 1 | 3 | 256 | ASN |
| 1 | 3 | 280 | GLN |
| 1 | 3 | 329 | GLN |
| 1 | 3 | 337 | ASN |
| 1 | 3 | 384 | GLN |
| 2 | 4 | 15 | GLN |
| 2 | 4 | 101 | ASN |
| 2 | 4 | 176 | GLN |
| 2 | 4 | 192 | HIS |
| 2 | 4 | 283 | HIS |
| 2 | 4 | 293 | ASN |
| 1 | 5 | 11 | GLN |
| 1 | 5 | 14 | ASN |
| 1 | 5 | 191 | GLN |
| 1 | 5 | 195 | ASN |
| 1 | 5 | 204 | ASN |
| 1 | 5 | 227 | HIS |
| 1 | 5 | 247 | ASN |
| 1 | 5 | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 298 | ASN |
| 1 | 5 | 329 | GLN |
| 1 | 5 | 334 | GLN |
| 1 | 5 | 337 | ASN |
| 1 | 5 | 348 | ASN |
| 1 | 5 | 396 | HIS |
| 1 | 5 | 414 | ASN |
| 2 | 6 | 8 | HIS |
| 2 | 6 | 11 | GLN |
| 2 | 6 | 61 | HIS |
| 2 | 6 | 192 | HIS |
| 2 | 6 | 226 | ASN |
| 2 | 6 | 258 | ASN |
| 2 | 6 | 293 | ASN |
| 1 | 7 | 14 | ASN |
| 1 | 7 | 37 | HIS |
| 1 | 7 | 99 | ASN |
| 1 | 7 | 190 | HIS |
| 1 | 7 | 247 | ASN |
| 1 | 7 | 334 | GLN |
| 1 | 7 | 335 | ASN |
| 1 | 7 | 337 | ASN |
| 1 | 7 | 348 | ASN |
| 1 | 7 | 414 | ASN |
| 2 | 8 | 8 | HIS |
| 2 | 8 | 85 | GLN |
| 2 | 8 | 88 | HIS |
| 2 | 8 | 102 | ASN |
| 2 | 8 | 133 | GLN |
| 2 | 8 | 258 | ASN |
| 2 | 8 | 285 | GLN |
| 2 | 8 | 293 | ASN |
| 2 | 8 | 309 | HIS |
| 2 | 8 | 329 | ASN |
| 2 | 8 | 372 | GLN |
| 1 | 9 | 8 | GLN |
| 1 | 9 | 14 | ASN |
| 1 | 9 | 227 | HIS |
| 1 | 9 | 247 | ASN |
| 1 | 9 | 329 | GLN |
| 1 | 9 | 334 | GLN |
| 1 | 9 | 348 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A0 | 8 | HIS |
| 2 | A0 | 11 | GLN |
| 2 | A0 | 101 | ASN |
| 2 | A0 | 128 | ASN |
| 2 | A0 | 192 | HIS |
| 2 | A0 | 226 | ASN |
| 2 | A0 | 283 | HIS |
| 2 | A0 | 293 | ASN |
| 1 | A1 | 6 | HIS |
| 1 | A1 | 14 | ASN |
| 1 | A1 | 99 | ASN |
| 1 | A1 | 190 | HIS |
| 1 | A1 | 279 | GLN |
| 1 | A1 | 292 | GLN |
| 1 | A1 | 329 | GLN |
| 1 | A1 | 334 | GLN |
| 1 | A1 | 337 | ASN |
| 1 | A1 | 348 | ASN |
| 2 | A2 | 85 | GLN |
| 2 | A2 | 283 | HIS |
| 2 | A2 | 329 | ASN |
| 2 | A2 | 372 | GLN |
| 1 | A3 | 14 | ASN |
| 1 | A3 | 15 | GLN |
| 1 | A3 | 131 | GLN |
| 1 | A3 | 137 | HIS |
| 1 | A3 | 227 | HIS |
| 1 | A3 | 334 | GLN |
| 1 | A3 | 335 | ASN |
| 1 | A3 | 337 | ASN |
| 2 | A4 | 88 | HIS |
| 2 | A4 | 101 | ASN |
| 2 | A4 | 197 | HIS |
| 2 | A4 | 258 | ASN |
| 2 | A4 | 283 | HIS |
| 2 | A4 | 293 | ASN |
| 2 | A4 | 309 | HIS |
| 1 | A5 | 14 | ASN |
| 1 | A5 | 256 | ASN |
| 1 | A5 | 280 | GLN |
| 1 | A5 | 292 | GLN |
| 1 | A5 | 329 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A5 | 348 | ASN |
| 1 | A5 | 375 | GLN |
| 1 | A5 | 414 | ASN |
| 1 | A5 | 426 | GLN |
| 1 | A7 | 6 | HIS |
| 1 | A7 | 89 | ASN |
| 1 | A7 | 99 | ASN |
| 1 | A7 | 280 | GLN |
| 1 | A7 | 329 | GLN |
| 1 | A7 | 396 | HIS |
| 2 | A8 | 61 | HIS |
| 2 | A8 | 133 | GLN |
| 2 | A8 | 249 | ASN |
| 2 | A8 | 256 | GLN |
| 2 | A8 | 258 | ASN |
| 2 | A8 | 309 | HIS |
| 2 | A8 | 329 | ASN |
| 2 | A8 | 393 | HIS |
| 1 | A9 | 37 | HIS |
| 1 | A9 | 256 | ASN |
| 1 | A9 | 280 | GLN |
| 1 | A9 | 329 | GLN |
| 1 | A9 | 334 | GLN |
| 1 | A9 | 384 | GLN |
| 1 | A9 | 396 | HIS |
| 2 | B0 | 61 | HIS |
| 2 | B0 | 101 | ASN |
| 2 | B0 | 206 | ASN |
| 2 | B0 | 256 | GLN |
| 2 | B0 | 258 | ASN |
| 2 | B0 | 283 | HIS |
| 2 | B0 | 309 | HIS |
| 2 | B0 | 406 | HIS |
| 1 | B1 | 11 | GLN |
| 1 | B1 | 14 | ASN |
| 1 | B1 | 329 | GLN |
| 1 | B1 | 334 | GLN |
| 1 | B1 | 348 | ASN |
| 1 | B1 | 396 | HIS |
| 1 | B1 | 423 | GLN |
| 2 | B2 | 61 | HIS |
| 2 | B2 | 88 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B2 | 197 | HIS |
| 2 | B2 | 258 | ASN |
| 2 | B2 | 309 | HIS |
| 1 | B3 | 8 | GLN |
| 1 | B3 | 14 | ASN |
| 1 | B3 | 204 | ASN |
| 1 | B3 | 256 | ASN |
| 1 | B3 | 334 | GLN |
| 1 | B3 | 337 | ASN |
| 2 | B4 | 61 | HIS |
| 2 | B4 | 128 | ASN |
| 2 | B4 | 206 | ASN |
| 2 | B4 | 233 | GLN |
| 2 | B4 | 249 | ASN |
| 2 | B4 | 406 | HIS |
| 1 | B5 | 11 | GLN |
| 1 | B5 | 14 | ASN |
| 1 | B5 | 28 | HIS |
| 1 | B5 | 48 | ASN |
| 1 | B5 | 134 | GLN |
| 1 | B5 | 245 | GLN |
| 1 | B5 | 334 | GLN |
| 1 | B5 | 348 | ASN |
| 1 | B5 | 396 | HIS |
| 1 | B5 | 423 | GLN |
| 2 | B7 | 15 | GLN |
| 2 | B7 | 61 | HIS |
| 2 | B7 | 128 | ASN |
| 2 | B7 | 133 | GLN |
| 2 | B7 | 206 | ASN |
| 2 | B7 | 285 | GLN |
| 1 | B8 | 89 | ASN |
| 1 | B8 | 99 | ASN |
| 1 | B8 | 190 | HIS |
| 1 | B8 | 256 | ASN |
| 1 | B8 | 279 | GLN |
| 1 | B8 | 329 | GLN |
| 1 | B8 | 348 | ASN |
| 1 | B8 | 423 | GLN |
| 2 | B9 | 15 | GLN |
| 2 | B9 | 61 | HIS |
| 2 | B9 | 107 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B9 | 128 | ASN |
| 2 | B9 | 197 | HIS |
| 2 | B9 | 206 | ASN |
| 2 | B9 | 226 | ASN |
| 1 | C0 | 14 | ASN |
| 1 | C0 | 131 | GLN |
| 1 | C0 | 190 | HIS |
| 1 | C0 | 292 | GLN |
| 1 | C0 | 332 | ASN |
| 1 | C0 | 334 | GLN |
| 1 | C0 | 348 | ASN |
| 1 | C0 | 396 | HIS |
| 2 | C1 | 15 | GLN |
| 2 | C1 | 61 | HIS |
| 2 | C1 | 85 | GLN |
| 2 | C1 | 128 | ASN |
| 2 | C1 | 206 | ASN |
| 2 | C1 | 226 | ASN |
| 2 | C1 | 258 | ASN |
| 2 | C1 | 393 | HIS |
| 1 | C2 | 8 | GLN |
| 1 | C2 | 14 | ASN |
| 1 | C2 | 37 | HIS |
| 1 | C2 | 256 | ASN |
| 1 | C2 | 292 | GLN |
| 1 | C2 | 332 | ASN |
| 1 | C2 | 334 | GLN |
| 1 | C2 | 384 | GLN |
| 1 | C2 | 423 | GLN |
| 1 | C4 | 6 | HIS |
| 1 | C4 | 8 | GLN |
| 1 | C4 | 14 | ASN |
| 1 | C4 | 99 | ASN |
| 1 | C4 | 227 | HIS |
| 1 | C4 | 247 | ASN |
| 1 | C4 | 256 | ASN |
| 1 | C4 | 334 | GLN |
| 2 | C5 | 61 | HIS |
| 2 | C5 | 197 | HIS |
| 2 | C5 | 226 | ASN |
| 2 | C5 | 249 | ASN |
| 2 | C5 | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C5 | 309 | HIS |
| 2 | C5 | 329 | ASN |
| 1 | C6 | 6 | HIS |
| 1 | C6 | 83 | GLN |
| 1 | C6 | 89 | ASN |
| 1 | C6 | 99 | ASN |
| 1 | C6 | 131 | GLN |
| 1 | C6 | 204 | ASN |
| 1 | C6 | 245 | GLN |
| 1 | C6 | 256 | ASN |
| 1 | C6 | 264 | HIS |
| 2 | C7 | 85 | GLN |
| 2 | C7 | 88 | HIS |
| 2 | C7 | 192 | HIS |
| 2 | C7 | 226 | ASN |
| 2 | C7 | 233 | GLN |
| 2 | C7 | 256 | GLN |
| 2 | C7 | 258 | ASN |
| 2 | C7 | 285 | GLN |
| 2 | C7 | 372 | GLN |
| 1 | C8 | 6 | HIS |
| 1 | C8 | 11 | GLN |
| 1 | C8 | 89 | ASN |
| 1 | C8 | 99 | ASN |
| 1 | C8 | 184 | ASN |
| 1 | C8 | 190 | HIS |
| 1 | C8 | 204 | ASN |
| 1 | C8 | 227 | HIS |
| 1 | C8 | 256 | ASN |
| 1 | C8 | 329 | GLN |
| 1 | C8 | 334 | GLN |
| 1 | C8 | 335 | ASN |
| 1 | C8 | 348 | ASN |
| 1 | C8 | 396 | HIS |
| 1 | C8 | 414 | ASN |
| 2 | C9 | 61 | HIS |
| 2 | C9 | 197 | HIS |
| 2 | C9 | 226 | ASN |
| 2 | C9 | 258 | ASN |
| 2 | C9 | 283 | HIS |
| 2 | C9 | 285 | GLN |
| 2 | C9 | 309 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C9 | 372 | GLN |
| 1 | D0 | 6 | HIS |
| 1 | D0 | 8 | GLN |
| 1 | D0 | 14 | ASN |
| 1 | D0 | 99 | ASN |
| 1 | D0 | 131 | GLN |
| 1 | D0 | 134 | GLN |
| 1 | D0 | 190 | HIS |
| 1 | D0 | 204 | ASN |
| 1 | D0 | 256 | ASN |
| 1 | D0 | 292 | GLN |
| 1 | D0 | 329 | GLN |
| 1 | D0 | 332 | ASN |
| 2 | D1 | 101 | ASN |
| 2 | D1 | 197 | HIS |
| 2 | D1 | 226 | ASN |
| 2 | D1 | 258 | ASN |
| 2 | D1 | 309 | HIS |
| 1 | D2 | 6 | HIS |
| 1 | D2 | 8 | GLN |
| 1 | D2 | 37 | HIS |
| 1 | D2 | 43 | GLN |
| 1 | D2 | 99 | ASN |
| 1 | D2 | 134 | GLN |
| 1 | D2 | 191 | GLN |
| 1 | D2 | 204 | ASN |
| 1 | D2 | 247 | ASN |
| 1 | D2 | 256 | ASN |
| 1 | D2 | 414 | ASN |
| 2 | D3 | 28 | HIS |
| 2 | D3 | 31 | GLN |
| 2 | D3 | 258 | ASN |
| 2 | D3 | 285 | GLN |
| 2 | D3 | 372 | GLN |
| 1 | D4 | 6 | HIS |
| 1 | D4 | 99 | ASN |
| 1 | D4 | 190 | HIS |
| 1 | D4 | 204 | ASN |
| 1 | D4 | 227 | HIS |
| 1 | D4 | 256 | ASN |
| 1 | D4 | 396 | HIS |
| 2 | D5 | 226 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D5 | 285 | GLN |
| 2 | D5 | 309 | HIS |
| 1 | D6 | 6 | HIS |
| 1 | D6 | 8 | GLN |
| 1 | D6 | 195 | ASN |
| 1 | D6 | 204 | ASN |
| 1 | D6 | 256 | ASN |
| 1 | D6 | 334 | GLN |
| 1 | D6 | 337 | ASN |
| 1 | D6 | 348 | ASN |
| 1 | D6 | 414 | ASN |
| 1 | D6 | 416 | ASN |
| 2 | D7 | 197 | HIS |
| 2 | D7 | 226 | ASN |
| 2 | D7 | 233 | GLN |
| 2 | D7 | 256 | GLN |
| 2 | D7 | 283 | HIS |
| 2 | D7 | 393 | HIS |
| 1 | D8 | 37 | HIS |
| 1 | D8 | 131 | GLN |
| 1 | D8 | 191 | GLN |
| 1 | D8 | 227 | HIS |
| 1 | D8 | 256 | ASN |
| 1 | D8 | 416 | ASN |
| 1 | E0 | 37 | HIS |
| 1 | E0 | 99 | ASN |
| 1 | E0 | 204 | ASN |
| 1 | E0 | 227 | HIS |
| 1 | E0 | 347 | ASN |
| 1 | E0 | 414 | ASN |
| 1 | E0 | 416 | ASN |
| 2 | E1 | 18 | ASN |
| 2 | E1 | 28 | HIS |
| 2 | E1 | 61 | HIS |
| 2 | E1 | 85 | GLN |
| 2 | E1 | 133 | GLN |
| 2 | E1 | 226 | ASN |
| 2 | E1 | 228 | ASN |
| 2 | E1 | 233 | GLN |
| 2 | E1 | 258 | ASN |
| 2 | E1 | 283 | HIS |
| 2 | E1 | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E2 | 190 | HIS |
| 1 | E2 | 204 | ASN |
| 1 | E2 | 227 | HIS |
| 1 | E2 | 329 | GLN |
| 1 | E2 | 334 | GLN |
| 1 | E2 | 337 | ASN |
| 2 | E3 | 8 | HIS |
| 2 | E3 | 18 | ASN |
| 2 | E3 | 197 | HIS |
| 2 | E3 | 226 | ASN |
| 2 | E3 | 256 | GLN |
| 2 | E3 | 258 | ASN |
| 1 | E4 | 11 | GLN |
| 1 | E4 | 14 | ASN |
| 1 | E4 | 99 | ASN |
| 1 | E4 | 131 | GLN |
| 1 | E4 | 190 | HIS |
| 1 | E4 | 204 | ASN |
| 1 | E4 | 227 | HIS |
| 1 | E4 | 245 | GLN |
| 1 | E4 | 256 | ASN |
| 1 | E4 | 292 | GLN |
| 1 | E4 | 334 | GLN |
| 1 | E4 | 348 | ASN |
| 1 | E4 | 396 | HIS |
| 2 | E5 | 8 | HIS |
| 2 | E5 | 15 | GLN |
| 2 | E5 | 192 | HIS |
| 2 | E5 | 226 | ASN |
| 2 | E5 | 228 | ASN |
| 2 | E5 | 258 | ASN |
| 2 | E5 | 309 | HIS |
| 2 | E5 | 329 | ASN |
| 1 | E6 | 11 | GLN |
| 1 | E6 | 15 | GLN |
| 1 | E6 | 99 | ASN |
| 1 | E6 | 131 | GLN |
| 1 | E6 | 190 | HIS |
| 1 | E6 | 204 | ASN |
| 1 | E6 | 227 | HIS |
| 1 | E6 | 256 | ASN |
| 1 | E6 | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E6 | 396 | HIS |
| 2 | E7 | 50 | ASN |
| 2 | E7 | 61 | HIS |
| 2 | E7 | 133 | GLN |
| 2 | E7 | 258 | ASN |
| 2 | E7 | 283 | HIS |
| 2 | E7 | 356 | ASN |
| 1 | E8 | 8 | GLN |
| 1 | E8 | 83 | GLN |
| 1 | E8 | 99 | ASN |
| 1 | E8 | 190 | HIS |
| 1 | E8 | 204 | ASN |
| 1 | E8 | 227 | HIS |
| 1 | E8 | 291 | GLN |
| 1 | E8 | 334 | GLN |
| 1 | E8 | 396 | HIS |
| 2 | E9 | 8 | HIS |
| 2 | E9 | 85 | GLN |
| 2 | E9 | 128 | ASN |
| 2 | E9 | 228 | ASN |
| 2 | E9 | 233 | GLN |
| 2 | E9 | 258 | ASN |
| 2 | E9 | 309 | HIS |
| 2 | E9 | 356 | ASN |
| 2 | E9 | 358 | GLN |
| 2 | E9 | 393 | HIS |
| 1 | F0 | 6 | HIS |
| 1 | F0 | 14 | ASN |
| 1 | F0 | 37 | HIS |
| 1 | F0 | 48 | ASN |
| 1 | F0 | 99 | ASN |
| 1 | F0 | 134 | GLN |
| 1 | F0 | 190 | HIS |
| 1 | F0 | 227 | HIS |
| 1 | F0 | 245 | GLN |
| 1 | F0 | 280 | GLN |
| 1 | F0 | 348 | ASN |
| 1 | F0 | 396 | HIS |
| 2 | F1 | 197 | HIS |
| 2 | F1 | 228 | ASN |
| 2 | F1 | 233 | GLN |
| 2 | F1 | 258 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F1 | 293 | ASN |
| 2 | F1 | 309 | HIS |
| 2 | F1 | 356 | ASN |
| 1 | F2 | 99 | ASN |
| 1 | F2 | 131 | GLN |
| 1 | F2 | 195 | ASN |
| 1 | F2 | 227 | HIS |
| 1 | F2 | 256 | ASN |
| 1 | F2 | 280 | GLN |
| 1 | F2 | 334 | GLN |
| 1 | F2 | 348 | ASN |
| 1 | F2 | 370 | ASN |
| 1 | F2 | 396 | HIS |
| 2 | F3 | 11 | GLN |
| 2 | F3 | 61 | HIS |
| 2 | F3 | 88 | HIS |
| 2 | F3 | 101 | ASN |
| 2 | F3 | 128 | ASN |
| 2 | F3 | 176 | GLN |
| 2 | F3 | 226 | ASN |
| 2 | F3 | 233 | GLN |
| 2 | F3 | 258 | ASN |
| 2 | F3 | 309 | HIS |
| 2 | F3 | 329 | ASN |
| 2 | F5 | 31 | GLN |
| 2 | F5 | 101 | ASN |
| 2 | F5 | 186 | ASN |
| 2 | F5 | 249 | ASN |
| 2 | F5 | 342 | GLN |
| 2 | F5 | 356 | ASN |
| 1 | F6 | 15 | GLN |
| 1 | F6 | 190 | HIS |
| 1 | F6 | 291 | GLN |
| 1 | F6 | 347 | ASN |
| 1 | F6 | 396 | HIS |
| 1 | F6 | 416 | ASN |
| 2 | F7 | 8 | HIS |
| 2 | F7 | 88 | HIS |
| 2 | F7 | 101 | ASN |
| 2 | F7 | 133 | GLN |
| 2 | F7 | 258 | ASN |
| 2 | F7 | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F7 | 293 | ASN |
| 2 | F7 | 406 | HIS |
| 1 | F8 | 6 | HIS |
| 1 | F8 | 11 | GLN |
| 1 | F8 | 204 | ASN |
| 1 | F8 | 279 | GLN |
| 1 | F8 | 298 | ASN |
| 1 | F8 | 335 | ASN |
| 1 | F8 | 348 | ASN |
| 1 | F8 | 396 | HIS |
| 2 | F9 | 8 | HIS |
| 2 | F9 | 11 | GLN |
| 2 | F9 | 101 | ASN |
| 2 | F9 | 256 | GLN |
| 2 | F9 | 293 | ASN |
| 2 | F9 | 309 | HIS |
| 1 | G0 | 99 | ASN |
| 1 | G0 | 105 | HIS |
| 1 | G0 | 137 | HIS |
| 1 | G0 | 184 | ASN |
| 1 | G0 | 190 | HIS |
| 1 | G0 | 279 | GLN |
| 1 | G0 | 280 | GLN |
| 1 | G0 | 334 | GLN |
| 1 | G0 | 348 | ASN |
| 1 | G0 | 396 | HIS |
| 2 | G1 | 133 | GLN |
| 2 | G1 | 258 | ASN |
| 2 | G1 | 293 | ASN |
| 2 | G1 | 309 | HIS |
| 1 | G2 | 14 | ASN |
| 1 | G2 | 204 | ASN |
| 1 | G2 | 256 | ASN |
| 1 | G2 | 347 | ASN |
| 1 | G2 | 384 | GLN |
| 1 | G2 | 396 | HIS |
| 1 | G2 | 416 | ASN |
| 2 | G3 | 8 | HIS |
| 2 | G3 | 85 | GLN |
| 2 | G3 | 101 | ASN |
| 2 | G3 | 256 | GLN |
| 2 | G3 | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G3 | 309 | HIS |
| 1 | G4 | 6 | HIS |
| 1 | G4 | 37 | HIS |
| 1 | G4 | 204 | ASN |
| 1 | G4 | 334 | GLN |
| 1 | G4 | 335 | ASN |
| 1 | G4 | 348 | ASN |
| 1 | G4 | 396 | HIS |
| 2 | G5 | 8 | HIS |
| 2 | G5 | 107 | HIS |
| 2 | G5 | 228 | ASN |
| 2 | G5 | 233 | GLN |
| 2 | G5 | 293 | ASN |
| 2 | G5 | 309 | HIS |
| 2 | G5 | 372 | GLN |
| 1 | G6 | 137 | HIS |
| 1 | G6 | 256 | ASN |
| 1 | G6 | 334 | GLN |
| 1 | G6 | 347 | ASN |
| 1 | G6 | 384 | GLN |
| 1 | G6 | 396 | HIS |
| 2 | G7 | 88 | HIS |
| 2 | G7 | 186 | ASN |
| 2 | G7 | 256 | GLN |
| 2 | G7 | 258 | ASN |
| 2 | G7 | 293 | ASN |
| 2 | G7 | 372 | GLN |
| 1 | G8 | 14 | ASN |
| 1 | G8 | 137 | HIS |
| 1 | G8 | 184 | ASN |
| 1 | G8 | 204 | ASN |
| 1 | G8 | 247 | ASN |
| 1 | G8 | 256 | ASN |
| 1 | G8 | 298 | ASN |
| 1 | G8 | 334 | GLN |
| 1 | G8 | 347 | ASN |
| 1 | G8 | 348 | ASN |
| 1 | G8 | 396 | HIS |
| 2 | G9 | 8 | HIS |
| 2 | G9 | 11 | GLN |
| 2 | G9 | 61 | HIS |
| 2 | G9 | 101 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G9 | 192 | HIS |
| 2 | G9 | 226 | ASN |
| 2 | G9 | 228 | ASN |
| 2 | G9 | 258 | ASN |
| 2 | G9 | 293 | ASN |
| 2 | G9 | 329 | ASN |
| 2 | G9 | 406 | HIS |
| 2 | H1 | 88 | HIS |
| 2 | H1 | 101 | ASN |
| 2 | H1 | 133 | GLN |
| 2 | H1 | 192 | HIS |
| 2 | H1 | 258 | ASN |
| 2 | H1 | 293 | ASN |
| 2 | H1 | 406 | HIS |
| 1 | H2 | 6 | HIS |
| 1 | H2 | 14 | ASN |
| 1 | H2 | 256 | ASN |
| 1 | H2 | 334 | GLN |
| 1 | H2 | 335 | ASN |
| 1 | H2 | 396 | HIS |
| 2 | H3 | 88 | HIS |
| 2 | H3 | 101 | ASN |
| 2 | H3 | 186 | ASN |
| 2 | H3 | 256 | GLN |
| 2 | H3 | 285 | GLN |
| 2 | H3 | 293 | ASN |
| 2 | H3 | 309 | HIS |
| 1 | H4 | 14 | ASN |
| 1 | H4 | 190 | HIS |
| 1 | H4 | 334 | GLN |
| 1 | H4 | 335 | ASN |
| 1 | H4 | 396 | HIS |
| 1 | H4 | 414 | ASN |
| 2 | H5 | 293 | ASN |
| 2 | H5 | 309 | HIS |
| 2 | H5 | 329 | ASN |
| 1 | H6 | 14 | ASN |
| 1 | H6 | 190 | HIS |
| 1 | H6 | 247 | ASN |
| 1 | H6 | 256 | ASN |
| 1 | H6 | 334 | GLN |
| 1 | H6 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H7 | 15 | GLN |
| 2 | H7 | 293 | ASN |
| 2 | H7 | 309 | HIS |
| 2 | H7 | 406 | HIS |
| 1 | H8 | 99 | ASN |
| 1 | H8 | 190 | HIS |
| 1 | H8 | 334 | GLN |
| 1 | H8 | 396 | HIS |
| 1 | H8 | 414 | ASN |
| 2 | H9 | 15 | GLN |
| 2 | H9 | 293 | ASN |
| 2 | H9 | 309 | HIS |
| 1 | I0 | 14 | ASN |
| 1 | I0 | 184 | ASN |
| 1 | I0 | 292 | GLN |
| 1 | I0 | 384 | GLN |
| 1 | I0 | 396 | HIS |
| 1 | I0 | 423 | GLN |
| 2 | I1 | 11 | GLN |
| 2 | I1 | 15 | GLN |
| 2 | I1 | 88 | HIS |
| 2 | I1 | 91 | GLN |
| 2 | I1 | 101 | ASN |
| 2 | I1 | 256 | GLN |
| 2 | I1 | 258 | ASN |
| 2 | I1 | 293 | ASN |
| 2 | I1 | 309 | HIS |
| 2 | I1 | 406 | HIS |
| 1 | I2 | 14 | ASN |
| 1 | I2 | 131 | GLN |
| 1 | I2 | 184 | ASN |
| 1 | I2 | 247 | ASN |
| 1 | I2 | 334 | GLN |
| 1 | I2 | 384 | GLN |
| 1 | I2 | 396 | HIS |
| 2 | I3 | 256 | GLN |
| 2 | I3 | 293 | ASN |
| 2 | I3 | 309 | HIS |
| 2 | I3 | 329 | ASN |
| 1 | I4 | 6 | HIS |
| 1 | I4 | 190 | HIS |
| 1 | I4 | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I4 | 396 | HIS |
| 2 | I5 | 8 | HIS |
| 2 | I5 | 226 | ASN |
| 2 | I5 | 293 | ASN |
| 2 | I5 | 309 | HIS |
| 2 | I5 | 393 | HIS |
| 2 | I5 | 406 | HIS |
| 2 | I7 | 61 | HIS |
| 2 | I7 | 285 | GLN |
| 2 | I7 | 293 | ASN |
| 2 | I7 | 309 | HIS |
| 1 | I8 | 190 | HIS |
| 1 | I8 | 292 | GLN |
| 1 | I8 | 334 | GLN |
| 1 | I8 | 396 | HIS |
| 2 | I9 | 197 | HIS |
| 2 | I9 | 206 | ASN |
| 2 | I9 | 258 | ASN |
| 2 | I9 | 285 | GLN |
| 2 | I9 | 293 | ASN |
| 2 | I9 | 329 | ASN |
| 1 | J0 | 43 | GLN |
| 1 | J0 | 131 | GLN |
| 1 | J0 | 245 | GLN |
| 1 | J0 | 334 | GLN |
| 1 | J0 | 335 | ASN |
| 2 | J1 | 11 | GLN |
| 2 | J1 | 133 | GLN |
| 2 | J1 | 258 | ASN |
| 2 | J1 | 285 | GLN |
| 2 | J1 | 309 | HIS |
| 1 | J2 | 14 | ASN |
| 1 | J2 | 94 | GLN |
| 1 | J2 | 247 | ASN |
| 1 | J2 | 264 | HIS |
| 1 | J2 | 348 | ASN |
| 1 | J2 | 396 | HIS |
| 2 | J3 | 15 | GLN |
| 2 | J3 | 88 | HIS |
| 2 | J3 | 128 | ASN |
| 2 | J3 | 283 | HIS |
| 2 | J3 | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | J3 | 309 | HIS |
| 1 | J4 | 6 | HIS |
| 1 | J4 | 14 | ASN |
| 1 | J4 | 43 | GLN |
| 1 | J4 | 89 | ASN |
| 1 | J4 | 99 | ASN |
| 1 | J4 | 227 | HIS |
| 1 | J4 | 247 | ASN |
| 1 | J4 | 292 | GLN |
| 1 | J4 | 334 | GLN |
| 1 | J4 | 335 | ASN |
| 1 | J4 | 396 | HIS |
| 2 | J5 | 258 | ASN |
| 2 | J5 | 309 | HIS |
| 2 | J5 | 329 | ASN |
| 2 | J5 | 342 | GLN |
| 2 | J5 | 372 | GLN |
| 1 | J6 | 14 | ASN |
| 1 | J6 | 37 | HIS |
| 1 | J6 | 99 | ASN |
| 1 | J6 | 131 | GLN |
| 1 | J6 | 190 | HIS |
| 1 | J6 | 227 | HIS |
| 1 | J6 | 245 | GLN |
| 1 | J6 | 256 | ASN |
| 1 | J6 | 291 | GLN |
| 1 | J6 | 334 | GLN |
| 1 | J6 | 347 | ASN |
| 1 | J6 | 348 | ASN |
| 1 | J6 | 396 | HIS |
| 2 | J7 | 11 | GLN |
| 2 | J7 | 31 | GLN |
| 2 | J7 | 258 | ASN |
| 2 | J7 | 309 | HIS |
| 2 | J7 | 358 | GLN |
| 1 | J8 | 14 | ASN |
| 1 | J8 | 89 | ASN |
| 1 | J8 | 227 | HIS |
| 1 | J8 | 245 | GLN |
| 1 | J8 | 247 | ASN |
| 1 | J8 | 256 | ASN |
| 1 | J8 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | J9 | 28 | HIS |
| 2 | J9 | 61 | HIS |
| 2 | J9 | 256 | GLN |
| 2 | J9 | 283 | HIS |
| 2 | J9 | 309 | HIS |
| 1 | K0 | 6 | HIS |
| 1 | K0 | 14 | ASN |
| 1 | K0 | 190 | HIS |
| 1 | K0 | 245 | GLN |
| 1 | K0 | 256 | ASN |
| 1 | K0 | 264 | HIS |
| 1 | K0 | 334 | GLN |
| 1 | K0 | 335 | ASN |
| 1 | K0 | 396 | HIS |
| 2 | K1 | 8 | HIS |
| 2 | K1 | 28 | HIS |
| 2 | K1 | 31 | GLN |
| 2 | K1 | 107 | HIS |
| 2 | K1 | 133 | GLN |
| 2 | K1 | 192 | HIS |
| 2 | K1 | 258 | ASN |
| 2 | K1 | 309 | HIS |
| 2 | K1 | 342 | GLN |
| 2 | K3 | 8 | HIS |
| 2 | K3 | 192 | HIS |
| 2 | K3 | 285 | GLN |
| 2 | K3 | 293 | ASN |
| 2 | K3 | 309 | HIS |
| 2 | K3 | 372 | GLN |
| 1 | K4 | 190 | HIS |
| 1 | K4 | 245 | GLN |
| 1 | K4 | 292 | GLN |
| 1 | K4 | 334 | GLN |
| 1 | K4 | 347 | ASN |
| 1 | K4 | 396 | HIS |
| 1 | K4 | 414 | ASN |
| 2 | K5 | 8 | HIS |
| 2 | K5 | 18 | ASN |
| 2 | K5 | 309 | HIS |
| 1 | K6 | 184 | ASN |
| 1 | K6 | 329 | GLN |
| 1 | K6 | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K6 | 348 | ASN |
| 1 | K6 | 384 | GLN |
| 1 | K6 | 396 | HIS |
| 2 | K7 | 8 | HIS |
| 2 | K7 | 293 | ASN |
| 2 | K7 | 342 | GLN |
| 1 | K8 | 14 | ASN |
| 1 | K8 | 131 | GLN |
| 1 | K8 | 190 | HIS |
| 1 | K8 | 247 | ASN |
| 1 | K8 | 334 | GLN |
| 1 | K8 | 347 | ASN |
| 1 | K8 | 384 | GLN |
| 1 | K8 | 396 | HIS |
| 2 | K9 | 8 | HIS |
| 2 | K9 | 283 | HIS |
| 2 | K9 | 309 | HIS |
| 2 | K9 | 329 | ASN |
| 2 | K9 | 342 | GLN |
| 1 | L0 | 14 | ASN |
| 1 | L0 | 190 | HIS |
| 1 | L0 | 264 | HIS |
| 1 | L0 | 334 | GLN |
| 1 | L0 | 348 | ASN |
| 1 | L0 | 396 | HIS |
| 2 | L1 | 8 | HIS |
| 2 | L1 | 102 | ASN |
| 2 | L1 | 226 | ASN |
| 2 | L1 | 258 | ASN |
| 2 | L1 | 293 | ASN |
| 2 | L1 | 309 | HIS |
| 2 | L1 | 372 | GLN |
| 1 | L2 | 99 | ASN |
| 1 | L2 | 191 | GLN |
| 1 | L2 | 195 | ASN |
| 1 | L2 | 247 | ASN |
| 1 | L2 | 256 | ASN |
| 1 | L2 | 292 | GLN |
| 1 | L2 | 329 | GLN |
| 1 | L2 | 334 | GLN |
| 1 | L2 | 384 | GLN |
| 1 | L2 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L3 | 8 | HIS |
| 2 | L3 | 88 | HIS |
| 2 | L3 | 226 | ASN |
| 2 | L3 | 258 | ASN |
| 2 | L3 | 329 | ASN |
| 2 | L3 | 372 | GLN |
| 1 | L4 | 14 | ASN |
| 1 | L4 | 15 | GLN |
| 1 | L4 | 204 | ASN |
| 1 | L4 | 256 | ASN |
| 1 | L4 | 334 | GLN |
| 2 | L5 | 18 | ASN |
| 2 | L5 | 197 | HIS |
| 2 | L5 | 293 | ASN |
| 1 | L6 | 11 | GLN |
| 1 | L6 | 43 | GLN |
| 1 | L6 | 99 | ASN |
| 1 | L6 | 190 | HIS |
| 1 | L6 | 245 | GLN |
| 1 | L6 | 247 | ASN |
| 1 | L6 | 256 | ASN |
| 1 | L6 | 280 | GLN |
| 1 | L6 | 334 | GLN |
| 1 | L6 | 348 | ASN |
| 1 | L6 | 396 | HIS |
| 1 | L6 | 414 | ASN |
| 2 | L7 | 8 | HIS |
| 2 | L7 | 233 | GLN |
| 2 | L7 | 258 | ASN |
| 2 | L7 | 283 | HIS |
| 2 | L7 | 293 | ASN |
| 2 | L7 | 329 | ASN |
| 2 | L9 | 293 | ASN |
| 2 | L9 | 309 | HIS |
| 1 | M0 | 14 | ASN |
| 1 | M0 | 89 | ASN |
| 1 | M0 | 247 | ASN |
| 1 | M0 | 256 | ASN |
| 1 | M0 | 292 | GLN |
| 1 | M0 | 329 | GLN |
| 1 | M0 | 334 | GLN |
| 1 | M0 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M1 | 18 | ASN |
| 2 | M1 | 85 | GLN |
| 2 | M1 | 133 | GLN |
| 2 | M1 | 176 | GLN |
| 2 | M1 | 258 | ASN |
| 2 | M1 | 309 | HIS |
| 1 | M2 | 14 | ASN |
| 1 | M2 | 89 | ASN |
| 1 | M2 | 195 | ASN |
| 1 | M2 | 256 | ASN |
| 1 | M2 | 334 | GLN |
| 1 | M2 | 348 | ASN |
| 2 | M3 | 61 | HIS |
| 2 | M3 | 226 | ASN |
| 2 | M3 | 258 | ASN |
| 2 | M3 | 309 | HIS |
| 1 | M4 | 89 | ASN |
| 1 | M4 | 105 | HIS |
| 1 | M4 | 227 | HIS |
| 1 | M4 | 256 | ASN |
| 1 | M4 | 292 | GLN |
| 1 | M4 | 334 | GLN |
| 1 | M4 | 396 | HIS |
| 2 | M5 | 8 | HIS |
| 2 | M5 | 18 | ASN |
| 2 | M5 | 88 | HIS |
| 2 | M5 | 293 | ASN |
| 2 | M5 | 309 | HIS |
| 1 | M6 | 14 | ASN |
| 1 | M6 | 37 | HIS |
| 1 | M6 | 89 | ASN |
| 1 | M6 | 105 | HIS |
| 1 | M6 | 334 | GLN |
| 1 | M6 | 396 | HIS |
| 2 | M7 | 15 | GLN |
| 2 | M7 | 50 | ASN |
| 2 | M7 | 61 | HIS |
| 2 | M7 | 91 | GLN |
| 2 | M7 | 101 | ASN |
| 2 | M7 | 206 | ASN |
| 2 | M7 | 283 | HIS |
| 2 | M7 | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M7 | 309 | HIS |
| 1 | M8 | 89 | ASN |
| 1 | M8 | 190 | HIS |
| 1 | M8 | 292 | GLN |
| 1 | M8 | 348 | ASN |
| 2 | M9 | 61 | HIS |
| 2 | M9 | 197 | HIS |
| 2 | M9 | 233 | GLN |
| 2 | M9 | 293 | ASN |
| 1 | N0 | 14 | ASN |
| 1 | N0 | 89 | ASN |
| 1 | N0 | 334 | GLN |
| 1 | N0 | 396 | HIS |
| 2 | N1 | 8 | HIS |
| 2 | N1 | 28 | HIS |
| 2 | N1 | 101 | ASN |
| 2 | N1 | 197 | HIS |
| 2 | N1 | 293 | ASN |
| 2 | N1 | 309 | HIS |
| 1 | N2 | 89 | ASN |
| 1 | N2 | 256 | ASN |
| 1 | N2 | 292 | GLN |
| 1 | N2 | 348 | ASN |
| 1 | N2 | 396 | HIS |
| 1 | N2 | 423 | GLN |
| 2 | N3 | 8 | HIS |
| 2 | N3 | 15 | GLN |
| 2 | N3 | 18 | ASN |
| 2 | N3 | 88 | HIS |
| 2 | N3 | 102 | ASN |
| 2 | N3 | 133 | GLN |
| 2 | N3 | 226 | ASN |
| 2 | N3 | 258 | ASN |
| 2 | N3 | 285 | GLN |
| 2 | N3 | 293 | ASN |
| 2 | N3 | 309 | HIS |
| 2 | N3 | 356 | ASN |
| 2 | N5 | 18 | ASN |
| 2 | N5 | 88 | HIS |
| 2 | N5 | 192 | HIS |
| 2 | N5 | 283 | HIS |
| 2 | N5 | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | N5 | 309 | HIS |
| 2 | N5 | 356 | ASN |
| 1 | N6 | 48 | ASN |
| 1 | N6 | 99 | ASN |
| 1 | N6 | 105 | HIS |
| 1 | N6 | 191 | GLN |
| 1 | N6 | 204 | ASN |
| 1 | N6 | 227 | HIS |
| 1 | N6 | 256 | ASN |
| 1 | N6 | 279 | GLN |
| 1 | N6 | 396 | HIS |
| 2 | N7 | 226 | ASN |
| 2 | N7 | 258 | ASN |
| 2 | N7 | 293 | ASN |
| 2 | N7 | 309 | HIS |
| 2 | N7 | 356 | ASN |
| 1 | N8 | 14 | ASN |
| 1 | N8 | 99 | ASN |
| 1 | N8 | 190 | HIS |
| 1 | N8 | 204 | ASN |
| 1 | N8 | 227 | HIS |
| 1 | N8 | 256 | ASN |
| 1 | N8 | 334 | GLN |
| 1 | N8 | 347 | ASN |
| 1 | N8 | 348 | ASN |
| 1 | N8 | 396 | HIS |
| 2 | N9 | 233 | GLN |
| 2 | N9 | 258 | ASN |
| 2 | N9 | 293 | ASN |
| 2 | N9 | 309 | HIS |
| 2 | N9 | 356 | ASN |
| 1 | O0 | 6 | HIS |
| 1 | O0 | 8 | GLN |
| 1 | O0 | 89 | ASN |
| 1 | O0 | 99 | ASN |
| 1 | O0 | 131 | GLN |
| 1 | O0 | 190 | HIS |
| 1 | O0 | 227 | HIS |
| 1 | O0 | 245 | GLN |
| 1 | O0 | 256 | ASN |
| 1 | O0 | 264 | HIS |
| 1 | O0 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O0 | 416 | ASN |
| 2 | O1 | 233 | GLN |
| 2 | O1 | 256 | GLN |
| 2 | O1 | 258 | ASN |
| 2 | O1 | 283 | HIS |
| 2 | O1 | 309 | HIS |
| 1 | O2 | 6 | HIS |
| 1 | O2 | 14 | ASN |
| 1 | O2 | 15 | GLN |
| 1 | O2 | 99 | ASN |
| 1 | O2 | 131 | GLN |
| 1 | O2 | 204 | ASN |
| 1 | O2 | 227 | HIS |
| 1 | O2 | 245 | GLN |
| 1 | O2 | 337 | ASN |
| 2 | O3 | 50 | ASN |
| 2 | O3 | 128 | ASN |
| 2 | O3 | 249 | ASN |
| 2 | O3 | 258 | ASN |
| 2 | O3 | 309 | HIS |
| 2 | O3 | 329 | ASN |
| 1 | O4 | 6 | HIS |
| 1 | O4 | 89 | ASN |
| 1 | O4 | 131 | GLN |
| 1 | O4 | 190 | HIS |
| 1 | O4 | 227 | HIS |
| 1 | O4 | 256 | ASN |
| 1 | O4 | 279 | GLN |
| 1 | O4 | 396 | HIS |
| 2 | O5 | 15 | GLN |
| 2 | O5 | 31 | GLN |
| 2 | O5 | 128 | ASN |
| 2 | O5 | 285 | GLN |
| 2 | O5 | 309 | HIS |
| 2 | O5 | 329 | ASN |
| 1 | O6 | 6 | HIS |
| 1 | O6 | 89 | ASN |
| 1 | O6 | 131 | GLN |
| 1 | O6 | 134 | GLN |
| 1 | O6 | 195 | ASN |
| 1 | O6 | 245 | GLN |
| 1 | O6 | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O6 | 396 | HIS |
| 2 | O7 | 28 | HIS |
| 2 | O7 | 85 | GLN |
| 2 | O7 | 88 | HIS |
| 2 | O7 | 197 | HIS |
| 2 | O7 | 258 | ASN |
| 2 | O7 | 329 | ASN |
| 2 | O7 | 358 | GLN |
| 1 | O8 | 99 | ASN |
| 1 | O8 | 131 | GLN |
| 1 | O8 | 227 | HIS |
| 1 | O8 | 245 | GLN |
| 1 | O8 | 256 | ASN |
| 1 | O8 | 292 | GLN |
| 1 | O8 | 347 | ASN |
| 1 | O8 | 396 | HIS |
| 2 | O9 | 28 | HIS |
| 2 | O9 | 101 | ASN |
| 2 | O9 | 258 | ASN |
| 2 | O9 | 285 | GLN |
| 2 | P3 | 8 | HIS |
| 2 | P3 | 18 | ASN |
| 2 | P3 | 133 | GLN |
| 2 | P3 | 226 | ASN |
| 2 | P3 | 293 | ASN |
| 2 | P3 | 309 | HIS |
| 2 | P3 | 356 | ASN |
| 1 | P4 | 14 | ASN |
| 1 | P4 | 137 | HIS |
| 1 | P4 | 204 | ASN |
| 1 | P4 | 256 | ASN |
| 1 | P4 | 329 | GLN |
| 1 | P4 | 416 | ASN |
| 2 | P5 | 8 | HIS |
| 2 | P5 | 197 | HIS |
| 2 | P5 | 228 | ASN |
| 2 | P5 | 283 | HIS |
| 2 | P5 | 309 | HIS |
| 2 | P5 | 329 | ASN |
| 1 | P6 | 89 | ASN |
| 1 | P6 | 137 | HIS |
| 1 | P6 | 190 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P6 | 204 | ASN |
| 1 | P6 | 256 | ASN |
| 1 | P6 | 334 | GLN |
| 1 | P6 | 347 | ASN |
| 1 | P6 | 384 | GLN |
| 1 | P6 | 396 | HIS |
| 1 | P6 | 414 | ASN |
| 1 | P6 | 416 | ASN |
| 2 | P7 | 88 | HIS |
| 2 | P7 | 107 | HIS |
| 2 | P7 | 133 | GLN |
| 2 | P7 | 192 | HIS |
| 2 | P7 | 309 | HIS |
| 2 | P7 | 342 | GLN |
| 1 | P8 | 11 | GLN |
| 1 | P8 | 14 | ASN |
| 1 | P8 | 37 | HIS |
| 1 | P8 | 99 | ASN |
| 1 | P8 | 137 | HIS |
| 1 | P8 | 204 | ASN |
| 1 | P8 | 256 | ASN |
| 1 | P8 | 298 | ASN |
| 1 | P8 | 334 | GLN |
| 1 | P8 | 423 | GLN |
| 2 | P9 | 8 | HIS |
| 2 | P9 | 18 | ASN |
| 2 | P9 | 31 | GLN |
| 2 | P9 | 107 | HIS |
| 2 | P9 | 133 | GLN |
| 2 | P9 | 228 | ASN |
| 2 | P9 | 258 | ASN |
| 2 | P9 | 309 | HIS |
| 1 | Q0 | 14 | ASN |
| 1 | Q0 | 131 | GLN |
| 1 | Q0 | 190 | HIS |
| 1 | Q0 | 204 | ASN |
| 1 | Q0 | 227 | HIS |
| 1 | Q0 | 247 | ASN |
| 1 | Q0 | 256 | ASN |
| 1 | Q0 | 292 | GLN |
| 1 | Q0 | 329 | GLN |
| 1 | Q0 | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q0 | 347 | ASN |
| 1 | Q0 | 348 | ASN |
| 1 | Q0 | 396 | HIS |
| 1 | Q0 | 416 | ASN |
| 1 | Q0 | 423 | GLN |
| 2 | Q1 | 8 | HIS |
| 2 | Q1 | 197 | HIS |
| 2 | Q1 | 258 | ASN |
| 2 | Q1 | 309 | HIS |
| 1 | Q2 | 99 | ASN |
| 1 | Q2 | 190 | HIS |
| 1 | Q2 | 204 | ASN |
| 1 | Q2 | 247 | ASN |
| 1 | Q2 | 334 | GLN |
| 1 | Q2 | 396 | HIS |
| 1 | Q2 | 423 | GLN |
| 2 | Q3 | 8 | HIS |
| 2 | Q3 | 88 | HIS |
| 2 | Q3 | 258 | ASN |
| 2 | Q3 | 309 | HIS |
| 1 | Q4 | 6 | HIS |
| 1 | Q4 | 8 | GLN |
| 1 | Q4 | 11 | GLN |
| 1 | Q4 | 14 | ASN |
| 1 | Q4 | 134 | GLN |
| 1 | Q4 | 204 | ASN |
| 1 | Q4 | 227 | HIS |
| 1 | Q4 | 245 | GLN |
| 1 | Q4 | 256 | ASN |
| 1 | Q4 | 348 | ASN |
| 1 | Q4 | 396 | HIS |
| 2 | Q5 | 8 | HIS |
| 2 | Q5 | 133 | GLN |
| 2 | Q5 | 226 | ASN |
| 2 | Q5 | 256 | GLN |
| 2 | Q5 | 309 | HIS |
| 2 | Q5 | 329 | ASN |
| 1 | Q6 | 14 | ASN |
| 1 | Q6 | 137 | HIS |
| 1 | Q6 | 190 | HIS |
| 1 | Q6 | 204 | ASN |
| 1 | Q6 | 227 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q6 | 256 | ASN |
| 1 | Q6 | 279 | GLN |
| 1 | Q6 | 298 | ASN |
| 1 | Q6 | 329 | GLN |
| 1 | Q6 | 334 | GLN |
| 1 | Q6 | 348 | ASN |
| 1 | Q6 | 384 | GLN |
| 1 | Q6 | 423 | GLN |
| 1 | Q8 | 11 | GLN |
| 1 | Q8 | 28 | HIS |
| 1 | Q8 | 43 | GLN |
| 1 | Q8 | 99 | ASN |
| 1 | Q8 | 396 | HIS |
| 2 | Q9 | 256 | GLN |
| 2 | Q9 | 258 | ASN |
| 2 | Q9 | 406 | HIS |
| 1 | R0 | 6 | HIS |
| 1 | R0 | 256 | ASN |
| 1 | R0 | 291 | GLN |
| 1 | R0 | 337 | ASN |
| 1 | R0 | 384 | GLN |
| 1 | R0 | 396 | HIS |
| 1 | R0 | 424 | GLN |
| 2 | R1 | 197 | HIS |
| 2 | R1 | 258 | ASN |
| 2 | R1 | 293 | ASN |
| 2 | R1 | 309 | HIS |
| 2 | R1 | 329 | ASN |
| 1 | R2 | 11 | GLN |
| 1 | R2 | 94 | GLN |
| 1 | R2 | 190 | HIS |
| 1 | R2 | 247 | ASN |
| 1 | R2 | 256 | ASN |
| 1 | R2 | 329 | GLN |
| 1 | R2 | 334 | GLN |
| 1 | R2 | 348 | ASN |
| 1 | R2 | 396 | HIS |
| 1 | R2 | 423 | GLN |
| 2 | R3 | 15 | GLN |
| 2 | R3 | 18 | ASN |
| 2 | R3 | 61 | HIS |
| 2 | R3 | 102 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | R3 | 192 | HIS |
| 2 | R3 | 226 | ASN |
| 2 | R3 | 309 | HIS |
| 2 | R3 | 372 | GLN |
| 1 | R4 | 6 | HIS |
| 1 | R4 | 14 | ASN |
| 1 | R4 | 190 | HIS |
| 1 | R4 | 334 | GLN |
| 1 | R4 | 335 | ASN |
| 1 | R4 | 384 | GLN |
| 1 | R4 | 414 | ASN |
| 1 | R4 | 424 | GLN |
| 1 | R4 | 426 | GLN |
| 2 | R5 | 8 | HIS |
| 2 | R5 | 88 | HIS |
| 2 | R5 | 197 | HIS |
| 2 | R5 | 258 | ASN |
| 2 | R5 | 293 | ASN |
| 2 | R5 | 309 | HIS |
| 2 | R5 | 329 | ASN |
| 1 | R6 | 11 | GLN |
| 1 | R6 | 14 | ASN |
| 1 | R6 | 190 | HIS |
| 1 | R6 | 191 | GLN |
| 1 | R6 | 195 | ASN |
| 1 | R6 | 247 | ASN |
| 1 | R6 | 256 | ASN |
| 1 | R6 | 329 | GLN |
| 1 | R6 | 396 | HIS |
| 1 | R6 | 414 | ASN |
| 1 | R6 | 423 | GLN |
| 2 | R7 | 8 | HIS |
| 2 | R7 | 31 | GLN |
| 2 | R7 | 293 | ASN |
| 2 | R7 | 356 | ASN |
| 2 | R7 | 372 | GLN |
| 1 | R8 | 89 | ASN |
| 1 | R8 | 94 | GLN |
| 1 | R8 | 99 | ASN |
| 1 | R8 | 204 | ASN |
| 1 | R8 | 245 | GLN |
| 1 | R8 | 247 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | R8 | 256 | ASN |
| 1 | R8 | 292 | GLN |
| 1 | R8 | 384 | GLN |
| 1 | R8 | 424 | GLN |
| 2 | R9 | 8 | HIS |
| 2 | R9 | 197 | HIS |
| 2 | R9 | 258 | ASN |
| 2 | R9 | 283 | HIS |
| 2 | R9 | 309 | HIS |
| 2 | R9 | 329 | ASN |
| 1 | S0 | 11 | GLN |
| 1 | S0 | 14 | ASN |
| 1 | S0 | 89 | ASN |
| 1 | S0 | 94 | GLN |
| 1 | S0 | 190 | HIS |
| 1 | S0 | 195 | ASN |
| 1 | S0 | 245 | GLN |
| 1 | S0 | 256 | ASN |
| 1 | S0 | 292 | GLN |
| 1 | S0 | 334 | GLN |
| 1 | S0 | 347 | ASN |
| 1 | S0 | 348 | ASN |
| 1 | S0 | 396 | HIS |
| 1 | S0 | 423 | GLN |
| 2 | S1 | 88 | HIS |
| 2 | S1 | 91 | GLN |
| 2 | S1 | 197 | HIS |
| 2 | S1 | 309 | HIS |
| 2 | S1 | 356 | ASN |
| 1 | S2 | 6 | HIS |
| 1 | S2 | 14 | ASN |
| 1 | S2 | 37 | HIS |
| 1 | S2 | 94 | GLN |
| 1 | S2 | 190 | HIS |
| 1 | S2 | 204 | ASN |
| 1 | S2 | 247 | ASN |
| 1 | S2 | 329 | GLN |
| 1 | S2 | 332 | ASN |
| 1 | S2 | 384 | GLN |
| 1 | S2 | 424 | GLN |
| 1 | S4 | 6 | HIS |
| 1 | S4 | 11 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S4 | 14 | ASN |
| 1 | S4 | 89 | ASN |
| 1 | S4 | 99 | ASN |
| 1 | S4 | 184 | ASN |
| 1 | S4 | 190 | HIS |
| 1 | S4 | 245 | GLN |
| 1 | S4 | 292 | GLN |
| 1 | S4 | 329 | GLN |
| 1 | S4 | 332 | ASN |
| 1 | S4 | 334 | GLN |
| 1 | S4 | 396 | HIS |
| 1 | S4 | 414 | ASN |
| 2 | S5 | 176 | GLN |
| 2 | S5 | 192 | HIS |
| 2 | S5 | 233 | GLN |
| 2 | S5 | 258 | ASN |
| 2 | S5 | 309 | HIS |
| 2 | S5 | 342 | GLN |
| 1 | S6 | 6 | HIS |
| 1 | S6 | 37 | HIS |
| 1 | S6 | 89 | ASN |
| 1 | S6 | 227 | HIS |
| 1 | S6 | 256 | ASN |
| 1 | S6 | 329 | GLN |
| 1 | S6 | 384 | GLN |
| 2 | S7 | 11 | GLN |
| 2 | S7 | 88 | HIS |
| 2 | S7 | 192 | HIS |
| 2 | S7 | 309 | HIS |
| 2 | S7 | 329 | ASN |
| 1 | S8 | 6 | HIS |
| 1 | S8 | 11 | GLN |
| 1 | S8 | 89 | ASN |
| 1 | S8 | 99 | ASN |
| 1 | S8 | 131 | GLN |
| 1 | S8 | 195 | ASN |
| 1 | S8 | 247 | ASN |
| 1 | S8 | 256 | ASN |
| 1 | S8 | 329 | GLN |
| 1 | S8 | 334 | GLN |
| 1 | S8 | 337 | ASN |
| 1 | S8 | 348 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S8 | 396 | HIS |
| 2 | S9 | 15 | GLN |
| 2 | S9 | 18 | ASN |
| 2 | S9 | 88 | HIS |
| 2 | S9 | 101 | ASN |
| 2 | S9 | 258 | ASN |
| 2 | S9 | 309 | HIS |
| 1 | T0 | 14 | ASN |
| 1 | T0 | 28 | HIS |
| 1 | T0 | 89 | ASN |
| 1 | T0 | 190 | HIS |
| 1 | T0 | 195 | ASN |
| 1 | T0 | 247 | ASN |
| 1 | T0 | 256 | ASN |
| 1 | T0 | 292 | GLN |
| 2 | T1 | 8 | HIS |
| 2 | T1 | 35 | GLN |
| 2 | T1 | 256 | GLN |
| 2 | T1 | 283 | HIS |
| 2 | T1 | 309 | HIS |
| 2 | T1 | 329 | ASN |
| 1 | T2 | 6 | HIS |
| 1 | T2 | 11 | GLN |
| 1 | T2 | 43 | GLN |
| 1 | T2 | 245 | GLN |
| 1 | T2 | 292 | GLN |
| 1 | T2 | 298 | ASN |
| 1 | T2 | 334 | GLN |
| 1 | T2 | 337 | ASN |
| 1 | T2 | 348 | ASN |
| 1 | T2 | 396 | HIS |
| 2 | T3 | 8 | HIS |
| 2 | T3 | 18 | ASN |
| 2 | T3 | 197 | HIS |
| 2 | T3 | 309 | HIS |
| 2 | T3 | 342 | GLN |
| 2 | T3 | 372 | GLN |
| 2 | T3 | 393 | HIS |
| 1 | T4 | 14 | ASN |
| 1 | T4 | 89 | ASN |
| 1 | T4 | 190 | HIS |
| 1 | T4 | 204 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | T4 | 245 | GLN |
| 1 | T4 | 298 | ASN |
| 1 | T4 | 329 | GLN |
| 1 | T4 | 334 | GLN |
| 1 | T4 | 384 | GLN |
| 1 | T4 | 423 | GLN |
| 2 | T5 | 15 | GLN |
| 2 | T5 | 133 | GLN |
| 2 | T5 | 192 | HIS |
| 2 | T5 | 197 | HIS |
| 2 | T5 | 309 | HIS |
| 2 | T5 | 329 | ASN |
| 2 | T5 | 406 | HIS |
| 1 | T6 | 6 | HIS |
| 1 | T6 | 11 | GLN |
| 1 | T6 | 14 | ASN |
| 1 | T6 | 37 | HIS |
| 1 | T6 | 190 | HIS |
| 1 | T6 | 227 | HIS |
| 1 | T6 | 256 | ASN |
| 1 | T6 | 298 | ASN |
| 1 | T6 | 334 | GLN |
| 1 | T6 | 335 | ASN |
| 1 | T6 | 337 | ASN |
| 1 | T6 | 348 | ASN |
| 1 | T6 | 396 | HIS |
| 1 | T6 | 414 | ASN |
| 1 | T6 | 423 | GLN |
| 2 | T7 | 8 | HIS |
| 2 | T7 | 88 | HIS |
| 2 | T7 | 133 | GLN |
| 2 | T7 | 228 | ASN |
| 2 | T7 | 293 | ASN |
| 2 | T7 | 342 | GLN |
| 2 | T7 | 372 | GLN |
| 1 | T8 | 14 | ASN |
| 1 | T8 | 89 | ASN |
| 1 | T8 | 204 | ASN |
| 1 | T8 | 227 | HIS |
| 1 | T8 | 256 | ASN |
| 1 | T8 | 291 | GLN |
| 1 | T8 | 292 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | T8 | 329 | GLN |
| 1 | T8 | 334 | GLN |
| 1 | T8 | 347 | ASN |
| 1 | T8 | 348 | ASN |
| 1 | T8 | 384 | GLN |
| 1 | T8 | 396 | HIS |
| 2 | U1 | 15 | GLN |
| 2 | U1 | 101 | ASN |
| 2 | U1 | 133 | GLN |
| 2 | U1 | 293 | ASN |
| 2 | U1 | 309 | HIS |
| 1 | U2 | 190 | HIS |
| 1 | U2 | 226 | ASN |
| 1 | U2 | 307 | HIS |
| 1 | U2 | 334 | GLN |
| 1 | U2 | 347 | ASN |
| 1 | U2 | 396 | HIS |
| 1 | U2 | 423 | GLN |
| 2 | U3 | 15 | GLN |
| 2 | U3 | 101 | ASN |
| 2 | U3 | 228 | ASN |
| 2 | U3 | 258 | ASN |
| 1 | U4 | 14 | ASN |
| 1 | U4 | 334 | GLN |
| 1 | U4 | 348 | ASN |
| 1 | U4 | 396 | HIS |
| 1 | U4 | 423 | GLN |
| 2 | U5 | 101 | ASN |
| 2 | U5 | 133 | GLN |
| 2 | U5 | 206 | ASN |
| 2 | U5 | 228 | ASN |
| 2 | U5 | 258 | ASN |
| 2 | U5 | 285 | GLN |
| 2 | U5 | 309 | HIS |
| 1 | U6 | 11 | GLN |
| 1 | U6 | 226 | ASN |
| 1 | U6 | 245 | GLN |
| 1 | U6 | 292 | GLN |
| 1 | U6 | 307 | HIS |
| 1 | U6 | 329 | GLN |
| 1 | U6 | 332 | ASN |
| 1 | U6 | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | U6 | 347 | ASN |
| 1 | U6 | 396 | HIS |
| 2 | U7 | 15 | GLN |
| 2 | U7 | 101 | ASN |
| 2 | U7 | 133 | GLN |
| 2 | U7 | 206 | ASN |
| 2 | U7 | 285 | GLN |
| 2 | U7 | 293 | ASN |
| 2 | U7 | 309 | HIS |
| 2 | U7 | 329 | ASN |
| 2 | U7 | 406 | HIS |
| 1 | U8 | 332 | ASN |
| 1 | U8 | 335 | ASN |
| 2 | U9 | 15 | GLN |
| 2 | U9 | 101 | ASN |
| 2 | U9 | 133 | GLN |
| 2 | U9 | 176 | GLN |
| 2 | U9 | 206 | ASN |
| 2 | U9 | 249 | ASN |
| 2 | U9 | 285 | GLN |
| 2 | U9 | 293 | ASN |
| 2 | U9 | 309 | HIS |
| 1 | V0 | 190 | HIS |
| 1 | V0 | 256 | ASN |
| 1 | V0 | 347 | ASN |
| 1 | V0 | 396 | HIS |
| 1 | V0 | 423 | GLN |
| 2 | V1 | 8 | HIS |
| 2 | V1 | 61 | HIS |
| 2 | V1 | 88 | HIS |
| 2 | V1 | 133 | GLN |
| 2 | V1 | 176 | GLN |
| 2 | V1 | 258 | ASN |
| 2 | V1 | 285 | GLN |
| 2 | V1 | 309 | HIS |
| 2 | V1 | 406 | HIS |
| 1 | V2 | 105 | HIS |
| 1 | V2 | 190 | HIS |
| 1 | V2 | 396 | HIS |
| 2 | V3 | 8 | HIS |
| 2 | V3 | 15 | GLN |
| 2 | V3 | 88 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | V3 | 101 | ASN |
| 2 | V3 | 249 | ASN |
| 2 | V3 | 285 | GLN |
| 2 | V3 | 309 | HIS |
| 2 | V3 | 329 | ASN |
| 2 | V3 | 356 | ASN |
| 1 | V4 | 190 | HIS |
| 1 | V4 | 195 | ASN |
| 1 | V4 | 226 | ASN |
| 1 | V4 | 329 | GLN |
| 1 | V4 | 335 | ASN |
| 1 | V4 | 396 | HIS |
| 1 | V6 | 6 | HIS |
| 1 | V6 | 14 | ASN |
| 1 | V6 | 99 | ASN |
| 1 | V6 | 134 | GLN |
| 1 | V6 | 292 | GLN |
| 1 | V6 | 347 | ASN |
| 1 | V6 | 348 | ASN |
| 1 | V6 | 396 | HIS |
| 2 | V7 | 15 | GLN |
| 2 | V7 | 31 | GLN |
| 2 | V7 | 283 | HIS |
| 2 | V7 | 293 | ASN |
| 2 | V7 | 329 | ASN |
| 1 | V8 | 105 | HIS |
| 1 | V8 | 227 | HIS |
| 1 | V8 | 245 | GLN |
| 1 | V8 | 256 | ASN |
| 1 | V8 | 292 | GLN |
| 1 | V8 | 334 | GLN |
| 1 | V8 | 348 | ASN |
| 1 | V8 | 396 | HIS |
| 2 | V9 | 8 | HIS |
| 2 | V9 | 15 | GLN |
| 2 | V9 | 61 | HIS |
| 2 | V9 | 91 | GLN |
| 2 | V9 | 309 | HIS |
| 1 | W0 | 14 | ASN |
| 1 | W0 | 37 | HIS |
| 1 | W0 | 184 | ASN |
| 1 | W0 | 227 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | W0 | 245 | GLN |
| 1 | W0 | 292 | GLN |
| 1 | W0 | 332 | ASN |
| 1 | W0 | 334 | GLN |
| 1 | W0 | 347 | ASN |
| 1 | W0 | 396 | HIS |
| 2 | W1 | 15 | GLN |
| 2 | W1 | 31 | GLN |
| 2 | W1 | 258 | ASN |
| 2 | W1 | 309 | HIS |
| 2 | W1 | 342 | GLN |
| 1 | W2 | 37 | HIS |
| 1 | W2 | 89 | ASN |
| 1 | W2 | 105 | HIS |
| 1 | W2 | 245 | GLN |
| 1 | W2 | 256 | ASN |
| 1 | W2 | 347 | ASN |
| 1 | W2 | 396 | HIS |
| 2 | W3 | 15 | GLN |
| 2 | W3 | 31 | GLN |
| 2 | W3 | 61 | HIS |
| 2 | W3 | 88 | HIS |
| 2 | W3 | 258 | ASN |
| 2 | W3 | 293 | ASN |
| 2 | W3 | 309 | HIS |
| 1 | W4 | 6 | HIS |
| 1 | W4 | 14 | ASN |
| 1 | W4 | 227 | HIS |
| 1 | W4 | 256 | ASN |
| 1 | W4 | 292 | GLN |
| 1 | W4 | 332 | ASN |
| 1 | W4 | 334 | GLN |
| 1 | W4 | 347 | ASN |
| 1 | W4 | 348 | ASN |
| 1 | W4 | 396 | HIS |
| 2 | W5 | 15 | GLN |
| 2 | W5 | 31 | GLN |
| 2 | W5 | 61 | HIS |
| 2 | W5 | 309 | HIS |
| 1 | W6 | 14 | ASN |
| 1 | W6 | 247 | ASN |
| 1 | W6 | 292 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | W6 | 334 | GLN |
| 1 | W6 | 396 | HIS |
| 2 | W7 | 8 | HIS |
| 2 | W7 | 15 | GLN |
| 2 | W7 | 31 | GLN |
| 2 | W7 | 61 | HIS |
| 2 | W7 | 88 | HIS |
| 2 | W7 | 133 | GLN |
| 2 | W7 | 176 | GLN |
| 2 | W7 | 283 | HIS |
| 2 | W7 | 309 | HIS |
| 2 | W7 | 329 | ASN |
| 1 | W8 | 37 | HIS |
| 1 | W8 | 131 | GLN |
| 1 | W8 | 190 | HIS |
| 1 | W8 | 245 | GLN |
| 1 | W8 | 292 | GLN |
| 1 | W8 | 334 | GLN |
| 1 | W8 | 348 | ASN |
| 1 | W8 | 396 | HIS |
| 2 | W9 | 11 | GLN |
| 2 | W9 | 15 | GLN |
| 2 | W9 | 258 | ASN |
| 2 | W9 | 309 | HIS |
| 1 | X0 | 14 | ASN |
| 1 | X0 | 43 | GLN |
| 1 | X0 | 190 | HIS |
| 1 | X0 | 245 | GLN |
| 1 | X0 | 247 | ASN |
| 1 | X0 | 256 | ASN |
| 1 | X0 | 280 | GLN |
| 1 | X0 | 334 | GLN |
| 1 | X0 | 414 | ASN |
| 1 | X0 | 423 | GLN |
| 1 | X2 | 99 | ASN |
| 1 | X2 | 134 | GLN |
| 1 | X2 | 191 | GLN |
| 1 | X2 | 227 | HIS |
| 1 | X2 | 247 | ASN |
| 1 | X2 | 279 | GLN |
| 1 | X2 | 280 | GLN |
| 1 | X2 | 292 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | X2 | 329 | GLN |
| 1 | X2 | 334 | GLN |
| 1 | X2 | 337 | ASN |
| 1 | X2 | 348 | ASN |
| 1 | X2 | 396 | HIS |
| 1 | X2 | 416 | ASN |
| 2 | X3 | 233 | GLN |
| 2 | X3 | 258 | ASN |
| 2 | X3 | 293 | ASN |
| 2 | X3 | 329 | ASN |
| 1 | X4 | 48 | ASN |
| 1 | X4 | 99 | ASN |
| 1 | X4 | 134 | GLN |
| 1 | X4 | 190 | HIS |
| 1 | X4 | 195 | ASN |
| 1 | X4 | 204 | ASN |
| 1 | X4 | 227 | HIS |
| 1 | X4 | 256 | ASN |
| 1 | X4 | 396 | HIS |
| 1 | X4 | 416 | ASN |
| 2 | X5 | 28 | HIS |
| 2 | X5 | 309 | HIS |
| 1 | X6 | 99 | ASN |
| 1 | X6 | 134 | GLN |
| 1 | X6 | 190 | HIS |
| 1 | X6 | 227 | HIS |
| 1 | X6 | 256 | ASN |
| 1 | X6 | 279 | GLN |
| 1 | X6 | 280 | GLN |
| 1 | X6 | 334 | GLN |
| 1 | X6 | 348 | ASN |
| 2 | X7 | 233 | GLN |
| 2 | X7 | 258 | ASN |
| 2 | X7 | 293 | ASN |
| 2 | X7 | 329 | ASN |
| 1 | X8 | 14 | ASN |
| 1 | X8 | 99 | ASN |
| 1 | X8 | 131 | GLN |
| 1 | X8 | 190 | HIS |
| 1 | X8 | 204 | ASN |
| 1 | X8 | 227 | HIS |
| 1 | X8 | 245 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | X8 | 256 | ASN |
| 1 | X8 | 396 | HIS |
| 2 | X9 | 61 | HIS |
| 2 | X9 | 226 | ASN |
| 2 | X9 | 283 | HIS |
| 2 | X9 | 309 | HIS |
| 1 | Y0 | 99 | ASN |
| 1 | Y0 | 131 | GLN |
| 1 | Y0 | 190 | HIS |
| 1 | Y0 | 191 | GLN |
| 1 | Y0 | 227 | HIS |
| 1 | Y0 | 256 | ASN |
| 1 | Y0 | 280 | GLN |
| 1 | Y0 | 347 | ASN |
| 1 | Y0 | 396 | HIS |
| 1 | Y0 | 416 | ASN |
| 2 | Y1 | 31 | GLN |
| 1 | Y2 | 37 | HIS |
| 1 | Y2 | 99 | ASN |
| 1 | Y2 | 227 | HIS |
| 1 | Y2 | 256 | ASN |
| 1 | Y2 | 264 | HIS |
| 1 | Y2 | 292 | GLN |
| 1 | Y2 | 332 | ASN |
| 1 | Y2 | 348 | ASN |
| 1 | Y2 | 396 | HIS |
| 2 | Y3 | 31 | GLN |
| 2 | Y3 | 88 | HIS |
| 2 | Y3 | 176 | GLN |
| 2 | Y3 | 233 | GLN |
| 2 | Y3 | 258 | ASN |
| 2 | Y3 | 372 | GLN |
| 1 | Y4 | 227 | HIS |
| 1 | Y4 | 245 | GLN |
| 1 | Y4 | 256 | ASN |
| 1 | Y4 | 347 | ASN |
| 1 | Y4 | 348 | ASN |
| 1 | Y4 | 396 | HIS |
| 2 | Y5 | 31 | GLN |
| 2 | Y5 | 88 | HIS |
| 2 | Y5 | 258 | ASN |
| 2 | Y5 | 309 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y6 | 14 | ASN |
| 1 | Y6 | 227 | HIS |
| 1 | Y6 | 256 | ASN |
| 1 | Y6 | 280 | GLN |
| 1 | Y6 | 332 | ASN |
| 1 | Y6 | 334 | GLN |
| 1 | Y6 | 335 | ASN |
| 1 | Y6 | 348 | ASN |
| 1 | Y6 | 416 | ASN |
| 1 | Y8 | 190 | HIS |
| 1 | Y8 | 292 | GLN |
| 1 | Y8 | 384 | GLN |
| 1 | Y8 | 396 | HIS |
| 1 | Y8 | 414 | ASN |
| 2 | Y9 | 11 | GLN |
| 2 | Y9 | 15 | GLN |
| 2 | Y9 | 258 | ASN |
| 2 | Y9 | 285 | GLN |
| 2 | Y9 | 380 | ASN |
| 2 | Y9 | 393 | HIS |
| 1 | Z0 | 37 | HIS |
| 1 | Z0 | 48 | ASN |
| 1 | Z0 | 131 | GLN |
| 1 | Z0 | 204 | ASN |
| 1 | Z0 | 256 | ASN |
| 1 | Z0 | 337 | ASN |
| 1 | Z0 | 348 | ASN |
| 1 | Z0 | 396 | HIS |
| 2 | Z1 | 18 | ASN |
| 2 | Z1 | 31 | GLN |
| 2 | Z1 | 107 | HIS |
| 2 | Z1 | 133 | GLN |
| 2 | Z1 | 233 | GLN |
| 2 | Z1 | 329 | ASN |
| 2 | Z1 | 393 | HIS |
| 1 | Z2 | 204 | ASN |
| 1 | Z2 | 245 | GLN |
| 1 | Z2 | 256 | ASN |
| 1 | Z2 | 332 | ASN |
| 1 | Z2 | 348 | ASN |
| 1 | Z2 | 384 | GLN |
| 1 | Z2 | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Z2 | 416 | ASN |
| 2 | Z3 | 11 | GLN |
| 2 | Z3 | 61 | HIS |
| 2 | Z3 | 228 | ASN |
| 2 | Z3 | 285 | GLN |
| 2 | Z3 | 309 | HIS |
| 1 | Z4 | 14 | ASN |
| 1 | Z4 | 204 | ASN |
| 1 | Z4 | 227 | HIS |
| 1 | Z4 | 256 | ASN |
| 1 | Z4 | 396 | HIS |
| 2 | Z5 | 8 | HIS |
| 2 | Z5 | 18 | ASN |
| 2 | Z5 | 88 | HIS |
| 2 | Z5 | 226 | ASN |
| 2 | Z5 | 228 | ASN |
| 2 | Z5 | 309 | HIS |
| 1 | Z6 | 14 | ASN |
| 1 | Z6 | 131 | GLN |
| 1 | Z6 | 204 | ASN |
| 1 | Z6 | 227 | HIS |
| 1 | Z6 | 256 | ASN |
| 1 | Z6 | 334 | GLN |
| 1 | Z6 | 396 | HIS |
| 2 | Z7 | 11 | GLN |
| 2 | Z7 | 18 | ASN |
| 2 | Z7 | 28 | HIS |
| 2 | Z7 | 101 | ASN |
| 2 | Z7 | 107 | HIS |
| 2 | Z7 | 128 | ASN |
| 2 | Z7 | 133 | GLN |
| 2 | Z7 | 192 | HIS |
| 2 | Z7 | 226 | ASN |
| 2 | Z7 | 309 | HIS |
| 2 | Z7 | 329 | ASN |
| 2 | Z7 | 393 | HIS |
| 1 | Z8 | 131 | GLN |
| 1 | Z8 | 204 | ASN |
| 1 | Z8 | 227 | HIS |
| 1 | Z8 | 256 | ASN |
| 1 | Z8 | 396 | HIS |
| 2 | Z9 | 101 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z9 | 133 | GLN |
| 2 | Z9 | 283 | HIS |
| 2 | Z9 | 393 | HIS |
| 1 | 0A | 6 | HIS |
| 1 | 0A | 204 | ASN |
| 1 | 0A | 227 | HIS |
| 1 | 0A | 256 | ASN |
| 1 | 0A | 334 | GLN |
| 1 | 0A | 335 | ASN |
| 1 | 0A | 396 | HIS |
| 1 | 0A | 416 | ASN |
| 2 | 0B | 11 | GLN |
| 2 | 0B | 15 | GLN |
| 2 | 0B | 61 | HIS |
| 2 | 0B | 233 | GLN |
| 2 | 0B | 393 | HIS |
| 1 | 0C | 6 | HIS |
| 1 | 0C | 8 | GLN |
| 1 | 0C | 94 | GLN |
| 1 | 0C | 204 | ASN |
| 1 | 0C | 227 | HIS |
| 1 | 0C | 247 | ASN |
| 1 | 0C | 334 | GLN |
| 1 | 0C | 335 | ASN |
| 1 | 0C | 347 | ASN |
| 1 | 0C | 348 | ASN |
| 1 | 0C | 384 | GLN |
| 1 | 0E | 11 | GLN |
| 1 | 0E | 190 | HIS |
| 1 | 0E | 247 | ASN |
| 1 | 0E | 292 | GLN |
| 1 | 0E | 329 | GLN |
| 1 | 0E | 334 | GLN |
| 1 | 0E | 414 | ASN |
| 2 | 0F | 8 | HIS |
| 2 | 0F | 133 | GLN |
| 2 | 0F | 293 | ASN |
| 2 | 0F | 309 | HIS |
| 2 | 0F | 356 | ASN |
| 1 | 0G | 8 | GLN |
| 1 | 0G | 37 | HIS |
| 1 | 0G | 105 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0G | 190 | HIS |
| 1 | 0G | 334 | GLN |
| 1 | 0G | 348 | ASN |
| 1 | 0G | 384 | GLN |
| 1 | 0G | 396 | HIS |
| 2 | 0H | 8 | HIS |
| 2 | 0H | 11 | GLN |
| 2 | 0H | 101 | ASN |
| 2 | 0H | 107 | HIS |
| 2 | 0H | 133 | GLN |
| 2 | 0H | 228 | ASN |
| 2 | 0H | 293 | ASN |
| 2 | 0H | 309 | HIS |
| 2 | 0H | 356 | ASN |
| 1 | 0I | 131 | GLN |
| 1 | 0I | 190 | HIS |
| 1 | 0I | 204 | ASN |
| 1 | 0I | 247 | ASN |
| 1 | 0I | 292 | GLN |
| 1 | 0I | 334 | GLN |
| 1 | 0I | 335 | ASN |
| 1 | 0I | 396 | HIS |
| 2 | 0J | 8 | HIS |
| 2 | 0J | 228 | ASN |
| 2 | 0J | 258 | ASN |
| 2 | 0J | 342 | GLN |
| 2 | 0J | 406 | HIS |
| 1 | 0K | 11 | GLN |
| 1 | 0K | 190 | HIS |
| 1 | 0K | 204 | ASN |
| 1 | 0K | 226 | ASN |
| 1 | 0K | 256 | ASN |
| 2 | 0L | 8 | HIS |
| 2 | 0L | 107 | HIS |
| 2 | 0L | 192 | HIS |
| 2 | 0L | 258 | ASN |
| 2 | 0L | 293 | ASN |
| 2 | 0L | 309 | HIS |
| 2 | 0L | 356 | ASN |
| 2 | 0L | 406 | HIS |
| 1 | 0M | 14 | ASN |
| 1 | 0M | 190 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0M | 204 | ASN |
| 1 | 0M | 247 | ASN |
| 1 | 0M | 292 | GLN |
| 1 | 0M | 334 | GLN |
| 1 | 0M | 335 | ASN |
| 1 | 0M | 396 | HIS |
| 2 | 0N | 8 | HIS |
| 2 | 0N | 11 | GLN |
| 2 | 0N | 101 | ASN |
| 2 | 0N | 107 | HIS |
| 2 | 0N | 283 | HIS |
| 2 | 0N | 293 | ASN |
| 2 | 0N | 309 | HIS |
| 2 | 0N | 406 | HIS |
| 1 | 0O | 99 | ASN |
| 1 | 0O | 134 | GLN |
| 1 | 0O | 190 | HIS |
| 1 | 0O | 204 | ASN |
| 1 | 0O | 256 | ASN |
| 1 | 0O | 334 | GLN |
| 1 | 0O | 348 | ASN |
| 1 | 0O | 384 | GLN |
| 1 | 0O | 396 | HIS |
| 2 | 0P | 258 | ASN |
| 2 | 0P | 283 | HIS |
| 2 | 0P | 293 | ASN |
| 2 | 0P | 309 | HIS |
| 2 | 0P | 329 | ASN |
| 1 | 0Q | 8 | GLN |
| 1 | 0Q | 190 | HIS |
| 1 | 0Q | 245 | GLN |
| 1 | 0Q | 247 | ASN |
| 1 | 0Q | 291 | GLN |
| 1 | 0Q | 292 | GLN |
| 1 | 0Q | 334 | GLN |
| 1 | 0Q | 348 | ASN |
| 1 | 0Q | 396 | HIS |
| 2 | 0R | 8 | HIS |
| 2 | 0R | 101 | ASN |
| 2 | 0R | 133 | GLN |
| 2 | 0R | 293 | ASN |
| 2 | 0R | 309 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 0R | 356 | ASN |
| 1 | 0S | 6 | HIS |
| 1 | 0S | 99 | ASN |
| 1 | 0S | 105 | HIS |
| 1 | 0S | 131 | GLN |
| 1 | 0S | 247 | ASN |
| 1 | 0S | 292 | GLN |
| 1 | 0S | 334 | GLN |
| 1 | 0S | 335 | ASN |
| 1 | 0S | 384 | GLN |
| 1 | 0U | 137 | HIS |
| 1 | 0U | 184 | ASN |
| 1 | 0U | 190 | HIS |
| 1 | 0U | 247 | ASN |
| 1 | 0U | 256 | ASN |
| 1 | 0U | 292 | GLN |
| 1 | 0U | 334 | GLN |
| 2 | 0V | 101 | ASN |
| 2 | 0V | 258 | ASN |
| 2 | 0V | 293 | ASN |
| 2 | 0V | 309 | HIS |
| 2 | 0V | 342 | GLN |
| 1 | 0W | 190 | HIS |
| 1 | 0W | 292 | GLN |
| 1 | 0W | 334 | GLN |
| 1 | 0W | 348 | ASN |
| 1 | 0W | 384 | GLN |
| 1 | 0W | 396 | HIS |
| 1 | 0W | 423 | GLN |
| 2 | 0X | 101 | ASN |
| 2 | 0X | 256 | GLN |
| 2 | 0X | 285 | GLN |
| 2 | 0X | 293 | ASN |
| 1 | 0Y | 11 | GLN |
| 1 | 0Y | 48 | ASN |
| 1 | 0Y | 332 | ASN |
| 1 | 0Y | 334 | GLN |
| 1 | 0Y | 396 | HIS |
| 2 | 0Z | 88 | HIS |
| 2 | 0Z | 128 | ASN |
| 2 | 0Z | 293 | ASN |
| 2 | 0Z | 329 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 6 | HIS |
| 1 | 1A | 14 | ASN |
| 1 | 1A | 137 | HIS |
| 1 | 1A | 190 | HIS |
| 1 | 1A | 204 | ASN |
| 1 | 1A | 247 | ASN |
| 1 | 1A | 291 | GLN |
| 1 | 1A | 292 | GLN |
| 1 | 1A | 334 | GLN |
| 1 | 1A | 335 | ASN |
| 1 | 1A | 348 | ASN |
| 1 | 1A | 384 | GLN |
| 2 | 1B | 133 | GLN |
| 2 | 1B | 258 | ASN |
| 2 | 1B | 283 | HIS |
| 2 | 1B | 293 | ASN |
| 2 | 1B | 329 | ASN |
| 2 | 1B | 406 | HIS |
| 1 | 1C | 14 | ASN |
| 1 | 1C | 89 | ASN |
| 1 | 1C | 184 | ASN |
| 1 | 1C | 190 | HIS |
| 1 | 1C | 292 | GLN |
| 1 | 1C | 334 | GLN |
| 1 | 1C | 335 | ASN |
| 1 | 1C | 384 | GLN |
| 1 | 1C | 396 | HIS |
| 2 | 1D | 28 | HIS |
| 2 | 1D | 107 | HIS |
| 2 | 1D | 256 | GLN |
| 2 | 1D | 258 | ASN |
| 2 | 1D | 309 | HIS |
| 2 | 1D | 342 | GLN |
| 1 | 1E | 14 | ASN |
| 1 | 1E | 137 | HIS |
| 1 | 1E | 190 | HIS |
| 1 | 1E | 247 | ASN |
| 1 | 1E | 264 | HIS |
| 1 | 1E | 298 | ASN |
| 1 | 1E | 332 | ASN |
| 1 | 1E | 334 | GLN |
| 1 | 1E | 348 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1E | 396 | HIS |
| 2 | 1F | 8 | HIS |
| 2 | 1F | 11 | GLN |
| 2 | 1F | 88 | HIS |
| 2 | 1F | 101 | ASN |
| 2 | 1F | 258 | ASN |
| 2 | 1F | 293 | ASN |
| 1 | 1G | 264 | HIS |
| 1 | 1G | 332 | ASN |
| 1 | 1G | 334 | GLN |
| 1 | 1G | 335 | ASN |
| 1 | 1G | 348 | ASN |
| 1 | 1G | 396 | HIS |
| 2 | 1H | 8 | HIS |
| 2 | 1H | 11 | GLN |
| 2 | 1H | 50 | ASN |
| 2 | 1H | 101 | ASN |
| 2 | 1H | 285 | GLN |
| 2 | 1H | 293 | ASN |
| 2 | 1H | 406 | HIS |
| 1 | 1K | 6 | HIS |
| 1 | 1K | 14 | ASN |
| 1 | 1K | 89 | ASN |
| 1 | 1K | 184 | ASN |
| 1 | 1K | 190 | HIS |
| 1 | 1K | 247 | ASN |
| 1 | 1K | 256 | ASN |
| 1 | 1K | 298 | ASN |
| 1 | 1K | 334 | GLN |
| 1 | 1K | 396 | HIS |
| 2 | 1L | 31 | GLN |
| 2 | 1L | 88 | HIS |
| 2 | 1L | 192 | HIS |
| 2 | 1L | 249 | ASN |
| 2 | 1L | 293 | ASN |
| 2 | 1L | 309 | HIS |
| 2 | 1L | 406 | HIS |
| 1 | 1M | 6 | HIS |
| 1 | 1M | 14 | ASN |
| 1 | 1M | 190 | HIS |
| 1 | 1M | 195 | ASN |
| 1 | 1M | 245 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1M | 264 | HIS |
| 1 | 1M | 279 | GLN |
| 1 | 1M | 292 | GLN |
| 1 | 1M | 334 | GLN |
| 1 | 1M | 335 | ASN |
| 1 | 1M | 384 | GLN |
| 1 | 1M | 396 | HIS |
| 2 | 1N | 15 | GLN |
| 2 | 1N | 28 | HIS |
| 2 | 1N | 85 | GLN |
| 2 | 1N | 133 | GLN |
| 2 | 1N | 258 | ASN |
| 2 | 1N | 293 | ASN |
| 1 | 1O | 137 | HIS |
| 1 | 1O | 190 | HIS |
| 1 | 1O | 195 | ASN |
| 1 | 1O | 227 | HIS |
| 1 | 1O | 334 | GLN |
| 1 | 1O | 347 | ASN |
| 1 | 1O | 396 | HIS |
| 2 | 1P | 258 | ASN |
| 2 | 1P | 309 | HIS |
| 2 | 1P | 372 | GLN |
| 2 | 1P | 406 | HIS |
| 1 | 1Q | 190 | HIS |
| 1 | 1Q | 264 | HIS |
| 1 | 1Q | 292 | GLN |
| 1 | 1Q | 334 | GLN |
| 1 | 1Q | 396 | HIS |
| 2 | 1R | 88 | HIS |
| 2 | 1R | 258 | ASN |
| 2 | 1R | 293 | ASN |
| 2 | 1R | 309 | HIS |
| 2 | 1R | 329 | ASN |
| 1 | 1S | 14 | ASN |
| 1 | 1S | 190 | HIS |
| 1 | 1S | 334 | GLN |
| 1 | 1S | 335 | ASN |
| 1 | 1S | 348 | ASN |
| 1 | 1S | 396 | HIS |
| 2 | 1T | 233 | GLN |
| 2 | 1T | 249 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1T | 258 | ASN |
| 2 | 1T | 283 | HIS |
| 2 | 1T | 293 | ASN |
| 2 | 1T | 309 | HIS |
| 2 | 1T | 329 | ASN |
| 2 | 1T | 406 | HIS |
| 1 | 1U | 6 | HIS |
| 1 | 1U | 14 | ASN |
| 1 | 1U | 245 | GLN |
| 1 | 1U | 292 | GLN |
| 1 | 1U | 332 | ASN |
| 1 | 1U | 334 | GLN |
| 2 | 1V | 88 | HIS |
| 2 | 1V | 283 | HIS |
| 2 | 1V | 293 | ASN |
| 2 | 1V | 309 | HIS |
| 2 | 1V | 329 | ASN |
| 1 | 1W | 14 | ASN |
| 1 | 1W | 89 | ASN |
| 1 | 1W | 190 | HIS |
| 1 | 1W | 191 | GLN |
| 1 | 1W | 245 | GLN |
| 1 | 1W | 247 | ASN |
| 1 | 1W | 292 | GLN |
| 1 | 1W | 334 | GLN |
| 1 | 1W | 335 | ASN |
| 1 | 1W | 396 | HIS |
| 2 | 1X | 8 | HIS |
| 2 | 1X | 101 | ASN |
| 2 | 1X | 102 | ASN |
| 2 | 1X | 133 | GLN |
| 2 | 1X | 192 | HIS |
| 2 | 1X | 293 | ASN |
| 2 | 1X | 309 | HIS |
| 2 | 1X | 358 | GLN |
| 2 | 1Z | 11 | GLN |
| 2 | 1Z | 88 | HIS |
| 2 | 1Z | 101 | ASN |
| 2 | 1Z | 133 | GLN |
| 2 | 1Z | 192 | HIS |
| 2 | 1Z | 258 | ASN |
| 2 | 1Z | 293 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 14 | ASN |
| 1 | 2A | 131 | GLN |
| 1 | 2A | 190 | HIS |
| 1 | 2A | 204 | ASN |
| 1 | 2A | 347 | ASN |
| 1 | 2A | 348 | ASN |
| 1 | 2A | 396 | HIS |
| 2 | 2B | 293 | ASN |
| 2 | 2B | 309 | HIS |
| 1 | 2C | 256 | ASN |
| 1 | 2C | 334 | GLN |
| 1 | 2C | 335 | ASN |
| 1 | 2C | 348 | ASN |
| 1 | 2C | 396 | HIS |
| 2 | 2D | 11 | GLN |
| 2 | 2D | 18 | ASN |
| 2 | 2D | 88 | HIS |
| 2 | 2D | 293 | ASN |
| 2 | 2D | 309 | HIS |
| 2 | 2D | 372 | GLN |
| 1 | 2E | 94 | GLN |
| 1 | 2E | 195 | ASN |
| 1 | 2E | 247 | ASN |
| 1 | 2E | 256 | ASN |
| 1 | 2E | 292 | GLN |
| 1 | 2E | 329 | GLN |
| 1 | 2E | 335 | ASN |
| 1 | 2E | 348 | ASN |
| 1 | 2E | 396 | HIS |
| 2 | 2F | 258 | ASN |
| 2 | 2F | 285 | GLN |
| 2 | 2F | 293 | ASN |
| 2 | 2F | 309 | HIS |
| 2 | 2F | 356 | ASN |
| 1 | 2G | 14 | ASN |
| 1 | 2G | 15 | GLN |
| 1 | 2G | 83 | GLN |
| 1 | 2G | 190 | HIS |
| 1 | 2G | 204 | ASN |
| 1 | 2G | 247 | ASN |
| 1 | 2G | 292 | GLN |
| 1 | 2G | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2H | 8 | HIS |
| 2 | 2H | 18 | ASN |
| 2 | 2H | 88 | HIS |
| 2 | 2H | 285 | GLN |
| 2 | 2H | 293 | ASN |
| 1 | 2I | 14 | ASN |
| 1 | 2I | 134 | GLN |
| 1 | 2I | 396 | HIS |
| 2 | 2J | 11 | GLN |
| 2 | 2J | 293 | ASN |
| 2 | 2J | 309 | HIS |
| 1 | 2K | 134 | GLN |
| 1 | 2K | 256 | ASN |
| 1 | 2K | 280 | GLN |
| 1 | 2K | 292 | GLN |
| 1 | 2K | 347 | ASN |
| 1 | 2K | 396 | HIS |
| 1 | 2K | 414 | ASN |
| 2 | 2L | 8 | HIS |
| 2 | 2L | 61 | HIS |
| 2 | 2L | 249 | ASN |
| 2 | 2L | 258 | ASN |
| 2 | 2L | 293 | ASN |
| 2 | 2L | 309 | HIS |
| 1 | 2M | 190 | HIS |
| 1 | 2M | 247 | ASN |
| 1 | 2M | 396 | HIS |
| 1 | 2M | 414 | ASN |
| 2 | 2N | 8 | HIS |
| 2 | 2N | 61 | HIS |
| 2 | 2N | 101 | ASN |
| 2 | 2N | 285 | GLN |
| 2 | 2N | 293 | ASN |
| 2 | 2N | 309 | HIS |
| 2 | 2P | 197 | HIS |
| 2 | 2P | 293 | ASN |
| 2 | 2P | 358 | GLN |
| 1 | 2Q | 6 | HIS |
| 1 | 2Q | 105 | HIS |
| 1 | 2Q | 247 | ASN |
| 1 | 2Q | 256 | ASN |
| 1 | 2Q | 291 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2Q | 292 | GLN |
| 1 | 2Q | 307 | HIS |
| 1 | 2Q | 332 | ASN |
| 1 | 2Q | 334 | GLN |
| 1 | 2Q | 348 | ASN |
| 1 | 2Q | 396 | HIS |
| 2 | 2R | 11 | GLN |
| 2 | 2R | 128 | ASN |
| 2 | 2R | 285 | GLN |
| 2 | 2R | 309 | HIS |
| 1 | 2S | 105 | HIS |
| 1 | 2S | 247 | ASN |
| 1 | 2S | 256 | ASN |
| 1 | 2S | 292 | GLN |
| 1 | 2S | 334 | GLN |
| 1 | 2S | 348 | ASN |
| 1 | 2S | 396 | HIS |
| 2 | 2T | 258 | ASN |
| 2 | 2T | 329 | ASN |
| 2 | 2T | 358 | GLN |
| 2 | 2T | 372 | GLN |
| 1 | 2U | 14 | ASN |
| 1 | 2U | 245 | GLN |
| 1 | 2U | 292 | GLN |
| 1 | 2U | 334 | GLN |
| 1 | 2U | 348 | ASN |
| 1 | 2U | 396 | HIS |
| 2 | 2V | 11 | GLN |
| 2 | 2V | 197 | HIS |
| 2 | 2V | 309 | HIS |
| 1 | 2W | 15 | GLN |
| 1 | 2W | 99 | ASN |
| 1 | 2W | 247 | ASN |
| 1 | 2W | 329 | GLN |
| 1 | 2W | 334 | GLN |
| 1 | 2W | 396 | HIS |
| 2 | 2X | 11 | GLN |
| 2 | 2X | 88 | HIS |
| 2 | 2X | 133 | GLN |
| 2 | 2X | 358 | GLN |
| 1 | 2Y | 14 | ASN |
| 1 | 2Y | 43 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2Y | 99 | ASN |
| 1 | 2Y | 247 | ASN |
| 1 | 2Y | 256 | ASN |
| 1 | 2Y | 334 | GLN |
| 1 | 2Y | 396 | HIS |
| 1 | 2Y | 426 | GLN |
| 2 | 2Z | 61 | HIS |
| 2 | 2Z | 91 | GLN |
| 2 | 2Z | 309 | HIS |
| 1 | 3A | 48 | ASN |
| 1 | 3A | 83 | GLN |
| 1 | 3A | 247 | ASN |
| 1 | 3A | 279 | GLN |
| 1 | 3A | 329 | GLN |
| 1 | 3A | 332 | ASN |
| 1 | 3A | 334 | GLN |
| 1 | 3A | 348 | ASN |
| 1 | 3A | 396 | HIS |
| 2 | 3B | 15 | GLN |
| 2 | 3B | 85 | GLN |
| 2 | 3B | 133 | GLN |
| 2 | 3B | 283 | HIS |
| 2 | 3B | 309 | HIS |
| 2 | 3B | 358 | GLN |
| 2 | 3B | 372 | GLN |
| 2 | 3B | 393 | HIS |
| 1 | 3C | 6 | HIS |
| 1 | 3C | 14 | ASN |
| 1 | 3C | 37 | HIS |
| 1 | 3C | 94 | GLN |
| 1 | 3C | 105 | HIS |
| 1 | 3C | 190 | HIS |
| 1 | 3C | 245 | GLN |
| 1 | 3C | 332 | ASN |
| 1 | 3C | 334 | GLN |
| 1 | 3C | 347 | ASN |
| 1 | 3C | 396 | HIS |
| 2 | 3D | 61 | HIS |
| 2 | 3D | 258 | ASN |
| 2 | 3D | 285 | GLN |
| 2 | 3D | 329 | ASN |
| 2 | 3F | 15 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 3F | 88 | HIS |
| 2 | 3F | 197 | HIS |
| 2 | 3F | 283 | HIS |
| 2 | 3F | 309 | HIS |
| 1 | 3G | 6 | HIS |
| 1 | 3G | 14 | ASN |
| 1 | 3G | 94 | GLN |
| 1 | 3G | 134 | GLN |
| 1 | 3G | 190 | HIS |
| 1 | 3G | 227 | HIS |
| 1 | 3G | 334 | GLN |
| 1 | 3G | 347 | ASN |
| 1 | 3G | 396 | HIS |
| 2 | 3H | 283 | HIS |
| 2 | 3H | 285 | GLN |
| 2 | 3H | 309 | HIS |
| 1 | 3I | 6 | HIS |
| 1 | 3I | 52 | ASN |
| 1 | 3I | 134 | GLN |
| 1 | 3I | 190 | HIS |
| 1 | 3I | 227 | HIS |
| 1 | 3I | 247 | ASN |
| 1 | 3I | 292 | GLN |
| 1 | 3I | 348 | ASN |
| 1 | 3I | 396 | HIS |
| 1 | 3I | 423 | GLN |
| 2 | 3J | 11 | GLN |
| 2 | 3J | 206 | ASN |
| 2 | 3J | 249 | ASN |
| 2 | 3J | 293 | ASN |
| 1 | 3K | 227 | HIS |
| 1 | 3K | 247 | ASN |
| 1 | 3K | 334 | GLN |
| 1 | 3K | 396 | HIS |
| 2 | 3L | 293 | ASN |
| 2 | 3L | 309 | HIS |
| 1 | 3M | 14 | ASN |
| 1 | 3M | 52 | ASN |
| 1 | 3M | 195 | ASN |
| 1 | 3M | 204 | ASN |
| 1 | 3M | 247 | ASN |
| 1 | 3M | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 3M | 292 | GLN |
| 1 | 3M | 334 | GLN |
| 1 | 3M | 396 | HIS |
| 2 | 3N | 91 | GLN |
| 2 | 3N | 309 | HIS |
| 2 | 3N | 372 | GLN |
| 1 | 3O | 37 | HIS |
| 1 | 3O | 99 | ASN |
| 1 | 3O | 227 | HIS |
| 1 | 3O | 256 | ASN |
| 1 | 3O | 329 | GLN |
| 1 | 3O | 396 | HIS |
| 2 | 3P | 11 | GLN |
| 2 | 3P | 233 | GLN |
| 2 | 3P | 309 | HIS |
| 1 | 3Q | 99 | ASN |
| 1 | 3Q | 190 | HIS |
| 1 | 3Q | 227 | HIS |
| 1 | 3Q | 247 | ASN |
| 1 | 3Q | 292 | GLN |
| 1 | 3Q | 396 | HIS |
| 2 | 3R | 15 | GLN |
| 2 | 3R | 61 | HIS |
| 2 | 3R | 197 | HIS |
| 2 | 3R | 283 | HIS |
| 2 | 3R | 293 | ASN |
| 2 | 3R | 309 | HIS |
| 2 | 3R | 356 | ASN |
| 2 | 3R | 358 | GLN |
| 1 | 3S | 6 | HIS |
| 1 | 3S | 190 | HIS |
| 1 | 3S | 227 | HIS |
| 1 | 3S | 247 | ASN |
| 1 | 3S | 292 | GLN |
| 1 | 3S | 334 | GLN |
| 1 | 3S | 335 | ASN |
| 1 | 3S | 348 | ASN |
| 1 | 3S | 396 | HIS |
| 2 | 3T | 61 | HIS |
| 2 | 3T | 206 | ASN |
| 2 | 3T | 356 | ASN |
| 2 | 3T | 372 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 3V | 16 | ASN |
| 3 | 3V | 28 | ASN |
| 3 | 3V | 49 | HIS |
| 3 | 3V | 156 | HIS |
| 4 | 3W | 7 | GLN |
| 4 | 3W | 109 | GLN |
| 4 | 3W | 157 | HIS |
| 4 | 3W | 159 | ASN |
| 3 | 3X | 16 | ASN |
| 3 | 3X | 28 | ASN |
| 3 | 3X | 156 | HIS |
| 4 | 3Y | 7 | GLN |
| 4 | 3Y | 109 | GLN |
| 4 | 3Y | 157 | HIS |
| 4 | 3Y | 159 | ASN |
| 3 | 3Z | 16 | ASN |
| 3 | 3Z | 28 | ASN |
| 3 | 3Z | 156 | HIS |
| 4 | 4A | 7 | GLN |
| 4 | 4A | 109 | GLN |
| 4 | 4A | 157 | HIS |
| 4 | 4A | 159 | ASN |
| 3 | 4B | 16 | ASN |
| 3 | 4B | 28 | ASN |
| 3 | 4B | 156 | HIS |
| 4 | 4C | 7 | GLN |
| 4 | 4C | 109 | GLN |
| 4 | 4C | 157 | HIS |
| 4 | 4C | 159 | ASN |
| 3 | 4D | 16 | ASN |
| 3 | 4D | 28 | ASN |
| 3 | 4D | 49 | HIS |
| 3 | 4D | 156 | HIS |
| 4 | 4E | 7 | GLN |
| 4 | 4E | 109 | GLN |
| 4 | 4E | 157 | HIS |
| 4 | 4E | 159 | ASN |
| 3 | 4F | 16 | ASN |
| 3 | 4F | 28 | ASN |
| 3 | 4F | 156 | HIS |
| 4 | 4G | 7 | GLN |
| 4 | 4G | 109 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 4G | 157 | HIS |
| 4 | 4G | 159 | ASN |
| 3 | 4H | 16 | ASN |
| 3 | 4H | 28 | ASN |
| 3 | 4H | 156 | HIS |
| 4 | 4I | 7 | GLN |
| 4 | 4I | 52 | GLN |
| 4 | 4I | 109 | GLN |
| 4 | 4I | 157 | HIS |
| 4 | 4I | 159 | ASN |
| 3 | 4J | 247 | ASN |
| 3 | 4J | 264 | GLN |
| 3 | 4J | 283 | GLN |
| 5 | 4L | 267 | ASN |
| 5 | 4L | 290 | GLN |
| 5 | 4L | 320 | GLN |
| 5 | 4M | 177 | HIS |
| 5 | 4M | 212 | GLN |
| 5 | 4M | 267 | ASN |
| 5 | 4M | 271 | GLN |
| 6 | 4O | 332 | ASN |
| 6 | 4P | 43 | ASN |
| 7 | 4R | 70 | GLN |
| 7 | 4R | 174 | HIS |
| 7 | 4R | 361 | GLN |
| 7 | 4T | 336 | GLN |
| 7 | 4T | 352 | ASN |
| 7 | 4U | 92 | GLN |
| 7 | 4U | 121 | ASN |
| 7 | 4U | 262 | HIS |
| 8 | 4V | 430 | GLN |
| 8 | 4V | 469 | GLN |
| 8 | 4W | 151 | GLN |
| 8 | 4W | 187 | HIS |
| 8 | 4W | 267 | ASN |
| 8 | 4X | 116 | ASN |
| 9 | 4Y | 329 | GLN |
| 9 | 4Y | 332 | GLN |
| 9 | 4Y | 388 | GLN |
| 9 | 4Z | 112 | HIS |
| 9 | 4Z | 164 | GLN |
| 9 | 4Z | 291 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 4Z | 329 | GLN |
| 9 | 4Z | 405 | GLN |
| 10 | 5A | 468 | GLN |
| 10 | 5C | 172 | GLN |
| 10 | 5C | 237 | GLN |
| 10 | 5C | 384 | GLN |
| 10 | 5D | 172 | GLN |
| 11 | 5E | 85 | ASN |
| 11 | 5E | 106 | GLN |
| 12 | 5F | 53 | HIS |
| 12 | 5F | 78 | HIS |
| 12 | 5F | 140 | GLN |
| 12 | 5F | 311 | HIS |
| 12 | 5F | 316 | GLN |
| 12 | 5G | 311 | HIS |
| 12 | 5G | 316 | GLN |
| 12 | 5G | 331 | ASN |
| 13 | 5H | 9 | GLN |
| 13 | 5H | 12 | HIS |
| 13 | 5H | 99 | ASN |
| 13 | 5H | 117 | ASN |
| 13 | 5I | 9 | GLN |
| 13 | 5I | 99 | ASN |
| 13 | 5I | 117 | ASN |
| 13 | 5J | 9 | GLN |
| 13 | 5J | 21 | ASN |
| 13 | 5J | 99 | ASN |
| 13 | 5K | 99 | ASN |
| 14 | 5L | 138 | ASN |
| 14 | 5L | 146 | ASN |
| 14 | 5L | 237 | ASN |
| 14 | 5L | 239 | GLN |
| 14 | 5L | 412 | GLN |
| 14 | 5L | 424 | HIS |
| 14 | 5L | 473 | ASN |
| 14 | 5M | 138 | ASN |
| 14 | 5M | 146 | ASN |
| 14 | 5M | 237 | ASN |
| 14 | 5M | 239 | GLN |
| 14 | 5M | 412 | GLN |
| 14 | 5M | 424 | HIS |
| 14 | 5M | 473 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | 5M | 510 | ASN |
| 14 | 5N | 138 | ASN |
| 14 | 5N | 146 | ASN |
| 14 | 5N | 220 | GLN |
| 14 | 5N | 237 | ASN |
| 14 | 5N | 239 | GLN |
| 14 | 5N | 424 | HIS |
| 14 | 5N | 473 | ASN |
| 15 | 5O | 4 | ASN |
| 15 | 5O | 25 | GLN |
| 15 | 5O | 182 | ASN |
| 15 | 5O | 203 | ASN |
| 15 | 5O | 325 | GLN |
| 15 | 5O | 357 | HIS |
| 15 | 5O | 370 | ASN |
| 15 | 5P | 42 | ASN |
| 15 | 5P | 72 | GLN |
| 15 | 5P | 295 | ASN |
| 16 | 5Q | 81 | HIS |
| 16 | 5Q | 89 | HIS |
| 16 | 5Q | 136 | HIS |
| 16 | 5Q | 186 | HIS |
| 17 | 5S | 101 | ASN |
| 17 | 5S | 129 | GLN |
| 17 | 5T | 101 | ASN |
| 17 | 5T | 129 | GLN |
| 17 | 5T | 179 | GLN |
| 17 | 5T | 180 | GLN |
| 17 | 5U | 101 | ASN |
| 17 | 5U | 129 | GLN |
| 17 | 5V | 179 | GLN |
| 17 | 5V | 193 | ASN |
| 18 | 5X | 17 | HIS |
| 18 | 5X | 173 | HIS |
| 18 | 5X | 181 | GLN |
| 18 | 5Y | 17 | HIS |
| 18 | 5Y | 173 | HIS |
| 18 | 5Z | 17 | HIS |
| 18 | 5Z | 173 | HIS |
| 18 | 6A | 17 | HIS |
| 18 | 6A | 173 | HIS |
| 18 | 6B | 17 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 6B | 173 | HIS |
| 18 | 6C | 17 | HIS |
| 18 | 6C | 44 | HIS |
| 18 | 6C | 173 | HIS |
| 18 | 6D | 17 | HIS |
| 18 | 6D | 173 | HIS |
| 19 | 6E | 14 | GLN |
| 19 | 6E | 67 | HIS |
| 19 | 6E | 73 | HIS |
| 19 | 6E | 79 | HIS |
| 20 | 6F | 143 | GLN |
| 20 | 6F | 150 | HIS |
| 20 | 6F | 210 | GLN |
| 20 | 6F | 391 | ASN |
| 21 | 6H | 61 | HIS |
| 21 | 6H | 127 | HIS |
| 21 | 6H | 136 | GLN |
| 22 | 6I | 125 | ASN |
| 22 | 6I | 181 | ASN |
| 22 | 6I | 182 | ASN |
| 22 | 6I | 203 | HIS |
| 22 | 6I | 351 | ASN |
| 22 | 6J | 87 | GLN |
| 22 | 6J | 92 | GLN |
| 22 | 6J | 134 | ASN |
| 22 | 6J | 148 | ASN |
| 22 | 6J | 182 | ASN |
| 22 | 6J | 209 | ASN |
| 22 | 6J | 264 | GLN |
| 22 | 6J | 278 | GLN |
| 22 | 6K | 92 | GLN |
| 22 | 6K | 134 | ASN |
| 22 | 6K | 148 | ASN |
| 22 | 6K | 181 | ASN |
| 22 | 6K | 196 | ASN |
| 22 | 6K | 203 | HIS |
| 22 | 6K | 264 | GLN |
| 22 | 6L | 87 | GLN |
| 22 | 6L | 134 | ASN |
| 22 | 6L | 136 | ASN |
| 22 | 6L | 148 | ASN |
| 22 | 6L | 155 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 6L | 181 | ASN |
| 22 | 6L | 182 | ASN |
| 22 | 6L | 264 | GLN |
| 22 | 6L | 278 | GLN |
| 22 | 6M | 87 | GLN |
| 22 | 6M | 134 | ASN |
| 22 | 6M | 182 | ASN |
| 22 | 6M | 209 | ASN |
| 22 | 6M | 264 | GLN |
| 22 | 6M | 351 | ASN |
| 22 | 6N | 92 | GLN |
| 22 | 6N | 134 | ASN |
| 22 | 6N | 136 | ASN |
| 22 | 6N | 148 | ASN |
| 22 | 6N | 182 | ASN |
| 22 | 6N | 203 | HIS |
| 22 | 6N | 264 | GLN |
| 22 | 6O | 125 | ASN |
| 22 | 6O | 134 | ASN |
| 22 | 6O | 209 | ASN |
| 22 | 6O | 264 | GLN |
| 22 | 6O | 278 | GLN |
| 22 | 6O | 308 | HIS |
| 22 | 6P | 101 | ASN |
| 22 | 6P | 136 | ASN |
| 23 | 6R | 57 | HIS |
| 24 | 6T | 37 | ASN |
| 24 | 6T | 91 | ASN |
| 24 | 6T | 110 | ASN |
| 24 | 6T | 137 | GLN |
| 24 | 6T | 269 | ASN |
| 24 | 6T | 360 | ASN |
| 24 | 6T | 369 | HIS |
| 24 | 6T | 422 | ASN |
| 24 | 6T | 458 | HIS |
| 24 | 6T | 527 | ASN |
| 24 | 6T | 545 | ASN |
| 24 | 6U | 91 | ASN |
| 24 | 6U | 137 | GLN |
| 24 | 6U | 360 | ASN |
| 24 | 6U | 440 | ASN |
| 24 | 6U | 458 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 6U | 460 | HIS |
| 24 | 6U | 527 | ASN |
| 24 | 6U | 545 | ASN |
| 24 | 6V | 37 | ASN |
| 24 | 6V | 91 | ASN |
| 24 | 6V | 110 | ASN |
| 24 | 6V | 131 | HIS |
| 24 | 6V | 137 | GLN |
| 24 | 6V | 421 | GLN |
| 24 | 6V | 422 | ASN |
| 24 | 6V | 440 | ASN |
| 24 | 6V | 458 | HIS |
| 24 | 6V | 527 | ASN |
| 24 | 6V | 545 | ASN |
| 24 | 6W | 31 | GLN |
| 24 | 6W | 37 | ASN |
| 24 | 6W | 91 | ASN |
| 24 | 6W | 110 | ASN |
| 24 | 6W | 137 | GLN |
| 24 | 6W | 269 | ASN |
| 24 | 6W | 346 | GLN |
| 24 | 6W | 440 | ASN |
| 24 | 6W | 458 | HIS |
| 24 | 6W | 527 | ASN |
| 24 | 6W | 545 | ASN |
| 24 | 6W | 565 | GLN |
| 24 | 6X | 37 | ASN |
| 24 | 6X | 91 | ASN |
| 24 | 6X | 131 | HIS |
| 24 | 6X | 137 | GLN |
| 24 | 6X | 139 | ASN |
| 24 | 6X | 295 | HIS |
| 24 | 6X | 311 | ASN |
| 24 | 6X | 377 | GLN |
| 24 | 6X | 440 | ASN |
| 24 | 6X | 458 | HIS |
| 24 | 6X | 460 | HIS |
| 24 | 6X | 489 | ASN |
| 24 | 6X | 527 | ASN |
| 24 | 6X | 545 | ASN |
| 24 | 6Y | 20 | GLN |
| 24 | 6Y | 31 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 6Y | 40 | GLN |
| 24 | 6Y | 91 | ASN |
| 24 | 6Y | 131 | HIS |
| 24 | 6Y | 137 | GLN |
| 24 | 6Y | 295 | HIS |
| 24 | 6Y | 346 | GLN |
| 24 | 6Y | 440 | ASN |
| 24 | 6Y | 458 | HIS |
| 24 | 6Y | 480 | ASN |
| 24 | 6Y | 527 | ASN |
| 24 | 6Y | 545 | ASN |
| 24 | 6Y | 619 | ASN |
| 24 | 6Z | 31 | GLN |
| 24 | 6Z | 91 | ASN |
| 24 | 6Z | 131 | HIS |
| 24 | 6Z | 137 | GLN |
| 24 | 6Z | 346 | GLN |
| 24 | 6Z | 440 | ASN |
| 24 | 6Z | 458 | HIS |
| 24 | 6Z | 489 | ASN |
| 24 | 6Z | 527 | ASN |
| 24 | 6Z | 545 | ASN |
| 24 | 7A | 91 | ASN |
| 24 | 7A | 137 | GLN |
| 12 | 7B | 78 | HIS |
| 26 | 7D | 87 | HIS |
| 26 | 7D | 91 | HIS |
| 26 | 7E | 87 | HIS |
| 26 | 7E | 91 | HIS |
| 26 | 7F | 67 | GLN |
| 26 | 7F | 69 | HIS |
| 26 | 7F | 87 | HIS |
| 26 | 7F | 91 | HIS |
| 26 | 7F | 116 | GLN |
| 27 | 7G | 49 | HIS |
| 27 | 7G | 54 | HIS |
| 27 | 7G | 108 | ASN |
| 27 | 7G | 199 | ASN |
| 29 | 7I | 19 | ASN |
| 29 | 7I | 224 | GLN |
| 29 | 7I | 241 | ASN |
| 29 | 7J | 102 | HIS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | 7J | 117 | ASN |
| 29 | 7J | 144 | GLN |
| 29 | 7J | 224 | GLN |
| 29 | 7J | 238 | GLN |
| 29 | 7J | 379 | ASN |
| 29 | 7J | 471 | HIS |
| 30 | 7K | 19 | GLN |
| 30 | 7K | 61 | HIS |
| 30 | 7K | 186 | HIS |
| 30 | 7K | 247 | HIS |
| 30 | 7K | 320 | ASN |
| 30 | 7K | 350 | ASN |
| 30 | 7L | 276 | HIS |
| 30 | 7L | 390 | GLN |
| 30 | 7L | 453 | GLN |
| 31 | 7M | 66 | HIS |
| 31 | 7M | 68 | HIS |
| 31 | 7N | 66 | HIS |
| 31 | 7N | 78 | HIS |
| 31 | 7N | 115 | GLN |
| 32 | 7P | 22 | ASN |
| 32 | 7P | 86 | HIS |
| 32 | 7P | 140 | GLN |
| 32 | 7P | 213 | GLN |
| 33 | 7Q | 132 | GLN |
| 34 | 7R | 97 | ASN |
| 34 | 7R | 140 | ASN |
| 34 | 7R | 213 | HIS |
| 34 | 7S | 140 | ASN |
| 34 | 7S | 213 | HIS |
| 34 | 7S | 242 | ASN |
| 35 | 7T | 129 | GLN |
| 35 | 7T | 137 | ASN |
| 35 | 7T | 147 | ASN |
| 35 | 7T | 153 | ASN |
| 35 | 7T | 194 | GLN |
| 35 | 7U | 74 | ASN |
| 35 | 7U | 147 | ASN |
| 35 | 7U | 153 | ASN |
| 35 | 7U | 194 | GLN |
| 35 | 7U | 221 | GLN |
| 36 | 7V | 103 | ASN |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | 7W | 103 | ASN |
| 28 | 7X | 355 | ASN |
| 28 | 7X | 408 | GLN |
| 37 | 7Y | 33 | GLN |
| 37 | 7Y | 215 | HIS |
| 37 | 7Y | 239 | HIS |
| 37 | 7Y | 250 | GLN |
| 38 | 7Z | 27 | HIS |
| 38 | 8A | 91 | GLN |
| 38 | 8A | 110 | ASN |
| 38 | 8A | 161 | GLN |
| 38 | 8B | 116 | GLN |
| 38 | 8B | 125 | ASN |
| 38 | 8B | 214 | HIS |
| 38 | 8C | 2 | ASN |
| 38 | 8C | 30 | GLN |
| 38 | 8C | 110 | ASN |
| 38 | 8C | 125 | ASN |
| 38 | 8C | 161 | GLN |
| 38 | 8C | 204 | GLN |
| 38 | 8C | 214 | HIS |
| 38 | 8D | 125 | ASN |
| 38 | 8D | 209 | HIS |
| 38 | 8D | 214 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 510 ligands modelled in this entry, 170 are monoatomic - leaving 340 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | 8 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | W8 | 503 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 41 | GTP | K0 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | Q4 | 501 | 40 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.38 | 5 (14%) |
| 41 | GTP | A4 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.36 | 6 (17%) |
| 41 | GTP | L4 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | 2Y | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.20 | 3 (10%) |
| 41 | GTP | G5 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | N0 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | F5 | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.24 | 4 (11%) |
| 41 | GTP | C8 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.36 | 4 (11%) |
| 41 | GTP | 1L | 501 | 40 | 29,34,34 | 1.24 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | W4 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.21 | 5 (16%) |
| 41 | GTP | 2Y | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | 1Q | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.16 | 3 (10%) |
| 41 | GTP | B7 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | Y0 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.37 | 4 (11%) |
| 39 | GDP | 1E | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 39 | GDP | H4 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 39 | GDP | I8 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | O4 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.35 | 4 (11%) |
| 39 | GDP | C4 | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.21 | 3 (10%) |
| 41 | GTP | L6 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | K4 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | M4 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | T4 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.16 | 3 (10%) |
| 41 | GTP | D3 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.33 | 3 (8%) |
| 39 | GDP | G2 | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.17 | 2 (6%) |
| 41 | GTP | 2A | 501 | 40 | 29,34,34 | 1.17 | 1 (3%) | 35,54,54 | 1.27 | 3 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 39 | GDP | G6 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.19 | 2 (6%) |
| 39 | GDP | Q8 | 501 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.26 | 4 (13%) |
| 39 | GDP | F0 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | A3 | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.24 | 4 (13%) |
| 39 | GDP | 2M | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | Y4 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | Z3 | 501 | 40 | 29,34,34 | 1.26 | 1 (3%) | 35,54,54 | 1.33 | 4 (11%) |
| 41 | GTP | N3 | 501 | 40 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | 9 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | V3 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 41 | GTP | P8 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | X2 | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | 1K | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.15 | 3 (10%) |
| 39 | GDP | 0Y | 502 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.19 | 2 (6%) |
| 39 | GDP | 2E | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | L2 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 39 | GDP | X6 | 502 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 39 | GDP | A7 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 39 | GDP | P6 | 503 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 41 | GTP | O8 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.29 | 3 (8%) |
| 39 | GDP | C8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 39 | GDP | 5 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | 0U | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.20 | 4 (13%) |
| 41 | GTP | F8 | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | C9 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.36 | 3 (8%) |
| 39 | GDP | 1A | 503 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.13 | 4 (13%) |
| 41 | GTP | 2N | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | O9 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.32 | 3 (8%) |
| 39 | GDP | 2S | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.23 | 5 (16%) |
| 39 | GDP | R2 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 41 | GTP | 2G | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | A9 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 41 | GTP | M2 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | N6 | 503 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | 0S | 502 | - | 25,30,30 | 1.03 | 2 (8%) | 30,47,47 | 1.13 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | I0 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | L6 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | 2K | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | Z6 | 502 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 39 | GDP | N0 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | Q6 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | V0 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | 2L | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | 0C | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | B5 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | 3A | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.35 | 4 (11%) |
| 41 | GTP | 3M | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.37 | 4 (11%) |
| 39 | GDP | X0 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.10 | 1 (3%) |
| 41 | GTP | H3 | 501 | 40 | 29,34,34 | 1.24 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | W8 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | P9 | 501 | 40 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.42 | 5 (14%) |
| 41 | GTP | K1 | 501 | 40 | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.28 | 3 (8%) |
| 41 | GTP | R4 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | U4 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.13 | 3 (10%) |
| 39 | GDP | 0G | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | N2 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.15 | 3 (10%) |
| 41 | GTP | Y1 | 501 | 40 | 29,34,34 | 1.19 | 1 (3%) | 35,54,54 | 1.39 | 4 (11%) |
| 39 | GDP | K6 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.17 | 2 (6%) |
| 39 | GDP | V4 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.19 | 3 (10%) |
| 39 | GDP | S2 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 41 | GTP | B0 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | 2G | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | J2 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | 3I | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 41 | GTP | 2S | 501 | 40 | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | 0Q | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.16 | 3 (10%) |
| 39 | GDP | 1U | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | G7 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | S4 | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 39 | GDP | K8 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | 1G | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.26 | 4 (11%) |
| 41 | GTP | X4 | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.43 | 5 (14%) |
| 39 | GDP | 0O | 502 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.19 | 4 (13%) |
| 39 | GDP | Q2 | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | S8 | 502 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.19 | 2 (6%) |
| 41 | GTP | 1T | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | 3A | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.19 | 3 (10%) |
| 39 | GDP | 1O | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | G9 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.24 | 4 (11%) |
| 41 | GTP | P4 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 41 | GTP | K6 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | K4 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.23 | 4 (11%) |
| 39 | GDP | 2C | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 41 | GTP | S9 | 501 | 40 | 29,34,34 | 1.00 | 3 (10%) | 35,54,54 | 1.13 | 2 (5%) |
| 39 | GDP | F6 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | Z0 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.15 | 3 (10%) |
| 39 | GDP | C2 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.12 | 3 (10%) |
| 41 | GTP | F1 | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | K0 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.18 | 4 (13%) |
| 41 | GTP | D1 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.47 | 6 (17%) |
| 41 | GTP | J8 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | B5 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 39 | GDP | T2 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 39 | GDP | X4 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.11 | 3 (10%) |
| 41 | GTP | E8 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.33 | 3 (8%) |
| 39 | GDP | A5 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | M2 | 502 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 41 | GTP | U7 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 39 | GDP | W6 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 41 | GTP | H8 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | 3C | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.16 | 4 (13%) |
| 39 | GDP | 1C | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.17 | 2 (6%) |
| 41 | GTP | 3O | 501 | 40 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.36 | 4 (11%) |
| 41 | GTP | Z6 | 501 | 40 | 29,34,34 | 1.26 | 1 (3%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | D4 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.23 | 3 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | S5 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.42 | 6 (17%) |
| 39 | GDP | Y8 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | 1Q | 501 | 40 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.32 | 4 (11%) |
| 41 | GTP | K9 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | P4 | 503 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.20 | 3 (10%) |
| 39 | GDP | U2 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 41 | GTP | I8 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | 1S | 501 | 40 | 29,34,34 | 1.24 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | 2Q | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.24 | 5 (16%) |
| 41 | GTP | T8 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.36 | 4 (11%) |
| 41 | GTP | C1 | 501 | 40 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | G1 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.36 | 4 (11%) |
| 41 | GTP | 0S | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | 2U | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | 0I | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | 7 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | E1 | 501 | 40 | 29,34,34 | 1.24 | 1 (3%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | 0W | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.19 | 2 (6%) |
| 41 | GTP | D7 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.30 | 3 (8%) |
| 41 | GTP | L7 | 501 | 40 | 29,34,34 | 1.30 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | C5 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | W4 | 501 | 40 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | 2I | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.15 | 3 (10%) |
| 41 | GTP | 3T | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | Y6 | 501 | 40 | 29,34,34 | 1.16 | 1 (3%) | 35,54,54 | 1.29 | 3 (8%) |
| 39 | GDP | I2 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.13 | 3 (10%) |
| 39 | GDP | Q0 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.15 | 4 (13%) |
| 39 | GDP | Y4 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | N6 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | 3 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 41 | GTP | 3D | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | W5 | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | 0Y | 501 | 40 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 41 | GTP | Z2 | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | I4 | 501 | 40 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.27 | 4 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 39 | GDP | F8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | T8 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 41 | GTP | 3P | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.44 | 6 (17%) |
| 41 | GTP | M6 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.35 | 4 (11%) |
| 39 | GDP | D8 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | I5 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | M0 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.13 | 3 (10%) |
| 41 | GTP | L2 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | 3M | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.18 | 2 (6%) |
| 39 | GDP | 0I | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | 3K | 503 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | T0 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 3 (10%) |
| 41 | GTP | 0O | 501 | 40 | 29,34,34 | 1.24 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | Q2 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.38 | 5 (14%) |
| 41 | GTP | S8 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | R6 | 503 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.26 | 5 (16%) |
| 41 | GTP | U9 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | 1H | 501 | 40 | 29,34,34 | 1.17 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 41 | GTP | T6 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.39 | 4 (11%) |
| 41 | GTP | 2E | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.27 | 3 (8%) |
| 39 | GDP | N8 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | V8 | 501 | 40 | 29,34,34 | 1.17 | 1 (3%) | 35,54,54 | 1.29 | 3 (8%) |
| 41 | GTP | 1W | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | T6 | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 41 | GTP | J6 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.33 | 4 (11%) |
| 41 | GTP | S2 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.35 | 5 (14%) |
| 39 | GDP | 3Q | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | J2 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | 0Q | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | E0 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 39 | GDP | 2U | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.20 | 4 (13%) |
| 41 | GTP | R8 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | 0E | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 39 | GDP | I4 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | Q4 | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | 3G | 501 | 40 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | M6 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.25 | 5 (16%) |
| 41 | GTP | 0F | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.29 | 3 (8%) |
| 41 | GTP | G0 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.27 | 4 (11%) |
| 39 | GDP | Y6 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | C6 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | 3S | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 41 | GTP | U4 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 39 | GDP | Z2 | 503 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | E4 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | H6 | 502 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 39 | GDP | R8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.18 | 4 (13%) |
| 39 | GDP | V6 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | H2 | 503 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 41 | GTP | K7 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | 1W | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 39 | GDP | X8 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | E6 | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | I1 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | B8 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.25 | 4 (13%) |
| 39 | GDP | D0 | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.21 | 3 (10%) |
| 39 | GDP | 1G | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 39 | GDP | P8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 41 | GTP | U2 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | A2 | 501 | 40 | 29,34,34 | 1.26 | 1 (3%) | 35,54,54 | 1.47 | 5 (14%) |
| 39 | GDP | B1 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 41 | GTP | W0 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 39 | GDP | J4 | 503 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 3 (10%) |
| 41 | GTP | 2C | 501 | 40 | 29,34,34 | 1.20 | 1 (3%) | 35,54,54 | 1.29 | 3 (8%) |
| 41 | GTP | G4 | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | O0 | 503 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 39 | GDP | Z4 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |
| 39 | GDP | H8 | 503 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | E4 | 502 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 39 | GDP | O4 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | 7 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | V2 | 503 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 3 (10%) |
| 39 | GDP | Z8 | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 41 | GTP | 0M | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.34 | 4 (11%) |
| 41 | GTP | F0 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.26 | 4 (11%) |
| 41 | GTP | 2W | 501 | 40 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.36 | 4 (11%) |
| 41 | GTP | 1X | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | X7 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.52 | 5 (14%) |
| 41 | GTP | H2 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | A1 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | 3O | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | 2Q | 501 | 40 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | E8 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | R0 | 501 | 40 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | V8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 3 (10%) |
| 39 | GDP | A9 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 39 | GDP | G4 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 39 | GDP | W0 | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 39 | GDP | Y0 | 502 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | 3K | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 41 | GTP | 1N | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 41 | GTP | 1A | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | M0 | 501 | 40 | 29,34,34 | 1.20 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | C0 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | R6 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.39 | 5 (14%) |
| 39 | GDP | W2 | 503 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 3 (10%) |
| 39 | GDP | M4 | 502 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | 3G | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.19 | 3 (10%) |
| 41 | GTP | O6 | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.35 | 3 (8%) |
| 41 | GTP | U6 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | 2 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 39 | GDP | G0 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.17 | 2 (6%) |
| 41 | GTP | E6 | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.30 | 3 (8%) |
| 41 | GTP | 1D | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | G8 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 41 | GTP | 0V | 501 | 40 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 41 | GTP | 0K | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.26 | 4 (11%) |
| 39 | GDP | 2W | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.22 | 4 (13%) |
| 39 | GDP | O2 | 502 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.17 | 2 (6%) |
| 41 | GTP | 3 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | B2 | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | F3 | 501 | 40 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | S0 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.23 | 4 (13%) |
| 41 | GTP | W2 | 501 | 40 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.27 | 3 (8%) |
| 39 | GDP | M8 | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | O2 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.47 | 6 (17%) |
| 41 | GTP | 4 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 41 | GTP | Z7 | 501 | 40 | 29,34,34 | 1.26 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | T2 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.39 | 4 (11%) |
| 41 | GTP | 2K | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.27 | 4 (11%) |
| 39 | GDP | F2 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | B3 | 501 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 41 | GTP | X6 | 501 | 40 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.44 | 5 (14%) |
| 41 | GTP | 3C | 501 | 40 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.33 | 4 (11%) |
| 41 | GTP | X0 | 501 | 40 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.32 | 4 (11%) |
| 41 | GTP | 0A | 501 | 40 | 29,34,34 | 1.27 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | 0M | 502 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.18 | 1 (3%) |
| 39 | GDP | U8 | 501 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | 2I | 501 | 40 | 29,34,34 | 1.22 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 39 | GDP | C0 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | 3S | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 41 | GTP | 0C | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | O6 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.22 | 3 (10%) |
| 41 | GTP | N1 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 41 | GTP | N8 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 41 | GTP | 3I | 501 | 40 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.37 | 3 (8%) |
| 39 | GDP | R4 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 39 | GDP | O8 | 503 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.22 | 3 (10%) |
| 39 | GDP | D2 | 501 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 39 | GDP | L0 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.16 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 39 | GDP | R0 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 39 | GDP | 0A | 503 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.21 | 1 (3%) |
| 39 | GDP | 0K | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.18 | 1 (3%) |
| 41 | GTP | M7 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 41 | GTP | P6 | 501 | 40 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | J8 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.23 | 3 (10%) |
| 41 | GTP | J0 | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.32 | 5 (14%) |
| 39 | GDP | S6 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.13 | 2 (6%) |
| 41 | GTP | R2 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 39 | GDP | I0 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 39 | GDP | J6 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.18 | 4 (13%) |
| 39 | GDP | J0 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.14 | 2 (6%) |
| 41 | GTP | D5 | 501 | 40 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | D6 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.18 | 2 (6%) |
| 41 | GTP | J4 | 501 | 40 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 39 | GDP | 1M | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.18 | 3 (10%) |
| 41 | GTP | 1C | 501 | 40 | 29,34,34 | 1.23 | 1 (3%) | 35,54,54 | 1.27 | 4 (11%) |
| 39 | GDP | Q6 | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 39 | GDP | U6 | 502 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 41 | GTP | O0 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | A1 | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 41 | GTP | S0 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 39 | GDP | 2A | 502 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 41 | GTP | V2 | 501 | 40 | 29,34,34 | 1.19 | 1 (3%) | 35,54,54 | 1.29 | 4 (11%) |
| 39 | GDP | L4 | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.12 | 3 (10%) |
| 39 | GDP | E2 | 501 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 39 | GDP | 1S | 502 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.20 | 2 (6%) |
| 41 | GTP | H6 | 501 | 40 | 29,34,34 | 1.25 | 1 (3%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | Z0 | 501 | 40 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 41 | GTP | T4 | 501 | 40 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 39 | GDP | Y2 | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.12 | 3 (10%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | 8 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 39 | GDP | W8 | 503 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | K0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | Q4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | A4 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | L4 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2Y | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 41 | GTP | G5 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | N0 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | F5 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | C8 | 501 | 40 | - | 2/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1L | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | W4 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2Y | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 1Q | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | B7 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | Y0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 1E | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | H4 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | I8 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | O4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | C4 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | L6 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | K4 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | M4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | T4 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | D3 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | G2 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2A | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | G6 | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | Q8 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | F0 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | A3 | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | 2M | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | Y4 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | Z3 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | N3 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 9 | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 41 | GTP | V3 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | P8 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | X2 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1K | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0Y | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | 2E | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | L2 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | X6 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | A7 | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | P6 | 503 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | O8 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | C8 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | 5 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0U | 501 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | F8 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | C9 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 39 | GDP | 1A | 503 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2N | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | O9 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2S | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | R2 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2G | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | A9 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | M2 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | N6 | 503 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0S | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | I0 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | L6 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | 2K | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | Z6 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | N0 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | Q6 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | V0 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2L | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 39 | GDP | 0C | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | B5 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | 3A | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | 3M | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | X0 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | H3 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | W8 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | P9 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | K1 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | R4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | U4 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0G | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | N2 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | Y1 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | K6 | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | V4 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | S2 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | B0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2G | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | J2 | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 39 | GDP | 3I | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2S | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 0Q | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1U | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | G7 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | S4 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | K8 | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 1G | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | X4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 0O | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | Q2 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | S8 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | 1T | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3A | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1O | 501 | - | - | 1/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | G9 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | P4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | K6 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | K4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2C | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | S9 | 501 | 40 | - | 3/18/38/38 | 0/3/3/3 |
| 39 | GDP | F6 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | Z0 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | C2 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | F1 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | K0 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | D1 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 41 | GTP | J8 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | B5 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | T2 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | X4 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | E8 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 39 | GDP | A5 | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 39 | GDP | M2 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | U7 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | W6 | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 41 | GTP | H8 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3C | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1C | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3O | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | Z6 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | D4 | 501 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | S5 | 501 | 40 | - | 4/18/38/38 | 0/3/3/3 |
| 39 | GDP | Y8 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 1Q | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | K9 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | P4 | 503 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | U2 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | I8 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1S | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 39 | GDP | 2Q | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | T8 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | C1 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | G1 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0S | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 2U | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0I | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 7 | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | E1 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | 0W | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | D7 | 501 | 40 | - | 4/18/38/38 | 0/3/3/3 |
| 41 | GTP | L7 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | C5 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | W4 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2I | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3T | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | Y6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | I2 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | Q0 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | Y4 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | N6 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3D | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | W5 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0Y | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | Z2 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | I4 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | F8 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | T8 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3P | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | M6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | D8 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | I5 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | M0 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | L2 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3M | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0I | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | 3K | 503 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | T0 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | 0O | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | Q2 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | S8 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | R6 | 503 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | U9 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1H | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | T6 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 41 | GTP | 2E | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | N8 | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 41 | GTP | V8 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1W | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | T6 | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 41 | GTP | J6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | S2 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3Q | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | J2 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0Q | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | E0 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | 2U | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | R8 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | 0E | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | I4 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | Q4 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3G | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | M6 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 0F | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | G0 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | Y6 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | C6 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 39 | GDP | 3S | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | U4 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | Z2 | 503 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | E4 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | H6 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | R8 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | V6 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | H2 | 503 | - | - | 0/12/32/32 | 0/3/3/3 |
| 41 | GTP | K7 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 1W | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | X8 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | E6 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | I1 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | B8 | 501 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | D0 | 501 | - | - | 8/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1G | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 39 | GDP | P8 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | U2 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | A2 | 501 | 40 | - | 2/18/38/38 | 0/3/3/3 |
| 39 | GDP | B1 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | W0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | J4 | 503 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2C | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | G4 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | O0 | 503 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | Z4 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | H8 | 503 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | E4 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | O4 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | 7 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | V2 | 503 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | Z8 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | 0M | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | F0 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | 2W | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | 1X | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | X7 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | H2 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | A1 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 3O | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2Q | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | E8 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | R0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | V8 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | A9 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | G4 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | W0 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | Y0 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3K | 501 | 40 | - | 4/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1N | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1A | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | M0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | C0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | R6 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | W2 | 503 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | M4 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 3G | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | O6 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | U6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2 | 501 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | G0 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | E6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 1D | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | G8 | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | 0V | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0K | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2W | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | O2 | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 41 | GTP | B2 | 501 | 40 | - | 4/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | GTP | F3 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 39 | GDP | S0 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | W2 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | M8 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | O2 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | 4 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | Z7 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | T2 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | 2K | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | F2 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 39 | GDP | B3 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | X6 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | 3C | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | X0 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0A | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 39 | GDP | 0M | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | U8 | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 2I | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 39 | GDP | C0 | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 41 | GTP | 3S | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | 0C | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | O6 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 41 | GTP | N1 | 501 | 40 | - | 7/18/38/38 | 0/3/3/3 |
| 41 | GTP | N8 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | 3I | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | R4 | 502 | - | - | 7/12/32/32 | 0/3/3/3 |
| 39 | GDP | O8 | 503 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | D2 | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | L0 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 39 | GDP | R0 | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0A | 503 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | 0K | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | M7 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | P6 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 39 | GDP | J8 | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | J0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | S6 | 501 | - | - | 7/12/32/32 | 0/3/3/3 |
| 41 | GTP | R2 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | I0 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | J6 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | J0 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | D5 | 501 | 40 | - | 4/18/38/38 | 0/3/3/3 |
| 39 | GDP | D6 | 501 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | J4 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | 1M | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | 1C | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | Q6 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 39 | GDP | U6 | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 41 | GTP | O0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | A1 | 502 | - | - | 6/12/32/32 | 0/3/3/3 |
| 41 | GTP | S0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 39 | GDP | 2A | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 41 | GTP | V2 | 501 | 40 | - | 6/18/38/38 | 0/3/3/3 |
| 39 | GDP | L4 | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 39 | GDP | E2 | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 39 | GDP | 1S | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 41 | GTP | H6 | 501 | 40 | - | 9/18/38/38 | 0/3/3/3 |
| 41 | GTP | Z0 | 501 | 40 | - | 8/18/38/38 | 0/3/3/3 |
| 41 | GTP | T4 | 501 | 40 | - | 5/18/38/38 | 0/3/3/3 |
| 39 | GDP | Y2 | 501 | - | - | 2/12/32/32 | 0/3/3/3 |

All (470) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | R0 | 501 | GTP | C5-C6 | -4.90 | 1.37 | 1.47 |
| 41 | P4 | 501 | GTP | C5-C6 | -4.87 | 1.37 | 1.47 |
| 41 | Z3 | 501 | GTP | C5-C6 | -4.86 | 1.37 | 1.47 |
| 41 | P6 | 501 | GTP | C5-C6 | -4.86 | 1.37 | 1.47 |
| 41 | 2S | 501 | GTP | C5-C6 | -4.83 | 1.37 | 1.47 |
| 41 | Q4 | 501 | GTP | C5-C6 | -4.83 | 1.37 | 1.47 |
| 41 | P9 | 501 | GTP | C5-C6 | -4.83 | 1.37 | 1.47 |
| 41 | I0 | 501 | GTP | C5-C6 | -4.83 | 1.37 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | T6 | 501 | GTP | C5-C6 | -4.82 | 1.37 | 1.47 |
| 41 | P8 | 501 | GTP | C5-C6 | -4.81 | 1.37 | 1.47 |
| 41 | S2 | 501 | GTP | C5-C6 | -4.81 | 1.37 | 1.47 |
| 41 | 8 | 501 | GTP | C5-C6 | -4.80 | 1.38 | 1.47 |
| 41 | I1 | 501 | GTP | C5-C6 | -4.80 | 1.38 | 1.47 |
| 41 | Q6 | 501 | GTP | C5-C6 | -4.79 | 1.38 | 1.47 |
| 41 | 2W | 501 | GTP | C5-C6 | -4.78 | 1.38 | 1.47 |
| 41 | 3A | 501 | GTP | C5-C6 | -4.78 | 1.38 | 1.47 |
| 41 | K9 | 501 | GTP | C5-C6 | -4.76 | 1.38 | 1.47 |
| 41 | S0 | 501 | GTP | C5-C6 | -4.76 | 1.38 | 1.47 |
| 41 | N1 | 501 | GTP | C5-C6 | -4.75 | 1.38 | 1.47 |
| 41 | R8 | 501 | GTP | C5-C6 | -4.75 | 1.38 | 1.47 |
| 41 | J4 | 501 | GTP | C5-C6 | -4.74 | 1.38 | 1.47 |
| 41 | T2 | 501 | GTP | C5-C6 | -4.74 | 1.38 | 1.47 |
| 41 | Q2 | 501 | GTP | C5-C6 | -4.73 | 1.38 | 1.47 |
| 41 | H6 | 501 | GTP | C5-C6 | -4.73 | 1.38 | 1.47 |
| 41 | N0 | 501 | GTP | C5-C6 | -4.72 | 1.38 | 1.47 |
| 41 | 4 | 501 | GTP | C5-C6 | -4.72 | 1.38 | 1.47 |
| 41 | G4 | 501 | GTP | C5-C6 | -4.71 | 1.38 | 1.47 |
| 41 | M6 | 501 | GTP | C5-C6 | -4.71 | 1.38 | 1.47 |
| 41 | 2Q | 501 | GTP | C5-C6 | -4.71 | 1.38 | 1.47 |
| 41 | S5 | 501 | GTP | C5-C6 | -4.70 | 1.38 | 1.47 |
| 41 | 7 | 501 | GTP | C5-C6 | -4.69 | 1.38 | 1.47 |
| 41 | 3O | 501 | GTP | C5-C6 | -4.69 | 1.38 | 1.47 |
| 41 | H8 | 501 | GTP | C5-C6 | -4.69 | 1.38 | 1.47 |
| 41 | G5 | 501 | GTP | C5-C6 | -4.69 | 1.38 | 1.47 |
| 41 | I4 | 501 | GTP | C5-C6 | -4.68 | 1.38 | 1.47 |
| 41 | E1 | 501 | GTP | C5-C6 | -4.68 | 1.38 | 1.47 |
| 41 | R2 | 501 | GTP | C5-C6 | -4.68 | 1.38 | 1.47 |
| 41 | U7 | 501 | GTP | C5-C6 | -4.68 | 1.38 | 1.47 |
| 41 | R4 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | T4 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | M7 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | Z7 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | H3 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | L2 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | S8 | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 41 | Z6 | 501 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |
| 41 | 1Q | 501 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |
| 41 | 1A | 501 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |
| 41 | J6 | 501 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |
| 41 | 0A | 501 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | A9 | 501 | GTP | C5-C6 | -4.65 | 1.38 | 1.47 |
| 41 | 3 | 501 | GTP | C5-C6 | -4.65 | 1.38 | 1.47 |
| 41 | 1W | 501 | GTP | C5-C6 | -4.65 | 1.38 | 1.47 |
| 41 | 3C | 501 | GTP | C5-C6 | -4.64 | 1.38 | 1.47 |
| 41 | N8 | 501 | GTP | C5-C6 | -4.64 | 1.38 | 1.47 |
| 41 | H2 | 501 | GTP | C5-C6 | -4.63 | 1.38 | 1.47 |
| 41 | 0M | 501 | GTP | C5-C6 | -4.63 | 1.38 | 1.47 |
| 41 | R6 | 501 | GTP | C5-C6 | -4.63 | 1.38 | 1.47 |
| 41 | F8 | 501 | GTP | C5-C6 | -4.62 | 1.38 | 1.47 |
| 41 | G1 | 501 | GTP | C5-C6 | -4.62 | 1.38 | 1.47 |
| 41 | O2 | 501 | GTP | C5-C6 | -4.62 | 1.38 | 1.47 |
| 41 | A2 | 501 | GTP | C5-C6 | -4.62 | 1.38 | 1.47 |
| 41 | 3G | 501 | GTP | C5-C6 | -4.61 | 1.38 | 1.47 |
| 41 | F1 | 501 | GTP | C5-C6 | -4.61 | 1.38 | 1.47 |
| 41 | 1N | 501 | GTP | C5-C6 | -4.61 | 1.38 | 1.47 |
| 41 | O0 | 501 | GTP | C5-C6 | -4.61 | 1.38 | 1.47 |
| 41 | F5 | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | M4 | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | 1S | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | E6 | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | 0K | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | C5 | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 41 | 3P | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 41 | B2 | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 41 | U2 | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 41 | T8 | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 41 | A1 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | M2 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | G7 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | K6 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | B5 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | K0 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | J0 | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 41 | 3M | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 41 | B0 | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 41 | W8 | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 41 | J2 | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | D5 | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | D1 | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | 1L | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | U9 | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | Z0 | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | 2U | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 41 | 3S | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 41 | N6 | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 41 | 2Y | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 41 | O8 | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 41 | V3 | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 41 | Y4 | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 41 | A4 | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | 1C | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | E8 | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | 1D | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | L4 | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | F0 | 501 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 41 | I8 | 501 | GTP | C5-C6 | -4.52 | 1.38 | 1.47 |
| 41 | 3I | 501 | GTP | C5-C6 | -4.52 | 1.38 | 1.47 |
| 41 | 0I | 501 | GTP | C5-C6 | -4.51 | 1.38 | 1.47 |
| 41 | 3K | 501 | GTP | C5-C6 | -4.51 | 1.38 | 1.47 |
| 41 | O4 | 501 | GTP | C5-C6 | -4.51 | 1.38 | 1.47 |
| 41 | G0 | 501 | GTP | C5-C6 | -4.51 | 1.38 | 1.47 |
| 41 | M0 | 501 | GTP | C5-C6 | -4.51 | 1.38 | 1.47 |
| 41 | O9 | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 41 | Z2 | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 41 | E4 | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 41 | L7 | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 41 | U4 | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 41 | 1T | 501 | GTP | C5-C6 | -4.49 | 1.38 | 1.47 |
| 41 | U6 | 501 | GTP | C5-C6 | -4.49 | 1.38 | 1.47 |
| 41 | W5 | 501 | GTP | C5-C6 | -4.49 | 1.38 | 1.47 |
| 41 | 0Q | 501 | GTP | C5-C6 | -4.49 | 1.38 | 1.47 |
| 41 | L6 | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | D7 | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | K7 | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | 2I | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | I5 | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | 2K | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | B7 | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | 0O | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 41 | K1 | 501 | GTP | C5-C6 | -4.47 | 1.38 | 1.47 |
| 41 | 2G | 501 | GTP | C5-C6 | -4.47 | 1.38 | 1.47 |
| 41 | C8 | 501 | GTP | C5-C6 | -4.46 | 1.38 | 1.47 |
| 41 | K4 | 501 | GTP | C5-C6 | -4.46 | 1.38 | 1.47 |
| 41 | G9 | 501 | GTP | C5-C6 | -4.45 | 1.38 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | V2 | 501 | GTP | C5-C6 | -4.45 | 1.38 | 1.47 |
| 41 | 0V | 501 | GTP | C5-C6 | -4.44 | 1.38 | 1.47 |
| 41 | D3 | 501 | GTP | C5-C6 | -4.44 | 1.38 | 1.47 |
| 41 | C9 | 501 | GTP | C5-C6 | -4.43 | 1.38 | 1.47 |
| 41 | C1 | 501 | GTP | C5-C6 | -4.43 | 1.38 | 1.47 |
| 41 | 0F | 501 | GTP | C5-C6 | -4.42 | 1.38 | 1.47 |
| 41 | C0 | 501 | GTP | C5-C6 | -4.42 | 1.38 | 1.47 |
| 41 | 2L | 501 | GTP | C5-C6 | -4.42 | 1.38 | 1.47 |
| 41 | J8 | 501 | GTP | C5-C6 | -4.41 | 1.38 | 1.47 |
| 41 | 1X | 501 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 41 | 1G | 501 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 41 | 0C | 501 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 41 | 0Y | 501 | GTP | C5-C6 | -4.38 | 1.38 | 1.47 |
| 41 | 3T | 501 | GTP | C5-C6 | -4.38 | 1.38 | 1.47 |
| 41 | W2 | 501 | GTP | C5-C6 | -4.38 | 1.38 | 1.47 |
| 41 | Y1 | 501 | GTP | C5-C6 | -4.37 | 1.38 | 1.47 |
| 41 | 2E | 501 | GTP | C5-C6 | -4.37 | 1.38 | 1.47 |
| 41 | Y0 | 501 | GTP | C5-C6 | -4.37 | 1.38 | 1.47 |
| 41 | X4 | 501 | GTP | C5-C6 | -4.37 | 1.38 | 1.47 |
| 41 | W4 | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 41 | O6 | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 41 | 2C | 501 | GTP | C5-C6 | -4.35 | 1.38 | 1.47 |
| 41 | 0S | 501 | GTP | C5-C6 | -4.35 | 1.38 | 1.47 |
| 41 | W0 | 501 | GTP | C5-C6 | -4.33 | 1.38 | 1.47 |
| 41 | 3D | 501 | GTP | C5-C6 | -4.32 | 1.38 | 1.47 |
| 41 | X6 | 501 | GTP | C5-C6 | -4.31 | 1.38 | 1.47 |
| 41 | X0 | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 41 | F3 | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 41 | 2N | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 41 | V8 | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 41 | 1H | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 41 | X7 | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 41 | 2A | 501 | GTP | C5-C6 | -4.17 | 1.39 | 1.47 |
| 41 | Y6 | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 41 | N3 | 501 | GTP | C5-C6 | -4.10 | 1.39 | 1.47 |
| 39 | O2 | 502 | GDP | C6-N1 | -2.99 | 1.33 | 1.37 |
| 39 | 2S | 502 | GDP | C6-N1 | -2.93 | 1.33 | 1.37 |
| 39 | T6 | 502 | GDP | C6-N1 | -2.93 | 1.33 | 1.37 |
| 39 | P6 | 503 | GDP | C6-N1 | -2.91 | 1.33 | 1.37 |
| 39 | 2U | 502 | GDP | C6-N1 | -2.88 | 1.33 | 1.37 |
| 39 | Q2 | 502 | GDP | C6-N1 | -2.87 | 1.33 | 1.37 |
| 39 | 3C | 502 | GDP | C6-N1 | -2.85 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 39 | 2G | 502 | GDP | C6-N1 | -2.85 | 1.33 | 1.37 |
| 39 | R4 | 502 | GDP | C6-N1 | -2.85 | 1.33 | 1.37 |
| 39 | S6 | 501 | GDP | C6-N1 | -2.84 | 1.33 | 1.37 |
| 39 | 3I | 502 | GDP | C6-N1 | -2.84 | 1.33 | 1.37 |
| 39 | Q4 | 502 | GDP | C6-N1 | -2.84 | 1.33 | 1.37 |
| 39 | 9 | 501 | GDP | C6-N1 | -2.82 | 1.33 | 1.37 |
| 39 | L4 | 502 | GDP | C6-N1 | -2.82 | 1.33 | 1.37 |
| 39 | 2W | 502 | GDP | C6-N1 | -2.82 | 1.33 | 1.37 |
| 39 | 3A | 502 | GDP | C6-N1 | -2.81 | 1.33 | 1.37 |
| 39 | G2 | 501 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | 1C | 502 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | J8 | 502 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | F2 | 501 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | O8 | 503 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | R6 | 503 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | E4 | 502 | GDP | C6-N1 | -2.80 | 1.33 | 1.37 |
| 39 | H8 | 503 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | N8 | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | 2C | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | 2Q | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | Q6 | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | S2 | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | D2 | 501 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | E6 | 502 | GDP | C6-N1 | -2.79 | 1.33 | 1.37 |
| 39 | S0 | 502 | GDP | C6-N1 | -2.78 | 1.33 | 1.37 |
| 39 | 2E | 502 | GDP | C6-N1 | -2.78 | 1.33 | 1.37 |
| 39 | P8 | 502 | GDP | C6-N1 | -2.78 | 1.33 | 1.37 |
| 39 | R8 | 502 | GDP | C6-N1 | -2.78 | 1.33 | 1.37 |
| 39 | 1A | 503 | GDP | C6-N1 | -2.78 | 1.33 | 1.37 |
| 39 | H2 | 503 | GDP | C6-N1 | -2.77 | 1.33 | 1.37 |
| 39 | B3 | 501 | GDP | C6-N1 | -2.77 | 1.33 | 1.37 |
| 39 | N0 | 502 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | Q0 | 501 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | 5 | 501 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | P4 | 503 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | 1S | 502 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | 3G | 502 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | 2Y | 502 | GDP | C6-N1 | -2.76 | 1.33 | 1.37 |
| 39 | J6 | 502 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | N2 | 501 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | R0 | 502 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | 3K | 503 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 39 | J4 | 503 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | 2A | 502 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | 7 | 502 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | C6 | 501 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | G0 | 502 | GDP | C6-N1 | -2.75 | 1.33 | 1.37 |
| 39 | R2 | 502 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | G8 | 501 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 41 | S9 | 501 | GTP | C5-C6 | -2.74 | 1.42 | 1.47 |
| 39 | J2 | 502 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | 2K | 502 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | H4 | 501 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | V6 | 501 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | 0M | 502 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | T4 | 502 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | W2 | 503 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | O0 | 503 | GDP | C6-N1 | -2.74 | 1.33 | 1.37 |
| 39 | 3Q | 501 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | F6 | 501 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | U4 | 502 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | C4 | 501 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | B5 | 502 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | O6 | 502 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | D6 | 501 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | T0 | 501 | GDP | C6-N1 | -2.73 | 1.33 | 1.37 |
| 39 | J0 | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | U2 | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | K8 | 501 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | 3S | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | O4 | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | 1G | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | F0 | 502 | GDP | C6-N1 | -2.72 | 1.33 | 1.37 |
| 39 | L0 | 501 | GDP | C6-N1 | -2.71 | 1.33 | 1.37 |
| 39 | 3O | 502 | GDP | C6-N1 | -2.71 | 1.33 | 1.37 |
| 39 | 3 | 502 | GDP | C6-N1 | -2.71 | 1.33 | 1.37 |
| 39 | I8 | 502 | GDP | C6-N1 | -2.71 | 1.33 | 1.37 |
| 39 | 1M | 501 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | A1 | 502 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | M0 | 502 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | E0 | 501 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | I4 | 502 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | F8 | 502 | GDP | C6-N1 | -2.70 | 1.33 | 1.37 |
| 39 | V4 | 501 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 39 | H6 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | K6 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | W4 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 1E | 501 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | D4 | 501 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | I0 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 2I | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | L6 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | W0 | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 0O | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 1O | 501 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 3M | 502 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | 1K | 501 | GDP | C6-N1 | -2.69 | 1.33 | 1.37 |
| 39 | V8 | 502 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | 1W | 502 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | D0 | 501 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | T8 | 502 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | L2 | 502 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | B8 | 501 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 39 | C8 | 502 | GDP | C6-N1 | -2.67 | 1.33 | 1.37 |
| 39 | 1U | 501 | GDP | C6-N1 | -2.67 | 1.33 | 1.37 |
| 39 | 2 | 501 | GDP | C6-N1 | -2.67 | 1.33 | 1.37 |
| 39 | Y2 | 501 | GDP | C6-N1 | -2.67 | 1.33 | 1.37 |
| 39 | K0 | 502 | GDP | C6-N1 | -2.67 | 1.33 | 1.37 |
| 39 | B1 | 501 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | A5 | 501 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | C0 | 502 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | E8 | 502 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | V2 | 503 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | I2 | 501 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | E2 | 501 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | 0W | 502 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | 2M | 501 | GDP | C6-N1 | -2.66 | 1.33 | 1.37 |
| 39 | S8 | 502 | GDP | C6-N1 | -2.64 | 1.33 | 1.37 |
| 39 | T2 | 502 | GDP | C6-N1 | -2.64 | 1.33 | 1.37 |
| 39 | X2 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | C2 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | U6 | 502 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | G6 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | V0 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | Y6 | 502 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | 0A | 503 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 39 | U8 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | A3 | 501 | GDP | C6-N1 | -2.63 | 1.33 | 1.37 |
| 39 | N6 | 503 | GDP | C6-N1 | -2.62 | 1.33 | 1.37 |
| 39 | W6 | 501 | GDP | C6-N1 | -2.62 | 1.33 | 1.37 |
| 39 | K4 | 502 | GDP | C6-N1 | -2.62 | 1.33 | 1.37 |
| 39 | A9 | 502 | GDP | C6-N1 | -2.61 | 1.33 | 1.37 |
| 39 | 1Q | 502 | GDP | C6-N1 | -2.61 | 1.33 | 1.37 |
| 39 | M6 | 502 | GDP | C6-N1 | -2.60 | 1.33 | 1.37 |
| 39 | Q8 | 501 | GDP | C6-N1 | -2.60 | 1.33 | 1.37 |
| 39 | W8 | 503 | GDP | C6-N1 | -2.60 | 1.33 | 1.37 |
| 39 | G4 | 502 | GDP | C6-N1 | -2.59 | 1.33 | 1.37 |
| 39 | 0U | 501 | GDP | C6-N1 | -2.59 | 1.33 | 1.37 |
| 39 | Y4 | 502 | GDP | C6-N1 | -2.58 | 1.33 | 1.37 |
| 39 | 0Y | 502 | GDP | C6-N1 | -2.58 | 1.33 | 1.37 |
| 39 | Z6 | 502 | GDP | C6-N1 | -2.57 | 1.33 | 1.37 |
| 39 | A7 | 501 | GDP | C6-N1 | -2.56 | 1.33 | 1.37 |
| 39 | M8 | 501 | GDP | C6-N1 | -2.56 | 1.33 | 1.37 |
| 39 | 0Q | 502 | GDP | C6-N1 | -2.56 | 1.33 | 1.37 |
| 39 | S4 | 501 | GDP | C6-N1 | -2.55 | 1.33 | 1.37 |
| 39 | 0K | 502 | GDP | C6-N1 | -2.55 | 1.33 | 1.37 |
| 39 | X8 | 501 | GDP | C6-N1 | -2.55 | 1.33 | 1.37 |
| 39 | 0G | 501 | GDP | C6-N1 | -2.54 | 1.33 | 1.37 |
| 39 | D8 | 501 | GDP | C6-N1 | -2.53 | 1.33 | 1.37 |
| 39 | X6 | 502 | GDP | C6-N1 | -2.53 | 1.33 | 1.37 |
| 39 | X0 | 502 | GDP | C6-N1 | -2.53 | 1.33 | 1.37 |
| 39 | M2 | 502 | GDP | C6-N1 | -2.53 | 1.33 | 1.37 |
| 39 | Y0 | 502 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 39 | 0S | 502 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 39 | M4 | 502 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 39 | 0I | 502 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 39 | 0C | 502 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |
| 39 | Z8 | 501 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |
| 39 | X4 | 502 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 39 | Z4 | 501 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 39 | 0E | 501 | GDP | C6-N1 | -2.44 | 1.34 | 1.37 |
| 39 | Z2 | 503 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 39 | Y8 | 501 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 39 | Z0 | 502 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 41 | D1 | 501 | GTP | C5-C4 | -2.23 | 1.37 | 1.43 |
| 41 | C9 | 501 | GTP | C5-C4 | -2.23 | 1.37 | 1.43 |
| 41 | 2W | 501 | GTP | C5-C4 | -2.23 | 1.37 | 1.43 |
| 41 | 2S | 501 | GTP | C5-C4 | -2.21 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | C8 | 501 | GTP | C5-C4 | -2.20 | 1.37 | 1.43 |
| 41 | 2N | 501 | GTP | C2-N3 | 2.19 | 1.38 | 1.33 |
| 41 | Q6 | 501 | GTP | C5-C4 | -2.18 | 1.37 | 1.43 |
| 41 | L7 | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 41 | T6 | 501 | GTP | C5-C4 | -2.17 | 1.37 | 1.43 |
| 41 | 3A | 501 | GTP | C5-C4 | -2.17 | 1.37 | 1.43 |
| 41 | 1H | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 41 | N3 | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 41 | D5 | 501 | GTP | C5-C4 | -2.15 | 1.37 | 1.43 |
| 41 | P9 | 501 | GTP | C5-C4 | -2.15 | 1.37 | 1.43 |
| 41 | T2 | 501 | GTP | C5-C4 | -2.15 | 1.37 | 1.43 |
| 41 | 1T | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 41 | P6 | 501 | GTP | C5-C4 | -2.14 | 1.37 | 1.43 |
| 41 | L6 | 501 | GTP | C5-C4 | -2.14 | 1.37 | 1.43 |
| 41 | O4 | 501 | GTP | C5-C4 | -2.14 | 1.37 | 1.43 |
| 41 | 3O | 501 | GTP | C5-C4 | -2.14 | 1.37 | 1.43 |
| 41 | P4 | 501 | GTP | C5-C4 | -2.13 | 1.37 | 1.43 |
| 41 | 1X | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 41 | 3S | 501 | GTP | C5-C4 | -2.13 | 1.37 | 1.43 |
| 41 | Q2 | 501 | GTP | C5-C4 | -2.13 | 1.37 | 1.43 |
| 41 | C5 | 501 | GTP | C5-C4 | -2.12 | 1.37 | 1.43 |
| 41 | L2 | 501 | GTP | C5-C4 | -2.12 | 1.37 | 1.43 |
| 41 | S9 | 501 | GTP | C8-N7 | -2.12 | 1.31 | 1.34 |
| 41 | T4 | 501 | GTP | C5-C4 | -2.11 | 1.37 | 1.43 |
| 41 | 3C | 501 | GTP | C5-C4 | -2.11 | 1.37 | 1.43 |
| 41 | U6 | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 41 | 7 | 501 | GTP | C5-C4 | -2.11 | 1.37 | 1.43 |
| 41 | 3P | 501 | GTP | C5-C4 | -2.11 | 1.37 | 1.43 |
| 41 | N1 | 501 | GTP | C5-C4 | -2.11 | 1.37 | 1.43 |
| 41 | S8 | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | 3T | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 41 | 2U | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | 3I | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | W2 | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 41 | 2Y | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | K9 | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | 0Y | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 41 | 8 | 501 | GTP | C5-C4 | -2.10 | 1.37 | 1.43 |
| 41 | U4 | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 41 | W0 | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 41 | 4 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |
| 41 | Q4 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | O2 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |
| 41 | R8 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |
| 41 | R6 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |
| 41 | M6 | 501 | GTP | C5-C4 | -2.09 | 1.38 | 1.43 |
| 41 | U7 | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 41 | 1Q | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 41 | O8 | 501 | GTP | C5-C4 | -2.08 | 1.38 | 1.43 |
| 41 | 2Q | 501 | GTP | C5-C4 | -2.08 | 1.38 | 1.43 |
| 41 | 1Q | 501 | GTP | C5-C4 | -2.08 | 1.38 | 1.43 |
| 41 | 2E | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 41 | 3D | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 41 | G1 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | R4 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | 3K | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | J4 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | N0 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | V3 | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 41 | D3 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | L4 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | 3 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | S5 | 501 | GTP | C5-C4 | -2.07 | 1.38 | 1.43 |
| 41 | 0S | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 41 | M4 | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | M7 | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | C0 | 501 | GTP | C2-N3 | 2.06 | 1.38 | 1.33 |
| 41 | 3G | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | N8 | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | A9 | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | 3M | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | S0 | 501 | GTP | C5-C4 | -2.06 | 1.38 | 1.43 |
| 41 | K6 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | X6 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | R0 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | T8 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | 3C | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 41 | F3 | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 41 | S9 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | J8 | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 41 | 2G | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 41 | R2 | 501 | GTP | C5-C4 | -2.05 | 1.38 | 1.43 |
| 41 | 2L | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 41 | 1N | 501 | GTP | C5-C4 | -2.04 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | Y0 | 501 | GTP | C5-C4 | -2.04 | 1.38 | 1.43 |
| 41 | M2 | 501 | GTP | C5-C4 | -2.04 | 1.38 | 1.43 |
| 41 | U2 | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 41 | 2Q | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 41 | B5 | 501 | GTP | C5-C4 | -2.04 | 1.38 | 1.43 |
| 41 | U9 | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 41 | C1 | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 41 | K0 | 501 | GTP | C5-C4 | -2.04 | 1.38 | 1.43 |
| 39 | 0S | 502 | GDP | O4'-C1' | 2.03 | 1.43 | 1.40 |
| 41 | D7 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | K1 | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 41 | P8 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | O0 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | O6 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | B2 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | N6 | 501 | GTP | C5-C4 | -2.03 | 1.38 | 1.43 |
| 41 | O9 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | 0V | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 41 | N3 | 501 | GTP | PA-O3A | 2.02 | 1.61 | 1.59 |
| 41 | B0 | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 41 | A1 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | A4 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | G5 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | I4 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | Z0 | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 41 | I1 | 501 | GTP | C5-C4 | -2.02 | 1.38 | 1.43 |
| 41 | W4 | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 41 | S2 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | B7 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | H8 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | I0 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | K7 | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | X7 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | 1D | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | 1A | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | W5 | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | I8 | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | H2 | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 41 | Y4 | 501 | GTP | C5-C4 | -2.01 | 1.38 | 1.43 |
| 41 | 3O | 501 | GTP | C2-N3 | 2.00 | 1.38 | 1.33 |
| 41 | I4 | 501 | GTP | C2-N3 | 2.00 | 1.38 | 1.33 |
| 41 | 3G | 501 | GTP | C2-N3 | 2.00 | 1.38 | 1.33 |

