



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 07:32 PM EST

PDB ID : 7ML4
EMDB ID : EMD-23908
Title : RNA polymerase II initially transcribing complex (ITC)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 3.10 Å(reported)
Based on initial model : 5OQJ

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

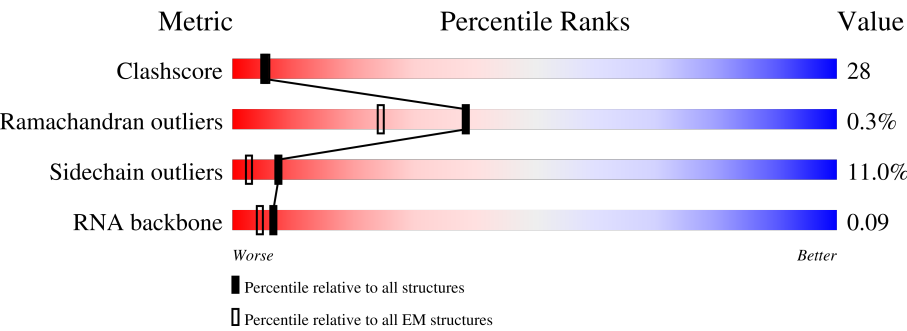
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 3.10 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 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 $\leq 5\%$. 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 | Q | 735 | <div><div>7% 11% . 80%</div></div> |
| 2 | R | 398 | <div><div>5% 18% 18% . 61%</div></div> |
| 3 | D | 221 | <div><div>30% 27% 41% . 29%</div></div> |
| 4 | G | 171 | <div><div>18% 32% 60% 8%</div></div> |
| 5 | M | 345 | <div><div>11% 26% 36% 5% . 32%</div></div> |
| 6 | A | 1733 | <div><div>36% 38% 7% 19%</div></div> |
| 7 | B | 1224 | <div><div>45% 38% 8% 9%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | C | 318 | |
| 9 | E | 215 | |
| 10 | F | 155 | |
| 11 | H | 146 | |
| 12 | I | 122 | |
| 13 | J | 70 | |
| 14 | K | 120 | |
| 15 | L | 70 | |
| 16 | 3 | 321 | |
| 17 | 0 | 778 | |
| 18 | 4 | 338 | |
| 19 | 6 | 461 | |
| 20 | 1 | 543 | |
| 21 | 7 | 843 | |
| 22 | 5 | 72 | |
| 23 | 2 | 513 | |
| 24 | X | 328 | |
| 25 | U | 286 | |
| 26 | V | 122 | |
| 27 | N | 38 | |
| 28 | T | 148 | |
| 29 | O | 240 | |
| 30 | W | 482 | |
| 31 | P | 5 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 34 | SF4 | 0 | 801 | - | - | X | - |

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 62733 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 Transcription initiation factor IIF subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | Q | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 731 | 195 | 212 | 3 | | |

- Molecule 2 is a protein called Transcription initiation factor IIF subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | R | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1039 | 652 | 190 | 193 | 4 | | |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | D | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1253 | 779 | 220 | 252 | 2 | | |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | G | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1340 | 861 | 222 | 249 | 8 | | |

- Molecule 5 is a protein called Transcription initiation factor IIB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | M | 234 | Total | C | N | O | S | 0 | 0 |
| | | | 1805 | 1152 | 304 | 333 | 16 | | |

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6 | A | 1405 | Total | C | N | O | S | 0 | 0 |
| | | | 11039 | 6962 | 1935 | 2081 | 61 | | |

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 7 | B | 1114 | Total | C | N | O | S | 0 | 0 |
| | | | 8861 | 5610 | 1549 | 1647 | 55 | | |

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | C | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2095 | 1317 | 348 | 417 | 13 | | |

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | E | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1752 | 1111 | 309 | 321 | 11 | | |

- Molecule 10 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | F | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 688 | 439 | 116 | 130 | 3 | | |

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | H | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1068 | 673 | 180 | 211 | 4 | | |

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12 | I | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 596 | 179 | 186 | 10 | | |

- Molecule 13 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13 | J | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 532 | 339 | 93 | 94 | 6 | | |

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | K | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 919 | 590 | 156 | 171 | 2 | | |

- Molecule 15 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15 | L | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 363 | 224 | 72 | 63 | 4 | | |

- Molecule 16 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16 | 3 | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 361 | 215 | 72 | 74 | | | |

- Molecule 17 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 17 | 0 | 754 | Total | C | N | O | S | 0 | 0 |
| | | | 6108 | 3891 | 1032 | 1147 | 38 | | |

- Molecule 18 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18 | 4 | 284 | Total | C | N | O | S | 0 | 0 |
| | | | 2041 | 1310 | 343 | 376 | 12 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| 4 | 113 | UNK | ASP | conflict | UNP A0A7I9C5C2 |
| 4 | 114 | UNK | MET | conflict | UNP A0A7I9C5C2 |

- Molecule 19 is a protein called General transcription and DNA repair factor IIIH.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19 | 6 | 351 | Total | C | N | O | S | 0 | 0 |
| | | | 2527 | 1590 | 454 | 456 | 27 | | |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| 6 | 412 | UNK | ILE | conflict | UNP A0A7I9FQL5 |
| 6 | 413 | UNK | LEU | conflict | UNP A0A7I9FQL5 |
| 6 | 414 | UNK | LYS | conflict | UNP A0A7I9FQL5 |
| 6 | 415 | UNK | ASN | conflict | UNP A0A7I9FQL5 |
| 6 | 416 | UNK | HIS | conflict | UNP A0A7I9FQL5 |
| 6 | 417 | UNK | LYS | conflict | UNP A0A7I9FQL5 |
| 6 | 418 | UNK | ASN | conflict | UNP A0A7I9FQL5 |
| 6 | 419 | UNK | ASP | conflict | UNP A0A7I9FQL5 |
| 6 | 420 | UNK | LYS | conflict | UNP A0A7I9FQL5 |
| 6 | 421 | UNK | LEU | conflict | UNP A0A7I9FQL5 |
| 6 | 422 | UNK | LEU | conflict | UNP A0A7I9FQL5 |
| 6 | 423 | UNK | THR | conflict | UNP A0A7I9FQL5 |
| 6 | 424 | UNK | SER | conflict | UNP A0A7I9FQL5 |

- Molecule 20 is a protein called Tfb1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20 | 1 | 367 | Total | C | N | O | S | 0 | 0 |
| | | | 2411 | 1536 | 438 | 430 | 7 | | |

- Molecule 21 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21 | 7 | 634 | Total | C | N | O | S | 0 | 0 |
| | | | 4447 | 2722 | 827 | 874 | 24 | | |

- Molecule 22 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22 | 5 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 498 | 314 | 89 | 93 | 2 | | |

- Molecule 23 is a protein called RNA polymerase II transcription factor B subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23 | 2 | 460 | Total | C | N | O | S | 0 | 0 |
| | | | 3011 | 1856 | 562 | 584 | 9 | | |

- Molecule 24 is a protein called Transcription initiation factor IIE subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | X | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 921 | 569 | 168 | 180 | 4 | | |

- Molecule 25 is a protein called Transcription initiation factor IIA large subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25 | U | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 383 | 242 | 67 | 71 | 3 | | |

- Molecule 26 is a protein called Transcription initiation factor IIA subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26 | V | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 381 | 241 | 63 | 74 | 3 | | |

- Molecule 27 is a DNA chain called non-template strand DNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 27 | N | 38 | Total | C | N | O | P | 0 | 0 |
| | | | 791 | 376 | 161 | 216 | 38 | | |

- Molecule 28 is a DNA chain called template strand DNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 28 | T | 48 | Total | C | N | O | P | 0 | 0 |
| | | | 968 | 468 | 150 | 302 | 48 | | |

- Molecule 29 is a protein called TATA-box-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | O | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1416 | 921 | 242 | 247 | 6 | | |

- Molecule 30 is a protein called Transcription initiation factor IIE subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | W | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1469 | 932 | 254 | 277 | 6 | | |

- Molecule 31 is a RNA chain called RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 31 | P | 5 | Total | C | N | O | P | 0 | 0 |
| | | | 110 | 50 | 25 | 31 | 4 | | |

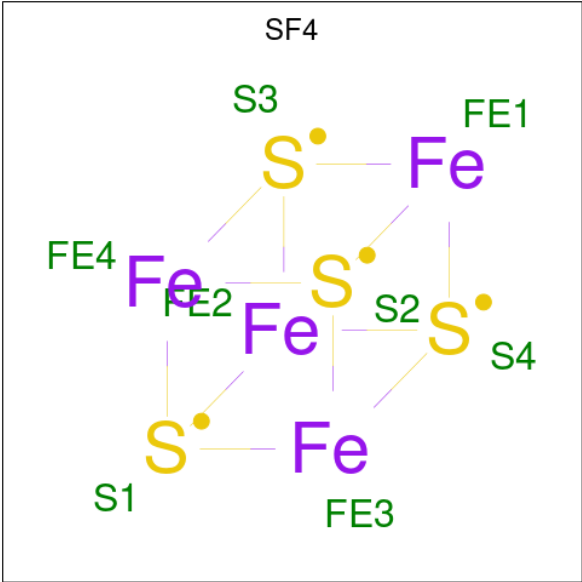
- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 32 | M | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | A | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 32 | B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | C | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | I | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 32 | J | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | L | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 32 | 6 | 4 | Total | Zn | 0 |
| | | | 4 | 4 | |
| 32 | W | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 33 | A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

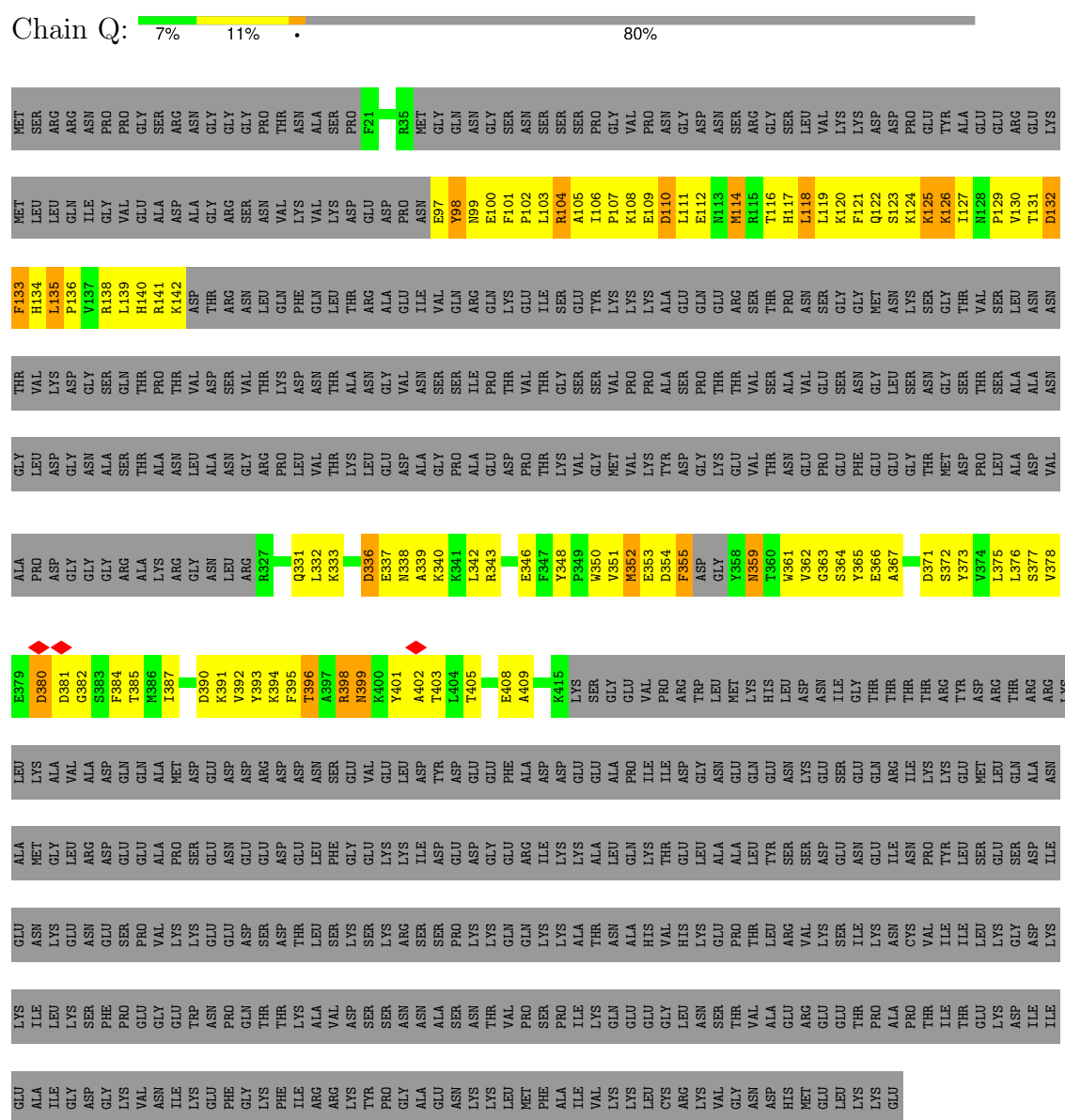


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 34 | 0 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

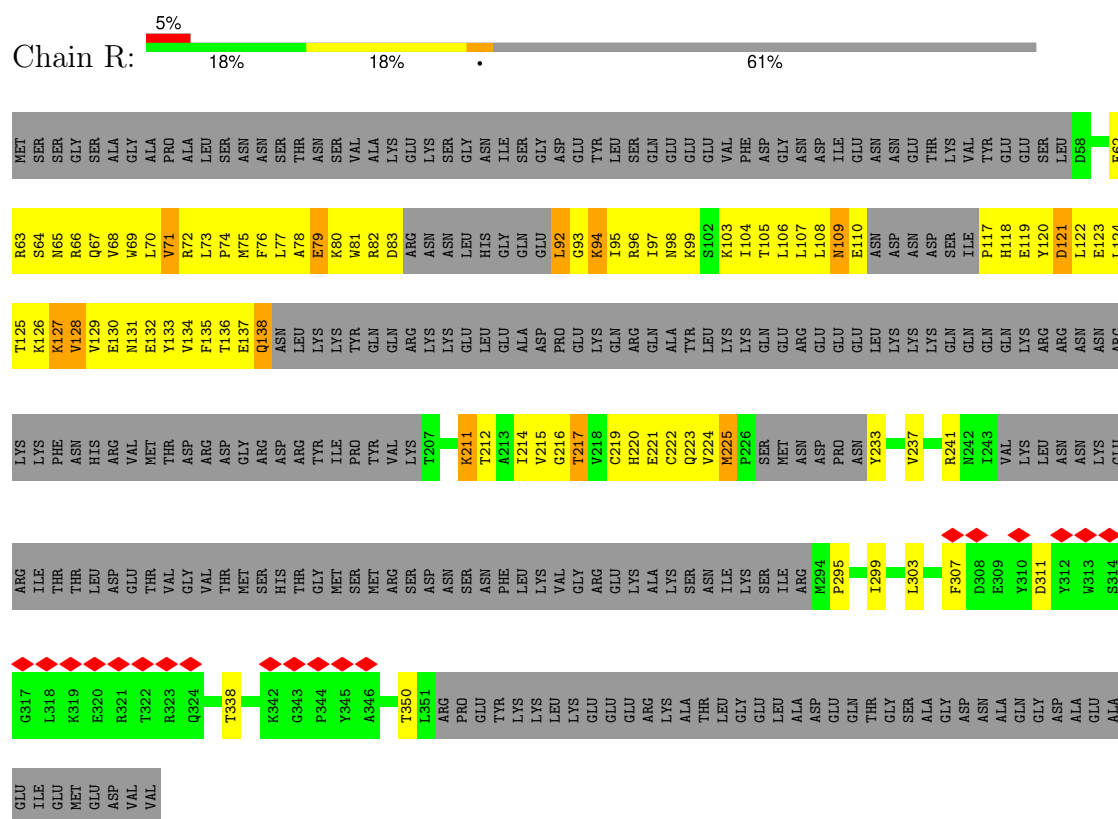
3 Residue-property plots

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.

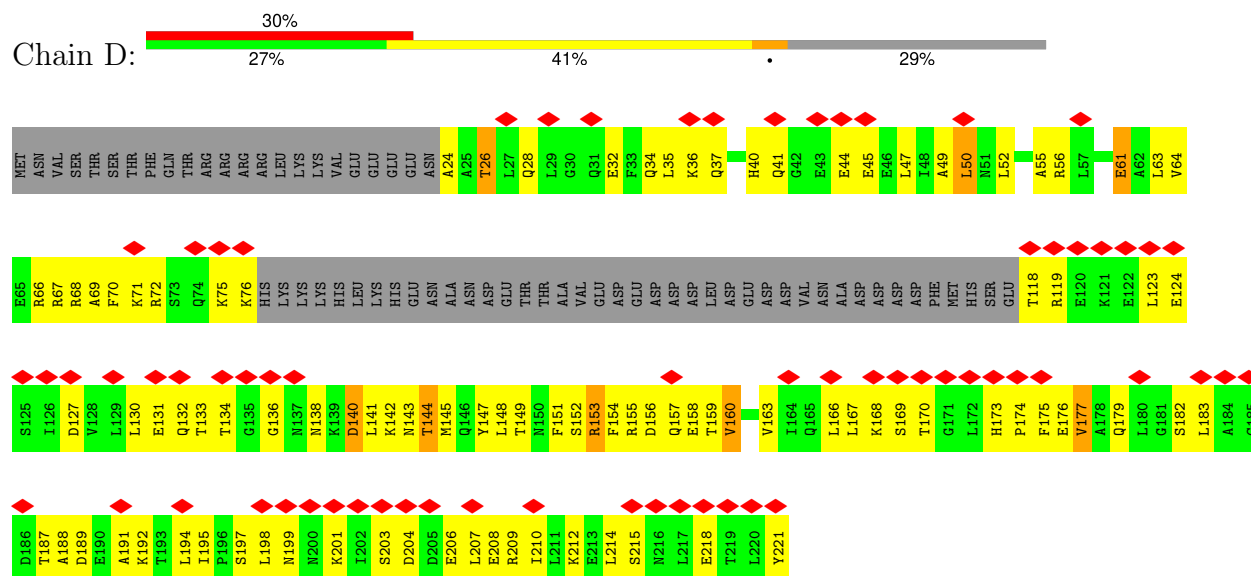
- Molecule 1: Transcription initiation factor IIF subunit alpha



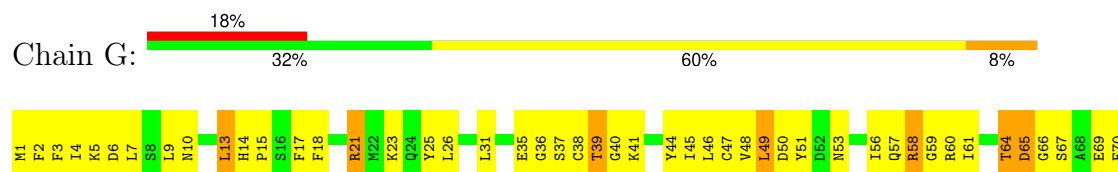
- Molecule 2: Transcription initiation factor IIF subunit beta

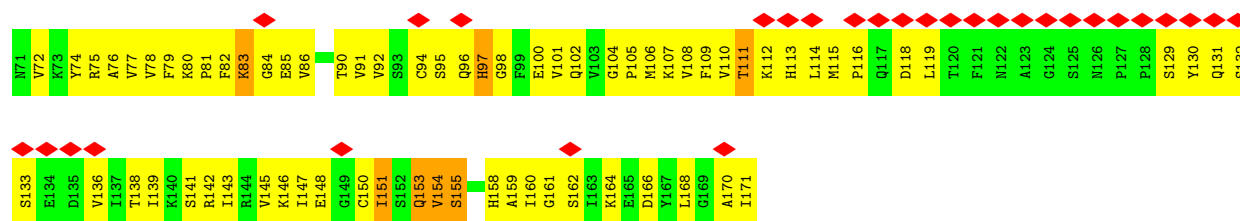


- Molecule 3: DNA-directed RNA polymerase II subunit RPB4

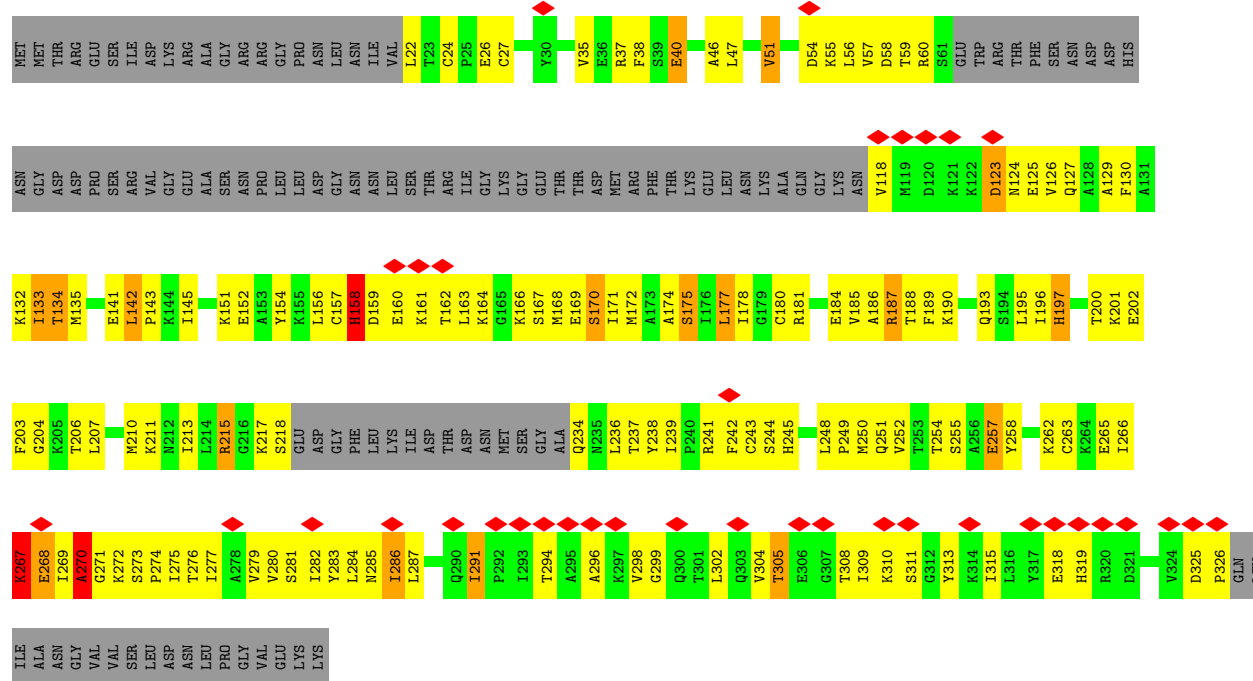
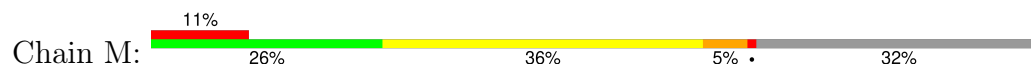


- Molecule 4: DNA-directed RNA polymerase II subunit RPB7

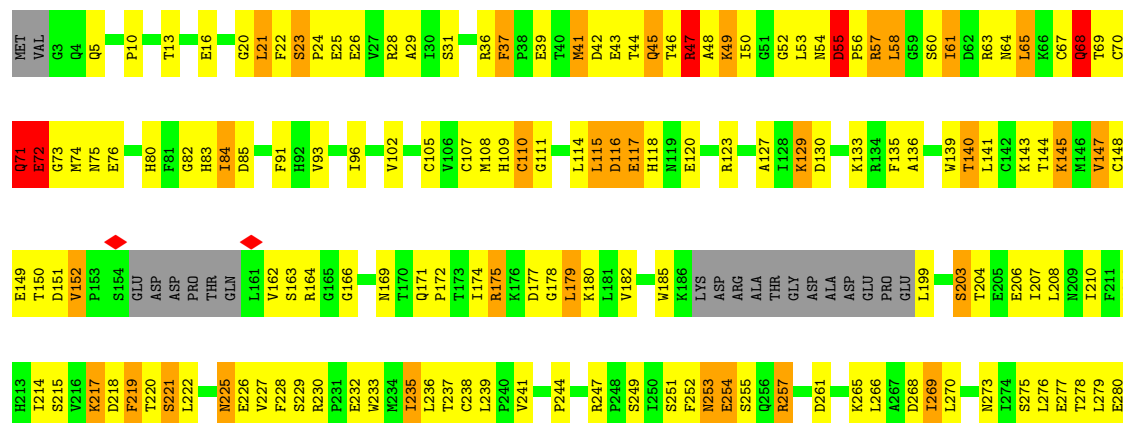




• Molecule 5: Transcription initiation factor IIB

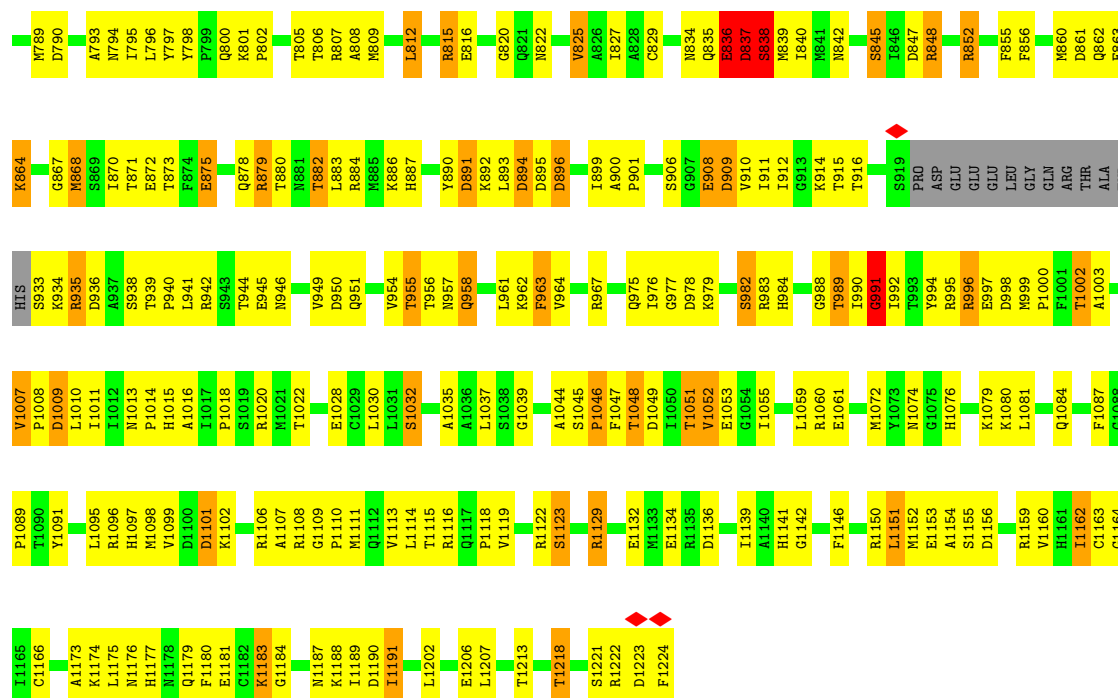


• Molecule 6: DNA-directed RNA polymerase subunit



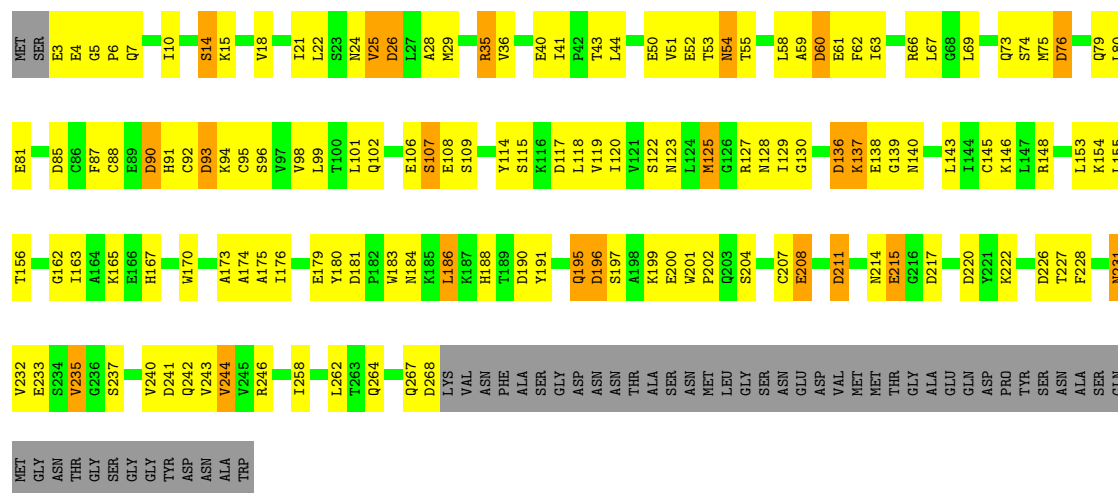






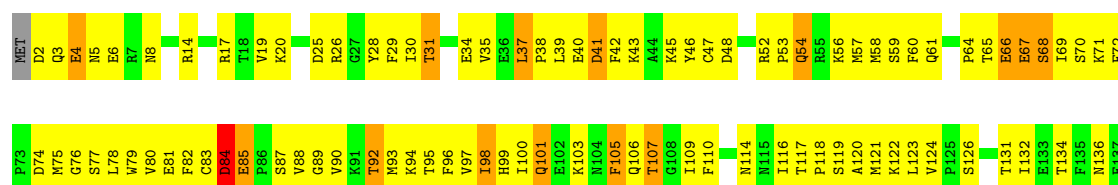
• Molecule 8: DNA-directed RNA polymerase II subunit RPB3

Chain C: 39% 37% 7% 16%



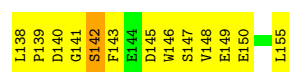
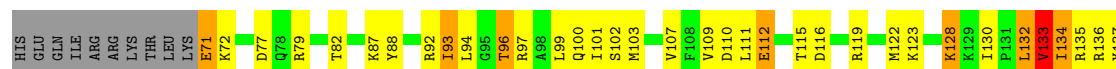
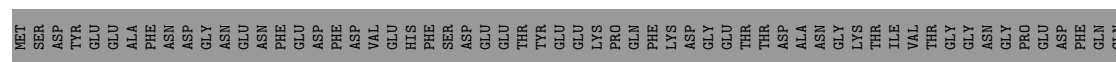
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 40% 50% 8%

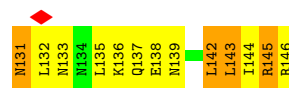
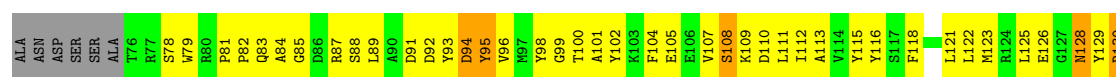
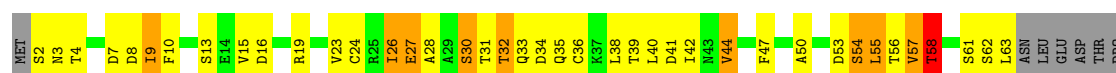




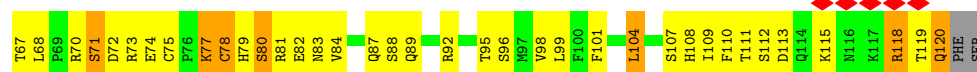
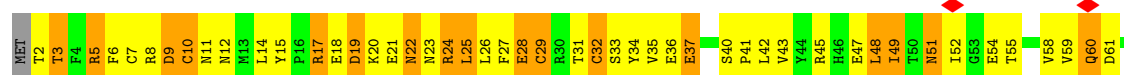
- Molecule 10: DNA-directed RNA polymerases I,II,and III subunit RPABC2



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3



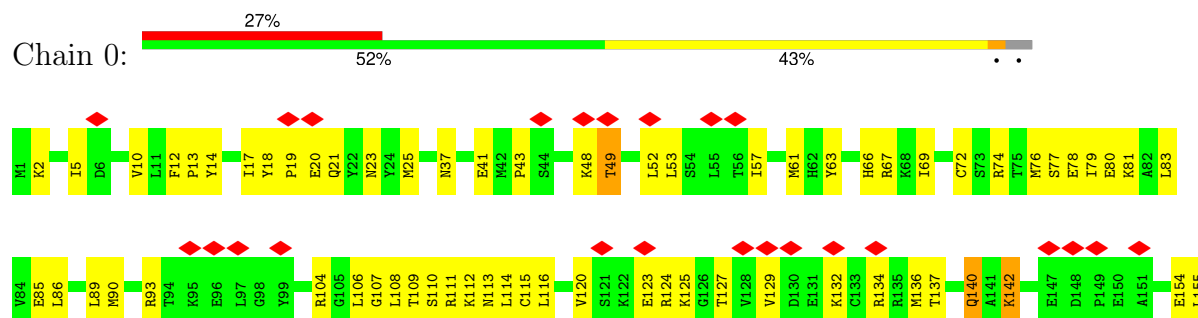
- Molecule 12: DNA-directed RNA polymerase II subunit RPB9

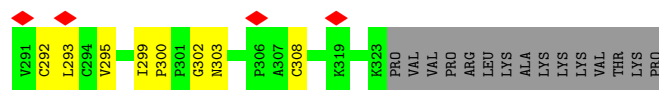


- Molecule 13: DNA-directed RNA polymerases II subunit RPABC5

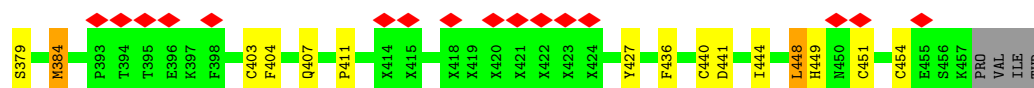
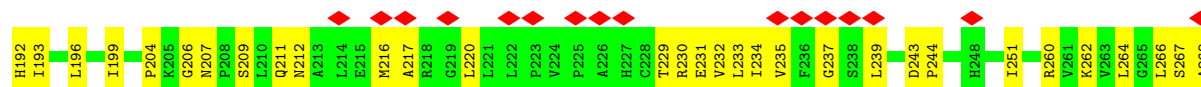
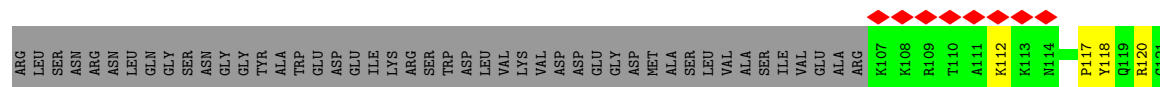
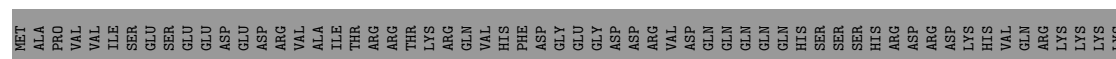


- Molecule 14: DNA-directed RNA polymerase II subunit RPB11

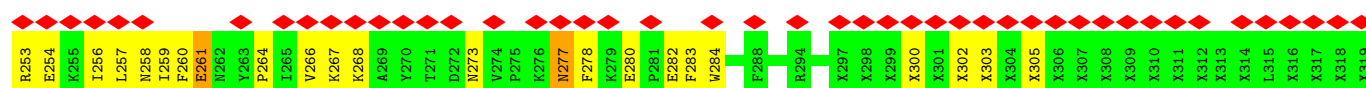
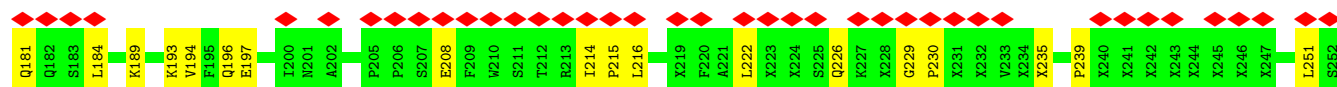
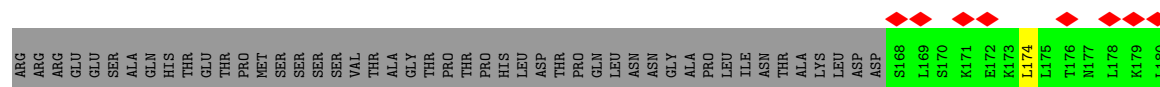
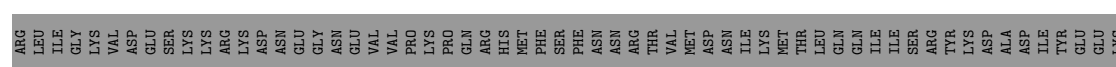


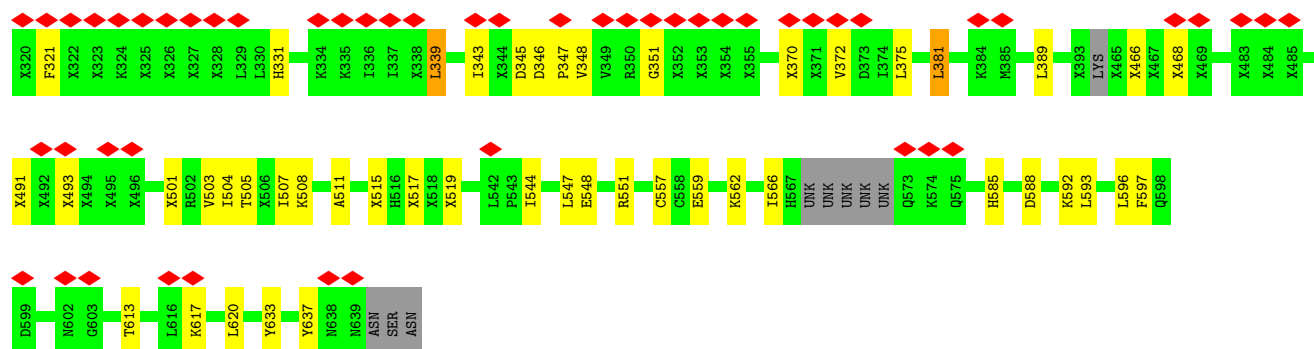


• Molecule 19: General transcription and DNA repair factor IIH

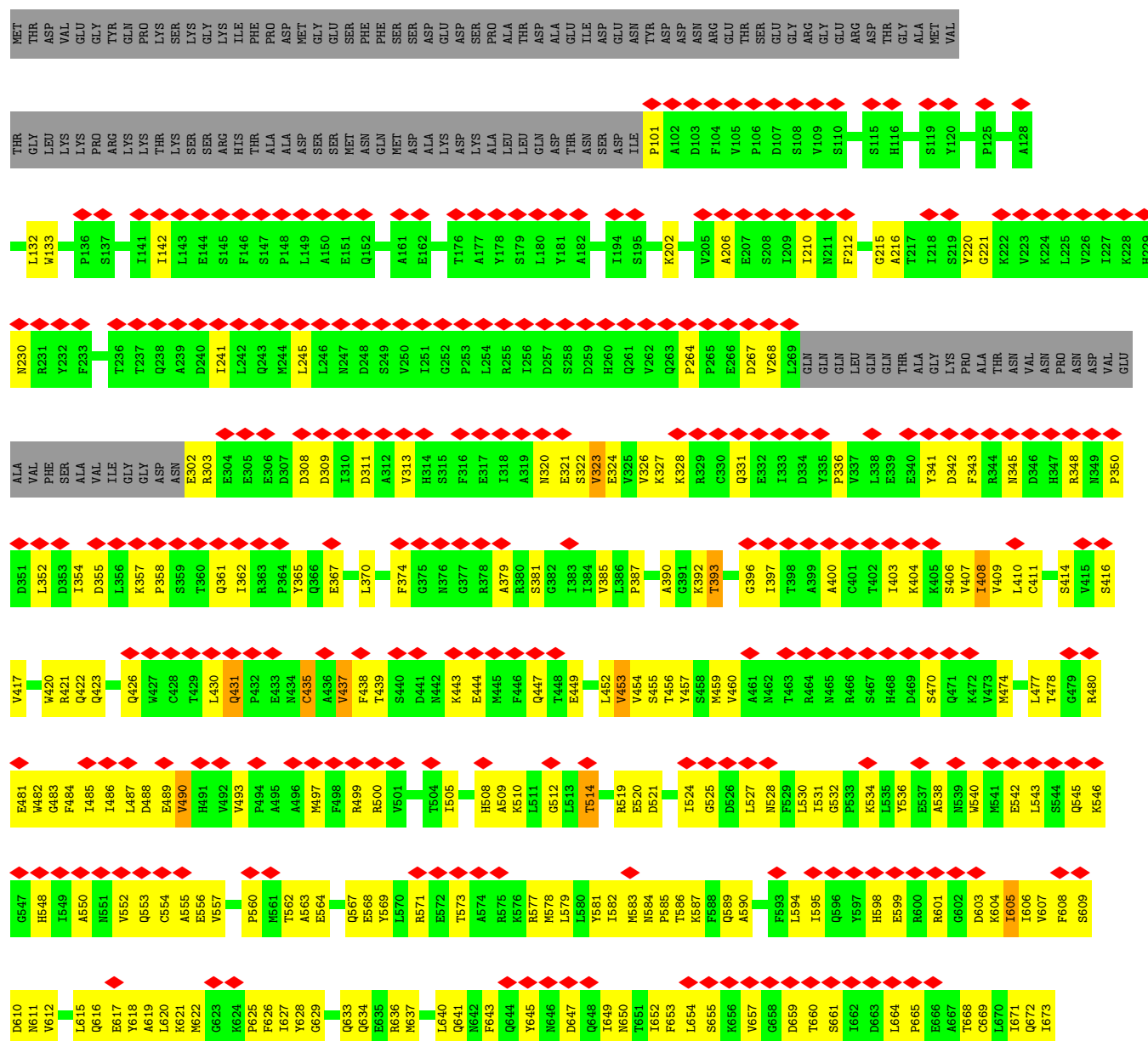
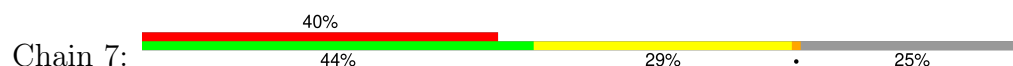


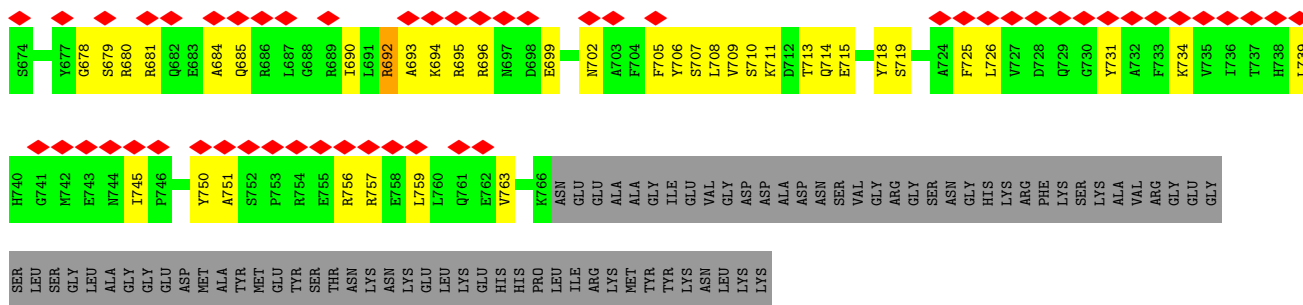
• Molecule 20: Tfb1



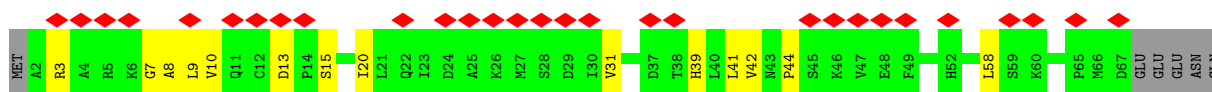
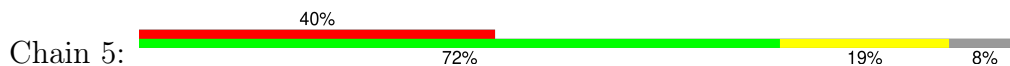


- Molecule 21: General transcription and DNA repair factor IIH helicase subunit XPB

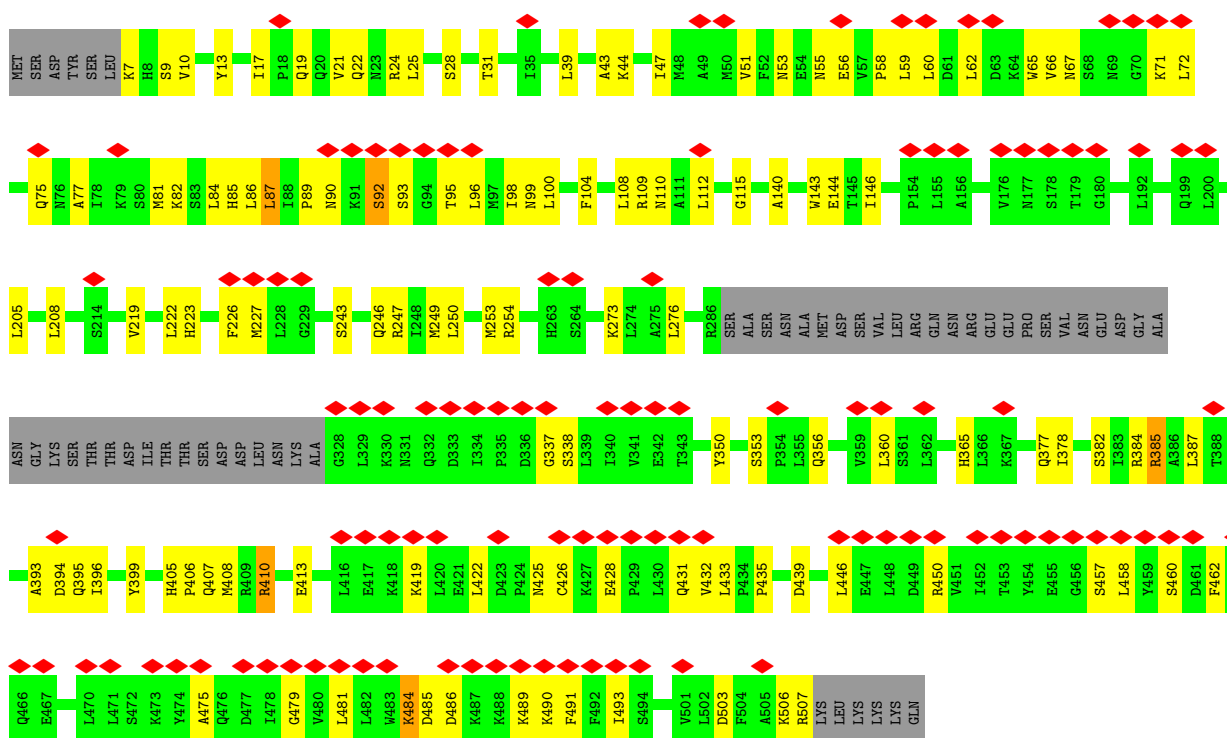




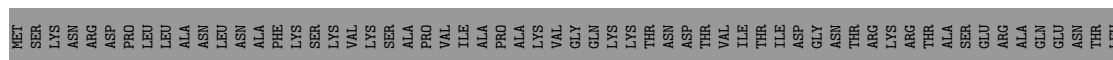
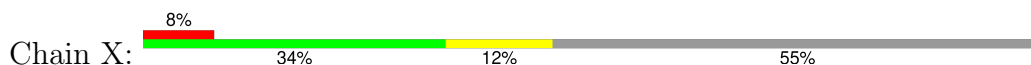
- Molecule 22: General transcription and DNA repair factor IIH subunit TFB5

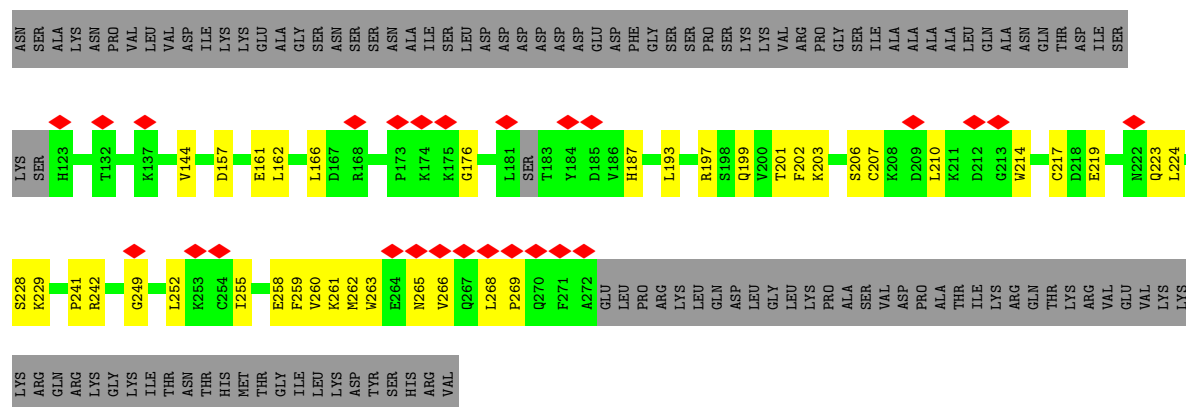


- Molecule 23: RNA polymerase II transcription factor B subunit 2

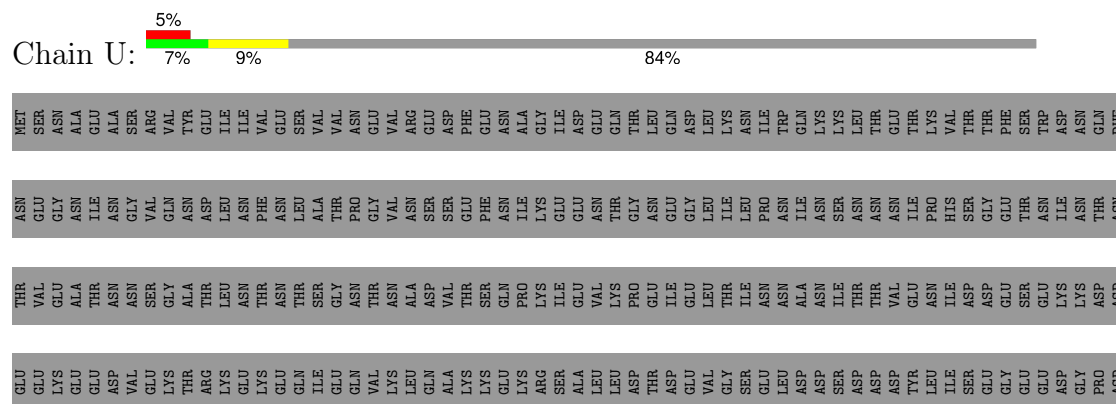


- Molecule 24: Transcription initiation factor IIE subunit beta

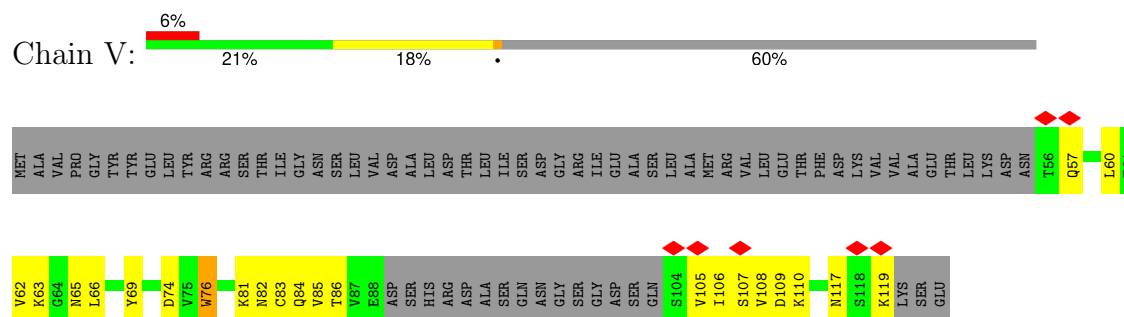




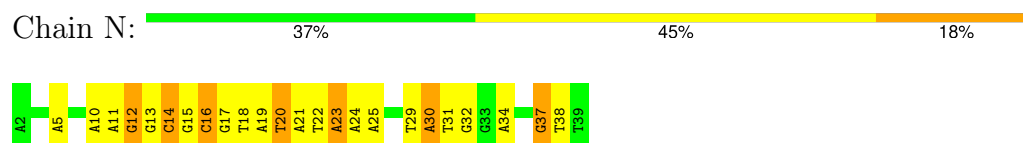
- Molecule 25: Transcription initiation factor IIA large subunit



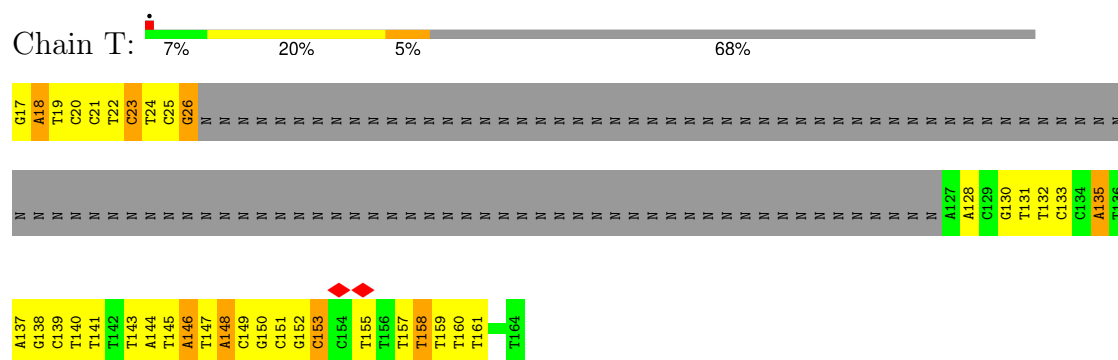
- Molecule 26: Transcription initiation factor IIA subunit 2



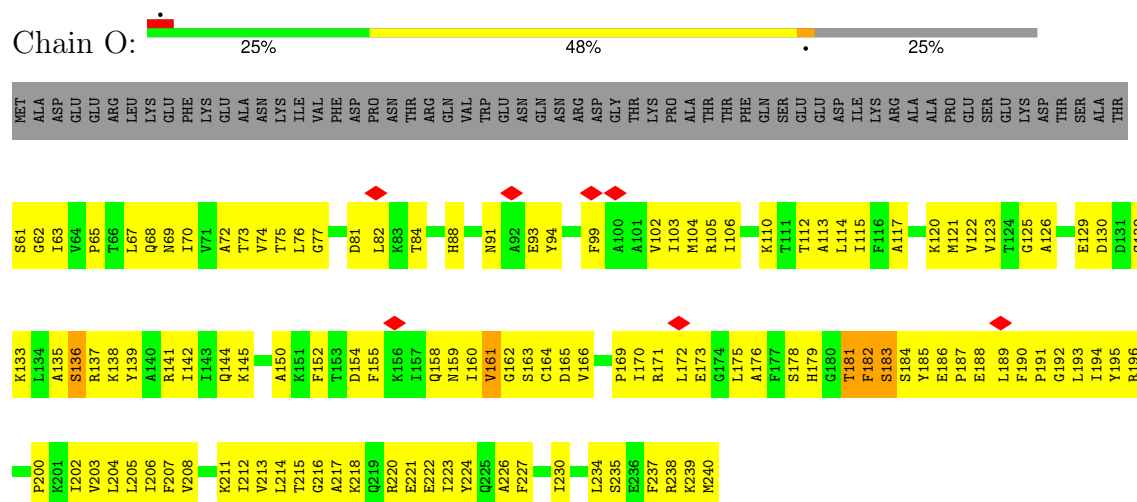
- Molecule 27: non-template strand DNA



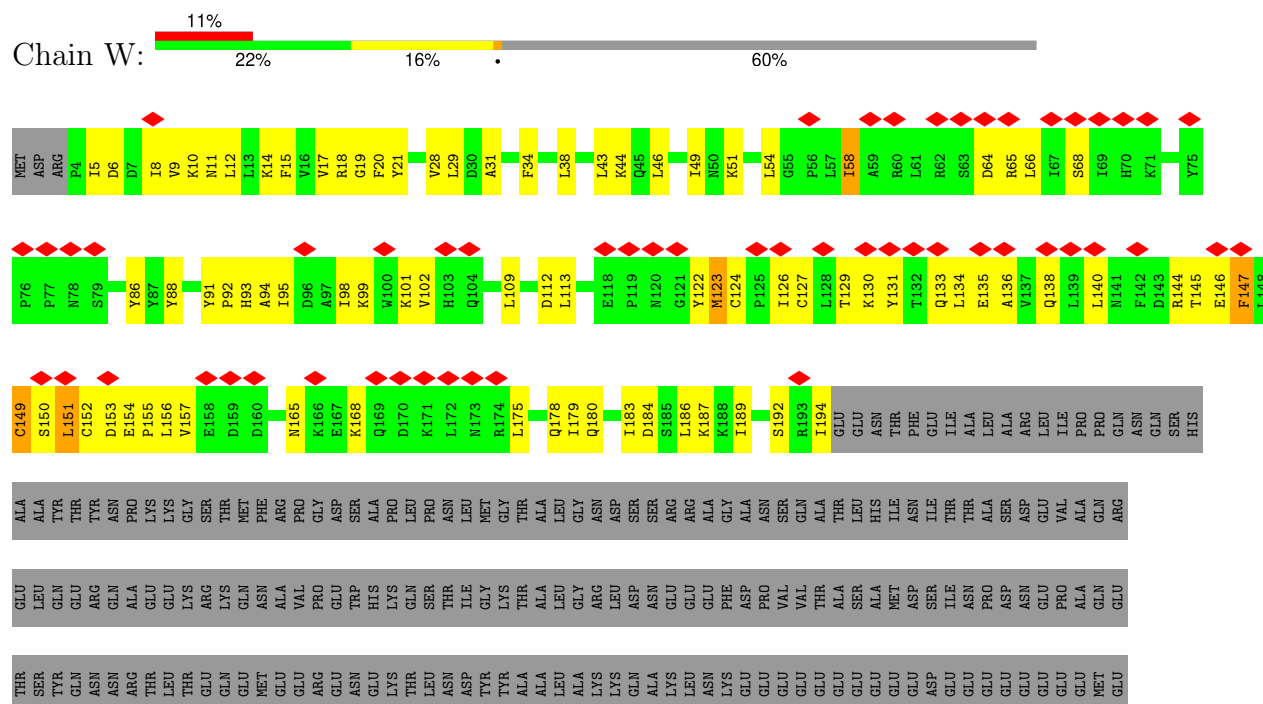
- Molecule 28: template strand DNA



• Molecule 29: TATA-box-binding protein



• Molecule 30: Transcription initiation factor IIE subunit alpha



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

PRO SER ALA ASN LYS PRO ASN ASP GLY ASP ASP ASP ASP ASP ASP ASP MET ASP THR ILE GLU PHE GLU VAL

● Molecule 31: RNA



G6 A7 G8 G9 A10

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 254448 | 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 ($e^-/\text{\AA}^2$) | 45 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.057 | Depositor |
| Minimum map value | -0.001 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.015 | Depositor |
| Map size (Å) | 444.13998, 503.49997, 508.8 | wwPDB |
| Map dimensions | 419, 475, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.06, 1.06, 1.06 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SF4

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 | Q | 0.49 | 0/1165 | 0.55 | 0/1576 |
| 2 | R | 0.35 | 0/1047 | 0.50 | 0/1422 |
| 3 | D | 0.32 | 0/1262 | 0.52 | 0/1693 |
| 4 | G | 0.53 | 0/1368 | 0.57 | 0/1844 |
| 5 | M | 0.40 | 0/1828 | 0.54 | 0/2459 |
| 6 | A | 1.01 | 5/11237 (0.0%) | 0.74 | 4/15195 (0.0%) |
| 7 | B | 1.08 | 0/9033 | 0.73 | 1/12181 (0.0%) |
| 8 | C | 0.98 | 0/2133 | 0.71 | 0/2891 |
| 9 | E | 0.94 | 0/1788 | 0.65 | 1/2406 (0.0%) |
| 10 | F | 1.17 | 0/700 | 0.76 | 1/945 (0.1%) |
| 11 | H | 0.95 | 0/1086 | 0.74 | 0/1470 |
| 12 | I | 0.76 | 0/989 | 0.63 | 0/1331 |
| 13 | J | 1.19 | 0/541 | 0.79 | 0/727 |
| 14 | K | 0.94 | 0/937 | 0.66 | 0/1265 |
| 15 | L | 0.82 | 0/365 | 0.77 | 0/485 |
| 16 | 3 | 0.23 | 0/360 | 0.35 | 0/501 |
| 17 | 0 | 0.25 | 0/6226 | 0.43 | 0/8407 |
| 18 | 4 | 0.26 | 0/2062 | 0.46 | 0/2805 |
| 19 | 6 | 0.25 | 0/2506 | 0.44 | 0/3402 |
| 20 | 1 | 0.24 | 0/1896 | 0.39 | 0/2543 |
| 21 | 7 | 0.25 | 0/4521 | 0.43 | 0/6036 |
| 22 | 5 | 0.23 | 0/502 | 0.42 | 0/677 |
| 23 | 2 | 0.24 | 0/3057 | 0.42 | 0/4071 |
| 24 | X | 0.25 | 0/929 | 0.43 | 0/1272 |
| 25 | U | 0.25 | 0/389 | 0.48 | 0/523 |
| 26 | V | 0.26 | 0/384 | 0.44 | 0/518 |
| 27 | N | 0.53 | 0/893 | 1.35 | 16/1377 (1.2%) |
| 28 | T | 0.51 | 0/1076 | 1.45 | 24/1654 (1.5%) |
| 29 | O | 0.29 | 0/1443 | 0.47 | 0/1942 |
| 30 | W | 0.27 | 0/1490 | 0.44 | 0/2014 |
| 31 | P | 0.69 | 0/124 | 1.59 | 3/193 (1.6%) |
| All | All | 0.73 | 5/63337 (0.0%) | 0.65 | 50/85825 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | Q | 0 | 1 |
| 4 | G | 0 | 1 |
| 5 | M | 0 | 3 |
| 6 | A | 0 | 9 |
| 7 | B | 0 | 5 |
| 10 | F | 0 | 1 |
| 11 | H | 0 | 3 |
| All | All | 0 | 23 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | A | 786 | HIS | CA-C | -5.82 | 1.37 | 1.52 |
| 6 | A | 656 | TRP | CB-CG | -5.68 | 1.40 | 1.50 |
| 6 | A | 55 | ASP | C-N | -5.65 | 1.23 | 1.34 |
| 6 | A | 512 | VAL | C-N | -5.34 | 1.21 | 1.34 |
| 6 | A | 556 | TRP | CB-CG | -5.17 | 1.41 | 1.50 |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 27 | N | 23 | DA | O4'-C4'-C3' | -12.58 | 98.45 | 106.00 |
| 28 | T | 20 | DC | O4'-C4'-C3' | -8.81 | 100.72 | 106.00 |
| 27 | N | 23 | DA | C4'-C3'-C2' | -8.56 | 95.39 | 103.10 |
| 27 | N | 16 | DC | O4'-C1'-N1 | 8.37 | 113.86 | 108.00 |
| 28 | T | 19 | DT | O4'-C4'-C3' | -8.21 | 101.07 | 106.00 |
| 28 | T | 23 | DC | N1-C2-O2 | -8.12 | 114.03 | 118.90 |
| 28 | T | 23 | DC | N3-C2-O2 | 7.81 | 127.37 | 121.90 |
| 28 | T | 19 | DT | C4'-C3'-C2' | -7.66 | 96.21 | 103.10 |
| 28 | T | 146 | DA | O4'-C4'-C3' | -7.23 | 101.61 | 104.50 |
| 31 | P | 9 | G | O4'-C1'-N9 | -7.13 | 102.49 | 108.20 |
| 28 | T | 153 | DC | O4'-C1'-N1 | 7.11 | 112.97 | 108.00 |
| 27 | N | 16 | DC | C3'-C2'-C1' | -6.93 | 94.19 | 102.50 |
| 27 | N | 16 | DC | O4'-C1'-C2' | -6.74 | 100.50 | 105.90 |
| 27 | N | 25 | DA | C4'-C3'-C2' | -6.70 | 97.07 | 103.10 |
| 27 | N | 20 | DT | O4'-C4'-C3' | -6.39 | 101.94 | 104.50 |
| 27 | N | 30 | DA | O4'-C1'-N9 | 6.33 | 112.43 | 108.00 |
| 27 | N | 16 | DC | C4'-C3'-C2' | -6.29 | 97.44 | 103.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28 | T | 153 | DC | C1'-O4'-C4' | -6.17 | 103.92 | 110.10 |
| 10 | F | 133 | VAL | CG1-CB-CG2 | -6.12 | 101.12 | 110.90 |
| 28 | T | 133 | DC | C1'-O4'-C4' | -6.05 | 104.05 | 110.10 |
| 31 | P | 6 | G | O4'-C1'-N9 | 6.02 | 113.02 | 108.20 |
| 28 | T | 23 | DC | C3'-C2'-C1' | -6.02 | 95.28 | 102.50 |
| 9 | E | 84 | ASP | C-N-CA | -5.95 | 106.82 | 121.70 |
| 6 | A | 472 | LEU | CA-CB-CG | -5.95 | 101.62 | 115.30 |
| 28 | T | 18 | DA | O4'-C4'-C3' | -5.91 | 102.14 | 104.50 |
| 28 | T | 23 | DC | O4'-C1'-N1 | 5.90 | 112.13 | 108.00 |
| 27 | N | 23 | DA | C1'-O4'-C4' | -5.85 | 104.25 | 110.10 |
| 27 | N | 14 | DC | C3'-C2'-C1' | -5.80 | 95.53 | 102.50 |
| 31 | P | 9 | G | N9-C1'-C2' | 5.80 | 121.54 | 114.00 |
| 28 | T | 148 | DA | O4'-C1'-N9 | 5.76 | 112.03 | 108.00 |
| 28 | T | 148 | DA | C4'-C3'-C2' | -5.73 | 97.94 | 103.10 |
| 27 | N | 23 | DA | O4'-C1'-N9 | 5.67 | 111.97 | 108.00 |
| 28 | T | 139 | DC | C3'-C2'-C1' | -5.59 | 95.79 | 102.50 |
| 27 | N | 25 | DA | O4'-C4'-C3' | -5.53 | 102.29 | 104.50 |
| 28 | T | 133 | DC | O4'-C1'-N1 | 5.47 | 111.83 | 108.00 |
| 28 | T | 135 | DA | C3'-C2'-C1' | -5.42 | 96.00 | 102.50 |
| 28 | T | 26 | DG | O4'-C4'-C3' | -5.39 | 102.34 | 104.50 |
| 6 | A | 761 | MET | C-N-CA | -5.34 | 108.34 | 121.70 |
| 28 | T | 19 | DT | O4'-C1'-N1 | 5.26 | 111.68 | 108.00 |
| 6 | A | 1442 | ASP | CB-CA-C | -5.25 | 99.90 | 110.40 |
| 27 | N | 37 | DG | C3'-C2'-C1' | -5.18 | 96.28 | 102.50 |
| 28 | T | 158 | DT | O4'-C1'-N1 | 5.15 | 111.60 | 108.00 |
| 28 | T | 18 | DA | C4'-C3'-C2' | -5.14 | 98.47 | 103.10 |
| 28 | T | 26 | DG | C4'-C3'-C2' | -5.09 | 98.52 | 103.10 |
| 27 | N | 12 | DG | C1'-O4'-C4' | -5.06 | 105.04 | 110.10 |
| 7 | B | 624 | LEU | CA-CB-CG | 5.04 | 126.90 | 115.30 |
| 6 | A | 21 | LEU | CA-CB-CG | -5.03 | 103.73 | 115.30 |
| 28 | T | 23 | DC | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 27 | N | 14 | DC | C4'-C3'-C2' | -5.02 | 98.58 | 103.10 |
| 28 | T | 139 | DC | C4'-C3'-C2' | -5.02 | 98.58 | 103.10 |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 6 | A | 1441 | PHE | Peptide |
| 6 | A | 1443 | VAL | Peptide |
| 6 | A | 47 | ARG | Peptide |
| 6 | A | 524 | VAL | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 6 | A | 55 | ASP | Peptide |
| 6 | A | 568 | PRO | Peptide |
| 6 | A | 65 | LEU | Peptide |
| 6 | A | 71 | GLN | Peptide |
| 6 | A | 957 | PRO | Peptide |
| 7 | B | 648 | HIS | Peptide |
| 7 | B | 836 | GLU | Peptide |
| 7 | B | 837 | ASP | Peptide |
| 7 | B | 838 | SER | Peptide |
| 7 | B | 991 | GLY | Peptide |
| 10 | F | 133 | VAL | Peptide |
| 4 | G | 56 | ILE | Peptide |
| 11 | H | 131 | ASN | Peptide |
| 11 | H | 54 | SER | Peptide |
| 11 | H | 57 | VAL | Peptide |
| 5 | M | 267 | LYS | Peptide |
| 5 | M | 268 | GLU | Peptide |
| 5 | M | 270 | ALA | Peptide |
| 1 | Q | 125 | LYS | Peptide |

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 | Q | 1141 | 0 | 1027 | 130 | 0 |
| 2 | R | 1039 | 0 | 857 | 124 | 0 |
| 3 | D | 1253 | 0 | 1275 | 102 | 0 |
| 4 | G | 1340 | 0 | 1357 | 118 | 0 |
| 5 | M | 1805 | 0 | 1895 | 115 | 0 |
| 6 | A | 11039 | 0 | 11122 | 727 | 0 |
| 7 | B | 8861 | 0 | 8884 | 494 | 0 |
| 8 | C | 2095 | 0 | 2051 | 112 | 0 |
| 9 | E | 1752 | 0 | 1776 | 112 | 0 |
| 10 | F | 688 | 0 | 707 | 73 | 0 |
| 11 | H | 1068 | 0 | 1040 | 123 | 0 |
| 12 | I | 971 | 0 | 927 | 96 | 0 |
| 13 | J | 532 | 0 | 542 | 27 | 0 |
| 14 | K | 919 | 0 | 929 | 47 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15 | L | 363 | 0 | 389 | 50 | 0 |
| 16 | 3 | 361 | 0 | 150 | 4 | 0 |
| 17 | 0 | 6108 | 0 | 6167 | 270 | 0 |
| 18 | 4 | 2041 | 0 | 1954 | 108 | 0 |
| 19 | 6 | 2527 | 0 | 2321 | 96 | 0 |
| 20 | 1 | 2411 | 0 | 1879 | 57 | 0 |
| 21 | 7 | 4447 | 0 | 3905 | 197 | 0 |
| 22 | 5 | 498 | 0 | 506 | 11 | 0 |
| 23 | 2 | 3011 | 0 | 2600 | 82 | 0 |
| 24 | X | 921 | 0 | 650 | 33 | 0 |
| 25 | U | 383 | 0 | 384 | 26 | 0 |
| 26 | V | 381 | 0 | 388 | 22 | 0 |
| 27 | N | 791 | 0 | 426 | 40 | 0 |
| 28 | T | 968 | 0 | 552 | 55 | 0 |
| 29 | O | 1416 | 0 | 1493 | 151 | 0 |
| 30 | W | 1469 | 0 | 1433 | 88 | 0 |
| 31 | P | 110 | 0 | 56 | 13 | 0 |
| 32 | 4 | 1 | 0 | 0 | 0 | 0 |
| 32 | 6 | 4 | 0 | 0 | 0 | 0 |
| 32 | A | 2 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |
| 32 | C | 1 | 0 | 0 | 0 | 0 |
| 32 | I | 2 | 0 | 0 | 0 | 0 |
| 32 | J | 1 | 0 | 0 | 0 | 0 |
| 32 | L | 1 | 0 | 0 | 0 | 0 |
| 32 | M | 1 | 0 | 0 | 0 | 0 |
| 32 | W | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 1 | 0 | 0 | 0 | 0 |
| 34 | 0 | 8 | 0 | 0 | 2 | 0 |
| All | All | 62733 | 0 | 59642 | 3374 | 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 28.