All (1099) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 41 | S9 | 501 | GTP | C4'-O4'-C1' | -4.69 | 105.63 | 109.92 |
| 41 | X7 | 501 | GTP | C4'-O4'-C1' | -3.87 | 106.38 | 109.92 |
| 41 | 2C | 501 | GTP | C8-N7-C5 | 3.87 | 109.13 | 102.55 |
| 41 | J8 | 501 | GTP | C8-N7-C5 | 3.83 | 109.07 | 102.55 |
| 41 | L4 | 501 | GTP | C8-N7-C5 | 3.83 | 109.07 | 102.55 |
| 41 | 2K | 501 | GTP | C8-N7-C5 | 3.82 | 109.05 | 102.55 |
| 41 | C9 | 501 | GTP | C8-N7-C5 | 3.81 | 109.04 | 102.55 |
| 41 | 2A | 501 | GTP | C8-N7-C5 | 3.80 | 109.03 | 102.55 |
| 41 | 0S | 501 | GTP | C8-N7-C5 | 3.79 | 109.01 | 102.55 |
| 41 | 2I | 501 | GTP | C8-N7-C5 | 3.77 | 108.97 | 102.55 |
| 41 | A1 | 501 | GTP | C8-N7-C5 | 3.77 | 108.97 | 102.55 |
| 41 | O6 | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | 2G | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | O9 | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | 3C | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | 3I | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | W4 | 501 | GTP | C8-N7-C5 | 3.76 | 108.95 | 102.55 |
| 41 | 3D | 501 | GTP | C8-N7-C5 | 3.76 | 108.94 | 102.55 |
| 41 | 2Y | 501 | GTP | C8-N7-C5 | 3.75 | 108.94 | 102.55 |
| 41 | J0 | 501 | GTP | C8-N7-C5 | 3.74 | 108.91 | 102.55 |
| 41 | K0 | 501 | GTP | C8-N7-C5 | 3.73 | 108.91 | 102.55 |
| 41 | M2 | 501 | GTP | C8-N7-C5 | 3.73 | 108.91 | 102.55 |
| 41 | 3M | 501 | GTP | C8-N7-C5 | 3.73 | 108.90 | 102.55 |
| 41 | C8 | 501 | GTP | C8-N7-C5 | 3.73 | 108.90 | 102.55 |
| 41 | A9 | 501 | GTP | C8-N7-C5 | 3.73 | 108.89 | 102.55 |
| 41 | W2 | 501 | GTP | C8-N7-C5 | 3.72 | 108.89 | 102.55 |
| 41 | X0 | 501 | GTP | C8-N7-C5 | 3.72 | 108.89 | 102.55 |
| 41 | T2 | 501 | GTP | C8-N7-C5 | 3.72 | 108.88 | 102.55 |
| 41 | W5 | 501 | GTP | C8-N7-C5 | 3.72 | 108.88 | 102.55 |
| 41 | 3K | 501 | GTP | C8-N7-C5 | 3.72 | 108.88 | 102.55 |
| 41 | C1 | 501 | GTP | C8-N7-C5 | 3.72 | 108.88 | 102.55 |
| 41 | O4 | 501 | GTP | C8-N7-C5 | 3.71 | 108.87 | 102.55 |
| 41 | O8 | 501 | GTP | C8-N7-C5 | 3.71 | 108.87 | 102.55 |
| 41 | R6 | 501 | GTP | C8-N7-C5 | 3.71 | 108.87 | 102.55 |
| 41 | 3O | 501 | GTP | C8-N7-C5 | 3.71 | 108.86 | 102.55 |
| 41 | 2N | 501 | GTP | C8-N7-C5 | 3.71 | 108.86 | 102.55 |
| 41 | I8 | 501 | GTP | C8-N7-C5 | 3.71 | 108.86 | 102.55 |
| 41 | W0 | 501 | GTP | C8-N7-C5 | 3.70 | 108.86 | 102.55 |
| 41 | L6 | 501 | GTP | C8-N7-C5 | 3.70 | 108.85 | 102.55 |
| 41 | B7 | 501 | GTP | C8-N7-C5 | 3.70 | 108.85 | 102.55 |
| 41 | 2W | 501 | GTP | C8-N7-C5 | 3.69 | 108.84 | 102.55 |
| 41 | C5 | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | V8 | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 41 | K6 | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 41 | 2L | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 41 | G0 | 501 | GTP | C8-N7-C5 | 3.68 | 108.82 | 102.55 |
| 41 | 1X | 501 | GTP | C8-N7-C5 | 3.68 | 108.82 | 102.55 |
| 41 | C0 | 501 | GTP | C8-N7-C5 | 3.68 | 108.82 | 102.55 |
| 41 | 2E | 501 | GTP | C8-N7-C5 | 3.68 | 108.82 | 102.55 |
| 41 | R8 | 501 | GTP | C8-N7-C5 | 3.68 | 108.82 | 102.55 |
| 41 | 2U | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 41 | B2 | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 41 | T6 | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 41 | 1C | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 41 | 3G | 501 | GTP | C8-N7-C5 | 3.67 | 108.81 | 102.55 |
| 41 | M6 | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 41 | 2Q | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 41 | 0Q | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 41 | M7 | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 41 | 1S | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 41 | D3 | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 41 | X7 | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 41 | 3S | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 41 | X6 | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 41 | L2 | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 41 | B0 | 501 | GTP | C8-N7-C5 | 3.66 | 108.77 | 102.55 |
| 41 | V3 | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | K7 | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | 0M | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | J2 | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | Y6 | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | 1Q | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 41 | N0 | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 41 | P9 | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 41 | M0 | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 41 | 0O | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 41 | W8 | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 41 | R4 | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 41 | U4 | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 41 | D1 | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 41 | Q4 | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 41 | F8 | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 41 | 0I | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 41 | S5 | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | V2 | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 41 | J4 | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 41 | T8 | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 41 | 1T | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 41 | J6 | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 41 | G1 | 501 | GTP | C8-N7-C5 | 3.62 | 108.70 | 102.55 |
| 41 | P8 | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 41 | 1L | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 41 | 1H | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 41 | 3P | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 41 | F3 | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 41 | S8 | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 41 | M4 | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 41 | 3 | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 41 | Q6 | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 41 | 3A | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 41 | G7 | 501 | GTP | C8-N7-C5 | 3.60 | 108.69 | 102.55 |
| 41 | O2 | 501 | GTP | C8-N7-C5 | 3.60 | 108.69 | 102.55 |
| 41 | Q2 | 501 | GTP | C8-N7-C5 | 3.60 | 108.69 | 102.55 |
| 41 | K9 | 501 | GTP | C8-N7-C5 | 3.60 | 108.68 | 102.55 |
| 41 | 8 | 501 | GTP | C8-N7-C5 | 3.60 | 108.67 | 102.55 |
| 41 | N3 | 501 | GTP | C8-N7-C5 | 3.60 | 108.67 | 102.55 |
| 41 | 0K | 501 | GTP | C8-N7-C5 | 3.60 | 108.67 | 102.55 |
| 41 | P6 | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 41 | Y1 | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 41 | 1D | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 41 | S0 | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 41 | P4 | 501 | GTP | C8-N7-C5 | 3.59 | 108.65 | 102.55 |
| 41 | 0C | 501 | GTP | C8-N7-C5 | 3.59 | 108.65 | 102.55 |
| 41 | D5 | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 41 | I1 | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 41 | 0V | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 41 | 1W | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 41 | B5 | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | G4 | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | 1G | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | K4 | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | U6 | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | H8 | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 41 | 4 | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 41 | A4 | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 41 | T4 | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | U2 | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 41 | G9 | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 41 | A2 | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 41 | K1 | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 41 | 2S | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 41 | 0F | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 41 | 3T | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 41 | O0 | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 41 | R0 | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 41 | R2 | 501 | GTP | C8-N7-C5 | 3.56 | 108.60 | 102.55 |
| 41 | 1N | 501 | GTP | C8-N7-C5 | 3.55 | 108.60 | 102.55 |
| 41 | 7 | 501 | GTP | C8-N7-C5 | 3.55 | 108.60 | 102.55 |
| 41 | H3 | 501 | GTP | C8-N7-C5 | 3.55 | 108.60 | 102.55 |
| 41 | D7 | 501 | GTP | C8-N7-C5 | 3.55 | 108.60 | 102.55 |
| 41 | Y0 | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 41 | Y4 | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 41 | 0Y | 501 | GTP | C8-N7-C5 | 3.55 | 108.58 | 102.55 |
| 41 | I0 | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 41 | I4 | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 41 | N8 | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 41 | G5 | 501 | GTP | C8-N7-C5 | 3.53 | 108.55 | 102.55 |
| 41 | I5 | 501 | GTP | C8-N7-C5 | 3.53 | 108.55 | 102.55 |
| 41 | S2 | 501 | GTP | C8-N7-C5 | 3.52 | 108.54 | 102.55 |
| 41 | N1 | 501 | GTP | C8-N7-C5 | 3.52 | 108.54 | 102.55 |
| 41 | 1A | 501 | GTP | C8-N7-C5 | 3.52 | 108.54 | 102.55 |
| 41 | H6 | 501 | GTP | C8-N7-C5 | 3.51 | 108.53 | 102.55 |
| 41 | U7 | 501 | GTP | C8-N7-C5 | 3.50 | 108.51 | 102.55 |
| 41 | E4 | 501 | GTP | C8-N7-C5 | 3.50 | 108.50 | 102.55 |
| 41 | Z2 | 501 | GTP | C8-N7-C5 | 3.50 | 108.50 | 102.55 |
| 41 | U9 | 501 | GTP | C8-N7-C5 | 3.48 | 108.47 | 102.55 |
| 41 | L7 | 501 | GTP | C8-N7-C5 | 3.47 | 108.46 | 102.55 |
| 41 | F0 | 501 | GTP | C8-N7-C5 | 3.47 | 108.45 | 102.55 |
| 41 | H2 | 501 | GTP | C8-N7-C5 | 3.46 | 108.44 | 102.55 |
| 41 | E6 | 501 | GTP | C8-N7-C5 | 3.46 | 108.44 | 102.55 |
| 41 | F5 | 501 | GTP | C8-N7-C5 | 3.46 | 108.44 | 102.55 |
| 41 | 3M | 501 | GTP | C2-N1-C6 | -3.44 | 118.81 | 125.11 |
| 41 | N6 | 501 | GTP | C8-N7-C5 | 3.44 | 108.41 | 102.55 |
| 41 | E1 | 501 | GTP | C8-N7-C5 | 3.44 | 108.40 | 102.55 |
| 41 | Z7 | 501 | GTP | C8-N7-C5 | 3.42 | 108.37 | 102.55 |
| 41 | Z0 | 501 | GTP | C8-N7-C5 | 3.42 | 108.36 | 102.55 |
| 41 | 3C | 501 | GTP | C2-N1-C6 | -3.41 | 118.87 | 125.11 |
| 41 | 3P | 501 | GTP | C2-N1-C6 | -3.41 | 118.88 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | F1 | 501 | GTP | C8-N7-C5 | 3.40 | 108.34 | 102.55 |
| 41 | E8 | 501 | GTP | C8-N7-C5 | 3.40 | 108.33 | 102.55 |
| 41 | 0A | 501 | GTP | C8-N7-C5 | 3.39 | 108.32 | 102.55 |
| 41 | W0 | 501 | GTP | C2-N1-C6 | -3.39 | 118.91 | 125.11 |
| 41 | 3S | 501 | GTP | C2-N1-C6 | -3.38 | 118.92 | 125.11 |
| 41 | 3O | 501 | GTP | C2-N1-C6 | -3.38 | 118.93 | 125.11 |
| 41 | C9 | 501 | GTP | C2-N1-C6 | -3.36 | 118.96 | 125.11 |
| 41 | Z3 | 501 | GTP | C8-N7-C5 | 3.36 | 108.27 | 102.55 |
| 41 | Z6 | 501 | GTP | C8-N7-C5 | 3.35 | 108.25 | 102.55 |
| 41 | 3A | 501 | GTP | C2-N1-C6 | -3.34 | 119.00 | 125.11 |
| 41 | 1Q | 501 | GTP | C2-N1-C6 | -3.32 | 119.03 | 125.11 |
| 41 | 3C | 501 | GTP | C5-C6-N1 | 3.32 | 120.40 | 114.07 |
| 41 | C9 | 501 | GTP | C5-C6-N1 | 3.31 | 120.38 | 114.07 |
| 41 | 3I | 501 | GTP | C2-N1-C6 | -3.31 | 119.06 | 125.11 |
| 41 | W4 | 501 | GTP | C2-N1-C6 | -3.29 | 119.08 | 125.11 |
| 41 | 7 | 501 | GTP | C2-N1-C6 | -3.29 | 119.08 | 125.11 |
| 41 | 3A | 501 | GTP | C5-C6-N1 | 3.29 | 120.35 | 114.07 |
| 41 | 2S | 501 | GTP | C2-N1-C6 | -3.29 | 119.09 | 125.11 |
| 41 | 2Q | 501 | GTP | C2-N1-C6 | -3.29 | 119.09 | 125.11 |
| 41 | 8 | 501 | GTP | C2-N1-C6 | -3.28 | 119.10 | 125.11 |
| 41 | 2Q | 501 | GTP | C5-C6-N1 | 3.28 | 120.33 | 114.07 |
| 41 | J8 | 501 | GTP | C2-N1-C6 | -3.28 | 119.11 | 125.11 |
| 41 | B0 | 501 | GTP | C2-N1-C6 | -3.28 | 119.11 | 125.11 |
| 41 | 3D | 501 | GTP | C2-N1-C6 | -3.28 | 119.11 | 125.11 |
| 41 | 2W | 501 | GTP | C2-N1-C6 | -3.27 | 119.12 | 125.11 |
| 41 | 1T | 501 | GTP | C2-N1-C6 | -3.27 | 119.12 | 125.11 |
| 41 | X4 | 501 | GTP | C8-N7-C5 | 3.27 | 108.11 | 102.55 |
| 41 | 2Y | 501 | GTP | C2-N1-C6 | -3.27 | 119.13 | 125.11 |
| 41 | J0 | 501 | GTP | C2-N1-C6 | -3.26 | 119.15 | 125.11 |
| 41 | E6 | 501 | GTP | C5-C6-N1 | 3.25 | 120.28 | 114.07 |
| 41 | A9 | 501 | GTP | C2-N1-C6 | -3.25 | 119.15 | 125.11 |
| 41 | G1 | 501 | GTP | C5-C6-N1 | 3.25 | 120.28 | 114.07 |
| 41 | T4 | 501 | GTP | C2-N1-C6 | -3.25 | 119.16 | 125.11 |
| 41 | Z3 | 501 | GTP | C5-C6-N1 | 3.25 | 120.27 | 114.07 |
| 41 | S5 | 501 | GTP | C5-C6-N1 | 3.25 | 120.26 | 114.07 |
| 41 | 0F | 501 | GTP | C5-C6-N1 | 3.24 | 120.26 | 114.07 |
| 41 | 2W | 501 | GTP | C5-C6-N1 | 3.24 | 120.25 | 114.07 |
| 41 | L7 | 501 | GTP | C2-N1-C6 | -3.24 | 119.18 | 125.11 |
| 41 | 3T | 501 | GTP | C2-N1-C6 | -3.24 | 119.18 | 125.11 |
| 41 | 3G | 501 | GTP | C2-N1-C6 | -3.24 | 119.18 | 125.11 |
| 41 | W2 | 501 | GTP | C2-N1-C6 | -3.24 | 119.19 | 125.11 |
| 41 | 4 | 501 | GTP | C2-N1-C6 | -3.23 | 119.19 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | 2U | 501 | GTP | C2-N1-C6 | -3.23 | 119.20 | 125.11 |
| 41 | I8 | 501 | GTP | C2-N1-C6 | -3.23 | 119.20 | 125.11 |
| 41 | 1Q | 501 | GTP | C5-C6-N1 | 3.23 | 120.23 | 114.07 |
| 41 | Z2 | 501 | GTP | C5-C6-N1 | 3.23 | 120.23 | 114.07 |
| 41 | C1 | 501 | GTP | C2-N1-C6 | -3.23 | 119.21 | 125.11 |
| 41 | 2S | 501 | GTP | C5-C6-N1 | 3.22 | 120.22 | 114.07 |
| 41 | S8 | 501 | GTP | C2-N1-C6 | -3.22 | 119.21 | 125.11 |
| 41 | W5 | 501 | GTP | C2-N1-C6 | -3.22 | 119.21 | 125.11 |
| 41 | P9 | 501 | GTP | C5-C6-N1 | 3.22 | 120.21 | 114.07 |
| 41 | 1N | 501 | GTP | C5-C6-N1 | 3.22 | 120.21 | 114.07 |
| 41 | T4 | 501 | GTP | C5-C6-N1 | 3.21 | 120.20 | 114.07 |
| 41 | C0 | 501 | GTP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 41 | D1 | 501 | GTP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 41 | S5 | 501 | GTP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 41 | T6 | 501 | GTP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 41 | E1 | 501 | GTP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 41 | D1 | 501 | GTP | C5-C6-N1 | 3.21 | 120.20 | 114.07 |
| 39 | 0M | 502 | GDP | C8-N7-C5 | 3.21 | 108.01 | 102.55 |
| 41 | 3 | 501 | GTP | C2-N1-C6 | -3.21 | 119.24 | 125.11 |
| 39 | 0O | 502 | GDP | C8-N7-C5 | 3.21 | 108.01 | 102.55 |
| 41 | O6 | 501 | GTP | C2-N1-C6 | -3.21 | 119.24 | 125.11 |
| 41 | 1X | 501 | GTP | C2-N1-C6 | -3.20 | 119.25 | 125.11 |
| 41 | 3K | 501 | GTP | C2-N1-C6 | -3.20 | 119.25 | 125.11 |
| 41 | V8 | 501 | GTP | C2-N1-C6 | -3.20 | 119.26 | 125.11 |
| 41 | 1T | 501 | GTP | C5-C6-N1 | 3.20 | 120.17 | 114.07 |
| 41 | C8 | 501 | GTP | C2-N1-C6 | -3.19 | 119.26 | 125.11 |
| 41 | P9 | 501 | GTP | C2-N1-C6 | -3.19 | 119.26 | 125.11 |
| 41 | R4 | 501 | GTP | C2-N1-C6 | -3.19 | 119.26 | 125.11 |
| 41 | T8 | 501 | GTP | C2-N1-C6 | -3.19 | 119.26 | 125.11 |
| 41 | T2 | 501 | GTP | C2-N1-C6 | -3.19 | 119.27 | 125.11 |
| 41 | T6 | 501 | GTP | C5-C6-N1 | 3.19 | 120.15 | 114.07 |
| 41 | 2K | 501 | GTP | C2-N1-C6 | -3.19 | 119.28 | 125.11 |
| 41 | K0 | 501 | GTP | C2-N1-C6 | -3.18 | 119.28 | 125.11 |
| 41 | 3O | 501 | GTP | C5-C6-N1 | 3.18 | 120.15 | 114.07 |
| 41 | Q2 | 501 | GTP | C5-C6-N1 | 3.18 | 120.15 | 114.07 |
| 41 | Q2 | 501 | GTP | C2-N1-C6 | -3.18 | 119.28 | 125.11 |
| 41 | O8 | 501 | GTP | C2-N1-C6 | -3.18 | 119.29 | 125.11 |
| 41 | Q6 | 501 | GTP | C5-C6-N1 | 3.18 | 120.14 | 114.07 |
| 41 | F3 | 501 | GTP | C2-N1-C6 | -3.18 | 119.30 | 125.11 |
| 41 | 1N | 501 | GTP | C2-N1-C6 | -3.18 | 119.30 | 125.11 |
| 41 | L7 | 501 | GTP | C5-C6-N1 | 3.17 | 120.12 | 114.07 |
| 41 | V3 | 501 | GTP | C2-N1-C6 | -3.17 | 119.30 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | 0A | 501 | GTP | C5-C6-N1 | 3.17 | 120.12 | 114.07 |
| 41 | P6 | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | 2I | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | 2C | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | L6 | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | M0 | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | R4 | 501 | GTP | C5-C6-N1 | 3.17 | 120.11 | 114.07 |
| 41 | A1 | 501 | GTP | C2-N1-C6 | -3.17 | 119.31 | 125.11 |
| 41 | 3I | 501 | GTP | C5-C6-N1 | 3.17 | 120.11 | 114.07 |
| 41 | M2 | 501 | GTP | C2-N1-C6 | -3.17 | 119.32 | 125.11 |
| 41 | X0 | 501 | GTP | C2-N1-C6 | -3.16 | 119.32 | 125.11 |
| 41 | E1 | 501 | GTP | C5-C6-N1 | 3.16 | 120.11 | 114.07 |
| 41 | 3P | 501 | GTP | C5-C6-N1 | 3.16 | 120.11 | 114.07 |
| 41 | Q6 | 501 | GTP | C2-N1-C6 | -3.16 | 119.32 | 125.11 |
| 41 | W8 | 501 | GTP | C2-N1-C6 | -3.16 | 119.32 | 125.11 |
| 41 | 1S | 501 | GTP | C2-N1-C6 | -3.16 | 119.32 | 125.11 |
| 41 | J4 | 501 | GTP | C5-C6-N1 | 3.16 | 120.10 | 114.07 |
| 41 | T8 | 501 | GTP | C5-C6-N1 | 3.16 | 120.10 | 114.07 |
| 41 | 2U | 501 | GTP | C5-C6-N1 | 3.16 | 120.09 | 114.07 |
| 41 | K7 | 501 | GTP | C2-N1-C6 | -3.16 | 119.33 | 125.11 |
| 41 | J8 | 501 | GTP | C5-C6-N1 | 3.16 | 120.09 | 114.07 |
| 41 | B0 | 501 | GTP | C5-C6-N1 | 3.15 | 120.09 | 114.07 |
| 41 | G1 | 501 | GTP | C2-N1-C6 | -3.15 | 119.34 | 125.11 |
| 41 | A9 | 501 | GTP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 41 | N8 | 501 | GTP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 41 | P4 | 501 | GTP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 41 | V3 | 501 | GTP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 41 | S8 | 501 | GTP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 41 | J2 | 501 | GTP | C2-N1-C6 | -3.15 | 119.35 | 125.11 |
| 41 | C8 | 501 | GTP | C5-C6-N1 | 3.15 | 120.07 | 114.07 |
| 41 | 4 | 501 | GTP | C5-C6-N1 | 3.15 | 120.07 | 114.07 |
| 41 | N8 | 501 | GTP | C2-N1-C6 | -3.14 | 119.35 | 125.11 |
| 41 | 3M | 501 | GTP | C5-C6-N1 | 3.14 | 120.07 | 114.07 |
| 41 | R2 | 501 | GTP | C5-C6-N1 | 3.14 | 120.07 | 114.07 |
| 41 | 7 | 501 | GTP | C5-C6-N1 | 3.14 | 120.07 | 114.07 |
| 41 | Z6 | 501 | GTP | C2-N1-C6 | -3.14 | 119.36 | 125.11 |
| 41 | M4 | 501 | GTP | C2-N1-C6 | -3.14 | 119.36 | 125.11 |
| 41 | L6 | 501 | GTP | C5-C6-N1 | 3.14 | 120.06 | 114.07 |
| 41 | E8 | 501 | GTP | C2-N1-C6 | -3.14 | 119.37 | 125.11 |
| 41 | M6 | 501 | GTP | C2-N1-C6 | -3.14 | 119.37 | 125.11 |
| 41 | P6 | 501 | GTP | C5-C6-N1 | 3.14 | 120.06 | 114.07 |
| 41 | O4 | 501 | GTP | C2-N1-C6 | -3.14 | 119.37 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | C1 | 501 | GTP | C5-C6-N1 | 3.14 | 120.06 | 114.07 |
| 41 | R2 | 501 | GTP | C2-N1-C6 | -3.14 | 119.37 | 125.11 |
| 41 | O9 | 501 | GTP | C5-C6-N1 | 3.14 | 120.05 | 114.07 |
| 41 | O9 | 501 | GTP | C2-N1-C6 | -3.13 | 119.37 | 125.11 |
| 41 | C0 | 501 | GTP | C5-C6-N1 | 3.13 | 120.05 | 114.07 |
| 41 | D7 | 501 | GTP | C2-N1-C6 | -3.13 | 119.38 | 125.11 |
| 41 | Y4 | 501 | GTP | C5-C6-N1 | 3.13 | 120.05 | 114.07 |
| 41 | L4 | 501 | GTP | C2-N1-C6 | -3.13 | 119.38 | 125.11 |
| 41 | 2A | 501 | GTP | C2-N1-C6 | -3.13 | 119.38 | 125.11 |
| 41 | 2N | 501 | GTP | C2-N1-C6 | -3.13 | 119.39 | 125.11 |
| 41 | D5 | 501 | GTP | C2-N1-C6 | -3.13 | 119.39 | 125.11 |
| 41 | G7 | 501 | GTP | C5-C6-N1 | 3.13 | 120.03 | 114.07 |
| 41 | M6 | 501 | GTP | C5-C6-N1 | 3.13 | 120.03 | 114.07 |
| 41 | 1X | 501 | GTP | C5-C6-N1 | 3.13 | 120.03 | 114.07 |
| 41 | T2 | 501 | GTP | C5-C6-N1 | 3.13 | 120.03 | 114.07 |
| 41 | 2L | 501 | GTP | C2-N1-C6 | -3.12 | 119.39 | 125.11 |
| 41 | J4 | 501 | GTP | C2-N1-C6 | -3.12 | 119.40 | 125.11 |
| 41 | 1L | 501 | GTP | C2-N1-C6 | -3.12 | 119.40 | 125.11 |
| 41 | J6 | 501 | GTP | C5-C6-N1 | 3.12 | 120.02 | 114.07 |
| 41 | E8 | 501 | GTP | C5-C6-N1 | 3.12 | 120.02 | 114.07 |
| 41 | O2 | 501 | GTP | C5-C6-N1 | 3.12 | 120.02 | 114.07 |
| 41 | R0 | 501 | GTP | C2-N1-C6 | -3.12 | 119.41 | 125.11 |
| 41 | R8 | 501 | GTP | C5-C6-N1 | 3.12 | 120.02 | 114.07 |
| 41 | L2 | 501 | GTP | C2-N1-C6 | -3.12 | 119.41 | 125.11 |
| 41 | N6 | 501 | GTP | C2-N1-C6 | -3.11 | 119.41 | 125.11 |
| 41 | R6 | 501 | GTP | C5-C6-N1 | 3.11 | 120.01 | 114.07 |
| 41 | 8 | 501 | GTP | C5-C6-N1 | 3.11 | 120.01 | 114.07 |
| 41 | K1 | 501 | GTP | C5-C6-N1 | 3.11 | 120.01 | 114.07 |
| 41 | J6 | 501 | GTP | C2-N1-C6 | -3.11 | 119.42 | 125.11 |
| 41 | N1 | 501 | GTP | C5-C6-N1 | 3.11 | 120.00 | 114.07 |
| 41 | N1 | 501 | GTP | C2-N1-C6 | -3.11 | 119.42 | 125.11 |
| 41 | L4 | 501 | GTP | C5-C6-N1 | 3.11 | 120.00 | 114.07 |
| 41 | H2 | 501 | GTP | C2-N1-C6 | -3.11 | 119.42 | 125.11 |
| 41 | Y4 | 501 | GTP | C2-N1-C6 | -3.11 | 119.42 | 125.11 |
| 41 | 3S | 501 | GTP | C5-C6-N1 | 3.10 | 119.99 | 114.07 |
| 41 | I8 | 501 | GTP | C5-C6-N1 | 3.10 | 119.99 | 114.07 |
| 41 | J0 | 501 | GTP | C5-C6-N1 | 3.10 | 119.99 | 114.07 |
| 41 | R8 | 501 | GTP | C2-N1-C6 | -3.10 | 119.44 | 125.11 |
| 41 | S0 | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 41 | M0 | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 41 | 0C | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 41 | E6 | 501 | GTP | C2-N1-C6 | -3.10 | 119.44 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | R0 | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 41 | 1L | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 41 | 2Y | 501 | GTP | C5-C6-N1 | 3.09 | 119.97 | 114.07 |
| 41 | 3G | 501 | GTP | C5-C6-N1 | 3.09 | 119.97 | 114.07 |
| 41 | F1 | 501 | GTP | C2-N1-C6 | -3.09 | 119.45 | 125.11 |
| 41 | L2 | 501 | GTP | C5-C6-N1 | 3.09 | 119.97 | 114.07 |
| 41 | P4 | 501 | GTP | C2-N1-C6 | -3.09 | 119.45 | 125.11 |
| 41 | Z6 | 501 | GTP | C5-C6-N1 | 3.09 | 119.97 | 114.07 |
| 41 | O4 | 501 | GTP | C5-C6-N1 | 3.09 | 119.96 | 114.07 |
| 41 | Z7 | 501 | GTP | C5-C6-N1 | 3.09 | 119.96 | 114.07 |
| 41 | D3 | 501 | GTP | C2-N1-C6 | -3.09 | 119.46 | 125.11 |
| 41 | 1W | 501 | GTP | C2-N1-C6 | -3.09 | 119.46 | 125.11 |
| 41 | B5 | 501 | GTP | C2-N1-C6 | -3.08 | 119.46 | 125.11 |
| 41 | U9 | 501 | GTP | C5-C6-N1 | 3.08 | 119.95 | 114.07 |
| 41 | K4 | 501 | GTP | C2-N1-C6 | -3.08 | 119.47 | 125.11 |
| 41 | V2 | 501 | GTP | C5-C6-N1 | 3.08 | 119.95 | 114.07 |
| 41 | 0S | 501 | GTP | C5-C6-N1 | 3.08 | 119.95 | 114.07 |
| 41 | E4 | 501 | GTP | C2-N1-C6 | -3.08 | 119.47 | 125.11 |
| 41 | M7 | 501 | GTP | C2-N1-C6 | -3.08 | 119.47 | 125.11 |
| 41 | M7 | 501 | GTP | C5-C6-N1 | 3.08 | 119.94 | 114.07 |
| 41 | 3D | 501 | GTP | C5-C6-N1 | 3.08 | 119.94 | 114.07 |
| 41 | A2 | 501 | GTP | C2-N1-C6 | -3.08 | 119.48 | 125.11 |
| 41 | F0 | 501 | GTP | C2-N1-C6 | -3.08 | 119.48 | 125.11 |
| 41 | D7 | 501 | GTP | C5-C6-N1 | 3.08 | 119.94 | 114.07 |
| 41 | 2G | 501 | GTP | C2-N1-C6 | -3.07 | 119.48 | 125.11 |
| 41 | Q4 | 501 | GTP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 41 | X0 | 501 | GTP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 41 | 1D | 501 | GTP | C2-N1-C6 | -3.07 | 119.49 | 125.11 |
| 41 | 0Q | 501 | GTP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 41 | G5 | 501 | GTP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 41 | 3T | 501 | GTP | C5-C6-N1 | 3.07 | 119.92 | 114.07 |
| 41 | O2 | 501 | GTP | C2-N1-C6 | -3.07 | 119.49 | 125.11 |
| 41 | U9 | 501 | GTP | C2-N1-C6 | -3.07 | 119.50 | 125.11 |
| 41 | I4 | 501 | GTP | C2-N1-C6 | -3.07 | 119.50 | 125.11 |
| 41 | U2 | 501 | GTP | C2-N1-C6 | -3.07 | 119.50 | 125.11 |
| 41 | H3 | 501 | GTP | C2-N1-C6 | -3.06 | 119.50 | 125.11 |
| 41 | I4 | 501 | GTP | C5-C6-N1 | 3.06 | 119.92 | 114.07 |
| 41 | 3K | 501 | GTP | C5-C6-N1 | 3.06 | 119.92 | 114.07 |
| 41 | Q4 | 501 | GTP | C2-N1-C6 | -3.06 | 119.50 | 125.11 |
| 41 | N0 | 501 | GTP | C2-N1-C6 | -3.06 | 119.50 | 125.11 |
| 41 | K0 | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 41 | 2N | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | V2 | 501 | GTP | C2-N1-C6 | -3.06 | 119.50 | 125.11 |
| 41 | I5 | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 41 | K1 | 501 | GTP | C2-N1-C6 | -3.06 | 119.51 | 125.11 |
| 41 | G7 | 501 | GTP | C2-N1-C6 | -3.06 | 119.51 | 125.11 |
| 41 | A2 | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 41 | F0 | 501 | GTP | C5-C6-N1 | 3.06 | 119.90 | 114.07 |
| 41 | 0A | 501 | GTP | C2-N1-C6 | -3.06 | 119.52 | 125.11 |
| 41 | R6 | 501 | GTP | C2-N1-C6 | -3.05 | 119.52 | 125.11 |
| 41 | B5 | 501 | GTP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 41 | F8 | 501 | GTP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 41 | M2 | 501 | GTP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 41 | F8 | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 41 | X4 | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 39 | O6 | 502 | GDP | C8-N7-C5 | 3.05 | 107.74 | 102.55 |
| 41 | 3 | 501 | GTP | C5-C6-N1 | 3.05 | 119.88 | 114.07 |
| 41 | K6 | 501 | GTP | C5-C6-N1 | 3.05 | 119.88 | 114.07 |
| 41 | Y0 | 501 | GTP | C5-C6-N1 | 3.05 | 119.88 | 114.07 |
| 41 | O6 | 501 | GTP | C5-C6-N1 | 3.05 | 119.88 | 114.07 |
| 41 | I1 | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 41 | H3 | 501 | GTP | C5-C6-N1 | 3.04 | 119.88 | 114.07 |
| 41 | 1S | 501 | GTP | C5-C6-N1 | 3.04 | 119.88 | 114.07 |
| 41 | Z2 | 501 | GTP | C2-N1-C6 | -3.04 | 119.54 | 125.11 |
| 41 | O0 | 501 | GTP | C2-N1-C6 | -3.04 | 119.54 | 125.11 |
| 41 | 2E | 501 | GTP | C2-N1-C6 | -3.04 | 119.54 | 125.11 |
| 41 | 1H | 501 | GTP | C2-N1-C6 | -3.04 | 119.54 | 125.11 |
| 41 | 0Y | 501 | GTP | C2-N1-C6 | -3.04 | 119.54 | 125.11 |
| 41 | 0Q | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | K6 | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | W0 | 501 | GTP | C5-C6-N1 | 3.04 | 119.87 | 114.07 |
| 41 | I5 | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | 2L | 501 | GTP | C5-C6-N1 | 3.04 | 119.86 | 114.07 |
| 41 | 0S | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | P8 | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | 0C | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 41 | H8 | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 41 | S0 | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 41 | X6 | 501 | GTP | C4'-O4'-C1' | -3.03 | 107.15 | 109.92 |
| 41 | P8 | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 41 | N0 | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 41 | X4 | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 41 | D3 | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 41 | 1W | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | H6 | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 41 | H2 | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 41 | M4 | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 41 | J2 | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 41 | A1 | 501 | GTP | C5-C6-N1 | 3.03 | 119.84 | 114.07 |
| 41 | O0 | 501 | GTP | C5-C6-N1 | 3.03 | 119.84 | 114.07 |
| 41 | U4 | 501 | GTP | C2-N1-C6 | -3.02 | 119.57 | 125.11 |
| 41 | F1 | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 41 | 2K | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 41 | E4 | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 41 | Y1 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | 0F | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 41 | K7 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | K9 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | H8 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | C5 | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 41 | U6 | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 41 | F3 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | 0M | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | W2 | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 41 | U7 | 501 | GTP | C2-N1-C6 | -3.02 | 119.59 | 125.11 |
| 41 | O8 | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 41 | 0K | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 41 | U2 | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 39 | O2 | 502 | GDP | C8-N7-C5 | 3.01 | 107.67 | 102.55 |
| 41 | X7 | 501 | GTP | O4'-C1'-N9 | 3.01 | 112.73 | 108.75 |
| 41 | F5 | 501 | GTP | C2-N1-C6 | -3.01 | 119.60 | 125.11 |
| 41 | Z7 | 501 | GTP | C2-N1-C6 | -3.01 | 119.61 | 125.11 |
| 41 | 2I | 501 | GTP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 39 | 0A | 503 | GDP | C8-N7-C5 | 3.00 | 107.67 | 102.55 |
| 41 | I0 | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 41 | Y6 | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 39 | 3A | 502 | GDP | C8-N7-C5 | 3.00 | 107.66 | 102.55 |
| 39 | 0W | 502 | GDP | C8-N7-C5 | 3.00 | 107.66 | 102.55 |
| 41 | D5 | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 41 | 0O | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 39 | 2C | 502 | GDP | C8-N7-C5 | 3.00 | 107.66 | 102.55 |
| 39 | 2G | 502 | GDP | C8-N7-C5 | 3.00 | 107.66 | 102.55 |
| 41 | X6 | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 41 | B7 | 501 | GTP | C2-N1-C6 | -3.00 | 119.62 | 125.11 |
| 39 | O8 | 503 | GDP | C8-N7-C5 | 3.00 | 107.66 | 102.55 |
| 41 | Y6 | 501 | GTP | C2-N1-C6 | -3.00 | 119.62 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | U6 | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 41 | Z3 | 501 | GTP | C2-N1-C6 | -3.00 | 119.62 | 125.11 |
| 39 | 2I | 502 | GDP | C8-N7-C5 | 3.00 | 107.65 | 102.55 |
| 41 | 0O | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 41 | N6 | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 41 | S2 | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 39 | 2E | 502 | GDP | C8-N7-C5 | 2.99 | 107.64 | 102.55 |
| 41 | S2 | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 41 | X6 | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 41 | I0 | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 41 | B2 | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 39 | 2K | 502 | GDP | C8-N7-C5 | 2.99 | 107.64 | 102.55 |
| 41 | 1A | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 41 | 0V | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 41 | F5 | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 41 | I1 | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 39 | B5 | 502 | GDP | C8-N7-C5 | 2.99 | 107.63 | 102.55 |
| 41 | 1A | 501 | GTP | C2-N1-C6 | -2.98 | 119.65 | 125.11 |
| 41 | H6 | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 41 | 2C | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 41 | Y0 | 501 | GTP | C2-N1-C6 | -2.98 | 119.65 | 125.11 |
| 41 | Z0 | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 41 | W5 | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 39 | U8 | 501 | GDP | C8-N7-C5 | 2.98 | 107.62 | 102.55 |
| 41 | 0Y | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 41 | G5 | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 41 | K9 | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 39 | E6 | 502 | GDP | C8-N7-C5 | 2.97 | 107.60 | 102.55 |
| 41 | 2A | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 41 | G0 | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 41 | 0I | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 41 | B2 | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 39 | V6 | 501 | GDP | C8-N7-C5 | 2.96 | 107.58 | 102.55 |
| 41 | W8 | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 41 | X7 | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 41 | X7 | 501 | GTP | C2-N1-C6 | -2.96 | 119.70 | 125.11 |
| 39 | 9 | 501 | GDP | C8-N7-C5 | 2.96 | 107.58 | 102.55 |
| 41 | U4 | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 39 | L2 | 502 | GDP | C8-N7-C5 | 2.95 | 107.58 | 102.55 |
| 39 | 2M | 501 | GDP | C8-N7-C5 | 2.95 | 107.58 | 102.55 |
| 41 | W4 | 501 | GTP | C5-C6-N1 | 2.95 | 119.71 | 114.07 |
| 41 | 2G | 501 | GTP | C5-C6-N1 | 2.95 | 119.71 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | V8 | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 41 | U7 | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 41 | G4 | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 39 | A3 | 501 | GDP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 39 | 1A | 503 | GDP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 39 | 1E | 501 | GDP | C8-N7-C5 | 2.94 | 107.56 | 102.55 |
| 41 | C5 | 501 | GTP | C5-C6-N1 | 2.94 | 119.69 | 114.07 |
| 41 | 0V | 501 | GTP | C5-C6-N1 | 2.94 | 119.69 | 114.07 |
| 41 | B7 | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 39 | U6 | 502 | GDP | C8-N7-C5 | 2.94 | 107.56 | 102.55 |
| 41 | 1G | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 41 | P9 | 501 | GTP | C4'-O4'-C1' | -2.93 | 107.24 | 109.92 |
| 41 | G9 | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 39 | W4 | 502 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 39 | V4 | 501 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 41 | Y1 | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 41 | G4 | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 41 | A4 | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 41 | 1C | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 39 | V2 | 503 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 41 | 1D | 501 | GTP | C5-C6-N1 | 2.93 | 119.65 | 114.07 |
| 39 | 2A | 502 | GDP | C8-N7-C5 | 2.92 | 107.53 | 102.55 |
| 41 | G9 | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 41 | G0 | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 41 | 0K | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 39 | D8 | 501 | GDP | C8-N7-C5 | 2.92 | 107.51 | 102.55 |
| 39 | J8 | 502 | GDP | C8-N7-C5 | 2.92 | 107.51 | 102.55 |
| 39 | 7 | 502 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 41 | 1H | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 39 | F8 | 502 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 39 | W6 | 501 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 41 | K4 | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 41 | 2E | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 39 | N2 | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 39 | G2 | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 39 | 2Y | 502 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 39 | W2 | 503 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 39 | P8 | 502 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 41 | A2 | 501 | GTP | O2B-PB-O3A | 2.90 | 115.12 | 107.27 |
| 39 | K6 | 502 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 39 | H8 | 503 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 39 | 2W | 502 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | G8 | 501 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 39 | N6 | 503 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 41 | 1C | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 39 | O4 | 502 | GDP | C8-N7-C5 | 2.89 | 107.48 | 102.55 |
| 39 | T2 | 502 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 39 | 2 | 501 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 41 | 0I | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 39 | 5 | 501 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 39 | C0 | 502 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 39 | V8 | 502 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 39 | I8 | 502 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 39 | S8 | 502 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 41 | N3 | 501 | GTP | C5-C6-N1 | 2.89 | 119.58 | 114.07 |
| 39 | B8 | 501 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 39 | Q0 | 501 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 39 | 2S | 502 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 39 | H4 | 501 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 39 | 1W | 502 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 39 | I0 | 502 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 39 | L0 | 501 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 39 | 3C | 502 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 39 | C6 | 501 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 39 | R2 | 502 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 39 | K8 | 501 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 39 | R8 | 502 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | 0S | 502 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | P4 | 503 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | G6 | 501 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | 0I | 502 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 41 | Z0 | 501 | GTP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 39 | H2 | 503 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | R6 | 503 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | V0 | 501 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 39 | 3I | 502 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 41 | A4 | 501 | GTP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 39 | 1M | 501 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | M6 | 502 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | M8 | 501 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | P6 | 503 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | M0 | 502 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | W0 | 502 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 39 | A7 | 501 | GDP | C8-N7-C5 | 2.86 | 107.43 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | J4 | 503 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 39 | C4 | 501 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 39 | 1U | 501 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 39 | K0 | 502 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 39 | W8 | 503 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 39 | K4 | 502 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 39 | 3O | 502 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 41 | 1G | 501 | GTP | C5-C6-N1 | 2.86 | 119.52 | 114.07 |
| 39 | X0 | 502 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 39 | 2U | 502 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 41 | N3 | 501 | GTP | C2-N1-C6 | -2.85 | 119.89 | 125.11 |
| 39 | B3 | 501 | GDP | C8-N7-C5 | 2.85 | 107.41 | 102.55 |
| 39 | X2 | 501 | GDP | C8-N7-C5 | 2.85 | 107.41 | 102.55 |
| 39 | H6 | 502 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 39 | 1G | 502 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 39 | Y2 | 501 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 39 | 1C | 502 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 39 | J6 | 502 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 39 | R4 | 502 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 39 | C2 | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | B1 | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | J0 | 502 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | I2 | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | 1O | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | R0 | 502 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 39 | A1 | 502 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 41 | 0M | 501 | GTP | C2-N1-C6 | -2.83 | 119.93 | 125.11 |
| 39 | 0U | 501 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 39 | Q8 | 501 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 39 | X6 | 502 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 39 | 0Q | 502 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 39 | Y8 | 501 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 39 | S0 | 502 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 39 | Y4 | 502 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 39 | N0 | 502 | GDP | C8-N7-C5 | 2.82 | 107.36 | 102.55 |
| 39 | D2 | 501 | GDP | C8-N7-C5 | 2.82 | 107.36 | 102.55 |
| 39 | J2 | 502 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 39 | 0C | 502 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 39 | 3M | 502 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 39 | L4 | 502 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 39 | U2 | 502 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 39 | Q6 | 502 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | 1K | 501 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 39 | Q2 | 502 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 39 | U4 | 502 | GDP | C8-N7-C5 | 2.81 | 107.34 | 102.55 |
| 39 | G4 | 502 | GDP | C8-N7-C5 | 2.81 | 107.34 | 102.55 |
| 39 | 0E | 501 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 39 | Q4 | 502 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 39 | Y6 | 502 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 39 | S6 | 501 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 39 | 3S | 502 | GDP | C8-N7-C5 | 2.79 | 107.31 | 102.55 |
| 39 | C8 | 502 | GDP | C8-N7-C5 | 2.79 | 107.31 | 102.55 |
| 39 | 0Y | 502 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | S2 | 502 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | L6 | 502 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | 3K | 503 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | A5 | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | D0 | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 39 | E4 | 502 | GDP | C8-N7-C5 | 2.79 | 107.29 | 102.55 |
| 39 | F6 | 501 | GDP | C8-N7-C5 | 2.78 | 107.29 | 102.55 |
| 39 | F0 | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 39 | 0G | 501 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 39 | 3 | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 39 | 2Q | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 39 | E2 | 501 | GDP | C8-N7-C5 | 2.78 | 107.27 | 102.55 |
| 39 | G0 | 502 | GDP | C8-N7-C5 | 2.77 | 107.27 | 102.55 |
| 39 | M2 | 502 | GDP | C8-N7-C5 | 2.77 | 107.27 | 102.55 |
| 39 | N8 | 502 | GDP | C8-N7-C5 | 2.77 | 107.27 | 102.55 |
| 39 | 1Q | 502 | GDP | C8-N7-C5 | 2.77 | 107.27 | 102.55 |
| 39 | S4 | 501 | GDP | C8-N7-C5 | 2.77 | 107.26 | 102.55 |
| 39 | X8 | 501 | GDP | C8-N7-C5 | 2.77 | 107.26 | 102.55 |
| 39 | Z0 | 502 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 39 | M4 | 502 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 39 | 1S | 502 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 39 | D4 | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 39 | T4 | 502 | GDP | C8-N7-C5 | 2.76 | 107.24 | 102.55 |
| 39 | Z2 | 503 | GDP | C8-N7-C5 | 2.76 | 107.24 | 102.55 |
| 39 | 3G | 502 | GDP | C8-N7-C5 | 2.76 | 107.24 | 102.55 |
| 41 | X6 | 501 | GTP | O4'-C1'-N9 | 2.75 | 112.40 | 108.75 |
| 39 | T6 | 502 | GDP | C8-N7-C5 | 2.75 | 107.23 | 102.55 |
| 39 | 3Q | 501 | GDP | C8-N7-C5 | 2.75 | 107.23 | 102.55 |
| 39 | T0 | 501 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 39 | I4 | 502 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 39 | O0 | 503 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | 0K | 502 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 39 | X4 | 502 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 39 | F2 | 501 | GDP | C8-N7-C5 | 2.73 | 107.20 | 102.55 |
| 39 | Z4 | 501 | GDP | C8-N7-C5 | 2.73 | 107.19 | 102.55 |
| 39 | Y0 | 502 | GDP | C8-N7-C5 | 2.72 | 107.17 | 102.55 |
| 39 | D6 | 501 | GDP | C8-N7-C5 | 2.71 | 107.17 | 102.55 |
| 39 | Z8 | 501 | GDP | C8-N7-C5 | 2.71 | 107.17 | 102.55 |
| 39 | A9 | 502 | GDP | C8-N7-C5 | 2.71 | 107.16 | 102.55 |
| 39 | E8 | 502 | GDP | C8-N7-C5 | 2.70 | 107.15 | 102.55 |
| 39 | T8 | 502 | GDP | C8-N7-C5 | 2.69 | 107.12 | 102.55 |
| 41 | X4 | 501 | GTP | C4'-O4'-C1' | -2.68 | 107.47 | 109.92 |
| 39 | Z6 | 502 | GDP | C8-N7-C5 | 2.68 | 107.10 | 102.55 |
| 41 | Y1 | 501 | GTP | O4'-C1'-N9 | 2.66 | 112.28 | 108.75 |
| 41 | Z3 | 501 | GTP | O6-C6-C5 | -2.62 | 119.12 | 124.32 |
| 39 | E0 | 501 | GDP | C8-N7-C5 | 2.61 | 106.99 | 102.55 |
| 39 | D4 | 501 | GDP | C4'-O4'-C1' | -2.61 | 107.54 | 109.92 |
| 41 | O2 | 501 | GTP | O4'-C1'-N9 | 2.59 | 112.18 | 108.75 |
| 41 | D1 | 501 | GTP | C4'-O4'-C1' | -2.58 | 107.56 | 109.92 |
| 41 | 0A | 501 | GTP | O6-C6-C5 | -2.57 | 119.22 | 124.32 |
| 41 | Z0 | 501 | GTP | O6-C6-C5 | -2.56 | 119.24 | 124.32 |
| 41 | Z7 | 501 | GTP | O6-C6-C5 | -2.53 | 119.31 | 124.32 |
| 39 | B8 | 501 | GDP | C4'-O4'-C1' | -2.51 | 107.63 | 109.92 |
| 41 | Q4 | 501 | GTP | C4'-O4'-C1' | -2.51 | 107.63 | 109.92 |
| 41 | D1 | 501 | GTP | O4'-C1'-N9 | 2.50 | 112.06 | 108.75 |
| 39 | C4 | 501 | GDP | O4'-C1'-N9 | 2.50 | 112.06 | 108.75 |
| 39 | Q8 | 501 | GDP | C4'-O4'-C1' | -2.49 | 107.64 | 109.92 |
| 39 | 2Q | 502 | GDP | C5-C6-N1 | 2.47 | 118.79 | 114.07 |
| 41 | 3P | 501 | GTP | C4'-O4'-C1' | -2.46 | 107.67 | 109.92 |
| 41 | Z6 | 501 | GTP | O6-C6-C5 | -2.46 | 119.45 | 124.32 |
| 41 | R4 | 501 | GTP | O6-C6-C5 | -2.45 | 119.46 | 124.32 |
| 41 | V3 | 501 | GTP | O6-C6-C5 | -2.45 | 119.47 | 124.32 |
| 41 | 1Q | 501 | GTP | O6-C6-C5 | -2.45 | 119.47 | 124.32 |
| 39 | D0 | 501 | GDP | C4'-O4'-C1' | -2.45 | 107.68 | 109.92 |
| 41 | O2 | 501 | GTP | C4'-O4'-C1' | -2.44 | 107.69 | 109.92 |
| 41 | 2Q | 501 | GTP | O6-C6-C5 | -2.42 | 119.52 | 124.32 |
| 41 | M6 | 501 | GTP | O6-C6-C5 | -2.39 | 119.58 | 124.32 |
| 41 | N1 | 501 | GTP | O6-C6-C5 | -2.39 | 119.59 | 124.32 |
| 39 | 2S | 502 | GDP | C5-C6-N1 | 2.38 | 118.61 | 114.07 |
| 41 | G5 | 501 | GTP | O6-C6-C5 | -2.38 | 119.61 | 124.32 |
| 41 | R6 | 501 | GTP | C4'-O4'-C1' | -2.37 | 107.75 | 109.92 |
| 41 | I0 | 501 | GTP | O6-C6-C5 | -2.37 | 119.62 | 124.32 |
| 41 | G4 | 501 | GTP | O6-C6-C5 | -2.37 | 119.63 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | 0M | 501 | GTP | O6-C6-C5 | -2.37 | 119.63 | 124.32 |
| 41 | U7 | 501 | GTP | O6-C6-C5 | -2.37 | 119.63 | 124.32 |
| 41 | H8 | 501 | GTP | O6-C6-C5 | -2.36 | 119.64 | 124.32 |
| 39 | 2W | 502 | GDP | C5-C6-N1 | 2.36 | 118.58 | 114.07 |
| 41 | F0 | 501 | GTP | O6-C6-C5 | -2.36 | 119.64 | 124.32 |
| 41 | I1 | 501 | GTP | O6-C6-C5 | -2.36 | 119.64 | 124.32 |
| 41 | 2S | 501 | GTP | O6-C6-C5 | -2.36 | 119.65 | 124.32 |
| 39 | 2W | 502 | GDP | O2A-PA-O3A | 2.35 | 113.64 | 107.27 |
| 39 | 3I | 502 | GDP | C5-C6-N1 | 2.35 | 118.56 | 114.07 |
| 41 | R2 | 501 | GTP | O6-C6-C5 | -2.35 | 119.66 | 124.32 |
| 39 | F2 | 501 | GDP | C5-C6-N1 | 2.35 | 118.55 | 114.07 |
| 41 | 8 | 501 | GTP | O6-C6-C5 | -2.35 | 119.67 | 124.32 |
| 41 | 3P | 501 | GTP | O4'-C1'-N9 | 2.34 | 111.85 | 108.75 |
| 39 | 2U | 502 | GDP | C5-C6-N1 | 2.34 | 118.54 | 114.07 |
| 41 | H6 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | P6 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | R8 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | I4 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | S5 | 501 | GTP | C4'-O4'-C1' | -2.34 | 107.78 | 109.92 |
| 41 | T6 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | L7 | 501 | GTP | O6-C6-C5 | -2.34 | 119.68 | 124.32 |
| 41 | R0 | 501 | GTP | O6-C6-C5 | -2.34 | 119.69 | 124.32 |
| 41 | G1 | 501 | GTP | O6-C6-C5 | -2.34 | 119.69 | 124.32 |
| 41 | P4 | 501 | GTP | O6-C6-C5 | -2.33 | 119.69 | 124.32 |
| 39 | R8 | 502 | GDP | C5-C6-N1 | 2.33 | 118.52 | 114.07 |
| 41 | 1A | 501 | GTP | O6-C6-C5 | -2.33 | 119.70 | 124.32 |
| 41 | 0K | 501 | GTP | O6-C6-C5 | -2.33 | 119.70 | 124.32 |
| 39 | A3 | 501 | GDP | O3B-PB-O3A | 2.32 | 112.43 | 104.64 |
| 41 | P8 | 501 | GTP | O6-C6-C5 | -2.32 | 119.72 | 124.32 |
| 41 | F1 | 501 | GTP | O6-C6-C5 | -2.32 | 119.73 | 124.32 |
| 41 | Q4 | 501 | GTP | O6-C6-C5 | -2.32 | 119.73 | 124.32 |
| 41 | 3A | 501 | GTP | O6-C6-C5 | -2.32 | 119.73 | 124.32 |
| 41 | S0 | 501 | GTP | O6-C6-C5 | -2.31 | 119.73 | 124.32 |
| 39 | O8 | 503 | GDP | O4'-C1'-N9 | 2.31 | 111.81 | 108.75 |
| 41 | E1 | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 41 | 1S | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 39 | R6 | 503 | GDP | C4'-O4'-C1' | -2.31 | 107.81 | 109.92 |
| 41 | 3 | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 39 | M6 | 502 | GDP | O2A-PA-O3A | 2.31 | 113.51 | 107.27 |
| 41 | Q2 | 501 | GTP | O6-C6-C5 | -2.31 | 119.75 | 124.32 |
| 39 | B8 | 501 | GDP | O4'-C1'-N9 | 2.31 | 111.80 | 108.75 |
| 41 | K9 | 501 | GTP | O6-C6-C5 | -2.30 | 119.75 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | S5 | 501 | GTP | O6-C6-C5 | -2.30 | 119.75 | 124.32 |
| 41 | P9 | 501 | GTP | O6-C6-C5 | -2.30 | 119.76 | 124.32 |
| 41 | G7 | 501 | GTP | O6-C6-C5 | -2.30 | 119.76 | 124.32 |
| 41 | H2 | 501 | GTP | O6-C6-C5 | -2.30 | 119.76 | 124.32 |
| 39 | 3A | 502 | GDP | C5-C6-N1 | 2.30 | 118.45 | 114.07 |
| 39 | Q6 | 502 | GDP | C5-C6-N1 | 2.30 | 118.45 | 114.07 |
| 39 | T6 | 502 | GDP | C5-C6-N1 | 2.29 | 118.45 | 114.07 |
| 41 | T8 | 501 | GTP | O6-C6-C5 | -2.29 | 119.77 | 124.32 |
| 39 | T4 | 502 | GDP | C5-C6-N1 | 2.29 | 118.45 | 114.07 |
| 41 | T4 | 501 | GTP | O6-C6-C5 | -2.29 | 119.78 | 124.32 |
| 41 | 7 | 501 | GTP | O6-C6-C5 | -2.28 | 119.80 | 124.32 |
| 39 | 0U | 501 | GDP | C5-C6-N1 | 2.28 | 118.42 | 114.07 |
| 39 | W4 | 502 | GDP | O4'-C1'-N9 | 2.28 | 111.77 | 108.75 |
| 39 | R6 | 503 | GDP | C5-C6-N1 | 2.28 | 118.41 | 114.07 |
| 39 | R4 | 502 | GDP | C5-C6-N1 | 2.28 | 118.41 | 114.07 |
| 41 | N0 | 501 | GTP | O6-C6-C5 | -2.28 | 119.81 | 124.32 |
| 41 | V2 | 501 | GTP | O6-C6-C5 | -2.27 | 119.81 | 124.32 |
| 41 | 0C | 501 | GTP | O6-C6-C5 | -2.27 | 119.81 | 124.32 |
| 39 | L0 | 501 | GDP | C5-C6-N1 | 2.27 | 118.41 | 114.07 |
| 41 | S8 | 501 | GTP | O6-C6-C5 | -2.27 | 119.82 | 124.32 |
| 39 | S2 | 502 | GDP | C5-C6-N1 | 2.27 | 118.40 | 114.07 |
| 41 | F5 | 501 | GTP | O6-C6-C5 | -2.27 | 119.82 | 124.32 |
| 39 | L6 | 502 | GDP | C5-C6-N1 | 2.27 | 118.39 | 114.07 |
| 41 | 4 | 501 | GTP | O6-C6-C5 | -2.26 | 119.84 | 124.32 |
| 39 | E0 | 501 | GDP | C5-C6-N1 | 2.26 | 118.38 | 114.07 |
| 41 | S2 | 501 | GTP | O6-C6-C5 | -2.26 | 119.84 | 124.32 |
| 41 | 1W | 501 | GTP | O6-C6-C5 | -2.26 | 119.84 | 124.32 |
| 41 | Z2 | 501 | GTP | O6-C6-C5 | -2.26 | 119.84 | 124.32 |
| 39 | 2W | 502 | GDP | O3B-PB-O3A | 2.26 | 112.20 | 104.64 |
| 41 | 0O | 501 | GTP | O6-C6-C5 | -2.26 | 119.85 | 124.32 |
| 39 | 2U | 502 | GDP | O3B-PB-O3A | 2.25 | 112.20 | 104.64 |
| 41 | A2 | 501 | GTP | O6-C6-C5 | -2.25 | 119.85 | 124.32 |
| 39 | P4 | 503 | GDP | C5-C6-N1 | 2.25 | 118.37 | 114.07 |
| 39 | 0O | 502 | GDP | O2A-PA-O3A | 2.25 | 113.36 | 107.27 |
| 39 | 2Q | 502 | GDP | O3B-PB-O3A | 2.25 | 112.18 | 104.64 |
| 39 | Q0 | 501 | GDP | C5-C6-N1 | 2.25 | 118.36 | 114.07 |
| 39 | F6 | 501 | GDP | C5-C6-N1 | 2.25 | 118.36 | 114.07 |
| 41 | 2W | 501 | GTP | O6-C6-C5 | -2.25 | 119.87 | 124.32 |
| 41 | 0Q | 501 | GTP | O6-C6-C5 | -2.25 | 119.87 | 124.32 |
| 41 | B5 | 501 | GTP | O6-C6-C5 | -2.24 | 119.87 | 124.32 |
| 39 | G0 | 502 | GDP | C5-C6-N1 | 2.24 | 118.35 | 114.07 |
| 39 | 2A | 502 | GDP | C5-C6-N1 | 2.24 | 118.35 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | 3C | 502 | GDP | C5-C6-N1 | 2.24 | 118.35 | 114.07 |
| 39 | S6 | 501 | GDP | C5-C6-N1 | 2.24 | 118.35 | 114.07 |
| 41 | N8 | 501 | GTP | O6-C6-C5 | -2.24 | 119.89 | 124.32 |
| 39 | G2 | 501 | GDP | C5-C6-N1 | 2.24 | 118.34 | 114.07 |
| 39 | P8 | 502 | GDP | O2A-PA-O3A | 2.24 | 113.32 | 107.27 |
| 41 | J4 | 501 | GTP | O6-C6-C5 | -2.23 | 119.89 | 124.32 |
| 39 | 5 | 501 | GDP | C5-C6-N1 | 2.23 | 118.33 | 114.07 |
| 39 | F0 | 502 | GDP | C5-C6-N1 | 2.23 | 118.33 | 114.07 |
| 39 | 2I | 502 | GDP | C5-C6-N1 | 2.23 | 118.33 | 114.07 |
| 39 | O0 | 503 | GDP | C5-C6-N1 | 2.23 | 118.32 | 114.07 |
| 39 | 2Q | 502 | GDP | O2A-PA-O3A | 2.23 | 113.30 | 107.27 |
| 39 | Y6 | 502 | GDP | C5-C6-N1 | 2.23 | 118.32 | 114.07 |
| 41 | 0I | 501 | GTP | O6-C6-C5 | -2.23 | 119.91 | 124.32 |
| 39 | 2G | 502 | GDP | C5-C6-N1 | 2.23 | 118.32 | 114.07 |
| 39 | S0 | 502 | GDP | O3B-PB-O3A | 2.23 | 112.10 | 104.64 |
| 41 | U6 | 501 | GTP | O6-C6-C5 | -2.22 | 119.91 | 124.32 |
| 41 | 1D | 501 | GTP | O6-C6-C5 | -2.22 | 119.91 | 124.32 |
| 41 | M4 | 501 | GTP | O6-C6-C5 | -2.22 | 119.91 | 124.32 |
| 41 | H3 | 501 | GTP | O6-C6-C5 | -2.22 | 119.92 | 124.32 |
| 39 | S0 | 502 | GDP | C5-C6-N1 | 2.22 | 118.30 | 114.07 |
| 41 | G0 | 501 | GTP | O6-C6-C5 | -2.22 | 119.92 | 124.32 |
| 41 | 3C | 501 | GTP | O6-C6-C5 | -2.22 | 119.92 | 124.32 |
| 39 | D2 | 501 | GDP | C5-C6-N1 | 2.22 | 118.30 | 114.07 |
| 41 | O0 | 501 | GTP | O6-C6-C5 | -2.22 | 119.92 | 124.32 |
| 41 | 1X | 501 | GTP | O6-C6-C5 | -2.22 | 119.93 | 124.32 |
| 41 | L2 | 501 | GTP | O6-C6-C5 | -2.21 | 119.93 | 124.32 |
| 41 | U2 | 501 | GTP | O6-C6-C5 | -2.21 | 119.93 | 124.32 |
| 39 | K0 | 502 | GDP | O3B-PB-O3A | 2.21 | 112.06 | 104.64 |
| 39 | 1M | 501 | GDP | C5-C6-N1 | 2.21 | 118.29 | 114.07 |
| 41 | A9 | 501 | GTP | O6-C6-C5 | -2.21 | 119.94 | 124.32 |
| 39 | H2 | 503 | GDP | C5-C6-N1 | 2.21 | 118.29 | 114.07 |
| 39 | Q2 | 502 | GDP | C5-C6-N1 | 2.21 | 118.29 | 114.07 |
| 39 | P6 | 503 | GDP | C5-C6-N1 | 2.21 | 118.28 | 114.07 |
| 41 | B0 | 501 | GTP | O6-C6-C5 | -2.21 | 119.94 | 124.32 |
| 39 | 0W | 502 | GDP | C5-C6-N1 | 2.21 | 118.28 | 114.07 |
| 39 | 2C | 502 | GDP | C5-C6-N1 | 2.21 | 118.28 | 114.07 |
| 41 | I5 | 501 | GTP | O6-C6-C5 | -2.21 | 119.95 | 124.32 |
| 41 | T2 | 501 | GTP | O6-C6-C5 | -2.21 | 119.95 | 124.32 |
| 39 | 2Y | 502 | GDP | C5-C6-N1 | 2.20 | 118.28 | 114.07 |
| 39 | Q8 | 501 | GDP | C5-C6-N1 | 2.20 | 118.27 | 114.07 |
| 41 | 1L | 501 | GTP | O6-C6-C5 | -2.20 | 119.96 | 124.32 |
| 41 | 1T | 501 | GTP | O6-C6-C5 | -2.20 | 119.96 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | V6 | 501 | GDP | C5-C6-N1 | 2.20 | 118.27 | 114.07 |
| 41 | 3G | 501 | GTP | O6-C6-C5 | -2.20 | 119.96 | 124.32 |
| 41 | M2 | 501 | GTP | O6-C6-C5 | -2.20 | 119.96 | 124.32 |
| 39 | B8 | 501 | GDP | C5-C6-N1 | 2.20 | 118.26 | 114.07 |
| 39 | C2 | 501 | GDP | C5-C6-N1 | 2.20 | 118.26 | 114.07 |
| 39 | K0 | 502 | GDP | C5-C6-N1 | 2.20 | 118.26 | 114.07 |
| 39 | V4 | 501 | GDP | C5-C6-N1 | 2.20 | 118.26 | 114.07 |
| 39 | 2U | 502 | GDP | O2A-PA-O3A | 2.20 | 113.21 | 107.27 |
| 41 | F8 | 501 | GTP | O6-C6-C5 | -2.20 | 119.97 | 124.32 |
| 41 | U4 | 501 | GTP | O6-C6-C5 | -2.20 | 119.97 | 124.32 |
| 39 | P8 | 502 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | U4 | 502 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | T0 | 501 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | 1K | 501 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | K8 | 501 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | U8 | 501 | GDP | C5-C6-N1 | 2.19 | 118.25 | 114.07 |
| 39 | V0 | 501 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | 3K | 503 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | U6 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | L4 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | Q4 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | V8 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | 2E | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 41 | Y0 | 501 | GTP | O4'-C1'-N9 | 2.19 | 111.64 | 108.75 |
| 39 | J6 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | J8 | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | 1G | 502 | GDP | C5-C6-N1 | 2.19 | 118.24 | 114.07 |
| 39 | 3I | 502 | GDP | O3B-PB-O3A | 2.19 | 111.97 | 104.64 |
| 41 | S5 | 501 | GTP | O4'-C1'-N9 | 2.19 | 111.64 | 108.75 |
| 39 | E2 | 501 | GDP | C5-C6-N1 | 2.18 | 118.24 | 114.07 |
| 39 | G8 | 501 | GDP | C5-C6-N1 | 2.18 | 118.24 | 114.07 |
| 39 | A9 | 502 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | H4 | 501 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | V2 | 503 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | I2 | 501 | GDP | O4'-C1'-N9 | 2.18 | 111.64 | 108.75 |
| 39 | U4 | 502 | GDP | O3B-PB-O3A | 2.18 | 111.95 | 104.64 |
| 39 | 3O | 502 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 41 | U9 | 501 | GTP | O6-C6-C5 | -2.18 | 120.00 | 124.32 |
| 39 | K6 | 502 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | 2K | 502 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | Y2 | 501 | GDP | C5-C6-N1 | 2.18 | 118.23 | 114.07 |
| 39 | 1A | 503 | GDP | C5-C6-N1 | 2.18 | 118.22 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | A1 | 502 | GDP | C5-C6-N1 | 2.18 | 118.22 | 114.07 |
| 39 | J8 | 502 | GDP | O3B-PB-O3A | 2.18 | 111.94 | 104.64 |
| 39 | H8 | 503 | GDP | C5-C6-N1 | 2.18 | 118.22 | 114.07 |
| 39 | R6 | 503 | GDP | O2A-PA-O3A | 2.17 | 113.15 | 107.27 |
| 39 | R2 | 502 | GDP | C5-C6-N1 | 2.17 | 118.22 | 114.07 |
| 41 | W8 | 501 | GTP | O6-C6-C5 | -2.17 | 120.01 | 124.32 |
| 39 | S0 | 502 | GDP | O2A-PA-O3A | 2.17 | 113.14 | 107.27 |
| 41 | C1 | 501 | GTP | O6-C6-C5 | -2.17 | 120.02 | 124.32 |
| 39 | 2 | 501 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | 1E | 501 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | 3M | 502 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | F8 | 502 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | O2 | 502 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | X8 | 501 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 41 | F3 | 501 | GTP | O6-C6-C5 | -2.17 | 120.02 | 124.32 |
| 39 | 0Q | 502 | GDP | C5-C6-N1 | 2.17 | 118.21 | 114.07 |
| 39 | S4 | 501 | GDP | O2A-PA-O3A | 2.17 | 113.14 | 107.27 |
| 39 | M6 | 502 | GDP | O4'-C1'-N9 | 2.17 | 111.62 | 108.75 |
| 39 | T2 | 502 | GDP | C5-C6-N1 | 2.17 | 118.20 | 114.07 |
| 39 | B3 | 501 | GDP | O4'-C1'-N9 | 2.17 | 111.62 | 108.75 |
| 41 | Q2 | 501 | GTP | C4'-O4'-C1' | -2.17 | 107.94 | 109.92 |
| 39 | E4 | 502 | GDP | C5-C6-N1 | 2.16 | 118.20 | 114.07 |
| 39 | 1U | 501 | GDP | C5-C6-N1 | 2.16 | 118.20 | 114.07 |
| 39 | Y4 | 502 | GDP | C5-C6-N1 | 2.16 | 118.19 | 114.07 |
| 39 | S8 | 502 | GDP | C5-C6-N1 | 2.16 | 118.19 | 114.07 |
| 39 | Y0 | 502 | GDP | C5-C6-N1 | 2.16 | 118.19 | 114.07 |
| 41 | Q6 | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 39 | J0 | 502 | GDP | C5-C6-N1 | 2.16 | 118.18 | 114.07 |
| 39 | R6 | 503 | GDP | O3B-PB-O3A | 2.16 | 111.87 | 104.64 |
| 39 | S4 | 501 | GDP | C5-C6-N1 | 2.16 | 118.18 | 114.07 |
| 39 | A7 | 501 | GDP | C5-C6-N1 | 2.16 | 118.18 | 114.07 |
| 39 | R2 | 502 | GDP | O2A-PA-O3A | 2.15 | 113.09 | 107.27 |
| 39 | H6 | 502 | GDP | C5-C6-N1 | 2.15 | 118.18 | 114.07 |
| 41 | K0 | 501 | GTP | O6-C6-C5 | -2.15 | 120.06 | 124.32 |
| 39 | 3G | 502 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 41 | M7 | 501 | GTP | O6-C6-C5 | -2.15 | 120.06 | 124.32 |
| 39 | 3 | 502 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 39 | B1 | 501 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 39 | W0 | 502 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 39 | I2 | 501 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 39 | 0Y | 502 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 41 | D1 | 501 | GTP | O6-C6-C5 | -2.15 | 120.06 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | I0 | 502 | GDP | C5-C6-N1 | 2.15 | 118.16 | 114.07 |
| 39 | I4 | 502 | GDP | C5-C6-N1 | 2.15 | 118.16 | 114.07 |
| 39 | A3 | 501 | GDP | C5-C6-N1 | 2.15 | 118.16 | 114.07 |
| 39 | W4 | 502 | GDP | O3B-PB-O3A | 2.14 | 111.82 | 104.64 |
| 41 | R6 | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 39 | C6 | 501 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 39 | J4 | 503 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 39 | T8 | 502 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 39 | M0 | 502 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 39 | M6 | 502 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 39 | B3 | 501 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 41 | A4 | 501 | GTP | O4'-C1'-N9 | 2.14 | 111.58 | 108.75 |
| 39 | J4 | 503 | GDP | O3B-PB-O3A | 2.14 | 111.80 | 104.64 |
| 39 | 2M | 501 | GDP | C5-C6-N1 | 2.14 | 118.14 | 114.07 |
| 41 | 2G | 501 | GTP | O6-C6-C5 | -2.14 | 120.09 | 124.32 |
| 39 | D0 | 501 | GDP | C5-C6-N1 | 2.13 | 118.14 | 114.07 |
| 41 | C5 | 501 | GTP | O6-C6-C5 | -2.13 | 120.09 | 124.32 |
| 39 | 0E | 501 | GDP | C5-C6-N1 | 2.13 | 118.14 | 114.07 |
| 39 | N2 | 501 | GDP | C5-C6-N1 | 2.13 | 118.14 | 114.07 |
| 39 | 1C | 502 | GDP | C5-C6-N1 | 2.13 | 118.13 | 114.07 |
| 39 | E6 | 502 | GDP | C5-C6-N1 | 2.13 | 118.13 | 114.07 |
| 39 | K4 | 502 | GDP | C5-C6-N1 | 2.13 | 118.13 | 114.07 |
| 39 | N2 | 501 | GDP | O3B-PB-O3A | 2.13 | 111.77 | 104.64 |
| 39 | U2 | 502 | GDP | C5-C6-N1 | 2.13 | 118.13 | 114.07 |
| 39 | O6 | 502 | GDP | C5-C6-N1 | 2.13 | 118.13 | 114.07 |
| 39 | 3Q | 501 | GDP | C5-C6-N1 | 2.13 | 118.12 | 114.07 |
| 41 | 0Y | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 41 | 3T | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 39 | J2 | 502 | GDP | C5-C6-N1 | 2.12 | 118.12 | 114.07 |
| 39 | 3A | 502 | GDP | O3B-PB-O3A | 2.12 | 111.75 | 104.64 |
| 39 | D8 | 501 | GDP | C5-C6-N1 | 2.12 | 118.11 | 114.07 |
| 41 | L4 | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 39 | I8 | 502 | GDP | C5-C6-N1 | 2.12 | 118.11 | 114.07 |
| 41 | J6 | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 39 | Q8 | 501 | GDP | O4'-C1'-N9 | 2.12 | 111.55 | 108.75 |
| 39 | R8 | 502 | GDP | O3B-PB-O3A | 2.12 | 111.73 | 104.64 |
| 39 | 1W | 502 | GDP | C5-C6-N1 | 2.12 | 118.11 | 114.07 |
| 39 | M6 | 502 | GDP | O3B-PB-O3A | 2.12 | 111.73 | 104.64 |
| 39 | C0 | 502 | GDP | C5-C6-N1 | 2.12 | 118.11 | 114.07 |
| 41 | O2 | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 41 | X0 | 501 | GTP | O2G-PG-O3B | 2.11 | 111.72 | 104.64 |
| 39 | D6 | 501 | GDP | C5-C6-N1 | 2.11 | 118.10 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | J0 | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 39 | T4 | 502 | GDP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 39 | G4 | 502 | GDP | C5-C6-N1 | 2.11 | 118.10 | 114.07 |
| 39 | O8 | 503 | GDP | C5-C6-N1 | 2.11 | 118.10 | 114.07 |
| 41 | E4 | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 39 | 2Y | 502 | GDP | O4'-C1'-N9 | 2.11 | 111.54 | 108.75 |
| 41 | M0 | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 39 | 0O | 502 | GDP | O3B-PB-O3A | 2.10 | 111.69 | 104.64 |
| 41 | B2 | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 39 | L2 | 502 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 39 | 3S | 502 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 39 | B5 | 502 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 39 | O4 | 502 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 39 | X2 | 501 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 39 | 0S | 502 | GDP | C2'-C3'-C4' | 2.10 | 106.66 | 102.61 |
| 39 | M8 | 501 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 41 | 2U | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 39 | R0 | 502 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 39 | E8 | 502 | GDP | C5-C6-N1 | 2.09 | 118.06 | 114.07 |
| 39 | N0 | 502 | GDP | C5-C6-N1 | 2.09 | 118.06 | 114.07 |
| 41 | 3P | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 39 | 1A | 503 | GDP | O3B-PB-O3A | 2.09 | 111.64 | 104.64 |
| 39 | 9 | 501 | GDP | C5-C6-N1 | 2.09 | 118.05 | 114.07 |
| 39 | 3C | 502 | GDP | O3B-PB-O3A | 2.09 | 111.64 | 104.64 |
| 39 | Y8 | 501 | GDP | C5-C6-N1 | 2.09 | 118.05 | 114.07 |
| 41 | G9 | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 41 | J2 | 501 | GTP | O6-C6-C5 | -2.09 | 120.19 | 124.32 |
| 41 | 3O | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 41 | 3M | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 39 | Z8 | 501 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 39 | 0G | 501 | GDP | O2A-PA-O3A | 2.08 | 112.90 | 107.27 |
| 39 | 7 | 502 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 39 | 0I | 502 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 41 | 1G | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 39 | Q0 | 501 | GDP | O2A-PA-O3A | 2.08 | 112.89 | 107.27 |
| 39 | M2 | 502 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 41 | N3 | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 41 | K6 | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 39 | K0 | 502 | GDP | O2A-PA-O3A | 2.08 | 112.89 | 107.27 |
| 39 | 0C | 502 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 39 | 1Q | 502 | GDP | O3B-PB-O3A | 2.08 | 111.59 | 104.64 |
| 39 | 1M | 501 | GDP | O3B-PB-O3A | 2.07 | 111.58 | 104.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | W6 | 501 | GDP | O4'-C1'-N9 | 2.07 | 111.49 | 108.75 |
| 41 | A4 | 501 | GTP | C4'-O4'-C1' | -2.07 | 108.03 | 109.92 |
| 39 | W2 | 503 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 41 | K7 | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 39 | G6 | 501 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 39 | X4 | 502 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 39 | X6 | 502 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 41 | 2Y | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 41 | 3S | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 41 | 1N | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 39 | 0U | 501 | GDP | O3B-PB-O3A | 2.06 | 111.56 | 104.64 |
| 41 | I8 | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 41 | W0 | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 39 | 2S | 502 | GDP | O2A-PA-O3A | 2.06 | 112.84 | 107.27 |
| 41 | 0S | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 41 | 2L | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 39 | W6 | 501 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 39 | Q0 | 501 | GDP | O3B-PB-O3A | 2.06 | 111.54 | 104.64 |
| 39 | C8 | 502 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 41 | X4 | 501 | GTP | O4'-C1'-N9 | 2.06 | 111.48 | 108.75 |
| 41 | C0 | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 39 | X4 | 502 | GDP | C2'-C3'-C4' | 2.06 | 106.58 | 102.61 |
| 39 | 1S | 502 | GDP | C5-C6-N1 | 2.06 | 117.99 | 114.07 |
| 41 | 2K | 501 | GTP | O6-C6-C5 | -2.06 | 120.25 | 124.32 |
| 39 | P4 | 503 | GDP | O4'-C1'-N9 | -2.06 | 106.02 | 108.75 |
| 39 | 1Q | 502 | GDP | C5-C6-N1 | 2.06 | 117.99 | 114.07 |
| 39 | 1K | 501 | GDP | O2A-PA-O3A | 2.05 | 112.83 | 107.27 |
| 41 | J0 | 501 | GTP | O2B-PB-O3B | 2.05 | 112.83 | 107.27 |
| 41 | J8 | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 39 | J6 | 502 | GDP | O3B-PB-O3A | 2.05 | 111.52 | 104.64 |
| 39 | 2S | 502 | GDP | C4'-O4'-C1' | -2.05 | 108.05 | 109.92 |
| 39 | V4 | 501 | GDP | O3B-PB-O3A | 2.05 | 111.52 | 104.64 |
| 41 | 2I | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 39 | M0 | 502 | GDP | O3B-PB-O3A | 2.05 | 111.52 | 104.64 |
| 41 | S9 | 501 | GTP | O6-C6-C5 | 2.05 | 128.39 | 124.32 |
| 41 | B7 | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 39 | V8 | 502 | GDP | O3B-PB-O3A | 2.05 | 111.51 | 104.64 |
| 39 | N8 | 502 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 41 | Y4 | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 41 | W5 | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 39 | J6 | 502 | GDP | O2A-PA-O3A | 2.05 | 112.81 | 107.27 |
| 39 | W8 | 503 | GDP | C5-C6-N1 | 2.05 | 117.97 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | S2 | 501 | GTP | C4'-O4'-C1' | -2.05 | 108.05 | 109.92 |
| 41 | D5 | 501 | GTP | O6-C6-C5 | -2.05 | 120.27 | 124.32 |
| 39 | C2 | 501 | GDP | O3B-PB-O3A | 2.05 | 111.50 | 104.64 |
| 39 | Z4 | 501 | GDP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 41 | 0V | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 39 | 2Q | 502 | GDP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 39 | 1O | 501 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 39 | M4 | 502 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 41 | C8 | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 41 | K4 | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 41 | O4 | 501 | GTP | O2B-PB-O3B | 2.04 | 112.79 | 107.27 |
| 41 | A4 | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 41 | 3D | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 39 | Y2 | 501 | GDP | O4'-C1'-N9 | 2.04 | 111.45 | 108.75 |
| 39 | A5 | 501 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 39 | Z2 | 503 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 41 | 3K | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 39 | T0 | 501 | GDP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 39 | 3G | 502 | GDP | O3B-PB-O3A | 2.04 | 111.46 | 104.64 |
| 39 | W4 | 502 | GDP | O2A-PA-O3A | 2.04 | 112.78 | 107.27 |
| 39 | 0E | 501 | GDP | O2A-PA-O3A | 2.04 | 112.78 | 107.27 |
| 39 | 2S | 502 | GDP | O3B-PB-O3A | 2.03 | 111.45 | 104.64 |
| 39 | W2 | 503 | GDP | O3B-PB-O3A | 2.03 | 111.45 | 104.64 |
| 41 | 1C | 501 | GTP | O6-C6-C5 | -2.03 | 120.29 | 124.32 |
| 39 | D4 | 501 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 41 | 1H | 501 | GTP | O6-C6-C5 | -2.03 | 120.30 | 124.32 |
| 41 | W4 | 501 | GTP | O6-C6-C5 | -2.03 | 120.30 | 124.32 |
| 41 | A9 | 501 | GTP | O2B-PB-O3B | 2.03 | 112.75 | 107.27 |
| 41 | 2N | 501 | GTP | O6-C6-C5 | -2.03 | 120.30 | 124.32 |
| 39 | 0Q | 502 | GDP | O2A-PA-O3A | 2.03 | 112.75 | 107.27 |
| 41 | A1 | 501 | GTP | O6-C6-C5 | -2.02 | 120.31 | 124.32 |
| 39 | V2 | 503 | GDP | O3B-PB-O3A | 2.02 | 111.41 | 104.64 |
| 41 | N6 | 501 | GTP | O6-C6-C5 | -2.02 | 120.32 | 124.32 |
| 39 | 0O | 502 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 39 | 2I | 502 | GDP | C2'-C3'-C4' | 2.02 | 106.51 | 102.61 |
| 39 | C4 | 501 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 39 | R8 | 502 | GDP | O2A-PA-O3A | 2.02 | 112.72 | 107.27 |
| 39 | L4 | 502 | GDP | O3B-PB-O3A | 2.01 | 111.39 | 104.64 |
| 39 | N6 | 503 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 39 | O6 | 502 | GDP | O4'-C1'-N9 | 2.01 | 111.41 | 108.75 |
| 39 | Z0 | 502 | GDP | O2A-PA-O3A | 2.01 | 112.70 | 107.27 |
| 39 | W4 | 502 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | A3 | 501 | GDP | O2A-PA-O3A | 2.01 | 112.70 | 107.27 |
| 39 | 0U | 501 | GDP | O6-C6-C5 | -2.01 | 120.34 | 124.32 |
| 41 | L6 | 501 | GTP | O6-C6-C5 | -2.01 | 120.34 | 124.32 |
| 39 | Z0 | 502 | GDP | C5-C6-N1 | 2.00 | 117.89 | 114.07 |
| 39 | Z6 | 502 | GDP | C5-C6-N1 | 2.00 | 117.89 | 114.07 |
| 39 | 3C | 502 | GDP | O2A-PA-O3A | 2.00 | 112.68 | 107.27 |
| 39 | 1A | 503 | GDP | O2A-PA-O3A | 2.00 | 112.68 | 107.27 |

There are no chirality outliers.

All (1774) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | 2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | 2 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | 2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 3 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 3 | 502 | GDP | C5'-O5'-PA-O2A |
| 39 | 5 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | 7 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | A1 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | A1 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | A1 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | A1 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | A3 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | A7 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | A9 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | A9 | 502 | GDP | C5'-O5'-PA-O2A |
| 39 | B3 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | B5 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | B5 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | B8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | B8 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | B8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | C0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | C2 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | C2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | C4 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | C6 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | C8 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | D0 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | D0 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | D0 | 501 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | D0 | 501 | GDP | C5'-O5'-PA-O2A |
| 39 | D0 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | D2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | D2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | D4 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | D4 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | D4 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | D6 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | D6 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | D6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | D8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | E0 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | E0 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | E2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | E2 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | E4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | E4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | E6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | E6 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | E6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | E8 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | E8 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | E8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | F0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | F2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | F2 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | F6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | F8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | G0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | G2 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | G2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | G4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | G6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | H4 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | H4 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | H8 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | I0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | I8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | J0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | J2 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | J2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | J4 | 503 | GDP | PA-O3A-PB-O3B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | J4 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | K0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | K4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | K6 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | K8 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | K8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | L0 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | L0 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | L2 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | L2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | L4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | L6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | L6 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | M0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | M2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | M4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | M6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | M6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | M8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | M8 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | M8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | N2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | N6 | 503 | GDP | PA-O3A-PB-O3B |
| 39 | N6 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | N8 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | N8 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | N8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | O0 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | O2 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | O2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | O4 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | O4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | O4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | O4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | O6 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | O6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | O6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | P4 | 503 | GDP | PA-O3A-PB-O3B |
| 39 | P4 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | P6 | 503 | GDP | PA-O3A-PB-O2B |
| 39 | P6 | 503 | GDP | PA-O3A-PB-O3B |
| 39 | P6 | 503 | GDP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | P6 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | Q0 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | Q0 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | Q0 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | Q2 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | Q2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Q4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Q4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | Q4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Q6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Q6 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | Q6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | Q8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | R0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | R2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | R4 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | R4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | R4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | R4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | R8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | S0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | S2 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | S2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | S4 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | S6 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | S6 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | S6 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | S6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | S8 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | T0 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | T0 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | T2 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | T2 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | T2 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | T2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | T4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | T6 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | T6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | T6 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | T6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | T8 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | T8 | 502 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | U2 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | U4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | U4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | U6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | U8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | V0 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | V2 | 503 | GDP | C5'-O5'-PA-O3A |
| 39 | V2 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | V4 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | V4 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | V8 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | W0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | W4 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | W4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | X2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | X4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | X6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | X8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | Y0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Y2 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | Y4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Y4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Y6 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Y8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | Z0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | Z4 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | Z6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Z8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 0A | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | 0C | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 0E | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 0I | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 0K | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 0K | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 0M | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 0Q | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 0S | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 0U | 501 | GDP | PA-O3A-PB-O3B |
| 39 | 0U | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | 0W | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 1A | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | 1C | 502 | GDP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | 1C | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 1K | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | 1K | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 1Q | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 1S | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 1U | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 2C | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2G | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 2I | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 2I | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2K | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2Q | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2S | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2U | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 2U | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2W | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 2W | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2Y | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 2Y | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 2Y | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 3A | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 3C | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 3C | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3I | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3K | 503 | GDP | PA-O3A-PB-O3B |
| 39 | 3M | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 3M | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 3M | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3O | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 3Q | 501 | GDP | PA-O3A-PB-O3B |
| 39 | 3S | 502 | GDP | PA-O3A-PB-O3B |
| 41 | 3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 8 | 501 | GTP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | A1 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | A1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | A1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | A1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | A4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | A4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | A4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | A9 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | A9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | A9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | A9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | B0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | B0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | B0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | B5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | B5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | B5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | B7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | B7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | B7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | C0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | C0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | C1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | C1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | C1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | C5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | C5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | C5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | C8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | C9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | C9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | C9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | D1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | D1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | D3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | D3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | D3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | D5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | D5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | D5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | E1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | E1 | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | E1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | E4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | E4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | E4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | E6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | E6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | E6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | E8 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | E8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | E8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | F0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | F0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | F1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | F1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | F1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | F3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | F3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | F3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | F5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | F5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | F8 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | F8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | F8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | F8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G0 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | G0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | G0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | G1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | G4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G5 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | G5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | G7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | G9 | 501 | GTP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | H2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | H2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | H2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | H3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | H3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | H3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | H6 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | H6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | H6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | H6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | H8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | H8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | H8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | I0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | I0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | I1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | I1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | I4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | I4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I5 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | I5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | I5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | I8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | I8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | J0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | J0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | J2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | J2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | J4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | J6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | J6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | J6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | J8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K0 | 501 | GTP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | K0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | K1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | K1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | K4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | K4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | K6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | K6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | K7 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | K7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | K7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | K9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | K9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | K9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | L2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | L2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | L2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | L4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | L4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | L4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | L6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | L6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | L7 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | L7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | L7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | M0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | M0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | M0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | M2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | M2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | M2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | M4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | M4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | M4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | M6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | M6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | M6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | M7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | M7 | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | M7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | N0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | N0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | N0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | N1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | N1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | N1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | N3 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | N3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | N3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | N3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | N6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | N6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | N6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | N8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | N8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | N8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O2 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | O2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | O4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | O9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | O9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | O9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | P4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | P4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | P6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | P6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | P6 | 501 | GTP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | P8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | P8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | P8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | P9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | P9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | P9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Q2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Q2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Q2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Q4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Q4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Q4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Q6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Q6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Q6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | R0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | R0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | R0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | R2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | R2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | R2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | R4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | R4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | R4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | R6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | R6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | R6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | R8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | R8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | R8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | S0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | S0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | S0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | S2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | S2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | S2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | S5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | S5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | S5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | S8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | S8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | S8 | 501 | GTP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | S9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | S9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | S9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | T2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | T2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | T2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | T4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | T4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | T4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | T6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | T6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | T6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | T8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | T8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | U2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | U2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | U2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | U4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | U4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | U6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | U6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | U7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | U7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | U9 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | U9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | U9 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | V2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | V2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | V2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | V3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | V3 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | V8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | V8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | V8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | W0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | W0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | W0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | W2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | W2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | W2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | W4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | W4 | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | W4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | W5 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | W5 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | W5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | W8 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | W8 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | W8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | X0 | 501 | GTP | PB-O3B-PG-O2G |
| 41 | X0 | 501 | GTP | PB-O3B-PG-O3G |
| 41 | X0 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | X4 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | X4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | X4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | X4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | X6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | X6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | X6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | X7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | X7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | X7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Y0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Y0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Y0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Y1 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Y1 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Y1 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Y4 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | Y4 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Y4 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Y4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Y6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Y6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Y6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Z0 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Z0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Z2 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | Z2 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Z2 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Z2 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Z3 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Z3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Z6 | 501 | GTP | PB-O3A-PA-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | Z6 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Z6 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Z6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | Z7 | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | Z7 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | Z7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0A | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0A | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0A | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0C | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0C | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0C | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0F | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0F | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0F | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0I | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0I | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0I | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0I | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0K | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0K | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0M | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0M | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0M | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0O | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0O | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0O | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0O | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0Q | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0Q | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0S | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0S | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0S | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0V | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0V | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0V | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0Y | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0Y | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 0Y | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 0Y | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1A | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1A | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 1A | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1C | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1C | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1C | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1D | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1D | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1G | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1G | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1G | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1H | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1H | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1H | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1H | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1L | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1L | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1N | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1N | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1N | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1Q | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1Q | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1S | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1S | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1T | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1T | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1T | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1W | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1W | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1W | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1X | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 1X | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 1X | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2A | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2A | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2A | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2C | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2C | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2C | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2E | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 2E | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2E | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2E | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2G | 501 | GTP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 2G | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2G | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2I | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2I | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2I | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2K | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2K | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2K | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2L | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2L | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2L | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2N | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 2N | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2N | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2Q | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 2Q | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2Q | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2Q | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2S | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2S | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2S | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2U | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2U | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2U | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2W | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2W | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2W | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 2Y | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 2Y | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 2Y | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3A | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3A | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3C | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3C | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3D | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3D | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3G | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 3G | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3G | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3G | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3I | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3I | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 3I | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3K | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3K | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3K | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3M | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3M | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3M | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3O | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3O | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3O | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3P | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 3P | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3P | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3P | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3P | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 3S | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3S | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3T | 501 | GTP | C5'-O5'-PA-O3A |
| 41 | 3T | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | 3T | 501 | GTP | C5'-O5'-PA-O2A |
| 39 | A1 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | D4 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | D4 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | D6 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | D6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | E2 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | E6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | Q4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | Q4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | Q6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | R4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | S2 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | S2 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | T4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | T4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0C | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 0C | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0U | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | 2S | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2Y | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3M | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 3M | 502 | GDP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | 3O | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3S | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | A9 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | B2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | C8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | I5 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | I5 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | O2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | O6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | X0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | X0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | X4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | X6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | X6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | X7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0I | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0I | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0O | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0O | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0Q | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0Q | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3A | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 3A | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3P | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | M4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | M4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | O2 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | O2 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | R4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | R8 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | S6 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | S6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0U | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3A | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 3A | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3S | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | A9 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | B2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | I1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | I1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | J8 | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | O0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | O0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | O6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | U2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U9 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | U9 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | W0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | W0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | W8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | W8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0M | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0S | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0S | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1L | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1L | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2Q | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2Q | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3D | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | N8 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | Y6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2S | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | J8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Y4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0M | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2E | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2E | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3D | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | C6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | D0 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | H4 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | J2 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | L6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | M6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | O4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | U4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2W | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3O | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | C0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | F5 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | I4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | K0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M0 | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | N0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | N3 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | O4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Q4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | V8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Y0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Y1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z3 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0A | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0F | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0Y | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1T | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3G | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3T | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | A3 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | B8 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | R8 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | X4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | X6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | Y6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 3I | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | F5 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | H3 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | I0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | K4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | L4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | N3 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Q4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | R4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | S0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Y4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Y6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z3 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Z7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0F | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0V | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0Y | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1A | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 1N | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1Q | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2S | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | H4 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | L6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | N8 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | V4 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | Y4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2G | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2I | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2U | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | A1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | C0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | G4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | J2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | K0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | M0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | M4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | N8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | O8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | U7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Y0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Z0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 0K | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1H | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2N | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2U | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2W | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | A3 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | E4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | G2 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | K8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | L6 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | R6 | 503 | GDP | PA-O3A-PB-O1B |
| 39 | U4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | V6 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | 2S | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3G | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3I | 502 | GDP | PA-O3A-PB-O1B |
| 39 | C6 | 501 | GDP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | N6 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | T6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | B0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | F1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | G9 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | I4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | J0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | R0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Y1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Z6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1G | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3G | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 3T | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | E4 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | G9 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | P4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Z3 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | A4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | B5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | J2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | N1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | R4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | R6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | V8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | W0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | W2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3G | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3M | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3O | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3P | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | J2 | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | I0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | N0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | O4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | R4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0A | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1N | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1T | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | A9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | B0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | B7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | C0 | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | C1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | E6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | H8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | I0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | I1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | I8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | J0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | J6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | M0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | M2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | M6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | M7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | N0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Q6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | R2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | S2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | T2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | T6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | U2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | W4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | W5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | W8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Y0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Z0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2W | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2Y | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3I | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | T0 | 501 | GDP | C3'-C4'-C5'-O5' |
| 41 | G4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | L7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | V8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0V | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | B7 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | G1 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | G7 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | G9 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | H3 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | H8 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | I1 | 501 | GTP | PB-O3A-PA-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | L6 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | N0 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | N6 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | P4 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | P6 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | P8 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | R4 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | S2 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | T8 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | W0 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | X7 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | Z0 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | Z3 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0A | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0V | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1A | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1C | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1D | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1G | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 1W | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 2C | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 2L | 501 | GTP | PB-O3A-PA-O5' |
| 41 | S8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | U9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Y4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1N | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | E4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | G6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | O4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | V6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 41 | D7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | H6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | I8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | S0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | S8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1A | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | O0 | 503 | GDP | PA-O3A-PB-O1B |
| 39 | Q6 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | S2 | 502 | GDP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | 3S | 502 | GDP | PA-O3A-PB-O1B |
| 39 | E2 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | J2 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | J4 | 503 | GDP | PA-O3A-PB-O2B |
| 39 | K8 | 501 | GDP | PA-O3A-PB-O3B |
| 39 | M8 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | N8 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | R0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | R6 | 503 | GDP | PA-O3A-PB-O3B |
| 39 | S8 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | U2 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | U4 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | W0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | X2 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | Y8 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | 3G | 502 | GDP | PA-O3A-PB-O3B |
| 39 | 3Q | 501 | GDP | PA-O3A-PB-O2B |
| 39 | 2 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | A7 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | B3 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | F6 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | U4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 1K | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 1U | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2W | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | 7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | B5 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | E6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | H2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | H3 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | K1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | K6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | N1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | W2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1D | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1Q | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2C | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2L | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2S | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2Y | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3C | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 3I | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | A1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | C9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | A1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | B2 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | C5 | 501 | GTP | PB-O3A-PA-O2A |
| 41 | C9 | 501 | GTP | PB-O3A-PA-O2A |
| 41 | E8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | F3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | F5 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | F8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | G4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | H3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | H6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | I0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | I1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | I5 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | I8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | L7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | N0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | N1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | N6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | P6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | R4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | S2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | T6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | U2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | V8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | W2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0A | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0F | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0I | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0M | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0O | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0S | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0V | 501 | GTP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 1C | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1W | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2E | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2L | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2N | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2Q | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3G | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3P | 501 | GTP | PA-O3A-PB-O2B |
| 39 | H8 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | U8 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | Z0 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0M | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0Q | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | G0 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | J2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | L4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | P9 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | Z0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0C | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1C | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1X | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2G | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | D7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | E8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | F3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | F5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | I4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | J8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | L6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | M4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | N8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | R8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | T8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | U7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | V2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Z7 | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 0V | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0Y | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1A | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1C | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1D | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1H | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1L | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2A | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2C | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2K | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2L | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3A | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3T | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | A3 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | B8 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | M6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | W0 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | X6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | X8 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 3I | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | A1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | F1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | G9 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | J0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | K4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | K7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | M4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | M7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | N8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | O8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | P4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | R0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | U7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | Y6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0K | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1H | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2N | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2U | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2W | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | 3 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 5 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 7 | 502 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | A3 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | A9 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | B1 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | B3 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | B5 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | C0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | C6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | C8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | D2 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | E6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | G6 | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | G8 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | H6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | H8 | 503 | GDP | C5'-O5'-PA-O3A |
| 39 | I4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | J2 | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | J6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | J8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | K0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | K6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | L6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | M4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | N0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | N2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | O8 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | P8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Q6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | R0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | R6 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | S8 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | T4 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | U2 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | V6 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | W0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | W8 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | X0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | X2 | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | Y0 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Y6 | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | Z2 | 503 | GDP | C5'-O5'-PA-O1A |
| 39 | 0G | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 0O | 502 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | 0Q | 502 | GDP | C5'-O5'-PA-O3A |
| 39 | 0U | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 0Y | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 1E | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 1M | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 1O | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 1U | 501 | GDP | C5'-O5'-PA-O3A |
| 39 | 1W | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2E | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2G | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 2M | 501 | GDP | C5'-O5'-PA-O1A |
| 39 | 2Y | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3A | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3G | 502 | GDP | C5'-O5'-PA-O1A |
| 39 | 3O | 502 | GDP | C5'-O5'-PA-O1A |
| 41 | 7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | C0 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | F0 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | F5 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | G9 | 501 | GTP | C5'-O5'-PA-O1A |
| 41 | I4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | J8 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | U4 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | U6 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | U7 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | V3 | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0K | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 0Q | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1L | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1Q | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 1S | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3A | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3C | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3D | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3S | 501 | GTP | C5'-O5'-PA-O2A |
| 41 | 3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | A2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | B2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | D1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | D3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | E1 | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | F0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | F1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | F8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | G7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | H2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | H3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | H6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | I5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | J4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K1 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | K6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | L2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | L4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | L7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | N3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | N6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | O8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | P4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | P6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | P8 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | P9 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Q2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Q4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | R0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | S0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | S5 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | T4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | U4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | U6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | V3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | X0 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | X4 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | X6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | X7 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Y1 | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | Y6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Z2 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Z3 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | Z6 | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0A | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0C | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0F | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0I | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0K | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0M | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0O | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0Q | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 0S | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1G | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1Q | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1S | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1T | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1W | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 1X | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2E | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2G | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2I | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2N | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2Q | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2S | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 2U | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3C | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3D | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3K | 501 | GTP | C4'-C5'-O5'-PA |
| 41 | 3S | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | D2 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | E0 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | F6 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | G6 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | L2 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | N2 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | Q4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 0U | 501 | GDP | PA-O3A-PB-O1B |
| 39 | 2U | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | H8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | J6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | L7 | 501 | GTP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | Z2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1G | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2K | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3S | 501 | GTP | C3'-C4'-C5'-O5' |
| 39 | P8 | 502 | GDP | PB-O3A-PA-O2A |
| 39 | 1A | 503 | GDP | PB-O3A-PA-O2A |
| 41 | 4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | A4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | A9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | B7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | C0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | C1 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | E1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | E6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | F0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G5 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | H2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | H8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | I4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | J0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | J2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | L2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | L6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | M6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | M7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | N3 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | N8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | P8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | P9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Q2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Q4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Q6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | R2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | R6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | R8 | 501 | GTP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | S0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | T8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | U6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | U7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | U9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | V2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | V3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | W0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | W8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | X7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | X7 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | Y4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Z2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0C | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0K | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0Q | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0Y | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1A | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1D | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1G | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1H | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2A | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2C | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2I | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2S | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2W | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3D | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3I | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3M | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3O | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3T | 501 | GTP | PA-O3A-PB-O2B |
| 39 | 3K | 503 | GDP | C3'-C4'-C5'-O5' |
| 41 | C1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | J4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | T8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2A | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | C5 | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | K0 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | P4 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | V4 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | Y0 | 502 | GDP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | T2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | W4 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2I | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 7 | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | B1 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | C4 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | D6 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | 2Q | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3C | 502 | GDP | PA-O3A-PB-O1B |
| 39 | E8 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 2G | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | G1 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | U6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | K8 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | N6 | 503 | GDP | O4'-C4'-C5'-O5' |
| 39 | O0 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | T6 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | V6 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | X4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | Y4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 2I | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | B0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | B5 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | B7 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | E6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | H6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | I8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | K1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | S8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | V3 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1D | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2C | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2L | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | B0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | E6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | J6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | L6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | M2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | N3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | O0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | O8 | 501 | GTP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | P4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | T4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | T8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | U4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | X4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | X7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Y0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Y1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1G | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1H | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 1N | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2Y | 501 | GTP | PA-O3A-PB-O2B |
| 41 | K1 | 501 | GTP | PB-O3A-PA-O5' |
| 41 | 0F | 501 | GTP | PB-O3A-PA-O5' |
| 39 | 2 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | A7 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | G6 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | T0 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | T8 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | W4 | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | 7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | G0 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | H2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | K6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | M6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | P4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | P9 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | W2 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1X | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 3C | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 3I | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | E4 | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | F6 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | U6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 41 | L2 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1W | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 2G | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | B8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | D0 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | D8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | E2 | 501 | GDP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | J2 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | K0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | N6 | 503 | GDP | PA-O3A-PB-O1B |
| 39 | N8 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | R0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | R4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | S6 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | S8 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | T6 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | U2 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | V8 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | W0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | W2 | 503 | GDP | PA-O3A-PB-O1B |
| 39 | X2 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | X4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | Y0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | Y2 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | Y4 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | Y8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | 2I | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 2U | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 2W | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3Q | 501 | GDP | PA-O3A-PB-O1B |
| 39 | 2 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | A1 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | A7 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | B5 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | C0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | C8 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | D0 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | D4 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | E6 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | F0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | F2 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | M0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | M0 | 502 | GDP | PA-O3A-PB-O3B |
| 39 | N6 | 503 | GDP | PA-O3A-PB-O2B |
| 39 | O2 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | P4 | 503 | GDP | PA-O3A-PB-O2B |
| 39 | Q8 | 501 | GDP | PA-O3A-PB-O2B |
| 39 | S0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | V8 | 502 | GDP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | X6 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | Y0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | Y4 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | Y6 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | Z0 | 502 | GDP | PA-O3A-PB-O2B |
| 39 | 0S | 502 | GDP | PA-O3A-PB-O2B |
| 39 | 2Y | 502 | GDP | PA-O3A-PB-O2B |
| 39 | 3K | 503 | GDP | PA-O3A-PB-O2B |
| 39 | 3M | 502 | GDP | PA-O3A-PB-O2B |
| 41 | E4 | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | O6 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | Q0 | 501 | GDP | C3'-C4'-C5'-O5' |
| 39 | 1U | 501 | GDP | O4'-C4'-C5'-O5' |
| 41 | K7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | N1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 0C | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 1C | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2Y | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | J4 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | Q2 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | V2 | 503 | GDP | C3'-C4'-C5'-O5' |
| 39 | 0Q | 502 | GDP | O4'-C4'-C5'-O5' |
| 39 | 0W | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | 1K | 501 | GDP | O4'-C4'-C5'-O5' |
| 41 | G5 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | K9 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | P6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3M | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 3S | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | W4 | 502 | GDP | C4'-C5'-O5'-PA |
| 39 | P8 | 502 | GDP | PB-O3A-PA-O1A |
| 39 | 1A | 503 | GDP | PB-O3A-PA-O1A |
| 41 | 3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | A1 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | A2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | A4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | A9 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | B0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | B5 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | C0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | C5 | 501 | GTP | PB-O3A-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | D1 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | D1 | 501 | GTP | PB-O3A-PA-O2A |
| 41 | D3 | 501 | GTP | PB-O3A-PA-O2A |
| 41 | E4 | 501 | GTP | PB-O3A-PA-O2A |
| 41 | F1 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | F8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G1 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | G5 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | G7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | H6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | H8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | I1 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | I5 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | J2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | J6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | K7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | L4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | L7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | M6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | N0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | O0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | O2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | O2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | O4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | O6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | O8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | O9 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | O9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | P6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | P8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Q4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Q6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | R0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | R0 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | R2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | S0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | T2 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | U6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | U7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | U9 | 501 | GTP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | V2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | V3 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | W4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | W4 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | W5 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | W5 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | X4 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | X6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Y0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Y4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Y6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Y6 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Z6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0A | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0C | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0F | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0I | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0O | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0Q | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0S | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0V | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 0Y | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1N | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1T | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2E | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2G | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2I | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2K | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2K | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2N | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2U | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2U | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2W | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2Y | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 3I | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 3O | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 3P | 501 | GTP | PA-O3A-PB-O1B |
| 39 | B3 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | S0 | 502 | GDP | C3'-C4'-C5'-O5' |
| 39 | W8 | 503 | GDP | C4'-C5'-O5'-PA |
| 39 | A7 | 501 | GDP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | F0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | J8 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | M6 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | Q8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | S0 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | X8 | 501 | GDP | PA-O3A-PB-O1B |
| 39 | Y6 | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 2Y | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3K | 503 | GDP | PA-O3A-PB-O1B |
| 39 | 3M | 502 | GDP | PA-O3A-PB-O1B |
| 39 | 3O | 502 | GDP | PA-O3A-PB-O1B |
| 39 | U8 | 501 | GDP | O4'-C4'-C5'-O5' |
| 39 | 0E | 501 | GDP | C3'-C4'-C5'-O5' |
| 41 | C5 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | F8 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | G1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | H8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | J6 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | T8 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2A | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | 2K | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | D7 | 501 | GTP | O4'-C4'-C5'-O5' |
| 39 | I2 | 501 | GDP | C4'-C5'-O5'-PA |
| 41 | D5 | 501 | GTP | C4'-C5'-O5'-PA |
| 39 | 0G | 501 | GDP | PB-O3A-PA-O2A |
| 41 | 7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | B7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | D3 | 501 | GTP | PB-O3A-PA-O1A |
| 41 | D7 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | E1 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | F0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | G0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | G9 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | H2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | I4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | J0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | K4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | L2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M0 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | M7 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | N8 | 501 | GTP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | O4 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | P9 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | Q2 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | R6 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | R8 | 501 | GTP | PA-O3A-PB-O1B |
| 41 | S8 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | Z3 | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 0K | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1A | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 1X | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 2A | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2C | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 2S | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 3D | 501 | GTP | PA-O3A-PB-O1B |
| 41 | 3S | 501 | GTP | PA-O3A-PB-O2B |
| 41 | 3T | 501 | GTP | PA-O3A-PB-O1B |
| 39 | H8 | 503 | GDP | O4'-C4'-C5'-O5' |
| 39 | Z0 | 502 | GDP | O4'-C4'-C5'-O5' |
| 41 | C1 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | J4 | 501 | GTP | O4'-C4'-C5'-O5' |
| 41 | N6 | 501 | GTP | C3'-C4'-C5'-O5' |
| 41 | 1S | 501 | GTP | C3'-C4'-C5'-O5' |

There are no ring outliers.

241 monomers are involved in 397 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 41 | 8 | 501 | GTP | 1 | 0 |
| 39 | W8 | 503 | GDP | 2 | 0 |
| 41 | K0 | 501 | GTP | 2 | 0 |
| 41 | Q4 | 501 | GTP | 1 | 0 |
| 41 | A4 | 501 | GTP | 2 | 0 |
| 41 | L4 | 501 | GTP | 3 | 0 |
| 41 | G5 | 501 | GTP | 3 | 0 |
| 41 | N0 | 501 | GTP | 1 | 0 |
| 41 | F5 | 501 | GTP | 2 | 0 |
| 41 | C8 | 501 | GTP | 1 | 0 |
| 41 | 1L | 501 | GTP | 1 | 0 |
| 39 | 1Q | 502 | GDP | 1 | 0 |
| 41 | B7 | 501 | GTP | 1 | 0 |
| 41 | Y0 | 501 | GTP | 3 | 0 |
| 39 | H4 | 501 | GDP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 41 | O4 | 501 | GTP | 2 | 0 |
| 39 | C4 | 501 | GDP | 3 | 0 |
| 41 | L6 | 501 | GTP | 1 | 0 |
| 39 | K4 | 502 | GDP | 1 | 0 |
| 41 | D3 | 501 | GTP | 2 | 0 |
| 39 | F0 | 502 | GDP | 2 | 0 |
| 39 | 2M | 501 | GDP | 2 | 0 |
| 41 | Y4 | 501 | GTP | 2 | 0 |
| 41 | Z3 | 501 | GTP | 2 | 0 |
| 39 | 9 | 501 | GDP | 1 | 0 |
| 41 | P8 | 501 | GTP | 2 | 0 |
| 39 | X2 | 501 | GDP | 3 | 0 |
| 39 | 1K | 501 | GDP | 1 | 0 |
| 39 | 0Y | 502 | GDP | 1 | 0 |
| 39 | 2E | 502 | GDP | 1 | 0 |
| 39 | L2 | 502 | GDP | 1 | 0 |
| 39 | X6 | 502 | GDP | 3 | 0 |
| 39 | A7 | 501 | GDP | 2 | 0 |
| 41 | O8 | 501 | GTP | 1 | 0 |
| 39 | C8 | 502 | GDP | 3 | 0 |
| 39 | 5 | 501 | GDP | 1 | 0 |
| 39 | 0U | 501 | GDP | 1 | 0 |
| 41 | F8 | 501 | GTP | 1 | 0 |
| 41 | C9 | 501 | GTP | 5 | 0 |
| 39 | 1A | 503 | GDP | 2 | 0 |
| 41 | 2N | 501 | GTP | 1 | 0 |
| 41 | O9 | 501 | GTP | 1 | 0 |
| 41 | 2G | 501 | GTP | 2 | 0 |
| 41 | A9 | 501 | GTP | 1 | 0 |
| 39 | N6 | 503 | GDP | 2 | 0 |
| 39 | 0S | 502 | GDP | 2 | 0 |
| 41 | I0 | 501 | GTP | 1 | 0 |
| 39 | L6 | 502 | GDP | 1 | 0 |
| 39 | 2K | 502 | GDP | 2 | 0 |
| 39 | Z6 | 502 | GDP | 2 | 0 |
| 41 | Q6 | 501 | GTP | 1 | 0 |
| 41 | 2L | 501 | GTP | 1 | 0 |
| 39 | 0C | 502 | GDP | 2 | 0 |
| 41 | B5 | 501 | GTP | 2 | 0 |
| 41 | 3M | 501 | GTP | 1 | 0 |
| 39 | X0 | 502 | GDP | 2 | 0 |
| 41 | H3 | 501 | GTP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 41 | P9 | 501 | GTP | 2 | 0 |
| 39 | 0G | 501 | GDP | 2 | 0 |
| 39 | N2 | 501 | GDP | 1 | 0 |
| 41 | Y1 | 501 | GTP | 2 | 0 |
| 39 | V4 | 501 | GDP | 1 | 0 |
| 39 | S2 | 502 | GDP | 1 | 0 |
| 41 | B0 | 501 | GTP | 2 | 0 |
| 39 | 2G | 502 | GDP | 3 | 0 |
| 39 | J2 | 502 | GDP | 1 | 0 |
| 39 | 3I | 502 | GDP | 1 | 0 |
| 39 | 0Q | 502 | GDP | 1 | 0 |
| 41 | G7 | 501 | GTP | 2 | 0 |
| 39 | S4 | 501 | GDP | 1 | 0 |
| 41 | 1G | 501 | GTP | 1 | 0 |
| 41 | X4 | 501 | GTP | 3 | 0 |
| 39 | 0O | 502 | GDP | 1 | 0 |
| 39 | Q2 | 502 | GDP | 1 | 0 |
| 39 | S8 | 502 | GDP | 1 | 0 |
| 41 | 1T | 501 | GTP | 1 | 0 |
| 39 | 3A | 502 | GDP | 1 | 0 |
| 39 | 1O | 501 | GDP | 1 | 0 |
| 41 | G9 | 501 | GTP | 1 | 0 |
| 41 | P4 | 501 | GTP | 3 | 0 |
| 41 | K6 | 501 | GTP | 3 | 0 |
| 41 | K4 | 501 | GTP | 2 | 0 |
| 39 | 2C | 502 | GDP | 1 | 0 |
| 41 | S9 | 501 | GTP | 2 | 0 |
| 39 | Z0 | 502 | GDP | 2 | 0 |
| 41 | F1 | 501 | GTP | 1 | 0 |
| 41 | D1 | 501 | GTP | 1 | 0 |
| 41 | J8 | 501 | GTP | 1 | 0 |
| 39 | X4 | 502 | GDP | 2 | 0 |
| 41 | E8 | 501 | GTP | 3 | 0 |
| 39 | A5 | 501 | GDP | 1 | 0 |
| 41 | H8 | 501 | GTP | 1 | 0 |
| 39 | 3C | 502 | GDP | 1 | 0 |
| 39 | 1C | 502 | GDP | 1 | 0 |
| 41 | 3O | 501 | GTP | 1 | 0 |
| 41 | Z6 | 501 | GTP | 2 | 0 |
| 39 | D4 | 501 | GDP | 3 | 0 |
| 39 | Y8 | 501 | GDP | 2 | 0 |
| 41 | 1Q | 501 | GTP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 41 | K9 | 501 | GTP | 2 | 0 |
| 39 | P4 | 503 | GDP | 1 | 0 |
| 39 | U2 | 502 | GDP | 1 | 0 |
| 41 | I8 | 501 | GTP | 1 | 0 |
| 41 | 1S | 501 | GTP | 1 | 0 |
| 41 | T8 | 501 | GTP | 2 | 0 |
| 41 | C1 | 501 | GTP | 2 | 0 |
| 41 | G1 | 501 | GTP | 2 | 0 |
| 41 | 0S | 501 | GTP | 2 | 0 |
| 41 | 2U | 501 | GTP | 1 | 0 |
| 41 | 0I | 501 | GTP | 3 | 0 |
| 39 | 7 | 502 | GDP | 3 | 0 |
| 41 | E1 | 501 | GTP | 3 | 0 |
| 39 | 0W | 502 | GDP | 2 | 0 |
| 41 | D7 | 501 | GTP | 2 | 0 |
| 41 | C5 | 501 | GTP | 2 | 0 |
| 41 | Y6 | 501 | GTP | 2 | 0 |
| 39 | Y4 | 502 | GDP | 3 | 0 |
| 41 | N6 | 501 | GTP | 3 | 0 |
| 39 | 3 | 502 | GDP | 2 | 0 |
| 41 | 3D | 501 | GTP | 2 | 0 |
| 41 | W5 | 501 | GTP | 1 | 0 |
| 41 | 0Y | 501 | GTP | 1 | 0 |
| 41 | Z2 | 501 | GTP | 2 | 0 |
| 41 | I4 | 501 | GTP | 2 | 0 |
| 39 | D8 | 501 | GDP | 1 | 0 |
| 41 | L2 | 501 | GTP | 2 | 0 |
| 39 | 0I | 502 | GDP | 1 | 0 |
| 39 | 3K | 503 | GDP | 1 | 0 |
| 39 | T0 | 501 | GDP | 2 | 0 |
| 41 | 0O | 501 | GTP | 2 | 0 |
| 41 | Q2 | 501 | GTP | 1 | 0 |
| 41 | S8 | 501 | GTP | 1 | 0 |
| 39 | R6 | 503 | GDP | 1 | 0 |
| 41 | 1H | 501 | GTP | 2 | 0 |
| 41 | T6 | 501 | GTP | 3 | 0 |
| 41 | 2E | 501 | GTP | 2 | 0 |
| 39 | N8 | 502 | GDP | 3 | 0 |
| 41 | 1W | 501 | GTP | 1 | 0 |
| 39 | T6 | 502 | GDP | 3 | 0 |
| 41 | J6 | 501 | GTP | 1 | 0 |
| 41 | S2 | 501 | GTP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 39 | 3Q | 501 | GDP | 1 | 0 |
| 41 | J2 | 501 | GTP | 1 | 0 |
| 41 | 0Q | 501 | GTP | 3 | 0 |
| 39 | E0 | 501 | GDP | 4 | 0 |
| 39 | 0E | 501 | GDP | 3 | 0 |
| 39 | Q4 | 502 | GDP | 1 | 0 |
| 41 | 0F | 501 | GTP | 3 | 0 |
| 41 | G0 | 501 | GTP | 3 | 0 |
| 39 | Y6 | 502 | GDP | 2 | 0 |
| 39 | C6 | 501 | GDP | 3 | 0 |
| 39 | 3S | 502 | GDP | 1 | 0 |
| 41 | U4 | 501 | GTP | 1 | 0 |
| 39 | Z2 | 503 | GDP | 3 | 0 |
| 41 | E4 | 501 | GTP | 1 | 0 |
| 39 | H6 | 502 | GDP | 1 | 0 |
| 39 | V6 | 501 | GDP | 1 | 0 |
| 39 | H2 | 503 | GDP | 1 | 0 |
| 41 | K7 | 501 | GTP | 2 | 0 |
| 39 | 1W | 502 | GDP | 2 | 0 |
| 39 | X8 | 501 | GDP | 1 | 0 |
| 39 | E6 | 502 | GDP | 1 | 0 |
| 41 | I1 | 501 | GTP | 1 | 0 |
| 39 | B8 | 501 | GDP | 2 | 0 |
| 39 | D0 | 501 | GDP | 5 | 0 |
| 39 | P8 | 502 | GDP | 2 | 0 |
| 41 | A2 | 501 | GTP | 1 | 0 |
| 39 | B1 | 501 | GDP | 1 | 0 |
| 41 | 2C | 501 | GTP | 2 | 0 |
| 41 | G4 | 501 | GTP | 2 | 0 |
| 39 | Z4 | 501 | GDP | 1 | 0 |
| 39 | Z8 | 501 | GDP | 3 | 0 |
| 41 | 0M | 501 | GTP | 3 | 0 |
| 41 | F0 | 501 | GTP | 2 | 0 |
| 41 | 2W | 501 | GTP | 1 | 0 |
| 41 | 1X | 501 | GTP | 1 | 0 |
| 41 | X7 | 501 | GTP | 2 | 0 |
| 41 | H2 | 501 | GTP | 1 | 0 |
| 41 | A1 | 501 | GTP | 2 | 0 |
| 39 | 3O | 502 | GDP | 1 | 0 |
| 41 | 2Q | 501 | GTP | 1 | 0 |
| 39 | E8 | 502 | GDP | 1 | 0 |
| 41 | R0 | 501 | GTP | 1 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 39 | V8 | 502 | GDP | 1 | 0 |
| 39 | G4 | 502 | GDP | 1 | 0 |
| 39 | W0 | 502 | GDP | 2 | 0 |
| 39 | Y0 | 502 | GDP | 2 | 0 |
| 41 | 1N | 501 | GTP | 1 | 0 |
| 41 | 1A | 501 | GTP | 1 | 0 |
| 41 | C0 | 501 | GTP | 2 | 0 |
| 41 | R6 | 501 | GTP | 1 | 0 |
| 39 | W2 | 503 | GDP | 1 | 0 |
| 41 | O6 | 501 | GTP | 1 | 0 |
| 41 | U6 | 501 | GTP | 1 | 0 |
| 41 | E6 | 501 | GTP | 2 | 0 |
| 41 | 1D | 501 | GTP | 1 | 0 |
| 39 | G8 | 501 | GDP | 1 | 0 |
| 41 | 0V | 501 | GTP | 1 | 0 |
| 41 | 0K | 501 | GTP | 2 | 0 |
| 39 | O2 | 502 | GDP | 2 | 0 |
| 41 | 3 | 501 | GTP | 1 | 0 |
| 41 | F3 | 501 | GTP | 2 | 0 |
| 41 | 4 | 501 | GTP | 1 | 0 |
| 41 | Z7 | 501 | GTP | 2 | 0 |
| 41 | T2 | 501 | GTP | 2 | 0 |
| 39 | F2 | 501 | GDP | 3 | 0 |
| 39 | B3 | 501 | GDP | 1 | 0 |
| 41 | X6 | 501 | GTP | 3 | 0 |
| 41 | X0 | 501 | GTP | 1 | 0 |
| 41 | 0A | 501 | GTP | 2 | 0 |
| 39 | 0M | 502 | GDP | 1 | 0 |
| 41 | 2I | 501 | GTP | 1 | 0 |
| 41 | 0C | 501 | GTP | 3 | 0 |
| 39 | O6 | 502 | GDP | 1 | 0 |
| 41 | N8 | 501 | GTP | 2 | 0 |
| 39 | R4 | 502 | GDP | 1 | 0 |
| 39 | O8 | 503 | GDP | 1 | 0 |
| 39 | D2 | 501 | GDP | 2 | 0 |
| 39 | 0A | 503 | GDP | 1 | 0 |
| 39 | 0K | 502 | GDP | 1 | 0 |
| 41 | M7 | 501 | GTP | 1 | 0 |
| 41 | P6 | 501 | GTP | 2 | 0 |
| 39 | J8 | 502 | GDP | 1 | 0 |
| 41 | J0 | 501 | GTP | 1 | 0 |
| 41 | R2 | 501 | GTP | 1 | 0 |

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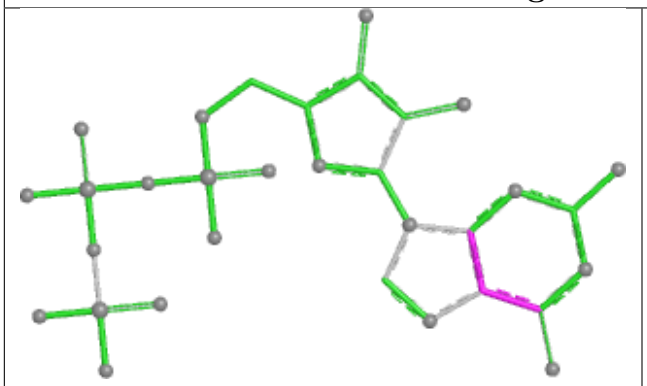
*Continued from previous page...*

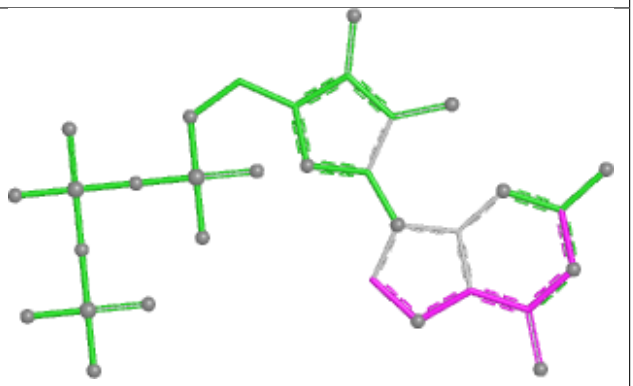
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 39 | J6 | 502 | GDP | 1 | 0 |
| 41 | D5 | 501 | GTP | 1 | 0 |
| 39 | D6 | 501 | GDP | 3 | 0 |
| 41 | J4 | 501 | GTP | 1 | 0 |
| 39 | 1M | 501 | GDP | 1 | 0 |
| 41 | 1C | 501 | GTP | 1 | 0 |
| 39 | Q6 | 502 | GDP | 2 | 0 |
| 41 | O0 | 501 | GTP | 1 | 0 |
| 41 | S0 | 501 | GTP | 1 | 0 |
| 39 | L4 | 502 | GDP | 2 | 0 |
| 39 | E2 | 501 | GDP | 2 | 0 |
| 39 | 1S | 502 | GDP | 1 | 0 |
| 41 | H6 | 501 | GTP | 1 | 0 |
| 41 | Z0 | 501 | GTP | 1 | 0 |
| 41 | T4 | 501 | GTP | 3 | 0 |
| 39 | Y2 | 501 | GDP | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

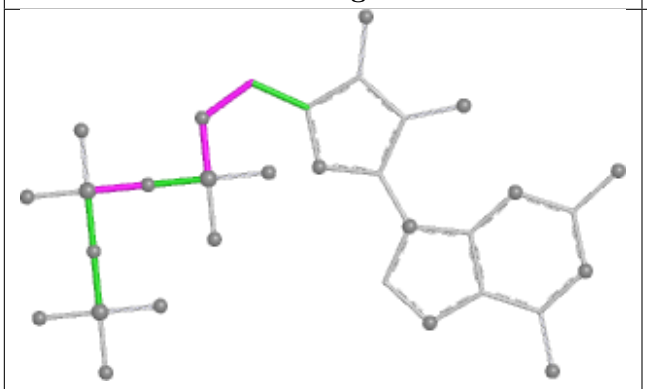
## Ligand GTP 8 501



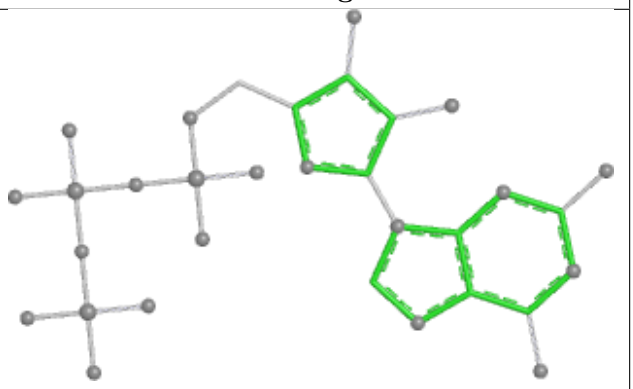
Bond lengths



Bond angles

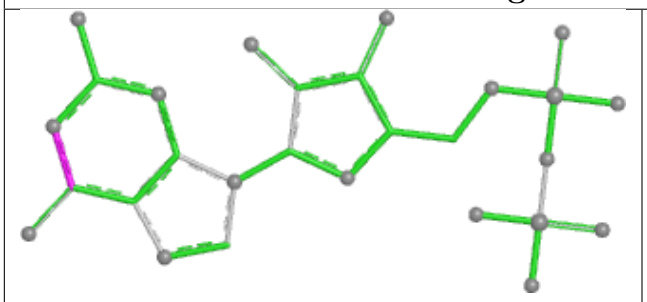


Torsions



Rings

## Ligand GDP W8 503



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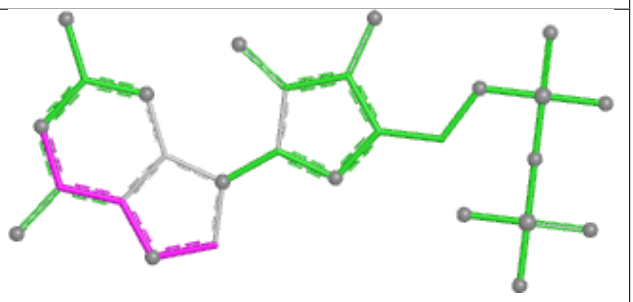
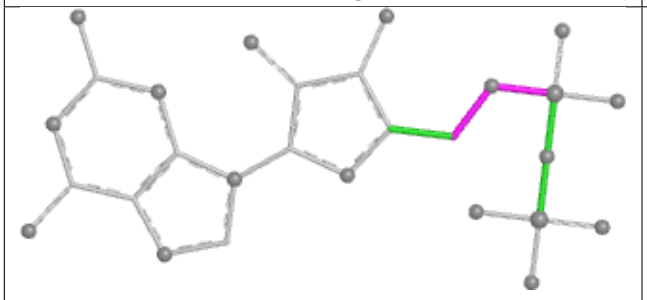
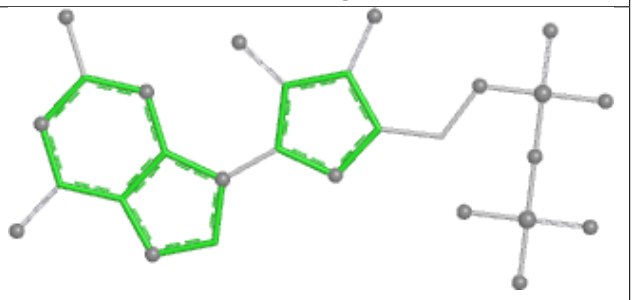


Bond angles

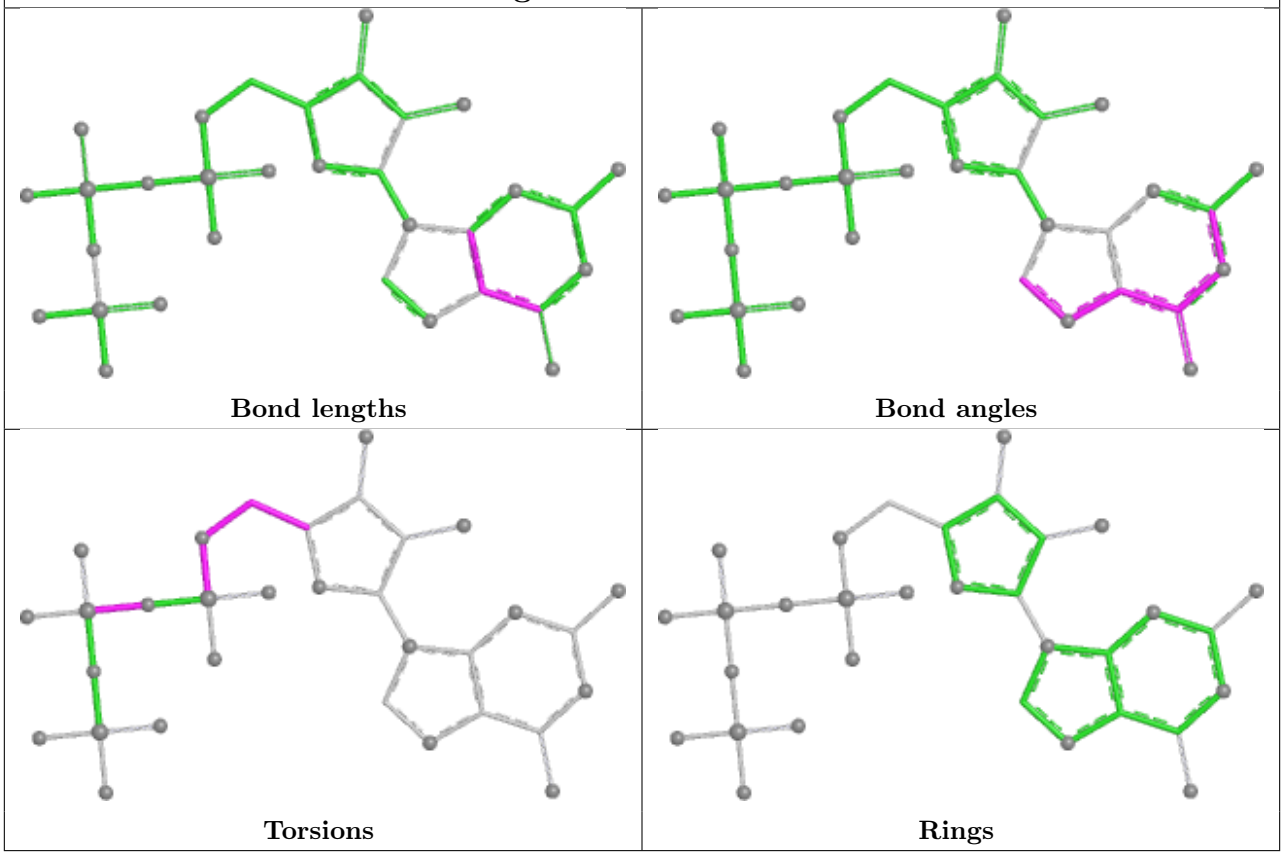


Torsions

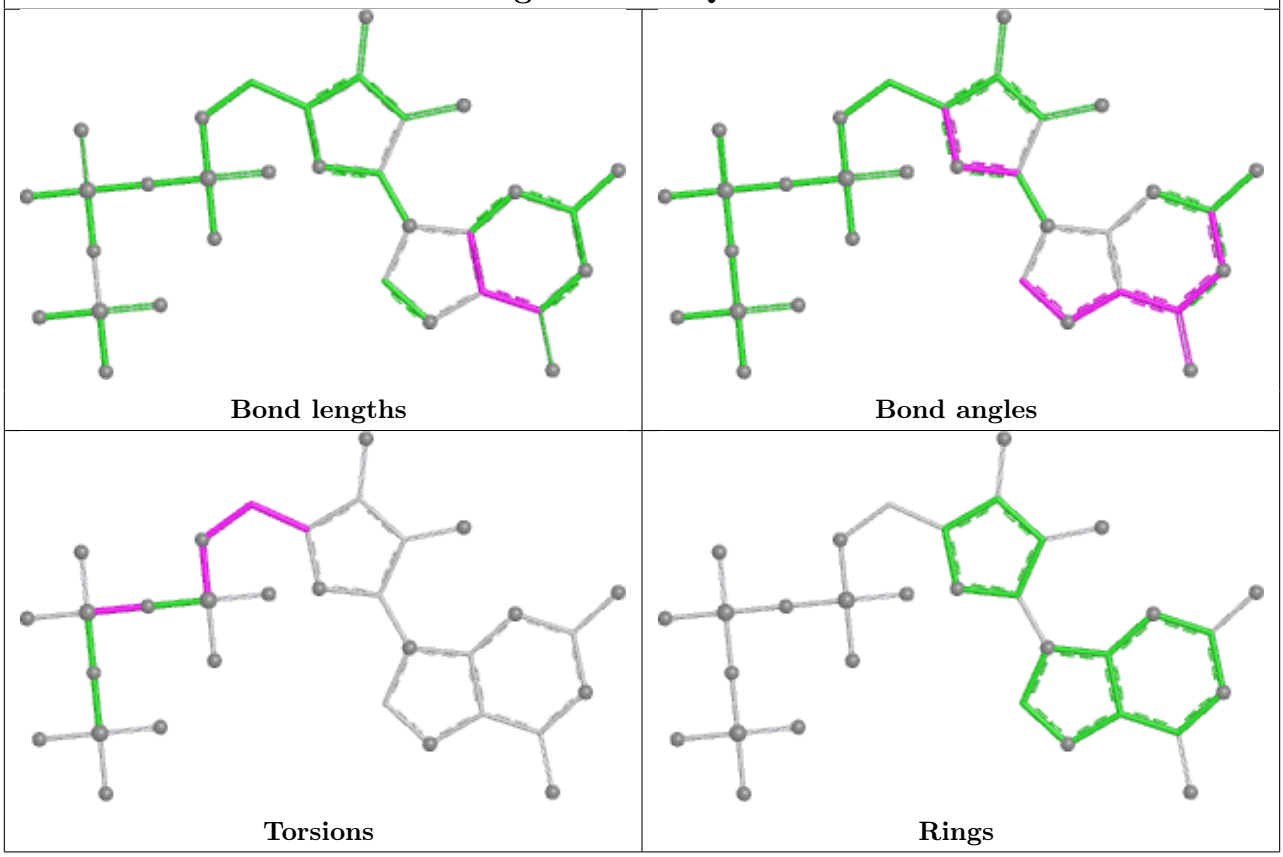


Rings

## Ligand GTP K0 501




## Ligand GTP Q4 501



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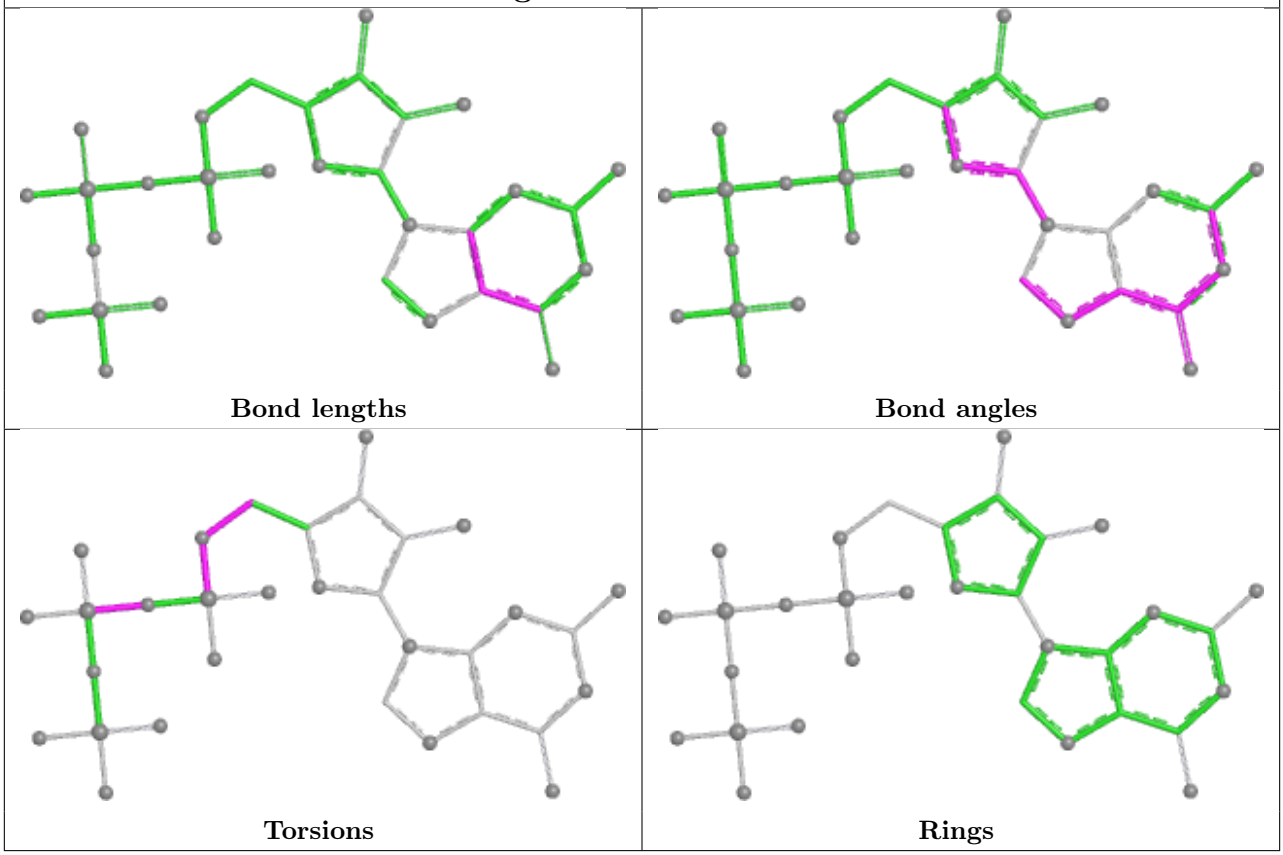


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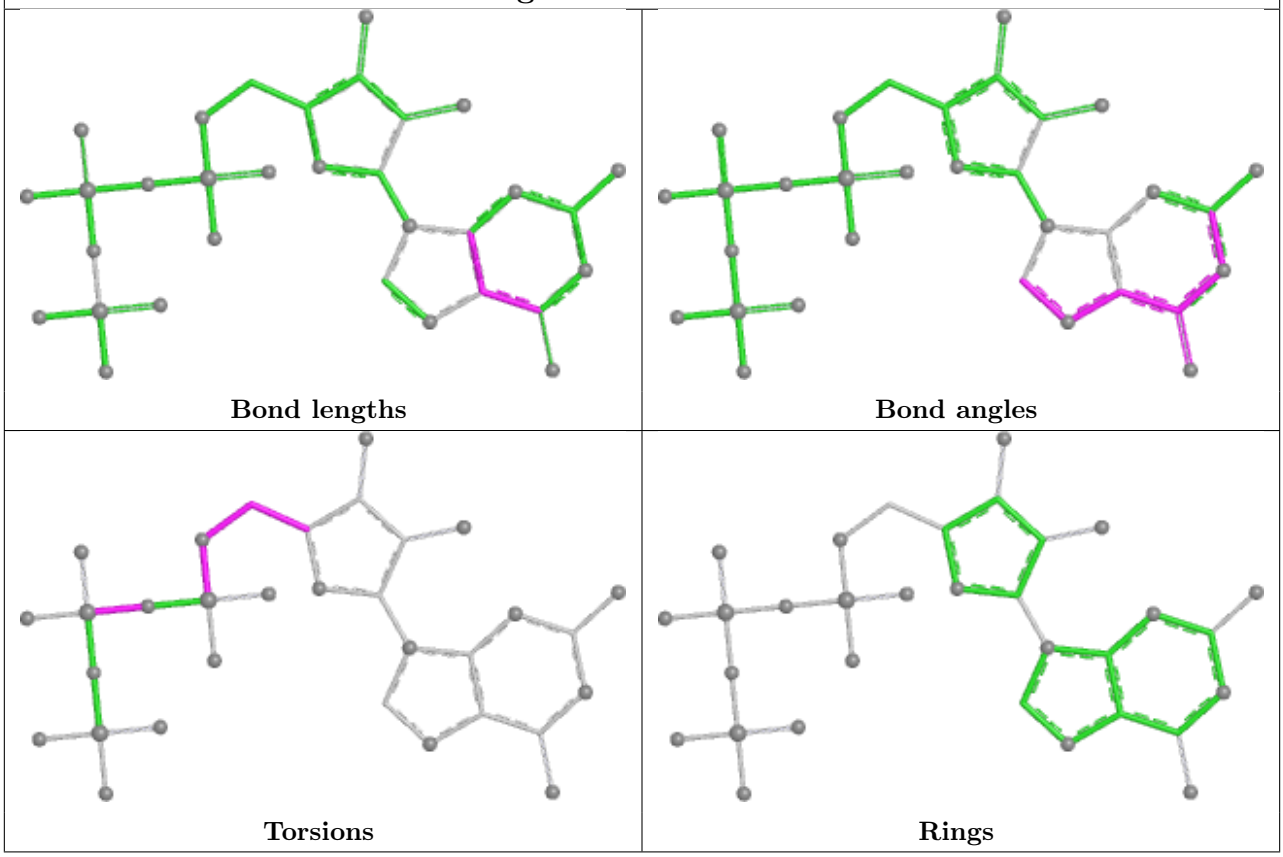

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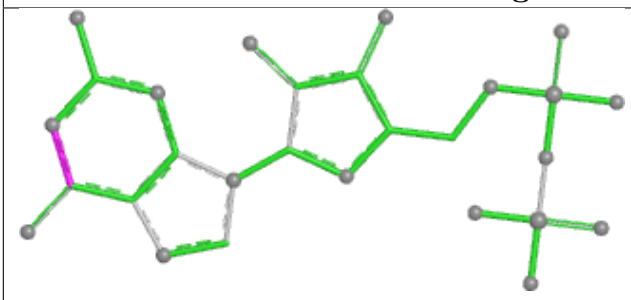
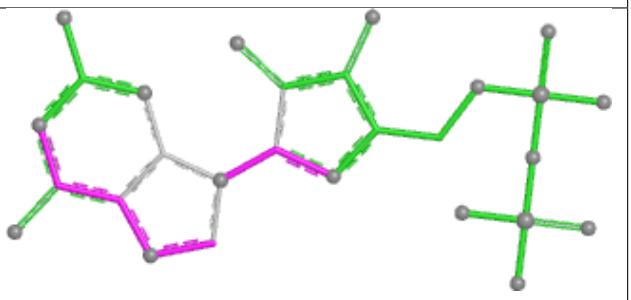
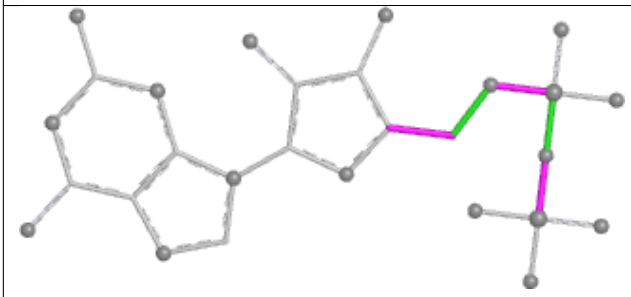


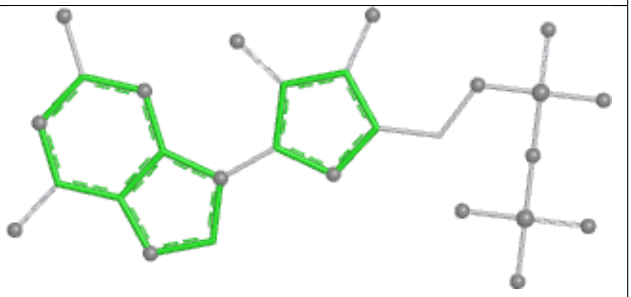
Bond lengths



Bond angles

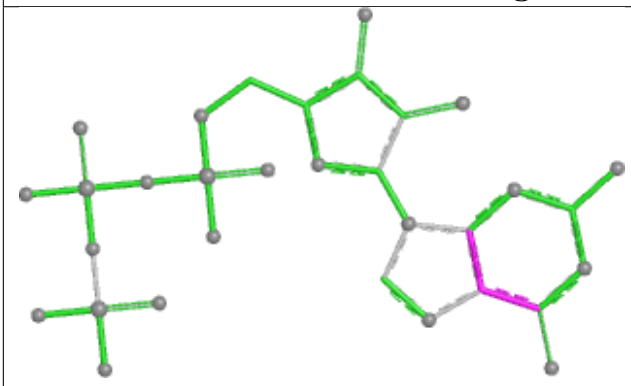


Torsions



Rings

## Ligand GTP G5 501



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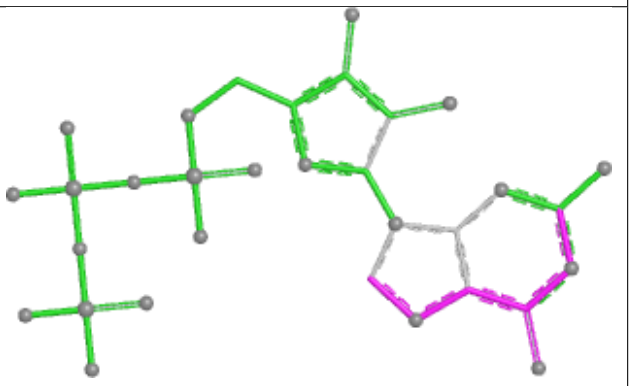
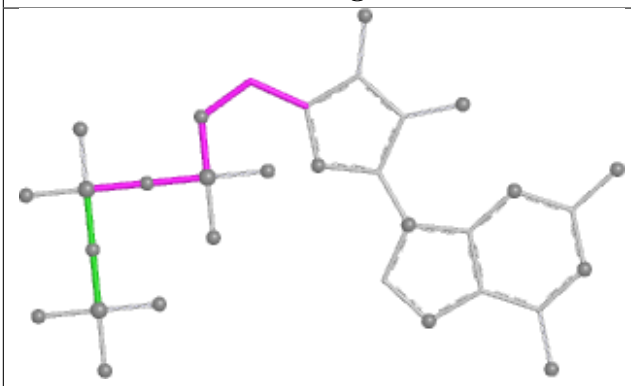


Bond angles



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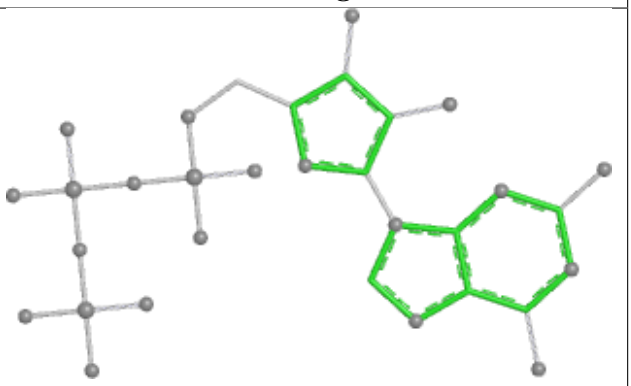

Rings

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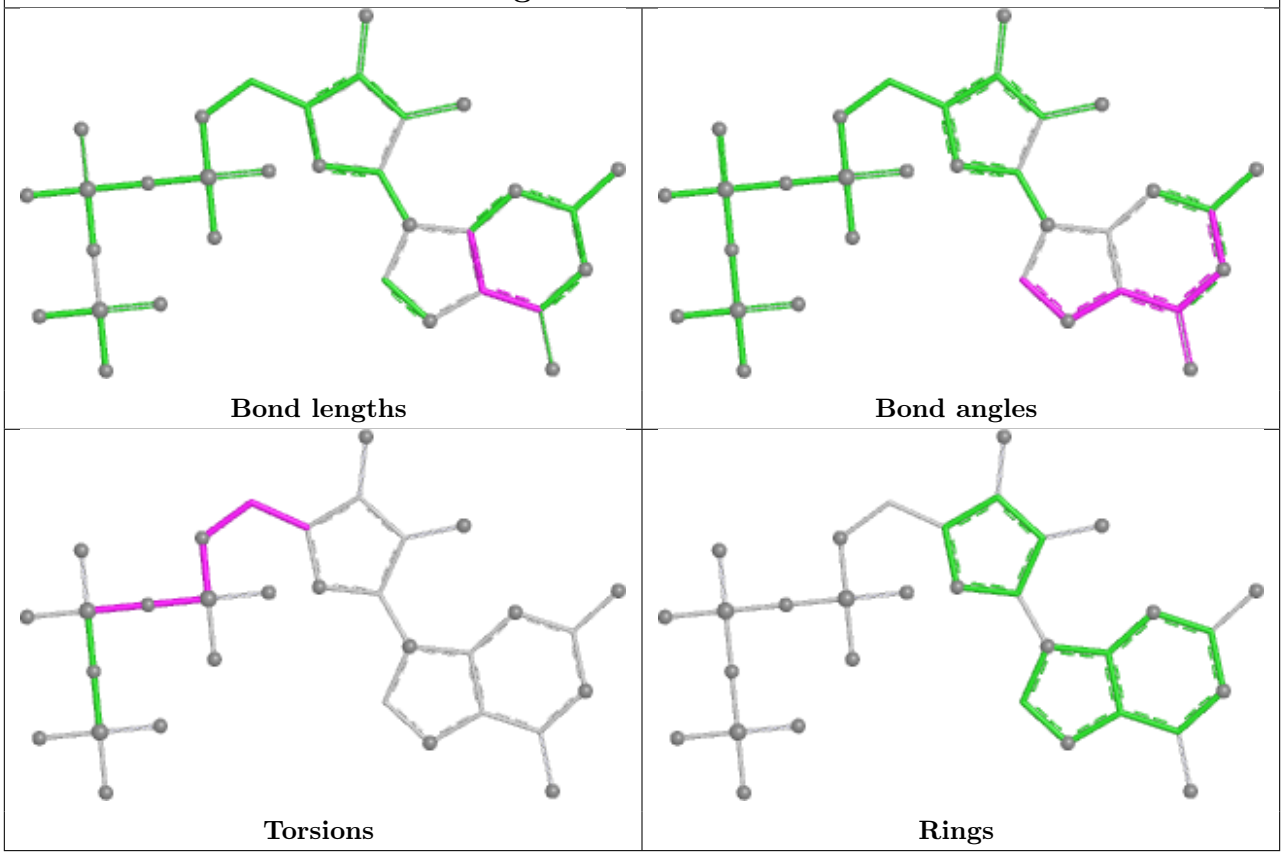


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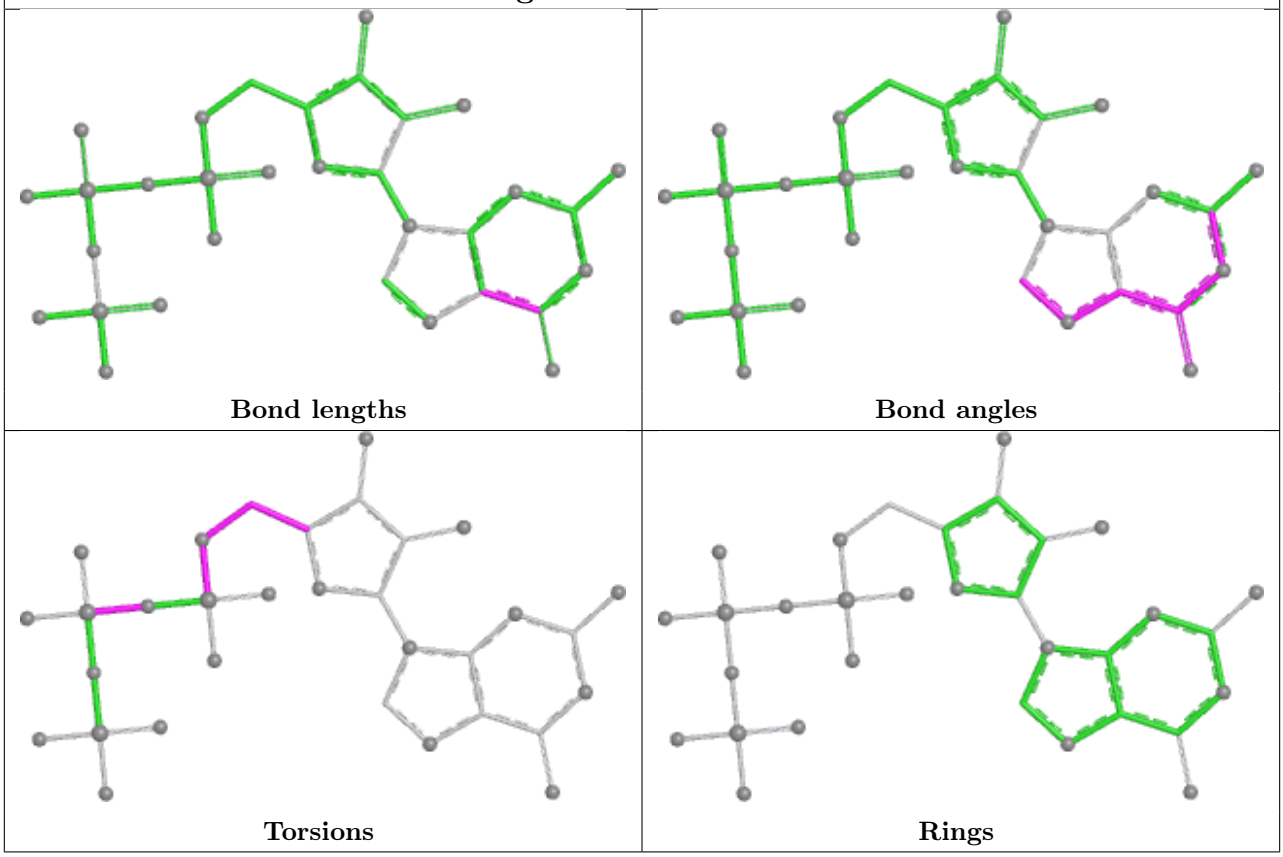
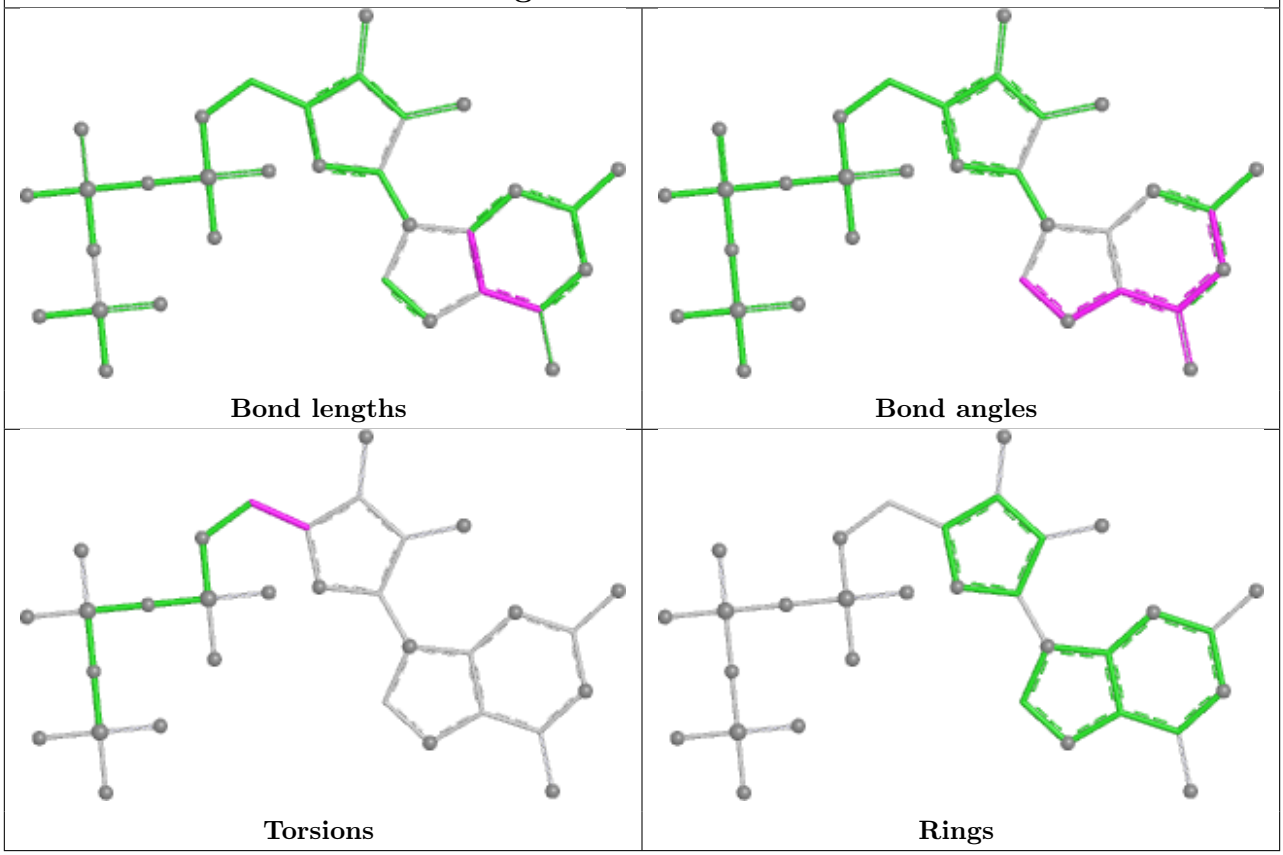
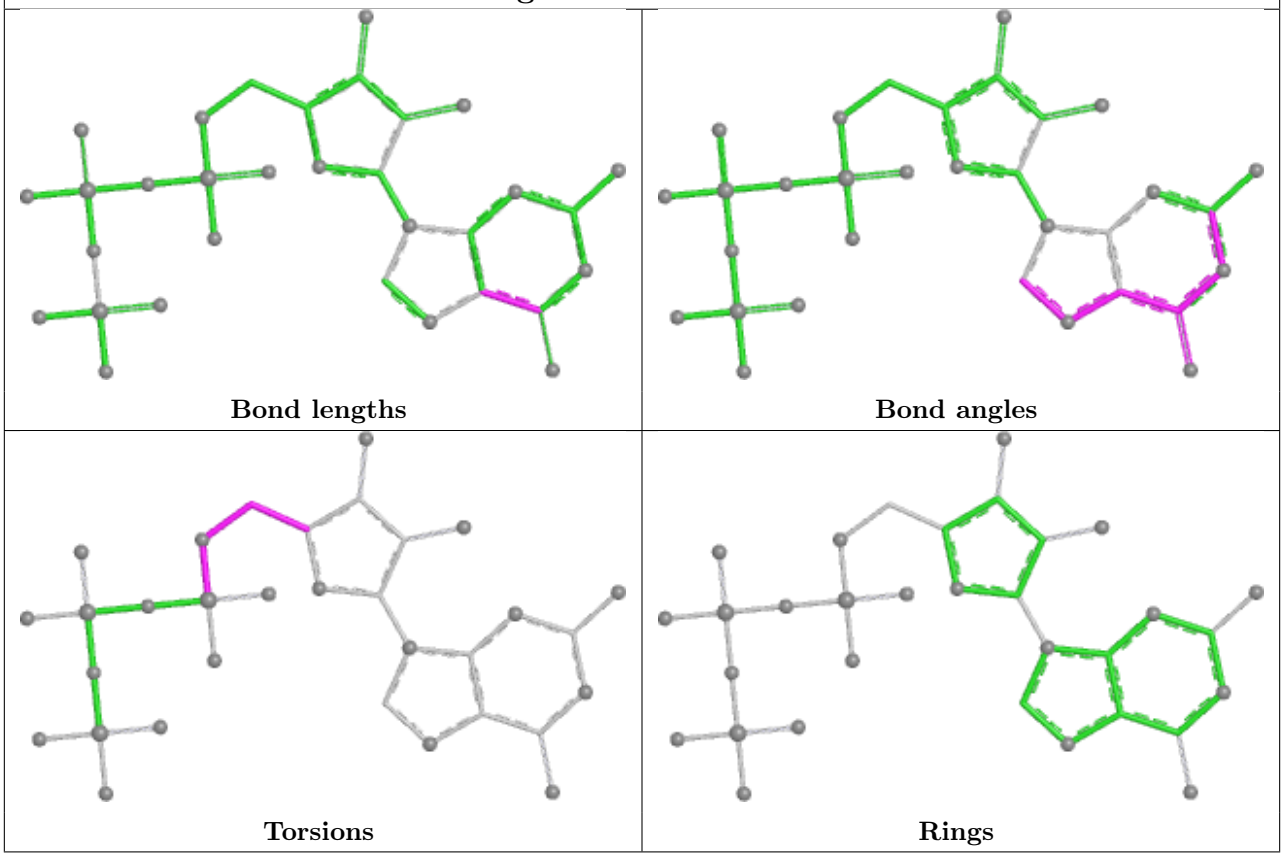


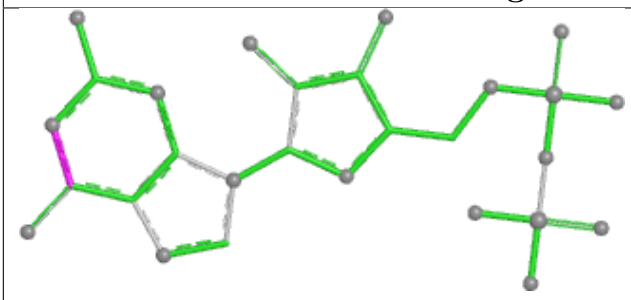
## Ligand GTP C8 501



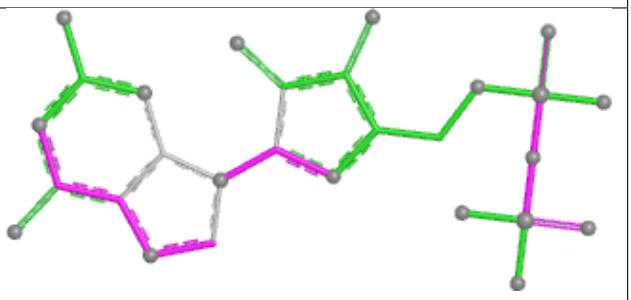

## Ligand GTP 1L 501



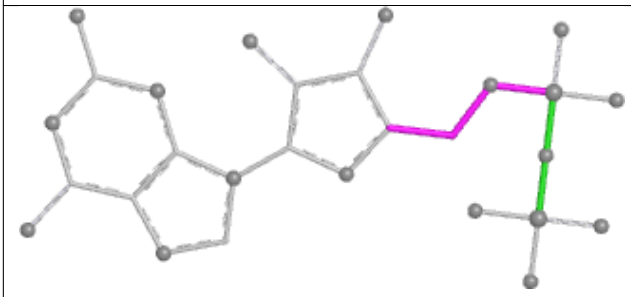
## Ligand GDP W4 502



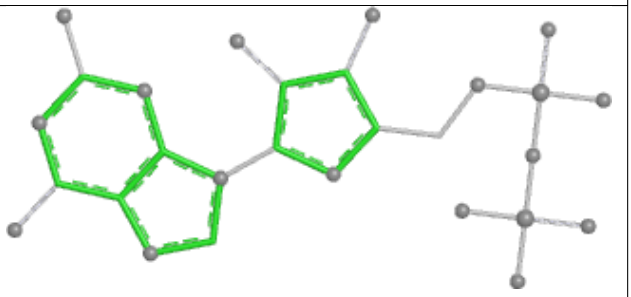
Bond lengths



Bond angles

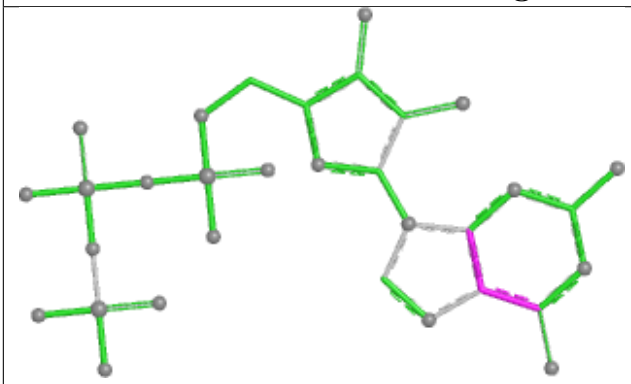


Torsions



Rings

## Ligand GTP 2Y 501



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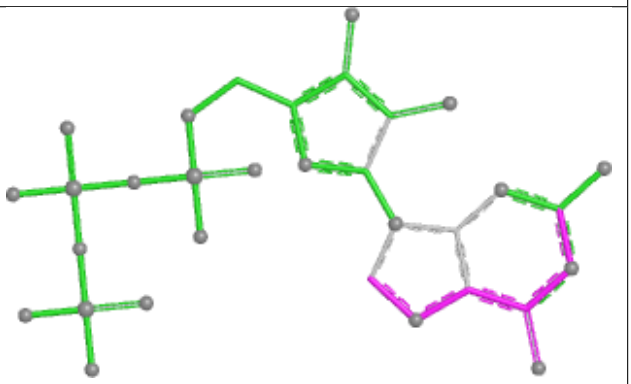

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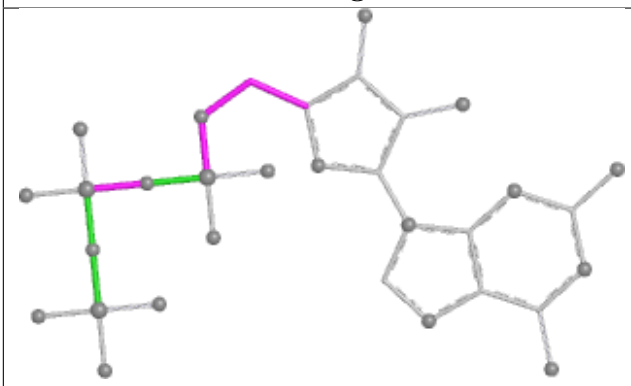
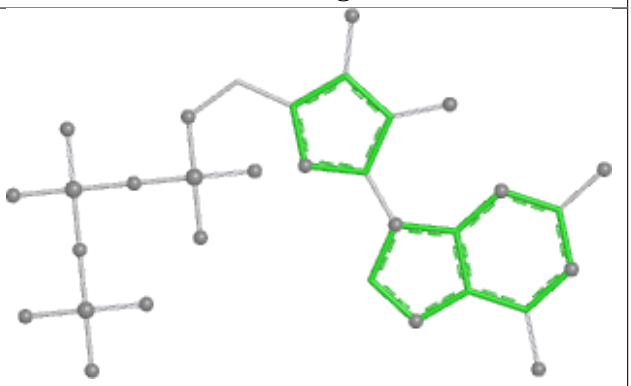
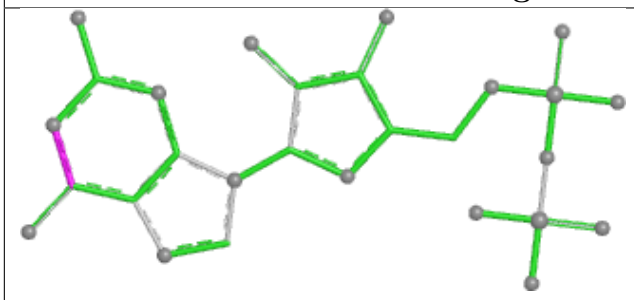


Torsions

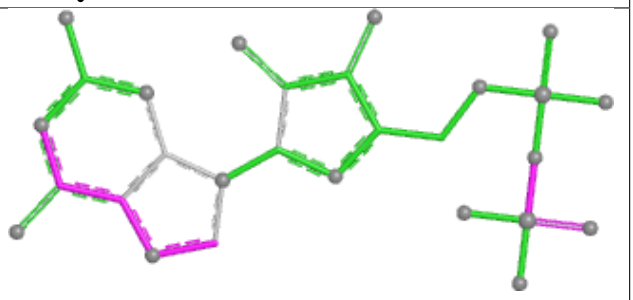


Rings

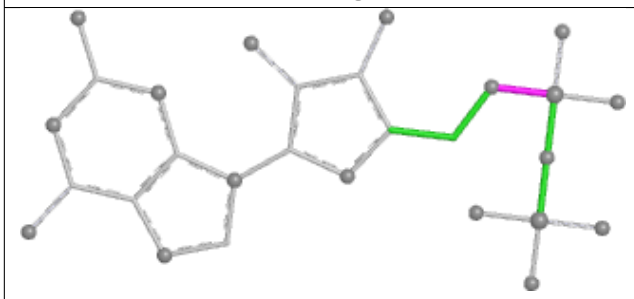
## Ligand GDP 1Q 502



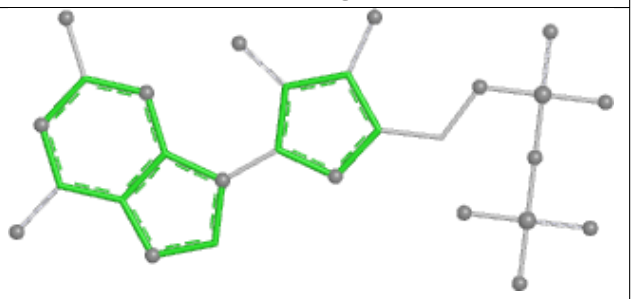
Bond lengths



Bond angles

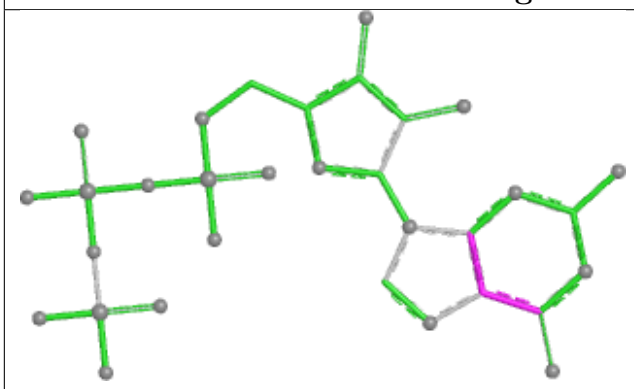


Torsions



Rings

## Ligand GTP B7 501



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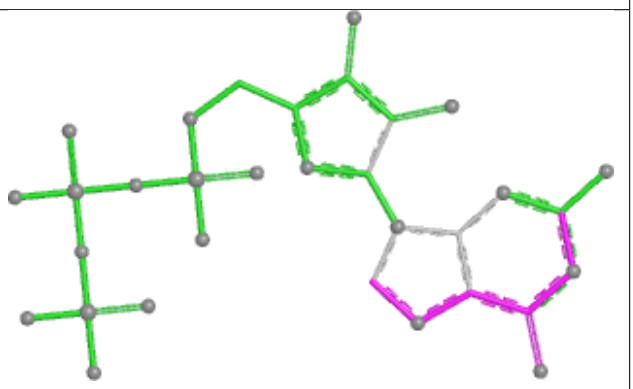
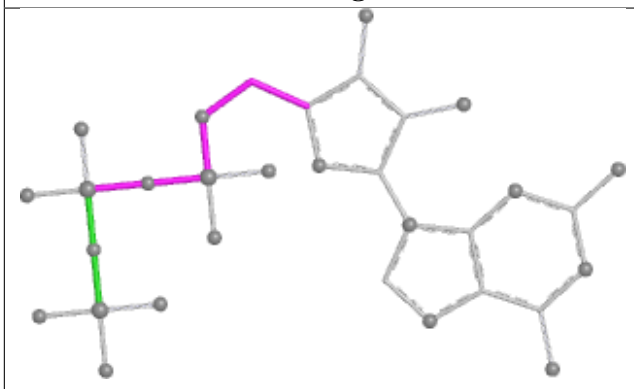


Bond angles



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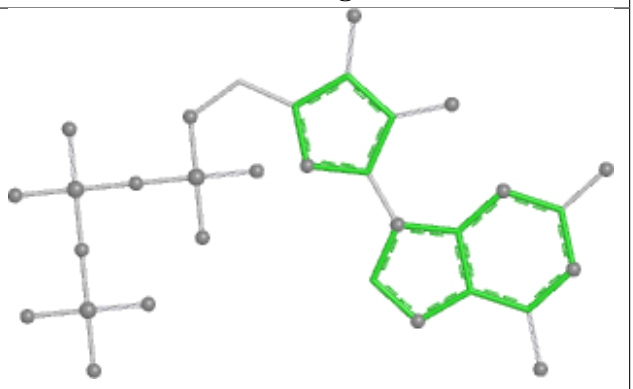