All (3374) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:A:68:GLN:NE2 | 6:A:80:HIS:ND1 | 1.92 | 1.16 |
| 11:H:55:LEU:H | 11:H:146:ARG:HA | 1.12 | 1.10 |
| 6:A:1444:MET:HA | 10:F:133:VAL:HA | 1.19 | 1.09 |
| 6:A:68:GLN:NE2 | 6:A:80:HIS:CE1 | 2.23 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:A:68:GLN:HE22 | 6:A:80:HIS:CG | 1.74 | 1.05 |
| 6:A:68:GLN:NE2 | 6:A:80:HIS:CG | 2.27 | 1.01 |
| 17:0:191:CYS:HB3 | 34:0:801:SF4:S3 | 2.00 | 1.00 |
| 15:L:31:CYS:SG | 15:L:34:CYS:N | 2.34 | 0.99 |
| 6:A:1423:GLY:O | 6:A:1427:ASN:ND2 | 1.99 | 0.95 |
| 5:M:271:GLY:HA2 | 5:M:277:ILE:HG13 | 1.48 | 0.95 |
| 7:B:757:PRO:HD3 | 7:B:983:ARG:HE | 1.32 | 0.94 |
| 18:4:228:THR:HG21 | 18:4:235:TYR:HB2 | 1.48 | 0.93 |
| 9:E:99:HIS:O | 9:E:103:LYS:NZ | 2.02 | 0.93 |
| 11:H:128:ASN:O | 11:H:131:ASN:ND2 | 2.02 | 0.93 |
| 1:Q:98:TYR:HA | 2:R:98:ASN:HA | 1.49 | 0.92 |
| 11:H:55:LEU:N | 11:H:146:ARG:HA | 1.83 | 0.92 |
| 21:7:411:CYS:H | 21:7:456:THR:HA | 1.33 | 0.92 |
| 8:C:66:ARG:NH2 | 13:J:3:VAL:O | 2.02 | 0.91 |
| 7:B:188:ASP:OD1 | 7:B:188:ASP:N | 2.00 | 0.91 |
| 1:Q:377:SER:HB3 | 1:Q:385:THR:H | 1.35 | 0.91 |
| 6:A:43:GLU:O | 6:A:45:GLN:NE2 | 2.03 | 0.90 |
| 9:E:41:ASP:OD1 | 9:E:41:ASP:N | 2.01 | 0.89 |
| 6:A:57:ARG:O | 6:A:68:GLN:HG2 | 1.69 | 0.89 |
| 6:A:68:GLN:HE22 | 6:A:80:HIS:CD2 | 1.89 | 0.89 |
| 12:I:19:ASP:HB3 | 12:I:24:ARG:H | 1.37 | 0.89 |
| 6:A:985:ASP:OD1 | 6:A:985:ASP:N | 2.04 | 0.89 |
| 7:B:838:SER:OG | 7:B:989:THR:N | 2.05 | 0.89 |
| 6:A:68:GLN:HE21 | 6:A:80:HIS:CE1 | 1.88 | 0.88 |
| 12:I:78:CYS:SG | 12:I:79:HIS:N | 2.46 | 0.88 |
| 7:B:195:CYS:HG | 7:B:783:THR:HG1 | 1.21 | 0.88 |
| 5:M:141:GLU:OE1 | 7:B:103:ASN:ND2 | 2.07 | 0.86 |
| 6:A:49:LYS:NZ | 6:A:55:ASP:O | 2.08 | 0.86 |
| 9:E:56:LYS:HE2 | 9:E:84:ASP:HB2 | 1.57 | 0.86 |
| 8:C:211:ASP:OD1 | 8:C:211:ASP:N | 2.07 | 0.86 |
| 7:B:668:ASP:N | 7:B:668:ASP:OD1 | 2.05 | 0.86 |
| 6:A:746:MET:HE3 | 7:B:1015:HIS:HA | 1.58 | 0.86 |
| 8:C:3:GLU:O | 8:C:7:GLN:NE2 | 2.08 | 0.86 |
| 11:H:54:SER:HB3 | 11:H:146:ARG:HB3 | 1.56 | 0.86 |
| 30:W:43:LEU:HG | 30:W:54:LEU:HD11 | 1.56 | 0.85 |
| 6:A:1232:ASN:ND2 | 6:A:1233:ASP:OD1 | 2.09 | 0.85 |
| 7:B:229:ALA:O | 7:B:261:ARG:NH2 | 2.09 | 0.85 |
| 15:L:50:ASP:OD1 | 15:L:50:ASP:N | 2.08 | 0.85 |
| 3:D:206:GLU:HG2 | 3:D:209:ARG:HE | 1.41 | 0.85 |
| 8:C:76:ASP:N | 8:C:76:ASP:OD1 | 2.08 | 0.85 |
| 6:A:1334:ASP:N | 6:A:1334:ASP:OD1 | 2.07 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:C:148:ARG:NH1 | 13:J:64:ASN:O | 2.11 | 0.84 |
| 6:A:767:GLN:NE2 | 6:A:768:GLN:O | 2.10 | 0.84 |
| 12:I:32:CYS:SG | 12:I:33:SER:N | 2.50 | 0.84 |
| 6:A:290:GLU:OE1 | 6:A:290:GLU:N | 2.09 | 0.84 |
| 6:A:383:TYR:HB3 | 10:F:115:THR:HG23 | 1.58 | 0.84 |
| 6:A:71:GLN:O | 6:A:73:GLY:N | 2.10 | 0.83 |
| 6:A:853:ASP:OD1 | 6:A:853:ASP:N | 2.11 | 0.83 |
| 6:A:362:ASP:OD2 | 6:A:459:ARG:NH1 | 2.11 | 0.83 |
| 6:A:1197:LEU:HD11 | 6:A:1238:ILE:HD11 | 1.60 | 0.83 |
| 11:H:131:ASN:O | 11:H:133:ASN:N | 2.12 | 0.83 |
| 30:W:149:CYS:SG | 30:W:150:SER:N | 2.52 | 0.83 |
| 6:A:567:LYS:HB2 | 11:H:96:VAL:H | 1.44 | 0.82 |
| 7:B:837:ASP:OD1 | 7:B:837:ASP:N | 2.09 | 0.82 |
| 7:B:167:ILE:HD11 | 7:B:453:ILE:HD12 | 1.60 | 0.82 |
| 5:M:215:ARG:HB3 | 29:O:181:THR:HG23 | 1.61 | 0.82 |
| 29:O:68:GLN:H | 29:O:162:GLY:HA2 | 1.45 | 0.82 |
| 6:A:1151:GLU:OE2 | 12:I:45:ARG:NH1 | 2.13 | 0.82 |
| 2:R:63:ARG:HE | 2:R:65:ASN:HB3 | 1.43 | 0.82 |
| 6:A:1158:PRO:HB3 | 6:A:1188:GLN:HE22 | 1.45 | 0.81 |
| 9:E:40:GLU:OE1 | 9:E:40:GLU:N | 2.13 | 0.81 |
| 6:A:674:PRO:O | 6:A:677:ARG:NH1 | 2.14 | 0.81 |
| 29:O:206:ILE:HG12 | 29:O:212:ILE:HG23 | 1.62 | 0.81 |
| 21:7:490:VAL:HB | 21:7:519:ARG:HH22 | 1.43 | 0.81 |
| 23:2:71:LYS:NZ | 23:2:75:GLN:OE1 | 2.14 | 0.81 |
| 27:N:23:DA:H2'' | 29:O:158:GLN:HB3 | 1.62 | 0.81 |
| 6:A:49:LYS:NZ | 6:A:55:ASP:OD2 | 2.12 | 0.81 |
| 6:A:120:GLU:OE2 | 6:A:123:ARG:NH1 | 2.13 | 0.81 |
| 6:A:1443:VAL:HG21 | 10:F:93:ILE:HD11 | 1.62 | 0.81 |
| 7:B:979:LYS:NZ | 31:P:9:G:O3' | 2.14 | 0.81 |
| 6:A:25:GLU:OE1 | 6:A:25:GLU:N | 2.10 | 0.81 |
| 12:I:7:CYS:O | 12:I:11:ASN:N | 2.12 | 0.81 |
| 3:D:55:ALA:HB3 | 3:D:148:LEU:HD21 | 1.61 | 0.81 |
| 4:G:95:SER:O | 4:G:130:TYR:OH | 1.99 | 0.81 |
| 6:A:1173:HIS:CE1 | 6:A:1228:TRP:H | 1.99 | 0.80 |
| 7:B:647:GLY:HA3 | 7:B:648:HIS:HB3 | 1.62 | 0.80 |
| 6:A:46:THR:O | 6:A:48:ALA:N | 2.14 | 0.80 |
| 6:A:127:ALA:O | 6:A:129:LYS:NZ | 2.14 | 0.80 |
| 6:A:567:LYS:O | 6:A:569:LYS:N | 2.14 | 0.80 |
| 9:E:54:GLN:OE1 | 9:E:57:MET:N | 2.15 | 0.80 |
| 13:J:10:CYS:SG | 13:J:43:ARG:NH2 | 2.52 | 0.80 |
| 6:A:37:PHE:HB2 | 6:A:39:GLU:HG2 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:848:ARG:NH1 | 13:J:8:PHE:O | 2.15 | 0.80 |
| 7:B:891:ASP:N | 7:B:891:ASP:OD1 | 2.10 | 0.80 |
| 2:R:138:GLN:NE2 | 2:R:138:GLN:H | 1.79 | 0.80 |
| 18:4:285:VAL:HA | 19:6:323:GLY:HA2 | 1.64 | 0.80 |
| 29:O:192:GLY:HA2 | 29:O:207:PHE:HA | 1.64 | 0.80 |
| 9:E:67:GLU:OE1 | 9:E:67:GLU:N | 2.15 | 0.79 |
| 11:H:135:LEU:O | 11:H:137:GLN:NE2 | 2.13 | 0.79 |
| 3:D:192:LYS:HG2 | 3:D:199:ASN:HA | 1.64 | 0.79 |
| 12:I:8:ARG:NH1 | 12:I:9:ASP:OD1 | 2.14 | 0.79 |
| 7:B:641:GLU:O | 7:B:650:GLU:N | 2.15 | 0.79 |
| 6:A:147:VAL:HG23 | 6:A:149:GLU:H | 1.45 | 0.79 |
| 7:B:763:GLN:HG2 | 7:B:765:PRO:HD2 | 1.64 | 0.79 |
| 7:B:708:GLU:OE1 | 7:B:708:GLU:N | 2.15 | 0.79 |
| 7:B:706:GLN:H | 7:B:710:LEU:HD23 | 1.48 | 0.79 |
| 23:2:7:LYS:HG2 | 23:2:9:SER:H | 1.48 | 0.79 |
| 1:Q:339:ALA:O | 1:Q:343:ARG:N | 2.14 | 0.79 |
| 6:A:590:ARG:NH1 | 6:A:592:ASP:OD1 | 2.16 | 0.79 |
| 6:A:1008:GLN:HB3 | 6:A:1012:ARG:HH22 | 1.47 | 0.79 |
| 7:B:199:MET:N | 7:B:199:MET:SD | 2.52 | 0.79 |
| 5:M:188:THR:HG22 | 5:M:190:LYS:H | 1.48 | 0.78 |
| 6:A:1215:ARG:NH2 | 6:A:1272:THR:O | 2.15 | 0.78 |
| 7:B:1218:THR:O | 7:B:1218:THR:OG1 | 2.01 | 0.78 |
| 6:A:5:GLN:O | 7:B:1159:ARG:NH2 | 2.16 | 0.78 |
| 6:A:1442:ASP:HB2 | 10:F:136:ARG:N | 1.99 | 0.78 |
| 19:6:126:LEU:HD11 | 19:6:233:LEU:HB2 | 1.66 | 0.78 |
| 6:A:438:ASP:OD1 | 6:A:438:ASP:N | 2.15 | 0.78 |
| 7:B:270:LYS:HB3 | 7:B:279:ASP:HB3 | 1.66 | 0.78 |
| 5:M:157:CYS:SG | 5:M:158:HIS:N | 2.54 | 0.78 |
| 7:B:1163:CYS:HB3 | 7:B:1166:CYS:SG | 2.24 | 0.78 |
| 6:A:1162:VAL:HG11 | 12:I:41:PRO:HG3 | 1.65 | 0.78 |
| 6:A:926:GLN:NE2 | 6:A:930:ASP:OD1 | 2.17 | 0.78 |
| 6:A:219:PHE:HD1 | 6:A:220:THR:H | 1.32 | 0.78 |
| 30:W:92:PRO:HA | 30:W:95:ILE:HD12 | 1.66 | 0.78 |
| 6:A:152:VAL:O | 6:A:162:VAL:N | 2.15 | 0.77 |
| 3:D:123:LEU:HD11 | 3:D:145:MET:HB3 | 1.66 | 0.77 |
| 18:4:79:TYR:HB3 | 18:4:140:ILE:HG23 | 1.65 | 0.77 |
| 29:O:102:VAL:HB | 29:O:115:ILE:HB | 1.66 | 0.77 |
| 6:A:67:CYS:SG | 6:A:80:HIS:CE1 | 2.78 | 0.77 |
| 7:B:997:GLU:OE2 | 7:B:997:GLU:N | 2.12 | 0.77 |
| 17:O:356:PRO:HG2 | 17:O:413:GLU:HA | 1.66 | 0.77 |
| 6:A:746:MET:HE1 | 7:B:1018:PRO:HG2 | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:1084:GLN:NE2 | 8:C:190:ASP:O | 2.17 | 0.77 |
| 7:B:957:ASN:OD1 | 7:B:958:GLN:N | 2.17 | 0.77 |
| 20:1:557:CYS:SG | 20:1:585:HIS:NE2 | 2.57 | 0.77 |
| 18:4:175:ARG:HE | 18:4:256:PRO:HG3 | 1.47 | 0.77 |
| 6:A:278:THR:HA | 6:A:281:HIS:NE2 | 1.99 | 0.77 |
| 8:C:14:SER:OG | 8:C:15:LYS:N | 2.14 | 0.77 |
| 3:D:151:PHE:O | 3:D:153:ARG:NH1 | 2.18 | 0.77 |
| 2:R:99:LYS:O | 2:R:103:LYS:N | 2.18 | 0.76 |
| 5:M:281:SER:O | 5:M:285:ASN:ND2 | 2.18 | 0.76 |
| 11:H:56:THR:O | 11:H:144:ILE:N | 2.18 | 0.76 |
| 27:N:23:DA:N6 | 28:T:143:DT:O4 | 2.18 | 0.76 |
| 4:G:64:THR:OG1 | 4:G:65:ASP:OD1 | 2.04 | 0.76 |
| 7:B:135:ARG:NH1 | 7:B:136:THR:O | 2.19 | 0.76 |
| 1:Q:337:GLU:OE2 | 1:Q:340:LYS:N | 2.18 | 0.76 |
| 7:B:235:SER:OG | 7:B:236:HIS:ND1 | 2.16 | 0.76 |
| 12:I:22:ASN:OD1 | 12:I:22:ASN:N | 2.19 | 0.76 |
| 7:B:1187:ASN:HD21 | 7:B:1190:ASP:HB3 | 1.49 | 0.76 |
| 25:U:253:ARG:NH1 | 28:T:144:DA:OP1 | 2.19 | 0.76 |
| 6:A:1062:GLU:OE1 | 10:F:88:TYR:OH | 2.04 | 0.76 |
| 7:B:1175:LEU:O | 7:B:1176:ASN:ND2 | 2.18 | 0.76 |
| 6:A:118:HIS:HA | 6:A:123:ARG:HH22 | 1.49 | 0.76 |
| 6:A:982:THR:N | 6:A:985:ASP:OD2 | 2.18 | 0.76 |
| 13:J:1:MET:O | 13:J:53:HIS:NE2 | 2.18 | 0.76 |
| 7:B:89:GLU:N | 7:B:135:ARG:O | 2.18 | 0.76 |
| 7:B:567:GLU:OE1 | 7:B:567:GLU:N | 2.18 | 0.76 |
| 6:A:1215:ARG:O | 6:A:1218:GLN:NE2 | 2.17 | 0.75 |
| 6:A:1215:ARG:O | 6:A:1219:THR:OG1 | 2.04 | 0.75 |
| 9:E:3:GLN:O | 9:E:6:GLU:N | 2.19 | 0.75 |
| 17:O:134:ARG:NH2 | 17:O:303:GLU:O | 2.19 | 0.75 |
| 29:O:191:PRO:HG2 | 29:O:207:PHE:HE1 | 1.51 | 0.75 |
| 5:M:24:CYS:SG | 5:M:27:CYS:N | 2.57 | 0.75 |
| 6:A:107:CYS:SG | 6:A:110:CYS:N | 2.59 | 0.75 |
| 12:I:17:ARG:O | 12:I:26:LEU:N | 2.18 | 0.75 |
| 25:U:262:LEU:HB2 | 25:U:279:ALA:HB3 | 1.68 | 0.75 |
| 7:B:996:ARG:HH22 | 8:C:173:ALA:HB1 | 1.51 | 0.75 |
| 8:C:60:ASP:OD1 | 8:C:60:ASP:N | 2.15 | 0.75 |
| 3:D:140:ASP:N | 3:D:140:ASP:OD1 | 2.16 | 0.75 |
| 5:M:193:GLN:HE22 | 5:M:197:HIS:HA | 1.51 | 0.75 |
| 18:4:136:GLU:HA | 18:4:140:ILE:HG13 | 1.68 | 0.75 |
| 18:4:84:LYS:HB3 | 18:4:132:LEU:HD12 | 1.67 | 0.75 |
| 3:D:119:ARG:HD2 | 3:D:155:ARG:HH22 | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:185:TRP:H | 6:A:199:LEU:HD12 | 1.53 | 0.74 |
| 7:B:864:LYS:HB3 | 7:B:872:GLU:H | 1.51 | 0.74 |
| 1:Q:132:ASP:N | 1:Q:132:ASP:OD1 | 2.21 | 0.74 |
| 4:G:46:LEU:HD12 | 4:G:77:VAL:HG12 | 1.70 | 0.74 |
| 15:L:48:CYS:O | 15:L:52:GLY:N | 2.17 | 0.74 |
| 6:A:1005:GLU:N | 6:A:1005:GLU:OE1 | 2.19 | 0.74 |
| 7:B:529:GLU:HA | 7:B:533:CYS:HB2 | 1.69 | 0.74 |
| 8:C:61:GLU:OE1 | 8:C:61:GLU:N | 2.18 | 0.74 |
| 2:R:75:MET:N | 2:R:75:MET:SD | 2.60 | 0.74 |
| 17:O:618:ARG:NH1 | 17:O:676:TYR:O | 2.20 | 0.74 |
| 1:Q:120:LYS:O | 1:Q:395:PHE:N | 2.15 | 0.74 |
| 19:6:132:CYS:HB2 | 19:6:175:ARG:HG2 | 1.68 | 0.74 |
| 28:T:144:DA:N3 | 29:O:69:ASN:ND2 | 2.35 | 0.74 |
| 17:O:74:ARG:NH1 | 17:O:239:ASN:OD1 | 2.21 | 0.74 |
| 20:1:214:ILE:HG13 | 20:1:215:PRO:HD3 | 1.70 | 0.74 |
| 29:O:73:THR:HG22 | 29:O:122:VAL:HG22 | 1.70 | 0.74 |
| 7:B:867:GLY:HA3 | 7:B:870:ILE:HB | 1.70 | 0.74 |
| 6:A:795:GLU:N | 6:A:795:GLU:OE1 | 2.20 | 0.73 |
| 7:B:642:ASP:OD1 | 7:B:642:ASP:N | 2.18 | 0.73 |
| 7:B:982:SER:OG | 7:B:983:ARG:N | 2.20 | 0.73 |
| 10:F:149:GLU:N | 10:F:149:GLU:OE2 | 2.20 | 0.73 |
| 30:W:123:MET:HA | 30:W:130:LYS:HA | 1.70 | 0.73 |
| 2:R:74:PRO:HD2 | 2:R:224:VAL:HB | 1.70 | 0.73 |
| 7:B:326:ASP:O | 7:B:329:THR:OG1 | 2.06 | 0.73 |
| 6:A:711:ARG:NH1 | 12:I:95:THR:O | 2.21 | 0.73 |
| 6:A:821:ARG:HH12 | 7:B:527:THR:HG21 | 1.53 | 0.73 |
| 12:I:27:PHE:N | 12:I:36:GLU:O | 2.21 | 0.73 |
| 6:A:1147:THR:HA | 6:A:1197:LEU:HA | 1.71 | 0.73 |
| 7:B:195:CYS:SG | 7:B:783:THR:OG1 | 2.43 | 0.73 |
| 9:E:48:ASP:OD1 | 9:E:52:ARG:N | 2.22 | 0.73 |
| 17:O:37:ASN:HB2 | 17:O:477:THR:HG22 | 1.70 | 0.73 |
| 6:A:951:GLU:O | 6:A:954:TRP:NE1 | 2.20 | 0.73 |
| 7:B:739:THR:OG1 | 7:B:740:HIS:ND1 | 2.20 | 0.73 |
| 9:E:52:ARG:HD3 | 9:E:53:PRO:HD2 | 1.70 | 0.73 |
| 6:A:232:GLU:OE1 | 6:A:232:GLU:N | 2.21 | 0.73 |
| 29:O:183:SER:HB3 | 29:O:193:LEU:HD11 | 1.69 | 0.73 |
| 6:A:939:ASP:OD2 | 6:A:1023:ARG:NH1 | 2.22 | 0.73 |
| 6:A:1157:ASP:OD1 | 6:A:1160:SER:N | 2.21 | 0.73 |
| 3:D:32:GLU:O | 4:G:5:LYS:NZ | 2.17 | 0.73 |
| 7:B:886:LYS:HE3 | 7:B:940:PRO:HD3 | 1.70 | 0.73 |
| 6:A:1426:GLU:OE1 | 6:A:1426:GLU:N | 2.22 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:411:CYS:HA | 21:7:488:ASP:HB2 | 1.71 | 0.73 |
| 4:G:57:GLN:OE1 | 4:G:57:GLN:N | 2.22 | 0.72 |
| 6:A:1278:ASN:HD22 | 6:A:1312:ASN:HB2 | 1.54 | 0.72 |
| 10:F:130:ILE:HG22 | 10:F:132:LEU:HD23 | 1.71 | 0.72 |
| 12:I:87:GLN:O | 12:I:89:GLN:NE2 | 2.22 | 0.72 |
| 21:7:381:SER:HB3 | 21:7:509:ALA:HB1 | 1.70 | 0.72 |
| 6:A:1197:LEU:HD12 | 6:A:1236:LEU:HB3 | 1.71 | 0.72 |
| 9:E:66:GLU:O | 9:E:69:ILE:N | 2.22 | 0.72 |
| 15:L:47:ARG:NH2 | 15:L:52:GLY:O | 2.22 | 0.72 |
| 17:0:140:GLN:NE2 | 17:0:386:ARG:O | 2.21 | 0.72 |
| 6:A:1167:GLU:O | 6:A:1171:GLN:NE2 | 2.17 | 0.72 |
| 3:D:119:ARG:NH1 | 3:D:152:SER:O | 2.21 | 0.72 |
| 11:H:83:GLN:O | 11:H:87:ARG:NH1 | 2.21 | 0.72 |
| 6:A:399:HIS:O | 6:A:401:GLY:N | 2.22 | 0.72 |
| 11:H:56:THR:HA | 11:H:145:ARG:NH1 | 2.04 | 0.72 |
| 11:H:94:ASP:OD1 | 11:H:94:ASP:N | 2.21 | 0.72 |
| 1:Q:375:LEU:HB3 | 1:Q:387:ILE:HB | 1.71 | 0.72 |
| 17:0:41:GLU:HB2 | 17:0:466:LEU:HD21 | 1.71 | 0.72 |
| 17:0:350:HIS:HA | 17:0:422:PRO:HD3 | 1.72 | 0.72 |
| 21:7:601:ARG:O | 21:7:696:ARG:NH2 | 2.22 | 0.72 |
| 2:R:127:LYS:HD3 | 2:R:220:HIS:CE1 | 2.25 | 0.72 |
| 6:A:47:ARG:HG2 | 6:A:257:ARG:HH12 | 1.54 | 0.72 |
| 6:A:359:LEU:O | 6:A:471:ASN:ND2 | 2.22 | 0.72 |
| 12:I:19:ASP:OD2 | 12:I:22:ASN:N | 2.22 | 0.72 |
| 19:6:262:LYS:HG3 | 19:6:287:PHE:HB3 | 1.70 | 0.72 |
| 23:2:82:LYS:HE2 | 23:2:89:PRO:HG3 | 1.72 | 0.72 |
| 7:B:816:GLU:OE1 | 7:B:816:GLU:N | 2.23 | 0.72 |
| 11:H:57:VAL:HA | 11:H:144:ILE:CA | 2.19 | 0.72 |
| 29:O:195:TYR:HB3 | 29:O:204:LEU:HB2 | 1.71 | 0.72 |
| 5:M:244:SER:HB3 | 7:B:108:VAL:HG13 | 1.71 | 0.72 |
| 14:K:108:GLU:O | 14:K:111:LEU:HB2 | 1.90 | 0.71 |
| 29:O:196:ARG:HG2 | 29:O:203:VAL:HG13 | 1.71 | 0.71 |
| 6:A:434:ARG:NH2 | 6:A:440:ASP:OD2 | 2.23 | 0.71 |
| 6:A:1208:THR:H | 6:A:1211:GLN:CD | 1.93 | 0.71 |
| 7:B:486:TYR:OH | 7:B:794:ASN:ND2 | 2.23 | 0.71 |
| 10:F:92:ARG:O | 10:F:96:THR:OG1 | 2.07 | 0.71 |
| 19:6:141:LEU:HD23 | 19:6:145:ARG:HA | 1.70 | 0.71 |
| 6:A:152:VAL:N | 6:A:162:VAL:O | 2.20 | 0.71 |
| 7:B:67:SER:HB2 | 7:B:92:PHE:HD2 | 1.56 | 0.71 |
| 17:0:446:ILE:HG21 | 17:0:473:LEU:HB3 | 1.72 | 0.71 |
| 29:O:193:LEU:O | 29:O:206:ILE:N | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:W:38:LEU:HD21 | 30:W:43:LEU:HD22 | 1.72 | 0.71 |
| 6:A:488:ASN:OD1 | 6:A:488:ASN:N | 2.18 | 0.71 |
| 7:B:1028:GLU:O | 7:B:1032:SER:OG | 2.08 | 0.71 |
| 6:A:1128:GLN:HG3 | 6:A:1284:MET:HE1 | 1.73 | 0.71 |
| 7:B:310:MET:HG3 | 7:B:386:LEU:HD12 | 1.73 | 0.71 |
| 21:7:603:ASP:OD1 | 21:7:696:ARG:NH1 | 2.24 | 0.71 |
| 6:A:918:GLU:OE1 | 6:A:918:GLU:N | 2.17 | 0.71 |
| 9:E:66:GLU:OE1 | 9:E:66:GLU:N | 2.23 | 0.71 |
| 17:0:66:HIS:ND1 | 17:0:229:ASP:O | 2.23 | 0.71 |
| 30:W:127:CYS:HB2 | 30:W:151:LEU:HD12 | 1.71 | 0.71 |
| 2:R:106:LEU:N | 2:R:120:TYR:O | 2.22 | 0.71 |
| 12:I:6:PHE:HA | 12:I:12:ASN:O | 1.91 | 0.71 |
| 29:O:104:MET:HB3 | 29:O:113:ALA:HB3 | 1.71 | 0.71 |
| 29:O:65:PRO:HA | 29:O:164:CYS:HB3 | 1.73 | 0.71 |
| 6:A:385:ILE:O | 6:A:389:THR:OG1 | 2.08 | 0.70 |
| 27:N:34:DA:H2 | 28:T:132:DT:H3 | 1.36 | 0.70 |
| 29:O:133:LYS:HD2 | 29:O:137:ARG:HH21 | 1.55 | 0.70 |
| 8:C:5:GLY:O | 8:C:24:ASN:ND2 | 2.25 | 0.70 |
| 11:H:2:SER:N | 11:H:61:SER:HG | 1.89 | 0.70 |
| 6:A:107:CYS:HA | 6:A:171:GLN:HE22 | 1.57 | 0.70 |
| 6:A:788:SER:OG | 6:A:789:LYS:N | 2.22 | 0.70 |
| 7:B:499:ASN:OD1 | 7:B:500:THR:N | 2.23 | 0.70 |
| 11:H:2:SER:OG | 11:H:3:ASN:N | 2.21 | 0.70 |
| 4:G:84:GLY:N | 4:G:147:ILE:O | 2.24 | 0.70 |
| 7:B:957:ASN:N | 7:B:961:LEU:O | 2.21 | 0.70 |
| 6:A:273:ASN:ND2 | 6:A:277:GLU:OE2 | 2.25 | 0.70 |
| 6:A:560:ILE:N | 11:H:78:SER:OG | 2.17 | 0.70 |
| 7:B:641:GLU:N | 7:B:650:GLU:O | 2.25 | 0.70 |
| 3:D:56:ARG:HH21 | 3:D:152:SER:HB3 | 1.55 | 0.70 |
| 6:A:1121:GLU:OE2 | 6:A:1124:HIS:ND1 | 2.24 | 0.70 |
| 9:E:59:SER:OG | 9:E:82:PHE:N | 2.23 | 0.70 |
| 9:E:159:ASP:N | 9:E:159:ASP:OD1 | 2.19 | 0.70 |
| 19:6:117:PRO:HB3 | 19:6:384:MET:HA | 1.74 | 0.70 |
| 5:M:130:PHE:O | 5:M:134:THR:OG1 | 2.09 | 0.70 |
| 6:A:496:GLU:OE1 | 6:A:496:GLU:N | 2.22 | 0.70 |
| 30:W:149:CYS:SG | 30:W:151:LEU:N | 2.65 | 0.70 |
| 4:G:45:ILE:HA | 4:G:78:VAL:HG12 | 1.71 | 0.70 |
| 8:C:53:THR:HG22 | 8:C:154:LYS:HB3 | 1.74 | 0.70 |
| 11:H:126:GLU:O | 11:H:130:ARG:NH2 | 2.25 | 0.70 |
| 12:I:74:GLU:OE2 | 12:I:79:HIS:ND1 | 2.25 | 0.70 |
| 14:K:108:GLU:HA | 14:K:111:LEU:HD13 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:A:1199:ARG:O | 6:A:1203:ASN:ND2 | 2.23 | 0.70 |
| 8:C:123:ASN:ND2 | 8:C:125:MET:SD | 2.65 | 0.70 |
| 19:6:165:PRO:HG2 | 19:6:375:HIS:HA | 1.72 | 0.70 |
| 21:7:355:ASP:H | 21:7:431:GLN:HE22 | 1.40 | 0.70 |
| 3:D:214:LEU:O | 3:D:218:GLU:N | 2.25 | 0.69 |
| 3:D:56:ARG:HB2 | 3:D:148:LEU:HD22 | 1.74 | 0.69 |
| 3:D:167:LEU:O | 3:D:170:THR:OG1 | 2.08 | 0.69 |
| 6:A:41:MET:SD | 6:A:42:ASP:N | 2.65 | 0.69 |
| 6:A:268:ASP:HB3 | 6:A:299:HIS:NE2 | 2.08 | 0.69 |
| 6:A:775:ILE:O | 6:A:797:LYS:NZ | 2.25 | 0.69 |
| 23:2:462:PHE:HB2 | 23:2:489:LYS:HB3 | 1.74 | 0.69 |
| 1:Q:375:LEU:N | 1:Q:387:ILE:O | 2.21 | 0.69 |
| 6:A:618:GLU:OE1 | 6:A:619:LYS:N | 2.25 | 0.69 |
| 7:B:896:ASP:N | 7:B:896:ASP:OD1 | 2.23 | 0.69 |
| 9:E:40:GLU:HA | 9:E:43:LYS:HE2 | 1.72 | 0.69 |
| 10:F:147:SER:N | 10:F:150:GLU:OE2 | 2.23 | 0.69 |
| 6:A:935:GLN:NE2 | 6:A:939:ASP:OD1 | 2.25 | 0.69 |
| 17:0:259:ARG:NH2 | 17:0:397:THR:OG1 | 2.25 | 0.69 |
| 2:R:94:LYS:NZ | 2:R:107:LEU:O | 2.24 | 0.69 |
| 3:D:148:LEU:O | 3:D:152:SER:N | 2.25 | 0.69 |
| 9:E:92:THR:O | 9:E:95:THR:OG1 | 2.10 | 0.69 |
| 21:7:557:VAL:HB | 21:7:708:LEU:HA | 1.75 | 0.69 |
| 26:V:84:GLN:HA | 26:V:107:SER:HA | 1.74 | 0.69 |
| 6:A:1174:PHE:H | 6:A:1174:PHE:HD1 | 1.40 | 0.69 |
| 3:D:127:ASP:HB3 | 3:D:142:LYS:HD2 | 1.74 | 0.69 |
| 6:A:1030:ARG:NH2 | 6:A:1035:TYR:OH | 2.25 | 0.69 |
| 6:A:1173:HIS:CG | 6:A:1227:ILE:HG23 | 2.28 | 0.69 |
| 19:6:136:MET:HA | 19:6:145:ARG:HD2 | 1.75 | 0.69 |
| 7:B:245:GLU:HG2 | 7:B:246:LYS:HG2 | 1.73 | 0.69 |
| 9:E:136:ASN:OD1 | 9:E:138:ALA:N | 2.26 | 0.69 |
| 10:F:133:VAL:O | 10:F:134:ILE:HG13 | 1.92 | 0.69 |
| 12:I:9:ASP:OD1 | 12:I:9:ASP:N | 2.24 | 0.69 |
| 17:0:727:PRO:HG3 | 19:6:289:LYS:HA | 1.75 | 0.69 |
| 19:6:269:GLN:HG3 | 19:6:288:TYR:HE2 | 1.57 | 0.69 |
| 8:C:75:MET:O | 8:C:246:ARG:NH2 | 2.20 | 0.69 |
| 11:H:98:TYR:OH | 11:H:138:GLU:OE2 | 2.07 | 0.69 |
| 21:7:587:LYS:HD3 | 21:7:673:ILE:HD12 | 1.74 | 0.69 |
| 6:A:23:SER:OG | 6:A:26:GLU:N | 2.22 | 0.69 |
| 6:A:219:PHE:HD1 | 6:A:220:THR:N | 1.91 | 0.69 |
| 7:B:63:ILE:O | 7:B:65:GLU:N | 2.25 | 0.69 |
| 6:A:56:PRO:HB2 | 6:A:57:ARG:NH1 | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1376:THR:O | 9:E:212:ARG:NH2 | 2.26 | 0.68 |
| 7:B:585:VAL:O | 7:B:587:HIS:ND1 | 2.26 | 0.68 |
| 29:O:186:GLU:O | 29:O:190:PHE:N | 2.26 | 0.68 |
| 5:M:263:CYS:HA | 5:M:266:ILE:HG22 | 1.75 | 0.68 |
| 6:A:1161:THR:HG21 | 6:A:1166:ASP:HB2 | 1.74 | 0.68 |
| 7:B:223:VAL:HG22 | 7:B:384:ARG:HH21 | 1.58 | 0.68 |
| 17:O:571:VAL:HG11 | 20:1:375:LEU:HD22 | 1.75 | 0.68 |
| 21:7:582:ILE:HG21 | 21:7:611:ASN:HD21 | 1.58 | 0.68 |
| 7:B:311:LEU:HA | 7:B:314:LEU:HD12 | 1.74 | 0.68 |
| 9:E:197:LYS:HE2 | 9:E:199:ILE:HD11 | 1.74 | 0.68 |
| 1:Q:99:ASN:HB3 | 2:R:97:ILE:HB | 1.73 | 0.68 |
| 1:Q:121:PHE:HB2 | 2:R:131:ASN:HD21 | 1.58 | 0.68 |
| 6:A:1134:ILE:O | 6:A:1137:ALA:N | 2.26 | 0.68 |
| 7:B:185:THR:N | 7:B:188:ASP:OD2 | 2.24 | 0.68 |
| 7:B:326:ASP:OD1 | 7:B:327:ARG:N | 2.26 | 0.68 |
| 7:B:975:GLN:N | 7:B:978:ASP:OD2 | 2.24 | 0.68 |
| 2:R:69:TRP:CD1 | 2:R:219:CYS:HB3 | 2.29 | 0.68 |
| 5:M:59:THR:H | 5:M:60:ARG:HH11 | 1.41 | 0.68 |
| 6:A:55:ASP:OD1 | 6:A:58:LEU:N | 2.26 | 0.68 |
| 6:A:1386:ARG:NE | 6:A:1404:GLU:OE2 | 2.24 | 0.68 |
| 7:B:800:GLN:OE1 | 7:B:822:ASN:ND2 | 2.22 | 0.68 |
| 21:7:489:GLU:OE1 | 21:7:685:GLN:NE2 | 2.26 | 0.68 |
| 7:B:1097:HIS:NE2 | 31:P:9:G:H4' | 2.09 | 0.68 |
| 15:L:66:GLN:OE1 | 15:L:67:PHE:N | 2.26 | 0.68 |
| 15:L:68:GLU:OE2 | 15:L:70:ARG:NH1 | 2.26 | 0.68 |
| 6:A:871:ASP:OD1 | 6:A:873:MET:N | 2.17 | 0.68 |
| 7:B:516:ASN:N | 7:B:516:ASN:OD1 | 2.21 | 0.68 |
| 9:E:26:ARG:NH1 | 9:E:188:LEU:O | 2.27 | 0.68 |
| 11:H:110:ASP:O | 11:H:128:ASN:HB2 | 1.94 | 0.68 |
| 7:B:990:ILE:HG22 | 7:B:991:GLY:H | 1.59 | 0.68 |
| 8:C:136:ASP:OD2 | 8:C:139:GLY:N | 2.26 | 0.68 |
| 9:E:67:GLU:CD | 9:E:67:GLU:H | 1.97 | 0.68 |
| 12:I:7:CYS:HB2 | 12:I:29:CYS:HB2 | 1.75 | 0.68 |
| 12:I:73:ARG:O | 12:I:83:ASN:ND2 | 2.26 | 0.68 |
| 4:G:90:THR:O | 4:G:102:GLN:N | 2.24 | 0.68 |
| 6:A:150:THR:HA | 6:A:166:GLY:O | 1.94 | 0.68 |
| 7:B:1000:PRO:HB2 | 7:B:1072:MET:HE2 | 1.74 | 0.68 |
| 8:C:196:ASP:OD2 | 8:C:199:LYS:N | 2.22 | 0.68 |
| 11:H:35:GLN:OE1 | 11:H:35:GLN:N | 2.20 | 0.68 |
| 6:A:526:ASP:HB2 | 7:B:835:GLN:OE1 | 1.93 | 0.68 |
| 7:B:1122:ARG:N | 28:T:23:DC:OP1 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:118:THR:OG1 | 3:D:119:ARG:N | 2.27 | 0.67 |
| 6:A:1396:ALA:N | 6:A:1419:ASP:OD2 | 2.26 | 0.67 |
| 18:4:53:VAL:HG13 | 18:4:179:LEU:HD23 | 1.76 | 0.67 |
| 12:I:5:ARG:HB2 | 12:I:14:LEU:HB2 | 1.75 | 0.67 |
| 21:7:487:LEU:HB2 | 21:7:512:GLY:HA2 | 1.74 | 0.67 |
| 1:Q:99:ASN:N | 2:R:97:ILE:O | 2.26 | 0.67 |
| 5:M:170:SER:HB3 | 5:M:206:THR:HG21 | 1.75 | 0.67 |
| 8:C:3:GLU:N | 8:C:6:PRO:O | 2.27 | 0.67 |
| 21:7:615:LEU:HD11 | 21:7:653:PHE:HB3 | 1.76 | 0.67 |
| 3:D:67:ARG:HA | 3:D:70:PHE:HB3 | 1.76 | 0.67 |
| 4:G:129:SER:OG | 4:G:131:GLN:NE2 | 2.26 | 0.67 |
| 8:C:92:CYS:SG | 8:C:94:LYS:N | 2.62 | 0.67 |
| 6:A:898:ARG:O | 6:A:1029:ARG:NH1 | 2.27 | 0.67 |
| 7:B:466:TRP:N | 7:B:476:ARG:O | 2.27 | 0.67 |
| 6:A:287:HIS:ND1 | 6:A:290:GLU:OE2 | 2.28 | 0.67 |
| 6:A:624:SER:O | 6:A:624:SER:OG | 2.08 | 0.67 |
| 6:A:881:GLN:NE2 | 6:A:957:PRO:O | 2.28 | 0.67 |
| 6:A:1148:ILE:HB | 6:A:1196:GLU:HG2 | 1.74 | 0.67 |
| 17:0:500:GLY:HA3 | 17:0:521:ASN:HD21 | 1.60 | 0.67 |
| 21:7:553:GLN:HB3 | 21:7:734:LYS:HE2 | 1.76 | 0.67 |
| 7:B:760:ASP:N | 7:B:760:ASP:OD1 | 2.26 | 0.67 |
| 23:2:458:LEU:HD11 | 23:2:490:LYS:HB3 | 1.77 | 0.67 |
| 6:A:1445:ILE:H | 10:F:133:VAL:HG23 | 1.60 | 0.67 |
| 18:4:289:CYS:SG | 18:4:290:SER:N | 2.68 | 0.67 |
| 4:G:146:LYS:NZ | 4:G:148:GLU:OE1 | 2.25 | 0.66 |
| 8:C:26:ASP:OD2 | 8:C:29:MET:N | 2.22 | 0.66 |
| 8:C:92:CYS:O | 8:C:96:SER:OG | 2.13 | 0.66 |
| 21:7:499:ARG:NH2 | 21:7:525:GLY:O | 2.27 | 0.66 |
| 6:A:874:ASP:OD1 | 6:A:875:ALA:N | 2.28 | 0.66 |
| 7:B:328:GLU:OE1 | 7:B:328:GLU:N | 2.24 | 0.66 |
| 29:O:93:GLU:O | 29:O:103:ILE:N | 2.18 | 0.66 |
| 2:R:68:VAL:O | 2:R:219:CYS:N | 2.27 | 0.66 |
| 3:D:154:PHE:CE2 | 3:D:163:VAL:HG21 | 2.31 | 0.66 |
| 4:G:96:GLN:H | 30:W:145:THR:HB | 1.60 | 0.66 |
| 18:4:175:ARG:NH1 | 18:4:252:MET:O | 2.28 | 0.66 |
| 29:O:162:GLY:O | 29:O:214:LEU:N | 2.23 | 0.66 |
| 4:G:101:VAL:N | 4:G:108:VAL:O | 2.28 | 0.66 |
| 5:M:186:ALA:HB3 | 5:M:241:ARG:HD2 | 1.76 | 0.66 |
| 5:M:201:LYS:HE3 | 27:N:19:DA:H3' | 1.76 | 0.66 |
| 6:A:56:PRO:O | 6:A:57:ARG:NH1 | 2.28 | 0.66 |
| 6:A:1329:THR:OG1 | 6:A:1330:ASN:N | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:178:ASN:O | 7:B:178:ASN:ND2 | 2.29 | 0.66 |
| 11:H:142:LEU:HG | 11:H:143:LEU:N | 2.10 | 0.66 |
| 15:L:30:ILE:HG23 | 15:L:36:SER:O | 1.95 | 0.66 |
| 17:O:288:LYS:O | 17:O:291:GLN:NE2 | 2.28 | 0.66 |
| 17:O:496:ILE:HD12 | 17:O:686:PHE:HB3 | 1.78 | 0.66 |
| 21:7:606:ILE:O | 21:7:671:ILE:N | 2.26 | 0.66 |
| 2:R:98:ASN:OD1 | 2:R:99:LYS:N | 2.23 | 0.66 |
| 4:G:110:VAL:HG13 | 4:G:162:SER:HA | 1.76 | 0.66 |
| 6:A:76:GLU:OE2 | 7:B:1159:ARG:NH1 | 2.28 | 0.66 |
| 17:O:112:LYS:NZ | 17:O:123:GLU:O | 2.28 | 0.66 |
| 19:6:209:SER:OG | 19:6:212:ASN:ND2 | 2.22 | 0.66 |
| 20:1:174:LEU:O | 20:1:181:GLN:NE2 | 2.26 | 0.66 |
| 7:B:708:GLU:CD | 7:B:709:ASP:H | 1.98 | 0.66 |
| 1:Q:343:ARG:NH2 | 1:Q:346:GLU:OE2 | 2.21 | 0.66 |
| 29:O:206:ILE:HD13 | 29:O:234:LEU:HD21 | 1.78 | 0.66 |
| 9:E:74:ASP:OD1 | 9:E:74:ASP:N | 2.24 | 0.66 |
| 11:H:57:VAL:HA | 11:H:144:ILE:HA | 1.77 | 0.66 |
| 14:K:24:ASP:OD1 | 14:K:25:THR:N | 2.29 | 0.66 |
| 17:O:69:ILE:HG23 | 17:O:231:ILE:HG23 | 1.77 | 0.66 |
| 21:7:579:LEU:HD22 | 21:7:611:ASN:HD22 | 1.60 | 0.66 |
| 24:X:187:HIS:HA | 24:X:214:TRP:HB2 | 1.77 | 0.66 |
| 1:Q:104:ARG:HD2 | 2:R:92:LEU:HB3 | 1.77 | 0.66 |
| 6:A:215:SER:OG | 6:A:217:LYS:N | 2.28 | 0.66 |
| 6:A:1063:MET:SD | 6:A:1436:ILE:HD12 | 2.36 | 0.66 |
| 6:A:1229:SER:N | 6:A:1237:ILE:O | 2.21 | 0.66 |
| 7:B:1139:ILE:O | 7:B:1142:GLY:N | 2.28 | 0.66 |
| 11:H:57:VAL:HG23 | 11:H:144:ILE:HA | 1.78 | 0.66 |
| 21:7:560:PRO:HA | 21:7:711:LYS:HE2 | 1.77 | 0.66 |
| 21:7:607:VAL:O | 21:7:654:LEU:N | 2.29 | 0.66 |
| 28:T:147:DT:O4 | 28:T:148:DA:N6 | 2.29 | 0.66 |
| 4:G:97:HIS:O | 4:G:112:LYS:N | 2.29 | 0.65 |
| 6:A:900:ASP:OD1 | 6:A:903:ASN:N | 2.29 | 0.65 |
| 6:A:1287:TYR:OH | 6:A:1307:GLU:OE2 | 2.10 | 0.65 |
| 7:B:137:TYR:HD1 | 7:B:137:TYR:H | 1.44 | 0.65 |
| 7:B:737:THR:O | 7:B:737:THR:OG1 | 2.10 | 0.65 |
| 12:I:34:TYR:OH | 12:I:36:GLU:OE2 | 2.13 | 0.65 |
| 27:N:37:DG:O6 | 28:T:128:DA:N6 | 2.29 | 0.65 |
| 5:M:234:GLN:NE2 | 29:O:173:GLU:OE2 | 2.27 | 0.65 |
| 7:B:1008:PRO:HB3 | 7:B:1087:PHE:HE1 | 1.60 | 0.65 |
| 2:R:73:LEU:HD12 | 2:R:74:PRO:HD2 | 1.78 | 0.65 |
| 2:R:98:ASN:HB3 | 2:R:103:LYS:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:36:GLY:N | 4:G:45:ILE:O | 2.30 | 0.65 |
| 29:O:163:SER:HA | 29:O:213:VAL:HA | 1.78 | 0.65 |
| 6:A:739:ASP:OD1 | 6:A:739:ASP:N | 2.27 | 0.65 |
| 7:B:213:ILE:O | 7:B:215:GLN:NE2 | 2.27 | 0.65 |
| 7:B:862:GLN:HB3 | 7:B:963:PHE:HB2 | 1.79 | 0.65 |
| 6:A:1436:ILE:O | 6:A:1439:GLY:N | 2.20 | 0.65 |
| 7:B:216:GLU:OE2 | 7:B:404:LYS:HG2 | 1.96 | 0.65 |
| 17:O:446:ILE:HG13 | 17:O:473:LEU:HD22 | 1.78 | 0.65 |
| 29:O:193:LEU:N | 29:O:206:ILE:O | 2.29 | 0.65 |
| 1:Q:352:MET:N | 1:Q:352:MET:SD | 2.70 | 0.65 |
| 9:E:29:PHE:HB2 | 9:E:65:THR:HG22 | 1.78 | 0.65 |
| 19:6:124:ARG:NH2 | 19:6:231:GLU:OE1 | 2.29 | 0.65 |
| 21:7:456:THR:HG23 | 21:7:459:MET:H | 1.61 | 0.65 |
| 29:O:136:SER:HB2 | 29:O:152:PHE:HE1 | 1.61 | 0.65 |
| 4:G:83:LYS:HD2 | 4:G:83:LYS:H | 1.62 | 0.65 |
| 6:A:16:GLU:OE2 | 7:B:1221:SER:N | 2.23 | 0.65 |
| 6:A:821:ARG:NH1 | 7:B:527:THR:HG21 | 2.12 | 0.65 |
| 7:B:253:THR:OG1 | 7:B:253:THR:O | 2.12 | 0.65 |
| 7:B:802:PRO:HG2 | 7:B:805:THR:HG22 | 1.78 | 0.65 |
| 27:N:19:DA:H2'' | 27:N:20:DT:H5' | 1.79 | 0.65 |
| 6:A:362:ASP:OD1 | 6:A:362:ASP:N | 2.22 | 0.65 |
| 18:4:255:ASP:O | 18:4:259:ARG:NH1 | 2.29 | 0.65 |
| 1:Q:380:ASP:OD1 | 1:Q:380:ASP:N | 2.27 | 0.65 |
| 7:B:825:VAL:HG23 | 7:B:1010:LEU:HB3 | 1.78 | 0.65 |
| 9:E:20:LYS:NZ | 9:E:34:GLU:O | 2.15 | 0.65 |
| 9:E:191:LYS:N | 9:E:194:GLU:OE1 | 2.25 | 0.65 |
| 23:2:350:TYR:N | 23:2:407:GLN:OE1 | 2.25 | 0.65 |
| 30:W:149:CYS:HB3 | 30:W:154:GLU:H | 1.62 | 0.65 |
| 6:A:1442:ASP:HA | 10:F:134:ILE:C | 2.17 | 0.64 |
| 7:B:104:GLU:OE2 | 15:L:54:ARG:NE | 2.30 | 0.64 |
| 7:B:280:ILE:HB | 7:B:285:ILE:HD11 | 1.77 | 0.64 |
| 17:O:534:PRO:HD3 | 17:O:721:LEU:HD21 | 1.78 | 0.64 |
| 6:A:82:GLY:O | 6:A:241:VAL:N | 2.28 | 0.64 |
| 6:A:1443:VAL:N | 10:F:134:ILE:O | 2.29 | 0.64 |
| 8:C:36:VAL:HG23 | 8:C:40:GLU:HB2 | 1.79 | 0.64 |
| 12:I:45:ARG:NH2 | 12:I:47:GLU:OE2 | 2.29 | 0.64 |
| 23:2:87:LEU:HD12 | 23:2:98:ILE:HG23 | 1.80 | 0.64 |
| 23:2:387:LEU:HD11 | 23:2:393:ALA:HB2 | 1.79 | 0.64 |
| 29:O:76:LEU:HD22 | 29:O:150:ALA:HB1 | 1.79 | 0.64 |
| 2:R:62:GLU:OE1 | 2:R:62:GLU:N | 2.28 | 0.64 |
| 6:A:43:GLU:O | 6:A:44:THR:OG1 | 2.16 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:609:ASP:OD1 | 6:A:610:GLY:N | 2.31 | 0.64 |
| 17:0:580:SER:HB3 | 20:1:339:LEU:H | 1.62 | 0.64 |
| 21:7:520:GLU:H | 21:7:681:ARG:HH12 | 1.45 | 0.64 |
| 29:O:179:HIS:HB3 | 29:O:182:PHE:HD2 | 1.63 | 0.64 |
| 1:Q:104:ARG:CZ | 1:Q:105:ALA:H | 2.10 | 0.64 |
| 1:Q:116:THR:O | 1:Q:117:HIS:ND1 | 2.31 | 0.64 |
| 6:A:1142:THR:O | 6:A:1145:SER:OG | 2.15 | 0.64 |
| 1:Q:373:TYR:H | 2:R:82:ARG:NH2 | 1.96 | 0.64 |
| 5:M:60:ARG:H | 5:M:60:ARG:HD2 | 1.62 | 0.64 |
| 6:A:401:GLY:O | 6:A:435:HIS:ND1 | 2.31 | 0.64 |
| 7:B:69:LEU:HD13 | 7:B:429:PHE:HB2 | 1.80 | 0.64 |
| 8:C:5:GLY:O | 8:C:7:GLN:NE2 | 2.31 | 0.64 |
| 17:0:293:LEU:HD13 | 17:0:319:GLU:HA | 1.79 | 0.64 |
| 18:4:51:ILE:O | 18:4:55:GLU:N | 2.20 | 0.64 |
| 19:6:130:LEU:N | 19:6:172:ILE:O | 2.30 | 0.64 |
| 19:6:322:MET:HB2 | 19:6:369:MET:HB2 | 1.79 | 0.64 |
| 1:Q:363:GLY:HA2 | 1:Q:395:PHE:HA | 1.80 | 0.64 |
| 6:A:471:ASN:OD1 | 6:A:472:LEU:N | 2.31 | 0.64 |
| 6:A:1297:GLU:OE1 | 6:A:1297:GLU:N | 2.23 | 0.64 |
| 7:B:20:ASP:OD2 | 7:B:22:SER:N | 2.31 | 0.64 |
| 7:B:618:ASP:OD1 | 7:B:621:GLU:N | 2.29 | 0.64 |
| 8:C:90:ASP:OD1 | 8:C:91:HIS:ND1 | 2.31 | 0.64 |
| 18:4:59:VAL:HB | 18:4:245:ILE:HD11 | 1.78 | 0.64 |
| 24:X:214:TRP:HD1 | 24:X:217:CYS:HG | 1.44 | 0.64 |
| 25:U:281:VAL:HG22 | 26:V:62:VAL:HB | 1.79 | 0.64 |
| 9:E:157:SER:OG | 9:E:159:ASP:OD1 | 2.13 | 0.64 |
| 1:Q:140:HIS:NE2 | 1:Q:353:GLU:OE2 | 2.30 | 0.64 |
| 12:I:82:GLU:OE1 | 12:I:82:GLU:N | 2.30 | 0.64 |
| 18:4:239:GLU:HG2 | 18:4:242:GLU:HB2 | 1.79 | 0.64 |
| 30:W:144:ARG:HH12 | 30:W:146:GLU:HB3 | 1.63 | 0.64 |
| 1:Q:117:HIS:HB2 | 2:R:135:PHE:CE1 | 2.33 | 0.64 |
| 6:A:225:ASN:OD1 | 6:A:228:PHE:N | 2.21 | 0.64 |
| 6:A:556:TRP:O | 14:K:26:LYS:NZ | 2.22 | 0.64 |
| 6:A:780:VAL:N | 7:B:699:GLU:OE1 | 2.29 | 0.64 |
| 7:B:979:LYS:NZ | 31:P:9:G:O2' | 2.31 | 0.64 |
| 9:E:4:GLU:O | 9:E:8:ASN:HB2 | 1.98 | 0.64 |
| 17:0:124:ARG:HH22 | 17:0:577:GLN:H | 1.46 | 0.64 |
| 18:4:82:GLY:H | 18:4:148:THR:HG21 | 1.63 | 0.64 |
| 30:W:65:ARG:HE | 30:W:93:HIS:HB3 | 1.62 | 0.64 |
| 8:C:3:GLU:OE2 | 14:K:104:ASN:HB2 | 1.97 | 0.64 |
| 17:0:113:ASN:ND2 | 20:1:346:ASP:OD1 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:571:VAL:HG22 | 17:0:599:LEU:HD21 | 1.80 | 0.64 |
| 7:B:1136:ASP:N | 7:B:1136:ASP:OD1 | 2.27 | 0.63 |
| 7:B:1187:ASN:OD1 | 7:B:1188:LYS:N | 2.31 | 0.63 |
| 11:H:32:THR:OG1 | 11:H:33:GLN:N | 2.29 | 0.63 |
| 18:4:29:ILE:HD11 | 18:4:156:GLY:HA3 | 1.80 | 0.63 |
| 21:7:303:ARG:HA | 21:7:320:ASN:HA | 1.78 | 0.63 |
| 30:W:21:TYR:OH | 30:W:64:ASP:OD2 | 2.16 | 0.63 |
| 6:A:316:GLN:O | 6:A:318:SER:OG | 2.14 | 0.63 |
| 6:A:1438:THR:O | 10:F:92:ARG:NH1 | 2.30 | 0.63 |
| 7:B:882:THR:HA | 7:B:934:LYS:O | 1.98 | 0.63 |
| 19:6:142:ARG:HB2 | 19:6:143:PRO:HD3 | 1.79 | 0.63 |
| 24:X:255:ILE:HD13 | 30:W:178:GLN:HB3 | 1.79 | 0.63 |
| 1:Q:101:PHE:CZ | 1:Q:382:GLY:HA3 | 2.32 | 0.63 |
| 1:Q:109:GLU:OE1 | 1:Q:109:GLU:N | 2.28 | 0.63 |
| 8:C:74:SER:OG | 8:C:237:SER:OG | 2.13 | 0.63 |
| 17:0:80:GLU:HA | 17:0:83:LEU:HB2 | 1.80 | 0.63 |
| 19:6:173:ILE:HD12 | 19:6:175:ARG:HD2 | 1.79 | 0.63 |
| 20:1:593:LEU:O | 20:1:597:PHE:N | 2.30 | 0.63 |
| 1:Q:332:LEU:HB2 | 7:B:429:PHE:CZ | 2.34 | 0.63 |
| 6:A:1234:GLU:OE1 | 6:A:1234:GLU:N | 2.32 | 0.63 |
| 7:B:65:GLU:O | 7:B:67:SER:N | 2.31 | 0.63 |
| 7:B:864:LYS:HG2 | 7:B:871:THR:HA | 1.79 | 0.63 |
| 9:E:46:TYR:CD1 | 9:E:58:MET:HG2 | 2.33 | 0.63 |
| 11:H:55:LEU:O | 11:H:146:ARG:NE | 2.31 | 0.63 |
| 17:0:722:ARG:HA | 19:6:267:SER:HB2 | 1.80 | 0.63 |
| 23:2:59:LEU:HD22 | 23:2:96:LEU:HD12 | 1.80 | 0.63 |
| 2:R:69:TRP:HD1 | 2:R:219:CYS:HB3 | 1.61 | 0.63 |
| 4:G:47:CYS:SG | 4:G:48:VAL:N | 2.72 | 0.63 |
| 4:G:49:LEU:HD21 | 4:G:77:VAL:HG23 | 1.81 | 0.63 |
| 6:A:21:LEU:HD12 | 6:A:229:SER:HB2 | 1.80 | 0.63 |
| 6:A:567:LYS:HB2 | 11:H:95:TYR:HA | 1.80 | 0.63 |
| 9:E:79:TRP:NE1 | 9:E:81:GLU:OE1 | 2.30 | 0.63 |
| 17:0:419:ILE:HG12 | 17:0:436:ARG:HB3 | 1.80 | 0.63 |
| 21:7:303:ARG:HB3 | 21:7:323:VAL:HG13 | 1.80 | 0.63 |
| 6:A:535:THR:HG21 | 6:A:617:VAL:H | 1.64 | 0.63 |
| 7:B:135:ARG:HH12 | 7:B:138:GLU:HB2 | 1.62 | 0.63 |
| 7:B:332:ASP:O | 7:B:348:ARG:NH1 | 2.32 | 0.63 |
| 7:B:977:GLY:HA3 | 7:B:1099:VAL:HG11 | 1.80 | 0.63 |
| 3:D:63:LEU:HB3 | 3:D:130:LEU:HD22 | 1.79 | 0.63 |
| 3:D:173:HIS:N | 3:D:176:GLU:OE2 | 2.32 | 0.63 |
| 21:7:365:TYR:OH | 21:7:390:ALA:O | 2.15 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1445:ILE:N | 10:F:133:VAL:HG23 | 2.13 | 0.63 |
| 7:B:1002:THR:OG1 | 7:B:1003:ALA:N | 2.32 | 0.63 |
| 9:E:101:GLN:H | 9:E:101:GLN:CD | 1.99 | 0.63 |
| 17:O:436:ARG:HE | 17:O:634:ILE:HG21 | 1.62 | 0.63 |
| 19:6:291:LEU:HA | 19:6:296:HIS:CD2 | 2.33 | 0.63 |
| 21:7:302:GLU:HG3 | 21:7:321:GLU:HB3 | 1.80 | 0.63 |
| 21:7:483:GLY:HA2 | 21:7:508:HIS:HB2 | 1.80 | 0.63 |
| 7:B:46:GLN:OE1 | 7:B:47:GLN:N | 2.32 | 0.63 |
| 7:B:282:ILE:O | 7:B:285:ILE:N | 2.31 | 0.63 |
| 21:7:599:GLU:HG2 | 21:7:650:ASN:HB2 | 1.80 | 0.63 |
| 23:2:246:GLN:O | 23:2:250:LEU:N | 2.26 | 0.63 |
| 29:O:129:GLU:OE1 | 29:O:220:ARG:NH2 | 2.32 | 0.63 |
| 29:O:171:ARG:N | 29:O:237:PHE:O | 2.26 | 0.63 |
| 1:Q:366:GLU:HB3 | 1:Q:392:VAL:HG13 | 1.80 | 0.62 |
| 6:A:65:LEU:O | 6:A:67:CYS:N | 2.30 | 0.62 |
| 6:A:136:ALA:O | 6:A:140:THR:OG1 | 2.16 | 0.62 |
| 6:A:420:ARG:HB3 | 6:A:423:ASP:HB3 | 1.81 | 0.62 |
| 7:B:895:ASP:N | 7:B:895:ASP:OD1 | 2.32 | 0.62 |
| 7:B:1098:MET:N | 7:B:1098:MET:SD | 2.72 | 0.62 |
| 7:B:1153:GLU:OE1 | 7:B:1153:GLU:N | 2.31 | 0.62 |
| 19:6:217:ALA:HB1 | 19:6:232:VAL:HG21 | 1.80 | 0.62 |
| 4:G:148:GLU:HB2 | 4:G:160:ILE:HG22 | 1.81 | 0.62 |
| 7:B:37:PHE:HD2 | 7:B:38:PHE:N | 1.97 | 0.62 |
| 4:G:60:ARG:O | 4:G:69:GLU:N | 2.31 | 0.62 |
| 5:M:255:SER:OG | 5:M:285:ASN:OD1 | 2.14 | 0.62 |
| 6:A:1082:ASN:OD1 | 6:A:1083:THR:N | 2.32 | 0.62 |
| 6:A:1123:GLY:HA3 | 6:A:1124:HIS:CG | 2.34 | 0.62 |
| 17:O:116:LEU:HD21 | 17:O:186:GLU:HA | 1.81 | 0.62 |
| 17:O:666:LEU:HD22 | 17:O:679:MET:HB3 | 1.81 | 0.62 |
| 19:6:188:ASN:O | 19:6:192:HIS:ND1 | 2.32 | 0.62 |
| 29:O:193:LEU:HB3 | 29:O:206:ILE:HB | 1.80 | 0.62 |
| 1:Q:103:LEU:HD21 | 2:R:95:ILE:HG22 | 1.81 | 0.62 |
| 2:R:106:LEU:HB2 | 2:R:120:TYR:HB2 | 1.82 | 0.62 |
| 6:A:903:ASN:OD1 | 6:A:904:THR:N | 2.32 | 0.62 |
| 11:H:55:LEU:O | 11:H:145:ARG:HD2 | 1.98 | 0.62 |
| 11:H:142:LEU:O | 11:H:143:LEU:HG | 1.98 | 0.62 |
| 12:I:19:ASP:N | 12:I:24:ARG:O | 2.32 | 0.62 |
| 17:O:79:ILE:HG23 | 17:O:207:ILE:HG22 | 1.79 | 0.62 |
| 17:O:378:SER:OG | 17:O:407:THR:OG1 | 2.17 | 0.62 |
| 5:M:37:ARG:HG3 | 6:A:416:ARG:HH21 | 1.64 | 0.62 |
| 6:A:67:CYS:H | 6:A:71:GLN:HA | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:982:THR:OG1 | 6:A:985:ASP:OD1 | 2.07 | 0.62 |
| 7:B:432:MET:O | 7:B:435:THR:OG1 | 2.14 | 0.62 |
| 7:B:757:PRO:HD3 | 7:B:983:ARG:NE | 2.10 | 0.62 |
| 11:H:82:PRO:HA | 11:H:87:ARG:HD2 | 1.81 | 0.62 |
| 7:B:705:MET:HE1 | 7:B:745:PRO:HB3 | 1.82 | 0.62 |
| 18:4:27:THR:HG22 | 18:4:74:ALA:HB3 | 1.80 | 0.62 |
| 21:7:308:ASP:OD1 | 21:7:309:ASP:N | 2.33 | 0.62 |
| 2:R:73:LEU:HD21 | 2:R:77:LEU:HG | 1.81 | 0.62 |
| 2:R:138:GLN:H | 2:R:138:GLN:HE21 | 1.45 | 0.62 |
| 8:C:214:ASN:ND2 | 8:C:217:ASP:OD1 | 2.32 | 0.62 |
| 12:I:19:ASP:HB3 | 12:I:24:ARG:N | 2.12 | 0.62 |
| 15:L:61:THR:OG1 | 15:L:62:LYS:N | 2.29 | 0.62 |
| 5:M:51:VAL:HG11 | 6:A:412:ARG:HB2 | 1.82 | 0.62 |
| 6:A:41:MET:O | 6:A:49:LYS:HA | 1.99 | 0.62 |
| 6:A:1442:ASP:OD2 | 10:F:135:ARG:HA | 1.99 | 0.62 |
| 12:I:92:ARG:O | 12:I:95:THR:OG1 | 2.13 | 0.62 |
| 18:4:200:ILE:HG12 | 18:4:227:THR:HG23 | 1.80 | 0.62 |
| 18:4:212:VAL:HG21 | 18:4:224:LEU:HB3 | 1.80 | 0.62 |
| 1:Q:120:LYS:HB2 | 1:Q:394:LYS:HD2 | 1.82 | 0.62 |
| 1:Q:131:THR:OG1 | 1:Q:132:ASP:OD1 | 2.13 | 0.62 |
| 5:M:35:VAL:HG23 | 5:M:46:ALA:HB2 | 1.81 | 0.62 |
| 17:0:339:ILE:HD12 | 17:0:342:LEU:HD21 | 1.82 | 0.62 |
| 21:7:365:TYR:HB3 | 21:7:543:LEU:HD21 | 1.81 | 0.62 |
| 2:R:69:TRP:NE1 | 2:R:220:HIS:HB3 | 2.15 | 0.62 |
| 5:M:158:HIS:ND1 | 5:M:158:HIS:O | 2.33 | 0.62 |
| 7:B:883:LEU:O | 7:B:884:ARG:NE | 2.33 | 0.62 |
| 18:4:29:ILE:HD13 | 18:4:153:MET:HA | 1.82 | 0.62 |
| 20:1:547:LEU:O | 20:1:551:ARG:N | 2.33 | 0.62 |
| 3:D:63:LEU:HD22 | 3:D:130:LEU:HB3 | 1.82 | 0.61 |
| 5:M:267:LYS:HE2 | 29:O:240:MET:HB2 | 1.81 | 0.61 |
| 6:A:310:GLY:O | 6:A:311:GLN:NE2 | 2.33 | 0.61 |
| 6:A:886:ILE:HD11 | 6:A:950:GLY:HA2 | 1.81 | 0.61 |
| 10:F:110:ASP:O | 10:F:123:LYS:NZ | 2.33 | 0.61 |
| 1:Q:119:LEU:HD12 | 2:R:133:TYR:HB2 | 1.82 | 0.61 |
| 6:A:1392:SER:OG | 6:A:1393:ASN:N | 2.32 | 0.61 |
| 8:C:262:LEU:HD11 | 14:K:87:LEU:HD23 | 1.80 | 0.61 |
| 18:4:273:ARG:HH11 | 19:6:373:SER:HB3 | 1.65 | 0.61 |
| 2:R:123:GLU:O | 2:R:222:CYS:HB3 | 2.00 | 0.61 |
| 3:D:41:GLN:OE1 | 3:D:41:GLN:N | 2.33 | 0.61 |
| 9:E:72:PHE:HB2 | 9:E:75:MET:HE2 | 1.82 | 0.61 |
| 11:H:110:ASP:OD1 | 11:H:110:ASP:N | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:4:289:CYS:HA | 19:6:319:LEU:HD12 | 1.82 | 0.61 |
| 23:2:84:LEU:HD11 | 23:2:86:LEU:HD23 | 1.81 | 0.61 |
| 29:O:93:GLU:HB3 | 29:O:103:ILE:HB | 1.82 | 0.61 |
| 29:O:235:SER:OG | 29:O:238:ARG:NH2 | 2.33 | 0.61 |
| 2:R:73:LEU:HD23 | 2:R:78:ALA:HA | 1.81 | 0.61 |
| 8:C:14:SER:HA | 14:K:114:LEU:HD13 | 1.81 | 0.61 |
| 10:F:133:VAL:O | 10:F:133:VAL:HG12 | 2.00 | 0.61 |
| 27:N:19:DA:H4' | 29:O:189:LEU:HG | 1.81 | 0.61 |
| 6:A:268:ASP:HB3 | 6:A:299:HIS:CD2 | 2.35 | 0.61 |
| 6:A:842:VAL:HG11 | 7:B:1136:ASP:OD2 | 2.01 | 0.61 |
| 7:B:838:SER:OG | 7:B:989:THR:O | 2.10 | 0.61 |
| 7:B:1180:PHE:HB3 | 7:B:1191:ILE:HD13 | 1.82 | 0.61 |
| 7:B:1187:ASN:OD1 | 7:B:1189:ILE:N | 2.28 | 0.61 |
| 8:C:76:ASP:OD2 | 8:C:128:ASN:N | 2.30 | 0.61 |
| 8:C:114:TYR:N | 8:C:117:ASP:OD2 | 2.32 | 0.61 |
| 21:7:608:PHE:HB3 | 21:7:672:GLN:HA | 1.83 | 0.61 |
| 6:A:68:GLN:HE22 | 6:A:80:HIS:CE1 | 2.06 | 0.61 |
| 29:O:207:PHE:HB2 | 29:O:211:LYS:HB2 | 1.82 | 0.61 |
| 1:Q:127:ILE:O | 2:R:133:TYR:OH | 2.18 | 0.61 |
| 1:Q:398:ARG:NH1 | 7:B:328:GLU:OE2 | 2.33 | 0.61 |
| 2:R:225:MET:N | 2:R:225:MET:SD | 2.74 | 0.61 |
| 6:A:130:ASP:O | 6:A:133:LYS:N | 2.33 | 0.61 |
| 7:B:385:LEU:HD23 | 7:B:386:LEU:HD23 | 1.82 | 0.61 |
| 11:H:57:VAL:HB | 11:H:145:ARG:CB | 2.30 | 0.61 |
| 18:4:202:SER:HA | 18:4:205:LYS:HB3 | 1.82 | 0.61 |
| 1:Q:102:PRO:HA | 2:R:93:GLY:O | 2.01 | 0.61 |
| 2:R:105:THR:HA | 2:R:121:ASP:HA | 1.83 | 0.61 |
| 5:M:251:GLN:OE1 | 5:M:251:GLN:N | 2.33 | 0.61 |