Rings

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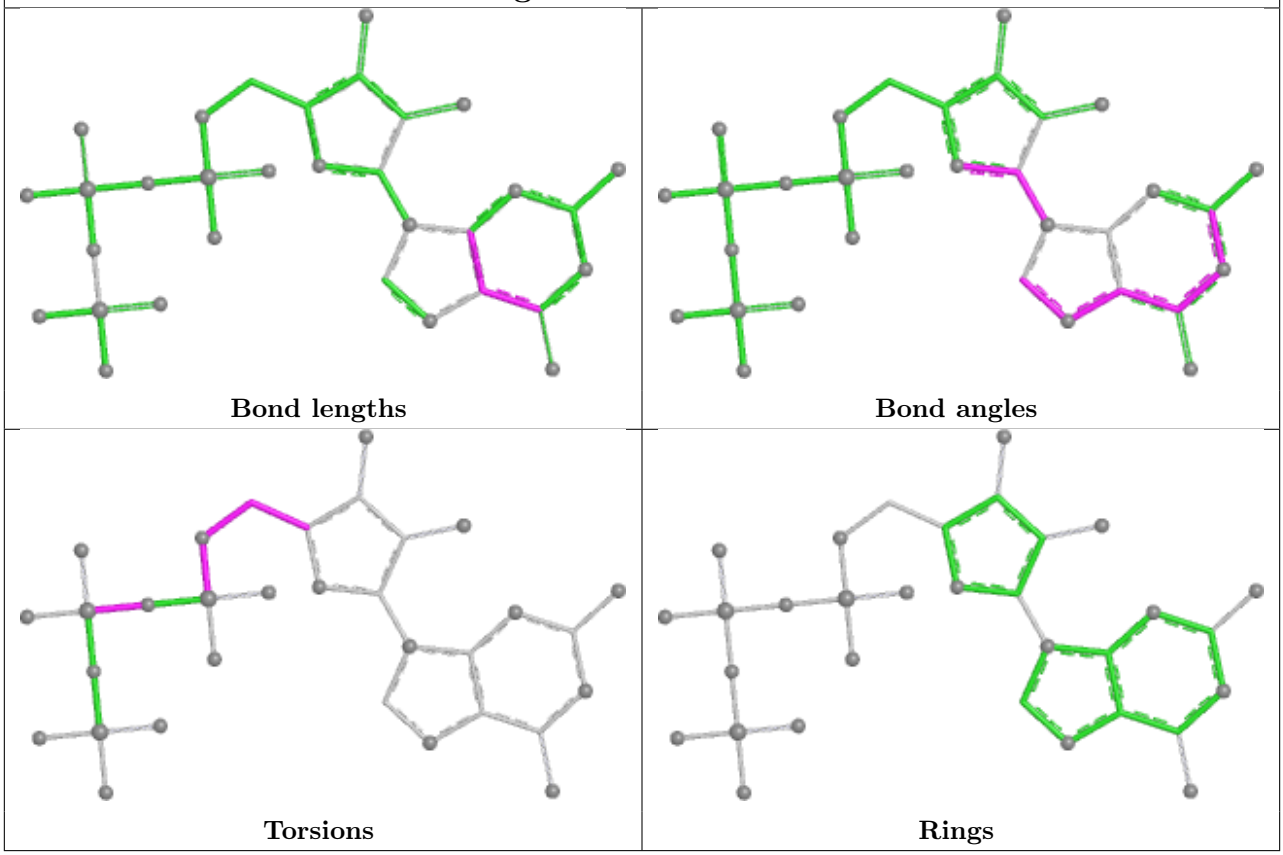
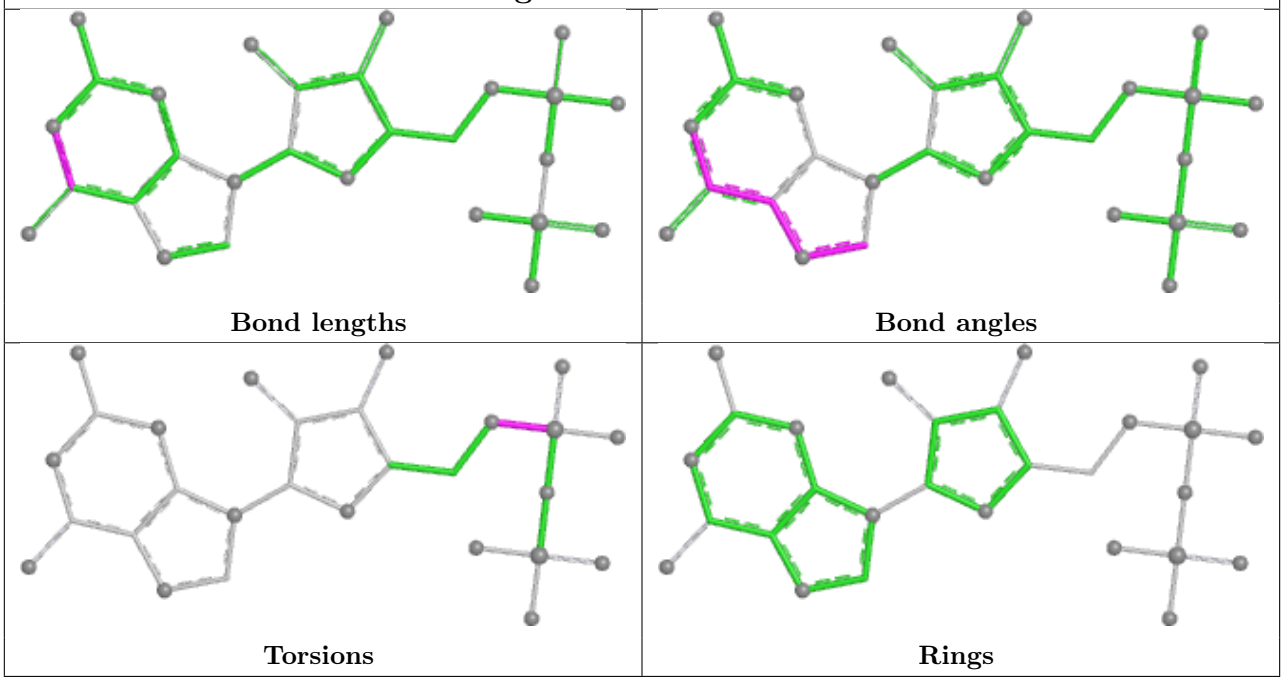
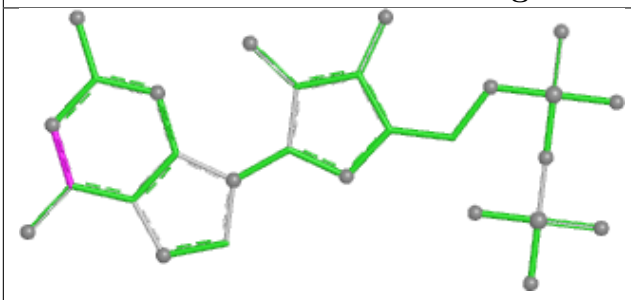


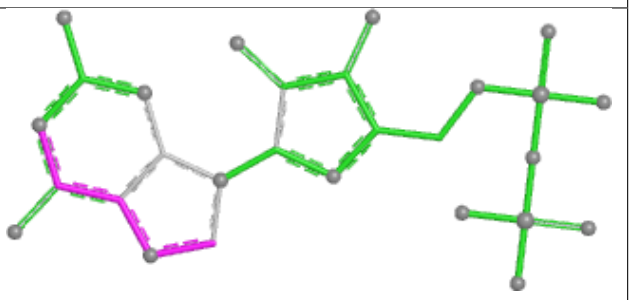

## Ligand GDP 1E 501



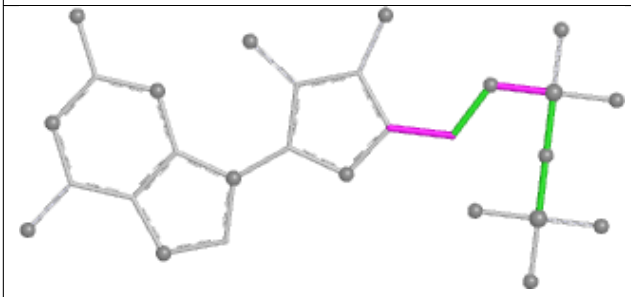
## Ligand GDP H4 501



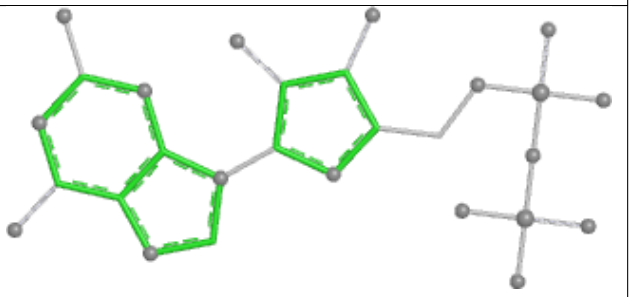
Bond lengths



Bond angles

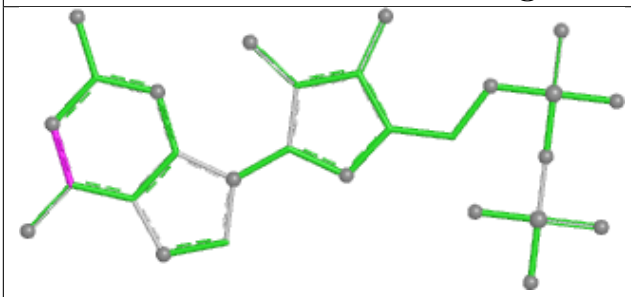


Torsions



Rings

## Ligand GDP I8 502



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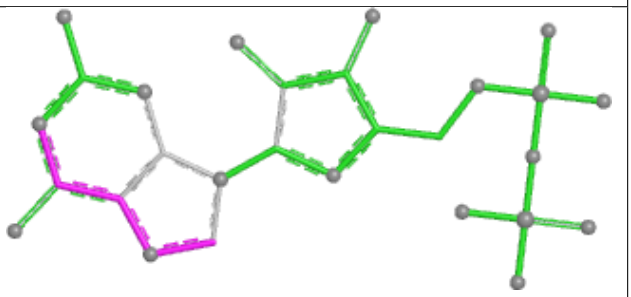

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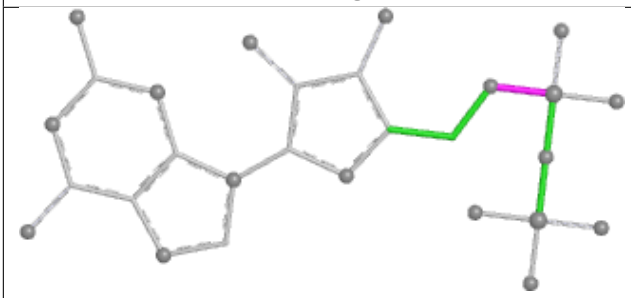

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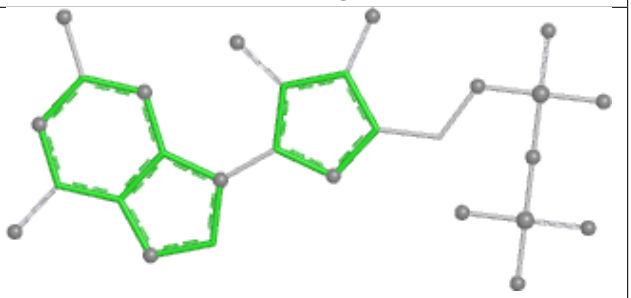

Rings

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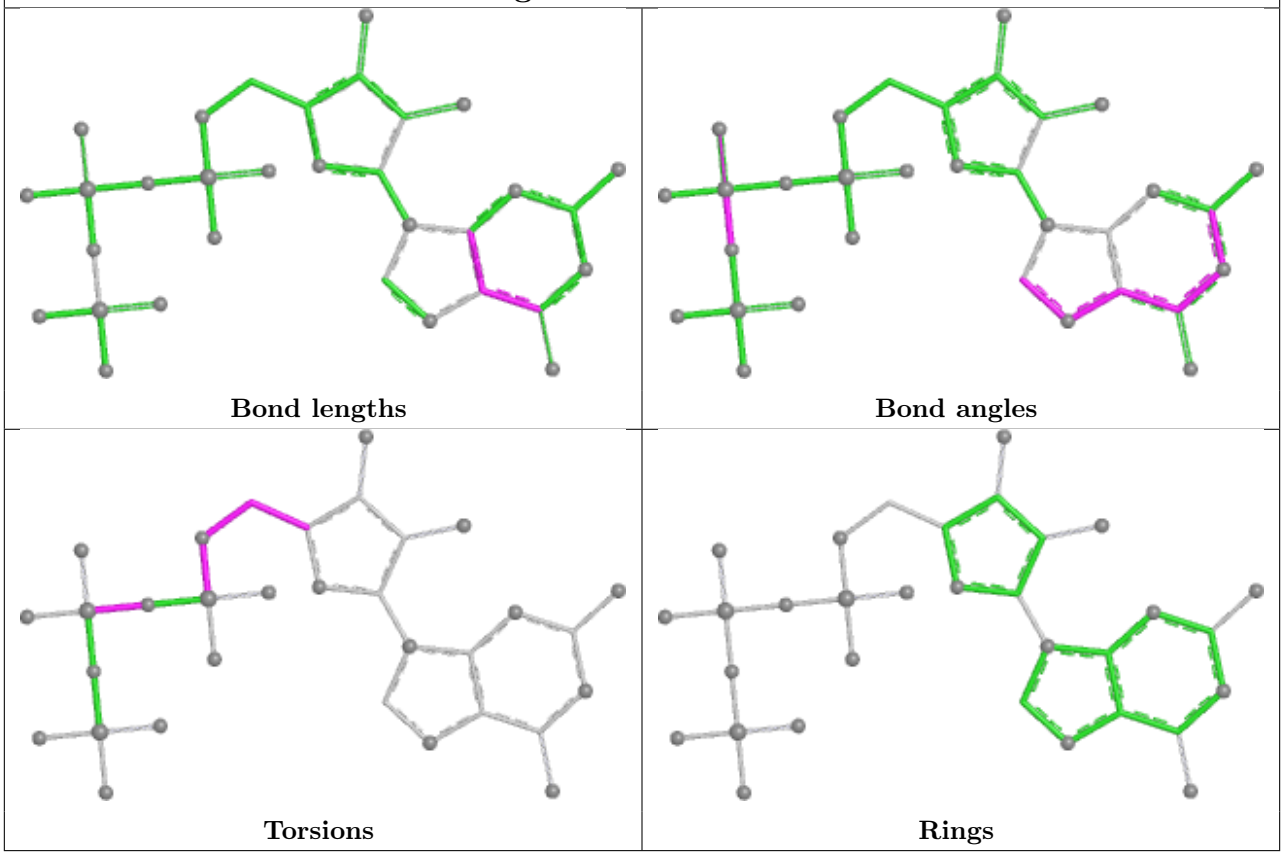


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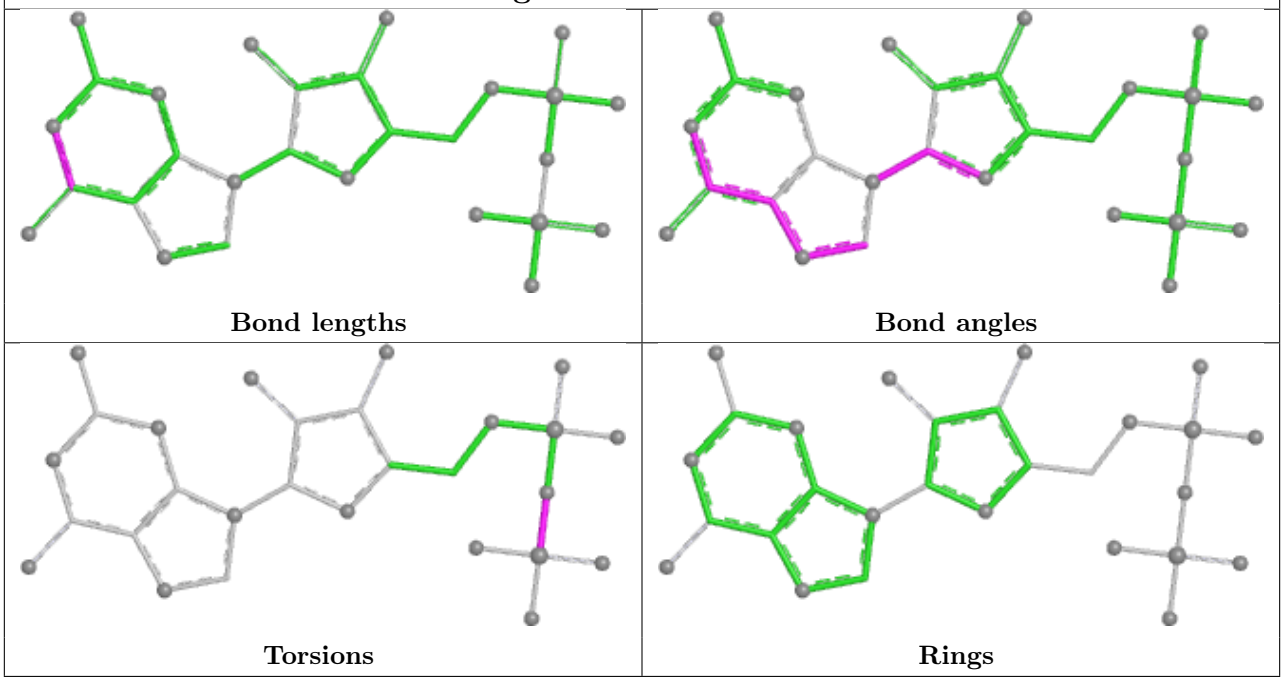

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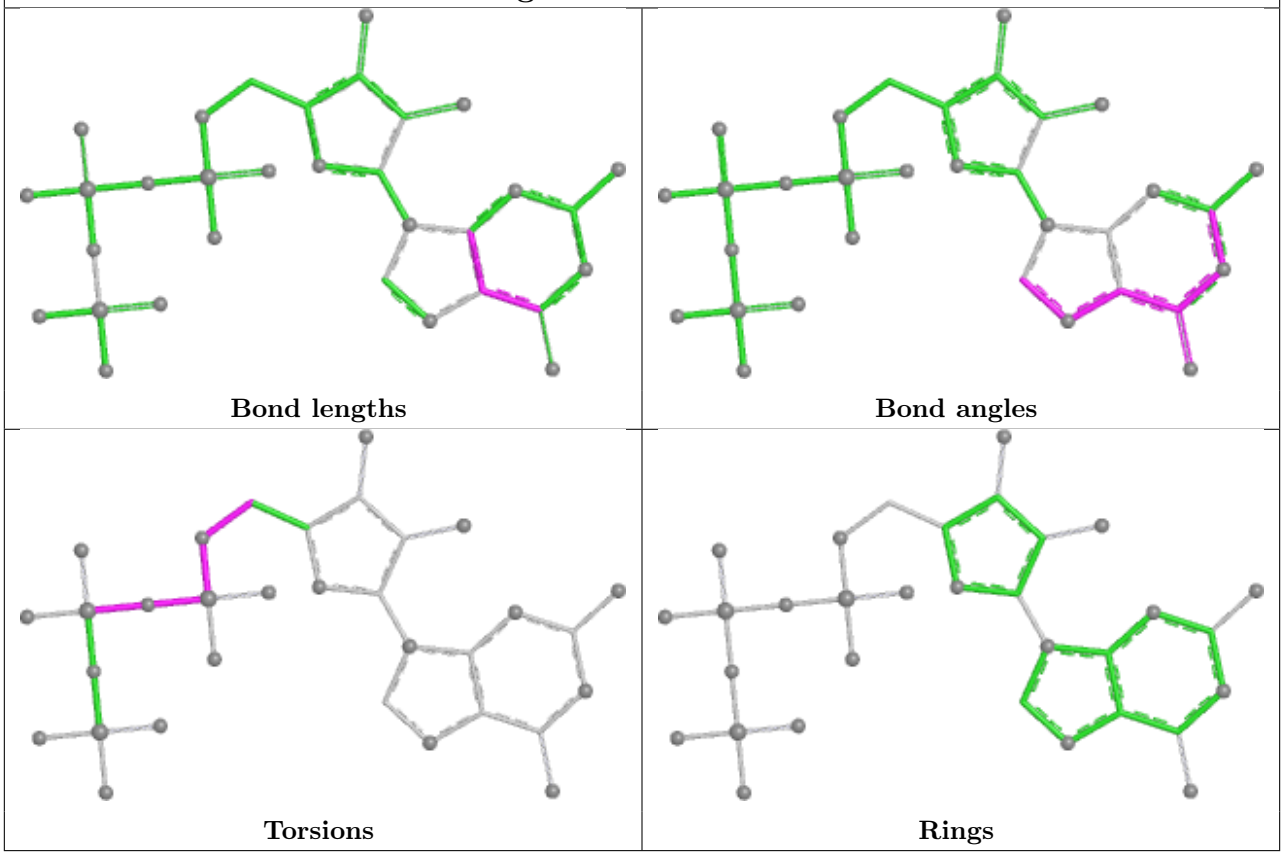


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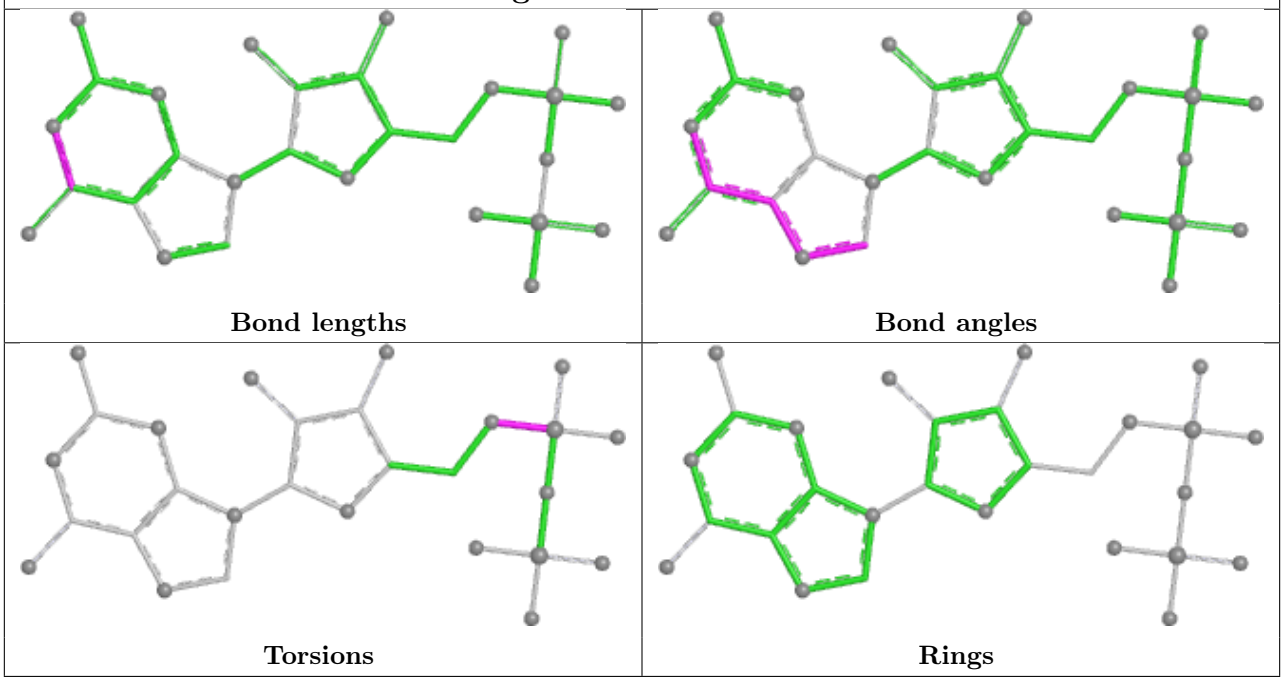

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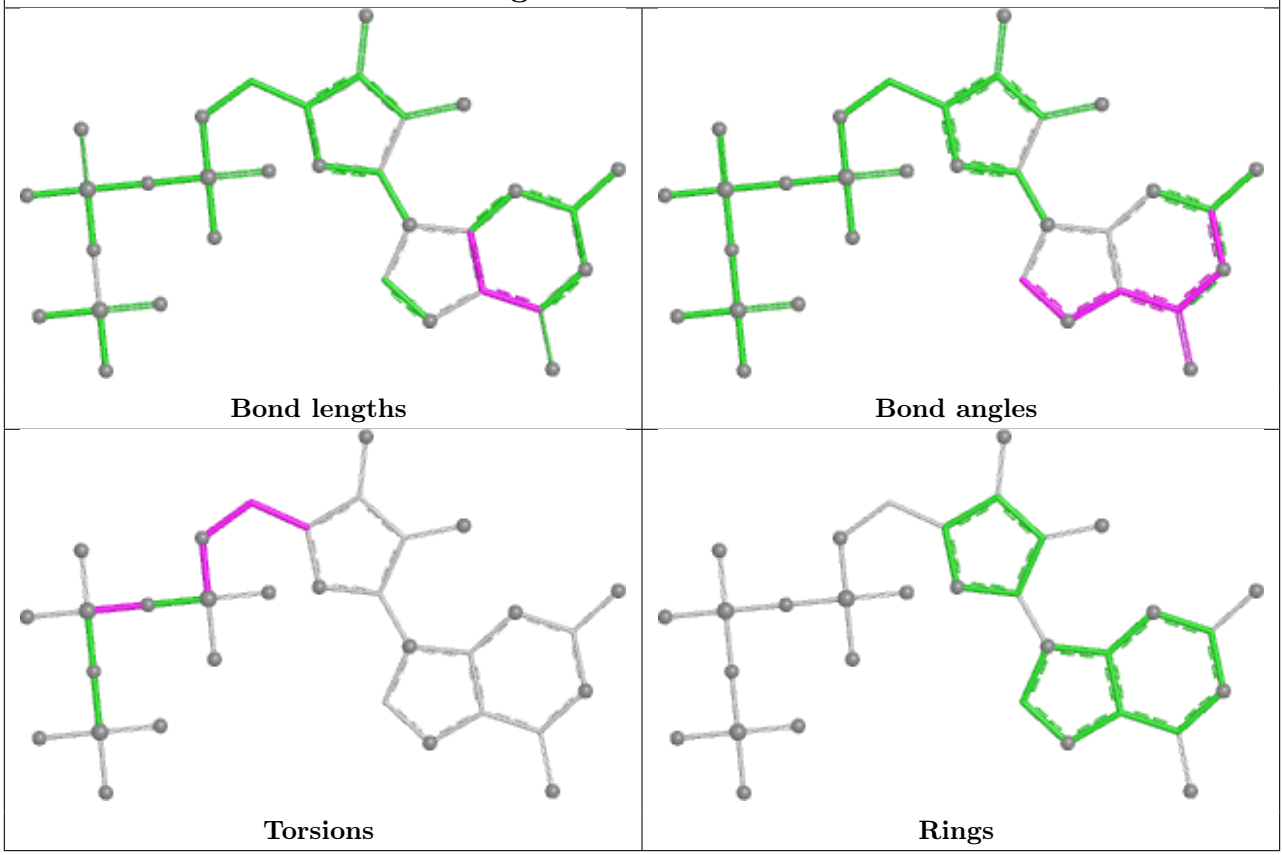


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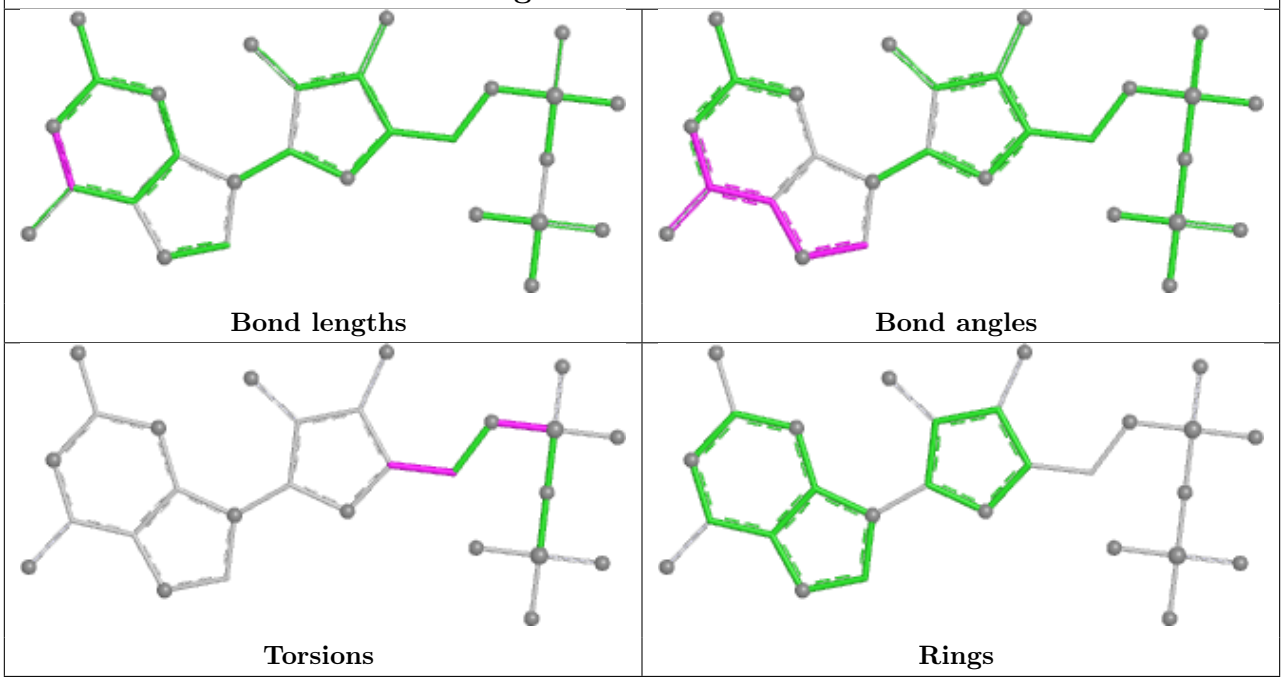

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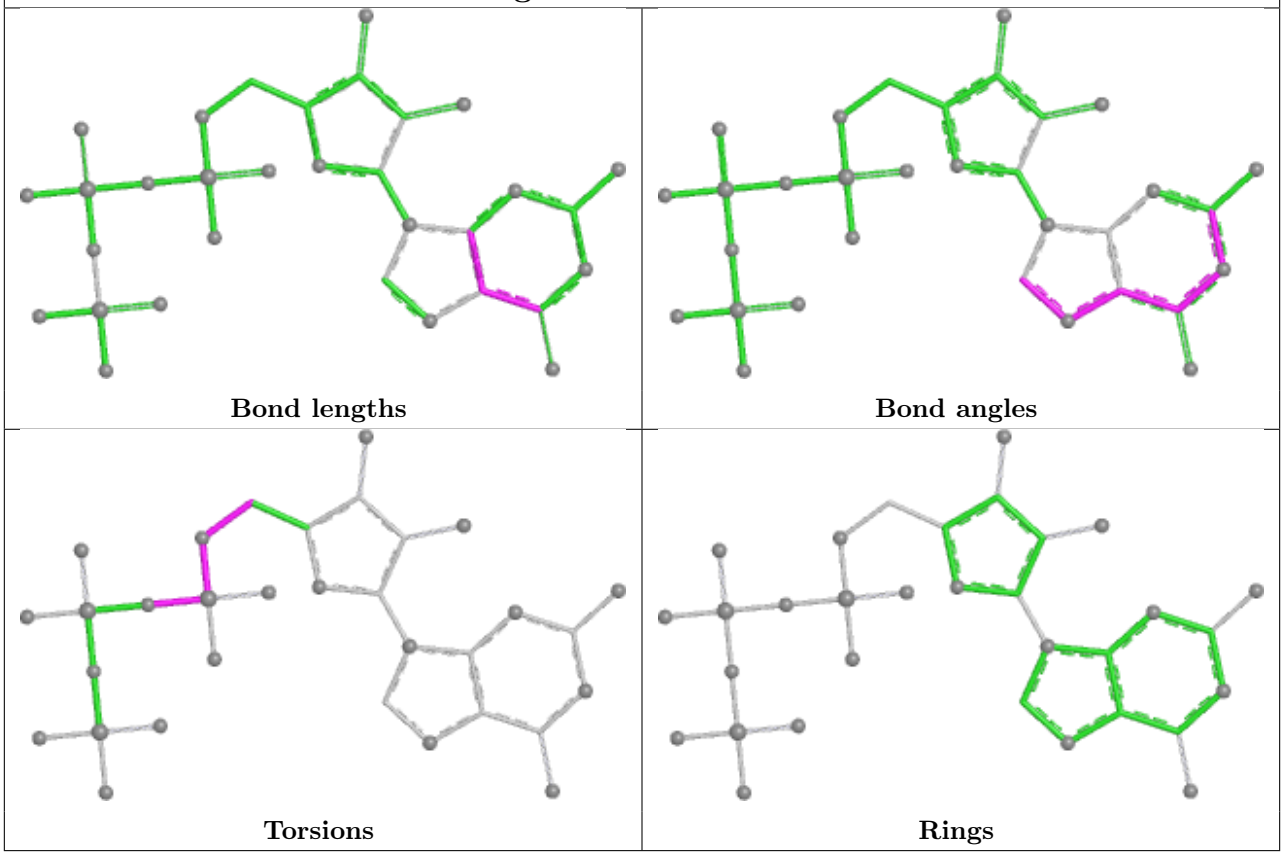


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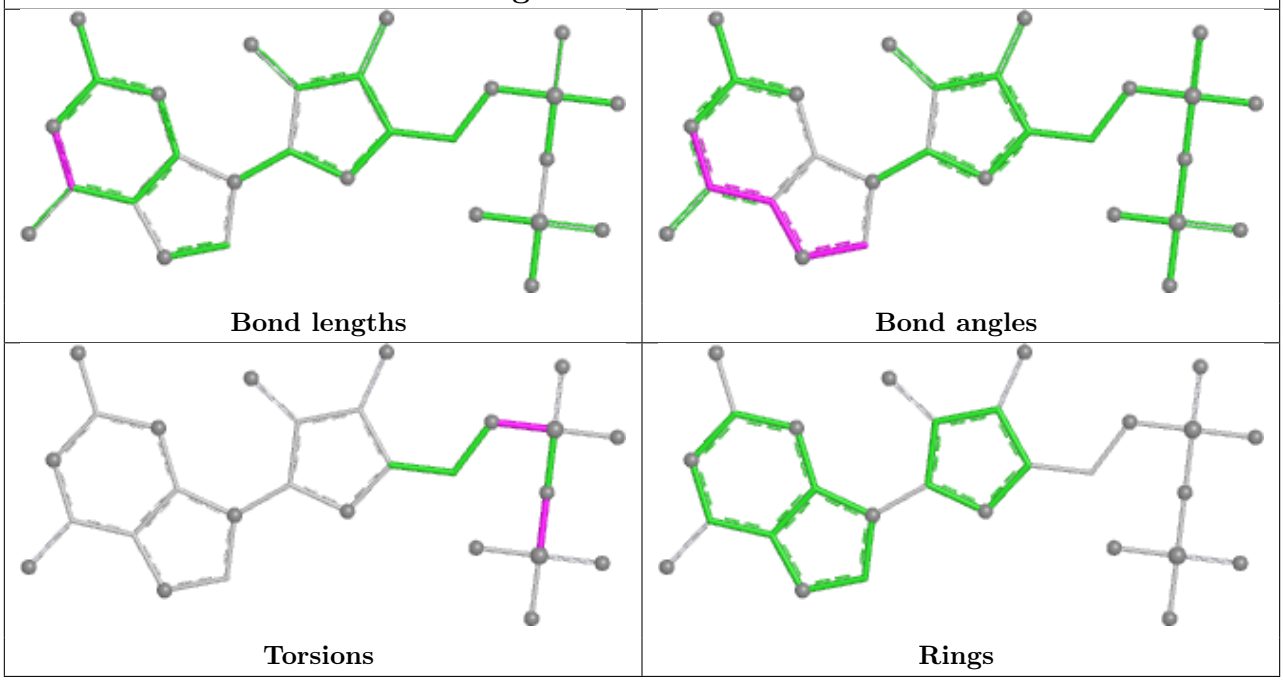

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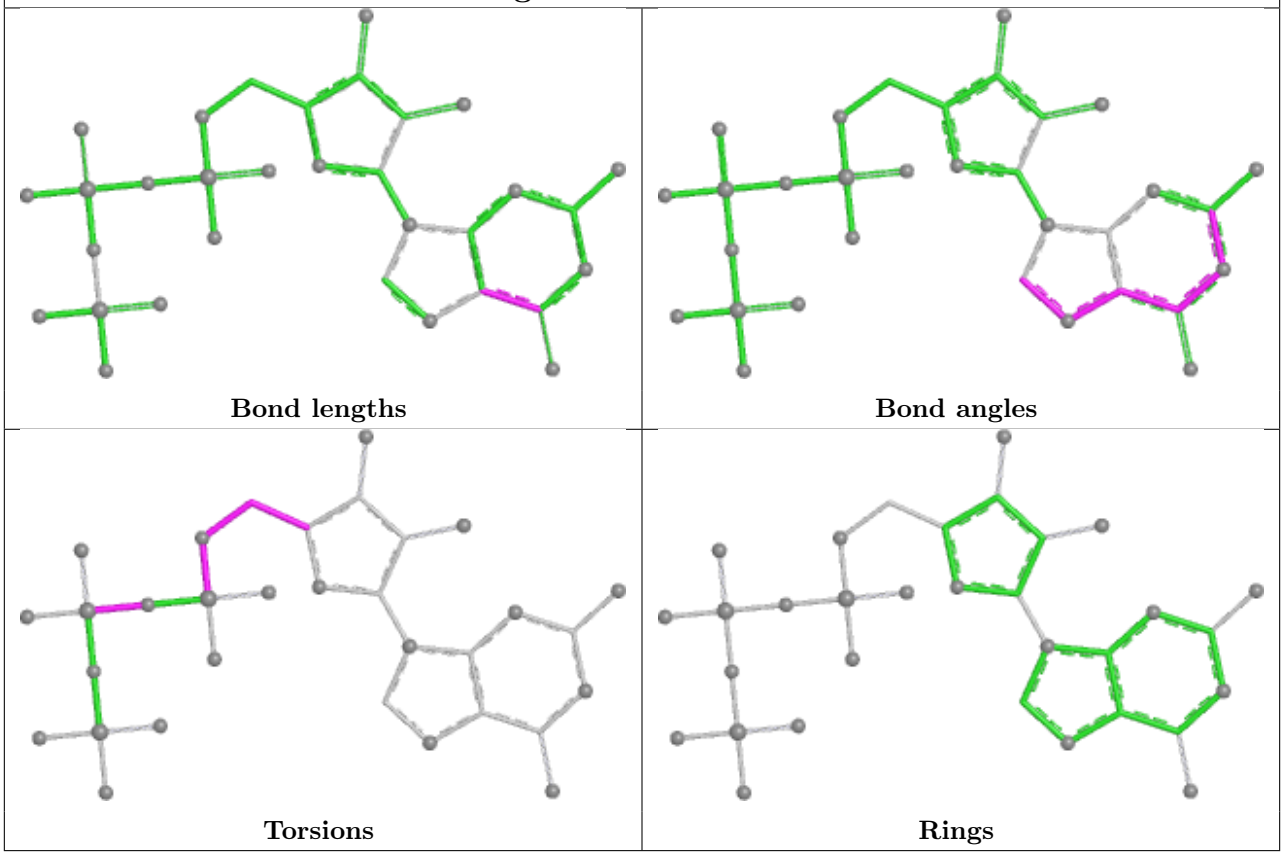


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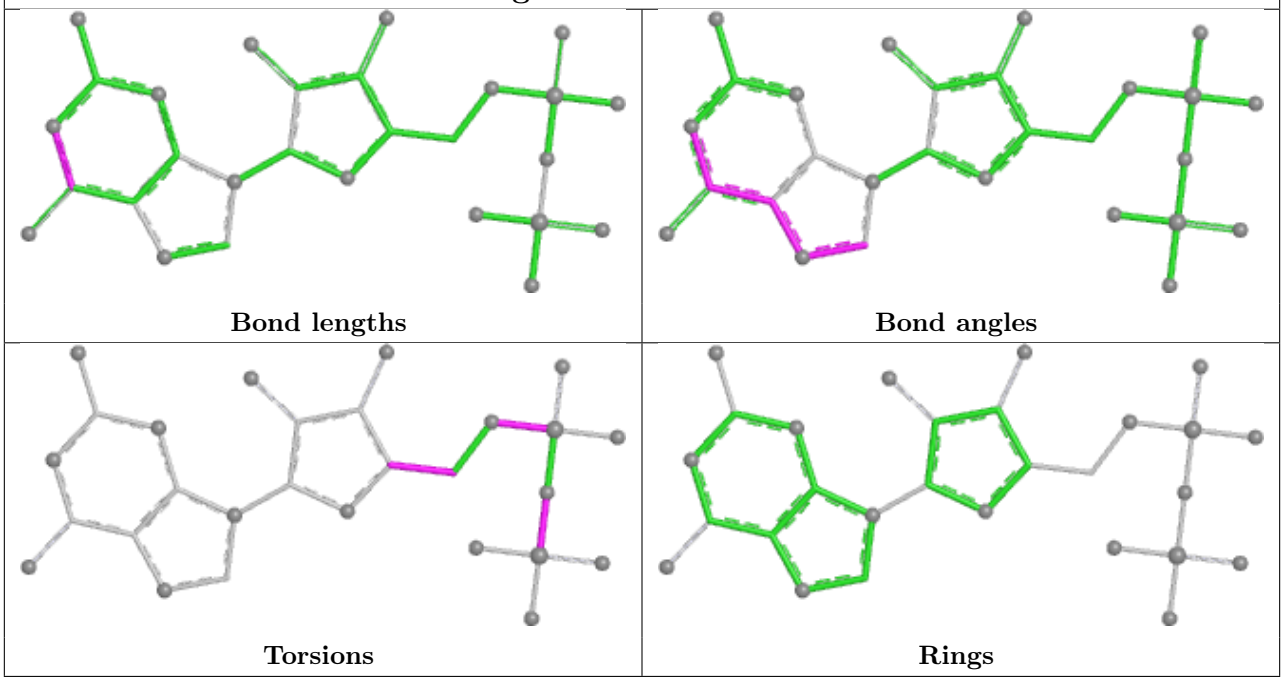

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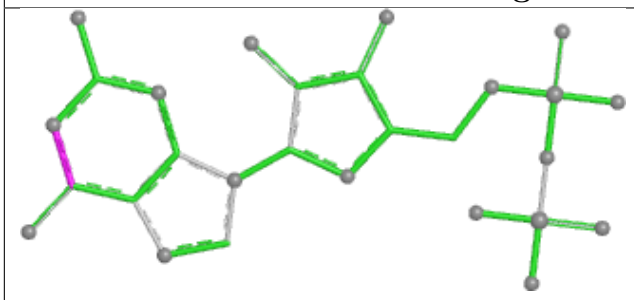

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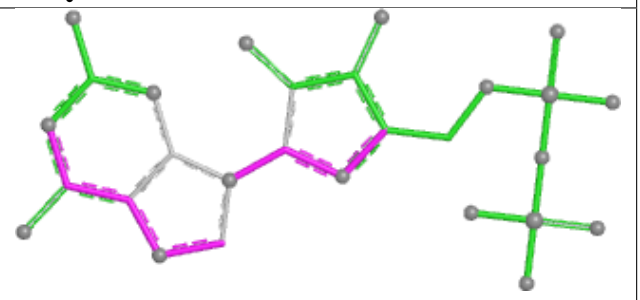
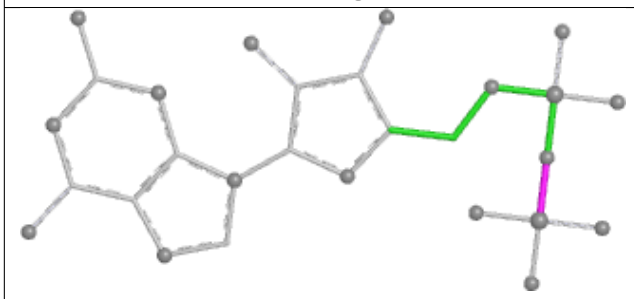
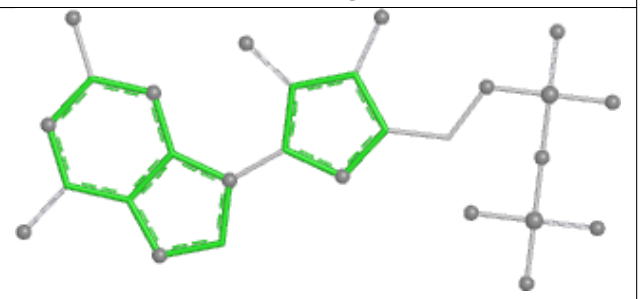


Bond angles

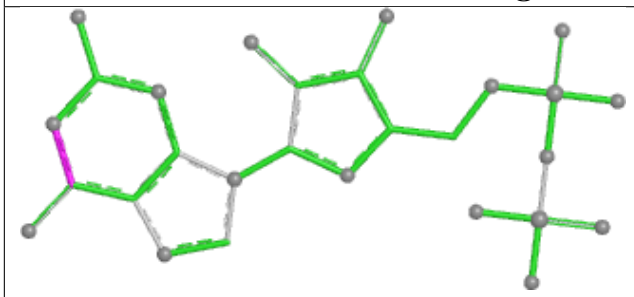


Torsions



Rings

## Ligand GDP F0 502



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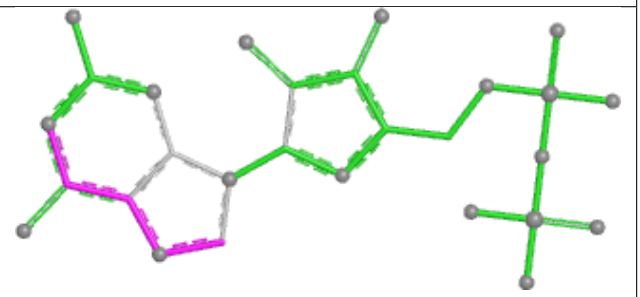

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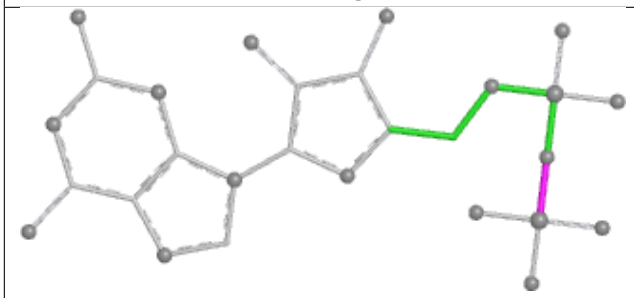

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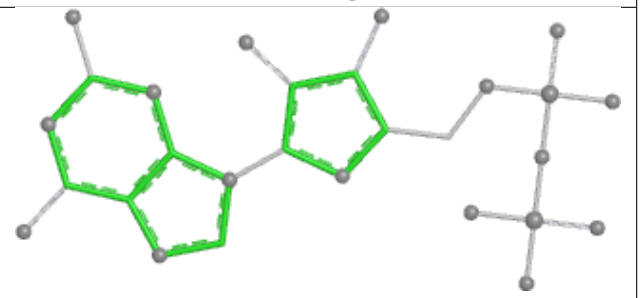

Rings

| Ligand GDP A3 501 | |
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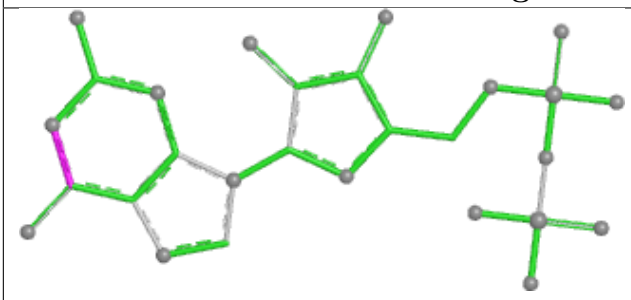
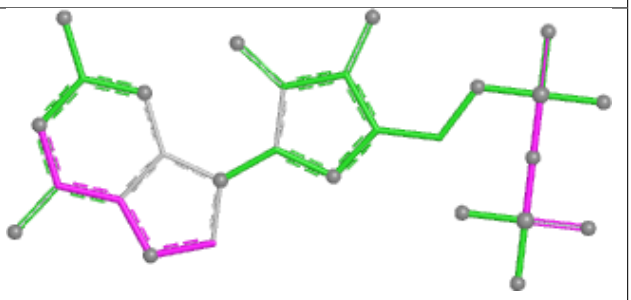
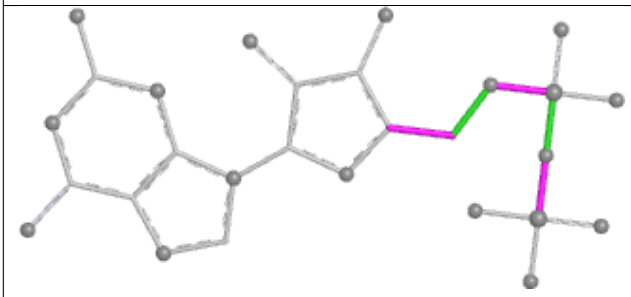
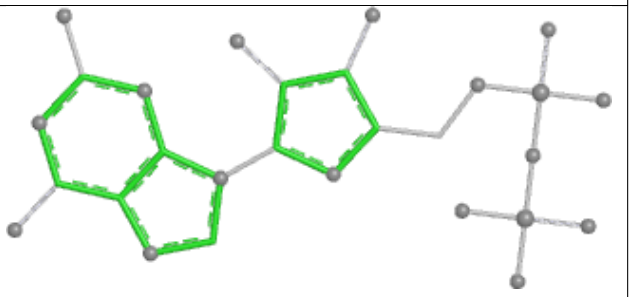
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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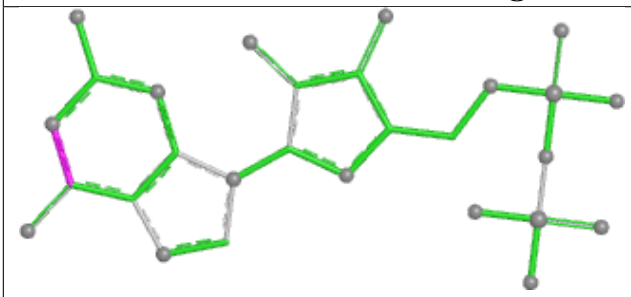
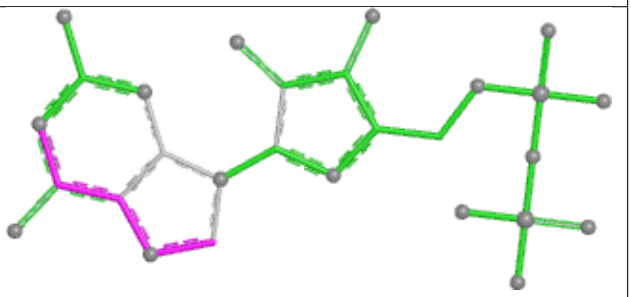
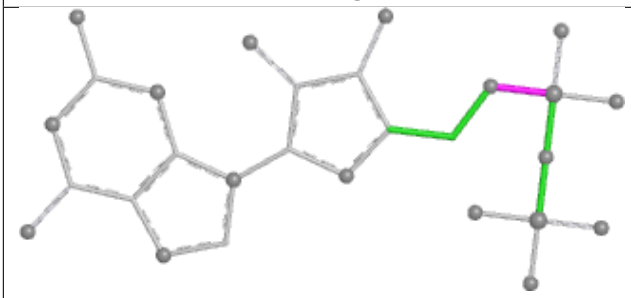
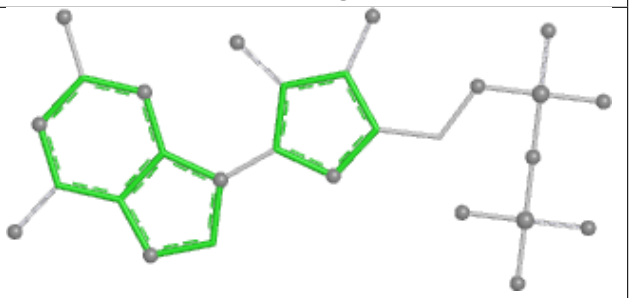
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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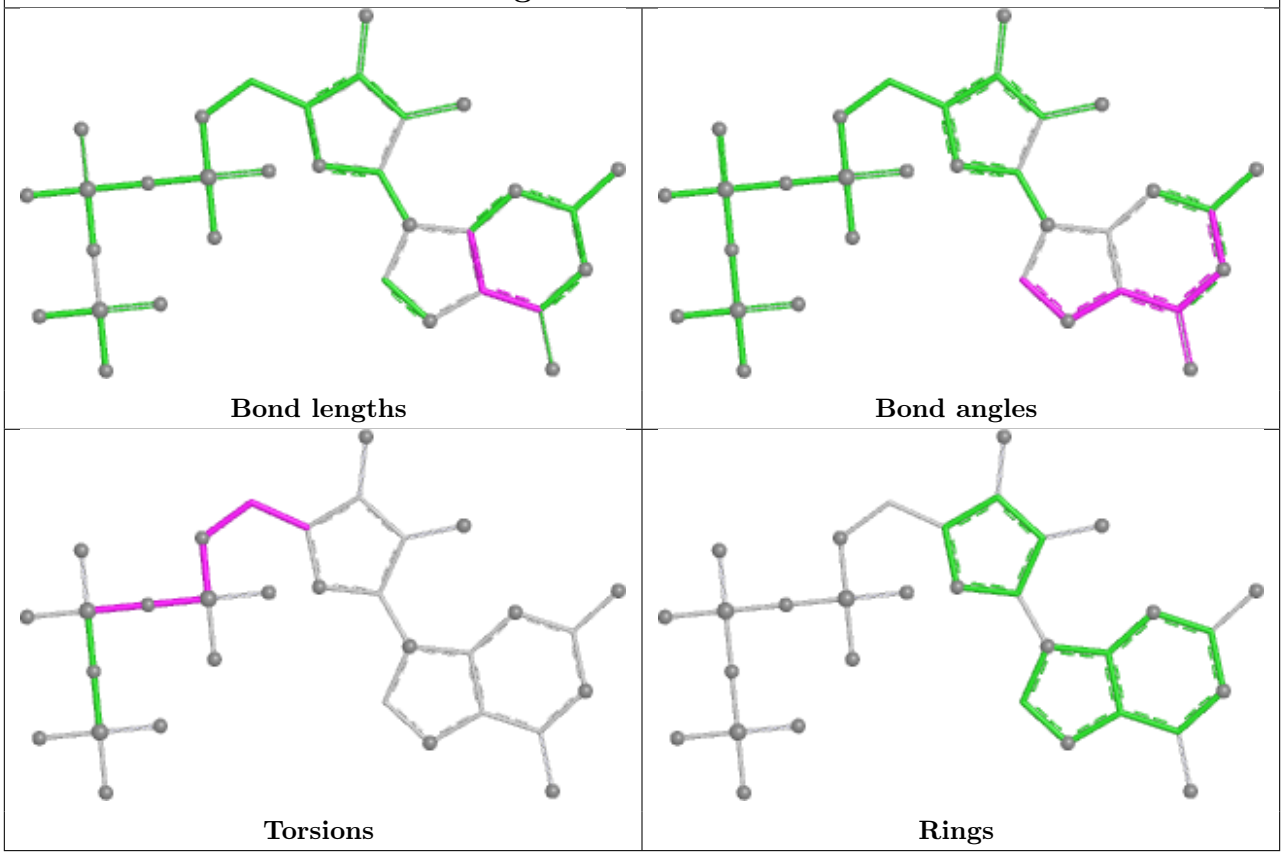
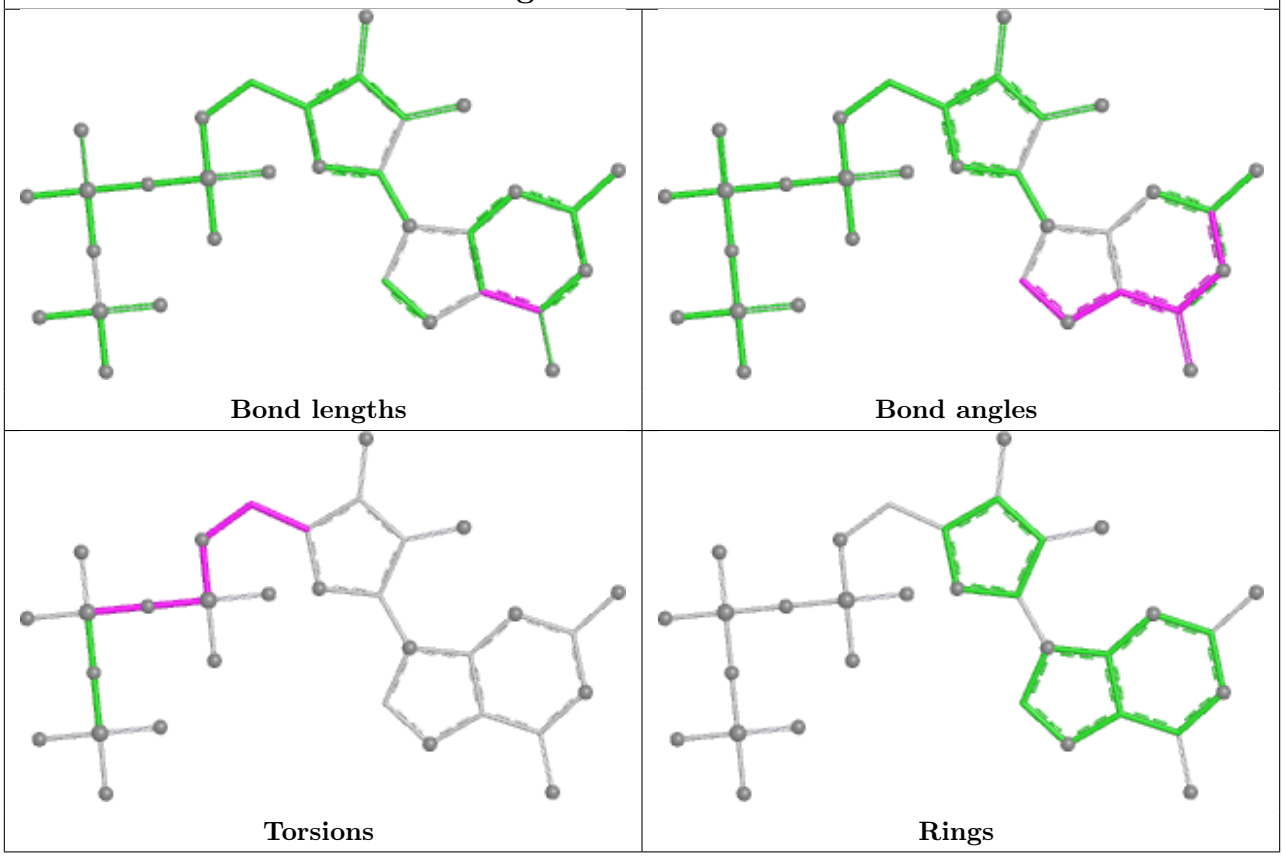



## Ligand GTP Z3 501



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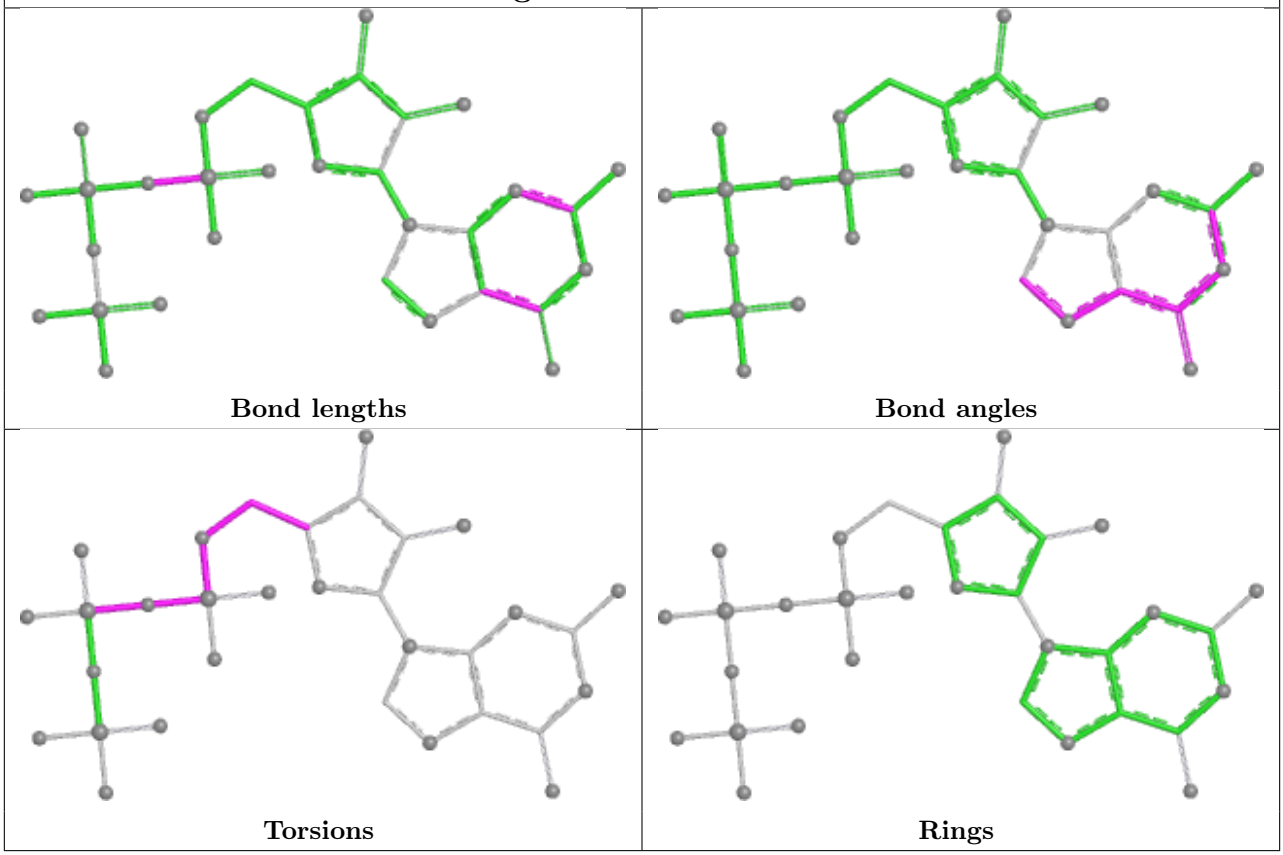


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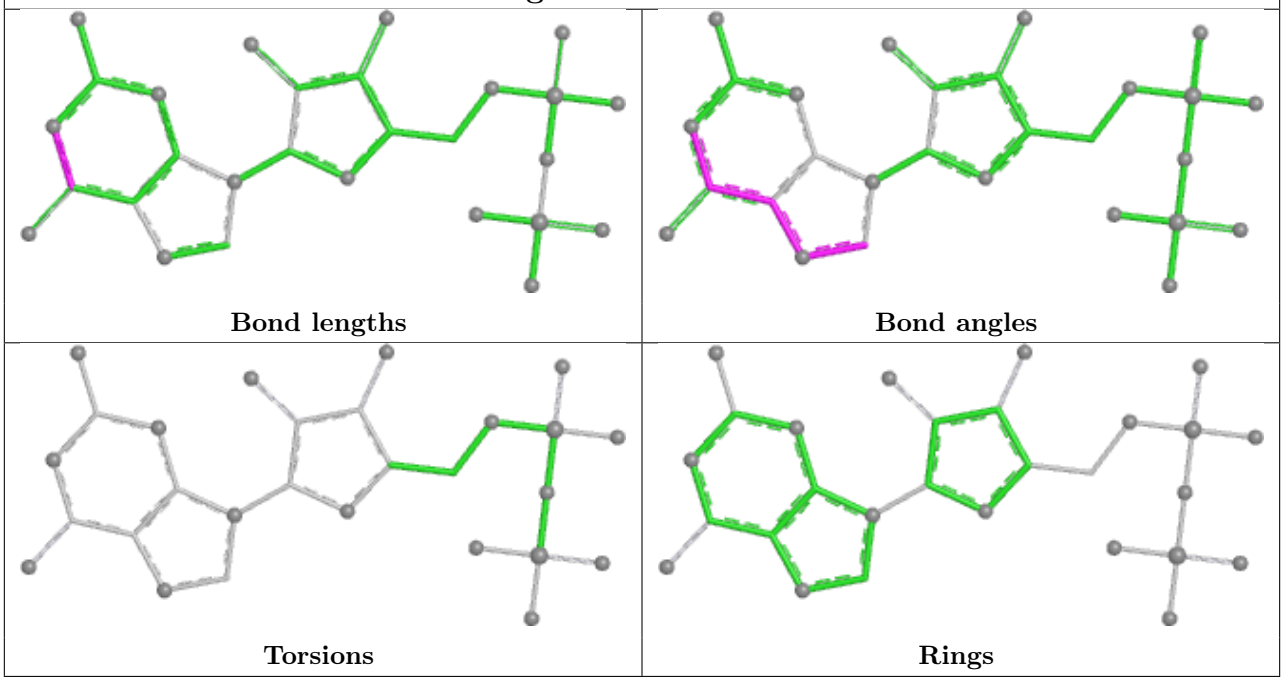

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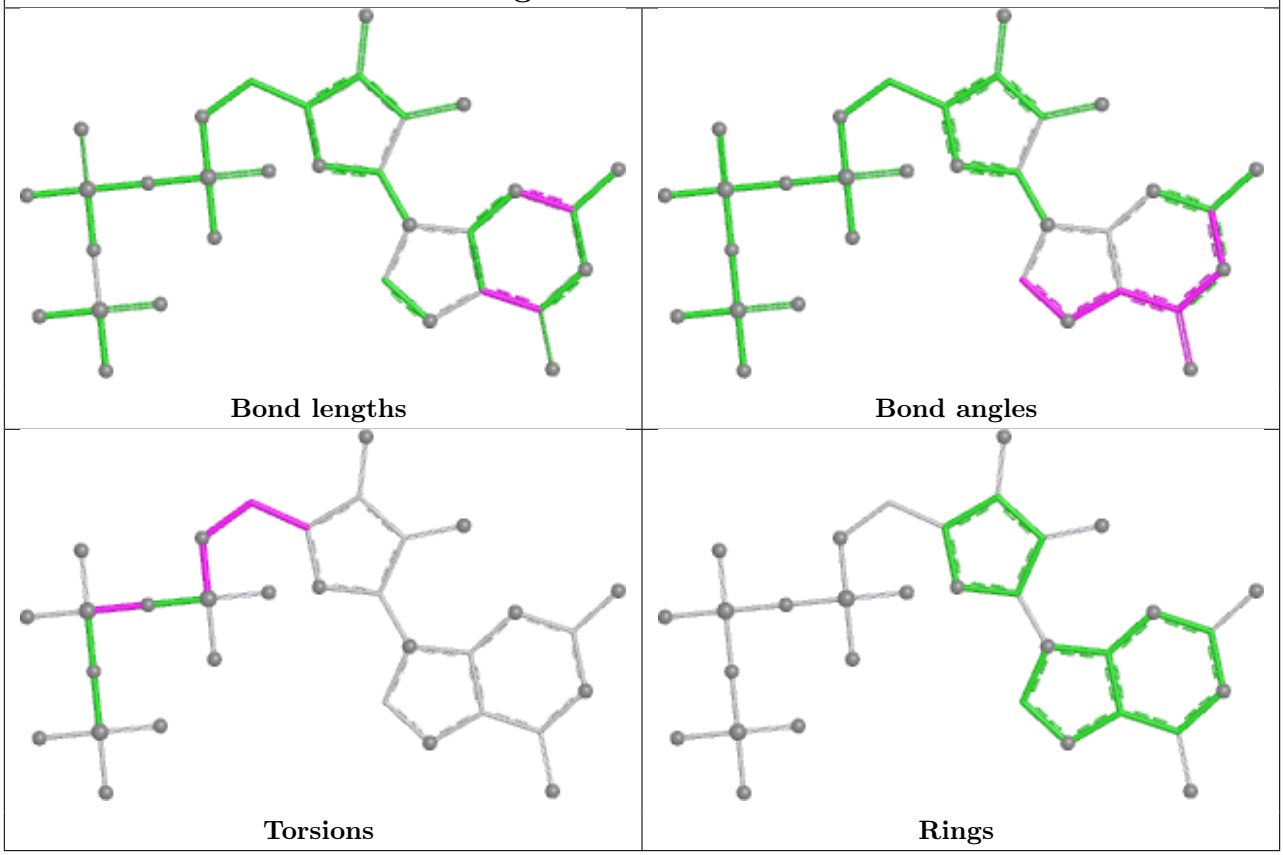


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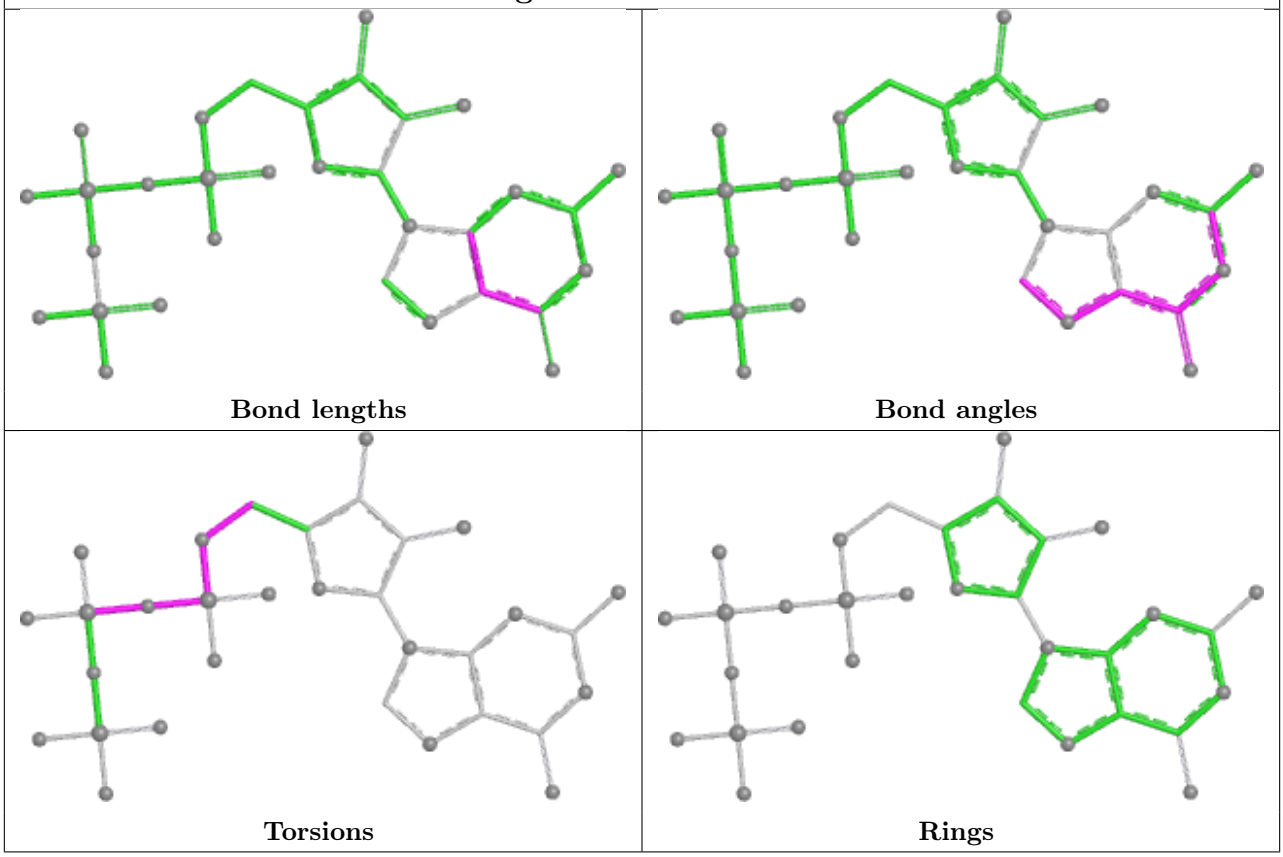

| Ligand GDP X2 501 | |
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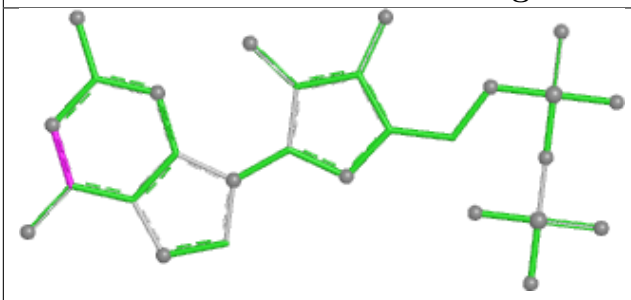
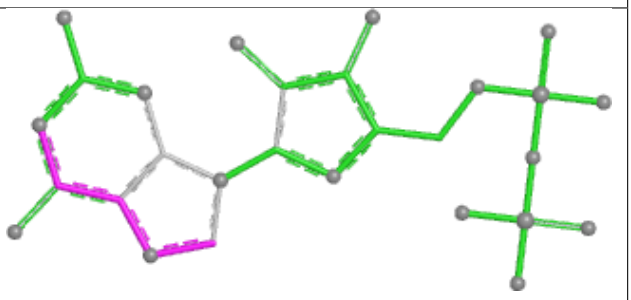
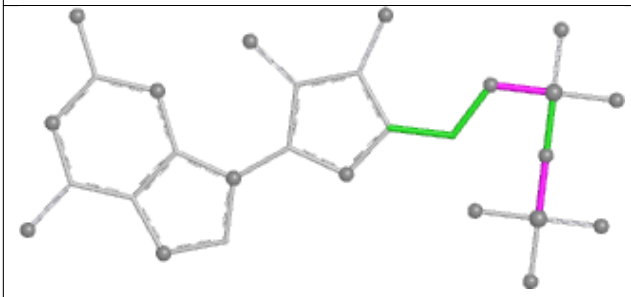
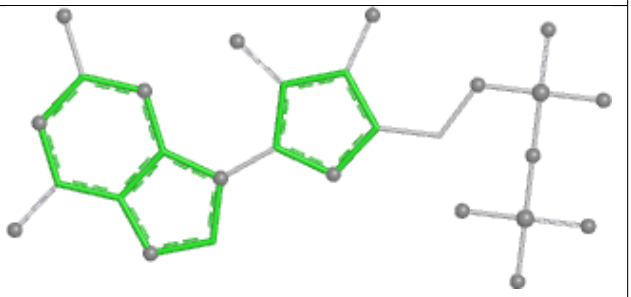
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 1K 501 | |
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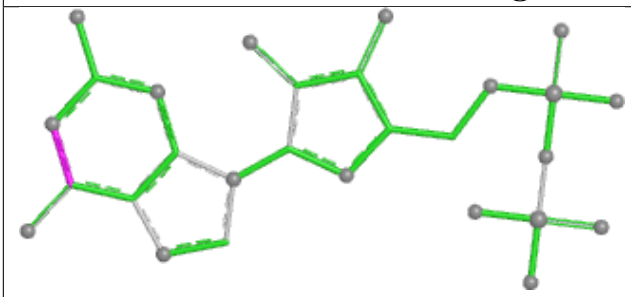
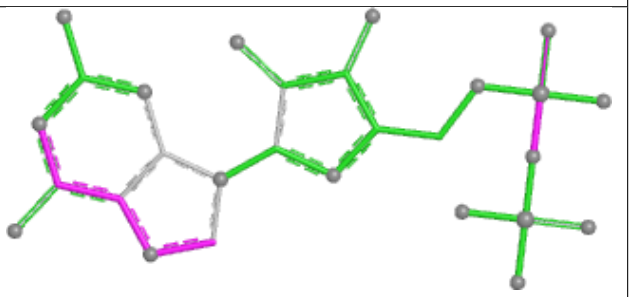
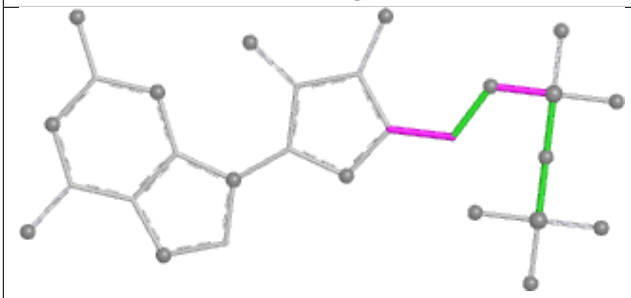
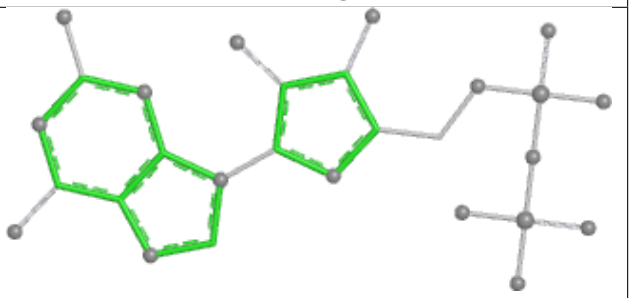
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 0Y 502 | |
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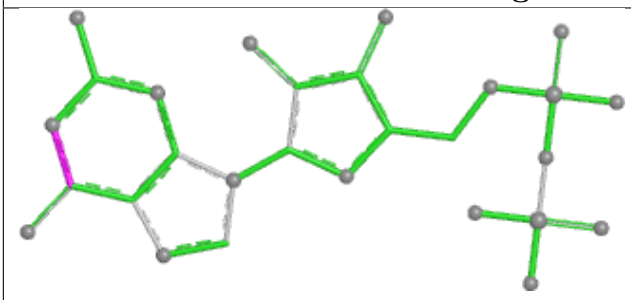
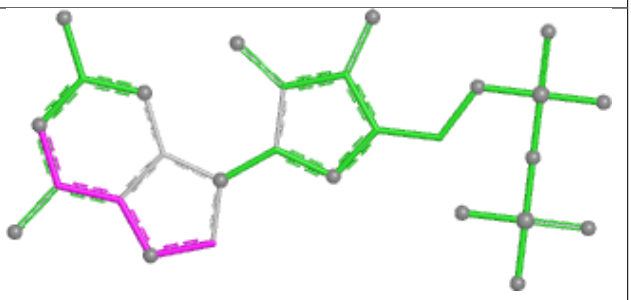
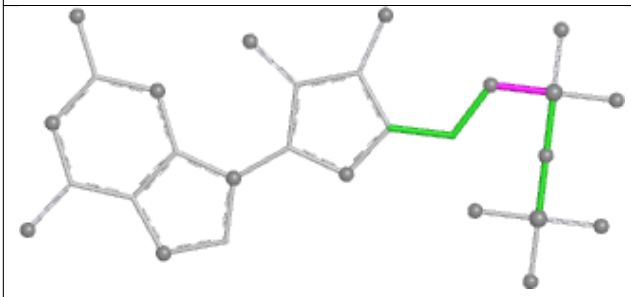
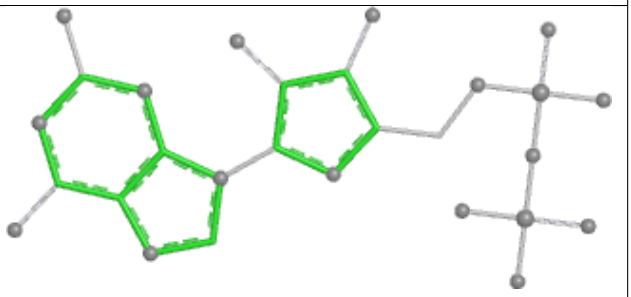
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 2E 502 | |
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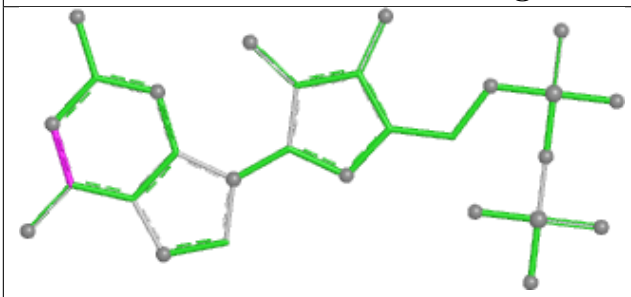
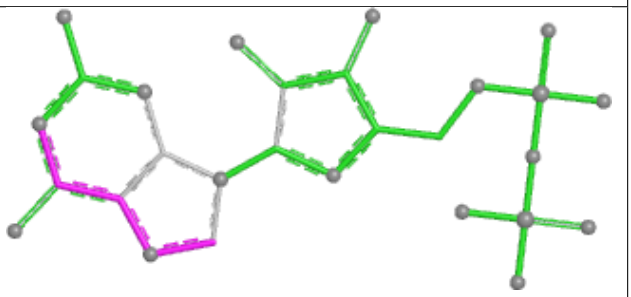
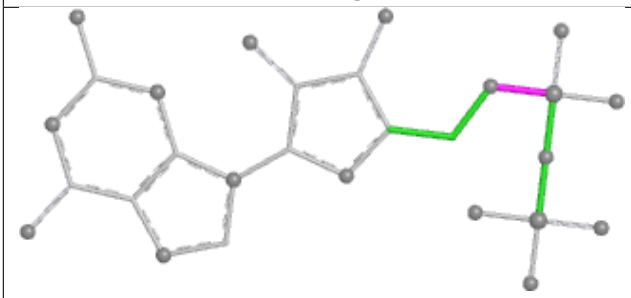
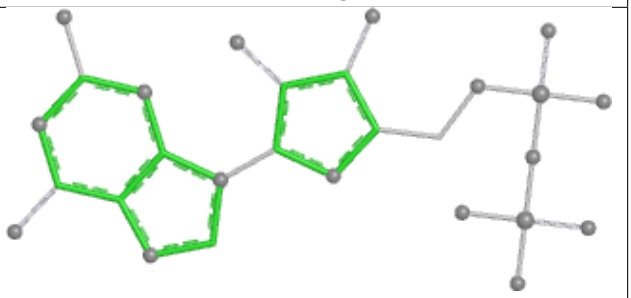
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP L2 502 | |
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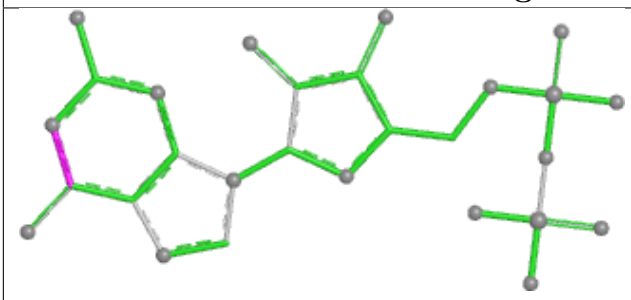
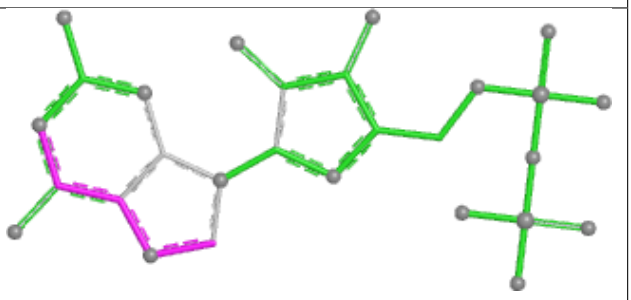
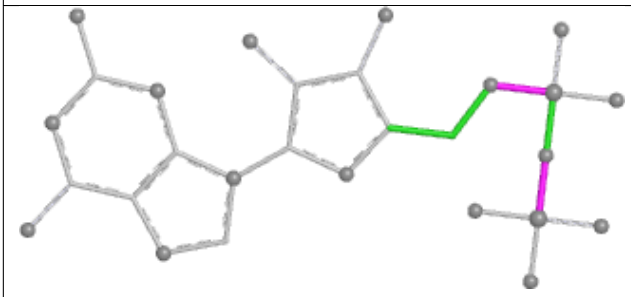
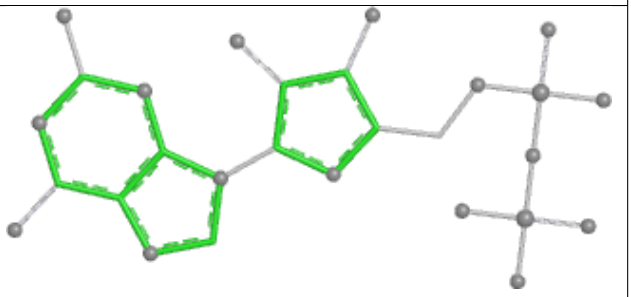
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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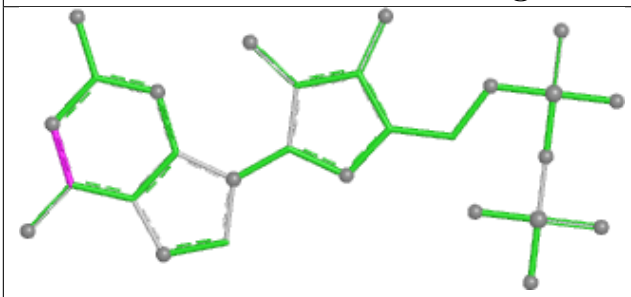
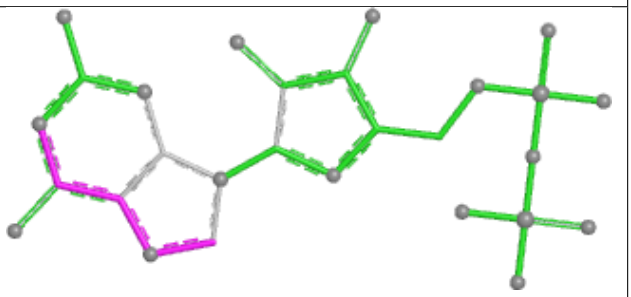
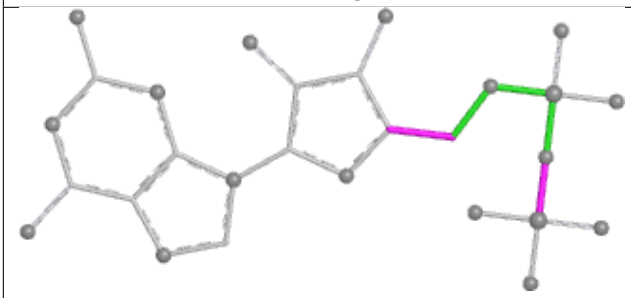
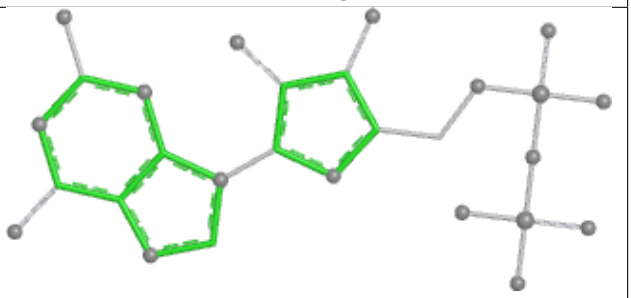
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP A7 501 | |
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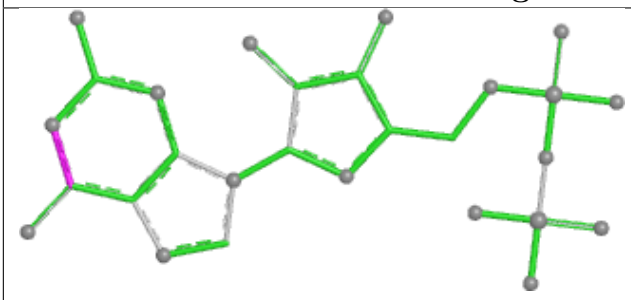
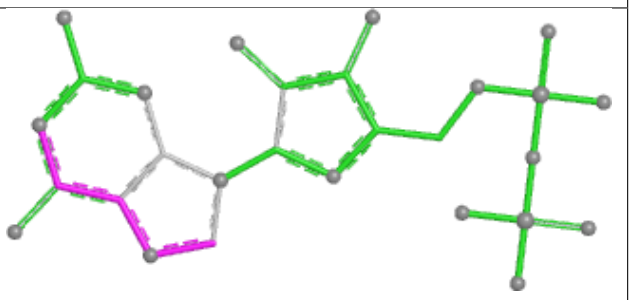
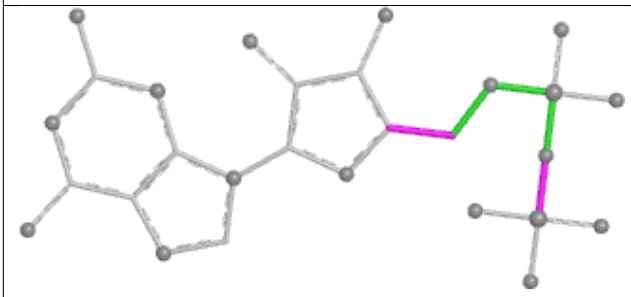
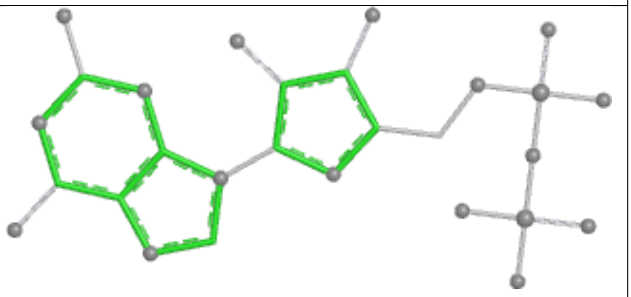
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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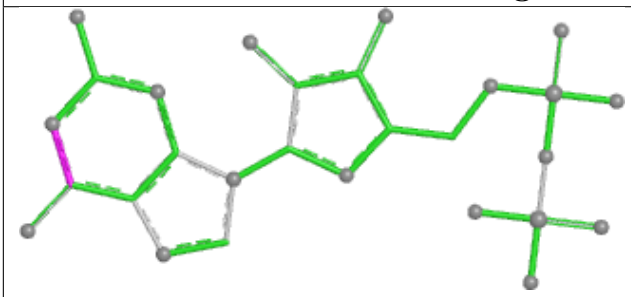
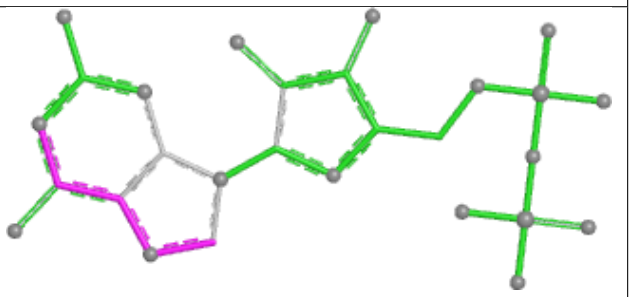
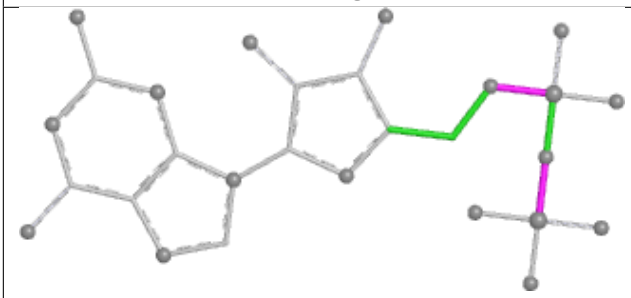
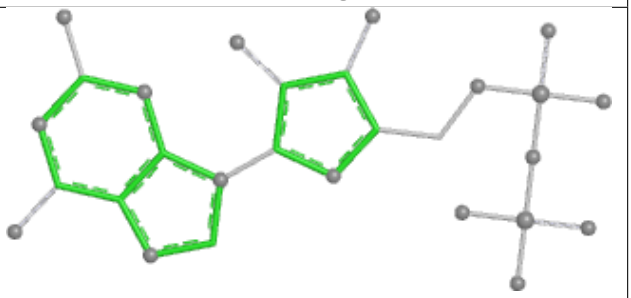
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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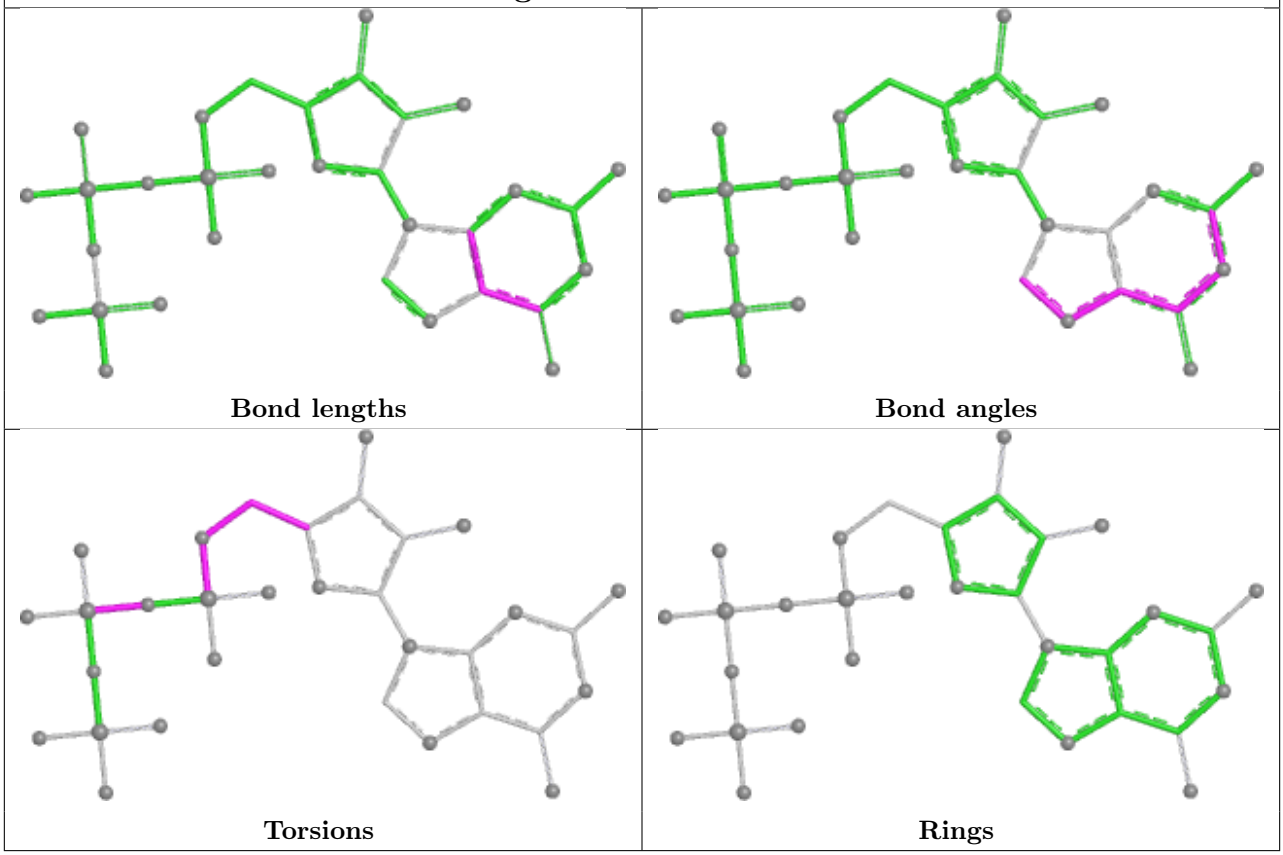


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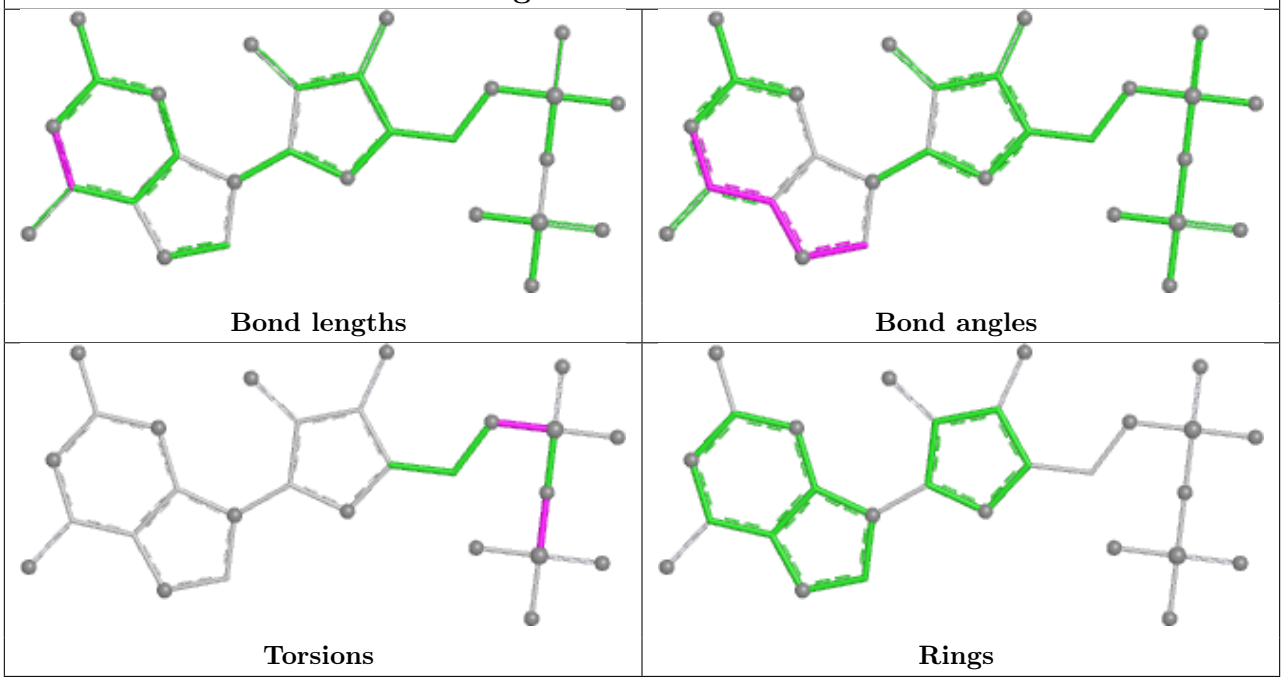

| Ligand GDP 5 501 | |
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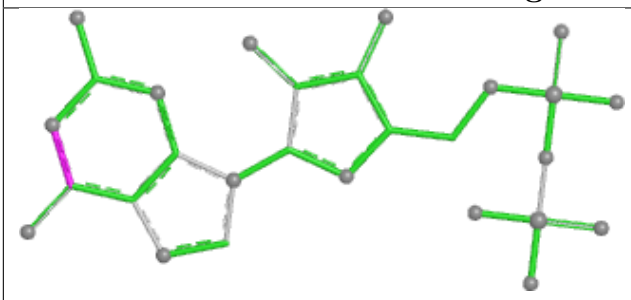
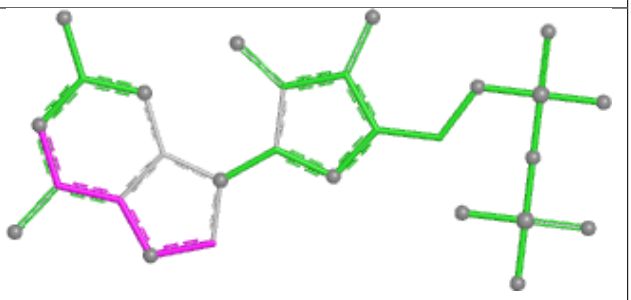
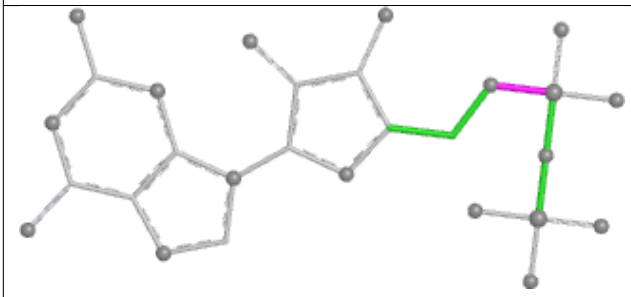
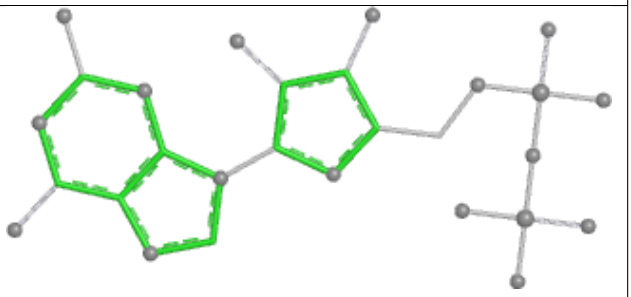
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 0U 501 | |
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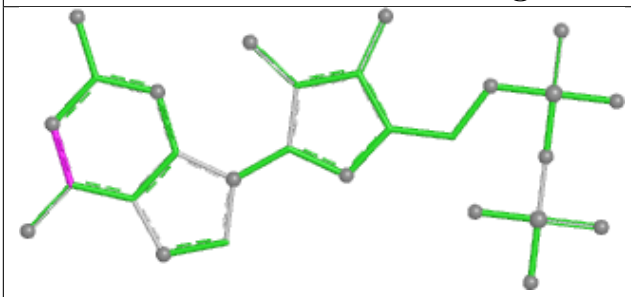
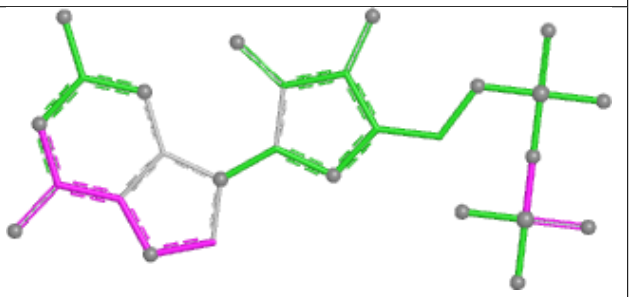
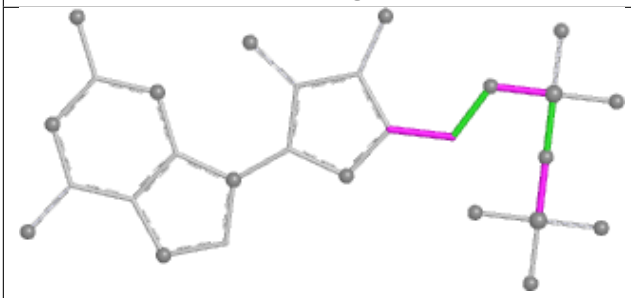
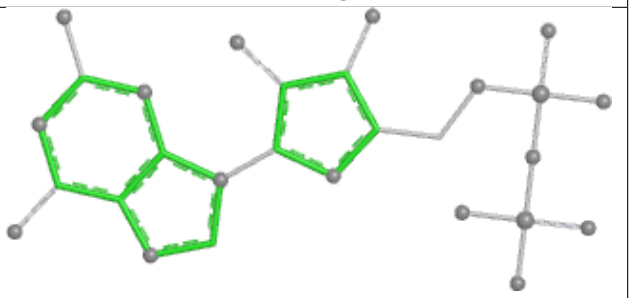
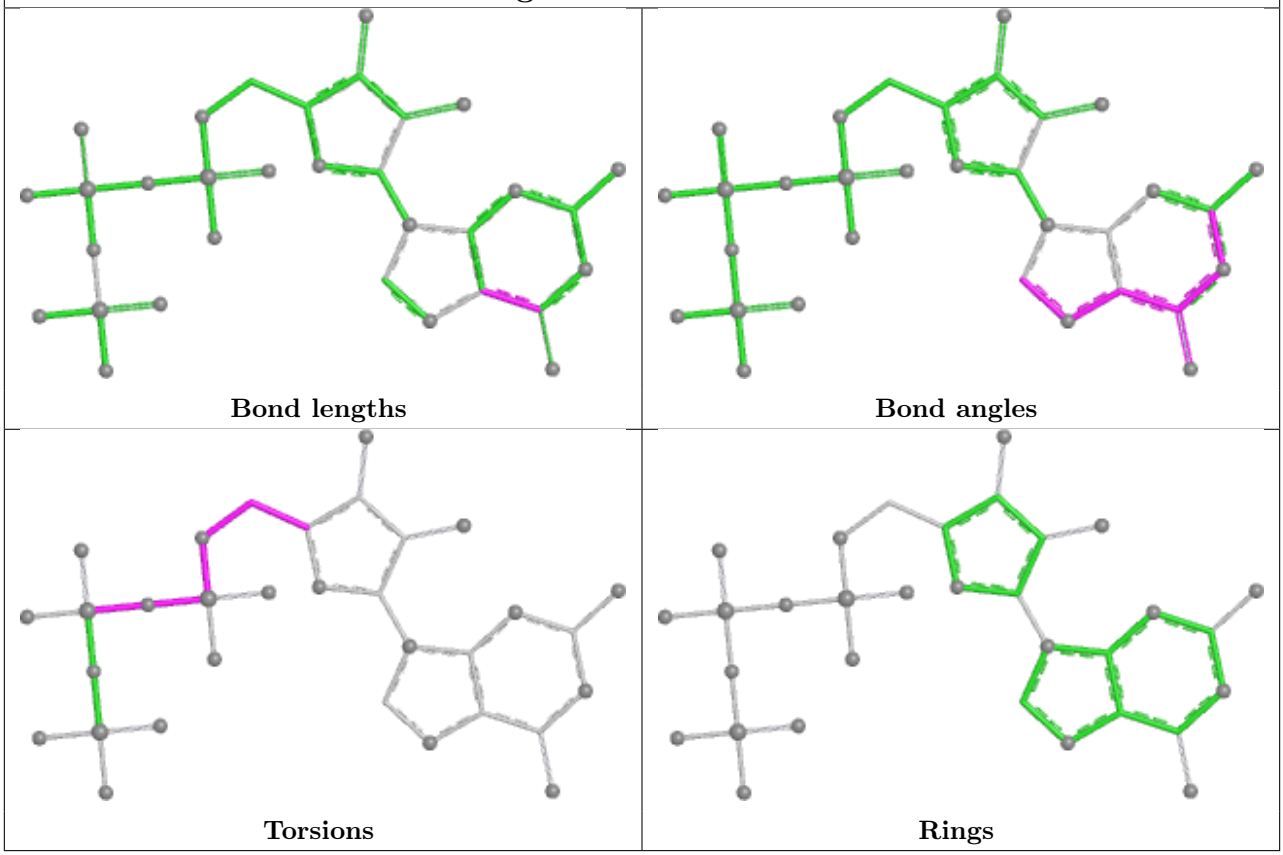
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand GTP F8 501

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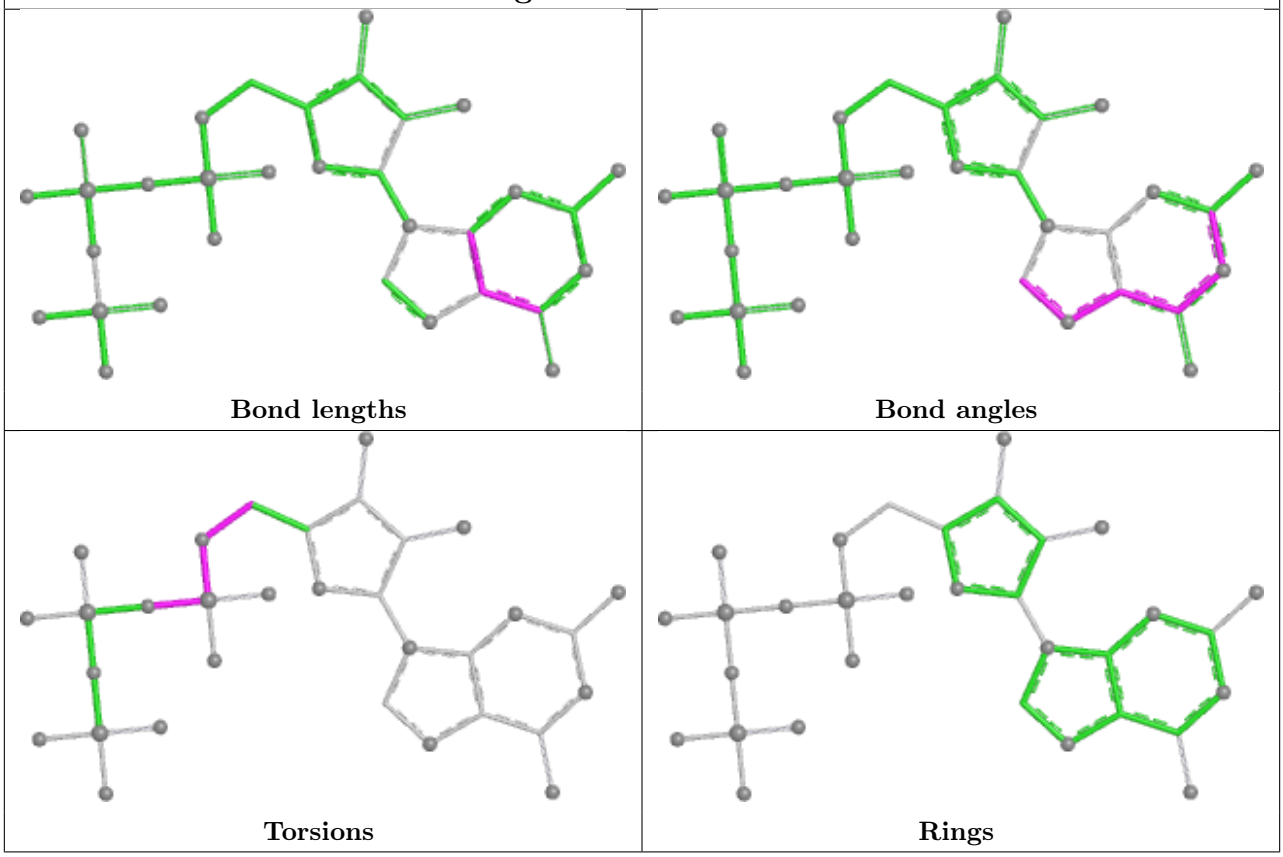
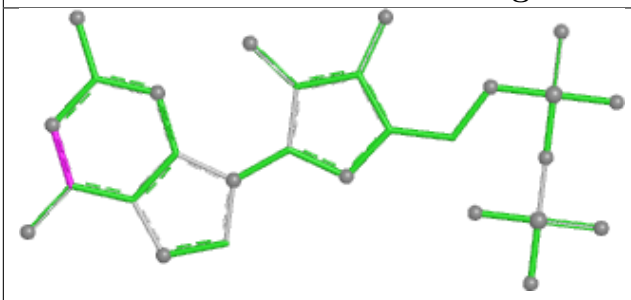
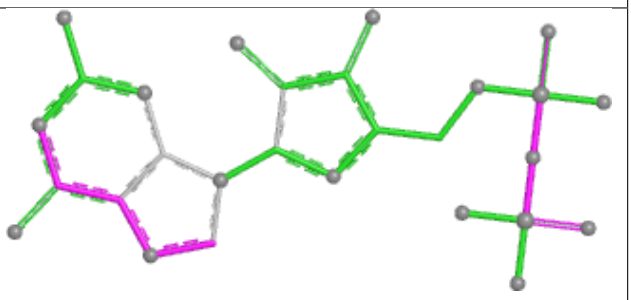


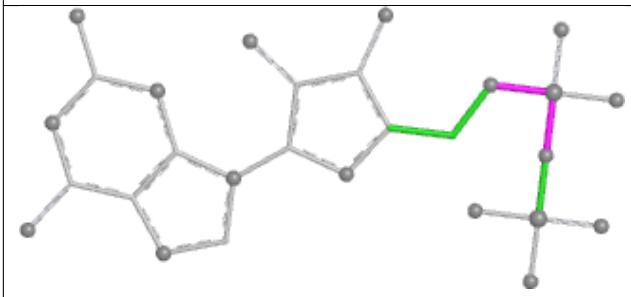
## Ligand GDP 1A 503



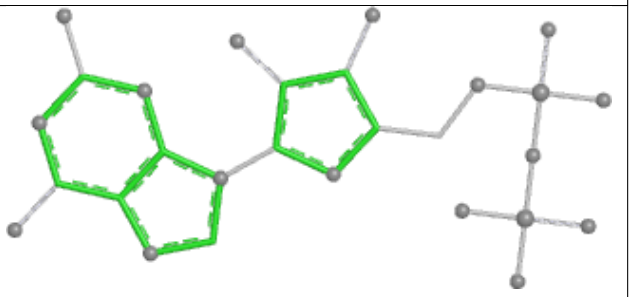
Bond lengths



Bond angles

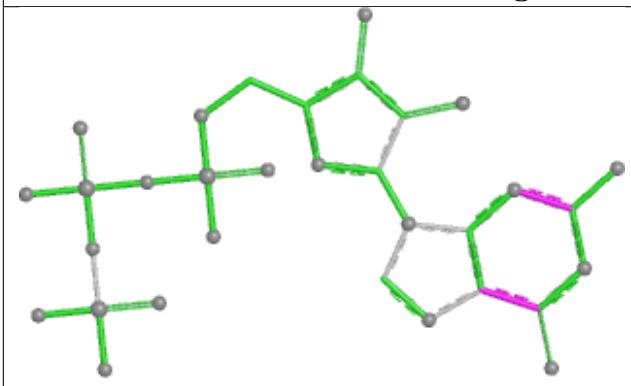


Torsions



Rings

## Ligand GTP 2N 501



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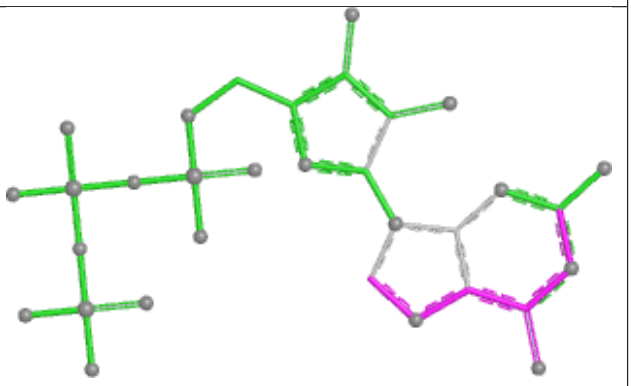

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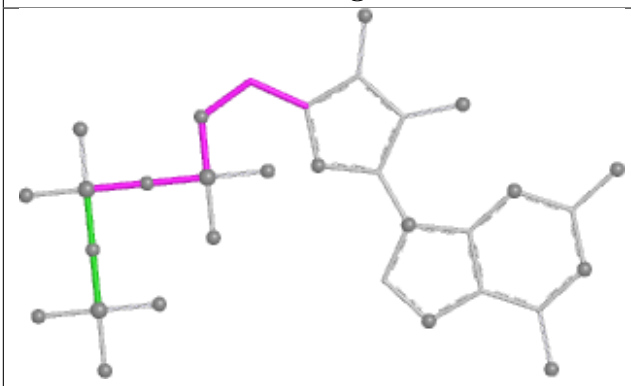

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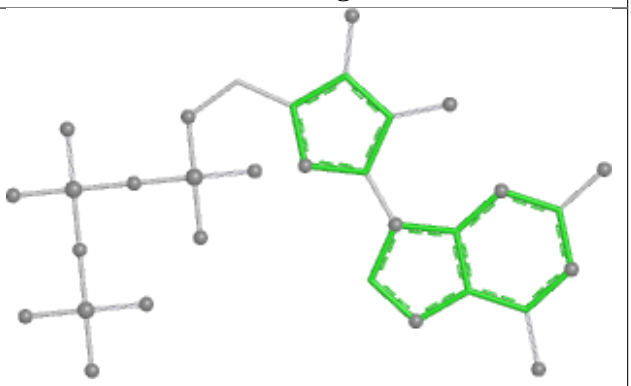

Rings

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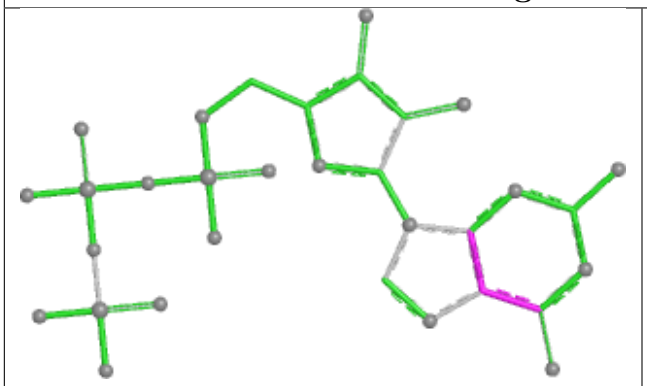

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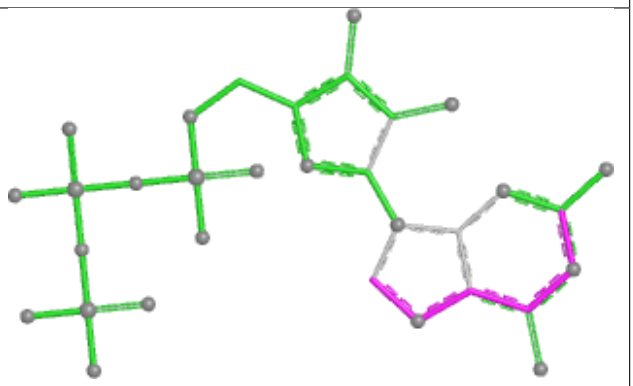

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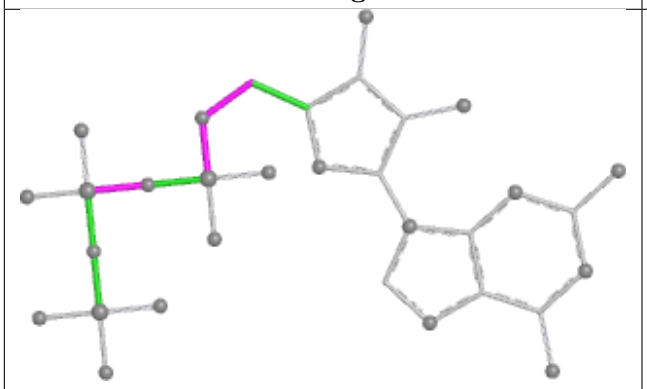

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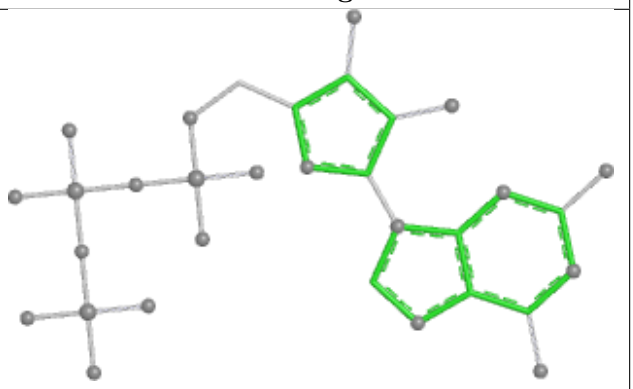
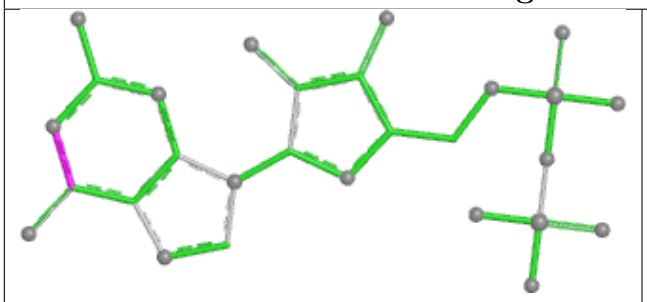


Rings

## Ligand GDP 2S 502



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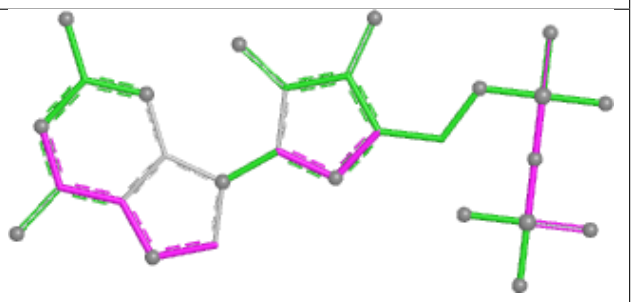

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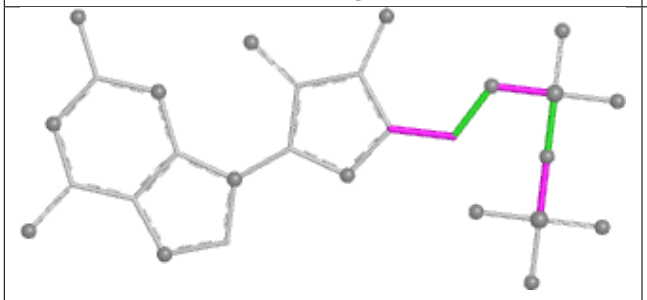

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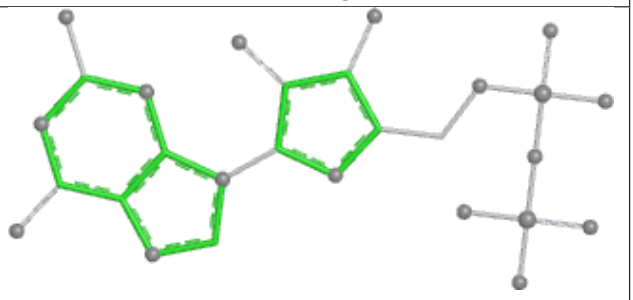

Rings

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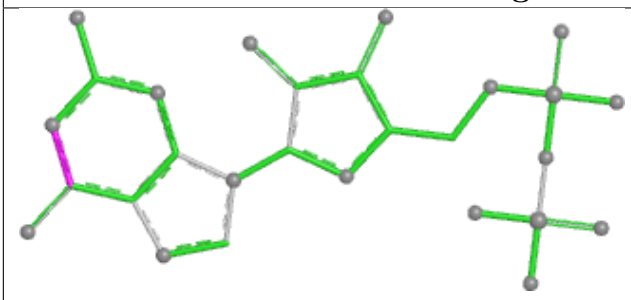

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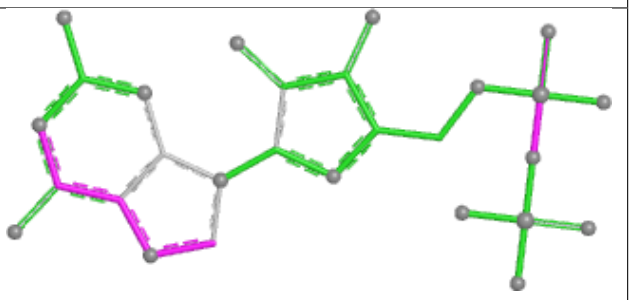

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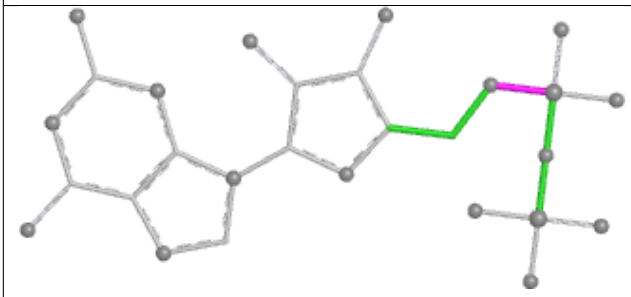

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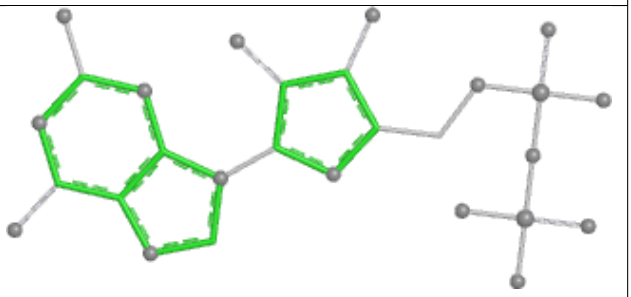
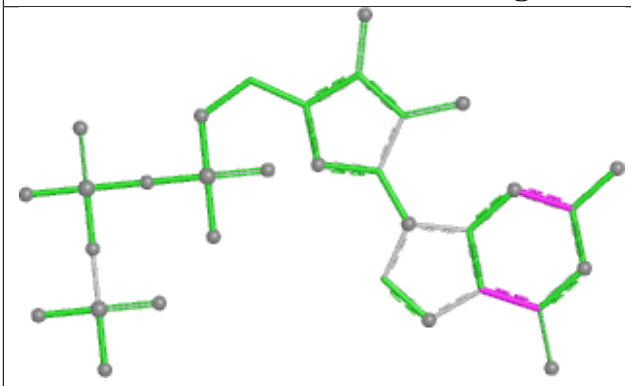


Rings

## Ligand GTP 2G 501



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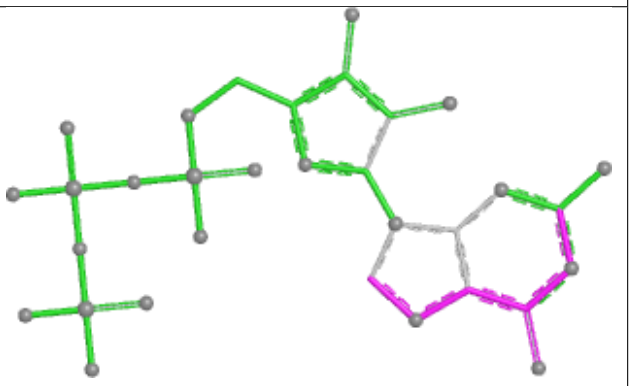

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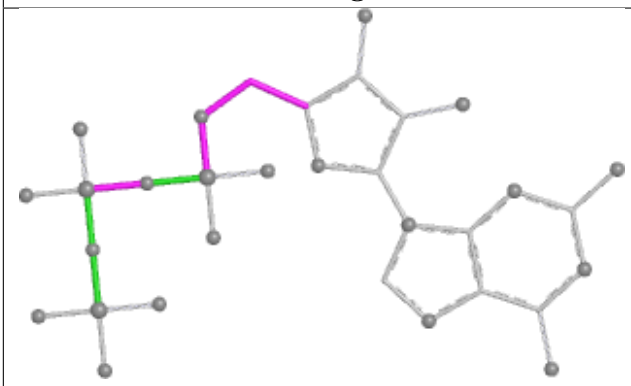

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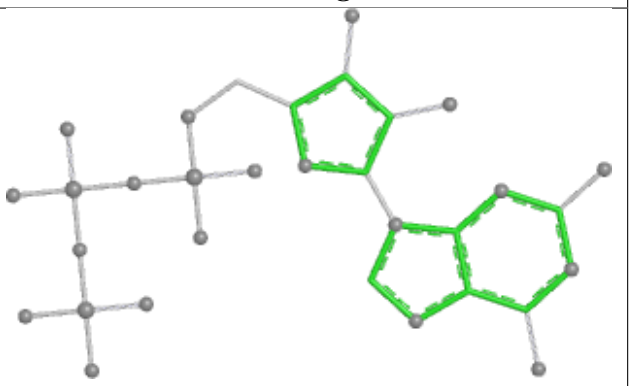
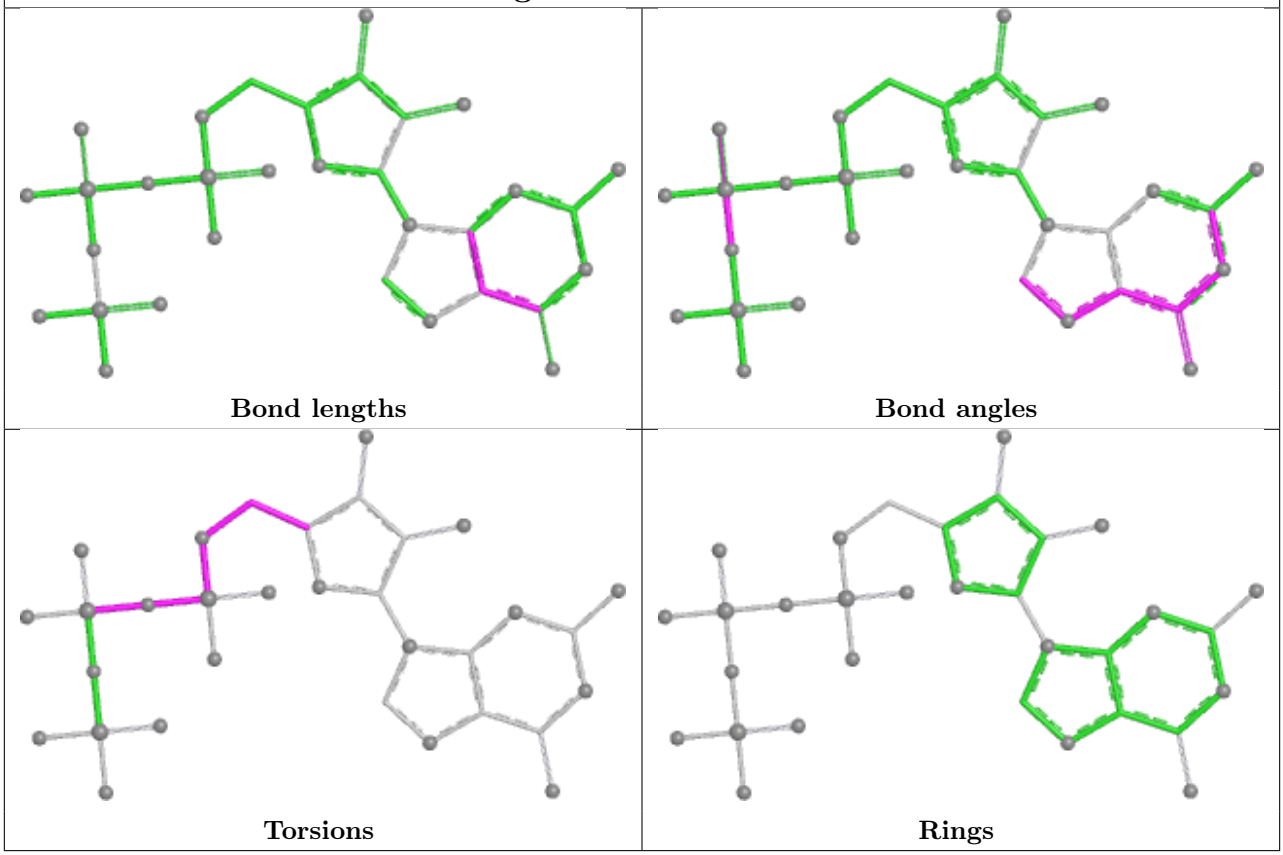
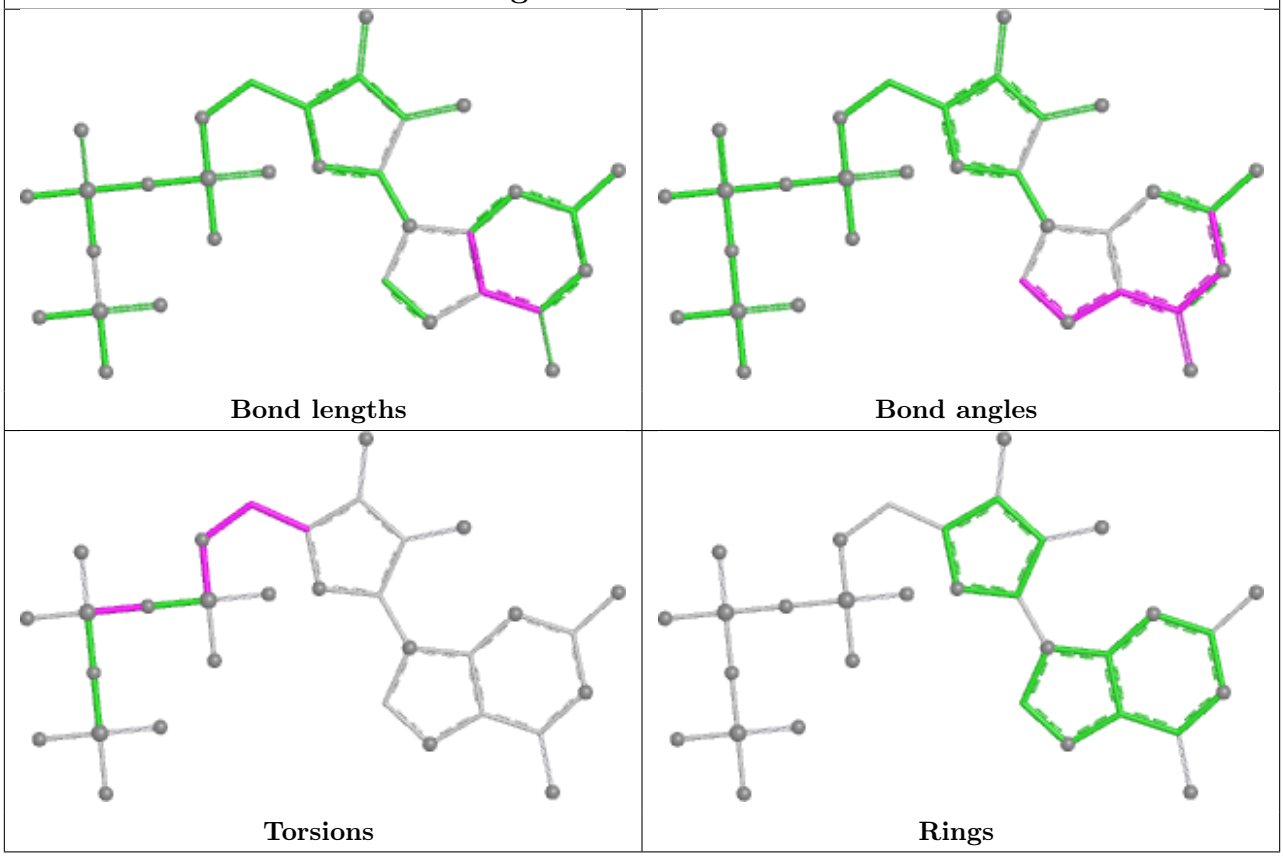


Rings

## Ligand GTP A9 501




## Ligand GTP M2 501



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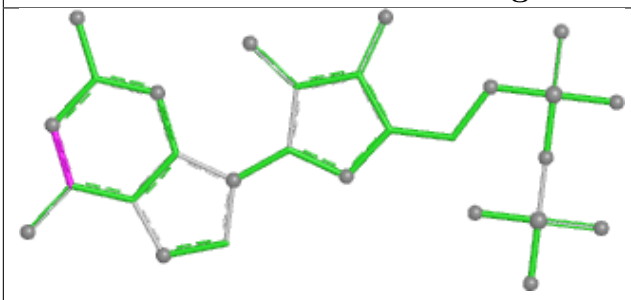
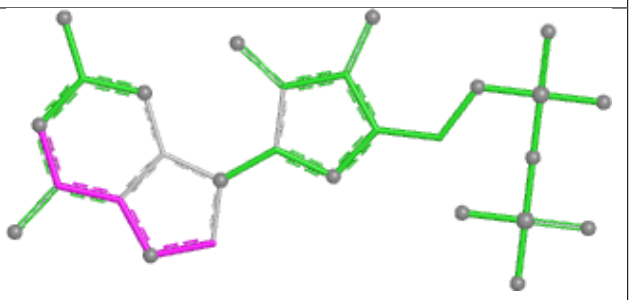
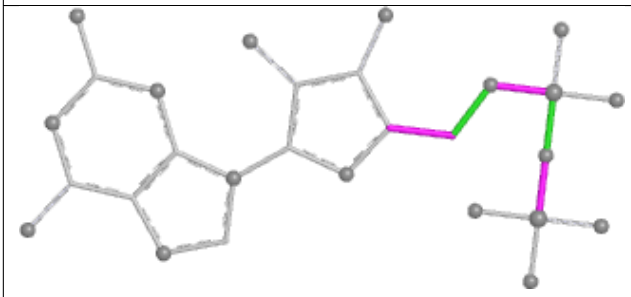
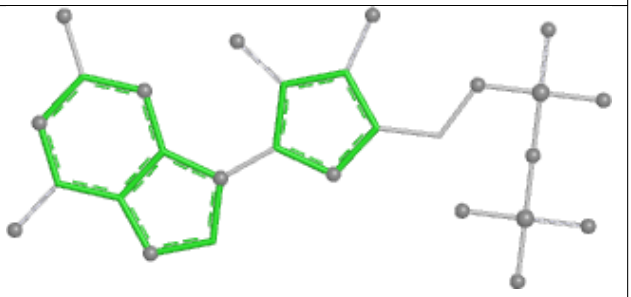
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 0S 502 | |
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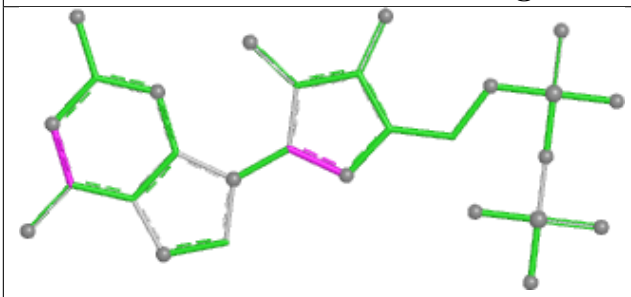
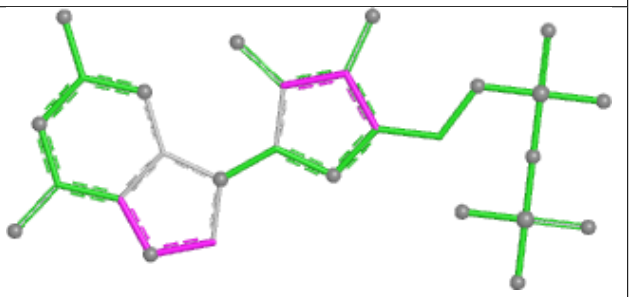
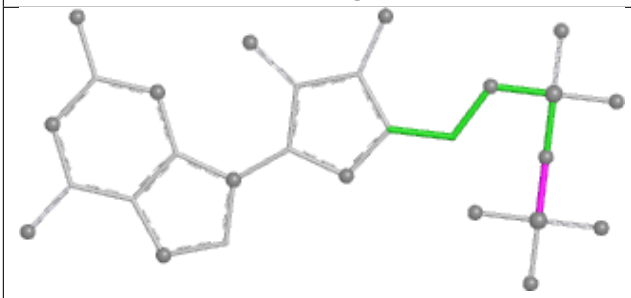
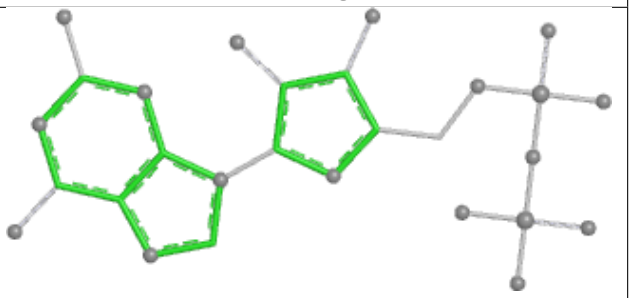
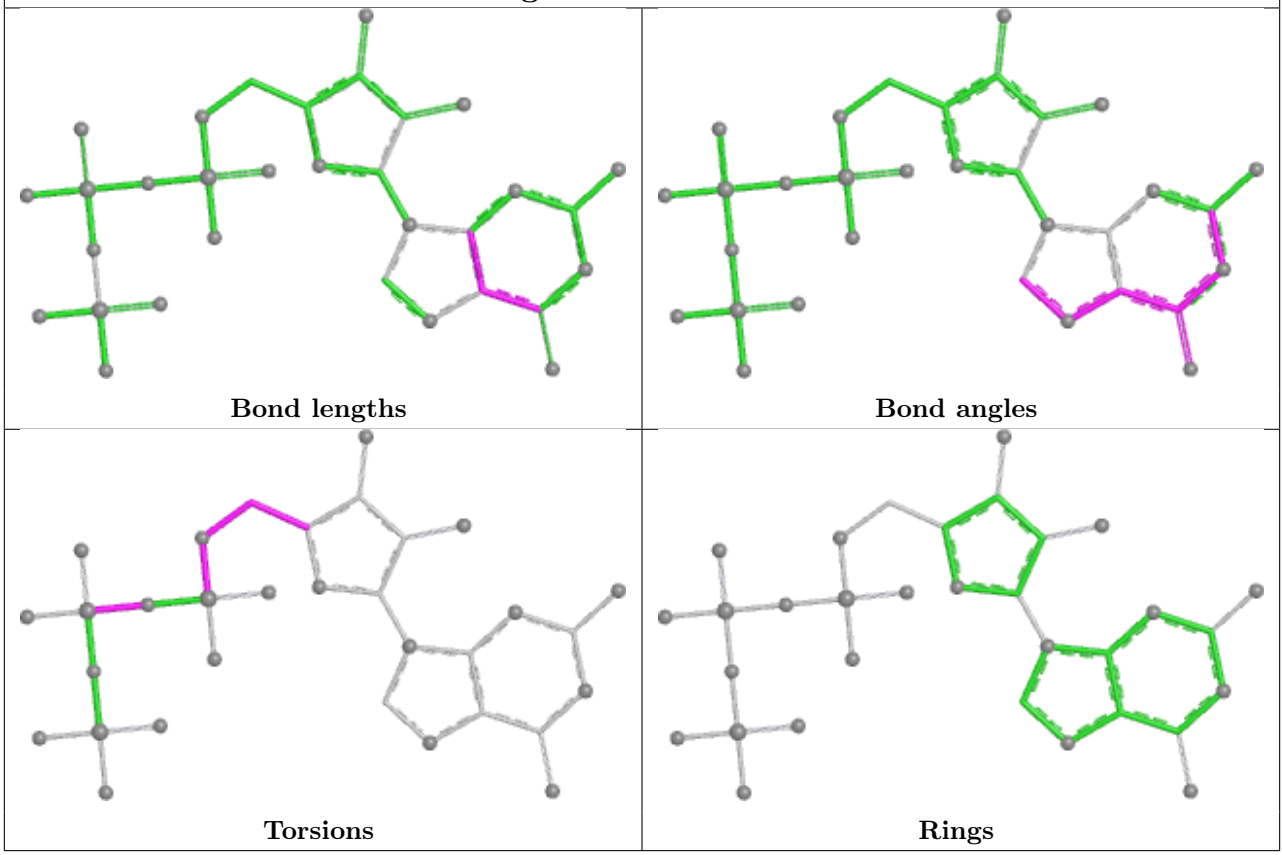
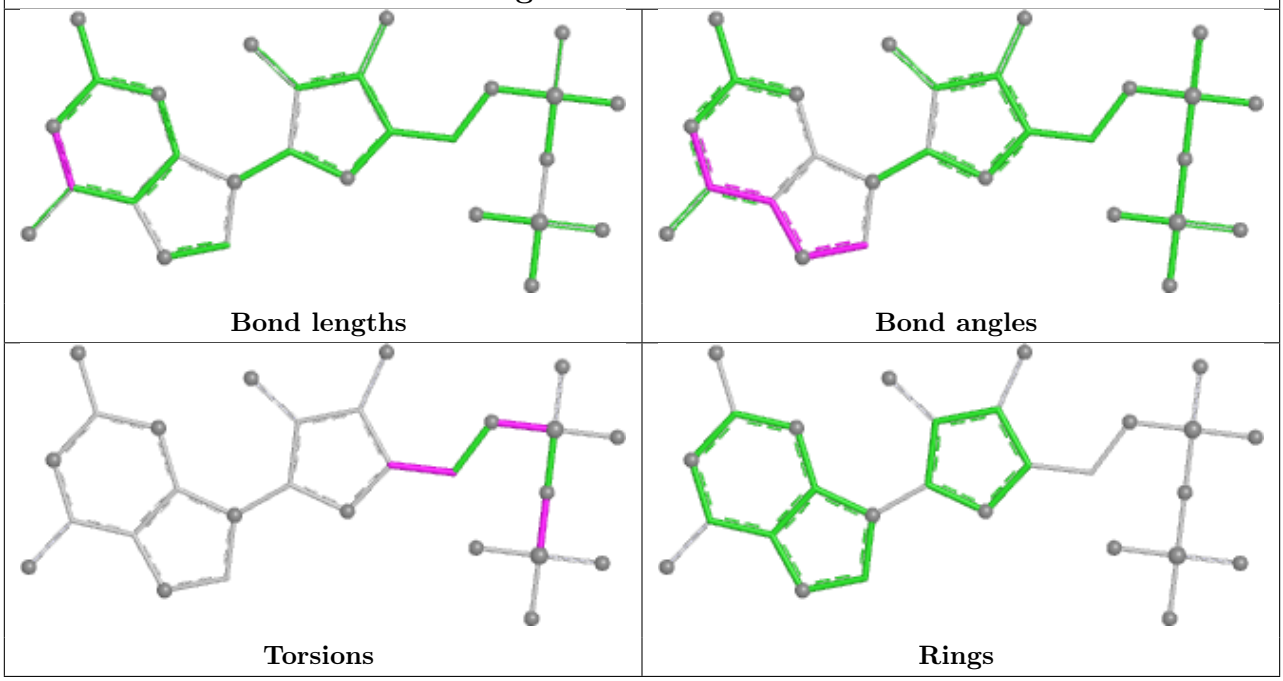
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand GTP I0 501




## Ligand GDP L6 502



| Ligand GDP 2K 502 | |
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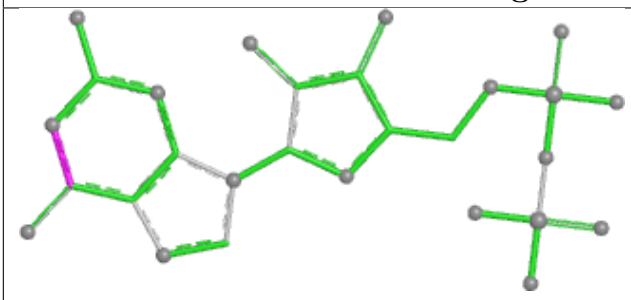
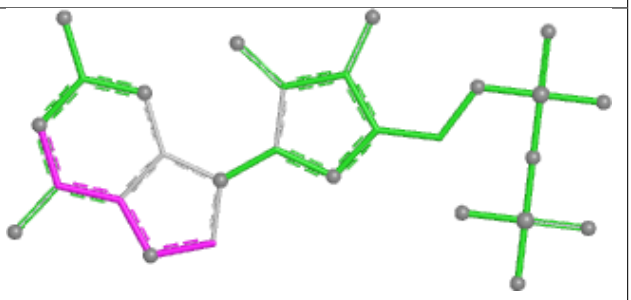
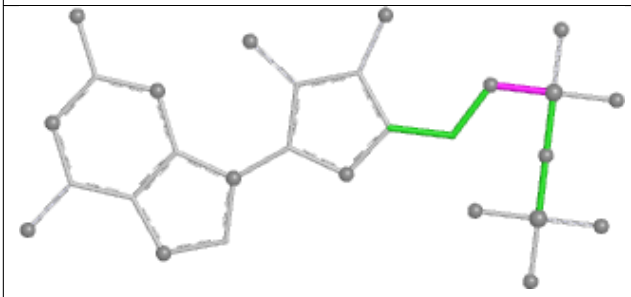
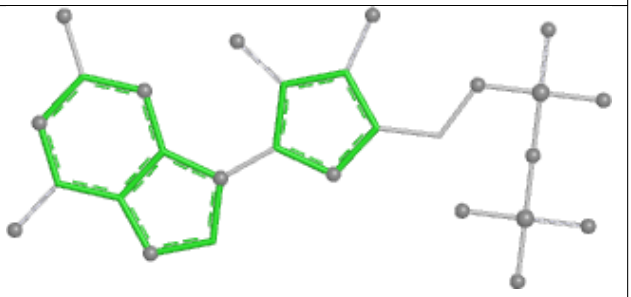
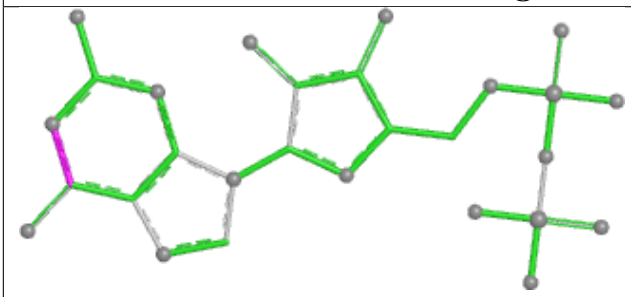
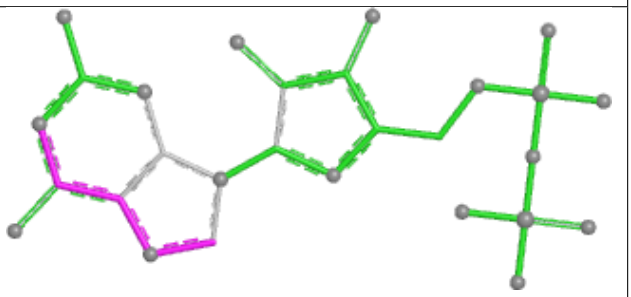
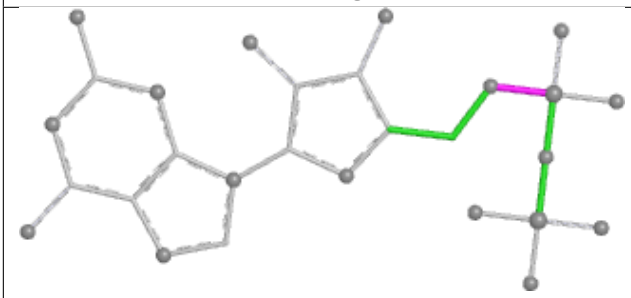
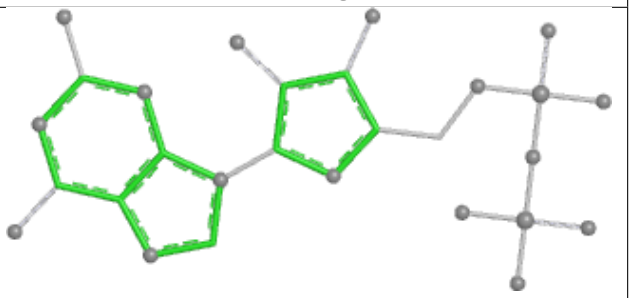
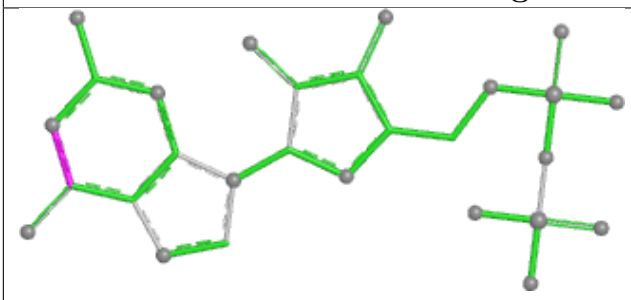
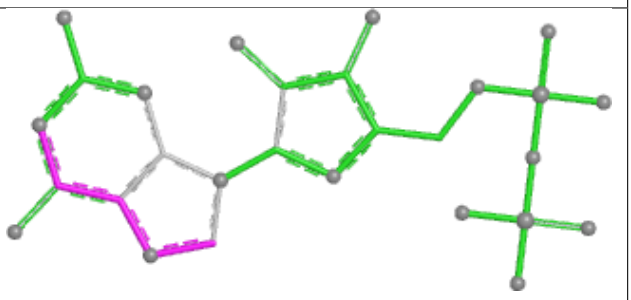
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP Z6 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

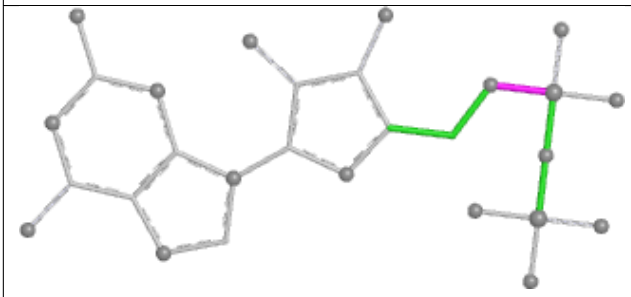
## Ligand GDP N0 502



Bond lengths



Bond angles



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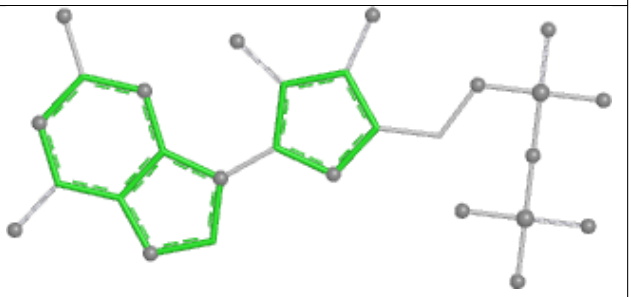
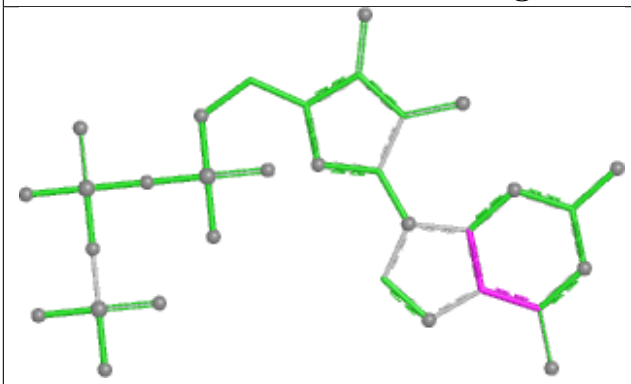


Rings

## Ligand GTP Q6 501



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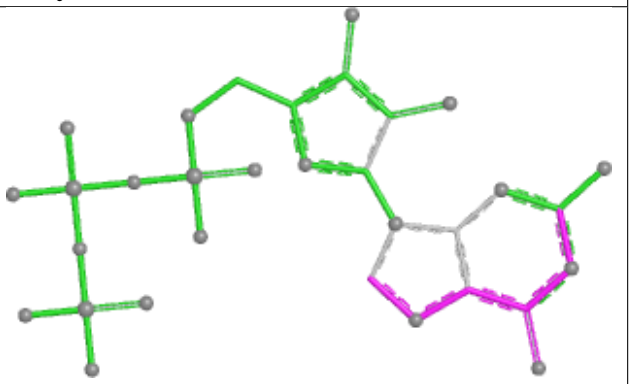
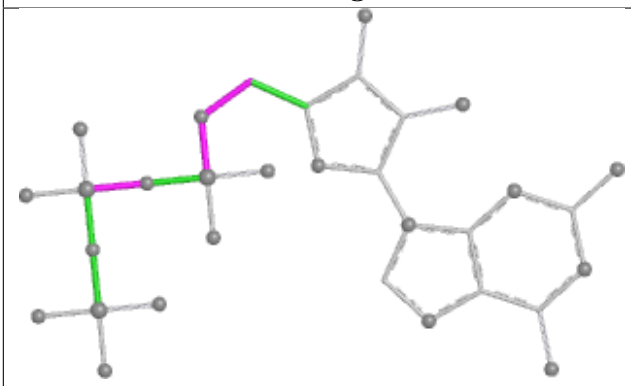


Bond angles



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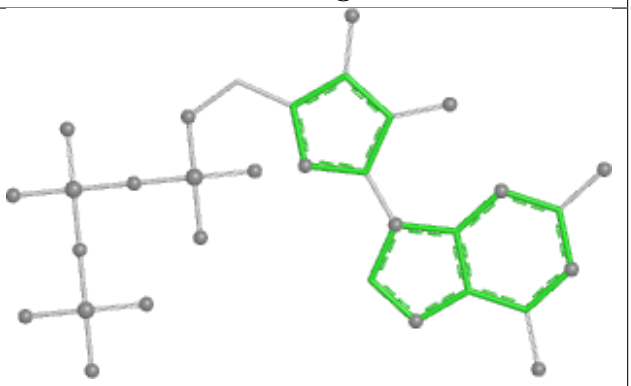
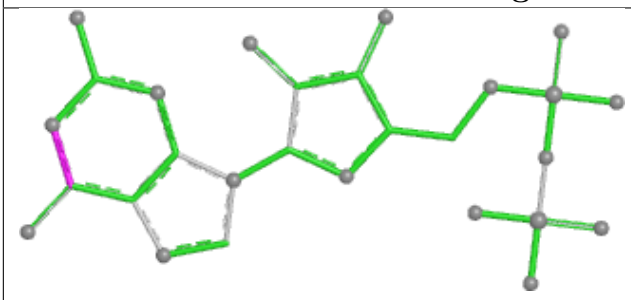


Rings

## Ligand GDP V0 501



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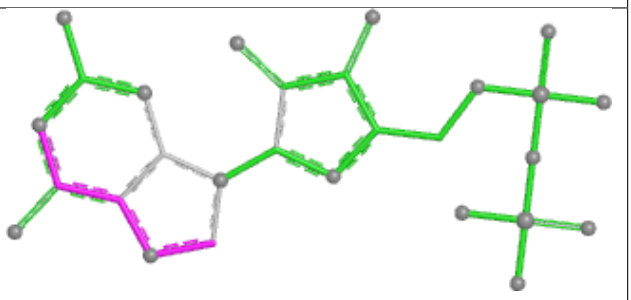
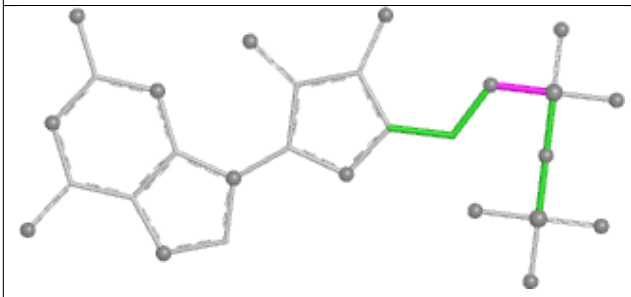


Bond angles



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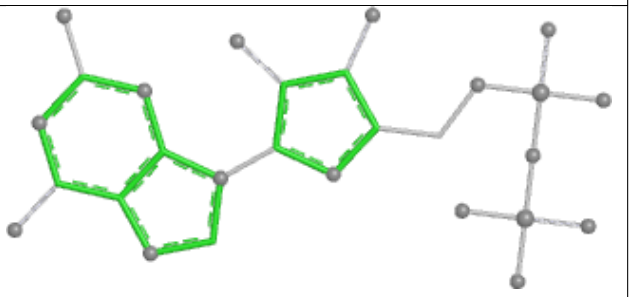
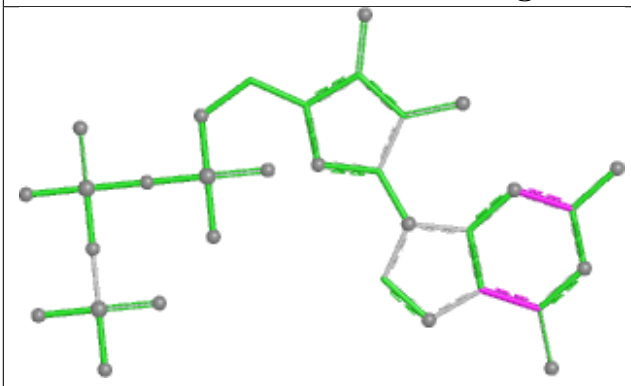


Rings

## Ligand GTP 2L 501



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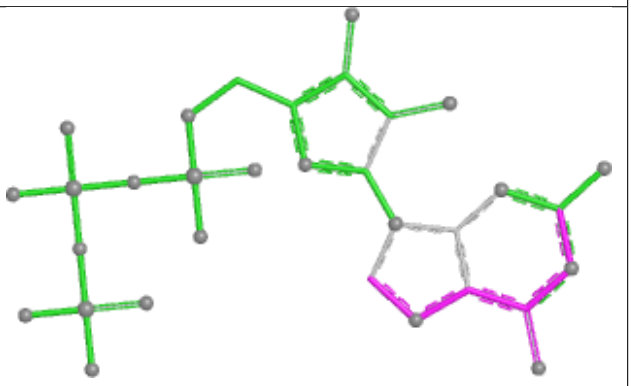

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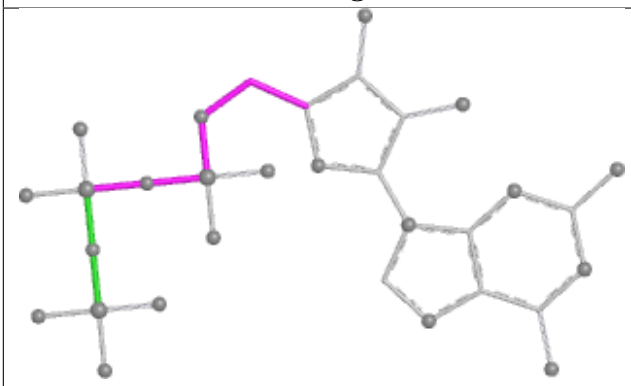

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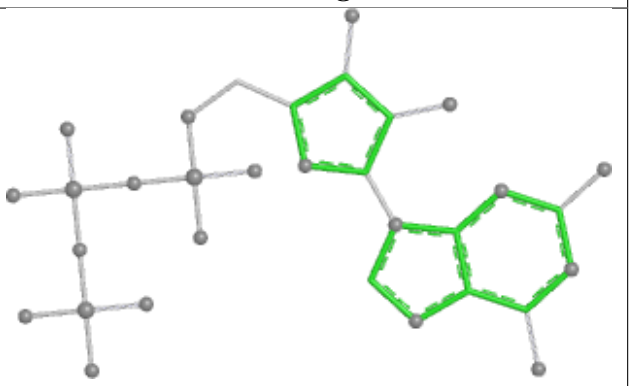
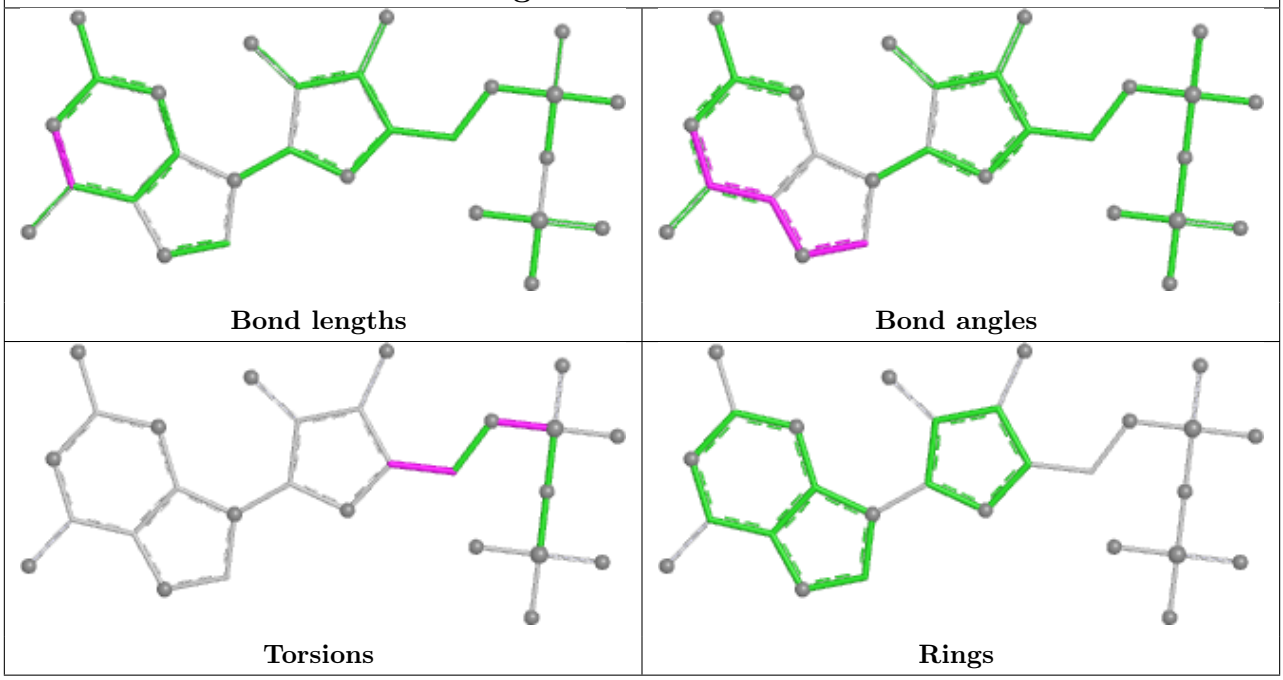


Rings

## Ligand GDP 0C 502

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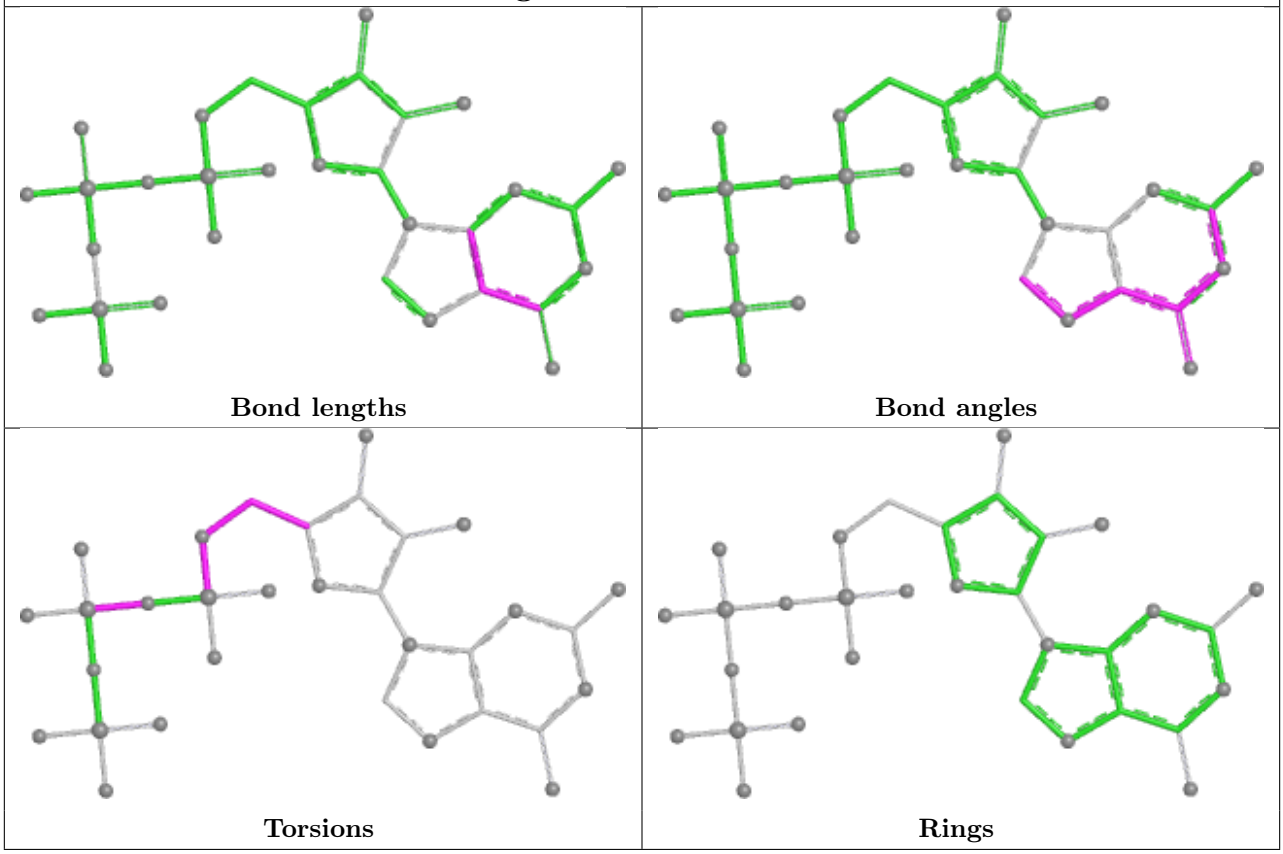

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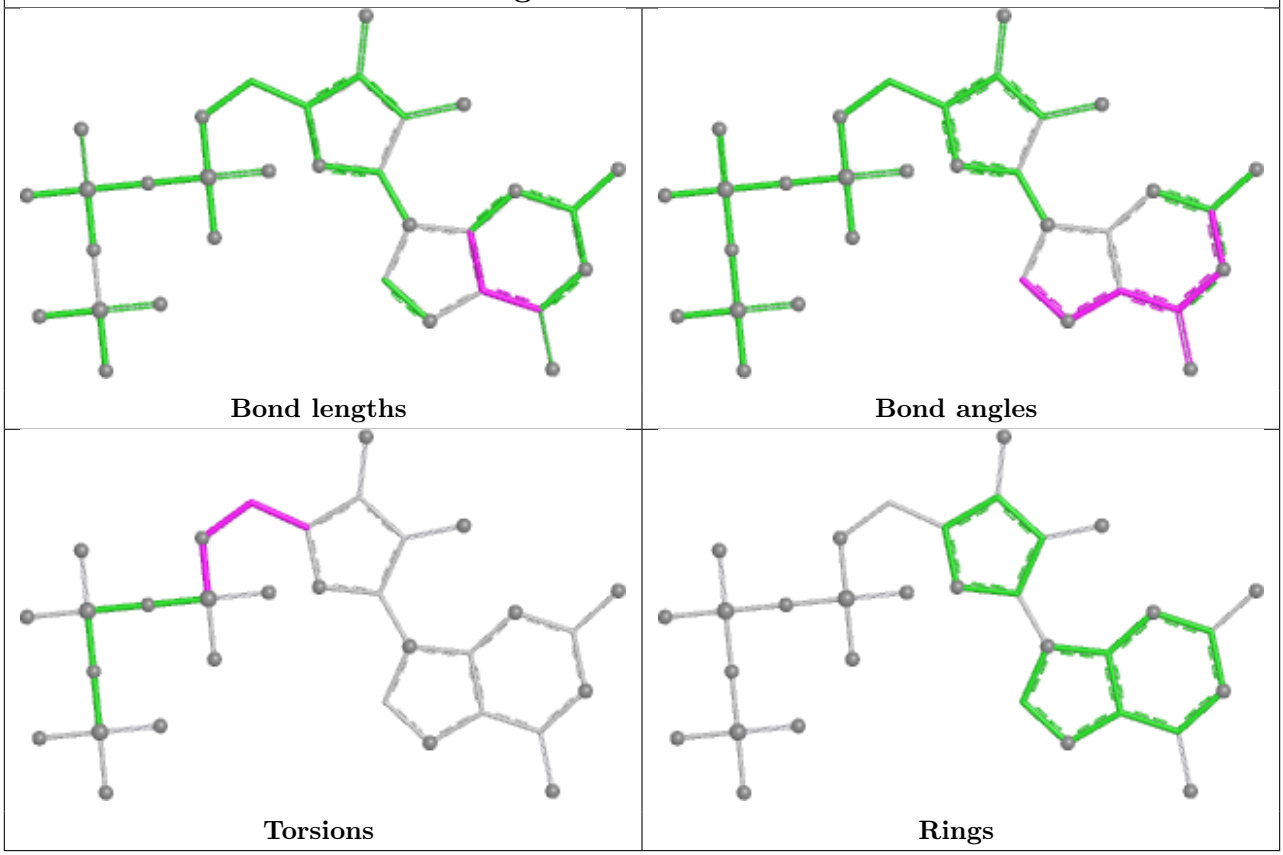


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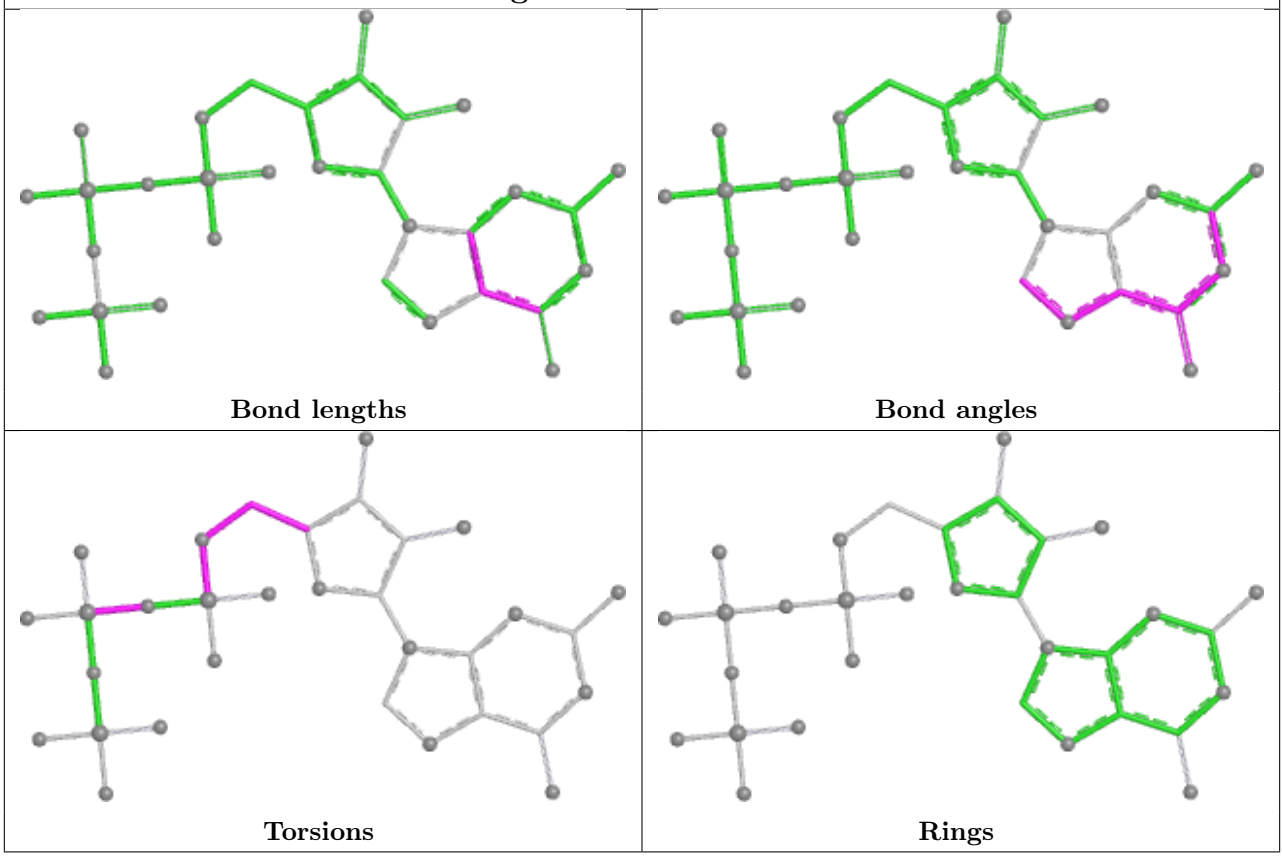

| Ligand GDP X0 502 | |
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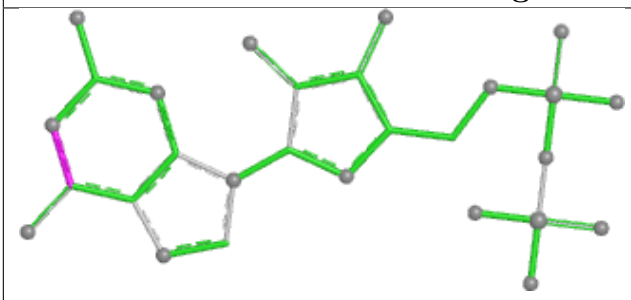
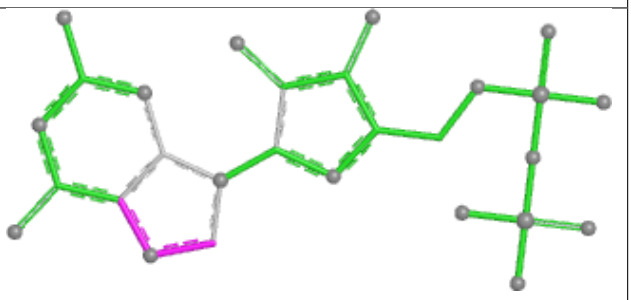
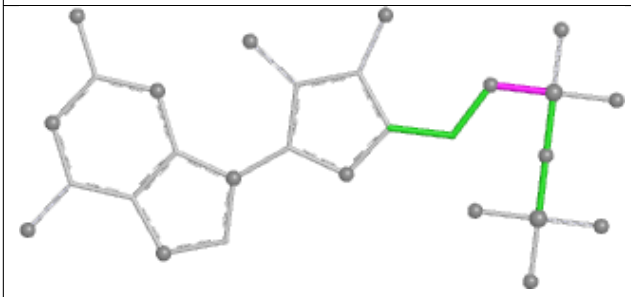
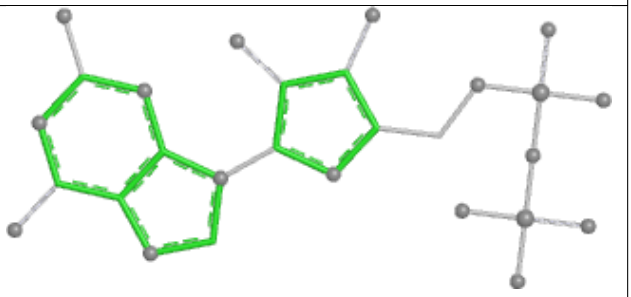
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GTP H3 501 | |
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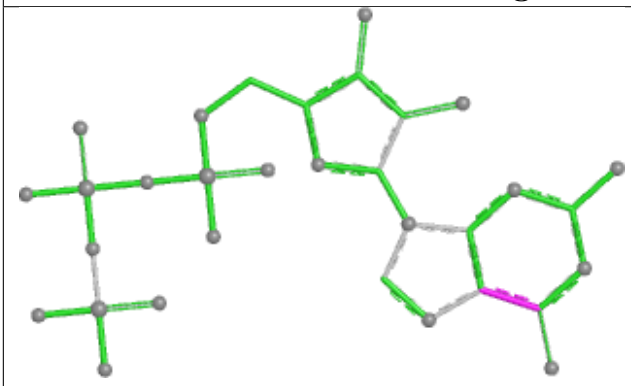
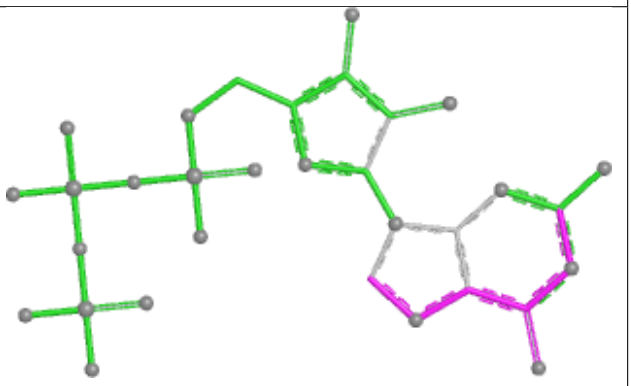
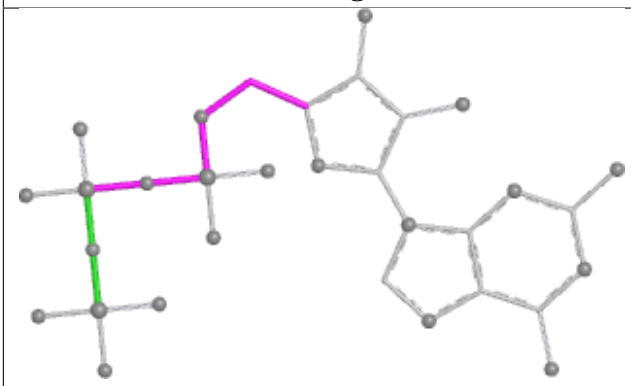
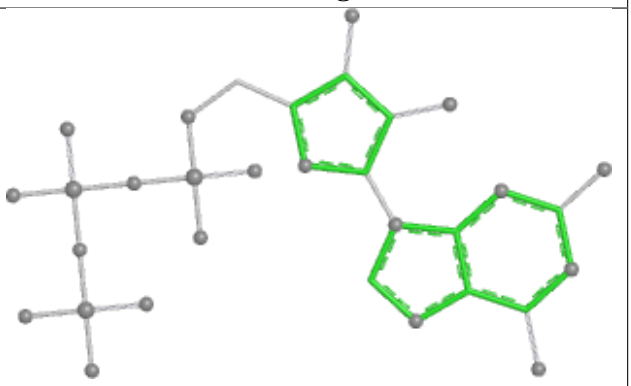
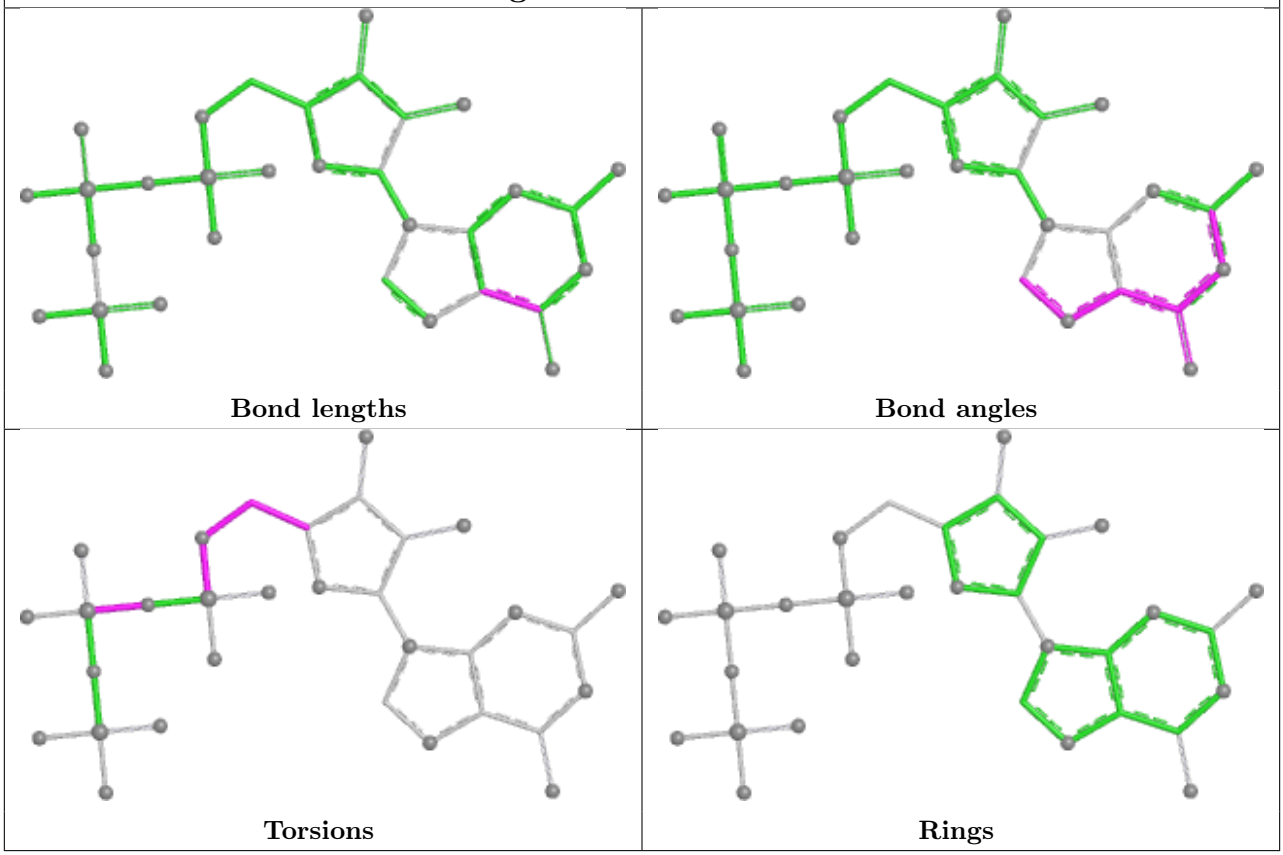
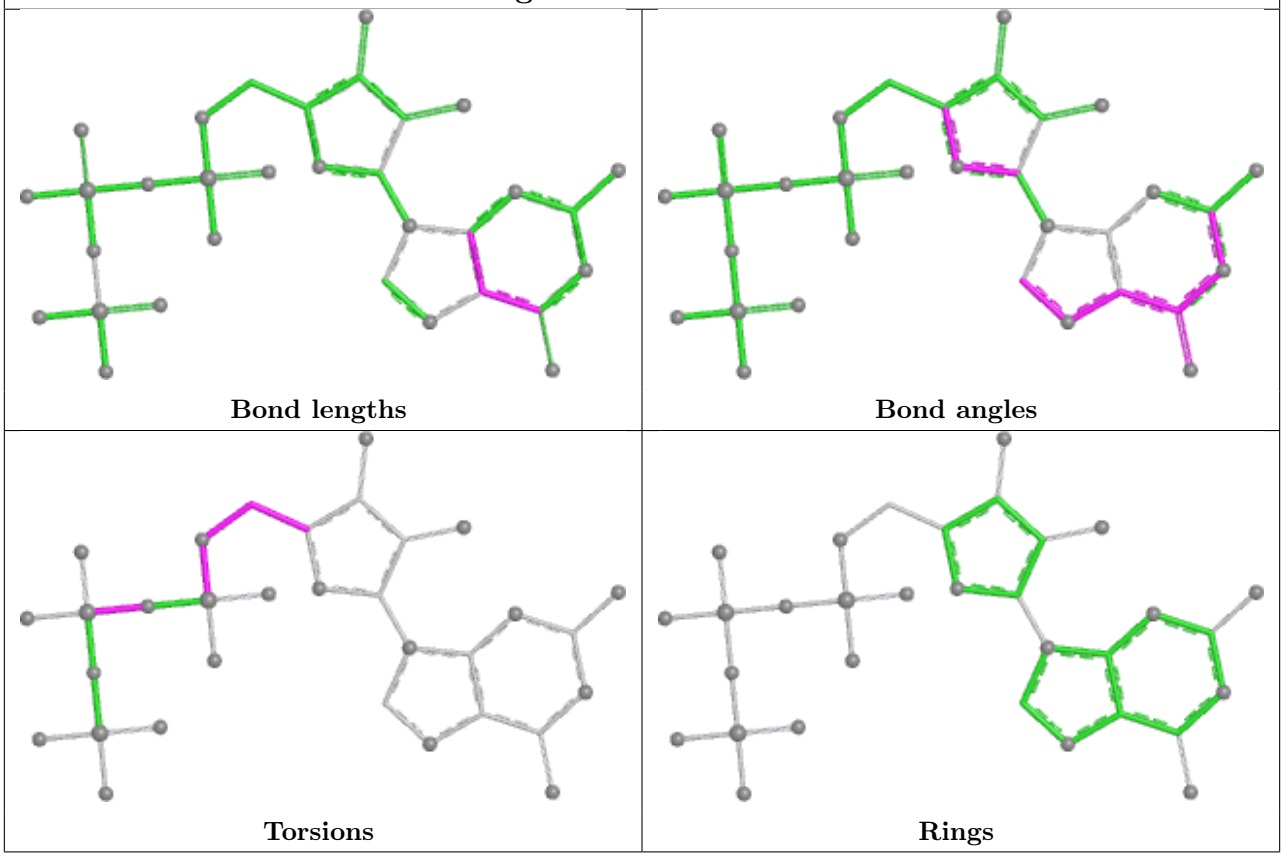
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

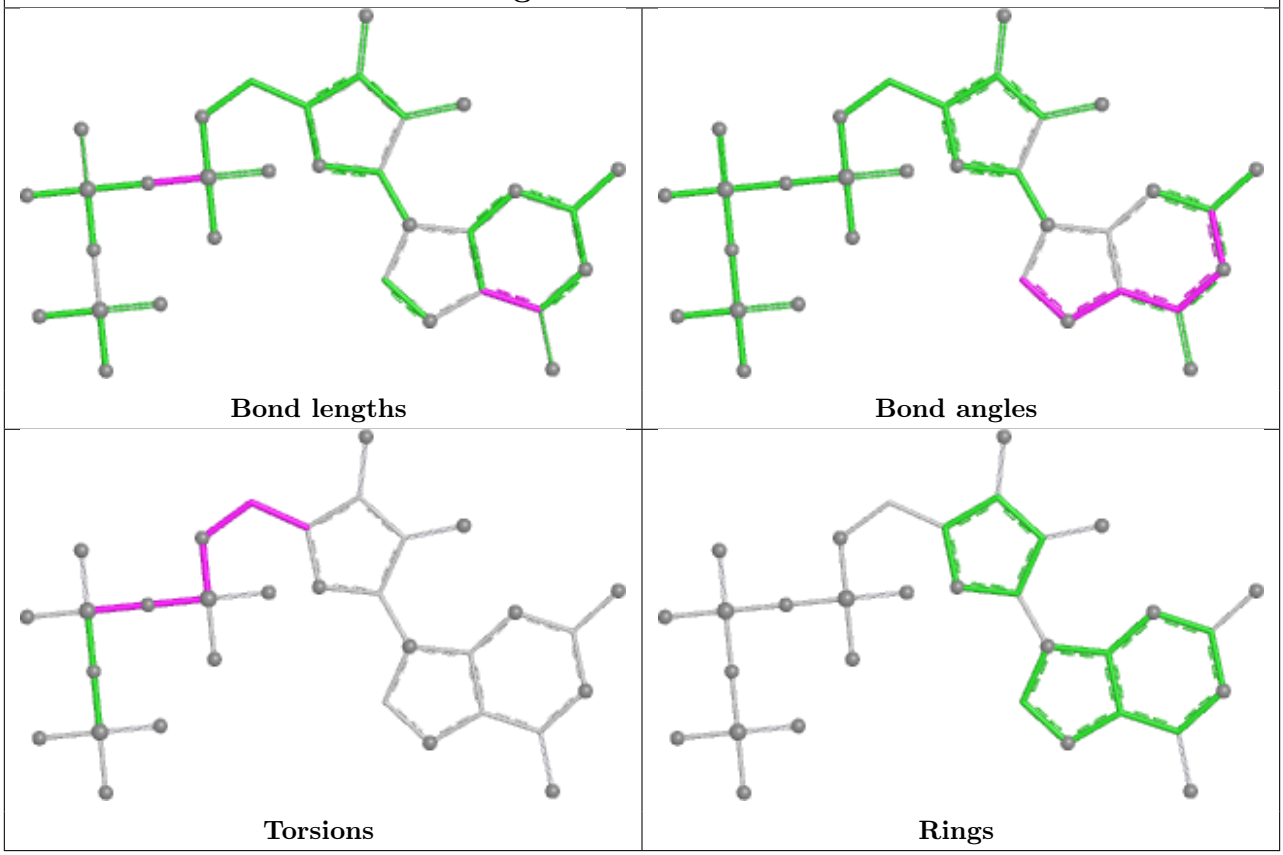
## Ligand GTP W8 501



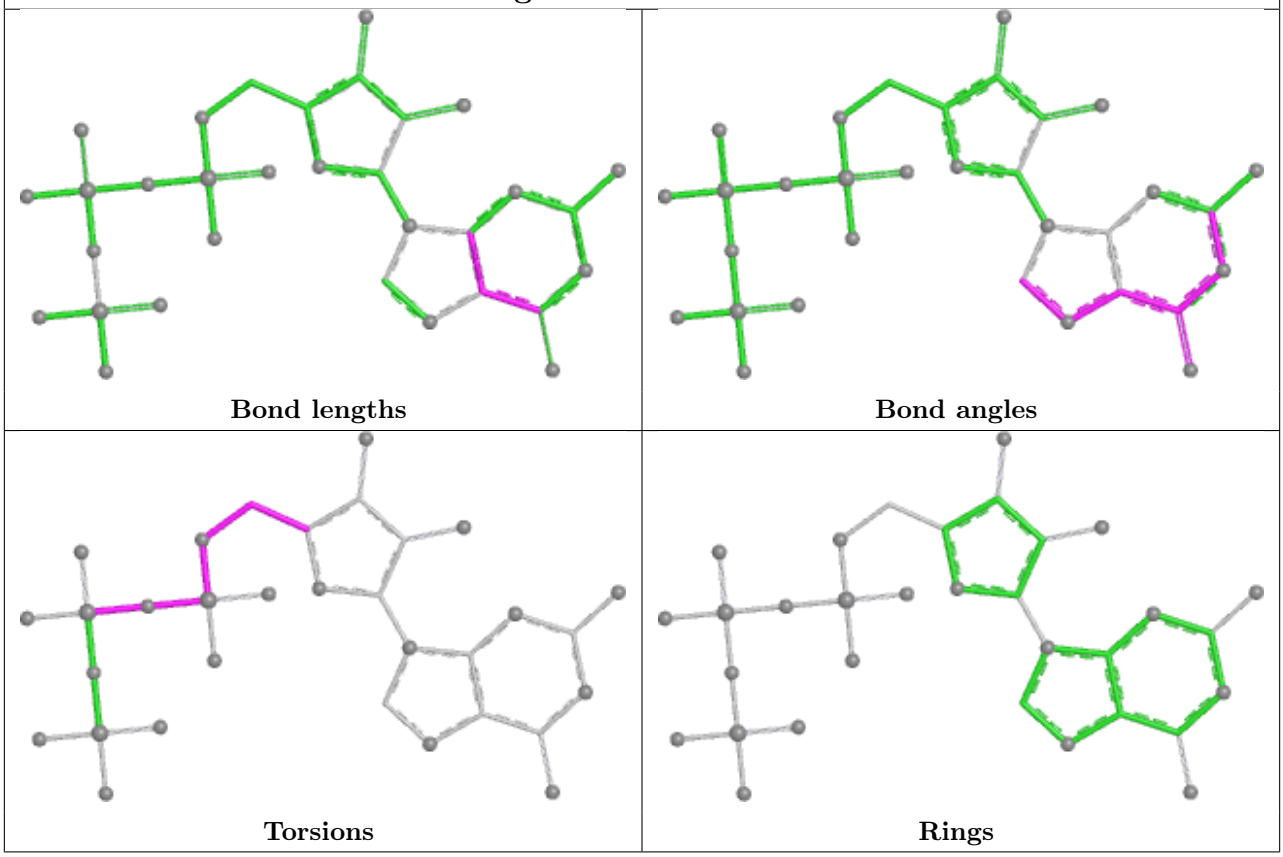

## Ligand GTP P9 501



## Ligand GTP K1 501




## Ligand GTP R4 501



| Ligand GDP U4 502 | |
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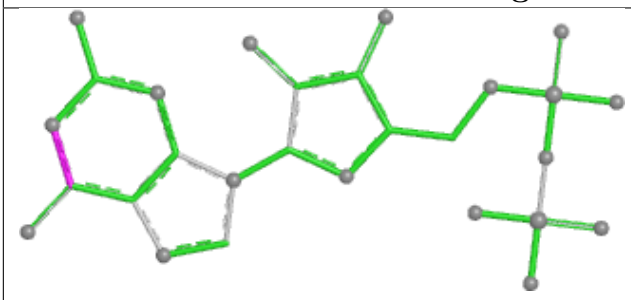
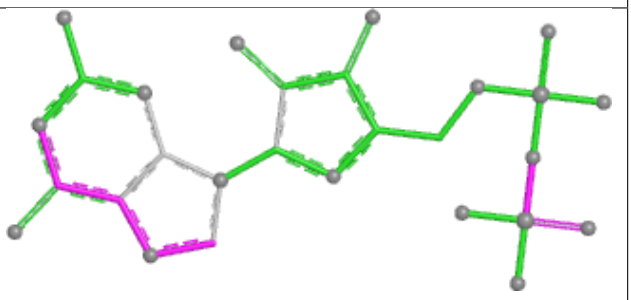
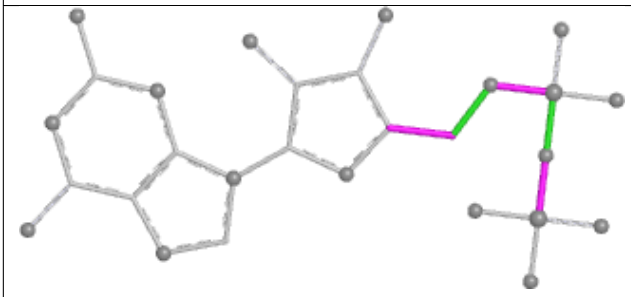
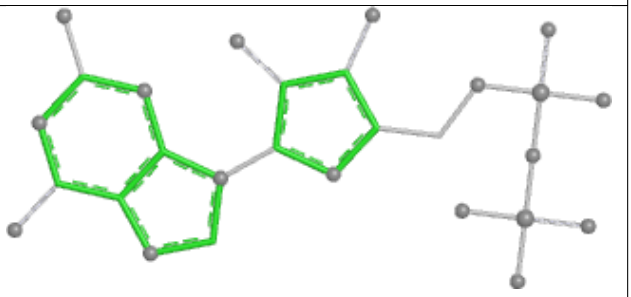
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 0G 501 | |
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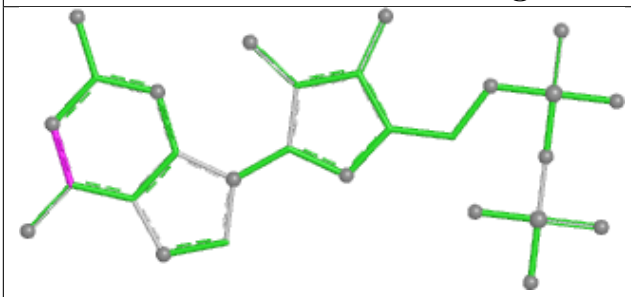
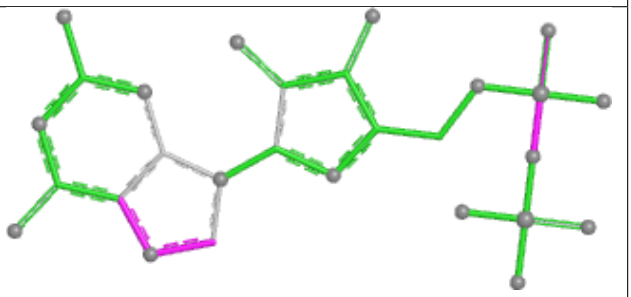
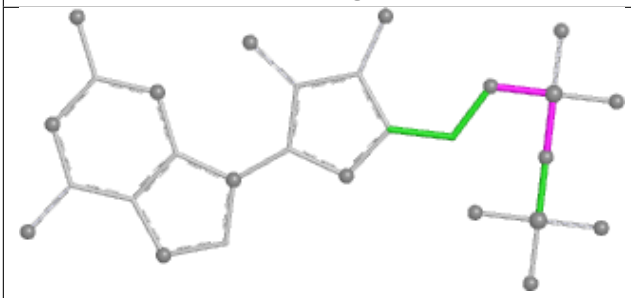
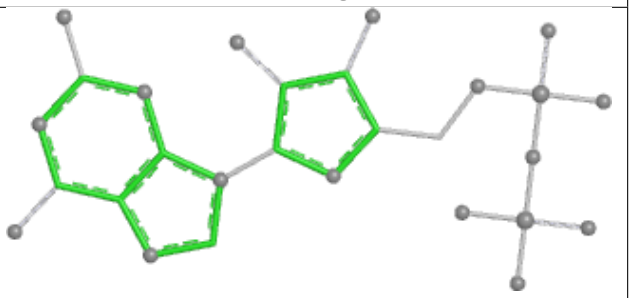
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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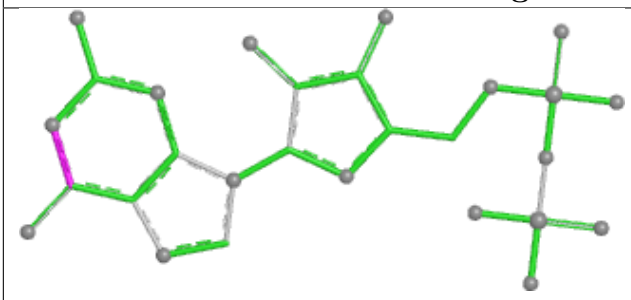

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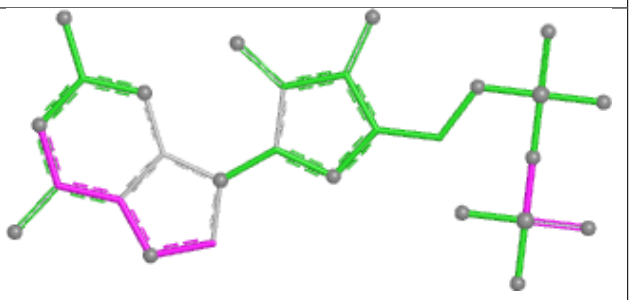

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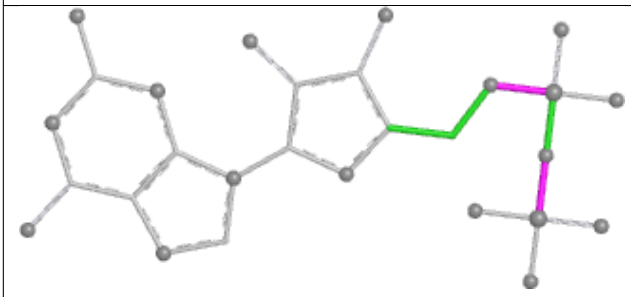

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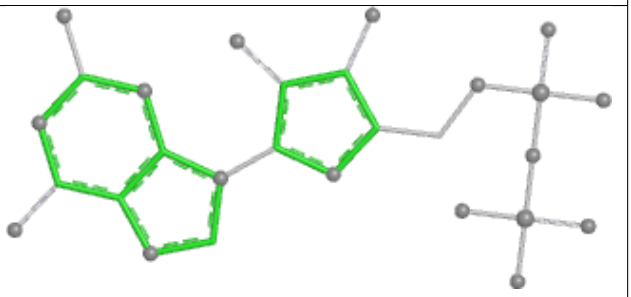
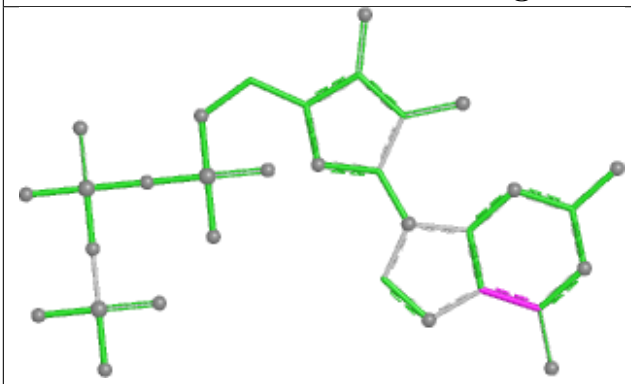


Rings

## Ligand GTP Y1 501



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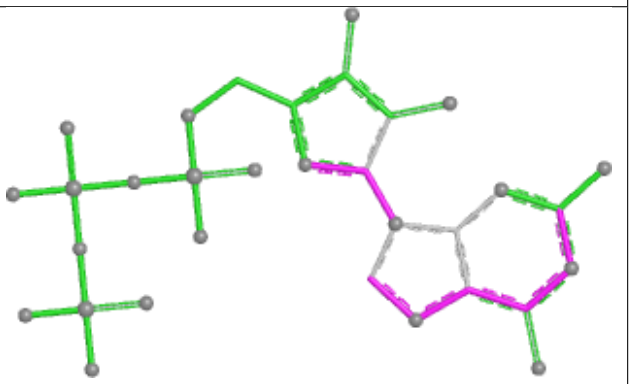

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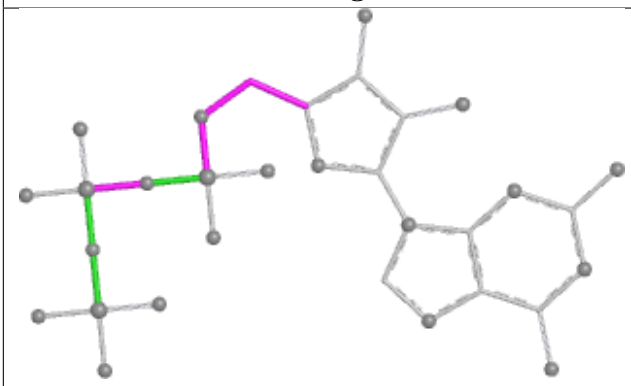

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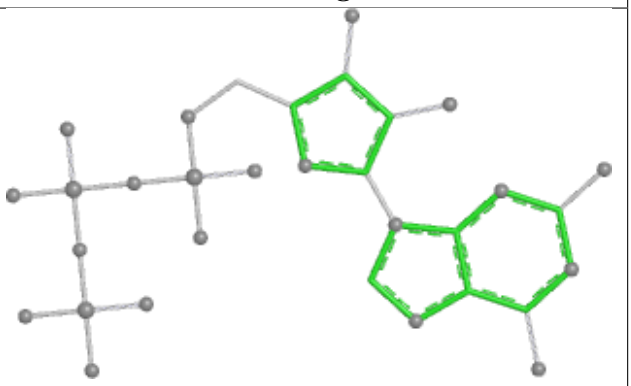

Rings

| Ligand GDP K6 502 | |
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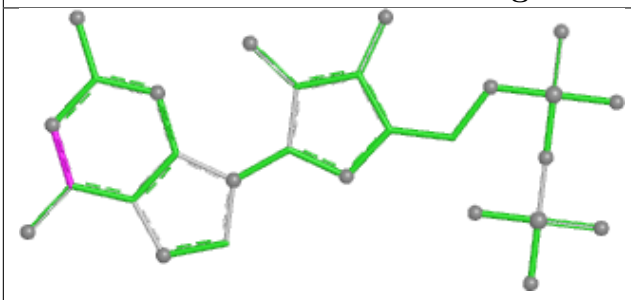
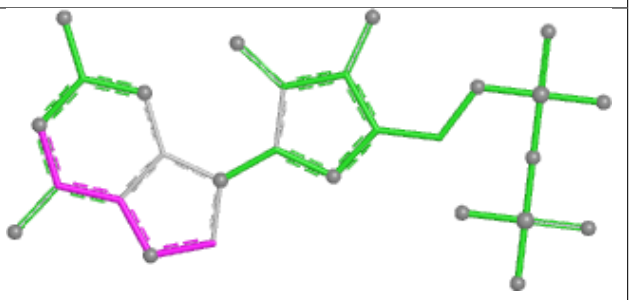
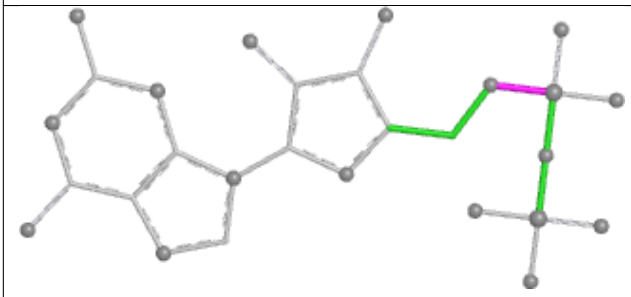
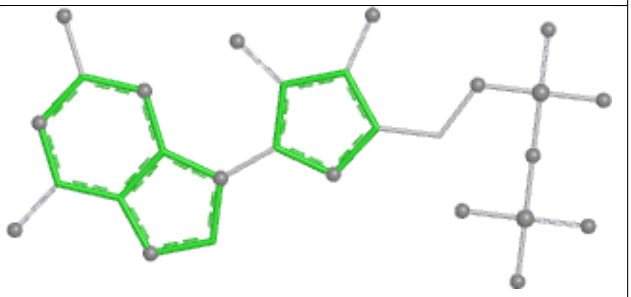
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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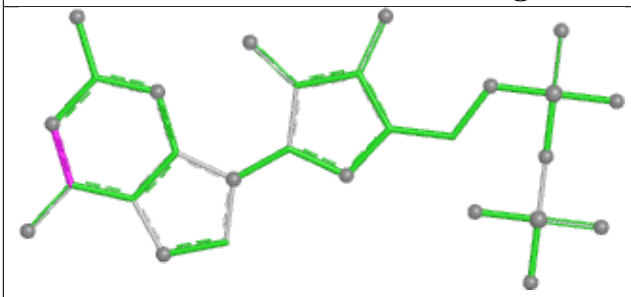
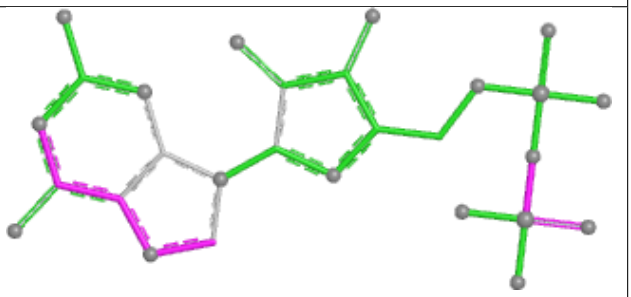
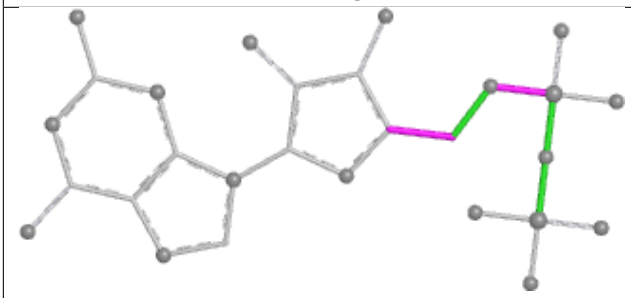
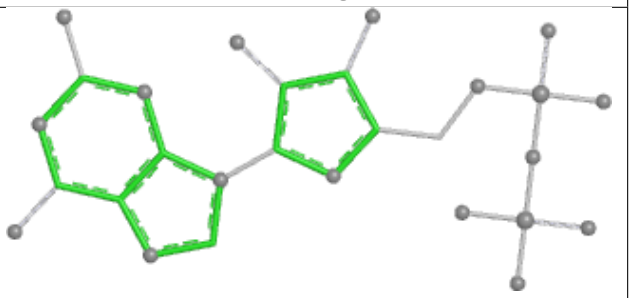
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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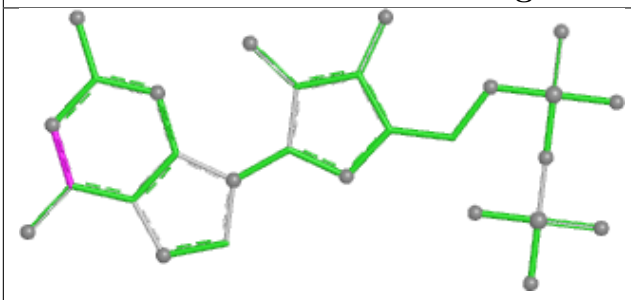

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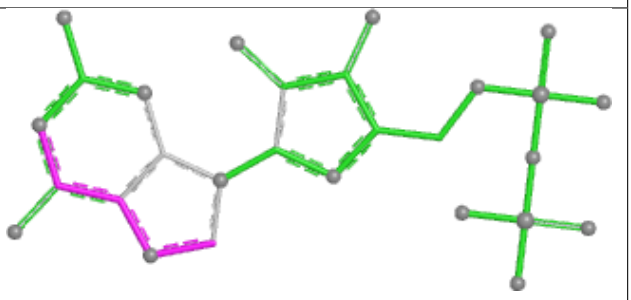
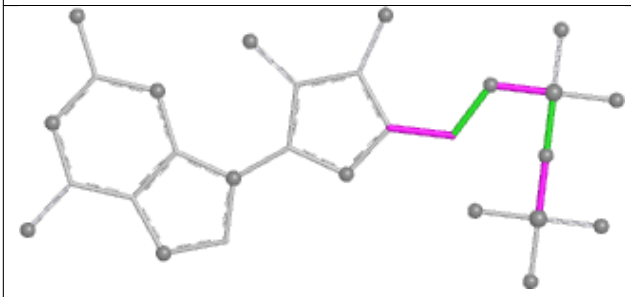


Bond angles



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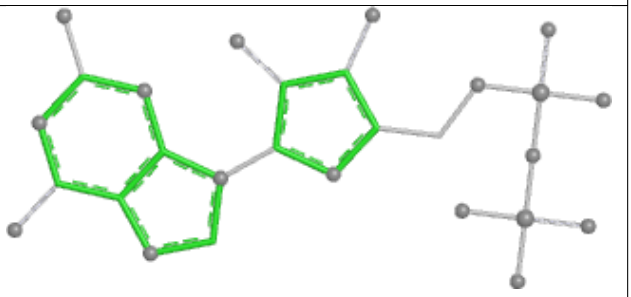
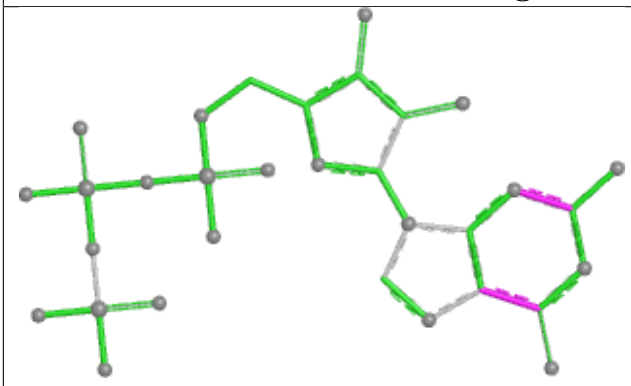


Rings

## Ligand GTP B0 501



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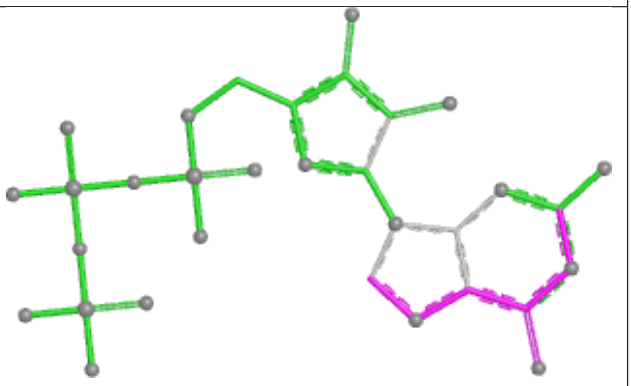

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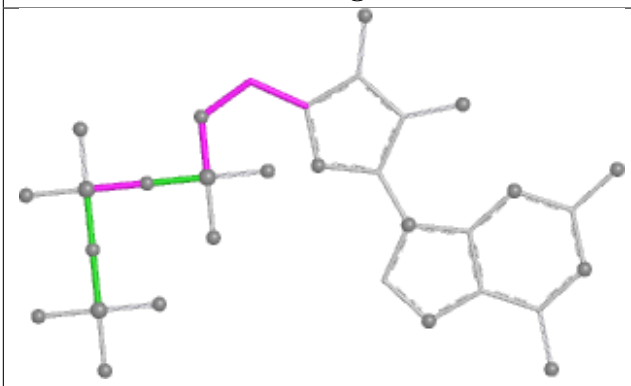

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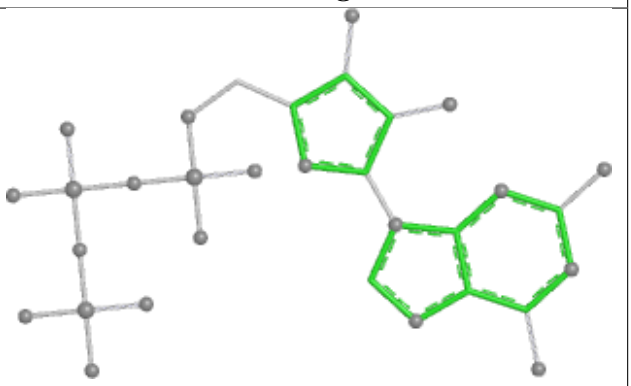

Rings

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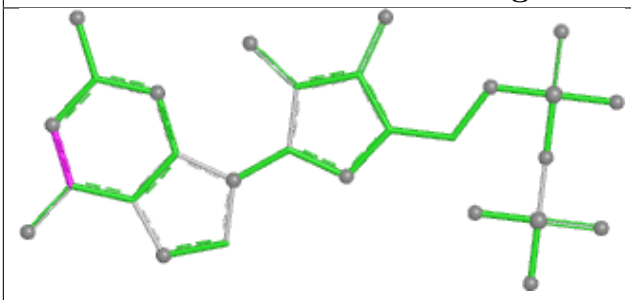
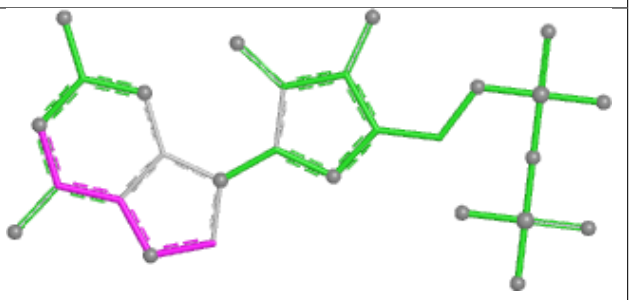
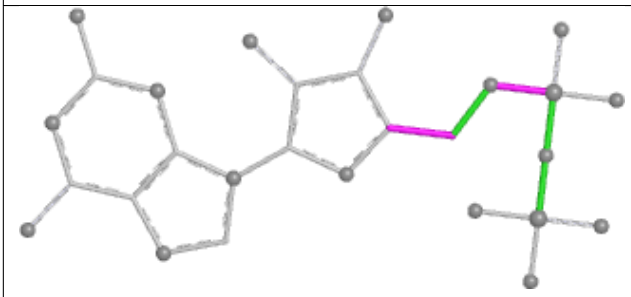
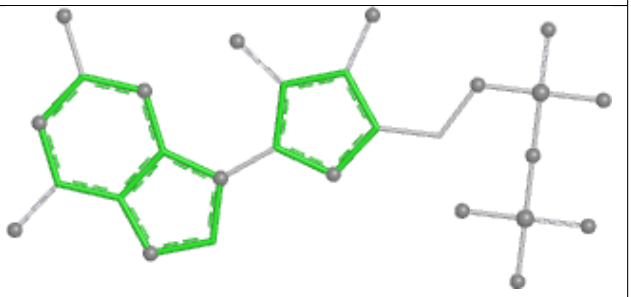
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP J2 502 | |
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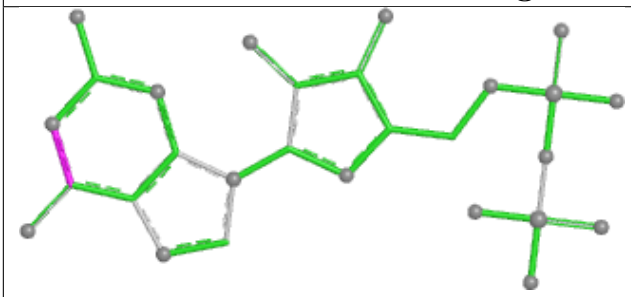
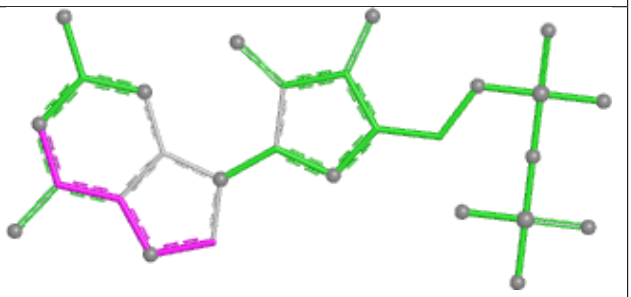
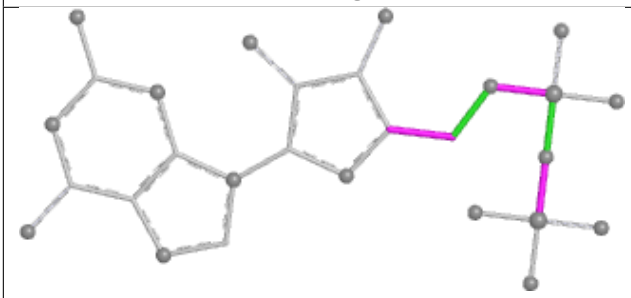
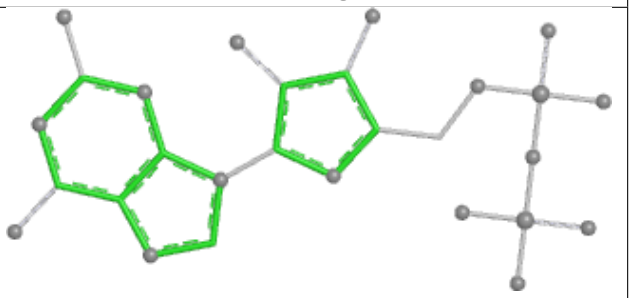
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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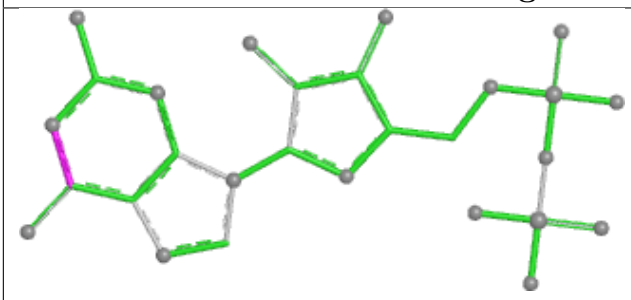

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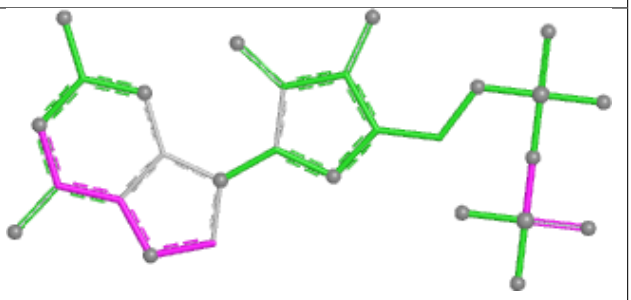

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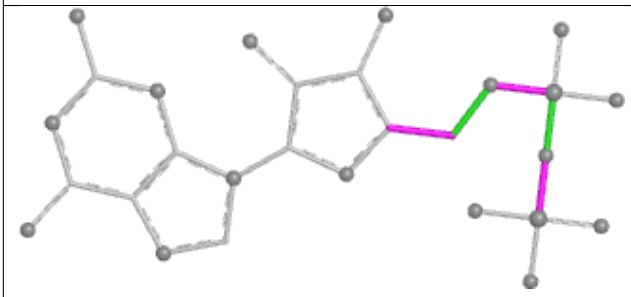

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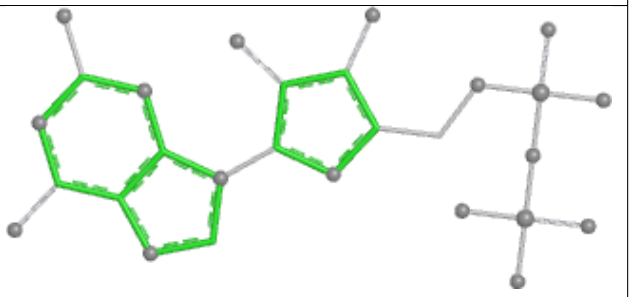
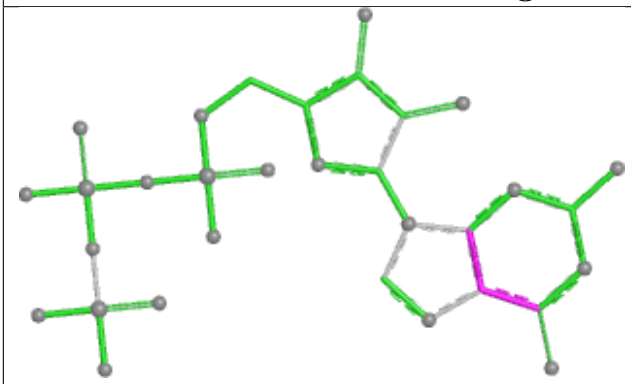


Rings

## Ligand GTP 2S 501



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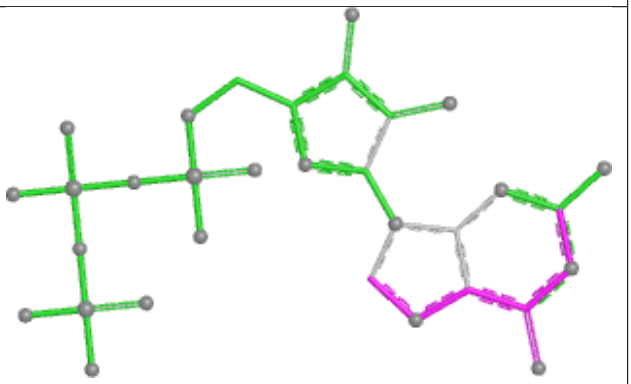

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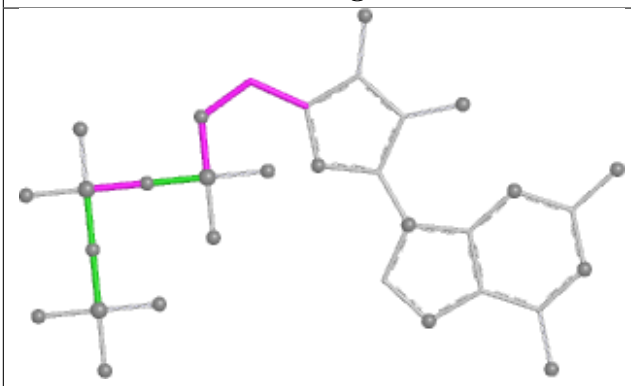

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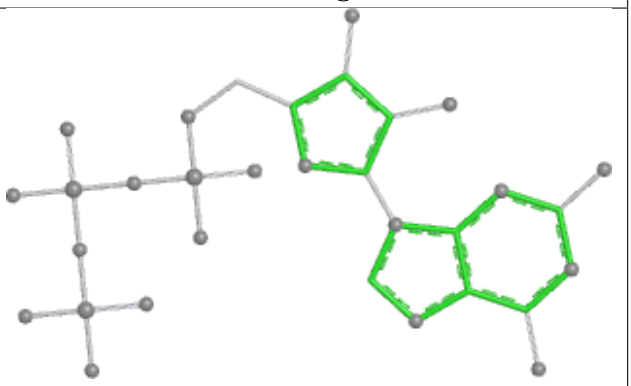

Rings

| Ligand GDP 0Q 502 | |
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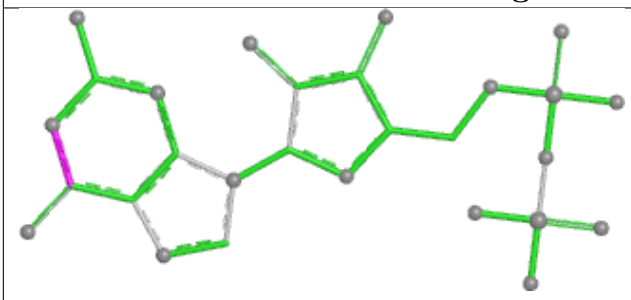
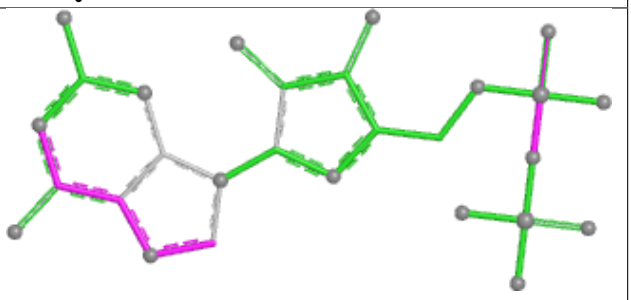
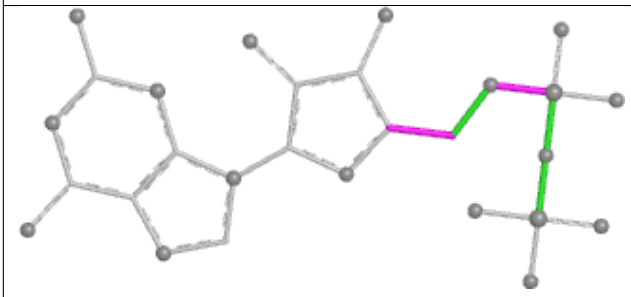
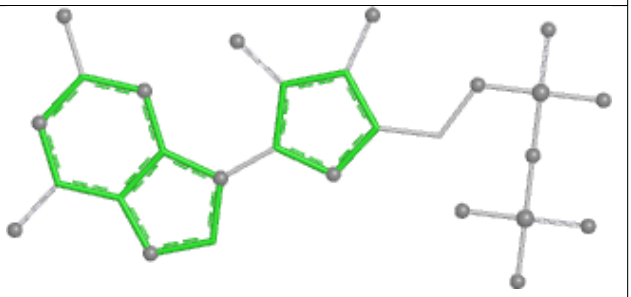
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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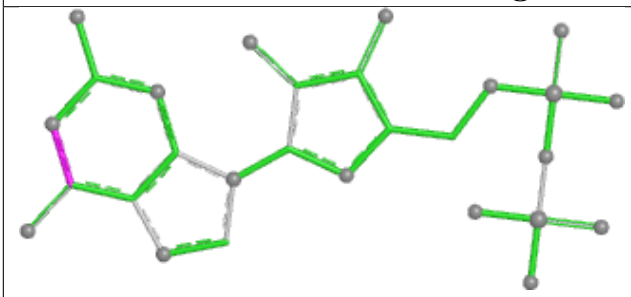
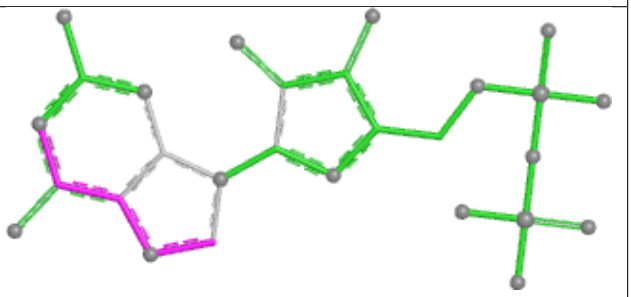
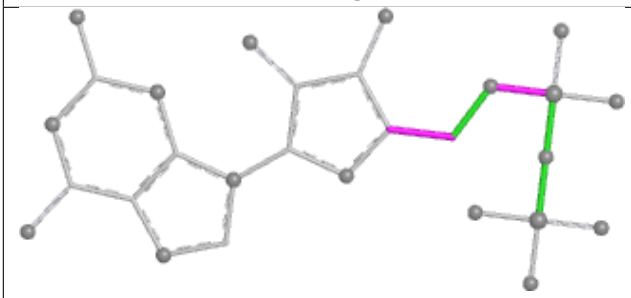
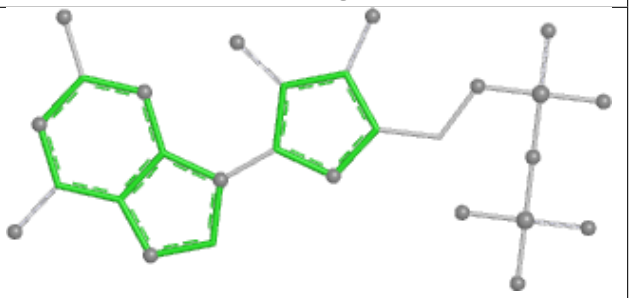
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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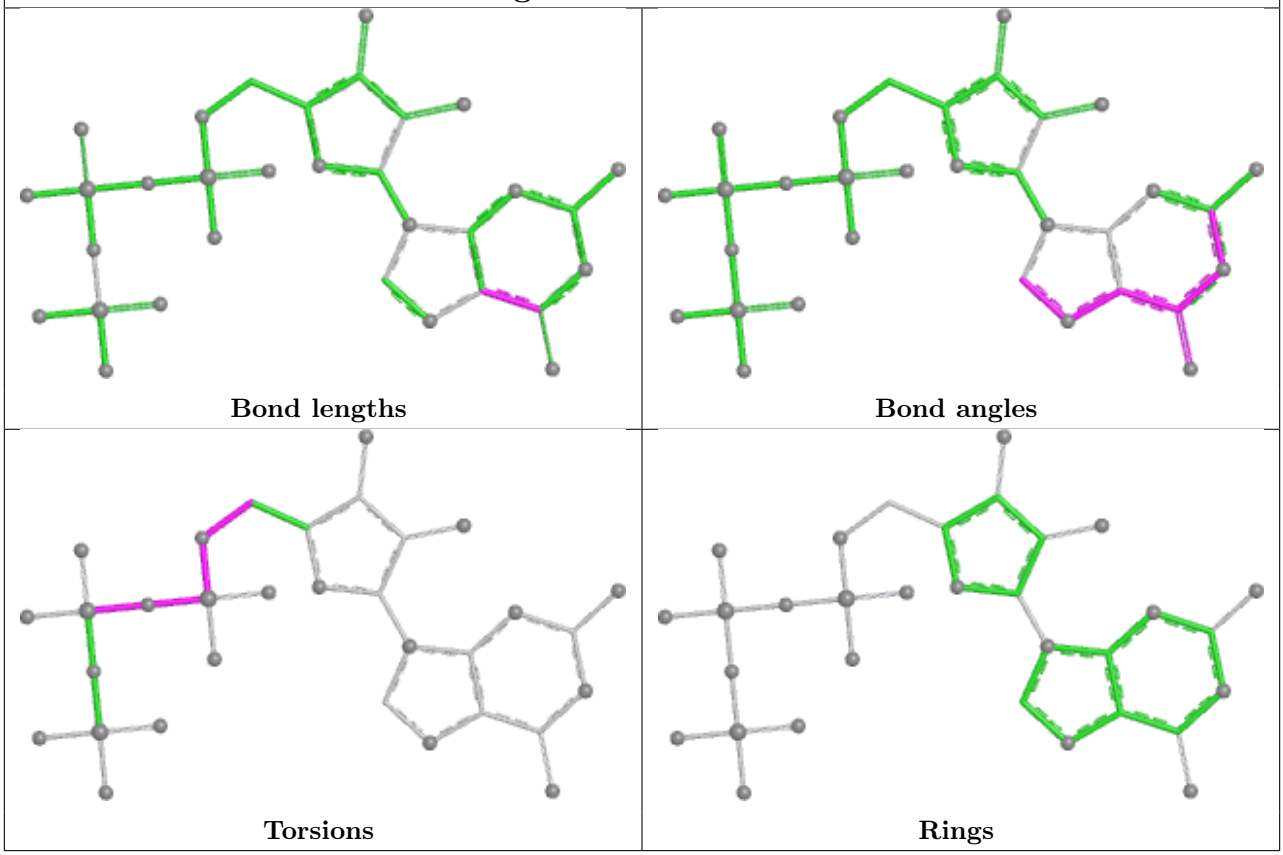


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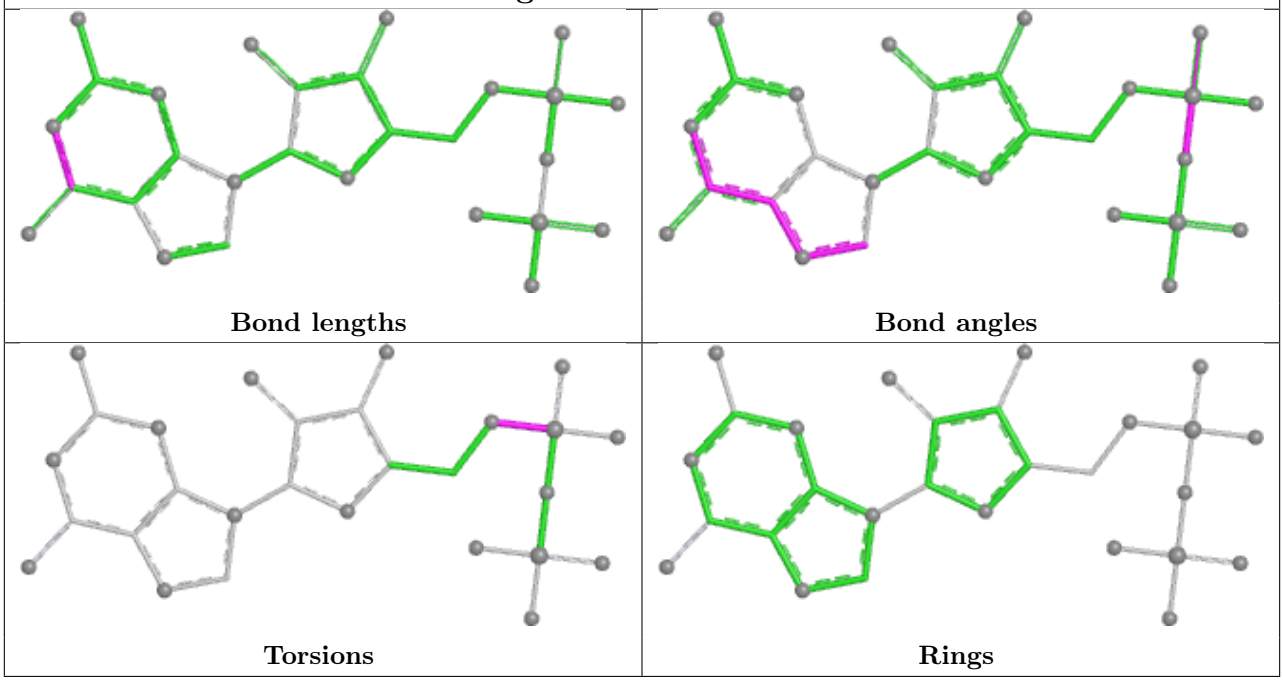

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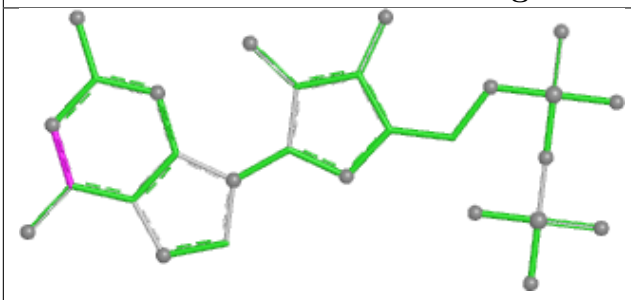

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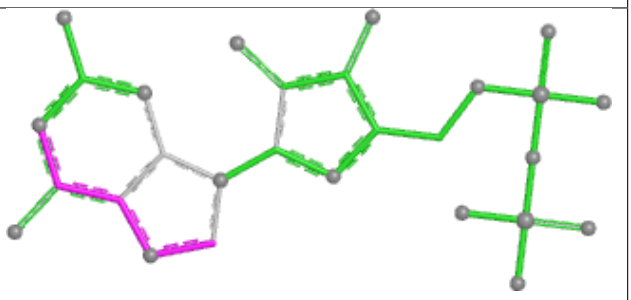

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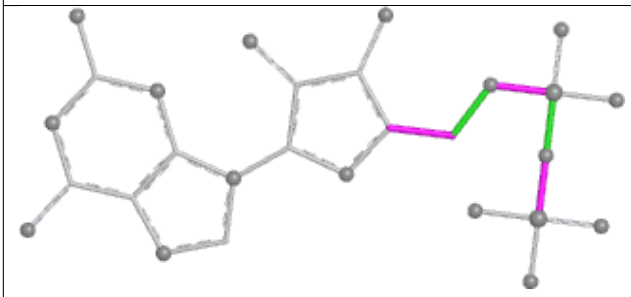

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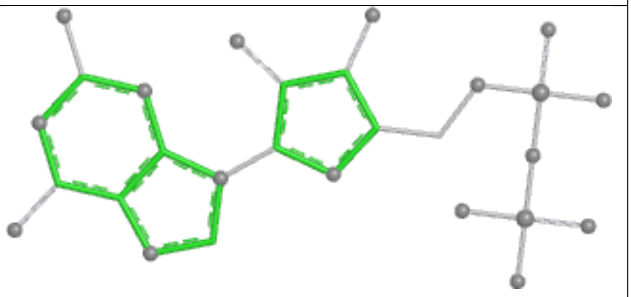

Rings

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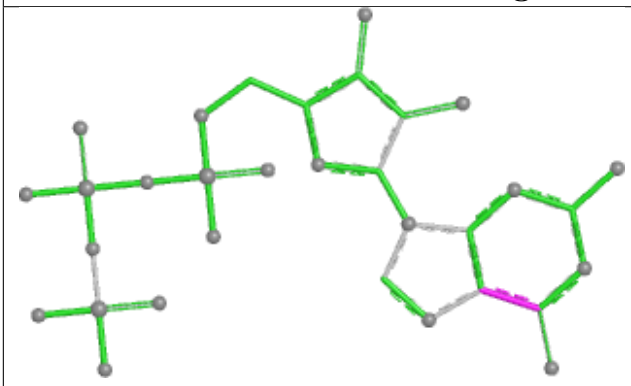

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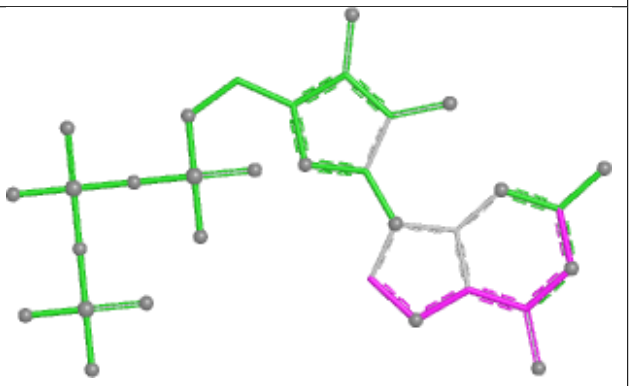

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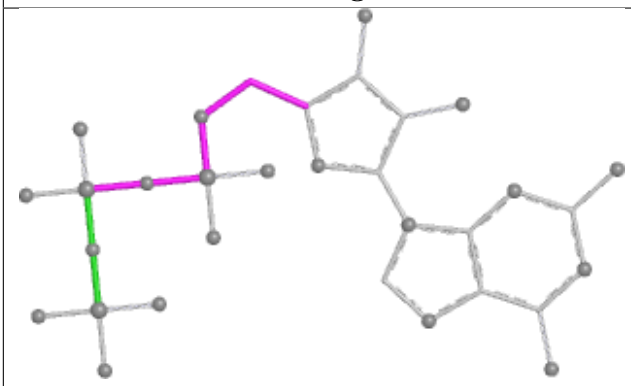

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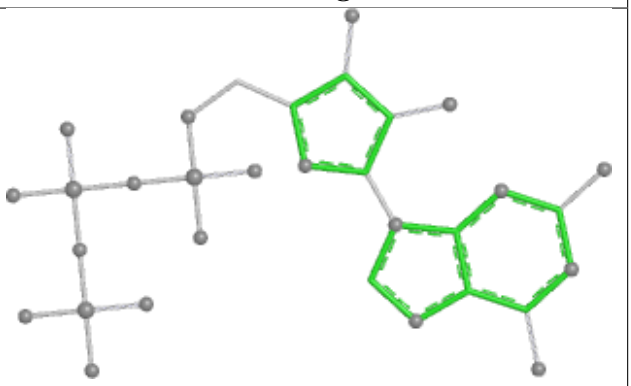

Rings

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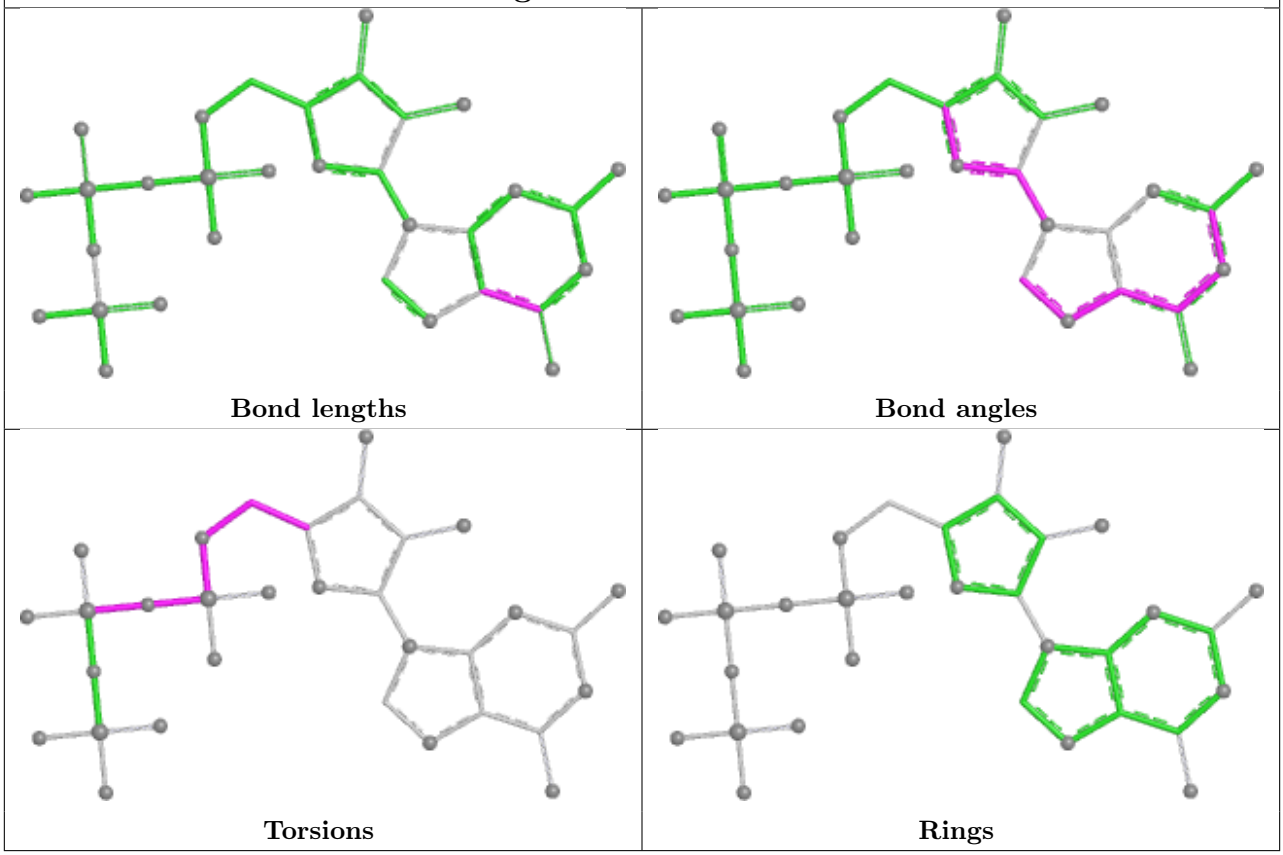


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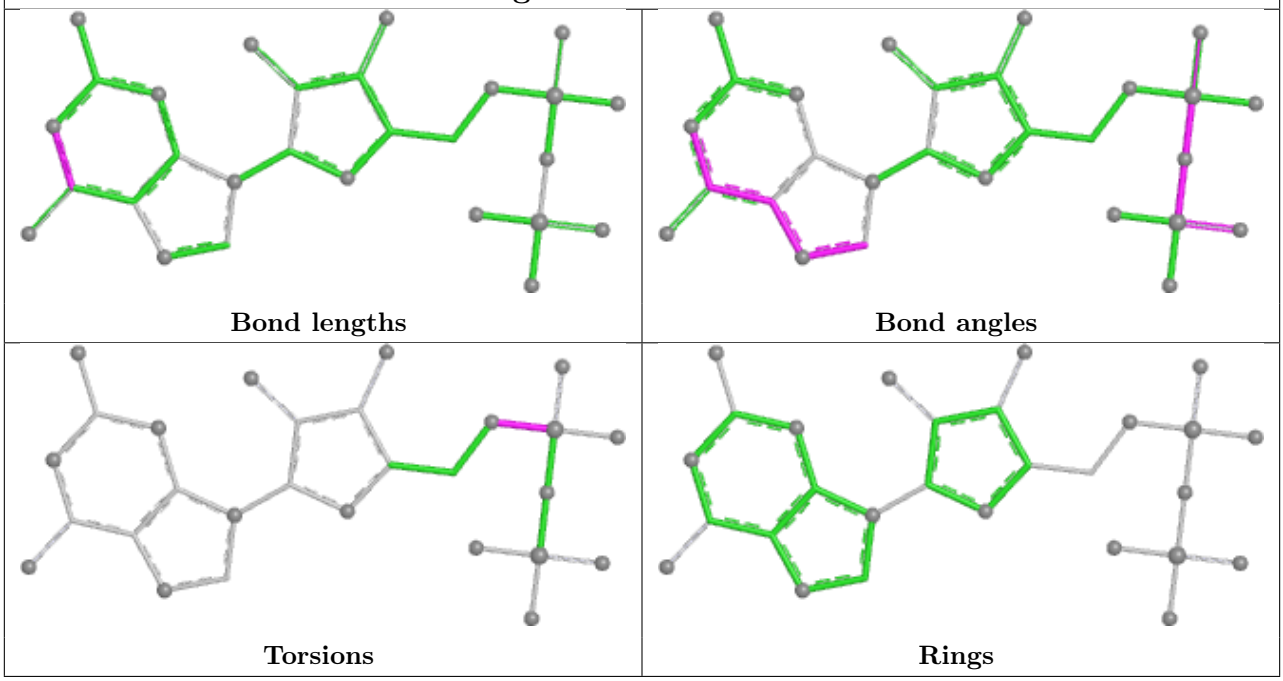

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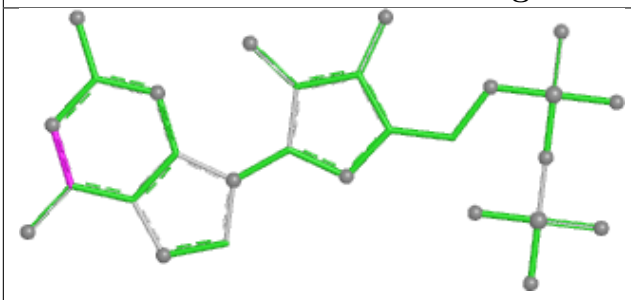
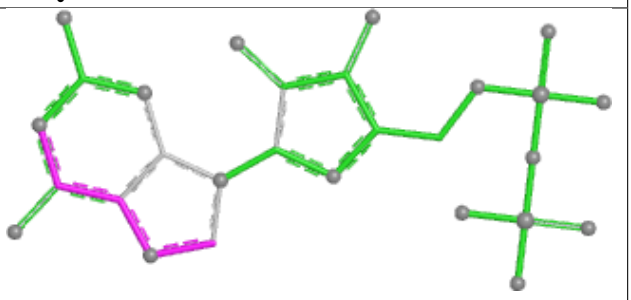
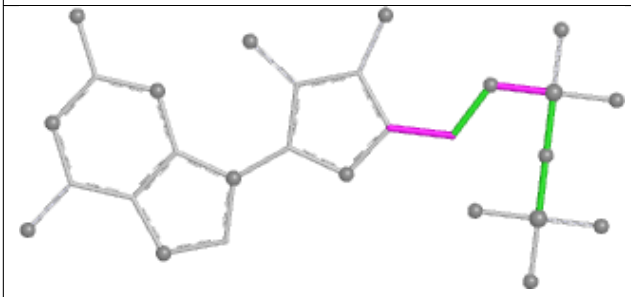
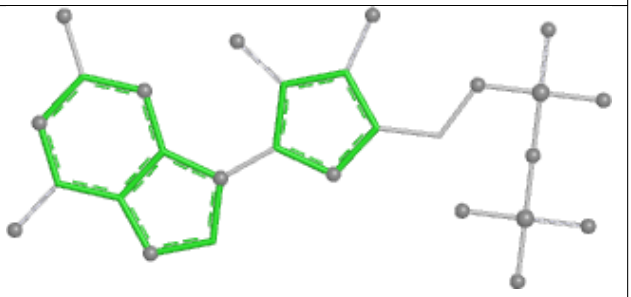
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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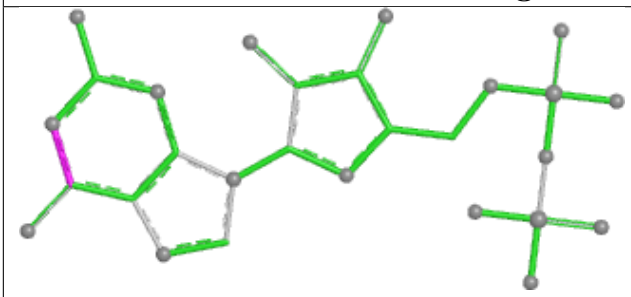
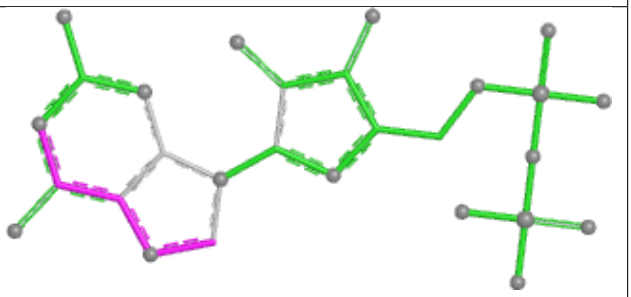
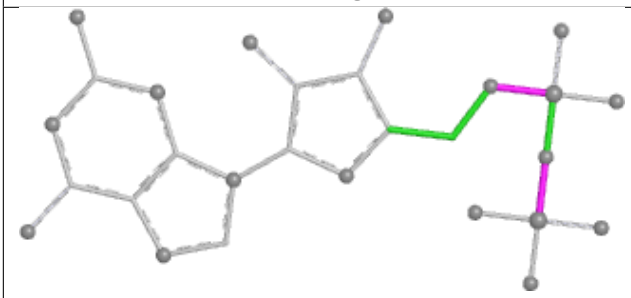
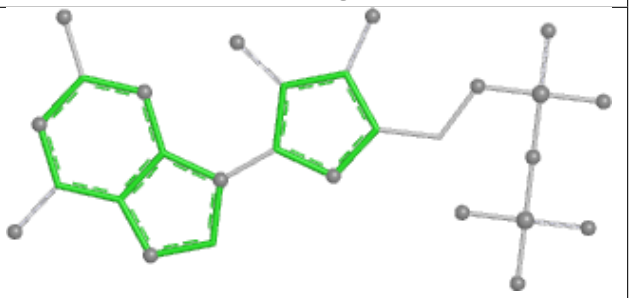
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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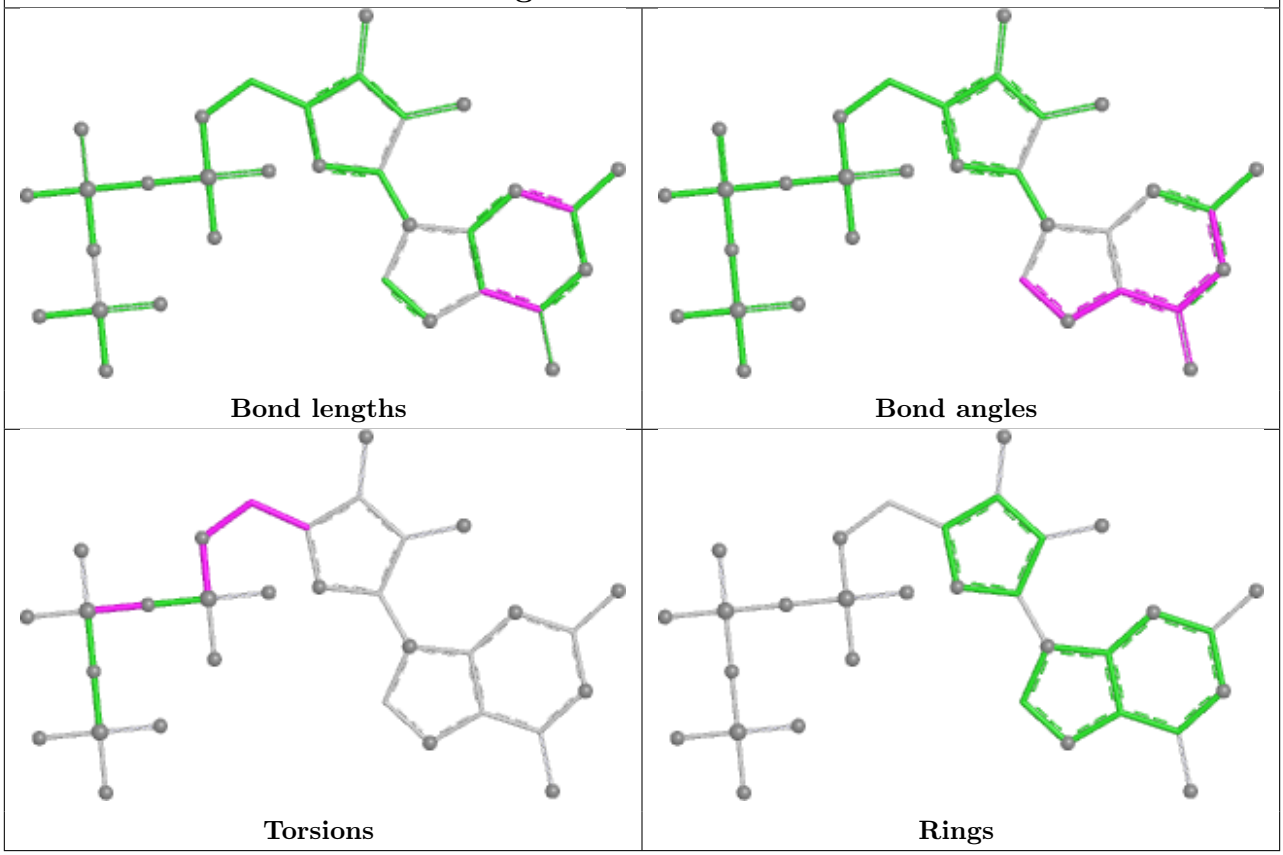


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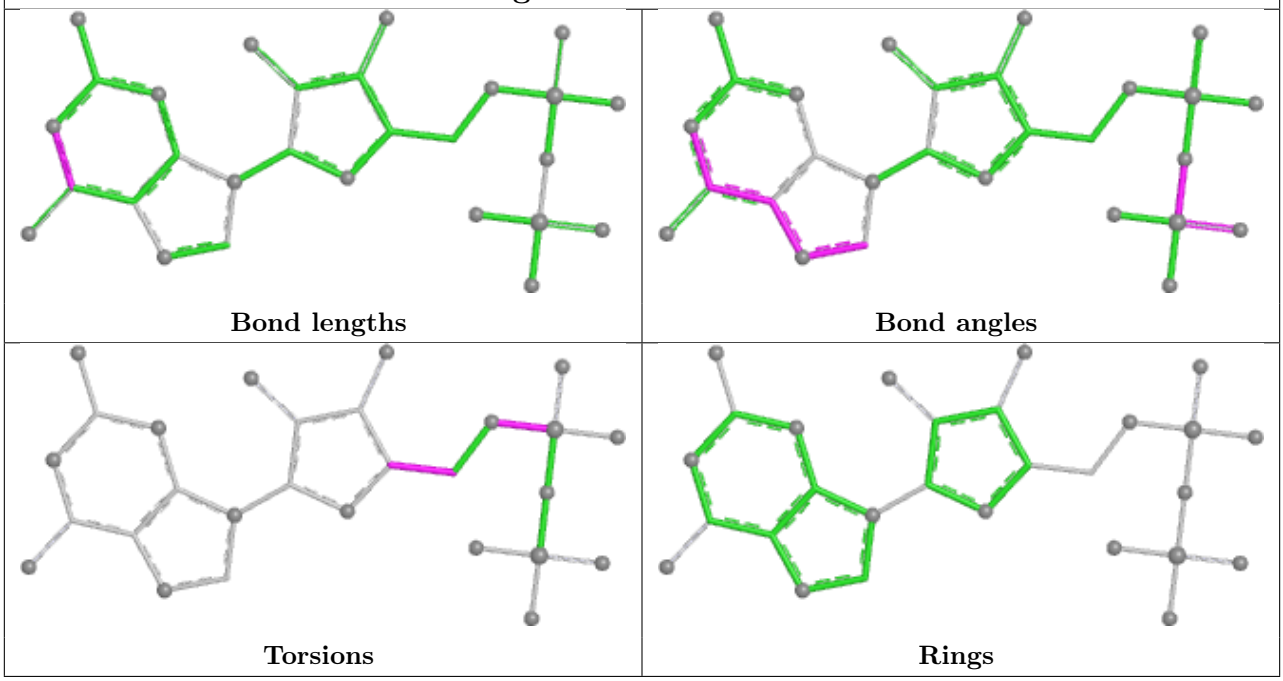

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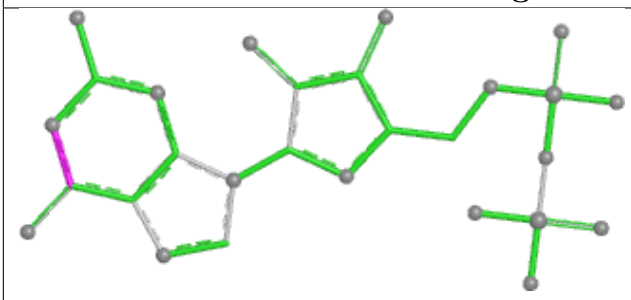
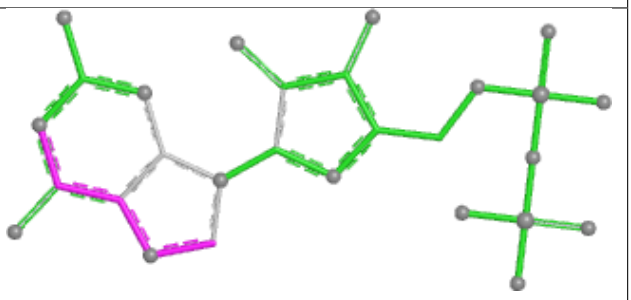
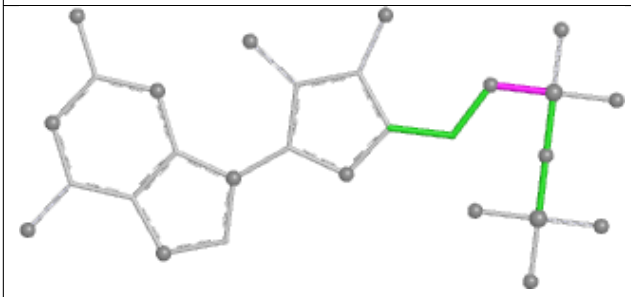


Bond lengths



Bond angles



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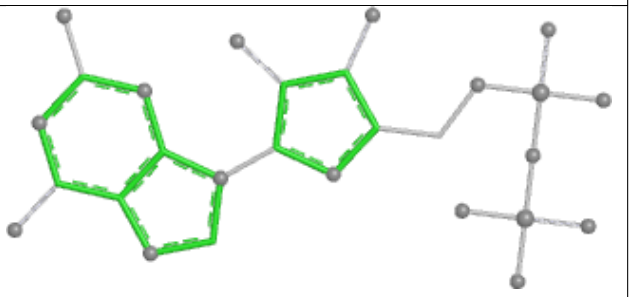
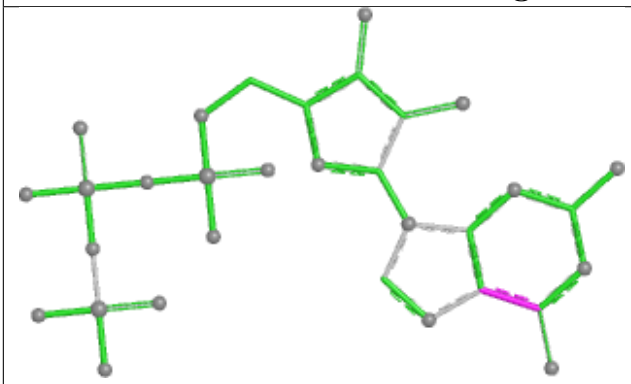


Rings

## Ligand GTP G9 501



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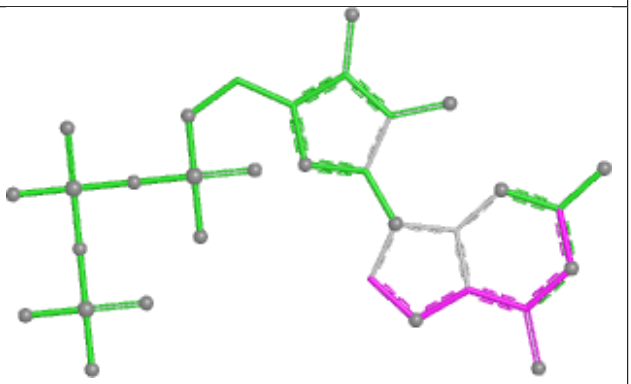

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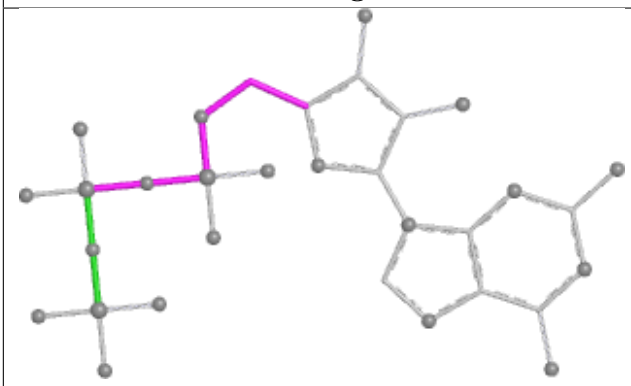

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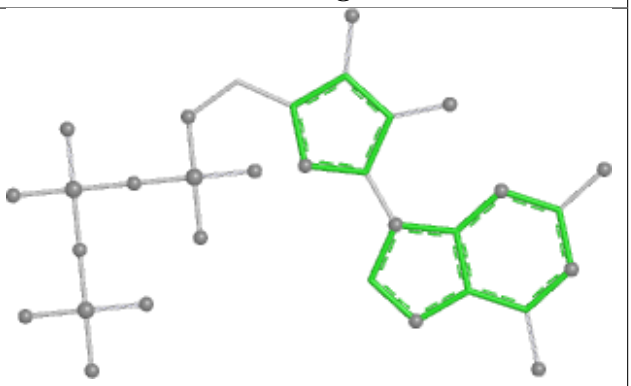

Rings

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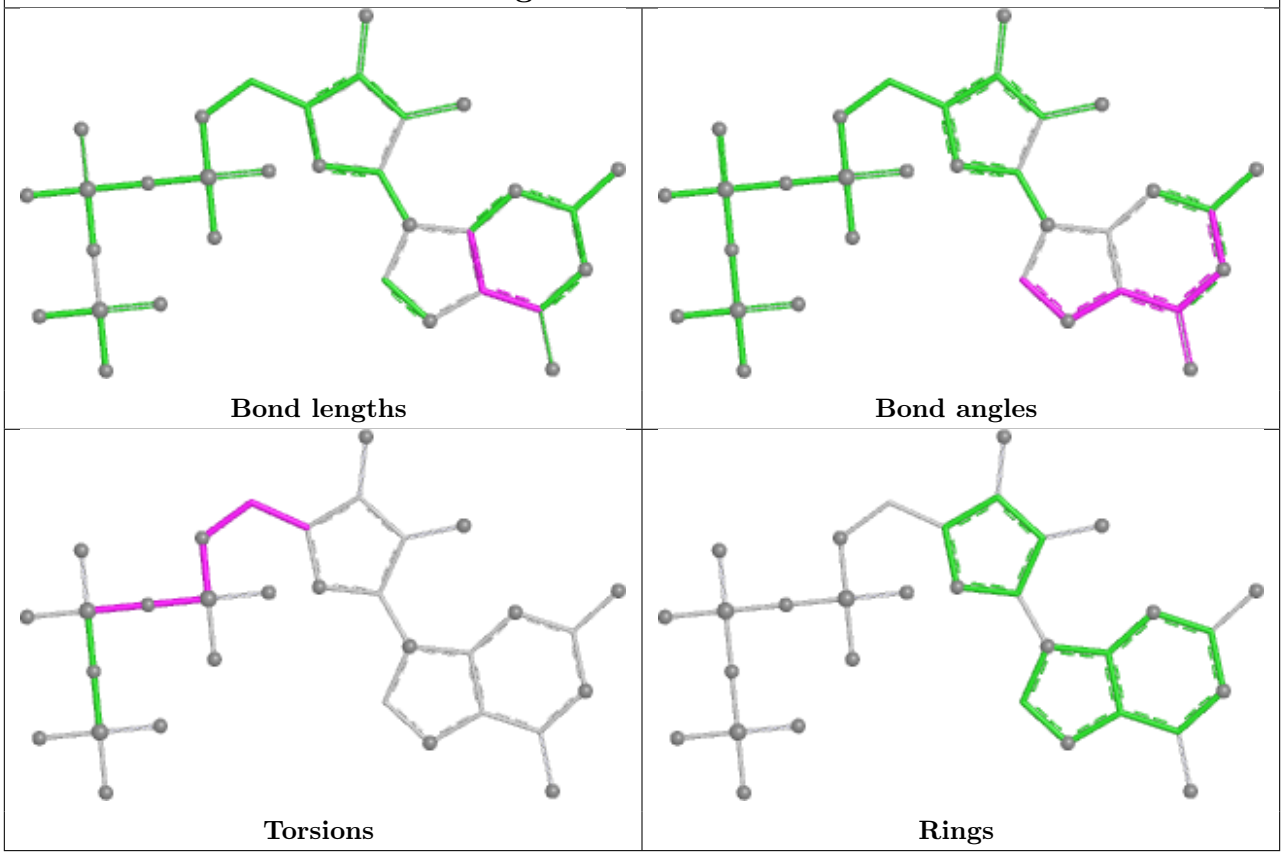


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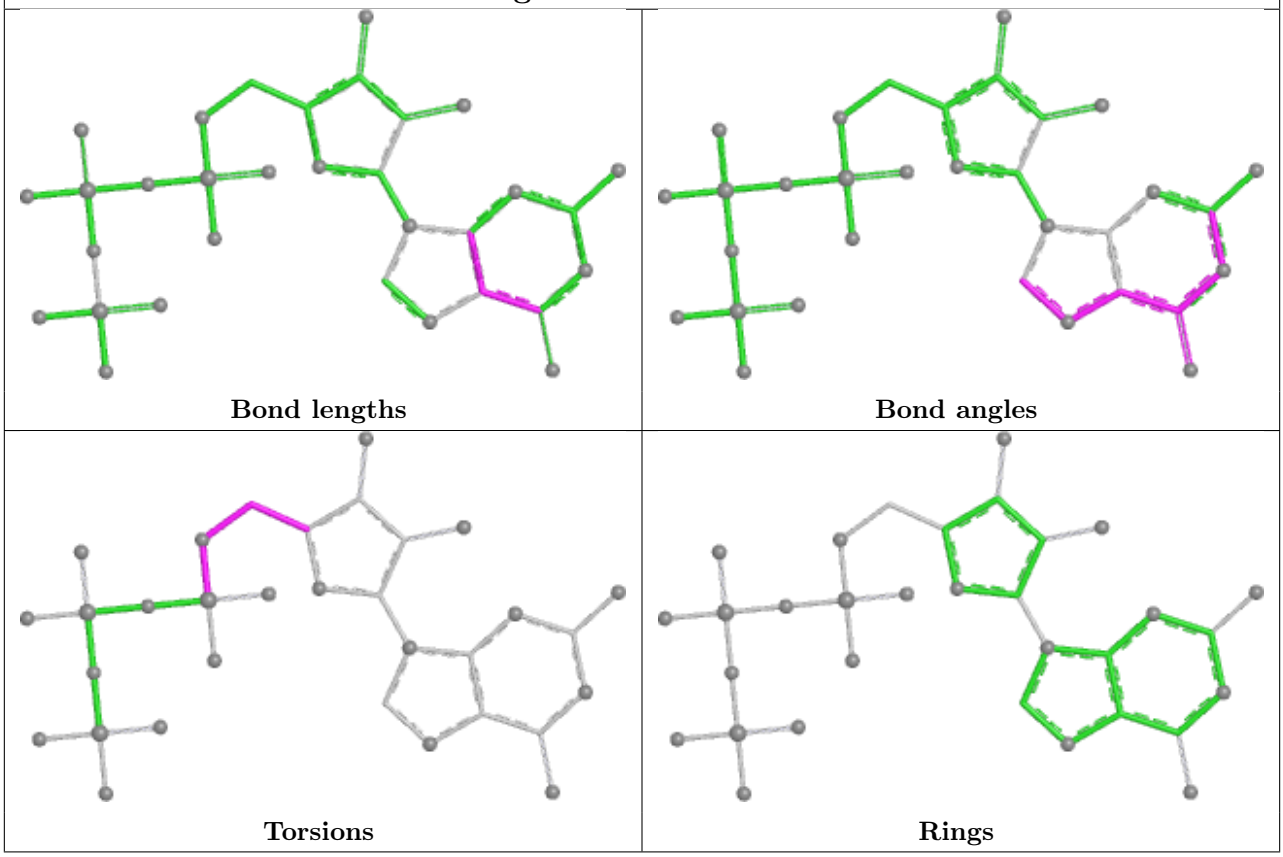

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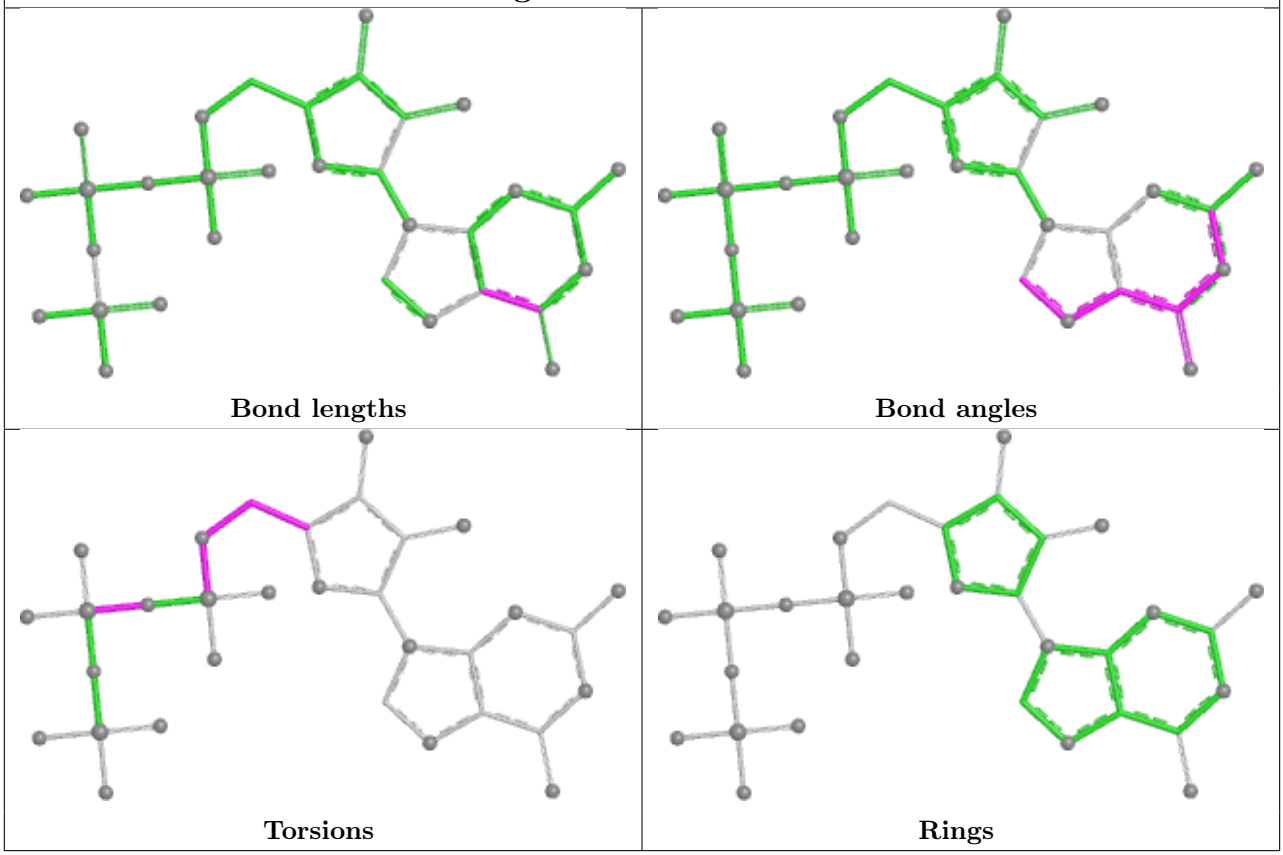


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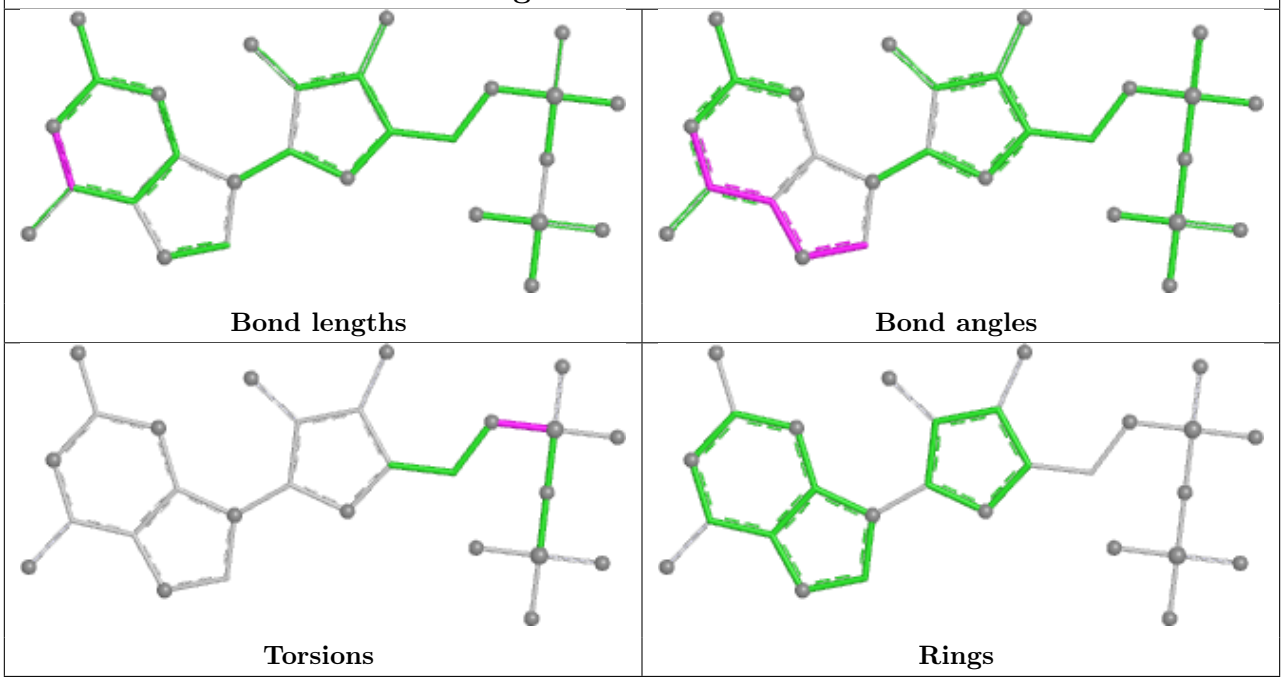

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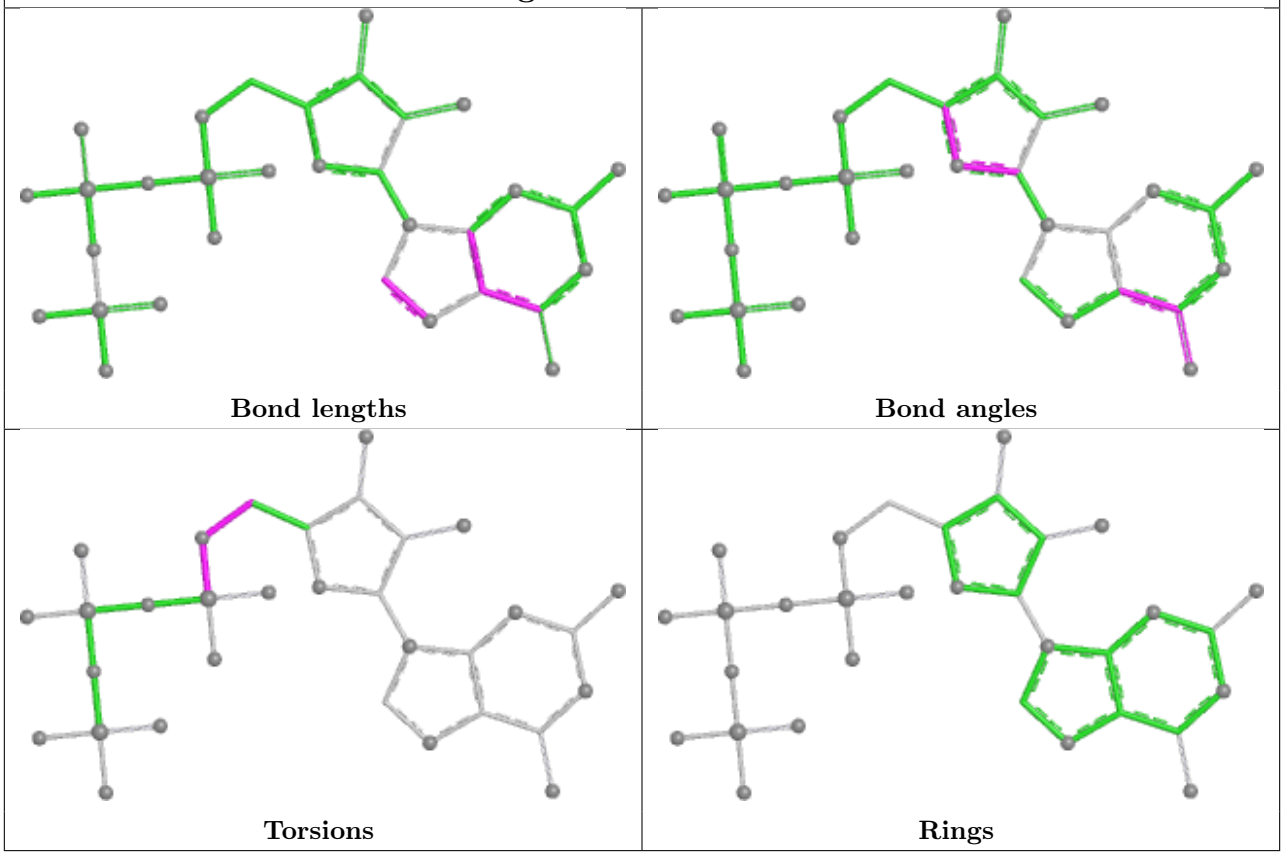


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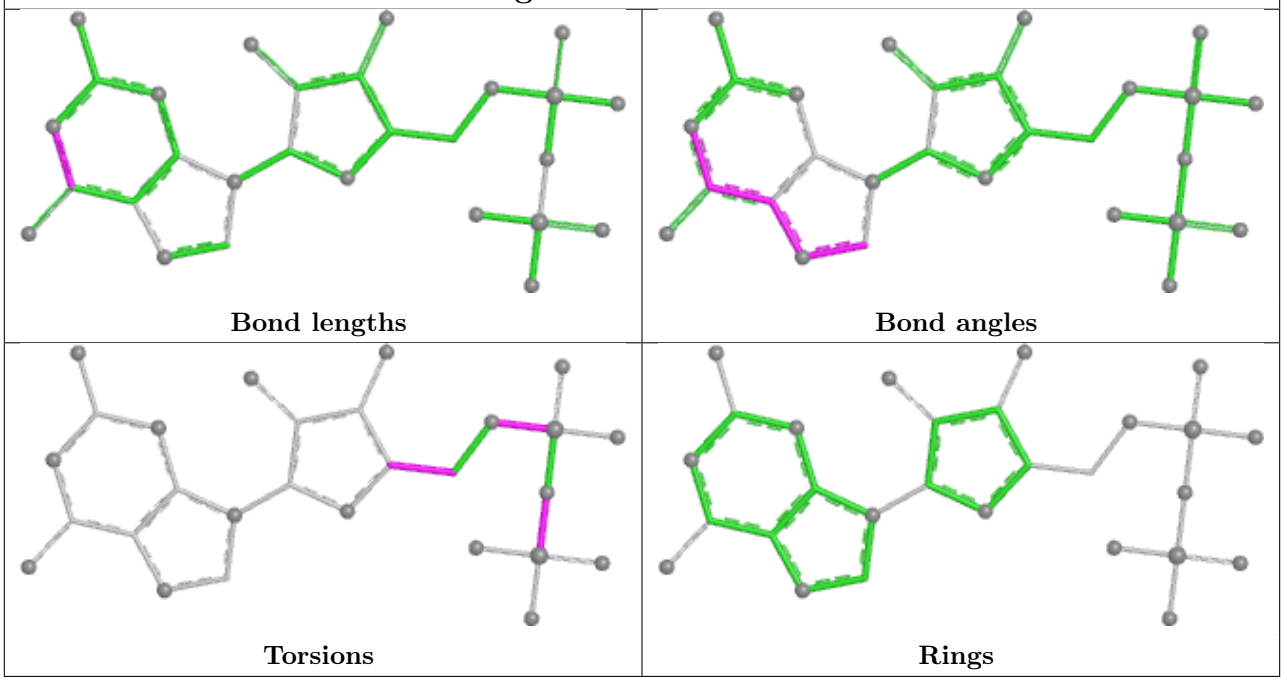

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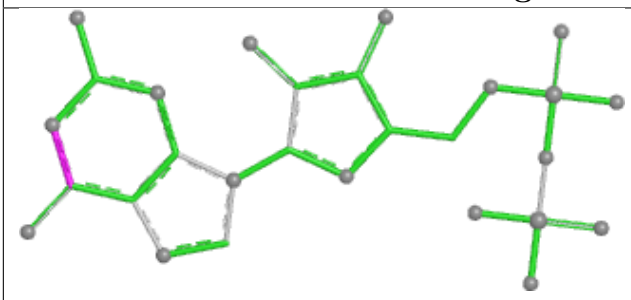
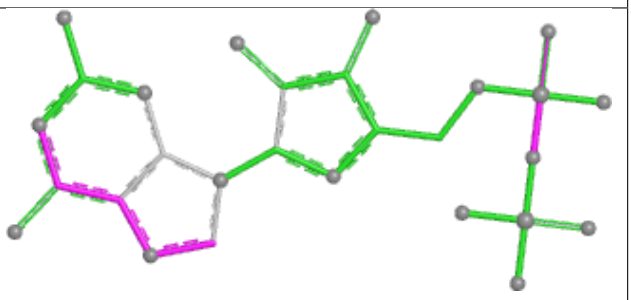
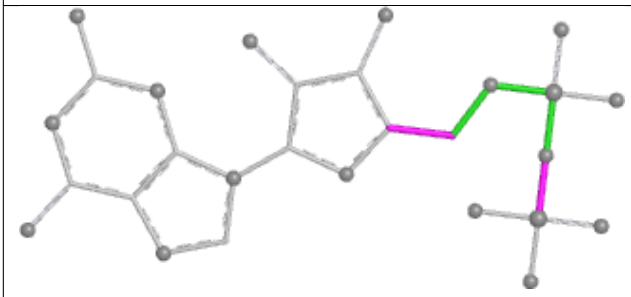
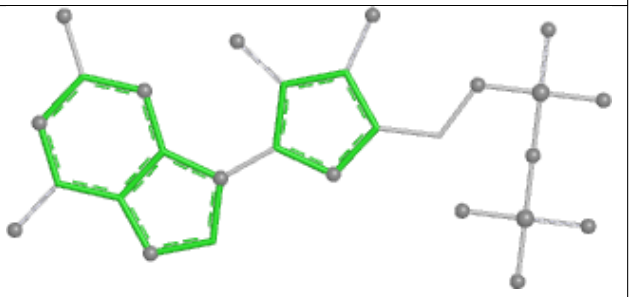
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP C2 501 | |
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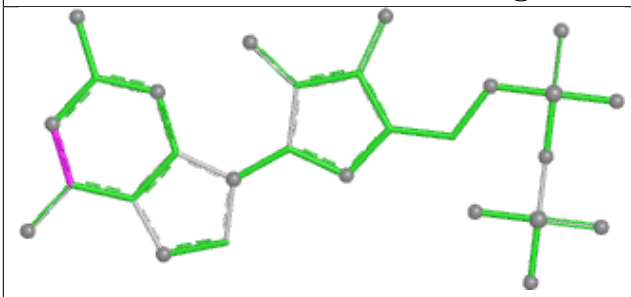
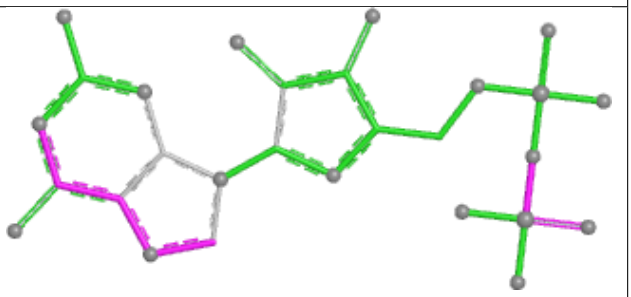
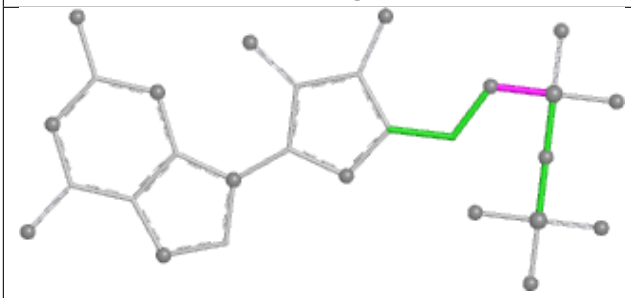
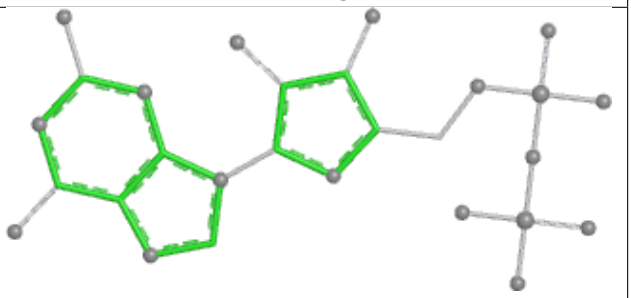
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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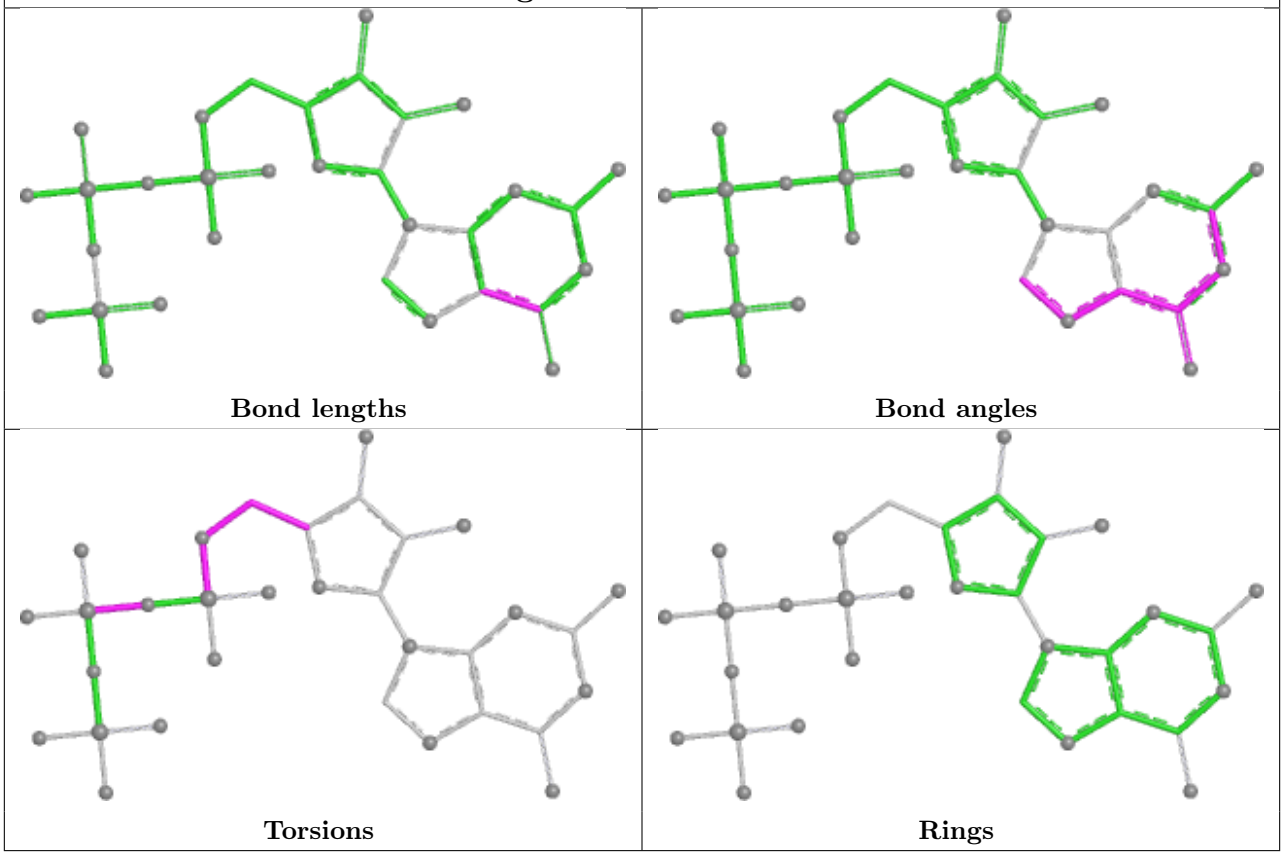
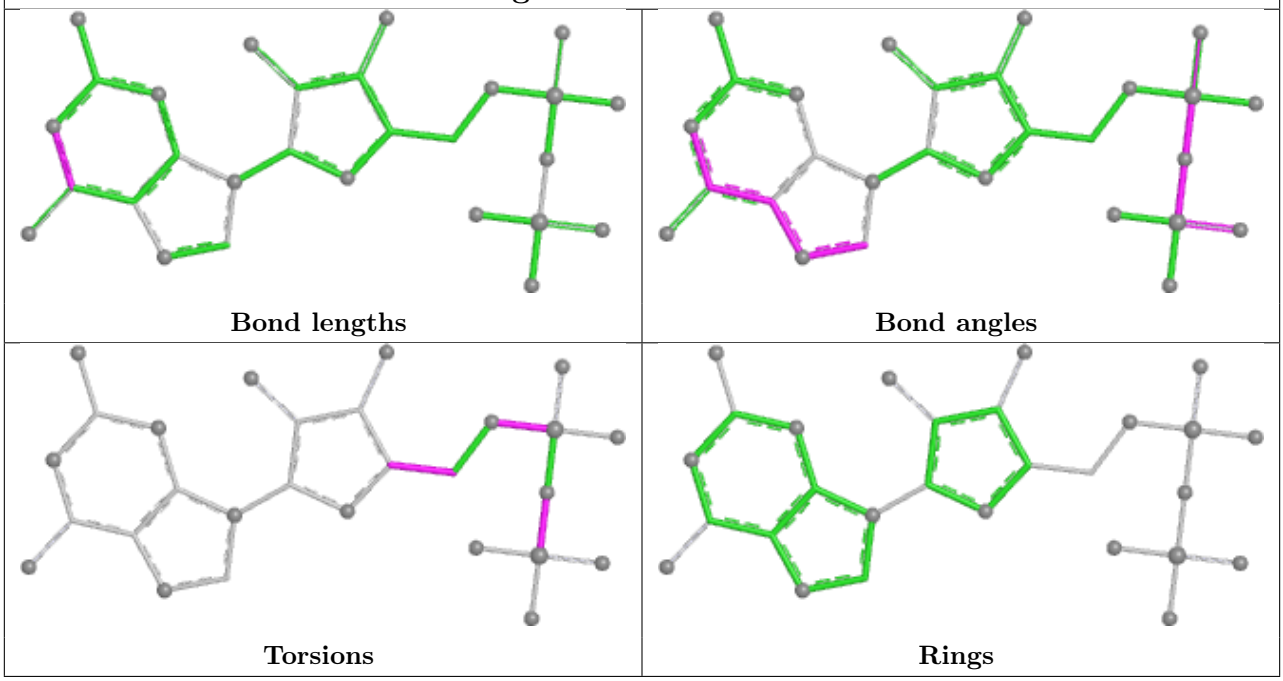



## Ligand GDP K0 502



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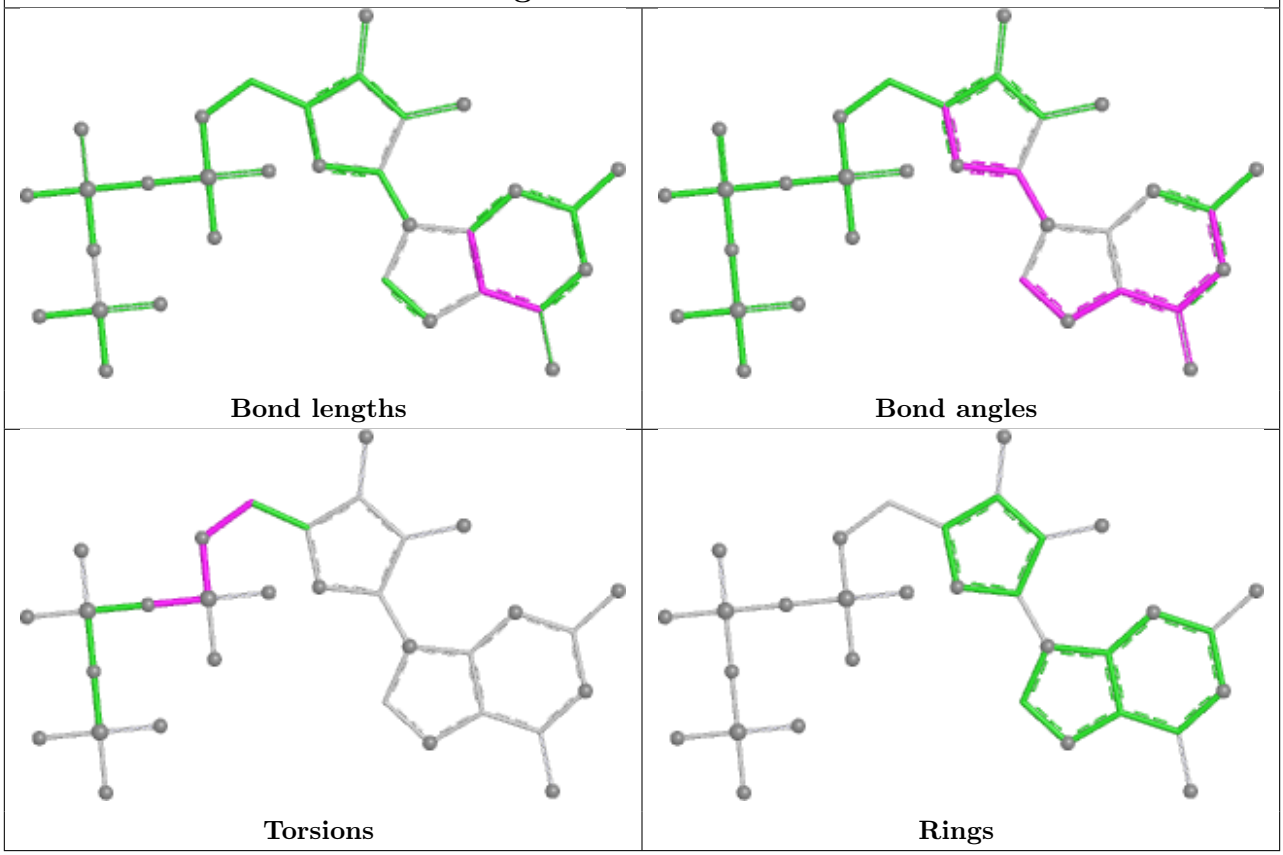


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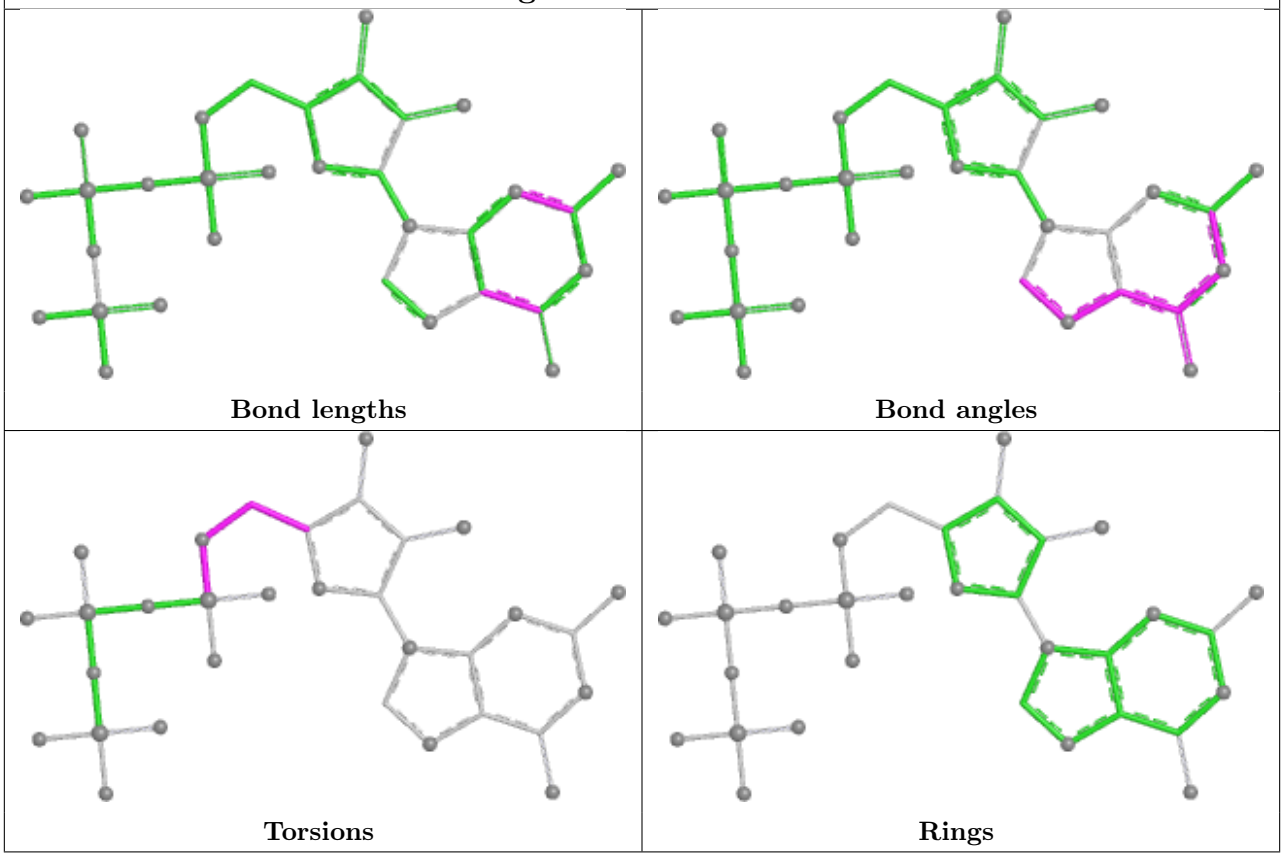

| Ligand GDP B5 502 | |
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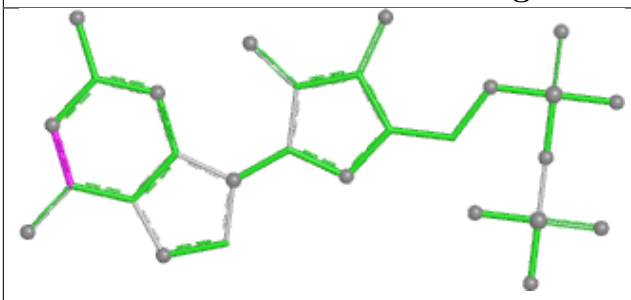
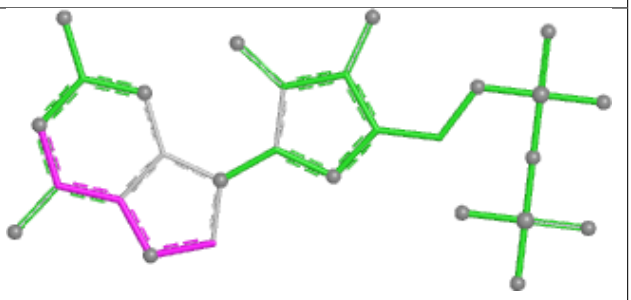
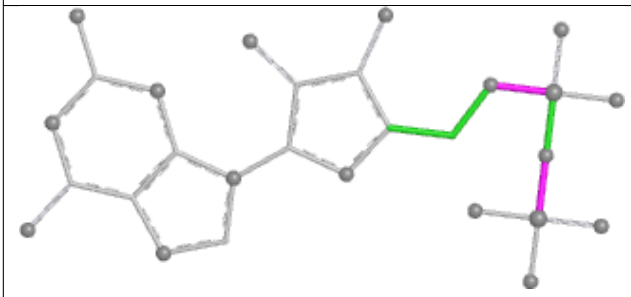
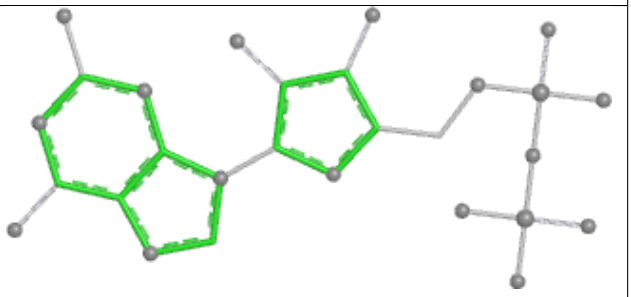
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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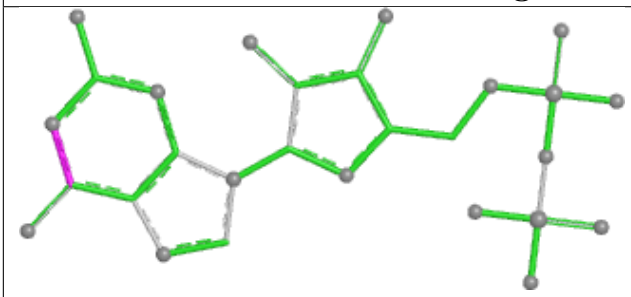
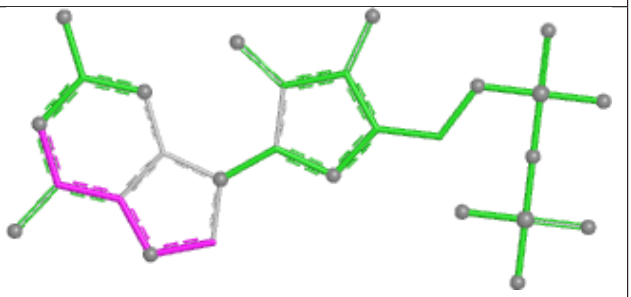
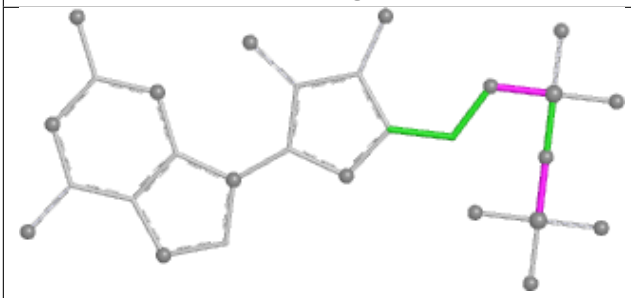
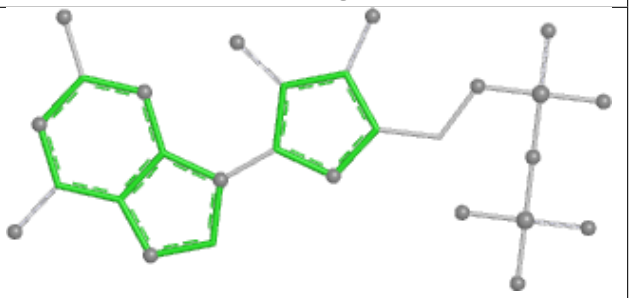
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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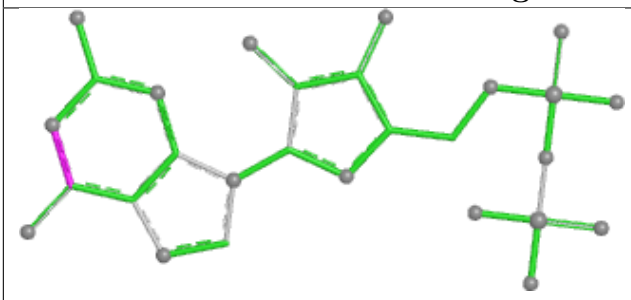

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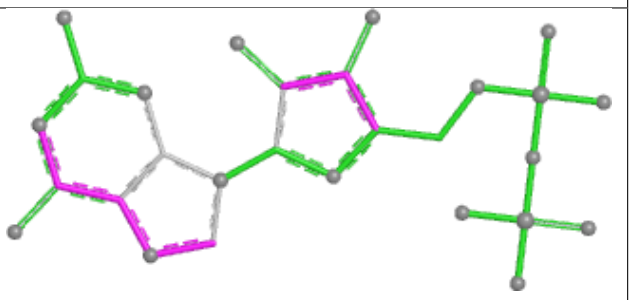

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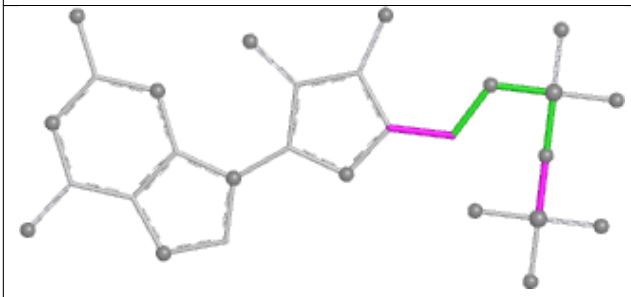

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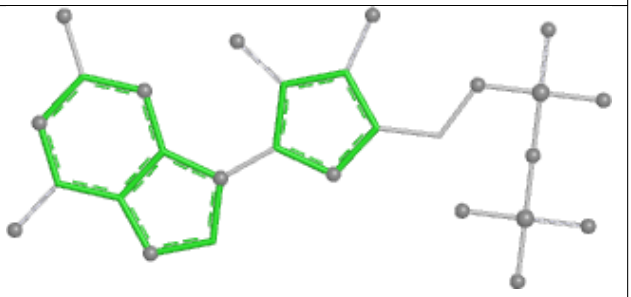

Rings

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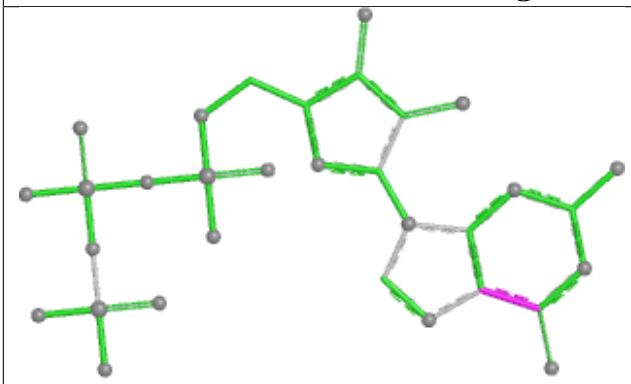

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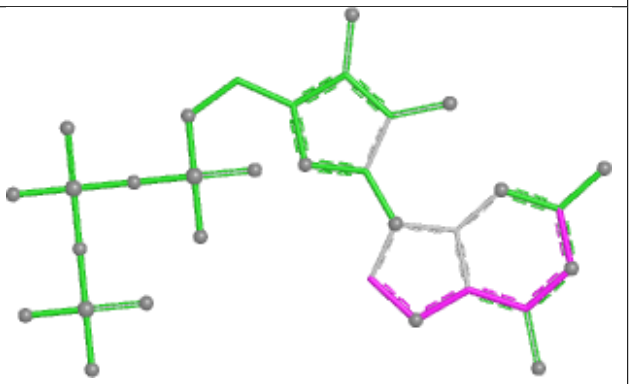

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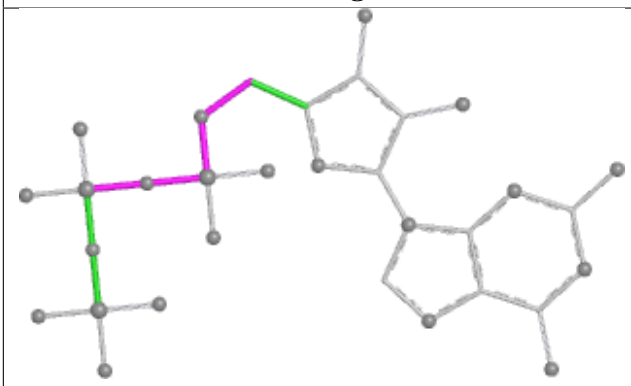

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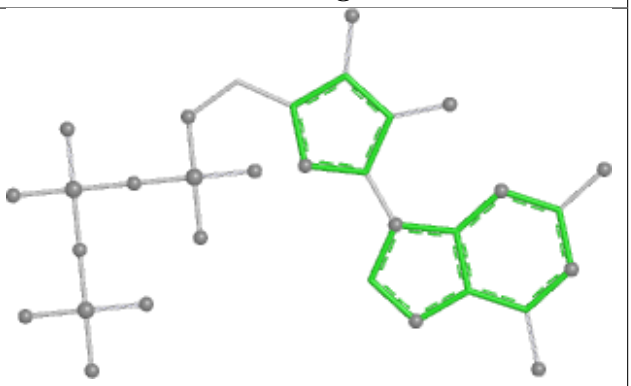

Rings

| Ligand GDP A5 501 | |
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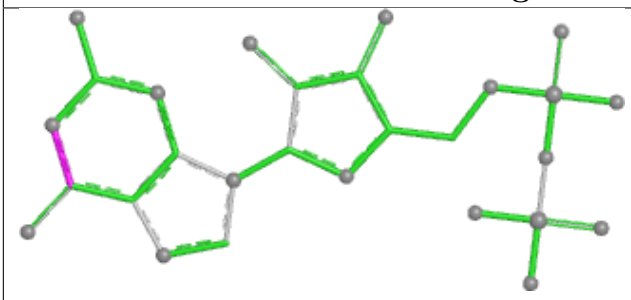
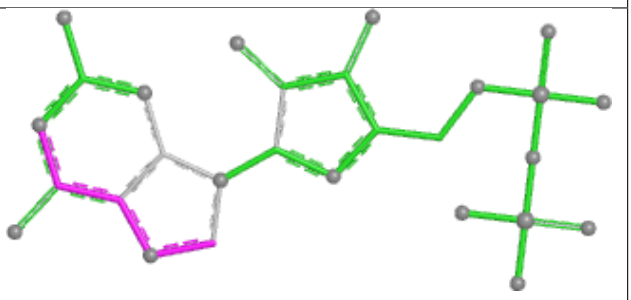
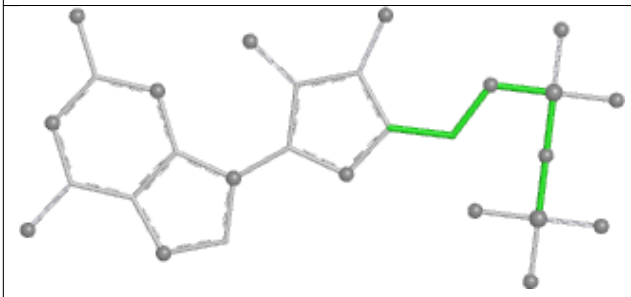
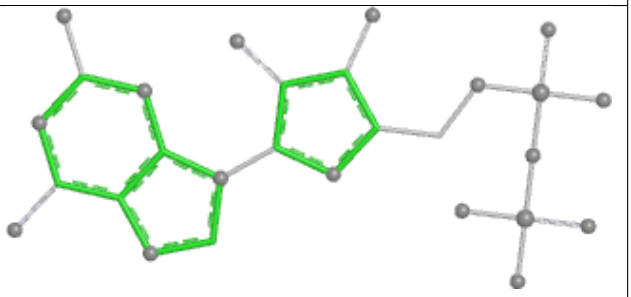
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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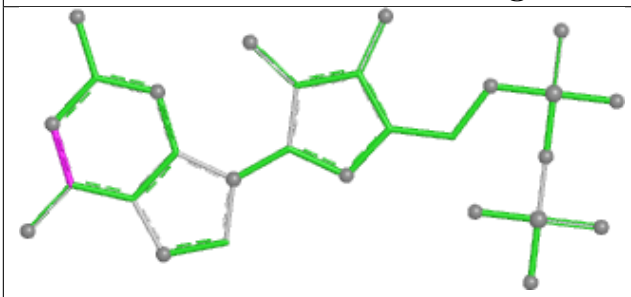
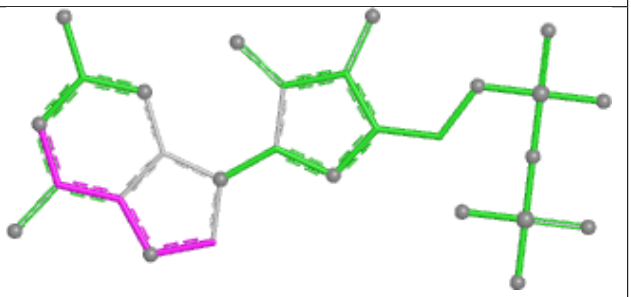
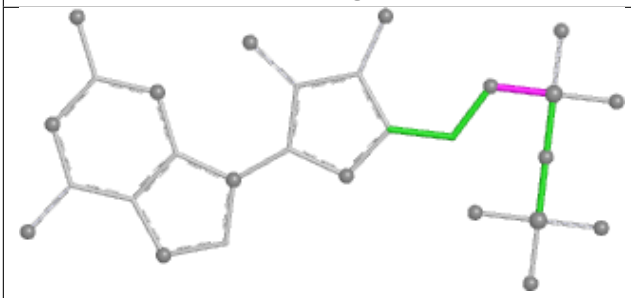
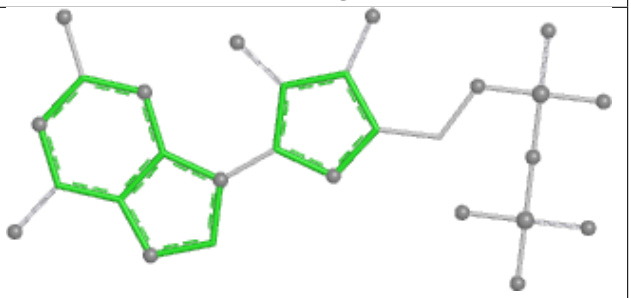
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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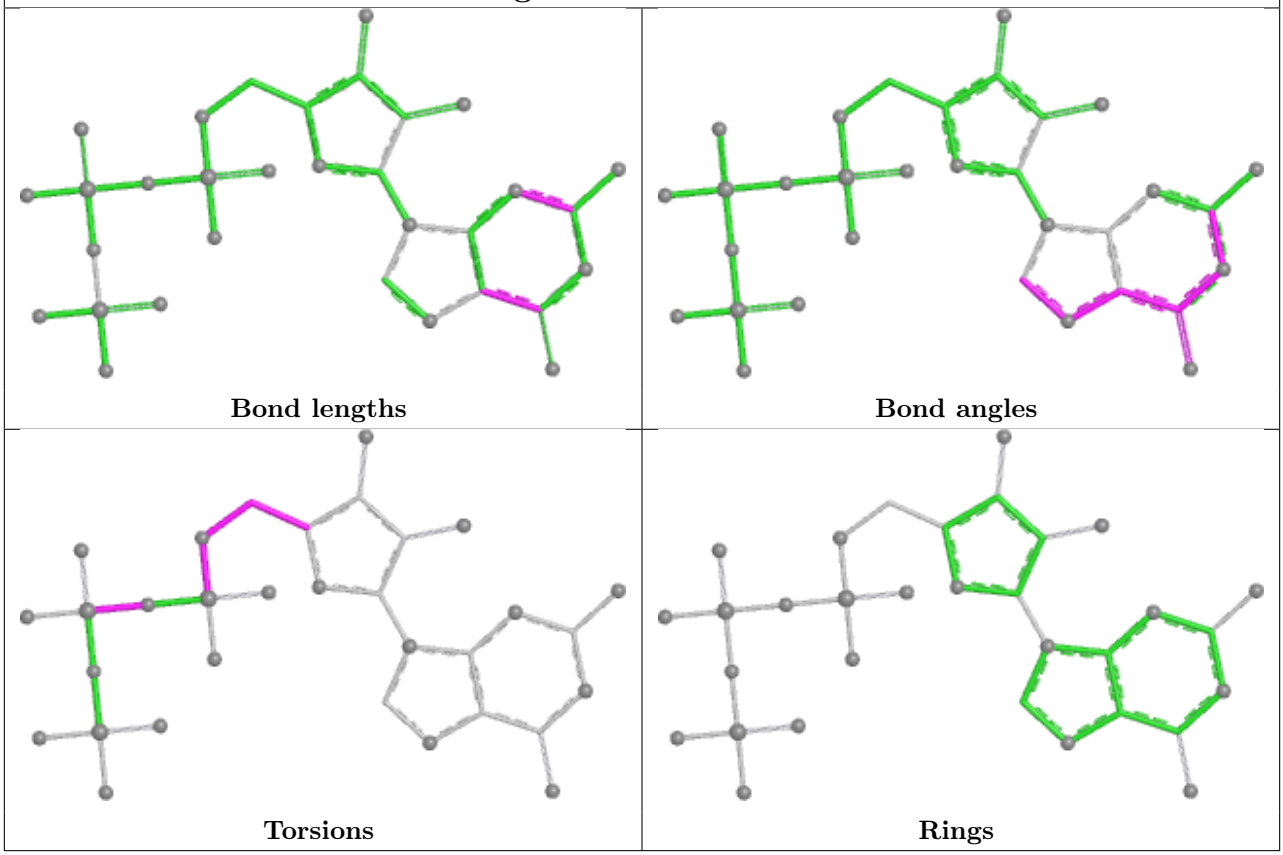
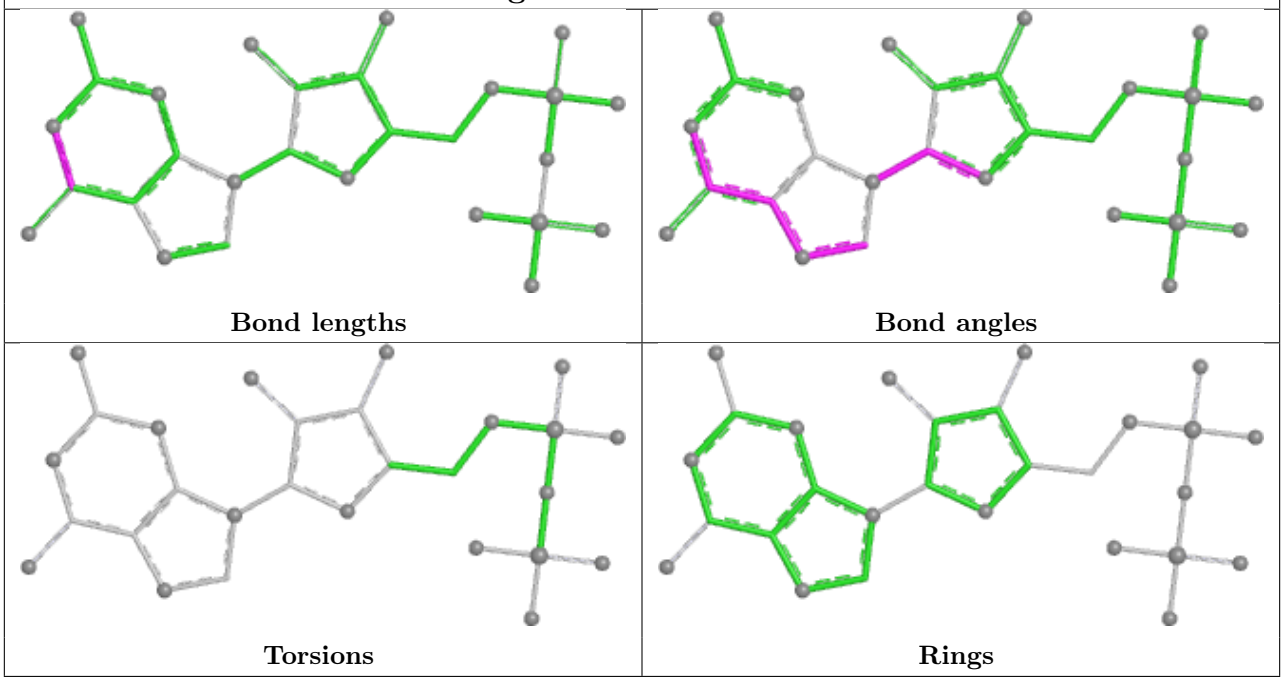



## Ligand GDP W6 501



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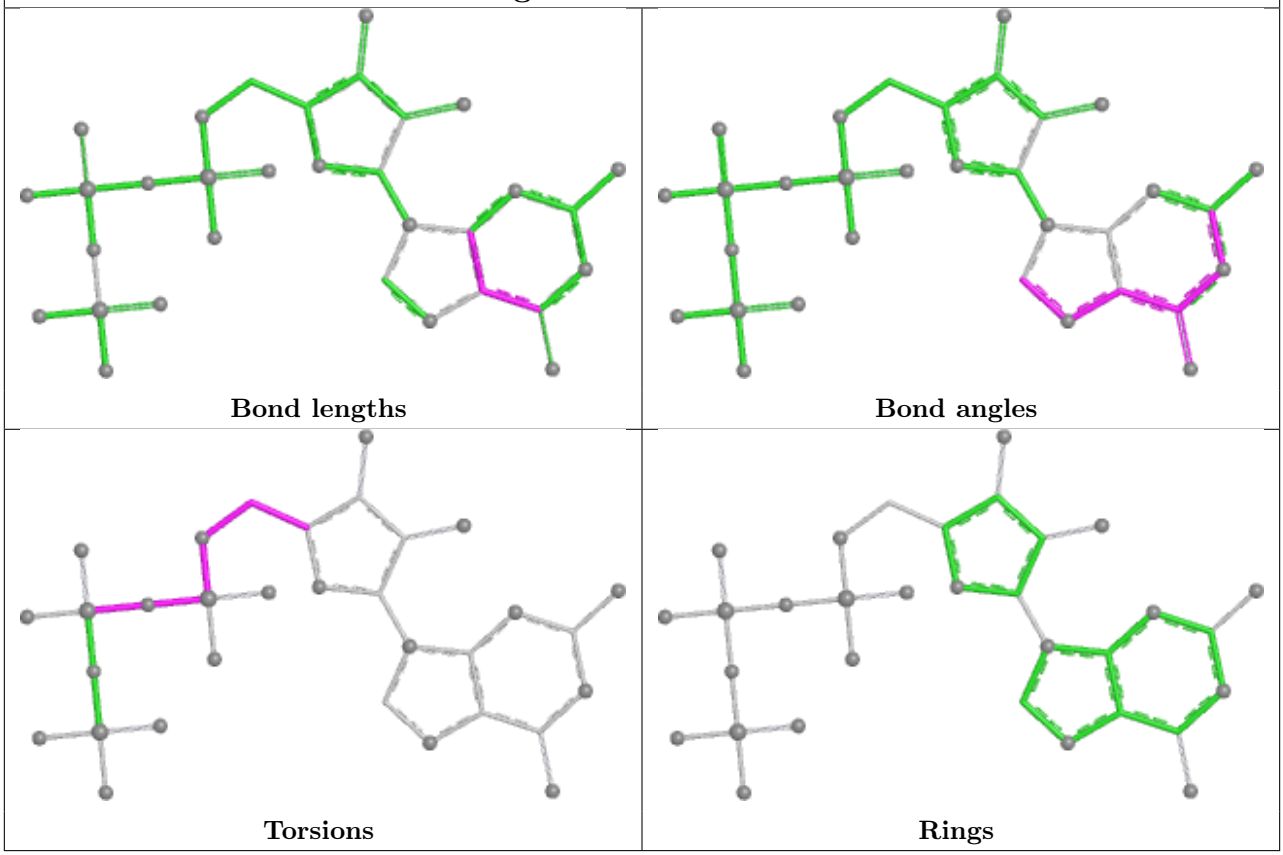


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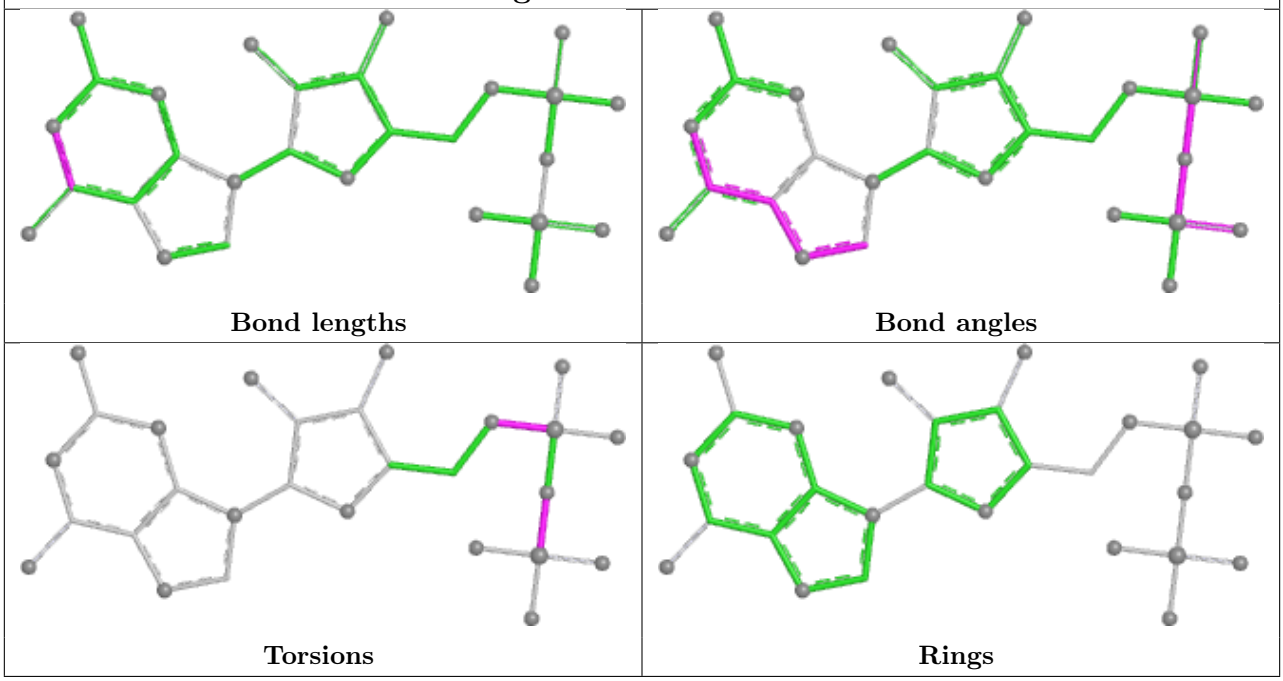

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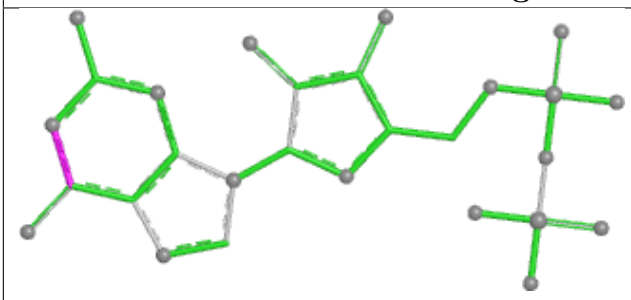
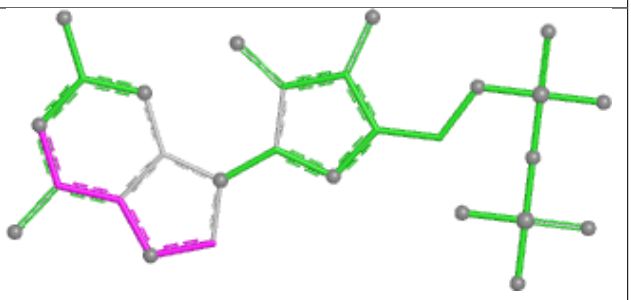
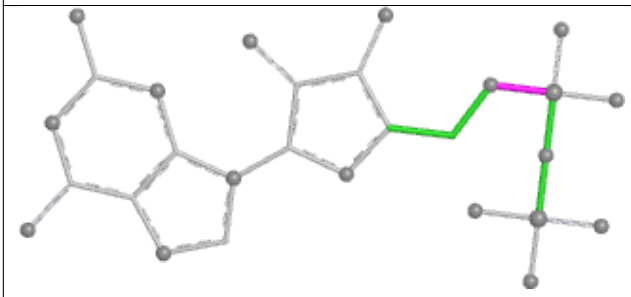


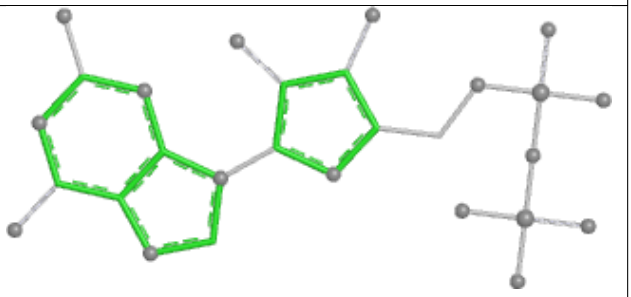
Bond lengths



Bond angles

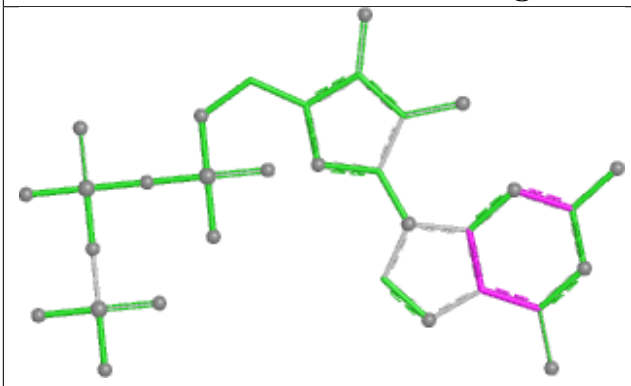


Torsions



Rings

## Ligand GTP 3O 501



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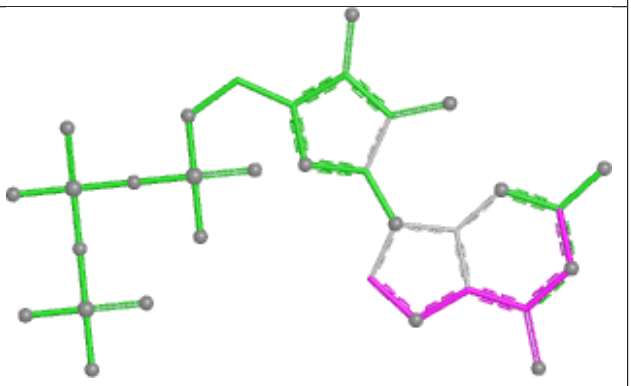

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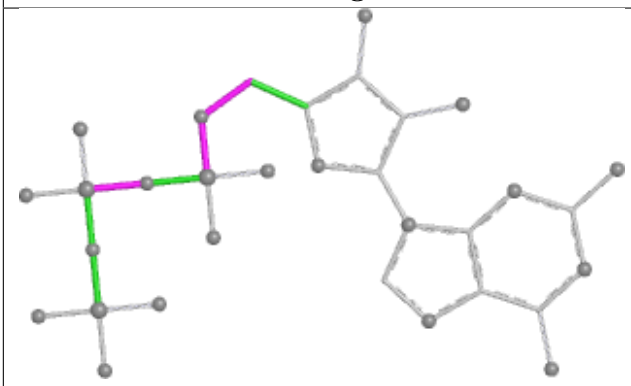

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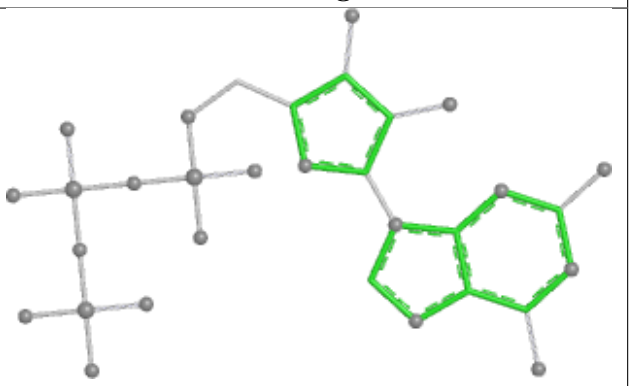

Rings

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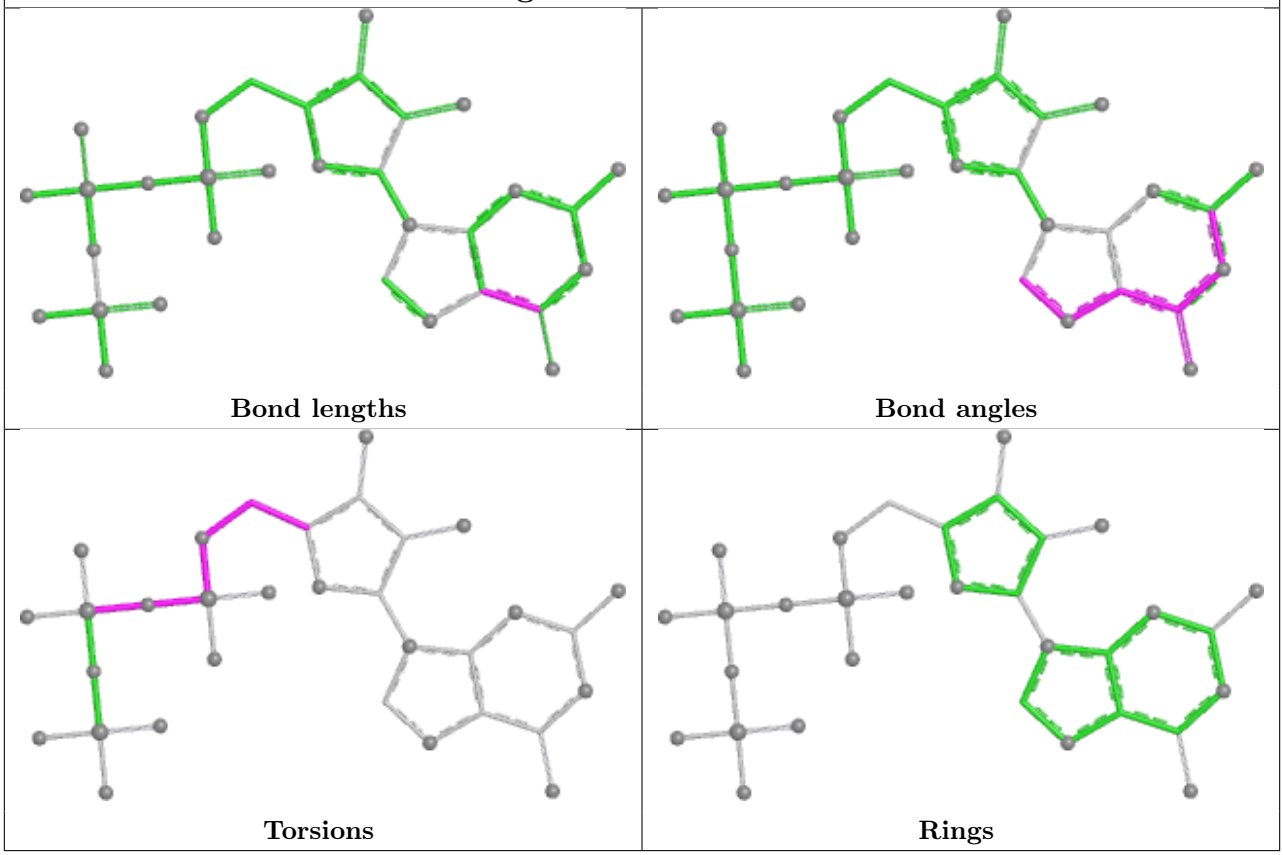