| 6:A:177:ASP:OD1 | 6:A:180:LYS:HB2 | 2.00 | 0.61 |
| 6:A:225:ASN:OD1 | 6:A:227:VAL:N | 2.34 | 0.61 |
| 6:A:626:ASN:O | 6:A:631:HIS:ND1 | 2.26 | 0.61 |
| 7:B:173:MET:O | 7:B:176:SER:OG | 2.12 | 0.61 |
| 7:B:911:ILE:HG13 | 7:B:912:ILE:HG13 | 1.81 | 0.61 |
| 17:0:315:ASP:OD1 | 17:0:315:ASP:N | 2.29 | 0.61 |
| 17:0:372:LYS:HA | 17:0:375:ARG:HD3 | 1.83 | 0.61 |
| 21:7:699:GLU:O | 21:7:702:ASN:ND2 | 2.34 | 0.61 |
| 29:O:68:GLN:N | 29:O:161:VAL:O | 2.34 | 0.61 |
| 6:A:57:ARG:HB2 | 6:A:68:GLN:HB3 | 1.83 | 0.61 |
| 6:A:665:GLY:N | 6:A:668:ASP:OD2 | 2.21 | 0.61 |
| 6:A:870:GLU:OE1 | 9:E:202:SER:HB2 | 2.01 | 0.61 |
| 6:A:1189:SER:OG | 6:A:1256:GLU:OE1 | 2.17 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1445:ILE:HB | 10:F:133:VAL:HG23 | 1.83 | 0.61 |
| 7:B:722:ASP:OD1 | 7:B:722:ASP:N | 2.34 | 0.61 |
| 21:7:607:VAL:HB | 21:7:653:PHE:HA | 1.82 | 0.61 |
| 30:W:122:TYR:N | 30:W:131:TYR:O | 2.33 | 0.61 |
| 2:R:69:TRP:CE2 | 2:R:220:HIS:HB3 | 2.36 | 0.61 |
| 7:B:37:PHE:HD2 | 7:B:38:PHE:H | 1.49 | 0.61 |
| 7:B:786:ASN:N | 7:B:786:ASN:OD1 | 2.24 | 0.61 |
| 17:O:159:HIS:NE2 | 17:O:303:GLU:OE2 | 2.34 | 0.61 |
| 17:O:673:LYS:NZ | 17:O:737:SER:OG | 2.34 | 0.61 |
| 29:O:179:HIS:O | 29:O:183:SER:N | 2.34 | 0.61 |
| 7:B:512:ARG:NH1 | 7:B:533:CYS:O | 2.33 | 0.60 |
| 7:B:901:PRO:HG2 | 15:L:60:ARG:HA | 1.82 | 0.60 |
| 12:I:71:SER:OG | 12:I:72:ASP:N | 2.32 | 0.60 |
| 17:O:507:SER:HG | 17:O:685:ARG:HH22 | 1.46 | 0.60 |
| 17:O:593:GLY:HA2 | 19:6:272:ILE:HG21 | 1.83 | 0.60 |
| 18:4:29:ILE:HB | 18:4:178:VAL:HG22 | 1.82 | 0.60 |
| 27:N:24:DA:N6 | 28:T:141:DT:O4 | 2.34 | 0.60 |
| 1:Q:401:TYR:CZ | 12:I:32:CYS:HB2 | 2.36 | 0.60 |
| 4:G:97:HIS:HA | 4:G:112:LYS:HD3 | 1.82 | 0.60 |
| 6:A:739:ASP:OD2 | 11:H:19:ARG:NE | 2.34 | 0.60 |
| 7:B:365:THR:HG21 | 7:B:370:PHE:CD2 | 2.37 | 0.60 |
| 8:C:73:GLN:O | 8:C:130:GLY:N | 2.24 | 0.60 |
| 9:E:98:ILE:HA | 9:E:101:GLN:HE22 | 1.66 | 0.60 |
| 12:I:59:VAL:HG23 | 12:I:61:ASP:H | 1.66 | 0.60 |
| 17:O:114:LEU:HB3 | 17:O:192:PRO:HG2 | 1.83 | 0.60 |
| 3:D:189:ASP:HA | 3:D:192:LYS:HE3 | 1.82 | 0.60 |
| 6:A:344:ARG:NH2 | 7:B:1118:PRO:O | 2.33 | 0.60 |
| 7:B:241:ARG:HG2 | 7:B:253:THR:HB | 1.83 | 0.60 |
| 8:C:43:THR:OG1 | 8:C:44:LEU:N | 2.30 | 0.60 |
| 11:H:107:VAL:N | 11:H:111:LEU:O | 2.34 | 0.60 |
| 23:2:384:ARG:HA | 23:2:387:LEU:HB2 | 1.82 | 0.60 |
| 5:M:243:CYS:HA | 5:M:248:LEU:HD12 | 1.84 | 0.60 |
| 6:A:230:ARG:HD2 | 6:A:233:TRP:CH2 | 2.36 | 0.60 |
| 6:A:1199:ARG:NH2 | 6:A:1233:ASP:O | 2.35 | 0.60 |
| 7:B:568:ASP:N | 7:B:568:ASP:OD1 | 2.33 | 0.60 |
| 7:B:936:ASP:OD1 | 7:B:938:SER:N | 2.34 | 0.60 |
| 18:4:119:ARG:O | 18:4:123:GLU:N | 2.27 | 0.60 |
| 19:6:349:CYS:HB3 | 19:6:352:CYS:SG | 2.40 | 0.60 |
| 21:7:671:ILE:HG23 | 21:7:708:LEU:HD13 | 1.83 | 0.60 |
| 6:A:386:ASP:N | 6:A:386:ASP:OD2 | 2.33 | 0.60 |
| 6:A:411:ASP:N | 6:A:411:ASP:OD1 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:771:GLU:N | 6:A:822:GLU:OE2 | 2.32 | 0.60 |
| 6:A:998:LEU:HA | 6:A:1011:GLN:HE22 | 1.67 | 0.60 |
| 6:A:1140:HIS:HB2 | 6:A:1276:VAL:O | 2.02 | 0.60 |
| 7:B:121:ASN:HA | 7:B:207:GLY:HA3 | 1.82 | 0.60 |
| 17:0:77:SER:OG | 17:0:81:LYS:NZ | 2.31 | 0.60 |
| 18:4:79:TYR:O | 18:4:148:THR:OG1 | 2.15 | 0.60 |
| 25:U:263:LYS:HZ3 | 25:U:278:LYS:HG2 | 1.66 | 0.60 |
| 1:Q:121:PHE:HB2 | 2:R:131:ASN:ND2 | 2.17 | 0.60 |
| 1:Q:129:PRO:HG2 | 1:Q:132:ASP:HB2 | 1.84 | 0.60 |
| 6:A:208:LEU:O | 6:A:212:LYS:HG3 | 2.02 | 0.60 |
| 7:B:680:THR:O | 7:B:683:SER:OG | 2.11 | 0.60 |
| 7:B:878:GLN:OE1 | 7:B:878:GLN:N | 2.35 | 0.60 |
| 14:K:58:PHE:HB3 | 14:K:76:GLN:HB3 | 1.83 | 0.60 |
| 18:4:114:UNK:C | 18:4:116:ARG:H | 2.15 | 0.60 |
| 21:7:421:ARG:HH11 | 21:7:437:VAL:HG11 | 1.67 | 0.60 |
| 4:G:15:PRO:HA | 4:G:18:PHE:CE1 | 2.37 | 0.60 |
| 6:A:148:CYS:H | 6:A:169:ASN:H | 1.49 | 0.60 |
| 6:A:175:ARG:N | 6:A:182:VAL:O | 2.33 | 0.60 |
| 6:A:206:GLU:O | 6:A:210:ILE:HG12 | 2.00 | 0.60 |
| 6:A:517:ASN:O | 6:A:517:ASN:ND2 | 2.35 | 0.60 |
| 6:A:587:HIS:NE2 | 6:A:969:GLN:HG3 | 2.17 | 0.60 |
| 7:B:1150:ARG:O | 7:B:1154:ALA:HB3 | 2.01 | 0.60 |
| 8:C:241:ASP:OD1 | 8:C:242:GLN:N | 2.33 | 0.60 |
| 18:4:190:ILE:HD12 | 18:4:277:TYR:HE1 | 1.66 | 0.60 |
| 20:1:259:ILE:HG22 | 20:1:266:VAL:HG11 | 1.82 | 0.60 |
| 21:7:664:LEU:HD12 | 21:7:690:ILE:HD13 | 1.84 | 0.60 |
| 1:Q:375:LEU:O | 1:Q:387:ILE:N | 2.23 | 0.60 |
| 4:G:97:HIS:HE1 | 30:W:146:GLU:HG3 | 1.66 | 0.60 |
| 7:B:277:LYS:NZ | 7:B:333:PHE:O | 2.27 | 0.60 |
| 19:6:130:LEU:HD23 | 19:6:235:VAL:HG21 | 1.84 | 0.60 |
| 6:A:475:THR:OG1 | 6:A:480:ALA:O | 2.19 | 0.60 |
| 6:A:1092:LYS:O | 6:A:1094:VAL:N | 2.34 | 0.60 |
| 6:A:1342:GLU:OE2 | 9:E:212:ARG:NH1 | 2.34 | 0.60 |
| 7:B:61:ASP:N | 7:B:61:ASP:OD1 | 2.34 | 0.60 |
| 7:B:365:THR:HG1 | 7:B:367:LEU:H | 1.50 | 0.60 |
| 7:B:801:LYS:O | 13:J:52:THR:OG1 | 2.20 | 0.60 |
| 11:H:56:THR:HB | 11:H:93:TYR:HB3 | 1.84 | 0.60 |
| 11:H:94:ASP:OD2 | 11:H:146:ARG:NH2 | 2.35 | 0.60 |
| 20:1:504:ILE:O | 20:1:508:LYS:N | 2.34 | 0.60 |
| 21:7:608:PHE:N | 21:7:671:ILE:O | 2.35 | 0.60 |
| 22:5:9:LEU:HD11 | 22:5:39:HIS:HB3 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:93:GLY:HA2 | 2:R:109:ASN:HB2 | 1.83 | 0.60 |
| 6:A:544:ASP:N | 6:A:544:ASP:OD1 | 2.30 | 0.60 |
| 6:A:1035:TYR:HB3 | 6:A:1037:LEU:HD21 | 1.84 | 0.60 |
| 17:0:112:LYS:HG2 | 20:1:345:ASP:HB3 | 1.83 | 0.60 |
| 17:0:241:ASP:OD1 | 17:0:241:ASP:N | 2.29 | 0.60 |
| 3:D:52:LEU:HD12 | 3:D:148:LEU:HD23 | 1.84 | 0.59 |
| 7:B:635:ARG:NH1 | 7:B:742:GLU:OE2 | 2.30 | 0.59 |
| 9:E:26:ARG:HH12 | 9:E:189:GLY:HA3 | 1.67 | 0.59 |
| 21:7:459:MET:O | 21:7:470:SER:OG | 2.14 | 0.59 |
| 6:A:575:LYS:O | 6:A:579:SER:OG | 2.19 | 0.59 |
| 6:A:830:LYS:HG3 | 6:A:1082:ASN:HB3 | 1.84 | 0.59 |
| 7:B:213:ILE:HG13 | 7:B:481:GLN:HE21 | 1.67 | 0.59 |
| 7:B:776:GLN:HB2 | 7:B:1095:LEU:HD22 | 1.82 | 0.59 |
| 17:0:346:MET:HG2 | 17:0:435:MET:HG2 | 1.84 | 0.59 |
| 1:Q:338:ASN:O | 1:Q:342:LEU:N | 2.28 | 0.59 |
| 3:D:195:ILE:HG22 | 3:D:198:LEU:H | 1.66 | 0.59 |
| 6:A:56:PRO:HB2 | 6:A:57:ARG:HH12 | 1.67 | 0.59 |
| 7:B:1129:ARG:HD3 | 28:T:21:DC:OP1 | 2.01 | 0.59 |
| 8:C:215:GLU:OE1 | 8:C:215:GLU:N | 2.33 | 0.59 |
| 17:0:20:GLU:HG2 | 17:0:43:PRO:HG2 | 1.84 | 0.59 |
| 17:0:61:MET:SD | 17:0:93:ARG:NH1 | 2.75 | 0.59 |
| 24:X:259:PHE:HE1 | 30:W:109:LEU:HD11 | 1.66 | 0.59 |
| 26:V:66:LEU:HD21 | 26:V:69:TYR:HB3 | 1.83 | 0.59 |
| 1:Q:120:LYS:HB3 | 1:Q:394:LYS:HZ2 | 1.67 | 0.59 |
| 2:R:63:ARG:HG2 | 2:R:65:ASN:H | 1.67 | 0.59 |
| 5:M:177:LEU:O | 5:M:181:ARG:HG2 | 2.02 | 0.59 |
| 5:M:187:ARG:O | 5:M:238:TYR:OH | 2.21 | 0.59 |
| 6:A:1214:GLU:O | 6:A:1218:GLN:HG3 | 2.03 | 0.59 |
| 11:H:58:THR:H | 11:H:143:LEU:C | 2.04 | 0.59 |
| 12:I:32:CYS:SG | 12:I:34:TYR:N | 2.62 | 0.59 |
| 30:W:144:ARG:NH1 | 30:W:146:GLU:O | 2.36 | 0.59 |
| 6:A:715:GLU:OE2 | 6:A:774:ARG:NE | 2.32 | 0.59 |
| 6:A:1442:ASP:OD1 | 6:A:1443:VAL:N | 2.35 | 0.59 |
| 11:H:8:ASP:OD1 | 11:H:9:ILE:N | 2.34 | 0.59 |
| 13:J:32:GLU:OE1 | 13:J:32:GLU:N | 2.22 | 0.59 |
| 21:7:714:GLN:HG2 | 21:7:718:TYR:HE2 | 1.67 | 0.59 |
| 29:O:206:ILE:HG23 | 29:O:212:ILE:HD12 | 1.85 | 0.59 |
| 6:A:219:PHE:O | 6:A:222:LEU:HG | 2.03 | 0.59 |
| 6:A:446:ARG:HG3 | 6:A:487:MET:HG2 | 1.83 | 0.59 |
| 7:B:486:TYR:CZ | 7:B:1096:ARG:HD2 | 2.37 | 0.59 |
| 17:0:155:LEU:HD12 | 17:0:160:GLU:HG3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:457:TYR:HB2 | 21:7:493:VAL:HG21 | 1.83 | 0.59 |
| 28:T:147:DT:H2' | 28:T:148:DA:H5'' | 1.85 | 0.59 |
| 6:A:609:ASP:O | 6:A:611:GLN:N | 2.36 | 0.59 |
| 6:A:790:ASP:N | 6:A:790:ASP:OD1 | 2.33 | 0.59 |
| 6:A:914:GLU:OE1 | 6:A:978:PRO:HB2 | 2.02 | 0.59 |
| 6:A:1151:GLU:HG2 | 12:I:45:ARG:HB2 | 1.84 | 0.59 |
| 6:A:1159:ARG:NH2 | 6:A:1175:SER:OG | 2.26 | 0.59 |
| 7:B:345:LYS:HB3 | 7:B:347:LYS:HG2 | 1.83 | 0.59 |
| 20:1:208:GLU:OE1 | 20:1:208:GLU:N | 2.33 | 0.59 |
| 21:7:101:PRO:O | 21:7:331:GLN:NE2 | 2.35 | 0.59 |
| 21:7:324:GLU:HA | 21:7:327:LYS:HE2 | 1.83 | 0.59 |
| 21:7:709:VAL:HG21 | 21:7:719:SER:HB3 | 1.83 | 0.59 |
| 24:X:261:LYS:O | 24:X:265:ASN:ND2 | 2.35 | 0.59 |
| 6:A:42:ASP:OD2 | 6:A:47:ARG:NE | 2.36 | 0.59 |
| 6:A:203:SER:N | 6:A:206:GLU:OE2 | 2.35 | 0.59 |
| 7:B:118:ARG:NH1 | 7:B:209:GLU:OE2 | 2.33 | 0.59 |
| 7:B:304:ASP:OD1 | 7:B:306:ASN:ND2 | 2.32 | 0.59 |
| 7:B:480:SER:O | 7:B:480:SER:OG | 2.20 | 0.59 |
| 17:0:69:ILE:HD12 | 17:0:205:ILE:HB | 1.85 | 0.59 |
| 17:0:440:LEU:HD22 | 17:0:638:ARG:HA | 1.84 | 0.59 |
| 21:7:328:LYS:O | 21:7:331:GLN:NE2 | 2.36 | 0.59 |
| 21:7:411:CYS:N | 21:7:456:THR:HA | 2.12 | 0.59 |
| 29:O:202:ILE:HD11 | 29:O:222:GLU:HB3 | 1.84 | 0.59 |
| 6:A:690:VAL:HG22 | 6:A:718:VAL:HG22 | 1.83 | 0.59 |
| 6:A:1153:TYR:CE1 | 6:A:1163:ILE:HD11 | 2.38 | 0.59 |
| 13:J:3:VAL:HG11 | 13:J:18:TRP:HB2 | 1.84 | 0.59 |
| 17:0:443:SER:HA | 17:0:446:ILE:HB | 1.85 | 0.59 |
| 18:4:261:ILE:HG13 | 23:2:66:VAL:HA | 1.84 | 0.59 |
| 6:A:1106:ASN:N | 6:A:1106:ASN:OD1 | 2.36 | 0.59 |
| 7:B:487:THR:O | 7:B:490:SER:N | 2.35 | 0.59 |
| 7:B:643:ASP:C | 7:B:645:SER:H | 2.07 | 0.59 |
| 9:E:87:SER:H | 9:E:114:ASN:HB2 | 1.67 | 0.59 |
| 14:K:77:THR:OG1 | 14:K:78:THR:O | 2.20 | 0.59 |
| 17:0:170:TYR:HA | 17:0:199:MET:HE1 | 1.84 | 0.59 |
| 17:0:353:SER:HB2 | 17:0:417:LEU:HD11 | 1.84 | 0.59 |
| 6:A:217:LYS:HG3 | 6:A:218:ASP:N | 2.18 | 0.58 |
| 6:A:793:SER:O | 6:A:796:SER:OG | 2.18 | 0.58 |
| 6:A:966:ASN:O | 6:A:970:THR:OG1 | 2.15 | 0.58 |
| 6:A:1407:GLU:CD | 6:A:1407:GLU:H | 2.06 | 0.58 |
| 7:B:909:ASP:OD1 | 7:B:909:ASP:N | 2.34 | 0.58 |
| 11:H:57:VAL:HB | 11:H:145:ARG:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:441:ASP:OD1 | 17:0:646:TYR:OH | 2.21 | 0.58 |
| 21:7:556:GLU:HG2 | 21:7:707:SER:HB3 | 1.84 | 0.58 |
| 6:A:1386:ARG:O | 6:A:1390:ASN:HB3 | 2.03 | 0.58 |
| 7:B:1037:LEU:O | 13:J:47:ARG:NH2 | 2.33 | 0.58 |
| 26:V:86:THR:HG23 | 26:V:105:VAL:HG22 | 1.85 | 0.58 |
| 29:O:105:ARG:NE | 29:O:112:THR:OG1 | 2.35 | 0.58 |
| 6:A:949:ASP:OD1 | 6:A:950:GLY:N | 2.36 | 0.58 |
| 11:H:50:ALA:N | 11:H:53:ASP:OD2 | 2.21 | 0.58 |
| 17:0:468:MET:SD | 17:0:471:ARG:NH1 | 2.77 | 0.58 |
| 4:G:60:ARG:HA | 10:F:133:VAL:HG11 | 1.85 | 0.58 |
| 4:G:111:THR:HB | 4:G:114:LEU:HD13 | 1.85 | 0.58 |
| 7:B:583:ASN:N | 7:B:583:ASN:OD1 | 2.34 | 0.58 |
| 7:B:706:GLN:O | 7:B:710:LEU:HB2 | 2.02 | 0.58 |
| 9:E:100:ILE:HG23 | 9:E:105:PHE:HB2 | 1.85 | 0.58 |
| 2:R:66:ARG:N | 2:R:216:GLY:HA3 | 2.18 | 0.58 |
| 5:M:244:SER:HB3 | 7:B:108:VAL:HA | 1.85 | 0.58 |
| 6:A:1229:SER:OG | 6:A:1237:ILE:N | 2.19 | 0.58 |
| 7:B:371:GLU:OE2 | 7:B:371:GLU:N | 2.22 | 0.58 |
| 14:K:53:ASP:OD1 | 14:K:54:ARG:N | 2.36 | 0.58 |
| 17:0:238:HIS:HB2 | 17:0:660:ARG:HD2 | 1.85 | 0.58 |
| 17:0:280:GLN:OE1 | 17:0:283:GLN:NE2 | 2.37 | 0.58 |
| 18:4:28:VAL:HB | 18:4:75:VAL:HA | 1.86 | 0.58 |
| 20:1:343:ILE:O | 20:1:345:ASP:N | 2.33 | 0.58 |
| 6:A:351:THR:HG22 | 6:A:352:VAL:H | 1.69 | 0.58 |
| 6:A:1002:GLY:H | 6:A:1007:ILE:HG21 | 1.69 | 0.58 |
| 7:B:216:GLU:OE1 | 7:B:500:THR:OG1 | 2.21 | 0.58 |
| 9:E:165:LEU:HD13 | 9:E:170:LEU:HB2 | 1.84 | 0.58 |
| 11:H:27:GLU:OE1 | 11:H:28:ALA:N | 2.36 | 0.58 |
| 17:0:286:TYR:O | 17:0:326:ARG:NH1 | 2.37 | 0.58 |
| 21:7:417:VAL:HG12 | 21:7:437:VAL:HG12 | 1.85 | 0.58 |
| 21:7:595:ILE:HA | 21:7:605:ILE:HD13 | 1.85 | 0.58 |
| 21:7:640:LEU:HA | 21:7:643:PHE:HB3 | 1.85 | 0.58 |
| 4:G:6:ASP:OD1 | 4:G:75:ARG:NH1 | 2.37 | 0.58 |
| 5:M:171:ILE:O | 5:M:175:SER:OG | 2.22 | 0.58 |
| 6:A:406:ILE:HB | 6:A:431:LYS:HB2 | 1.86 | 0.58 |
| 6:A:811:GLN:OE1 | 6:A:811:GLN:N | 2.28 | 0.58 |
| 6:A:1438:THR:HG23 | 10:F:92:ARG:HB2 | 1.85 | 0.58 |
| 7:B:590:HIS:NE2 | 7:B:592:ASN:O | 2.32 | 0.58 |
| 1:Q:405:THR:O | 1:Q:409:ALA:N | 2.25 | 0.58 |
| 2:R:62:GLU:OE1 | 2:R:214:ILE:N | 2.36 | 0.58 |
| 6:A:203:SER:OG | 6:A:204:THR:N | 2.37 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:880:THR:O | 7:B:933:SER:OG | 2.18 | 0.58 |
| 11:H:118:PHE:HB2 | 11:H:121:LEU:HB2 | 1.84 | 0.58 |
| 17:0:78:GLU:HA | 17:0:81:LYS:HD2 | 1.86 | 0.58 |
| 6:A:329:LEU:HD21 | 7:B:1206:GLU:OE1 | 2.04 | 0.58 |
| 6:A:452:LYS:HB2 | 7:B:1141:HIS:CE1 | 2.39 | 0.58 |
| 6:A:1095:THR:HG22 | 6:A:1100:ARG:HB2 | 1.84 | 0.58 |
| 6:A:1133:LEU:O | 6:A:1136:SER:OG | 2.16 | 0.58 |
| 7:B:639:ILE:HD11 | 7:B:691:GLU:HB2 | 1.84 | 0.58 |
| 9:E:169:ARG:HD3 | 10:F:140:ASP:OD2 | 2.03 | 0.58 |
| 4:G:111:THR:H | 4:G:114:LEU:HD22 | 1.69 | 0.58 |
| 6:A:269:ILE:HG13 | 6:A:299:HIS:HB3 | 1.83 | 0.58 |
| 6:A:399:HIS:O | 6:A:435:HIS:ND1 | 2.36 | 0.58 |
| 6:A:1148:ILE:O | 12:I:48:LEU:HG | 2.04 | 0.58 |
| 17:0:624:GLY:HA2 | 17:0:683:ASP:HB2 | 1.85 | 0.58 |
| 22:5:10:VAL:HG11 | 22:5:20:ILE:HG21 | 1.85 | 0.58 |
| 28:T:147:DT:H1' | 29:O:207:PHE:CZ | 2.38 | 0.58 |
| 1:Q:99:ASN:OD1 | 1:Q:100:GLU:N | 2.37 | 0.57 |
| 6:A:949:ASP:OD1 | 6:A:951:GLU:N | 2.37 | 0.57 |
| 7:B:861:ASP:OD1 | 7:B:862:GLN:N | 2.36 | 0.57 |
| 17:0:395:ASP:OD1 | 17:0:395:ASP:N | 2.30 | 0.57 |
| 18:4:273:ARG:NH1 | 19:6:373:SER:HB3 | 2.18 | 0.57 |
| 21:7:715:GLU:HA | 21:7:718:TYR:HD2 | 1.68 | 0.57 |
| 28:T:21:DC:H2' | 28:T:22:DT:C6 | 2.39 | 0.57 |
| 3:D:154:PHE:HE2 | 3:D:163:VAL:HG21 | 1.68 | 0.57 |
| 6:A:118:HIS:HA | 6:A:123:ARG:NH2 | 2.19 | 0.57 |
| 12:I:60:GLN:OE1 | 12:I:60:GLN:N | 2.20 | 0.57 |
| 12:I:101:PHE:HE1 | 12:I:112:SER:HB3 | 1.69 | 0.57 |
| 21:7:481:GLU:HB3 | 21:7:508:HIS:NE2 | 2.19 | 0.57 |
| 2:R:338:THR:N | 2:R:350:THR:O | 2.37 | 0.57 |
| 4:G:158:HIS:CE1 | 30:W:138:GLN:HE22 | 2.22 | 0.57 |
| 5:M:262:LYS:HA | 5:M:265:GLU:OE1 | 2.05 | 0.57 |
| 6:A:840:ARG:NH2 | 6:A:1106:ASN:OD1 | 2.37 | 0.57 |
| 7:B:861:ASP:OD1 | 7:B:914:LYS:NZ | 2.28 | 0.57 |
| 21:7:554:CYS:HB3 | 21:7:726:LEU:HD13 | 1.86 | 0.57 |
| 25:U:269:ILE:HG21 | 26:V:106:ILE:HG21 | 1.85 | 0.57 |
| 30:W:68:SER:O | 30:W:88:TYR:N | 2.33 | 0.57 |
| 6:A:107:CYS:SG | 6:A:109:HIS:N | 2.68 | 0.57 |
| 6:A:1147:THR:OG1 | 6:A:1196:GLU:O | 2.16 | 0.57 |
| 8:C:102:GLN:HG3 | 8:C:154:LYS:HG3 | 1.86 | 0.57 |
| 11:H:55:LEU:H | 11:H:146:ARG:CA | 2.01 | 0.57 |
| 15:L:44:ASP:OD2 | 15:L:46:VAL:N | 2.26 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:343:LYS:HG2 | 17:0:347:LYS:HZ2 | 1.69 | 0.57 |
| 18:4:221:SER:O | 18:4:225:GLN:N | 2.31 | 0.57 |
| 23:2:396:ILE:HD12 | 23:2:399:TYR:HB3 | 1.86 | 0.57 |
| 25:U:266:VAL:HG13 | 25:U:275:THR:HG22 | 1.86 | 0.57 |
| 7:B:756:ILE:HG12 | 7:B:770:GLN:HG2 | 1.86 | 0.57 |
| 7:B:1177:HIS:HB3 | 7:B:1179:GLN:NE2 | 2.18 | 0.57 |
| 18:4:245:ILE:HA | 18:4:248:LEU:HB2 | 1.86 | 0.57 |
| 19:6:196:LEU:HA | 19:6:199:ILE:HD12 | 1.87 | 0.57 |
| 3:D:154:PHE:HZ | 3:D:214:LEU:HD22 | 1.70 | 0.57 |
| 4:G:91:VAL:HB | 4:G:139:ILE:HA | 1.86 | 0.57 |
| 6:A:1148:ILE:HA | 12:I:49:ILE:HD11 | 1.86 | 0.57 |
| 9:E:123:LEU:O | 9:E:126:SER:OG | 2.20 | 0.57 |
| 20:1:503:VAL:O | 20:1:507:ILE:N | 2.37 | 0.57 |
| 21:7:604:LYS:H | 21:7:668:THR:HB | 1.70 | 0.57 |
| 22:5:31:VAL:HA | 22:5:42:VAL:HG13 | 1.86 | 0.57 |
| 25:U:260:CYS:N | 25:U:281:VAL:O | 2.28 | 0.57 |
| 4:G:4:ILE:HA | 4:G:77:VAL:HG22 | 1.87 | 0.57 |
| 5:M:188:THR:HG22 | 5:M:190:LYS:N | 2.18 | 0.57 |
| 6:A:781:ASP:OD1 | 6:A:781:ASP:N | 2.34 | 0.57 |
| 6:A:1210:GLY:O | 6:A:1214:GLU:HG2 | 2.05 | 0.57 |
| 7:B:1048:THR:OG1 | 7:B:1049:ASP:N | 2.30 | 0.57 |
| 11:H:7:ASP:OD1 | 11:H:8:ASP:N | 2.37 | 0.57 |
| 21:7:267:ASP:O | 21:7:348:ARG:NE | 2.36 | 0.57 |
| 21:7:311:ASP:OD1 | 21:7:311:ASP:N | 2.31 | 0.57 |
| 24:X:249:GLY:H | 30:W:18:ARG:NH2 | 2.02 | 0.57 |
| 2:R:95:ILE:HD13 | 2:R:106:LEU:HG | 1.85 | 0.57 |
| 3:D:175:PHE:O | 3:D:179:GLN:HG2 | 2.04 | 0.57 |
| 4:G:142:ARG:HB3 | 4:G:171:ILE:HD12 | 1.87 | 0.57 |
| 6:A:567:LYS:HB2 | 11:H:96:VAL:N | 2.18 | 0.57 |
| 6:A:635:ARG:HH11 | 6:A:635:ARG:HA | 1.69 | 0.57 |
| 6:A:786:HIS:N | 6:A:786:HIS:CD2 | 2.72 | 0.57 |
| 6:A:922:ASP:OD1 | 6:A:923:LEU:N | 2.37 | 0.57 |
| 10:F:79:ARG:NH1 | 10:F:145:ASP:O | 2.37 | 0.57 |
| 12:I:2:THR:OG1 | 12:I:3:THR:N | 2.38 | 0.57 |
| 15:L:61:THR:HG1 | 15:L:63:ARG:HH11 | 1.52 | 0.57 |
| 6:A:147:VAL:HG22 | 6:A:149:GLU:OE2 | 2.04 | 0.57 |
| 6:A:741:ASN:ND2 | 6:A:744:LYS:H | 2.03 | 0.57 |
| 7:B:60:GLN:OE1 | 7:B:95:ILE:HG22 | 2.05 | 0.57 |
| 7:B:324:ILE:HD11 | 7:B:333:PHE:HD2 | 1.69 | 0.57 |
| 7:B:650:GLU:OE2 | 7:B:651:LEU:N | 2.36 | 0.57 |
| 7:B:942:ARG:HB2 | 7:B:945:GLU:HG2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:H:83:GLN:HA | 14:K:54:ARG:NH2 | 2.20 | 0.57 |
| 21:7:636:ARG:HH22 | 21:7:657:VAL:HG21 | 1.70 | 0.57 |
| 28:T:22:DT:O4 | 28:T:23:DC:N4 | 2.38 | 0.57 |
| 28:T:146:DA:OP1 | 29:O:68:GLN:NE2 | 2.37 | 0.57 |
| 30:W:109:LEU:HD12 | 30:W:175:LEU:HD22 | 1.87 | 0.57 |
| 6:A:997:LEU:O | 6:A:1011:GLN:NE2 | 2.38 | 0.57 |
| 7:B:807:ARG:HG2 | 7:B:1045:SER:OG | 2.05 | 0.57 |
| 8:C:92:CYS:SG | 8:C:93:ASP:N | 2.78 | 0.57 |
| 17:0:104:ARG:HH22 | 17:0:171:LEU:HB2 | 1.68 | 0.57 |
| 17:0:224:ASN:HA | 17:0:227:SER:HB3 | 1.87 | 0.57 |
| 17:0:539:VAL:HG22 | 17:0:599:LEU:HA | 1.86 | 0.57 |
| 18:4:52:LYS:HD3 | 18:4:243:GLY:HA2 | 1.86 | 0.57 |
| 25:U:276:PHE:HB3 | 26:V:60:LEU:HG | 1.87 | 0.57 |
| 3:D:119:ARG:HD3 | 3:D:221:TYR:HB2 | 1.87 | 0.56 |
| 9:E:4:GLU:O | 9:E:8:ASN:CB | 2.53 | 0.56 |
| 12:I:11:ASN:O | 12:I:12:ASN:ND2 | 2.38 | 0.56 |
| 17:0:351:VAL:HG21 | 17:0:633:ARG:HD2 | 1.86 | 0.56 |
| 20:1:501:UNK:HA | 20:1:504:ILE:HB | 1.87 | 0.56 |
| 29:O:204:LEU:HD13 | 29:O:230:ILE:HG12 | 1.87 | 0.56 |
| 31:P:7:A:H3' | 31:P:8:G:O4' | 2.05 | 0.56 |
| 5:M:187:ARG:HA | 5:M:187:ARG:HE | 1.69 | 0.56 |
| 6:A:28:ARG:NH2 | 6:A:85:ASP:OD1 | 2.26 | 0.56 |
| 6:A:1157:ASP:OD1 | 6:A:1159:ARG:N | 2.37 | 0.56 |
| 8:C:51:VAL:HA | 8:C:155:LEU:HB3 | 1.87 | 0.56 |
| 17:0:104:ARG:NH1 | 17:0:171:LEU:O | 2.39 | 0.56 |
| 21:7:499:ARG:HH12 | 21:7:525:GLY:H | 1.52 | 0.56 |
| 24:X:263:TRP:HZ3 | 30:W:179:ILE:HD11 | 1.70 | 0.56 |
| 3:D:191:ALA:O | 3:D:195:ILE:N | 2.25 | 0.56 |
| 3:D:197:SER:O | 3:D:201:LYS:NZ | 2.29 | 0.56 |
| 4:G:94:CYS:SG | 4:G:95:SER:N | 2.78 | 0.56 |
| 5:M:249:PRO:HB2 | 5:M:251:GLN:HE22 | 1.70 | 0.56 |
| 6:A:1239:ARG:HH12 | 6:A:1241:ARG:HH12 | 1.50 | 0.56 |
| 7:B:955:THR:OG1 | 7:B:956:THR:N | 2.37 | 0.56 |
| 7:B:1099:VAL:O | 7:B:1102:LYS:N | 2.20 | 0.56 |
| 9:E:54:GLN:HE22 | 9:E:56:LYS:H | 1.53 | 0.56 |
| 12:I:7:CYS:SG | 12:I:10:CYS:N | 2.71 | 0.56 |
| 13:J:48:ARG:O | 13:J:52:THR:HG22 | 2.04 | 0.56 |
| 17:0:196:VAL:HA | 17:0:199:MET:HB2 | 1.87 | 0.56 |
| 21:7:585:PRO:HG2 | 21:7:756:ARG:HG2 | 1.87 | 0.56 |
| 28:T:145:DT:H4' | 29:O:68:GLN:HE21 | 1.69 | 0.56 |
| 2:R:63:ARG:HD3 | 2:R:66:ARG:HG3 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:69:TRP:HA | 2:R:220:HIS:O | 2.05 | 0.56 |
| 2:R:124:LEU:HD13 | 2:R:127:LYS:HD2 | 1.87 | 0.56 |
| 4:G:6:ASP:HA | 4:G:75:ARG:HA | 1.86 | 0.56 |
| 6:A:767:GLN:NE2 | 6:A:798:GLY:O | 2.38 | 0.56 |
| 6:A:884:ASP:OD1 | 6:A:884:ASP:N | 2.37 | 0.56 |
| 7:B:259:TYR:HE2 | 7:B:270:LYS:HB2 | 1.69 | 0.56 |
| 7:B:590:HIS:NE2 | 7:B:591:ARG:O | 2.38 | 0.56 |
| 9:E:47:CYS:HA | 9:E:53:PRO:HA | 1.86 | 0.56 |
| 11:H:113:ALA:HA | 11:H:125:LEU:O | 2.05 | 0.56 |
| 28:T:25:DC:H2' | 28:T:26:DG:C8 | 2.41 | 0.56 |
| 1:Q:371:ASP:OD1 | 1:Q:372:SER:N | 2.35 | 0.56 |
| 6:A:915:SER:O | 6:A:919:ILE:HG12 | 2.05 | 0.56 |
| 7:B:335:GLY:HA3 | 7:B:348:ARG:HH21 | 1.69 | 0.56 |
| 7:B:577:ALA:HB1 | 7:B:589:VAL:HB | 1.88 | 0.56 |
| 10:F:140:ASP:OD1 | 10:F:141:GLY:N | 2.39 | 0.56 |
| 17:O:257:LEU:HD22 | 17:O:346:MET:HE2 | 1.88 | 0.56 |
| 17:O:430:VAL:HG12 | 30:W:18:ARG:HH12 | 1.70 | 0.56 |
| 21:7:554:CYS:HA | 21:7:705:PHE:HB3 | 1.88 | 0.56 |
| 23:2:377:GLN:O | 23:2:382:SER:OG | 2.24 | 0.56 |
| 29:O:202:ILE:HG21 | 29:O:214:LEU:HD23 | 1.86 | 0.56 |
| 30:W:28:VAL:HG13 | 30:W:43:LEU:HD21 | 1.86 | 0.56 |
| 3:D:26:THR:OG1 | 3:D:28:GLN:NE2 | 2.39 | 0.56 |
| 6:A:253:ASN:ND2 | 6:A:255:SER:H | 2.03 | 0.56 |
| 7:B:629:ASP:OD1 | 7:B:630:ALA:N | 2.39 | 0.56 |
| 12:I:10:CYS:SG | 12:I:31:THR:OG1 | 2.63 | 0.56 |
| 17:O:310:PRO:HG3 | 17:O:404:THR:HG23 | 1.86 | 0.56 |
| 17:O:576:ALA:HB2 | 20:1:343:ILE:HD11 | 1.88 | 0.56 |
| 23:2:43:ALA:HB2 | 23:2:77:ALA:HB1 | 1.86 | 0.56 |
| 29:O:105:ARG:HG2 | 29:O:112:THR:HA | 1.87 | 0.56 |
| 7:B:272:THR:OG1 | 7:B:279:ASP:OD1 | 2.19 | 0.56 |
| 8:C:174:ALA:HB1 | 8:C:233:GLU:HG2 | 1.87 | 0.56 |
| 9:E:25:ASP:OD2 | 9:E:187:TYR:OH | 2.16 | 0.56 |
| 9:E:124:VAL:HA | 9:E:132:ILE:HD11 | 1.86 | 0.56 |
| 19:6:163:GLN:OE1 | 19:6:378:ARG:NH1 | 2.38 | 0.56 |
| 2:R:66:ARG:HD2 | 2:R:215:VAL:HG13 | 1.87 | 0.56 |
| 4:G:84:GLY:HA2 | 4:G:146:LYS:HZ3 | 1.70 | 0.56 |
| 4:G:113:HIS:O | 4:G:164:LYS:NZ | 2.22 | 0.56 |
| 6:A:42:ASP:OD1 | 6:A:47:ARG:NH2 | 2.39 | 0.56 |
| 7:B:98:THR:OG1 | 7:B:99:LYS:N | 2.38 | 0.56 |
| 7:B:739:THR:HG1 | 7:B:740:HIS:CE1 | 2.21 | 0.56 |
| 7:B:834:ASN:HB2 | 7:B:839:MET:HA | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:H:58:THR:N | 11:H:143:LEU:O | 2.38 | 0.56 |
| 12:I:51:ASN:N | 12:I:51:ASN:OD1 | 2.35 | 0.56 |
| 23:2:338:SER:O | 23:2:356:GLN:NE2 | 2.39 | 0.56 |
| 3:D:131:GLU:HG3 | 3:D:136:GLY:HA2 | 1.88 | 0.56 |
| 7:B:839:MET:HB2 | 7:B:1011:ILE:O | 2.06 | 0.56 |
| 18:4:254:ILE:HG22 | 18:4:259:ARG:HA | 1.88 | 0.56 |
| 30:W:140:LEU:HB2 | 30:W:147:PHE:CD1 | 2.41 | 0.56 |
| 2:R:67:GLN:C | 2:R:219:CYS:HB2 | 2.27 | 0.56 |
| 10:F:135:ARG:HD2 | 10:F:143:PHE:CE1 | 2.41 | 0.56 |
| 18:4:225:GLN:NE2 | 18:4:268:GLY:O | 2.39 | 0.56 |
| 26:V:81:LYS:HE2 | 26:V:110:LYS:HG3 | 1.87 | 0.56 |
| 29:O:171:ARG:HB2 | 29:O:237:PHE:HB3 | 1.87 | 0.56 |
| 29:O:178:SER:HB3 | 29:O:237:PHE:HZ | 1.70 | 0.56 |
| 1:Q:373:TYR:OH | 2:R:72:ARG:NH1 | 2.39 | 0.55 |
| 5:M:157:CYS:O | 5:M:159:ASP:N | 2.39 | 0.55 |
| 6:A:91:PHE:HA | 6:A:235:ILE:HG22 | 1.88 | 0.55 |
| 6:A:1166:ASP:HB3 | 6:A:1239:ARG:HD2 | 1.87 | 0.55 |
| 6:A:1443:VAL:HG12 | 10:F:132:LEU:O | 2.07 | 0.55 |
| 7:B:996:ARG:HD2 | 7:B:1007:VAL:HG11 | 1.87 | 0.55 |
| 17:0:198:ARG:NH1 | 17:0:199:MET:SD | 2.80 | 0.55 |
| 17:0:251:ASP:OD1 | 17:0:436:ARG:NH1 | 2.35 | 0.55 |
| 17:0:537:MET:SD | 17:0:567:LYS:NZ | 2.77 | 0.55 |
| 18:4:82:GLY:N | 18:4:148:THR:HG21 | 2.21 | 0.55 |
| 22:5:31:VAL:HG22 | 22:5:42:VAL:HG22 | 1.87 | 0.55 |
| 1:Q:99:ASN:O | 2:R:97:ILE:N | 2.38 | 0.55 |
| 1:Q:336:ASP:OD1 | 1:Q:337:GLU:N | 2.39 | 0.55 |
| 2:R:74:PRO:HB2 | 2:R:76:PHE:CD1 | 2.41 | 0.55 |
| 3:D:215:SER:HA | 3:D:218:GLU:HB2 | 1.87 | 0.55 |
| 5:M:213:ILE:O | 5:M:217:LYS:HG2 | 2.06 | 0.55 |
| 6:A:351:THR:HG22 | 6:A:352:VAL:N | 2.21 | 0.55 |
| 6:A:1199:ARG:HE | 6:A:1236:LEU:HD21 | 1.70 | 0.55 |
| 7:B:232:SER:O | 7:B:261:ARG:NH1 | 2.39 | 0.55 |
| 11:H:87:ARG:NE | 11:H:87:ARG:HA | 2.20 | 0.55 |
| 29:O:205:LEU:HB2 | 29:O:213:VAL:HB | 1.87 | 0.55 |
| 1:Q:138:ARG:HH22 | 1:Q:355:PHE:HB3 | 1.70 | 0.55 |
| 6:A:47:ARG:HG2 | 6:A:257:ARG:NH1 | 2.21 | 0.55 |
| 7:B:1134:GLU:N | 7:B:1134:GLU:OE1 | 2.33 | 0.55 |
| 17:0:162:LEU:HD12 | 17:0:166:GLU:HG2 | 1.88 | 0.55 |
| 17:0:499:LYS:HB3 | 17:0:503:GLN:HA | 1.87 | 0.55 |
| 18:4:59:VAL:O | 18:4:63:ALA:N | 2.30 | 0.55 |
| 18:4:75:VAL:HG12 | 18:4:86:LEU:HD23 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:221:GLY:H | 21:7:336:PRO:HG2 | 1.72 | 0.55 |
| 21:7:407:VAL:HB | 21:7:452:LEU:HD22 | 1.87 | 0.55 |
| 4:G:96:GLN:N | 30:W:145:THR:HB | 2.21 | 0.55 |
| 6:A:445:ASN:N | 6:A:445:ASN:OD1 | 2.38 | 0.55 |
| 6:A:1168:GLU:HA | 6:A:1171:GLN:HG2 | 1.89 | 0.55 |
| 6:A:1295:THR:OG1 | 6:A:1297:GLU:OE2 | 2.21 | 0.55 |
| 6:A:1318:THR:O | 9:E:14:ARG:NH2 | 2.38 | 0.55 |
| 6:A:1442:ASP:HA | 10:F:135:ARG:N | 2.22 | 0.55 |
| 7:B:512:ARG:NH2 | 7:B:531:GLN:O | 2.39 | 0.55 |
| 21:7:457:TYR:HE1 | 21:7:487:LEU:HD22 | 1.71 | 0.55 |
| 2:R:66:ARG:NH1 | 2:R:215:VAL:O | 2.37 | 0.55 |
| 5:M:161:LYS:O | 5:M:164:LYS:HB2 | 2.06 | 0.55 |
| 6:A:803:SER:OG | 6:A:805:LEU:N | 2.36 | 0.55 |
| 7:B:423:LYS:NZ | 7:B:468:GLU:OE2 | 2.29 | 0.55 |
| 12:I:77:LYS:HZ3 | 12:I:108:HIS:HB2 | 1.71 | 0.55 |
| 1:Q:124:LYS:HG2 | 1:Q:126:LYS:NZ | 2.21 | 0.55 |
| 1:Q:372:SER:OG | 2:R:73:LEU:N | 2.38 | 0.55 |
| 2:R:94:LYS:NZ | 2:R:94:LYS:O | 2.35 | 0.55 |
| 6:A:567:LYS:HZ2 | 6:A:568:PRO:N | 2.05 | 0.55 |
| 6:A:1329:THR:OG1 | 6:A:1331:SER:N | 2.32 | 0.55 |
| 11:H:54:SER:HB3 | 11:H:146:ARG:CB | 2.33 | 0.55 |
| 16:3:86:LYS:O | 16:3:90:ASN:N | 2.39 | 0.55 |
| 20:1:251:LEU:HB3 | 20:1:254:GLU:HB2 | 1.89 | 0.55 |
| 3:D:179:GLN:HB3 | 3:D:195:ILE:HD13 | 1.89 | 0.55 |
| 6:A:1154:TYR:HB2 | 6:A:1191:TRP:CZ3 | 2.41 | 0.55 |
| 6:A:1202:MET:HG3 | 6:A:1236:LEU:HD13 | 1.87 | 0.55 |
| 12:I:15:TYR:O | 12:I:27:PHE:HA | 2.07 | 0.55 |
| 12:I:29:CYS:SG | 12:I:31:THR:OG1 | 2.59 | 0.55 |
| 23:2:140:ALA:O | 23:2:144:GLU:N | 2.37 | 0.55 |
| 25:U:259:LYS:HA | 25:U:282:GLU:HG2 | 1.88 | 0.55 |
| 1:Q:362:VAL:O | 1:Q:396:THR:N | 2.35 | 0.55 |
| 2:R:211:LYS:H | 2:R:211:LYS:HD2 | 1.71 | 0.55 |
| 4:G:13:LEU:HD11 | 4:G:17:PHE:HB2 | 1.89 | 0.55 |
| 6:A:107:CYS:HA | 6:A:171:GLN:NE2 | 2.21 | 0.55 |
| 6:A:579:SER:HB3 | 6:A:611:GLN:HA | 1.88 | 0.55 |
| 18:4:88:PRO:HB2 | 19:6:407:GLN:NE2 | 2.22 | 0.55 |
| 18:4:137:LYS:HG3 | 18:4:139:GLN:HG3 | 1.89 | 0.55 |
| 19:6:122:ILE:HG21 | 19:6:379:SER:HB3 | 1.88 | 0.55 |
| 21:7:323:VAL:HA | 21:7:326:VAL:HB | 1.87 | 0.55 |
| 21:7:564:GLU:HA | 21:7:567:GLN:HB2 | 1.89 | 0.55 |
| 30:W:31:ALA:HA | 30:W:34:PHE:HB2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:1:MET:HB3 | 4:G:82:PHE:HE2 | 1.71 | 0.55 |
| 6:A:980:ASP:OD2 | 6:A:1039:LYS:HB3 | 2.06 | 0.55 |
| 7:B:946:ASN:OD1 | 7:B:946:ASN:N | 2.39 | 0.55 |
| 9:E:89:GLY:O | 9:E:92:THR:OG1 | 2.22 | 0.55 |
| 17:0:248:LEU:HB2 | 17:0:439:CYS:HB2 | 1.89 | 0.55 |
| 18:4:28:VAL:N | 18:4:74:ALA:O | 2.32 | 0.55 |
| 21:7:215:GLY:O | 21:7:220:TYR:N | 2.28 | 0.55 |
| 21:7:385:VAL:HG23 | 21:7:538:ALA:H | 1.72 | 0.55 |
| 1:Q:121:PHE:N | 2:R:131:ASN:OD1 | 2.39 | 0.55 |
| 4:G:115:MET:HE3 | 4:G:119:LEU:HD23 | 1.88 | 0.55 |
| 6:A:878:ILE:HG21 | 6:A:955:PRO:HB2 | 1.90 | 0.55 |
| 8:C:93:ASP:N | 8:C:93:ASP:OD1 | 2.40 | 0.55 |
| 11:H:47:PHE:HE1 | 11:H:94:ASP:HB2 | 1.72 | 0.55 |
| 26:V:69:TYR:HB2 | 26:V:76:TRP:CZ3 | 2.41 | 0.55 |
| 2:R:73:LEU:HD11 | 2:R:77:LEU:HD23 | 1.89 | 0.54 |
| 6:A:1116:LEU:HB2 | 6:A:1311:VAL:HG22 | 1.89 | 0.54 |
| 7:B:979:LYS:HZ3 | 31:P:10:A:P | 2.29 | 0.54 |
| 8:C:88:CYS:SG | 8:C:92:CYS:HB3 | 2.47 | 0.54 |
| 17:0:496:ILE:HG13 | 17:0:706:LEU:HD13 | 1.90 | 0.54 |
| 1:Q:127:ILE:HG23 | 1:Q:129:PRO:HD3 | 1.88 | 0.54 |
| 3:D:40:HIS:HE1 | 4:G:74:TYR:O | 1.91 | 0.54 |
| 6:A:596:THR:C | 6:A:598:LEU:H | 2.11 | 0.54 |
| 7:B:331:LEU:HD23 | 7:B:352:ALA:HB3 | 1.90 | 0.54 |
| 7:B:334:ILE:O | 7:B:348:ARG:NE | 2.41 | 0.54 |
| 18:4:75:VAL:H | 18:4:88:PRO:HD3 | 1.71 | 0.54 |
| 18:4:292:CYS:HB2 | 18:4:308:CYS:SG | 2.47 | 0.54 |
| 19:6:267:SER:HA | 19:6:290:ILE:HD12 | 1.89 | 0.54 |
| 21:7:435:CYS:HA | 21:7:453:VAL:HA | 1.89 | 0.54 |
| 6:A:419:LYS:NZ | 6:A:419:LYS:H | 2.04 | 0.54 |
| 6:A:798:GLY:HA2 | 6:A:815:PHE:CD2 | 2.43 | 0.54 |
| 6:A:1090:ALA:HA | 6:A:1093:LYS:HG3 | 1.89 | 0.54 |
| 6:A:1299:VAL:HG23 | 6:A:1300:LYS:O | 2.07 | 0.54 |
| 10:F:110:ASP:OD1 | 10:F:110:ASP:N | 2.38 | 0.54 |
| 17:0:280:GLN:HA | 17:0:283:GLN:HG2 | 1.89 | 0.54 |
| 18:4:77:ALA:HB3 | 18:4:132:LEU:HD11 | 1.87 | 0.54 |
| 21:7:569:TYR:HA | 21:7:577:ARG:HH11 | 1.71 | 0.54 |
| 21:7:617:GLU:O | 21:7:621:LYS:NZ | 2.40 | 0.54 |
| 4:G:85:GLU:HB3 | 4:G:147:ILE:HD12 | 1.88 | 0.54 |
| 8:C:98:VAL:H | 8:C:122:SER:HB3 | 1.73 | 0.54 |
| 11:H:58:THR:N | 11:H:143:LEU:HB2 | 2.22 | 0.54 |
| 17:0:493:LEU:HB2 | 17:0:678:VAL:HG13 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:516:PRO:HB2 | 21:7:358:PRO:HD2 | 1.89 | 0.54 |
| 23:2:486:ASP:O | 23:2:489:LYS:NZ | 2.27 | 0.54 |
| 30:W:9:VAL:HG11 | 30:W:91:TYR:HB3 | 1.90 | 0.54 |
| 30:W:149:CYS:SG | 30:W:152:CYS:N | 2.70 | 0.54 |
| 2:R:106:LEU:HD11 | 2:R:122:LEU:HB2 | 1.89 | 0.54 |
| 5:M:202:GLU:O | 5:M:206:THR:OG1 | 2.22 | 0.54 |
| 6:A:57:ARG:HG3 | 6:A:68:GLN:HB3 | 1.88 | 0.54 |
| 6:A:108:MET:HE2 | 6:A:171:GLN:HB3 | 1.90 | 0.54 |
| 6:A:298:PHE:O | 6:A:302:THR:HG22 | 2.07 | 0.54 |
| 6:A:1197:LEU:HB2 | 6:A:1236:LEU:HD12 | 1.89 | 0.54 |
| 7:B:862:GLN:CB | 7:B:963:PHE:HB2 | 2.36 | 0.54 |
| 11:H:128:ASN:O | 11:H:128:ASN:ND2 | 2.41 | 0.54 |
| 19:6:128:LEU:HA | 19:6:233:LEU:HB3 | 1.88 | 0.54 |
| 21:7:637:MET:HA | 21:7:640:LEU:HB2 | 1.88 | 0.54 |
| 23:2:62:LEU:HA | 23:2:65:TRP:HD1 | 1.72 | 0.54 |
| 26:V:83:CYS:O | 26:V:108:VAL:N | 2.34 | 0.54 |
| 29:O:215:THR:OG1 | 29:O:216:GLY:N | 2.40 | 0.54 |
| 30:W:123:MET:HG2 | 30:W:157:VAL:HB | 1.88 | 0.54 |
| 2:R:118:HIS:ND1 | 2:R:120:TYR:OH | 2.39 | 0.54 |
| 6:A:923:LEU:O | 6:A:927:VAL:HG12 | 2.08 | 0.54 |
| 7:B:355:ILE:HG22 | 7:B:356:LEU:HD23 | 1.90 | 0.54 |
| 7:B:954:VAL:HG22 | 7:B:964:VAL:HG22 | 1.89 | 0.54 |
| 13:J:6:ARG:HA | 13:J:12:LYS:O | 2.08 | 0.54 |
| 14:K:82:ASP:OD2 | 14:K:85:ASP:N | 2.36 | 0.54 |
| 18:4:234:VAL:HG11 | 18:4:252:MET:HG3 | 1.89 | 0.54 |
| 19:6:182:VAL:HG21 | 19:6:199:ILE:HD11 | 1.88 | 0.54 |
| 23:2:432:VAL:HG23 | 23:2:433:LEU:HD23 | 1.90 | 0.54 |
| 24:X:201:THR:HG22 | 30:W:34:PHE:HA | 1.88 | 0.54 |
| 30:W:66:LEU:HA | 30:W:94:ALA:HB2 | 1.89 | 0.54 |
| 2:R:237:VAL:O | 2:R:241:ARG:N | 2.39 | 0.54 |
| 5:M:143:PRO:HB2 | 5:M:145:ILE:HG22 | 1.90 | 0.54 |
| 6:A:215:SER:OG | 6:A:218:ASP:OD1 | 2.23 | 0.54 |
| 6:A:590:ARG:NH2 | 6:A:621:THR:OG1 | 2.40 | 0.54 |
| 6:A:606:LEU:HD21 | 6:A:608:ILE:HD11 | 1.88 | 0.54 |
| 6:A:1110:ASN:OD1 | 6:A:1110:ASN:N | 2.36 | 0.54 |
| 20:1:544:ILE:O | 20:1:548:GLU:N | 2.33 | 0.54 |
| 21:7:710:SER:O | 21:7:713:THR:OG1 | 2.25 | 0.54 |
| 28:T:158:DT:H2'' | 28:T:159:DT:O4' | 2.07 | 0.54 |
| 5:M:204:GLY:O | 5:M:207:LEU:HG | 2.08 | 0.54 |
| 6:A:494:SER:OG | 6:A:496:GLU:OE1 | 2.25 | 0.54 |
| 6:A:1148:ILE:N | 6:A:1196:GLU:O | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:C:29:MET:HE1 | 14:K:97:LYS:HD2 | 1.89 | 0.54 |
| 9:E:20:LYS:HE3 | 9:E:34:GLU:HG2 | 1.89 | 0.54 |
| 11:H:41:ASP:OD2 | 11:H:122:LEU:N | 2.29 | 0.54 |
| 15:L:62:LYS:H | 15:L:63:ARG:NH1 | 2.06 | 0.54 |
| 23:2:47:ILE:HD12 | 23:2:104:PHE:HE2 | 1.73 | 0.54 |
| 1:Q:120:LYS:HG2 | 2:R:132:GLU:OE1 | 2.08 | 0.54 |
| 6:A:257:ARG:H | 6:A:257:ARG:HE | 1.55 | 0.54 |
| 6:A:1021:LEU:O | 6:A:1024:SER:OG | 2.18 | 0.54 |
| 9:E:56:LYS:NZ | 9:E:84:ASP:H | 2.05 | 0.54 |
| 11:H:100:THR:HG23 | 11:H:138:GLU:HA | 1.88 | 0.54 |
| 17:0:245:ILE:HA | 17:0:439:CYS:HB3 | 1.90 | 0.54 |
| 20:1:511:ALA:O | 20:1:515:UNK:N | 2.40 | 0.54 |
| 24:X:199:GLN:HA | 24:X:202:PHE:HB2 | 1.90 | 0.54 |
| 1:Q:372:SER:HG | 2:R:73:LEU:H | 1.55 | 0.54 |
| 6:A:1043:ASP:N | 6:A:1043:ASP:OD1 | 2.40 | 0.54 |
| 6:A:1161:THR:HG22 | 6:A:1163:ILE:N | 2.23 | 0.54 |
| 6:A:1261:LYS:O | 6:A:1264:GLU:HG3 | 2.08 | 0.54 |
| 7:B:345:LYS:HA | 7:B:347:LYS:N | 2.23 | 0.54 |
| 7:B:361:LEU:HB3 | 7:B:364:ILE:HG13 | 1.89 | 0.54 |
| 17:0:322:PRO:HB3 | 17:0:376:PHE:HB2 | 1.89 | 0.54 |
| 18:4:122:ASP:HA | 18:4:125:LEU:HB2 | 1.90 | 0.54 |
| 21:7:637:MET:O | 21:7:641:GLN:N | 2.40 | 0.54 |
| 23:2:39:LEU:HD13 | 23:2:47:ILE:HG13 | 1.88 | 0.54 |
| 6:A:512:VAL:HA | 6:A:519:PRO:HA | 1.90 | 0.53 |
| 6:A:827:THR:O | 6:A:831:THR:HG23 | 2.09 | 0.53 |
| 6:A:1348:LEU:HD23 | 6:A:1372:VAL:HG22 | 1.89 | 0.53 |
| 10:F:77:ASP:OD2 | 10:F:77:ASP:N | 2.28 | 0.53 |
| 29:O:130:ASP:OD1 | 29:O:133:LYS:NZ | 2.33 | 0.53 |
| 1:Q:375:LEU:HD21 | 2:R:134:VAL:HG21 | 1.90 | 0.53 |
| 4:G:50:ASP:OD1 | 4:G:53:ASN:N | 2.35 | 0.53 |
| 5:M:236:LEU:O | 5:M:239:ILE:HG12 | 2.08 | 0.53 |
| 6:A:980:ASP:OD1 | 6:A:1039:LYS:N | 2.36 | 0.53 |
| 7:B:708:GLU:CD | 7:B:708:GLU:H | 2.09 | 0.53 |
| 7:B:808:ALA:O | 7:B:812:LEU:HD22 | 2.09 | 0.53 |
| 20:1:303:UNK:O | 20:1:305:UNK:N | 2.42 | 0.53 |
| 4:G:84:GLY:HA2 | 4:G:146:LYS:NZ | 2.23 | 0.53 |
| 6:A:31:SER:HB2 | 6:A:83:HIS:HB3 | 1.91 | 0.53 |
| 6:A:668:ASP:OD1 | 6:A:742:ASN:ND2 | 2.40 | 0.53 |
| 7:B:731:VAL:HG23 | 7:B:732:SER:H | 1.74 | 0.53 |
| 9:E:97:VAL:O | 9:E:101:GLN:NE2 | 2.41 | 0.53 |
| 9:E:143:ASN:OD1 | 9:E:145:THR:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:6:166:ILE:HG12 | 19:6:375:HIS:HB3 | 1.90 | 0.53 |
| 24:X:269:PRO:O | 30:W:65:ARG:NH2 | 2.41 | 0.53 |
| 6:A:39:GLU:HG3 | 6:A:50:ILE:HD13 | 1.91 | 0.53 |
| 6:A:302:THR:HA | 6:A:305:ASP:O | 2.09 | 0.53 |
| 8:C:107:SER:OG | 8:C:108:GLU:N | 2.42 | 0.53 |
| 10:F:99:LEU:O | 10:F:102:SER:OG | 2.22 | 0.53 |
| 16:3:82:VAL:O | 16:3:86:LYS:N | 2.31 | 0.53 |
| 17:0:79:ILE:HD12 | 17:0:207:ILE:HG22 | 1.91 | 0.53 |
| 21:7:497:MET:HA | 21:7:500:ARG:HE | 1.73 | 0.53 |
| 27:N:16:DC:H2'' | 27:N:17:DG:N7 | 2.23 | 0.53 |
| 3:D:35:LEU:O | 3:D:47:LEU:N | 2.41 | 0.53 |
| 3:D:68:ARG:HG2 | 3:D:72:ARG:HH22 | 1.72 | 0.53 |
| 6:A:414:ASP:OD1 | 6:A:416:ARG:N | 2.34 | 0.53 |
| 9:E:76:GLY:HA3 | 9:E:106:GLN:HB2 | 1.90 | 0.53 |
| 11:H:108:SER:OG | 11:H:110:ASP:OD1 | 2.25 | 0.53 |
| 17:0:422:PRO:HA | 17:0:433:PRO:HB3 | 1.91 | 0.53 |
| 23:2:24:ARG:HB3 | 23:2:219:VAL:HG11 | 1.90 | 0.53 |
| 27:N:5:DA:H61 | 28:T:161:DT:H3 | 1.55 | 0.53 |
| 29:O:141:ARG:NH1 | 29:O:144:GLN:OE1 | 2.38 | 0.53 |
| 29:O:176:ALA:HA | 29:O:183:SER:HB2 | 1.90 | 0.53 |
| 2:R:94:LYS:HE3 | 2:R:107:LEU:HG | 1.91 | 0.53 |
| 3:D:144:THR:HG23 | 4:G:105:PRO:HD3 | 1.91 | 0.53 |
| 4:G:10:ASN:HA | 4:G:70:PHE:O | 2.08 | 0.53 |
| 6:A:1209:MET:N | 6:A:1231:ASP:OD1 | 2.28 | 0.53 |
| 6:A:1444:MET:CG | 10:F:133:VAL:HG22 | 2.39 | 0.53 |
| 12:I:107:SER:O | 12:I:107:SER:OG | 2.26 | 0.53 |
| 15:L:61:THR:OG1 | 15:L:63:ARG:NH1 | 2.42 | 0.53 |
| 15:L:63:ARG:NE | 15:L:63:ARG:HA | 2.22 | 0.53 |
| 17:0:342:LEU:O | 17:0:346:MET:N | 2.41 | 0.53 |
| 24:X:203:LYS:HA | 30:W:46:LEU:HD13 | 1.90 | 0.53 |
| 29:O:81:ASP:HB3 | 29:O:84:THR:HB | 1.89 | 0.53 |
| 3:D:127:ASP:O | 3:D:142:LYS:NZ | 2.32 | 0.53 |
| 6:A:557:ASP:O | 14:K:26:LYS:HB3 | 2.08 | 0.53 |
| 6:A:1301:GLU:HG3 | 6:A:1302:PRO:HD2 | 1.91 | 0.53 |
| 7:B:408:LEU:HD11 | 7:B:545:ILE:HD12 | 1.89 | 0.53 |
| 7:B:643:ASP:C | 7:B:645:SER:N | 2.62 | 0.53 |
| 6:A:1441:PHE:HZ | 10:F:92:ARG:HB3 | 1.74 | 0.53 |
| 7:B:26:THR:N | 7:B:29:ASP:OD2 | 2.42 | 0.53 |
| 9:E:38:PRO:HB2 | 9:E:41:ASP:OD1 | 2.09 | 0.53 |
| 9:E:101:GLN:N | 9:E:101:GLN:OE1 | 2.42 | 0.53 |
| 12:I:7:CYS:O | 12:I:9:ASP:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:208:TYR:HE2 | 17:0:213:LEU:HB2 | 1.73 | 0.53 |
| 17:0:308:GLU:CD | 17:0:308:GLU:H | 2.12 | 0.53 |
| 18:4:54:LEU:O | 18:4:58:ILE:N | 2.42 | 0.53 |
| 21:7:552:VAL:HG21 | 21:7:731:TYR:HD2 | 1.74 | 0.53 |
| 21:7:647:ASP:O | 21:7:650:ASN:ND2 | 2.42 | 0.53 |
| 1:Q:333:LYS:HB2 | 7:B:70:ILE:HD11 | 1.90 | 0.53 |
| 2:R:134:VAL:N | 2:R:216:GLY:O | 2.32 | 0.53 |
| 3:D:195:ILE:HG21 | 3:D:198:LEU:HD12 | 1.89 | 0.53 |
| 6:A:254:GLU:OE1 | 7:B:935:ARG:NH1 | 2.42 | 0.53 |
| 7:B:892:LYS:NZ | 7:B:909:ASP:OD2 | 2.41 | 0.53 |
| 7:B:894:ASP:N | 7:B:894:ASP:OD1 | 2.41 | 0.53 |
| 12:I:18:GLU:HB3 | 12:I:20:LYS:HD3 | 1.91 | 0.53 |
| 18:4:78:ALA:HB2 | 18:4:152:ALA:HB2 | 1.90 | 0.53 |
| 19:6:291:LEU:HD13 | 19:6:297:LEU:HB3 | 1.91 | 0.53 |
| 30:W:124:CYS:N | 30:W:129:THR:O | 2.22 | 0.53 |
| 6:A:41:MET:O | 6:A:50:ILE:HG13 | 2.07 | 0.53 |
| 6:A:53:LEU:HD12 | 6:A:54:ASN:H | 1.73 | 0.53 |
| 6:A:420:ARG:NH2 | 6:A:423:ASP:OD2 | 2.27 | 0.53 |
| 6:A:1166:ASP:O | 6:A:1170:ILE:HG12 | 2.09 | 0.53 |
| 7:B:137:TYR:N | 7:B:137:TYR:CD1 | 2.76 | 0.53 |
| 7:B:345:LYS:N | 7:B:346:GLU:HB3 | 2.23 | 0.53 |
| 7:B:706:GLN:N | 7:B:710:LEU:HD23 | 2.21 | 0.53 |
| 11:H:84:ALA:H | 14:K:54:ARG:HH22 | 1.57 | 0.53 |
| 17:0:53:LEU:HD13 | 17:0:86:LEU:HB2 | 1.91 | 0.53 |
| 20:1:370:UNK:C | 20:1:372:VAL:H | 2.22 | 0.53 |
| 21:7:212:PHE:O | 21:7:216:ALA:N | 2.34 | 0.53 |
| 21:7:615:LEU:HD12 | 21:7:618:TYR:HD2 | 1.74 | 0.53 |
| 23:2:19:GLN:HE21 | 23:2:85:HIS:CE1 | 2.26 | 0.53 |
| 26:V:62:VAL:HA | 26:V:84:GLN:O | 2.09 | 0.53 |
| 1:Q:103:LEU:HA | 1:Q:384:PHE:O | 2.09 | 0.52 |
| 3:D:34:GLN:O | 3:D:47:LEU:HB2 | 2.09 | 0.52 |
| 3:D:154:PHE:O | 3:D:155:ARG:NE | 2.42 | 0.52 |
| 6:A:584:ASN:HA | 6:A:610:GLY:HA3 | 1.89 | 0.52 |
| 6:A:847:ASP:N | 6:A:847:ASP:OD1 | 2.40 | 0.52 |
| 7:B:1016:ALA:O | 7:B:1020:ARG:HD2 | 2.09 | 0.52 |
| 8:C:235:VAL:HG21 | 13:J:6:ARG:NH2 | 2.24 | 0.52 |
| 12:I:25:LEU:O | 12:I:37:GLU:HA | 2.09 | 0.52 |
| 17:0:21:GLN:O | 17:0:25:MET:N | 2.29 | 0.52 |
| 29:O:172:LEU:HD13 | 29:O:193:LEU:HB2 | 1.90 | 0.52 |
| 30:W:44:LYS:HA | 30:W:54:LEU:HD13 | 1.89 | 0.52 |
| 30:W:98:ILE:HB | 30:W:186:LEU:HD21 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:71:VAL:HA | 2:R:222:CYS:O | 2.08 | 0.52 |
| 4:G:92:VAL:HG23 | 4:G:102:GLN:HB2 | 1.90 | 0.52 |
| 5:M:60:ARG:HD2 | 5:M:60:ARG:N | 2.24 | 0.52 |
| 6:A:1212:VAL:O | 6:A:1216:ILE:HG13 | 2.09 | 0.52 |
| 9:E:56:LYS:HZ1 | 9:E:84:ASP:H | 1.56 | 0.52 |
| 12:I:7:CYS:H | 12:I:12:ASN:H | 1.58 | 0.52 |
| 17:O:137:THR:HA | 17:O:142:LYS:HB3 | 1.91 | 0.52 |
| 1:Q:100:GLU:HA | 2:R:95:ILE:O | 2.10 | 0.52 |
| 1:Q:103:LEU:HD12 | 1:Q:384:PHE:HB2 | 1.90 | 0.52 |
| 1:Q:133:PHE:HE1 | 1:Q:359:ASN:HB2 | 1.74 | 0.52 |
| 4:G:60:ARG:HA | 10:F:133:VAL:CG1 | 2.39 | 0.52 |
| 5:M:193:GLN:NE2 | 5:M:197:HIS:HA | 2.22 | 0.52 |
| 6:A:218:ASP:N | 6:A:218:ASP:OD1 | 2.42 | 0.52 |
| 6:A:1158:PRO:HB3 | 6:A:1188:GLN:NE2 | 2.22 | 0.52 |
| 6:A:1445:ILE:N | 10:F:132:LEU:O | 2.42 | 0.52 |
| 7:B:135:ARG:NH1 | 7:B:138:GLU:HB2 | 2.25 | 0.52 |
| 7:B:864:LYS:NZ | 7:B:867:GLY:O | 2.42 | 0.52 |
| 21:7:390:ALA:HB2 | 21:7:692:ARG:CZ | 2.39 | 0.52 |
| 21:7:655:SER:HB2 | 21:7:657:VAL:HG22 | 1.91 | 0.52 |
| 29:O:67:LEU:HD13 | 29:O:70:ILE:HD11 | 1.91 | 0.52 |
| 29:O:160:ILE:N | 29:O:217:ALA:O | 2.41 | 0.52 |
| 6:A:60:SER:OG | 6:A:65:LEU:O | 2.24 | 0.52 |
| 6:A:287:HIS:HA | 6:A:290:GLU:OE1 | 2.10 | 0.52 |
| 6:A:858:ASN:OD1 | 6:A:859:SER:N | 2.43 | 0.52 |
| 6:A:1037:LEU:HD12 | 6:A:1042:PHE:HD1 | 1.74 | 0.52 |
| 27:N:10:DA:H2" | 27:N:11:DA:N7 | 2.24 | 0.52 |
| 29:O:165:ASP:OD1 | 29:O:166:VAL:N | 2.42 | 0.52 |
| 2:R:99:LYS:HB2 | 2:R:103:LYS:HE2 | 1.91 | 0.52 |
| 3:D:206:GLU:O | 3:D:210:ILE:HG13 | 2.09 | 0.52 |
| 5:M:163:LEU:O | 5:M:166:LYS:HG2 | 2.09 | 0.52 |
| 12:I:17:ARG:N | 12:I:26:LEU:O | 2.42 | 0.52 |
| 17:O:125:LYS:HE2 | 17:O:127:THR:HG23 | 1.92 | 0.52 |
| 17:O:703:ASP:HA | 17:O:706:LEU:HD23 | 1.91 | 0.52 |
| 20:1:300:UNK:O | 20:1:302:UNK:N | 2.42 | 0.52 |
| 23:2:59:LEU:HB2 | 23:2:96:LEU:HB2 | 1.92 | 0.52 |
| 24:X:201:THR:HA | 30:W:34:PHE:HB3 | 1.91 | 0.52 |
| 25:U:282:GLU:HB2 | 26:V:63:LYS:HG2 | 1.92 | 0.52 |
| 29:O:170:ILE:HG21 | 29:O:234:LEU:HD22 | 1.90 | 0.52 |
| 30:W:98:ILE:HG22 | 30:W:186:LEU:HD11 | 1.92 | 0.52 |
| 6:A:858:ASN:OD1 | 6:A:860:LEU:N | 2.43 | 0.52 |
| 6:A:1129:GLU:O | 6:A:1133:LEU:HG | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1229:SER:HB3 | 6:A:1237:ILE:HD12 | 1.91 | 0.52 |
| 7:B:1097:HIS:CE1 | 31:P:9:G:H4' | 2.45 | 0.52 |
| 11:H:56:THR:HA | 11:H:145:ARG:HH11 | 1.72 | 0.52 |
| 24:X:207:CYS:HA | 24:X:210:LEU:HD12 | 1.91 | 0.52 |
| 30:W:144:ARG:NH2 | 30:W:145:THR:H | 2.07 | 0.52 |
| 4:G:9:LEU:O | 4:G:72:VAL:N | 2.42 | 0.52 |
| 5:M:271:GLY:HA2 | 5:M:277:ILE:CG1 | 2.33 | 0.52 |
| 6:A:23:SER:HG | 6:A:26:GLU:H | 1.53 | 0.52 |
| 6:A:72:GLU:O | 6:A:76:GLU:HB3 | 2.09 | 0.52 |
| 6:A:1228:TRP:HA | 6:A:1238:ILE:HA | 1.91 | 0.52 |
| 11:H:57:VAL:HB | 11:H:145:ARG:N | 2.24 | 0.52 |
| 18:4:217:GLY:O | 18:4:237:HIS:NE2 | 2.40 | 0.52 |
| 29:O:175:LEU:HD11 | 29:O:195:TYR:HE1 | 1.74 | 0.52 |
| 2:R:105:THR:OG1 | 2:R:119:GLU:OE2 | 2.14 | 0.52 |
| 3:D:63:LEU:HD13 | 3:D:130:LEU:HD13 | 1.92 | 0.52 |
| 6:A:353:ILE:HG13 | 6:A:482:PHE:HD1 | 1.75 | 0.52 |
| 6:A:860:LEU:HD11 | 6:A:1394:THR:HA | 1.91 | 0.52 |
| 7:B:232:SER:O | 7:B:261:ARG:NH2 | 2.42 | 0.52 |
| 7:B:950:ASP:OD2 | 7:B:967:ARG:NE | 2.42 | 0.52 |
| 9:E:119:SER:O | 9:E:122:LYS:HB2 | 2.10 | 0.52 |
| 11:H:57:VAL:HA | 11:H:144:ILE:N | 2.24 | 0.52 |
| 17:0:231:ILE:HA | 17:0:455:SER:HB2 | 1.92 | 0.52 |
| 29:O:84:THR:O | 29:O:88:HIS:ND1 | 2.43 | 0.52 |
| 6:A:244:PRO:O | 6:A:247:ARG:N | 2.40 | 0.52 |
| 6:A:821:ARG:HE | 7:B:514:LEU:HB2 | 1.75 | 0.52 |
| 8:C:22:LEU:HG | 8:C:25:VAL:HG21 | 1.91 | 0.52 |
| 14:K:12:LEU:HD11 | 14:K:18:LYS:HB2 | 1.90 | 0.52 |
| 17:0:657:ASP:O | 17:0:661:HIS:ND1 | 2.35 | 0.52 |
| 17:0:719:GLN:OE1 | 17:0:722:ARG:NH1 | 2.43 | 0.52 |
| 19:6:352:CYS:HB3 | 19:6:366:CYS:SG | 2.50 | 0.52 |
| 20:1:260:PHE:HE1 | 20:1:266:VAL:HG22 | 1.73 | 0.52 |
| 1:Q:381:ASP:OD1 | 1:Q:382:GLY:N | 2.43 | 0.52 |
| 3:D:167:LEU:HA | 3:D:170:THR:HG23 | 1.92 | 0.52 |
| 5:M:168:MET:O | 5:M:172:MET:HG2 | 2.10 | 0.52 |
| 6:A:630:ILE:O | 6:A:634:THR:OG1 | 2.28 | 0.52 |
| 7:B:46:GLN:OE1 | 7:B:47:GLN:HG2 | 2.10 | 0.52 |
| 7:B:647:GLY:C | 7:B:649:LYS:H | 2.11 | 0.52 |
| 7:B:936:ASP:OD1 | 7:B:938:SER:OG | 2.14 | 0.52 |
| 7:B:1155:SER:OG | 7:B:1156:ASP:N | 2.43 | 0.52 |
| 9:E:81:GLU:HB3 | 9:E:110:PHE:HA | 1.92 | 0.52 |
| 11:H:132:LEU:HB3 | 11:H:135:LEU:HD11 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:81:ARG:N | 12:I:82:GLU:OE1 | 2.43 | 0.52 |
| 17:O:23:ASN:OD1 | 17:O:752:LYS:NZ | 2.27 | 0.52 |
| 18:4:225:GLN:HE22 | 18:4:269:SER:HA | 1.73 | 0.52 |
| 21:7:556:GLU:HA | 21:7:707:SER:HB3 | 1.92 | 0.52 |
| 23:2:481:LEU:HA | 23:2:493:ILE:HG21 | 1.92 | 0.52 |
| 26:V:85:VAL:N | 26:V:106:ILE:O | 2.29 | 0.52 |
| 3:D:130:LEU:HA | 3:D:133:THR:HB | 1.92 | 0.51 |
| 7:B:294:ASP:OD1 | 7:B:294:ASP:N | 2.43 | 0.51 |
| 7:B:486:TYR:OH | 7:B:1096:ARG:HB3 | 2.09 | 0.51 |
| 10:F:146:TRP:HE3 | 10:F:150:GLU:HG3 | 1.74 | 0.51 |
| 12:I:51:ASN:HB3 | 12:I:118:ARG:NH2 | 2.25 | 0.51 |
| 17:O:497:ILE:HB | 17:O:682:ALA:HA | 1.91 | 0.51 |
| 21:7:350:PRO:HD2 | 21:7:480:ARG:HH12 | 1.75 | 0.51 |
| 21:7:607:VAL:N | 21:7:652:ILE:O | 2.31 | 0.51 |
| 2:R:127:LYS:HA | 2:R:220:HIS:ND1 | 2.25 | 0.51 |
| 2:R:129:VAL:HG11 | 2:R:220:HIS:HA | 1.90 | 0.51 |
| 5:M:210:MET:HE3 | 5:M:210:MET:O | 2.10 | 0.51 |
| 6:A:709:THR:N | 6:A:712:GLU:OE2 | 2.30 | 0.51 |
| 6:A:1173:HIS:NE2 | 6:A:1227:ILE:HA | 2.25 | 0.51 |
| 7:B:254:LEU:HG | 7:B:255:GLN:N | 2.24 | 0.51 |
| 10:F:135:ARG:HD2 | 10:F:143:PHE:CZ | 2.45 | 0.51 |
| 11:H:57:VAL:C | 11:H:143:LEU:HB2 | 2.31 | 0.51 |
| 12:I:26:LEU:HD23 | 12:I:37:GLU:HA | 1.93 | 0.51 |
| 17:O:124:ARG:HH12 | 17:O:577:GLN:HB2 | 1.75 | 0.51 |
| 1:Q:339:ALA:O | 1:Q:343:ARG:HG2 | 2.10 | 0.51 |
| 1:Q:367:ALA:HB3 | 7:B:369:GLY:O | 2.10 | 0.51 |
| 2:R:303:LEU:O | 2:R:307:PHE:N | 2.32 | 0.51 |
| 5:M:280:VAL:HG12 | 5:M:309:ILE:HA | 1.92 | 0.51 |
| 6:A:115:LEU:HD13 | 6:A:141:LEU:HB3 | 1.93 | 0.51 |
| 7:B:371:GLU:H | 7:B:371:GLU:CD | 2.08 | 0.51 |
| 7:B:422:LYS:O | 7:B:425:THR:OG1 | 2.26 | 0.51 |
| 12:I:75:CYS:SG | 12:I:78:CYS:N | 2.83 | 0.51 |
| 17:O:181:LEU:HG | 17:O:192:PRO:HB3 | 1.93 | 0.51 |
| 4:G:98:GLY:HA3 | 4:G:110:VAL:O | 2.11 | 0.51 |
| 6:A:67:CYS:SG | 6:A:80:HIS:HE1 | 2.16 | 0.51 |
| 6:A:1217:LYS:O | 6:A:1221:LYS:HG3 | 2.10 | 0.51 |
| 6:A:1359:ASP:OD1 | 6:A:1361:SER:N | 2.42 | 0.51 |
| 6:A:1444:MET:SD | 10:F:133:VAL:HG22 | 2.50 | 0.51 |
| 7:B:70:ILE:HD12 | 7:B:89:GLU:OE2 | 2.10 | 0.51 |
| 7:B:704:ALA:HB2 | 7:B:738:PHE:CD2 | 2.45 | 0.51 |
| 9:E:45:LYS:HB3 | 9:E:46:TYR:CE2 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:N:12:DG:N2 | 28:T:155:DT:O2 | 2.43 | 0.51 |
| 29:O:115:ILE:HG12 | 29:O:121:MET:HG2 | 1.93 | 0.51 |
| 4:G:131:GLN:HG3 | 4:G:136:VAL:HG22 | 1.92 | 0.51 |
| 5:M:325:ASP:HB3 | 5:M:326:PRO:HD3 | 1.93 | 0.51 |
| 6:A:1442:ASP:CG | 10:F:135:ARG:HA | 2.31 | 0.51 |
| 9:E:83:CYS:SG | 9:E:88:VAL:HG22 | 2.50 | 0.51 |
| 17:O:53:LEU:O | 17:O:57:ILE:N | 2.36 | 0.51 |
| 17:O:307:VAL:HG21 | 17:O:381:LEU:HB3 | 1.93 | 0.51 |
| 17:O:603:ARG:NH2 | 17:O:626:PRO:O | 2.43 | 0.51 |
| 18:4:66:ALA:HA | 18:4:117:ARG:NH2 | 2.25 | 0.51 |
| 18:4:84:LYS:HD3 | 18:4:132:LEU:HB2 | 1.93 | 0.51 |
| 21:7:264:PRO:O | 21:7:268:VAL:N | 2.43 | 0.51 |
| 23:2:92:SER:OG | 23:2:93:SER:N | 2.44 | 0.51 |
| 29:O:144:GLN:NE2 | 29:O:150:ALA:O | 2.43 | 0.51 |
| 3:D:64:VAL:HG22 | 3:D:67:ARG:HH22 | 1.76 | 0.51 |
| 6:A:172:PRO:HB3 | 6:A:185:TRP:CD2 | 2.44 | 0.51 |
| 6:A:596:THR:O | 6:A:598:LEU:N | 2.44 | 0.51 |
| 7:B:102:VAL:O | 7:B:109:THR:HA | 2.10 | 0.51 |
| 7:B:645:SER:HG | 7:B:648:HIS:CG | 2.29 | 0.51 |
| 12:I:19:ASP:OD2 | 12:I:21:GLU:N | 2.35 | 0.51 |
| 17:O:154:GLU:N | 17:O:154:GLU:OE1 | 2.43 | 0.51 |
| 17:O:694:PRO:HG2 | 17:O:697:ILE:HB | 1.92 | 0.51 |
| 3:D:69:ALA:HA | 3:D:72:ARG:HB3 | 1.92 | 0.51 |
| 6:A:771:GLU:O | 6:A:773:LYS:N | 2.39 | 0.51 |
| 8:C:6:PRO:HB2 | 14:K:101:LEU:HG | 1.93 | 0.51 |
| 9:E:88:VAL:HB | 9:E:116:ILE:HD13 | 1.92 | 0.51 |
| 9:E:117:THR:O | 9:E:120:ALA:N | 2.43 | 0.51 |
| 10:F:134:ILE:HG22 | 10:F:135:ARG:H | 1.75 | 0.51 |
| 11:H:57:VAL:HB | 11:H:145:ARG:CA | 2.40 | 0.51 |
| 17:O:643:ARG:HH11 | 17:O:650:GLU:HG3 | 1.75 | 0.51 |
| 25:U:285:TRP:HZ3 | 29:O:110:LYS:HE3 | 1.76 | 0.51 |
| 4:G:118:ASP:OD2 | 4:G:132:SER:OG | 2.26 | 0.51 |
| 5:M:274:PRO:HA | 5:M:277:ILE:HG12 | 1.92 | 0.51 |
| 6:A:226:GLU:OE2 | 6:A:230:ARG:NH2 | 2.42 | 0.51 |
| 6:A:727:ASP:OD1 | 6:A:727:ASP:N | 2.42 | 0.51 |
| 6:A:851:HIS:O | 6:A:854:ASN:N | 2.43 | 0.51 |
| 6:A:857:ARG:HD3 | 6:A:861:GLY:O | 2.11 | 0.51 |
| 7:B:360:PHE:O | 7:B:374:LYS:NZ | 2.37 | 0.51 |
| 11:H:95:TYR:O | 11:H:143:LEU:HD23 | 2.10 | 0.51 |
| 12:I:80:SER:HG | 12:I:82:GLU:H | 1.56 | 0.51 |
| 15:L:61:THR:OG1 | 15:L:63:ARG:HG2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:123:GLU:OE1 | 17:0:125:LYS:N | 2.43 | 0.51 |
| 17:0:227:SER:HG | 17:0:453:PHE:HE1 | 1.59 | 0.51 |
| 17:0:275:ARG:NH2 | 17:0:329:GLU:OE2 | 2.43 | 0.51 |
| 21:7:520:GLU:N | 21:7:681:ARG:HH12 | 2.09 | 0.51 |
| 30:W:112:ASP:HB2 | 30:W:168:LYS:HG3 | 1.93 | 0.51 |
| 4:G:101:VAL:HG13 | 4:G:143:ILE:HD13 | 1.93 | 0.51 |
| 6:A:1233:ASP:OD1 | 6:A:1233:ASP:N | 2.44 | 0.51 |
| 8:C:226:ASP:OD1 | 8:C:227:THR:OG1 | 2.25 | 0.51 |
| 12:I:8:ARG:CZ | 12:I:8:ARG:HB3 | 2.40 | 0.51 |
| 17:0:72:CYS:HB3 | 17:0:210:TYR:CD1 | 2.46 | 0.51 |
| 6:A:335:ARG:HD2 | 7:B:1202:LEU:HD23 | 1.92 | 0.51 |
| 6:A:603:ASN:N | 6:A:603:ASN:OD1 | 2.39 | 0.51 |
| 9:E:90:VAL:HA | 9:E:120:ALA:HB2 | 1.93 | 0.51 |
| 14:K:60:ALA:O | 14:K:73:LEU:HD12 | 2.10 | 0.51 |
| 17:0:502:ASP:OD1 | 17:0:521:ASN:ND2 | 2.44 | 0.51 |
| 18:4:58:ILE:HD12 | 18:4:125:LEU:HD13 | 1.93 | 0.51 |
| 19:6:120:ARG:HG2 | 19:6:309:PRO:HG3 | 1.92 | 0.51 |
| 19:6:159:GLU:O | 19:6:163:GLN:NE2 | 2.44 | 0.51 |
| 20:1:501:UNK:O | 20:1:505:THR:N | 2.32 | 0.51 |
| 21:7:626:PHE:HB2 | 21:7:653:PHE:CD1 | 2.46 | 0.51 |
| 23:2:95:THR:OG1 | 23:2:96:LEU:N | 2.44 | 0.51 |
| 4:G:23:LYS:HA | 4:G:26:LEU:HB2 | 1.93 | 0.50 |
| 6:A:737:LEU:HD13 | 6:A:741:ASN:ND2 | 2.26 | 0.50 |
| 7:B:652:LYS:HE3 | 7:B:689:LEU:HD23 | 1.92 | 0.50 |
| 8:C:35:ARG:HD3 | 14:K:41:THR:OG1 | 2.11 | 0.50 |
| 17:0:120:VAL:HG12 | 17:0:129:VAL:HG13 | 1.93 | 0.50 |
| 29:O:175:LEU:HD12 | 29:O:179:HIS:HB2 | 1.93 | 0.50 |
| 1:Q:133:PHE:CE1 | 1:Q:359:ASN:HB2 | 2.46 | 0.50 |
| 6:A:862:ASN:OD1 | 6:A:862:ASN:N | 2.41 | 0.50 |
| 9:E:59:SER:HG | 9:E:82:PHE:H | 1.53 | 0.50 |
| 18:4:202:SER:HB3 | 19:6:448:LEU:HD21 | 1.92 | 0.50 |
| 18:4:260:PRO:O | 23:2:67:ASN:ND2 | 2.43 | 0.50 |
| 21:7:416:SER:OG | 21:7:661:SER:OG | 2.23 | 0.50 |
| 23:2:25:LEU:HD21 | 23:2:226:PHE:HE2 | 1.75 | 0.50 |
| 6:A:1228:TRP:HB3 | 6:A:1238:ILE:HG23 | 1.92 | 0.50 |
| 7:B:708:GLU:N | 7:B:708:GLU:CD | 2.64 | 0.50 |
| 15:L:38:LEU:HD23 | 15:L:39:SER:N | 2.26 | 0.50 |
| 17:0:495:MET:HB2 | 17:0:680:VAL:HA | 1.91 | 0.50 |
| 18:4:50:ILE:O | 18:4:54:LEU:N | 2.38 | 0.50 |
| 18:4:193:TYR:HE2 | 18:4:274:THR:HG21 | 1.77 | 0.50 |
| 18:4:302:GLY:HA2 | 19:6:319:LEU:HD22 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:477:LEU:HB3 | 21:7:505:ILE:HG12 | 1.94 | 0.50 |
| 21:7:619:ALA:HB3 | 21:7:626:PHE:CG | 2.47 | 0.50 |
| 23:2:457:SER:N | 23:2:493:ILE:O | 2.41 | 0.50 |
| 27:N:11:DA:C5 | 27:N:12:DG:C6 | 2.99 | 0.50 |
| 4:G:97:HIS:CE1 | 30:W:146:GLU:HA | 2.46 | 0.50 |
| 6:A:587:HIS:HA | 6:A:607:ILE:O | 2.11 | 0.50 |
| 7:B:882:THR:O | 7:B:935:ARG:HA | 2.11 | 0.50 |
| 7:B:1107:ALA:O | 7:B:1108:ARG:HB3 | 2.12 | 0.50 |
| 8:C:79:GLN:OE1 | 8:C:79:GLN:N | 2.44 | 0.50 |
| 17:0:310:PRO:HB2 | 17:0:408:LEU:HD21 | 1.93 | 0.50 |
| 17:0:515:ASP:N | 17:0:515:ASP:OD1 | 2.45 | 0.50 |
| 17:0:555:GLN:HE22 | 17:0:564:TRP:HZ2 | 1.60 | 0.50 |
| 18:4:286:GLY:N | 19:6:322:MET:O | 2.44 | 0.50 |
| 19:6:137:LEU:HG | 19:6:204:PRO:HG2 | 1.93 | 0.50 |
| 21:7:564:GLU:OE2 | 21:7:756:ARG:HB2 | 2.11 | 0.50 |
| 1:Q:409:ALA:HB1 | 7:B:323:VAL:CG1 | 2.42 | 0.50 |
| 6:A:75:ASN:HA | 7:B:1116:ARG:HH12 | 1.77 | 0.50 |
| 6:A:164:ARG:O | 6:A:166:GLY:N | 2.42 | 0.50 |
| 7:B:93:GLY:N | 7:B:131:ASP:O | 2.42 | 0.50 |
| 11:H:84:ALA:HA | 11:H:87:ARG:HG2 | 1.94 | 0.50 |
| 17:0:237:ALA:N | 17:0:460:SER:OG | 2.45 | 0.50 |
| 18:4:258:LEU:HB3 | 18:4:260:PRO:HD3 | 1.93 | 0.50 |
| 19:6:266:LEU:HA | 19:6:291:LEU:HG | 1.92 | 0.50 |
| 21:7:385:VAL:HG12 | 21:7:514:THR:HB | 1.93 | 0.50 |
| 28:T:144:DA:H4' | 29:O:125:GLY:HA2 | 1.93 | 0.50 |
| 29:O:133:LYS:HD3 | 29:O:155:PHE:CE2 | 2.47 | 0.50 |
| 3:D:67:ARG:HH11 | 3:D:130:LEU:HD21 | 1.76 | 0.50 |
| 6:A:43:GLU:OE1 | 6:A:43:GLU:N | 2.36 | 0.50 |
| 6:A:1254:ALA:HB1 | 6:A:1256:GLU:HG3 | 1.93 | 0.50 |
| 7:B:327:ARG:O | 7:B:331:LEU:HD12 | 2.11 | 0.50 |
| 7:B:497:ARG:HG2 | 7:B:498:THR:H | 1.76 | 0.50 |
| 11:H:47:PHE:CE1 | 11:H:94:ASP:HB2 | 2.46 | 0.50 |
| 15:L:28:LYS:HG2 | 15:L:29:TYR:CE2 | 2.46 | 0.50 |
| 17:0:166:GLU:HG3 | 17:0:198:ARG:HH21 | 1.76 | 0.50 |
| 18:4:180:THR:OG1 | 18:4:214:LYS:NZ | 2.35 | 0.50 |
| 19:6:427:TYR:N | 19:6:436:PHE:O | 2.44 | 0.50 |
| 21:7:536:TYR:OH | 21:7:542:GLU:OE1 | 2.30 | 0.50 |
| 24:X:162:LEU:O | 24:X:166:LEU:N | 2.45 | 0.50 |
| 28:T:151:DC:H2'' | 28:T:152:DG:H8 | 1.77 | 0.50 |
| 29:O:162:GLY:N | 29:O:214:LEU:O | 2.44 | 0.50 |
| 29:O:178:SER:HB3 | 29:O:237:PHE:CZ | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:76:PHE:HZ | 2:R:120:TYR:HE2 | 1.59 | 0.50 |
| 4:G:100:GLU:HA | 4:G:109:PHE:HA | 1.94 | 0.50 |
| 5:M:57:VAL:HG11 | 7:B:1113:VAL:HG13 | 1.93 | 0.50 |
| 6:A:1130:GLN:HA | 6:A:1133:LEU:HD12 | 1.93 | 0.50 |
| 8:C:145:CYS:SG | 8:C:146:LYS:N | 2.85 | 0.50 |
| 9:E:79:TRP:HD1 | 9:E:96:PHE:HE1 | 1.58 | 0.50 |
| 14:K:14:GLU:OE1 | 14:K:14:GLU:N | 2.45 | 0.50 |
| 15:L:40:LEU:HG | 15:L:41:SER:O | 2.11 | 0.50 |
| 17:O:349:LEU:HD23 | 17:O:349:LEU:H | 1.77 | 0.50 |
| 17:O:360:LEU:HD11 | 17:O:410:SER:HA | 1.93 | 0.50 |
| 18:4:244:LEU:O | 18:4:248:LEU:N | 2.34 | 0.50 |
| 19:6:269:GLN:HG3 | 19:6:288:TYR:CE2 | 2.44 | 0.50 |
| 19:6:403:CYS:SG | 19:6:404:PHE:N | 2.84 | 0.50 |
| 29:O:73:THR:HG23 | 29:O:158:GLN:HG3 | 1.93 | 0.50 |
| 4:G:166:ASP:O | 4:G:168:LEU:HG | 2.12 | 0.50 |
| 5:M:267:LYS:NZ | 29:O:239:LYS:HB2 | 2.27 | 0.50 |
| 7:B:299:GLU:OE2 | 7:B:572:HIS:N | 2.33 | 0.50 |
| 7:B:1051:THR:OG1 | 7:B:1053:GLU:N | 2.45 | 0.50 |
| 9:E:77:SER:HG | 9:E:105:PHE:HD1 | 1.58 | 0.50 |
| 9:E:95:THR:O | 9:E:98:ILE:HG22 | 2.11 | 0.50 |
| 11:H:145:ARG:NH1 | 11:H:146:ARG:NH2 | 2.59 | 0.50 |
| 12:I:98:VAL:HG11 | 12:I:113:ASP:HB2 | 1.94 | 0.50 |
| 17:O:330:HIS:O | 17:O:333:SER:OG | 2.21 | 0.50 |
| 19:6:152:TYR:HD1 | 19:6:298:LYS:HD3 | 1.76 | 0.50 |
| 21:7:594:LEU:O | 21:7:598:HIS:ND1 | 2.45 | 0.50 |
| 21:7:627:ILE:HG12 | 21:7:636:ARG:HG3 | 1.94 | 0.50 |
| 23:2:10:VAL:HG12 | 23:2:205:LEU:HD11 | 1.94 | 0.50 |
| 1:Q:116:THR:O | 1:Q:390:ASP:HB3 | 2.12 | 0.50 |
| 7:B:137:TYR:O | 7:B:140:ILE:HG13 | 2.11 | 0.50 |
| 17:O:509:ARG:HH11 | 17:O:685:ARG:HD3 | 1.77 | 0.50 |
| 23:2:51:VAL:HG13 | 23:2:109:ARG:HD2 | 1.94 | 0.50 |
| 23:2:108:LEU:HG | 23:2:112:LEU:HD13 | 1.94 | 0.50 |
| 30:W:6:ASP:O | 30:W:10:LYS:HG3 | 2.12 | 0.50 |
| 3:D:194:LEU:HD22 | 4:G:86:VAL:HG11 | 1.93 | 0.49 |
| 4:G:35:GLU:OE2 | 4:G:48:VAL:N | 2.39 | 0.49 |
| 4:G:79:PHE:HE2 | 4:G:106:MET:HG2 | 1.77 | 0.49 |
| 5:M:273:SER:O | 5:M:276:THR:HG22 | 2.12 | 0.49 |
| 6:A:249:SER:O | 6:A:249:SER:OG | 2.27 | 0.49 |
| 6:A:269:ILE:HD11 | 6:A:300:VAL:HA | 1.94 | 0.49 |
| 6:A:390:GLN:O | 6:A:393:ARG:HB3 | 2.12 | 0.49 |
| 6:A:1364:ASN:OD1 | 6:A:1365:TYR:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:363:HIS:CG | 7:B:363:HIS:O | 2.64 | 0.49 |
| 7:B:1074:ASN:HB2 | 7:B:1081:LEU:HD21 | 1.94 | 0.49 |
| 7:B:1179:GLN:HB3 | 7:B:1181:GLU:OE2 | 2.12 | 0.49 |
| 9:E:60:PHE:CZ | 9:E:80:VAL:HG21 | 2.47 | 0.49 |
| 11:H:23:VAL:HA | 11:H:42:ILE:O | 2.11 | 0.49 |
| 12:I:19:ASP:OD2 | 12:I:23:ASN:N | 2.34 | 0.49 |
| 12:I:80:SER:OG | 12:I:82:GLU:OE1 | 2.23 | 0.49 |
| 15:L:47:ARG:HH22 | 15:L:54:ARG:CZ | 2.25 | 0.49 |
| 17:O:239:ASN:OD1 | 17:O:664:GLN:NE2 | 2.45 | 0.49 |
| 21:7:302:GLU:HG2 | 21:7:322:SER:HB2 | 1.94 | 0.49 |
| 21:7:759:LEU:O | 21:7:763:VAL:HG23 | 2.12 | 0.49 |
| 4:G:151:ILE:HB | 4:G:158:HIS:HB2 | 1.93 | 0.49 |
| 5:M:157:CYS:C | 5:M:159:ASP:H | 2.15 | 0.49 |
| 6:A:1163:ILE:HG22 | 6:A:1165:GLU:H | 1.76 | 0.49 |
| 6:A:1205:LYS:O | 6:A:1274:ARG:NH1 | 2.45 | 0.49 |
| 9:E:76:GLY:H | 9:E:106:GLN:HG2 | 1.77 | 0.49 |
| 9:E:79:TRP:HB2 | 9:E:105:PHE:CD2 | 2.47 | 0.49 |
| 15:L:47:ARG:HH12 | 15:L:54:ARG:NE | 2.10 | 0.49 |
| 21:7:589:GLN:HB3 | 21:7:745:ILE:HD11 | 1.94 | 0.49 |
| 21:7:684:ALA:HB2 | 21:7:725:PHE:HZ | 1.77 | 0.49 |
| 23:2:208:LEU:HD13 | 23:2:222:LEU:HD21 | 1.93 | 0.49 |
| 23:2:405:HIS:O | 23:2:408:MET:N | 2.45 | 0.49 |
| 6:A:594:GLY:O | 6:A:596:THR:HG23 | 2.12 | 0.49 |
| 6:A:943:LEU:O | 6:A:946:VAL:N | 2.45 | 0.49 |
| 7:B:183:GLU:OE1 | 7:B:184:ALA:N | 2.44 | 0.49 |
| 7:B:576:ASP:OD1 | 7:B:576:ASP:N | 2.42 | 0.49 |
| 8:C:264:GLN:O | 8:C:267:GLN:HB3 | 2.12 | 0.49 |
| 17:O:270:ARG:CZ | 17:O:390:VAL:HA | 2.42 | 0.49 |
| 17:O:564:TRP:CD2 | 20:1:239:PRO:HG3 | 2.46 | 0.49 |
| 27:N:12:DG:C5 | 27:N:13:DG:C6 | 3.00 | 0.49 |
| 30:W:140:LEU:HB2 | 30:W:147:PHE:HD1 | 1.76 | 0.49 |
| 1:Q:124:LYS:O | 1:Q:126:LYS:NZ | 2.28 | 0.49 |
| 2:R:98:ASN:OD1 | 2:R:103:LYS:HE3 | 2.12 | 0.49 |
| 3:D:24:ALA:N | 3:D:28:GLN:HB2 | 2.27 | 0.49 |
| 4:G:14:HIS:HB3 | 4:G:17:PHE:HE1 | 1.77 | 0.49 |
| 4:G:108:VAL:HG22 | 4:G:159:ALA:HB3 | 1.94 | 0.49 |
| 6:A:607:ILE:HG23 | 6:A:612:ILE:HA | 1.94 | 0.49 |
| 6:A:917:SER:OG | 6:A:918:GLU:N | 2.46 | 0.49 |
| 12:I:77:LYS:HG3 | 12:I:108:HIS:CD2 | 2.47 | 0.49 |
| 18:4:55:GLU:HA | 18:4:58:ILE:HB | 1.93 | 0.49 |
| 1:Q:343:ARG:NE | 1:Q:343:ARG:HA | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Q:405:THR:O | 1:Q:408:GLU:N | 2.46 | 0.49 |
| 6:A:425:GLN:O | 6:A:427:GLN:NE2 | 2.45 | 0.49 |
| 6:A:463:ILE:HD11 | 6:A:469:ARG:HG3 | 1.95 | 0.49 |
| 6:A:810:PRO:HG3 | 7:B:1047:PHE:CD1 | 2.47 | 0.49 |
| 6:A:982:THR:OG1 | 6:A:983:ILE:N | 2.44 | 0.49 |
| 7:B:994:TYR:HB2 | 7:B:999:MET:SD | 2.52 | 0.49 |
| 9:E:78:LEU:HD12 | 9:E:107:THR:O | 2.12 | 0.49 |
| 12:I:99:LEU:HB2 | 12:I:112:SER:HB3 | 1.95 | 0.49 |
| 15:L:28:LYS:HG2 | 15:L:29:TYR:CD2 | 2.47 | 0.49 |
| 17:0:619:THR:HG22 | 17:0:678:VAL:HB | 1.94 | 0.49 |
| 21:7:406:SER:HB3 | 21:7:482:TRP:CE3 | 2.48 | 0.49 |
| 26:V:60:LEU:HA | 26:V:86:THR:O | 2.12 | 0.49 |
| 29:O:185:TYR:CG | 29:O:187:PRO:HD3 | 2.48 | 0.49 |
| 29:O:204:LEU:HD23 | 29:O:214:LEU:HD11 | 1.92 | 0.49 |
| 3:D:61:GLU:O | 3:D:64:VAL:HB | 2.12 | 0.49 |
| 4:G:46:LEU:HD21 | 4:G:79:PHE:HB3 | 1.94 | 0.49 |
| 5:M:189:PHE:N | 29:O:188:GLU:OE1 | 2.37 | 0.49 |
| 6:A:515:GLN:HG2 | 6:A:516:SER:OG | 2.12 | 0.49 |
| 6:A:766:GLY:HA2 | 6:A:799:PHE:CE1 | 2.47 | 0.49 |
| 7:B:908:GLU:OE1 | 7:B:908:GLU:N | 2.45 | 0.49 |
| 7:B:1101:ASP:N | 7:B:1101:ASP:OD1 | 2.42 | 0.49 |
| 11:H:9:ILE:HD11 | 11:H:31:THR:HG21 | 1.95 | 0.49 |
| 11:H:84:ALA:H | 14:K:54:ARG:HH12 | 1.59 | 0.49 |
| 12:I:54:GLU:OE1 | 12:I:120:GLN:HA | 2.13 | 0.49 |
| 17:0:161:ASN:ND2 | 17:0:189:THR:O | 2.46 | 0.49 |
| 21:7:606:ILE:HA | 21:7:652:ILE:HG13 | 1.95 | 0.49 |
| 23:2:485:ASP:OD1 | 23:2:485:ASP:N | 2.45 | 0.49 |
| 29:O:184:SER:H | 29:O:193:LEU:HG | 1.78 | 0.49 |
| 1:Q:116:THR:HA | 2:R:136:THR:HG22 | 1.93 | 0.49 |
| 2:R:307:PHE:O | 2:R:311:ASP:N | 2.45 | 0.49 |
| 6:A:457:ALA:HB3 | 6:A:506:ALA:HA | 1.93 | 0.49 |
| 7:B:27:ALA:O | 7:B:30:SER:OG | 2.29 | 0.49 |
| 15:L:62:LYS:H | 15:L:63:ARG:HH12 | 1.60 | 0.49 |
| 17:0:312:LEU:O | 17:0:314:GLN:N | 2.44 | 0.49 |
| 17:0:318:THR:H | 17:0:375:ARG:HH11 | 1.60 | 0.49 |
| 17:0:564:TRP:CE2 | 20:1:239:PRO:HG3 | 2.47 | 0.49 |
| 21:7:564:GLU:O | 21:7:568:GLU:N | 2.42 | 0.49 |
| 3:D:49:ALA:O | 3:D:50:LEU:HD23 | 2.13 | 0.49 |
| 4:G:65:ASP:OD1 | 4:G:65:ASP:N | 2.46 | 0.49 |
| 5:M:126:VAL:HG13 | 5:M:154:TYR:HE2 | 1.76 | 0.49 |
| 6:A:870:GLU:O | 9:E:205:SER:OG | 2.14 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1436:ILE:O | 6:A:1437:GLY:C | 2.51 | 0.49 |
| 7:B:643:ASP:OD2 | 7:B:654:ARG:NH2 | 2.29 | 0.49 |
| 17:O:211:HIS:O | 17:O:215:ASP:N | 2.38 | 0.49 |
| 21:7:438:PHE:HB3 | 21:7:459:MET:HG3 | 1.94 | 0.49 |
| 29:O:169:PRO:HA | 29:O:208:VAL:O | 2.13 | 0.49 |
| 4:G:65:ASP:O | 4:G:67:SER:N | 2.46 | 0.49 |
| 6:A:741:ASN:HD22 | 6:A:744:LYS:HB2 | 1.78 | 0.49 |
| 6:A:1218:GLN:O | 6:A:1221:LYS:NZ | 2.46 | 0.49 |
| 7:B:307:ASP:O | 7:B:310:MET:N | 2.45 | 0.49 |
| 9:E:185:ALA:O | 9:E:189:GLY:N | 2.46 | 0.49 |
| 14:K:10:PHE:HA | 14:K:37:LYS:HB3 | 1.94 | 0.49 |
| 21:7:659:ASP:HB3 | 21:7:660:THR:HG22 | 1.95 | 0.49 |
| 25:U:253:ARG:HA | 25:U:257:ARG:O | 2.12 | 0.49 |
| 28:T:17:DG:H2' | 28:T:18:DA:C4 | 2.47 | 0.49 |
| 4:G:7:LEU:HB2 | 4:G:74:TYR:CZ | 2.48 | 0.49 |
| 5:M:180:CYS:SG | 5:M:181:ARG:N | 2.86 | 0.49 |
| 5:M:244:SER:CB | 7:B:108:VAL:HA | 2.43 | 0.49 |
| 6:A:36:ARG:O | 6:A:270:LEU:HD21 | 2.12 | 0.49 |
| 6:A:316:GLN:O | 6:A:318:SER:N | 2.45 | 0.49 |
| 7:B:1122:ARG:HG3 | 7:B:1123:SER:N | 2.26 | 0.49 |
| 7:B:1175:LEU:C | 7:B:1177:HIS:H | 2.16 | 0.49 |
| 8:C:91:HIS:HA | 8:C:95:CYS:SG | 2.53 | 0.49 |
| 9:E:67:GLU:O | 9:E:70:SER:OG | 2.25 | 0.49 |
| 19:6:129:THR:HG22 | 19:6:172:ILE:HD12 | 1.95 | 0.49 |
| 22:5:9:LEU:HD21 | 22:5:39:HIS:HD2 | 1.77 | 0.49 |
| 30:W:152:CYS:O | 30:W:154:GLU:HG3 | 2.13 | 0.49 |
| 1:Q:337:GLU:OE1 | 1:Q:339:ALA:N | 2.44 | 0.48 |
| 1:Q:377:SER:HB3 | 1:Q:385:THR:N | 2.16 | 0.48 |
| 2:R:220:HIS:CG | 2:R:221:GLU:N | 2.81 | 0.48 |
| 6:A:924:LYS:HE3 | 6:A:984:LYS:HZ2 | 1.77 | 0.48 |
| 6:A:1072:ILE:O | 6:A:1075:PRO:HD2 | 2.13 | 0.48 |
| 6:A:1225:PHE:CE2 | 6:A:1227:ILE:HD11 | 2.48 | 0.48 |
| 8:C:81:GLU:HG3 | 8:C:85:ASP:HB2 | 1.95 | 0.48 |
| 12:I:113:ASP:OD2 | 12:I:115:LYS:N | 2.46 | 0.48 |
| 17:O:294:HIS:ND1 | 17:O:383:LEU:HD12 | 2.28 | 0.48 |
| 17:O:473:LEU:HB2 | 17:O:475:PHE:CD1 | 2.48 | 0.48 |
| 27:N:15:DG:N2 | 28:T:152:DG:O4' | 2.45 | 0.48 |
| 1:Q:120:LYS:HG3 | 1:Q:393:TYR:O | 2.13 | 0.48 |
| 6:A:39:GLU:OE2 | 6:A:50:ILE:HG21 | 2.12 | 0.48 |
| 6:A:404:TYR:HB2 | 6:A:433:GLU:HG3 | 1.95 | 0.48 |
| 6:A:786:HIS:CD2 | 6:A:786:HIS:H | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1198:ASP:OD2 | 6:A:1201:ALA:N | 2.39 | 0.48 |
| 7:B:345:LYS:HA | 7:B:347:LYS:H | 1.78 | 0.48 |
| 12:I:18:GLU:O | 12:I:20:LYS:HE3 | 2.14 | 0.48 |
| 17:O:512:ILE:O | 17:O:513:ARG:NE | 2.43 | 0.48 |
| 17:O:690:ARG:HG3 | 17:O:701:LEU:HD23 | 1.94 | 0.48 |
| 21:7:354:ILE:HD12 | 21:7:404:LYS:HA | 1.95 | 0.48 |
| 26:V:82:ASN:HA | 26:V:109:ASP:HA | 1.93 | 0.48 |
| 29:O:196:ARG:HA | 29:O:203:VAL:HA | 1.95 | 0.48 |
| 1:Q:104:ARG:NH2 | 1:Q:105:ALA:HB3 | 2.28 | 0.48 |
| 3:D:159:THR:O | 3:D:163:VAL:HG23 | 2.13 | 0.48 |
| 6:A:332:LYS:O | 6:A:333:GLU:HB2 | 2.13 | 0.48 |
| 7:B:168:GLY:H | 7:B:450:ALA:HB1 | 1.79 | 0.48 |
| 11:H:96:VAL:HG22 | 11:H:143:LEU:HD21 | 1.94 | 0.48 |
| 12:I:54:GLU:N | 12:I:120:GLN:OE1 | 2.45 | 0.48 |
| 13:J:32:GLU:HA | 13:J:35:ALA:HB3 | 1.95 | 0.48 |
| 17:O:76:MET:HB3 | 17:O:178:PHE:HE2 | 1.78 | 0.48 |
| 17:O:232:VAL:HG21 | 17:O:453:PHE:CD2 | 2.48 | 0.48 |
| 17:O:252:LEU:HB2 | 17:O:435:MET:HB2 | 1.95 | 0.48 |
| 23:2:475:ALA:O | 23:2:479:GLY:N | 2.43 | 0.48 |
| 27:N:21:DA:H4' | 29:O:203:VAL:HG11 | 1.95 | 0.48 |
| 1:Q:375:LEU:HD21 | 2:R:68:VAL:HG21 | 1.94 | 0.48 |
| 5:M:129:ALA:O | 5:M:133:ILE:HB | 2.12 | 0.48 |
| 6:A:1163:ILE:HD12 | 6:A:1163:ILE:H | 1.78 | 0.48 |
| 7:B:40:GLU:OE2 | 7:B:681:TRP:HD1 | 1.96 | 0.48 |
| 7:B:643:ASP:O | 7:B:645:SER:N | 2.47 | 0.48 |
| 10:F:135:ARG:HD2 | 10:F:143:PHE:CD1 | 2.48 | 0.48 |
| 11:H:34:ASP:OD2 | 11:H:34:ASP:N | 2.45 | 0.48 |
| 17:O:190:LEU:HD12 | 17:O:195:ILE:HD11 | 1.94 | 0.48 |
| 17:O:244:CYS:O | 17:O:247:SER:OG | 2.30 | 0.48 |
| 21:7:414:SER:HB2 | 21:7:439:THR:HG23 | 1.95 | 0.48 |
| 21:7:555:ALA:N | 21:7:705:PHE:O | 2.46 | 0.48 |
| 23:2:53:ASN:ND2 | 23:2:55:ASN:OD1 | 2.47 | 0.48 |
| 29:O:114:LEU:HB2 | 29:O:122:VAL:HB | 1.96 | 0.48 |
| 4:G:151:ILE:N | 4:G:158:HIS:O | 2.40 | 0.48 |
| 5:M:185:VAL:HG22 | 7:B:106:ASP:HB2 | 1.95 | 0.48 |
| 6:A:286:HIS:O | 6:A:287:HIS:ND1 | 2.36 | 0.48 |
| 6:A:446:ARG:NH1 | 6:A:479:ASN:O | 2.46 | 0.48 |
| 6:A:1445:ILE:CB | 10:F:133:VAL:HG23 | 2.43 | 0.48 |
| 7:B:564:GLU:OE1 | 7:B:591:ARG:NE | 2.46 | 0.48 |
| 11:H:58:THR:O | 11:H:143:LEU:HD12 | 2.13 | 0.48 |
| 14:K:13:GLY:H | 14:K:16:GLU:HB2 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:407:VAL:HG13 | 21:7:484:PHE:HB3 | 1.94 | 0.48 |
| 24:X:214:TRP:HD1 | 24:X:217:CYS:SG | 2.37 | 0.48 |
| 3:D:71:LYS:O | 3:D:75:LYS:HG3 | 2.13 | 0.48 |
| 4:G:102:GLN:HA | 4:G:107:LYS:HA | 1.94 | 0.48 |
| 5:M:241:ARG:O | 5:M:245:HIS:ND1 | 2.47 | 0.48 |
| 6:A:896:ARG:HD2 | 6:A:897:TYR:CE2 | 2.49 | 0.48 |
| 6:A:1012:ARG:HB2 | 6:A:1012:ARG:CZ | 2.44 | 0.48 |
| 6:A:1198:ASP:OD1 | 6:A:1200:ALA:N | 2.46 | 0.48 |
| 9:E:56:LYS:HZ3 | 9:E:83:CYS:HA | 1.77 | 0.48 |
| 17:0:83:LEU:HB3 | 17:0:177:SER:HA | 1.96 | 0.48 |
| 17:0:244:CYS:HB2 | 17:0:442:ALA:HB1 | 1.95 | 0.48 |
| 17:0:431:PRO:HG3 | 24:X:252:LEU:HG | 1.96 | 0.48 |
| 17:0:496:ILE:HG12 | 17:0:701:LEU:HD11 | 1.96 | 0.48 |
| 21:7:579:LEU:HD22 | 21:7:611:ASN:ND2 | 2.28 | 0.48 |
| 23:2:223:HIS:O | 23:2:227:MET:N | 2.47 | 0.48 |
| 1:Q:398:ARG:HD3 | 7:B:326:ASP:OD2 | 2.13 | 0.48 |
| 4:G:21:ARG:HD2 | 4:G:25:TYR:CE2 | 2.48 | 0.48 |
| 5:M:211:LYS:NZ | 29:O:176:ALA:HB1 | 2.29 | 0.48 |
| 5:M:277:ILE:HA | 5:M:280:VAL:HG22 | 1.96 | 0.48 |
| 6:A:39:GLU:CG | 6:A:50:ILE:HD13 | 2.43 | 0.48 |
| 6:A:353:ILE:HG21 | 6:A:487:MET:SD | 2.53 | 0.48 |
| 6:A:1435:PRO:HA | 6:A:1439:GLY:O | 2.14 | 0.48 |
| 7:B:405:ARG:O | 7:B:406:LEU:HD23 | 2.14 | 0.48 |
| 7:B:586:TRP:NE1 | 7:B:588:GLY:O | 2.34 | 0.48 |
| 7:B:1009:ASP:OD1 | 7:B:1009:ASP:N | 2.34 | 0.48 |
| 11:H:33:GLN:HG3 | 11:H:129:TYR:CE1 | 2.49 | 0.48 |
| 11:H:81:PRO:O | 11:H:83:GLN:N | 2.47 | 0.48 |
| 17:0:537:MET:HB2 | 17:0:597:ILE:HG12 | 1.96 | 0.48 |
| 20:1:597:PHE:HE2 | 20:1:620:LEU:HD13 | 1.78 | 0.48 |
| 21:7:341:TYR:N | 21:7:379:ALA:O | 2.47 | 0.48 |
| 21:7:396:GLY:O | 21:7:400:ALA:N | 2.41 | 0.48 |
| 21:7:616:GLN:HE21 | 21:7:628:TYR:HD2 | 1.62 | 0.48 |
| 26:V:62:VAL:HG22 | 26:V:85:VAL:HG22 | 1.94 | 0.48 |
| 26:V:74:ASP:HB3 | 26:V:117:ASN:HB2 | 1.95 | 0.48 |
| 28:T:143:DT:O2 | 29:O:114:LEU:HD11 | 2.14 | 0.48 |
| 29:O:141:ARG:O | 29:O:145:LYS:N | 2.46 | 0.48 |
| 30:W:131:TYR:HD1 | 30:W:135:GLU:HB3 | 1.79 | 0.48 |
| 3:D:50:LEU:O | 4:G:2:PHE:HB2 | 2.14 | 0.48 |
| 4:G:7:LEU:N | 4:G:74:TYR:O | 2.40 | 0.48 |
| 4:G:148:GLU:N | 4:G:160:ILE:O | 2.33 | 0.48 |
| 6:A:151:ASP:HB3 | 6:A:163:SER:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:408:ASP:N | 6:A:408:ASP:OD1 | 2.44 | 0.48 |
| 6:A:408:ASP:O | 6:A:409:SER:OG | 2.20 | 0.48 |
| 6:A:678:GLU:HG2 | 6:A:732:LEU:HD13 | 1.96 | 0.48 |
| 6:A:1089:VAL:HG12 | 6:A:1091:SER:HB3 | 1.95 | 0.48 |
| 7:B:37:PHE:CD2 | 7:B:38:PHE:N | 2.81 | 0.48 |
| 7:B:569:TYR:CE2 | 7:B:571:PRO:HG3 | 2.49 | 0.48 |
| 17:0:85:GLU:O | 17:0:89:LEU:HD13 | 2.13 | 0.48 |
| 18:4:28:VAL:O | 18:4:76:ILE:N | 2.40 | 0.48 |
| 18:4:67:PHE:CE1 | 23:2:44:LYS:HB3 | 2.48 | 0.48 |
| 1:Q:364:SER:N | 1:Q:394:LYS:O | 2.46 | 0.48 |
| 4:G:114:LEU:HD23 | 4:G:161:GLY:O | 2.13 | 0.48 |
| 6:A:1139:GLU:O | 6:A:1275:GLY:HA3 | 2.13 | 0.48 |
| 6:A:1239:ARG:HH22 | 6:A:1241:ARG:HH22 | 1.60 | 0.48 |
| 7:B:275:TYR:O | 7:B:276:ILE:HD13 | 2.14 | 0.48 |
| 7:B:1051:THR:O | 7:B:1055:ILE:HG13 | 2.14 | 0.48 |
| 8:C:163:ILE:HG13 | 8:C:165:LYS:H | 1.78 | 0.48 |
| 11:H:56:THR:HB | 11:H:93:TYR:CD1 | 2.47 | 0.48 |
| 18:4:246:GLN:HG3 | 20:1:503:VAL:HG11 | 1.94 | 0.48 |
| 20:1:557:CYS:HG | 20:1:585:HIS:CD2 | 2.29 | 0.48 |
| 23:2:17:ILE:O | 23:2:22:GLN:NE2 | 2.46 | 0.48 |
| 24:X:266:VAL:HG21 | 30:W:101:LYS:HG2 | 1.96 | 0.48 |
| 25:U:285:TRP:CH2 | 29:O:105:ARG:HB3 | 2.49 | 0.48 |
| 27:N:22:DT:OP2 | 29:O:196:ARG:NH1 | 2.46 | 0.48 |
| 2:R:121:ASP:N | 2:R:225:MET:O | 2.36 | 0.48 |
| 3:D:40:HIS:CE1 | 4:G:74:TYR:N | 2.82 | 0.48 |
| 6:A:443:LEU:HD21 | 6:A:455:MET:HE2 | 1.96 | 0.48 |
| 6:A:483:ASP:O | 31:P:10:A:H5'' | 2.13 | 0.48 |
| 6:A:926:GLN:NE2 | 6:A:926:GLN:O | 2.46 | 0.48 |
| 7:B:128:LEU:HA | 7:B:128:LEU:HD23 | 1.53 | 0.48 |
| 7:B:603:LEU:HD23 | 7:B:603:LEU:HA | 1.58 | 0.48 |
| 8:C:186:LEU:HB3 | 8:C:188:HIS:CD2 | 2.49 | 0.48 |
| 17:0:346:MET:SD | 17:0:433:PRO:HG2 | 2.54 | 0.48 |
| 17:0:369:ILE:HG21 | 17:0:374:LEU:HD13 | 1.95 | 0.48 |
| 28:T:24:DT:H4' | 31:P:6:G:O6 | 2.13 | 0.48 |
| 1:Q:119:LEU:HD11 | 2:R:135:PHE:HB3 | 1.95 | 0.47 |
| 3:D:119:ARG:HB3 | 3:D:155:ARG:HH12 | 1.78 | 0.47 |
| 5:M:257:GLU:OE1 | 5:M:258:TYR:N | 2.47 | 0.47 |
| 5:M:294:THR:O | 5:M:296:ALA:N | 2.47 | 0.47 |
| 6:A:50:ILE:C | 6:A:52:GLY:H | 2.18 | 0.47 |
| 6:A:346:ASP:OD1 | 6:A:346:ASP:N | 2.46 | 0.47 |
| 6:A:446:ARG:HB2 | 6:A:487:MET:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:784:LEU:HD23 | 6:A:784:LEU:HA | 1.71 | 0.47 |
| 6:A:961:ARG:O | 6:A:965:GLN:HG2 | 2.14 | 0.47 |
| 6:A:1134:ILE:HD13 | 6:A:1322:ILE:HG22 | 1.96 | 0.47 |
| 7:B:875:GLU:OE2 | 7:B:915:THR:OG1 | 2.18 | 0.47 |
| 8:C:99:LEU:HD13 | 8:C:120:ILE:HA | 1.96 | 0.47 |
| 21:7:568:GLU:OE1 | 21:7:571:ARG:NH1 | 2.41 | 0.47 |
| 23:2:62:LEU:HA | 23:2:65:TRP:CD1 | 2.48 | 0.47 |
| 30:W:11:ASN:HA | 30:W:14:LYS:HD2 | 1.96 | 0.47 |
| 4:G:37:SER:O | 4:G:44:TYR:HA | 2.14 | 0.47 |
| 4:G:131:GLN:HG3 | 4:G:136:VAL:HG13 | 1.95 | 0.47 |
| 6:A:672:ASP:OD1 | 6:A:674:PRO:HD2 | 2.14 | 0.47 |
| 7:B:556:THR:O | 7:B:559:SER:OG | 2.30 | 0.47 |
| 7:B:834:ASN:HB3 | 7:B:840:ILE:HG13 | 1.95 | 0.47 |
| 7:B:1164:GLY:HA3 | 7:B:1190:ASP:OD2 | 2.14 | 0.47 |
| 11:H:55:LEU:HB2 | 11:H:144:ILE:O | 2.13 | 0.47 |
| 11:H:102:TYR:CZ | 11:H:115:TYR:HB3 | 2.49 | 0.47 |
| 11:H:116:TYR:HB2 | 11:H:123:MET:HE3 | 1.94 | 0.47 |
| 17:0:74:ARG:NH1 | 17:0:664:GLN:OE1 | 2.38 | 0.47 |
| 17:0:673:LYS:NZ | 17:0:737:SER:O | 2.40 | 0.47 |
| 18:4:71:ASN:OD1 | 18:4:71:ASN:N | 2.44 | 0.47 |
| 21:7:609:SER:O | 21:7:655:SER:HA | 2.14 | 0.47 |
| 1:Q:139:LEU:HD23 | 2:R:212:THR:HG21 | 1.97 | 0.47 |
| 2:R:76:PHE:HZ | 2:R:120:TYR:CE2 | 2.32 | 0.47 |
| 3:D:35:LEU:HG | 3:D:36:LYS:HG3 | 1.96 | 0.47 |
| 3:D:147:TYR:HB2 | 4:G:104:GLY:HA2 | 1.95 | 0.47 |
| 5:M:242:PHE:HB3 | 5:M:302:LEU:HD21 | 1.96 | 0.47 |
| 6:A:567:LYS:CB | 11:H:96:VAL:H | 2.22 | 0.47 |
| 6:A:885:THR:O | 6:A:940:ARG:NH1 | 2.42 | 0.47 |
| 6:A:1196:GLU:HA | 6:A:1236:LEU:O | 2.14 | 0.47 |
| 7:B:57:TYR:CD1 | 7:B:57:TYR:N | 2.83 | 0.47 |
| 7:B:770:GLN:HB2 | 7:B:984:HIS:O | 2.14 | 0.47 |
| 7:B:899:ILE:HD11 | 7:B:911:ILE:HA | 1.96 | 0.47 |
| 8:C:162:GLY:HA3 | 8:C:170:TRP:CE2 | 2.49 | 0.47 |
| 8:C:181:ASP:OD1 | 8:C:184:ASN:N | 2.46 | 0.47 |
| 14:K:99:GLY:O | 14:K:103:THR:HG23 | 2.15 | 0.47 |
| 17:0:726:GLN:HA | 19:6:290:ILE:HG12 | 1.96 | 0.47 |
| 19:6:129:THR:N | 19:6:233:LEU:O | 2.44 | 0.47 |
| 20:1:184:LEU:HD21 | 20:1:216:LEU:HB3 | 1.97 | 0.47 |
| 20:1:222:LEU:O | 20:1:226:GLN:N | 2.48 | 0.47 |
| 20:1:562:LYS:O | 20:1:566:ILE:N | 2.41 | 0.47 |
| 21:7:599:GLU:HG2 | 21:7:650:ASN:HD22 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:U:285:TRP:CZ3 | 29:O:110:LYS:HE3 | 2.50 | 0.47 |
| 29:O:159:ASN:ND2 | 29:O:161:VAL:HG22 | 2.29 | 0.47 |
| 1:Q:120:LYS:NZ | 1:Q:366:GLU:OE2 | 2.47 | 0.47 |
| 3:D:156:ASP:N | 3:D:156:ASP:OD1 | 2.46 | 0.47 |
| 3:D:158:GLU:OE1 | 3:D:158:GLU:N | 2.42 | 0.47 |
| 6:A:1207:LEU:HA | 6:A:1211:GLN:HE22 | 1.80 | 0.47 |
| 7:B:329:THR:O | 7:B:332:ASP:HB3 | 2.14 | 0.47 |
| 7:B:790:ASP:N | 7:B:790:ASP:OD1 | 2.44 | 0.47 |
| 7:B:1162:ILE:HA | 7:B:1162:ILE:HD13 | 1.60 | 0.47 |
| 9:E:93:MET:HE1 | 9:E:123:LEU:HD23 | 1.96 | 0.47 |
| 15:L:28:LYS:HB3 | 15:L:39:SER:HA | 1.97 | 0.47 |
| 17:O:333:SER:HB2 | 17:O:337:ARG:HH22 | 1.80 | 0.47 |
| 17:O:436:ARG:NE | 17:O:634:ILE:HG21 | 2.28 | 0.47 |
| 17:O:687:SER:HA | 17:O:706:LEU:HD12 | 1.96 | 0.47 |
| 20:1:593:LEU:HA | 20:1:596:LEU:HB2 | 1.95 | 0.47 |
| 1:Q:123:SER:HB3 | 1:Q:361:TRP:CH2 | 2.50 | 0.47 |
| 2:R:223:GLN:HG2 | 2:R:224:VAL:N | 2.30 | 0.47 |
| 3:D:140:ASP:HA | 3:D:143:ASN:ND2 | 2.30 | 0.47 |
| 4:G:81:PRO:HG3 | 4:G:106:MET:SD | 2.54 | 0.47 |
| 5:M:267:LYS:HA | 5:M:270:ALA:HB3 | 1.96 | 0.47 |
| 6:A:217:LYS:NZ | 6:A:221:SER:OG | 2.45 | 0.47 |
| 6:A:396:PRO:HG3 | 6:A:416:ARG:HG2 | 1.97 | 0.47 |
| 6:A:439:ASN:HA | 6:A:459:ARG:HB3 | 1.96 | 0.47 |
| 7:B:955:THR:HB | 15:L:55:ILE:HG22 | 1.96 | 0.47 |
| 9:E:78:LEU:HD11 | 9:E:109:ILE:HG12 | 1.97 | 0.47 |
| 12:I:51:ASN:HB3 | 12:I:118:ARG:CZ | 2.44 | 0.47 |
| 13:J:53:HIS:CD2 | 13:J:54:VAL:H | 2.32 | 0.47 |
| 17:O:325:ILE:HG22 | 17:O:331:PHE:HA | 1.95 | 0.47 |
| 17:O:476:LYS:NZ | 17:O:478:VAL:HG22 | 2.29 | 0.47 |
| 18:4:288:ILE:HD11 | 18:4:293:LEU:HD13 | 1.95 | 0.47 |
| 22:5:9:LEU:HD21 | 22:5:39:HIS:CD2 | 2.49 | 0.47 |
| 29:O:72:ALA:O | 29:O:123:VAL:N | 2.28 | 0.47 |
| 30:W:64:ASP:OD1 | 30:W:101:LYS:NZ | 2.48 | 0.47 |
| 30:W:184:ASP:OD1 | 30:W:187:LYS:NZ | 2.37 | 0.47 |
| 2:R:81:TRP:N | 2:R:81:TRP:CD1 | 2.81 | 0.47 |
| 3:D:119:ARG:HD2 | 3:D:155:ARG:NH2 | 2.25 | 0.47 |
| 5:M:249:PRO:HB2 | 5:M:251:GLN:NE2 | 2.29 | 0.47 |
| 6:A:24:PRO:HD2 | 6:A:233:TRP:CD1 | 2.50 | 0.47 |
| 6:A:251:SER:HA | 6:A:257:ARG:HA | 1.96 | 0.47 |
| 6:A:446:ARG:HD2 | 6:A:480:ALA:HB2 | 1.95 | 0.47 |
| 7:B:585:VAL:HB | 7:B:587:HIS:CE1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:984:HIS:CD2 | 7:B:984:HIS:N | 2.83 | 0.47 |
| 9:E:45:LYS:HB3 | 9:E:46:TYR:CD2 | 2.49 | 0.47 |
| 11:H:30:SER:HB3 | 11:H:36:CYS:O | 2.15 | 0.47 |
| 12:I:51:ASN:HD22 | 12:I:118:ARG:HH12 | 1.62 | 0.47 |
| 17:0:37:ASN:ND2 | 17:0:476:LYS:O | 2.47 | 0.47 |
| 17:0:643:ARG:HD2 | 17:0:650:GLU:HG3 | 1.97 | 0.47 |
| 19:6:171:ILE:HG21 | 19:6:196:LEU:HD11 | 1.95 | 0.47 |
| 20:1:491:UNK:O | 20:1:493:UNK:N | 2.47 | 0.47 |
| 21:7:206:ALA:O | 21:7:210:ILE:N | 2.32 | 0.47 |
| 21:7:510:LYS:HE3 | 21:7:531:ILE:HG12 | 1.96 | 0.47 |
| 21:7:527:LEU:HA | 21:7:530:LEU:HB2 | 1.97 | 0.47 |
| 21:7:607:VAL:HA | 21:7:671:ILE:HB | 1.97 | 0.47 |
| 24:X:252:LEU:HB3 | 30:W:19:GLY:HA2 | 1.96 | 0.47 |
| 24:X:263:TRP:CZ3 | 30:W:179:ILE:HD11 | 2.49 | 0.47 |
| 27:N:17:DG:C4 | 27:N:18:DT:C4 | 3.03 | 0.47 |
| 1:Q:106:ILE:HD13 | 1:Q:385:THR:HG21 | 1.97 | 0.47 |
| 4:G:39:THR:HG1 | 4:G:41:LYS:H | 1.60 | 0.47 |
| 6:A:525:GLN:OE1 | 7:B:836:GLU:N | 2.47 | 0.47 |
| 6:A:1209:MET:HA | 6:A:1212:VAL:HG23 | 1.95 | 0.47 |
| 6:A:1443:VAL:HG21 | 10:F:93:ILE:CD1 | 2.40 | 0.47 |
| 7:B:548:GLY:HA3 | 7:B:630:ALA:HB2 | 1.96 | 0.47 |
| 7:B:603:LEU:HB3 | 7:B:609:ILE:HG13 | 1.95 | 0.47 |
| 7:B:842:ASN:HB2 | 7:B:1009:ASP:HA | 1.97 | 0.47 |
| 7:B:880:THR:O | 7:B:880:THR:OG1 | 2.29 | 0.47 |
| 8:C:107:SER:OG | 8:C:109:SER:N | 2.48 | 0.47 |
| 10:F:93:ILE:HA | 10:F:93:ILE:HD13 | 1.45 | 0.47 |
| 11:H:138:GLU:OE1 | 11:H:139:ASN:N | 2.48 | 0.47 |
| 17:0:627:PHE:HD1 | 17:0:654:LEU:HD12 | 1.80 | 0.47 |
| 18:4:175:ARG:NH2 | 18:4:211:ASP:OD2 | 2.48 | 0.47 |
| 18:4:236:LEU:HB3 | 18:4:238:VAL:HG13 | 1.96 | 0.47 |
| 19:6:211:GLN:HB3 | 19:6:243:ASP:HA | 1.96 | 0.47 |
| 21:7:133:TRP:N | 21:7:142:ILE:O | 2.45 | 0.47 |
| 21:7:678:GLY:HA2 | 21:7:679:SER:HA | 1.67 | 0.47 |
| 23:2:250:LEU:O | 23:2:254:ARG:N | 2.37 | 0.47 |
| 25:U:258:TRP:CE2 | 26:V:66:LEU:HD23 | 2.50 | 0.47 |
| 29:O:141:ARG:HA | 29:O:141:ARG:HD2 | 1.79 | 0.47 |
| 30:W:149:CYS:O | 30:W:153:ASP:HA | 2.14 | 0.47 |
| 1:Q:375:LEU:HA | 1:Q:375:LEU:HD12 | 1.70 | 0.47 |
| 1:Q:377:SER:O | 1:Q:384:PHE:HD1 | 1.98 | 0.47 |
| 5:M:299:GLY:HA2 | 5:M:304:VAL:HG22 | 1.97 | 0.47 |
| 6:A:567:LYS:HZ2 | 6:A:568:PRO:CD | 2.27 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1257:ASP:N | 6:A:1257:ASP:OD1 | 2.47 | 0.47 |
| 6:A:1271:ILE:HG22 | 6:A:1273:LEU:HD12 | 1.97 | 0.47 |
| 7:B:46:GLN:H | 7:B:46:GLN:HG3 | 1.42 | 0.47 |
| 7:B:170:LEU:HD12 | 7:B:171:PRO:HD2 | 1.97 | 0.47 |
| 7:B:433:GLN:O | 7:B:436:VAL:HG13 | 2.14 | 0.47 |
| 7:B:750:GLY:O | 7:B:754:SER:OG | 2.33 | 0.47 |
| 7:B:794:ASN:OD1 | 7:B:855:PHE:HD1 | 1.98 | 0.47 |
| 8:C:90:ASP:O | 8:C:91:HIS:HB3 | 2.13 | 0.47 |
| 9:E:147:HIS:CD2 | 9:E:149:LEU:H | 2.32 | 0.47 |
| 12:I:36:GLU:HB3 | 12:I:37:GLU:OE2 | 2.15 | 0.47 |
| 12:I:74:GLU:HB2 | 12:I:81:ARG:NH1 | 2.30 | 0.47 |
| 17:O:12:PHE:HE2 | 17:O:14:TYR:HB2 | 1.78 | 0.47 |
| 17:O:104:ARG:CZ | 17:O:170:TYR:HB2 | 2.45 | 0.47 |
| 17:O:271:ILE:HA | 17:O:388:LEU:HD22 | 1.97 | 0.47 |
| 21:7:545:GLN:HA | 21:7:550:ALA:HA | 1.97 | 0.47 |
| 21:7:709:VAL:HG13 | 21:7:715:GLU:HB3 | 1.97 | 0.47 |
| 23:2:353:SER:HB2 | 23:2:356:GLN:HB2 | 1.97 | 0.47 |
| 30:W:144:ARG:NH1 | 30:W:155:PRO:HG3 | 2.29 | 0.47 |
| 1:Q:120:LYS:HD3 | 1:Q:394:LYS:HD2 | 1.95 | 0.47 |
| 2:R:80:LYS:HB3 | 2:R:81:TRP:HD1 | 1.79 | 0.47 |
| 3:D:66:ARG:HH12 | 4:G:35:GLU:CD | 2.18 | 0.47 |
| 3:D:130:LEU:O | 3:D:134:THR:N | 2.35 | 0.47 |
| 4:G:1:MET:N | 4:G:80:LYS:O | 2.35 | 0.47 |
| 5:M:267:LYS:HZ3 | 29:O:239:LYS:HB2 | 1.79 | 0.47 |
| 5:M:305:THR:HB | 5:M:308:THR:H | 1.80 | 0.47 |
| 6:A:871:ASP:OD1 | 6:A:872:GLY:N | 2.48 | 0.47 |
| 6:A:1397:LEU:HB2 | 6:A:1426:GLU:HG3 | 1.96 | 0.47 |
| 17:O:581:LEU:O | 17:O:585:THR:OG1 | 2.29 | 0.47 |
| 18:4:87:TYR:CE1 | 18:4:121:VAL:HG22 | 2.50 | 0.47 |
| 29:O:93:GLU:HG2 | 29:O:103:ILE:HD12 | 1.96 | 0.47 |
| 1:Q:117:HIS:ND1 | 1:Q:391:LYS:HB2 | 2.30 | 0.47 |
| 3:D:124:GLU:HA | 3:D:127:ASP:HB2 | 1.97 | 0.47 |
| 5:M:286:ILE:HG13 | 5:M:291:ILE:HB | 1.97 | 0.47 |
| 6:A:607:ILE:HG22 | 6:A:609:ASP:O | 2.14 | 0.47 |
| 6:A:878:ILE:HD12 | 6:A:878:ILE:HG23 | 1.75 | 0.47 |
| 6:A:1034:GLU:O | 6:A:1036:ARG:HG3 | 2.15 | 0.47 |
| 7:B:291:ILE:HD12 | 7:B:291:ILE:N | 2.30 | 0.47 |
| 7:B:307:ASP:OD2 | 7:B:310:MET:HE3 | 2.15 | 0.47 |
| 7:B:706:GLN:HB2 | 7:B:710:LEU:HD23 | 1.96 | 0.47 |
| 11:H:125:LEU:HD12 | 11:H:125:LEU:HA | 1.63 | 0.47 |
| 17:O:136:MET:HG3 | 17:O:154:GLU:HG2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:6:176:ASN:HA | 19:6:206:GLY:HA3 | 1.96 | 0.47 |
| 23:2:249:MET:O | 23:2:253:MET:N | 2.36 | 0.47 |
| 1:Q:106:ILE:HG13 | 1:Q:107:PRO:HD2 | 1.97 | 0.46 |
| 1:Q:142:LYS:O | 1:Q:142:LYS:HG2 | 2.15 | 0.46 |