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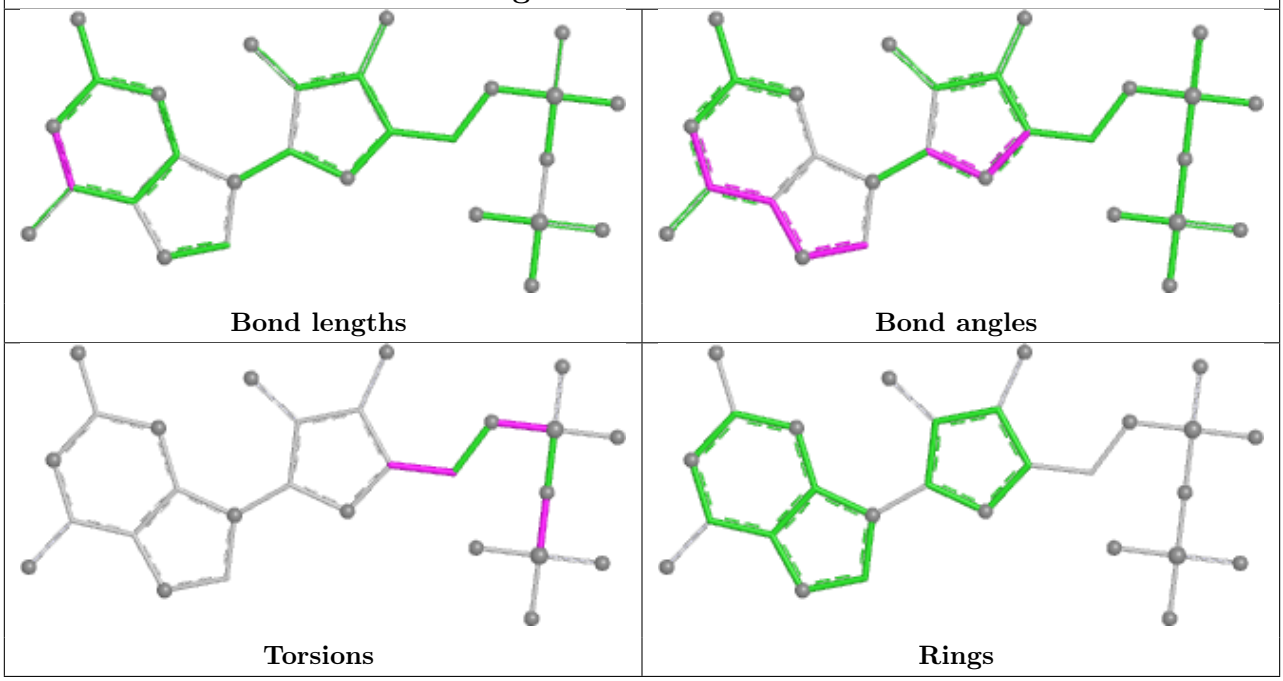

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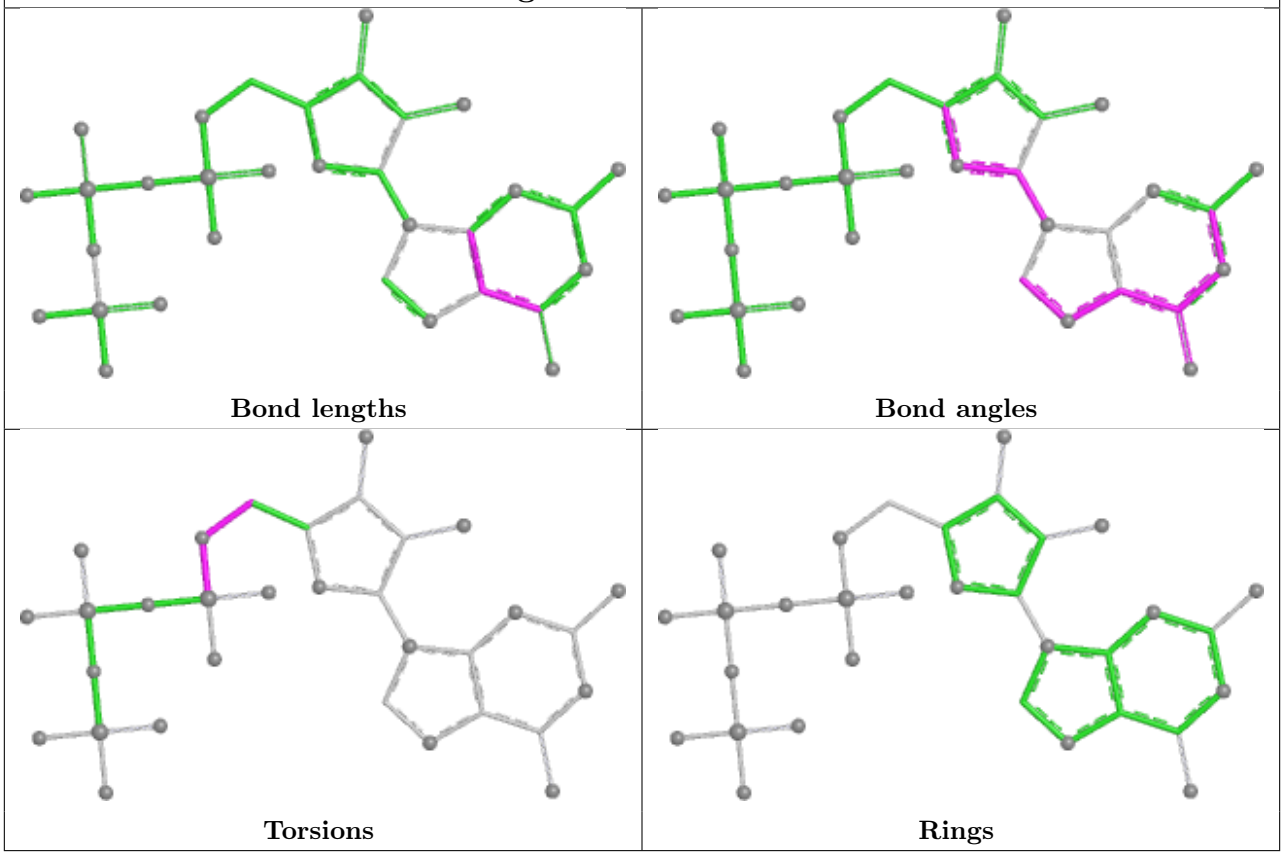


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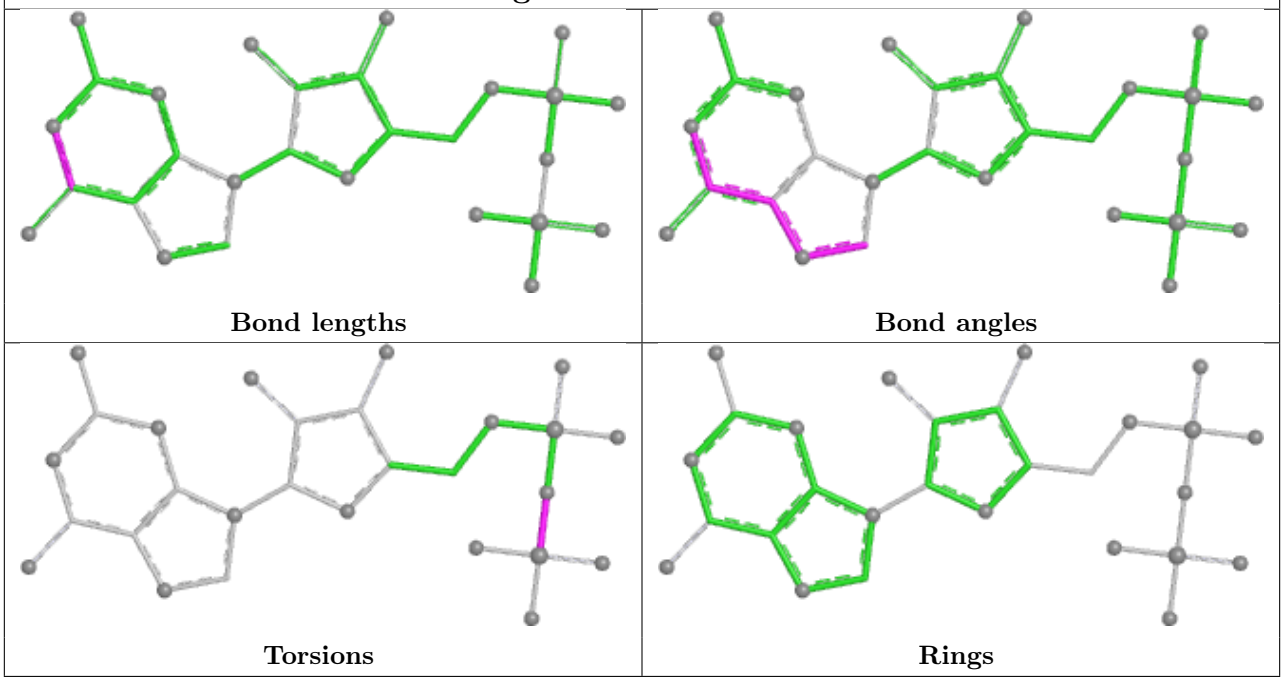

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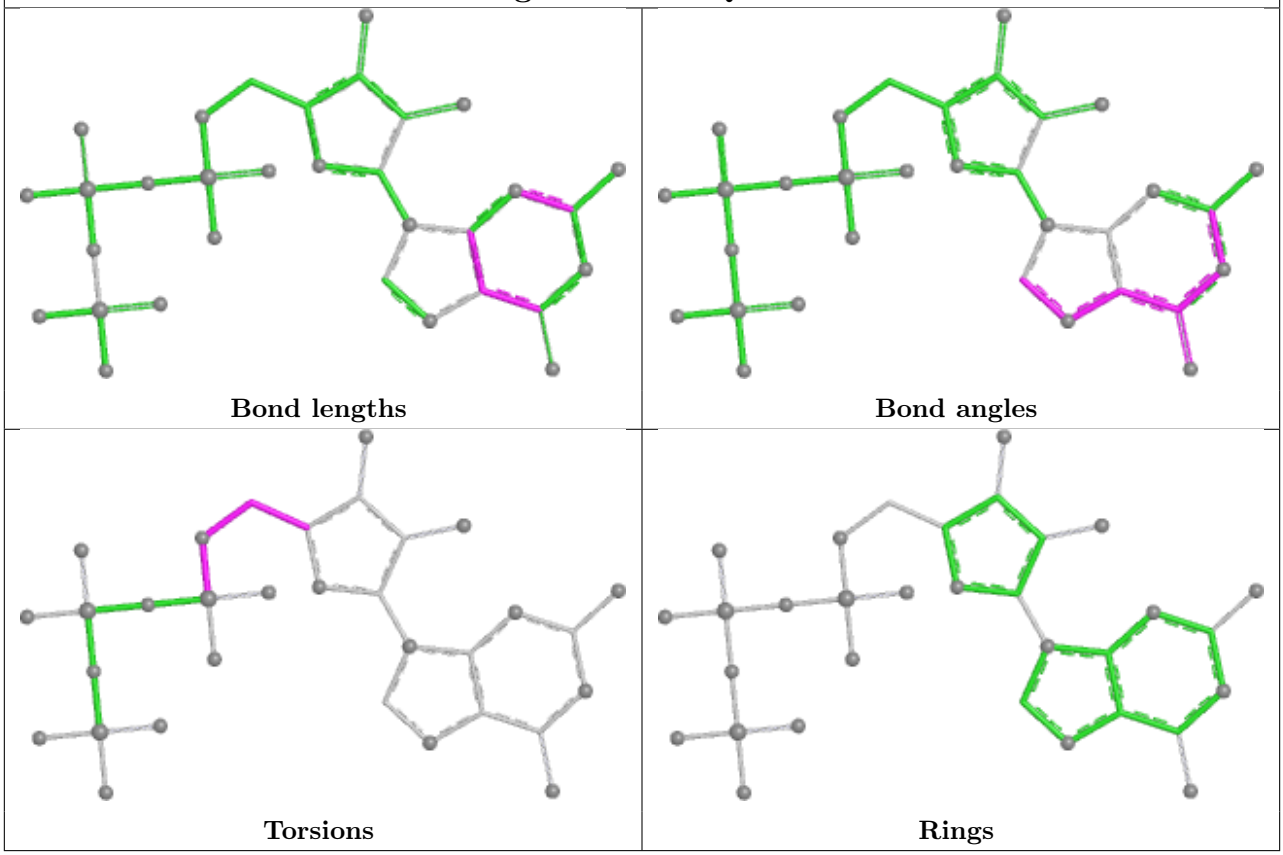


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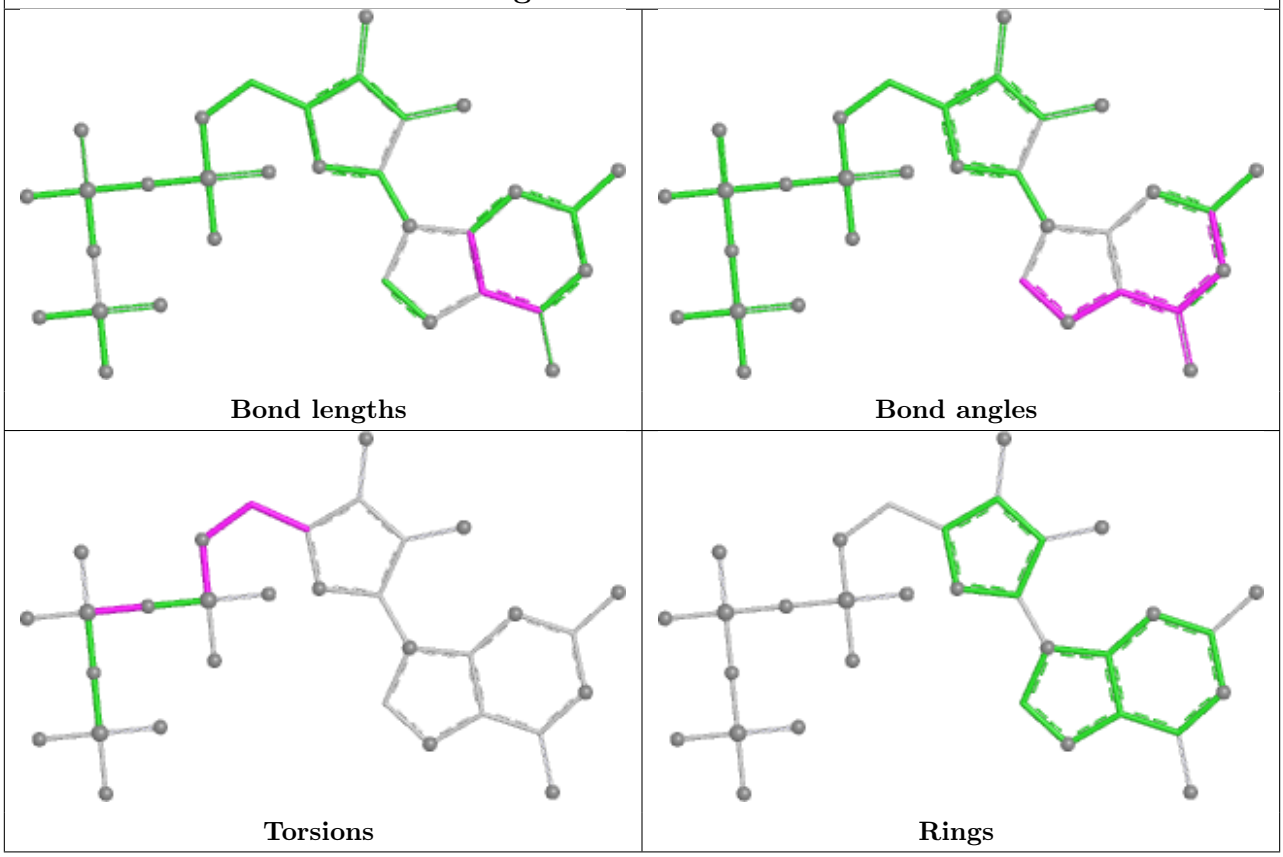

| Ligand GDP P4 503 | |
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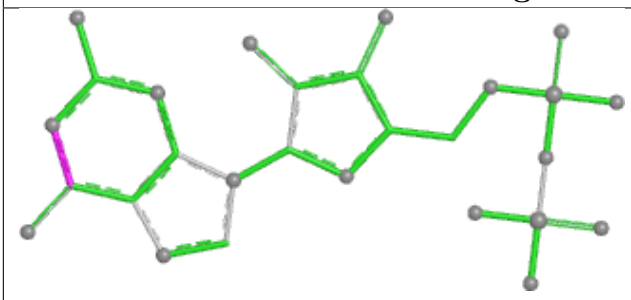
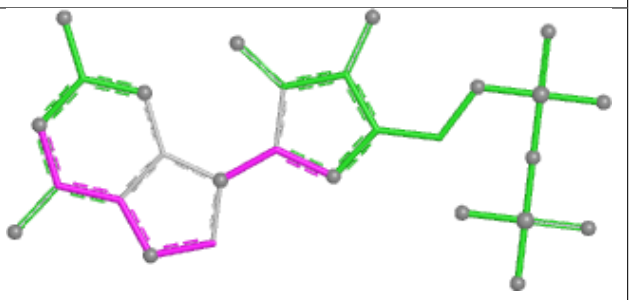
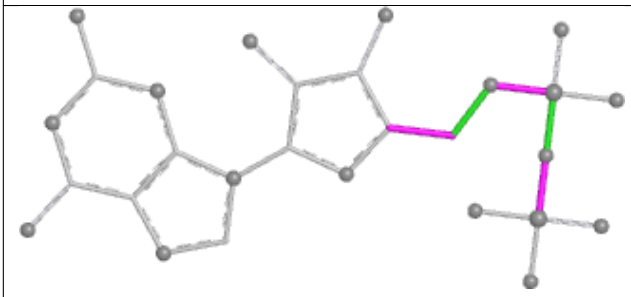
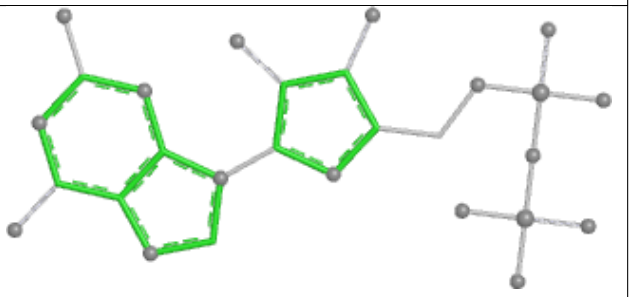
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP U2 502 | |
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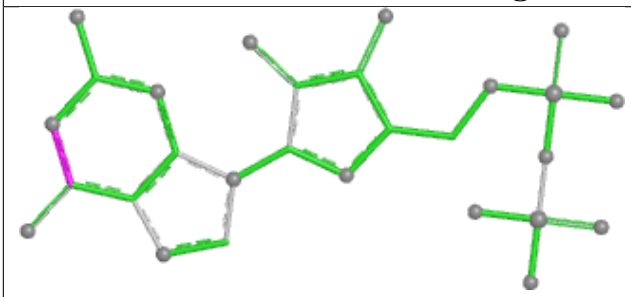
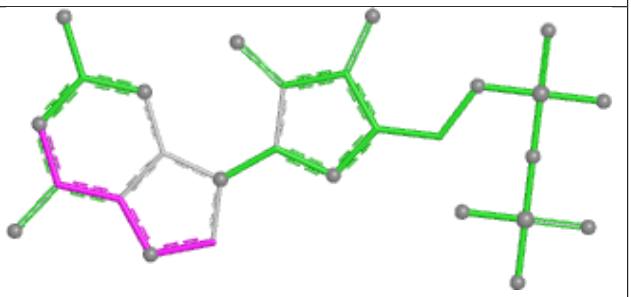
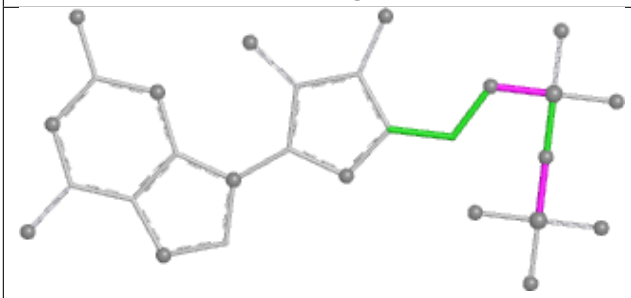
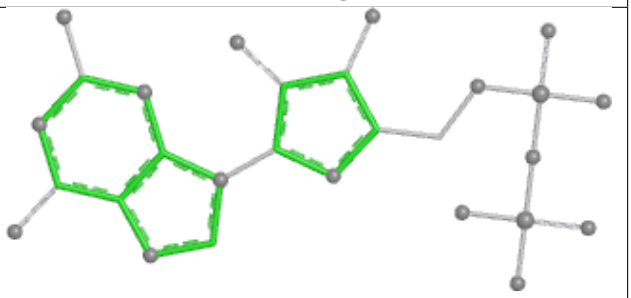
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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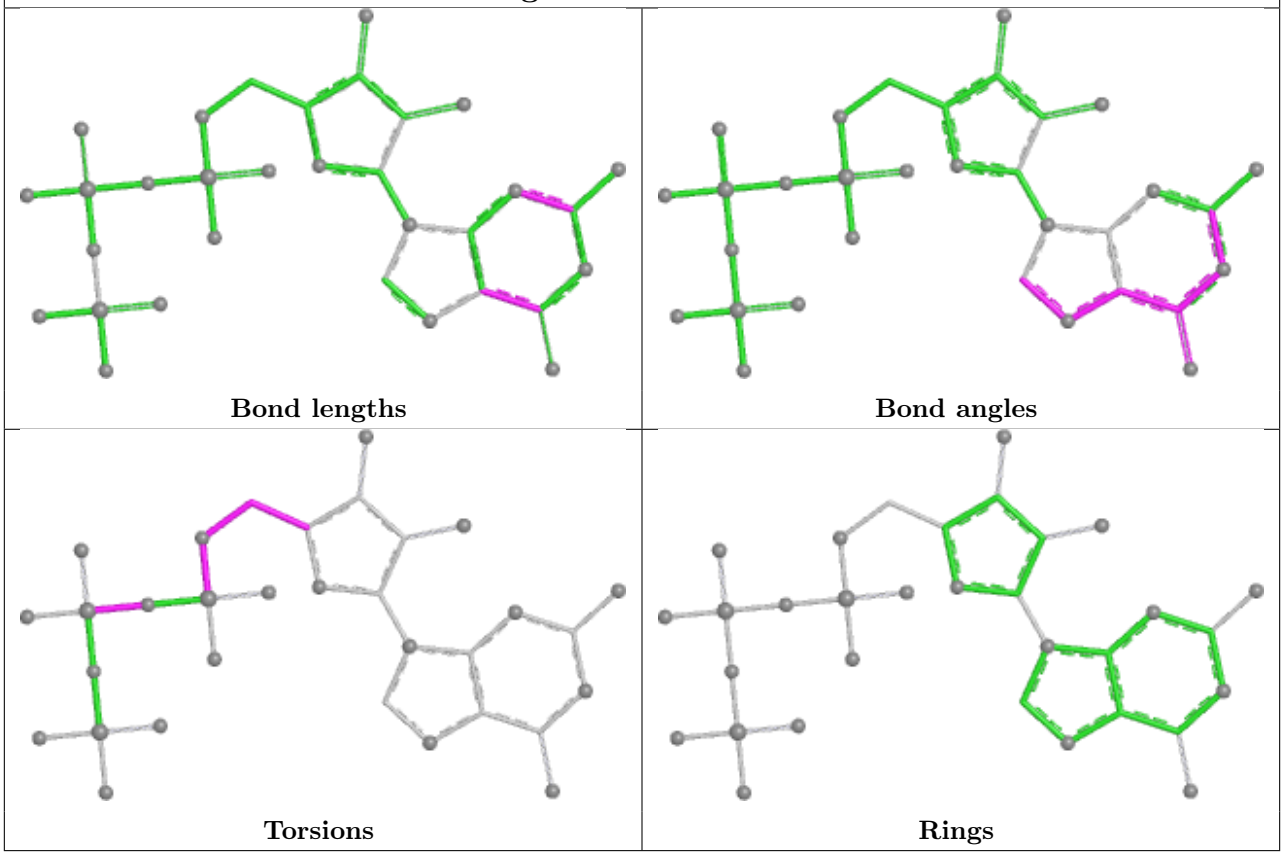


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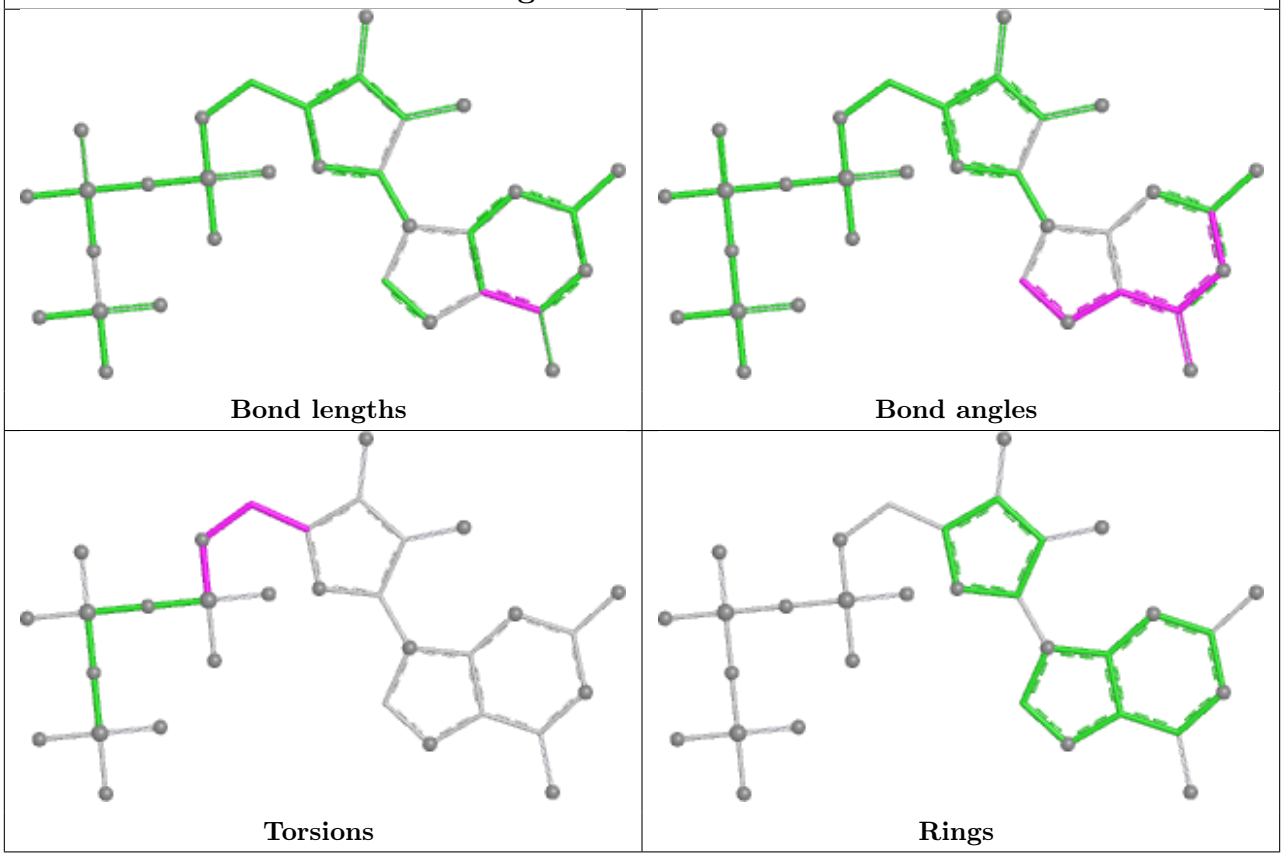

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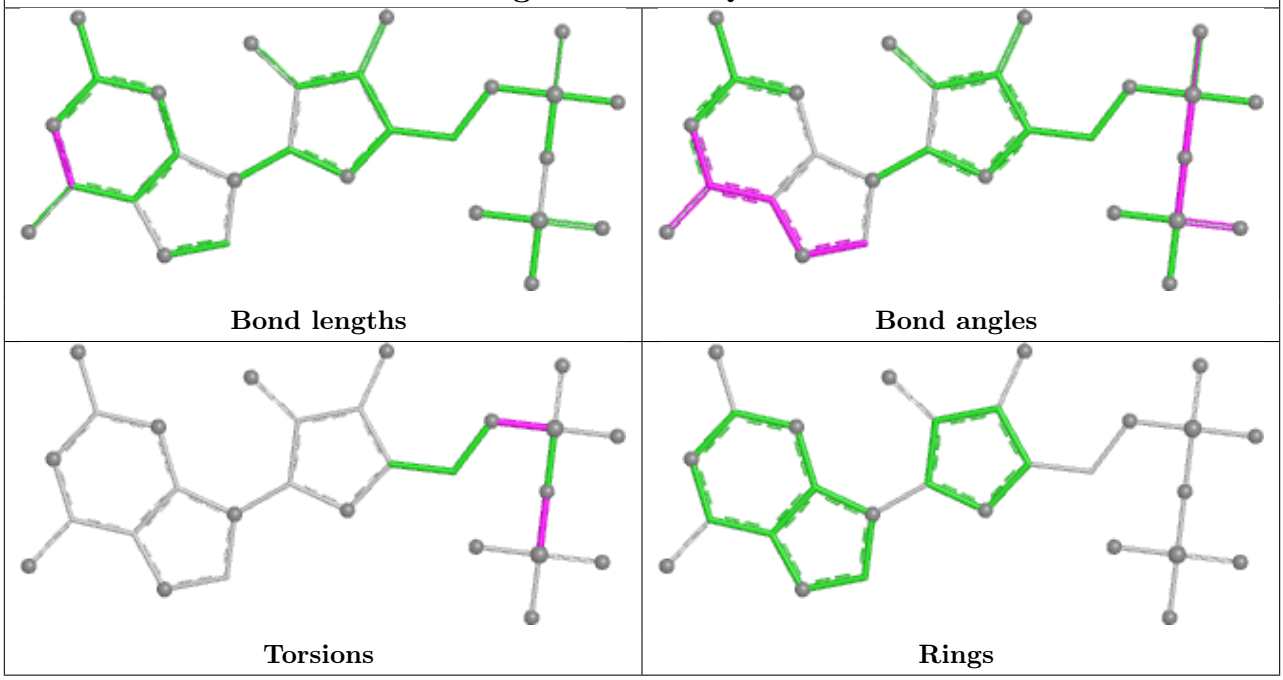


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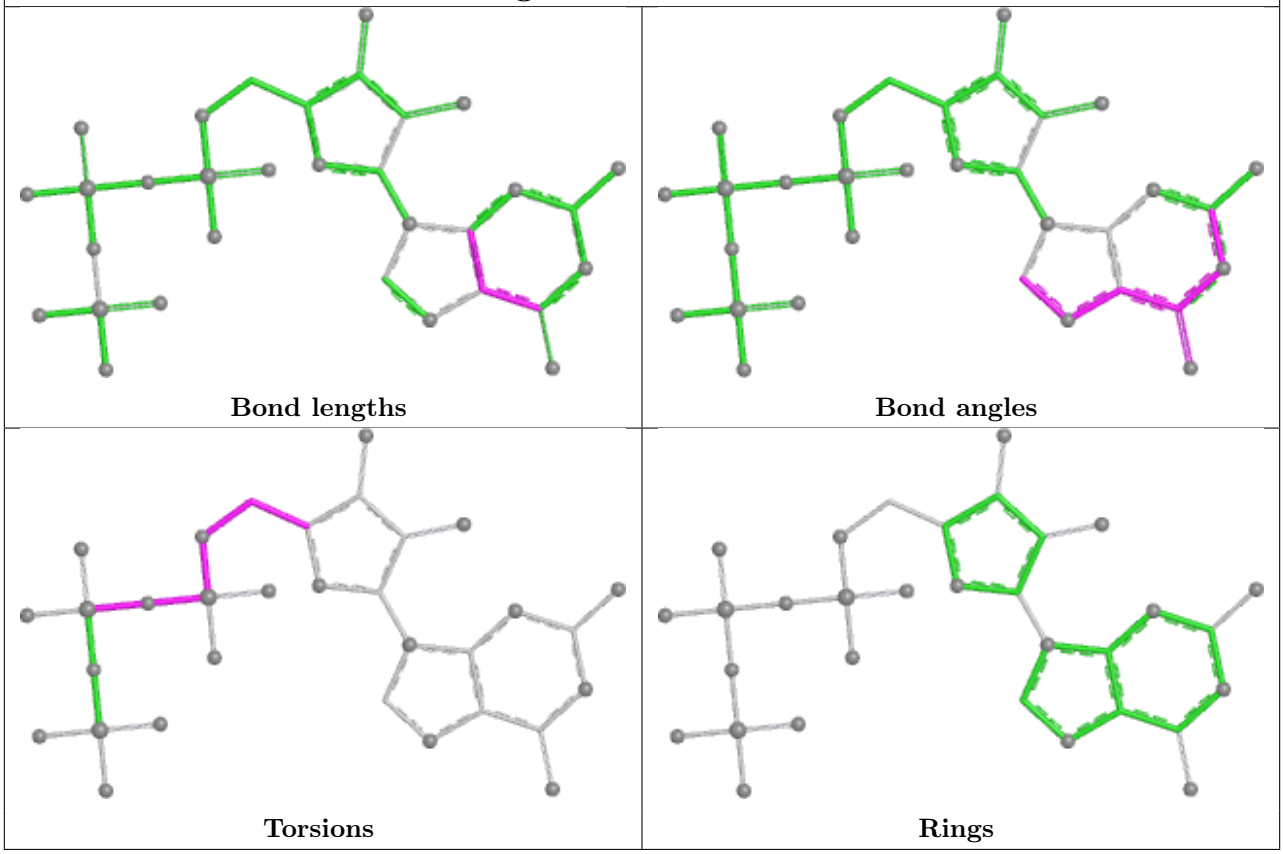
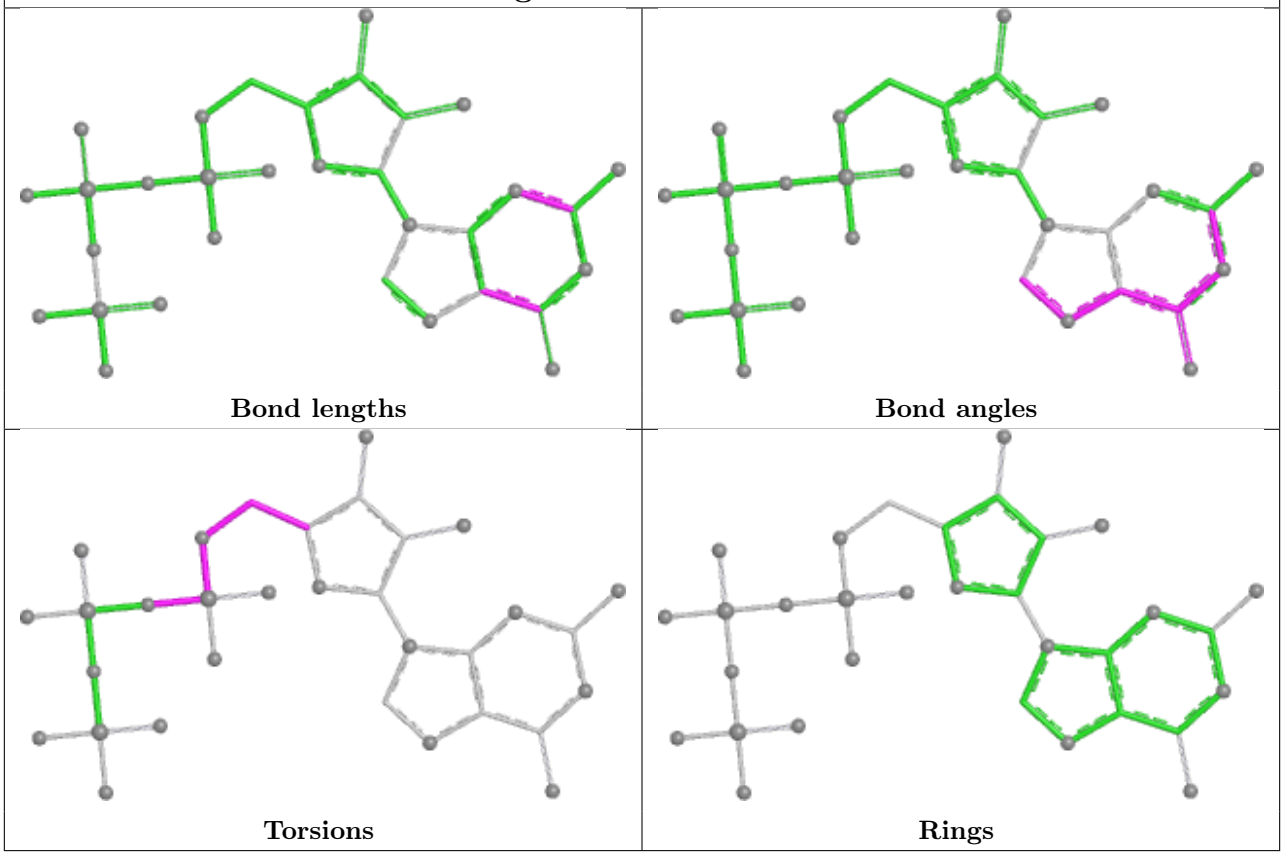
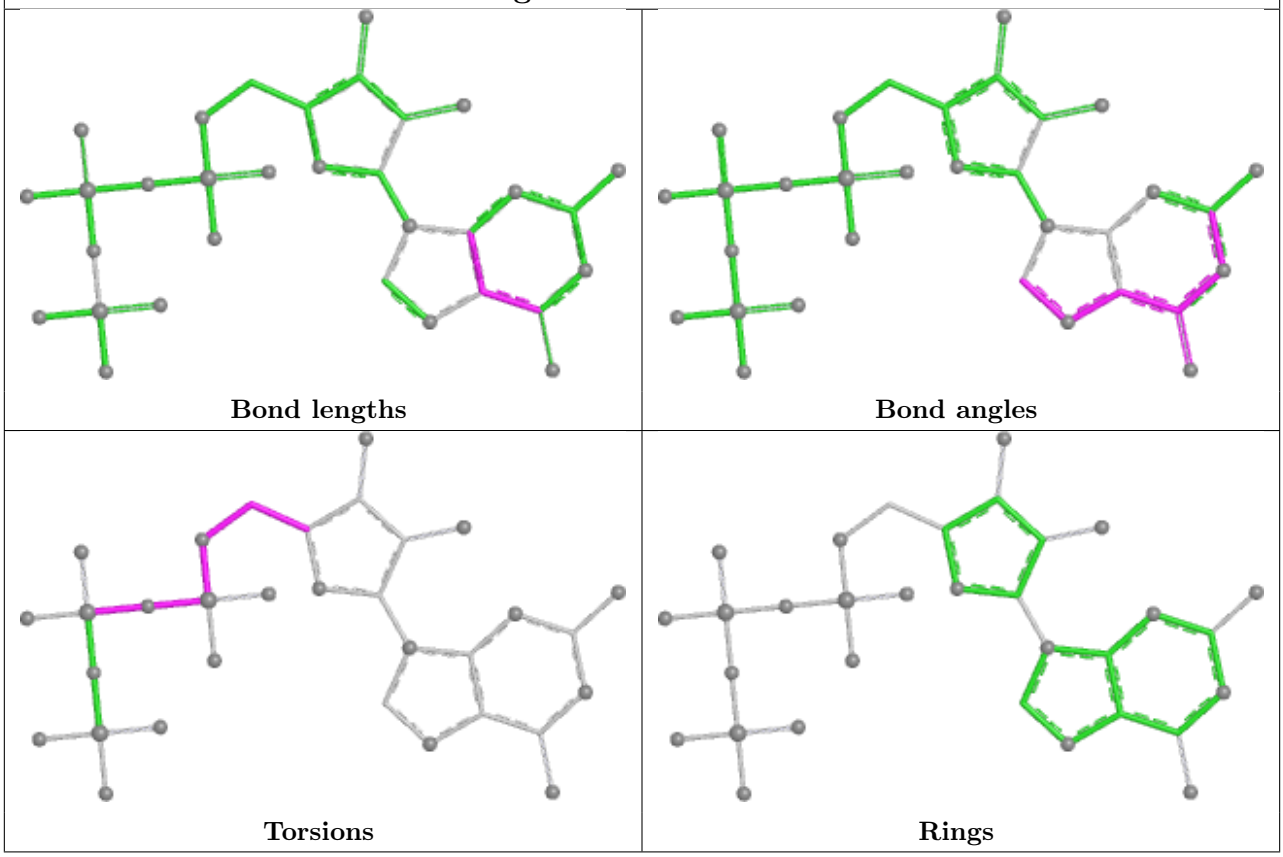


## Ligand GTP C1 501




## Ligand GTP G1 501



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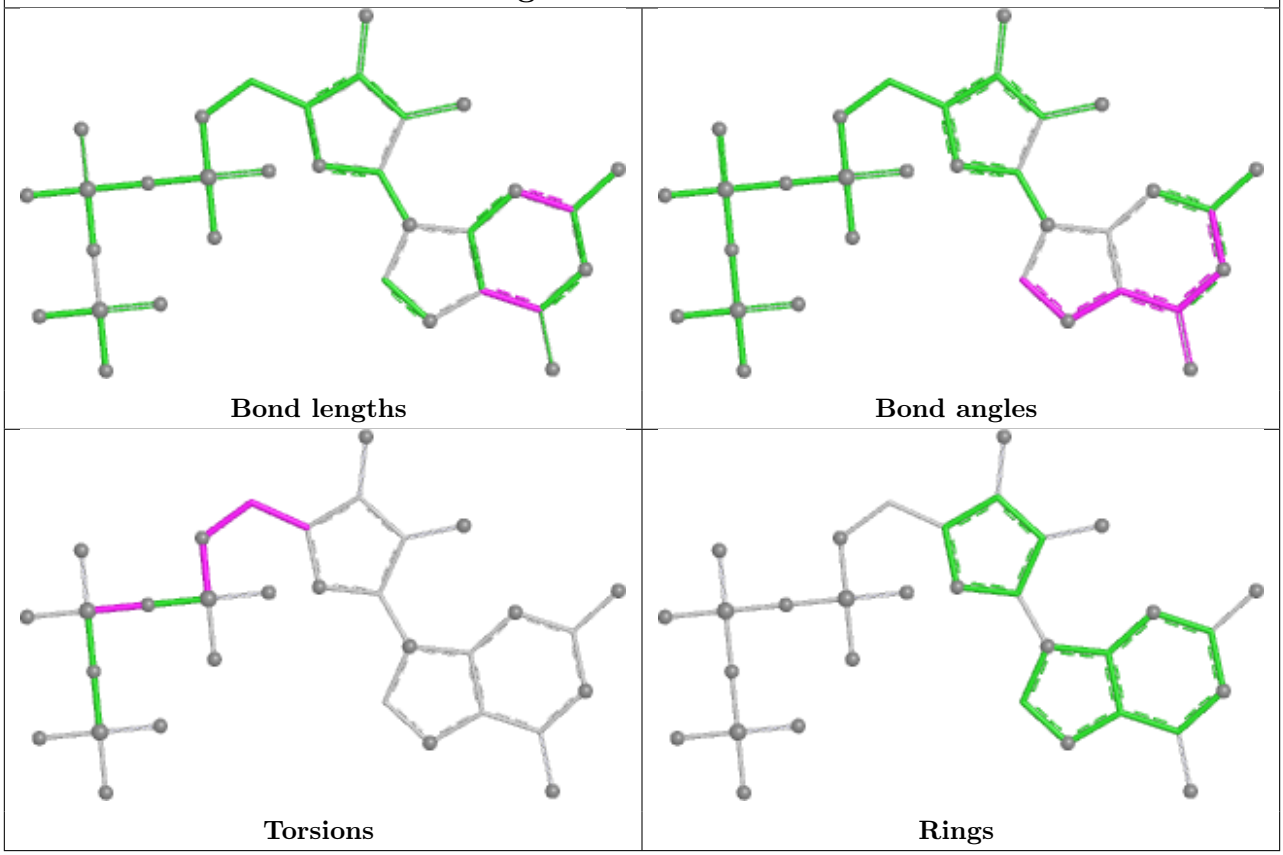


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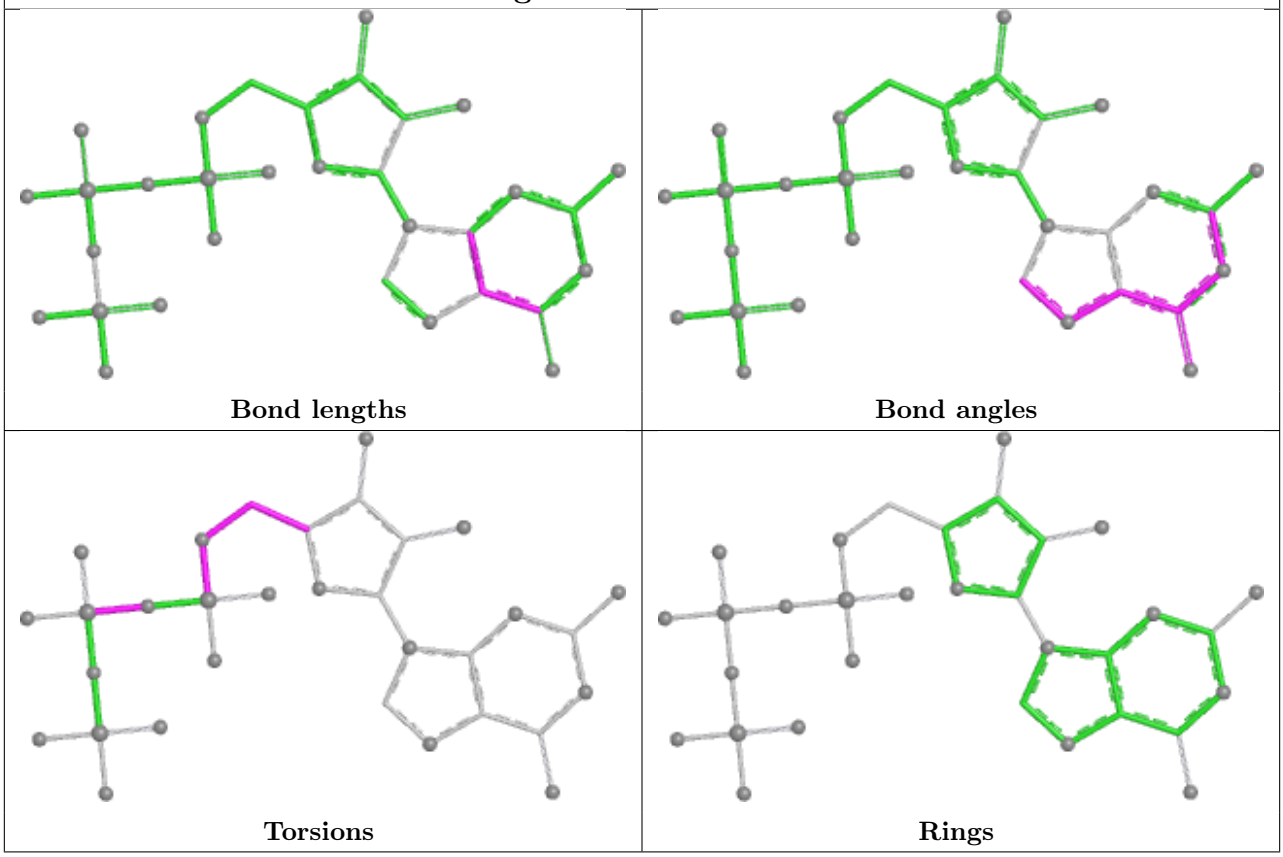

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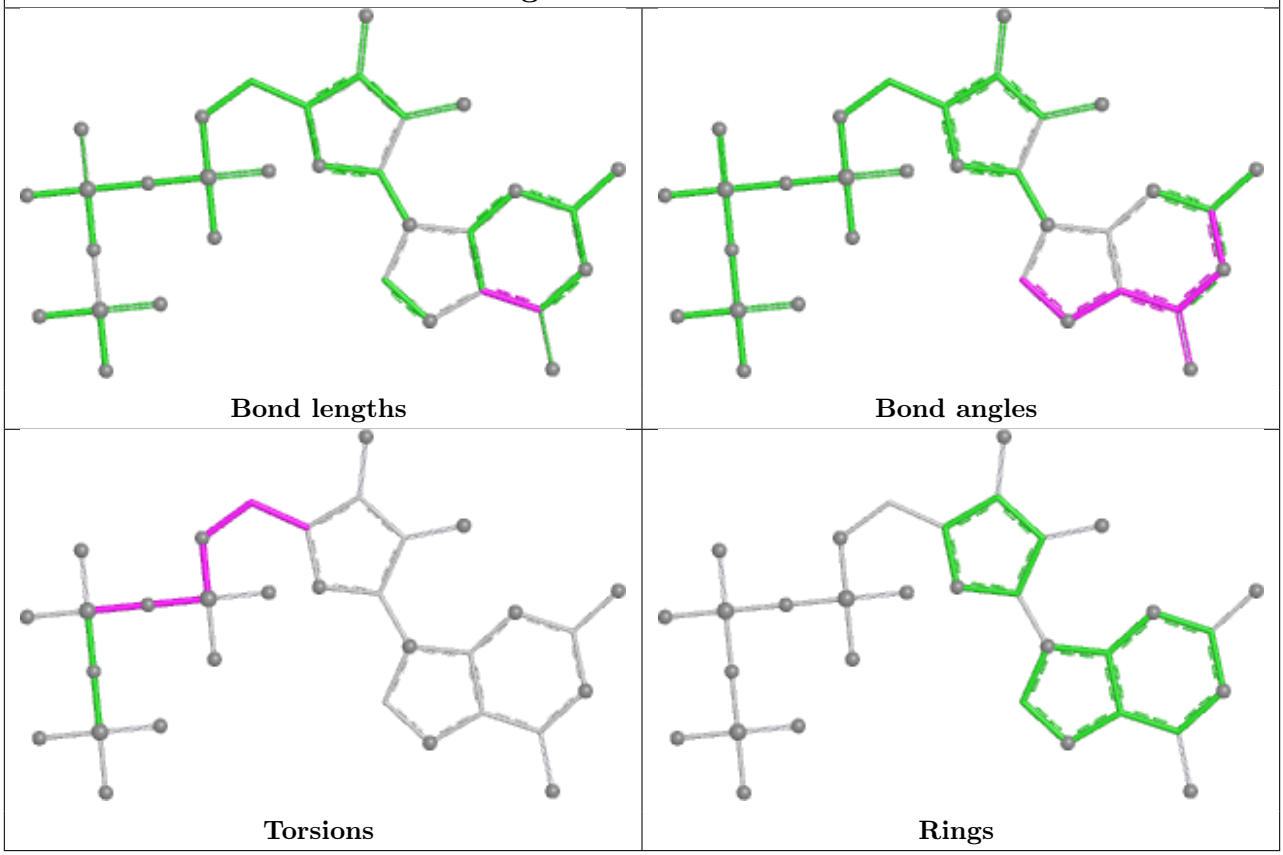


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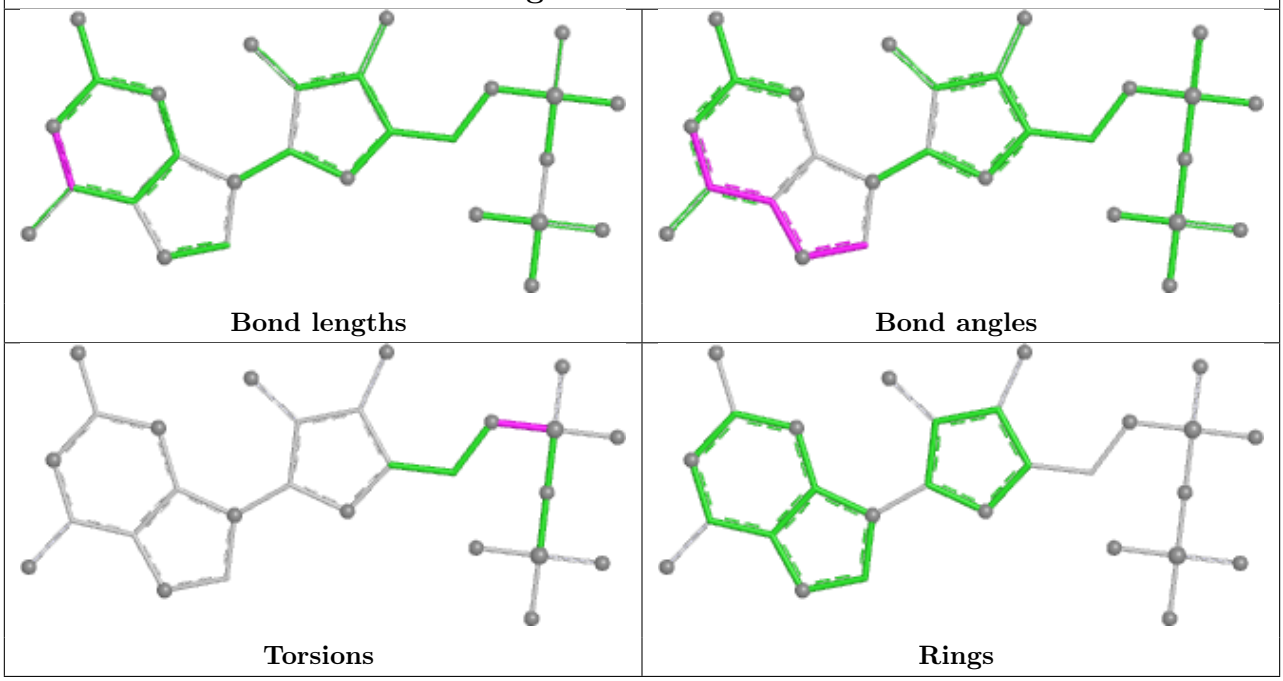

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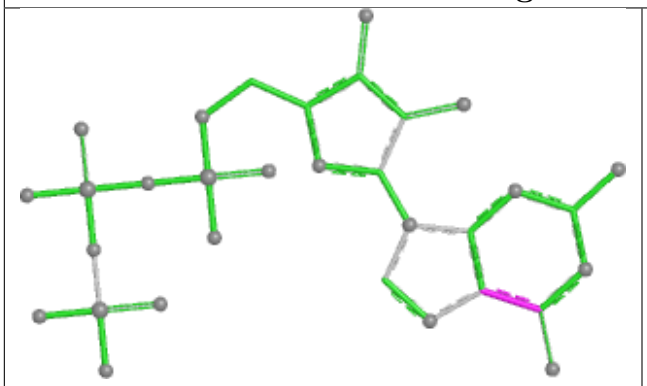

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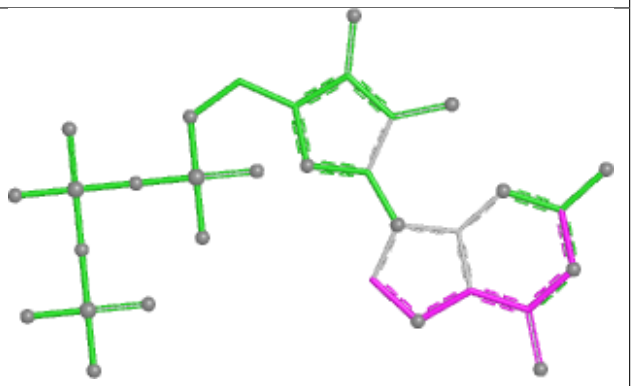

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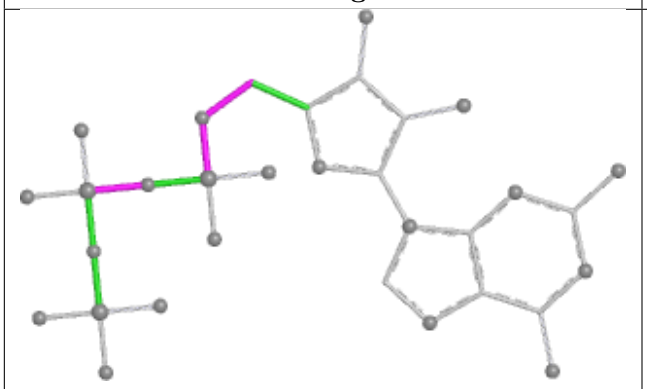
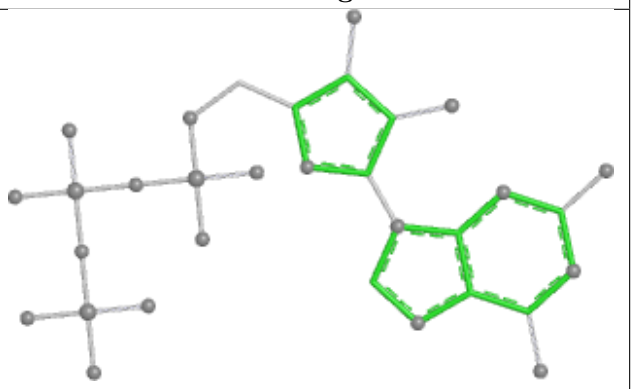
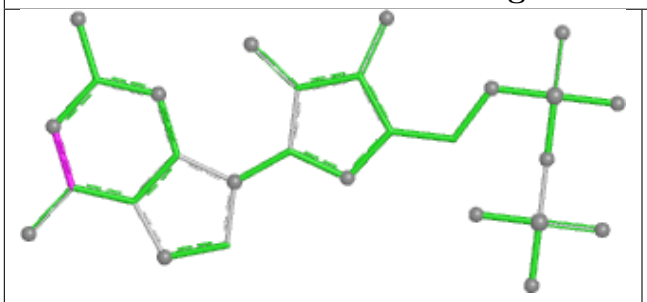


Torsions



Rings

## Ligand GDP 0W 502



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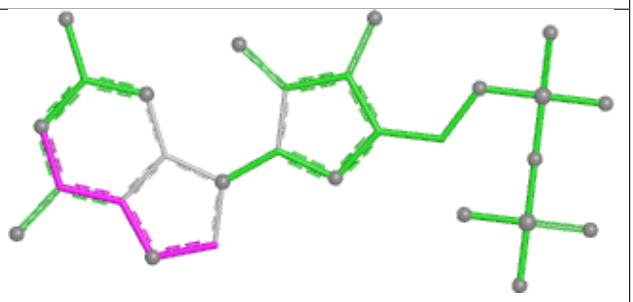

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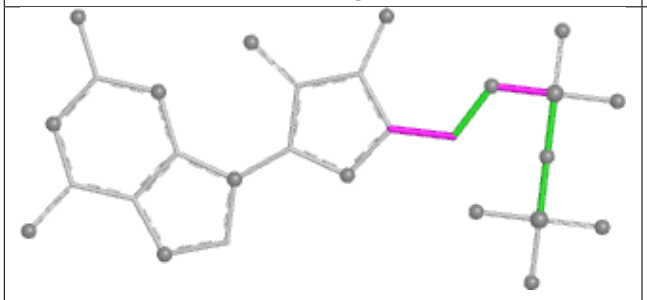

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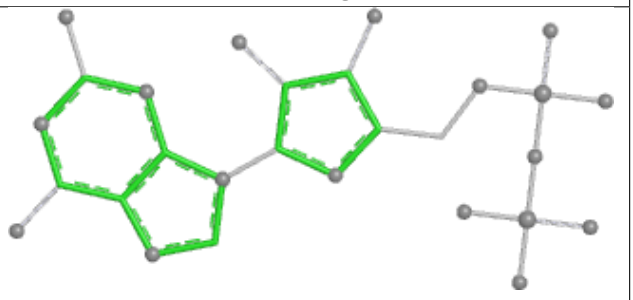
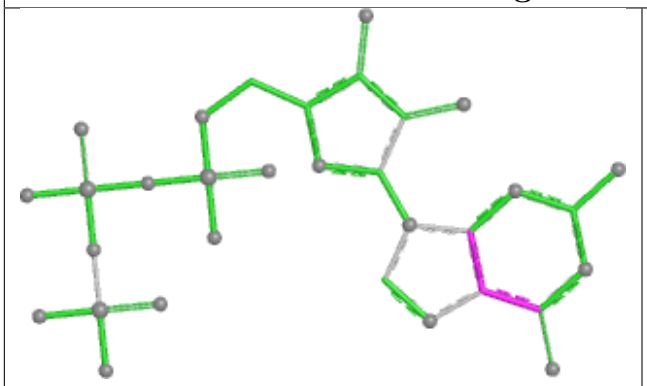


Rings

## Ligand GTP D7 501



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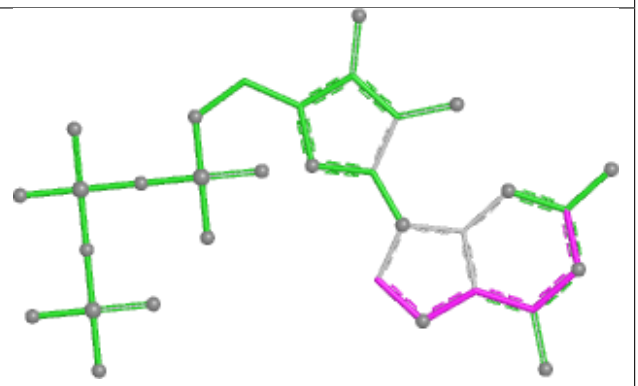

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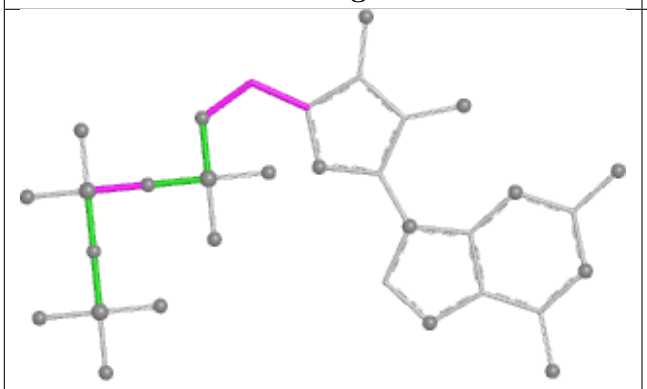

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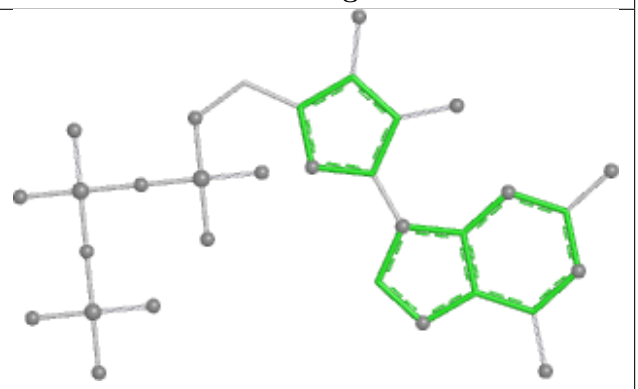
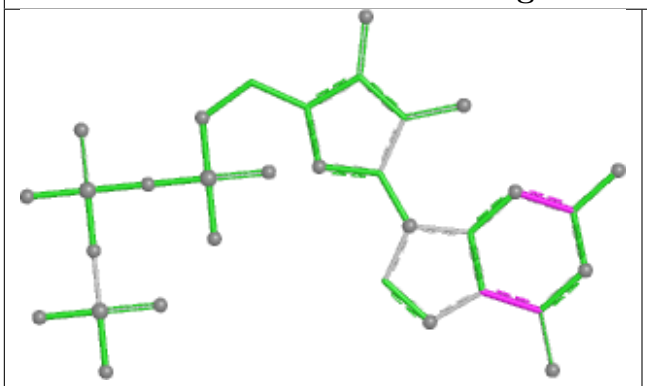


Rings

## Ligand GTP L7 501



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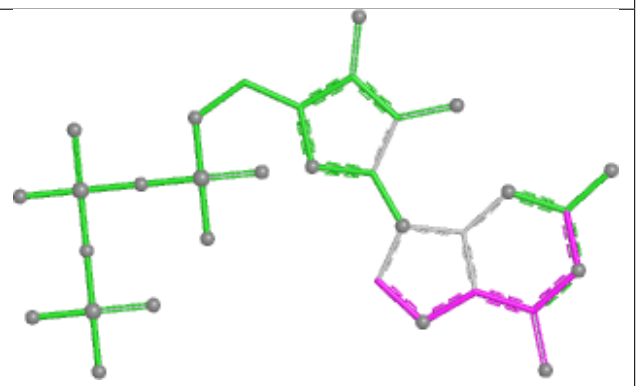

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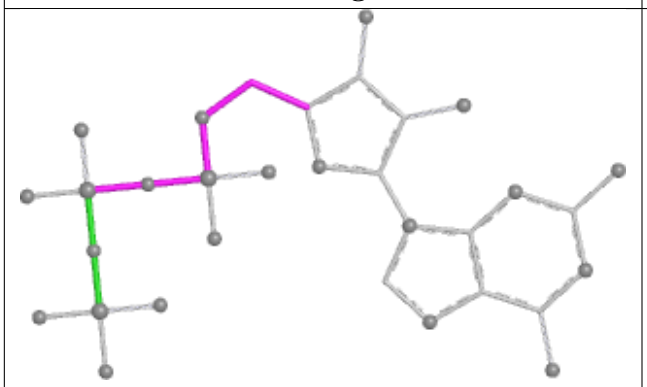

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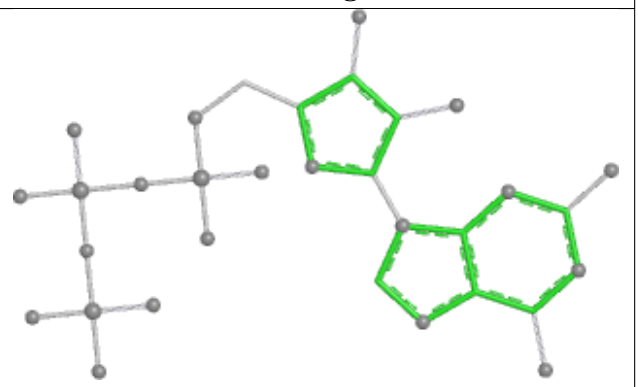

Rings

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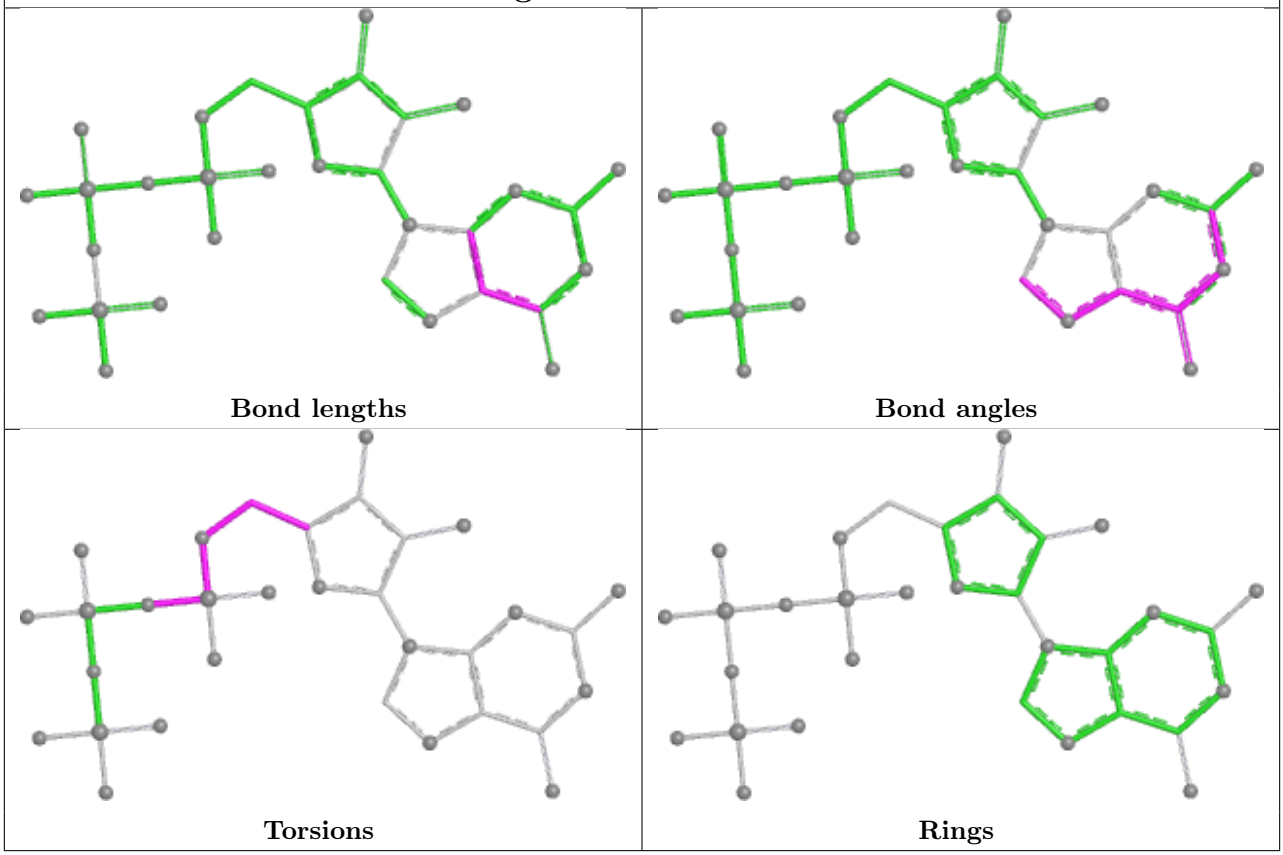


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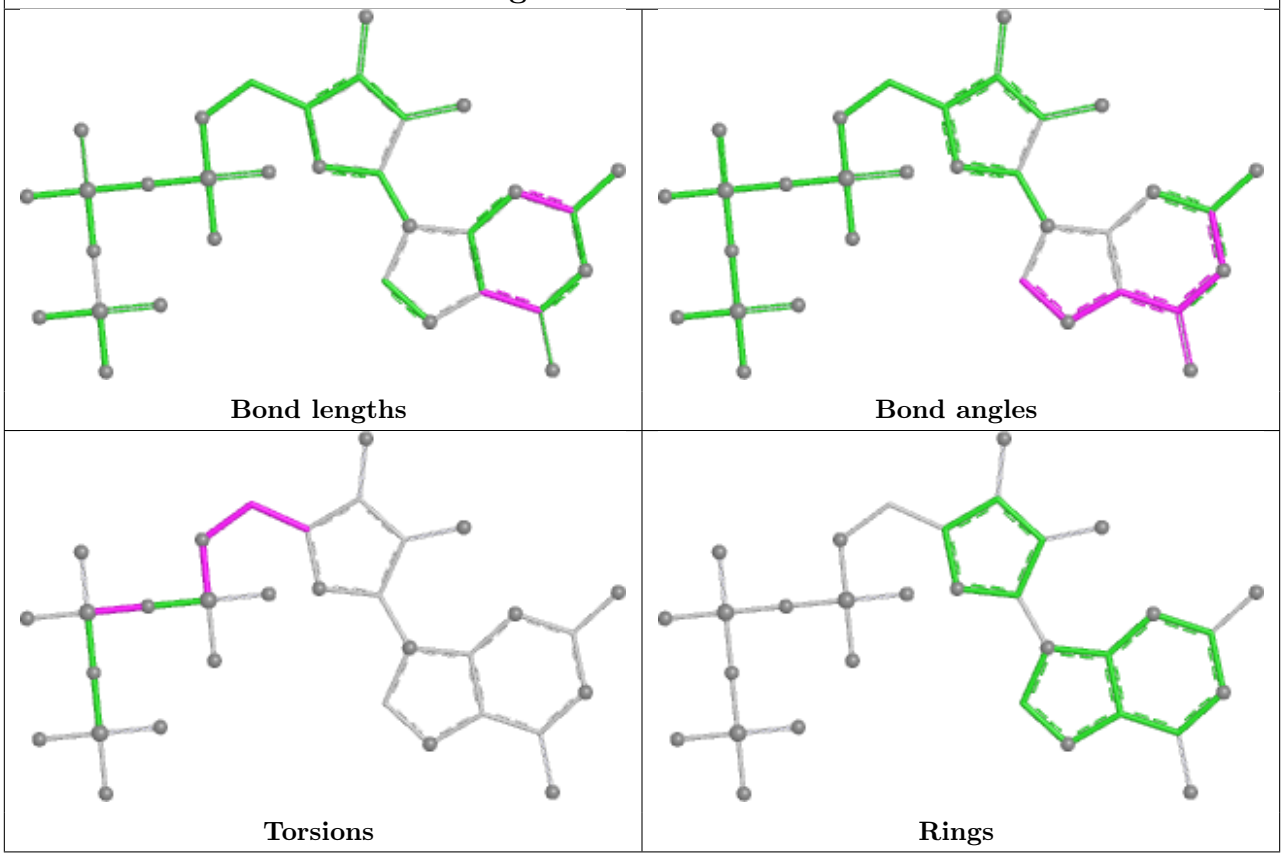

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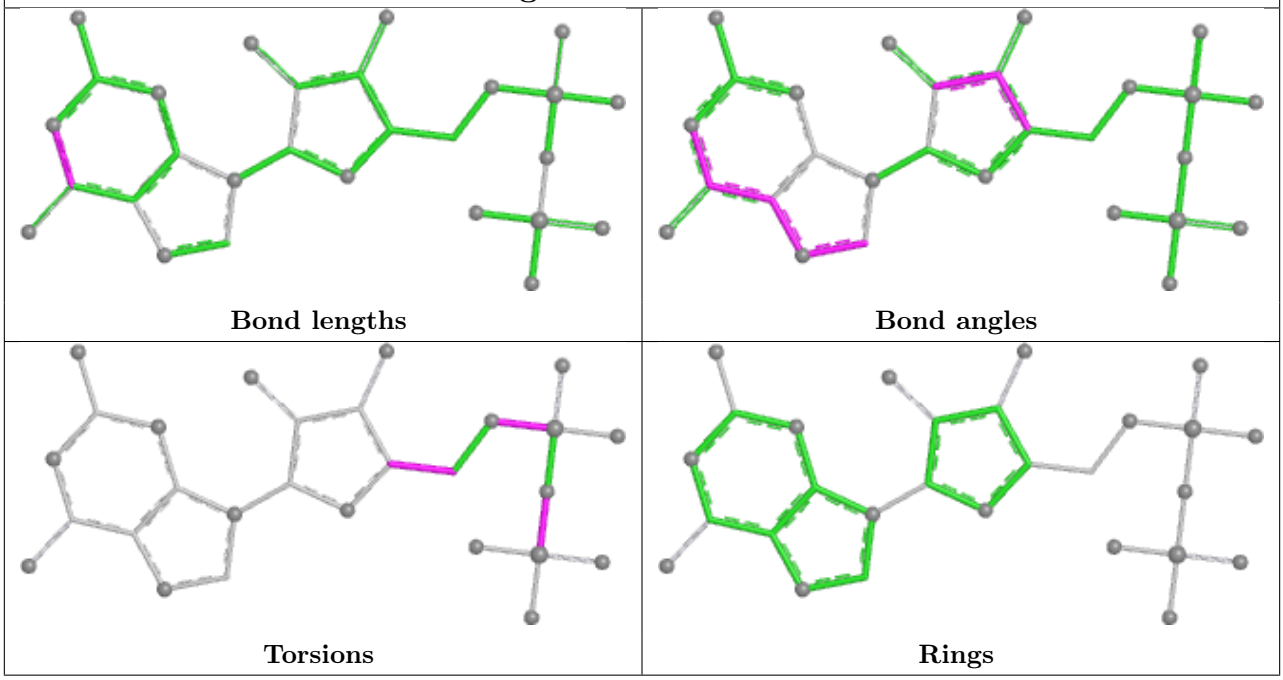


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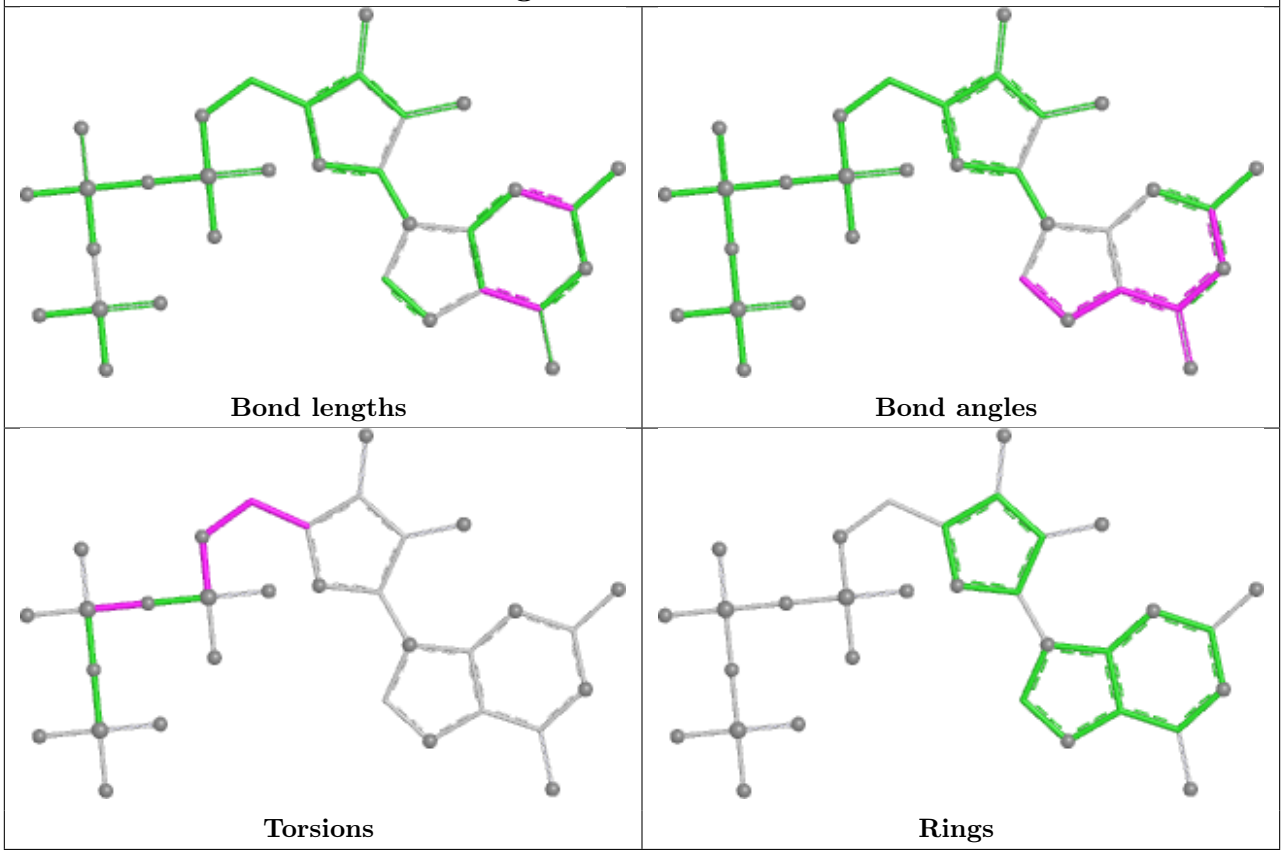

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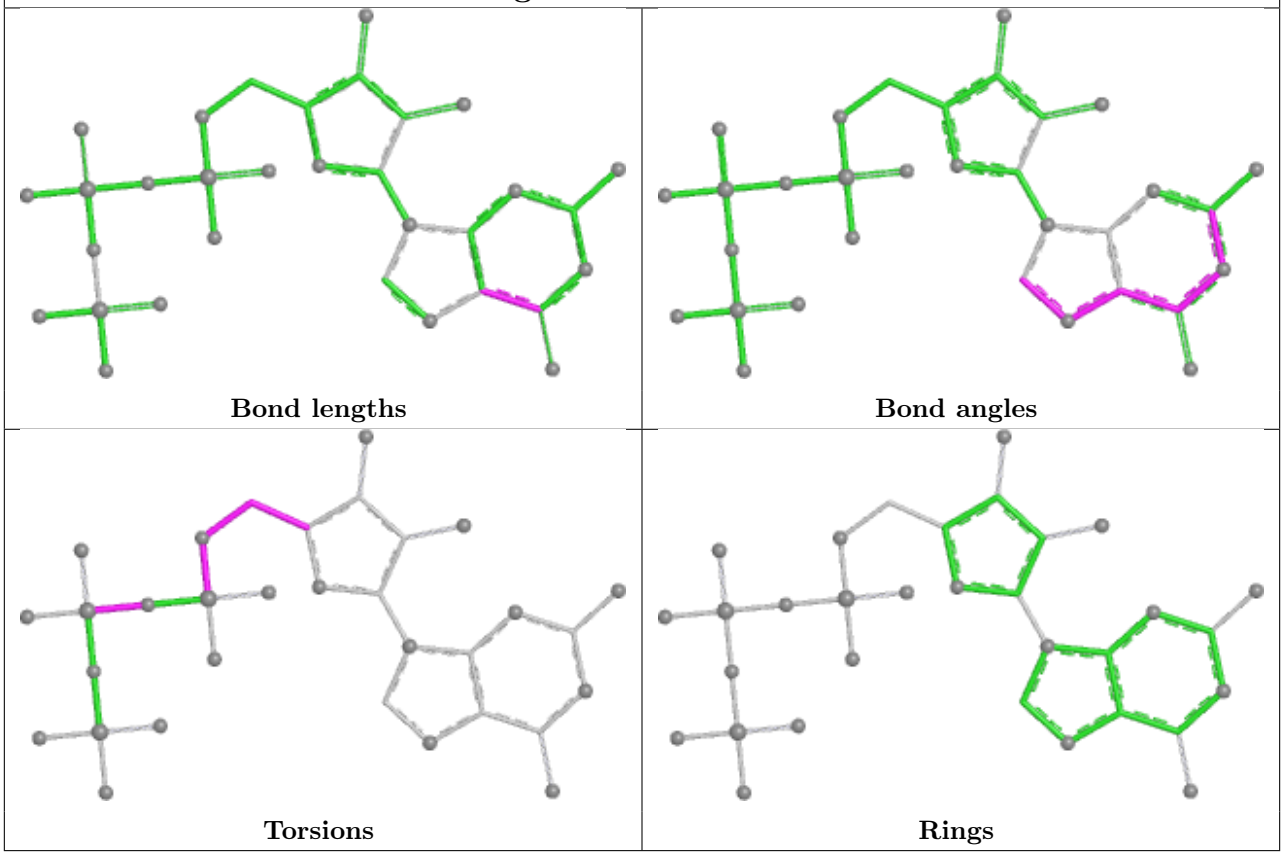


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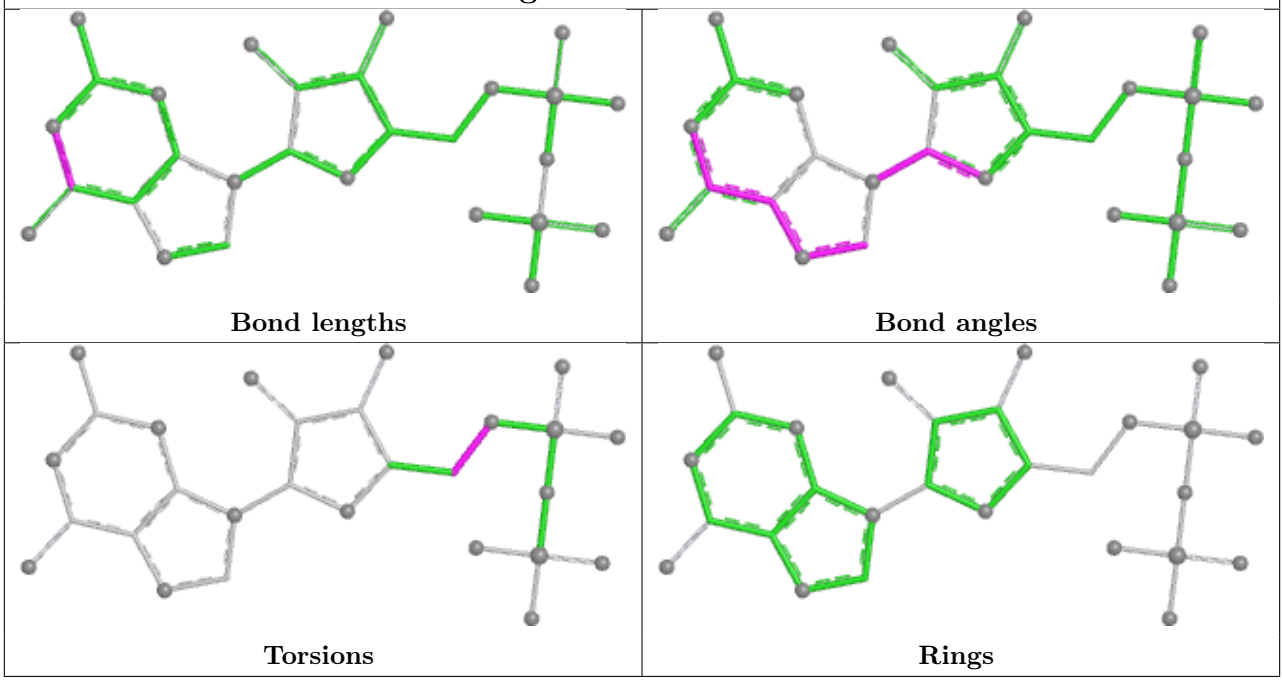

| Ligand GDP Q0 501 | |
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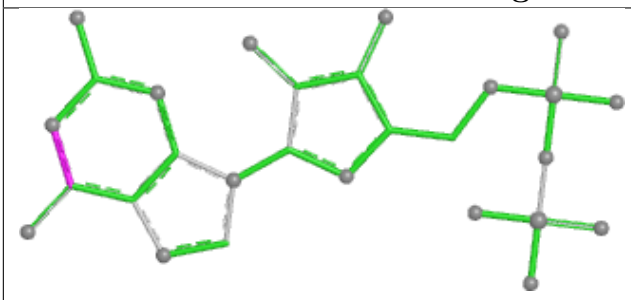
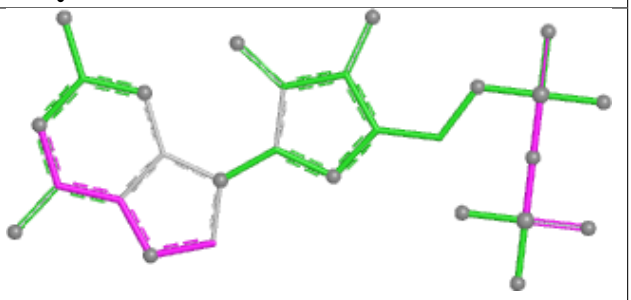
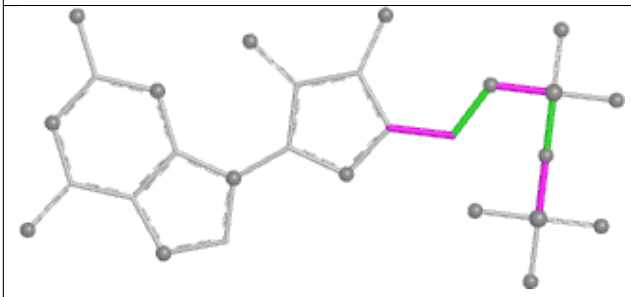
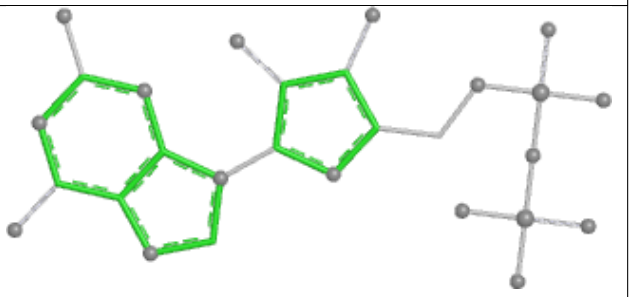
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP Y4 502 | |
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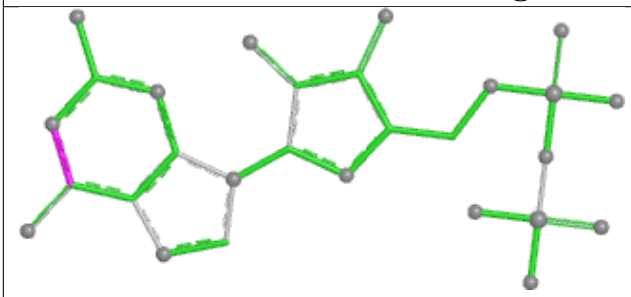
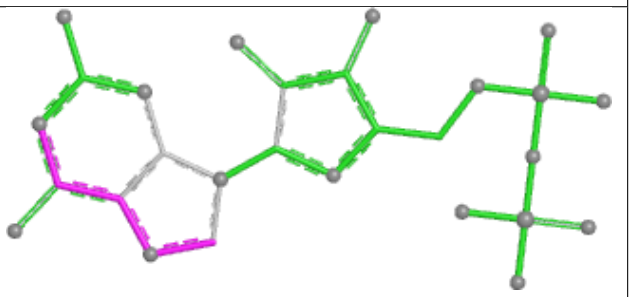
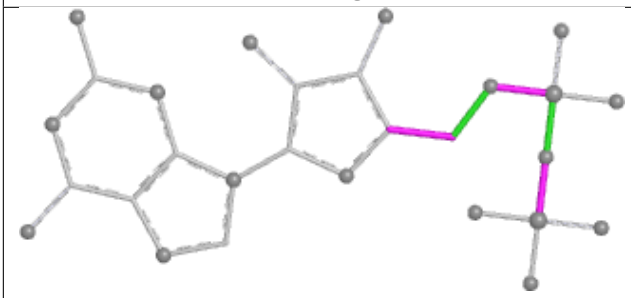
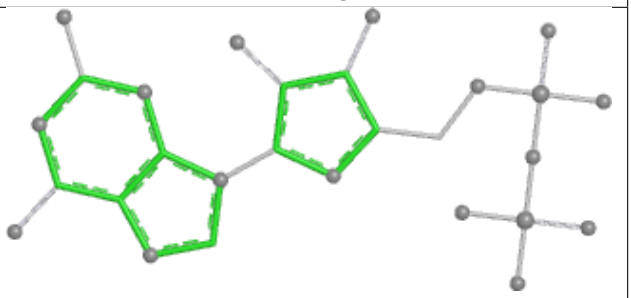
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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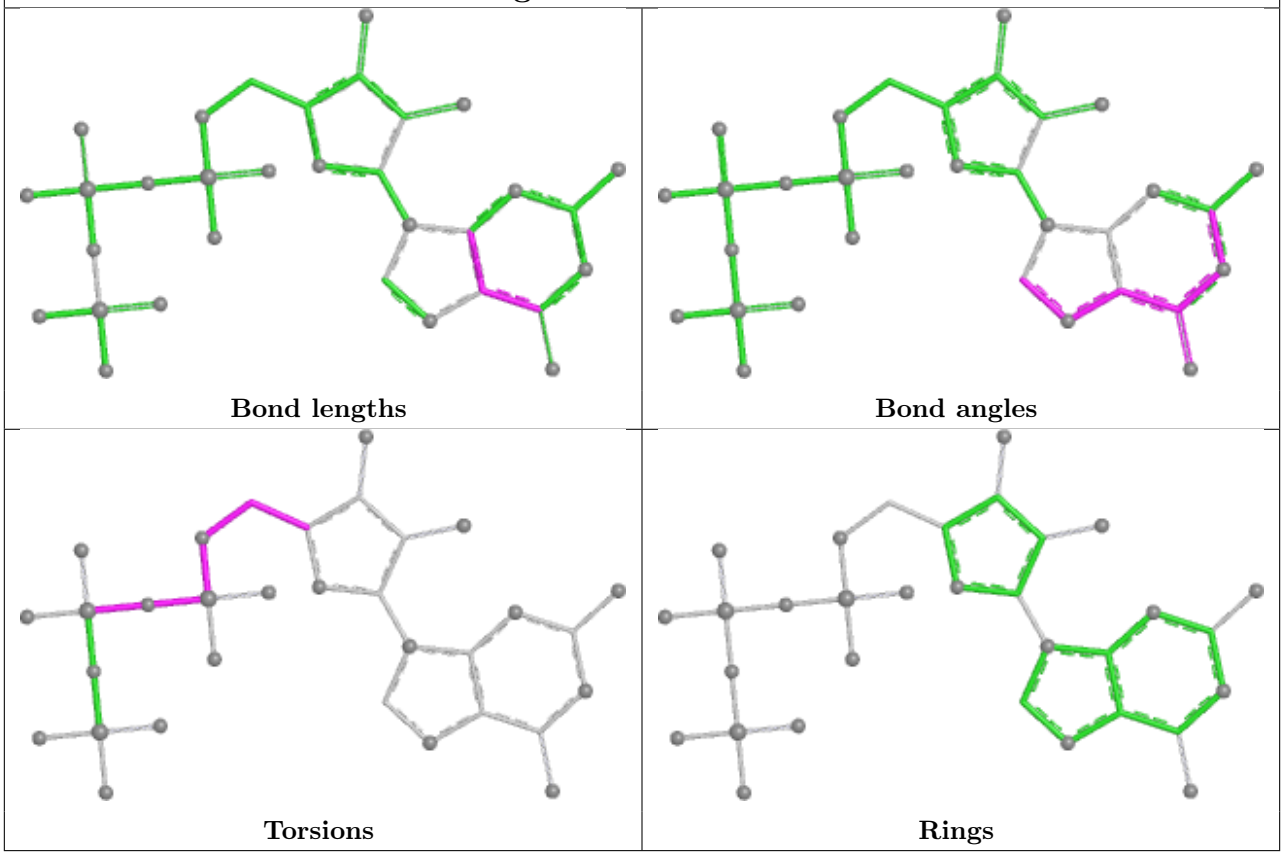


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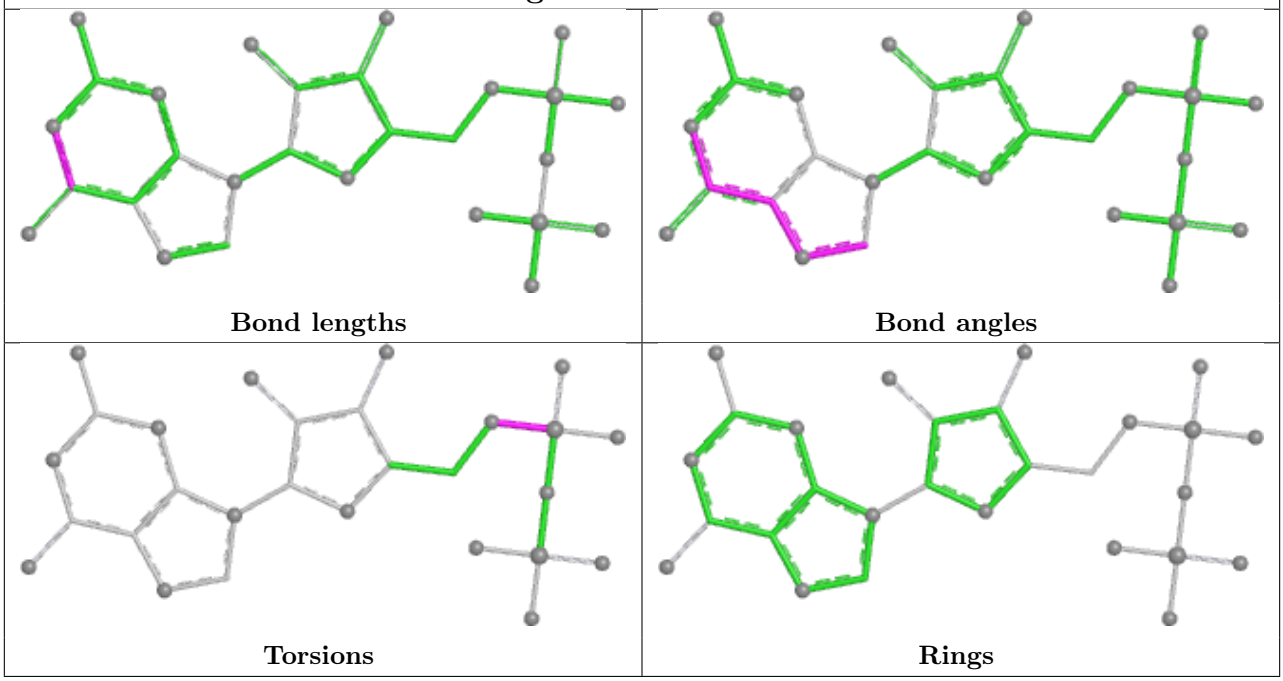

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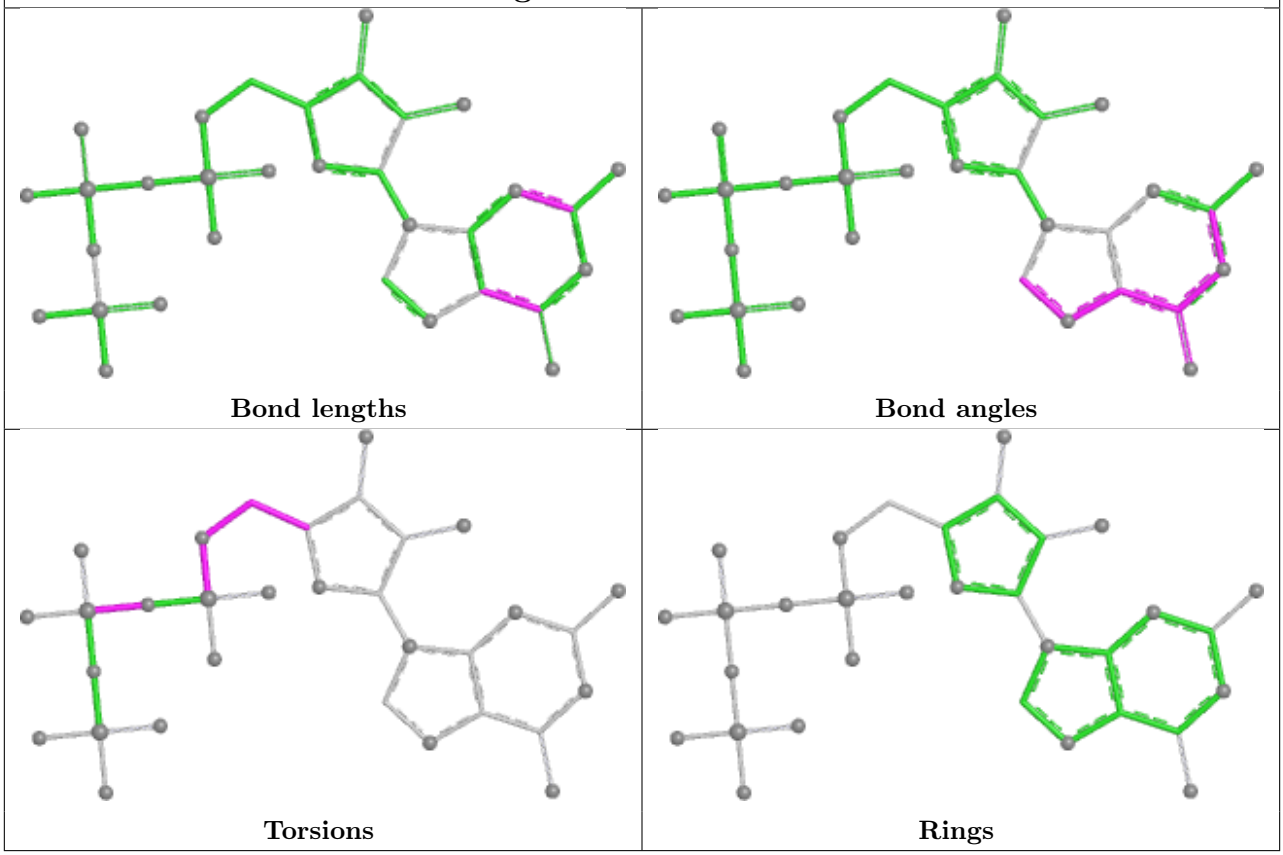


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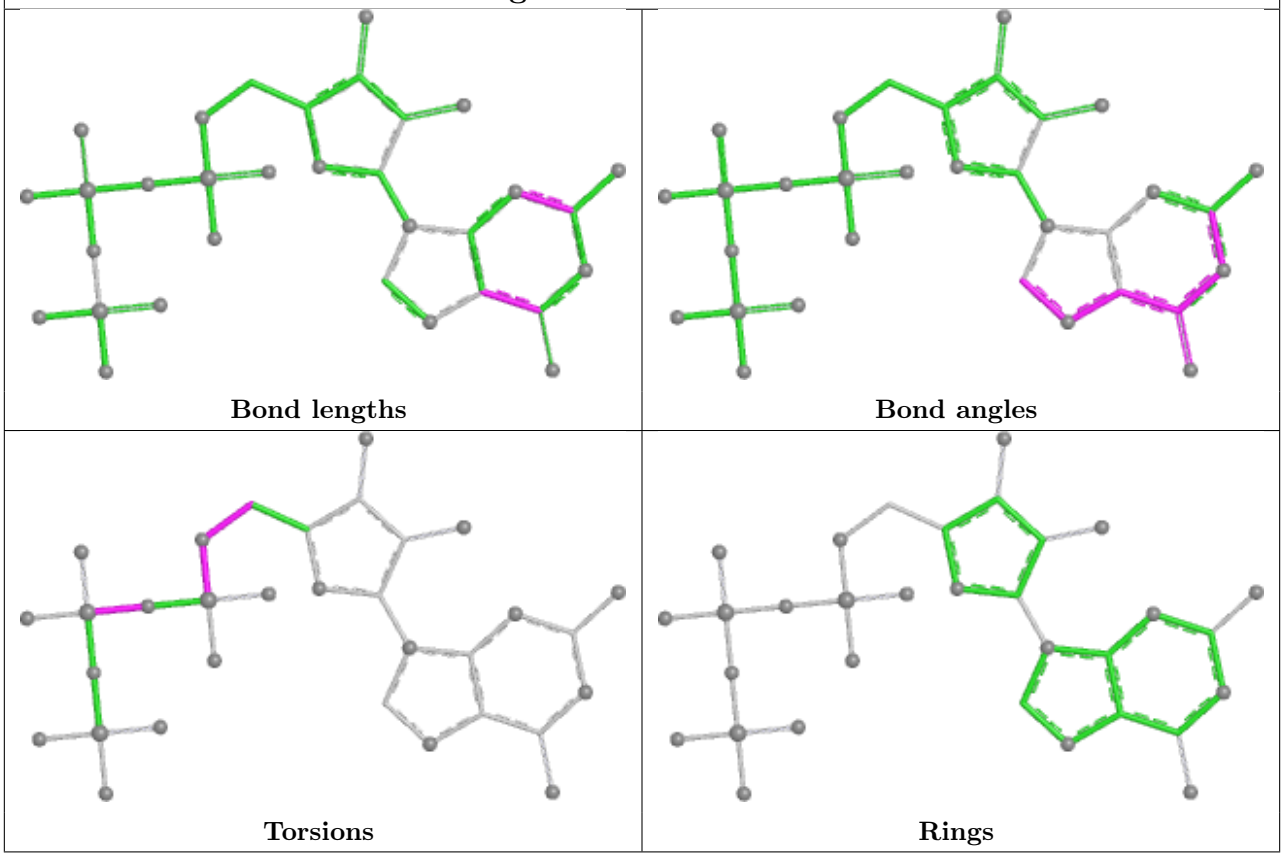

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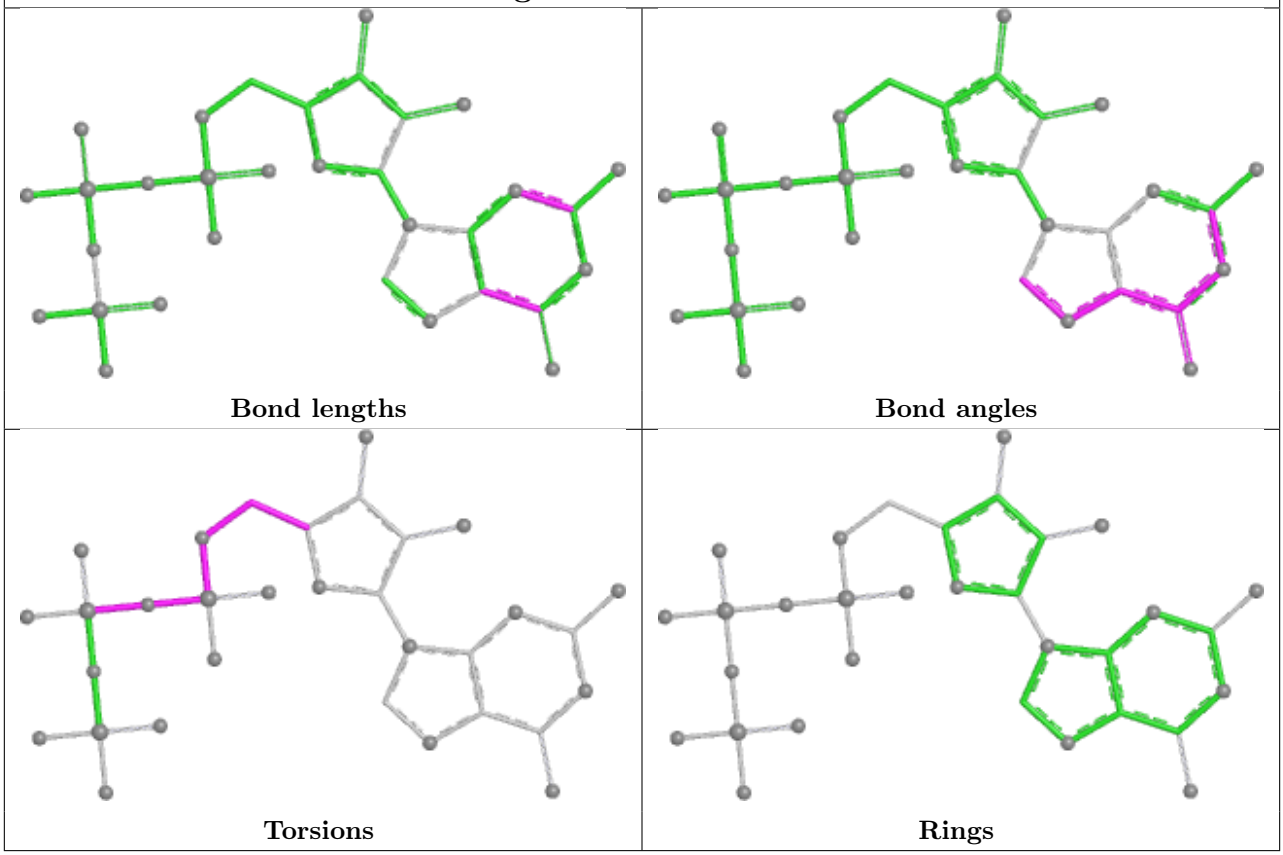


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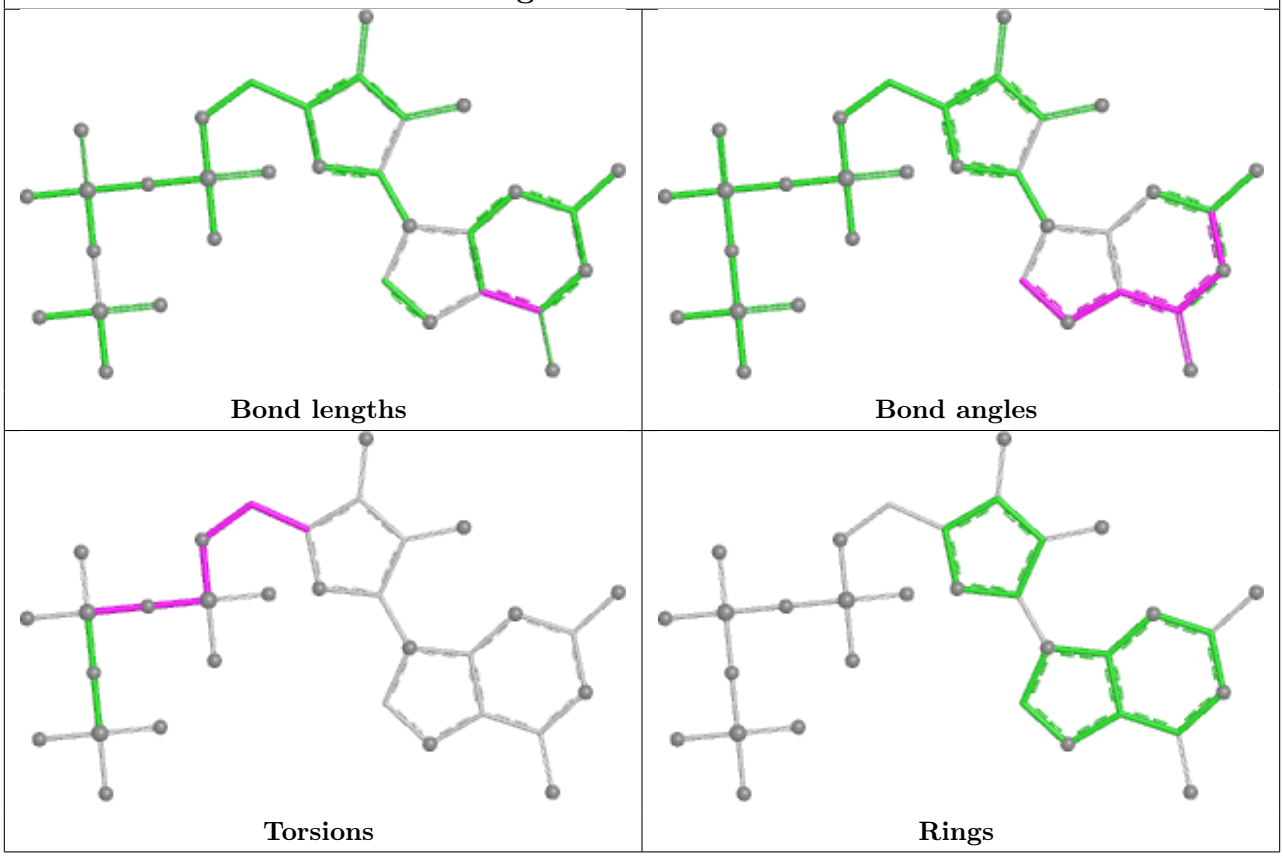

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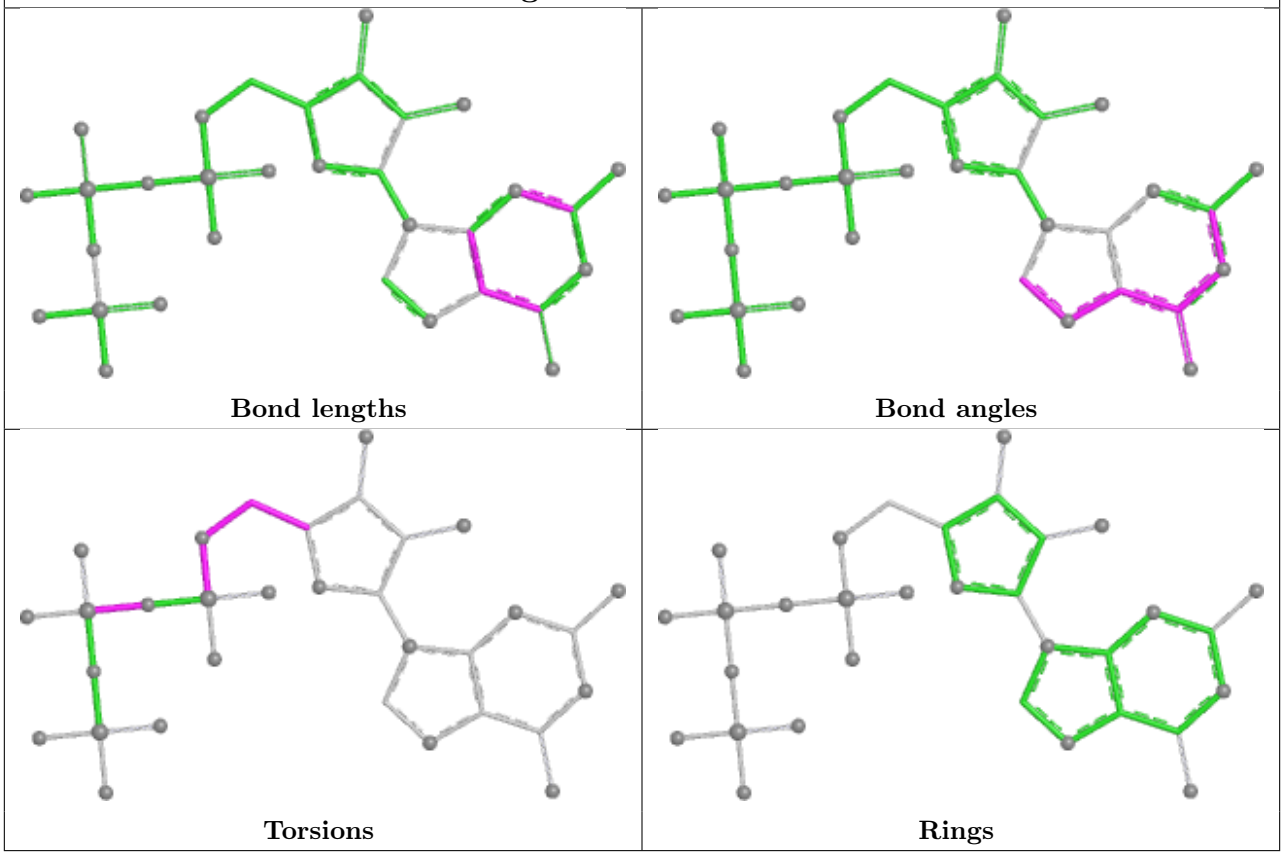
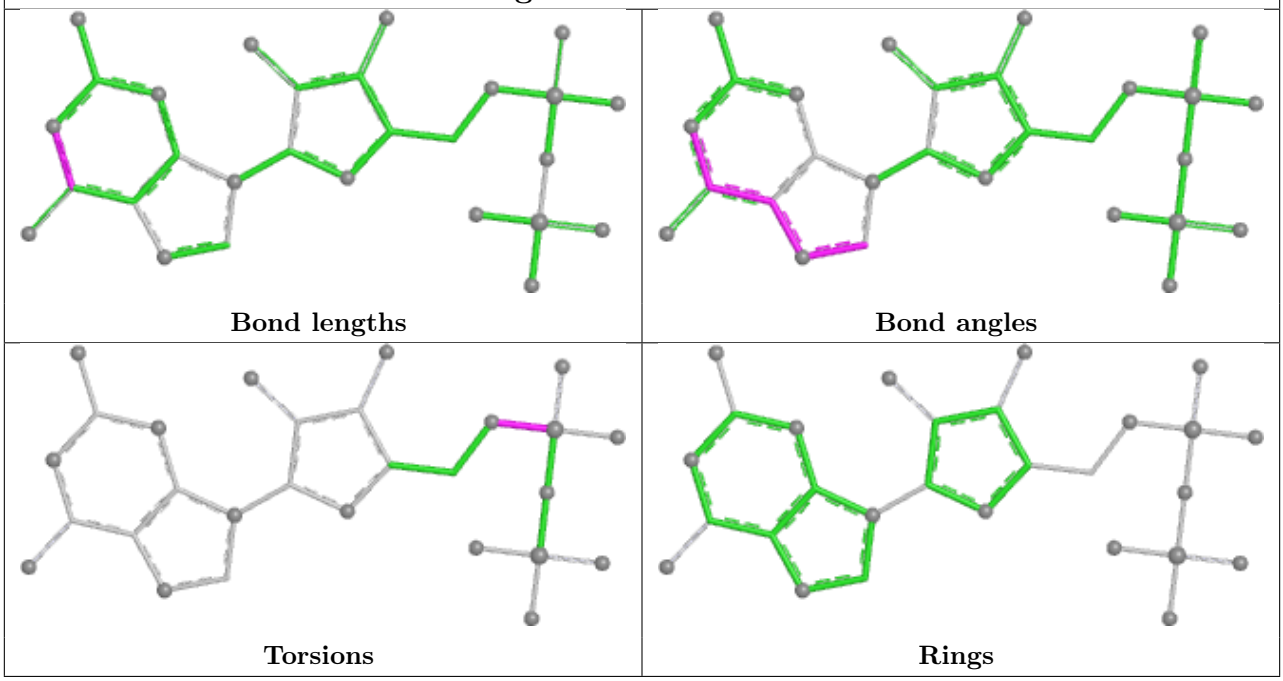



## Ligand GDP F8 502



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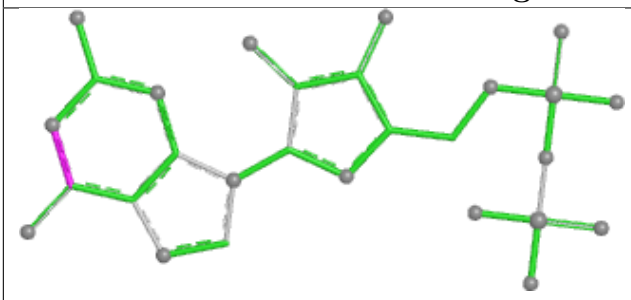

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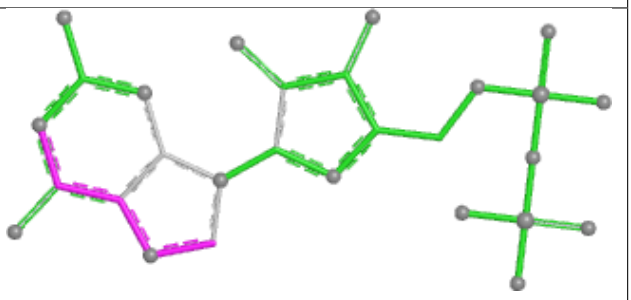
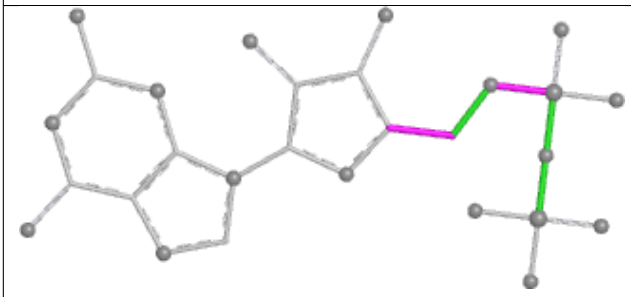
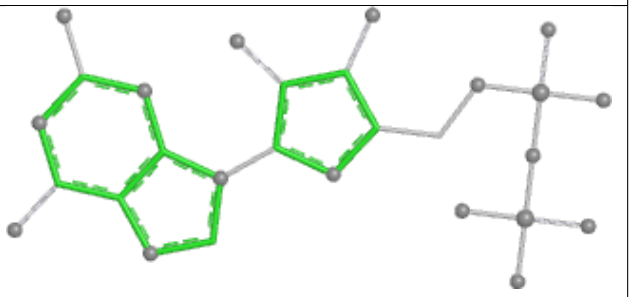


Bond angles

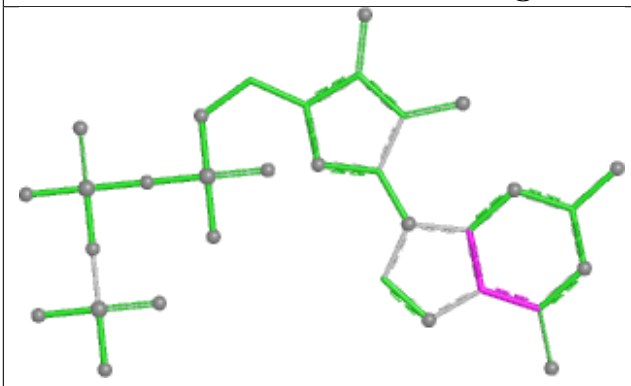


Torsions



Rings

## Ligand GTP 3P 501



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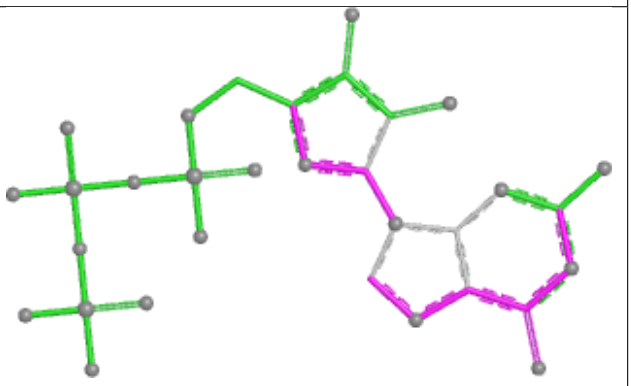

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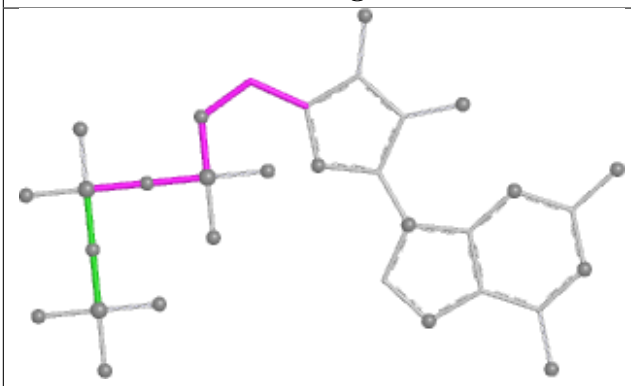

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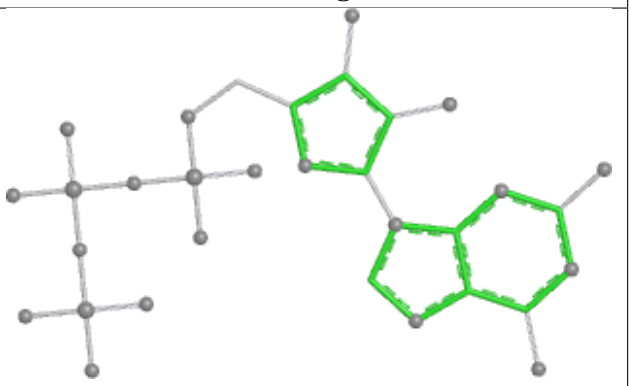
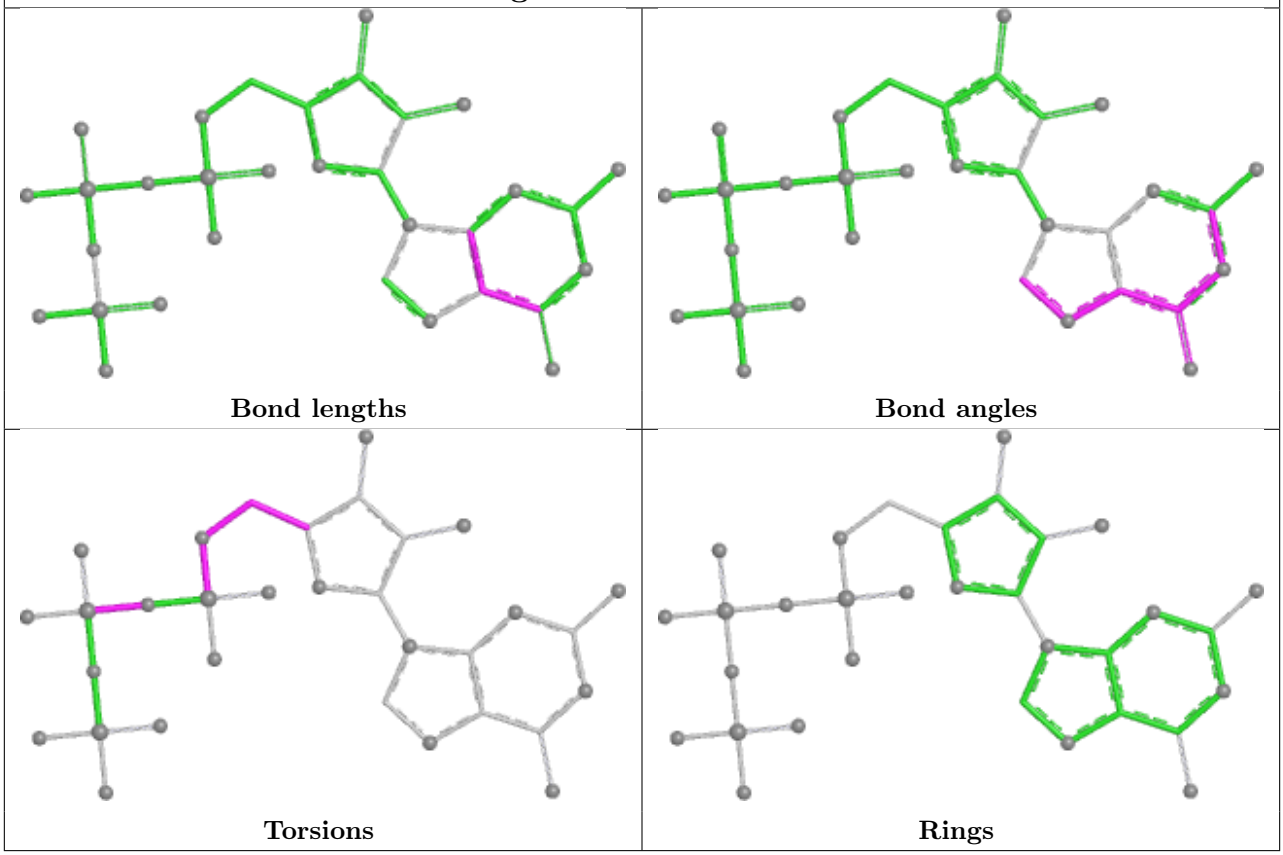
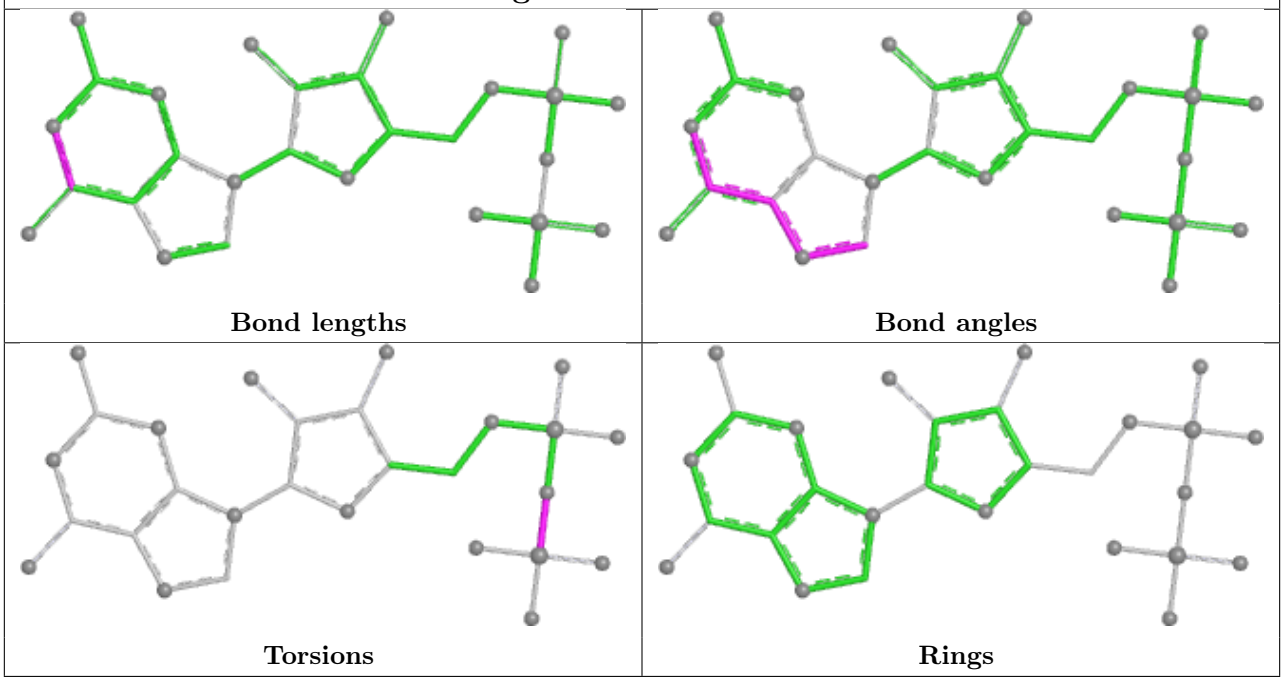


Rings

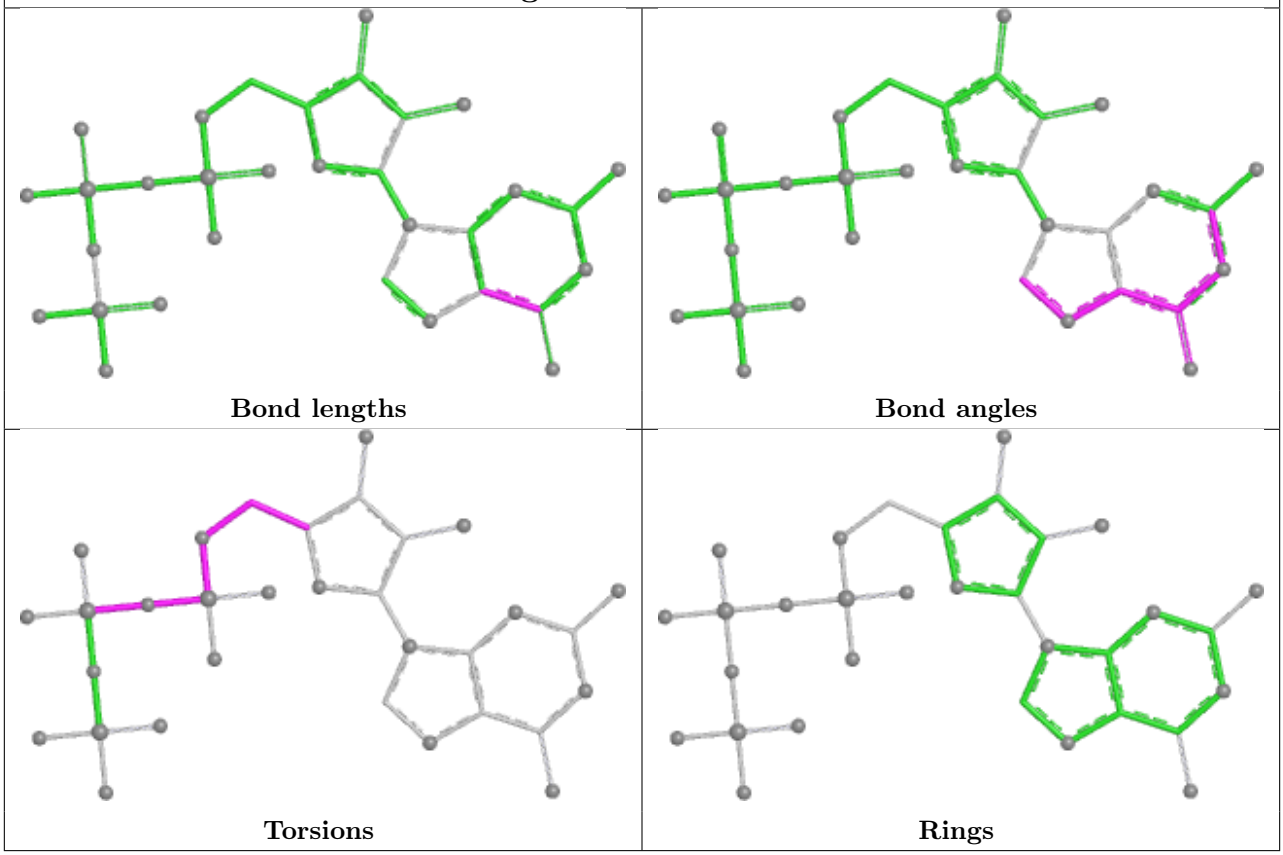
## Ligand GTP M6 501



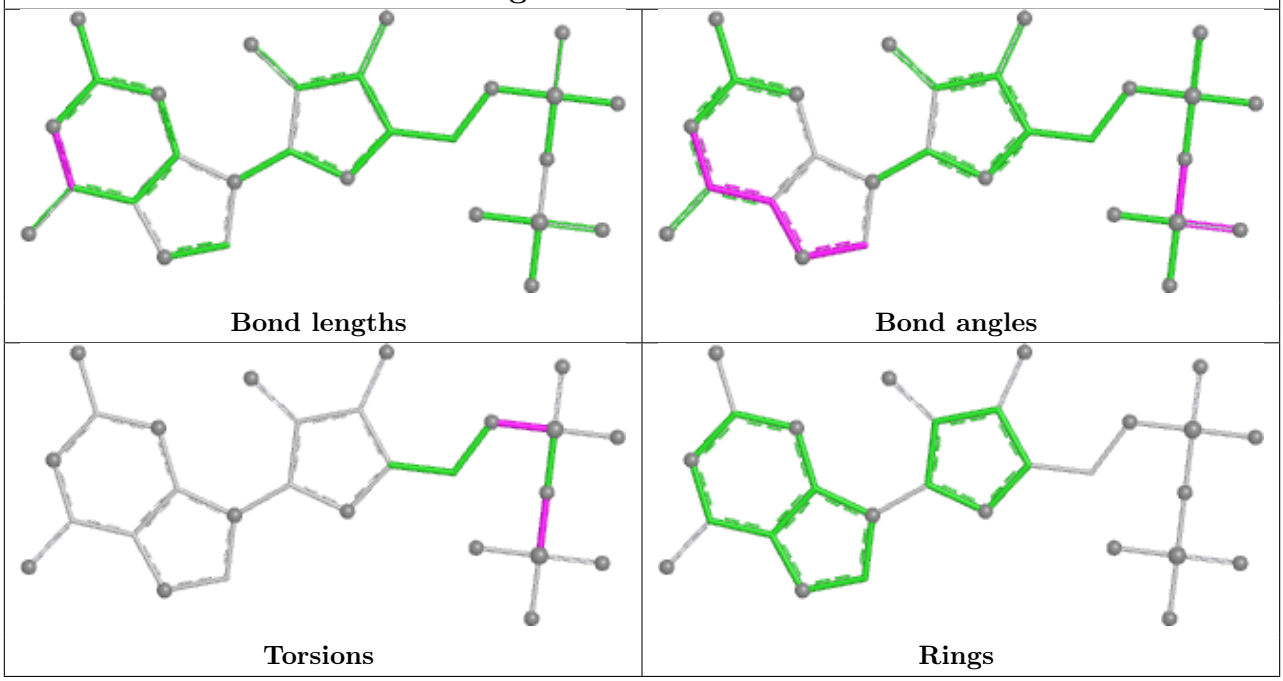

## Ligand GDP D8 501



## Ligand GTP I5 501




## Ligand GDP M0 502



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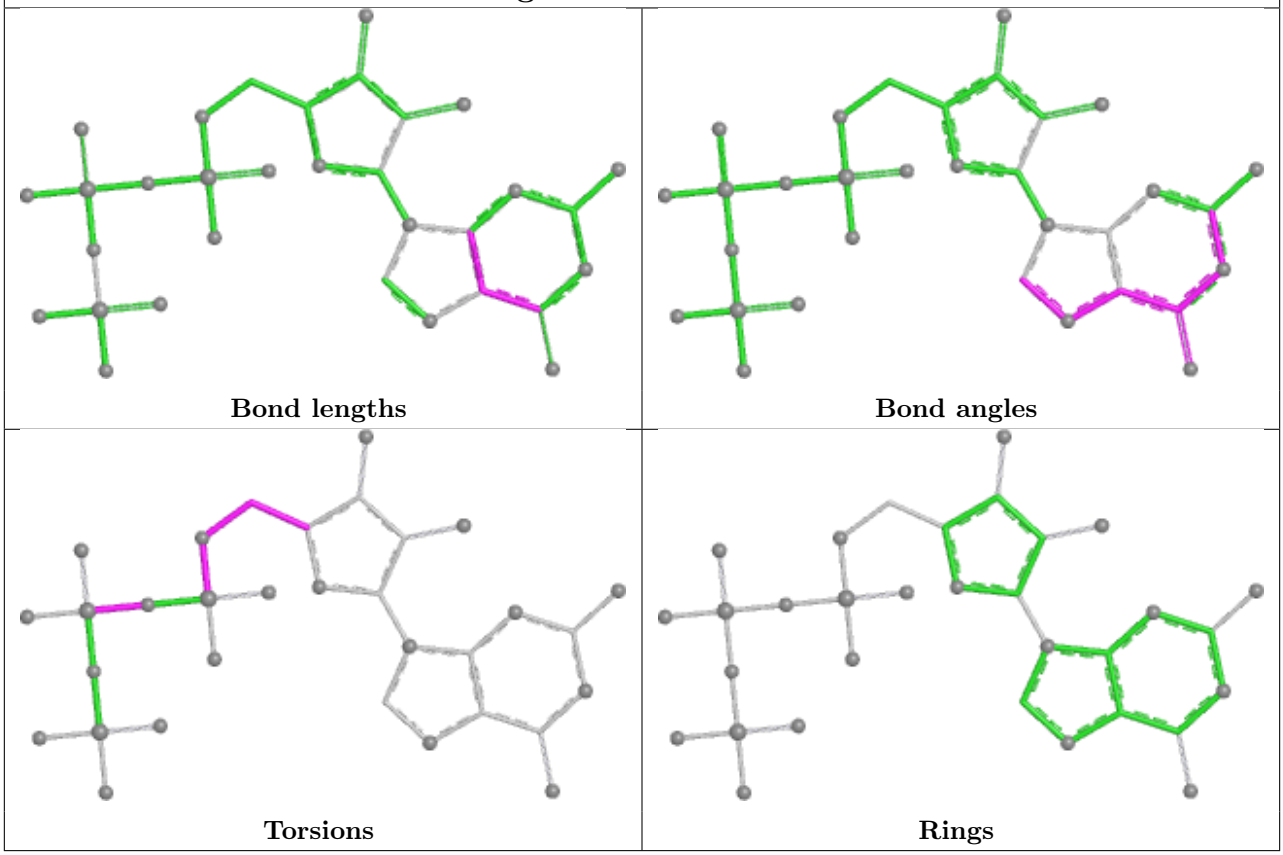


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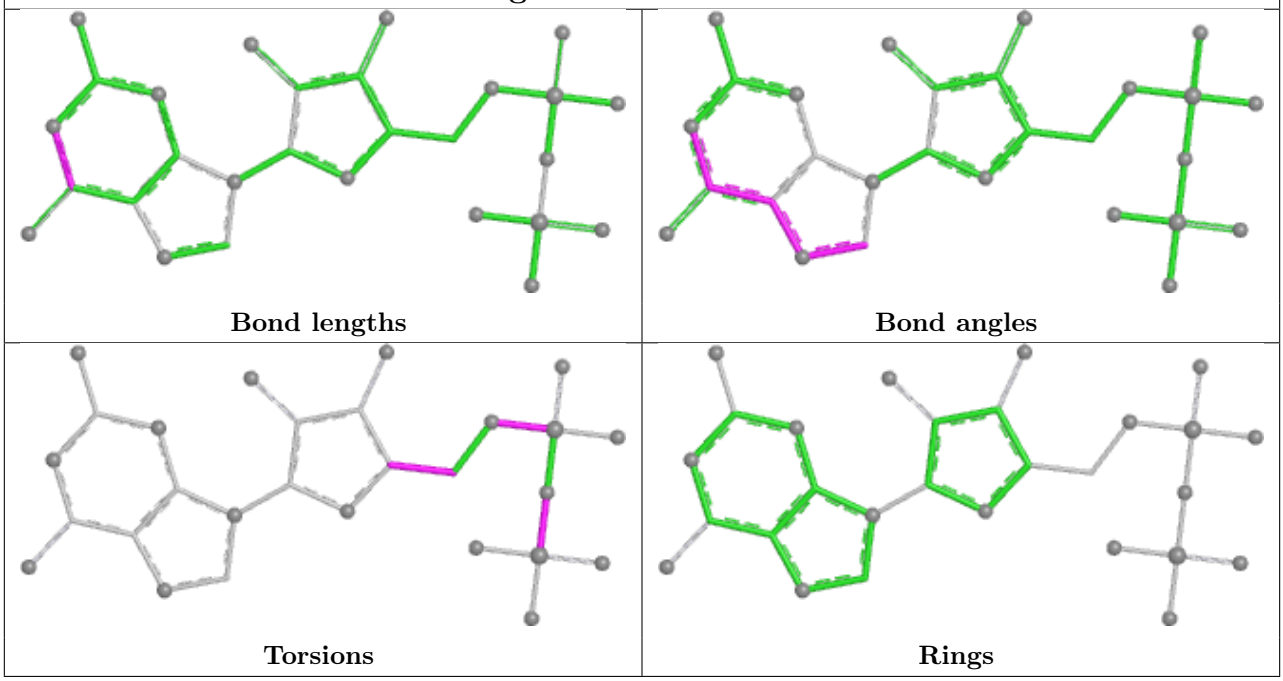

| Ligand GDP 0I 502 | |
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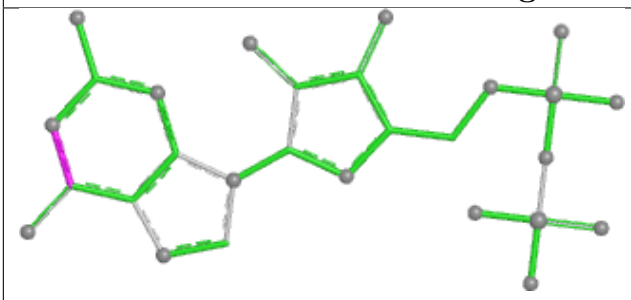
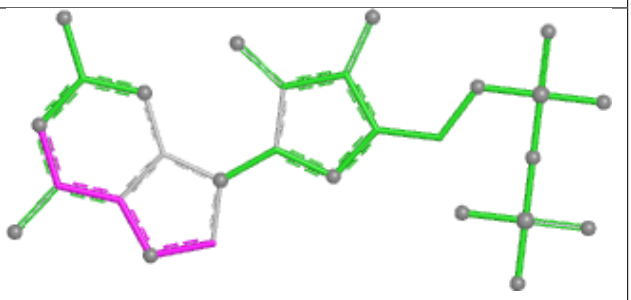
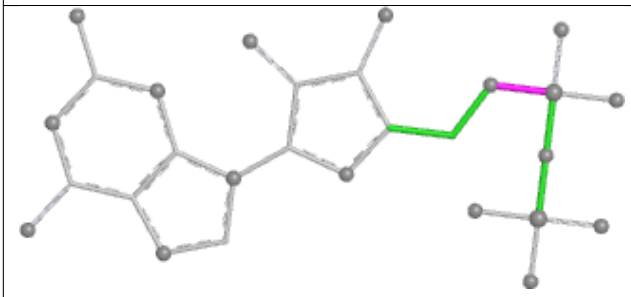
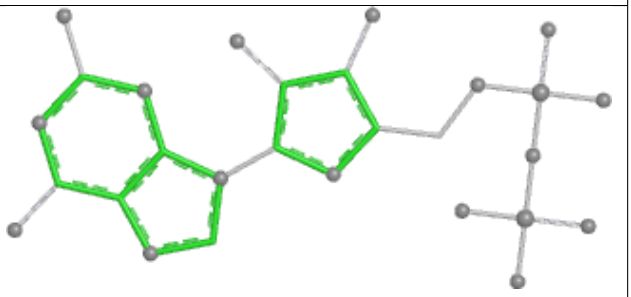
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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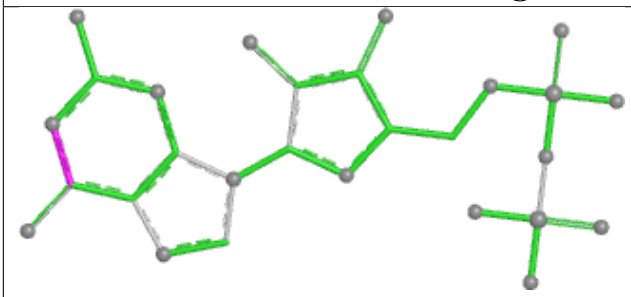
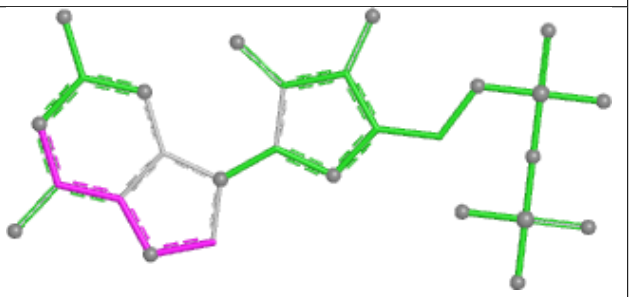
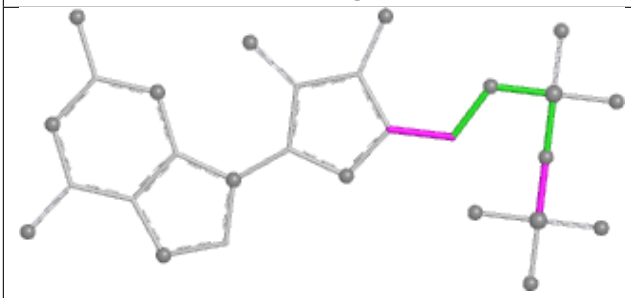
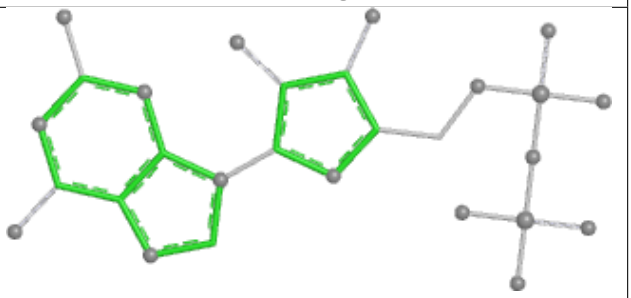
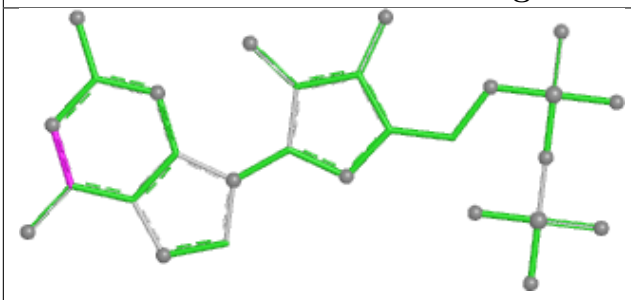
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand GDP T0 501



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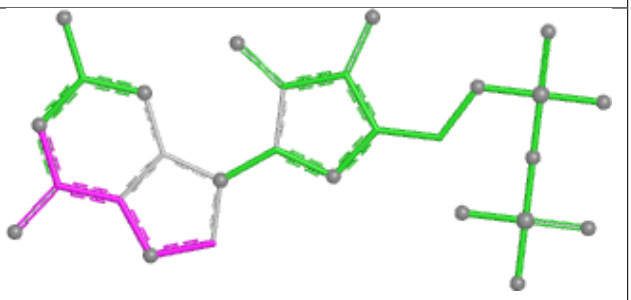

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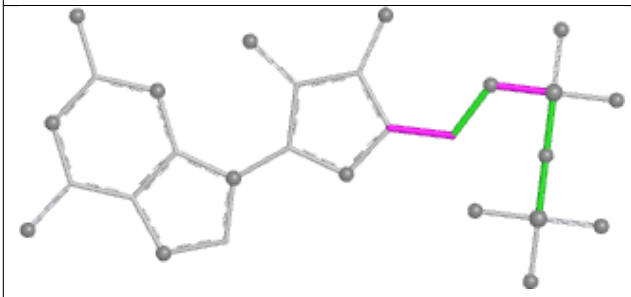

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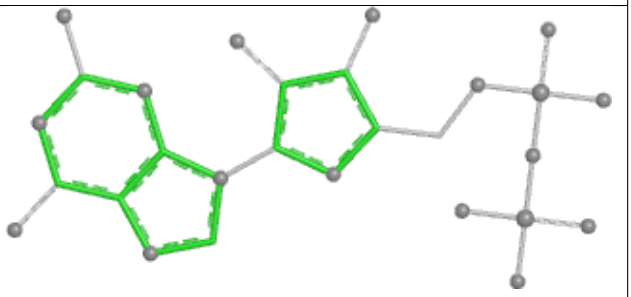
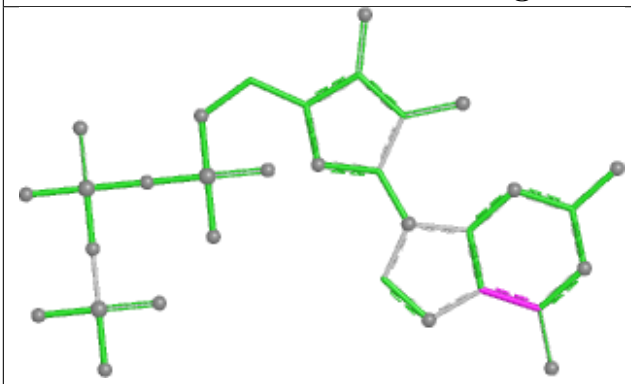


Rings

## Ligand GTP 0O 501



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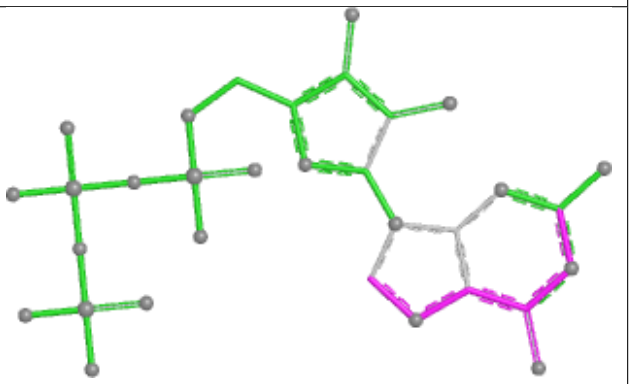

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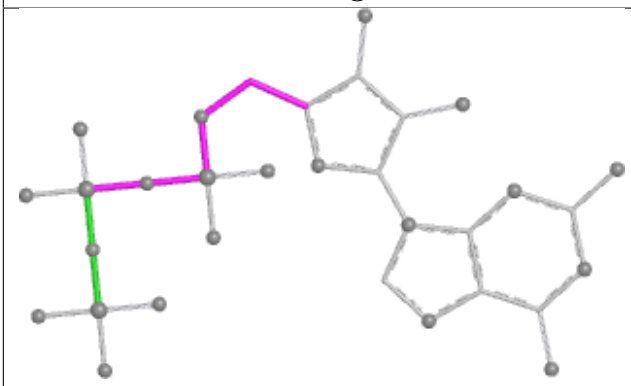

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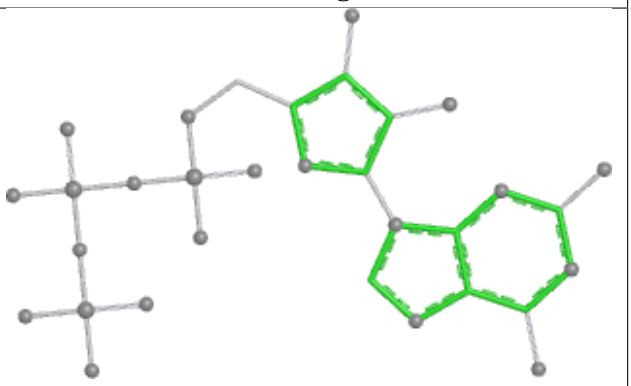

Rings

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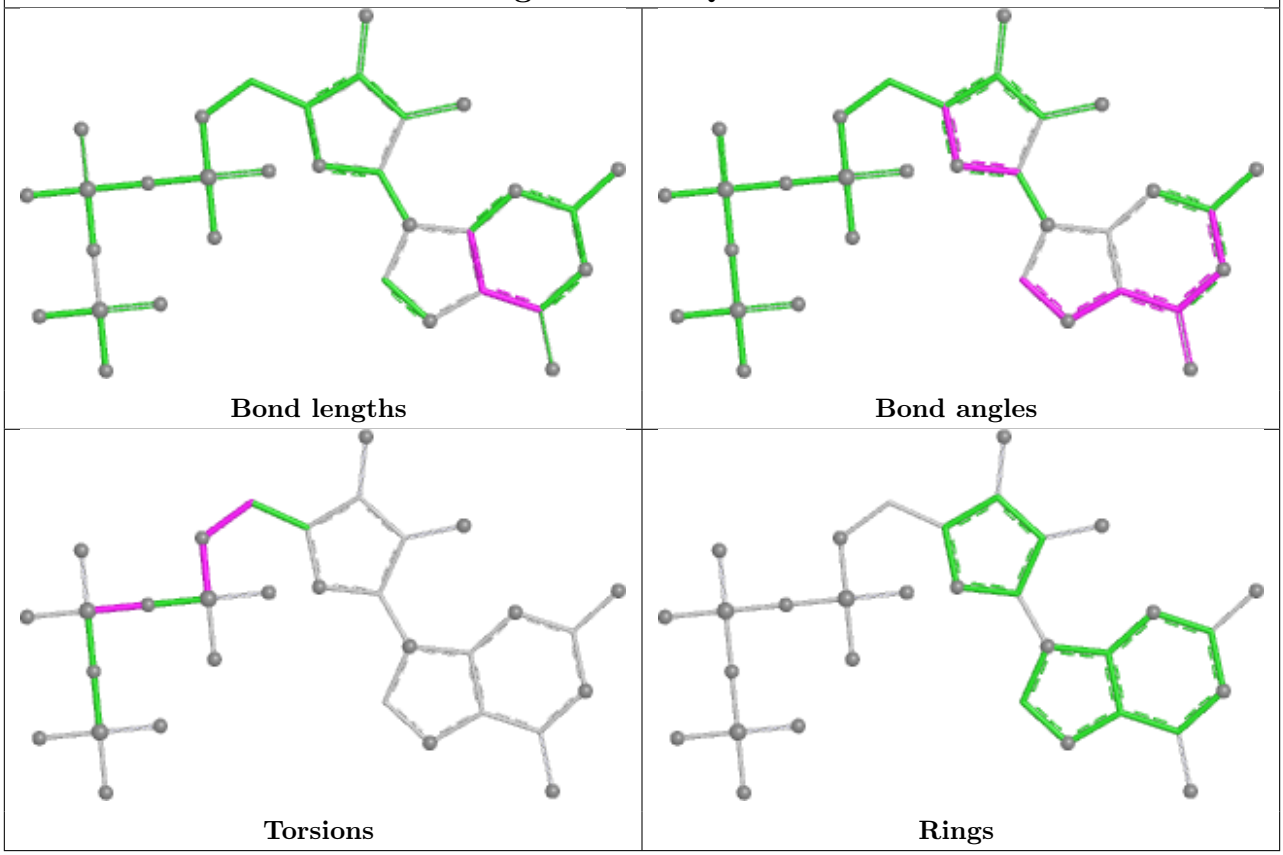


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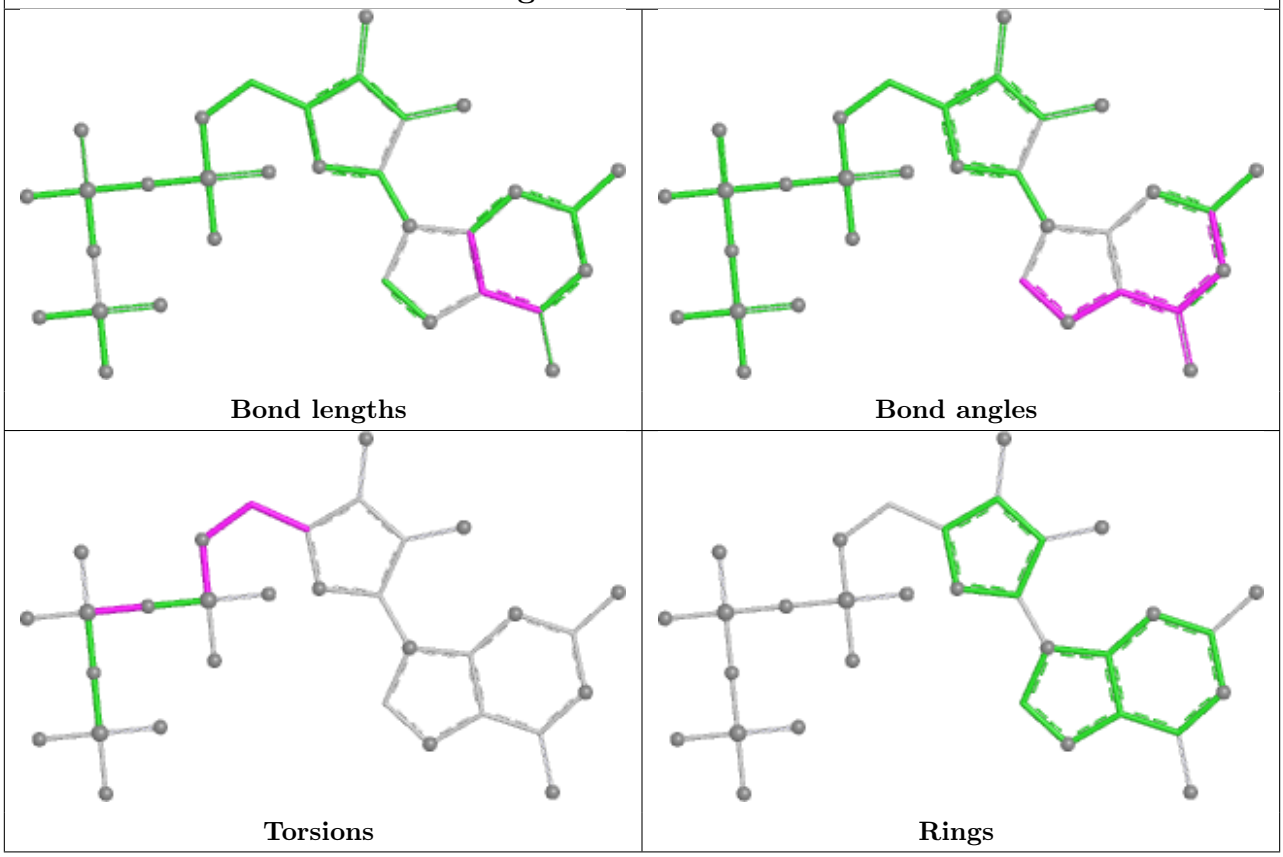
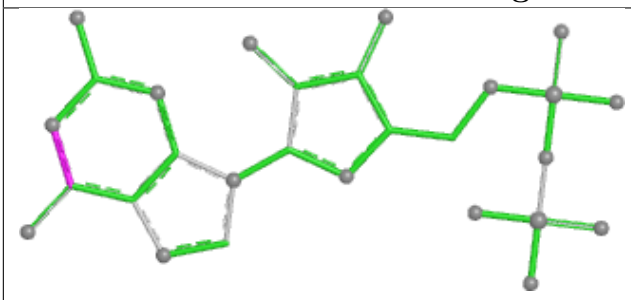


## Ligand GDP R6 503



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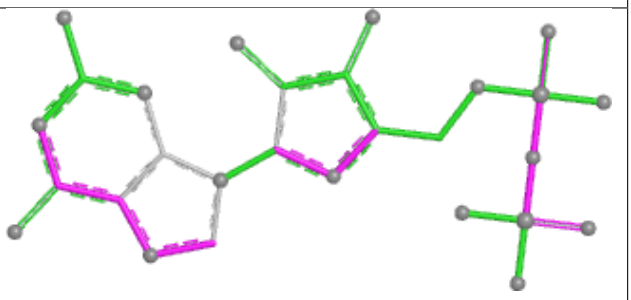
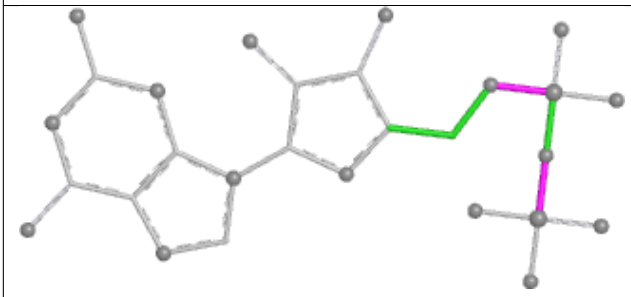


Bond angles



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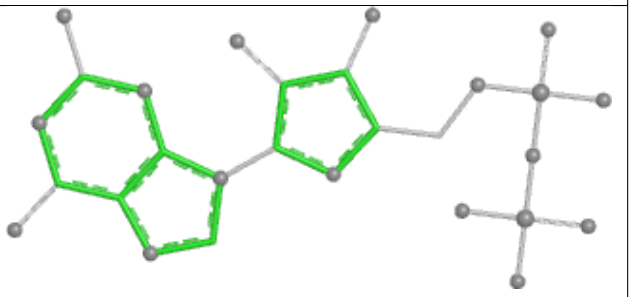

Rings

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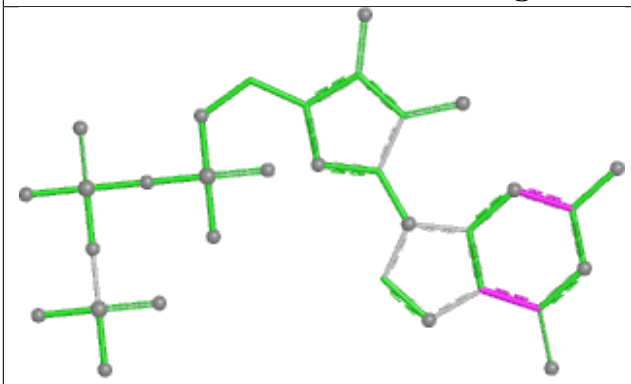

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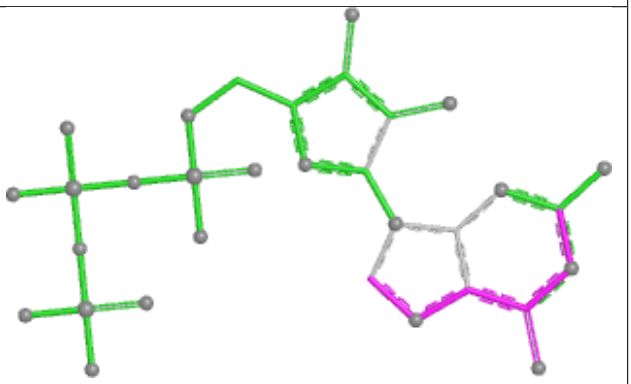

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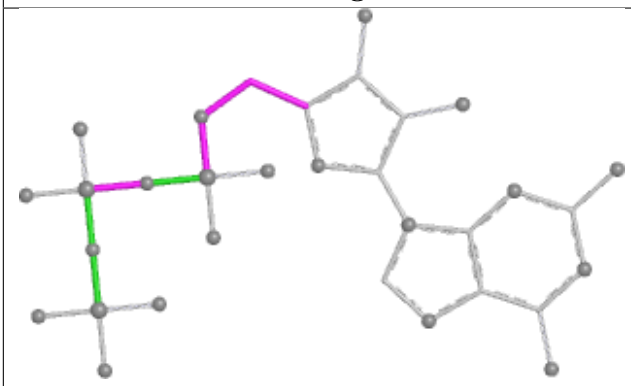

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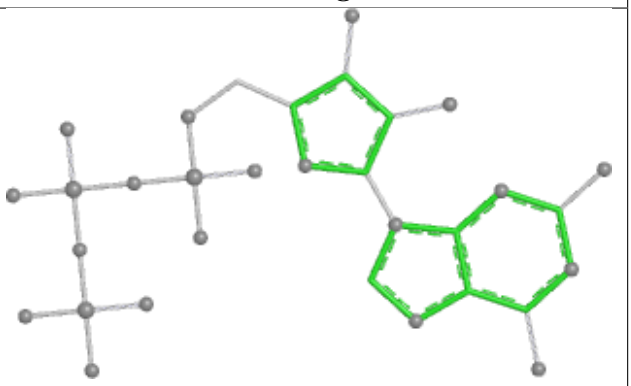

Rings

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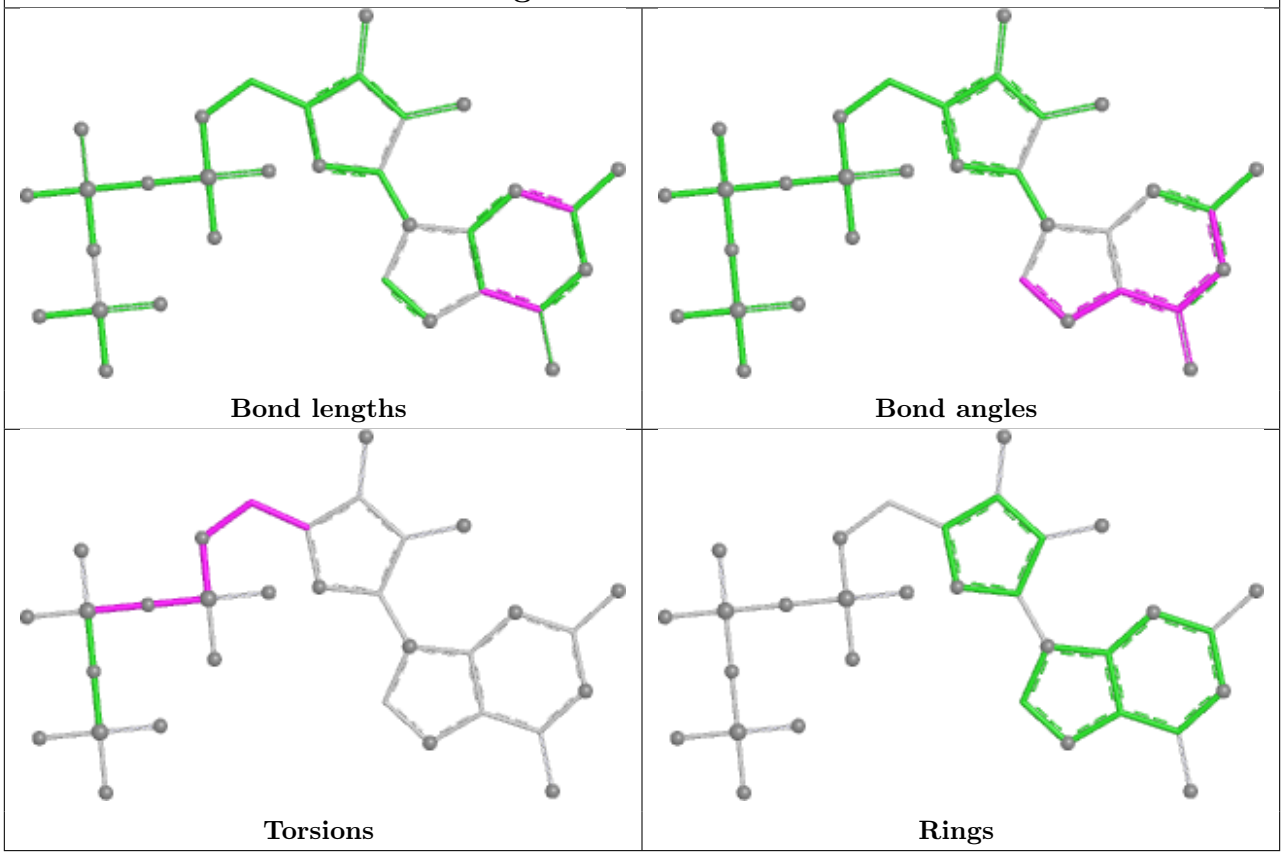


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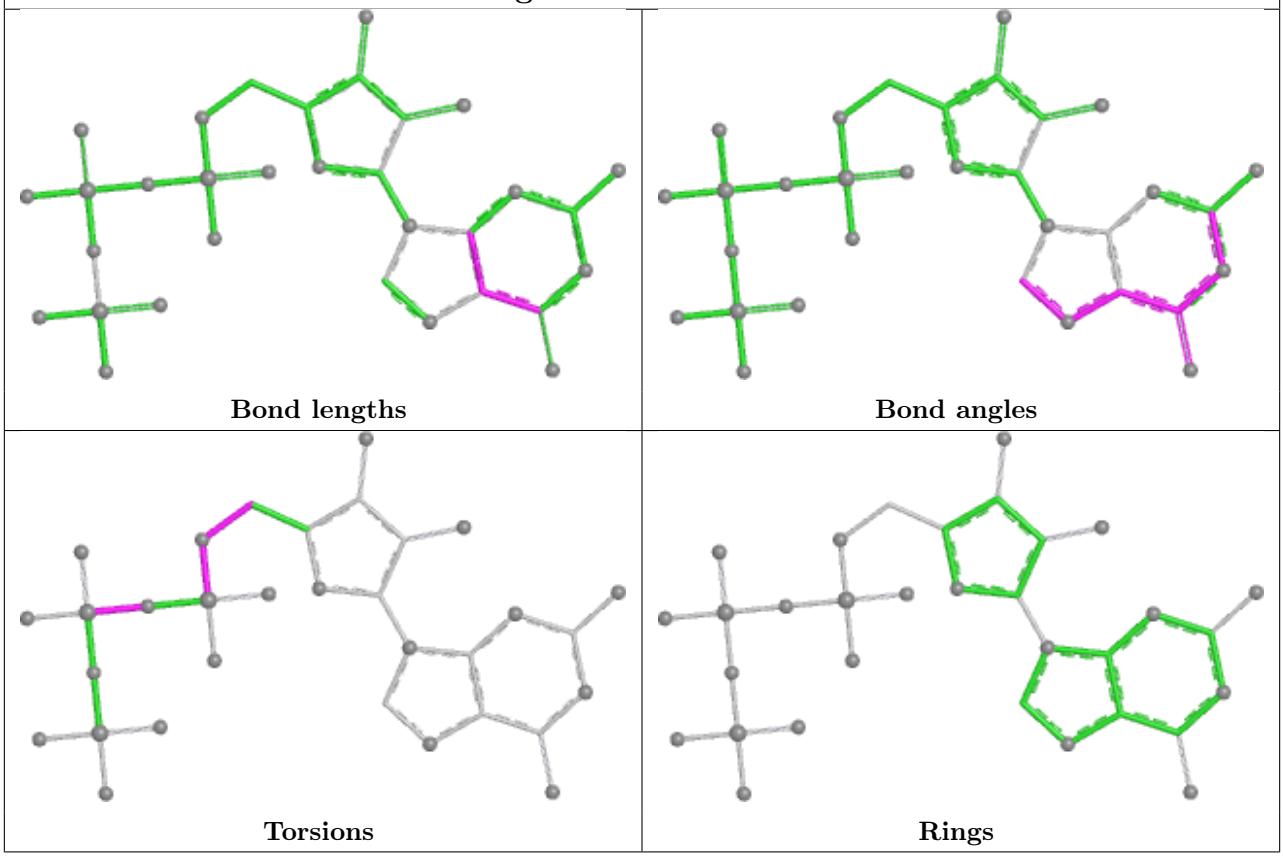

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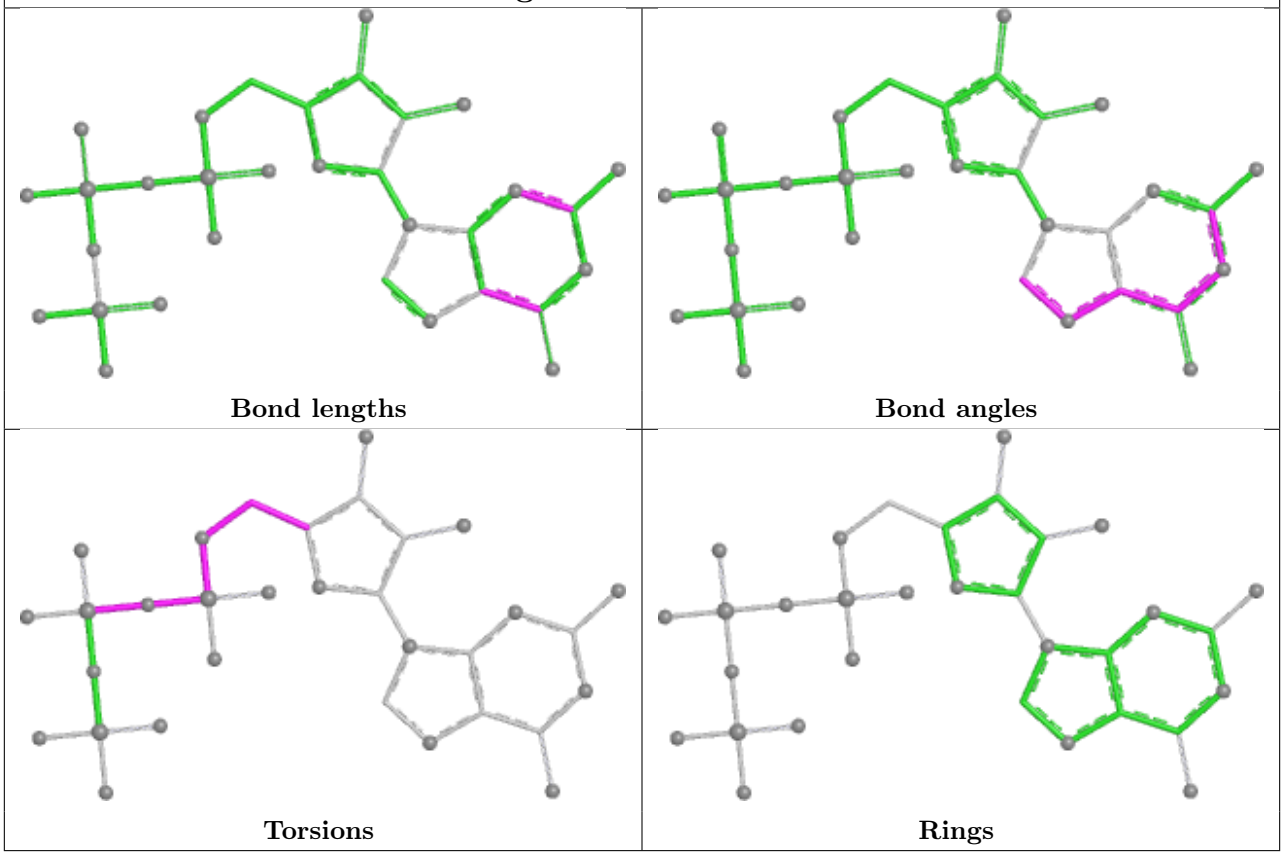


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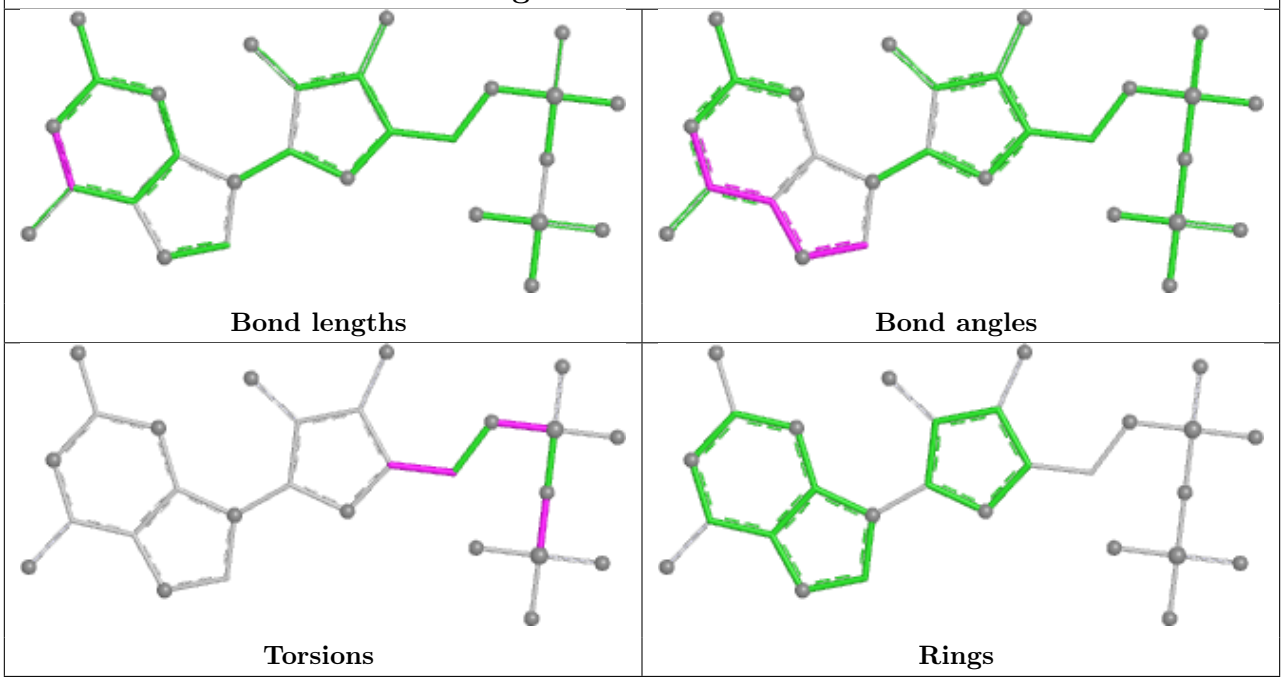

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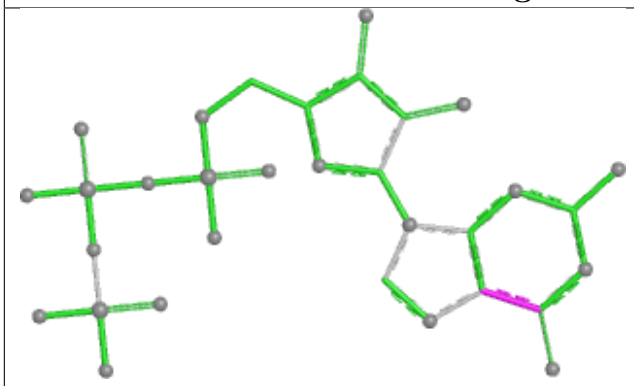

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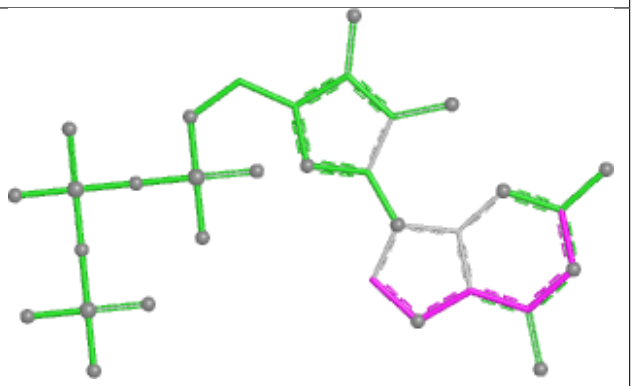

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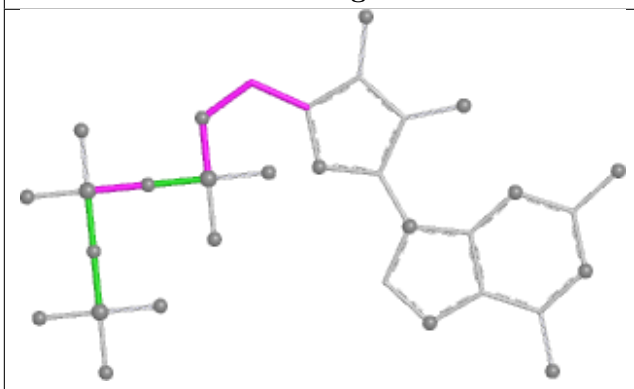
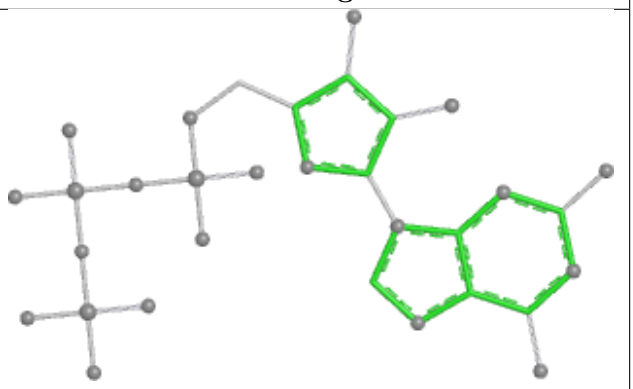


Torsions



Rings

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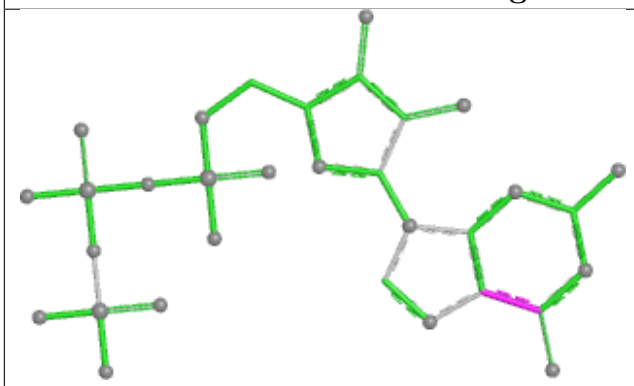

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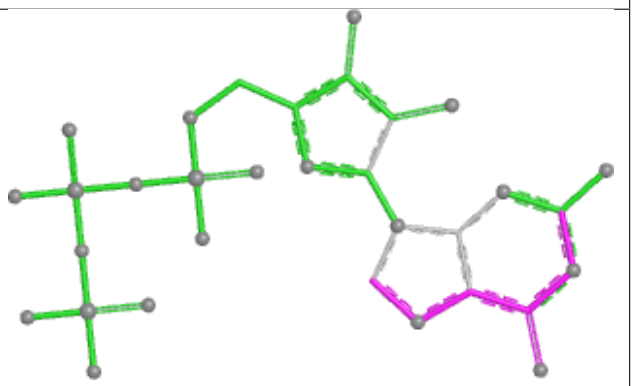

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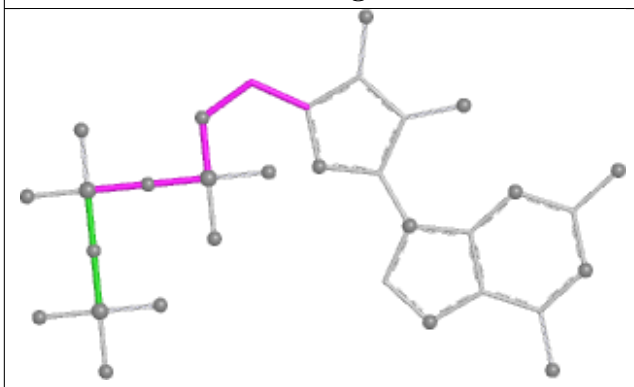

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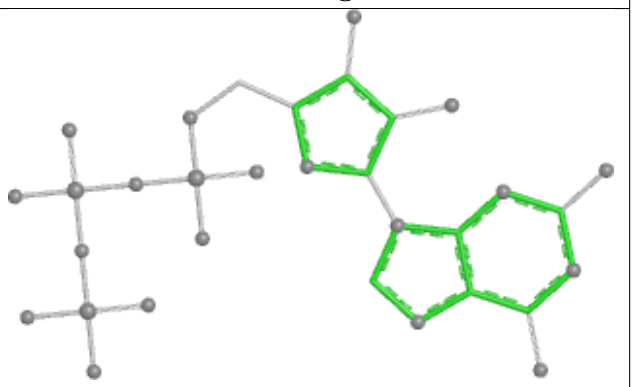

Rings

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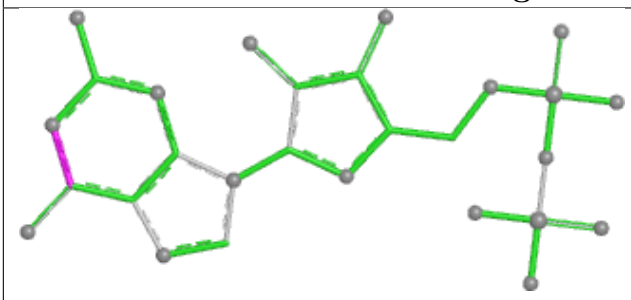

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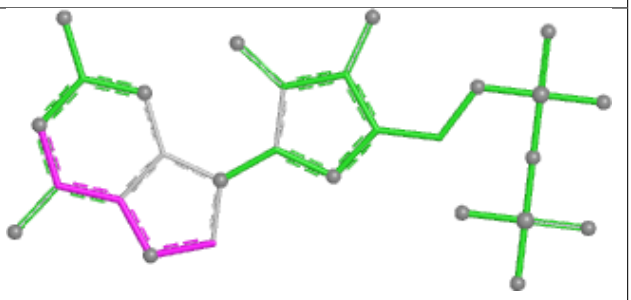

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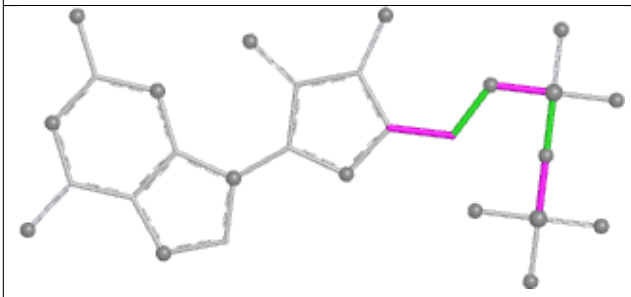

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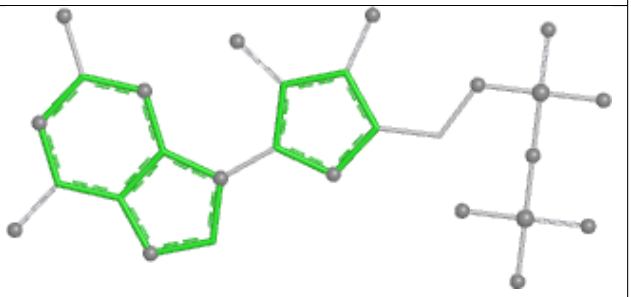

Rings

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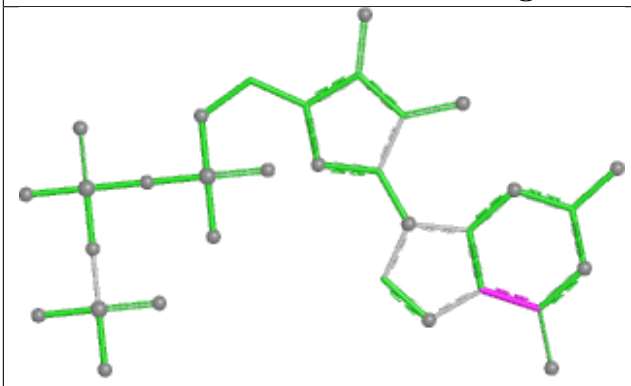

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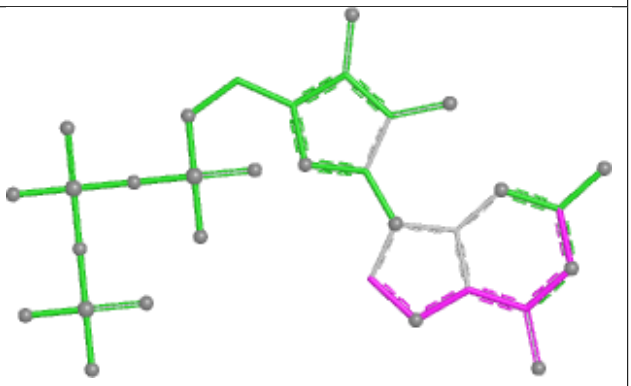

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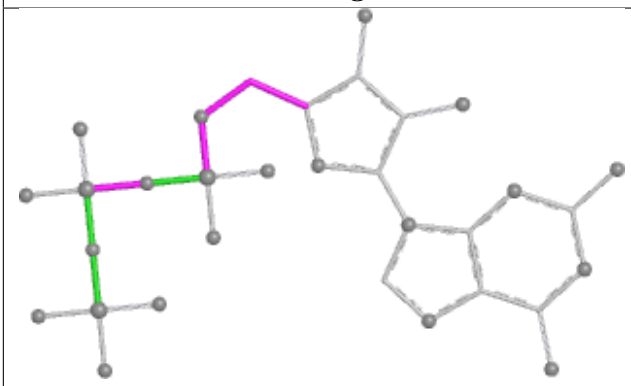

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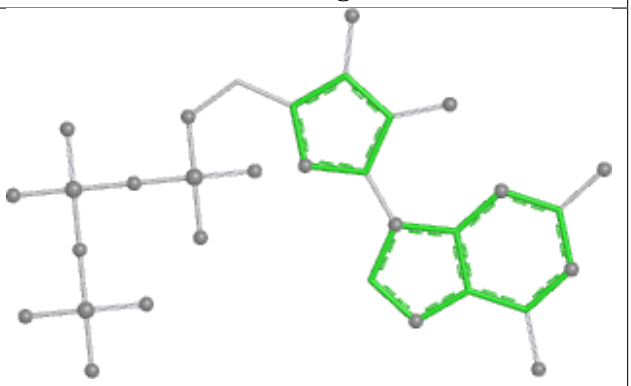

Rings

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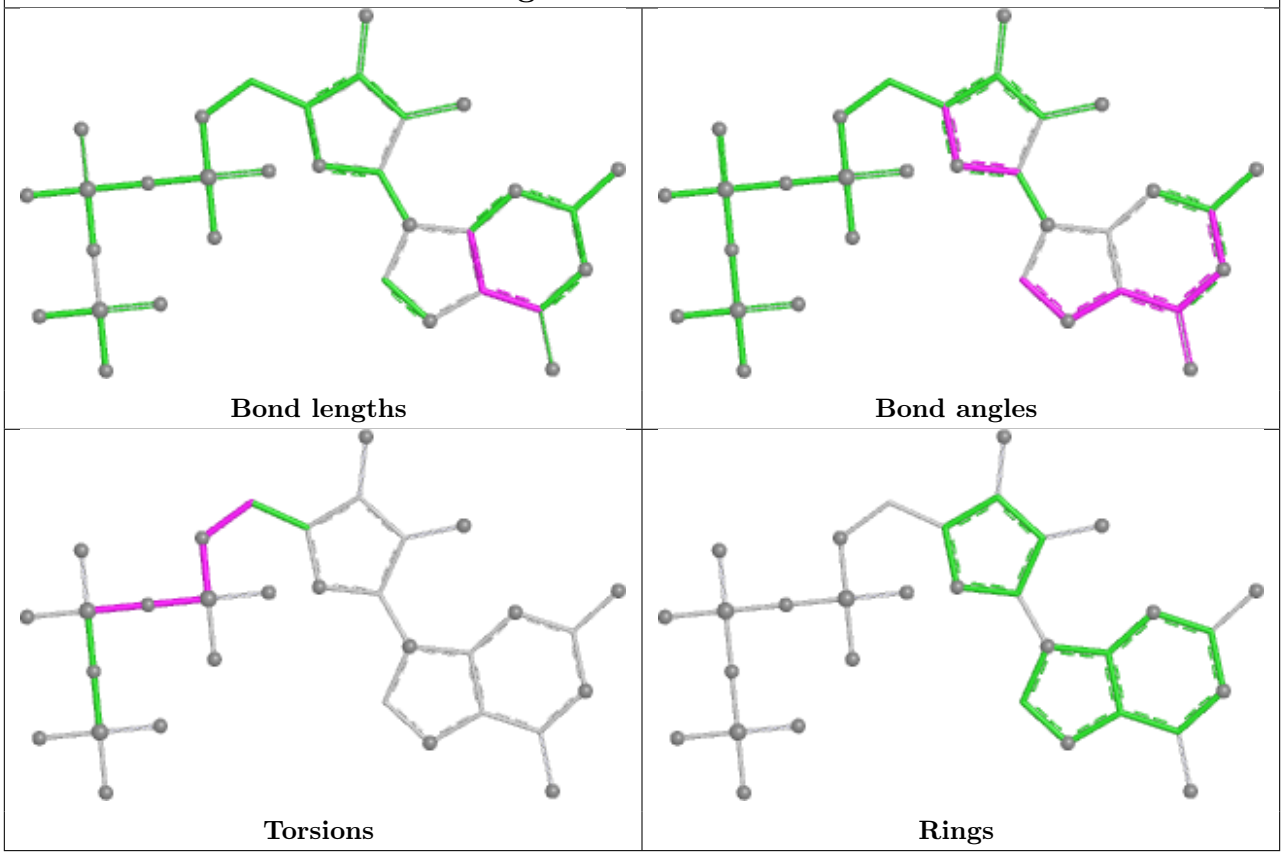
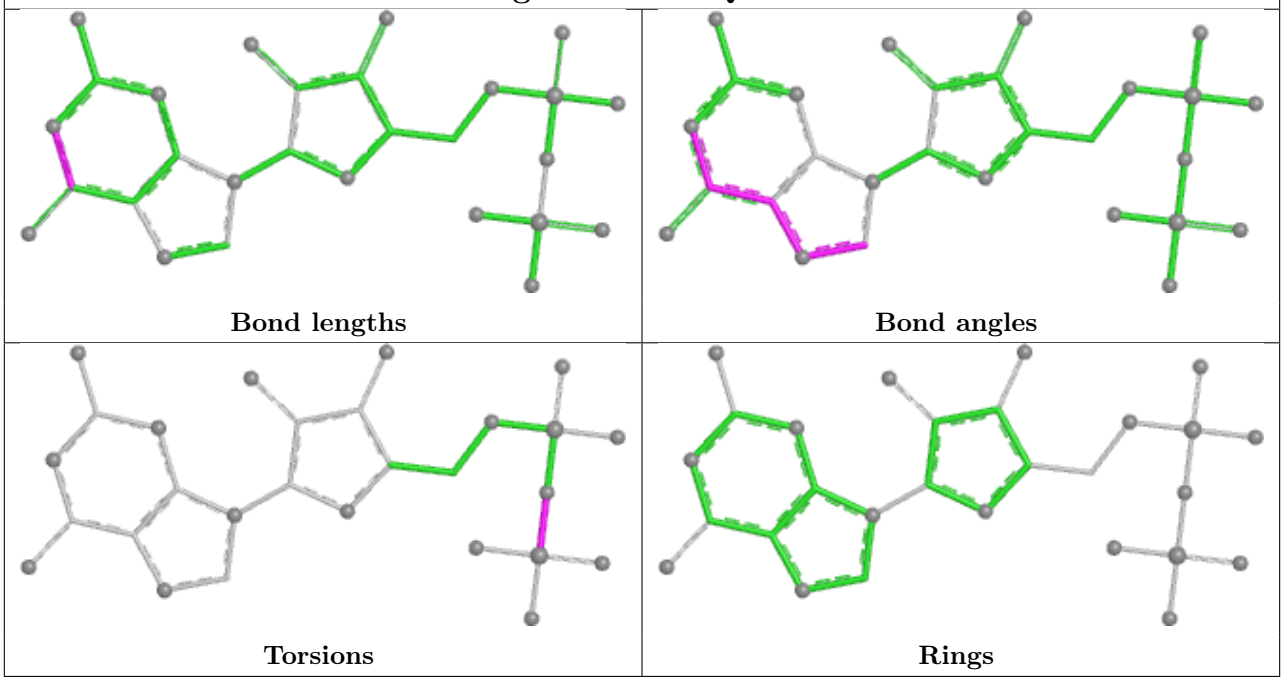



## Ligand GDP 3Q 501



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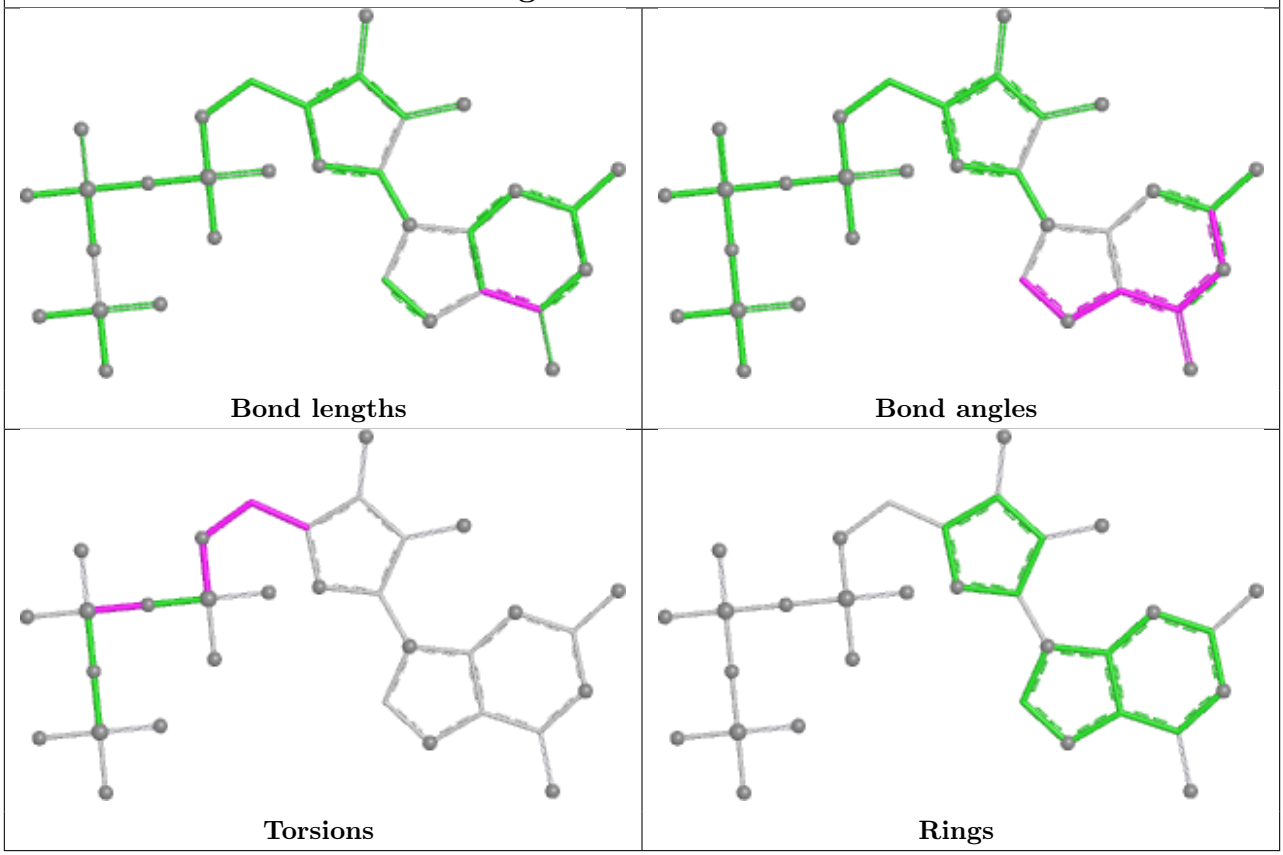


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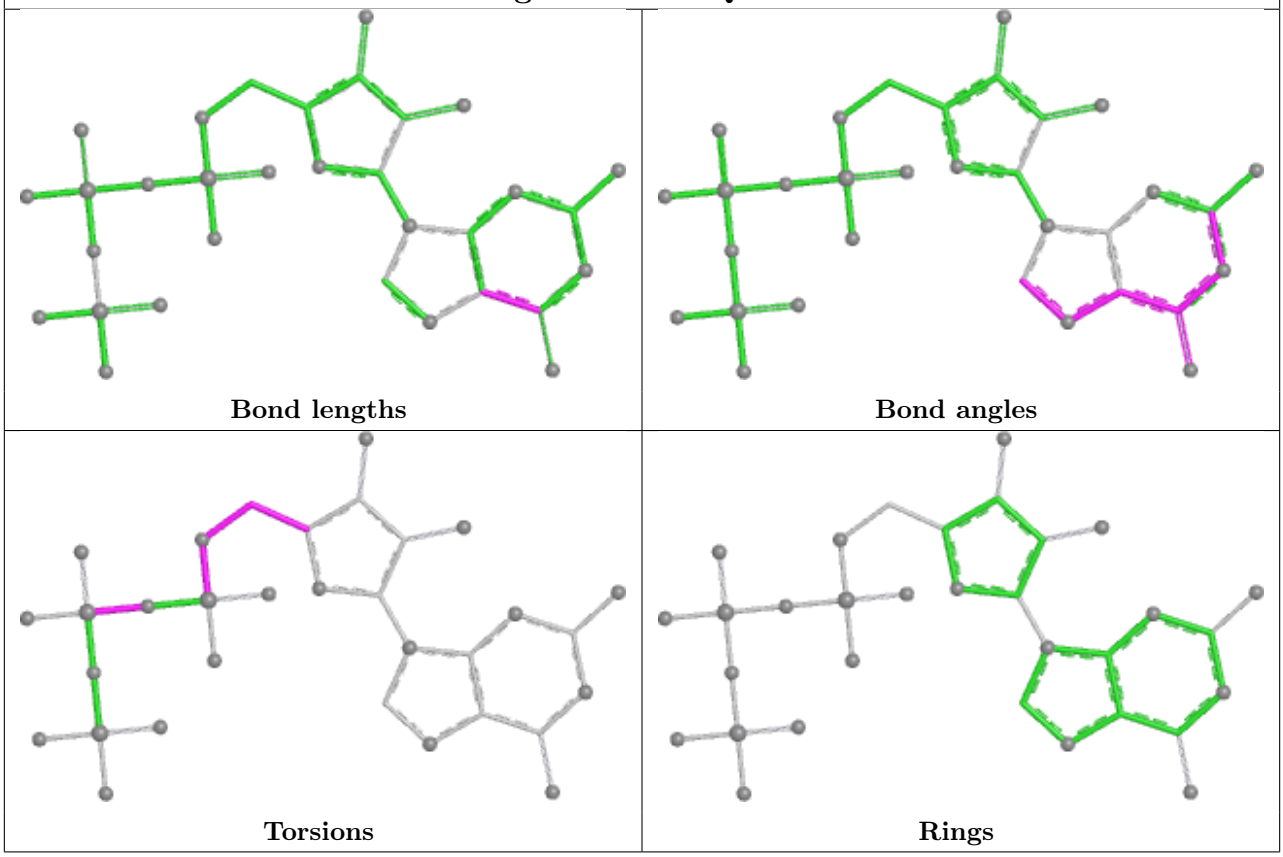

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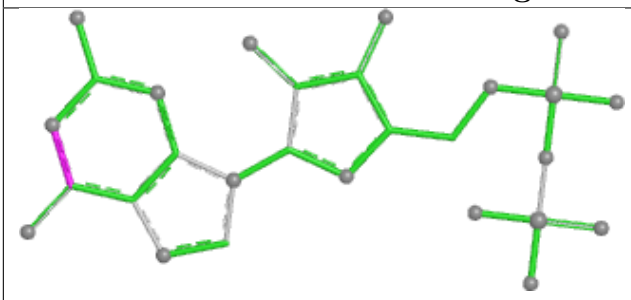
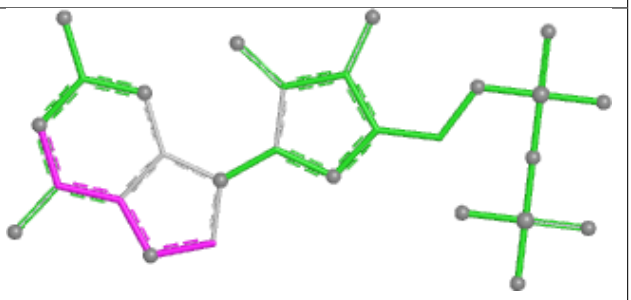
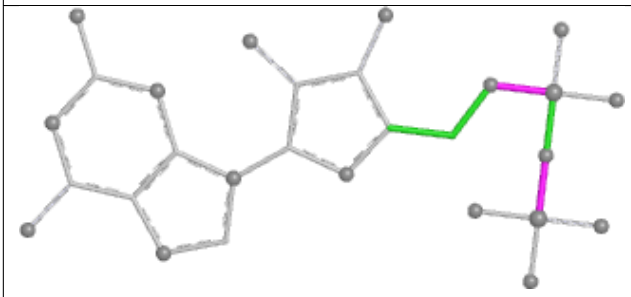
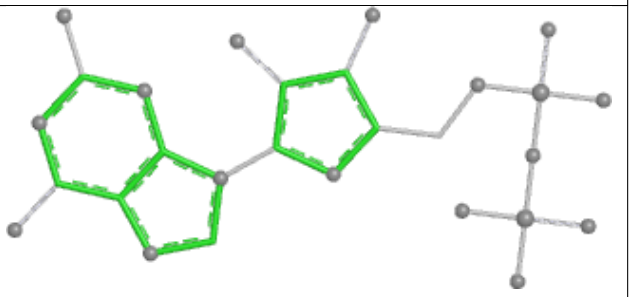
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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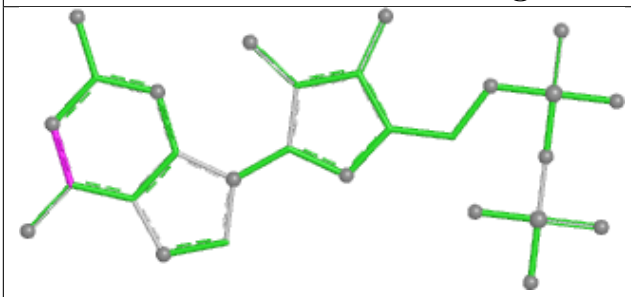
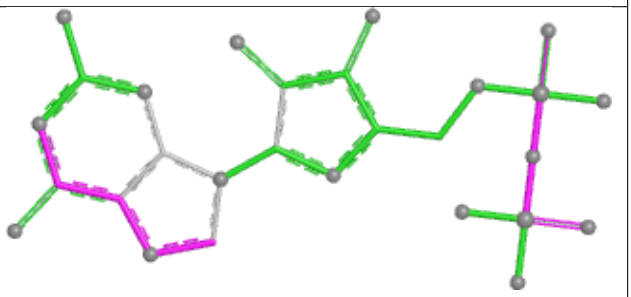
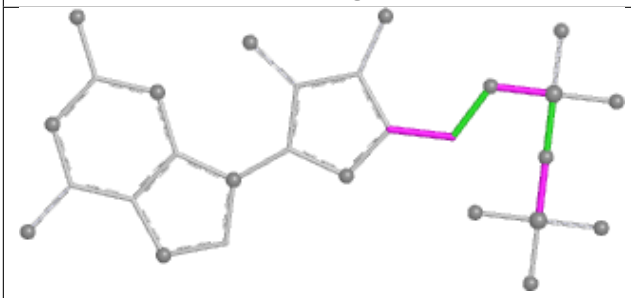
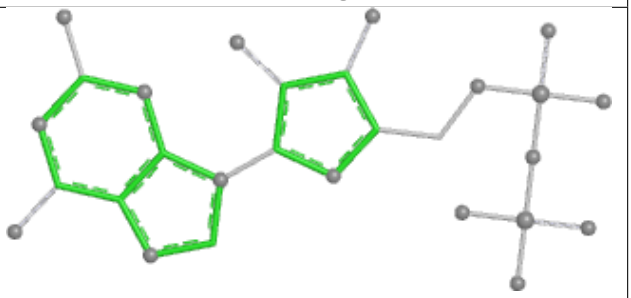
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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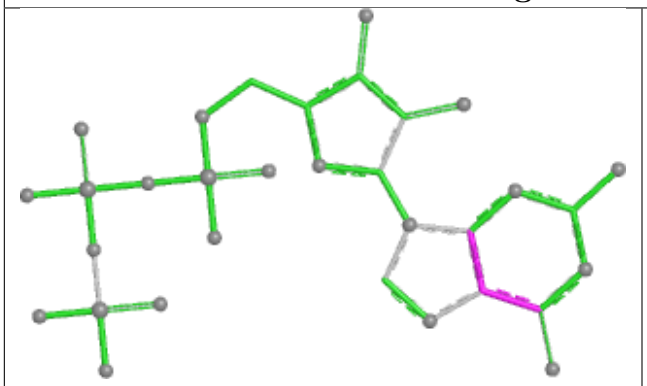

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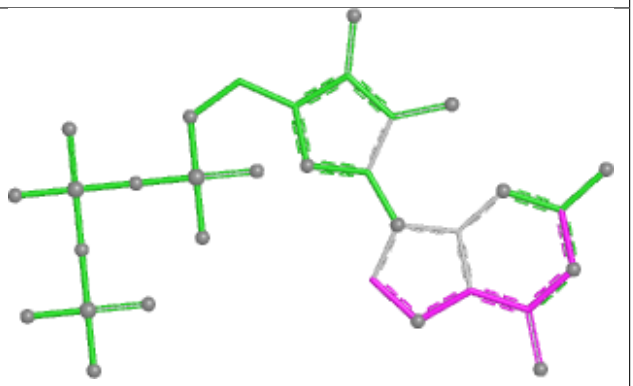

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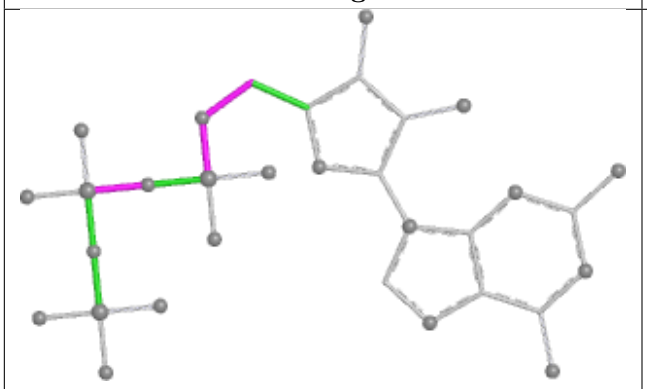

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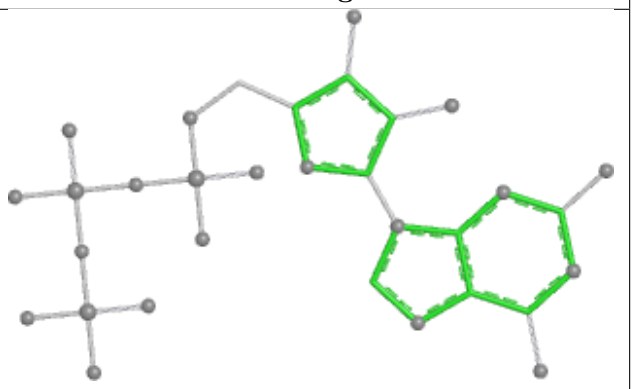

Rings

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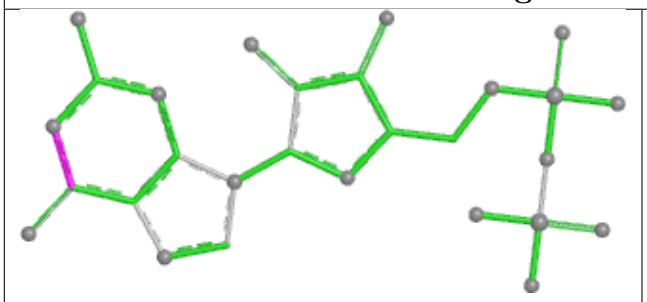

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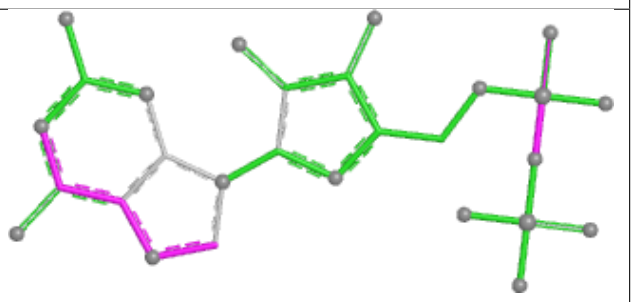

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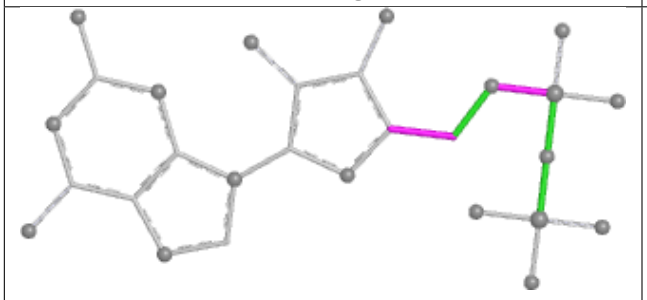

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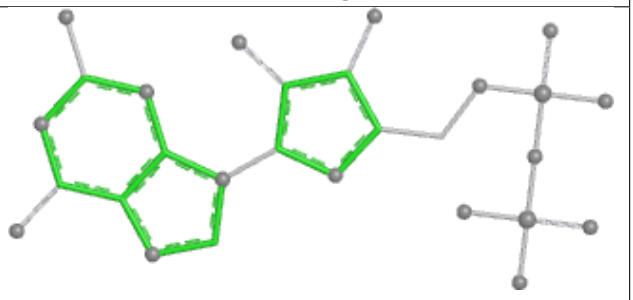

Rings

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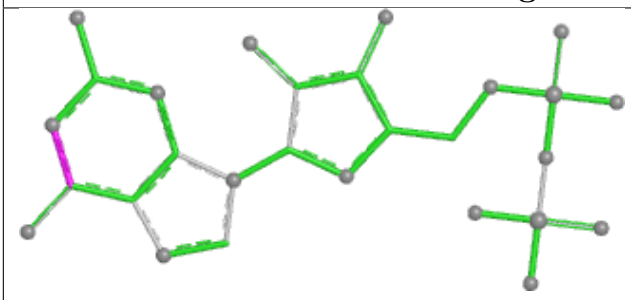

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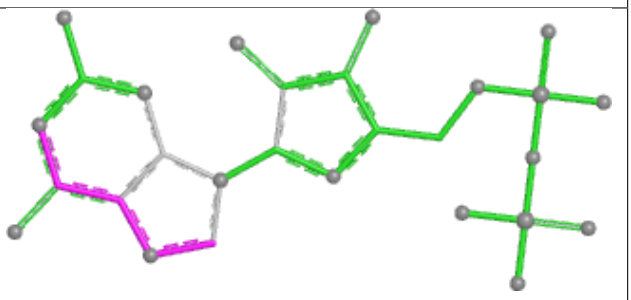

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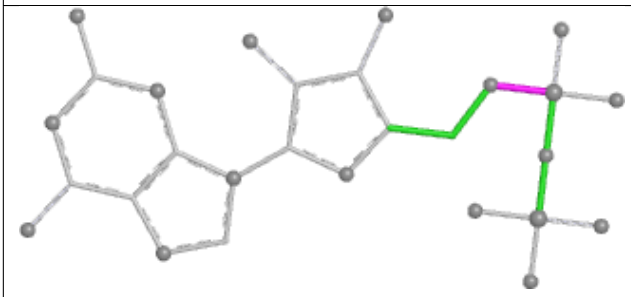

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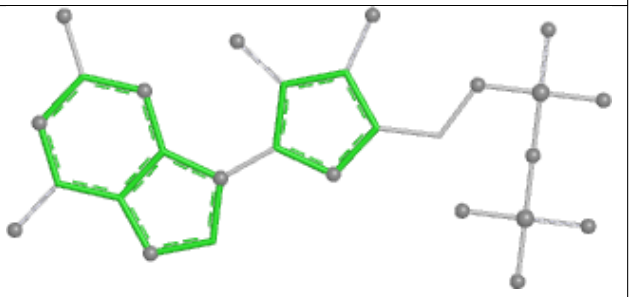

Rings

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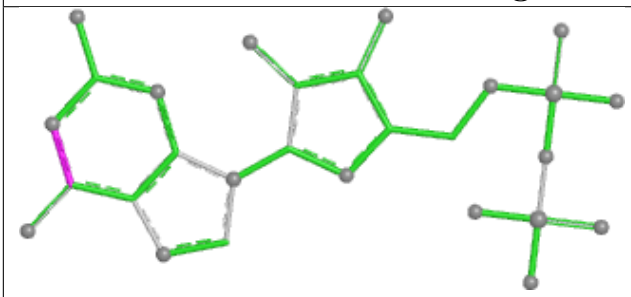

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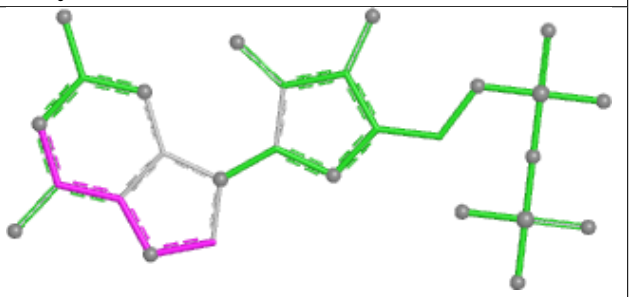

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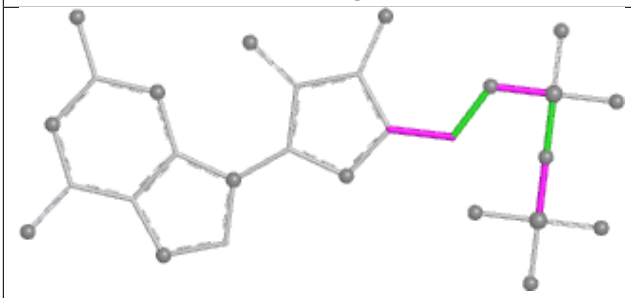

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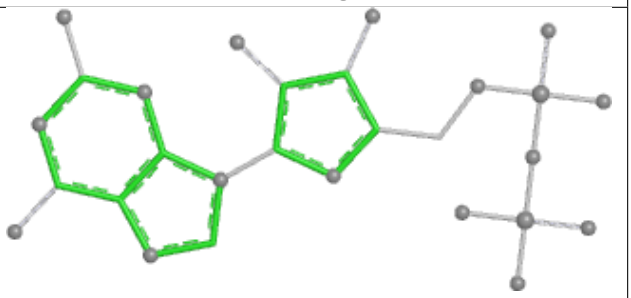

Rings

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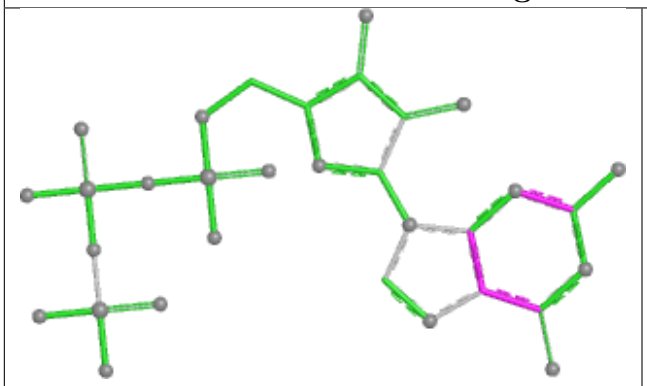

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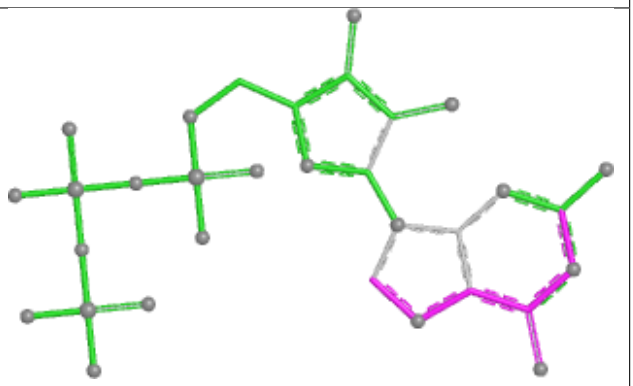

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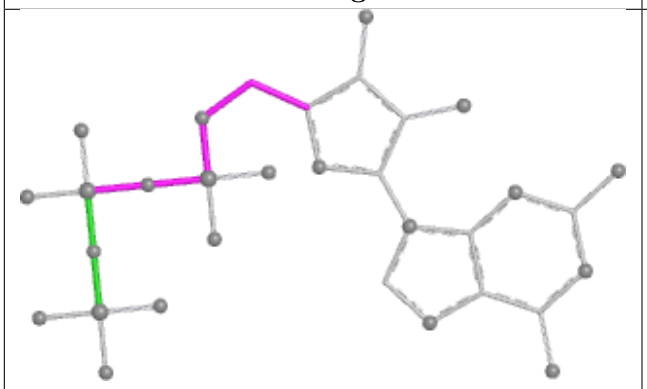

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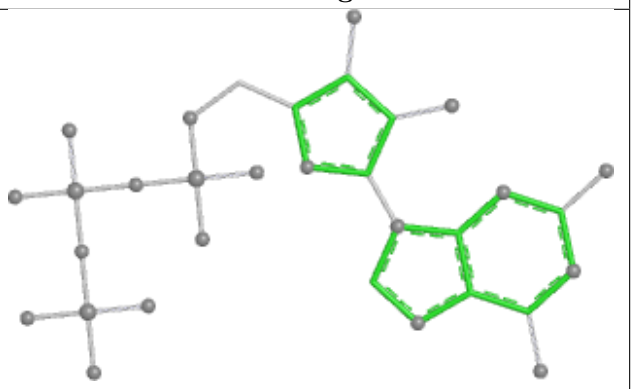

Rings

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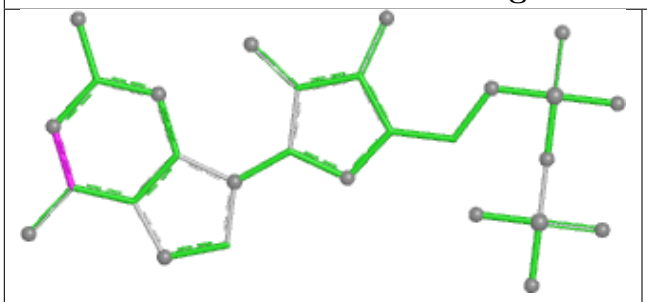

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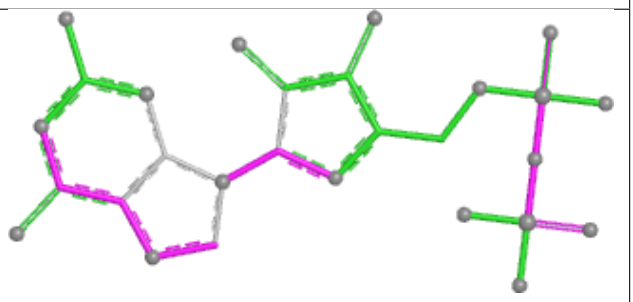

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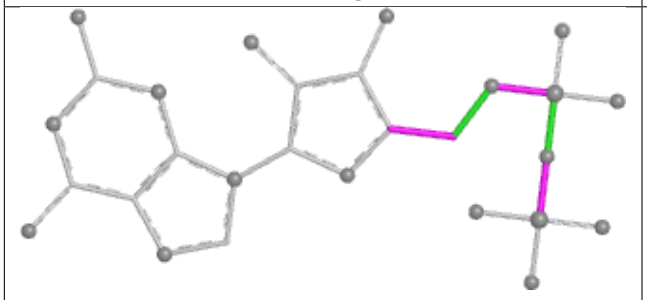

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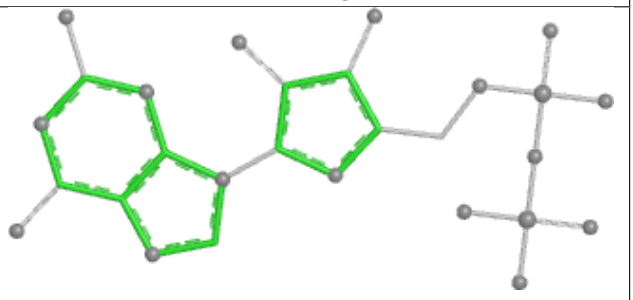

Rings

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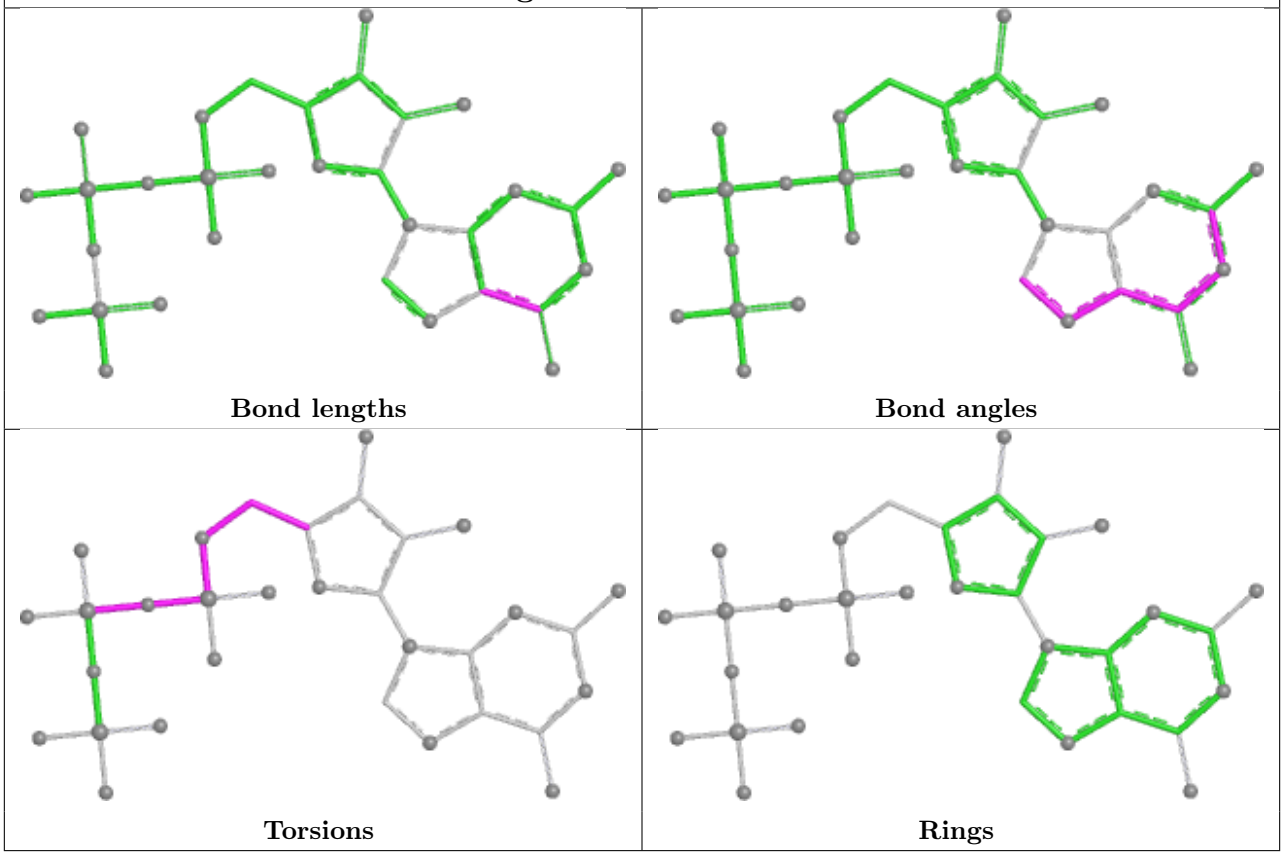


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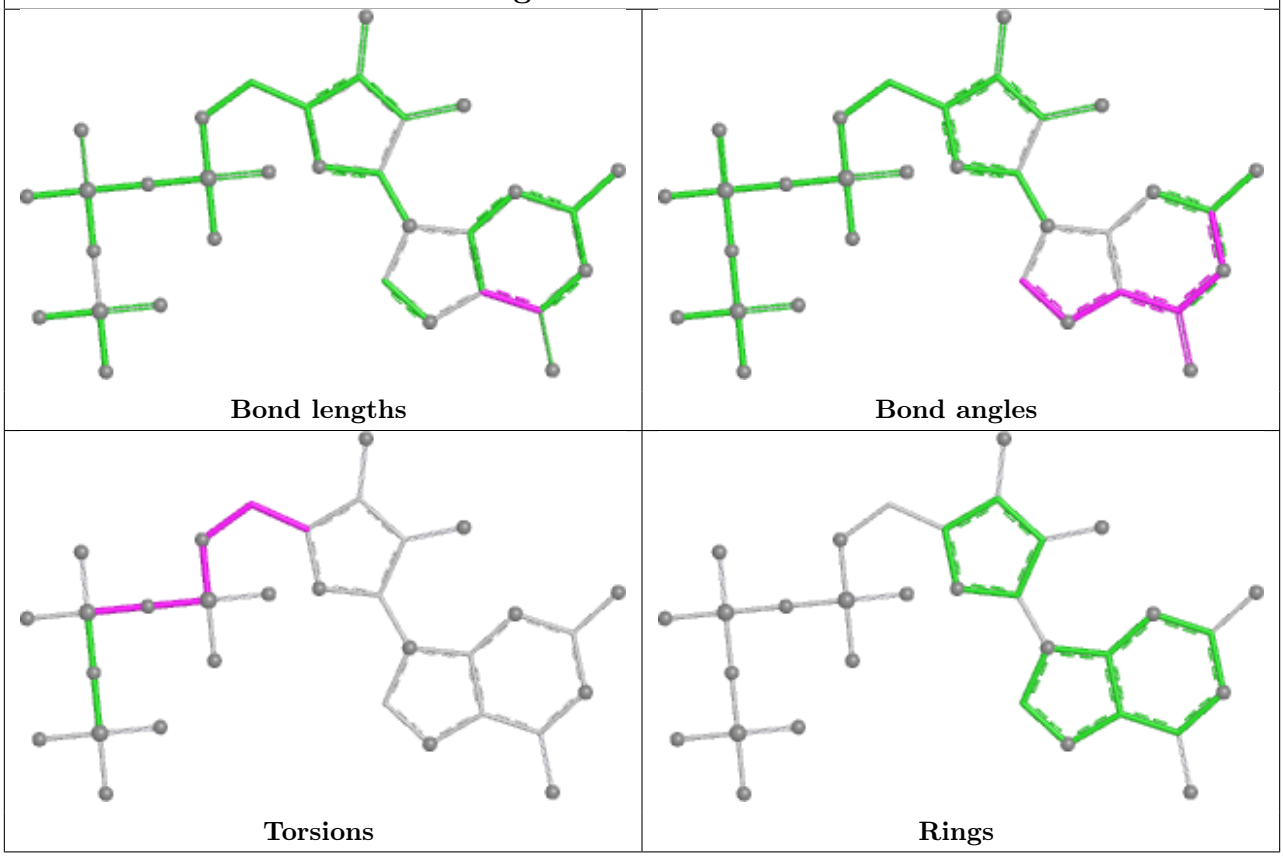

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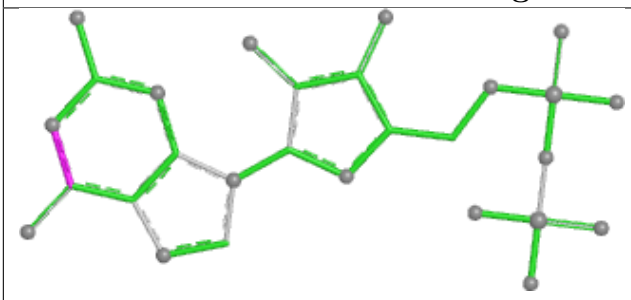
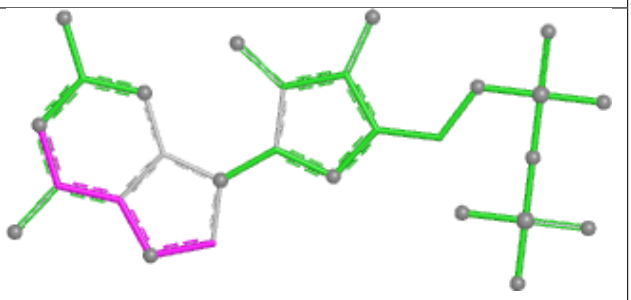
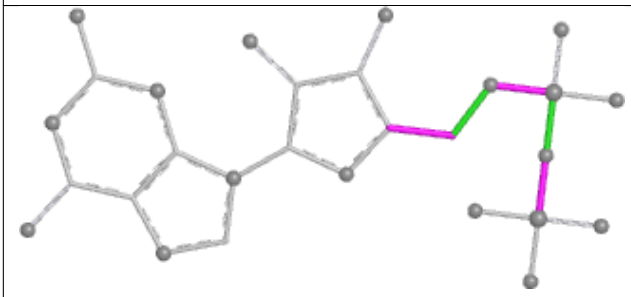
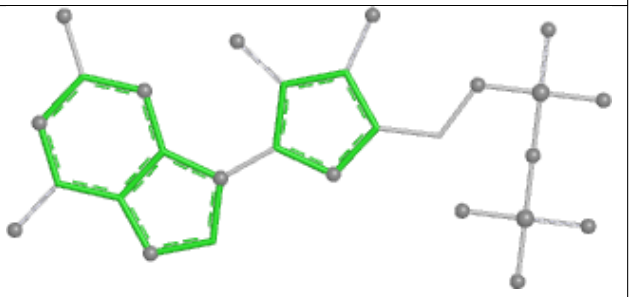
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP C6 501 | |
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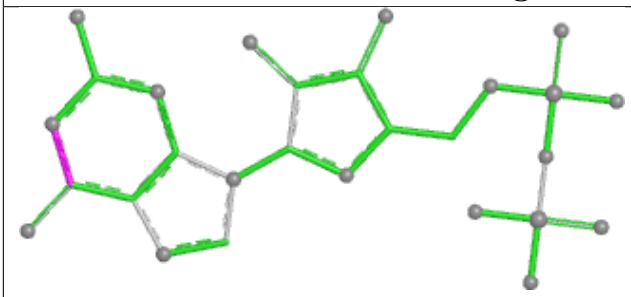
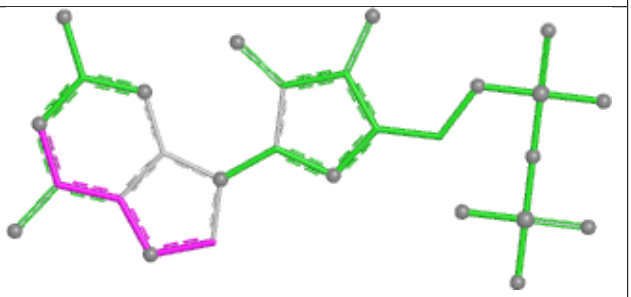
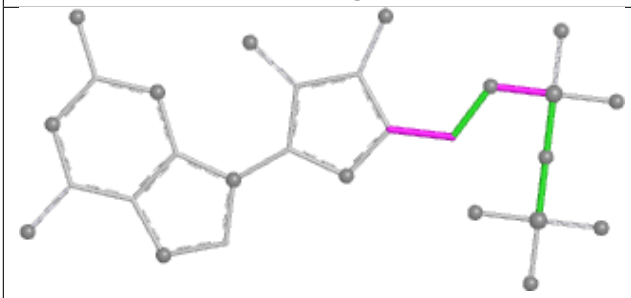
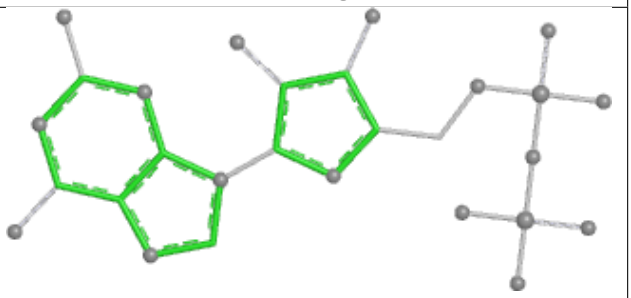
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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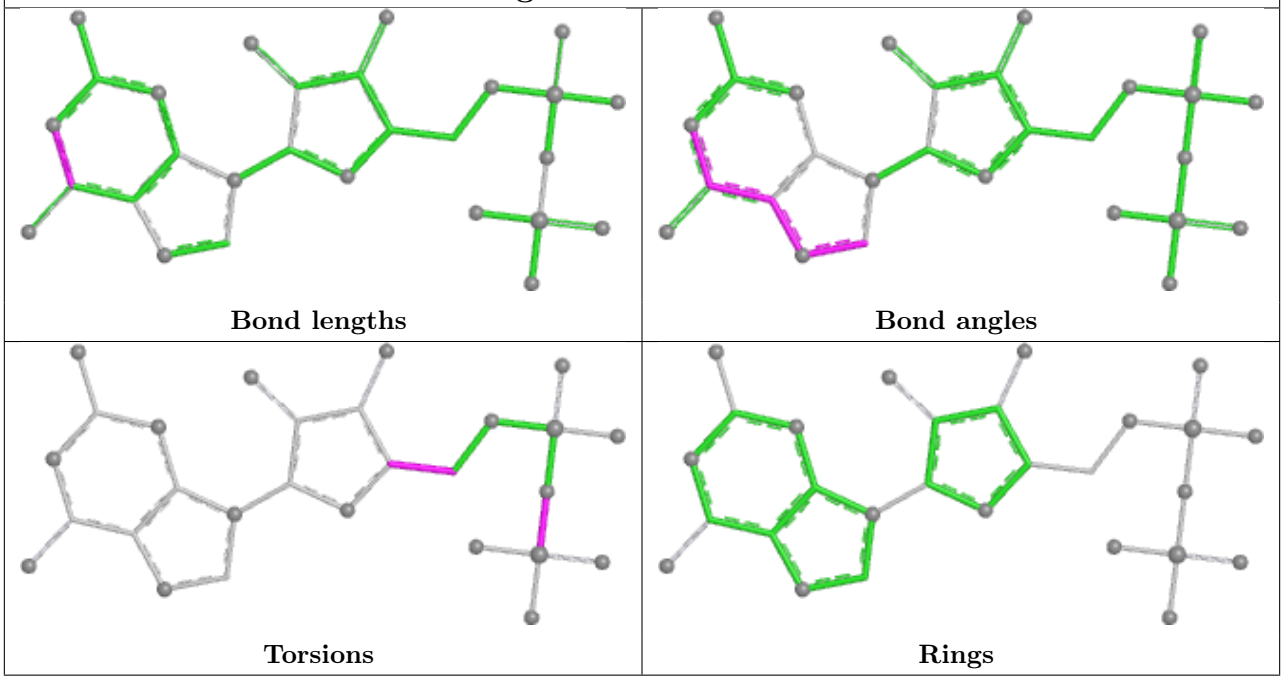


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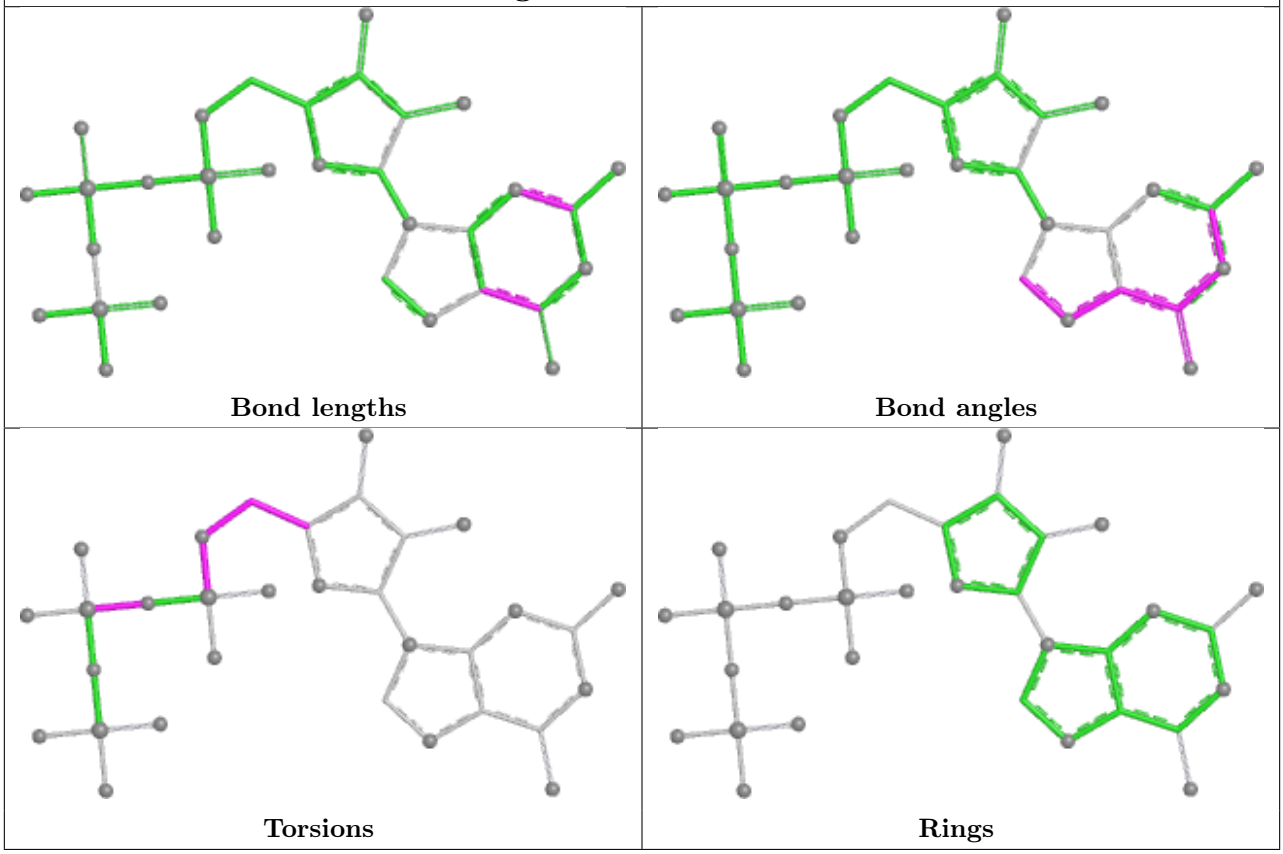

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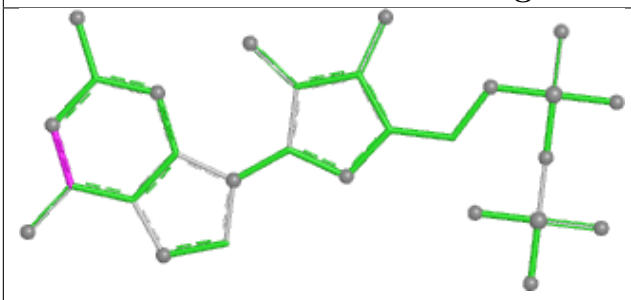
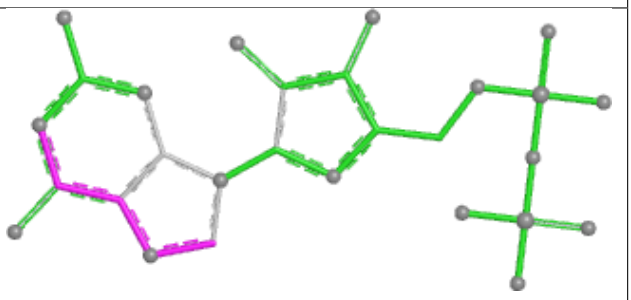
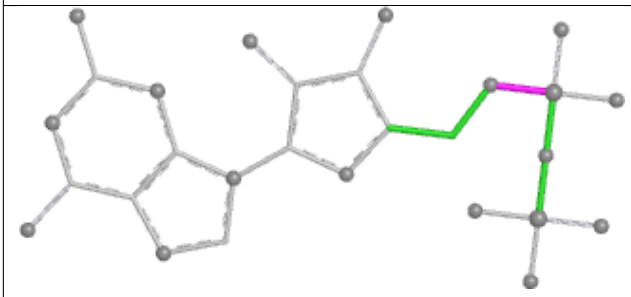


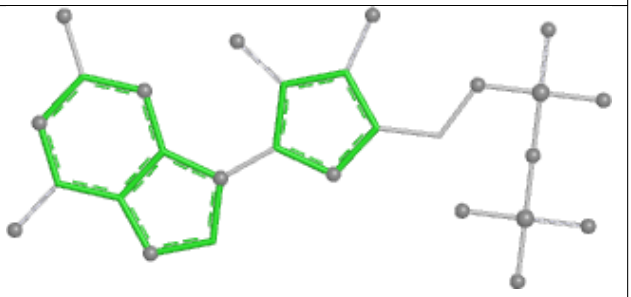
Bond lengths



Bond angles

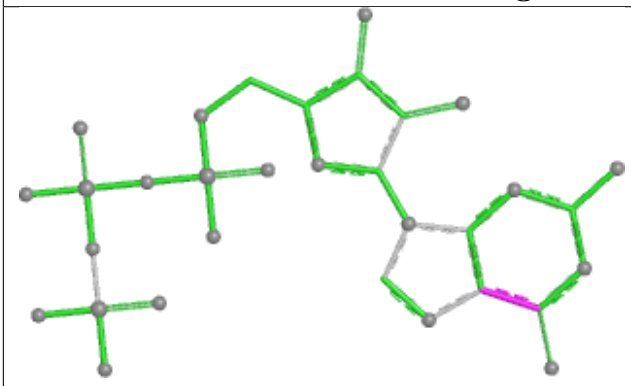


Torsions



Rings

## Ligand GTP E4 501



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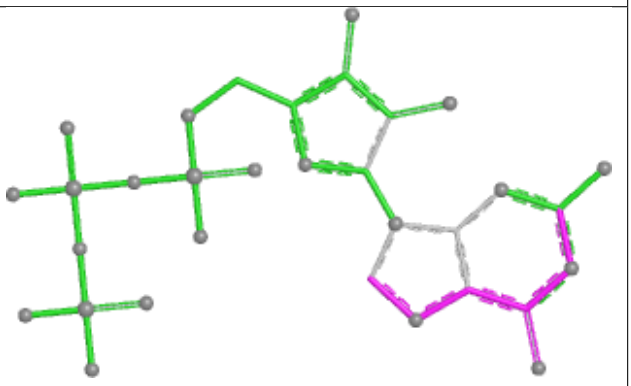
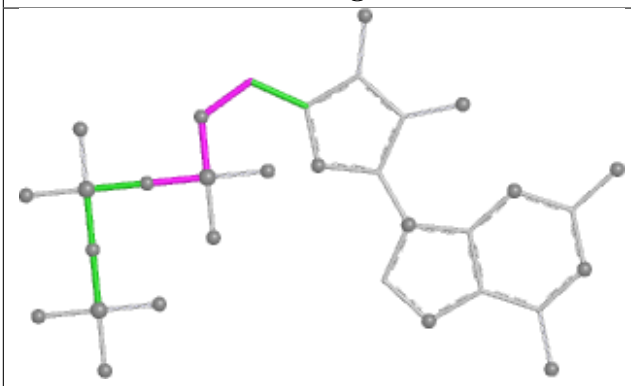


Bond angles



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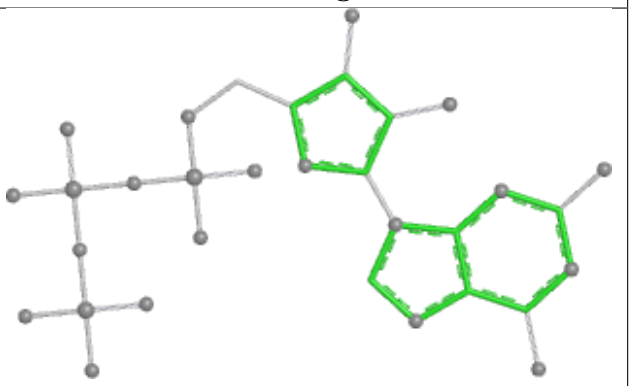

Rings

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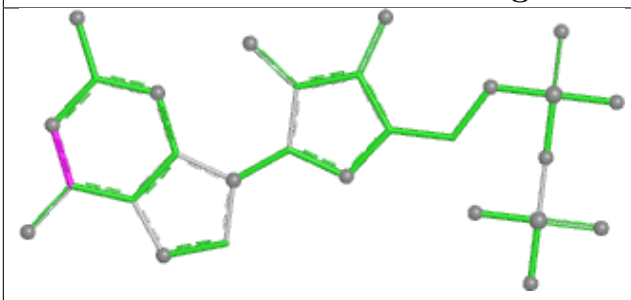

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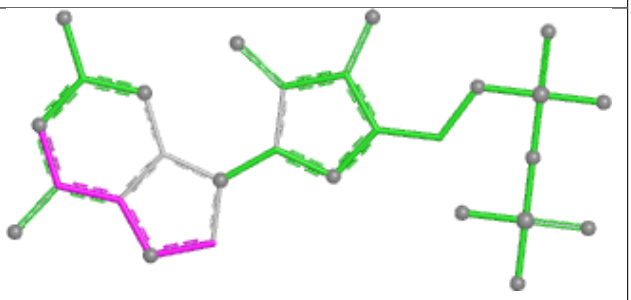
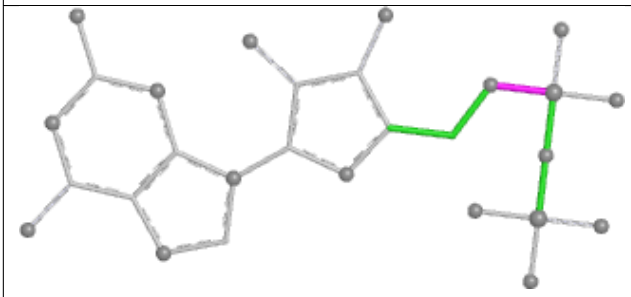
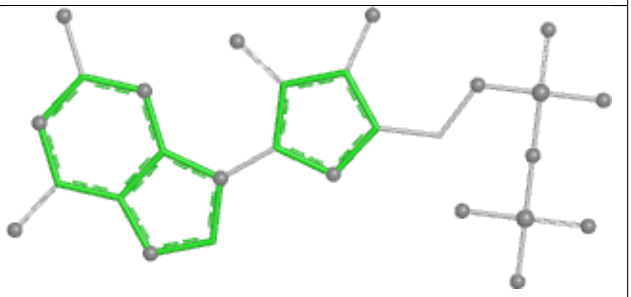


Bond angles

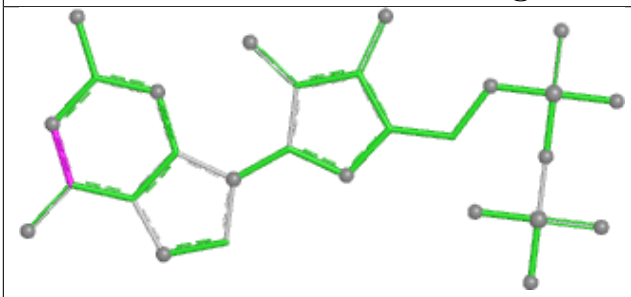


Torsions



Rings

## Ligand GDP R8 502



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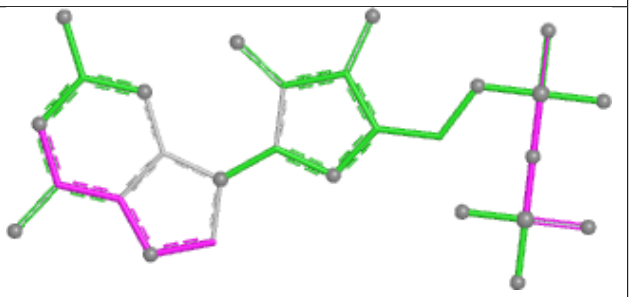

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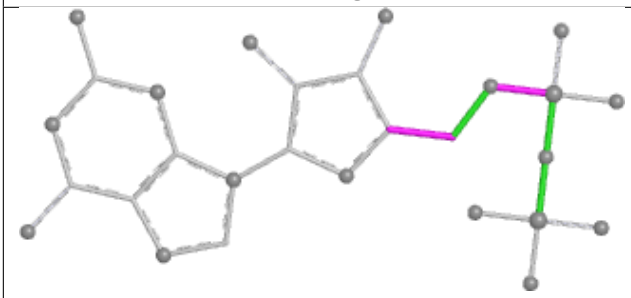

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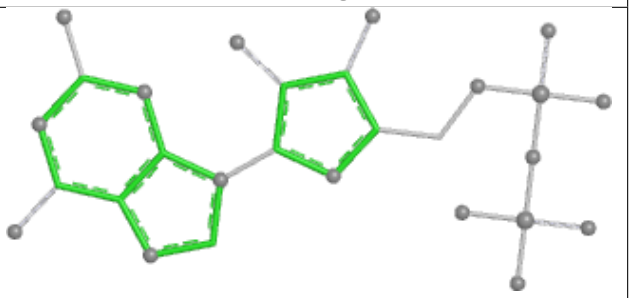

Rings

| Ligand GDP V6 501 | |
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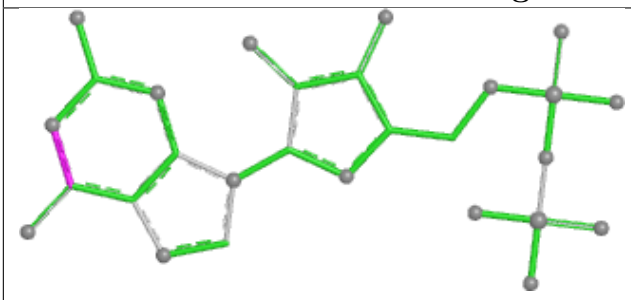
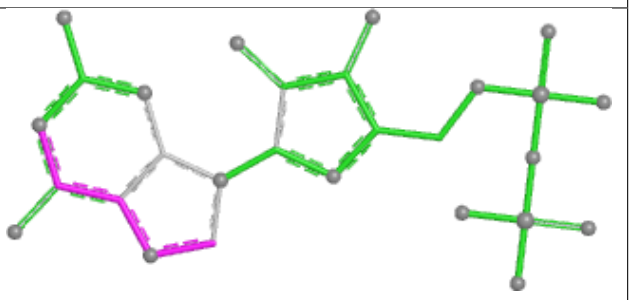
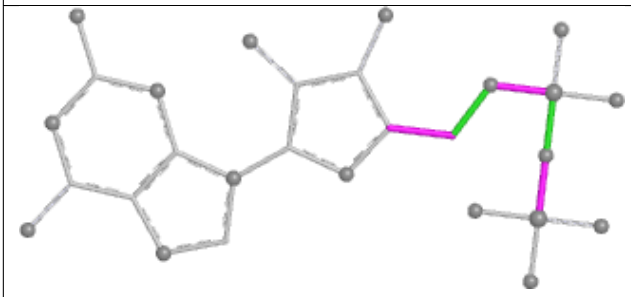
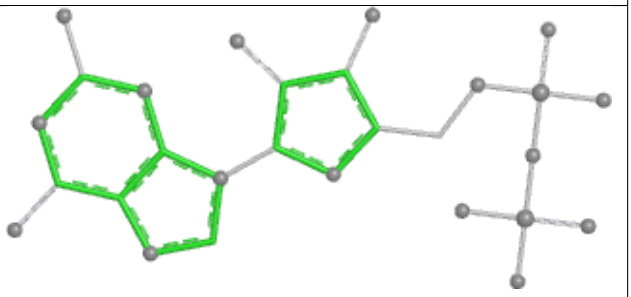
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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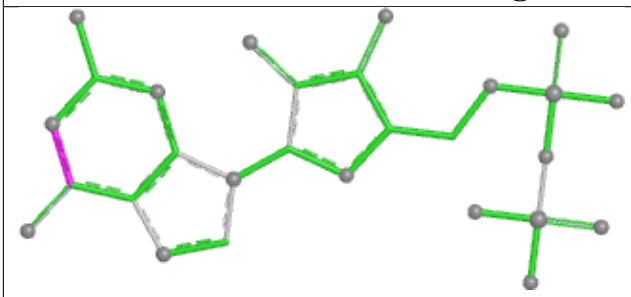
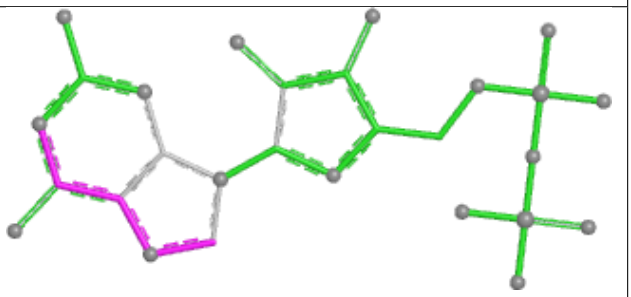
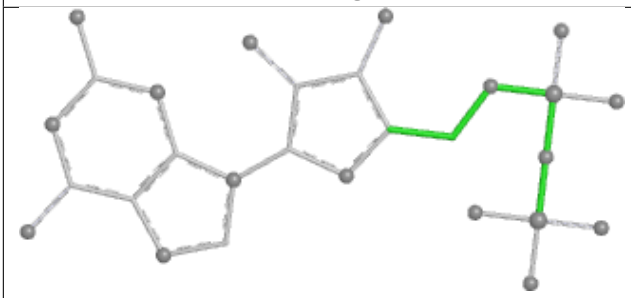
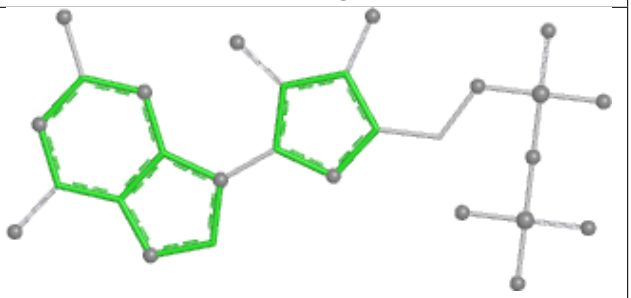
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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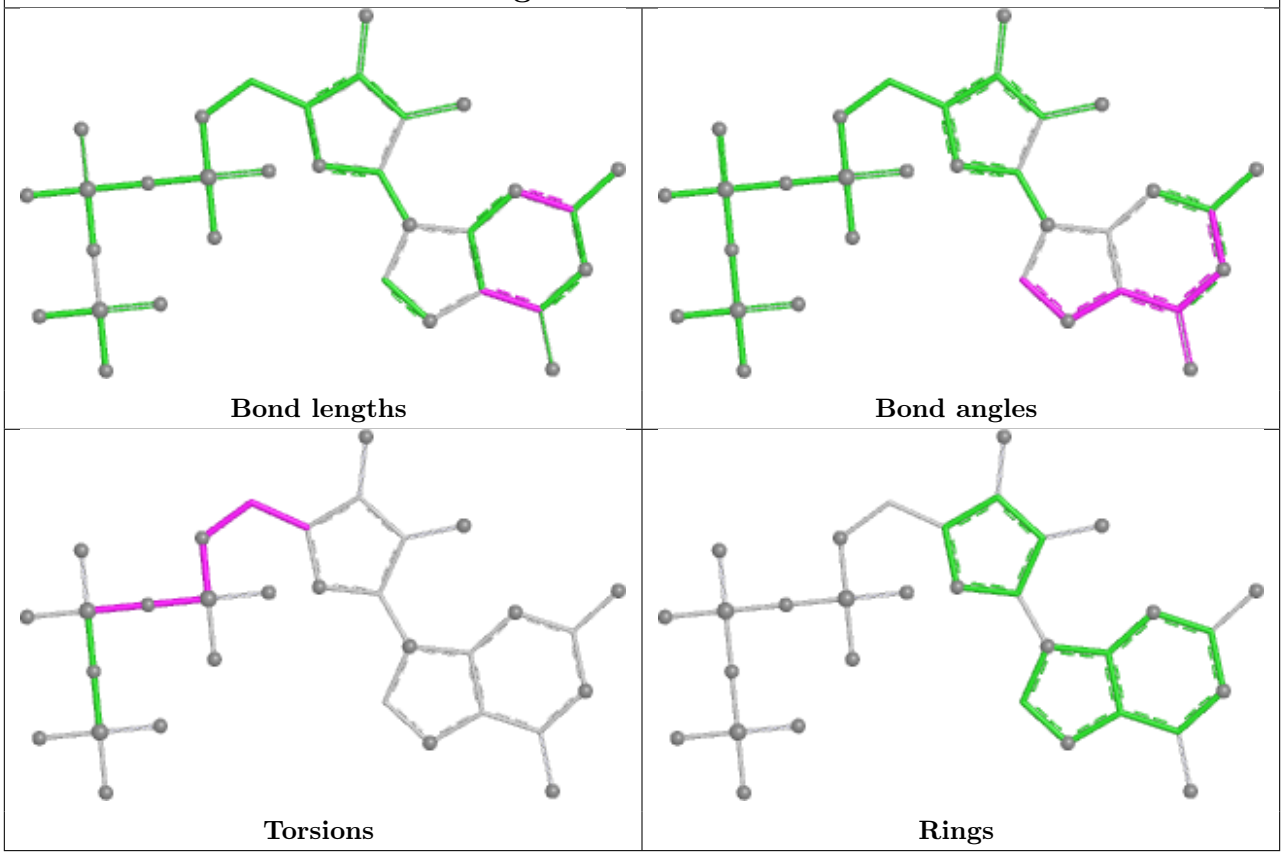


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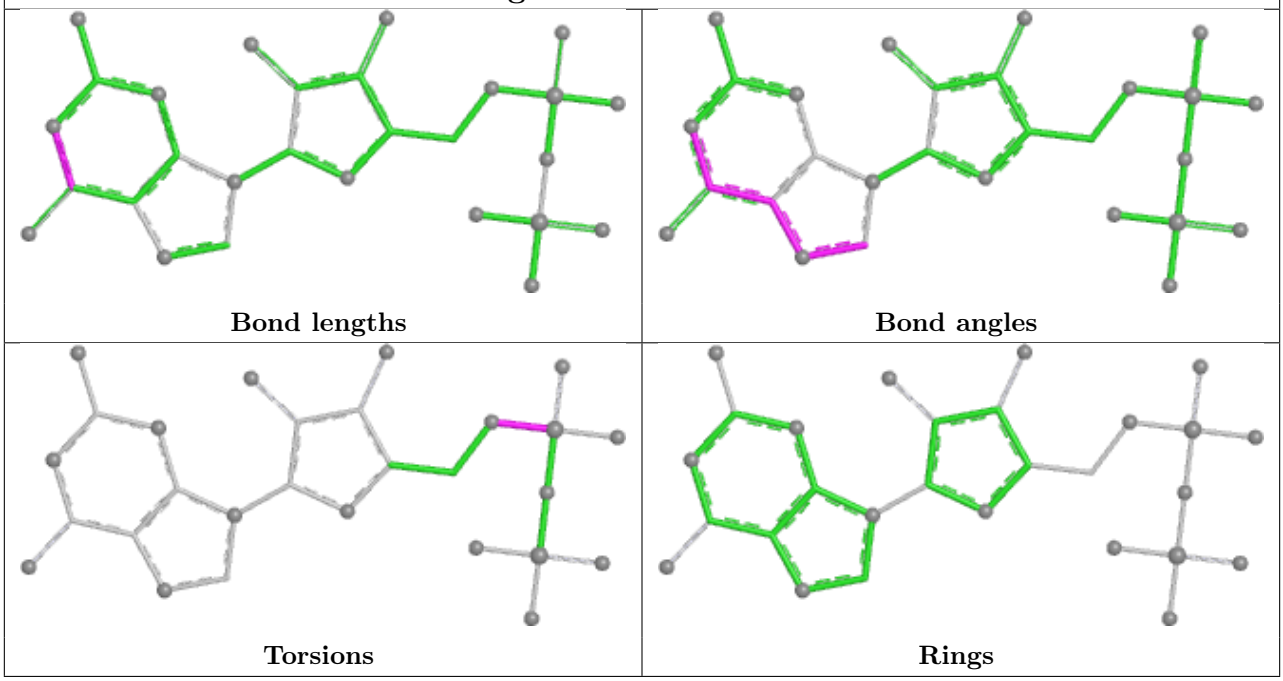

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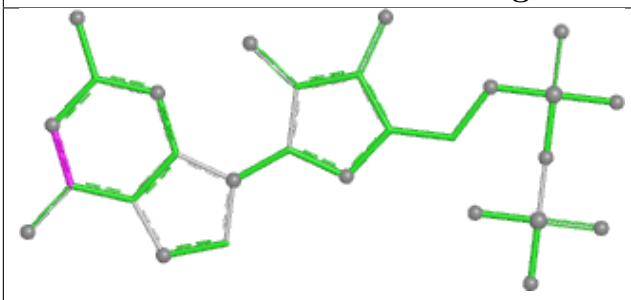
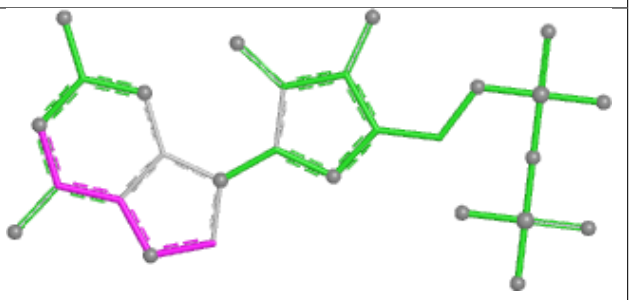


Bond lengths



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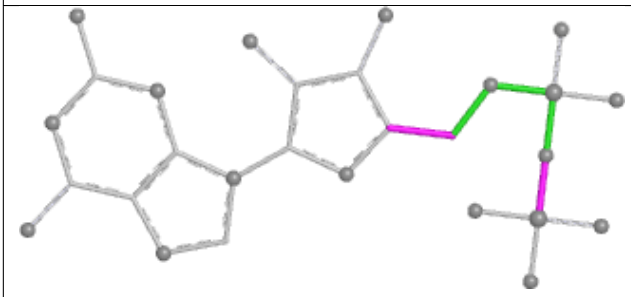
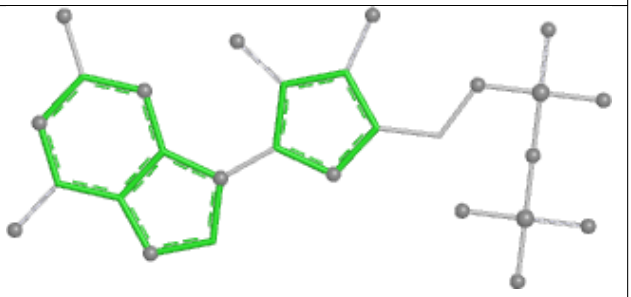
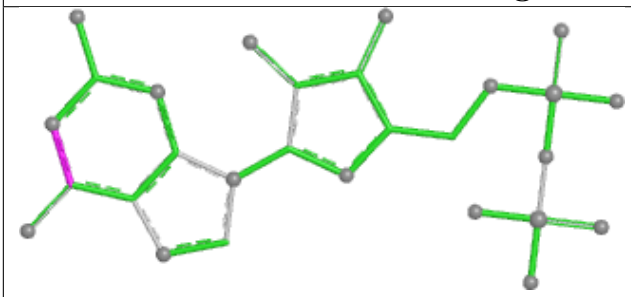


Torsions



Rings

## Ligand GDP E6 502



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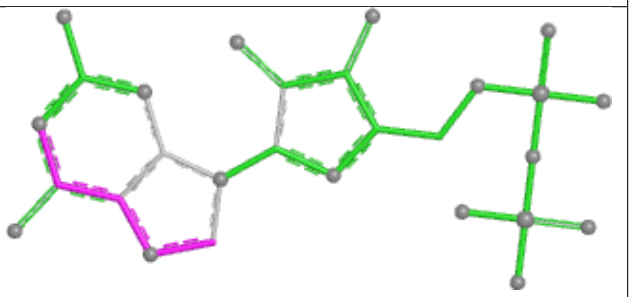

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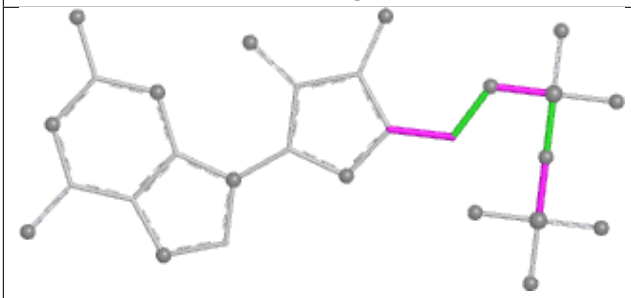

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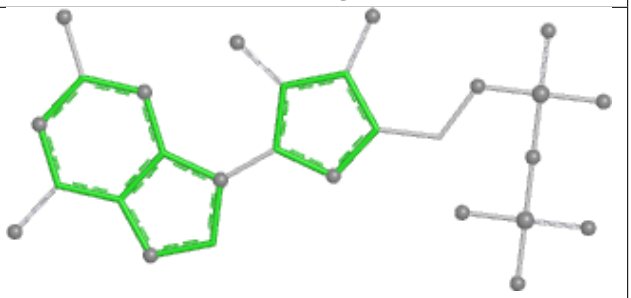
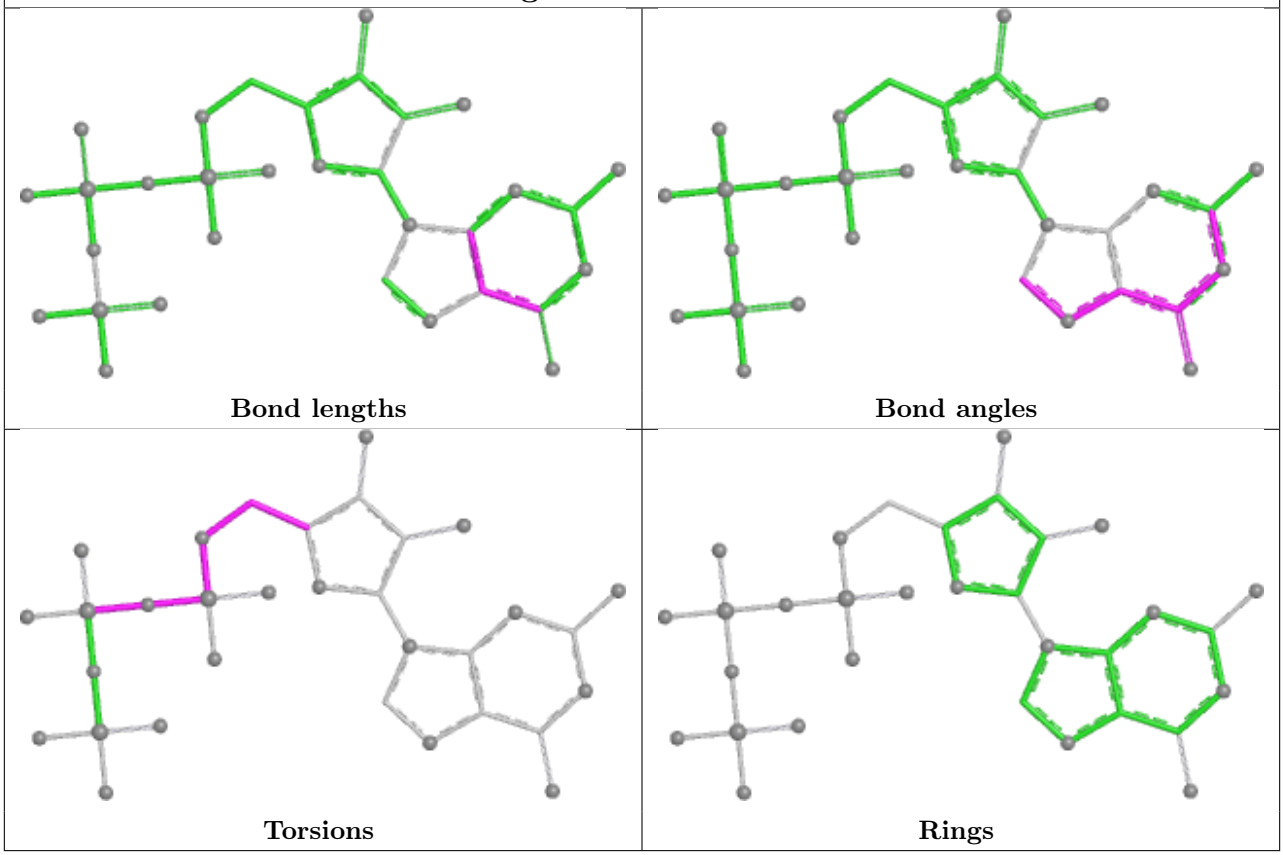


Rings

## Ligand GTP I1 501

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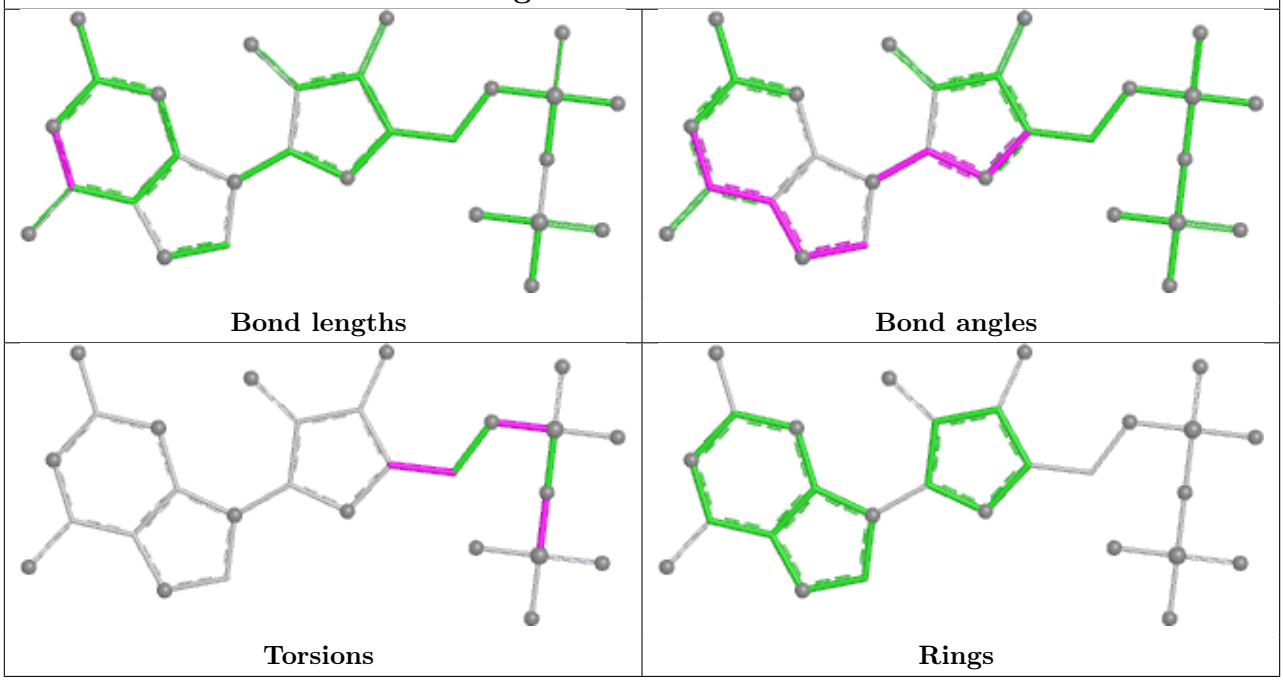

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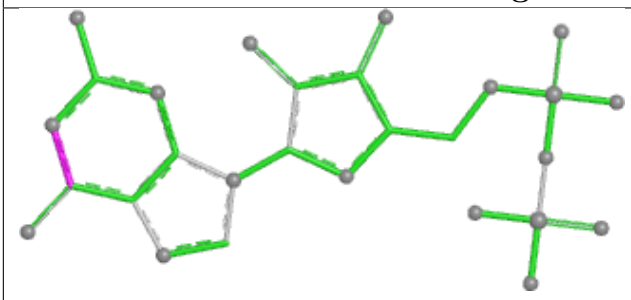

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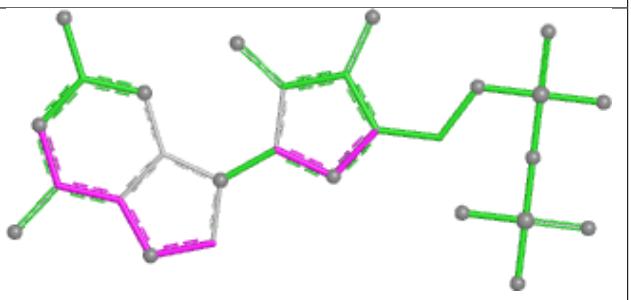

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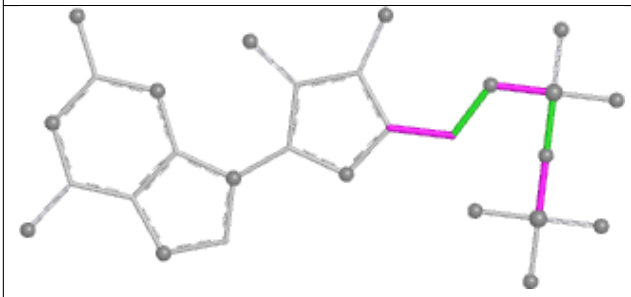

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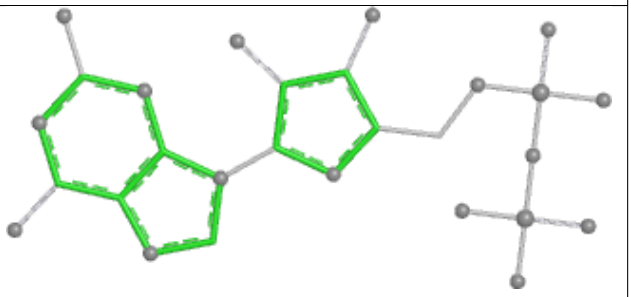
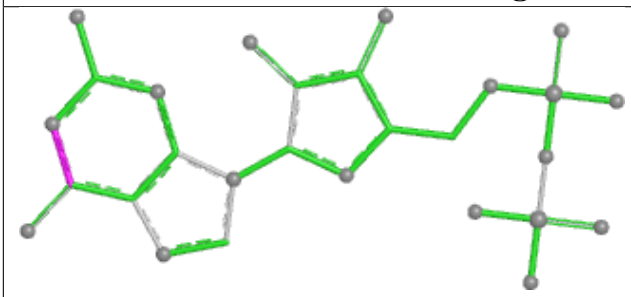


Rings

## Ligand GDP 1G 502



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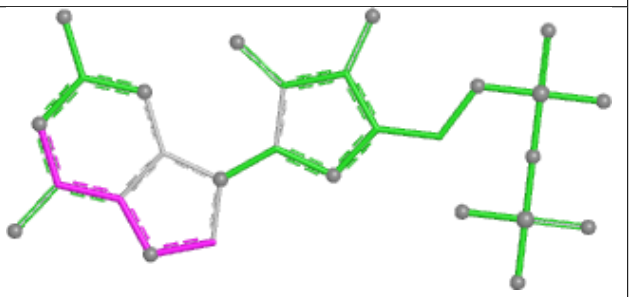

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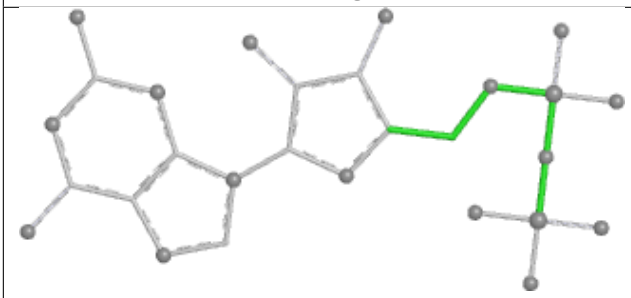

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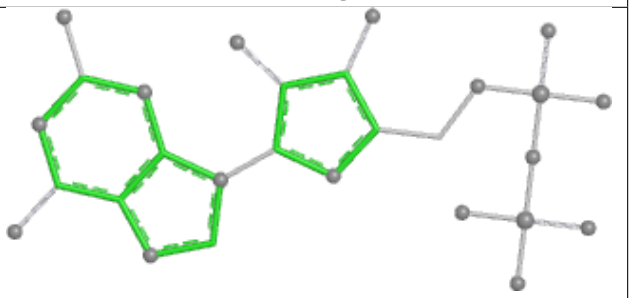
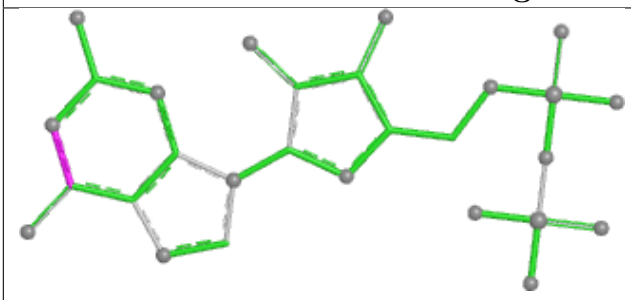


Rings

## Ligand GDP P8 502



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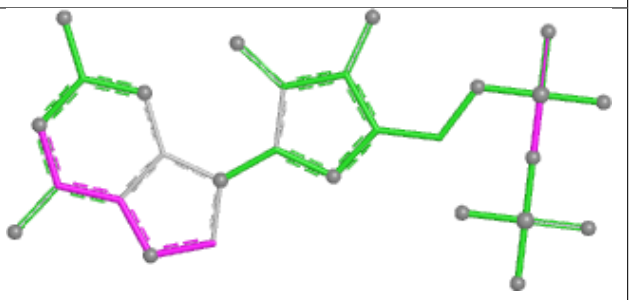

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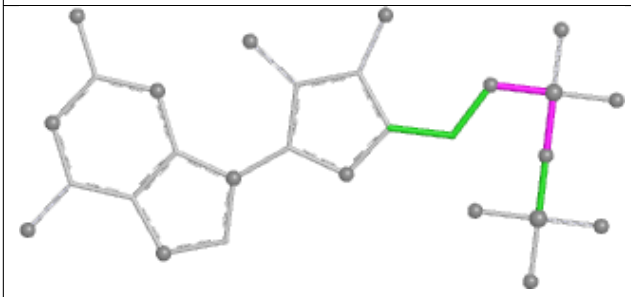

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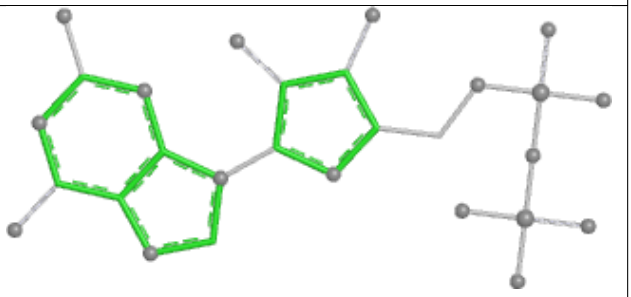
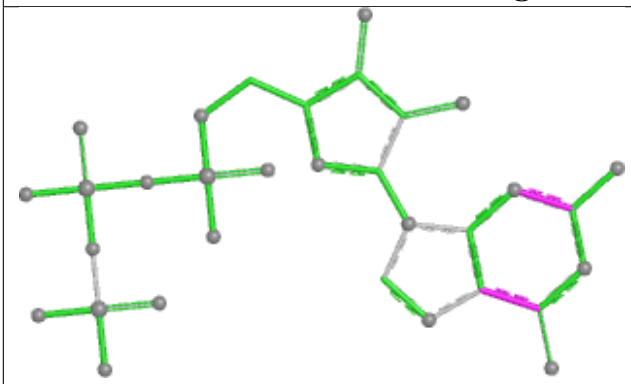


Rings

## Ligand GTP U2 501



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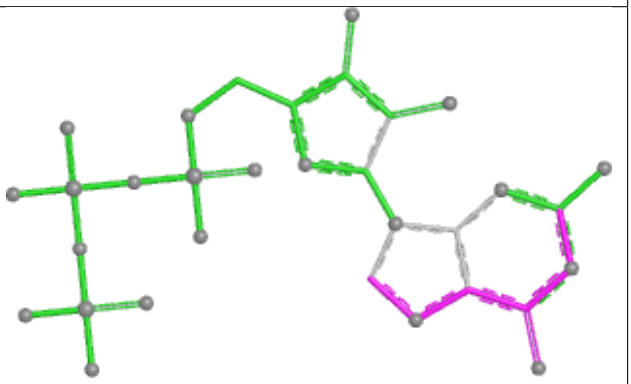

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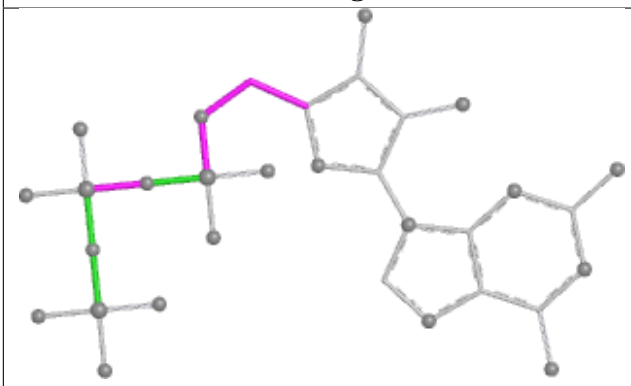

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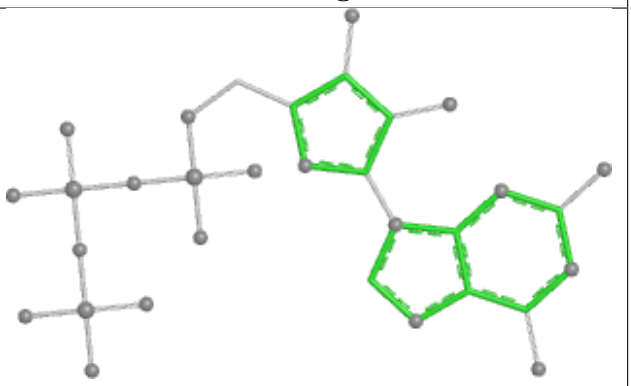

Rings

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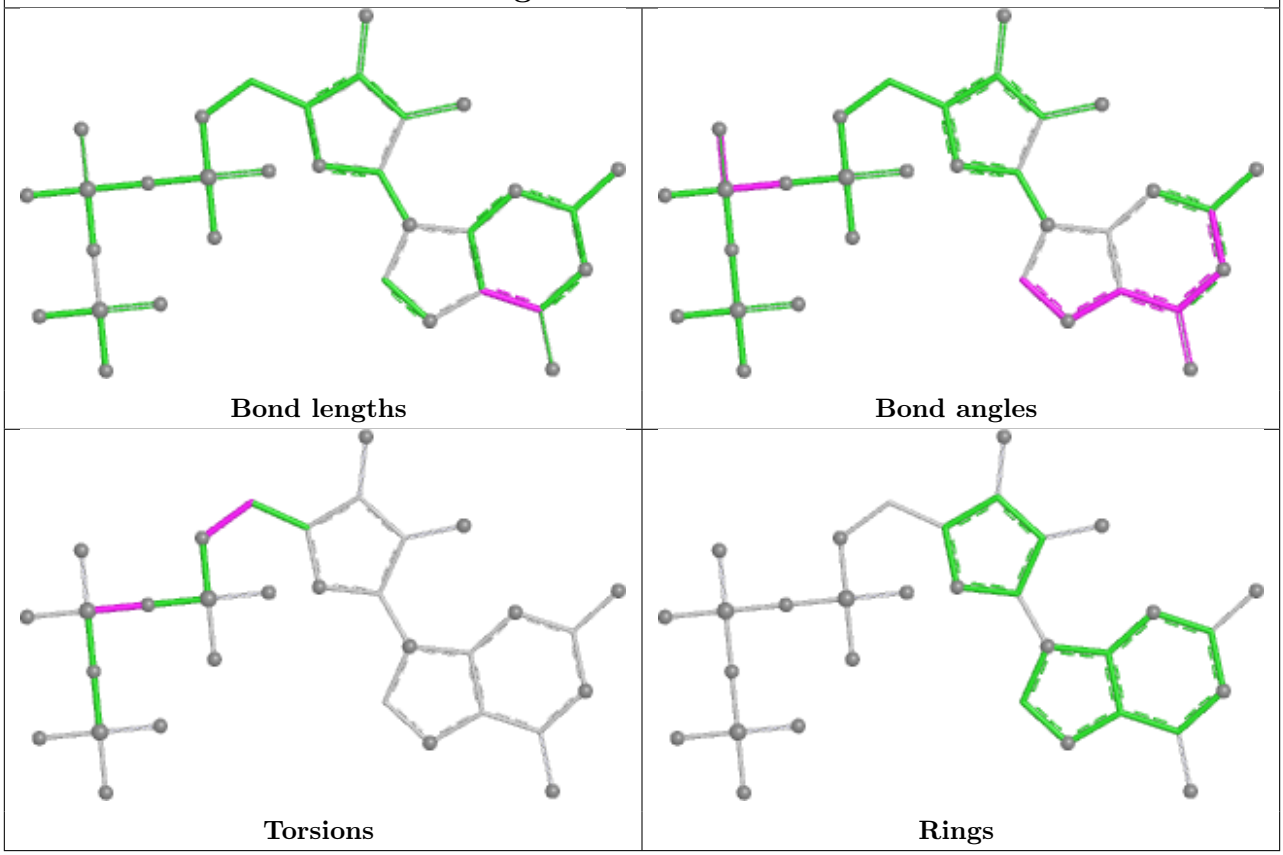


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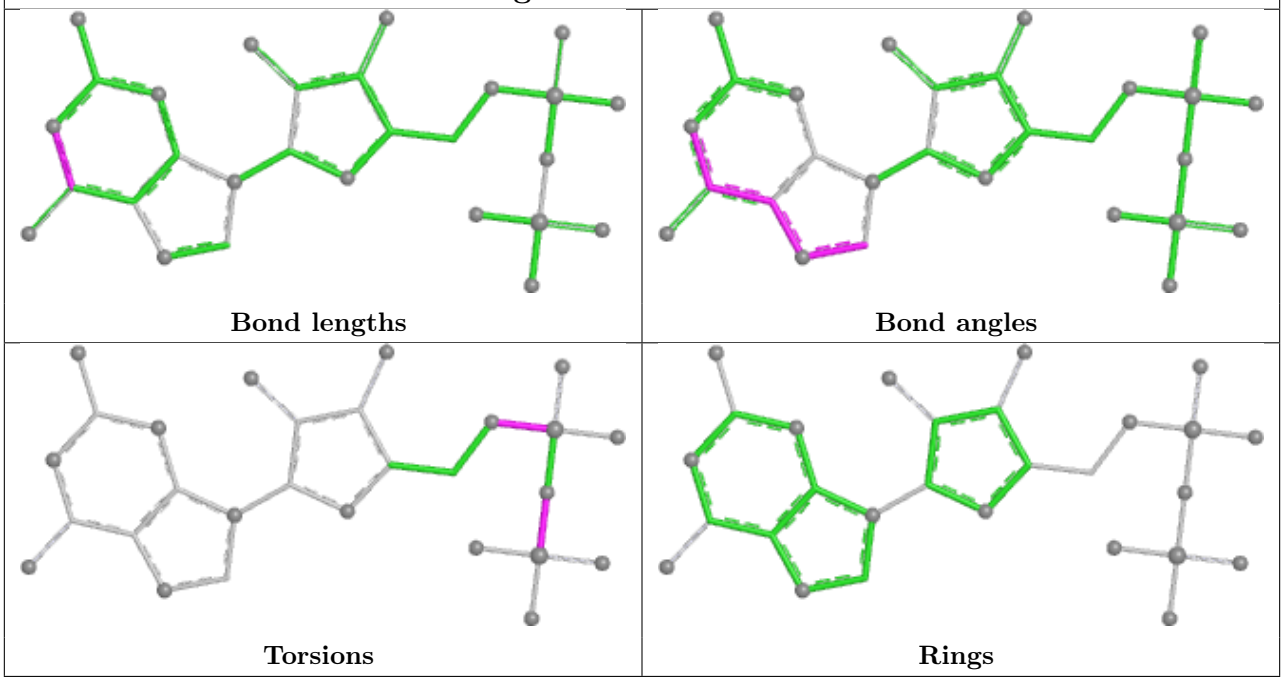

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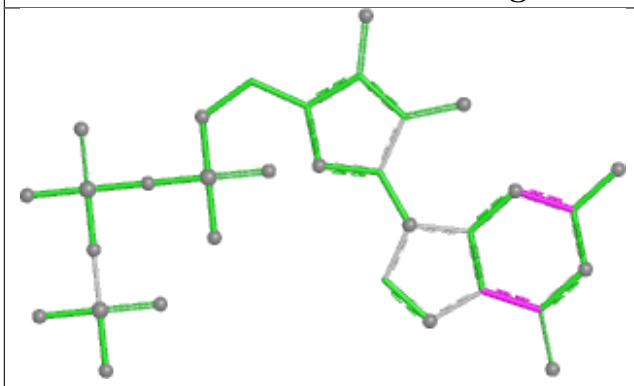

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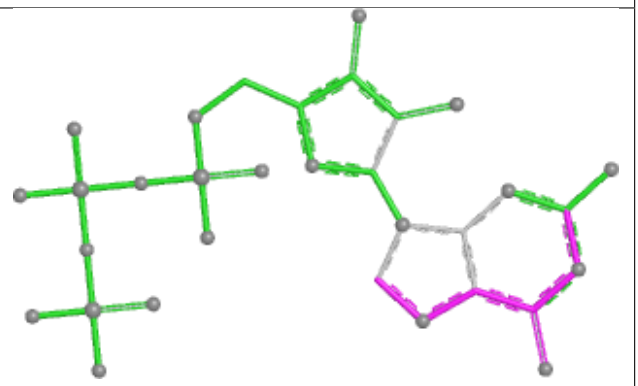

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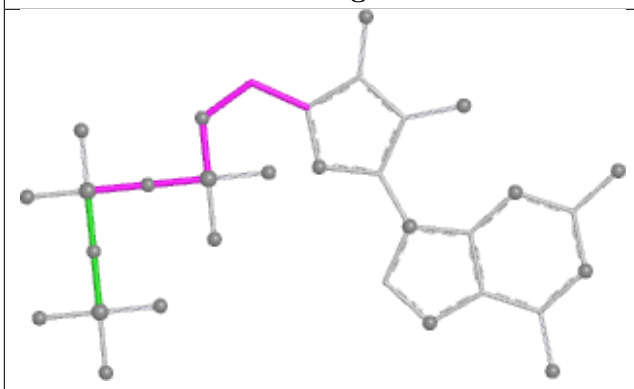

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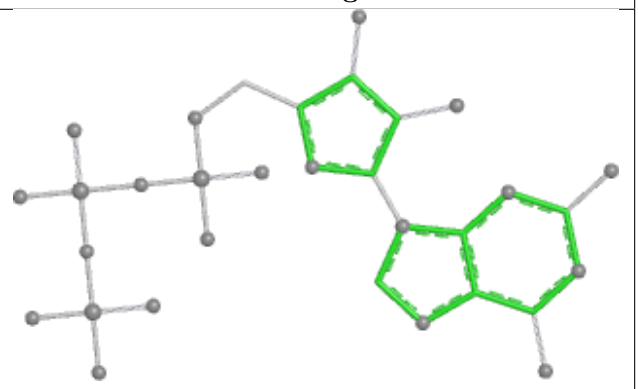

Rings

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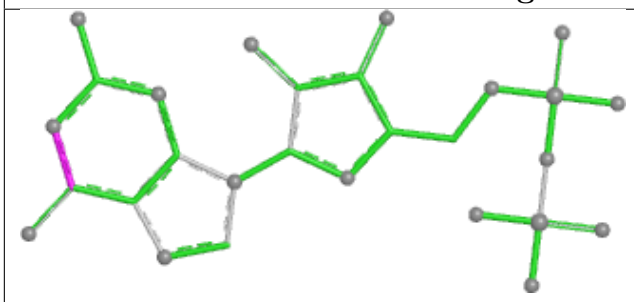

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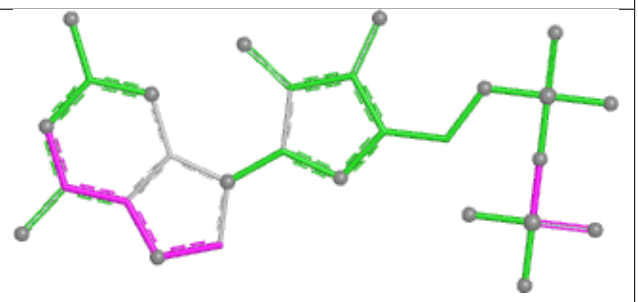
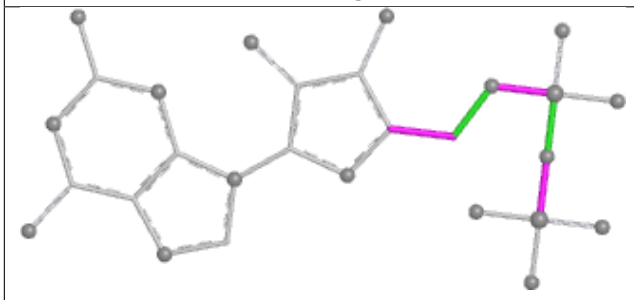


Bond angles



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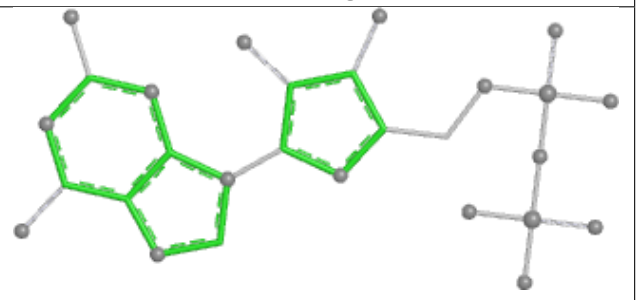

Rings

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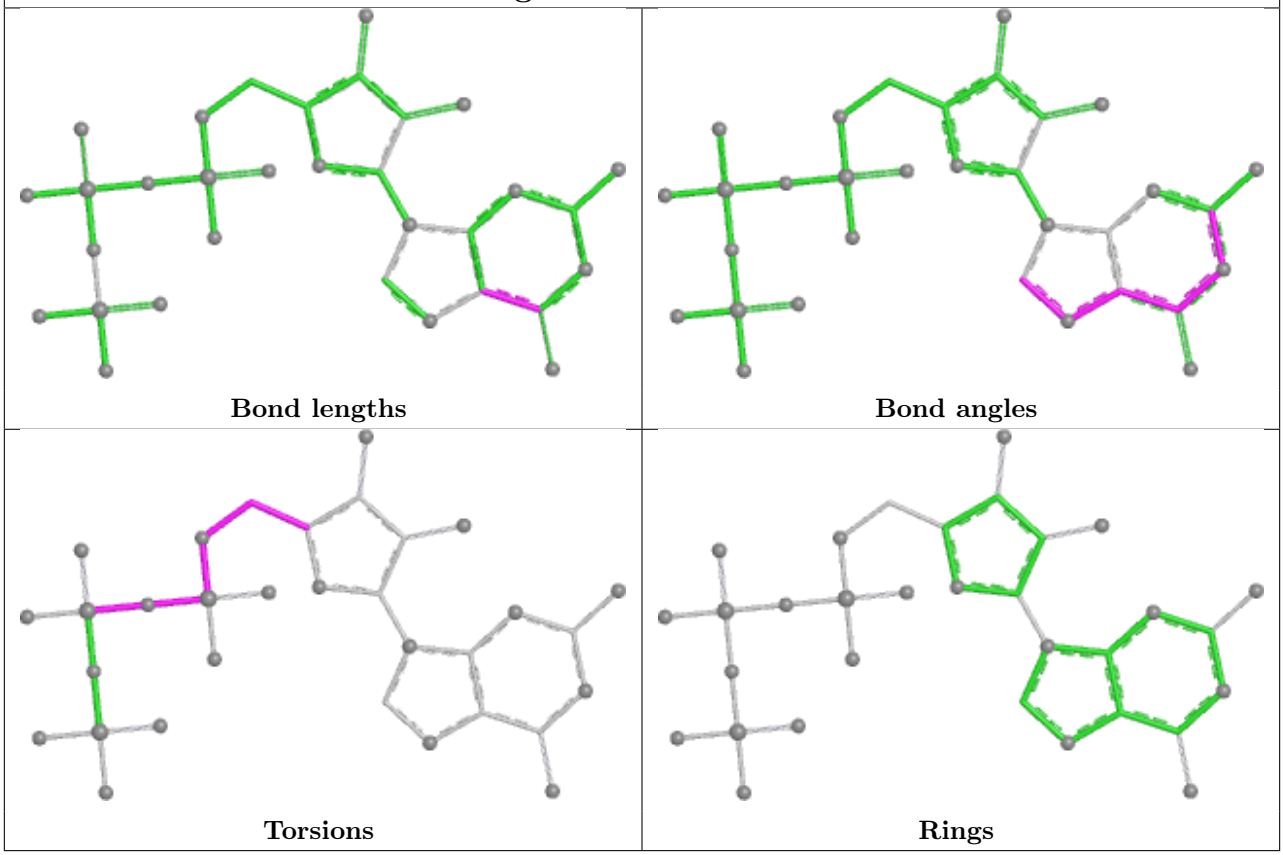


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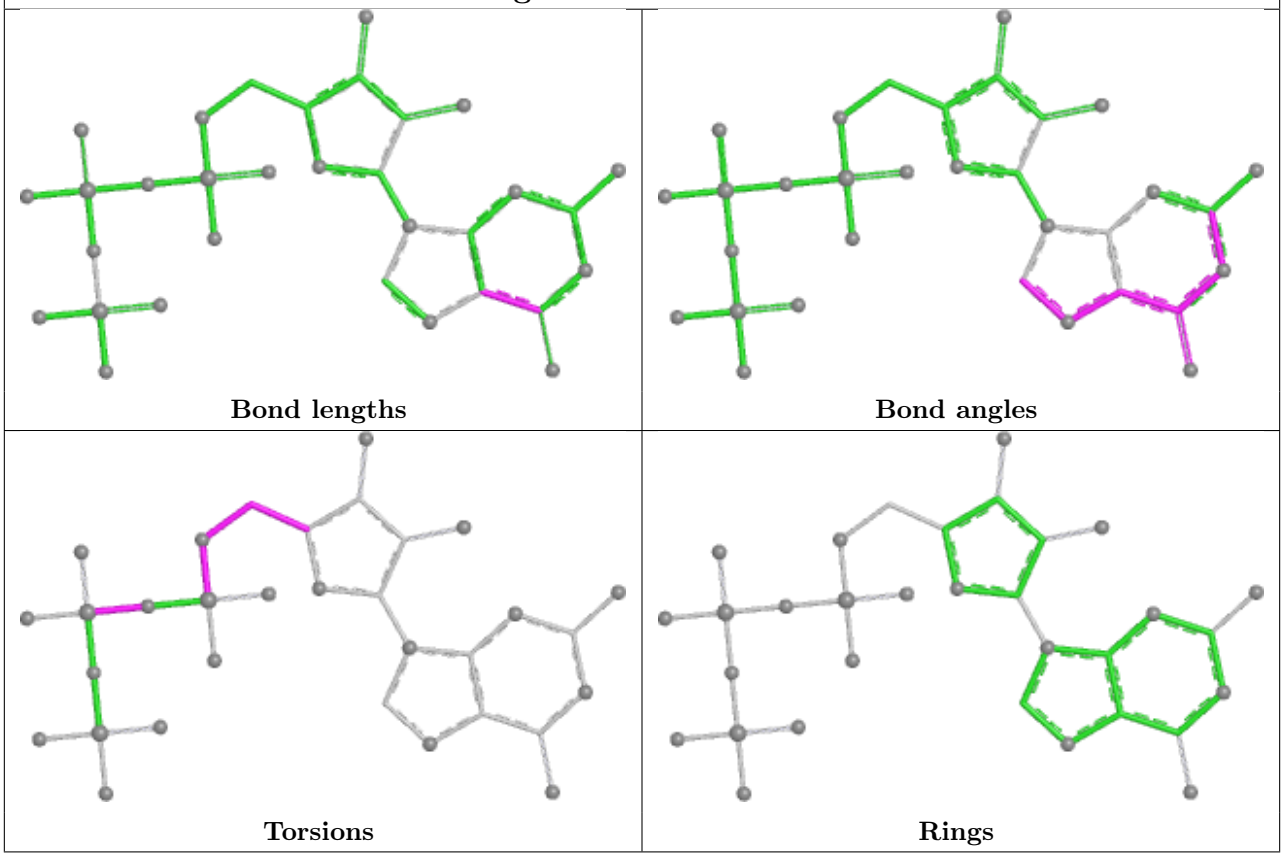

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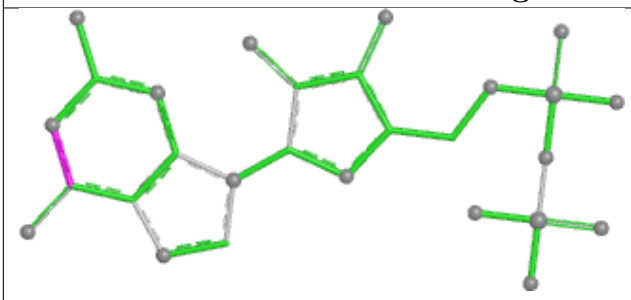
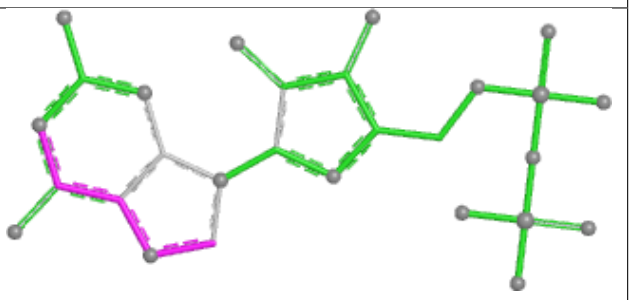
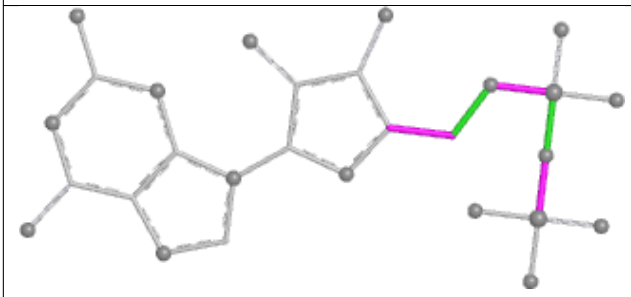
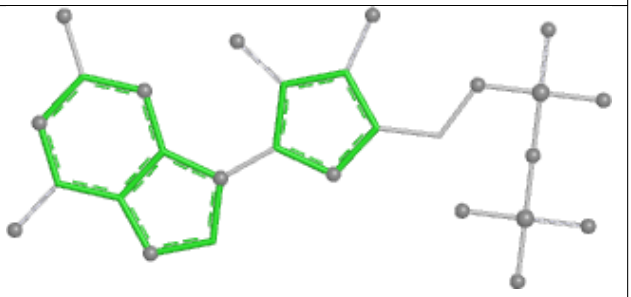
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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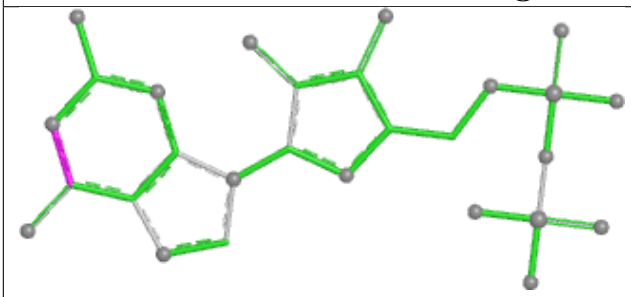
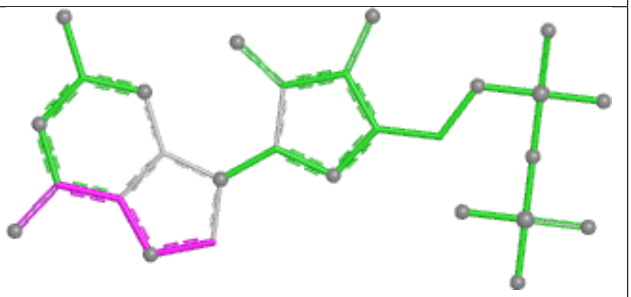
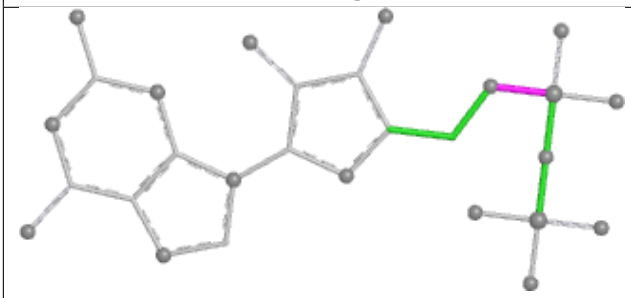
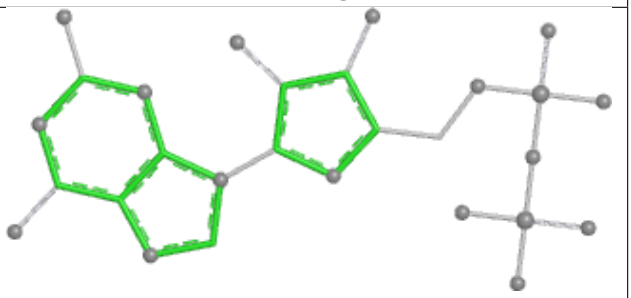
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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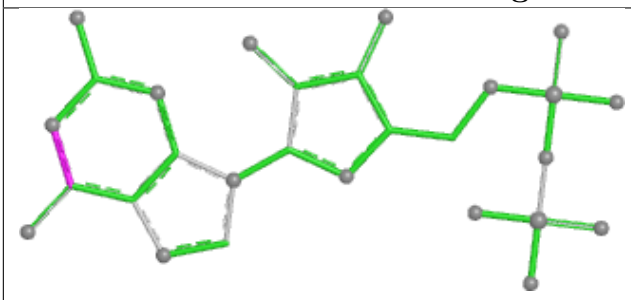
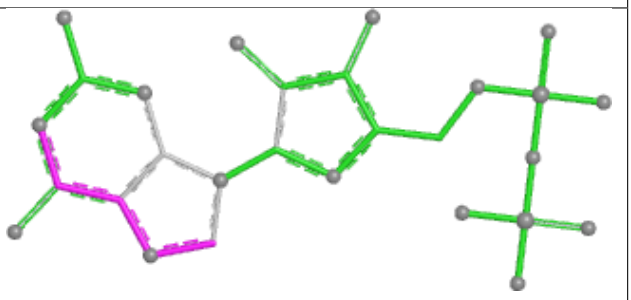
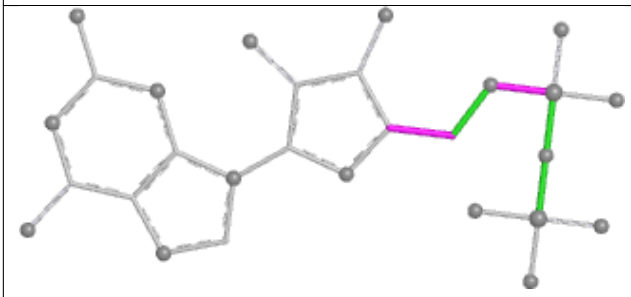
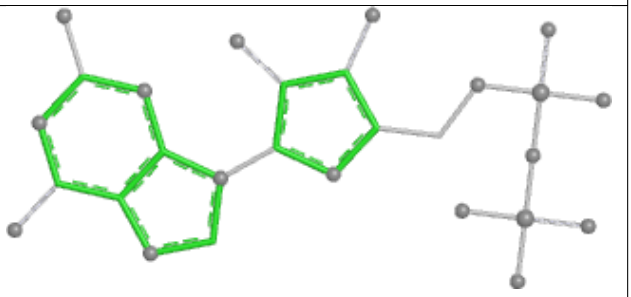
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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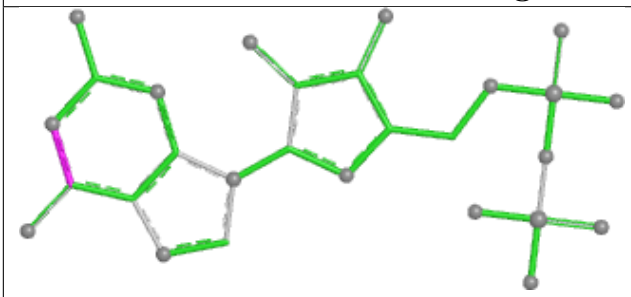
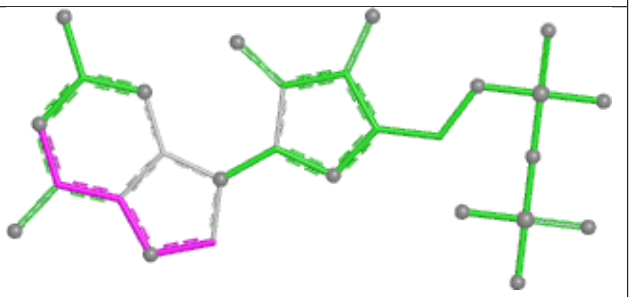
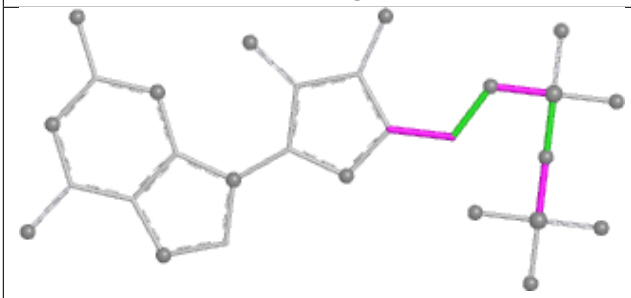
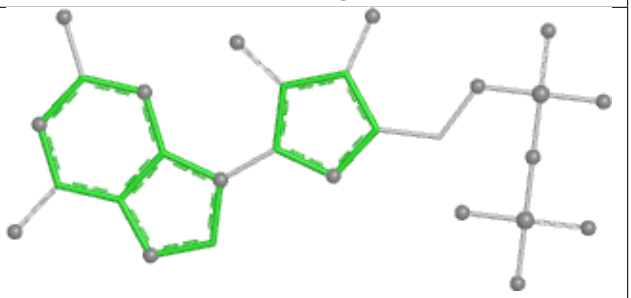
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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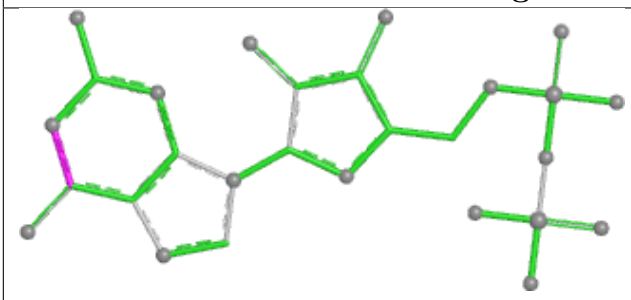

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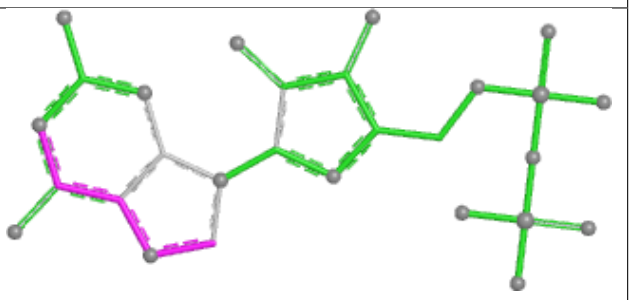

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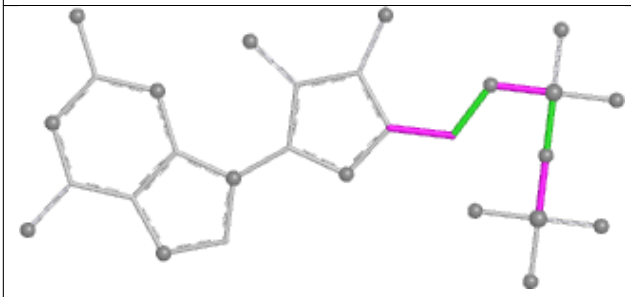

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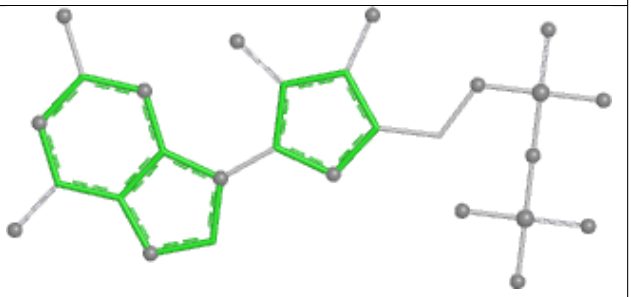
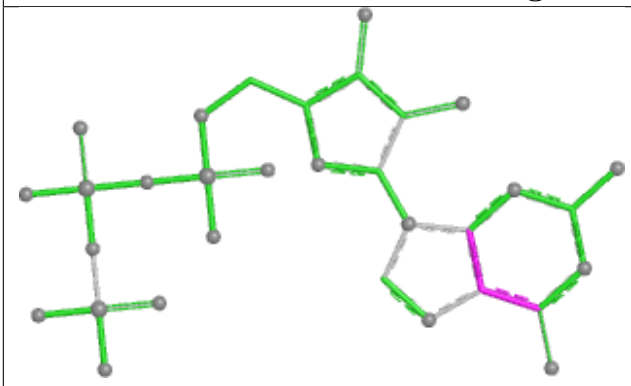


Rings

## Ligand GTP 7 501



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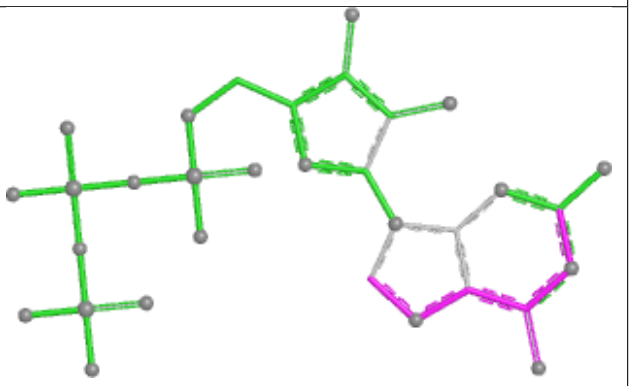

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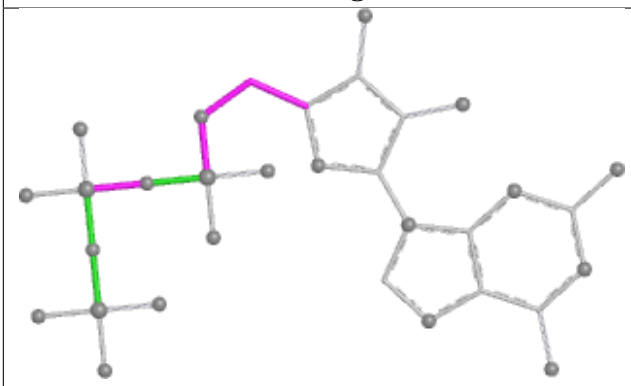

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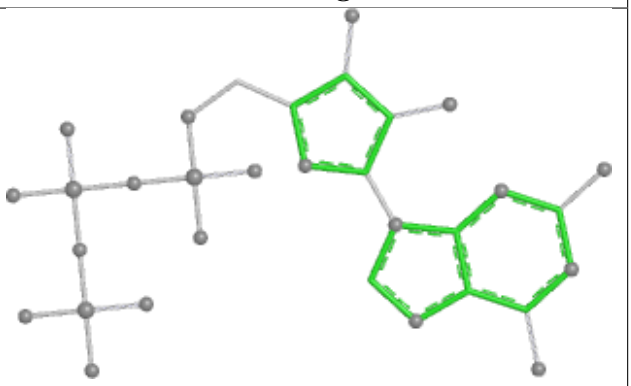

Rings

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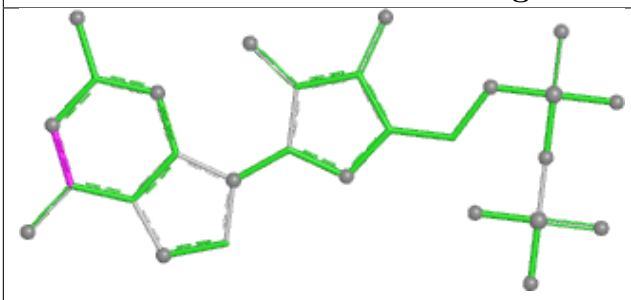
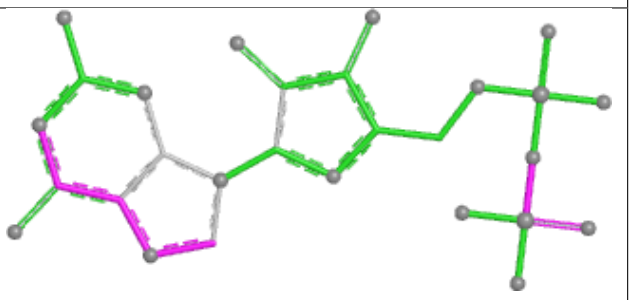
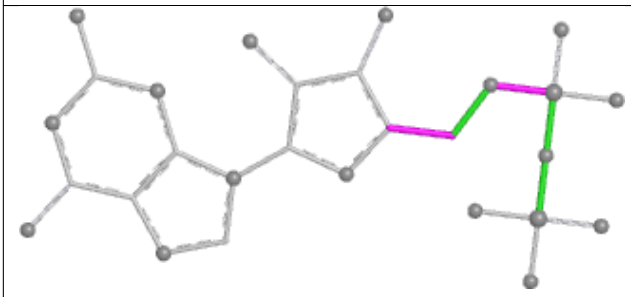
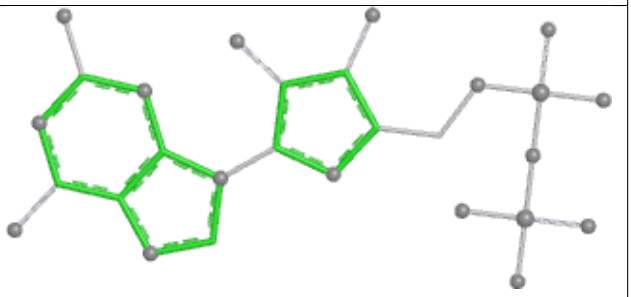
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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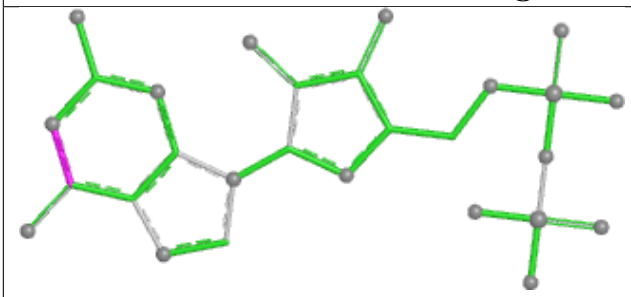
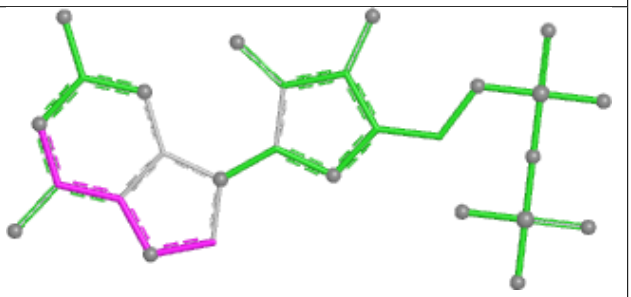
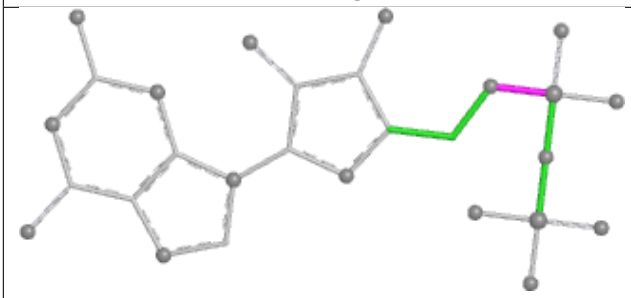
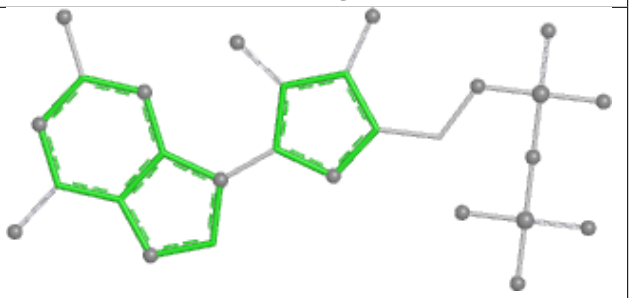
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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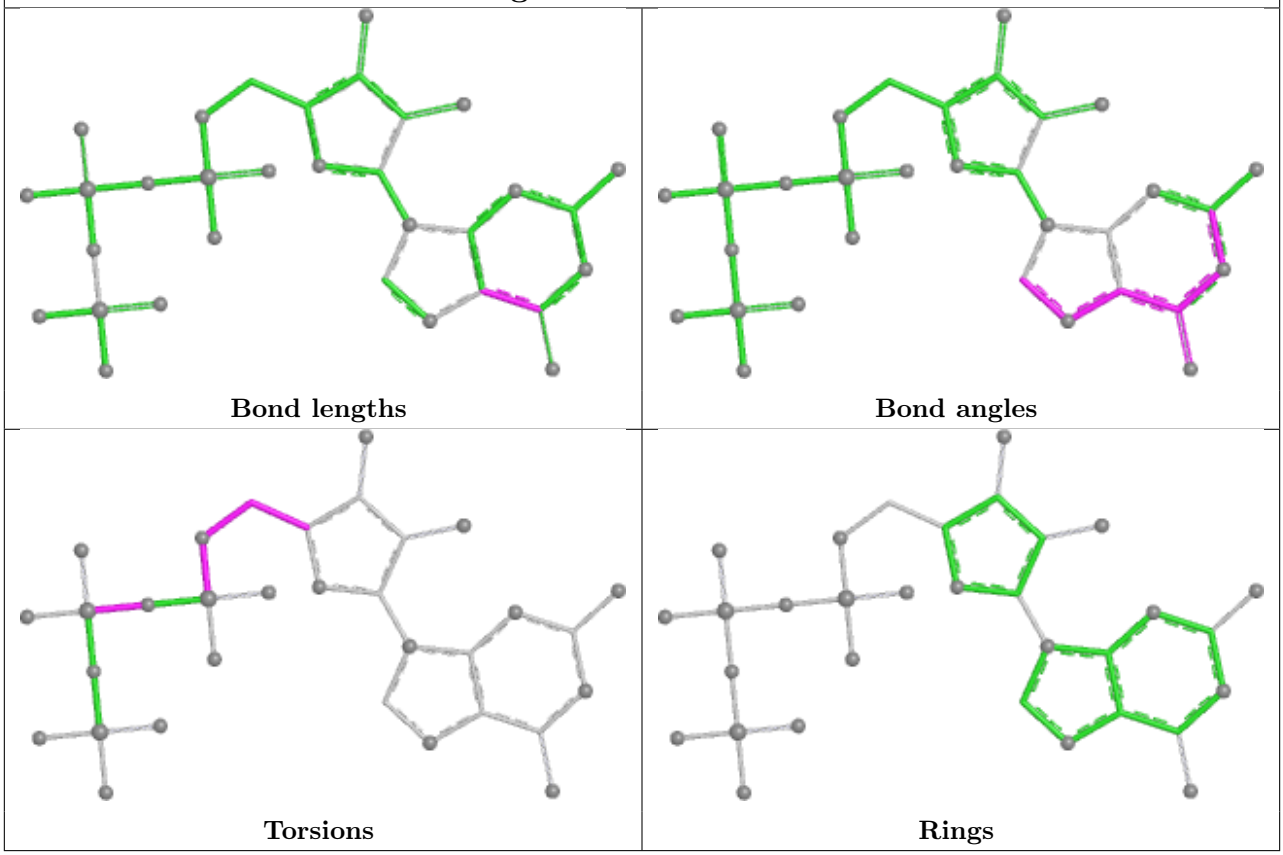


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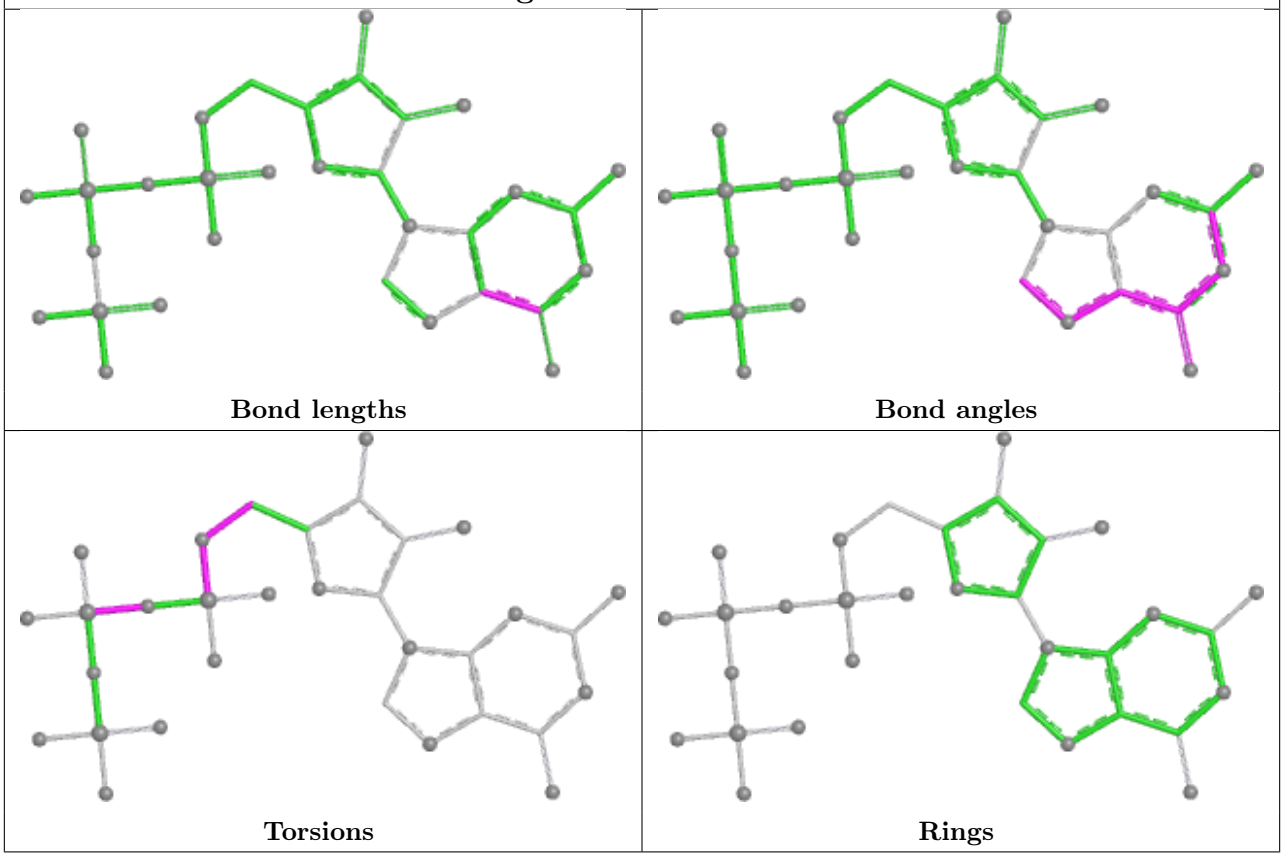

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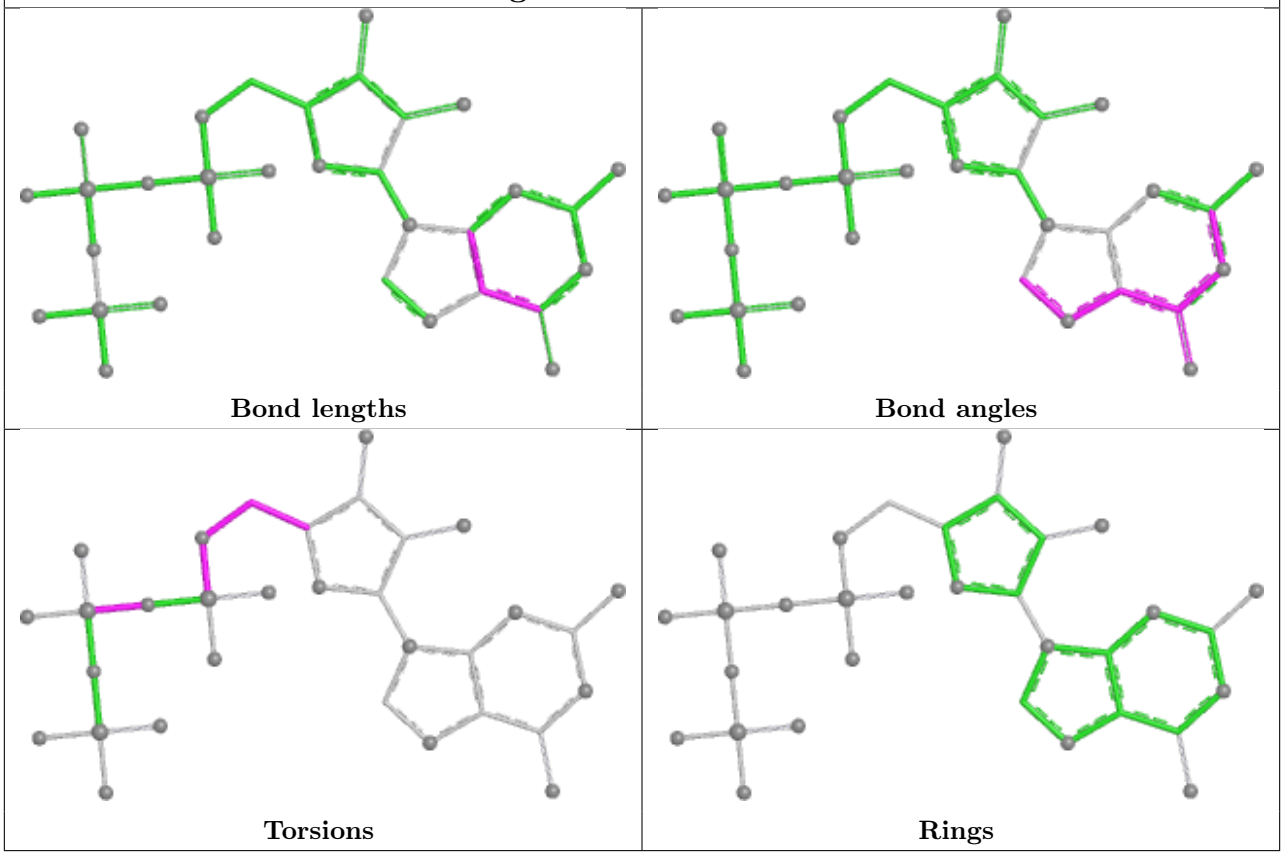


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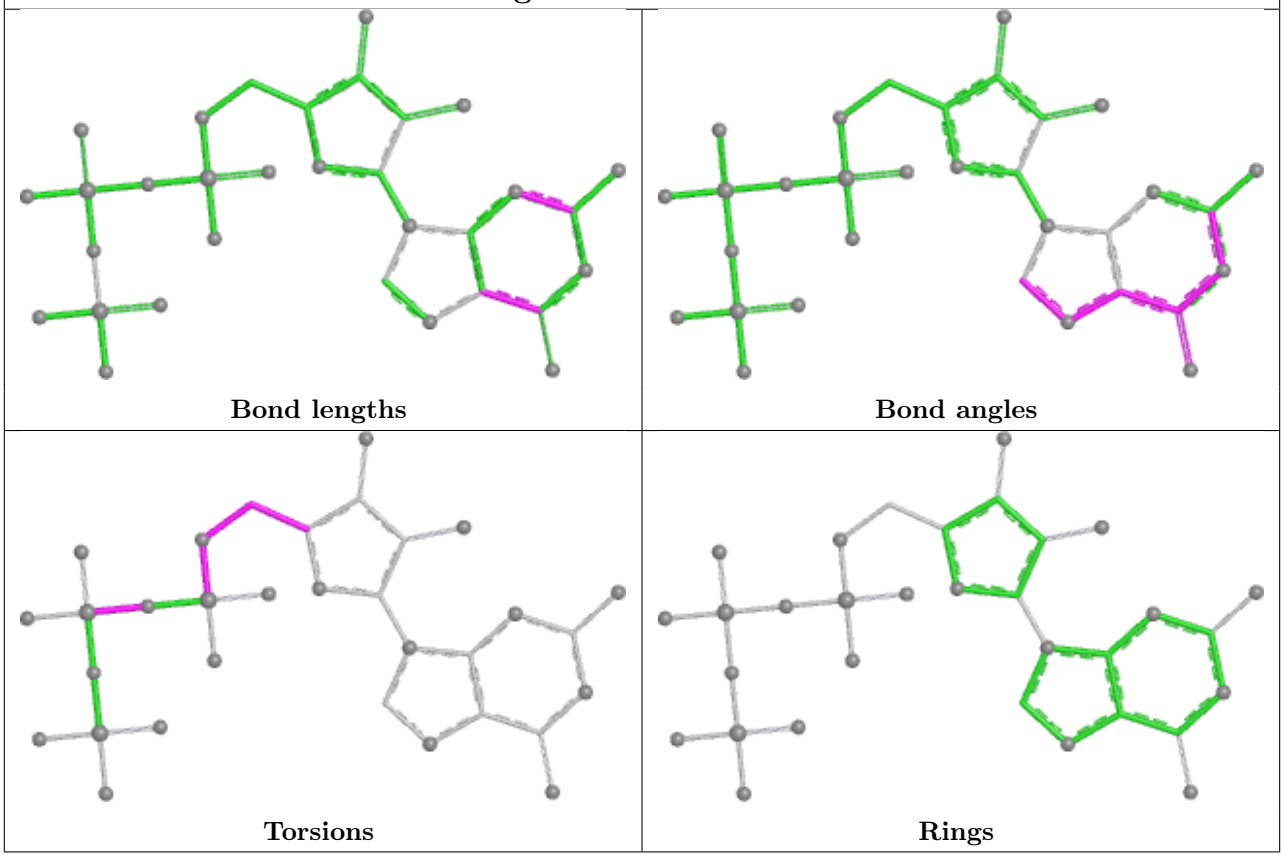

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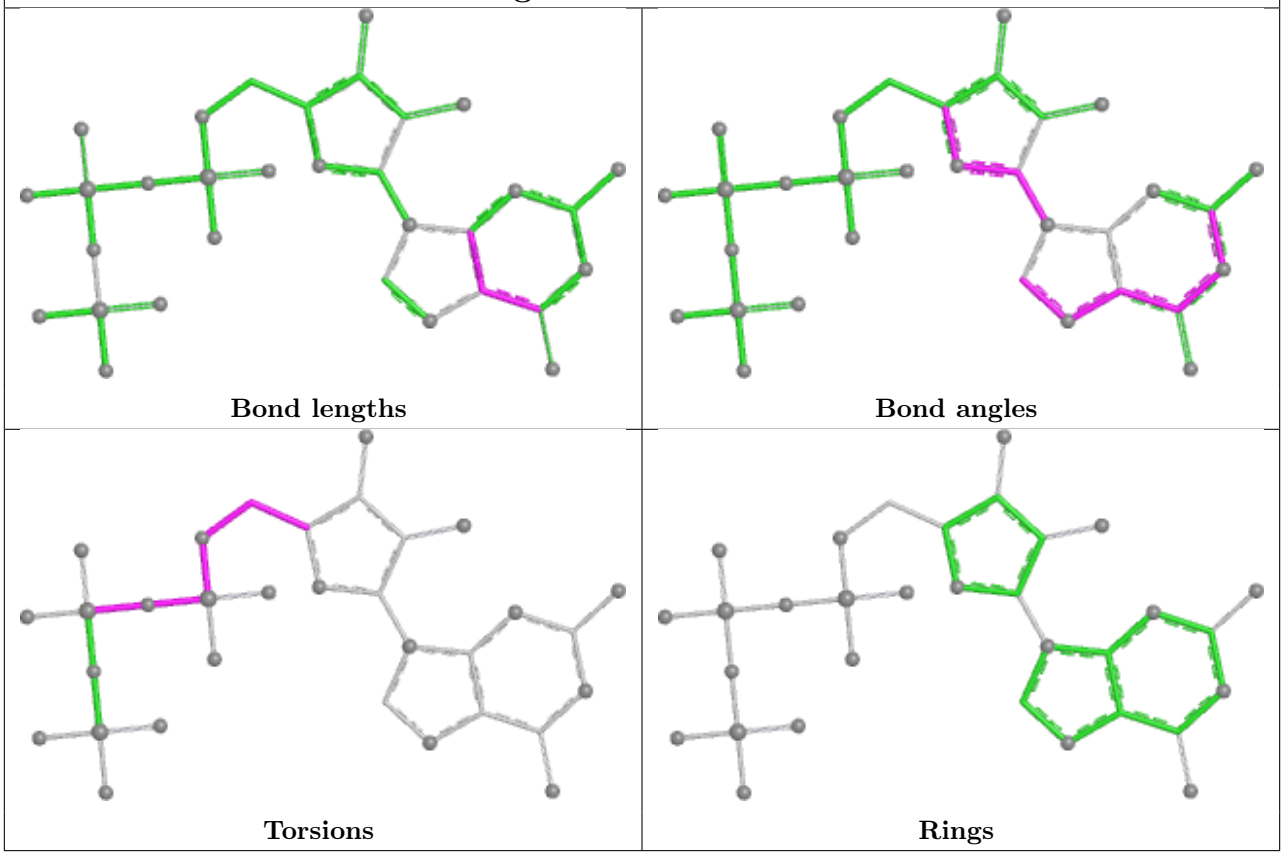