| 6:A:172:PRO:HB3 | 6:A:185:TRP:CE2 | 2.50 | 0.46 |
| 6:A:1121:GLU:O | 6:A:1123:GLY:N | 2.48 | 0.46 |
| 7:B:69:LEU:O | 7:B:89:GLU:HA | 2.15 | 0.46 |
| 7:B:547:VAL:N | 7:B:612:GLU:OE2 | 2.45 | 0.46 |
| 7:B:1051:THR:OG1 | 7:B:1052:VAL:N | 2.46 | 0.46 |
| 8:C:26:ASP:OD1 | 8:C:28:ALA:N | 2.41 | 0.46 |
| 9:E:20:LYS:HE2 | 9:E:35:VAL:HA | 1.96 | 0.46 |
| 15:L:47:ARG:HH22 | 15:L:54:ARG:NH1 | 2.13 | 0.46 |
| 17:0:416:PHE:HA | 17:0:440:LEU:HG | 1.97 | 0.46 |
| 18:4:130:TYR:O | 18:4:134:GLU:N | 2.48 | 0.46 |
| 18:4:303:ASN:N | 18:4:303:ASN:OD1 | 2.48 | 0.46 |
| 21:7:582:ILE:O | 21:7:587:LYS:HD2 | 2.15 | 0.46 |
| 29:O:175:LEU:HA | 29:O:237:PHE:CD2 | 2.49 | 0.46 |
| 30:W:122:TYR:CD2 | 30:W:156:LEU:HB2 | 2.49 | 0.46 |
| 2:R:118:HIS:HB2 | 2:R:120:TYR:CE1 | 2.51 | 0.46 |
| 6:A:261:ASP:OD1 | 6:A:322:VAL:HG13 | 2.16 | 0.46 |
| 6:A:770:VAL:HA | 6:A:822:GLU:OE1 | 2.15 | 0.46 |
| 6:A:873:MET:HE3 | 6:A:873:MET:HB3 | 1.75 | 0.46 |
| 6:A:1166:ASP:OD2 | 6:A:1194:ARG:NE | 2.34 | 0.46 |
| 6:A:1174:PHE:CD1 | 6:A:1175:SER:N | 2.79 | 0.46 |
| 6:A:1187:GLN:HE22 | 6:A:1188:GLN:NE2 | 2.13 | 0.46 |
| 7:B:805:THR:O | 7:B:1044:ALA:N | 2.35 | 0.46 |
| 7:B:990:ILE:HD12 | 7:B:990:ILE:HG23 | 1.65 | 0.46 |
| 7:B:1046:PRO:HB2 | 7:B:1047:PHE:CD2 | 2.50 | 0.46 |
| 15:L:27:LEU:HG | 15:L:37:LYS:NZ | 2.30 | 0.46 |
| 17:0:252:LEU:O | 17:0:434:ILE:HA | 2.16 | 0.46 |
| 17:0:534:PRO:HA | 19:6:239:LEU:HG | 1.97 | 0.46 |
| 18:4:64:HIS:O | 18:4:71:ASN:ND2 | 2.31 | 0.46 |
| 21:7:422:GLN:HA | 21:7:426:GLN:HE22 | 1.79 | 0.46 |
| 23:2:81:MET:HG2 | 23:2:86:LEU:HD11 | 1.97 | 0.46 |
| 25:U:253:ARG:HD3 | 25:U:255:LYS:H | 1.80 | 0.46 |
| 25:U:269:ILE:O | 25:U:272:ASN:ND2 | 2.48 | 0.46 |
| 29:O:175:LEU:HD11 | 29:O:195:TYR:CE1 | 2.51 | 0.46 |
| 1:Q:373:TYR:H | 2:R:82:ARG:HH21 | 1.60 | 0.46 |
| 5:M:123:ASP:N | 5:M:123:ASP:OD1 | 2.48 | 0.46 |
| 6:A:1406:VAL:HG13 | 6:A:1407:GLU:OE1 | 2.16 | 0.46 |
| 7:B:302:CYS:SG | 7:B:307:ASP:HB3 | 2.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:1221:SER:O | 7:B:1222:ARG:NE | 2.40 | 0.46 |
| 8:C:60:ASP:O | 8:C:63:ILE:N | 2.48 | 0.46 |
| 17:0:694:PRO:O | 17:0:698:ALA:N | 2.31 | 0.46 |
| 18:4:194:ILE:HB | 18:4:195:PRO:HD3 | 1.96 | 0.46 |
| 21:7:303:ARG:HB2 | 21:7:323:VAL:H | 1.79 | 0.46 |
| 29:O:82:LEU:HD11 | 29:O:117:ALA:HB2 | 1.97 | 0.46 |
| 30:W:65:ARG:NE | 30:W:93:HIS:HB3 | 2.30 | 0.46 |
| 2:R:138:GLN:H | 2:R:138:GLN:CD | 2.15 | 0.46 |
| 3:D:56:ARG:HE | 3:D:148:LEU:HB3 | 1.79 | 0.46 |
| 3:D:156:ASP:O | 3:D:158:GLU:N | 2.48 | 0.46 |
| 6:A:74:MET:O | 6:A:76:GLU:N | 2.48 | 0.46 |
| 6:A:120:GLU:OE1 | 6:A:123:ARG:HD2 | 2.15 | 0.46 |
| 6:A:441:PRO:HA | 6:A:458:HIS:O | 2.15 | 0.46 |
| 7:B:1181:GLU:HA | 7:B:1187:ASN:O | 2.16 | 0.46 |
| 8:C:231:ASN:C | 8:C:231:ASN:HD22 | 2.18 | 0.46 |
| 9:E:98:ILE:HA | 9:E:101:GLN:NE2 | 2.31 | 0.46 |
| 13:J:23:ASN:HB3 | 13:J:27:GLU:OE2 | 2.15 | 0.46 |
| 17:0:681:LEU:HB3 | 17:0:686:PHE:CE2 | 2.50 | 0.46 |
| 20:1:260:PHE:HD1 | 20:1:266:VAL:HG13 | 1.80 | 0.46 |
| 20:1:517:UNK:O | 20:1:519:UNK:N | 2.49 | 0.46 |
| 21:7:420:TRP:HE1 | 21:7:661:SER:HG | 0.57 | 0.46 |
| 21:7:660:THR:HA | 21:7:661:SER:HA | 1.75 | 0.46 |
| 28:T:145:DT:H1' | 28:T:146:DA:C8 | 2.50 | 0.46 |
| 2:R:118:HIS:HB2 | 2:R:120:TYR:CZ | 2.50 | 0.46 |
| 5:M:157:CYS:HB3 | 5:M:210:MET:CE | 2.45 | 0.46 |
| 6:A:683:ILE:O | 6:A:687:LYS:HG2 | 2.15 | 0.46 |
| 6:A:711:ARG:NH2 | 12:I:96:SER:O | 2.46 | 0.46 |
| 6:A:1218:GLN:HA | 6:A:1221:LYS:HD3 | 1.98 | 0.46 |
| 6:A:1441:PHE:CZ | 10:F:92:ARG:HB3 | 2.51 | 0.46 |
| 7:B:468:GLU:H | 7:B:471:LYS:HB2 | 1.80 | 0.46 |
| 7:B:1177:HIS:O | 7:B:1179:GLN:HG3 | 2.15 | 0.46 |
| 10:F:97:ARG:O | 10:F:101:ILE:HG13 | 2.16 | 0.46 |
| 11:H:36:CYS:HA | 11:H:126:GLU:O | 2.16 | 0.46 |
| 14:K:5:ASP:O | 14:K:8:GLU:HG2 | 2.14 | 0.46 |
| 17:0:13:PRO:HG3 | 17:0:89:LEU:HD11 | 1.96 | 0.46 |
| 17:0:252:LEU:HD12 | 17:0:435:MET:HG3 | 1.96 | 0.46 |
| 17:0:465:PRO:HD2 | 17:0:656:PHE:HD2 | 1.80 | 0.46 |
| 17:0:473:LEU:HB2 | 17:0:475:PHE:CE1 | 2.50 | 0.46 |
| 18:4:61:LEU:HD11 | 18:4:73:VAL:HB | 1.96 | 0.46 |
| 18:4:288:ILE:HB | 18:4:295:VAL:HG22 | 1.97 | 0.46 |
| 21:7:443:LYS:HD3 | 21:7:444:GLU:H | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:587:LYS:HG3 | 21:7:708:LEU:HD23 | 1.96 | 0.46 |
| 21:7:636:ARG:HH12 | 21:7:657:VAL:HG23 | 1.81 | 0.46 |
| 21:7:751:ALA:O | 21:7:756:ARG:NH2 | 2.46 | 0.46 |
| 23:2:243:SER:O | 23:2:247:ARG:N | 2.31 | 0.46 |
| 23:2:503:ASP:HA | 23:2:506:LYS:HG2 | 1.97 | 0.46 |
| 26:V:65:ASN:O | 26:V:81:LYS:N | 2.39 | 0.46 |
| 4:G:40:GLY:H | 4:G:154:VAL:HA | 1.81 | 0.46 |
| 6:A:84:ILE:HD11 | 6:A:270:LEU:HD12 | 1.98 | 0.46 |
| 6:A:998:LEU:HA | 6:A:1011:GLN:NE2 | 2.28 | 0.46 |
| 7:B:1114:LEU:HD12 | 7:B:1114:LEU:HA | 1.61 | 0.46 |
| 7:B:1183:LYS:HB2 | 7:B:1183:LYS:HE3 | 1.71 | 0.46 |
| 11:H:145:ARG:NH1 | 11:H:146:ARG:CZ | 2.79 | 0.46 |
| 13:J:58:GLU:O | 13:J:61:LEU:N | 2.48 | 0.46 |
| 21:7:552:VAL:HG11 | 21:7:731:TYR:CD2 | 2.50 | 0.46 |
| 21:7:692:ARG:NE | 21:7:692:ARG:HA | 2.30 | 0.46 |
| 28:T:159:DT:H2' | 28:T:160:DT:C6 | 2.51 | 0.46 |
| 29:O:202:ILE:HG13 | 29:O:222:GLU:O | 2.16 | 0.46 |
| 30:W:136:ALA:HB1 | 30:W:147:PHE:CD2 | 2.51 | 0.46 |
| 31:P:9:G:C6 | 31:P:10:A:C6 | 3.04 | 0.46 |
| 1:Q:104:ARG:HD2 | 1:Q:104:ARG:HA | 1.55 | 0.46 |
| 1:Q:365:TYR:CE2 | 1:Q:367:ALA:HB2 | 2.50 | 0.46 |
| 2:R:80:LYS:HB3 | 2:R:81:TRP:CD1 | 2.51 | 0.46 |
| 2:R:94:LYS:H | 2:R:94:LYS:HZ3 | 1.63 | 0.46 |
| 4:G:111:THR:HG22 | 4:G:112:LYS:H | 1.79 | 0.46 |
| 6:A:872:GLY:O | 6:A:1058:VAL:HG12 | 2.15 | 0.46 |
| 6:A:898:ARG:HB3 | 6:A:906:HIS:CD2 | 2.51 | 0.46 |
| 6:A:934:LYS:O | 6:A:937:VAL:HG22 | 2.15 | 0.46 |
| 6:A:956:LEU:HD23 | 6:A:956:LEU:HA | 1.63 | 0.46 |
| 9:E:39:LEU:O | 9:E:42:PHE:HB3 | 2.15 | 0.46 |
| 11:H:57:VAL:O | 11:H:58:THR:OG1 | 2.29 | 0.46 |
| 13:J:50:ILE:HA | 13:J:50:ILE:HD13 | 1.60 | 0.46 |
| 13:J:61:LEU:HD23 | 13:J:61:LEU:HA | 1.67 | 0.46 |
| 14:K:50:LEU:HD13 | 14:K:75:ILE:HD12 | 1.98 | 0.46 |
| 17:O:76:MET:HA | 17:O:79:ILE:HB | 1.97 | 0.46 |
| 19:6:164:ASN:ND2 | 19:6:305:VAL:O | 2.49 | 0.46 |
| 21:7:342:ASP:OD1 | 21:7:342:ASP:N | 2.46 | 0.46 |
| 21:7:438:PHE:HB2 | 21:7:455:SER:HB2 | 1.98 | 0.46 |
| 22:5:7:GLY:HA3 | 22:5:41:LEU:HD11 | 1.97 | 0.46 |
| 27:N:20:DT:C4 | 27:N:21:DA:N6 | 2.83 | 0.46 |
| 27:N:30:DA:C2 | 27:N:31:DT:C2 | 3.03 | 0.46 |
| 2:R:63:ARG:HG2 | 2:R:65:ASN:N | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:68:VAL:HG21 | 2:R:134:VAL:HG21 | 1.98 | 0.46 |
| 4:G:112:LYS:HA | 4:G:112:LYS:HD2 | 1.74 | 0.46 |
| 5:M:276:THR:HA | 5:M:279:VAL:HG12 | 1.98 | 0.46 |
| 6:A:882:SER:O | 6:A:1025:ARG:NH2 | 2.40 | 0.46 |
| 6:A:1147:THR:HG23 | 12:I:48:LEU:HD11 | 1.98 | 0.46 |
| 6:A:1239:ARG:HH12 | 6:A:1241:ARG:NH1 | 2.13 | 0.46 |
| 7:B:185:THR:OG1 | 7:B:188:ASP:OD1 | 2.24 | 0.46 |
| 7:B:546:SER:OG | 7:B:632:ARG:N | 2.49 | 0.46 |
| 7:B:863:GLU:OE2 | 7:B:873:THR:HA | 2.16 | 0.46 |
| 17:O:17:ILE:HG13 | 17:O:18:TYR:H | 1.79 | 0.46 |
| 17:O:729:ASP:O | 17:O:731:LYS:NZ | 2.40 | 0.46 |
| 19:6:444:ILE:O | 19:6:449:HIS:HA | 2.16 | 0.46 |
| 21:7:578:MET:HA | 21:7:581:TYR:CZ | 2.50 | 0.46 |
| 22:5:58:LEU:HD23 | 23:2:450:ARG:HH11 | 1.80 | 0.46 |
| 27:N:17:DG:H22 | 28:T:149:DC:H42 | 1.63 | 0.46 |
| 27:N:22:DT:H1' | 29:O:215:THR:OG1 | 2.16 | 0.46 |
| 29:O:67:LEU:HD11 | 29:O:220:ARG:HG3 | 1.98 | 0.46 |
| 29:O:161:VAL:HA | 29:O:215:THR:HB | 1.98 | 0.46 |
| 30:W:136:ALA:HB1 | 30:W:147:PHE:CG | 2.51 | 0.46 |
| 1:Q:337:GLU:CD | 1:Q:340:LYS:H | 2.16 | 0.46 |
| 2:R:73:LEU:HD12 | 2:R:74:PRO:CD | 2.46 | 0.46 |
| 2:R:74:PRO:HB2 | 2:R:76:PHE:HD1 | 1.80 | 0.46 |
| 6:A:578:LEU:HA | 6:A:578:LEU:HD12 | 1.56 | 0.46 |
| 6:A:1100:ARG:NH1 | 6:A:1103:GLU:OE1 | 2.37 | 0.46 |
| 6:A:1167:GLU:HA | 6:A:1170:ILE:HG12 | 1.97 | 0.46 |
| 6:A:1208:THR:OG1 | 6:A:1211:GLN:HG3 | 2.16 | 0.46 |
| 6:A:1221:LYS:HE2 | 6:A:1221:LYS:HB2 | 1.58 | 0.46 |
| 6:A:1286:LYS:HG3 | 6:A:1304:TRP:CH2 | 2.51 | 0.46 |
| 7:B:647:GLY:H | 7:B:648:HIS:C | 2.19 | 0.46 |
| 7:B:744:HIS:O | 7:B:747:MET:HG2 | 2.15 | 0.46 |
| 7:B:1099:VAL:O | 7:B:1101:ASP:N | 2.49 | 0.46 |
| 7:B:1221:SER:C | 7:B:1222:ARG:HE | 2.18 | 0.46 |
| 9:E:87:SER:N | 9:E:114:ASN:HB2 | 2.31 | 0.46 |
| 11:H:38:LEU:HD12 | 11:H:39:THR:N | 2.31 | 0.46 |
| 12:I:33:SER:O | 12:I:35:VAL:HG23 | 2.16 | 0.46 |
| 18:4:175:ARG:HH12 | 18:4:252:MET:HB3 | 1.80 | 0.46 |
| 23:2:10:VAL:HA | 23:2:13:TYR:HB3 | 1.98 | 0.46 |
| 2:R:62:GLU:HG2 | 2:R:63:ARG:N | 2.31 | 0.46 |
| 5:M:37:ARG:HG3 | 6:A:416:ARG:NH2 | 2.28 | 0.46 |
| 5:M:276:THR:O | 5:M:280:VAL:HG13 | 2.16 | 0.46 |
| 6:A:43:GLU:OE2 | 6:A:48:ALA:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:557:ASP:OD1 | 6:A:559:VAL:N | 2.48 | 0.46 |
| 6:A:809:THR:N | 6:A:812:GLU:OE2 | 2.40 | 0.46 |
| 6:A:1035:TYR:N | 6:A:1035:TYR:CD1 | 2.79 | 0.46 |
| 6:A:1266:THR:HG23 | 6:A:1270:ASN:OD1 | 2.16 | 0.46 |
| 7:B:365:THR:OG1 | 7:B:367:LEU:N | 2.38 | 0.46 |
| 7:B:416:LEU:HD12 | 7:B:416:LEU:HA | 1.69 | 0.46 |
| 7:B:487:THR:O | 7:B:488:TYR:C | 2.54 | 0.46 |
| 7:B:796:LEU:HD12 | 7:B:796:LEU:HA | 1.68 | 0.46 |
| 7:B:838:SER:HB2 | 7:B:839:MET:CG | 2.46 | 0.46 |
| 7:B:900:ALA:HB3 | 15:L:61:THR:HB | 1.98 | 0.46 |
| 7:B:906:SER:O | 7:B:941:LEU:HD21 | 2.16 | 0.46 |
| 17:0:527:VAL:HG22 | 17:0:531:LYS:HE3 | 1.98 | 0.46 |
| 28:T:149:DC:H2'' | 28:T:150:DG:C8 | 2.51 | 0.46 |
| 5:M:275:ILE:H | 5:M:275:ILE:HD12 | 1.81 | 0.45 |
| 6:A:658:LEU:HG | 6:A:659:HIS:ND1 | 2.31 | 0.45 |
| 6:A:1217:LYS:O | 6:A:1221:LYS:N | 2.49 | 0.45 |
| 7:B:234:ILE:H | 7:B:234:ILE:HG12 | 1.43 | 0.45 |
| 8:C:174:ALA:HB3 | 8:C:233:GLU:O | 2.16 | 0.45 |
| 9:E:119:SER:O | 9:E:123:LEU:HD22 | 2.16 | 0.45 |
| 17:0:106:LEU:HD12 | 17:0:199:MET:HG3 | 1.97 | 0.45 |
| 17:0:508:SER:HB2 | 17:0:546:TYR:CE1 | 2.51 | 0.45 |
| 19:6:188:ASN:ND2 | 19:6:191:ASP:OD2 | 2.49 | 0.45 |
| 21:7:132:LEU:O | 21:7:202:LYS:N | 2.44 | 0.45 |
| 21:7:241:ILE:O | 21:7:245:LEU:N | 2.39 | 0.45 |
| 21:7:604:LYS:O | 21:7:669:CYS:N | 2.50 | 0.45 |
| 1:Q:110:ASP:O | 1:Q:114:MET:HB2 | 2.16 | 0.45 |
| 1:Q:372:SER:HG | 2:R:73:LEU:N | 2.14 | 0.45 |
| 2:R:295:PRO:O | 2:R:299:ILE:N | 2.31 | 0.45 |
| 3:D:154:PHE:HB3 | 3:D:160:VAL:HG22 | 1.98 | 0.45 |
| 5:M:37:ARG:NH1 | 6:A:417:TYR:OH | 2.48 | 0.45 |
| 5:M:127:GLN:HA | 5:M:130:PHE:HB2 | 1.98 | 0.45 |
| 6:A:220:THR:OG1 | 6:A:221:SER:N | 2.50 | 0.45 |
| 6:A:382:PRO:HG3 | 6:A:428:TYR:CZ | 2.50 | 0.45 |
| 6:A:399:HIS:HB3 | 6:A:400:PRO:HD3 | 1.97 | 0.45 |
| 7:B:128:LEU:HB2 | 7:B:167:ILE:O | 2.16 | 0.45 |
| 9:E:37:LEU:HD23 | 9:E:38:PRO:HD2 | 1.98 | 0.45 |
| 9:E:157:SER:N | 9:E:160:GLU:OE1 | 2.49 | 0.45 |
| 10:F:136:ARG:O | 10:F:137:TYR:CG | 2.70 | 0.45 |
| 17:0:63:TYR:O | 17:0:67:ARG:NH2 | 2.49 | 0.45 |
| 17:0:257:LEU:HA | 17:0:260:ALA:HB3 | 1.97 | 0.45 |
| 17:0:446:ILE:HD12 | 17:0:473:LEU:HD13 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:6:251:ILE:HG12 | 19:6:276:LEU:HD13 | 1.99 | 0.45 |
| 20:1:466:UNK:O | 20:1:468:UNK:N | 2.49 | 0.45 |
| 21:7:362:ILE:HD11 | 21:7:367:GLU:HB3 | 1.98 | 0.45 |
| 2:R:70:LEU:HD12 | 2:R:71:VAL:H | 1.81 | 0.45 |
| 4:G:83:LYS:HE3 | 4:G:150:CYS:HB2 | 1.97 | 0.45 |
| 5:M:251:GLN:NE2 | 5:M:252:VAL:HG23 | 2.31 | 0.45 |
| 6:A:229:SER:O | 6:A:229:SER:OG | 2.33 | 0.45 |
| 6:A:276:LEU:HD23 | 6:A:276:LEU:HA | 1.56 | 0.45 |
| 6:A:559:VAL:HG13 | 11:H:78:SER:HA | 1.98 | 0.45 |
| 6:A:904:THR:O | 6:A:907:THR:HB | 2.16 | 0.45 |
| 7:B:68:THR:HA | 7:B:90:ILE:O | 2.17 | 0.45 |
| 7:B:140:ILE:HA | 7:B:141:ASP:HA | 1.68 | 0.45 |
| 7:B:219:ALA:HB3 | 7:B:222:ILE:HD12 | 1.99 | 0.45 |
| 7:B:880:THR:OG1 | 7:B:934:LYS:NZ | 2.33 | 0.45 |
| 7:B:1106:ARG:NH2 | 7:B:1109:GLY:O | 2.49 | 0.45 |
| 9:E:4:GLU:N | 9:E:4:GLU:OE1 | 2.49 | 0.45 |
| 9:E:94:LYS:HE3 | 9:E:123:LEU:HG | 1.99 | 0.45 |
| 14:K:82:ASP:OD1 | 14:K:84:LYS:HG3 | 2.16 | 0.45 |
| 17:0:49:THR:HA | 17:0:52:LEU:HB2 | 1.97 | 0.45 |
| 17:0:256:ALA:O | 17:0:260:ALA:N | 2.43 | 0.45 |
| 17:0:351:VAL:HB | 17:0:421:GLU:HG2 | 1.97 | 0.45 |
| 17:0:487:LEU:HG | 17:0:489:LYS:H | 1.82 | 0.45 |
| 19:6:347:TYR:N | 19:6:356:VAL:O | 2.39 | 0.45 |
| 23:2:356:GLN:HE22 | 23:2:360:LEU:HD11 | 1.81 | 0.45 |
| 24:X:144:VAL:N | 24:X:176:GLY:HA3 | 2.31 | 0.45 |
| 29:O:61:SER:OG | 29:O:62:GLY:N | 2.50 | 0.45 |
| 29:O:133:LYS:HB2 | 29:O:155:PHE:CZ | 2.52 | 0.45 |
| 1:Q:378:VAL:HB | 2:R:68:VAL:HA | 1.97 | 0.45 |
| 6:A:55:ASP:HA | 6:A:58:LEU:HD23 | 1.97 | 0.45 |
| 6:A:866:PHE:HE2 | 9:E:211:TYR:H | 1.65 | 0.45 |
| 6:A:1312:ASN:OD1 | 6:A:1315:GLU:HG2 | 2.16 | 0.45 |
| 7:B:641:GLU:HB2 | 7:B:652:LYS:HG3 | 1.99 | 0.45 |
| 11:H:58:THR:H | 11:H:143:LEU:HB2 | 1.80 | 0.45 |
| 15:L:31:CYS:HB2 | 15:L:48:CYS:HB2 | 1.57 | 0.45 |
| 17:0:217:LYS:HD3 | 17:0:308:GLU:HG3 | 1.98 | 0.45 |
| 18:4:146:ARG:HA | 18:4:191:PHE:CZ | 2.52 | 0.45 |
| 21:7:627:ILE:O | 21:7:653:PHE:HB2 | 2.17 | 0.45 |
| 29:O:70:ILE:HG12 | 29:O:160:ILE:HG23 | 1.98 | 0.45 |
| 5:M:152:GLU:OE1 | 7:B:868:MET:HB2 | 2.17 | 0.45 |
| 6:A:23:SER:OG | 6:A:23:SER:O | 2.33 | 0.45 |
| 6:A:555:ASP:N | 6:A:555:ASP:OD1 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:A:663:SER:OG | 7:B:827:ILE:O | 2.29 | 0.45 |
| 6:A:1038:THR:OG1 | 6:A:1040:GLN:N | 2.50 | 0.45 |
| 7:B:793:ALA:HB3 | 7:B:856:PHE:HB2 | 1.98 | 0.45 |
| 17:0:2:LYS:HA | 17:0:10:VAL:O | 2.17 | 0.45 |
| 17:0:90:MET:HB2 | 17:0:175:VAL:HG21 | 1.99 | 0.45 |
| 17:0:285:GLU:OE2 | 17:0:288:LYS:NZ | 2.31 | 0.45 |
| 17:0:507:SER:OG | 17:0:508:SER:N | 2.49 | 0.45 |
| 19:6:129:THR:OG1 | 19:6:234:ILE:HA | 2.17 | 0.45 |
| 19:6:153:ALA:HA | 19:6:156:PHE:HB3 | 1.97 | 0.45 |
| 21:7:519:ARG:NE | 21:7:521:ASP:HB2 | 2.32 | 0.45 |
| 21:7:590:ALA:HA | 21:7:739:LEU:HD11 | 1.99 | 0.45 |
| 21:7:625:PRO:HD2 | 21:7:649:ILE:HG12 | 1.98 | 0.45 |
| 23:2:28:SER:O | 23:2:31:THR:OG1 | 2.35 | 0.45 |
| 24:X:207:CYS:SG | 24:X:241:PRO:HA | 2.56 | 0.45 |
| 24:X:259:PHE:CE1 | 30:W:109:LEU:HD11 | 2.49 | 0.45 |
| 30:W:17:VAL:HG21 | 30:W:29:LEU:HD22 | 1.97 | 0.45 |
| 30:W:149:CYS:H | 30:W:154:GLU:N | 2.14 | 0.45 |
| 1:Q:102:PRO:O | 1:Q:103:LEU:HD13 | 2.16 | 0.45 |
| 2:R:63:ARG:HB3 | 2:R:66:ARG:NH1 | 2.32 | 0.45 |
| 3:D:141:LEU:O | 3:D:145:MET:HG2 | 2.16 | 0.45 |
| 4:G:5:LYS:O | 4:G:76:ALA:N | 2.31 | 0.45 |
| 4:G:142:ARG:O | 4:G:170:ALA:HA | 2.17 | 0.45 |
| 6:A:326:ARG:HG2 | 6:A:1406:VAL:HG11 | 1.98 | 0.45 |
| 6:A:352:VAL:HG21 | 7:B:1099:VAL:HG12 | 1.99 | 0.45 |
| 6:A:863:VAL:HG11 | 6:A:866:PHE:CE1 | 2.51 | 0.45 |
| 7:B:37:PHE:C | 7:B:39:ARG:H | 2.20 | 0.45 |
| 7:B:110:HIS:ND1 | 7:B:111:ALA:O | 2.43 | 0.45 |
| 7:B:254:LEU:HD13 | 7:B:360:PHE:HE1 | 1.82 | 0.45 |
| 7:B:979:LYS:HD3 | 31:P:10:A:OP1 | 2.17 | 0.45 |
| 7:B:1159:ARG:HG2 | 7:B:1160:VAL:N | 2.31 | 0.45 |
| 8:C:3:GLU:HG2 | 14:K:100:ALA:HB1 | 1.98 | 0.45 |
| 10:F:112:GLU:OE2 | 10:F:123:LYS:NZ | 2.40 | 0.45 |
| 25:U:263:LYS:NZ | 25:U:278:LYS:HG2 | 2.32 | 0.45 |
| 1:Q:378:VAL:HA | 1:Q:384:PHE:CE1 | 2.52 | 0.45 |
| 4:G:14:HIS:HB3 | 4:G:17:PHE:CE1 | 2.52 | 0.45 |
| 4:G:132:SER:OG | 4:G:133:SER:N | 2.50 | 0.45 |
| 5:M:251:GLN:HA | 5:M:254:THR:HG22 | 1.99 | 0.45 |
| 6:A:217:LYS:HE2 | 6:A:217:LYS:HB2 | 1.64 | 0.45 |
| 6:A:391:LEU:O | 6:A:394:ASN:N | 2.48 | 0.45 |
| 6:A:407:ARG:HA | 6:A:430:TRP:CG | 2.52 | 0.45 |
| 7:B:878:GLN:C | 7:B:879:ARG:HE | 2.20 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:C:3:GLU:C | 8:C:7:GLN:HE22 | 2.13 | 0.45 |
| 11:H:99:GLY:HA3 | 11:H:118:PHE:CD2 | 2.52 | 0.45 |
| 17:0:343:LYS:HG2 | 17:0:347:LYS:NZ | 2.31 | 0.45 |
| 19:6:239:LEU:HD11 | 19:6:268:ALA:HB1 | 1.99 | 0.45 |
| 20:1:193:LYS:O | 20:1:196:GLN:HG3 | 2.17 | 0.45 |
| 20:1:633:TYR:O | 20:1:637:TYR:N | 2.36 | 0.45 |
| 21:7:393:THR:HG23 | 21:7:486:ILE:HG21 | 1.98 | 0.45 |
| 28:T:147:DT:H1' | 29:O:207:PHE:CE1 | 2.51 | 0.45 |
| 29:O:172:LEU:HD21 | 29:O:206:ILE:HG22 | 1.99 | 0.45 |
| 29:O:214:LEU:HB3 | 29:O:223:ILE:HD12 | 1.97 | 0.45 |
| 30:W:134:LEU:O | 30:W:138:GLN:HG2 | 2.17 | 0.45 |
| 2:R:110:GLU:HG2 | 2:R:117:PRO:N | 2.32 | 0.45 |
| 3:D:26:THR:OG1 | 3:D:26:THR:O | 2.25 | 0.45 |
| 5:M:310:LYS:HA | 5:M:313:TYR:HB3 | 1.97 | 0.45 |
| 6:A:288:ALA:HA | 6:A:291:GLU:OE1 | 2.16 | 0.45 |
| 6:A:830:LYS:HB2 | 6:A:1082:ASN:ND2 | 2.32 | 0.45 |
| 6:A:841:LEU:HA | 6:A:841:LEU:HD23 | 1.59 | 0.45 |
| 6:A:1292:PRO:HA | 6:A:1298:TYR:HA | 1.97 | 0.45 |
| 7:B:872:GLU:HG2 | 7:B:916:THR:HG22 | 1.96 | 0.45 |
| 7:B:890:TYR:OH | 7:B:936:ASP:OD2 | 2.34 | 0.45 |
| 7:B:894:ASP:OD2 | 15:L:58:LYS:NZ | 2.36 | 0.45 |
| 12:I:78:CYS:SG | 12:I:80:SER:N | 2.76 | 0.45 |
| 13:J:22:LEU:O | 13:J:26:GLN:HG2 | 2.16 | 0.45 |
| 15:L:32:ALA:HB3 | 15:L:55:ILE:HG13 | 1.97 | 0.45 |
| 17:0:376:PHE:HB3 | 17:0:379:GLU:OE2 | 2.17 | 0.45 |
| 18:4:239:GLU:CD | 18:4:239:GLU:H | 2.20 | 0.45 |
| 29:O:69:ASN:HA | 29:O:126:ALA:O | 2.17 | 0.45 |
| 29:O:164:CYS:O | 29:O:211:LYS:HA | 2.17 | 0.45 |
| 29:O:164:CYS:SG | 29:O:212:ILE:HB | 2.56 | 0.45 |
| 30:W:99:LYS:HA | 30:W:186:LEU:HD13 | 1.98 | 0.45 |
| 6:A:333:GLU:HA | 6:A:338:GLY:HA3 | 1.97 | 0.45 |
| 6:A:1192:LEU:HD11 | 6:A:1194:ARG:HB2 | 1.99 | 0.45 |
| 6:A:1199:ARG:HA | 6:A:1236:LEU:HD11 | 1.98 | 0.45 |
| 6:A:1211:GLN:HG3 | 6:A:1211:GLN:H | 1.45 | 0.45 |
| 6:A:1441:PHE:HD2 | 6:A:1441:PHE:C | 2.20 | 0.45 |
| 7:B:333:PHE:O | 7:B:333:PHE:HD1 | 2.00 | 0.45 |
| 7:B:712:PRO:HD2 | 7:B:733:HIS:HD2 | 1.81 | 0.45 |
| 7:B:785:TYR:CD2 | 7:B:786:ASN:N | 2.85 | 0.45 |
| 8:C:208:GLU:H | 8:C:208:GLU:HG3 | 1.34 | 0.45 |
| 11:H:145:ARG:HD3 | 11:H:145:ARG:HA | 1.51 | 0.45 |
| 12:I:68:LEU:HA | 12:I:68:LEU:HD23 | 1.62 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:K:18:LYS:NZ | 14:K:38:GLU:OE2 | 2.26 | 0.45 |
| 15:L:62:LYS:HB2 | 15:L:63:ARG:HH22 | 1.82 | 0.45 |
| 17:O:79:ILE:HD13 | 17:O:79:ILE:HA | 1.85 | 0.45 |
| 18:4:29:ILE:O | 18:4:178:VAL:HA | 2.17 | 0.45 |
| 30:W:123:MET:CG | 30:W:157:VAL:HB | 2.47 | 0.45 |
| 1:Q:398:ARG:HE | 1:Q:398:ARG:HB2 | 1.59 | 0.45 |
| 5:M:130:PHE:CG | 5:M:151:LYS:HE2 | 2.52 | 0.45 |
| 5:M:215:ARG:HD3 | 5:M:215:ARG:HA | 1.56 | 0.45 |
| 5:M:282:ILE:O | 5:M:286:ILE:HG22 | 2.17 | 0.45 |
| 6:A:544:ASP:OD1 | 6:A:545:GLN:N | 2.47 | 0.45 |
| 7:B:70:ILE:HA | 7:B:89:GLU:OE2 | 2.17 | 0.45 |
| 7:B:238:ALA:HB2 | 7:B:385:LEU:HB2 | 1.98 | 0.45 |
| 7:B:294:ASP:H | 12:I:12:ASN:HD22 | 1.62 | 0.45 |
| 7:B:647:GLY:C | 7:B:649:LYS:N | 2.70 | 0.45 |
| 7:B:797:TYR:HB3 | 7:B:798:TYR:CD2 | 2.52 | 0.45 |
| 7:B:1095:LEU:HD23 | 7:B:1095:LEU:HA | 1.63 | 0.45 |
| 8:C:262:LEU:HA | 8:C:262:LEU:HD23 | 1.64 | 0.45 |
| 9:E:83:CYS:SG | 9:E:85:GLU:N | 2.90 | 0.45 |
| 17:O:656:PHE:HA | 17:O:692:GLN:HG2 | 1.98 | 0.45 |
| 18:4:86:LEU:HA | 18:4:128:GLU:HB3 | 1.98 | 0.45 |
| 19:6:154:ILE:HG23 | 19:6:193:ILE:HD12 | 2.00 | 0.45 |
| 20:1:588:ASP:O | 20:1:592:LYS:N | 2.35 | 0.45 |
| 23:2:25:LEU:HD21 | 23:2:226:PHE:CE2 | 2.51 | 0.45 |
| 23:2:56:GLU:OE1 | 23:2:99:ASN:HB3 | 2.17 | 0.45 |
| 27:N:13:DG:H2'' | 27:N:14:DC:O4' | 2.16 | 0.45 |
| 28:T:22:DT:H2' | 28:T:23:DC:H5' | 1.99 | 0.45 |
| 31:P:6:G:C2 | 31:P:7:A:C8 | 3.05 | 0.45 |
| 1:Q:120:LYS:HE2 | 1:Q:394:LYS:NZ | 2.32 | 0.44 |
| 2:R:99:LYS:HB2 | 2:R:103:LYS:CE | 2.46 | 0.44 |
| 4:G:35:GLU:CD | 4:G:47:CYS:HA | 2.37 | 0.44 |
| 6:A:219:PHE:CD1 | 6:A:220:THR:N | 2.79 | 0.44 |
| 6:A:549:MET:HE2 | 6:A:577:ILE:HG21 | 1.97 | 0.44 |
| 6:A:635:ARG:HA | 6:A:635:ARG:NH1 | 2.33 | 0.44 |
| 6:A:1025:ARG:HD3 | 6:A:1025:ARG:HA | 1.69 | 0.44 |
| 6:A:1034:GLU:HB2 | 6:A:1035:TYR:CD1 | 2.51 | 0.44 |
| 6:A:1098:VAL:N | 6:A:1099:PRO:HD2 | 2.32 | 0.44 |
| 6:A:1100:ARG:NH2 | 6:A:1351:GLU:OE1 | 2.42 | 0.44 |
| 6:A:1286:LYS:HG3 | 6:A:1304:TRP:CZ3 | 2.52 | 0.44 |
| 7:B:380:TYR:CZ | 7:B:384:ARG:HD3 | 2.51 | 0.44 |
| 7:B:492:LEU:HD23 | 7:B:492:LEU:HA | 1.68 | 0.44 |
| 7:B:820:GLY:N | 7:B:1091:TYR:OH | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:1152:MET:HE3 | 7:B:1152:MET:HB3 | 1.82 | 0.44 |
| 9:E:197:LYS:HA | 9:E:211:TYR:HD1 | 1.81 | 0.44 |
| 11:H:100:THR:OG1 | 11:H:138:GLU:HG2 | 2.18 | 0.44 |
| 15:L:47:ARG:HH12 | 15:L:54:ARG:CZ | 2.30 | 0.44 |
| 17:O:223:SER:HB2 | 17:O:226:VAL:HG22 | 1.99 | 0.44 |
| 17:O:333:SER:HB2 | 17:O:337:ARG:NH2 | 2.32 | 0.44 |
| 17:O:490:LYS:NZ | 17:O:700:GLY:HA2 | 2.32 | 0.44 |
| 17:O:694:PRO:HB2 | 17:O:696:TRP:CD1 | 2.52 | 0.44 |
| 18:4:247:TYR:CZ | 20:1:503:VAL:HG22 | 2.53 | 0.44 |
| 21:7:457:TYR:OH | 21:7:488:ASP:N | 2.50 | 0.44 |
| 21:7:524:ILE:H | 21:7:524:ILE:HD12 | 1.82 | 0.44 |
| 27:N:22:DT:O2 | 29:O:215:THR:OG1 | 2.21 | 0.44 |
| 29:O:170:ILE:HD13 | 29:O:234:LEU:HD22 | 1.99 | 0.44 |
| 29:O:227:PHE:HA | 29:O:230:ILE:HG22 | 1.98 | 0.44 |
| 30:W:5:ILE:O | 30:W:9:VAL:HG23 | 2.17 | 0.44 |
| 30:W:38:LEU:O | 30:W:86:TYR:HA | 2.17 | 0.44 |
| 3:D:138:ASN:O | 3:D:141:LEU:HB3 | 2.17 | 0.44 |
| 3:D:154:PHE:CD2 | 3:D:160:VAL:HG13 | 2.52 | 0.44 |
| 6:A:20:GLY:O | 7:B:1213:THR:OG1 | 2.31 | 0.44 |
| 6:A:29:ALA:HB1 | 7:B:1184:GLY:HA2 | 1.99 | 0.44 |
| 6:A:265:LYS:HD2 | 6:A:265:LYS:HA | 1.74 | 0.44 |
| 6:A:854:ASN:O | 6:A:867:ILE:HA | 2.16 | 0.44 |
| 6:A:993:LEU:HD23 | 6:A:1022:LEU:HD21 | 1.99 | 0.44 |
| 6:A:1277:GLU:OE1 | 6:A:1277:GLU:N | 2.47 | 0.44 |
| 7:B:98:THR:OG1 | 7:B:99:LYS:O | 2.31 | 0.44 |
| 8:C:62:PHE:CE1 | 8:C:66:ARG:HD2 | 2.51 | 0.44 |
| 11:H:62:SER:OG | 11:H:63:LEU:HG | 2.17 | 0.44 |
| 14:K:87:LEU:HD12 | 14:K:87:LEU:HA | 1.78 | 0.44 |
| 15:L:48:CYS:O | 15:L:48:CYS:SG | 2.76 | 0.44 |
| 17:O:436:ARG:HE | 17:O:634:ILE:CG2 | 2.30 | 0.44 |
| 20:1:235:UNK:HA | 20:1:381:LEU:HD11 | 1.99 | 0.44 |
| 21:7:557:VAL:N | 21:7:707:SER:O | 2.49 | 0.44 |
| 22:5:13:ASP:OD1 | 22:5:15:SER:OG | 2.30 | 0.44 |
| 25:U:249:ASP:OD1 | 26:V:119:LYS:NZ | 2.47 | 0.44 |
| 1:Q:117:HIS:HE1 | 1:Q:390:ASP:OD2 | 2.00 | 0.44 |
| 3:D:56:ARG:CB | 3:D:148:LEU:HD22 | 2.46 | 0.44 |
| 4:G:116:PRO:HD3 | 4:G:164:LYS:HA | 1.99 | 0.44 |
| 5:M:38:PHE:HD1 | 5:M:56:LEU:HD23 | 1.82 | 0.44 |
| 6:A:67:CYS:O | 6:A:71:GLN:N | 2.50 | 0.44 |
| 6:A:83:HIS:HD2 | 6:A:238:CYS:SG | 2.41 | 0.44 |
| 6:A:426:LEU:H | 6:A:426:LEU:HG | 1.54 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1223:ASP:HB2 | 6:A:1224:LEU:HD12 | 1.99 | 0.44 |
| 6:A:1441:PHE:C | 6:A:1441:PHE:CD2 | 2.90 | 0.44 |
| 7:B:95:ILE:HD12 | 7:B:129:PHE:O | 2.17 | 0.44 |
| 7:B:1060:ARG:HD2 | 7:B:1060:ARG:HA | 1.55 | 0.44 |
| 8:C:50:GLU:OE2 | 15:L:66:GLN:HA | 2.17 | 0.44 |
| 9:E:118:PRO:O | 9:E:121:MET:HB2 | 2.17 | 0.44 |
| 14:K:49:GLU:HG2 | 14:K:94:ILE:HG13 | 2.00 | 0.44 |
| 17:0:37:ASN:ND2 | 17:0:475:PHE:HD2 | 2.16 | 0.44 |
| 17:0:107:GLY:HA2 | 17:0:207:ILE:HB | 1.99 | 0.44 |
| 17:0:714:ILE:HA | 17:0:717:THR:HG22 | 1.99 | 0.44 |
| 17:0:734:GLU:O | 17:0:738:VAL:N | 2.51 | 0.44 |
| 19:6:244:PRO:HB3 | 20:1:230:PRO:HB3 | 2.00 | 0.44 |
| 19:6:441:ASP:HA | 19:6:444:ILE:HD12 | 2.00 | 0.44 |
| 20:1:280:GLU:HA | 20:1:284:TRP:CD1 | 2.52 | 0.44 |
| 21:7:622:MET:H | 21:7:622:MET:HG3 | 1.67 | 0.44 |
| 29:O:185:TYR:CD2 | 29:O:187:PRO:HD3 | 2.53 | 0.44 |
| 2:R:75:MET:CE | 2:R:75:MET:H | 2.30 | 0.44 |
| 2:R:119:GLU:HB3 | 2:R:233:TYR:N | 2.32 | 0.44 |
| 3:D:168:LYS:HD3 | 3:D:168:LYS:HA | 1.84 | 0.44 |
| 4:G:35:GLU:OE1 | 4:G:47:CYS:HA | 2.17 | 0.44 |
| 4:G:114:LEU:HD21 | 4:G:160:ILE:HG23 | 2.00 | 0.44 |
| 6:A:332:LYS:HG3 | 6:A:333:GLU:OE1 | 2.17 | 0.44 |
| 6:A:473:SER:OG | 6:A:650:GLN:NE2 | 2.50 | 0.44 |
| 6:A:965:GLN:HG2 | 6:A:965:GLN:H | 1.47 | 0.44 |
| 6:A:1059:HIS:ND1 | 10:F:87:LYS:HG2 | 2.33 | 0.44 |
| 7:B:240:ILE:O | 7:B:240:ILE:HG13 | 2.17 | 0.44 |
| 7:B:860:MET:SD | 7:B:861:ASP:N | 2.90 | 0.44 |
| 8:C:127:ARG:O | 8:C:129:ILE:N | 2.51 | 0.44 |
| 15:L:30:ILE:HG22 | 15:L:31:CYS:O | 2.18 | 0.44 |
| 17:0:110:SER:OG | 17:0:111:ARG:N | 2.51 | 0.44 |
| 23:2:431:GLN:NE2 | 23:2:435:PRO:HD2 | 2.31 | 0.44 |
| 1:Q:135:LEU:HD23 | 1:Q:136:PRO:HA | 1.99 | 0.44 |
| 3:D:76:LYS:HA | 3:D:76:LYS:HD2 | 1.68 | 0.44 |
| 6:A:332:LYS:HD2 | 6:A:332:LYS:HA | 1.59 | 0.44 |
| 6:A:1227:ILE:O | 6:A:1239:ARG:N | 2.30 | 0.44 |
| 6:A:1404:GLU:O | 6:A:1408:ILE:HG12 | 2.18 | 0.44 |
| 6:A:1443:VAL:HG12 | 6:A:1443:VAL:O | 2.16 | 0.44 |
| 7:B:901:PRO:O | 15:L:61:THR:HG22 | 2.17 | 0.44 |
| 7:B:911:ILE:HG12 | 7:B:939:THR:O | 2.18 | 0.44 |
| 7:B:1155:SER:OG | 7:B:1156:ASP:OD1 | 2.34 | 0.44 |
| 8:C:195:GLN:N | 8:C:200:GLU:OE2 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:E:69:ILE:HA | 9:E:72:PHE:O | 2.17 | 0.44 |
| 14:K:49:GLU:O | 14:K:52:ASN:HB2 | 2.16 | 0.44 |
| 14:K:57:LEU:N | 14:K:76:GLN:O | 2.44 | 0.44 |
| 17:0:666:LEU:HD11 | 17:0:681:LEU:HD21 | 1.99 | 0.44 |
| 21:7:606:ILE:HD13 | 21:7:665:PRO:HG2 | 1.99 | 0.44 |
| 23:2:90:ASN:ND2 | 23:2:99:ASN:OD1 | 2.51 | 0.44 |
| 25:U:258:TRP:NE1 | 26:V:66:LEU:HD23 | 2.32 | 0.44 |
| 1:Q:141:ARG:HB3 | 1:Q:348:TYR:CB | 2.47 | 0.44 |
| 3:D:52:LEU:O | 3:D:152:SER:OG | 2.25 | 0.44 |
| 4:G:153:GLN:HE21 | 4:G:153:GLN:HB2 | 1.48 | 0.44 |
| 5:M:268:GLU:HB3 | 5:M:315:ILE:HD11 | 2.00 | 0.44 |
| 6:A:1217:LYS:C | 6:A:1221:LYS:HG3 | 2.38 | 0.44 |
| 7:B:103:ASN:HB2 | 7:B:169:ARG:HH22 | 1.82 | 0.44 |
| 7:B:260:GLY:O | 7:B:267:ARG:HD3 | 2.18 | 0.44 |
| 8:C:59:ALA:O | 8:C:62:PHE:HB3 | 2.18 | 0.44 |
| 11:H:101:ALA:HB2 | 11:H:116:TYR:CE2 | 2.52 | 0.44 |
| 12:I:101:PHE:N | 12:I:110:PHE:O | 2.42 | 0.44 |
| 18:4:90:SER:HB3 | 19:6:407:GLN:NE2 | 2.32 | 0.44 |
| 20:1:264:PRO:O | 20:1:268:LYS:HG2 | 2.18 | 0.44 |
| 21:7:599:GLU:HA | 21:7:650:ASN:HD22 | 1.83 | 0.44 |
| 21:7:604:LYS:HD3 | 21:7:694:LYS:NZ | 2.33 | 0.44 |
| 21:7:612:VAL:HG13 | 21:7:629:GLY:HA3 | 2.00 | 0.44 |
| 23:2:109:ARG:NH1 | 23:2:109:ARG:HA | 2.33 | 0.44 |
| 24:X:201:THR:HA | 30:W:34:PHE:CB | 2.48 | 0.44 |
| 27:N:20:DT:H4' | 29:O:194:ILE:HD11 | 1.99 | 0.44 |
| 29:O:200:PRO:HG2 | 29:O:226:ALA:HB2 | 1.99 | 0.44 |
| 29:O:220:ARG:HG2 | 29:O:224:TYR:CE2 | 2.53 | 0.44 |
| 30:W:122:TYR:CZ | 30:W:147:PHE:HE2 | 2.35 | 0.44 |
| 1:Q:106:ILE:HG23 | 1:Q:107:PRO:O | 2.18 | 0.44 |
| 5:M:132:LYS:O | 5:M:135:MET:HG2 | 2.18 | 0.44 |
| 6:A:206:GLU:HG3 | 6:A:207:ILE:H | 1.82 | 0.44 |
| 6:A:526:ASP:OD1 | 7:B:1013:ASN:ND2 | 2.41 | 0.44 |
| 6:A:567:LYS:C | 6:A:567:LYS:HD3 | 2.38 | 0.44 |
| 6:A:878:ILE:HG22 | 6:A:879:GLU:N | 2.33 | 0.44 |
| 6:A:1207:LEU:HA | 6:A:1207:LEU:HD23 | 1.68 | 0.44 |
| 7:B:215:GLN:NE2 | 7:B:479:VAL:HG12 | 2.32 | 0.44 |
| 7:B:838:SER:HB2 | 7:B:839:MET:HG2 | 1.99 | 0.44 |
| 7:B:1110:PRO:O | 7:B:1119:VAL:HG13 | 2.16 | 0.44 |
| 12:I:42:LEU:HD12 | 12:I:43:VAL:N | 2.33 | 0.44 |
| 17:0:342:LEU:HA | 17:0:345:ARG:HB2 | 1.99 | 0.44 |
| 17:0:701:LEU:HD12 | 17:0:705:ASP:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:0:709:SER:O | 17:0:713:ALA:N | 2.42 | 0.44 |
| 18:4:136:GLU:HA | 18:4:140:ILE:CG1 | 2.44 | 0.44 |
| 19:6:164:ASN:O | 19:6:167:SER:OG | 2.31 | 0.44 |
| 19:6:349:CYS:SG | 19:6:368:LEU:HD11 | 2.58 | 0.44 |
| 20:1:260:PHE:CG | 20:1:267:LYS:HD3 | 2.53 | 0.44 |
| 24:X:219:GLU:O | 24:X:223:GLN:HG2 | 2.18 | 0.44 |
| 27:N:31:DT:C2 | 27:N:32:DG:C8 | 3.06 | 0.44 |
| 29:O:74:VAL:HG11 | 29:O:152:PHE:CE1 | 2.53 | 0.44 |
| 30:W:28:VAL:HG11 | 30:W:58:ILE:HD13 | 1.98 | 0.44 |
| 1:Q:104:ARG:HA | 2:R:92:LEU:HB3 | 2.00 | 0.44 |
| 2:R:94:LYS:NZ | 2:R:94:LYS:H | 2.15 | 0.44 |
| 3:D:67:ARG:HB3 | 3:D:67:ARG:CZ | 2.48 | 0.44 |
| 4:G:98:GLY:O | 4:G:130:TYR:OH | 2.36 | 0.44 |
| 4:G:148:GLU:HG3 | 4:G:162:SER:HB3 | 1.99 | 0.44 |
| 5:M:186:ALA:HB2 | 5:M:237:THR:OG1 | 2.17 | 0.44 |
| 5:M:186:ALA:HB1 | 5:M:238:TYR:CG | 2.53 | 0.44 |
| 6:A:286:HIS:C | 6:A:287:HIS:HD1 | 2.18 | 0.44 |
| 6:A:333:GLU:N | 6:A:333:GLU:OE2 | 2.50 | 0.44 |
| 6:A:598:LEU:HD23 | 6:A:598:LEU:HA | 1.77 | 0.44 |
| 6:A:811:GLN:O | 6:A:814:PHE:N | 2.51 | 0.44 |
| 7:B:370:PHE:HD1 | 7:B:373:ARG:HE | 1.61 | 0.44 |
| 7:B:461:LEU:HD23 | 7:B:461:LEU:HA | 1.70 | 0.44 |
| 10:F:128:LYS:NZ | 10:F:148:VAL:O | 2.49 | 0.44 |
| 12:I:108:HIS:CE1 | 12:I:110:PHE:HB3 | 2.53 | 0.44 |
| 17:0:276:LYS:HE2 | 17:0:276:LYS:HB2 | 1.89 | 0.44 |
| 21:7:695:ARG:HD3 | 21:7:695:ARG:HA | 1.80 | 0.44 |
| 25:U:258:TRP:HB2 | 25:U:283:ALA:H | 1.82 | 0.44 |
| 30:W:192:SER:HB3 | 30:W:194:ILE:HG13 | 1.99 | 0.44 |
| 3:D:37:GLN:CD | 4:G:5:LYS:HZ1 | 2.20 | 0.44 |
| 4:G:50:ASP:OD2 | 4:G:53:ASN:HB2 | 2.18 | 0.44 |
| 6:A:69:THR:HA | 6:A:71:GLN:NE2 | 2.32 | 0.44 |
| 6:A:276:LEU:HD11 | 6:A:293:GLU:HA | 2.00 | 0.44 |
| 6:A:372:LYS:HD3 | 6:A:397:ASN:O | 2.18 | 0.44 |
| 6:A:567:LYS:HG2 | 6:A:568:PRO:HD2 | 2.00 | 0.44 |
| 6:A:964:ILE:HD13 | 6:A:964:ILE:HA | 1.69 | 0.44 |
| 6:A:1084:PHE:CD2 | 6:A:1086:PHE:HB2 | 2.53 | 0.44 |
| 6:A:1377:THR:O | 6:A:1379:GLY:N | 2.51 | 0.44 |
| 6:A:1381:LEU:HA | 6:A:1381:LEU:HD23 | 1.77 | 0.44 |
| 7:B:68:THR:HG22 | 7:B:91:SER:HA | 1.99 | 0.44 |
| 7:B:1084:GLN:NE2 | 8:C:191:TYR:HA | 2.32 | 0.44 |
| 8:C:220:ASP:OD1 | 8:C:222:LYS:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:F:107:VAL:HG12 | 10:F:109:VAL:H | 1.83 | 0.44 |
| 11:H:13:SER:N | 11:H:27:GLU:O | 2.50 | 0.44 |
| 11:H:82:PRO:CA | 11:H:87:ARG:HD2 | 2.48 | 0.44 |
| 13:J:25:LEU:HA | 13:J:25:LEU:HD23 | 1.67 | 0.44 |
| 18:4:210:ILE:HD13 | 18:4:227:THR:HG21 | 1.99 | 0.44 |
| 24:X:268:LEU:HD21 | 30:W:101:LYS:HE3 | 1.99 | 0.44 |
| 27:N:21:DA:N3 | 29:O:205:LEU:HD11 | 2.32 | 0.44 |
| 30:W:9:VAL:HG22 | 30:W:189:ILE:HD13 | 1.99 | 0.44 |
| 6:A:141:LEU:HD23 | 6:A:141:LEU:HA | 1.79 | 0.43 |
| 6:A:1230:GLU:O | 6:A:1233:ASP:N | 2.43 | 0.43 |
| 7:B:129:PHE:CD1 | 7:B:166:PHE:HA | 2.52 | 0.43 |
| 7:B:408:LEU:HA | 7:B:408:LEU:HD23 | 1.56 | 0.43 |
| 11:H:111:LEU:HD23 | 11:H:111:LEU:HA | 1.60 | 0.43 |
| 12:I:58:VAL:HG11 | 12:I:109:ILE:HD11 | 1.99 | 0.43 |
| 12:I:99:LEU:HA | 12:I:99:LEU:HD23 | 1.74 | 0.43 |
| 12:I:104:LEU:HA | 12:I:104:LEU:HD13 | 1.55 | 0.43 |
| 19:6:134:GLU:N | 19:6:206:GLY:O | 2.45 | 0.43 |
| 21:7:409:VAL:HA | 21:7:486:ILE:HB | 2.00 | 0.43 |
| 23:2:146:ILE:HD12 | 23:2:146:ILE:HA | 1.89 | 0.43 |
| 24:X:157:ASP:O | 24:X:161:GLU:N | 2.45 | 0.43 |
| 3:D:66:ARG:HG2 | 3:D:133:THR:HG22 | 2.00 | 0.43 |
| 4:G:59:GLY:O | 10:F:133:VAL:HG11 | 2.18 | 0.43 |
| 6:A:445:ASN:HA | 6:A:454:SER:O | 2.18 | 0.43 |
| 6:A:732:LEU:HA | 6:A:732:LEU:HD23 | 1.69 | 0.43 |
| 6:A:781:ASP:HB3 | 6:A:790:ASP:OD1 | 2.18 | 0.43 |
| 6:A:785:PRO:HG2 | 6:A:786:HIS:CD2 | 2.53 | 0.43 |
| 6:A:1079:MET:HE2 | 6:A:1359:ASP:HB3 | 1.99 | 0.43 |
| 6:A:1161:THR:HG22 | 6:A:1163:ILE:H | 1.81 | 0.43 |
| 7:B:766:ARG:HD3 | 7:B:766:ARG:HA | 1.62 | 0.43 |
| 7:B:1037:LEU:HD23 | 7:B:1037:LEU:HA | 1.67 | 0.43 |
| 8:C:69:LEU:O | 13:J:6:ARG:HD2 | 2.18 | 0.43 |
| 9:E:30:ILE:HG23 | 9:E:34:GLU:OE1 | 2.18 | 0.43 |
| 17:0:195:ILE:O | 17:0:199:MET:HG2 | 2.18 | 0.43 |
| 17:0:224:ASN:HD21 | 17:0:228:LYS:NZ | 2.15 | 0.43 |
| 17:0:327:ARG:HB3 | 17:0:330:HIS:HB3 | 2.00 | 0.43 |
| 18:4:86:LEU:HD11 | 18:4:132:LEU:HD13 | 1.99 | 0.43 |
| 20:1:346:ASP:HB2 | 20:1:347:PRO:HD3 | 1.99 | 0.43 |
| 21:7:604:LYS:HD3 | 21:7:694:LYS:HZ1 | 1.83 | 0.43 |
| 5:M:174:ALA:O | 5:M:178:ILE:HG12 | 2.17 | 0.43 |
| 6:A:315:LEU:HA | 6:A:321:PRO:HA | 2.00 | 0.43 |
| 6:A:811:GLN:O | 6:A:812:GLU:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:901:LEU:HD22 | 6:A:919:ILE:HG22 | 2.00 | 0.43 |
| 6:A:1208:THR:N | 6:A:1211:GLN:OE1 | 2.40 | 0.43 |
| 7:B:230:ALA:N | 7:B:231:PRO:HD2 | 2.33 | 0.43 |
| 7:B:1084:GLN:HE22 | 8:C:191:TYR:HA | 1.82 | 0.43 |
| 14:K:14:GLU:N | 14:K:16:GLU:OE1 | 2.52 | 0.43 |
| 14:K:29:ASN:HD22 | 14:K:79:GLU:HA | 1.83 | 0.43 |
| 15:L:47:ARG:N | 15:L:53:HIS:O | 2.45 | 0.43 |
| 17:O:171:LEU:HD11 | 17:O:195:ILE:HG21 | 2.00 | 0.43 |
| 17:O:465:PRO:HD2 | 17:O:656:PHE:CD2 | 2.54 | 0.43 |
| 17:O:720:PHE:CZ | 17:O:724:MET:HG3 | 2.53 | 0.43 |
| 18:4:119:ARG:HH22 | 18:4:123:GLU:HG2 | 1.82 | 0.43 |
| 21:7:341:TYR:CD2 | 21:7:343:PHE:HD1 | 2.35 | 0.43 |
| 21:7:421:ARG:NH1 | 21:7:437:VAL:HG11 | 2.33 | 0.43 |
| 2:R:73:LEU:HA | 2:R:224:VAL:HB | 2.00 | 0.43 |
| 5:M:248:LEU:HA | 5:M:249:PRO:HD3 | 1.86 | 0.43 |
| 6:A:107:CYS:HB3 | 6:A:111:GLY:N | 2.34 | 0.43 |
| 6:A:130:ASP:CG | 6:A:133:LYS:HB2 | 2.39 | 0.43 |
| 6:A:657:LEU:HA | 6:A:657:LEU:HD12 | 1.68 | 0.43 |
| 6:A:673:GLY:O | 6:A:676:MET:N | 2.51 | 0.43 |
| 6:A:903:ASN:O | 6:A:907:THR:OG1 | 2.36 | 0.43 |
| 7:B:59:LEU:HD12 | 7:B:59:LEU:HA | 1.50 | 0.43 |
| 7:B:96:TYR:N | 7:B:129:PHE:O | 2.36 | 0.43 |
| 7:B:710:LEU:HA | 7:B:710:LEU:HD13 | 1.55 | 0.43 |
| 7:B:806:THR:OG1 | 7:B:809:MET:HG3 | 2.18 | 0.43 |
| 7:B:884:ARG:HB2 | 7:B:936:ASP:H | 1.83 | 0.43 |
| 7:B:1174:LYS:N | 7:B:1179:GLN:O | 2.51 | 0.43 |
| 8:C:22:LEU:HD12 | 8:C:22:LEU:HA | 1.52 | 0.43 |
| 8:C:67:LEU:HD23 | 8:C:67:LEU:HA | 1.64 | 0.43 |
| 9:E:28:TYR:HA | 9:E:64:PRO:HA | 1.99 | 0.43 |
| 9:E:46:TYR:O | 9:E:54:GLN:N | 2.48 | 0.43 |
| 11:H:93:TYR:CG | 11:H:143:LEU:HD22 | 2.53 | 0.43 |
| 17:O:116:LEU:HD23 | 17:O:158:TYR:CE2 | 2.53 | 0.43 |
| 17:O:460:SER:HB2 | 17:O:463:ILE:HG13 | 1.99 | 0.43 |
| 18:4:258:LEU:CB | 18:4:260:PRO:HD3 | 2.49 | 0.43 |
| 27:N:17:DG:H2'' | 27:N:18:DT:O4' | 2.18 | 0.43 |
| 27:N:17:DG:H2' | 27:N:18:DT:C6 | 2.53 | 0.43 |
| 28:T:146:DA:H5' | 29:O:68:GLN:CD | 2.39 | 0.43 |
| 28:T:150:DG:C4 | 28:T:151:DC:N3 | 2.87 | 0.43 |
| 3:D:153:ARG:HH22 | 3:D:182:SER:C | 2.22 | 0.43 |
| 4:G:4:ILE:HG23 | 4:G:49:LEU:HD11 | 2.01 | 0.43 |
| 5:M:156:LEU:HD23 | 5:M:156:LEU:HA | 1.76 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:944:ARG:NH1 | 6:A:1296:GLY:O | 2.49 | 0.43 |
| 7:B:605:ARG:NH2 | 7:B:691:GLU:OE2 | 2.50 | 0.43 |
| 7:B:614:SER:C | 7:B:615:MET:HG3 | 2.38 | 0.43 |
| 7:B:1096:ARG:O | 7:B:1097:HIS:CG | 2.72 | 0.43 |
| 8:C:10:ILE:HG13 | 14:K:108:GLU:HG2 | 2.01 | 0.43 |
| 10:F:146:TRP:CD1 | 10:F:146:TRP:N | 2.87 | 0.43 |
| 11:H:83:GLN:O | 11:H:85:GLY:N | 2.50 | 0.43 |
| 18:4:78:ALA:HB2 | 18:4:152:ALA:CB | 2.49 | 0.43 |
| 19:6:126:LEU:HB3 | 19:6:160:PHE:CZ | 2.54 | 0.43 |
| 19:6:237:GLY:HA2 | 19:6:266:LEU:HB2 | 2.01 | 0.43 |
| 23:2:378:ILE:HD12 | 23:2:382:SER:HB2 | 2.00 | 0.43 |
| 28:T:152:DG:C5 | 28:T:153:DC:C4 | 3.06 | 0.43 |
| 1:Q:399:ASN:OD1 | 1:Q:402:ALA:HA | 2.19 | 0.43 |
| 2:R:118:HIS:CG | 2:R:120:TYR:HH | 2.36 | 0.43 |
| 5:M:26:GLU:OE2 | 6:A:407:ARG:NH1 | 2.52 | 0.43 |
| 5:M:40:GLU:N | 5:M:40:GLU:OE2 | 2.52 | 0.43 |
| 6:A:359:LEU:HA | 6:A:359:LEU:HD12 | 1.60 | 0.43 |
| 6:A:450:LEU:O | 6:A:451:HIS:CD2 | 2.72 | 0.43 |
| 6:A:1046:LEU:HD12 | 6:A:1046:LEU:HA | 1.70 | 0.43 |
| 6:A:1256:GLU:C | 6:A:1258:HIS:H | 2.22 | 0.43 |
| 6:A:1333:ILE:HA | 6:A:1333:ILE:HD13 | 1.83 | 0.43 |
| 8:C:165:LYS:NZ | 14:K:9:LEU:O | 2.30 | 0.43 |
| 9:E:153:HIS:O | 9:E:154:ILE:HD13 | 2.19 | 0.43 |
| 12:I:19:ASP:CB | 12:I:24:ARG:H | 2.19 | 0.43 |
| 17:O:350:HIS:ND1 | 30:W:184:ASP:OD2 | 2.52 | 0.43 |
| 19:6:124:ARG:HA | 19:6:229:THR:N | 2.33 | 0.43 |
| 19:6:129:THR:HA | 19:6:172:ILE:HB | 2.00 | 0.43 |
| 21:7:546:LYS:HA | 21:7:546:LYS:HD2 | 1.84 | 0.43 |
| 28:T:137:DA:C2 | 28:T:138:DG:C4 | 3.07 | 0.43 |
| 29:O:205:LEU:O | 29:O:213:VAL:N | 2.41 | 0.43 |
| 4:G:97:HIS:H | 4:G:97:HIS:CD2 | 2.36 | 0.43 |
| 4:G:131:GLN:N | 4:G:131:GLN:OE1 | 2.51 | 0.43 |
| 6:A:118:HIS:C | 6:A:123:ARG:HH12 | 2.22 | 0.43 |
| 6:A:360:GLU:HB2 | 6:A:363:GLN:OE1 | 2.18 | 0.43 |
| 6:A:1191:TRP:HD1 | 6:A:1256:GLU:OE1 | 2.01 | 0.43 |
| 7:B:245:GLU:H | 7:B:245:GLU:CD | 2.18 | 0.43 |
| 7:B:355:ILE:HD13 | 7:B:355:ILE:HA | 1.79 | 0.43 |
| 7:B:706:GLN:H | 7:B:710:LEU:CD2 | 2.27 | 0.43 |
| 7:B:848:ARG:HB3 | 13:J:8:PHE:HD1 | 1.83 | 0.43 |
| 11:H:84:ALA:N | 14:K:54:ARG:HH12 | 2.17 | 0.43 |
| 15:L:33:GLU:HB2 | 15:L:53:HIS:NE2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:659:MET:HA | 17:0:662:ALA:HB3 | 1.99 | 0.43 |
| 25:U:262:LEU:O | 25:U:279:ALA:N | 2.49 | 0.43 |
| 28:T:137:DA:C4 | 28:T:138:DG:C8 | 3.07 | 0.43 |
| 1:Q:342:LEU:O | 1:Q:346:GLU:HG3 | 2.18 | 0.43 |
| 3:D:215:SER:HA | 3:D:218:GLU:HG2 | 2.01 | 0.43 |
| 6:A:935:GLN:NE2 | 6:A:935:GLN:O | 2.51 | 0.43 |
| 6:A:1047:SER:OG | 6:A:1048:ASN:N | 2.52 | 0.43 |
| 6:A:1333:ILE:HD13 | 6:A:1381:LEU:HD12 | 2.00 | 0.43 |
| 8:C:136:ASP:OD2 | 8:C:140:ASN:N | 2.52 | 0.43 |
| 11:H:61:SER:O | 11:H:139:ASN:ND2 | 2.48 | 0.43 |
| 13:J:22:LEU:HA | 13:J:22:LEU:HD23 | 1.70 | 0.43 |
| 18:4:28:VAL:HG13 | 18:4:57:LEU:HD21 | 2.00 | 0.43 |
| 19:6:231:GLU:HA | 19:6:260:ARG:O | 2.19 | 0.43 |
| 21:7:387:PRO:HB3 | 21:7:540:TRP:CH2 | 2.54 | 0.43 |
| 21:7:443:LYS:HD3 | 21:7:444:GLU:N | 2.34 | 0.43 |
| 21:7:584:ASN:HB3 | 21:7:587:LYS:HB3 | 2.01 | 0.43 |
| 23:2:428:GLU:OE1 | 23:2:428:GLU:N | 2.52 | 0.43 |
| 28:T:21:DC:H2' | 28:T:22:DT:H6 | 1.81 | 0.43 |
| 28:T:147:DT:H5' | 29:O:211:LYS:HE2 | 2.00 | 0.43 |
| 29:O:102:VAL:N | 29:O:115:ILE:O | 2.37 | 0.43 |
| 30:W:179:ILE:HG23 | 30:W:183:ILE:HG23 | 2.00 | 0.43 |
| 1:Q:353:GLU:OE1 | 1:Q:353:GLU:N | 2.52 | 0.43 |
| 1:Q:376:LEU:HD12 | 2:R:69:TRP:HB3 | 2.00 | 0.43 |
| 2:R:79:GLU:N | 2:R:79:GLU:OE1 | 2.52 | 0.43 |
| 3:D:142:LYS:HA | 3:D:142:LYS:HD3 | 1.74 | 0.43 |
| 4:G:138:THR:O | 4:G:141:SER:OG | 2.17 | 0.43 |
| 5:M:177:LEU:HD11 | 5:M:181:ARG:HH21 | 1.83 | 0.43 |
| 6:A:573:SER:OG | 6:A:574:GLY:N | 2.51 | 0.43 |
| 6:A:913:LEU:HD11 | 6:A:981:LEU:O | 2.18 | 0.43 |
| 7:B:102:VAL:CG1 | 7:B:112:LEU:HD22 | 2.48 | 0.43 |
| 8:C:143:LEU:HG | 13:J:2:ILE:HD11 | 2.00 | 0.43 |
| 8:C:215:GLU:N | 8:C:215:GLU:CD | 2.71 | 0.43 |