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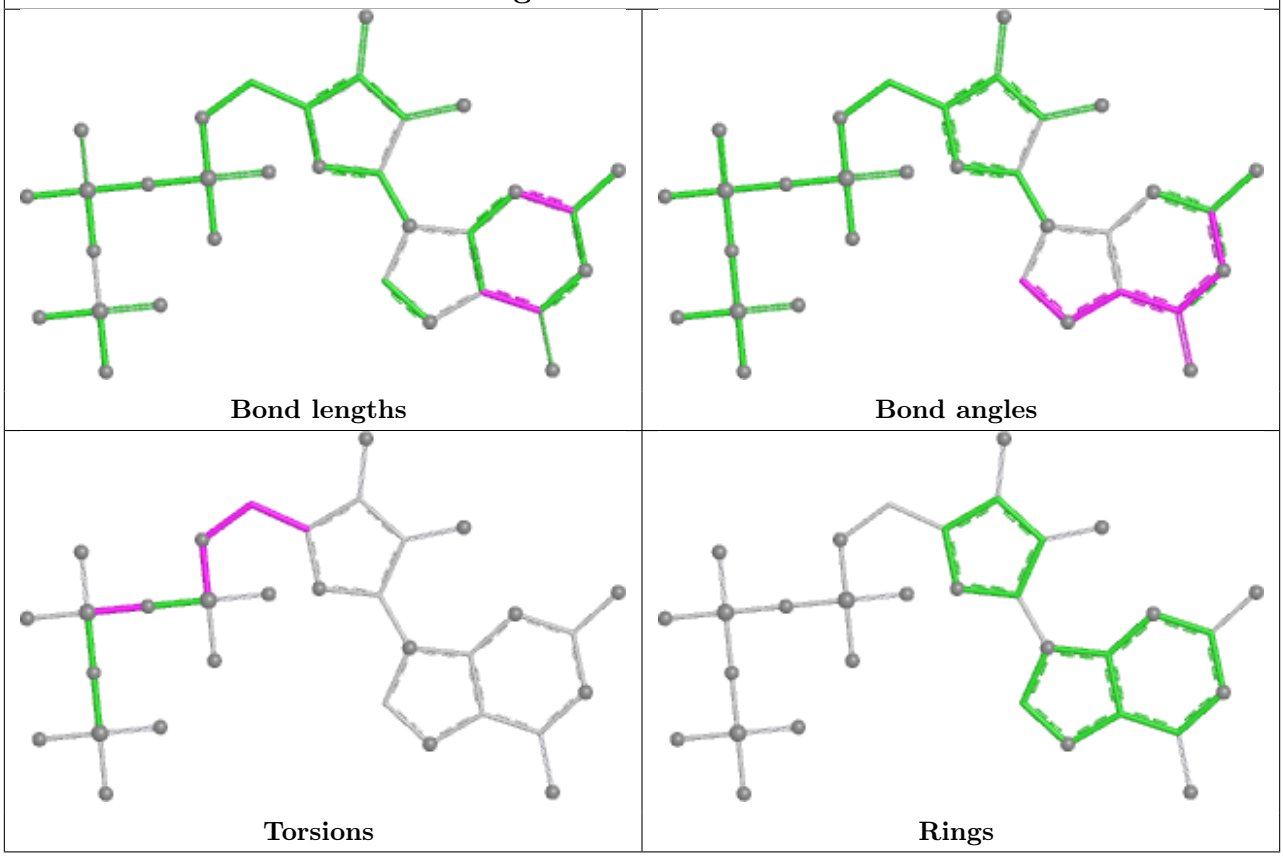

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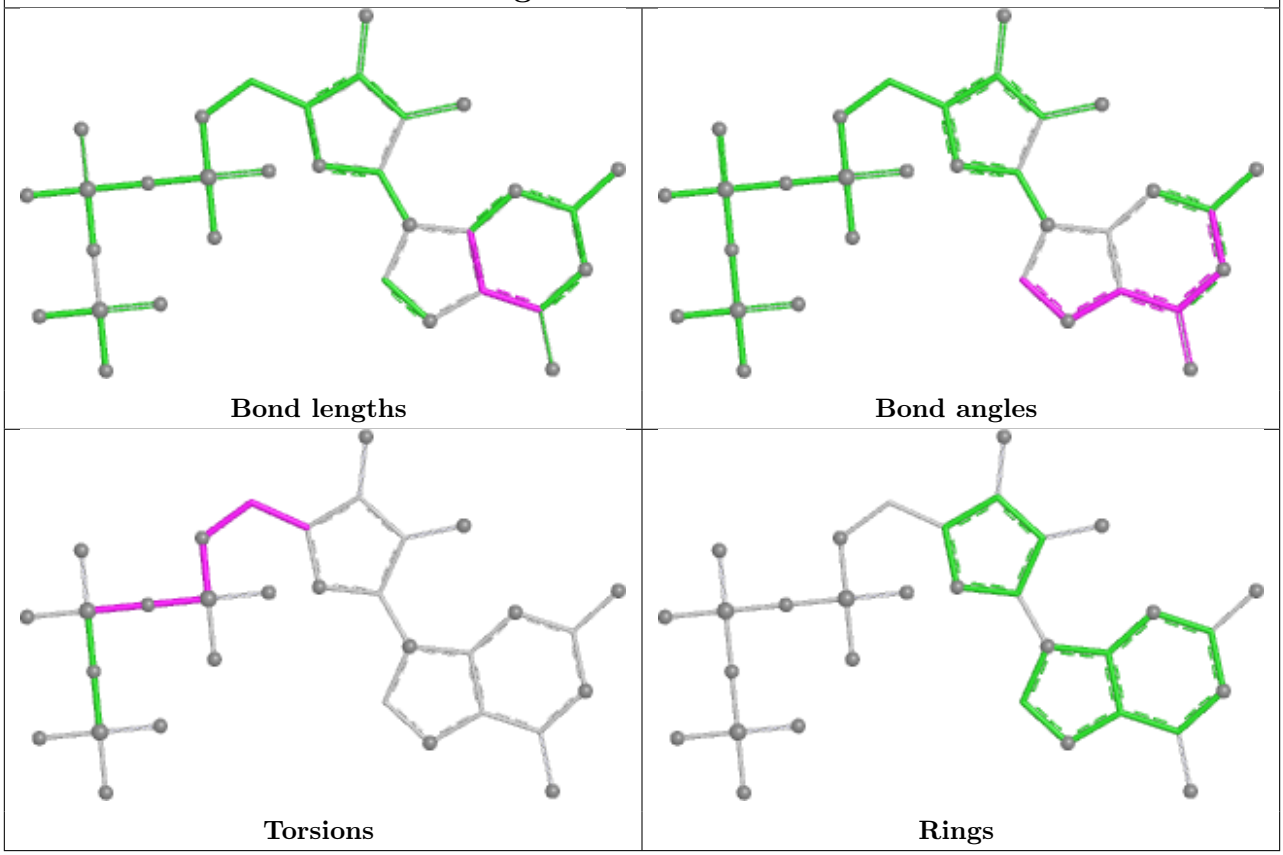


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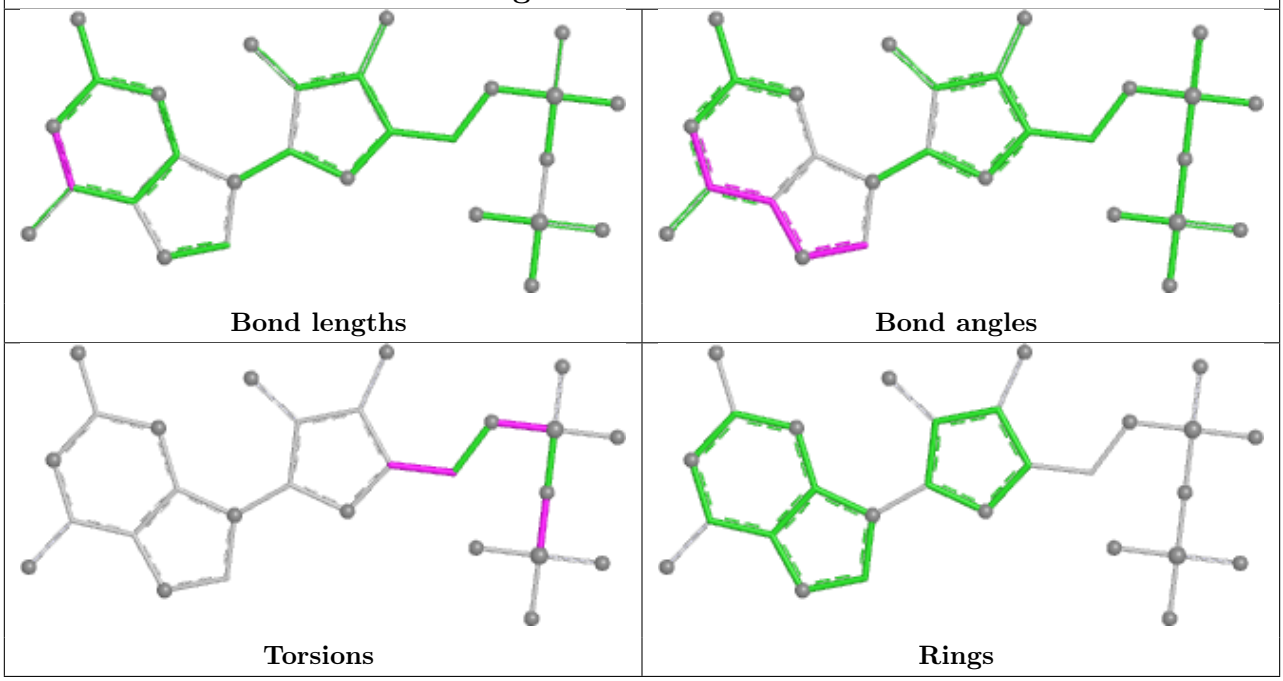

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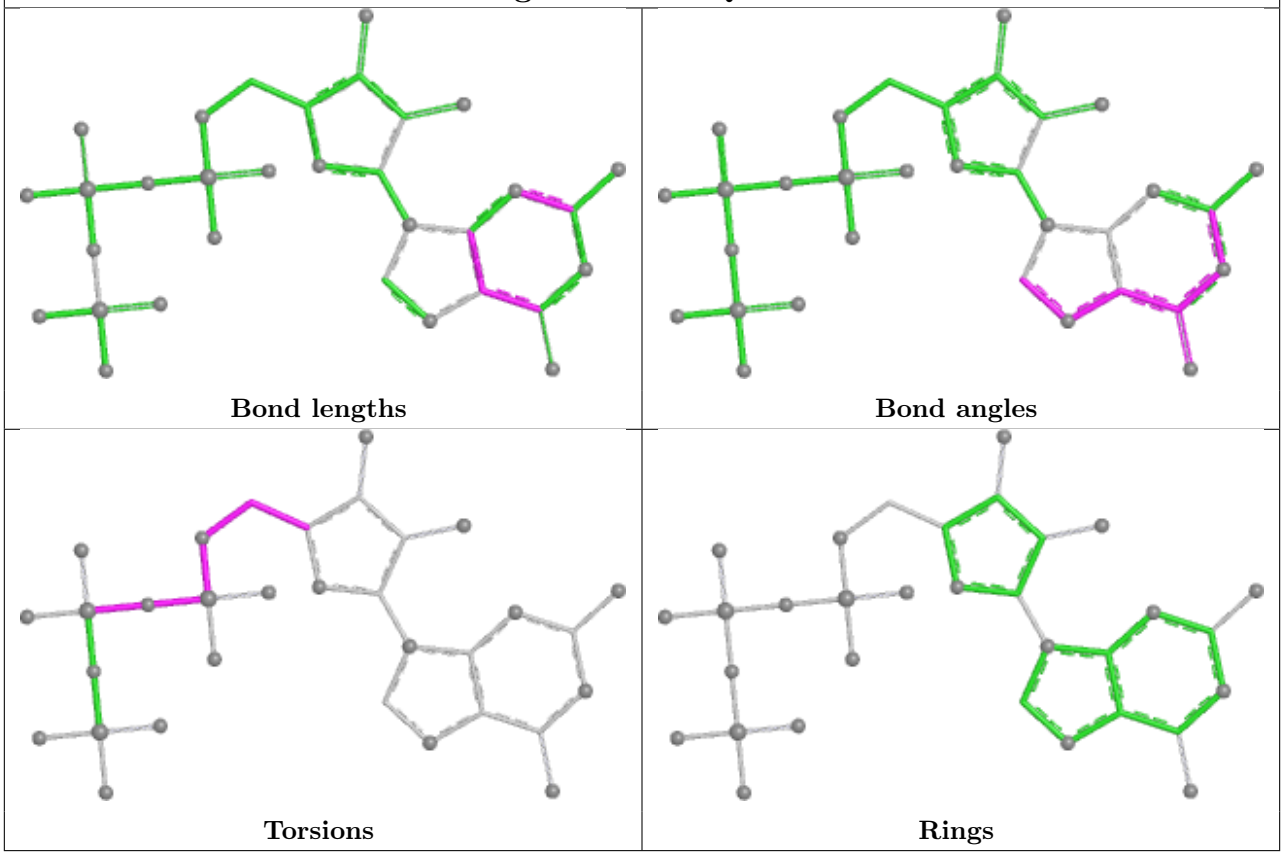


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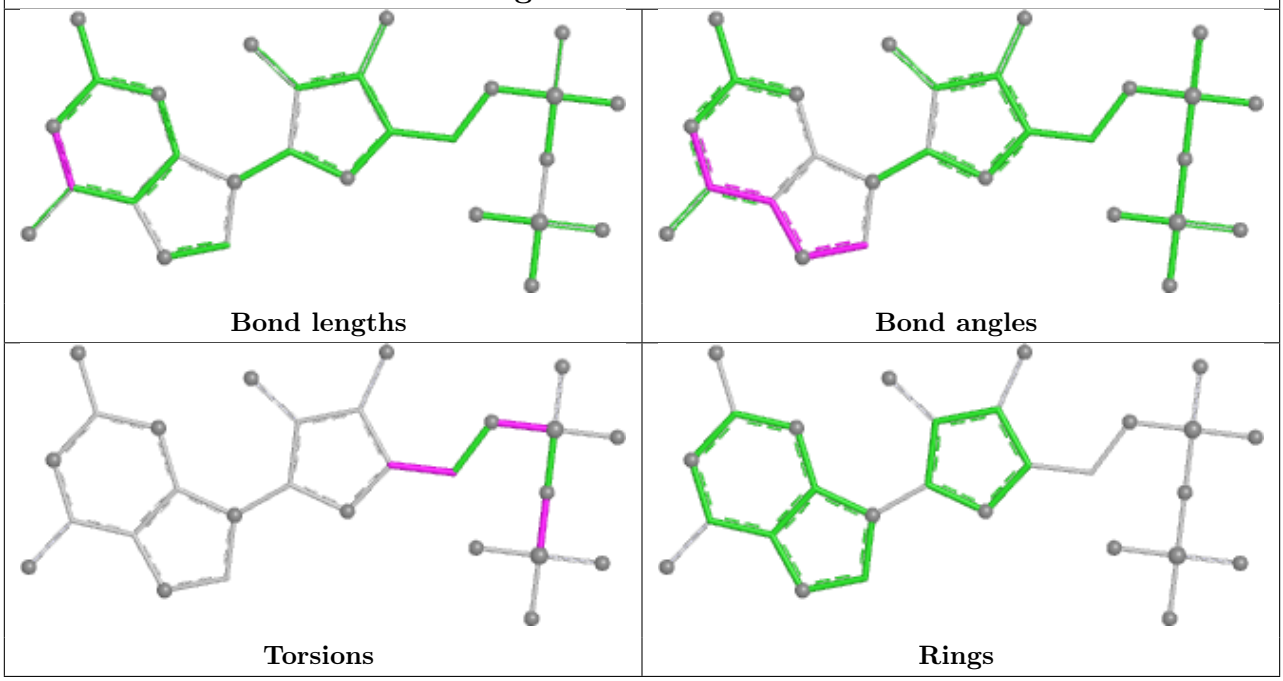

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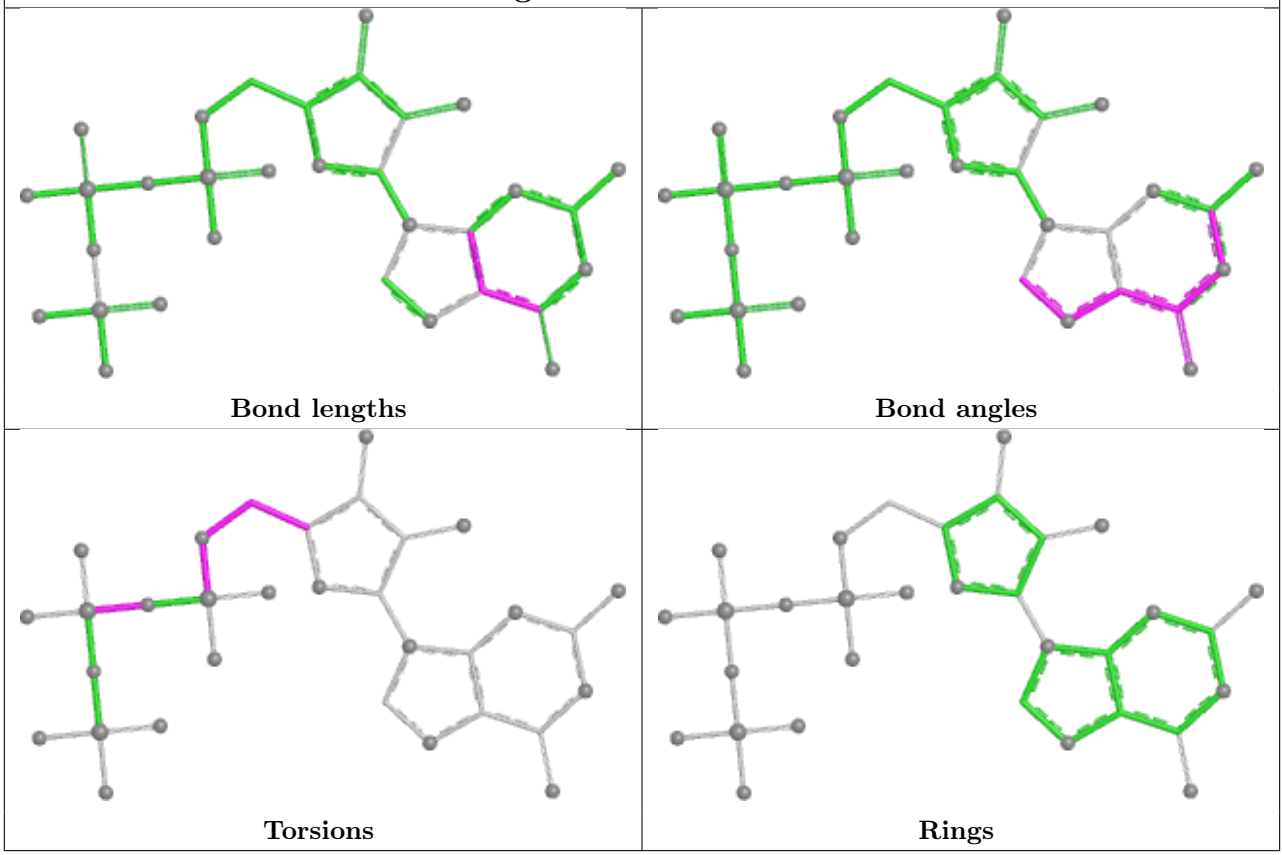


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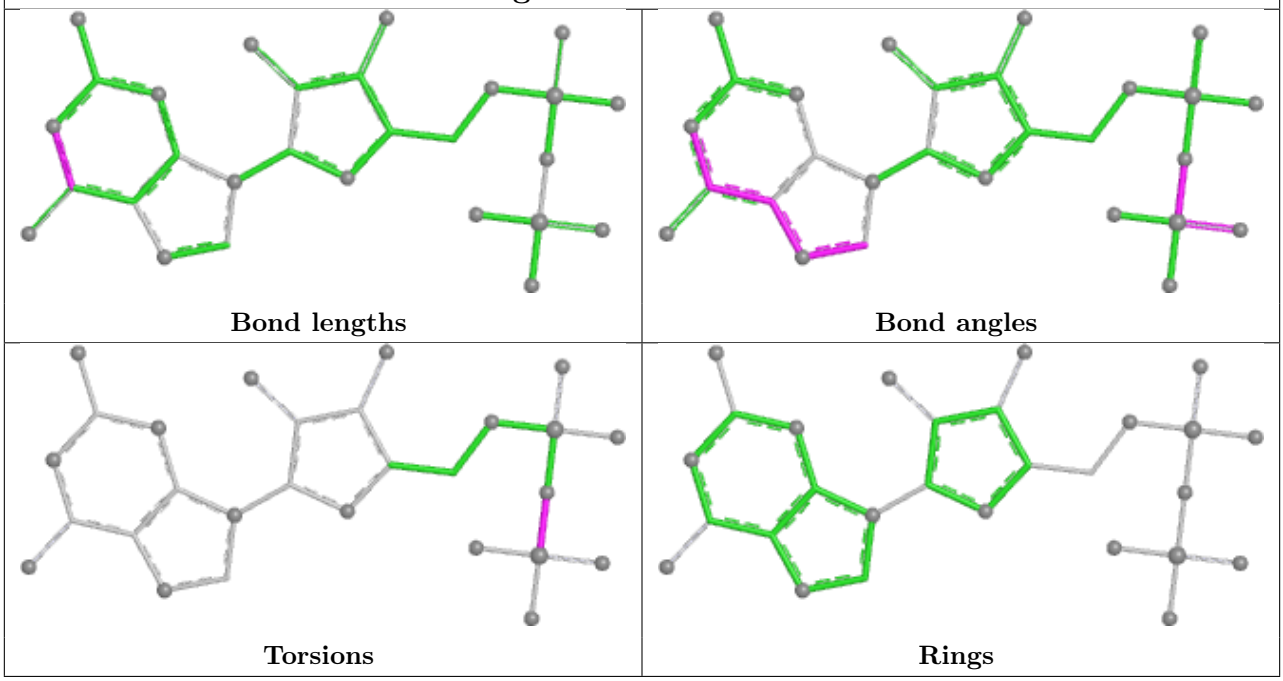

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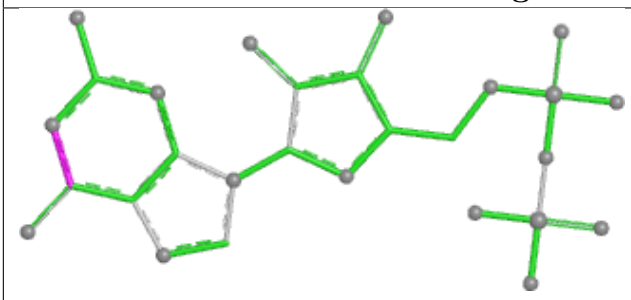
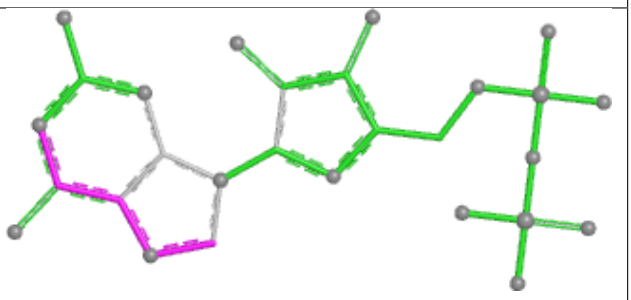
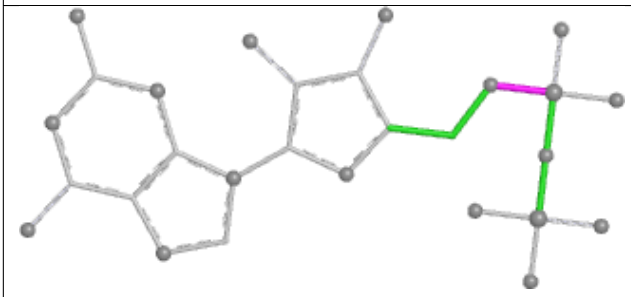
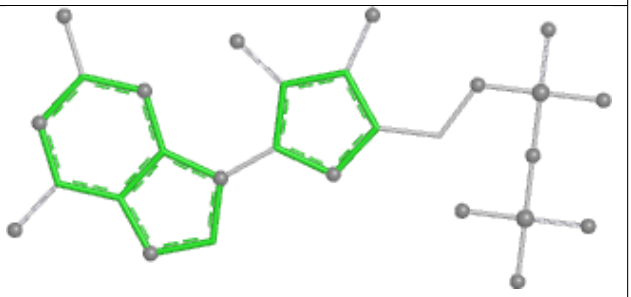
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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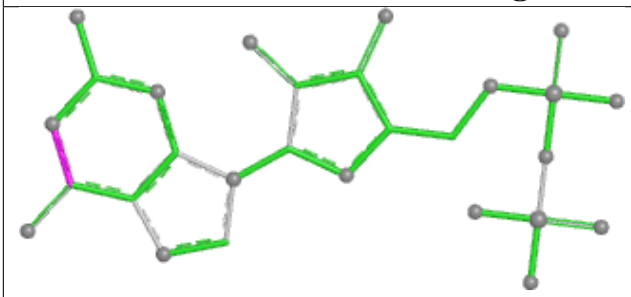
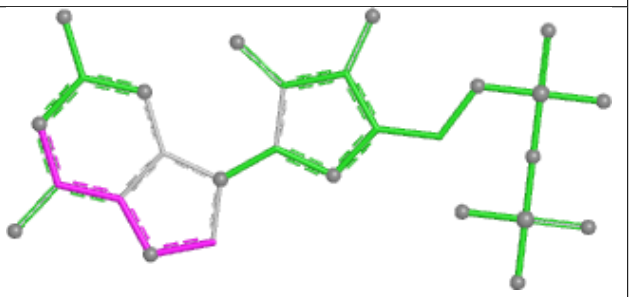
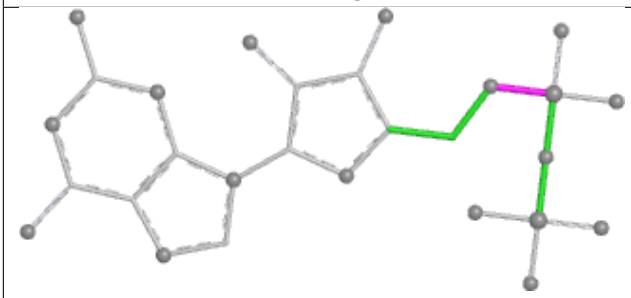
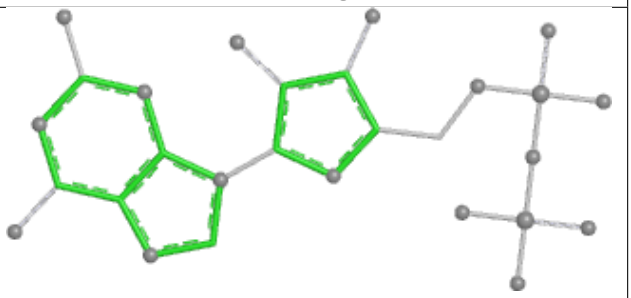
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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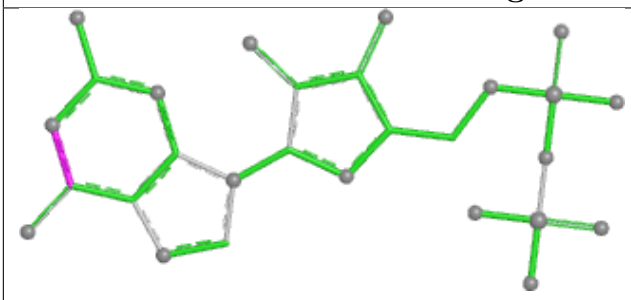
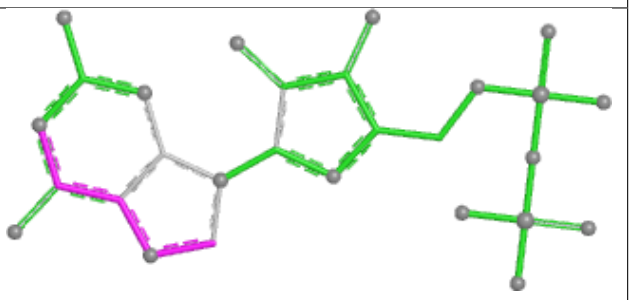
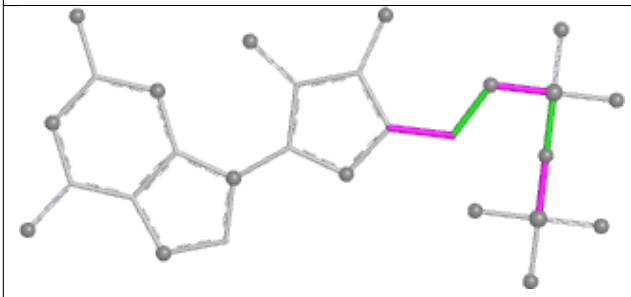
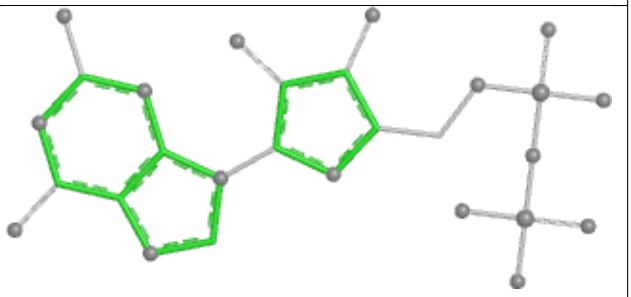
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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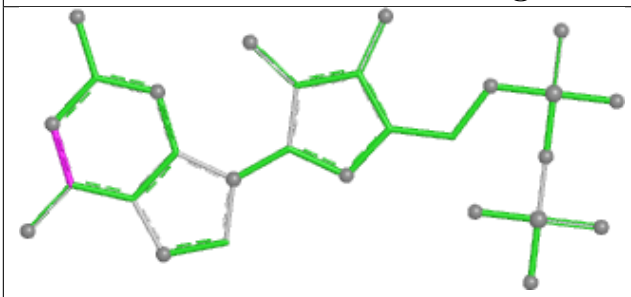
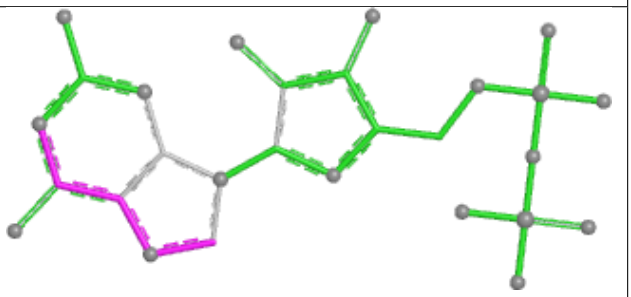
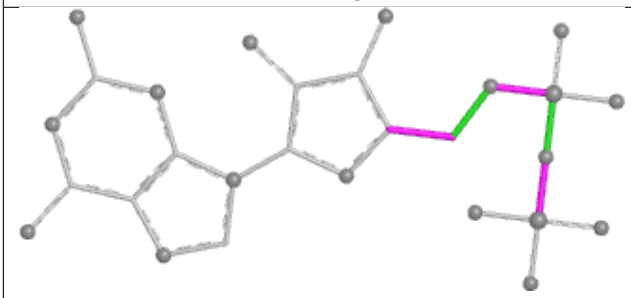
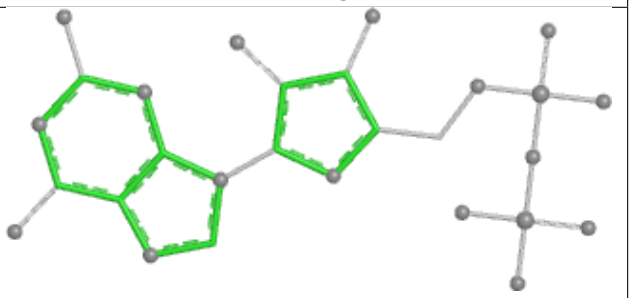
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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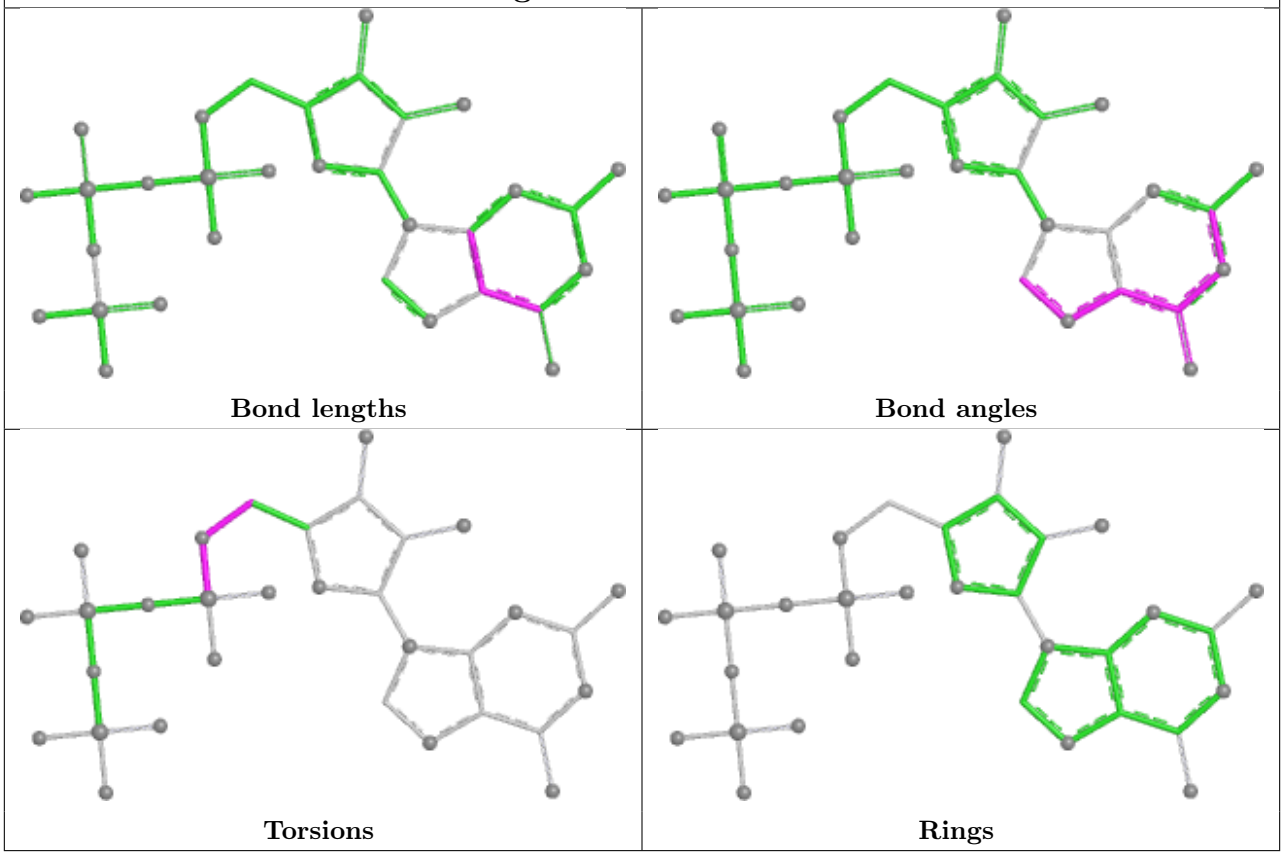


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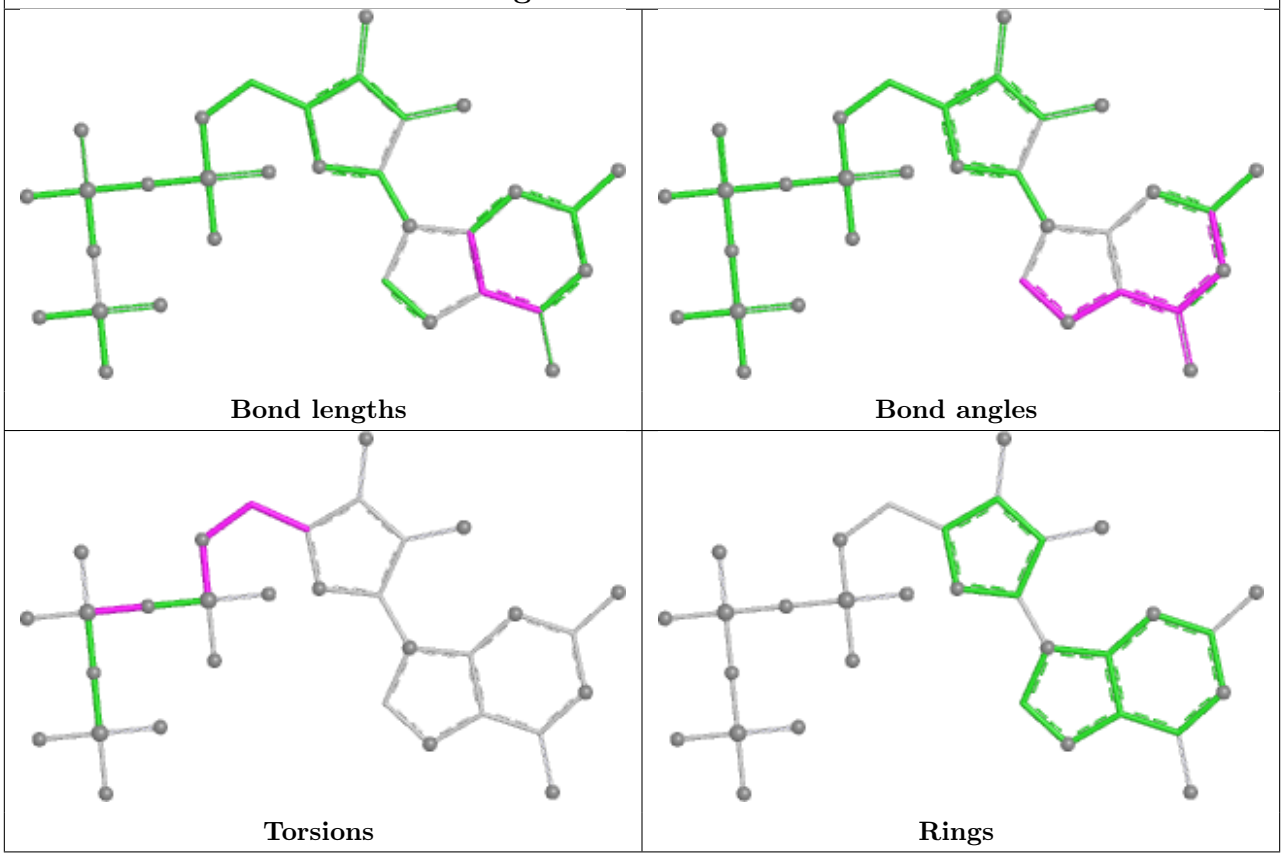

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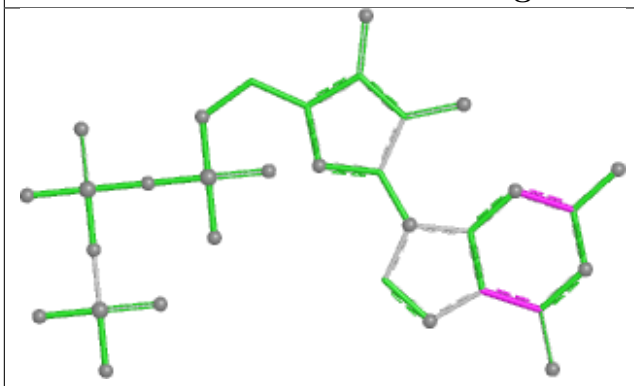

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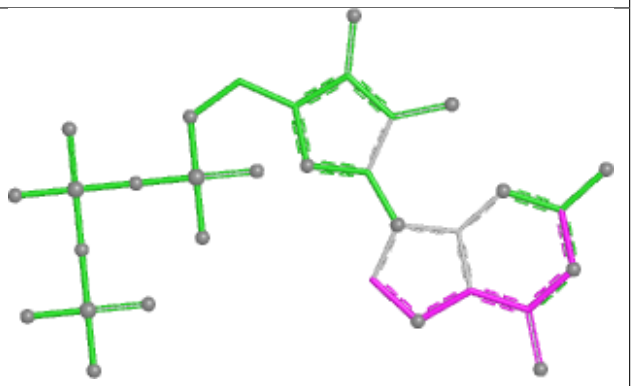
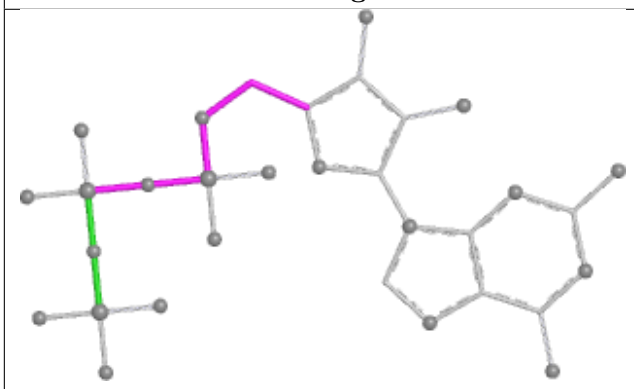


Bond angles



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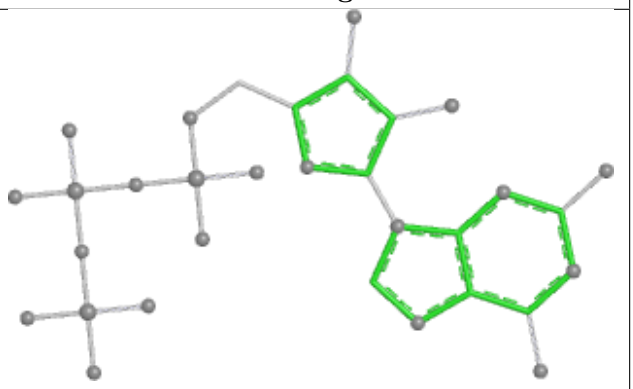

Rings

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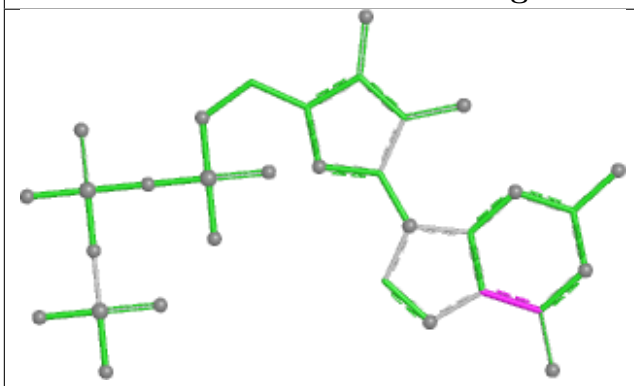

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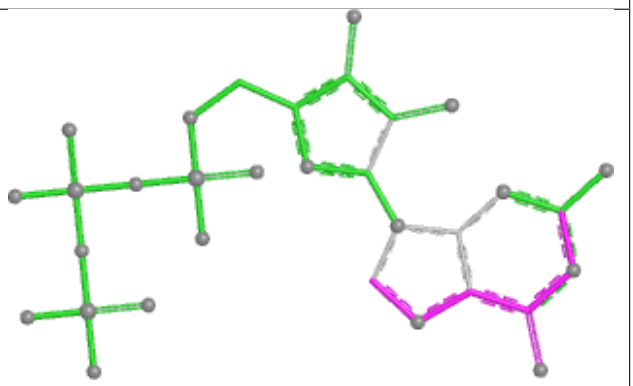

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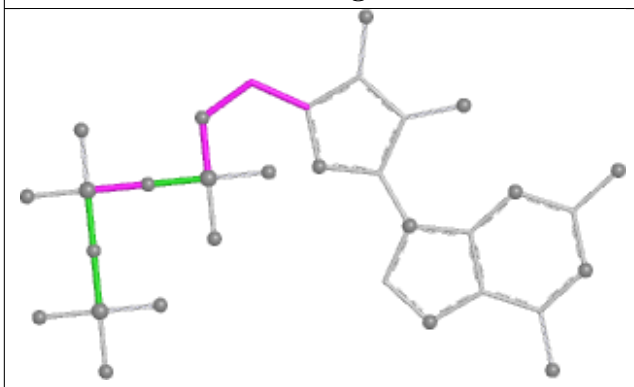

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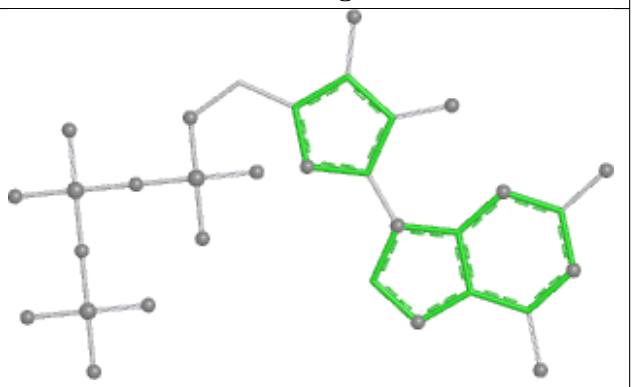

Rings

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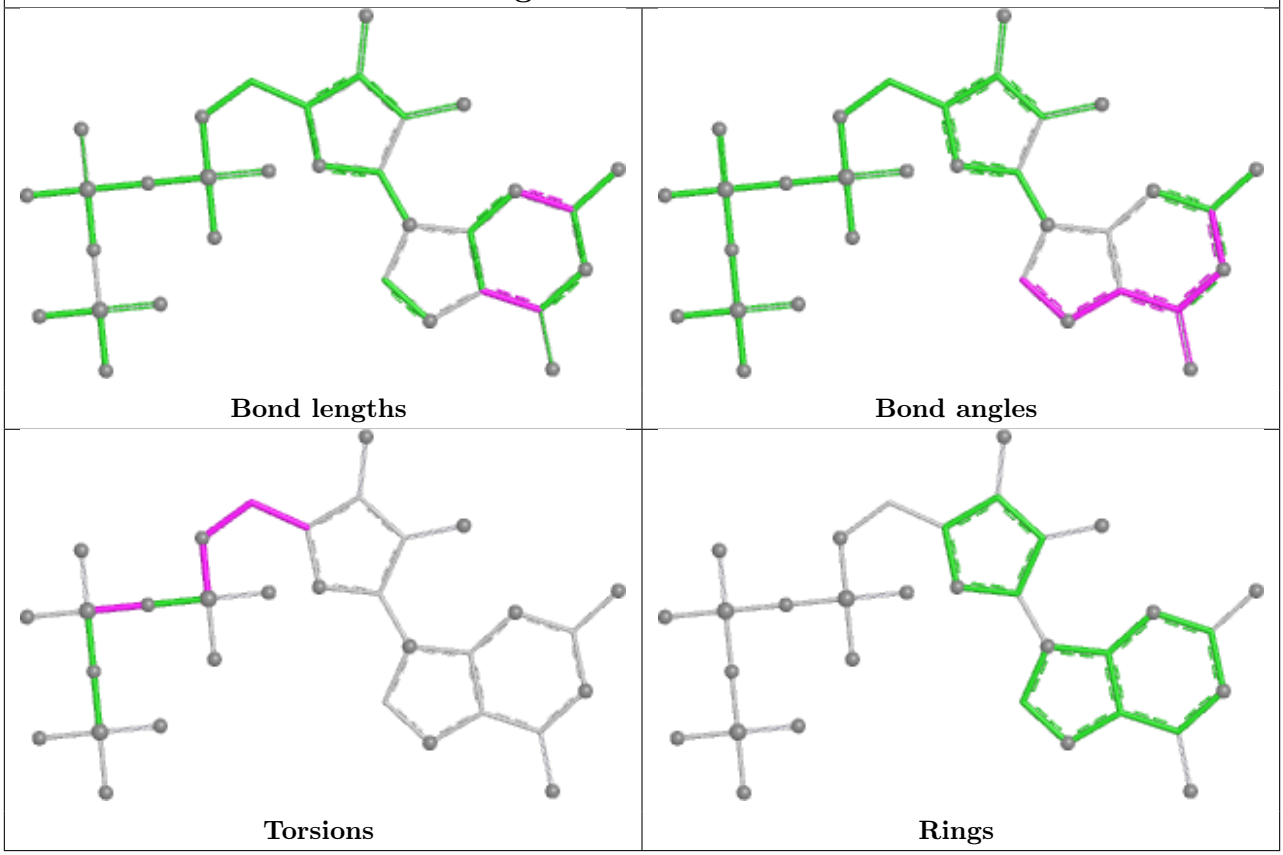


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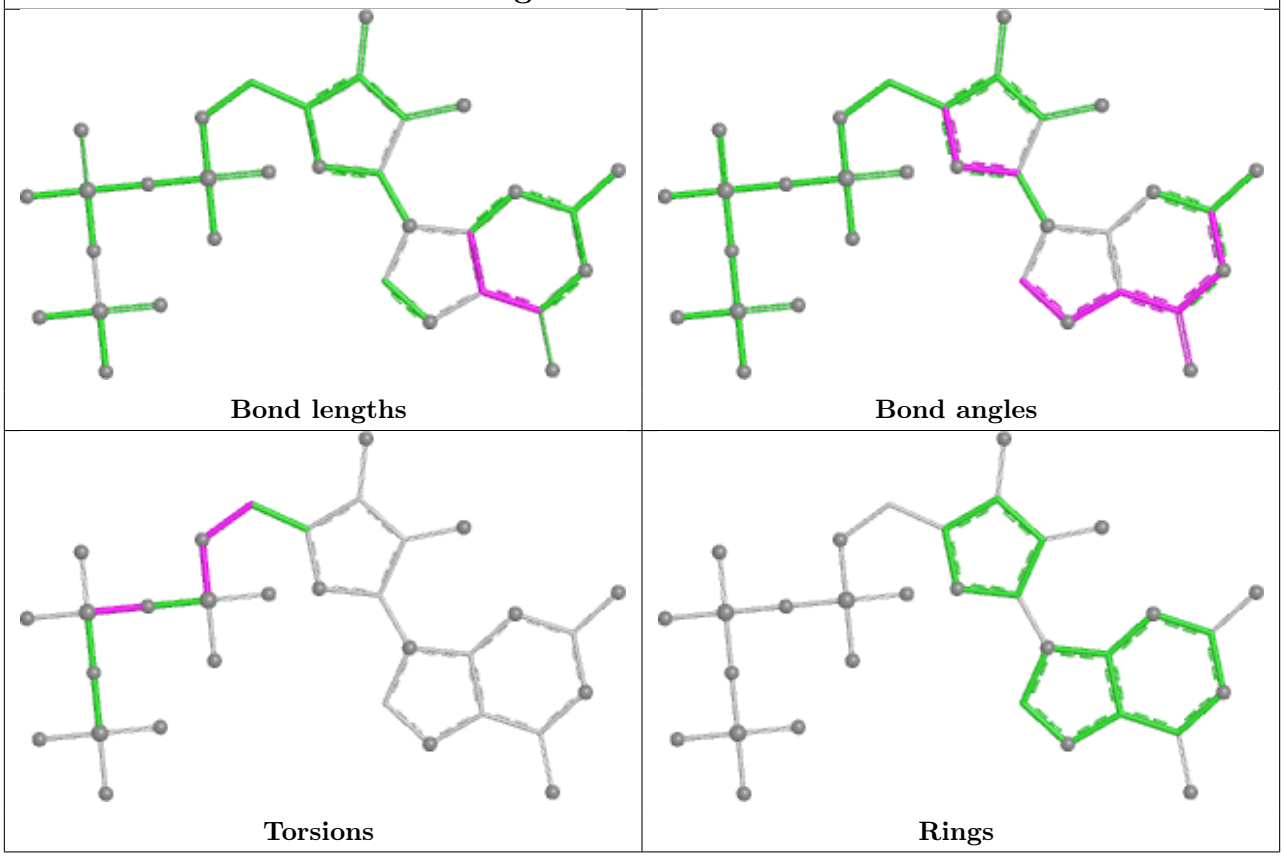

| Ligand GDP W2 503 | |
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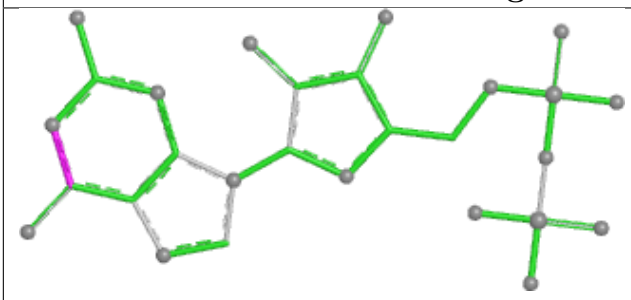
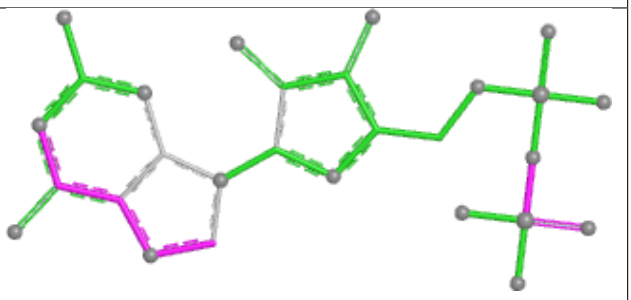
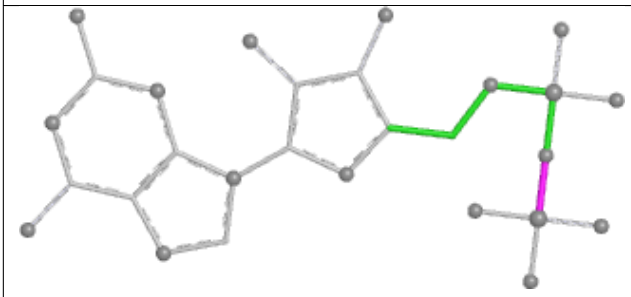
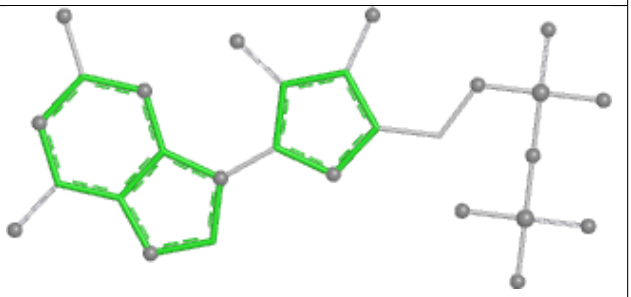
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP M4 502 | |
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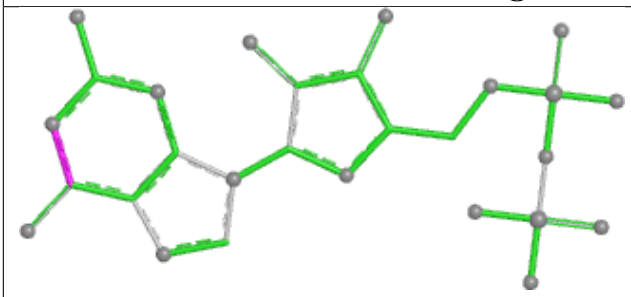
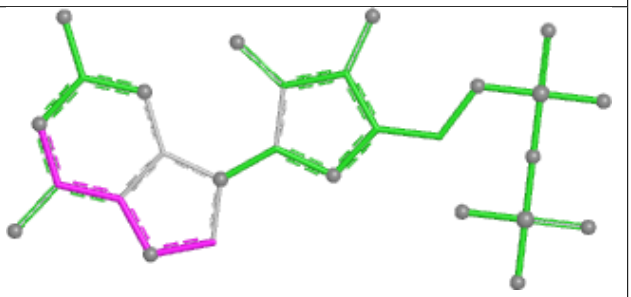
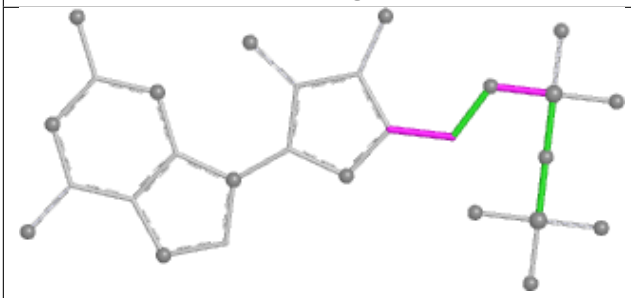
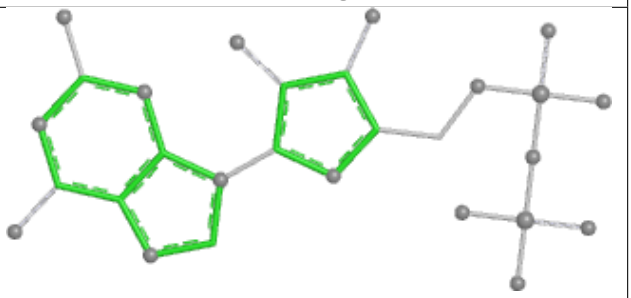
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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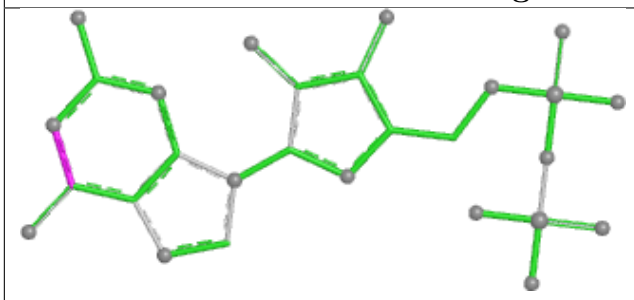

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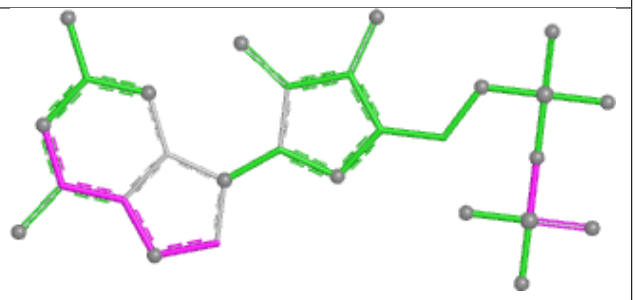

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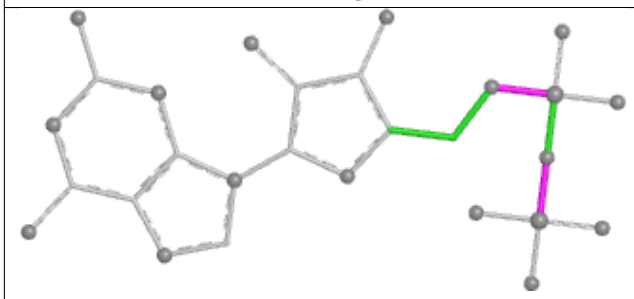

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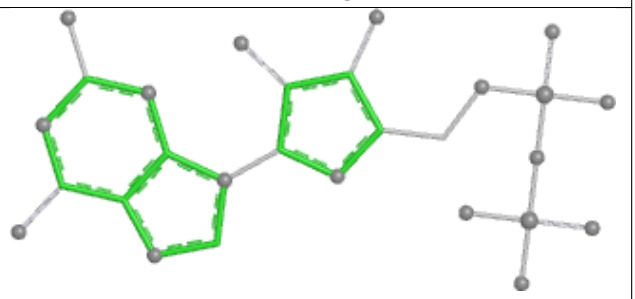
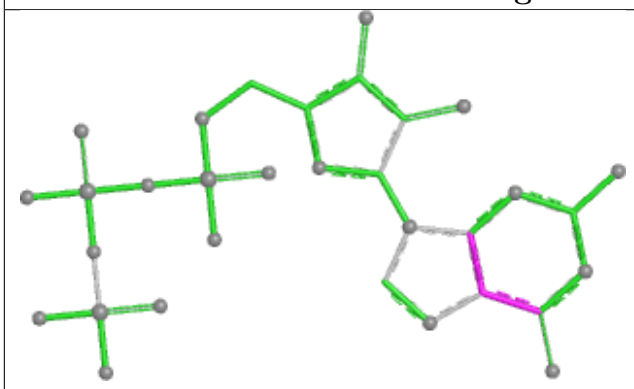


Rings

## Ligand GTP O6 501



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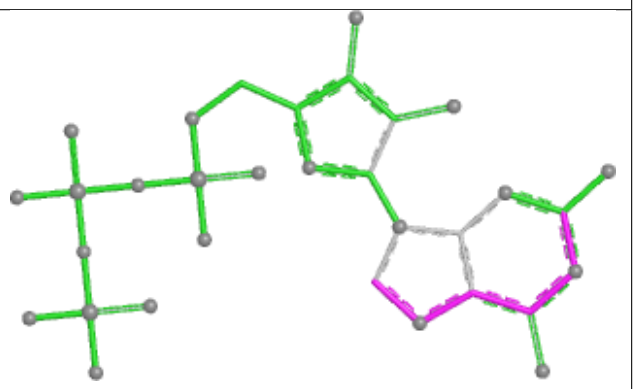

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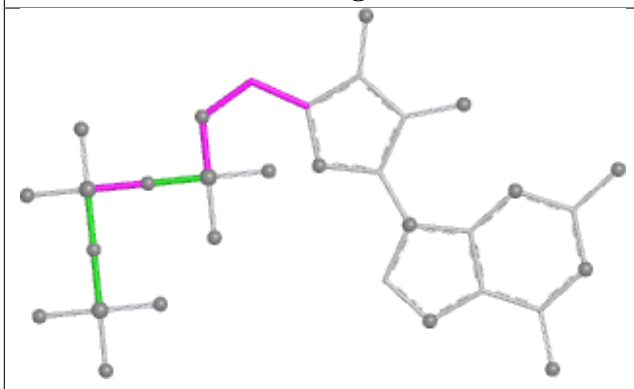

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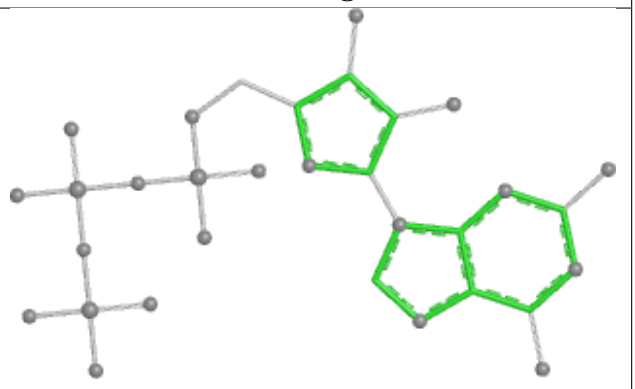

Rings

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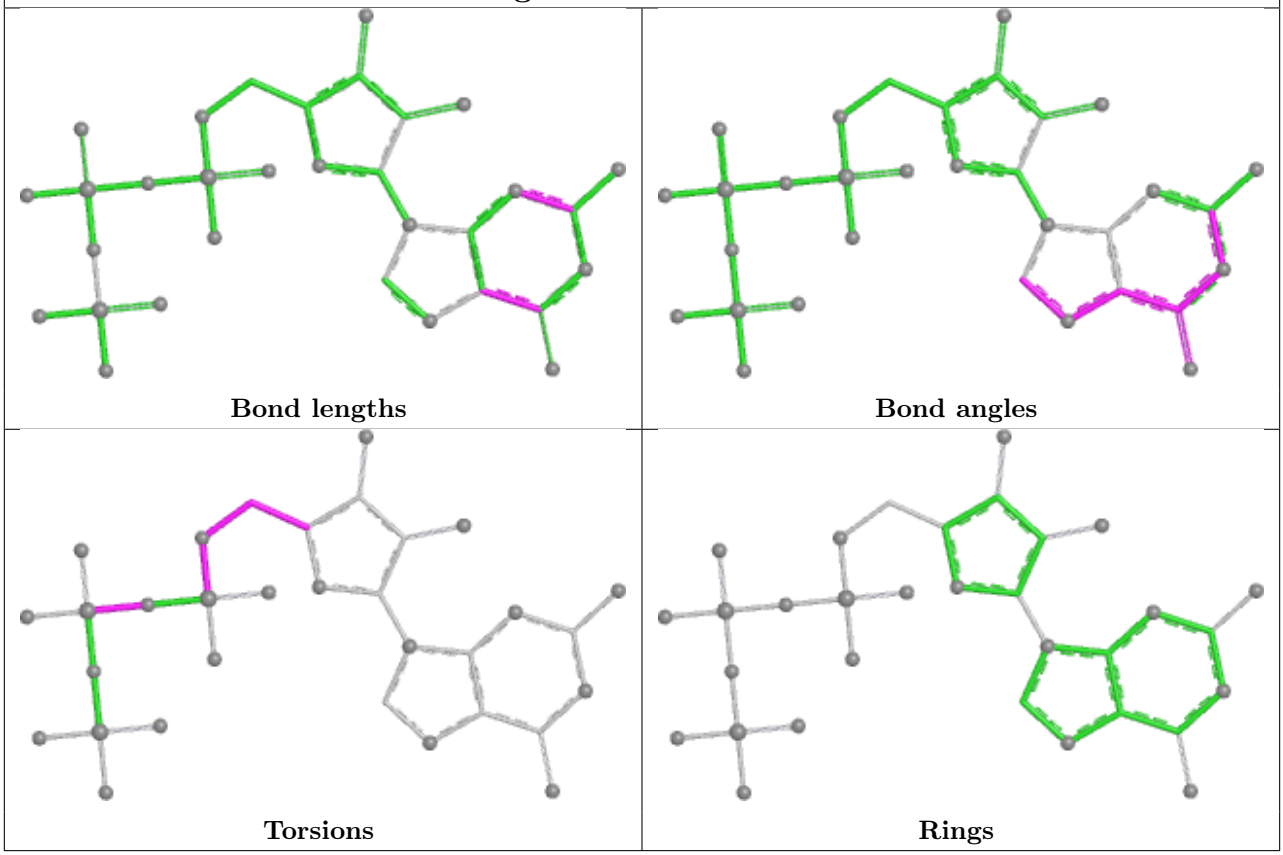
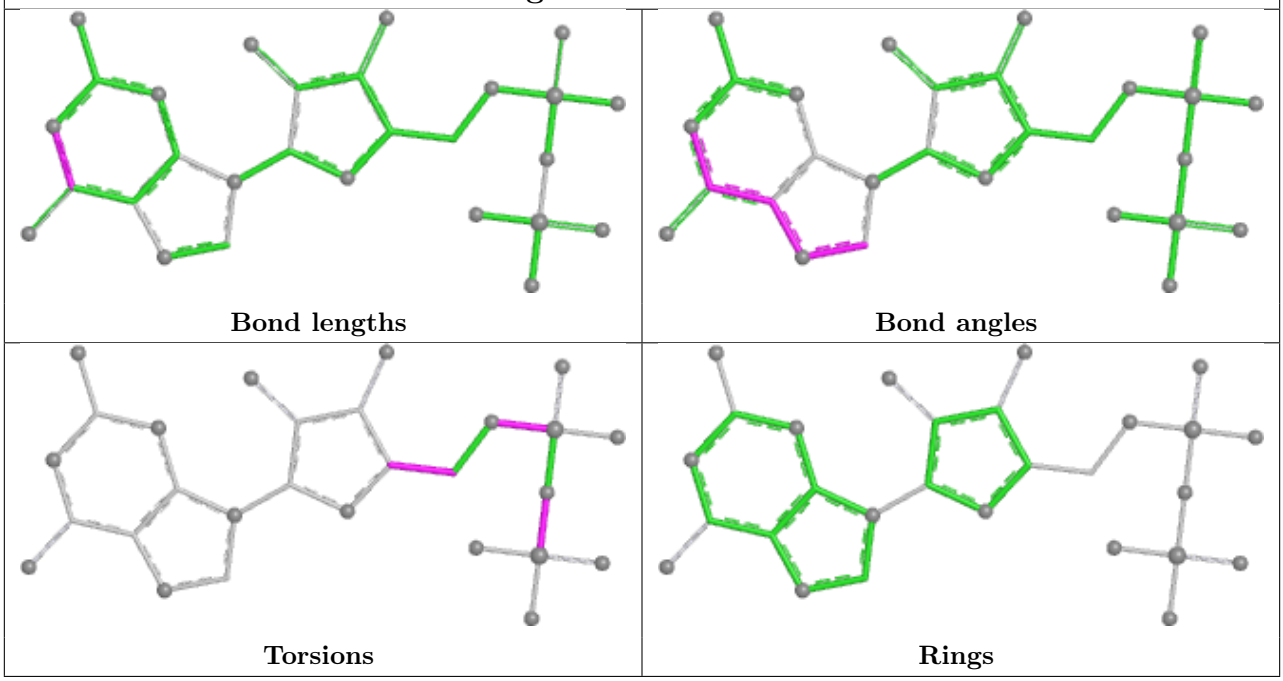



## Ligand GDP 2 501



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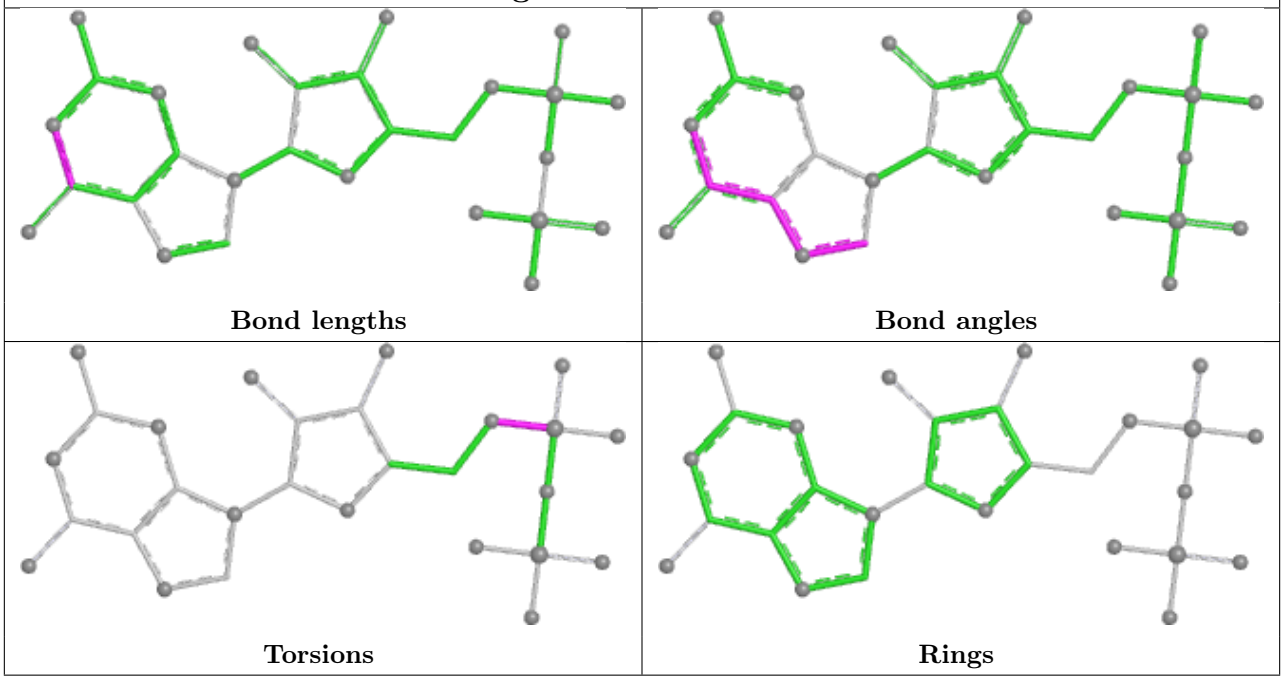


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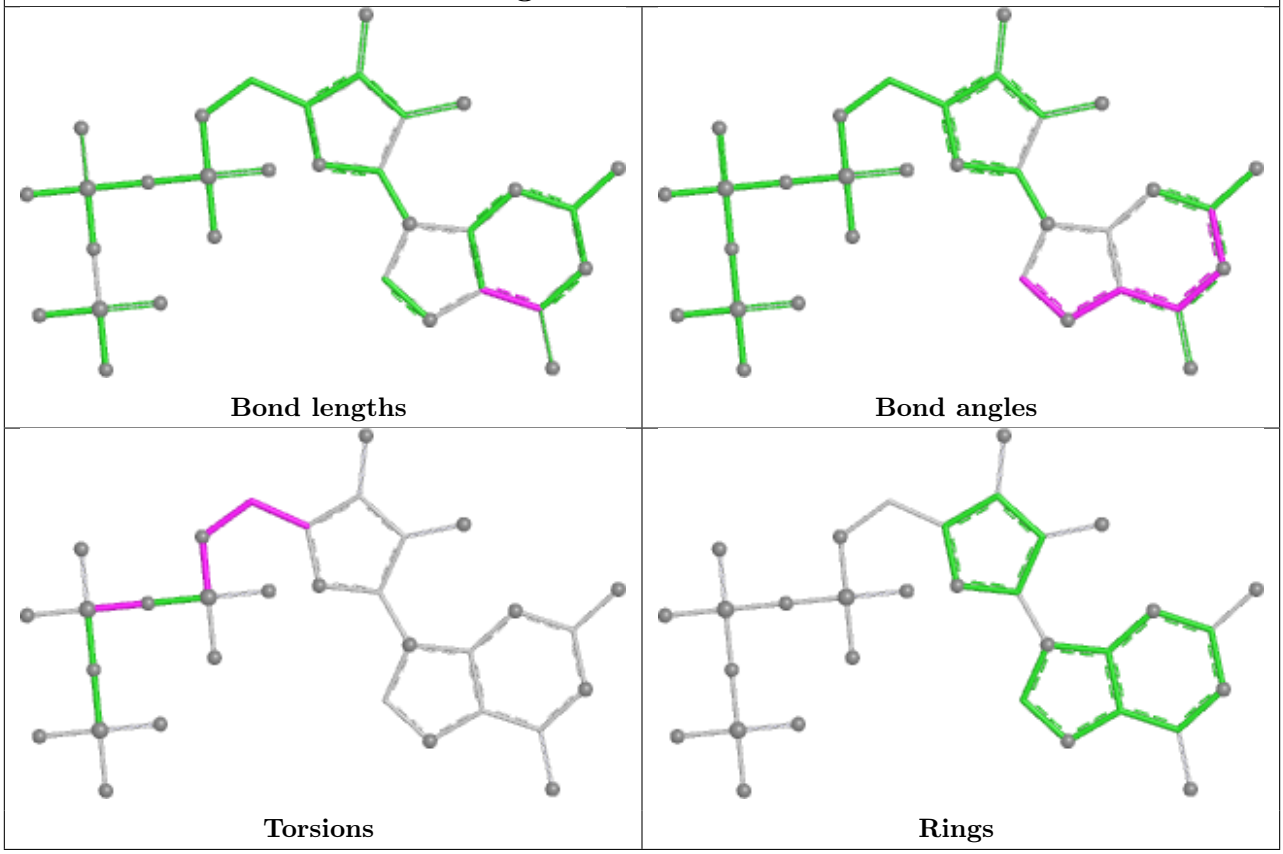

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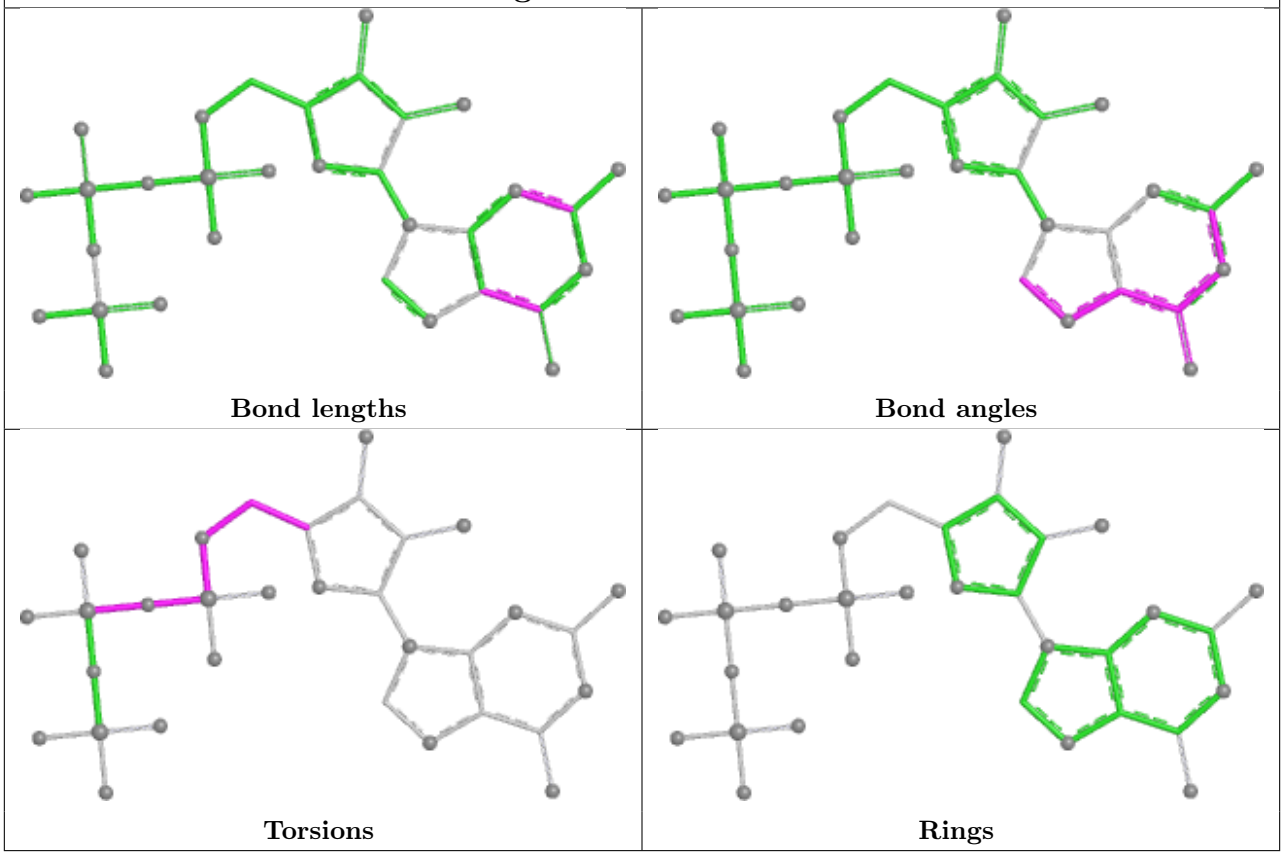


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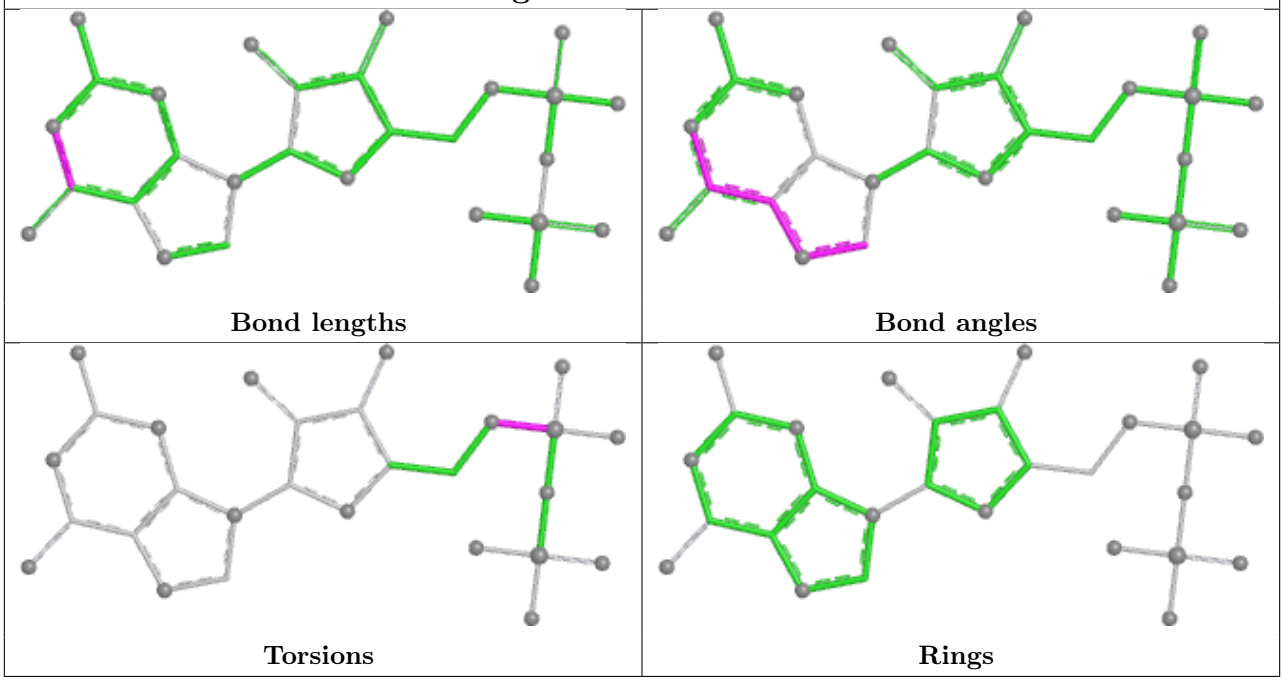

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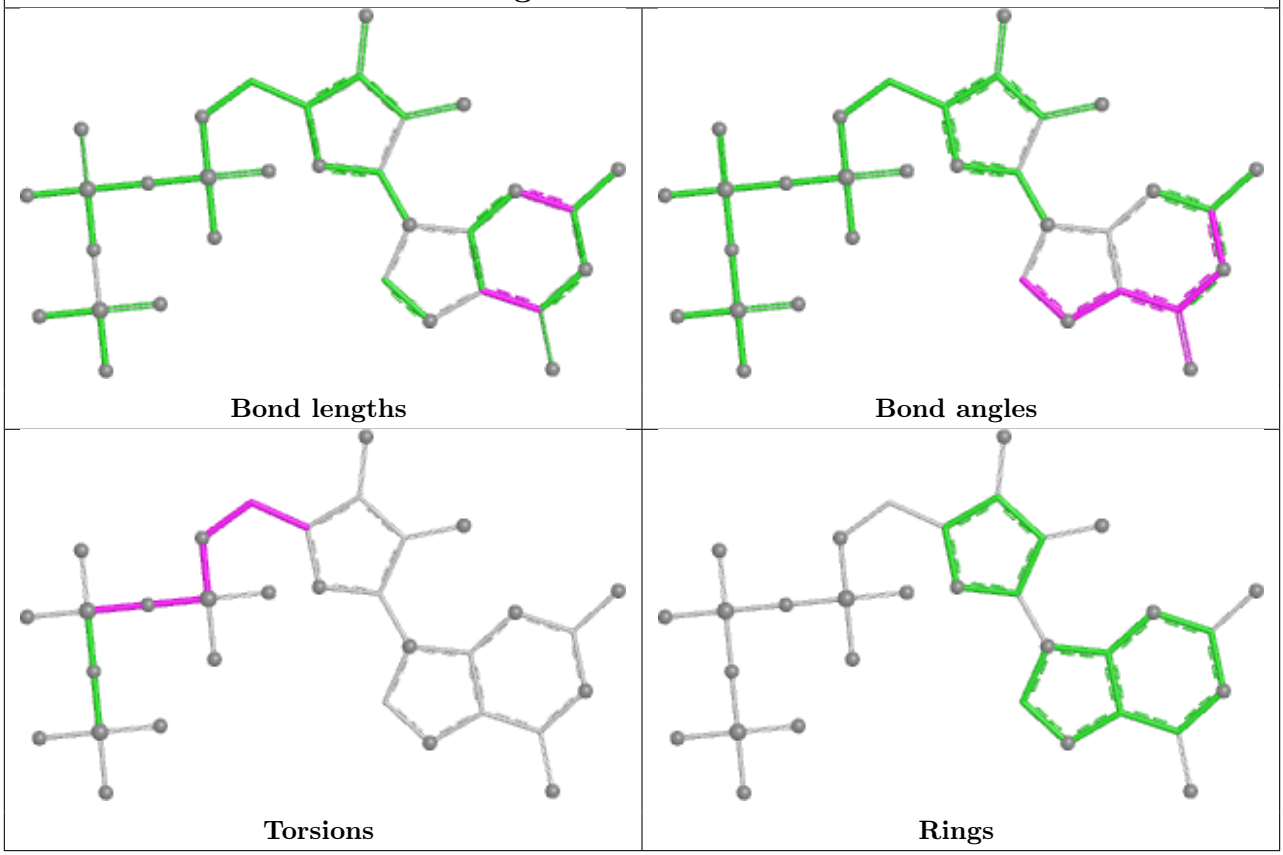


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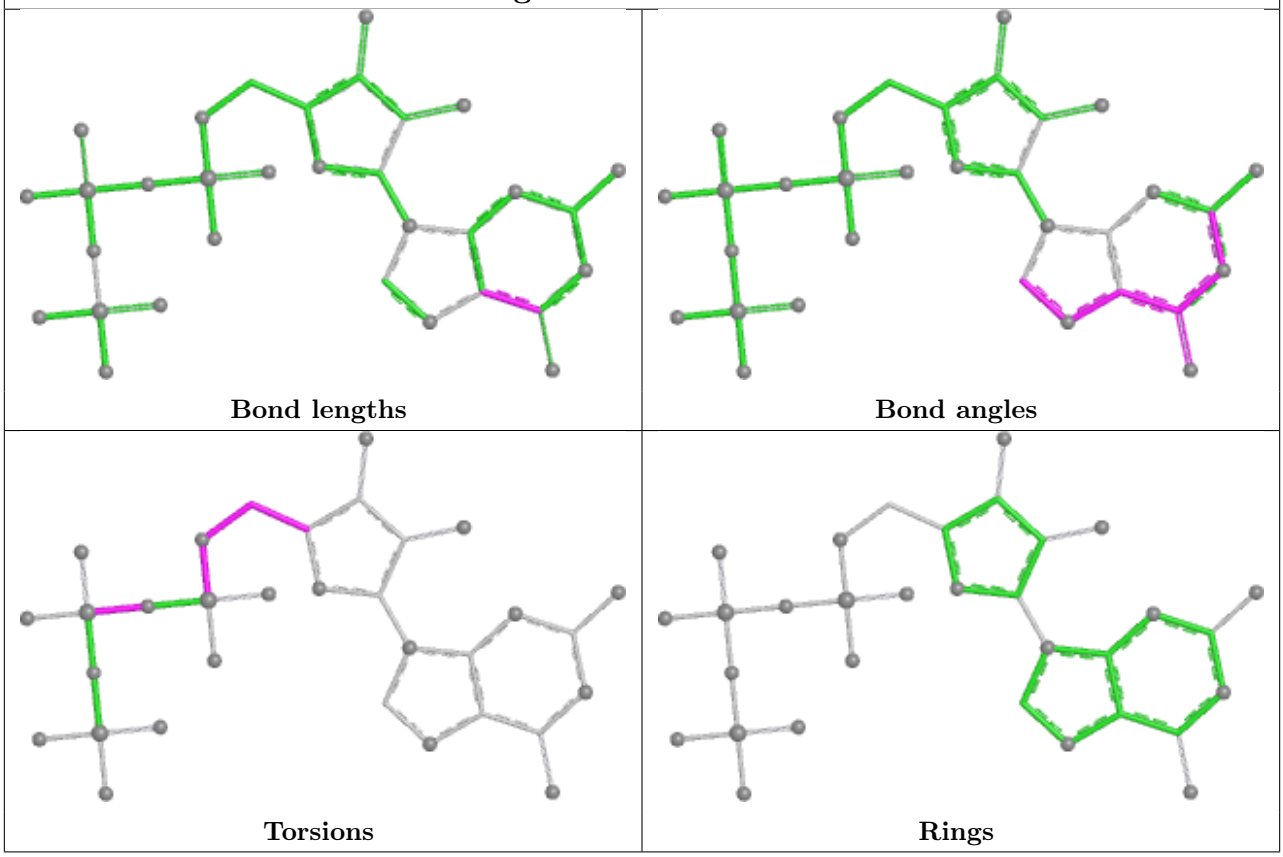

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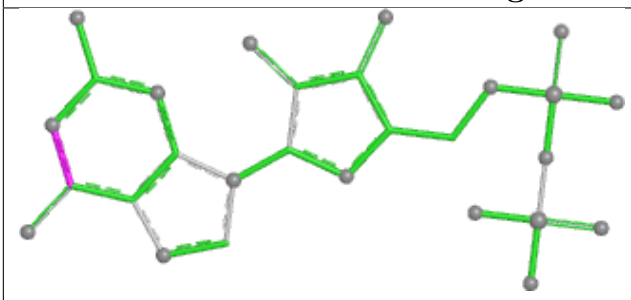
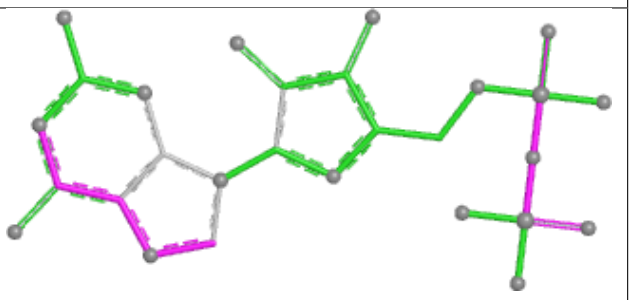
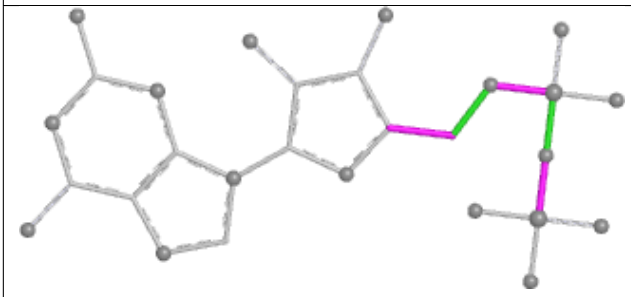
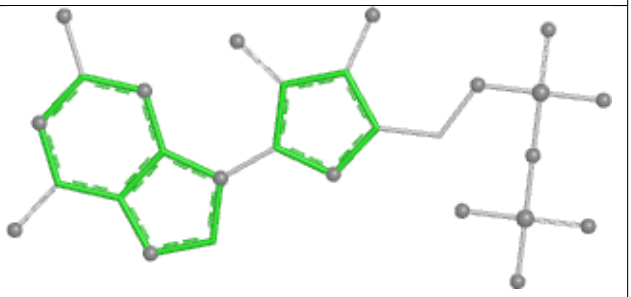
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP O2 502 | |
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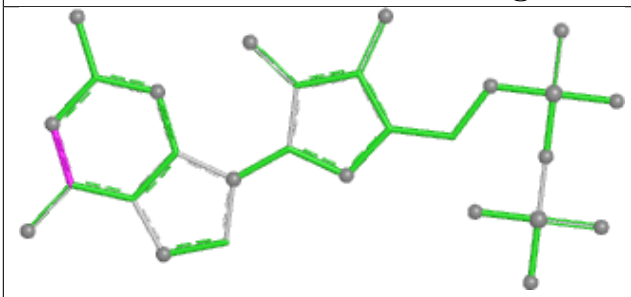
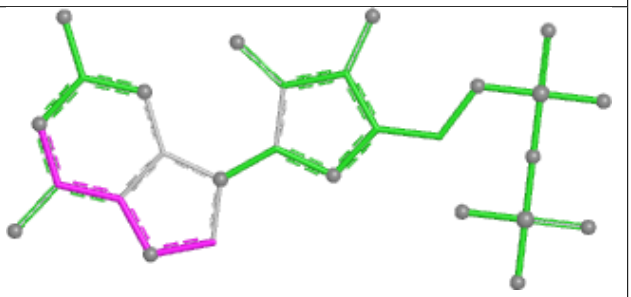
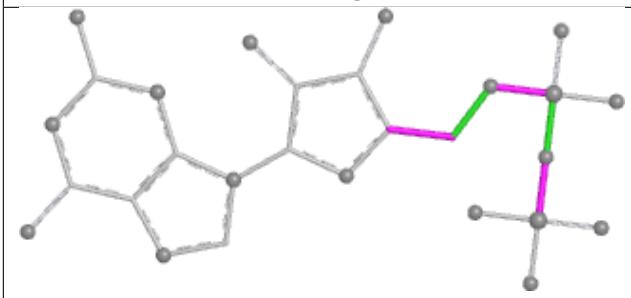
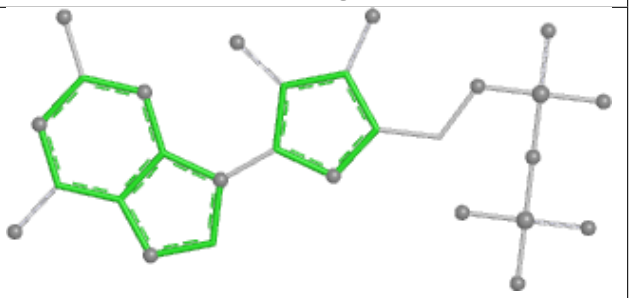
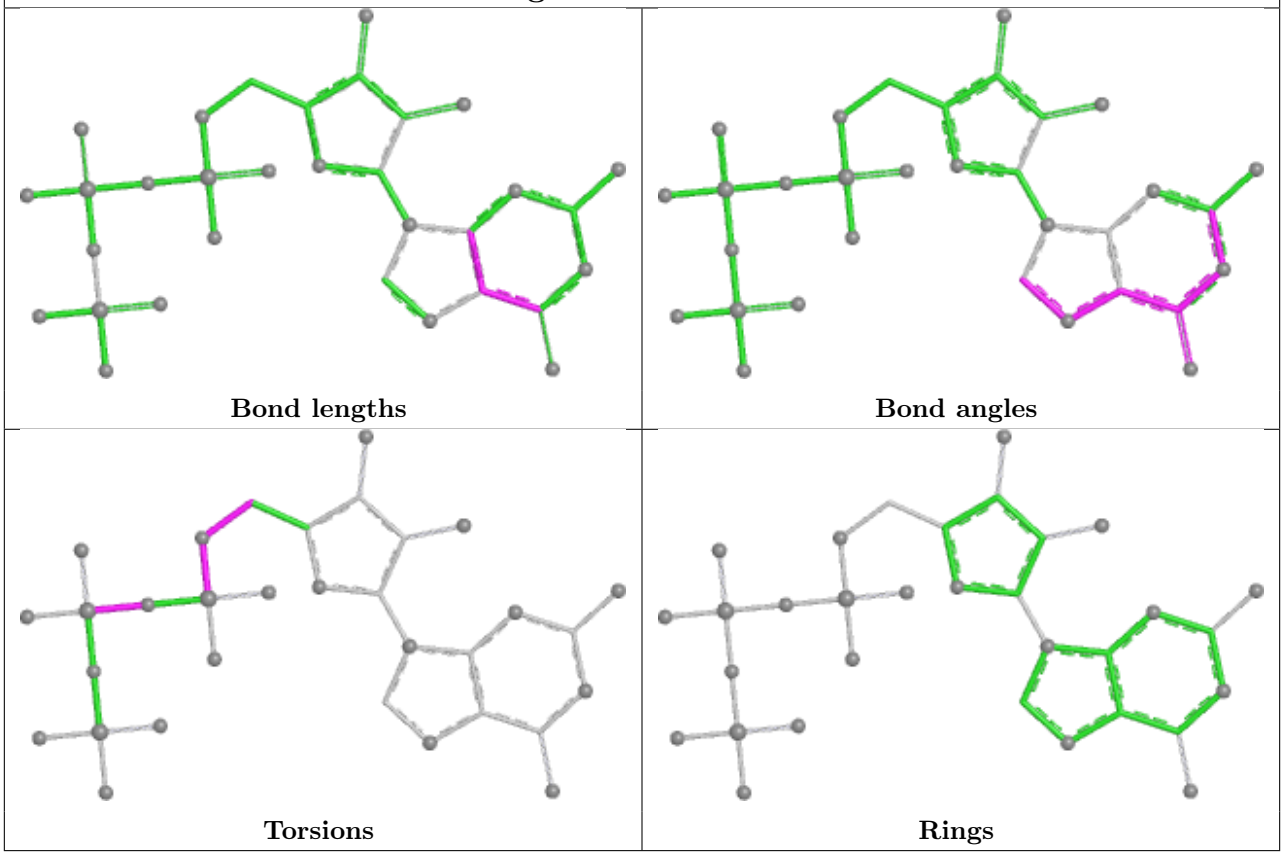
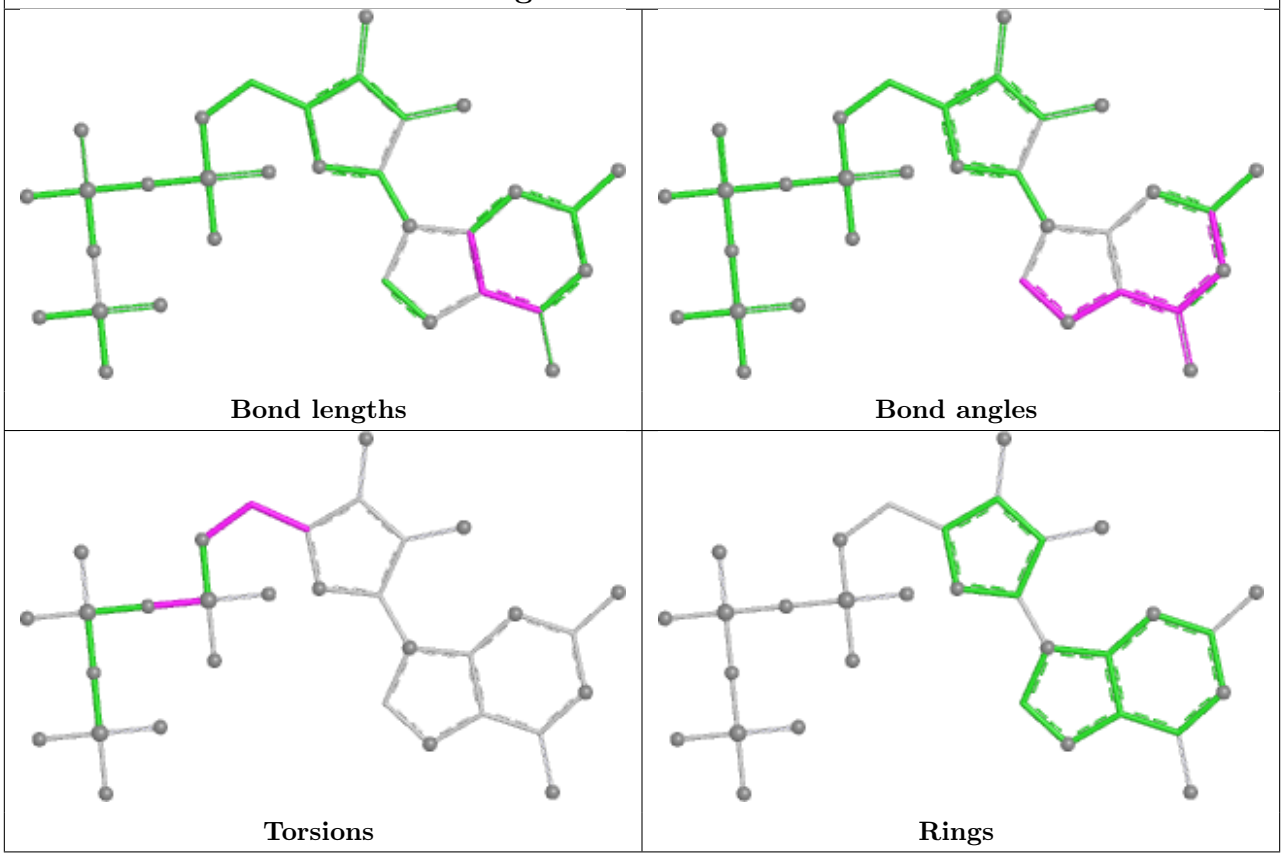
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand GTP 3 501




## Ligand GTP B2 501



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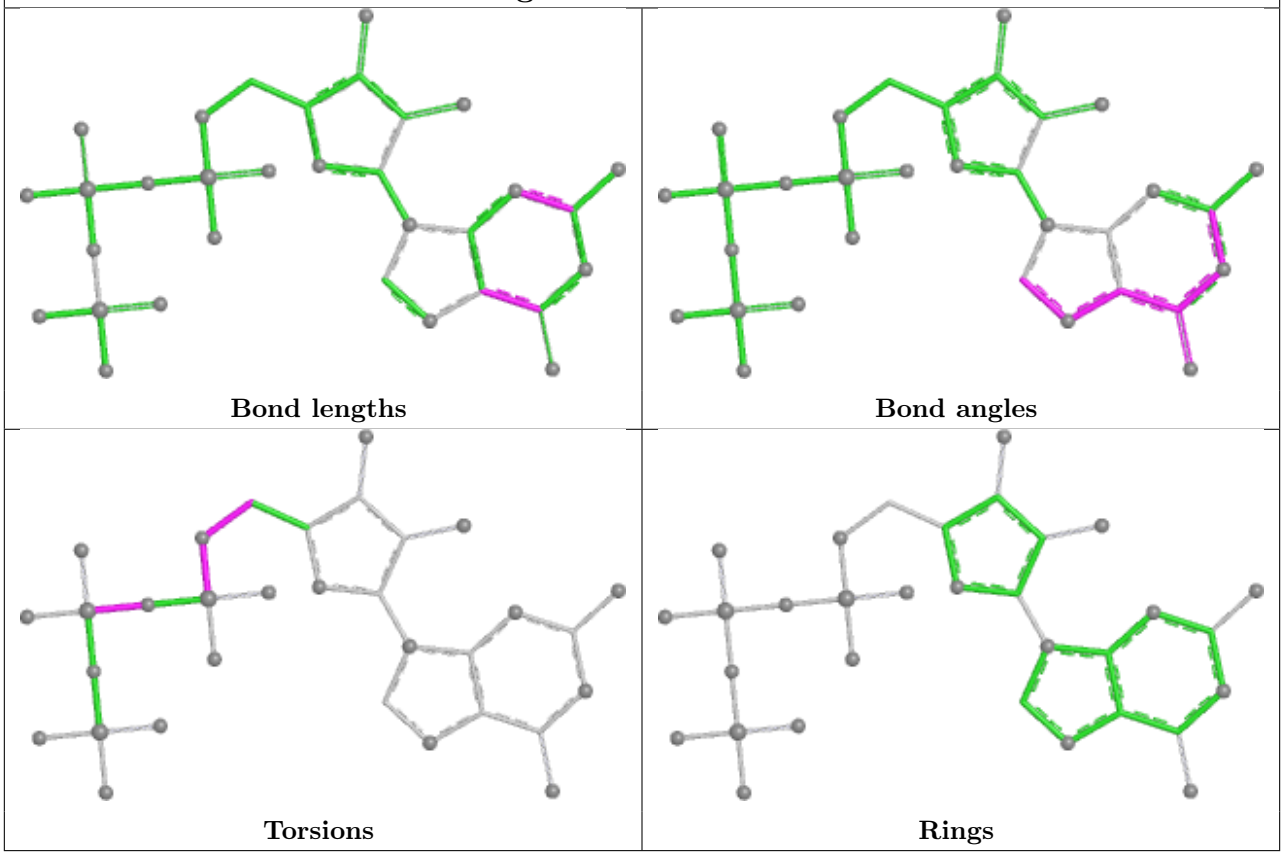
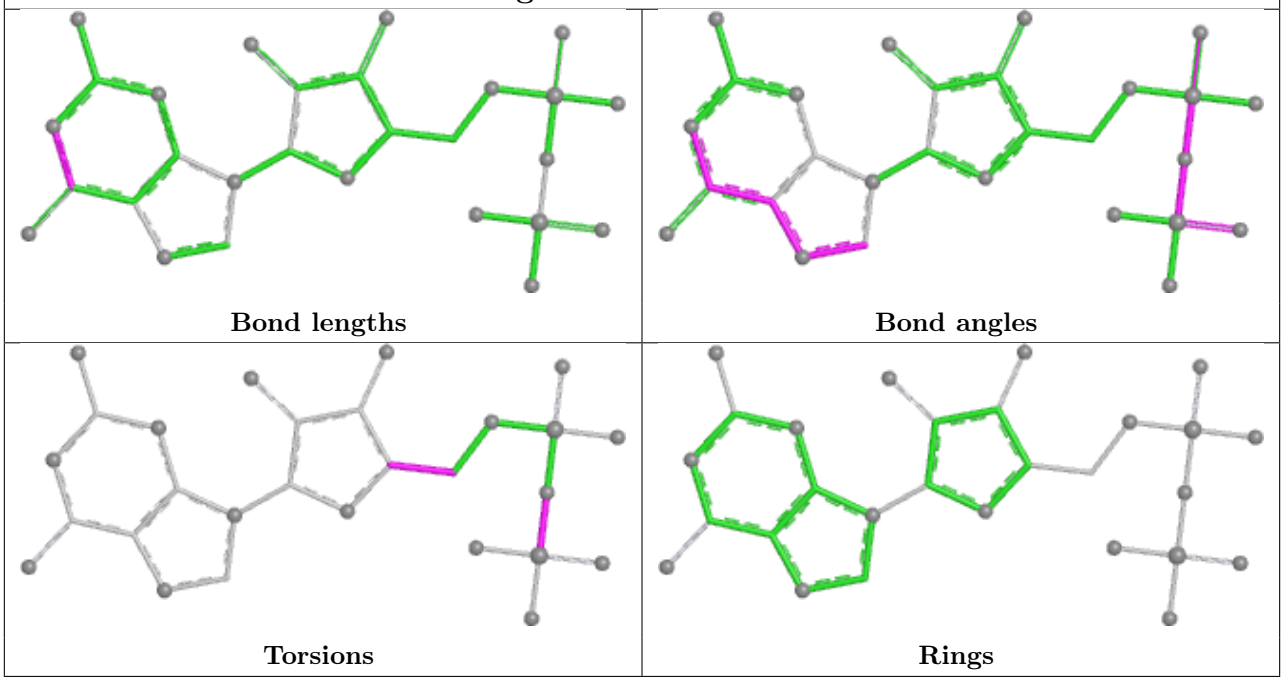
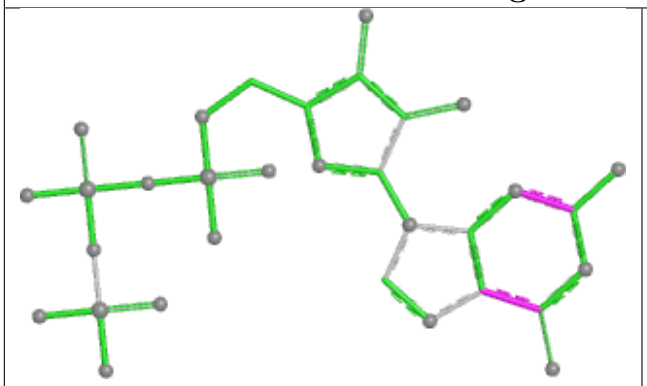


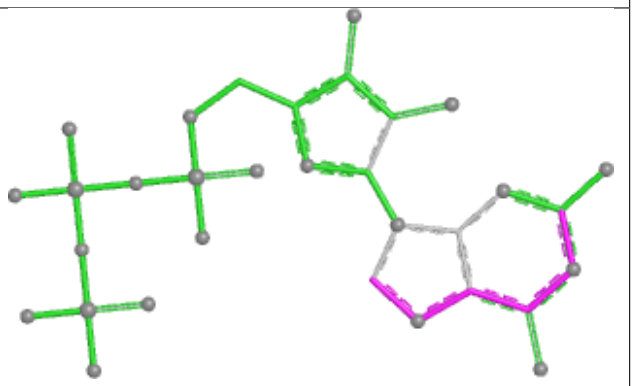

## Ligand GDP S0 502



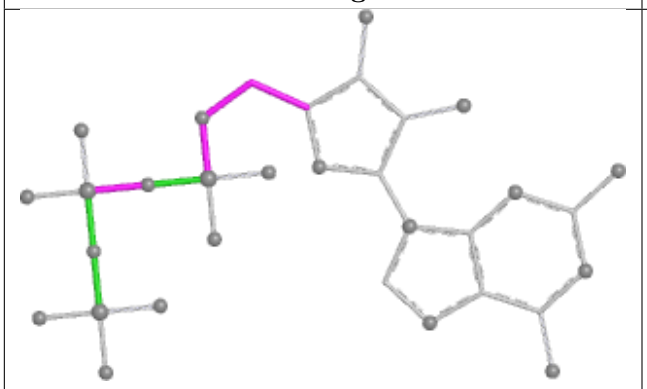
## Ligand GTP W2 501



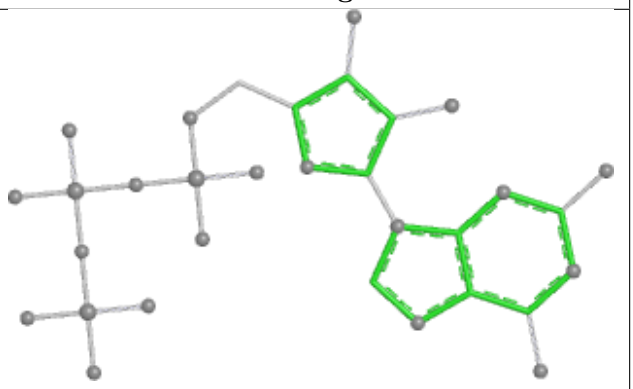
Bond lengths



Bond angles

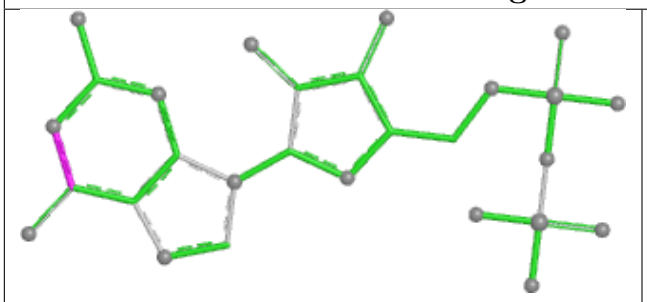


Torsions



Rings

## Ligand GDP M8 501



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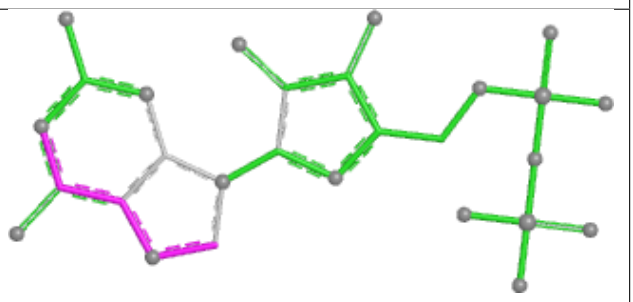

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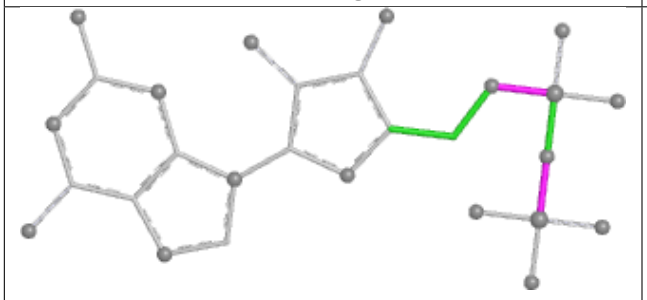

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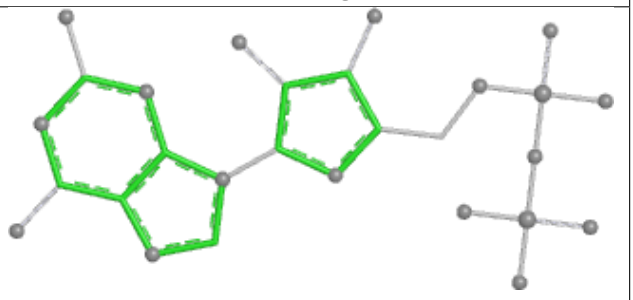
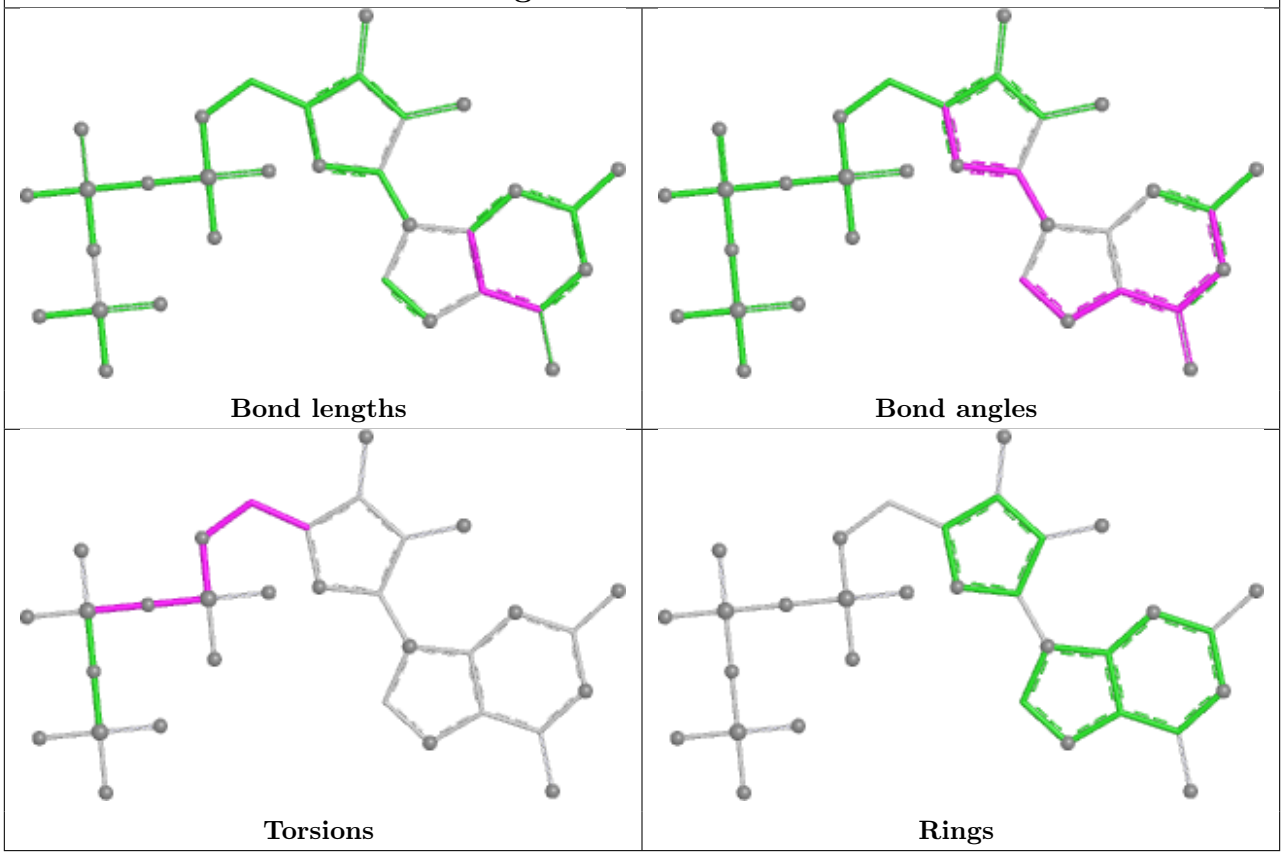
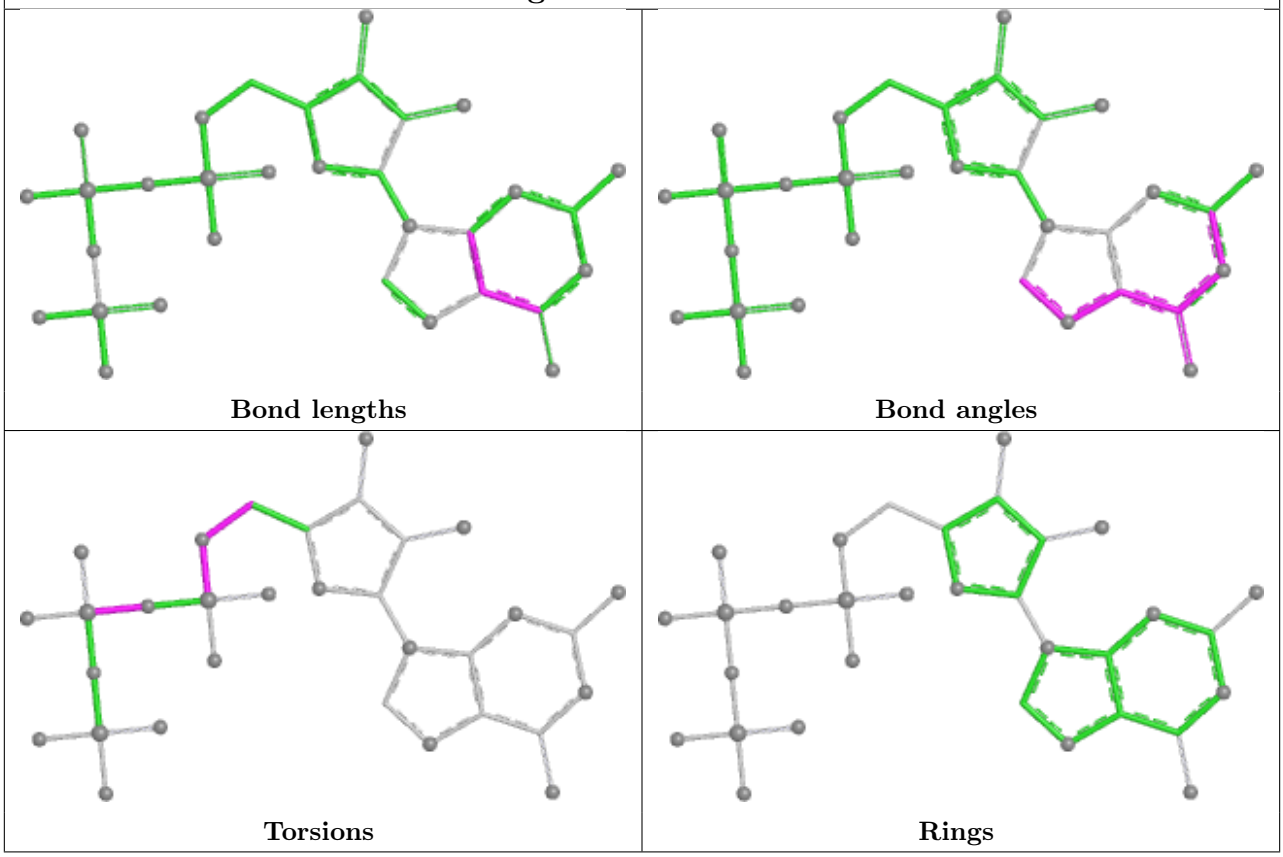


Rings

## Ligand GTP O2 501




## Ligand GTP 4 501



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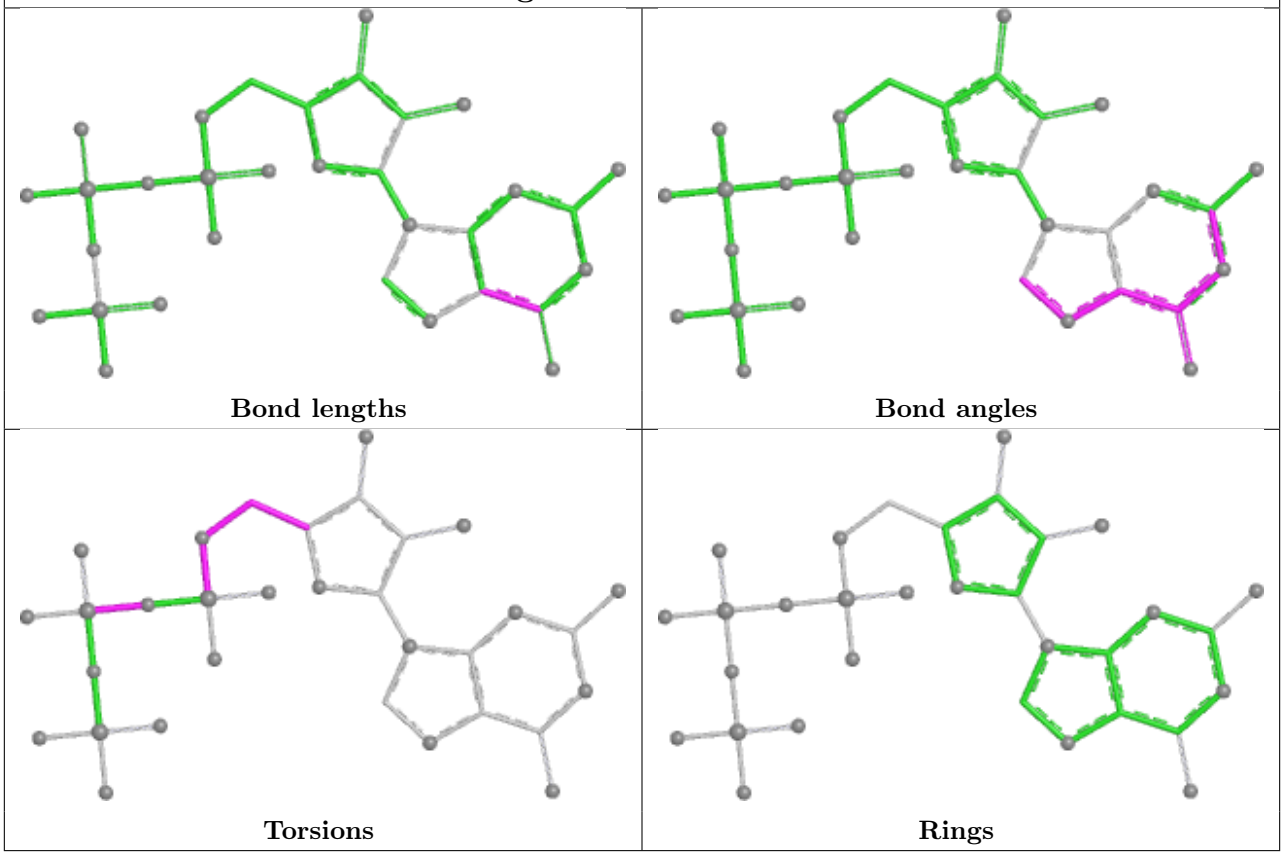


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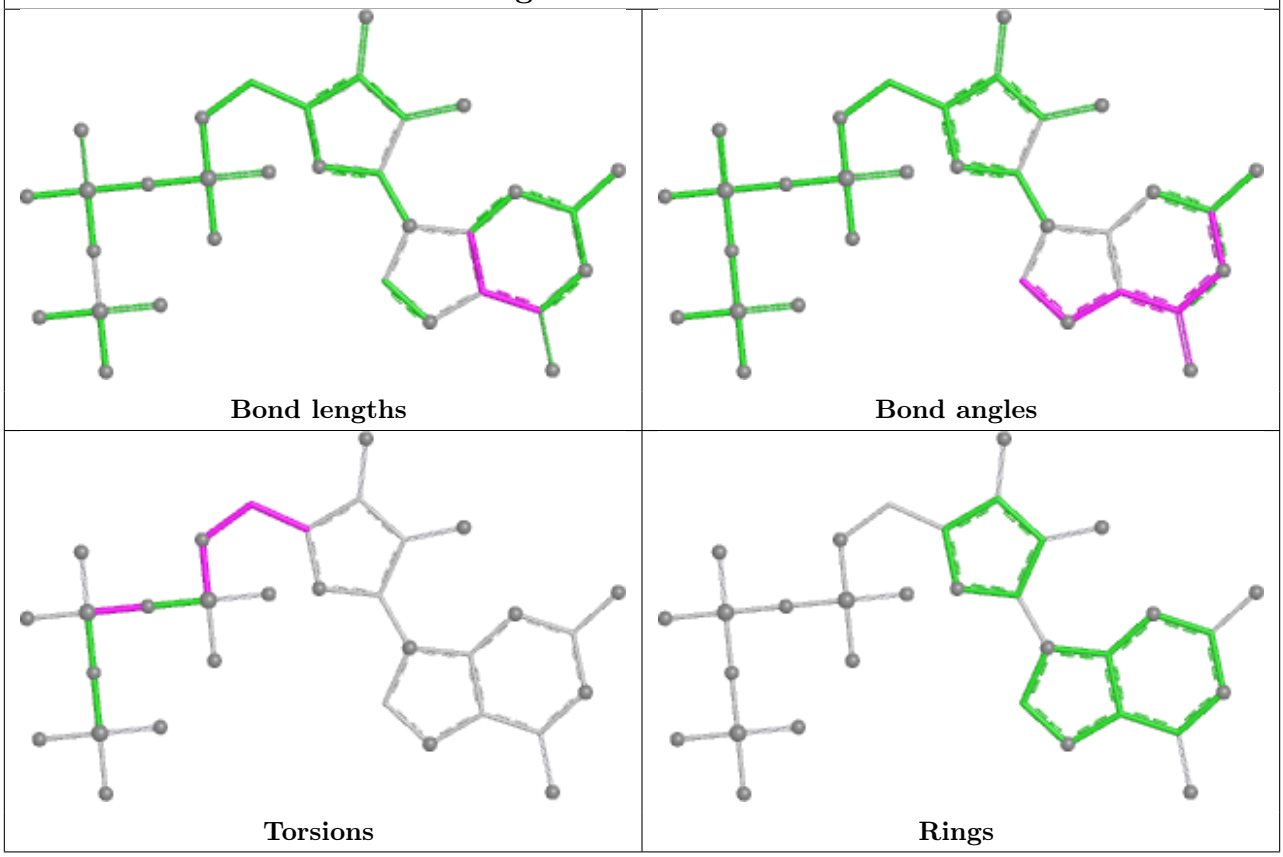

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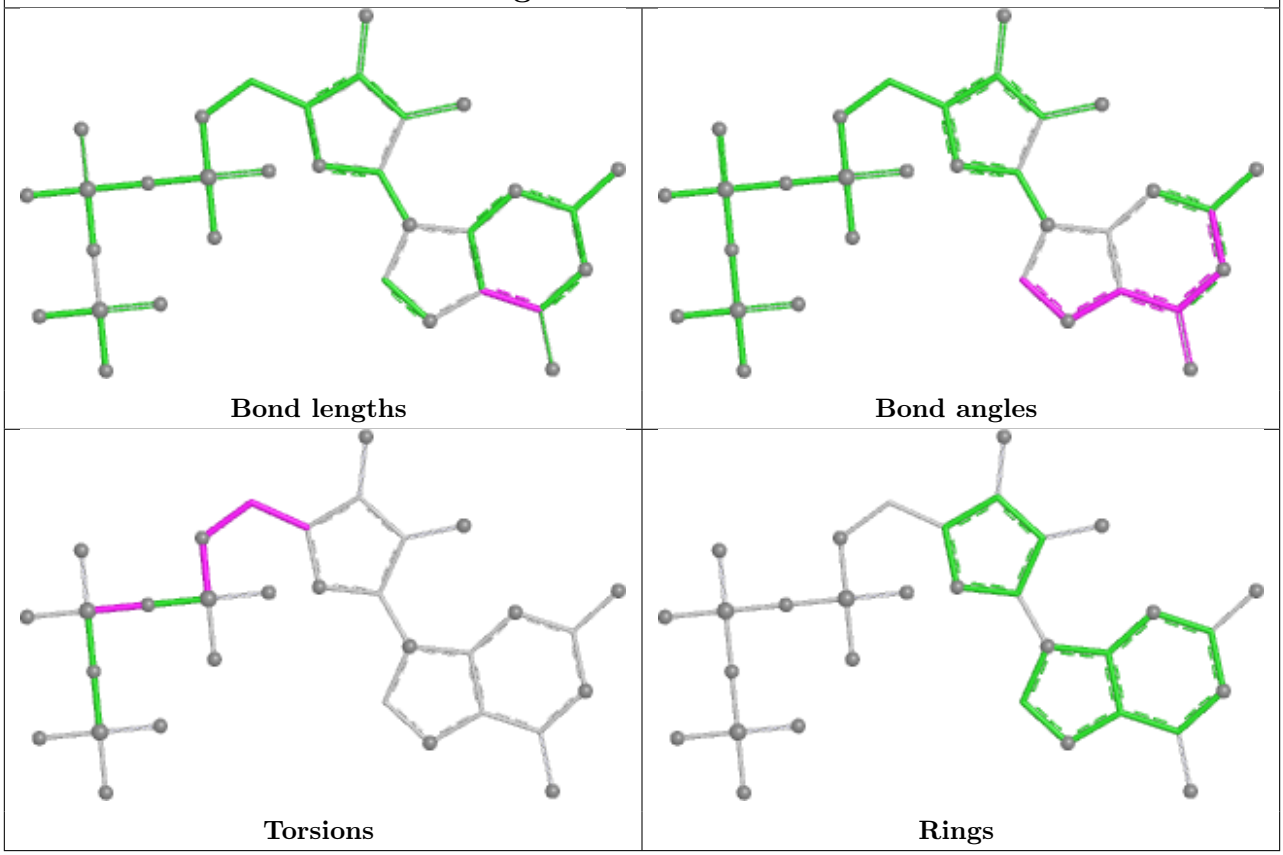


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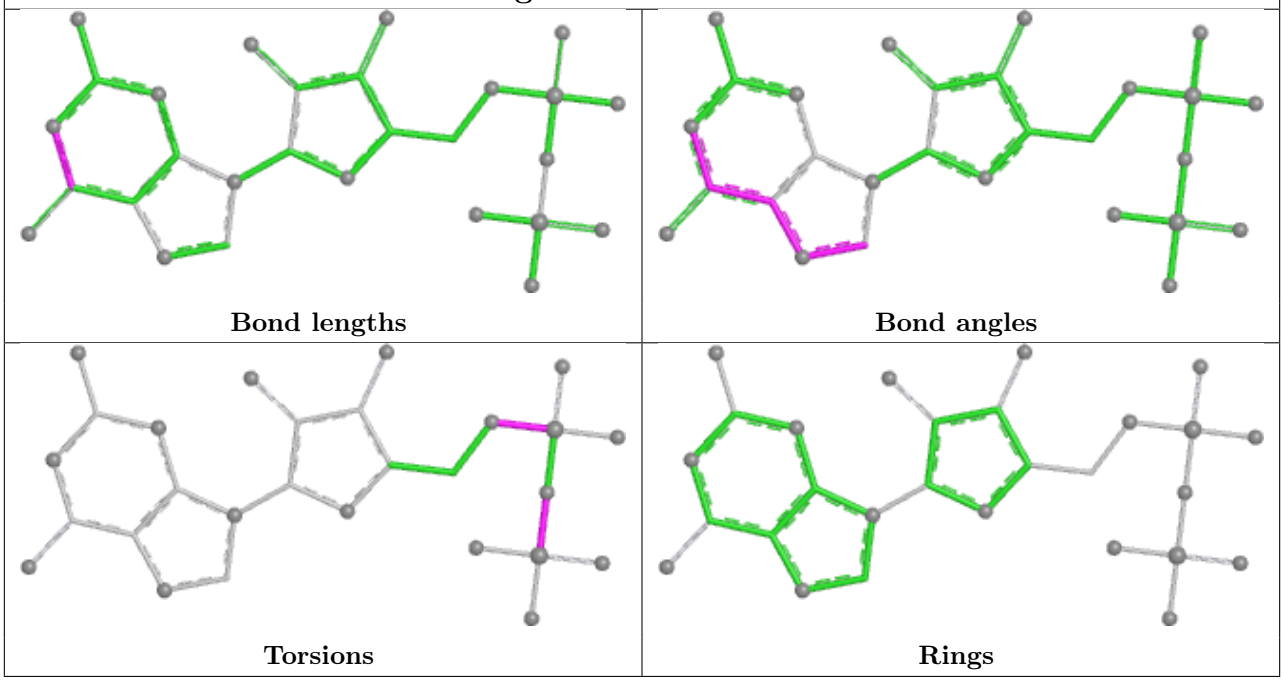
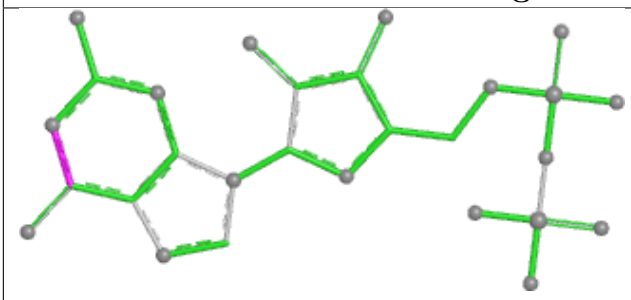
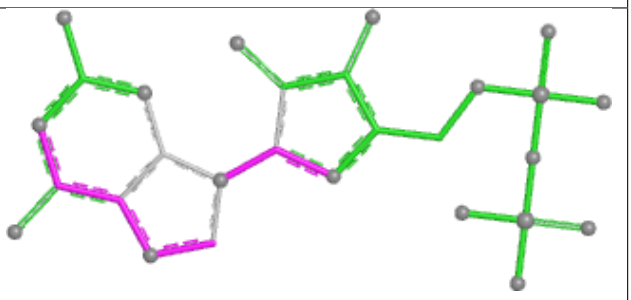


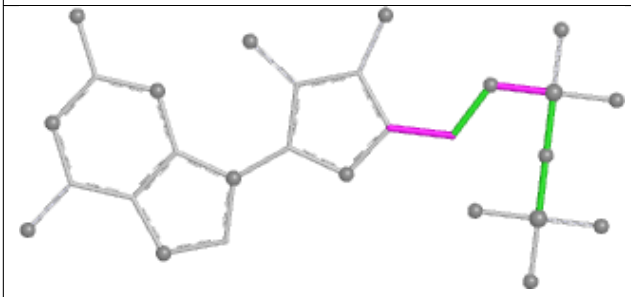
## Ligand GDP B3 501



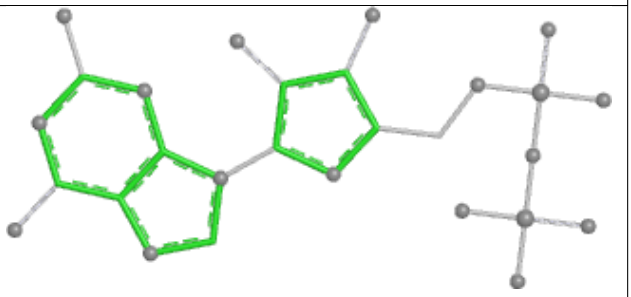
Bond lengths



Bond angles

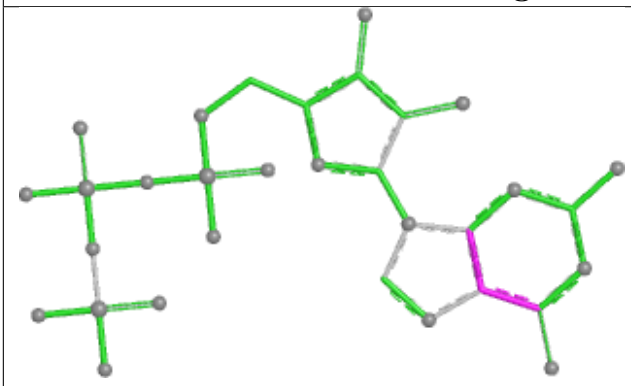


Torsions



Rings

## Ligand GTP X6 501



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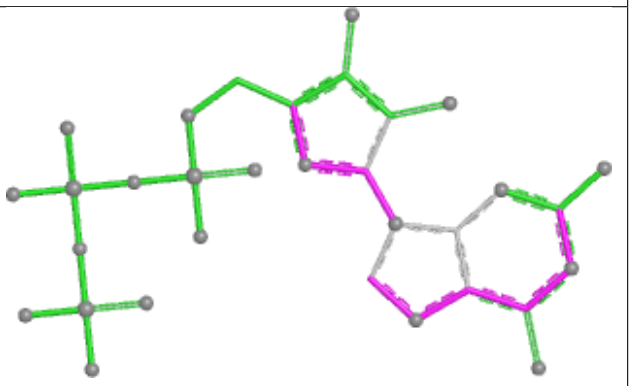

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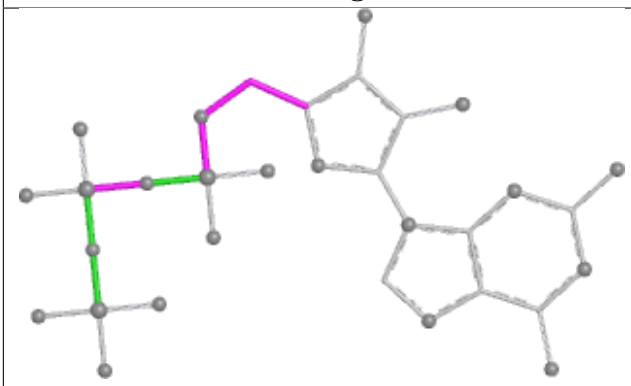

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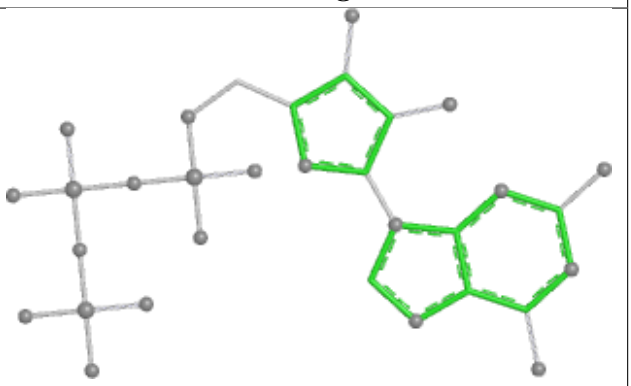

Rings

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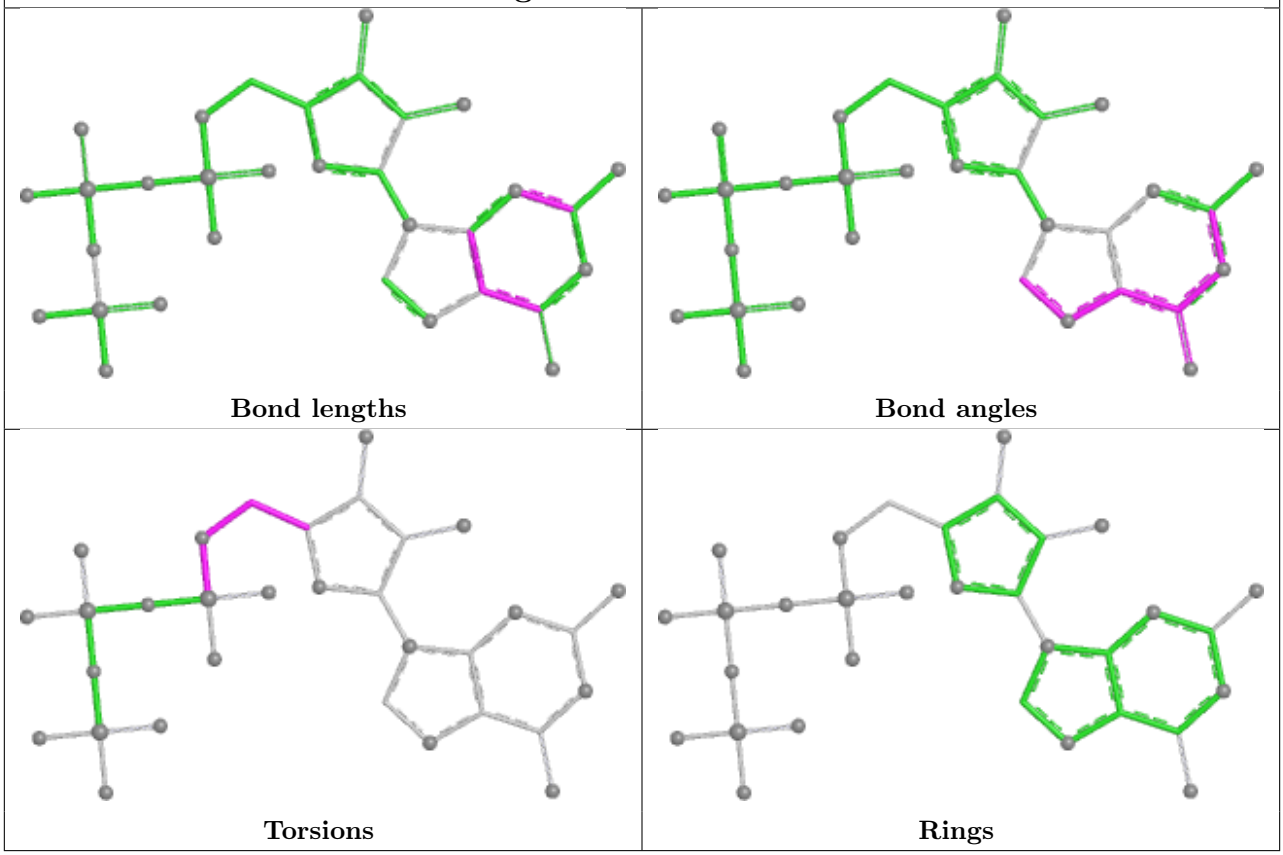


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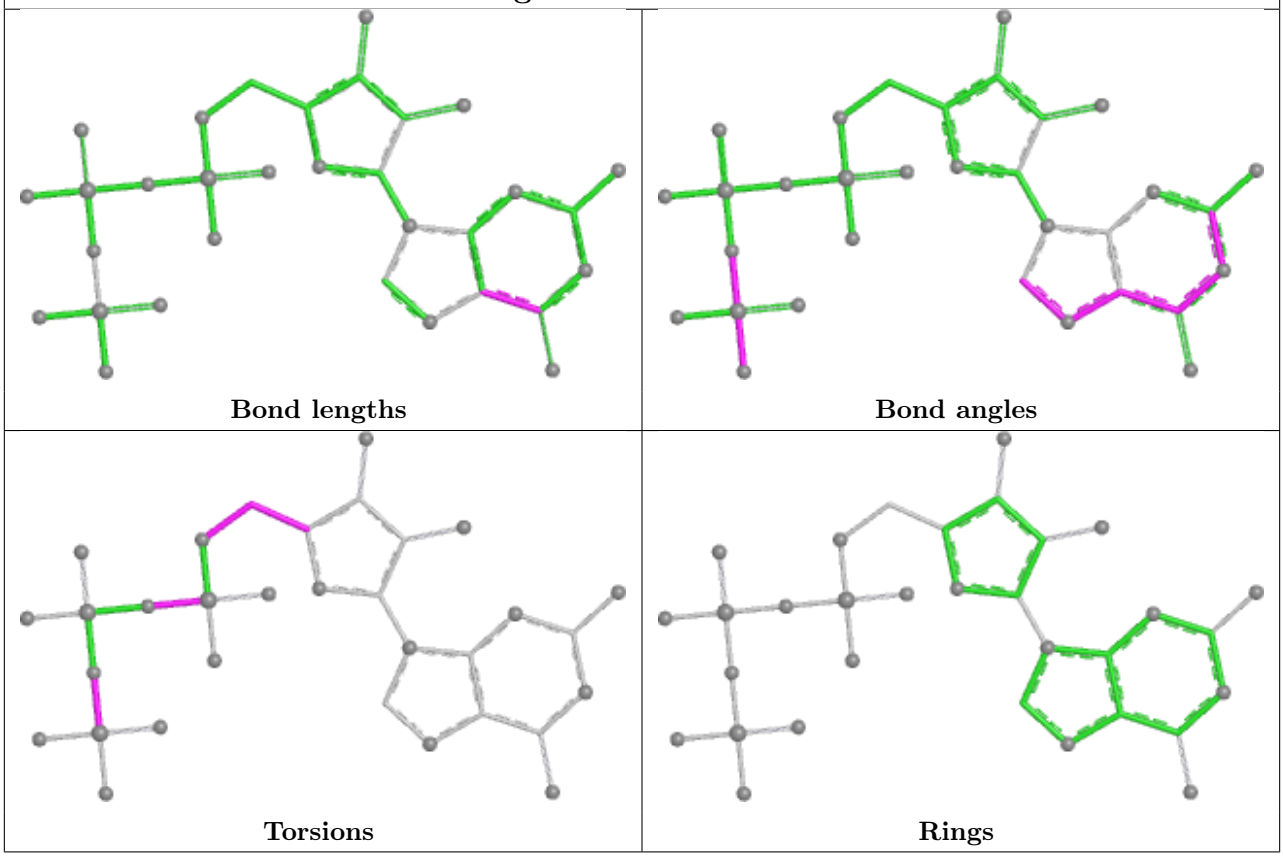
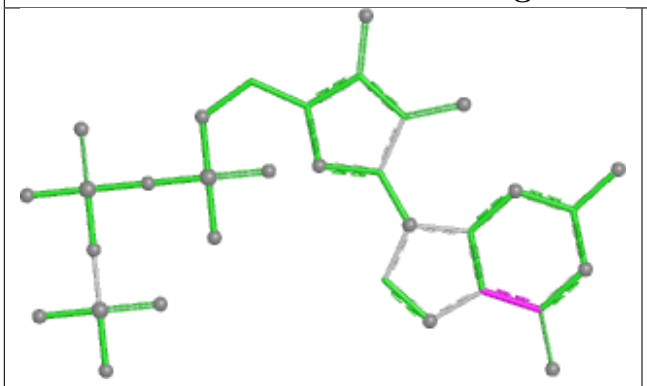
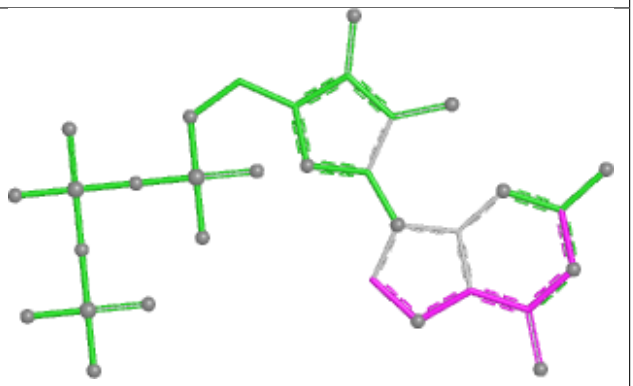


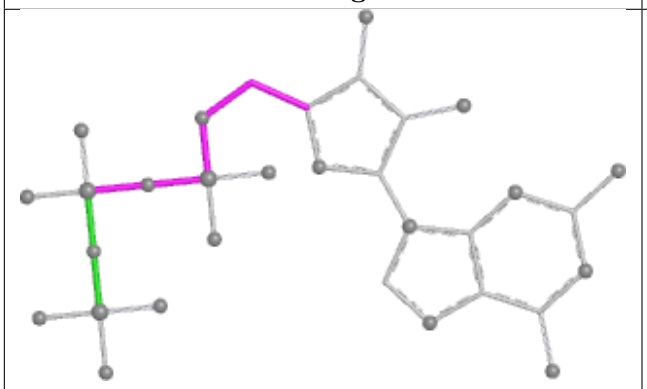
## Ligand GTP 0A 501



Bond lengths



Bond angles



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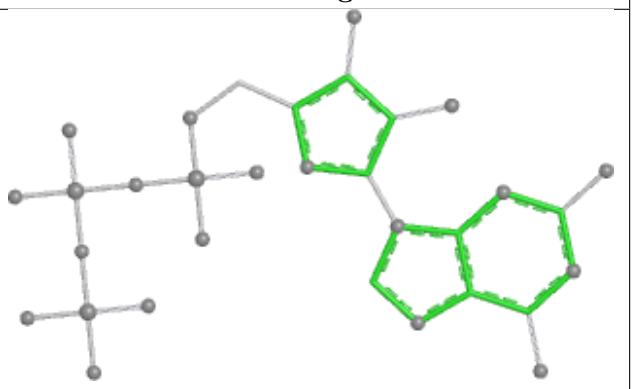

Rings

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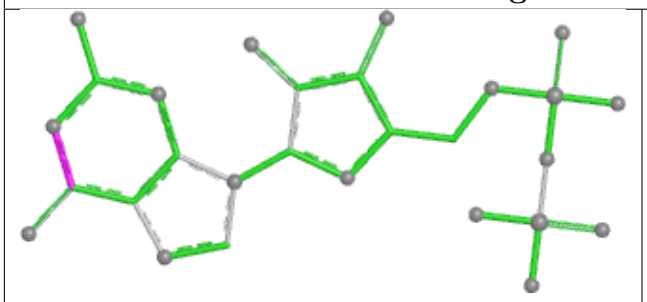

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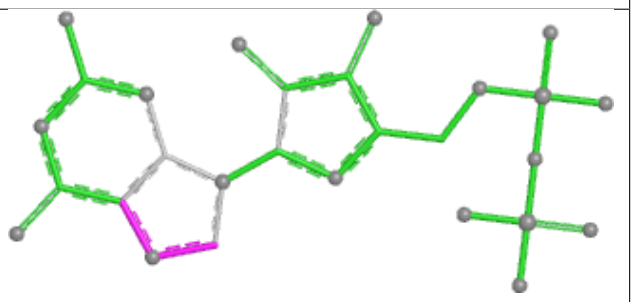

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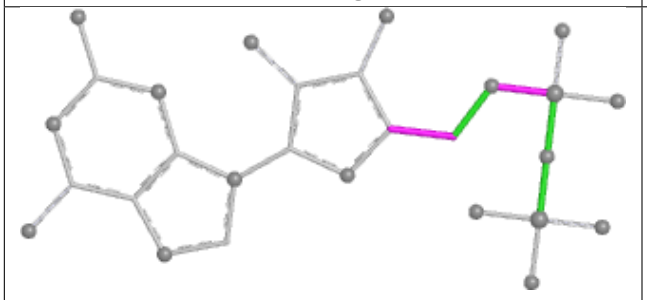

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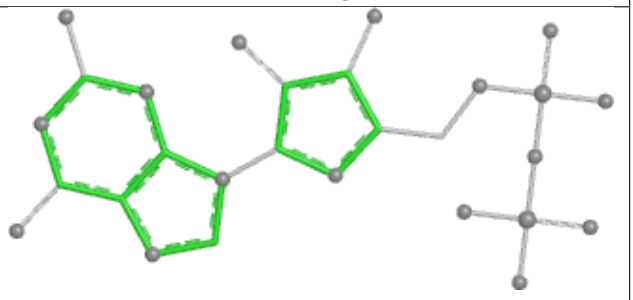
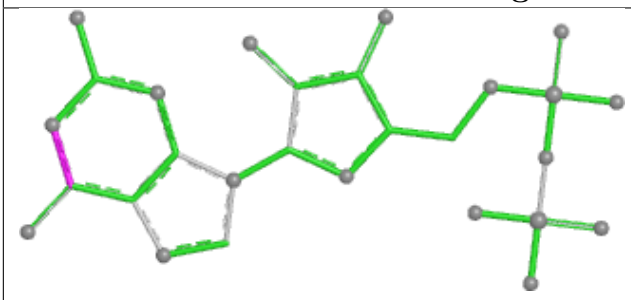


Rings

## Ligand GDP U8 501



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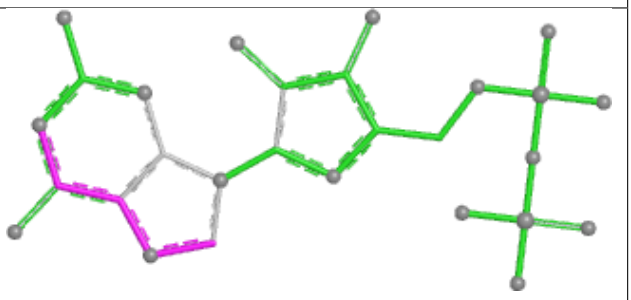
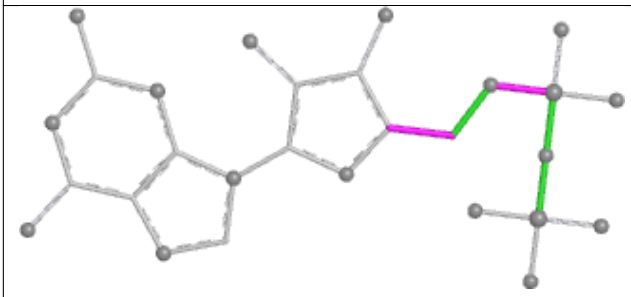


Bond angles



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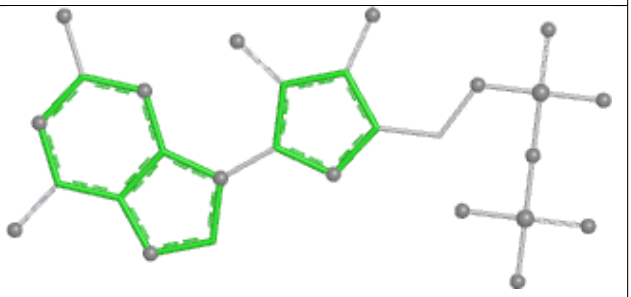
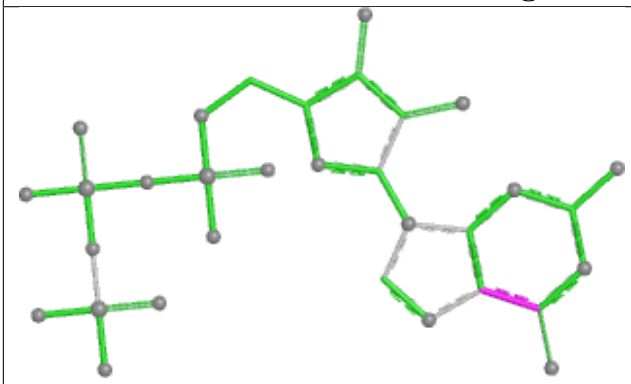


Rings

## Ligand GTP 2I 501



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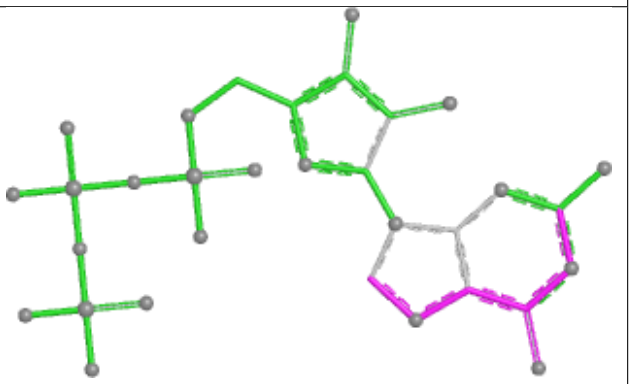

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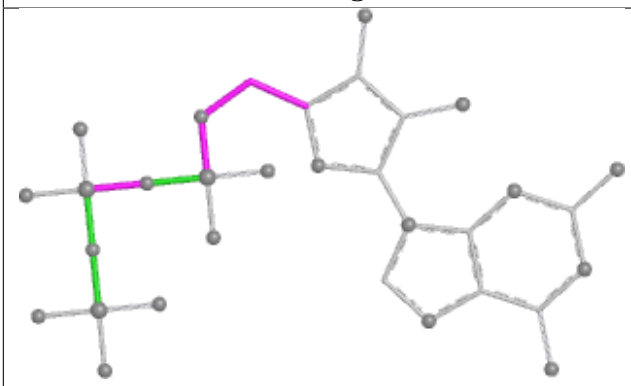

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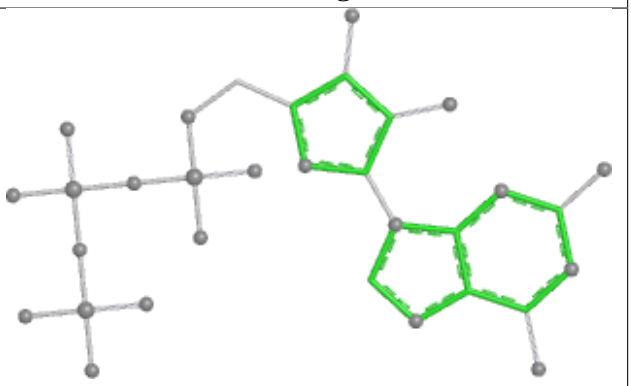
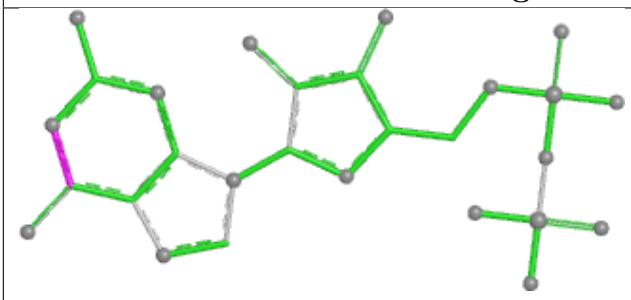


Rings

## Ligand GDP C0 502



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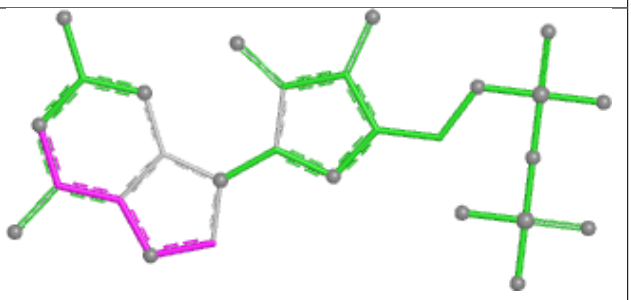

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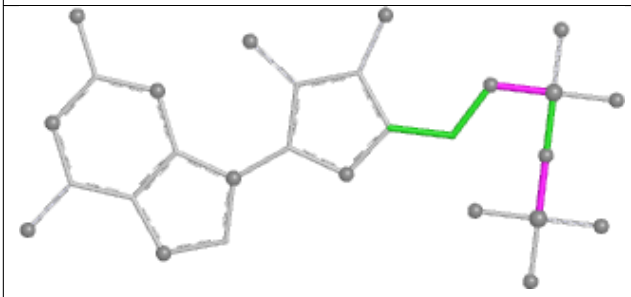

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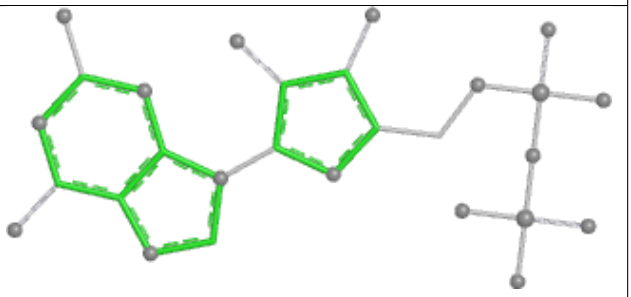
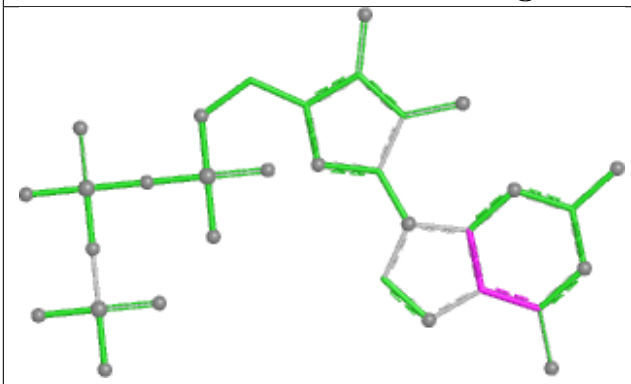


Rings

## Ligand GTP 3S 501



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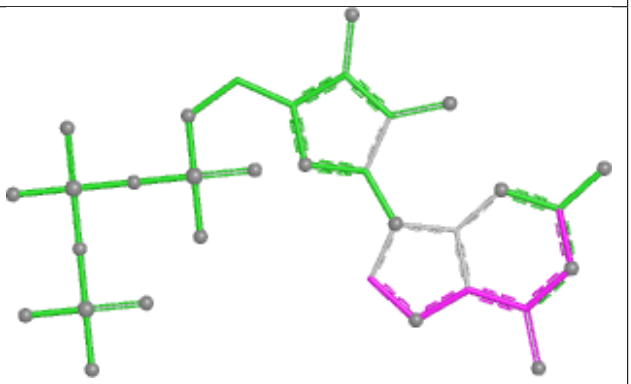

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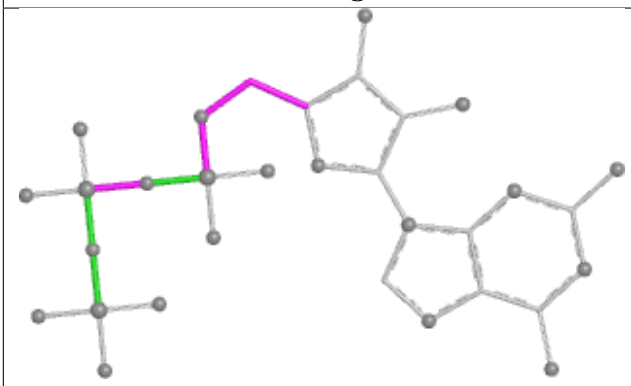

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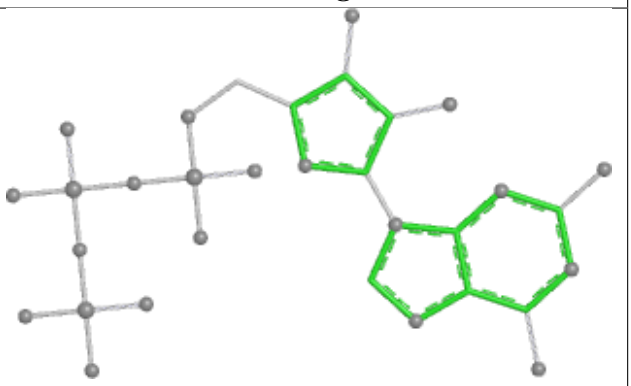
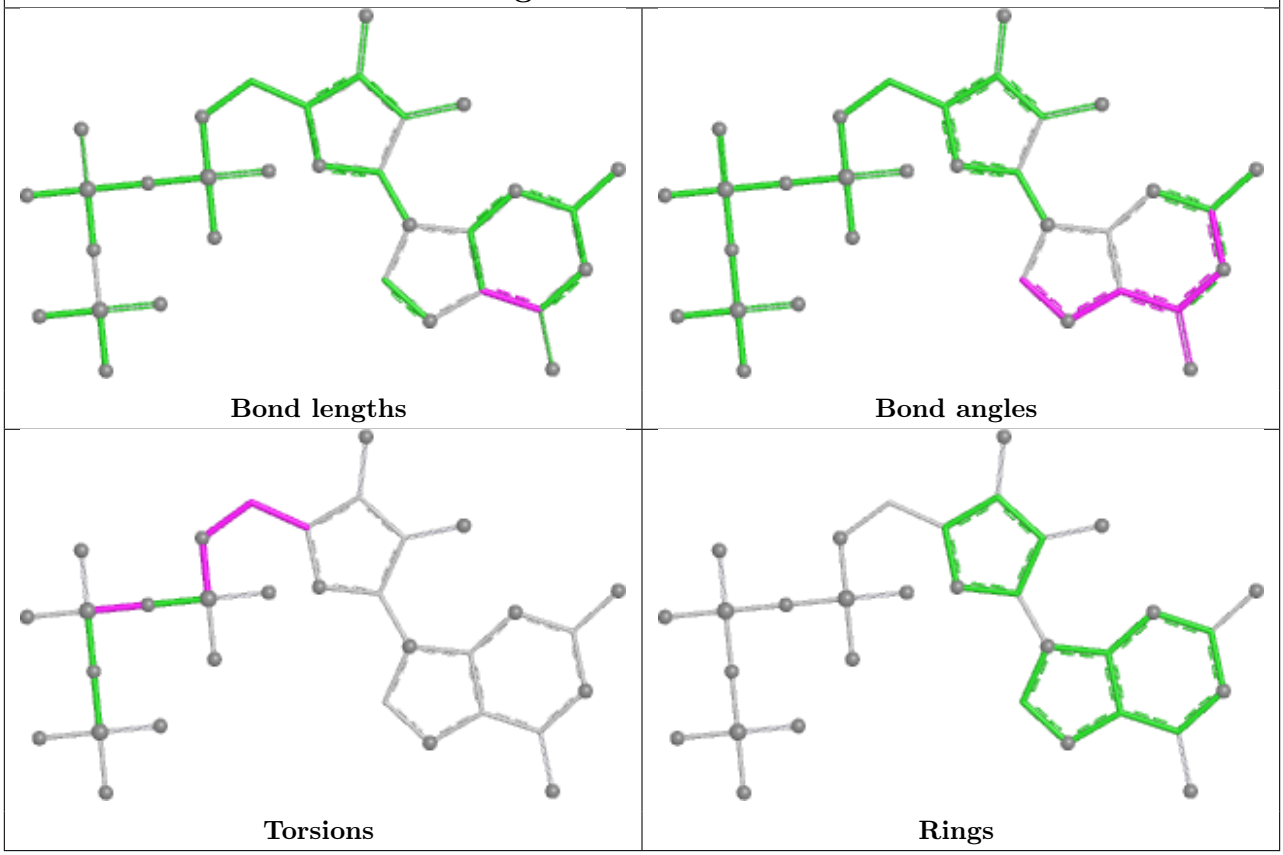


Rings

## Ligand GTP 0C 501

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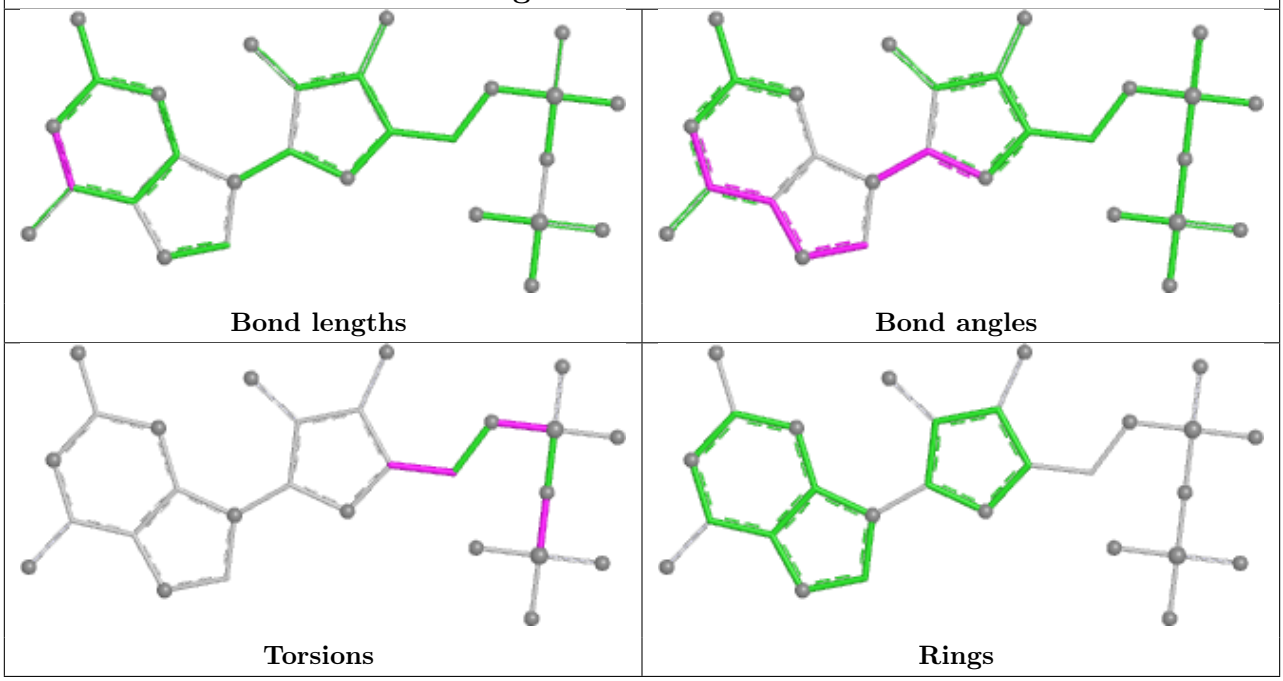

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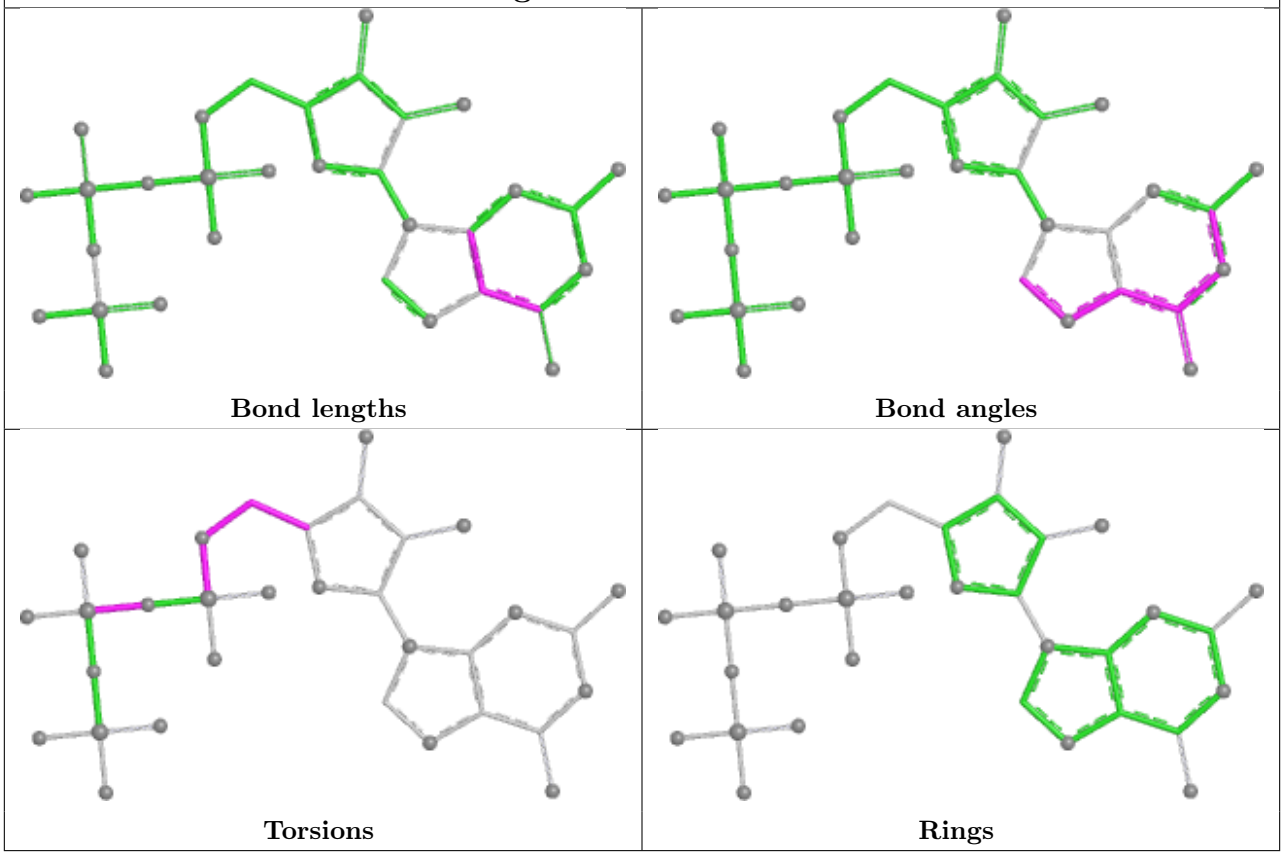


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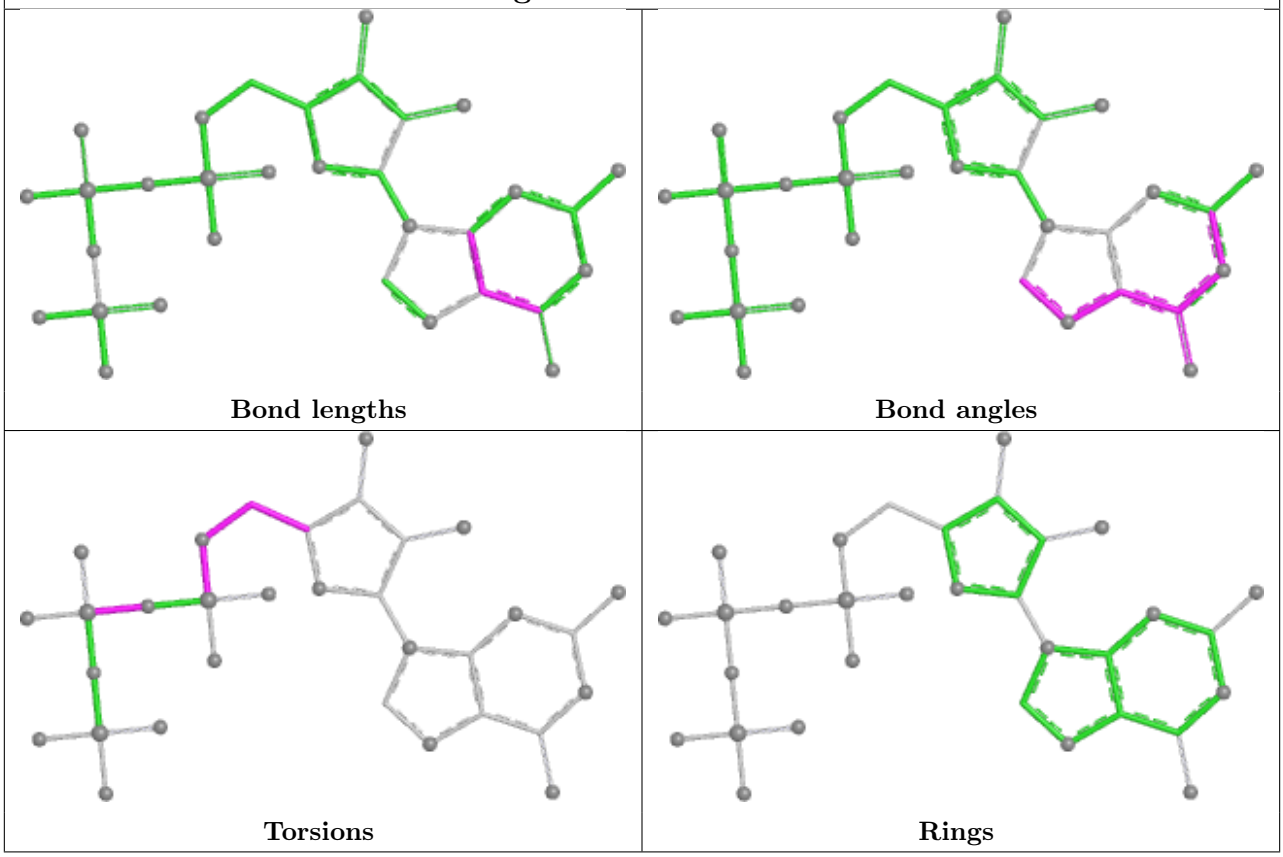

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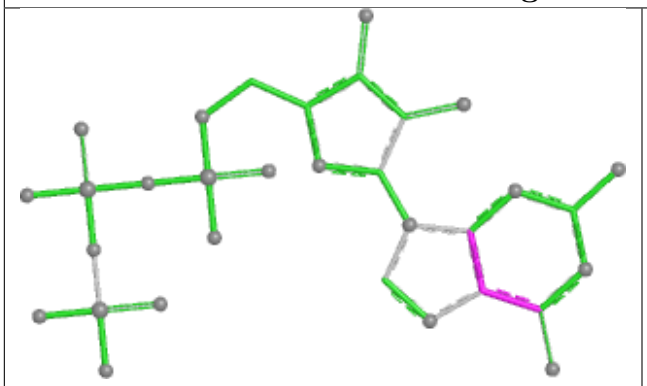
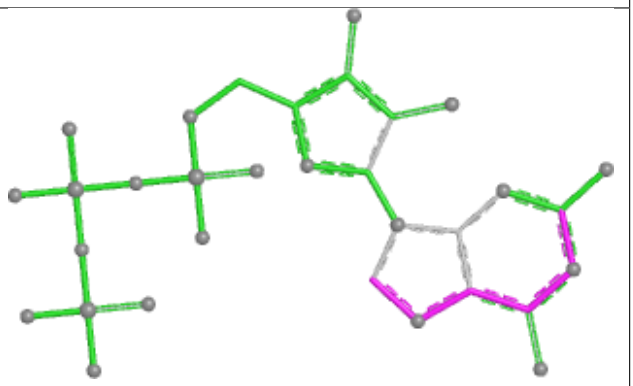
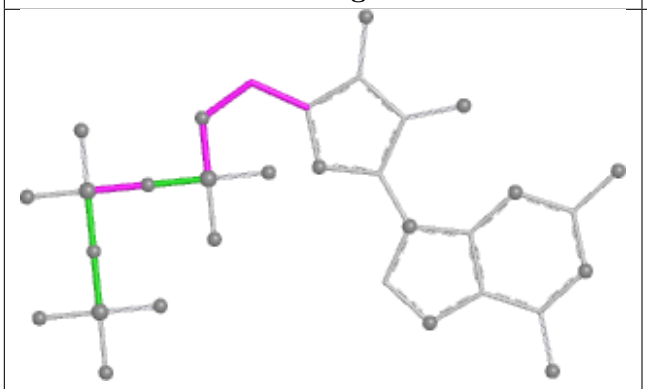


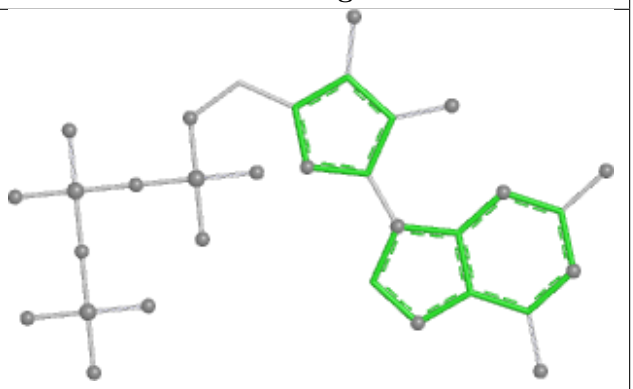
Bond lengths



Bond angles

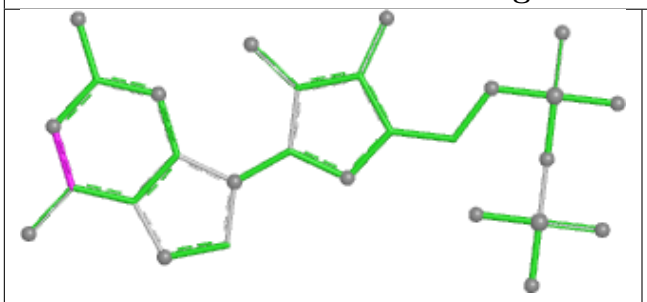


Torsions

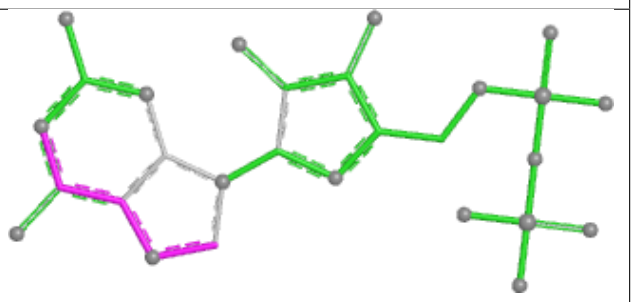


Rings

## Ligand GDP R4 502



Bond lengths



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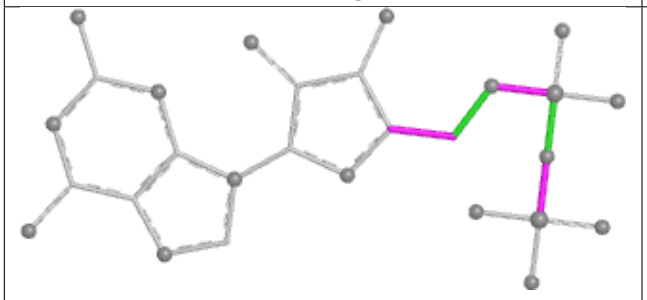

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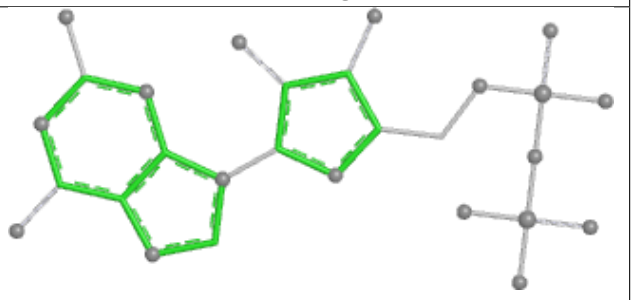

Rings

| Ligand GDP O8 503 | |
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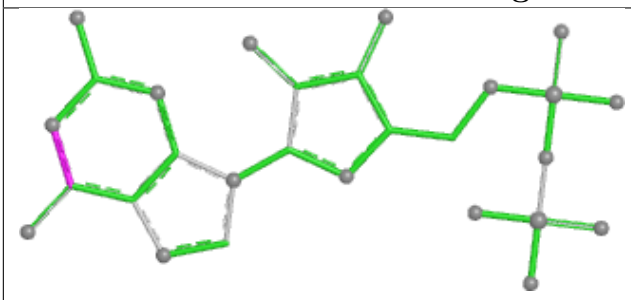
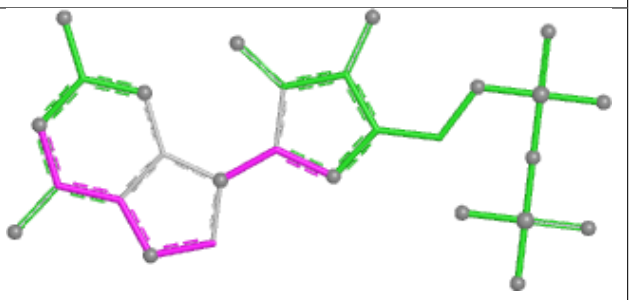
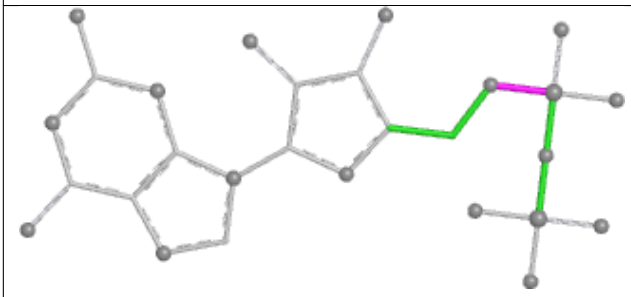
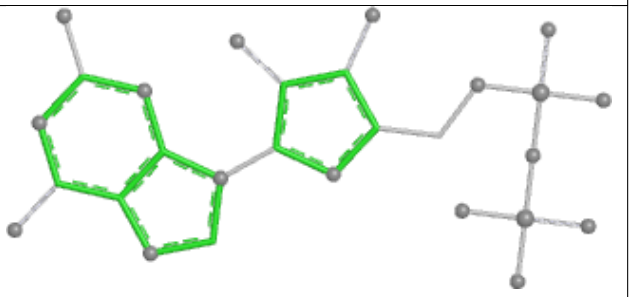
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP D2 501 | |
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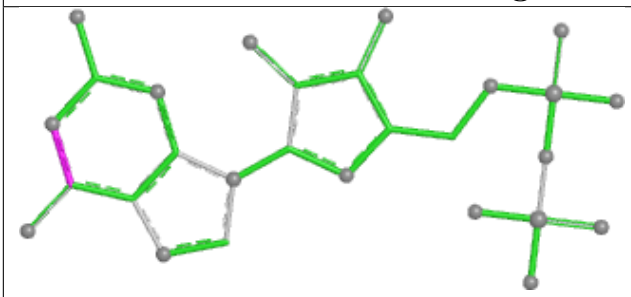
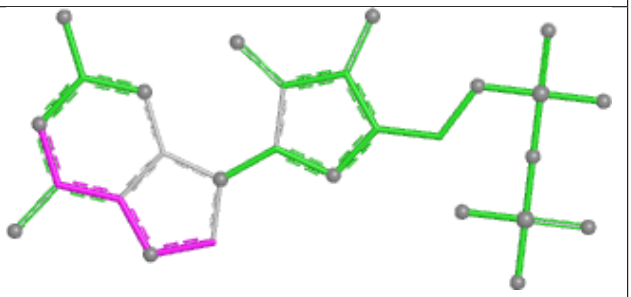
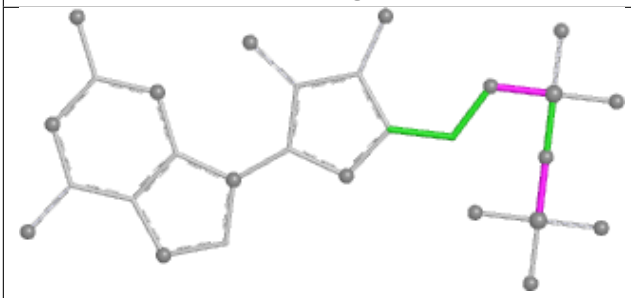
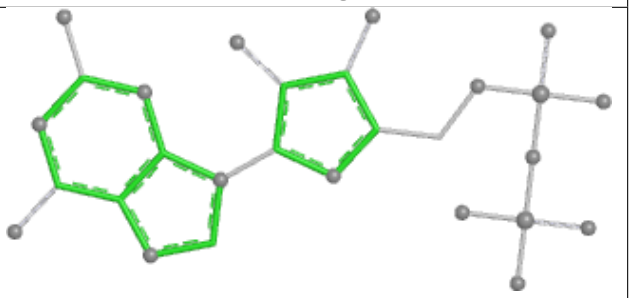
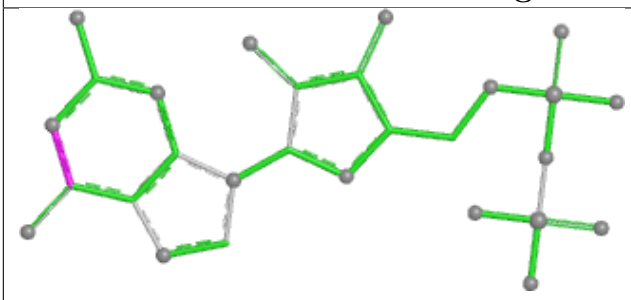
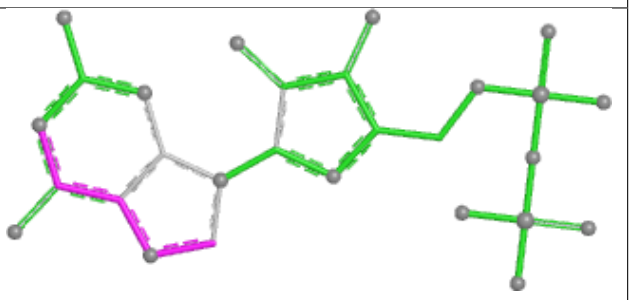
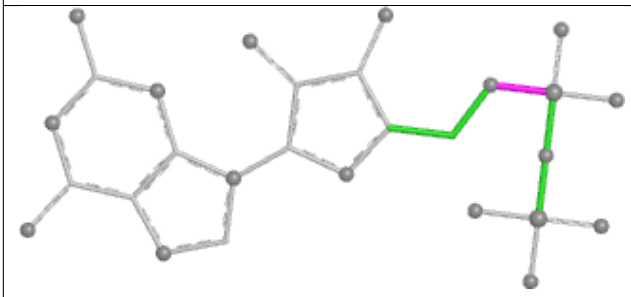
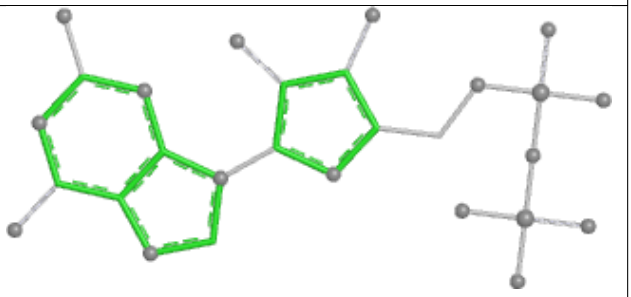
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP L0 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP R0 502 | |
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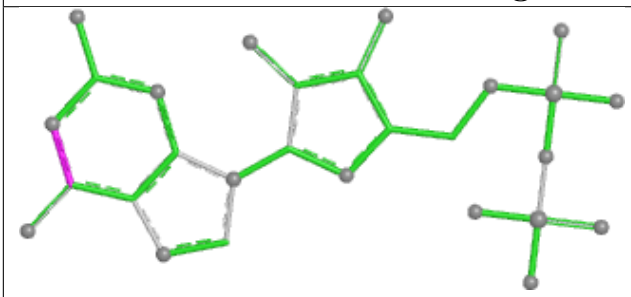
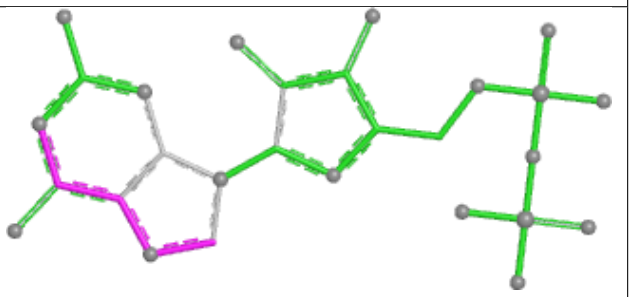
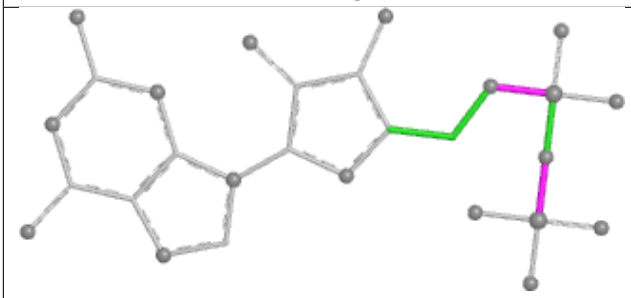
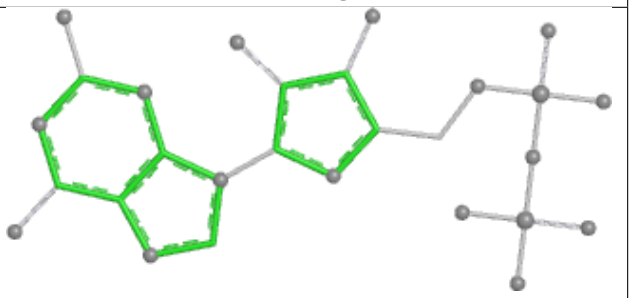
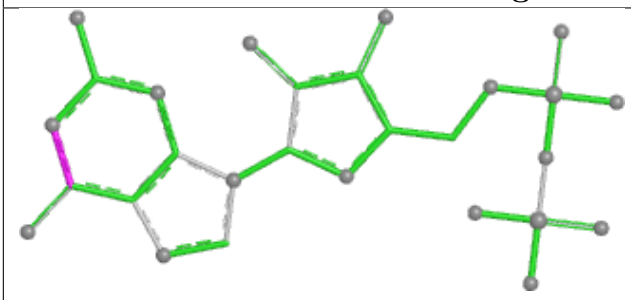
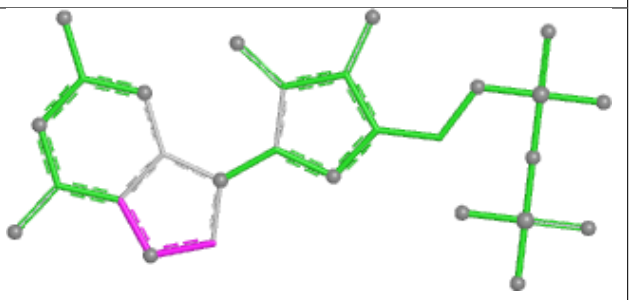
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

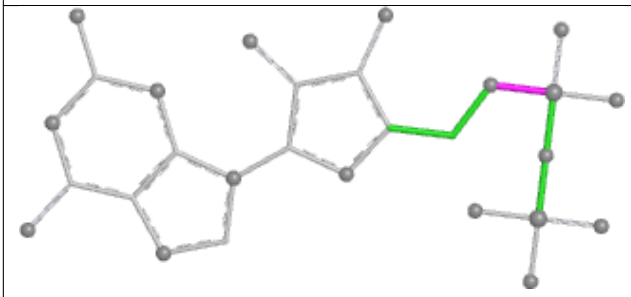
## Ligand GDP 0A 503



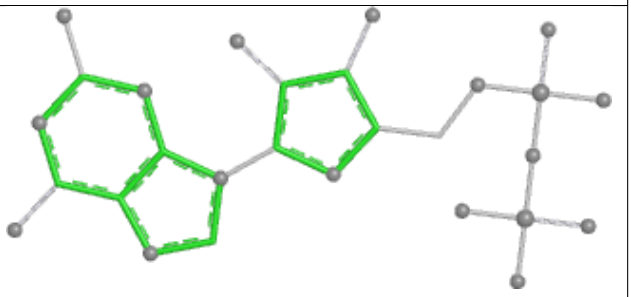
Bond lengths



Bond angles

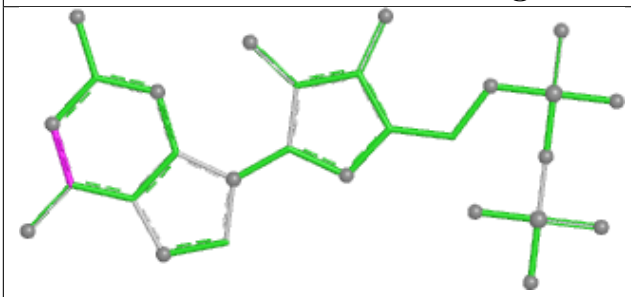


Torsions



Rings

## Ligand GDP 0K 502



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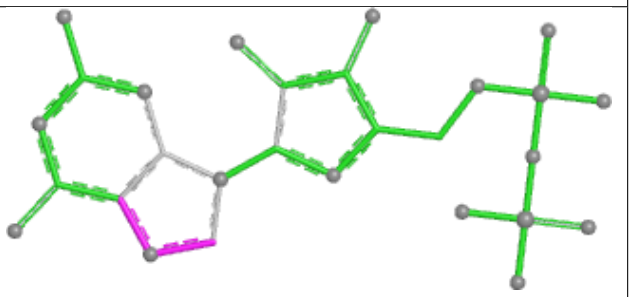

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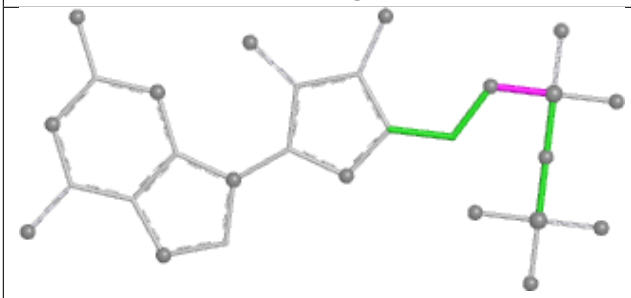

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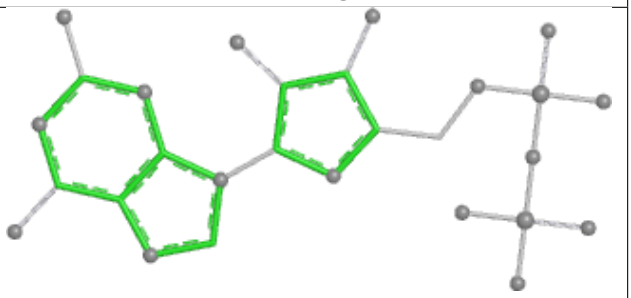
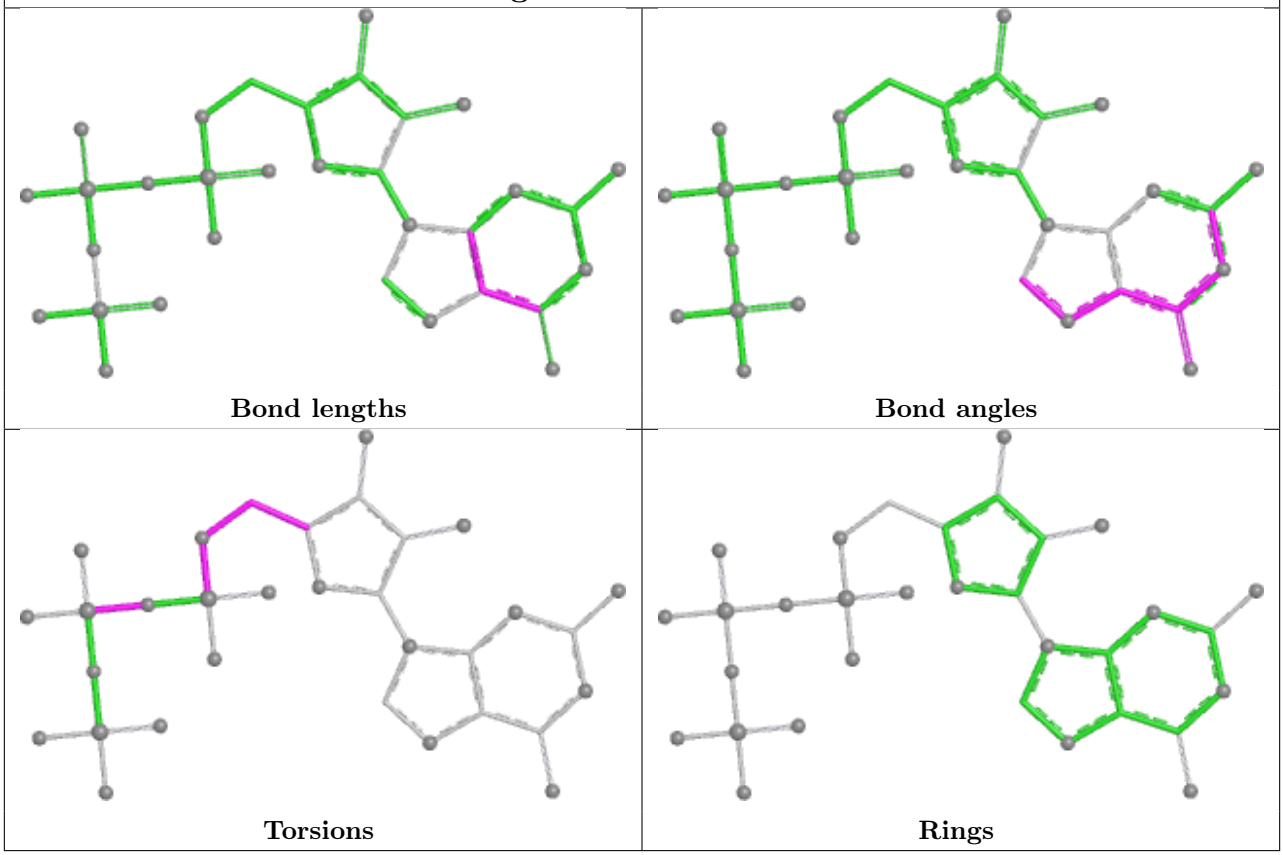
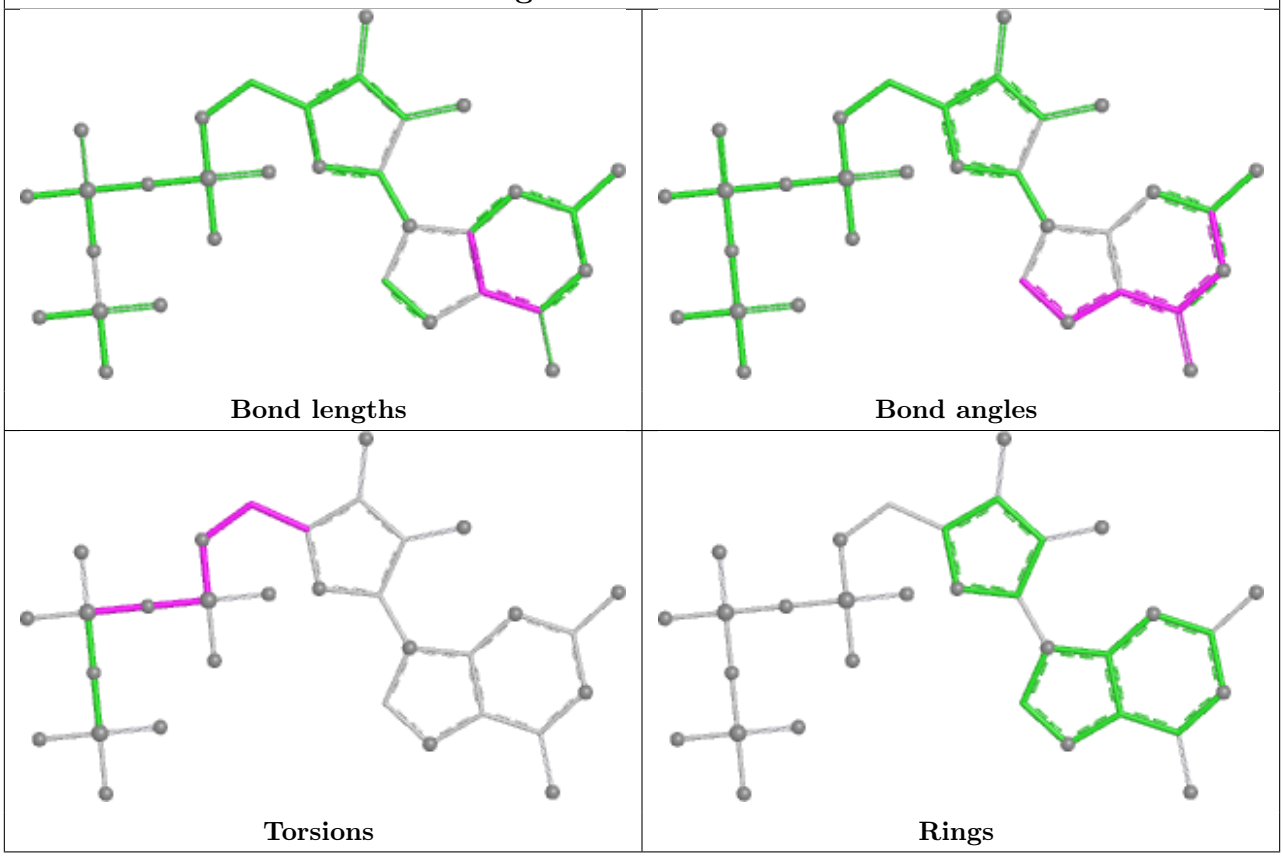


Rings

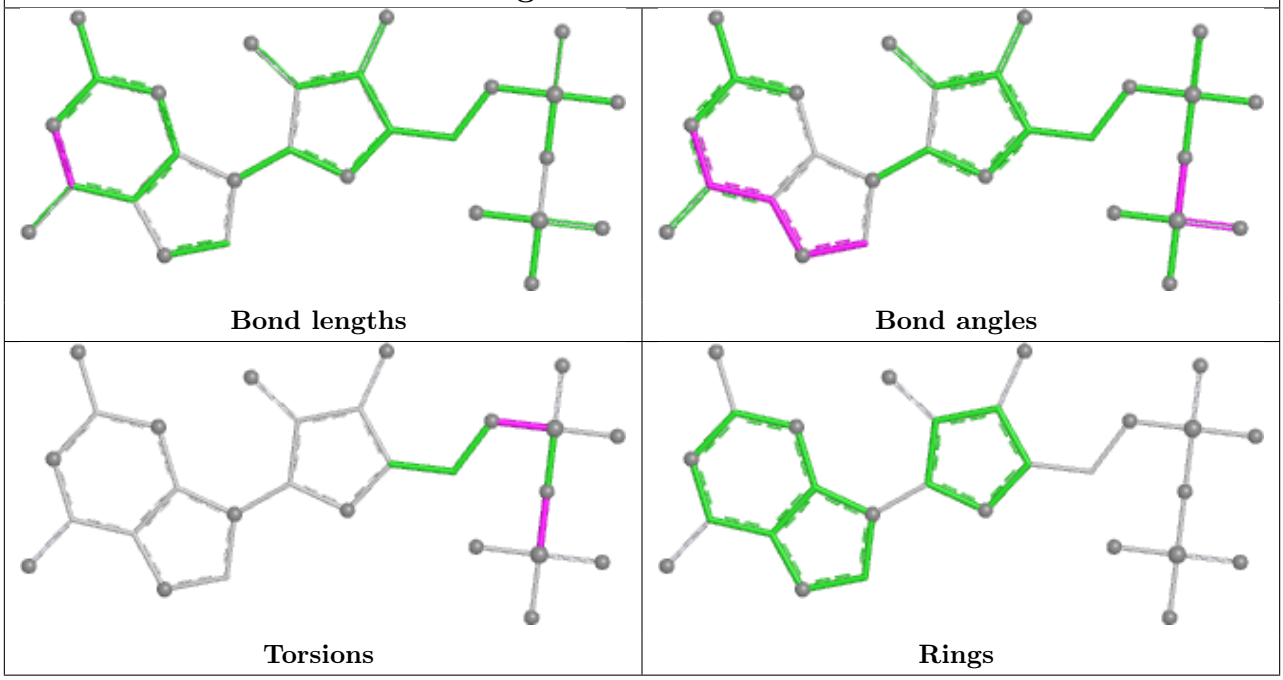
## Ligand GTP M7 501



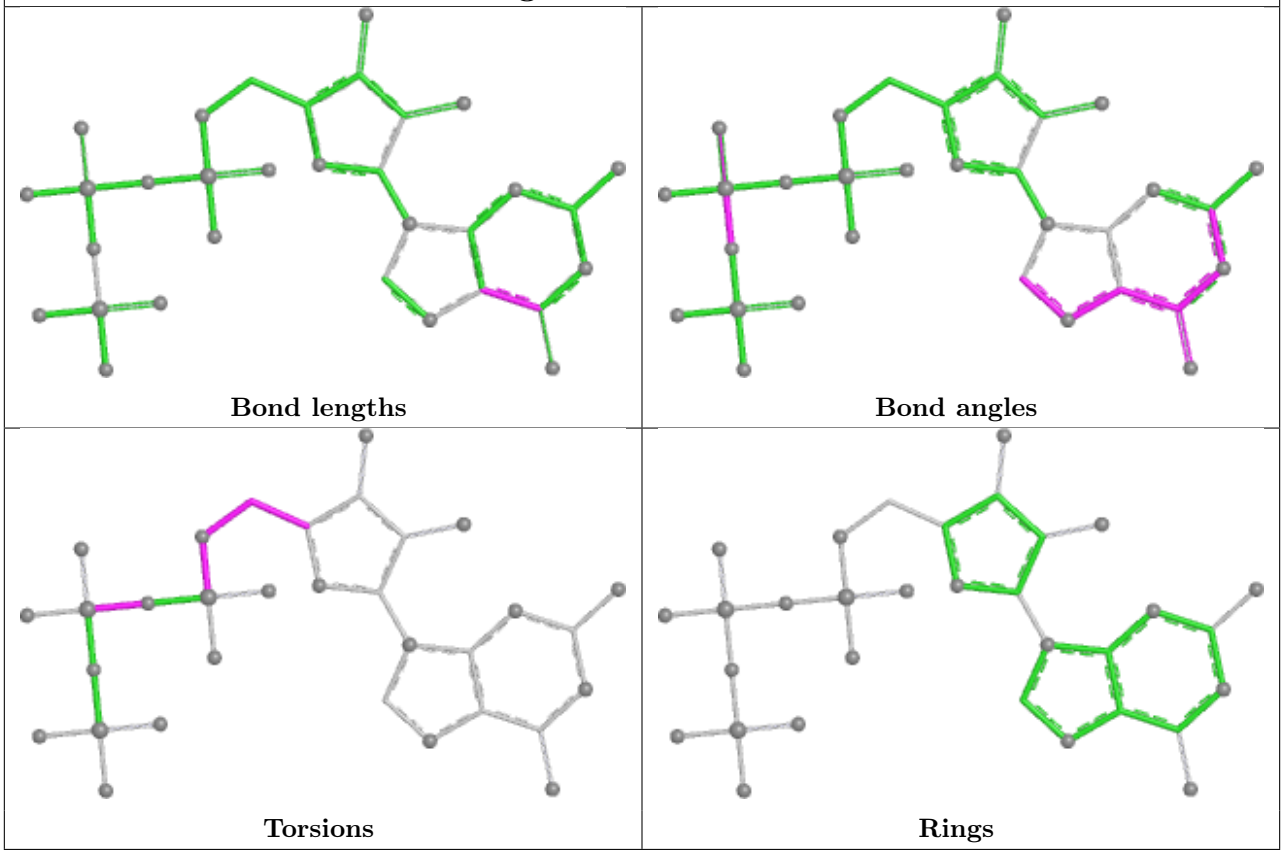

## Ligand GTP P6 501



## Ligand GDP J8 502




## Ligand GTP J0 501



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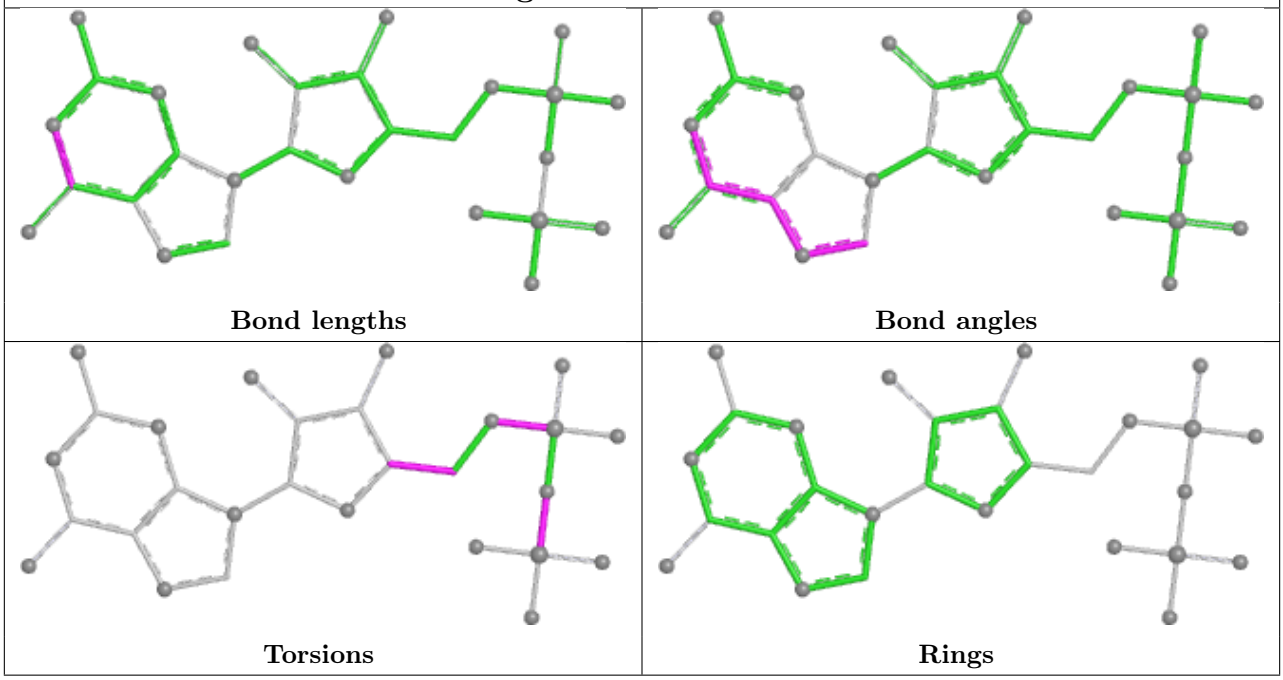
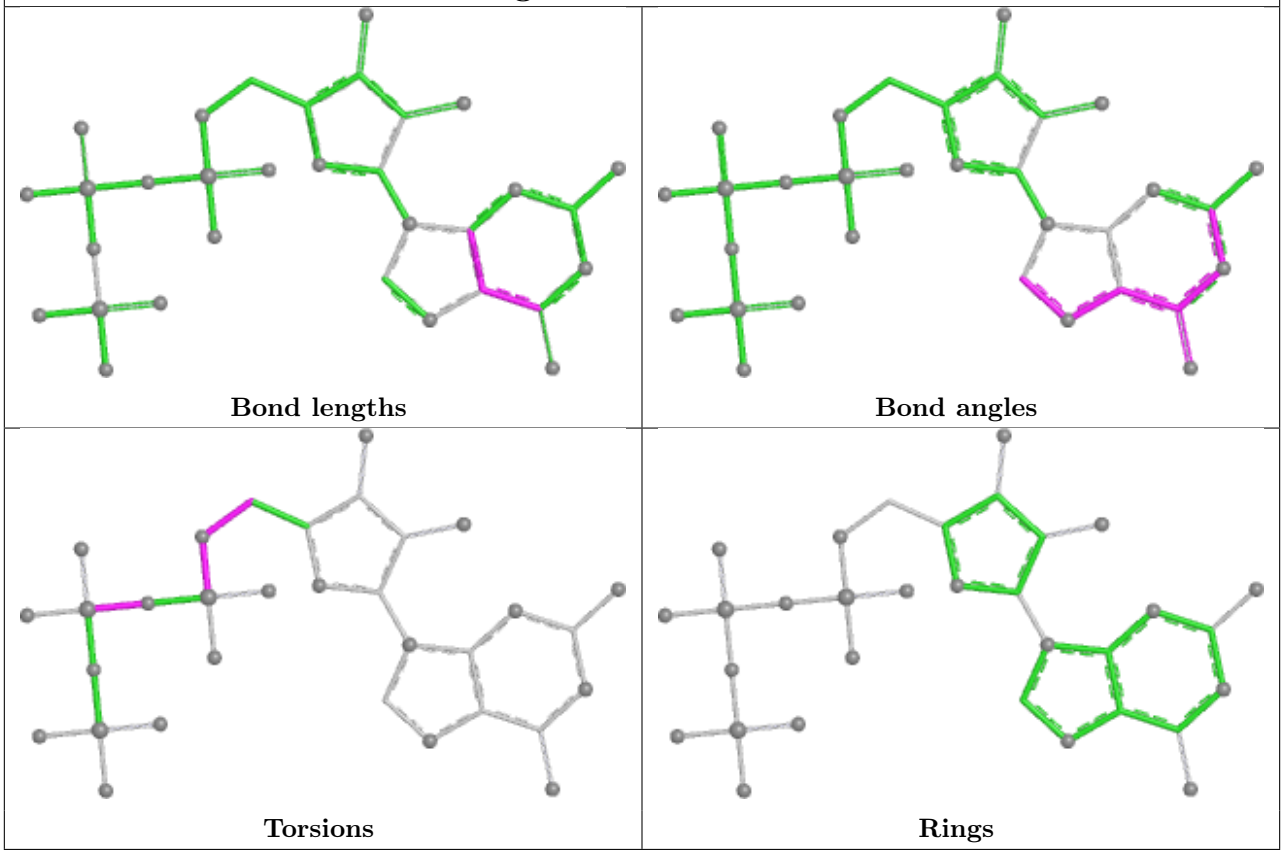



## Ligand GTP R2 501



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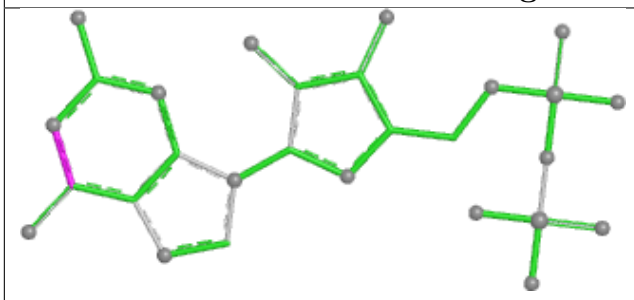
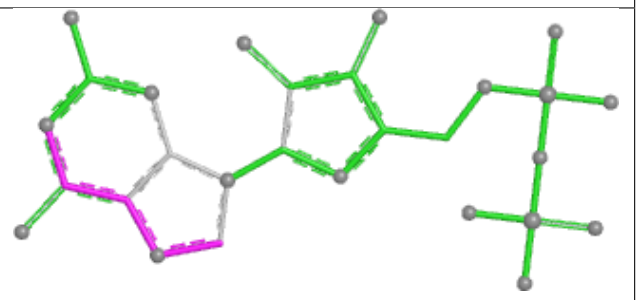
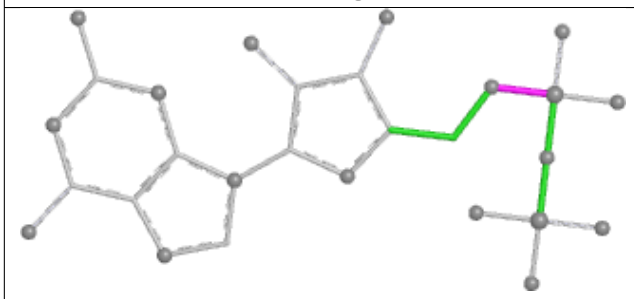


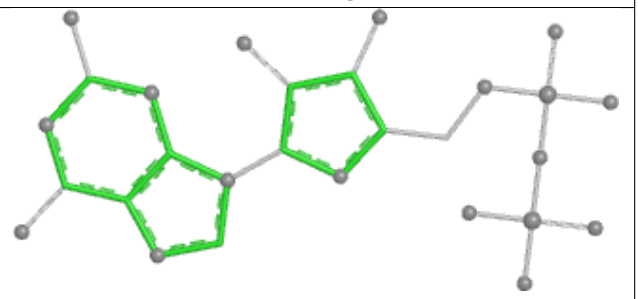
Bond lengths



Bond angles

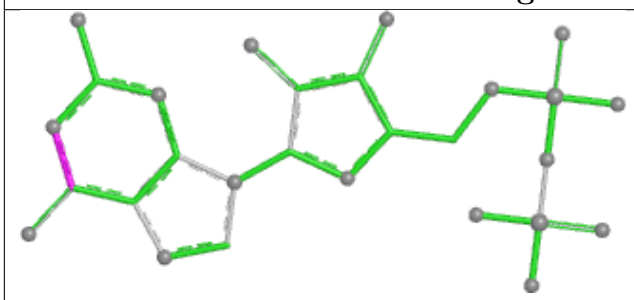


Torsions



Rings

## Ligand GDP J6 502



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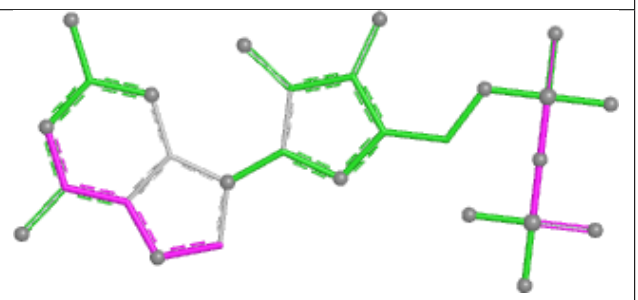

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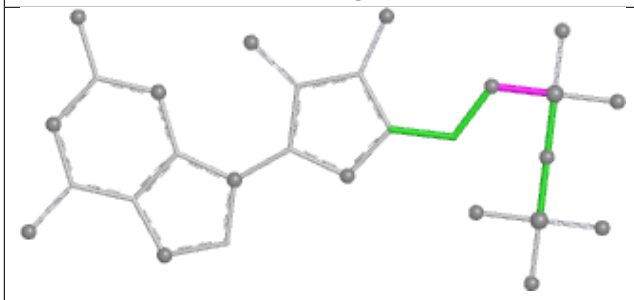

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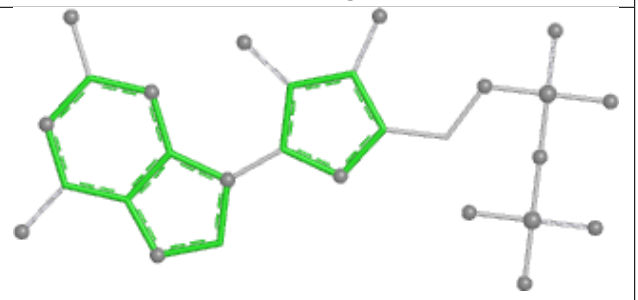
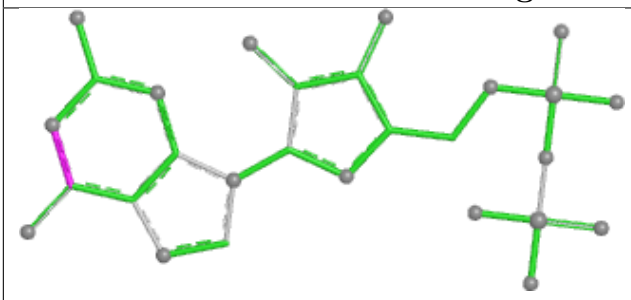


Rings

## Ligand GDP J0 502



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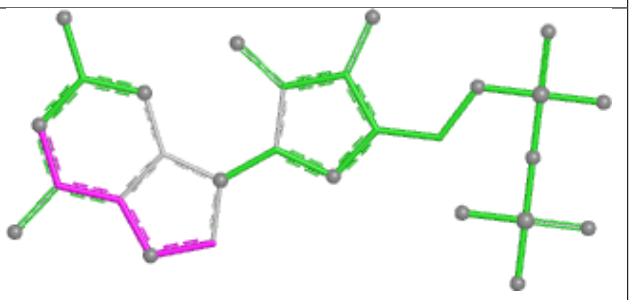
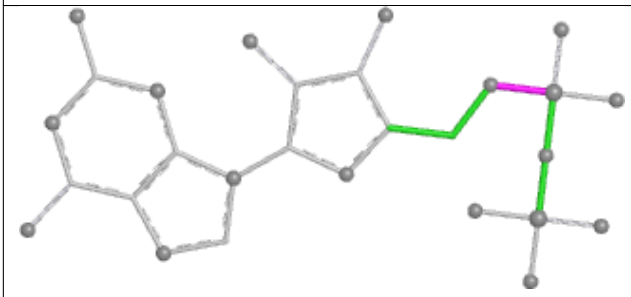


Bond angles



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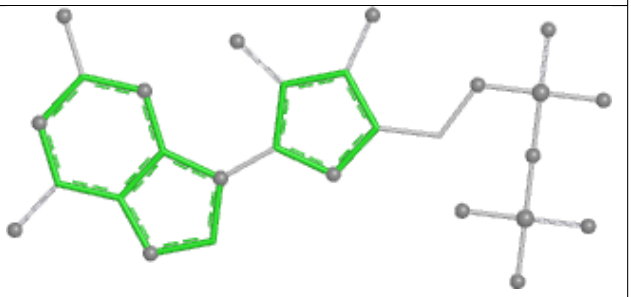
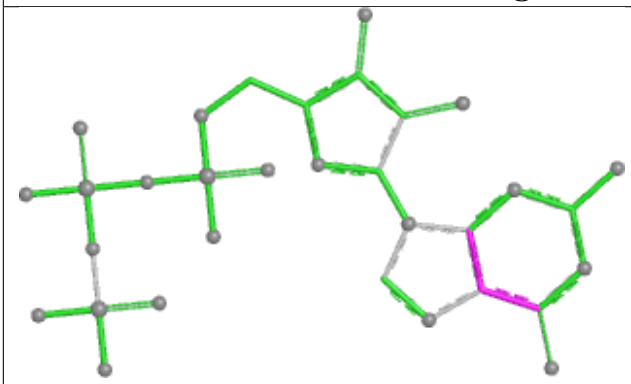
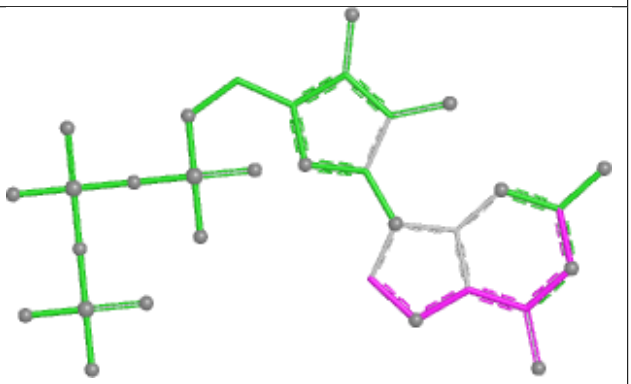


Rings

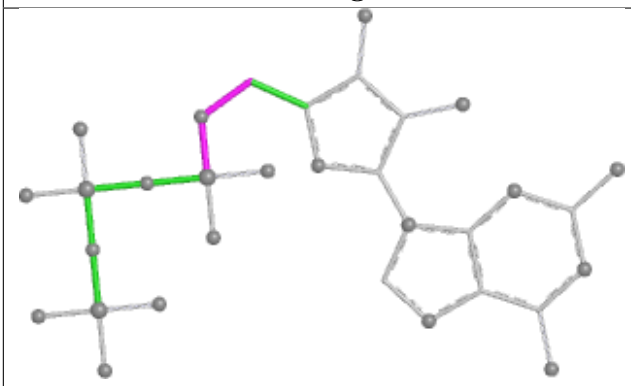
## Ligand GTP D5 501



Bond lengths



Bond angles



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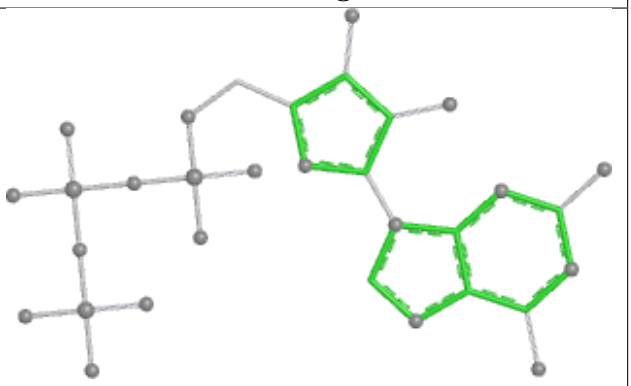
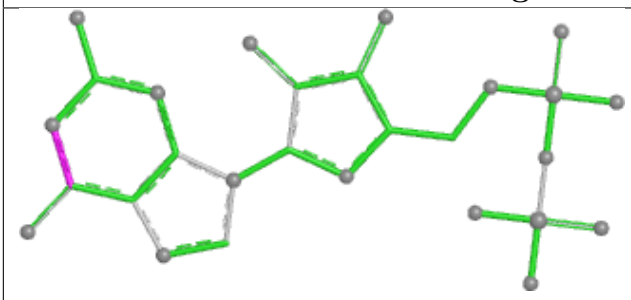
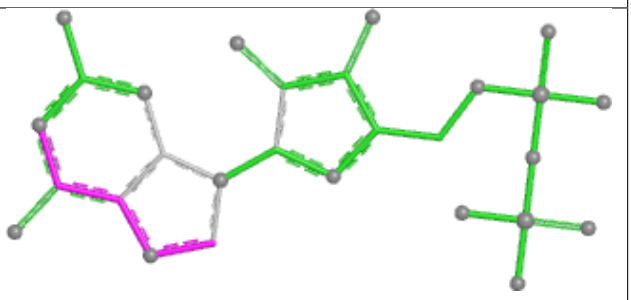


Rings

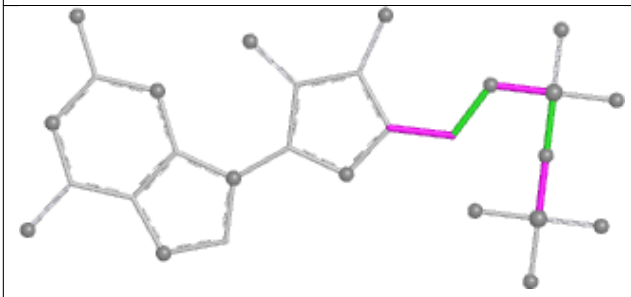
## Ligand GDP D6 501



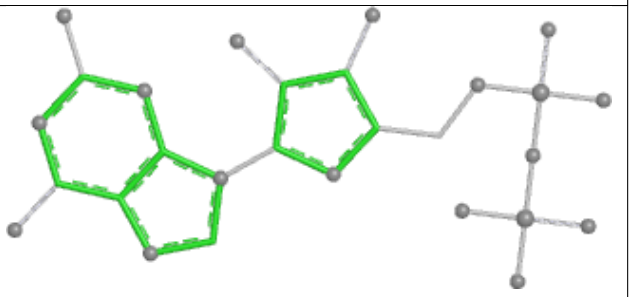
Bond lengths



Bond angles

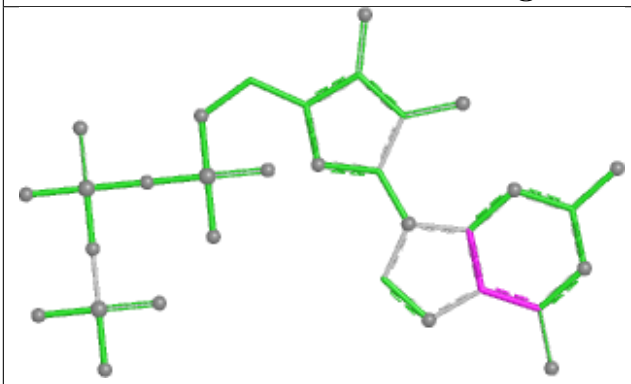


Torsions

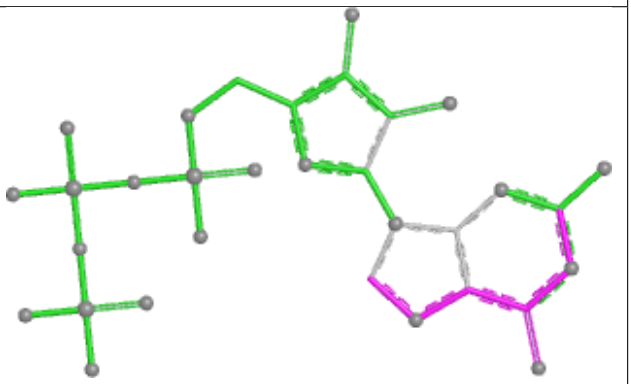


Rings

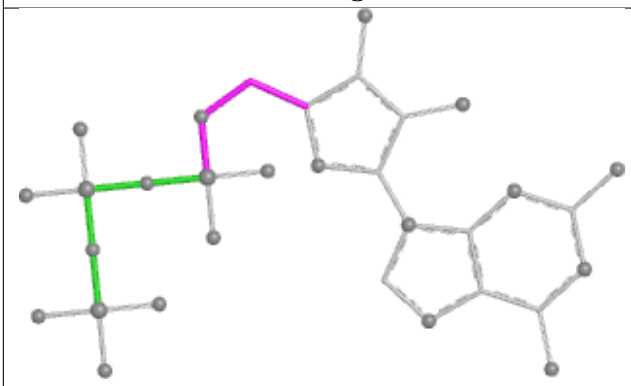
## Ligand GTP J4 501



Bond lengths



Bond angles



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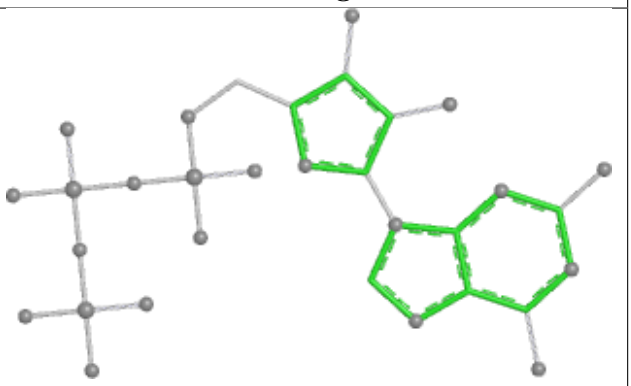
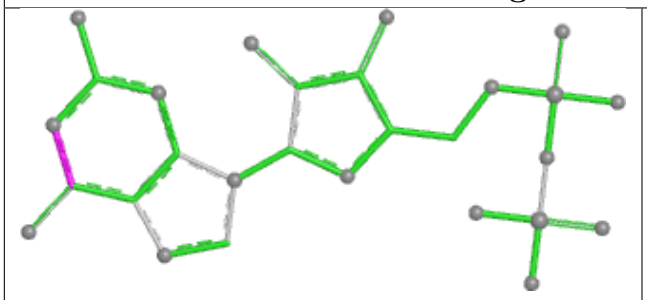
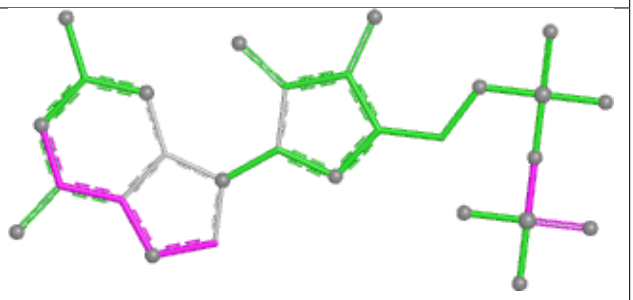


Rings

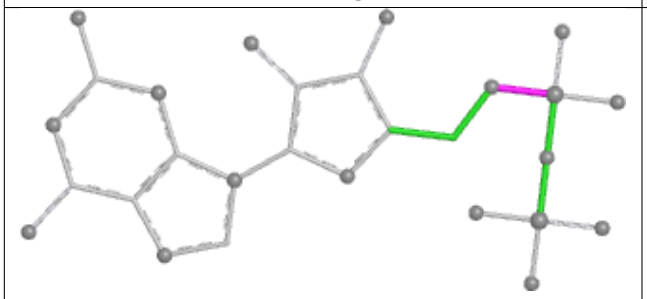
## Ligand GDP 1M 501



Bond lengths



Bond angles



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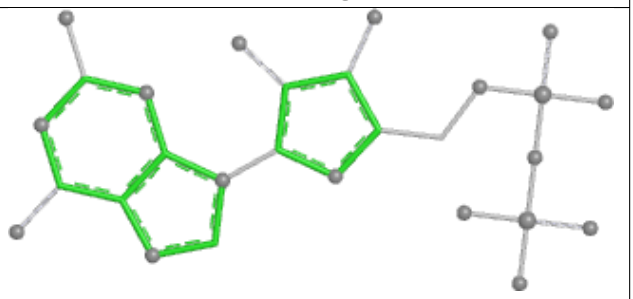
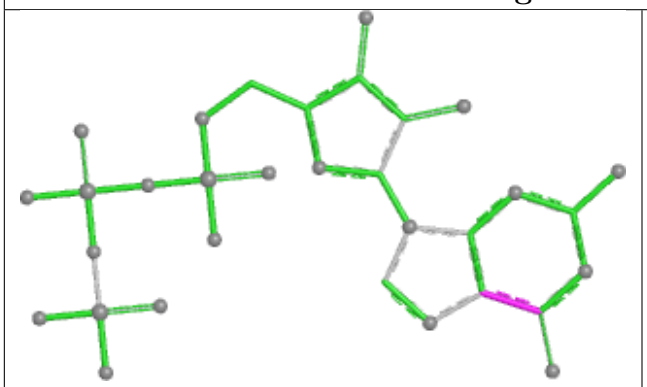
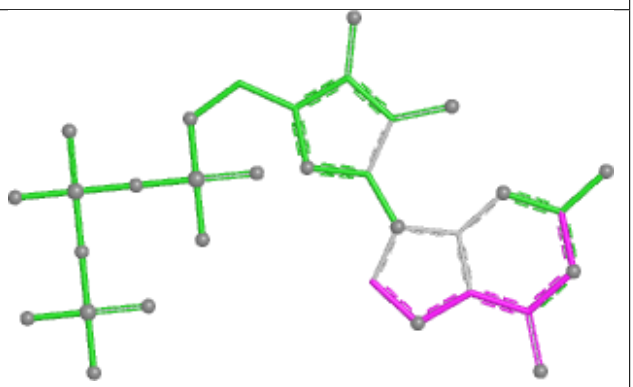


Rings

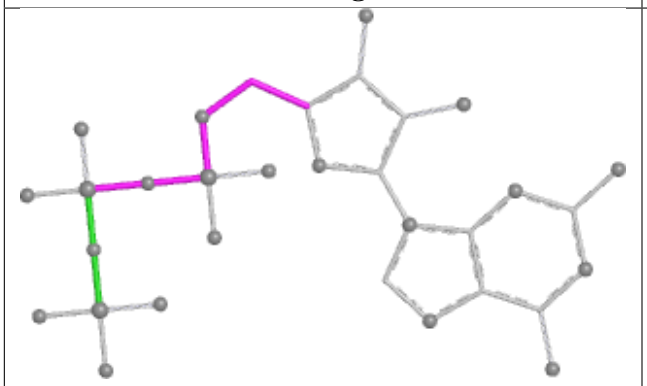
## Ligand GTP 1C 501



Bond lengths



Bond angles



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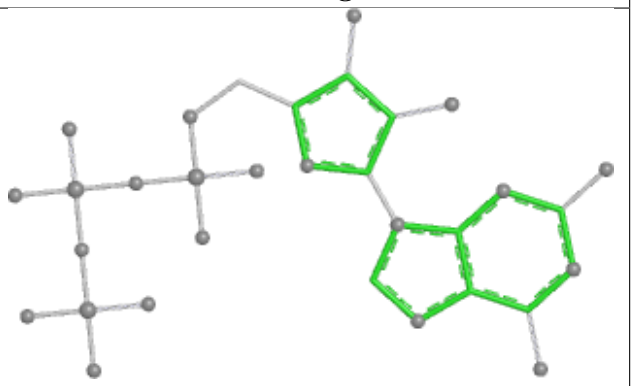
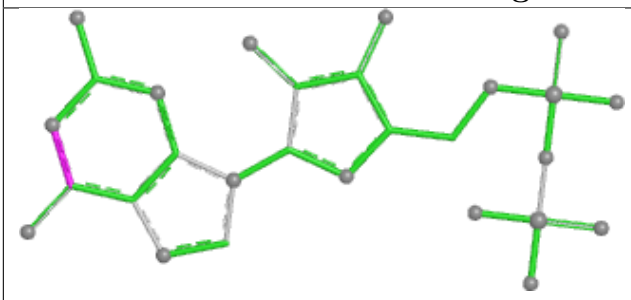
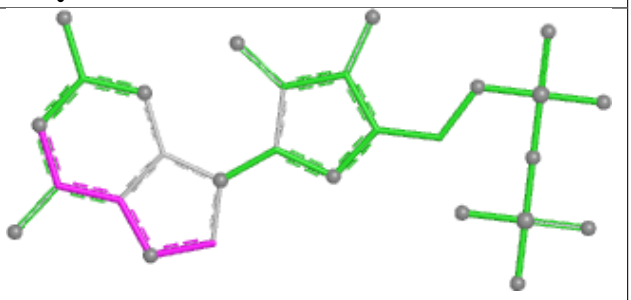
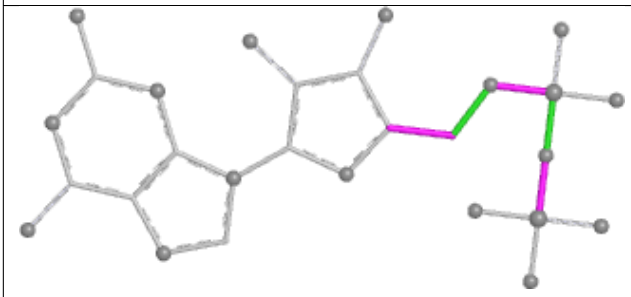
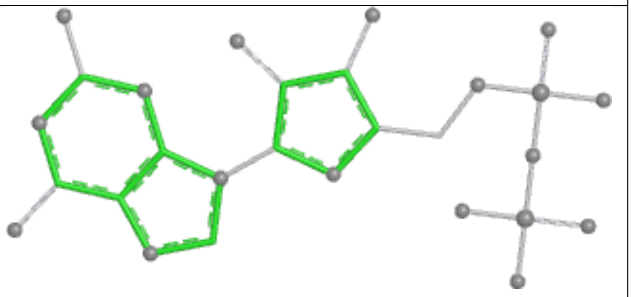
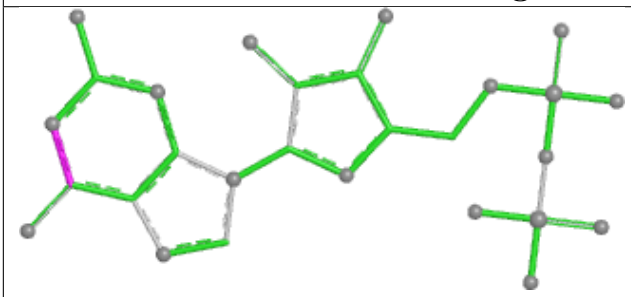
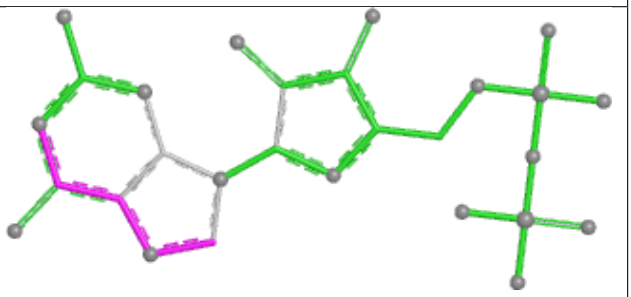
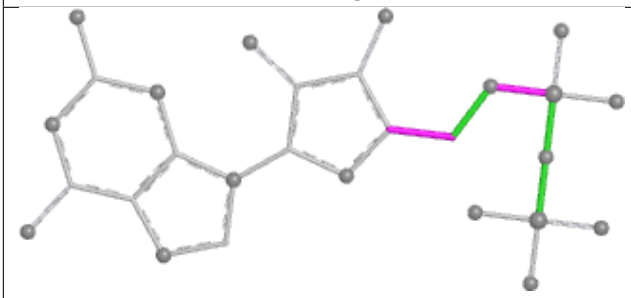
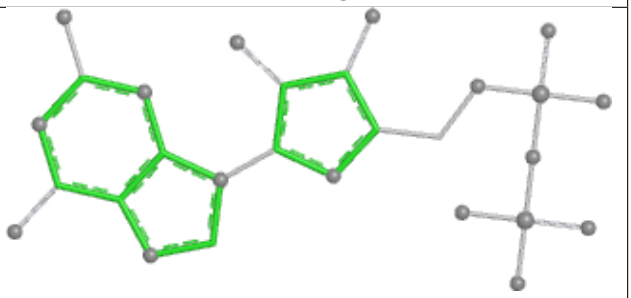
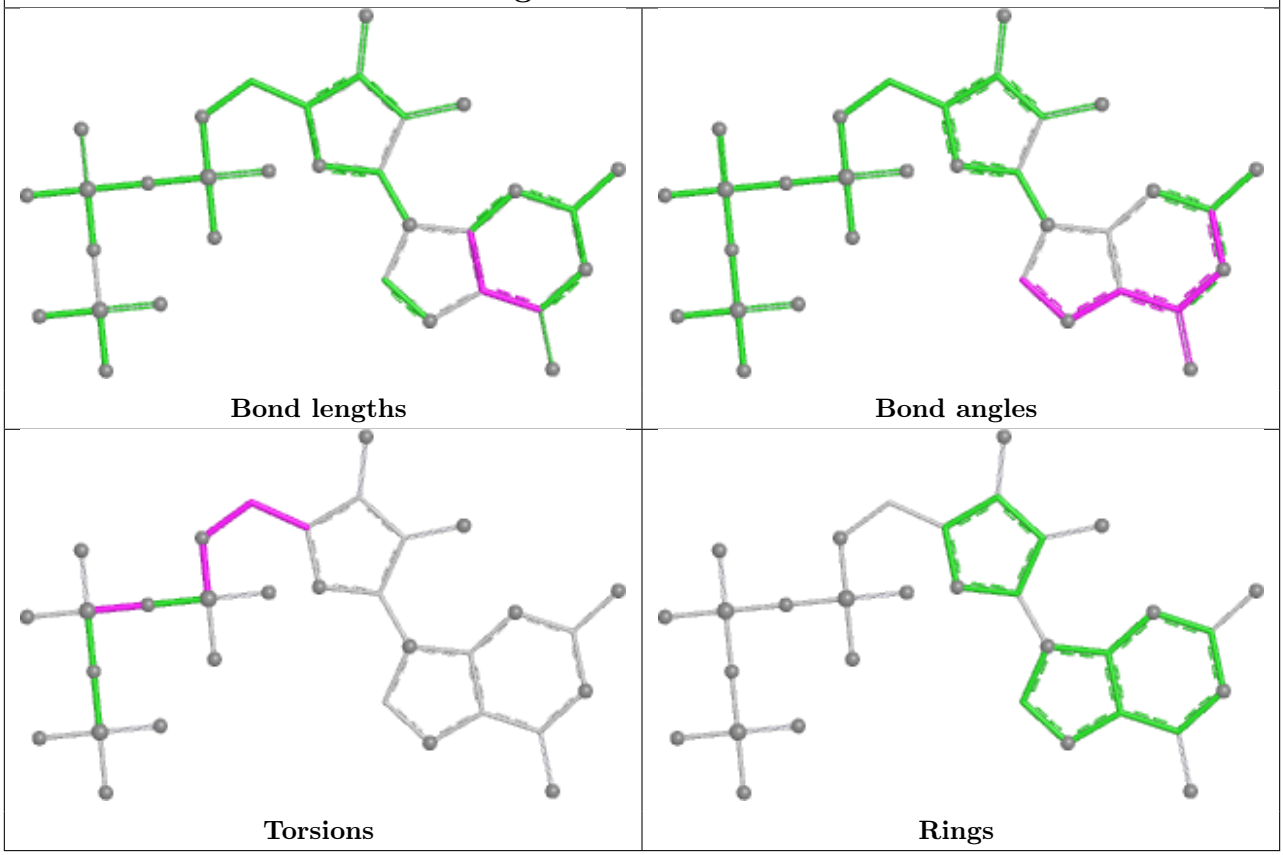


Rings

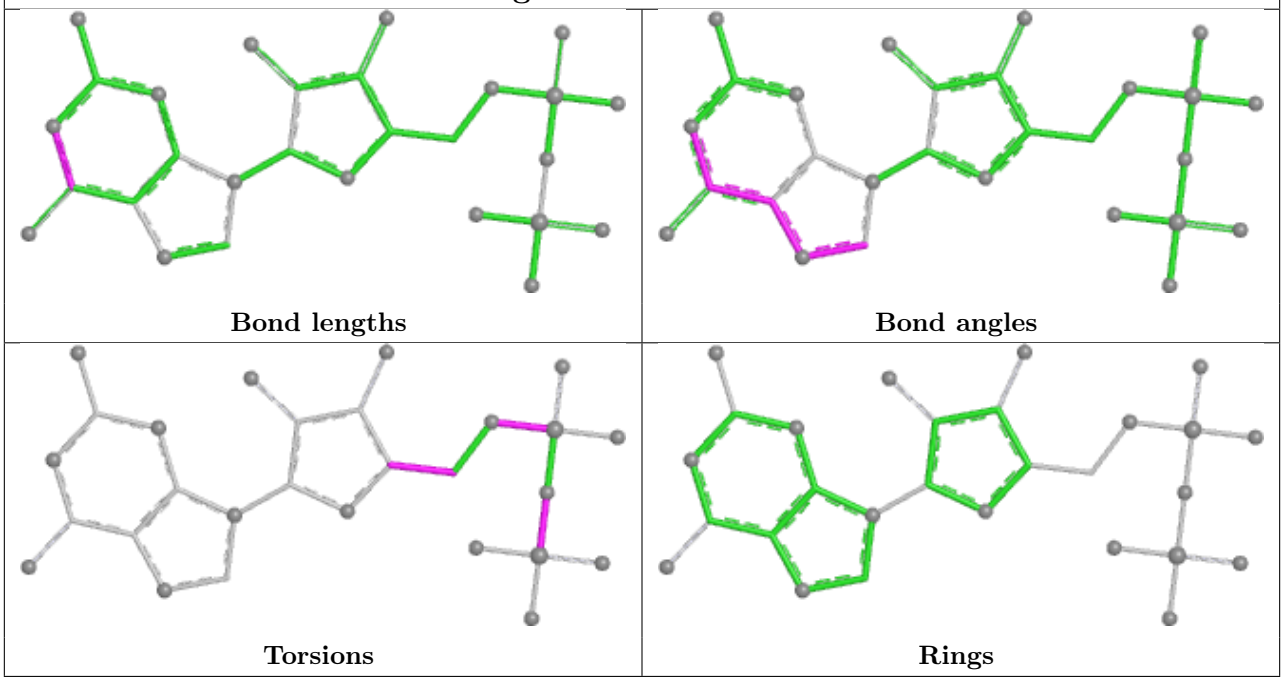
| Ligand GDP Q6 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP U6 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

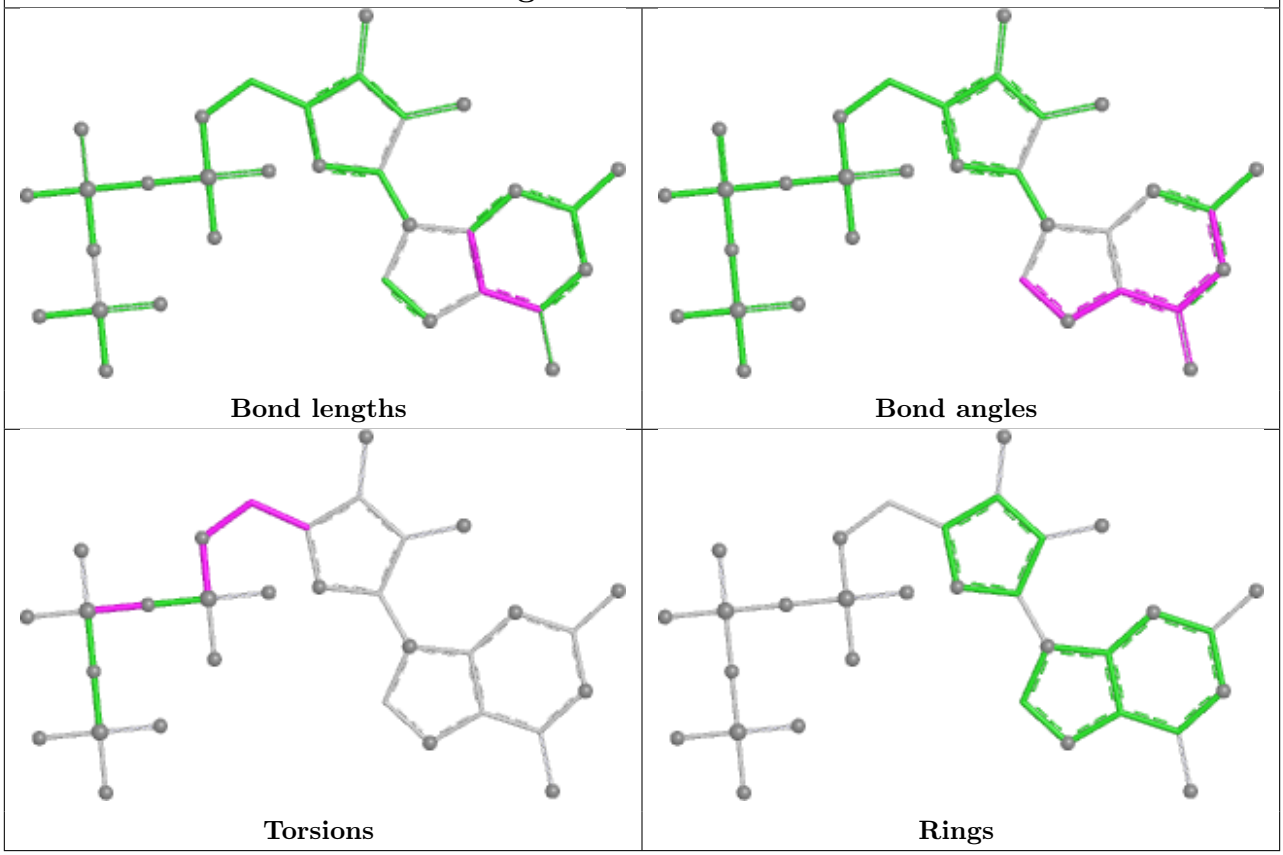
## Ligand GTP O0 501



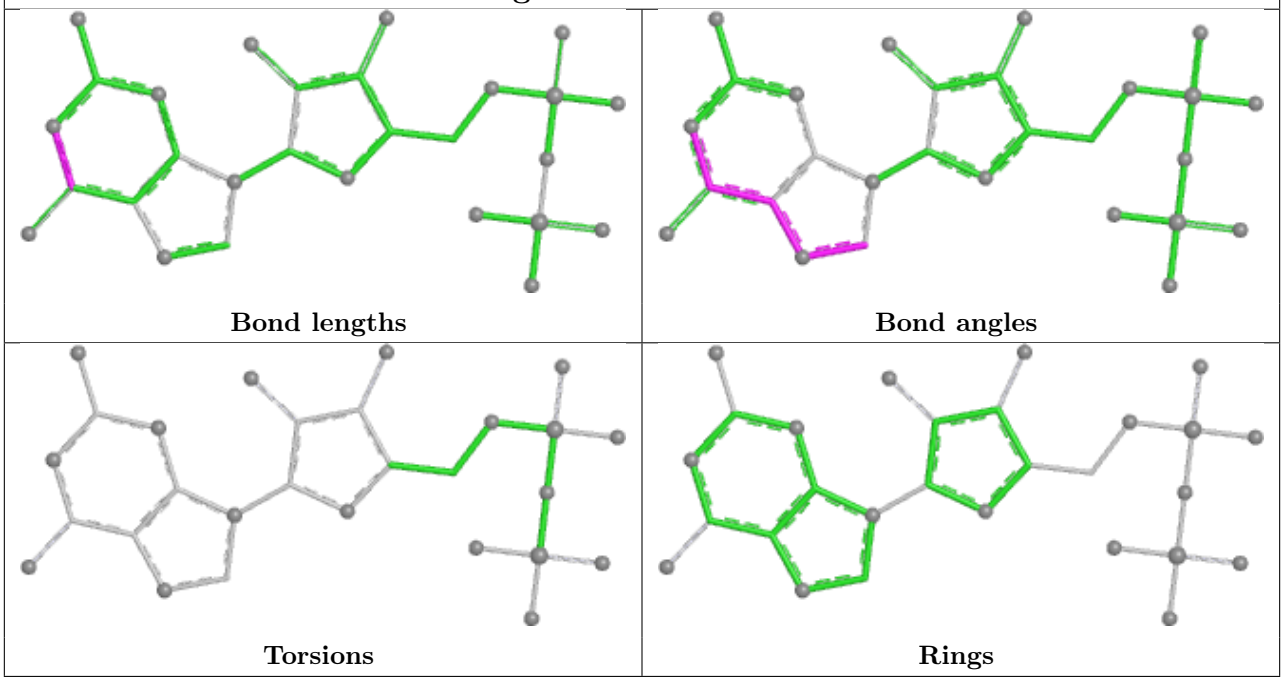

## Ligand GDP A1 502



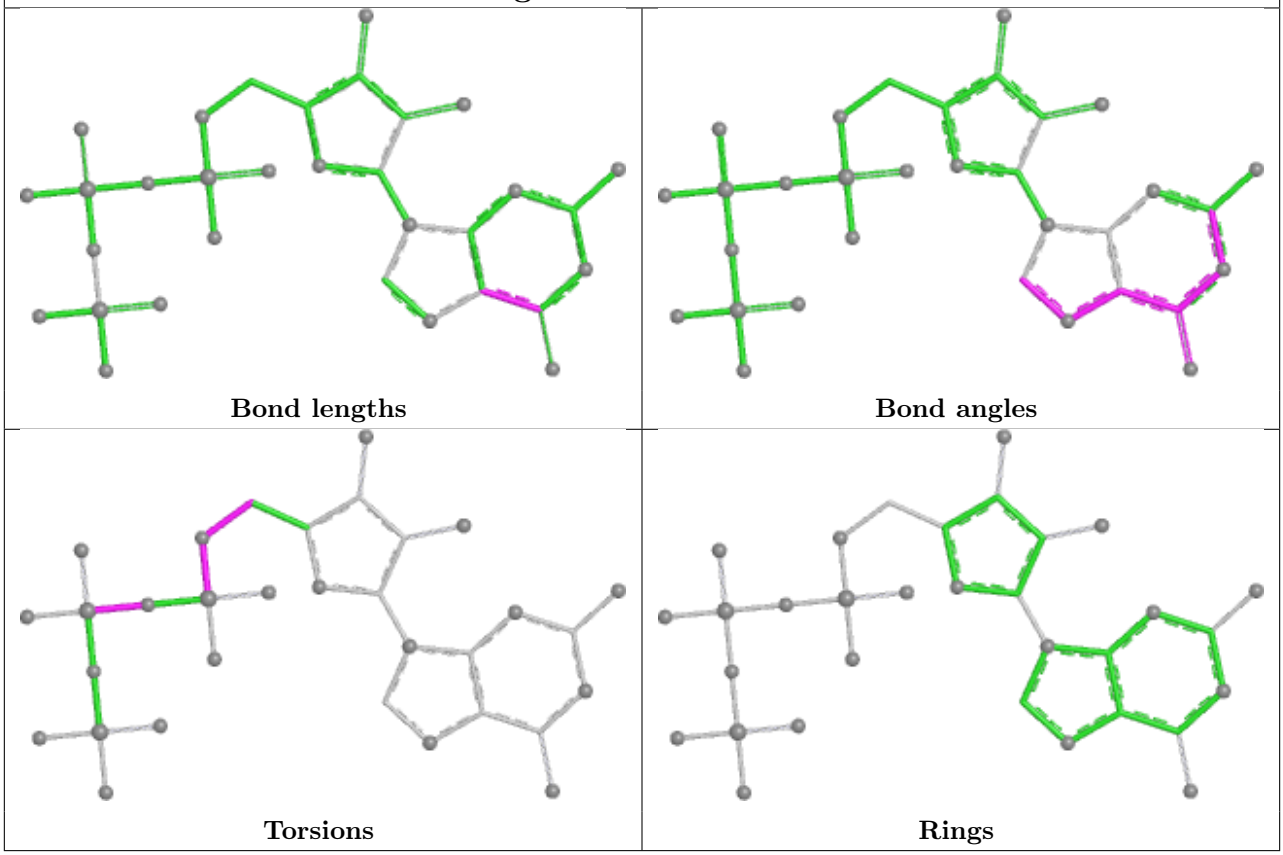
## Ligand GTP S0 501



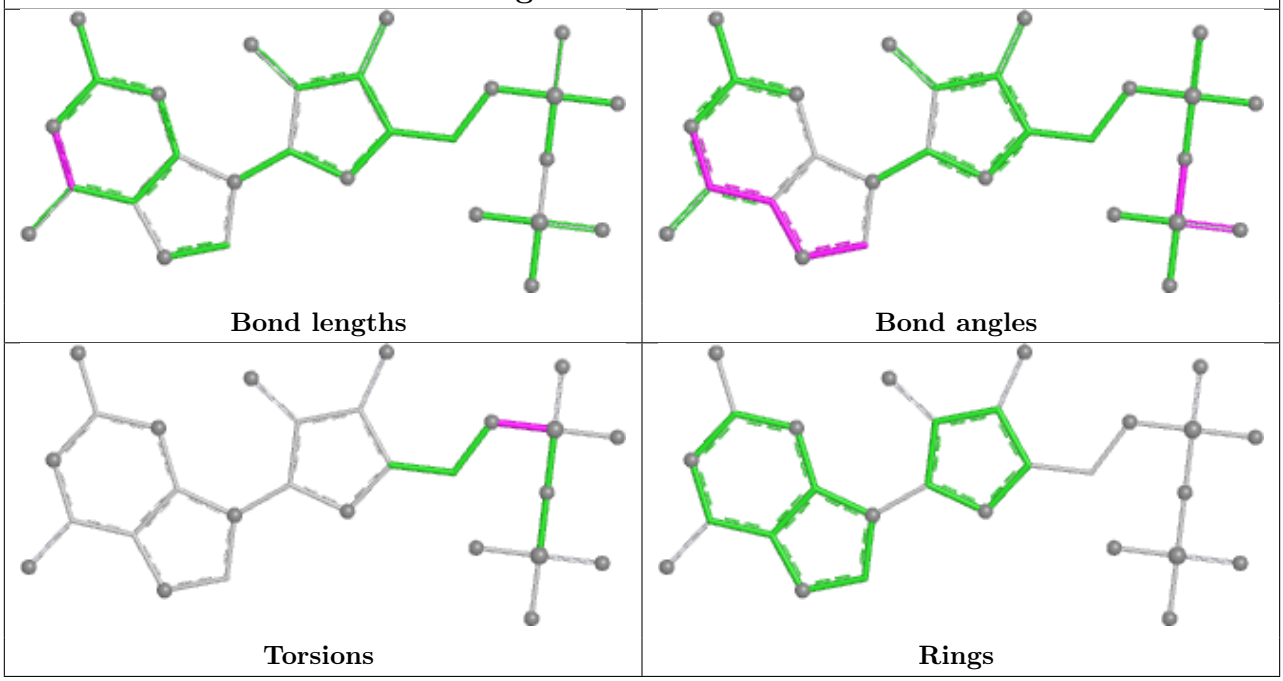

## Ligand GDP 2A 502

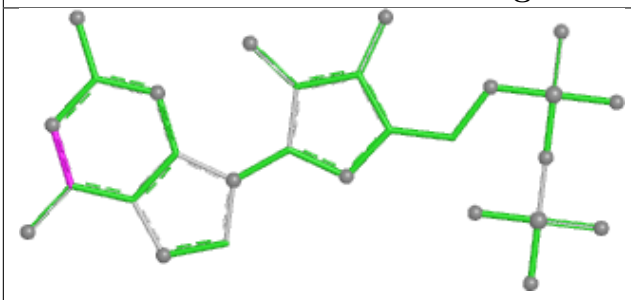
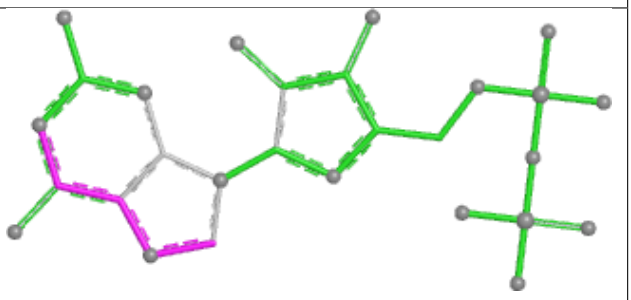
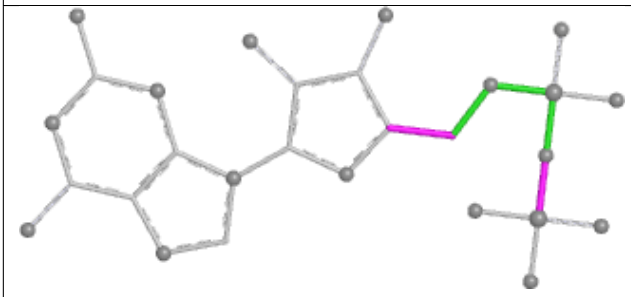
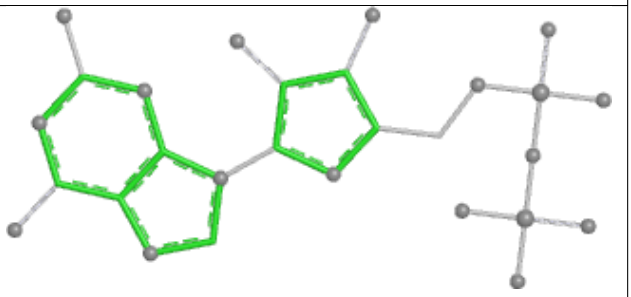


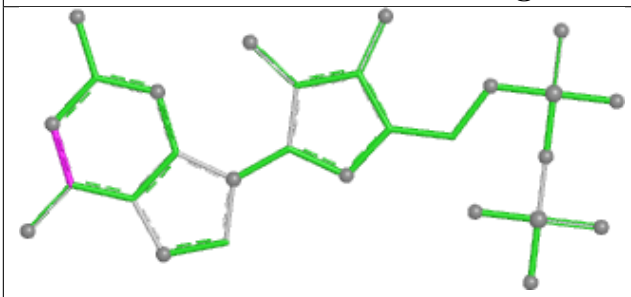
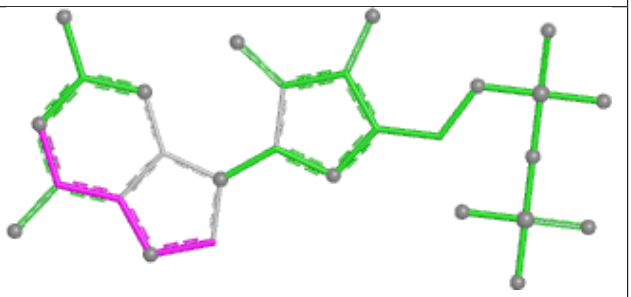
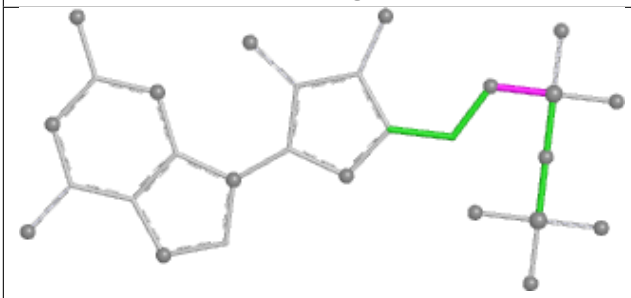
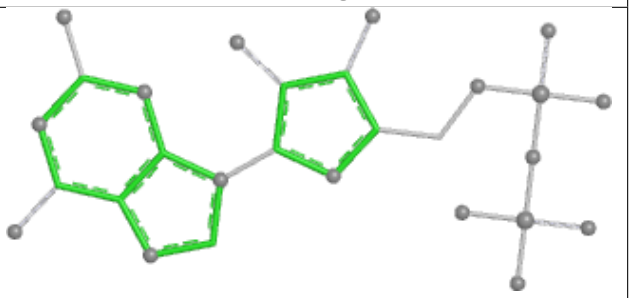
## Ligand GTP V2 501



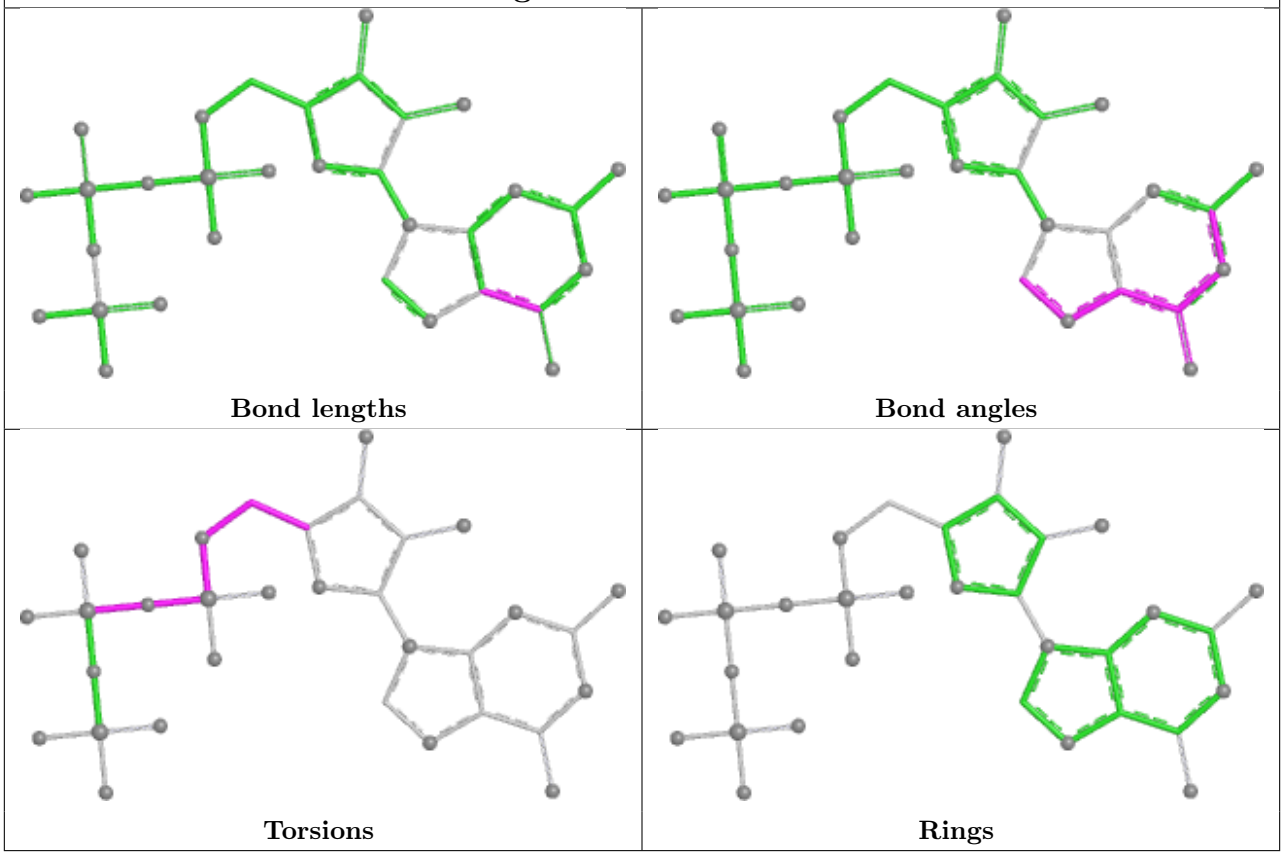

## Ligand GDP L4 502



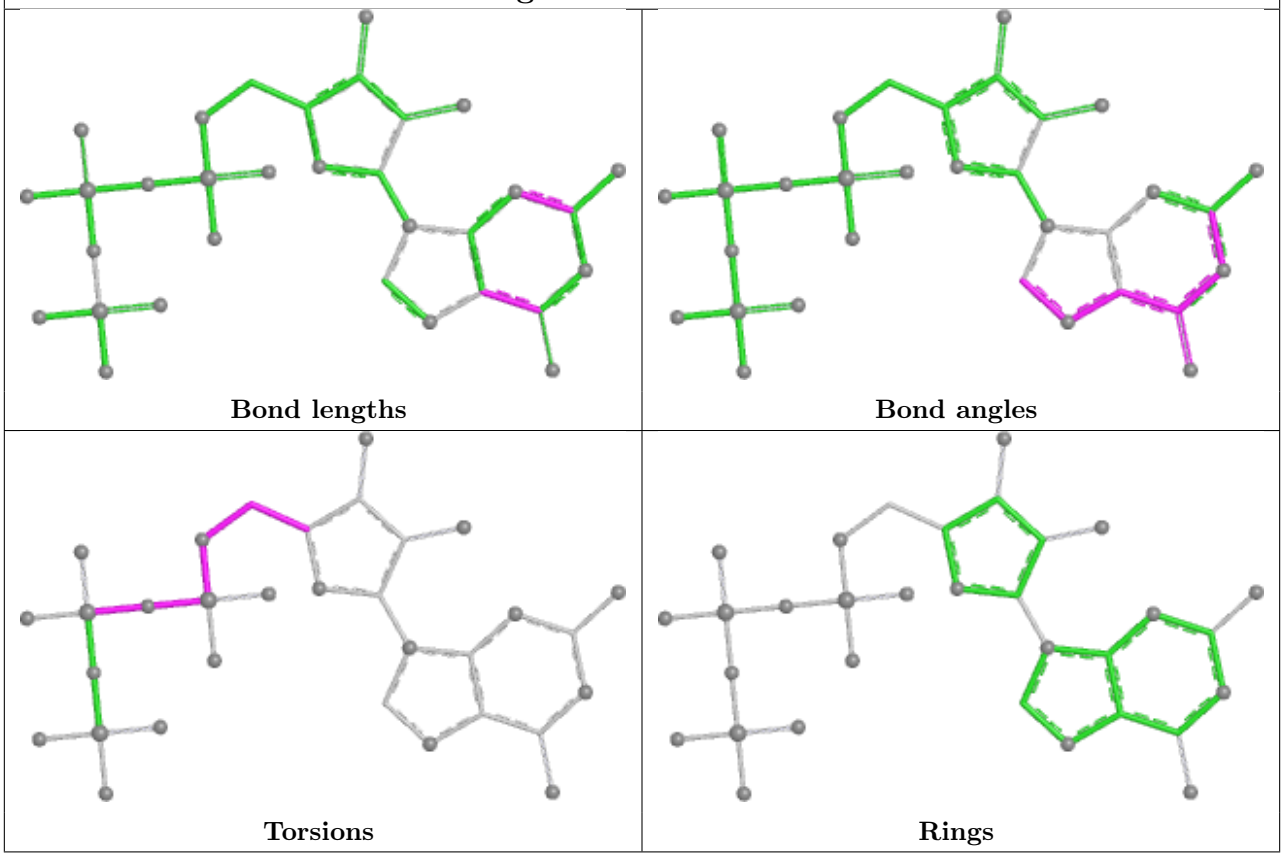
| Ligand GDP E2 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand GDP 1S 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

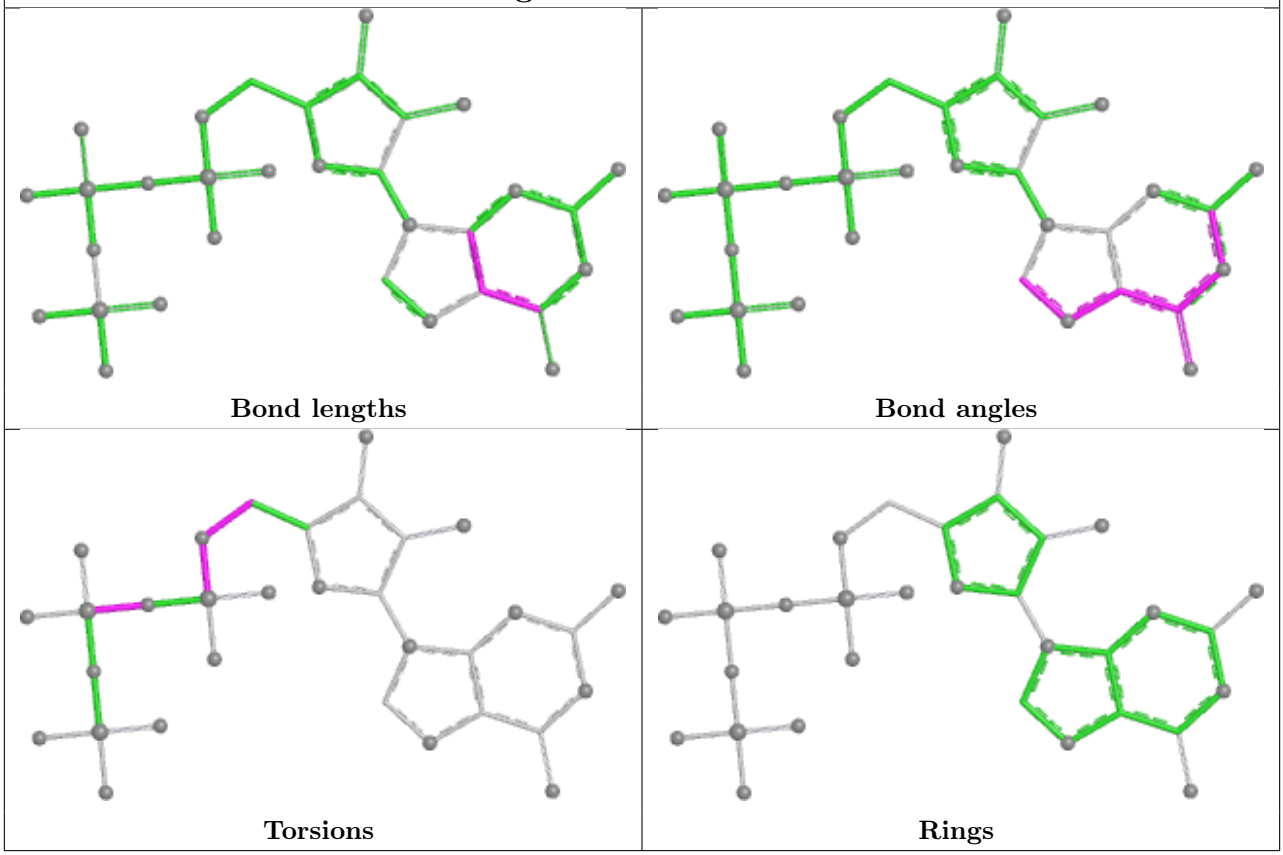
## Ligand GTP H6 501



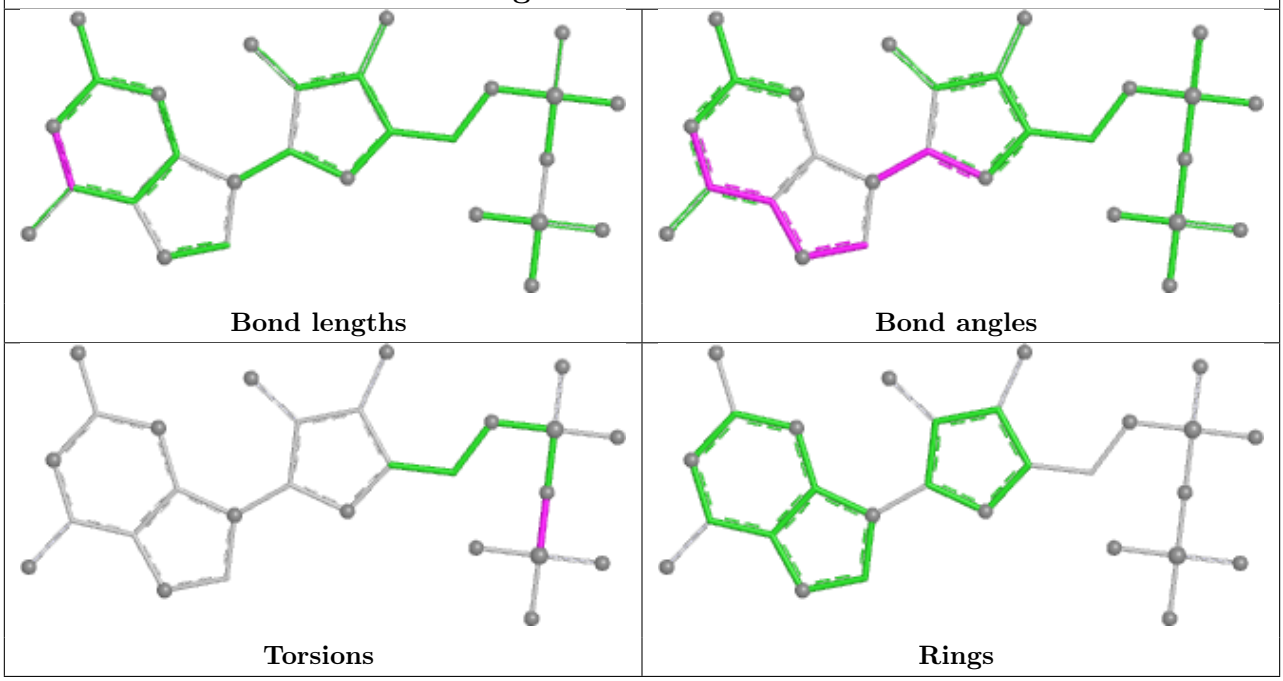

## Ligand GTP Z0 501



**Ligand GTP T4 501**




**Ligand GDP Y2 501**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

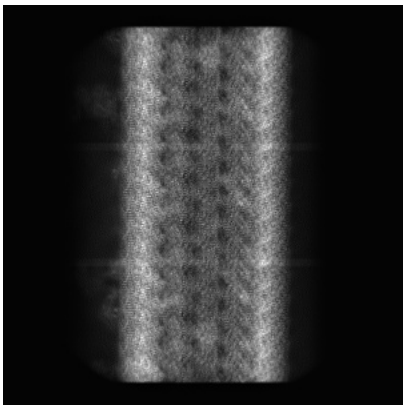
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20631. These allow visual inspection of the internal detail of the map and identification of artifacts.

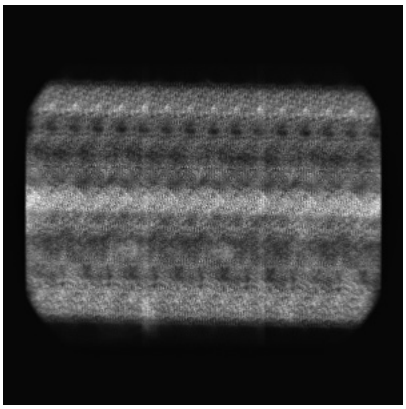
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

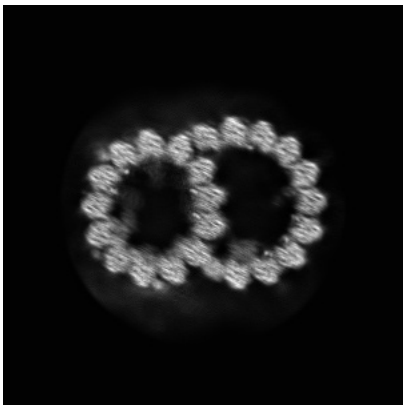
### 6.1.1 Primary map



X

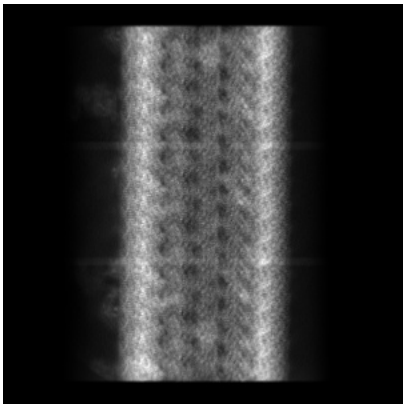


Y

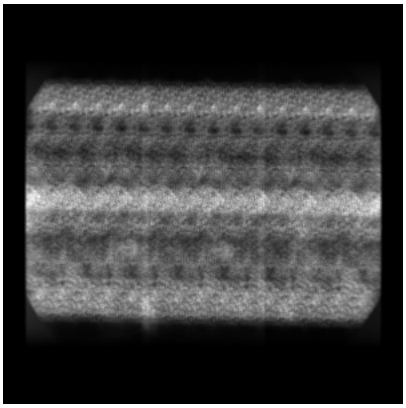


Z

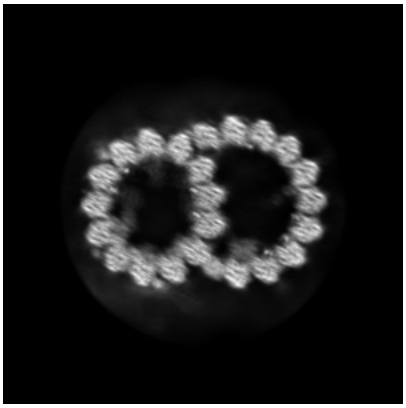
### 6.1.2 Raw map



X



Y

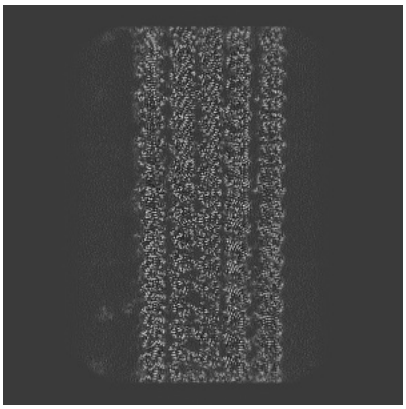


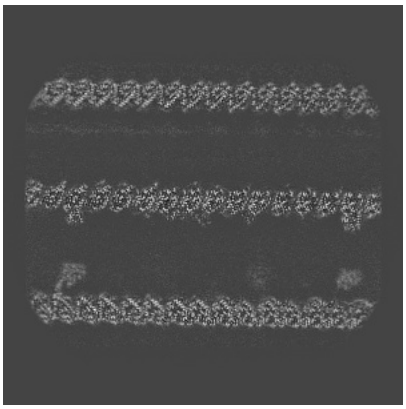
Z

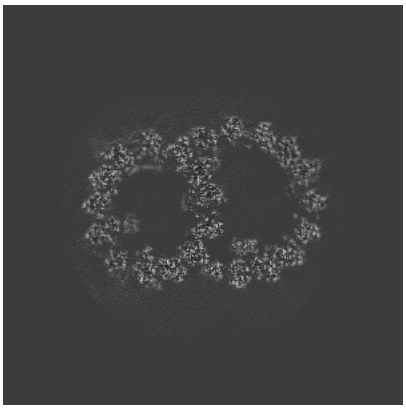
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

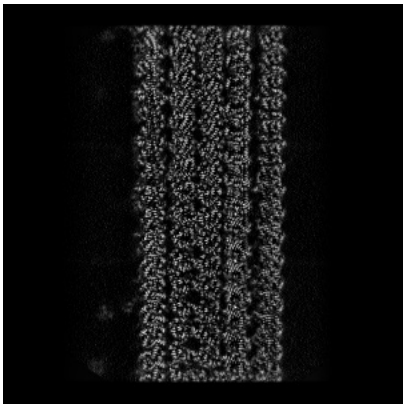
### 6.2.1 Primary map

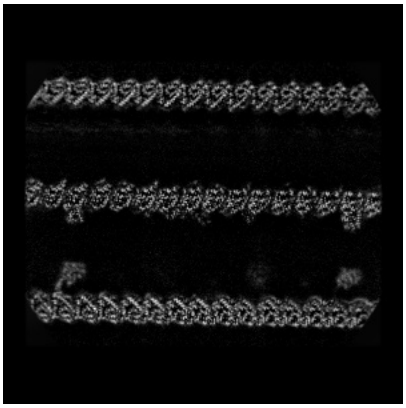

X Index: 256

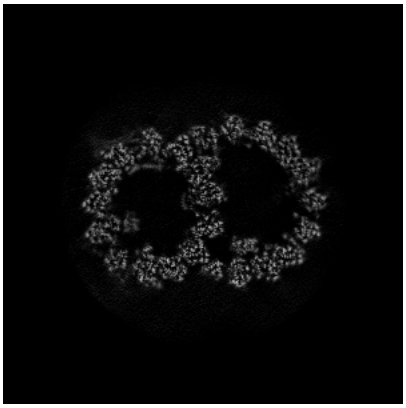

Y Index: 256


Z Index: 256

### 6.2.2 Raw map


X Index: 256

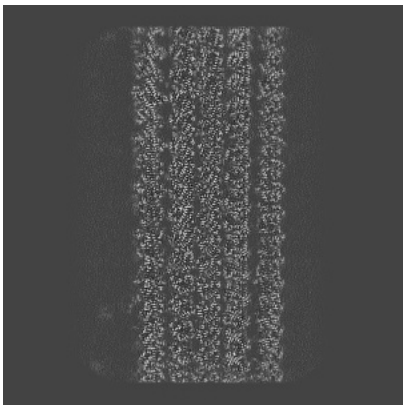

Y Index: 256

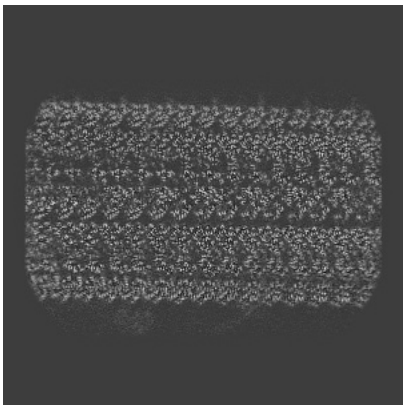

Z Index: 256

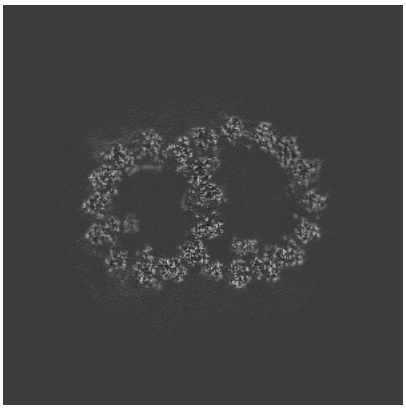
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

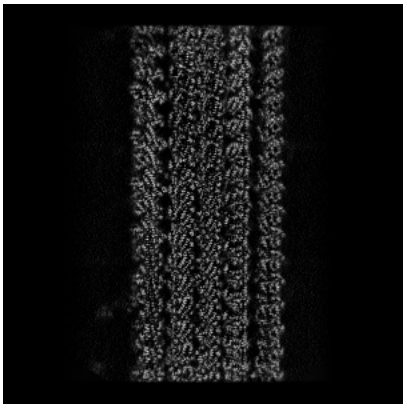
### 6.3.1 Primary map

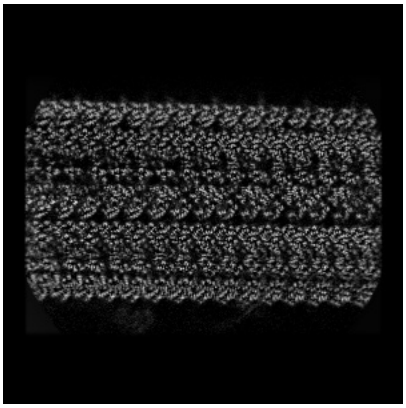

X Index: 258

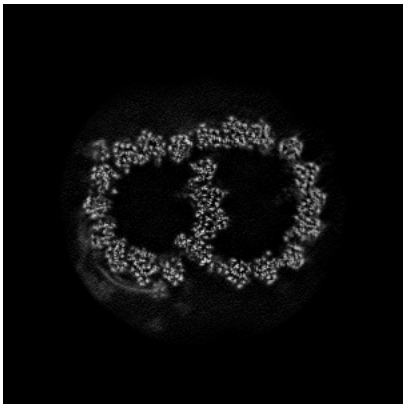

Y Index: 180


Z Index: 256

### 6.3.2 Raw map


X Index: 260

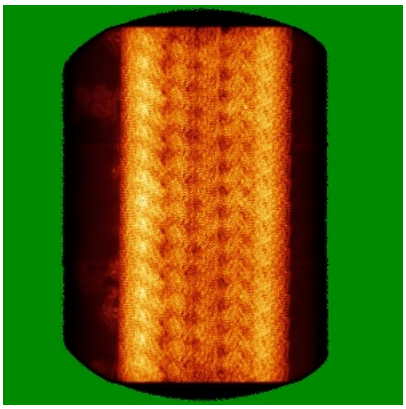

Y Index: 180

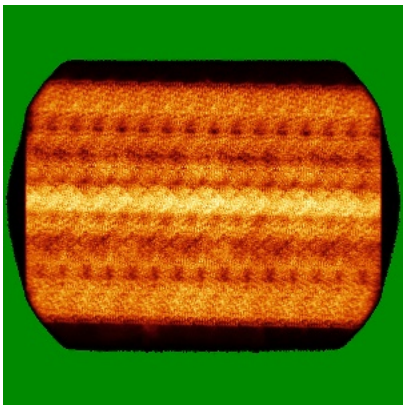

Z Index: 181

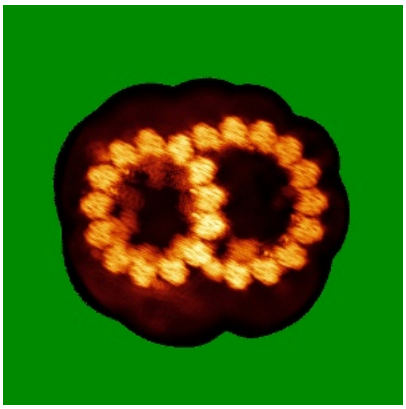
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

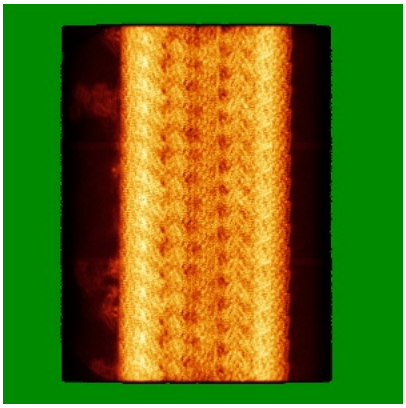
### 6.4.1 Primary map

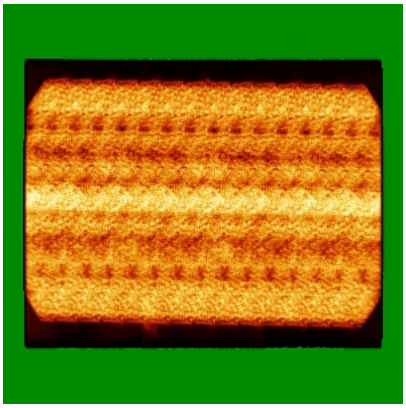

X


Y


Z

### 6.4.2 Raw map


X

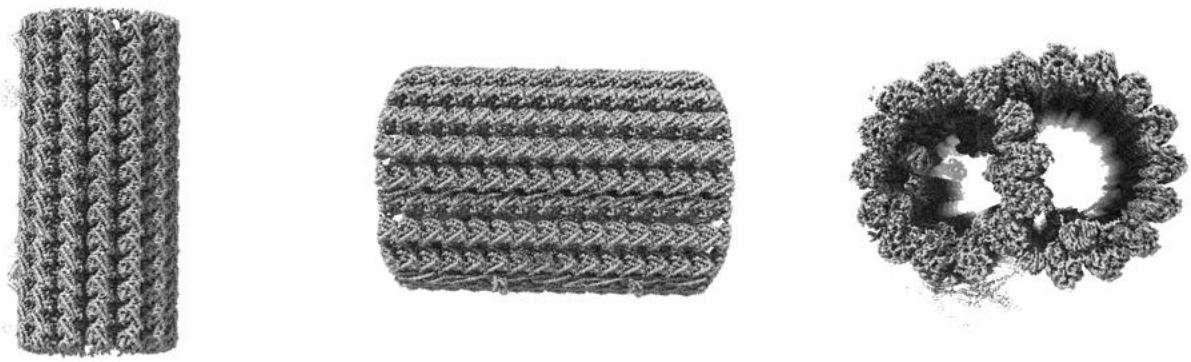

Y

Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

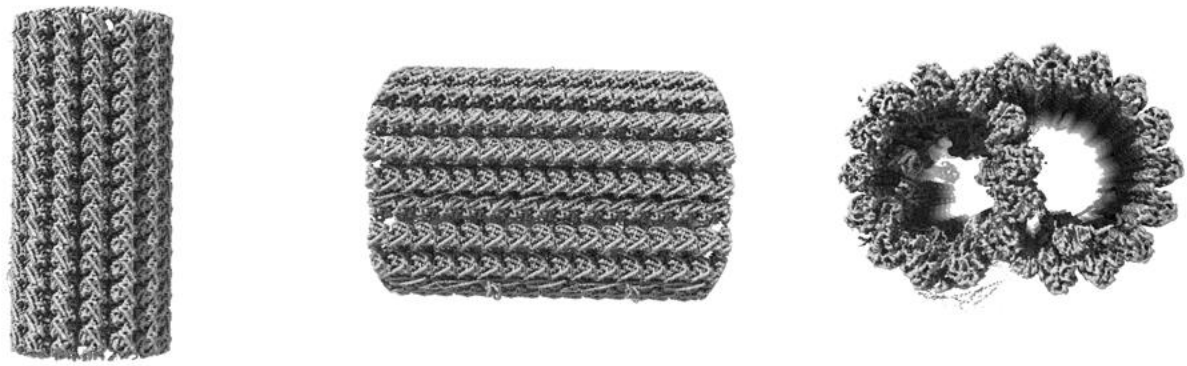
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

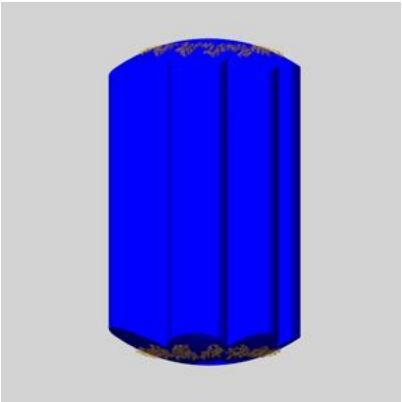
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

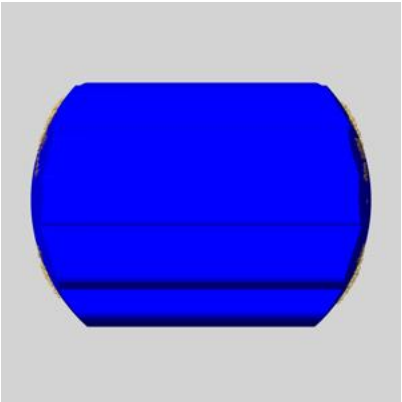
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

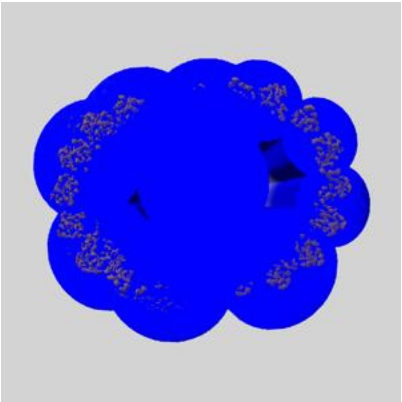
### 6.6.1 emd_20631_msk_1.map (i)



X



Y

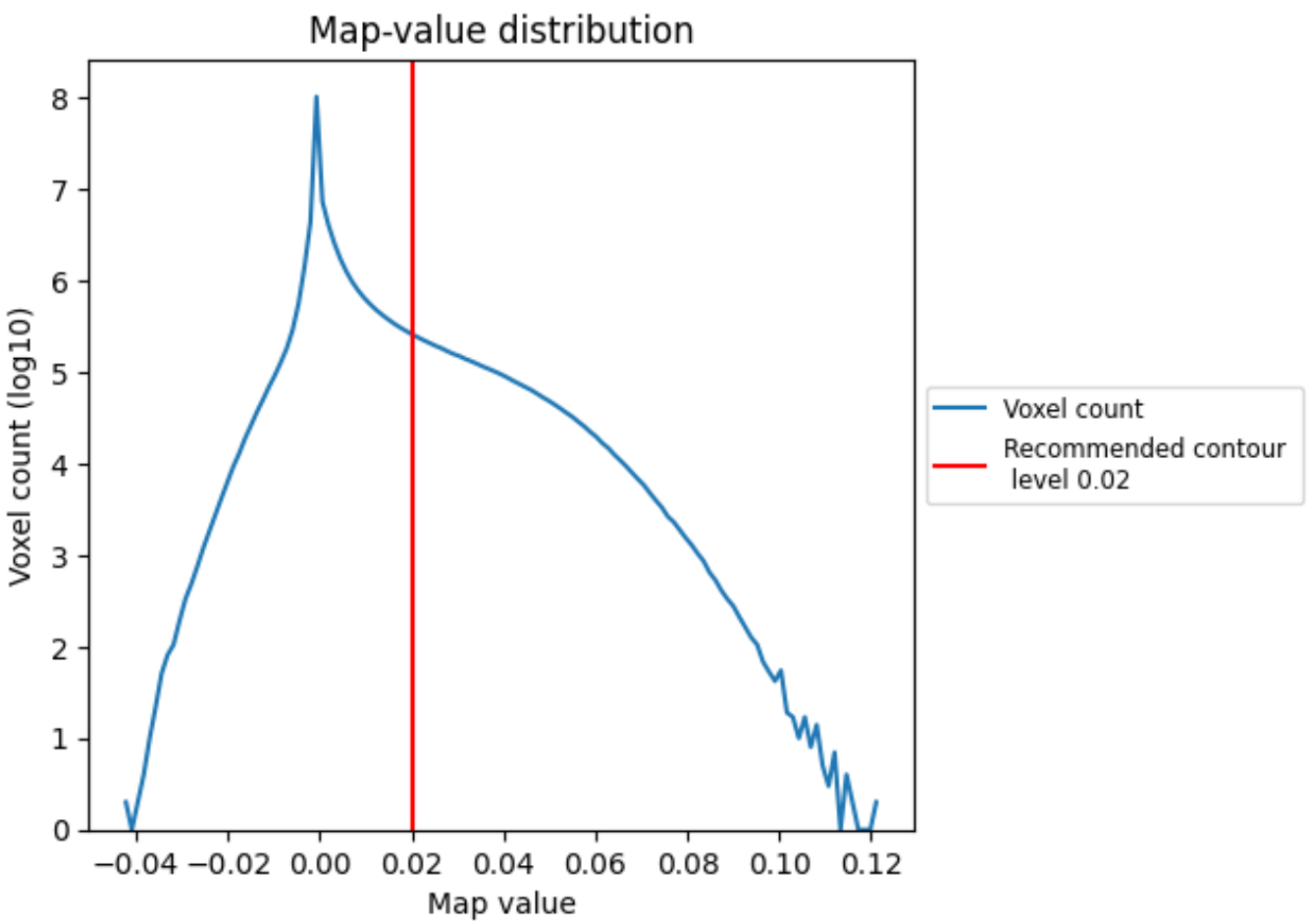


Z

# 7 Map analysis (i)

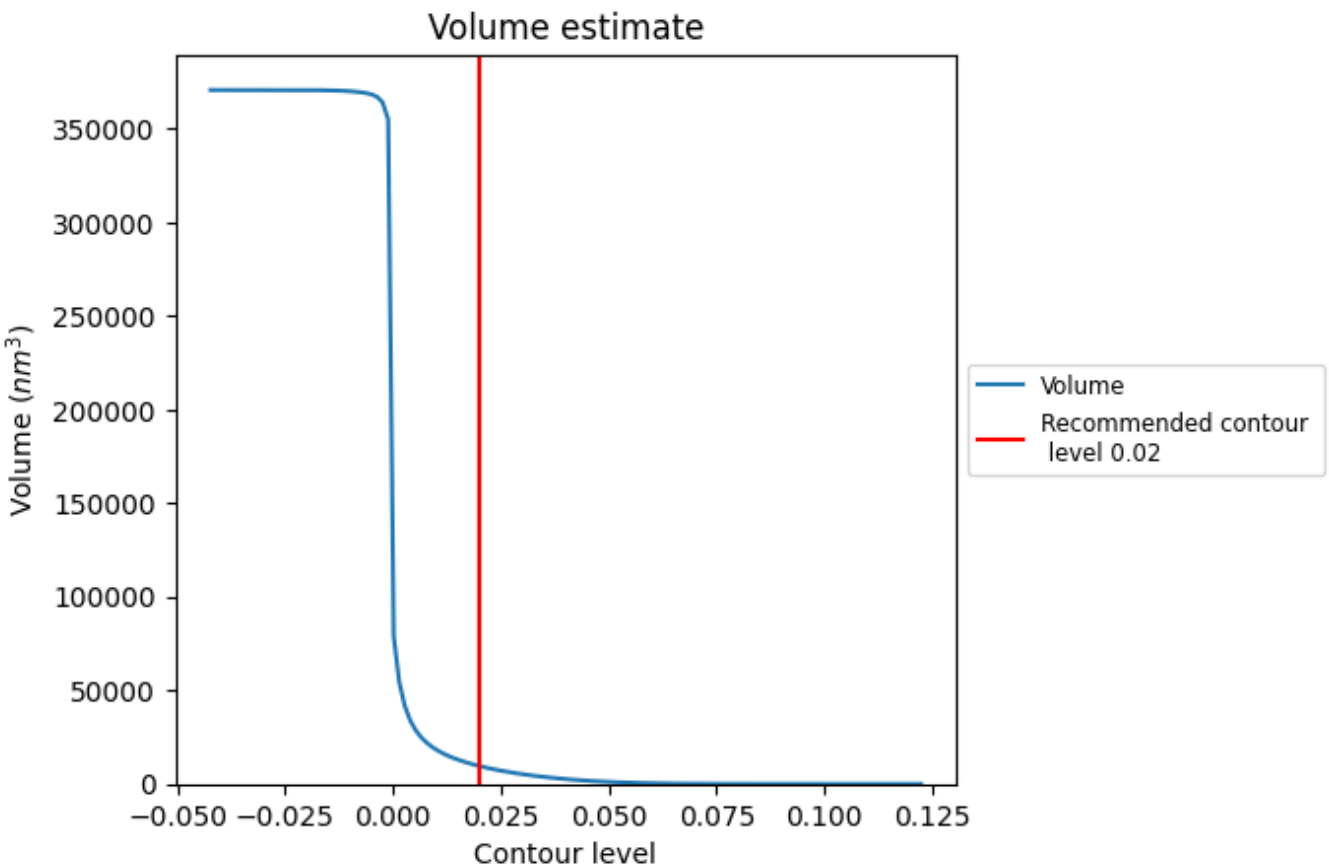
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

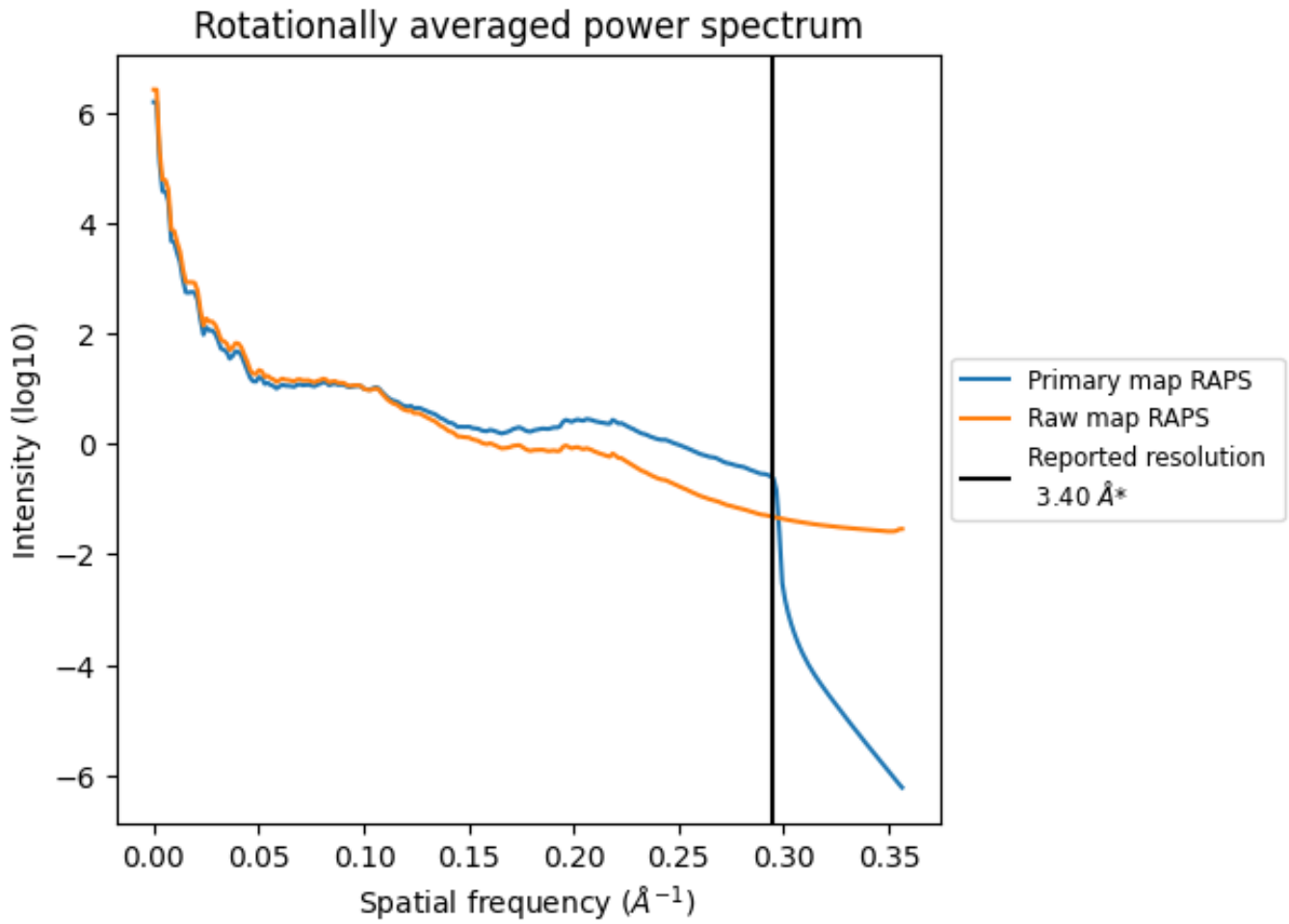
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 9602 $nm^3$; this corresponds to an approximate mass of 8673 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

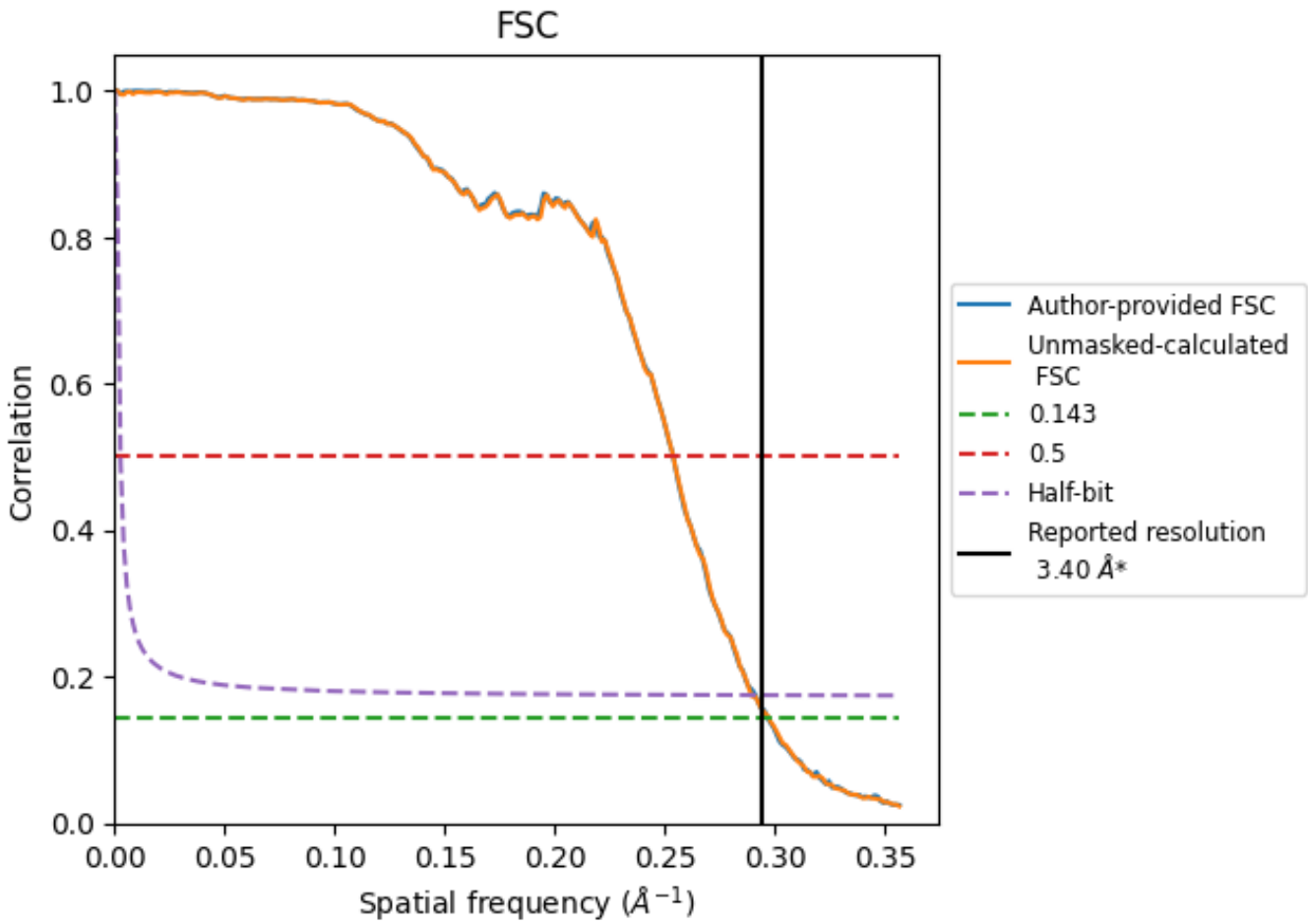



*Reported resolution corresponds to spatial frequency of 0.294 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.294 Å$^{-1}$

## 8.2 Resolution estimates (i)

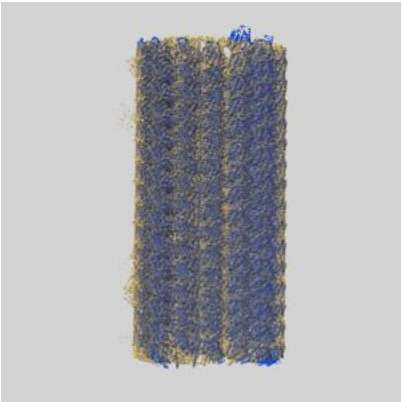
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.40 | - | - |
| Author-provided FSC curve | 3.37 | 3.94 | 3.44 |
| Unmasked-calculated* | 3.36 | 3.94 | 3.46 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

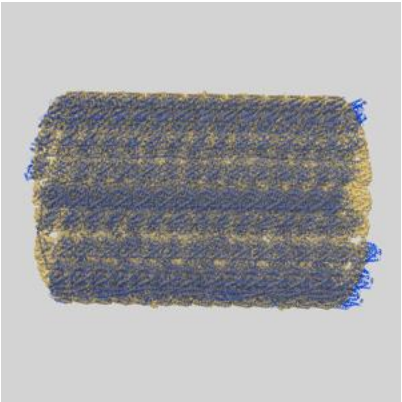
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20631 and PDB model 6U42. Per-residue inclusion information can be found in section 3 on page 72.

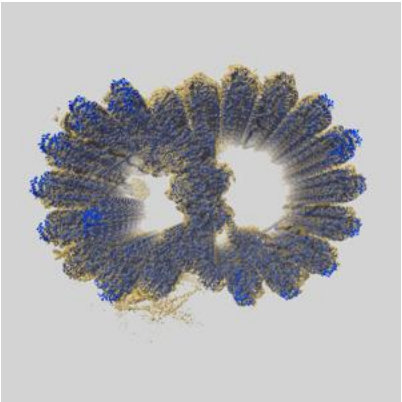
## 9.1 Map-model overlay (i)



X



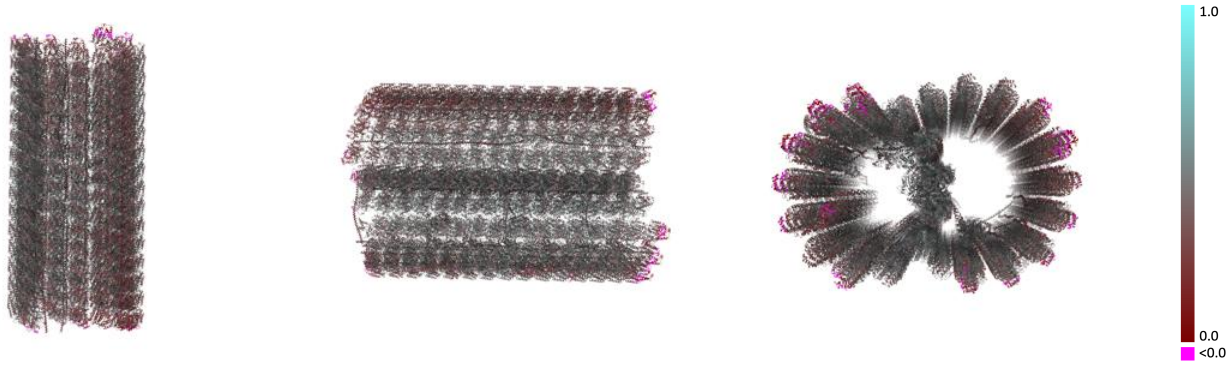
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

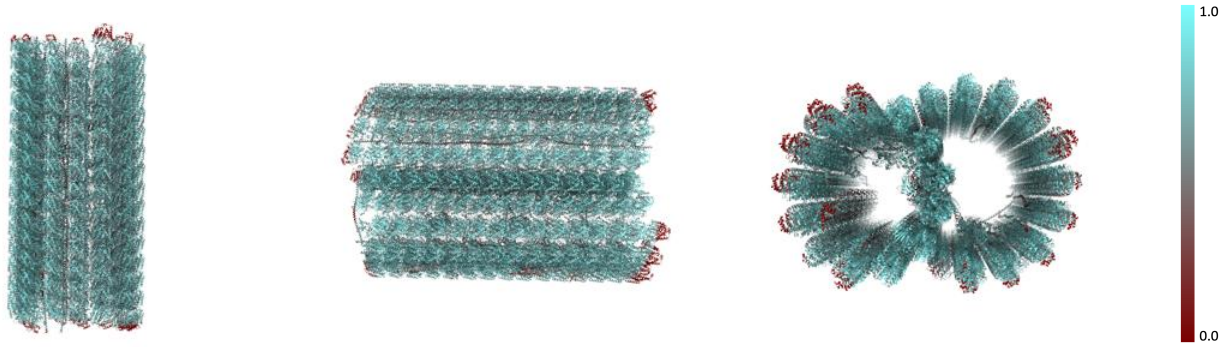
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

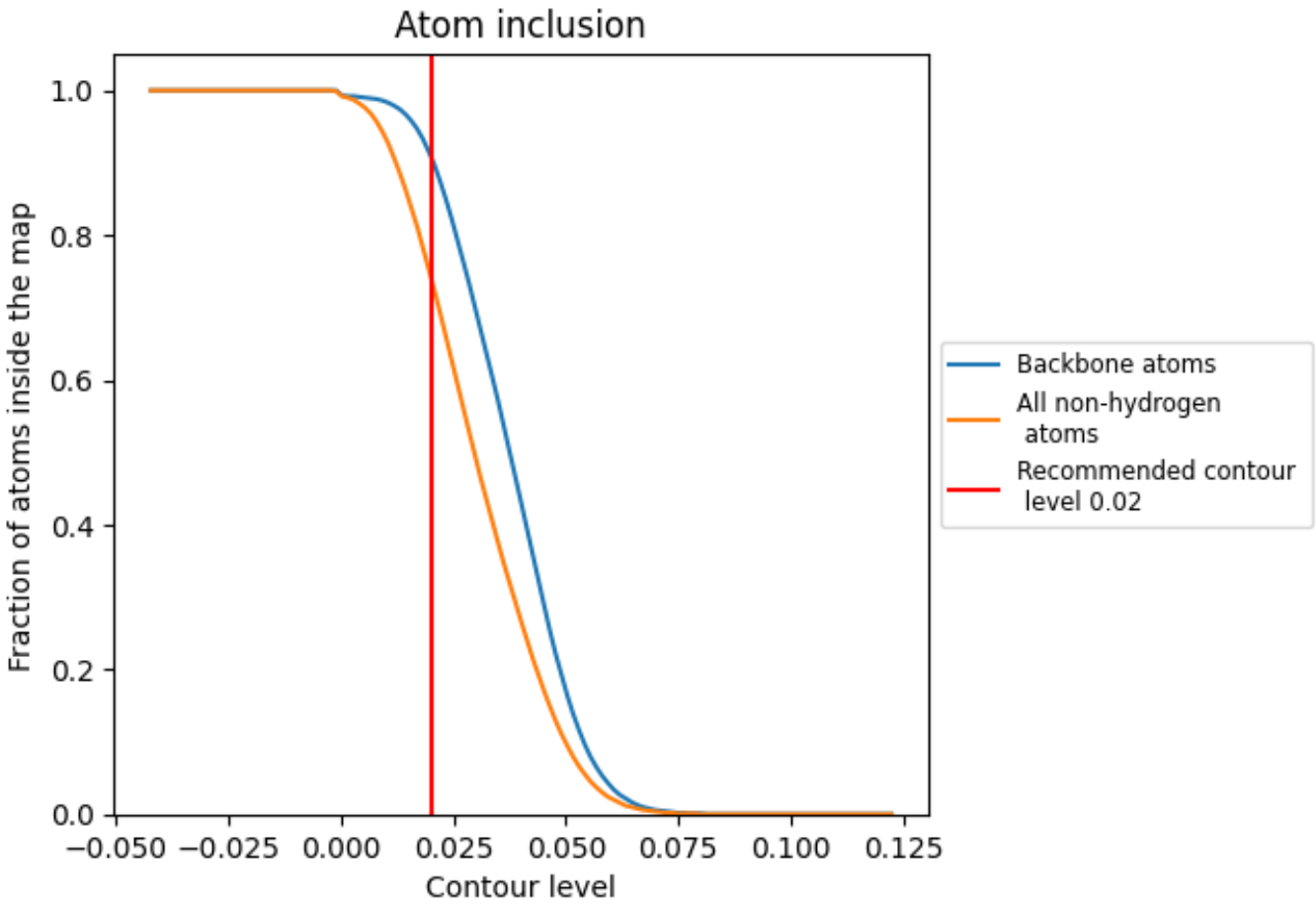
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion (i)




At the recommended contour level, 91% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7420 | 0.4300 |
| 0A | 0.7370 | 0.3560 |
| 0B | 0.7300 | 0.3380 |
| 0C | 0.6090 | 0.2820 |
| 0E | 0.6220 | 0.2650 |
| 0F | 0.7110 | 0.3210 |
| 0G | 0.7250 | 0.3350 |
| 0H | 0.7080 | 0.3340 |
| 0I | 0.7020 | 0.3280 |
| 0J | 0.6960 | 0.3710 |
| 0K | 0.7160 | 0.3810 |
| 0L | 0.7100 | 0.3780 |
| 0M | 0.7210 | 0.3860 |
| 0N | 0.6800 | 0.3580 |
| 0O | 0.7050 | 0.3580 |
| 0P | 0.7180 | 0.3690 |
| 0Q | 0.7280 | 0.3680 |
| 0R | 0.6960 | 0.3390 |
| 0S | 0.3710 | 0.1900 |
| 0U | 0.6160 | 0.3050 |
| 0V | 0.6750 | 0.3450 |
| 0W | 0.6970 | 0.3680 |
| 0X | 0.6900 | 0.3660 |
| 0Y | 0.6880 | 0.3750 |
| 0Z | 0.6990 | 0.4020 |
| 1 | 0.8460 | 0.4750 |
| 1A | 0.7080 | 0.4140 |
| 1B | 0.6970 | 0.4010 |
| 1C | 0.7020 | 0.4050 |
| 1D | 0.6760 | 0.3670 |
| 1E | 0.6920 | 0.3710 |
| 1F | 0.6760 | 0.3630 |
| 1G | 0.6810 | 0.3540 |
| 1H | 0.6020 | 0.3050 |
| 1K | 0.7220 | 0.3540 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 1L | 0.7570 | 0.4050 |
| 1M | 0.7560 | 0.4150 |
| 1N | 0.7490 | 0.4090 |
| 1O | 0.7350 | 0.4050 |
| 1P | 0.7560 | 0.4270 |
| 1Q | 0.7620 | 0.4410 |
| 1R | 0.7500 | 0.4280 |
| 1S | 0.7590 | 0.4280 |
| 1T | 0.7370 | 0.3960 |
| 1U | 0.7350 | 0.4000 |
| 1V | 0.7480 | 0.3950 |
| 1W | 0.7480 | 0.3900 |
| 1X | 0.6230 | 0.3180 |
| 1Z | 0.5680 | 0.3280 |
| 2 | 0.8290 | 0.4910 |
| 2A | 0.7580 | 0.3980 |
| 2B | 0.7750 | 0.4290 |
| 2C | 0.7720 | 0.4320 |
| 2D | 0.7590 | 0.4220 |
| 2E | 0.7580 | 0.4090 |
| 2F | 0.7880 | 0.4410 |
| 2G | 0.8020 | 0.4510 |
| 2H | 0.7920 | 0.4450 |
| 2I | 0.7920 | 0.4380 |
| 2J | 0.7650 | 0.4280 |
| 2K | 0.7690 | 0.4340 |
| 2L | 0.7770 | 0.4340 |
| 2M | 0.7770 | 0.4210 |
| 2N | 0.6510 | 0.3500 |
| 2P | 0.7520 | 0.4220 |
| 2Q | 0.7670 | 0.4430 |
| 2R | 0.7700 | 0.4550 |
| 2S | 0.7630 | 0.4540 |
| 2T | 0.7640 | 0.4410 |
| 2U | 0.7840 | 0.4560 |
| 2V | 0.7940 | 0.4650 |
| 2W | 0.8040 | 0.4760 |
| 2X | 0.7850 | 0.4630 |
| 2Y | 0.8010 | 0.4600 |
| 2Z | 0.7770 | 0.4590 |
| 3 | 0.8190 | 0.4990 |
| 3A | 0.7870 | 0.4640 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 3B | 0.7770 | 0.4490 |
| 3C | 0.7820 | 0.4420 |
| 3D | 0.6800 | 0.3770 |
| 3F | 0.7980 | 0.4370 |
| 3G | 0.8110 | 0.4600 |
| 3H | 0.8170 | 0.4660 |
| 3I | 0.8100 | 0.4710 |
| 3J | 0.8080 | 0.4530 |
| 3K | 0.8120 | 0.4600 |
| 3L | 0.8240 | 0.4740 |
| 3M | 0.8270 | 0.4790 |
| 3N | 0.8130 | 0.4610 |
| 3O | 0.8070 | 0.4530 |
| 3P | 0.8080 | 0.4590 |
| 3Q | 0.7960 | 0.4580 |
| 3R | 0.8040 | 0.4500 |
| 3S | 0.8000 | 0.4340 |
| 3T | 0.6390 | 0.3450 |
| 3V | 0.7570 | 0.4190 |
| 3W | 0.8250 | 0.4700 |
| 3X | 0.4290 | 0.4080 |
| 3Y | 0.8420 | 0.4940 |
| 3Z | 0.7490 | 0.4500 |
| 4 | 0.8180 | 0.5050 |
| 4A | 0.8370 | 0.4820 |
| 4B | 0.6770 | 0.4350 |
| 4C | 0.8400 | 0.4870 |
| 4D | 0.7600 | 0.4640 |
| 4E | 0.8240 | 0.4770 |
| 4F | 0.6740 | 0.4240 |
| 4G | 0.8180 | 0.4720 |
| 4H | 0.7500 | 0.4430 |
| 4I | 0.8100 | 0.4610 |
| 4J | 0.4450 | 0.4210 |
| 4L | 0.6120 | 0.3360 |
| 4M | 0.6680 | 0.3820 |
| 4N | 0.6150 | 0.3210 |
| 4O | 0.5690 | 0.3260 |
| 4P | 0.7030 | 0.4020 |
| 4Q | 0.7620 | 0.4420 |
| 4R | 0.7290 | 0.4650 |
| 4S | 0.7250 | 0.4290 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 4T | 0.7480 | 0.4530 |
| 4U | 0.7630 | 0.4690 |
| 4V | 0.5860 | 0.3590 |
| 4W | 0.4820 | 0.3340 |
| 4X | 0.7070 | 0.3980 |
| 4Y | 0.6020 | 0.3570 |
| 4Z | 0.5290 | 0.3180 |
| 5 | 0.8130 | 0.5050 |
| 5A | 0.5170 | 0.3020 |
| 5B | 0.5230 | 0.3210 |
| 5C | 0.5780 | 0.3700 |
| 5D | 0.5790 | 0.3640 |
| 5E | 0.4110 | 0.4750 |
| 5F | 0.7330 | 0.4860 |
| 5G | 0.7340 | 0.4760 |
| 5H | 0.7840 | 0.4550 |
| 5I | 0.7730 | 0.4790 |
| 5J | 0.7460 | 0.4650 |
| 5K | 0.7860 | 0.4650 |
| 5L | 0.7520 | 0.4530 |
| 5M | 0.7710 | 0.4660 |
| 5N | 0.7270 | 0.4380 |
| 5O | 0.6520 | 0.4170 |
| 5P | 0.7600 | 0.4460 |
| 5Q | 0.7260 | 0.4750 |
| 5R | 0.7440 | 0.4490 |
| 5S | 0.6280 | 0.4090 |
| 5T | 0.6360 | 0.4180 |
| 5U | 0.5900 | 0.4360 |
| 5V | 0.6240 | 0.4190 |
| 5X | 0.6870 | 0.4420 |
| 5Y | 0.6880 | 0.4480 |
| 5Z | 0.5550 | 0.4350 |
| 6 | 0.8280 | 0.5080 |
| 6A | 0.6660 | 0.4470 |
| 6B | 0.5020 | 0.4190 |
| 6C | 0.5750 | 0.4210 |
| 6D | 0.6180 | 0.4090 |
| 6E | 0.7370 | 0.4770 |
| 6F | 0.7860 | 0.4820 |
| 6G | 0.5490 | 0.4760 |
| 6H | 0.5180 | 0.4640 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 6I | 0.6550 | 0.3670 |
| 6J | 0.6510 | 0.4100 |
| 6K | 0.6410 | 0.4100 |
| 6L | 0.6480 | 0.4420 |
| 6M | 0.6410 | 0.4300 |
| 6N | 0.5920 | 0.4080 |
| 6O | 0.6220 | 0.4010 |
| 6P | 0.5000 | 0.3060 |
| 6Q | 0.6940 | 0.4520 |
| 6R | 0.7120 | 0.4470 |
| 6S | 0.6340 | 0.4170 |
| 6T | 0.7050 | 0.4190 |
| 6U | 0.7010 | 0.4500 |
| 6V | 0.7060 | 0.4470 |
| 6W | 0.7330 | 0.4860 |
| 6X | 0.7030 | 0.4560 |
| 6Y | 0.6740 | 0.4450 |
| 6Z | 0.6920 | 0.4280 |
| 7 | 0.8200 | 0.5030 |
| 7A | 0.7340 | 0.4460 |
| 7B | 0.7120 | 0.4780 |
| 7C | 0.6090 | 0.4370 |
| 7D | 0.7610 | 0.4860 |
| 7E | 0.7810 | 0.4910 |
| 7F | 0.5520 | 0.4700 |
| 7G | 0.6800 | 0.4610 |
| 7H | 0.6870 | 0.4210 |
| 7I | 0.6410 | 0.4360 |
| 7J | 0.7150 | 0.4510 |
| 7K | 0.6800 | 0.4330 |
| 7L | 0.7160 | 0.4460 |
| 7M | 0.6090 | 0.4630 |
| 7N | 0.5460 | 0.4640 |
| 7O | 0.7120 | 0.4240 |
| 7P | 0.6860 | 0.4690 |
| 7Q | 0.5990 | 0.4710 |
| 7R | 0.5080 | 0.3480 |
| 7S | 0.5430 | 0.3390 |
| 7T | 0.5130 | 0.3420 |
| 7U | 0.5160 | 0.3280 |
| 7V | 0.4630 | 0.2830 |
| 7W | 0.3500 | 0.2580 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 7X | 0.6080 | 0.3760 |
| 7Y | 0.4930 | 0.4670 |
| 7Z | 0.6180 | 0.4010 |
| 8 | 0.8340 | 0.5150 |
| 8A | 0.5740 | 0.4280 |
| 8B | 0.5720 | 0.4460 |
| 8C | 0.6410 | 0.4510 |
| 8D | 0.5470 | 0.4280 |
| 9 | 0.8260 | 0.5090 |
| A0 | 0.8080 | 0.4950 |
| A1 | 0.8130 | 0.4890 |
| A2 | 0.8150 | 0.5000 |
| A3 | 0.8150 | 0.5010 |
| A4 | 0.8140 | 0.4850 |
| A5 | 0.8230 | 0.4760 |
| A7 | 0.8250 | 0.4540 |
| A8 | 0.8240 | 0.4800 |
| A9 | 0.8320 | 0.5000 |
| B0 | 0.8210 | 0.4910 |
| B1 | 0.8230 | 0.4910 |
| B2 | 0.8260 | 0.4990 |
| B3 | 0.8380 | 0.5040 |
| B4 | 0.8210 | 0.5030 |
| B5 | 0.8300 | 0.5050 |
| B7 | 0.7970 | 0.4790 |
| B8 | 0.8050 | 0.4810 |
| B9 | 0.8140 | 0.4840 |
| C0 | 0.8210 | 0.4840 |
| C1 | 0.7940 | 0.4580 |
| C2 | 0.8070 | 0.4400 |
| C4 | 0.8190 | 0.4250 |
| C5 | 0.8300 | 0.4740 |
| C6 | 0.8300 | 0.4800 |
| C7 | 0.8170 | 0.4700 |
| C8 | 0.8200 | 0.4720 |
| C9 | 0.8200 | 0.4870 |
| D0 | 0.8320 | 0.4980 |
| D1 | 0.8170 | 0.4950 |
| D2 | 0.8100 | 0.4900 |
| D3 | 0.7770 | 0.4570 |
| D4 | 0.7820 | 0.4610 |
| D5 | 0.8130 | 0.4710 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| D6 | 0.8170 | 0.4670 |
| D7 | 0.7770 | 0.4310 |
| D8 | 0.6030 | 0.3340 |
| E0 | 0.7710 | 0.3970 |
| E1 | 0.7770 | 0.4380 |
| E2 | 0.7900 | 0.4500 |
| E3 | 0.7640 | 0.4440 |
| E4 | 0.7490 | 0.4130 |
| E5 | 0.7540 | 0.4420 |
| E6 | 0.7650 | 0.4450 |
| E7 | 0.7510 | 0.4420 |
| E8 | 0.7480 | 0.4360 |
| E9 | 0.6990 | 0.4040 |
| F0 | 0.7160 | 0.4180 |
| F1 | 0.7310 | 0.4140 |
| F2 | 0.7350 | 0.4050 |
| F3 | 0.6670 | 0.3580 |
| F5 | 0.3640 | 0.1850 |
| F6 | 0.7310 | 0.3650 |
| F7 | 0.7540 | 0.4080 |
| F8 | 0.7610 | 0.4210 |
| F9 | 0.7200 | 0.4040 |
| G0 | 0.7440 | 0.4010 |
| G1 | 0.7540 | 0.4320 |
| G2 | 0.7700 | 0.4420 |
| G3 | 0.7610 | 0.4330 |
| G4 | 0.7690 | 0.4290 |
| G5 | 0.7170 | 0.4070 |
| G6 | 0.7400 | 0.4190 |
| G7 | 0.7400 | 0.4040 |
| G8 | 0.7300 | 0.3980 |
| G9 | 0.5770 | 0.3110 |
| H1 | 0.5200 | 0.2780 |
| H2 | 0.7230 | 0.3820 |
| H3 | 0.7720 | 0.4350 |
| H4 | 0.7740 | 0.4360 |
| H5 | 0.7520 | 0.4130 |
| H6 | 0.7700 | 0.4190 |
| H7 | 0.7930 | 0.4490 |
| H8 | 0.7910 | 0.4550 |
| H9 | 0.7840 | 0.4440 |
| I0 | 0.7730 | 0.4390 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| I1 | 0.7530 | 0.4300 |
| I2 | 0.7640 | 0.4360 |
| I3 | 0.7500 | 0.4220 |
| I4 | 0.7380 | 0.4080 |
| I5 | 0.4760 | 0.2690 |
| I7 | 0.7090 | 0.3880 |
| I8 | 0.7800 | 0.4340 |
| I9 | 0.7970 | 0.4590 |
| J0 | 0.8060 | 0.4710 |
| J1 | 0.7750 | 0.4340 |
| J2 | 0.7990 | 0.4580 |
| J3 | 0.8050 | 0.4680 |
| J4 | 0.8200 | 0.4810 |
| J5 | 0.8070 | 0.4580 |
| J6 | 0.8090 | 0.4580 |
| J7 | 0.7850 | 0.4490 |
| J8 | 0.8010 | 0.4610 |
| J9 | 0.7760 | 0.4350 |
| K0 | 0.7730 | 0.4290 |
| K1 | 0.4200 | 0.2380 |
| K3 | 0.7840 | 0.4140 |
| K4 | 0.8080 | 0.4440 |
| K5 | 0.8090 | 0.4590 |
| K6 | 0.8110 | 0.4600 |
| K7 | 0.7850 | 0.4330 |
| K8 | 0.7950 | 0.4530 |
| K9 | 0.8070 | 0.4680 |
| L0 | 0.8200 | 0.4720 |
| L1 | 0.7950 | 0.4550 |
| L2 | 0.8060 | 0.4490 |
| L3 | 0.8020 | 0.4630 |
| L4 | 0.8250 | 0.4720 |
| L5 | 0.8050 | 0.4520 |
| L6 | 0.8090 | 0.4340 |
| L7 | 0.4370 | 0.2510 |
| L9 | 0.7920 | 0.4340 |
| M0 | 0.7990 | 0.4520 |
| M1 | 0.7950 | 0.4550 |
| M2 | 0.7690 | 0.4520 |
| M3 | 0.7670 | 0.4420 |
| M4 | 0.7760 | 0.4590 |
| M5 | 0.8030 | 0.4690 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| M6 | 0.7900 | 0.4690 |
| M7 | 0.7820 | 0.4560 |
| M8 | 0.7790 | 0.4540 |
| M9 | 0.7890 | 0.4680 |
| N0 | 0.8020 | 0.4700 |
| N1 | 0.7940 | 0.4490 |
| N2 | 0.8040 | 0.4370 |
| N3 | 0.4190 | 0.2430 |
| N5 | 0.8060 | 0.4260 |
| N6 | 0.8130 | 0.4580 |
| N7 | 0.8060 | 0.4600 |
| N8 | 0.8110 | 0.4730 |
| N9 | 0.7720 | 0.4520 |
| O0 | 0.8030 | 0.4610 |
| O1 | 0.8000 | 0.4640 |
| O2 | 0.8180 | 0.4810 |
| O3 | 0.8000 | 0.4660 |
| O4 | 0.8190 | 0.4720 |
| O5 | 0.8020 | 0.4630 |
| O6 | 0.8180 | 0.4820 |
| O7 | 0.8060 | 0.4670 |
| O8 | 0.8210 | 0.4640 |
| O9 | 0.8120 | 0.4370 |
| P3 | 0.8130 | 0.4570 |
| P4 | 0.7910 | 0.4720 |
| P5 | 0.7840 | 0.4730 |
| P6 | 0.7710 | 0.4670 |
| P7 | 0.7670 | 0.4630 |
| P8 | 0.7710 | 0.4690 |
| P9 | 0.7790 | 0.4740 |
| Q0 | 0.7880 | 0.4790 |
| Q1 | 0.7860 | 0.4740 |
| Q2 | 0.7910 | 0.4770 |
| Q3 | 0.7850 | 0.4770 |
| Q4 | 0.8040 | 0.4860 |
| Q5 | 0.7990 | 0.4820 |
| Q6 | 0.8150 | 0.4740 |
| Q8 | 0.4780 | 0.3100 |
| Q9 | 0.7840 | 0.4690 |
| R0 | 0.7770 | 0.4860 |
| R1 | 0.7580 | 0.4820 |
| R2 | 0.7630 | 0.4830 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| R3 | 0.7640 | 0.4780 |
| R4 | 0.7690 | 0.4930 |
| R5 | 0.7660 | 0.4890 |
| R6 | 0.7710 | 0.4880 |
| R7 | 0.7780 | 0.4950 |
| R8 | 0.7820 | 0.4880 |
| R9 | 0.7430 | 0.4760 |
| S0 | 0.7650 | 0.4840 |
| S1 | 0.7740 | 0.4820 |
| S2 | 0.7930 | 0.4720 |
| S4 | 0.6990 | 0.4180 |
| S5 | 0.8070 | 0.4810 |
| S6 | 0.7990 | 0.4910 |
| S7 | 0.7800 | 0.4800 |
| S8 | 0.7840 | 0.4990 |
| S9 | 0.7900 | 0.4940 |
| T0 | 0.8050 | 0.5010 |
| T1 | 0.8010 | 0.4940 |
| T2 | 0.8030 | 0.5020 |
| T3 | 0.8010 | 0.4950 |
| T4 | 0.7930 | 0.4910 |
| T5 | 0.7720 | 0.4850 |
| T6 | 0.7830 | 0.4830 |
| T7 | 0.7880 | 0.4780 |
| T8 | 0.8070 | 0.4720 |
| U1 | 0.7370 | 0.4110 |
| U2 | 0.7450 | 0.4330 |
| U3 | 0.7530 | 0.4410 |
| U4 | 0.7400 | 0.4470 |
| U5 | 0.7130 | 0.4290 |
| U6 | 0.7160 | 0.4420 |
| U7 | 0.7480 | 0.4550 |
| U8 | 0.7460 | 0.4600 |
| U9 | 0.7500 | 0.4570 |
| V0 | 0.7350 | 0.4470 |
| V1 | 0.7460 | 0.4530 |
| V2 | 0.7590 | 0.4580 |
| V3 | 0.7510 | 0.4490 |
| V4 | 0.7550 | 0.4490 |
| V6 | 0.5190 | 0.2730 |
| V7 | 0.7680 | 0.3980 |
| V8 | 0.7720 | 0.4180 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| V9 | 0.7720 | 0.4290 |
| W0 | 0.7810 | 0.4360 |
| W1 | 0.7720 | 0.4290 |
| W2 | 0.7920 | 0.4490 |
| W3 | 0.7920 | 0.4570 |
| W4 | 0.8090 | 0.4620 |
| W5 | 0.7900 | 0.4530 |
| W6 | 0.7900 | 0.4430 |
| W7 | 0.7950 | 0.4490 |
| W8 | 0.8080 | 0.4530 |
| W9 | 0.7920 | 0.4390 |
| X0 | 0.7890 | 0.4140 |
| X2 | 0.5910 | 0.2770 |
| X3 | 0.7280 | 0.3540 |
| X4 | 0.7310 | 0.3750 |
| X5 | 0.7300 | 0.3740 |
| X6 | 0.7390 | 0.3940 |
| X7 | 0.7310 | 0.3930 |
| X8 | 0.7470 | 0.4150 |
| X9 | 0.7610 | 0.4240 |
| Y0 | 0.7570 | 0.4320 |
| Y1 | 0.7270 | 0.4070 |
| Y2 | 0.7390 | 0.4020 |
| Y3 | 0.7550 | 0.4150 |
| Y4 | 0.7600 | 0.4230 |
| Y5 | 0.7510 | 0.4060 |
| Y6 | 0.7510 | 0.3900 |
| Y8 | 0.5500 | 0.2440 |
| Y9 | 0.6850 | 0.2980 |
| Z0 | 0.6910 | 0.3170 |
| Z1 | 0.6750 | 0.3180 |
| Z2 | 0.6700 | 0.3180 |
| Z3 | 0.6850 | 0.3580 |
| Z4 | 0.7150 | 0.3830 |
| Z5 | 0.7070 | 0.3800 |
| Z6 | 0.7170 | 0.3830 |
| Z7 | 0.6850 | 0.3560 |
| Z8 | 0.7020 | 0.3340 |
| Z9 | 0.7220 | 0.3560 |