| 9:E:215:MET:HE3 | 9:E:215:MET:HB3 | 1.91 | 0.43 |
| 11:H:24:CYS:HB2 | 11:H:44:VAL:HG11 | 2.01 | 0.43 |
| 15:L:29:TYR:O | 15:L:30:ILE:HD13 | 2.18 | 0.43 |
| 17:0:428:ALA:O | 17:0:430:VAL:HG13 | 2.19 | 0.43 |
| 18:4:25:LEU:HB3 | 18:4:174:SER:HB3 | 2.00 | 0.43 |
| 18:4:236:LEU:HD22 | 18:4:238:VAL:HG12 | 2.00 | 0.43 |
| 21:7:303:ARG:HG3 | 21:7:320:ASN:C | 2.39 | 0.43 |
| 21:7:385:VAL:HG23 | 21:7:538:ALA:N | 2.34 | 0.43 |
| 21:7:548:HIS:HB3 | 21:7:693:ALA:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:586:THR:O | 21:7:590:ALA:N | 2.37 | 0.43 |
| 24:X:260:VAL:HG22 | 30:W:20:PHE:HA | 2.01 | 0.43 |
| 1:Q:141:ARG:HB3 | 1:Q:348:TYR:HB2 | 2.00 | 0.43 |
| 1:Q:362:VAL:O | 1:Q:395:PHE:HA | 2.19 | 0.43 |
| 3:D:123:LEU:HD22 | 3:D:149:THR:HB | 2.00 | 0.43 |
| 3:D:188:ALA:O | 3:D:192:LYS:HG3 | 2.18 | 0.43 |
| 4:G:38:CYS:O | 4:G:155:SER:HA | 2.18 | 0.43 |
| 6:A:116:ASP:HA | 6:A:117:GLU:HA | 1.61 | 0.43 |
| 6:A:933:TYR:O | 6:A:937:VAL:HG13 | 2.18 | 0.43 |
| 6:A:981:LEU:HD21 | 6:A:1039:LYS:HA | 2.01 | 0.43 |
| 6:A:1032:LEU:HD23 | 6:A:1032:LEU:HA | 1.77 | 0.43 |
| 6:A:1032:LEU:O | 6:A:1036:ARG:HG2 | 2.18 | 0.43 |
| 9:E:180:ARG:HH12 | 9:E:192:ARG:HB2 | 1.83 | 0.43 |
| 12:I:55:THR:H | 12:I:120:GLN:CD | 2.22 | 0.43 |
| 14:K:108:GLU:HA | 14:K:111:LEU:HD22 | 2.00 | 0.43 |
| 17:0:524:SER:HA | 17:0:527:VAL:HG12 | 2.01 | 0.43 |
| 18:4:28:VAL:HG22 | 18:4:57:LEU:HD11 | 2.01 | 0.43 |
| 18:4:117:ARG:HA | 18:4:120:ASN:ND2 | 2.33 | 0.43 |
| 19:6:173:ILE:HG13 | 19:6:180:GLN:HB2 | 2.01 | 0.43 |
| 20:1:258:ASN:O | 20:1:261:GLU:HG3 | 2.18 | 0.43 |
| 29:O:132:SER:O | 29:O:136:SER:OG | 2.37 | 0.43 |
| 1:Q:108:LYS:HE2 | 1:Q:108:LYS:HB2 | 1.76 | 0.42 |
| 1:Q:127:ILE:HG12 | 1:Q:129:PRO:HD3 | 2.01 | 0.42 |
| 3:D:44:GLU:HG2 | 3:D:45:GLU:N | 2.34 | 0.42 |
| 3:D:208:GLU:C | 3:D:212:LYS:HZ3 | 2.22 | 0.42 |
| 6:A:70:CYS:O | 6:A:72:GLU:N | 2.47 | 0.42 |
| 6:A:1224:LEU:O | 6:A:1226:VAL:HG23 | 2.19 | 0.42 |
| 6:A:1436:ILE:HA | 6:A:1436:ILE:HD13 | 1.76 | 0.42 |
| 7:B:234:ILE:HG21 | 7:B:257:LYS:HB3 | 2.01 | 0.42 |
| 7:B:578:THR:HG23 | 7:B:622:LYS:C | 2.40 | 0.42 |
| 7:B:847:ASP:HB3 | 8:C:167:HIS:CE1 | 2.54 | 0.42 |
| 7:B:1010:LEU:HD12 | 7:B:1010:LEU:HA | 1.64 | 0.42 |
| 8:C:4:GLU:OE1 | 8:C:4:GLU:N | 2.51 | 0.42 |
| 8:C:179:GLU:HG2 | 8:C:180:TYR:N | 2.34 | 0.42 |
| 8:C:190:ASP:OD1 | 8:C:191:TYR:N | 2.52 | 0.42 |
| 9:E:81:GLU:HG2 | 9:E:96:PHE:CD1 | 2.54 | 0.42 |
| 10:F:99:LEU:O | 10:F:103:MET:HG3 | 2.18 | 0.42 |
| 21:7:230:ASN:O | 21:7:345:ASN:HB3 | 2.19 | 0.42 |
| 21:7:449:GLU:HG3 | 21:7:453:VAL:HG22 | 2.00 | 0.42 |
| 23:2:481:LEU:HD21 | 23:2:491:PHE:CG | 2.54 | 0.42 |
| 29:O:113:ALA:HB2 | 29:O:139:TYR:CE2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:O:123:VAL:HG21 | 29:O:136:SER:OG | 2.19 | 0.42 |
| 5:M:215:ARG:O | 5:M:218:SER:OG | 2.35 | 0.42 |
| 6:A:214:ILE:HG22 | 6:A:218:ASP:OD1 | 2.18 | 0.42 |
| 6:A:446:ARG:HB2 | 6:A:487:MET:CE | 2.49 | 0.42 |
| 6:A:457:ALA:O | 6:A:507:VAL:HG23 | 2.19 | 0.42 |
| 6:A:860:LEU:HB2 | 6:A:862:ASN:OD1 | 2.19 | 0.42 |
| 6:A:1022:LEU:HA | 6:A:1022:LEU:HD12 | 1.72 | 0.42 |
| 6:A:1104:ILE:HG22 | 6:A:1105:LEU:HD23 | 2.01 | 0.42 |
| 6:A:1263:ILE:O | 6:A:1267:MET:HG2 | 2.19 | 0.42 |
| 6:A:1442:ASP:HA | 10:F:134:ILE:O | 2.19 | 0.42 |
| 7:B:555:ILE:HA | 7:B:558:LEU:HD12 | 2.01 | 0.42 |
| 7:B:617:ARG:NH2 | 12:I:61:ASP:OD1 | 2.42 | 0.42 |
| 7:B:1072:MET:HE2 | 7:B:1072:MET:HB3 | 1.95 | 0.42 |
| 18:4:33:ALA:O | 18:4:37:TRP:N | 2.30 | 0.42 |
| 19:6:133:SER:HB2 | 19:6:207:ASN:HA | 2.01 | 0.42 |
| 20:1:613:THR:O | 20:1:617:LYS:N | 2.52 | 0.42 |
| 21:7:397:ILE:HD12 | 21:7:430:LEU:HD22 | 1.99 | 0.42 |
| 21:7:403:ILE:HD11 | 21:7:407:VAL:HG22 | 2.01 | 0.42 |
| 23:2:481:LEU:HD13 | 23:2:484:LYS:HB3 | 2.02 | 0.42 |
| 24:X:193:LEU:O | 24:X:197:ARG:HG3 | 2.19 | 0.42 |
| 30:W:8:ILE:O | 30:W:12:LEU:N | 2.52 | 0.42 |
| 1:Q:121:PHE:HD1 | 1:Q:361:TRP:CD2 | 2.37 | 0.42 |
| 4:G:64:THR:C | 4:G:66:GLY:H | 2.22 | 0.42 |
| 5:M:157:CYS:HB2 | 5:M:163:LEU:HD11 | 2.01 | 0.42 |
| 6:A:61:ILE:HA | 6:A:74:MET:HE1 | 2.02 | 0.42 |
| 6:A:436:ILE:HD12 | 6:A:436:ILE:HG23 | 1.71 | 0.42 |
| 6:A:1266:THR:HB | 6:A:1267:MET:HE2 | 2.01 | 0.42 |
| 7:B:334:ILE:H | 7:B:334:ILE:HG12 | 1.65 | 0.42 |
| 7:B:563:MET:HA | 7:B:589:VAL:O | 2.18 | 0.42 |
| 9:E:101:GLN:CD | 9:E:101:GLN:N | 2.70 | 0.42 |
| 10:F:96:THR:O | 10:F:100:GLN:HG3 | 2.19 | 0.42 |
| 11:H:42:ILE:HG23 | 11:H:95:TYR:CE2 | 2.55 | 0.42 |
| 11:H:54:SER:HB3 | 11:H:146:ARG:HD3 | 2.01 | 0.42 |
| 15:L:31:CYS:SG | 15:L:34:CYS:SG | 3.17 | 0.42 |
| 17:0:52:LEU:HD22 | 17:0:233:ILE:HD13 | 2.02 | 0.42 |
| 17:0:236:GLU:HB3 | 17:0:238:HIS:HE1 | 1.84 | 0.42 |
| 17:0:338:LEU:HD23 | 17:0:342:LEU:HD23 | 2.01 | 0.42 |
| 19:6:233:LEU:HA | 19:6:262:LYS:O | 2.20 | 0.42 |
| 19:6:233:LEU:HD21 | 19:6:264:LEU:HD22 | 2.01 | 0.42 |
| 20:1:256:ILE:HG13 | 20:1:257:LEU:N | 2.34 | 0.42 |
| 21:7:659:ASP:HA | 21:7:660:THR:HA | 1.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:2:110:ASN:O | 23:2:115:GLY:N | 2.52 | 0.42 |
| 29:O:175:LEU:HA | 29:O:237:PHE:CE2 | 2.54 | 0.42 |
| 2:R:126:LYS:HG2 | 2:R:128:VAL:O | 2.19 | 0.42 |
| 3:D:204:ASP:O | 3:D:207:LEU:HB2 | 2.19 | 0.42 |
| 4:G:146:LYS:O | 4:G:161:GLY:HA2 | 2.20 | 0.42 |
| 5:M:118:VAL:O | 5:M:124:ASN:HB3 | 2.19 | 0.42 |
| 6:A:367:PRO:HG3 | 6:A:466:SER:O | 2.19 | 0.42 |
| 6:A:501:LEU:HD23 | 6:A:501:LEU:HA | 1.65 | 0.42 |
| 6:A:562:THR:HA | 11:H:79:TRP:HB2 | 2.02 | 0.42 |
| 6:A:664:THR:OG1 | 6:A:668:ASP:OD2 | 2.28 | 0.42 |
| 7:B:933:SER:OG | 7:B:934:LYS:N | 2.52 | 0.42 |
| 7:B:1207:LEU:HD23 | 7:B:1207:LEU:HA | 1.57 | 0.42 |
| 17:O:173:LYS:HD2 | 17:O:173:LYS:HA | 1.86 | 0.42 |
| 17:0:349:LEU:HB3 | 30:W:180:GLN:HG2 | 2.01 | 0.42 |
| 17:0:372:LYS:HB2 | 17:0:373:PRO:HD3 | 2.01 | 0.42 |
| 19:6:216:MET:HE3 | 19:6:220:LEU:HD13 | 2.01 | 0.42 |
| 19:6:352:CYS:SG | 19:6:354:SER:OG | 2.57 | 0.42 |
| 21:7:606:ILE:HG12 | 21:7:652:ILE:HD11 | 2.01 | 0.42 |
| 23:2:410:ARG:HA | 23:2:413:GLU:HB2 | 2.01 | 0.42 |
| 25:U:252:THR:OG1 | 25:U:259:LYS:HB2 | 2.20 | 0.42 |
| 27:N:31:DT:O2 | 28:T:135:DA:H2 | 2.03 | 0.42 |
| 28:T:141:DT:H2" | 29:O:99:PHE:CG | 2.54 | 0.42 |
| 28:T:146:DA:C6 | 28:T:147:DT:C4 | 3.07 | 0.42 |
| 4:G:57:GLN:HG2 | 4:G:58:ARG:N | 2.34 | 0.42 |
| 6:A:123:ARG:NH1 | 6:A:123:ARG:HB2 | 2.33 | 0.42 |
| 6:A:135:PHE:HB2 | 6:A:222:LEU:O | 2.20 | 0.42 |
| 6:A:351:THR:O | 6:A:486:GLU:HB3 | 2.20 | 0.42 |
| 6:A:593:GLU:C | 6:A:593:GLU:CD | 2.77 | 0.42 |
| 6:A:1001:ARG:NH1 | 10:F:82:THR:HA | 2.33 | 0.42 |
| 6:A:1211:GLN:HA | 6:A:1214:GLU:HG2 | 2.00 | 0.42 |
| 6:A:1389:PHE:CG | 6:A:1390:ASN:N | 2.87 | 0.42 |
| 6:A:1390:ASN:O | 6:A:1399:ARG:HD2 | 2.20 | 0.42 |
| 7:B:757:PRO:CG | 7:B:983:ARG:HH21 | 2.32 | 0.42 |
| 8:C:241:ASP:OD2 | 14:K:109:TRP:NE1 | 2.53 | 0.42 |
| 9:E:186:LEU:O | 9:E:189:GLY:N | 2.52 | 0.42 |
| 10:F:71:GLU:HA | 10:F:72:LYS:HA | 1.74 | 0.42 |
| 11:H:135:LEU:HA | 11:H:135:LEU:HD23 | 1.66 | 0.42 |
| 12:I:5:ARG:HB3 | 12:I:5:ARG:CZ | 2.48 | 0.42 |
| 12:I:24:ARG:H | 12:I:24:ARG:HG3 | 1.72 | 0.42 |
| 12:I:77:LYS:HE2 | 12:I:77:LYS:HB3 | 1.69 | 0.42 |
| 16:3:140:ASN:O | 16:3:144:ILE:N | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:0:57:ILE:HG22 | 17:0:93:ARG:HH21 | 1.84 | 0.42 |
| 17:0:525:MET:O | 17:0:529:PHE:HD2 | 2.02 | 0.42 |
| 17:0:685:ARG:HB3 | 17:0:689:LYS:NZ | 2.35 | 0.42 |
| 18:4:279:THR:HG21 | 18:4:281:ARG:HE | 1.85 | 0.42 |
| 19:6:136:MET:O | 19:6:145:ARG:HB2 | 2.19 | 0.42 |
| 21:7:352:LEU:O | 21:7:404:LYS:NZ | 2.53 | 0.42 |
| 21:7:408:ILE:HG13 | 21:7:485:ILE:HG13 | 2.02 | 0.42 |
| 28:T:147:DT:H5' | 29:O:211:LYS:HG3 | 2.01 | 0.42 |
| 30:W:122:TYR:HD2 | 30:W:156:LEU:HB2 | 1.83 | 0.42 |
| 1:Q:114:MET:HA | 2:R:137:GLU:O | 2.19 | 0.42 |
| 1:Q:119:LEU:HB2 | 2:R:133:TYR:H | 1.85 | 0.42 |
| 1:Q:124:LYS:HG2 | 1:Q:126:LYS:HZ2 | 1.84 | 0.42 |
| 3:D:166:LEU:O | 3:D:170:THR:HG23 | 2.18 | 0.42 |
| 4:G:119:LEU:HA | 4:G:132:SER:HA | 2.00 | 0.42 |
| 5:M:200:THR:HA | 5:M:203:PHE:HB3 | 2.00 | 0.42 |
| 6:A:329:LEU:HD22 | 6:A:335:ARG:HB2 | 2.02 | 0.42 |
| 6:A:662:PHE:HD2 | 7:B:829:CYS:SG | 2.43 | 0.42 |
| 6:A:668:ASP:CG | 6:A:742:ASN:HD22 | 2.22 | 0.42 |
| 6:A:709:THR:HB | 6:A:712:GLU:HG3 | 2.01 | 0.42 |
| 6:A:1140:HIS:NE2 | 6:A:1272:THR:OG1 | 2.35 | 0.42 |
| 6:A:1359:ASP:OD1 | 6:A:1360:GLY:N | 2.52 | 0.42 |
| 7:B:1074:ASN:OD1 | 7:B:1076:HIS:N | 2.53 | 0.42 |
| 8:C:76:ASP:C | 8:C:129:ILE:HD11 | 2.40 | 0.42 |
| 10:F:116:ASP:HB3 | 10:F:119:ARG:CG | 2.49 | 0.42 |
| 10:F:140:ASP:OD1 | 10:F:142:SER:N | 2.35 | 0.42 |
| 12:I:21:GLU:N | 12:I:21:GLU:CD | 2.73 | 0.42 |
| 14:K:36:GLU:HB3 | 14:K:37:LYS:HE2 | 2.01 | 0.42 |
| 18:4:67:PHE:CD1 | 18:4:253:PHE:HZ | 2.37 | 0.42 |
| 21:7:350:PRO:HG2 | 21:7:480:ARG:HH22 | 1.85 | 0.42 |
| 21:7:355:ASP:OD2 | 21:7:357:LYS:NZ | 2.49 | 0.42 |
| 21:7:594:LEU:HD22 | 21:7:598:HIS:HE1 | 1.85 | 0.42 |
| 24:X:206:SER:OG | 24:X:207:CYS:N | 2.52 | 0.42 |
| 29:O:160:ILE:O | 29:O:215:THR:HA | 2.20 | 0.42 |
| 29:O:163:SER:HB3 | 29:O:213:VAL:HG13 | 2.01 | 0.42 |
| 4:G:26:LEU:HA | 4:G:26:LEU:HD23 | 1.64 | 0.42 |
| 5:M:268:GLU:C | 5:M:270:ALA:H | 2.23 | 0.42 |
| 6:A:149:GLU:O | 6:A:164:ARG:NH1 | 2.52 | 0.42 |
| 7:B:192:LEU:HD23 | 7:B:192:LEU:HA | 1.73 | 0.42 |
| 8:C:80:LEU:HD12 | 8:C:80:LEU:HA | 1.78 | 0.42 |
| 8:C:101:LEU:HD12 | 8:C:101:LEU:HA | 1.79 | 0.42 |
| 8:C:137:LYS:HE3 | 8:C:137:LYS:HB3 | 1.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:H:108:SER:OG | 11:H:109:LYS:N | 2.51 | 0.42 |
| 12:I:59:VAL:HG23 | 12:I:61:ASP:N | 2.34 | 0.42 |
| 14:K:16:GLU:OE1 | 14:K:16:GLU:N | 2.52 | 0.42 |
| 21:7:626:PHE:O | 21:7:628:TYR:HD1 | 2.03 | 0.42 |
| 1:Q:342:LEU:HB3 | 1:Q:343:ARG:HH22 | 1.85 | 0.42 |
| 2:R:92:LEU:HD12 | 2:R:93:GLY:O | 2.19 | 0.42 |
| 3:D:37:GLN:HG2 | 3:D:47:LEU:HA | 2.00 | 0.42 |
| 6:A:871:ASP:OD1 | 6:A:871:ASP:C | 2.57 | 0.42 |
| 6:A:912:LEU:O | 6:A:979:SER:HB3 | 2.20 | 0.42 |
| 6:A:1148:ILE:HG23 | 12:I:49:ILE:HG13 | 2.02 | 0.42 |
| 6:A:1172:LEU:O | 6:A:1174:PHE:N | 2.53 | 0.42 |
| 7:B:125:SER:HA | 7:B:171:PRO:HA | 2.01 | 0.42 |
| 7:B:590:HIS:CD2 | 7:B:591:ARG:O | 2.73 | 0.42 |
| 7:B:1132:GLU:H | 7:B:1132:GLU:HG2 | 1.62 | 0.42 |
| 8:C:214:ASN:HB3 | 8:C:217:ASP:OD2 | 2.19 | 0.42 |
| 9:E:79:TRP:CD1 | 9:E:96:PHE:HE1 | 2.36 | 0.42 |
| 11:H:26:ILE:HD13 | 11:H:26:ILE:HA | 1.56 | 0.42 |
| 11:H:50:ALA:H | 11:H:53:ASP:CG | 2.15 | 0.42 |
| 11:H:110:ASP:O | 11:H:111:LEU:HD23 | 2.19 | 0.42 |
| 15:L:31:CYS:SG | 15:L:34:CYS:CA | 3.06 | 0.42 |
| 15:L:34:CYS:SG | 15:L:36:SER:CB | 3.08 | 0.42 |
| 19:6:142:ARG:NH1 | 19:6:294:GLU:OE2 | 2.52 | 0.42 |
| 21:7:431:GLN:N | 21:7:431:GLN:OE1 | 2.53 | 0.42 |
| 21:7:477:LEU:HA | 21:7:482:TRP:NE1 | 2.34 | 0.42 |
| 23:2:19:GLN:HG3 | 23:2:85:HIS:CG | 2.55 | 0.42 |
| 29:O:63:ILE:HB | 29:O:227:PHE:CZ | 2.54 | 0.42 |
| 30:W:5:ILE:HG13 | 30:W:192:SER:OG | 2.20 | 0.42 |
| 3:D:174:PRO:O | 3:D:177:VAL:HG22 | 2.19 | 0.42 |
| 4:G:3:PHE:O | 4:G:77:VAL:HA | 2.20 | 0.42 |
| 5:M:166:LYS:HA | 5:M:166:LYS:HD3 | 1.83 | 0.42 |
| 6:A:10:PRO:HD2 | 7:B:1191:ILE:O | 2.20 | 0.42 |
| 6:A:21:LEU:HD11 | 6:A:1414:ALA:HA | 2.01 | 0.42 |
| 6:A:279:LEU:HB3 | 6:A:289:ILE:CD1 | 2.50 | 0.42 |
| 6:A:374:LEU:HA | 6:A:374:LEU:HD23 | 1.79 | 0.42 |
| 6:A:451:HIS:HB3 | 6:A:453:MET:N | 2.35 | 0.42 |
| 6:A:525:GLN:CD | 7:B:836:GLU:HG2 | 2.40 | 0.42 |
| 7:B:319:GLU:HG2 | 12:I:15:TYR:OH | 2.20 | 0.42 |
| 13:J:23:ASN:O | 13:J:27:GLU:HG2 | 2.20 | 0.42 |
| 14:K:19:LEU:HA | 14:K:19:LEU:HD23 | 1.74 | 0.42 |
| 17:0:360:LEU:O | 17:0:364:LYS:N | 2.46 | 0.42 |
| 19:6:451:CYS:HB3 | 19:6:454:CYS:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:7:581:TYR:CE1 | 21:7:714:GLN:HB3 | 2.55 | 0.42 |
| 27:N:23:DA:N1 | 28:T:144:DA:N6 | 2.68 | 0.42 |
| 28:T:157:DT:C4 | 28:T:158:DT:C4 | 3.07 | 0.42 |
| 3:D:40:HIS:CE1 | 4:G:6:ASP:HB3 | 2.54 | 0.42 |
| 4:G:64:THR:OG1 | 4:G:65:ASP:N | 2.53 | 0.42 |
| 5:M:54:ASP:OD1 | 5:M:55:LYS:N | 2.53 | 0.42 |
| 5:M:283:TYR:HA | 5:M:286:ILE:HG22 | 2.01 | 0.42 |
| 6:A:507:VAL:O | 6:A:510:GLN:N | 2.37 | 0.42 |
| 6:A:803:SER:HG | 6:A:805:LEU:H | 1.63 | 0.42 |
| 6:A:1111:MET:HB3 | 6:A:1111:MET:HE2 | 1.40 | 0.42 |
| 6:A:1153:TYR:CD1 | 6:A:1163:ILE:HD11 | 2.55 | 0.42 |
| 6:A:1409:LEU:HA | 6:A:1409:LEU:HD23 | 1.62 | 0.42 |
| 6:A:1442:ASP:HB2 | 10:F:136:ARG:CA | 2.50 | 0.42 |
| 7:B:852:ARG:HH11 | 7:B:852:ARG:HD3 | 1.69 | 0.42 |
| 8:C:5:GLY:HA3 | 8:C:6:PRO:HD3 | 1.87 | 0.42 |
| 9:E:88:VAL:HG21 | 9:E:110:PHE:HE1 | 1.83 | 0.42 |
| 11:H:79:TRP:CH2 | 11:H:81:PRO:HA | 2.54 | 0.42 |
| 17:0:428:ALA:O | 30:W:11:ASN:HB3 | 2.20 | 0.42 |
| 17:0:726:GLN:NE2 | 19:6:290:ILE:HG13 | 2.35 | 0.42 |
| 21:7:410:LEU:O | 21:7:488:ASP:N | 2.53 | 0.42 |
| 23:2:422:LEU:HA | 23:2:425:ASN:OD1 | 2.20 | 0.42 |
| 23:2:446:LEU:O | 23:2:450:ARG:N | 2.42 | 0.42 |
| 27:N:29:DT:C2 | 28:T:138:DG:C2 | 3.08 | 0.42 |
| 28:T:146:DA:H2 | 29:O:207:PHE:HZ | 1.68 | 0.42 |
| 29:O:179:HIS:CD2 | 29:O:237:PHE:HE2 | 2.38 | 0.42 |
| 2:R:99:LYS:HD2 | 2:R:99:LYS:HA | 1.89 | 0.41 |
| 3:D:176:GLU:H | 3:D:176:GLU:HG3 | 1.59 | 0.41 |
| 5:M:188:THR:HG23 | 29:O:188:GLU:CD | 2.41 | 0.41 |
| 6:A:129:LYS:HB2 | 6:A:129:LYS:HE2 | 1.84 | 0.41 |
| 6:A:968:GLN:O | 6:A:972:HIS:N | 2.53 | 0.41 |
| 6:A:1267:MET:HE2 | 6:A:1267:MET:N | 2.35 | 0.41 |
| 7:B:45:SER:OG | 7:B:46:GLN:N | 2.53 | 0.41 |
| 7:B:68:THR:O | 7:B:69:LEU:HD23 | 2.20 | 0.41 |
| 7:B:420:LEU:HD11 | 7:B:456:GLY:HA3 | 2.01 | 0.41 |
| 7:B:468:GLU:O | 7:B:471:LYS:N | 2.53 | 0.41 |
| 7:B:471:LYS:HB3 | 7:B:471:LYS:HE2 | 1.75 | 0.41 |
| 7:B:586:TRP:CD1 | 7:B:586:TRP:C | 2.91 | 0.41 |
| 7:B:647:GLY:N | 7:B:648:HIS:C | 2.73 | 0.41 |
| 7:B:910:VAL:HA | 7:B:940:PRO:HA | 2.02 | 0.41 |
| 11:H:58:THR:O | 11:H:143:LEU:N | 2.51 | 0.41 |
| 11:H:61:SER:HB2 | 11:H:139:ASN:HD21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:17:ARG:HD3 | 12:I:28:GLU:OE2 | 2.20 | 0.41 |
| 14:K:47:ARG:HE | 14:K:47:ARG:HB3 | 1.61 | 0.41 |
| 17:0:584:GLU:HG3 | 17:0:585:THR:N | 2.35 | 0.41 |
| 17:0:590:CYS:SG | 17:0:596:ALA:HB3 | 2.60 | 0.41 |
| 18:4:299:ILE:N | 18:4:300:PRO:HD2 | 2.34 | 0.41 |
| 21:7:420:TRP:O | 21:7:423:GLN:HG2 | 2.20 | 0.41 |
| 23:2:365:HIS:ND1 | 23:2:365:HIS:O | 2.53 | 0.41 |
| 23:2:503:ASP:OD1 | 23:2:507:ARG:NH1 | 2.53 | 0.41 |
| 29:O:106:ILE:HD11 | 29:O:135:ALA:HA | 2.02 | 0.41 |
| 1:Q:337:GLU:OE2 | 1:Q:339:ALA:HB3 | 2.20 | 0.41 |
| 3:D:40:HIS:CE1 | 4:G:74:TYR:H | 2.37 | 0.41 |
| 3:D:167:LEU:HA | 3:D:170:THR:CG2 | 2.50 | 0.41 |
| 3:D:188:ALA:HB1 | 3:D:207:LEU:HD12 | 2.02 | 0.41 |
| 6:A:57:ARG:HB2 | 6:A:68:GLN:CB | 2.50 | 0.41 |
| 6:A:102:VAL:O | 6:A:105:CYS:N | 2.49 | 0.41 |
| 6:A:239:LEU:HD12 | 6:A:239:LEU:HA | 1.76 | 0.41 |
| 6:A:496:GLU:H | 6:A:496:GLU:CD | 2.17 | 0.41 |
| 6:A:595:THR:H | 6:A:595:THR:HG23 | 1.55 | 0.41 |
| 6:A:1127:ASP:CG | 6:A:1130:GLN:H | 2.23 | 0.41 |
| 6:A:1150:SER:O | 12:I:45:ARG:HA | 2.20 | 0.41 |
| 6:A:1225:PHE:CZ | 6:A:1227:ILE:HD11 | 2.56 | 0.41 |
| 7:B:48:LEU:HA | 7:B:48:LEU:HD23 | 1.69 | 0.41 |
| 7:B:555:ILE:H | 7:B:555:ILE:HG13 | 1.42 | 0.41 |
| 7:B:710:LEU:O | 7:B:733:HIS:HB3 | 2.20 | 0.41 |
| 7:B:755:ILE:HD12 | 7:B:755:ILE:HG23 | 1.82 | 0.41 |
| 7:B:882:THR:O | 7:B:884:ARG:N | 2.53 | 0.41 |
| 9:E:43:LYS:O | 9:E:47:CYS:HB2 | 2.20 | 0.41 |
| 9:E:48:ASP:N | 9:E:52:ARG:O | 2.37 | 0.41 |
| 10:F:97:ARG:HD2 | 10:F:97:ARG:HA | 1.71 | 0.41 |
| 12:I:68:LEU:HB3 | 12:I:84:VAL:HG13 | 2.02 | 0.41 |
| 16:3:128:LYS:O | 16:3:132:LYS:N | 2.47 | 0.41 |
| 17:0:184:TYR:CE1 | 17:0:188:LYS:HG3 | 2.54 | 0.41 |
| 17:0:357:LYS:HB2 | 17:0:413:GLU:OE1 | 2.20 | 0.41 |
| 17:0:581:LEU:HA | 17:0:584:GLU:HG2 | 2.00 | 0.41 |
| 19:6:120:ARG:HE | 19:6:307:PRO:HB2 | 1.85 | 0.41 |
| 27:N:17:DG:N3 | 28:T:150:DG:N2 | 2.67 | 0.41 |
| 28:T:140:DT:H2' | 28:T:141:DT:H71 | 2.02 | 0.41 |
| 30:W:144:ARG:NH2 | 30:W:146:GLU:H | 2.17 | 0.41 |
| 31:P:6:G:C6 | 31:P:7:A:H1' | 2.55 | 0.41 |
| 1:Q:106:ILE:HB | 1:Q:385:THR:HG21 | 2.02 | 0.41 |
| 5:M:272:LYS:H | 29:O:208:VAL:HG11 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:49:LYS:HE3 | 6:A:49:LYS:HB3 | 1.86 | 0.41 |
| 6:A:49:LYS:HD3 | 6:A:55:ASP:O | 2.20 | 0.41 |
| 6:A:178:GLY:C | 6:A:179:LEU:HD13 | 2.40 | 0.41 |
| 6:A:664:THR:HG22 | 7:B:1014:PRO:HB3 | 2.02 | 0.41 |
| 6:A:982:THR:HG23 | 6:A:985:ASP:OD2 | 2.20 | 0.41 |
| 7:B:135:ARG:NH1 | 7:B:137:TYR:O | 2.53 | 0.41 |
| 7:B:782:LEU:HD23 | 7:B:782:LEU:HA | 1.67 | 0.41 |
| 7:B:842:ASN:HB3 | 7:B:845:SER:HB3 | 2.02 | 0.41 |
| 7:B:1187:ASN:HD21 | 7:B:1190:ASP:CB | 2.26 | 0.41 |
| 8:C:54:ASN:OD1 | 8:C:55:THR:N | 2.53 | 0.41 |
| 11:H:40:LEU:HD12 | 11:H:41:ASP:H | 1.85 | 0.41 |
| 12:I:74:GLU:HB2 | 12:I:81:ARG:CZ | 2.50 | 0.41 |
| 17:0:69:ILE:HB | 17:0:205:ILE:HG13 | 2.02 | 0.41 |
| 18:4:55:GLU:O | 18:4:59:VAL:HG23 | 2.21 | 0.41 |
| 18:4:114:UNK:C | 18:4:116:ARG:N | 2.83 | 0.41 |
| 30:W:65:ARG:HG2 | 30:W:93:HIS:HB3 | 2.03 | 0.41 |
| 5:M:318:GLU:OE1 | 5:M:319:HIS:ND1 | 2.53 | 0.41 |
| 6:A:72:GLU:OE2 | 6:A:80:HIS:NE2 | 2.52 | 0.41 |
| 6:A:1142:THR:OG1 | 6:A:1143:LEU:N | 2.52 | 0.41 |
| 6:A:1263:ILE:HD12 | 6:A:1263:ILE:HA | 1.84 | 0.41 |
| 7:B:89:GLU:O | 7:B:135:ARG:N | 2.48 | 0.41 |
| 7:B:120:ARG:HE | 7:B:120:ARG:HB3 | 1.67 | 0.41 |
| 7:B:585:VAL:HB | 7:B:587:HIS:HE1 | 1.84 | 0.41 |
| 7:B:794:ASN:C | 7:B:795:ILE:HD12 | 2.40 | 0.41 |
| 7:B:838:SER:HB3 | 7:B:988:GLY:HA3 | 2.02 | 0.41 |
| 7:B:976:ILE:CD1 | 7:B:992:ILE:HA | 2.51 | 0.41 |
| 7:B:997:GLU:HG2 | 7:B:998:ASP:N | 2.35 | 0.41 |
| 17:0:19:PRO:HG3 | 17:0:739:TRP:CE2 | 2.56 | 0.41 |
| 17:0:413:GLU:O | 17:0:414:GLU:HG3 | 2.20 | 0.41 |
| 17:0:495:MET:HA | 17:0:705:ASP:OD2 | 2.19 | 0.41 |
| 18:4:34:PRO:HD2 | 18:4:80:SER:CB | 2.50 | 0.41 |
| 18:4:175:ARG:NE | 18:4:256:PRO:HG3 | 2.26 | 0.41 |
| 21:7:564:GLU:OE1 | 21:7:757:ARG:HB2 | 2.21 | 0.41 |
| 22:5:8:ALA:HB2 | 22:5:44:PRO:HG3 | 2.02 | 0.41 |
| 23:2:394:ASP:OD1 | 23:2:395:GLN:N | 2.54 | 0.41 |
| 30:W:44:LYS:NZ | 30:W:51:LYS:HG2 | 2.34 | 0.41 |
| 1:Q:333:LYS:H | 7:B:70:ILE:HG12 | 1.84 | 0.41 |
| 1:Q:352:MET:HG2 | 1:Q:361:TRP:HB2 | 2.02 | 0.41 |
| 2:R:96:ARG:O | 2:R:104:ILE:HG23 | 2.20 | 0.41 |
| 3:D:183:LEU:HD12 | 3:D:195:ILE:HD11 | 2.03 | 0.41 |
| 4:G:110:VAL:HA | 4:G:161:GLY:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:414:ASP:OD1 | 6:A:415:LEU:N | 2.53 | 0.41 |
| 6:A:495:GLU:O | 6:A:498:ARG:HG3 | 2.21 | 0.41 |
| 6:A:618:GLU:OE1 | 6:A:620:LYS:N | 2.44 | 0.41 |
| 6:A:752:LYS:HD3 | 6:A:752:LYS:HA | 1.86 | 0.41 |
| 6:A:765:VAL:HG23 | 6:A:802:ASN:O | 2.20 | 0.41 |
| 6:A:843:LYS:HD2 | 6:A:843:LYS:HA | 1.71 | 0.41 |
| 6:A:1235:LYS:HB2 | 6:A:1237:ILE:HD11 | 2.03 | 0.41 |
| 6:A:1407:GLU:CD | 6:A:1407:GLU:N | 2.73 | 0.41 |
| 7:B:20:ASP:OD2 | 7:B:21:GLU:N | 2.52 | 0.41 |
| 7:B:1035:ALA:O | 7:B:1039:GLY:N | 2.53 | 0.41 |
| 8:C:201:TRP:HA | 8:C:202:PRO:HD3 | 1.96 | 0.41 |
| 10:F:147:SER:O | 10:F:149:GLU:N | 2.54 | 0.41 |
| 11:H:89:LEU:C | 11:H:91:ASP:H | 2.24 | 0.41 |
| 12:I:52:ILE:HA | 12:I:120:GLN:O | 2.20 | 0.41 |
| 14:K:7:PHE:HA | 14:K:10:PHE:CZ | 2.55 | 0.41 |
| 17:0:108:LEU:HD22 | 17:0:200:ILE:HD11 | 2.02 | 0.41 |
| 17:0:132:LYS:HE3 | 17:0:132:LYS:HB2 | 1.89 | 0.41 |
| 17:0:267:LEU:HD22 | 17:0:399:LEU:HD13 | 2.00 | 0.41 |
| 17:0:527:VAL:O | 17:0:531:LYS:HG3 | 2.20 | 0.41 |
| 17:0:575:ASP:OD1 | 17:0:575:ASP:N | 2.54 | 0.41 |
| 17:0:632:SER:OG | 17:0:633:ARG:N | 2.53 | 0.41 |
| 18:4:67:PHE:HE1 | 23:2:44:LYS:HB3 | 1.85 | 0.41 |
| 18:4:180:THR:HG23 | 18:4:214:LYS:HA | 2.01 | 0.41 |
| 23:2:100:LEU:HA | 23:2:100:LEU:HD23 | 1.79 | 0.41 |
| 24:X:193:LEU:HD21 | 24:X:228:SER:HA | 2.02 | 0.41 |
| 27:N:18:DT:C4 | 28:T:148:DA:N1 | 2.88 | 0.41 |
| 1:Q:104:ARG:O | 1:Q:385:THR:HG23 | 2.21 | 0.41 |
| 1:Q:134:HIS:HB3 | 1:Q:354:ASP:OD1 | 2.20 | 0.41 |
| 2:R:124:LEU:HD22 | 2:R:220:HIS:NE2 | 2.36 | 0.41 |
| 6:A:139:TRP:O | 6:A:143:LYS:HB3 | 2.19 | 0.41 |
| 6:A:217:LYS:HG3 | 6:A:218:ASP:H | 1.85 | 0.41 |
| 6:A:595:THR:HG21 | 6:A:604:GLY:HA3 | 2.02 | 0.41 |
| 6:A:726:ARG:HE | 6:A:726:ARG:HB3 | 1.60 | 0.41 |
| 6:A:1155:ASP:HB3 | 6:A:1241:ARG:HH21 | 1.86 | 0.41 |
| 7:B:301:ILE:HD13 | 7:B:382:ILE:HG21 | 2.02 | 0.41 |
| 7:B:523:CYS:HB2 | 7:B:750:GLY:HA3 | 2.02 | 0.41 |
| 10:F:138:LEU:HA | 10:F:138:LEU:HD13 | 1.56 | 0.41 |
| 10:F:147:SER:O | 10:F:150:GLU:HG2 | 2.20 | 0.41 |
| 11:H:95:TYR:HA | 11:H:95:TYR:HD1 | 1.73 | 0.41 |
| 11:H:136:LYS:HE2 | 11:H:136:LYS:HB2 | 1.80 | 0.41 |
| 17:0:709:SER:HB3 | 17:0:712:MET:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:4:228:THR:H | 18:4:228:THR:HG22 | 1.62 | 0.41 |
| 20:1:194:VAL:HA | 20:1:197:GLU:HG2 | 2.01 | 0.41 |
| 23:2:337:GLY:O | 23:2:406:PRO:HB2 | 2.21 | 0.41 |
| 23:2:419:LYS:NZ | 23:2:426:CYS:O | 2.35 | 0.41 |
| 23:2:435:PRO:O | 23:2:439:ASP:N | 2.40 | 0.41 |
| 2:R:66:ARG:O | 2:R:217:THR:N | 2.54 | 0.41 |
| 2:R:74:PRO:HB2 | 2:R:76:PHE:CE1 | 2.56 | 0.41 |
| 4:G:31:LEU:HD11 | 4:G:51:TYR:CE1 | 2.55 | 0.41 |
| 4:G:97:HIS:NE2 | 30:W:145:THR:O | 2.52 | 0.41 |
| 6:A:404:TYR:CD1 | 6:A:414:ASP:HA | 2.56 | 0.41 |
| 6:A:1435:PRO:O | 6:A:1436:ILE:HD13 | 2.21 | 0.41 |
| 7:B:356:LEU:HD23 | 7:B:356:LEU:N | 2.36 | 0.41 |
| 7:B:693:ILE:HA | 7:B:693:ILE:HD13 | 1.75 | 0.41 |
| 7:B:1151:LEU:HD12 | 7:B:1151:LEU:HA | 1.74 | 0.41 |
| 19:6:243:ASP:O | 20:1:389:LEU:HD22 | 2.20 | 0.41 |
| 21:7:562:THR:OG1 | 21:7:563:ALA:N | 2.52 | 0.41 |
| 24:X:258:GLU:O | 24:X:262:MET:N | 2.51 | 0.41 |
| 25:U:267:VAL:HG12 | 25:U:269:ILE:HG13 | 2.03 | 0.41 |
| 26:V:69:TYR:HB2 | 26:V:76:TRP:HZ3 | 1.83 | 0.41 |
| 27:N:37:DG:C2 | 27:N:38:DT:C2 | 3.08 | 0.41 |
| 28:T:18:DA:N3 | 28:T:18:DA:H3' | 2.36 | 0.41 |
| 1:Q:97:GLU:OE2 | 1:Q:99:ASN:N | 2.54 | 0.41 |
| 1:Q:125:LYS:O | 1:Q:127:ILE:N | 2.54 | 0.41 |
| 1:Q:141:ARG:NE | 1:Q:348:TYR:O | 2.53 | 0.41 |
| 1:Q:333:LYS:N | 7:B:70:ILE:HG12 | 2.36 | 0.41 |
| 6:A:369:SER:N | 14:K:2:ASN:OD1 | 2.40 | 0.41 |
| 6:A:839:ARG:O | 6:A:843:LYS:HG2 | 2.20 | 0.41 |
| 6:A:1067:LEU:HD12 | 6:A:1067:LEU:HA | 1.83 | 0.41 |
| 6:A:1193:LEU:HD12 | 6:A:1194:ARG:N | 2.35 | 0.41 |
| 6:A:1341:ILE:HD12 | 6:A:1341:ILE:HA | 1.85 | 0.41 |
| 6:A:1425:SER:O | 6:A:1429:ILE:HG13 | 2.21 | 0.41 |
| 6:A:1441:PHE:HZ | 10:F:92:ARG:CB | 2.33 | 0.41 |
| 7:B:239:GLU:HG2 | 7:B:240:ILE:N | 2.36 | 0.41 |
| 7:B:1079:LYS:HG2 | 7:B:1080:LYS:N | 2.36 | 0.41 |
| 7:B:1156:ASP:N | 7:B:1156:ASP:OD1 | 2.50 | 0.41 |
| 7:B:1173:ALA:O | 7:B:1175:LEU:N | 2.53 | 0.41 |
| 9:E:65:THR:O | 9:E:68:SER:OG | 2.25 | 0.41 |
| 13:J:30:LEU:HD12 | 13:J:30:LEU:HA | 1.52 | 0.41 |
| 17:0:120:VAL:HG21 | 34:0:801:SF4:S4 | 2.61 | 0.41 |
| 17:0:636:LYS:O | 17:0:640:GLU:HG2 | 2.21 | 0.41 |
| 19:6:137:LEU:HD23 | 19:6:137:LEU:HA | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:1:562:LYS:HD2 | 20:1:562:LYS:HA | 1.94 | 0.41 |
| 21:7:583:MET:HB3 | 21:7:763:VAL:HG21 | 2.02 | 0.41 |
| 21:7:633:GLN:O | 21:7:637:MET:HG2 | 2.21 | 0.41 |
| 23:2:273:LYS:HG3 | 23:2:276:LEU:HD23 | 2.03 | 0.41 |
| 24:X:224:LEU:O | 24:X:229:LYS:N | 2.53 | 0.41 |
| 27:N:19:DA:N6 | 28:T:146:DA:H61 | 2.19 | 0.41 |
| 28:T:144:DA:H1' | 29:O:69:ASN:ND2 | 2.36 | 0.41 |
| 29:O:74:VAL:HA | 29:O:154:ASP:O | 2.20 | 0.41 |
| 29:O:194:ILE:HD12 | 29:O:205:LEU:HD22 | 2.03 | 0.41 |
| 1:Q:106:ILE:HD12 | 1:Q:106:ILE:HA | 1.87 | 0.41 |
| 1:Q:376:LEU:O | 1:Q:378:VAL:N | 2.53 | 0.41 |
| 2:R:69:TRP:CH2 | 2:R:220:HIS:HD2 | 2.39 | 0.41 |
| 5:M:266:ILE:O | 5:M:266:ILE:HG23 | 2.21 | 0.41 |
| 6:A:147:VAL:HG23 | 6:A:148:CYS:N | 2.36 | 0.41 |
| 6:A:217:LYS:NZ | 6:A:218:ASP:HA | 2.36 | 0.41 |
| 6:A:340:LEU:HD13 | 6:A:1429:ILE:HG23 | 2.02 | 0.41 |
| 6:A:420:ARG:HB3 | 6:A:423:ASP:CB | 2.50 | 0.41 |
| 6:A:834:THR:HB | 6:A:1077:THR:HG22 | 2.01 | 0.41 |
| 6:A:857:ARG:CZ | 10:F:139:PRO:HG2 | 2.51 | 0.41 |
| 6:A:878:ILE:CG2 | 6:A:955:PRO:HB2 | 2.51 | 0.41 |
| 6:A:899:VAL:HG13 | 6:A:1029:ARG:HH11 | 1.85 | 0.41 |
| 6:A:1189:SER:HB3 | 6:A:1242:VAL:O | 2.21 | 0.41 |
| 6:A:1359:ASP:CG | 6:A:1361:SER:H | 2.24 | 0.41 |
| 7:B:69:LEU:HD23 | 7:B:69:LEU:HA | 1.70 | 0.41 |
| 7:B:193:LYS:HZ1 | 13:J:65:PRO:HD3 | 1.86 | 0.41 |
| 7:B:386:LEU:HD22 | 7:B:386:LEU:HA | 1.85 | 0.41 |
| 7:B:519:TRP:CD1 | 7:B:519:TRP:C | 2.94 | 0.41 |
| 7:B:637:LEU:HD23 | 7:B:637:LEU:HA | 1.63 | 0.41 |
| 7:B:644:GLU:HG2 | 7:B:648:HIS:NE2 | 2.36 | 0.41 |
| 7:B:815:ARG:HE | 7:B:815:ARG:HB3 | 1.39 | 0.41 |
| 8:C:29:MET:HE2 | 8:C:29:MET:HB2 | 1.92 | 0.41 |
| 8:C:51:VAL:HG13 | 15:L:65:VAL:HG13 | 2.03 | 0.41 |
| 8:C:58:LEU:HD23 | 8:C:58:LEU:HA | 1.79 | 0.41 |
| 8:C:106:GLU:H | 8:C:106:GLU:HG2 | 1.69 | 0.41 |
| 9:E:71:LYS:HE2 | 9:E:71:LYS:HB3 | 1.82 | 0.41 |
| 9:E:180:ARG:NH1 | 9:E:192:ARG:HB2 | 2.36 | 0.41 |
| 11:H:89:LEU:C | 11:H:91:ASP:N | 2.75 | 0.41 |
| 11:H:104:PHE:HE1 | 11:H:136:LYS:HD3 | 1.86 | 0.41 |
| 15:L:31:CYS:SG | 15:L:34:CYS:CB | 3.08 | 0.41 |
| 17:O:48:LYS:O | 17:O:52:LEU:HB2 | 2.21 | 0.41 |
| 19:6:365:CYS:O | 20:1:559:GLU:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:361:GLN:H | 21:7:361:GLN:HG2 | 1.68 | 0.41 |
| 21:7:528:ASN:O | 21:7:532:GLY:N | 2.53 | 0.41 |
| 21:7:671:ILE:HG13 | 21:7:706:TYR:HB2 | 2.02 | 0.41 |
| 23:2:143:TRP:O | 23:2:146:ILE:HG22 | 2.21 | 0.41 |
| 27:N:21:DA:H5'' | 29:O:196:ARG:HH22 | 1.86 | 0.41 |
| 28:T:130:DG:C2 | 28:T:131:DT:C2 | 3.08 | 0.41 |
| 29:O:73:THR:HG1 | 29:O:158:GLN:CD | 2.25 | 0.41 |
| 29:O:94:TYR:HB2 | 29:O:102:VAL:HA | 2.02 | 0.41 |
| 29:O:182:PHE:O | 29:O:195:TYR:HA | 2.21 | 0.41 |
| 29:O:204:LEU:HD22 | 29:O:230:ILE:HG21 | 2.02 | 0.41 |
| 29:O:206:ILE:HG23 | 29:O:212:ILE:CD1 | 2.49 | 0.41 |
| 30:W:113:LEU:HG | 30:W:165:ASN:OD1 | 2.21 | 0.41 |
| 1:Q:123:SER:H | 1:Q:361:TRP:HH2 | 1.69 | 0.41 |
| 2:R:64:SER:HA | 2:R:214:ILE:HG22 | 2.02 | 0.41 |
| 2:R:105:THR:OG1 | 2:R:120:TYR:O | 2.38 | 0.41 |
| 5:M:51:VAL:HG12 | 6:A:412:ARG:O | 2.21 | 0.41 |
| 5:M:132:LYS:HE3 | 5:M:132:LYS:HB2 | 1.89 | 0.41 |
| 6:A:84:ILE:O | 6:A:239:LEU:N | 2.50 | 0.41 |
| 6:A:151:ASP:HB3 | 6:A:162:VAL:O | 2.21 | 0.41 |
| 6:A:288:ALA:HA | 6:A:291:GLU:CD | 2.41 | 0.41 |
| 6:A:340:LEU:HD23 | 6:A:340:LEU:HA | 1.73 | 0.41 |
| 6:A:901:LEU:HA | 6:A:901:LEU:HD23 | 1.87 | 0.41 |
| 6:A:1284:MET:HE3 | 6:A:1284:MET:HB3 | 1.85 | 0.41 |
| 6:A:1444:MET:CE | 10:F:133:VAL:HG13 | 2.50 | 0.41 |
| 7:B:387:LEU:HD12 | 7:B:387:LEU:HA | 1.64 | 0.41 |
| 7:B:864:LYS:HA | 7:B:872:GLU:CD | 2.42 | 0.41 |
| 11:H:102:TYR:CE1 | 11:H:115:TYR:HB3 | 2.56 | 0.41 |
| 17:O:293:LEU:HD22 | 17:O:319:GLU:HG3 | 2.03 | 0.41 |
| 17:O:611:ASP:OD1 | 17:O:612:PHE:N | 2.54 | 0.41 |
| 19:6:346:GLY:HA2 | 19:6:358:SER:N | 2.36 | 0.41 |
| 21:7:370:LEU:HD22 | 21:7:374:PHE:CZ | 2.56 | 0.41 |
| 21:7:409:VAL:O | 21:7:455:SER:N | 2.40 | 0.41 |
| 21:7:417:VAL:HG13 | 21:7:454:VAL:HG22 | 2.02 | 0.41 |
| 27:N:23:DA:H4' | 29:O:158:GLN:O | 2.21 | 0.41 |
| 3:D:63:LEU:HB3 | 3:D:130:LEU:HD13 | 2.04 | 0.40 |
| 5:M:167:SER:C | 5:M:169:GLU:H | 2.24 | 0.40 |
| 6:A:114:LEU:HB3 | 6:A:145:LYS:HG2 | 2.03 | 0.40 |
| 6:A:220:THR:C | 6:A:222:LEU:N | 2.75 | 0.40 |
| 6:A:407:ARG:HA | 6:A:430:TRP:CD1 | 2.56 | 0.40 |
| 6:A:497:THR:HG22 | 7:B:1146:PHE:HA | 2.03 | 0.40 |
| 6:A:1077:THR:H | 6:A:1077:THR:HG23 | 1.64 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1109:LYS:HE2 | 6:A:1109:LYS:HB2 | 1.69 | 0.40 |
| 6:A:1224:LEU:HA | 6:A:1241:ARG:O | 2.22 | 0.40 |
| 6:A:1443:VAL:HG13 | 10:F:148:VAL:HG13 | 2.03 | 0.40 |
| 7:B:65:GLU:OE2 | 7:B:247:GLY:HA2 | 2.21 | 0.40 |
| 7:B:731:VAL:O | 7:B:732:SER:OG | 2.31 | 0.40 |
| 7:B:806:THR:HG22 | 7:B:1045:SER:HA | 2.02 | 0.40 |
| 7:B:901:PRO:HA | 7:B:949:VAL:HG12 | 2.04 | 0.40 |
| 8:C:153:LEU:HD11 | 8:C:155:LEU:HD23 | 2.01 | 0.40 |
| 11:H:4:THR:HG21 | 11:H:7:ASP:HB2 | 2.02 | 0.40 |
| 11:H:55:LEU:O | 11:H:146:ARG:CZ | 2.69 | 0.40 |
| 15:L:40:LEU:HD12 | 15:L:40:LEU:HA | 1.81 | 0.40 |
| 17:O:285:GLU:HA | 17:O:288:LYS:HD2 | 2.03 | 0.40 |
| 17:O:523:GLY:HA3 | 17:O:559:ILE:HG12 | 2.03 | 0.40 |
| 17:O:732:ASP:OD1 | 17:O:733:GLN:N | 2.54 | 0.40 |
| 20:1:253:ARG:HA | 20:1:256:ILE:HG12 | 2.03 | 0.40 |
| 20:1:273:ASN:HB3 | 20:1:277:ASN:O | 2.20 | 0.40 |
| 20:1:278:PHE:O | 20:1:283:PHE:HB2 | 2.21 | 0.40 |
| 23:2:382:SER:HA | 23:2:385:ARG:HH11 | 1.86 | 0.40 |
| 27:N:21:DA:H5'' | 29:O:196:ARG:NH2 | 2.37 | 0.40 |
| 29:O:172:LEU:O | 29:O:176:ALA:N | 2.54 | 0.40 |
| 29:O:185:TYR:CZ | 29:O:187:PRO:HB3 | 2.56 | 0.40 |
| 31:P:6:G:H3' | 31:P:6:G:N3 | 2.36 | 0.40 |
| 5:M:142:LEU:HD12 | 5:M:142:LEU:HA | 1.73 | 0.40 |
| 6:A:409:SER:OG | 6:A:411:ASP:OD1 | 2.38 | 0.40 |
| 6:A:849:MET:HB2 | 6:A:1063:MET:SD | 2.61 | 0.40 |
| 6:A:1017:LEU:HA | 6:A:1017:LEU:HD12 | 1.88 | 0.40 |
| 6:A:1242:VAL:HG12 | 6:A:1243:VAL:H | 1.86 | 0.40 |
| 7:B:232:SER:O | 7:B:261:ARG:CZ | 2.69 | 0.40 |
| 7:B:483:LEU:HA | 7:B:483:LEU:HD12 | 1.63 | 0.40 |
| 7:B:552:MET:HA | 7:B:555:ILE:CD1 | 2.51 | 0.40 |
| 7:B:861:ASP:CG | 7:B:914:LYS:HZ3 | 2.19 | 0.40 |
| 7:B:1030:LEU:HA | 7:B:1030:LEU:HD12 | 1.78 | 0.40 |
| 8:C:22:LEU:O | 8:C:228:PHE:N | 2.48 | 0.40 |
| 8:C:183:TRP:CZ2 | 8:C:207:CYS:HB3 | 2.56 | 0.40 |
| 9:E:52:ARG:HE | 9:E:52:ARG:HB2 | 1.70 | 0.40 |
| 11:H:24:CYS:SG | 11:H:44:VAL:HG11 | 2.61 | 0.40 |
| 12:I:19:ASP:HB2 | 12:I:24:ARG:NH1 | 2.36 | 0.40 |
| 17:O:210:TYR:OH | 17:O:235:ASP:O | 2.33 | 0.40 |
| 17:O:506:ILE:O | 17:O:683:ASP:HA | 2.21 | 0.40 |
| 18:4:138:LYS:O | 18:4:142:GLN:N | 2.55 | 0.40 |
| 19:6:144:ASN:HD21 | 19:6:146:HIS:HB3 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:6:181:LEU:HD11 | 19:6:184:GLN:HA | 2.02 | 0.40 |
| 21:7:409:VAL:HB | 21:7:454:VAL:HA | 2.02 | 0.40 |
| 21:7:460:VAL:HG13 | 21:7:474:MET:SD | 2.62 | 0.40 |
| 23:2:58:PRO:HB3 | 23:2:95:THR:HG21 | 2.02 | 0.40 |
| 25:U:250:LYS:O | 25:U:261:SER:N | 2.45 | 0.40 |
| 28:T:25:DC:H6 | 28:T:25:DC:H5" | 1.86 | 0.40 |
| 29:O:120:LYS:HA | 29:O:120:LYS:HD3 | 1.86 | 0.40 |
| 29:O:138:LYS:O | 29:O:142:ILE:HG13 | 2.21 | 0.40 |
| 6:A:525:GLN:NE2 | 7:B:836:GLU:HG2 | 2.36 | 0.40 |
| 6:A:927:VAL:HA | 6:A:930:ASP:OD2 | 2.22 | 0.40 |
| 6:A:1063:MET:SD | 6:A:1436:ILE:HG23 | 2.61 | 0.40 |
| 6:A:1084:PHE:HD2 | 6:A:1086:PHE:HB2 | 1.86 | 0.40 |
| 6:A:1153:TYR:HB2 | 6:A:1192:LEU:HD23 | 2.03 | 0.40 |
| 7:B:282:ILE:HG13 | 7:B:283:VAL:N | 2.36 | 0.40 |
| 7:B:1032:SER:HB2 | 7:B:1089:PRO:HG2 | 2.04 | 0.40 |
| 8:C:90:ASP:OD1 | 8:C:90:ASP:C | 2.60 | 0.40 |
| 9:E:31:THR:OG1 | 9:E:34:GLU:N | 2.41 | 0.40 |
| 9:E:140:LEU:HA | 9:E:140:LEU:HD23 | 1.81 | 0.40 |
| 15:L:25:ALA:HB3 | 15:L:37:LYS:NZ | 2.37 | 0.40 |
| 17:0:19:PRO:HG3 | 17:0:739:TRP:CD2 | 2.57 | 0.40 |
| 17:0:332:VAL:O | 17:0:336:LYS:HG3 | 2.21 | 0.40 |
| 17:0:375:ARG:HG3 | 17:0:410:SER:OG | 2.22 | 0.40 |
| 19:6:127:ILE:HG21 | 19:6:220:LEU:HD23 | 2.02 | 0.40 |
| 19:6:128:LEU:HD12 | 19:6:233:LEU:HD13 | 2.03 | 0.40 |
| 19:6:174:MET:HG2 | 19:6:209:SER:H | 1.87 | 0.40 |
| 19:6:298:LYS:HA | 19:6:298:LYS:HD2 | 1.82 | 0.40 |
| 21:7:585:PRO:HB3 | 21:7:750:TYR:HB2 | 2.03 | 0.40 |
| 22:5:3:ARG:HH11 | 23:2:460:SER:HB2 | 1.86 | 0.40 |
| 24:X:207:CYS:HB3 | 24:X:242:ARG:H | 1.86 | 0.40 |
| 26:V:84:GLN:HB3 | 26:V:105:VAL:HG12 | 2.02 | 0.40 |
| 2:R:76:PHE:CZ | 2:R:120:TYR:HE2 | 2.38 | 0.40 |
| 2:R:135:PHE:HA | 2:R:215:VAL:H | 1.86 | 0.40 |
| 3:D:68:ARG:HG2 | 3:D:72:ARG:NH2 | 2.36 | 0.40 |
| 4:G:61:ILE:HG12 | 10:F:133:VAL:HG12 | 2.03 | 0.40 |
| 4:G:151:ILE:HA | 4:G:151:ILE:HD13 | 1.80 | 0.40 |
| 5:M:37:ARG:HD2 | 5:M:37:ARG:HA | 1.53 | 0.40 |
| 5:M:283:TYR:O | 5:M:287:LEU:HG | 2.21 | 0.40 |
| 6:A:107:CYS:HB2 | 6:A:148:CYS:SG | 2.61 | 0.40 |
| 6:A:968:GLN:HA | 6:A:973:ILE:CD1 | 2.51 | 0.40 |
| 6:A:1143:LEU:O | 6:A:1146:VAL:HG12 | 2.21 | 0.40 |
| 6:A:1335:ILE:HA | 6:A:1335:ILE:HD13 | 1.77 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:B:258:LEU:HD13 | 7:B:269:ILE:HG12 | 2.02 | 0.40 |
| 7:B:399:ASP:O | 7:B:400:HIS:C | 2.60 | 0.40 |
| 7:B:1223:ASP:N | 7:B:1223:ASP:OD1 | 2.54 | 0.40 |
| 8:C:66:ARG:HH11 | 8:C:66:ARG:HD3 | 1.67 | 0.40 |
| 8:C:94:LYS:HE3 | 8:C:94:LYS:HB2 | 1.89 | 0.40 |
| 8:C:118:LEU:HA | 8:C:118:LEU:HD23 | 1.56 | 0.40 |
| 8:C:176:ILE:HG12 | 8:C:232:VAL:HG22 | 2.03 | 0.40 |
| 8:C:243:VAL:HG12 | 8:C:244:VAL:N | 2.37 | 0.40 |
| 9:E:77:SER:O | 9:E:106:GLN:HB3 | 2.20 | 0.40 |
| 9:E:178:ILE:HG23 | 9:E:214:CYS:HA | 2.03 | 0.40 |
| 10:F:140:ASP:OD1 | 10:F:142:SER:OG | 2.35 | 0.40 |
| 11:H:10:PHE:HB3 | 11:H:28:ALA:HB1 | 2.03 | 0.40 |
| 11:H:57:VAL:O | 11:H:93:TYR:CZ | 2.74 | 0.40 |
| 14:K:42:LEU:HA | 14:K:42:LEU:HD12 | 1.78 | 0.40 |
| 15:L:34:CYS:SG | 15:L:36:SER:HB3 | 2.62 | 0.40 |
| 15:L:61:THR:HG1 | 15:L:63:ARG:HG2 | 1.87 | 0.40 |
| 17:0:37:ASN:HD22 | 17:0:475:PHE:HD2 | 1.69 | 0.40 |
| 17:0:614:HIS:HB3 | 17:0:618:ARG:NH2 | 2.36 | 0.40 |
| 18:4:159:TYR:HE1 | 19:6:407:GLN:HB2 | 1.86 | 0.40 |
| 25:U:286:VAL:OXT | 29:O:110:LYS:HD2 | 2.21 | 0.40 |
| 29:O:75:THR:HG22 | 29:O:77:GLY:H | 1.86 | 0.40 |
| 1:Q:118:LEU:HB2 | 1:Q:392:VAL:HA | 2.04 | 0.40 |
| 1:Q:139:LEU:HA | 1:Q:351:VAL:O | 2.22 | 0.40 |
| 3:D:206:GLU:HA | 3:D:209:ARG:NE | 2.37 | 0.40 |
| 6:A:325:ILE:O | 6:A:328:ARG:N | 2.52 | 0.40 |
| 6:A:336:ILE:HG23 | 6:A:336:ILE:HD12 | 1.82 | 0.40 |
| 6:A:563:PRO:HB3 | 6:A:572:TRP:CE2 | 2.57 | 0.40 |
| 6:A:1348:LEU:HA | 6:A:1348:LEU:HD12 | 1.72 | 0.40 |
| 6:A:1442:ASP:OD1 | 6:A:1442:ASP:C | 2.60 | 0.40 |
| 7:B:126:SER:O | 7:B:170:LEU:N | 2.41 | 0.40 |
| 7:B:313:MET:HG3 | 7:B:390:LEU:HD21 | 2.02 | 0.40 |
| 7:B:1059:LEU:HD12 | 7:B:1059:LEU:HA | 1.80 | 0.40 |
| 8:C:62:PHE:HE1 | 8:C:66:ARG:HD2 | 1.87 | 0.40 |
| 8:C:231:ASN:C | 8:C:231:ASN:ND2 | 2.75 | 0.40 |
| 10:F:94:LEU:HD23 | 10:F:94:LEU:HA | 1.87 | 0.40 |
| 10:F:135:ARG:HD2 | 10:F:143:PHE:CE2 | 2.57 | 0.40 |
| 10:F:140:ASP:CG | 10:F:142:SER:HG | 2.25 | 0.40 |
| 15:L:26:THR:HA | 15:L:62:LYS:NZ | 2.36 | 0.40 |
| 17:0:57:ILE:HD11 | 17:0:86:LEU:HD11 | 2.03 | 0.40 |
| 17:0:565:LYS:HE3 | 17:0:565:LYS:HB2 | 1.86 | 0.40 |
| 17:0:620:VAL:O | 17:0:680:VAL:HG22 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:392:LYS:HE2 | 21:7:392:LYS:HB3 | 1.83 | 0.40 |
| 21:7:641:GLN:O | 21:7:645:TYR:HB3 | 2.22 | 0.40 |
| 27:N:19:DA:N3 | 29:O:190:PHE:HD1 | 2.18 | 0.40 |
| 28:T:148:DA:H2' | 28:T:148:DA:H5' | 1.89 | 0.40 |
| 29:O:136:SER:HB2 | 29:O:152:PHE:CE1 | 2.47 | 0.40 |
| 30:W:49:ILE:HD11 | 30:W:54:LEU:HD12 | 2.02 | 0.40 |
| 30:W:102:VAL:HG13 | 30:W:179:ILE:HG12 | 2.04 | 0.40 |
| 30:W:131:TYR:HA | 30:W:135:GLU:OE1 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran 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 backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1 | Q | 140/735 (19%) | 119 (85%) | 21 (15%) | 0 | 100 | 100 |
| 2 | R | 142/398 (36%) | 126 (89%) | 16 (11%) | 0 | 100 | 100 |
| 3 | D | 153/221 (69%) | 140 (92%) | 13 (8%) | 0 | 100 | 100 |
| 4 | G | 169/171 (99%) | 156 (92%) | 13 (8%) | 0 | 100 | 100 |
| 5 | M | 228/345 (66%) | 196 (86%) | 29 (13%) | 3 (1%) | 10 | 36 |
| 6 | A | 1395/1733 (80%) | 1227 (88%) | 161 (12%) | 7 (0%) | 25 | 58 |
| 7 | B | 1096/1224 (90%) | 942 (86%) | 149 (14%) | 5 (0%) | 25 | 58 |
| 8 | C | 264/318 (83%) | 241 (91%) | 22 (8%) | 1 (0%) | 30 | 63 |
| 9 | E | 212/215 (99%) | 199 (94%) | 13 (6%) | 0 | 100 | 100 |
| 10 | F | 83/155 (54%) | 73 (88%) | 10 (12%) | 0 | 100 | 100 |
| 11 | H | 129/146 (88%) | 97 (75%) | 31 (24%) | 1 (1%) | 16 | 48 |
| 12 | I | 117/122 (96%) | 95 (81%) | 22 (19%) | 0 | 100 | 100 |
| 13 | J | 63/70 (90%) | 52 (82%) | 11 (18%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|----------|-------------|-----|
| 14 | K | 112/120 (93%) | 101 (90%) | 11 (10%) | 0 | 100 | 100 |
| 15 | L | 44/70 (63%) | 30 (68%) | 14 (32%) | 0 | 100 | 100 |
| 16 | 3 | 70/321 (22%) | 65 (93%) | 5 (7%) | 0 | 100 | 100 |
| 17 | 0 | 752/778 (97%) | 701 (93%) | 51 (7%) | 0 | 100 | 100 |
| 18 | 4 | 279/338 (82%) | 246 (88%) | 33 (12%) | 0 | 100 | 100 |
| 19 | 6 | 336/461 (73%) | 295 (88%) | 39 (12%) | 2 (1%) | 22 | 53 |
| 20 | 1 | 256/543 (47%) | 237 (93%) | 17 (7%) | 2 (1%) | 16 | 48 |
| 21 | 7 | 630/843 (75%) | 578 (92%) | 52 (8%) | 0 | 100 | 100 |
| 22 | 5 | 64/72 (89%) | 59 (92%) | 5 (8%) | 0 | 100 | 100 |
| 23 | 2 | 456/513 (89%) | 412 (90%) | 44 (10%) | 0 | 100 | 100 |
| 24 | X | 145/328 (44%) | 126 (87%) | 19 (13%) | 0 | 100 | 100 |
| 25 | U | 44/286 (15%) | 39 (89%) | 5 (11%) | 0 | 100 | 100 |
| 26 | V | 45/122 (37%) | 45 (100%) | 0 | 0 | 100 | 100 |
| 29 | O | 178/240 (74%) | 165 (93%) | 13 (7%) | 0 | 100 | 100 |
| 30 | W | 189/482 (39%) | 179 (95%) | 10 (5%) | 0 | 100 | 100 |
| All | All | 7791/11370 (68%) | 6941 (89%) | 829 (11%) | 21 (0%) | 38 | 68 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | M | 269 | ILE |
| 5 | M | 270 | ALA |
| 6 | A | 68 | GLN |
| 6 | A | 72 | GLU |
| 6 | A | 609 | ASP |
| 7 | B | 837 | ASP |
| 7 | B | 838 | SER |
| 19 | 6 | 411 | PRO |
| 6 | A | 466 | SER |
| 11 | H | 58 | THR |
| 7 | B | 1046 | PRO |
| 5 | M | 158 | HIS |
| 6 | A | 47 | ARG |
| 8 | C | 175 | ALA |
| 6 | A | 958 | VAL |
| 7 | B | 991 | GLY |
| 19 | 6 | 112 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | 1 | 229 | GLY |
| 6 | A | 957 | PRO |
| 7 | B | 712 | PRO |
| 20 | 1 | 351 | GLY |

5.3.2 Protein sidechains ⓘ

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 | Q | 108/641 (17%) | 84 (78%) | 24 (22%) | 1 | 3 |
| 2 | R | 78/362 (22%) | 62 (80%) | 16 (20%) | 1 | 4 |
| 3 | D | 139/200 (70%) | 126 (91%) | 13 (9%) | 7 | 27 |
| 4 | G | 152/152 (100%) | 137 (90%) | 15 (10%) | 6 | 24 |
| 5 | M | 202/299 (68%) | 171 (85%) | 31 (15%) | 2 | 10 |
| 6 | A | 1224/1520 (80%) | 1032 (84%) | 192 (16%) | 2 | 9 |
| 7 | B | 967/1061 (91%) | 833 (86%) | 134 (14%) | 3 | 12 |
| 8 | C | 234/274 (85%) | 198 (85%) | 36 (15%) | 2 | 9 |
| 9 | E | 196/197 (100%) | 169 (86%) | 27 (14%) | 3 | 13 |
| 10 | F | 75/137 (55%) | 63 (84%) | 12 (16%) | 2 | 9 |
| 11 | H | 117/128 (91%) | 95 (81%) | 22 (19%) | 1 | 5 |
| 12 | I | 113/116 (97%) | 83 (74%) | 30 (26%) | 0 | 1 |
| 13 | J | 60/65 (92%) | 51 (85%) | 9 (15%) | 2 | 10 |
| 14 | K | 99/102 (97%) | 89 (90%) | 10 (10%) | 6 | 23 |
| 15 | L | 40/57 (70%) | 28 (70%) | 12 (30%) | 0 | 0 |
| 16 | 3 | 1/303 (0%) | 1 (100%) | 0 | 100 | 100 |
| 17 | 0 | 686/707 (97%) | 657 (96%) | 29 (4%) | 25 | 56 |
| 18 | 4 | 198/298 (66%) | 185 (93%) | 13 (7%) | 14 | 41 |
| 19 | 6 | 247/406 (61%) | 237 (96%) | 10 (4%) | 27 | 58 |
| 20 | 1 | 169/396 (43%) | 160 (95%) | 9 (5%) | 19 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 21 | 7 | 414/737 (56%) | 394 (95%) | 20 (5%) | 21 | 51 |
| 22 | 5 | 53/66 (80%) | 53 (100%) | 0 | 100 | 100 |
| 23 | 2 | 258/468 (55%) | 250 (97%) | 8 (3%) | 35 | 63 |
| 24 | X | 54/295 (18%) | 54 (100%) | 0 | 100 | 100 |
| 25 | U | 42/260 (16%) | 41 (98%) | 1 (2%) | 44 | 70 |
| 26 | V | 46/108 (43%) | 44 (96%) | 2 (4%) | 25 | 55 |
| 29 | O | 152/205 (74%) | 144 (95%) | 8 (5%) | 19 | 48 |
| 30 | W | 155/429 (36%) | 147 (95%) | 8 (5%) | 19 | 48 |
| All | All | 6279/9989 (63%) | 5588 (89%) | 691 (11%) | 7 | 21 |

All (691) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 98 | TYR |
| 1 | Q | 104 | ARG |
| 1 | Q | 110 | ASP |
| 1 | Q | 111 | LEU |
| 1 | Q | 112 | GLU |
| 1 | Q | 114 | MET |
| 1 | Q | 118 | LEU |
| 1 | Q | 122 | GLN |
| 1 | Q | 126 | LYS |
| 1 | Q | 130 | VAL |
| 1 | Q | 132 | ASP |
| 1 | Q | 133 | PHE |
| 1 | Q | 135 | LEU |
| 1 | Q | 331 | GLN |
| 1 | Q | 336 | ASP |
| 1 | Q | 350 | TRP |
| 1 | Q | 352 | MET |
| 1 | Q | 355 | PHE |
| 1 | Q | 359 | ASN |
| 1 | Q | 380 | ASP |
| 1 | Q | 396 | THR |
| 1 | Q | 398 | ARG |
| 1 | Q | 399 | ASN |
| 1 | Q | 403 | THR |
| 2 | R | 71 | VAL |
| 2 | R | 79 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 83 | ASP |
| 2 | R | 92 | LEU |
| 2 | R | 94 | LYS |
| 2 | R | 108 | LEU |
| 2 | R | 109 | ASN |
| 2 | R | 121 | ASP |
| 2 | R | 125 | THR |
| 2 | R | 127 | LYS |
| 2 | R | 128 | VAL |
| 2 | R | 130 | GLU |
| 2 | R | 138 | GLN |
| 2 | R | 211 | LYS |
| 2 | R | 217 | THR |
| 2 | R | 225 | MET |
| 3 | D | 26 | THR |
| 3 | D | 50 | LEU |
| 3 | D | 61 | GLU |
| 3 | D | 132 | GLN |
| 3 | D | 140 | ASP |
| 3 | D | 144 | THR |
| 3 | D | 153 | ARG |
| 3 | D | 157 | GLN |
| 3 | D | 160 | VAL |
| 3 | D | 169 | SER |
| 3 | D | 177 | VAL |
| 3 | D | 187 | THR |
| 3 | D | 203 | SER |
| 4 | G | 13 | LEU |
| 4 | G | 21 | ARG |
| 4 | G | 39 | THR |
| 4 | G | 49 | LEU |
| 4 | G | 58 | ARG |
| 4 | G | 64 | THR |
| 4 | G | 65 | ASP |
| 4 | G | 83 | LYS |
| 4 | G | 97 | HIS |
| 4 | G | 111 | THR |
| 4 | G | 145 | VAL |
| 4 | G | 151 | ILE |
| 4 | G | 153 | GLN |
| 4 | G | 154 | VAL |
| 4 | G | 155 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | M | 22 | LEU |
| 5 | M | 40 | GLU |
| 5 | M | 47 | LEU |
| 5 | M | 51 | VAL |
| 5 | M | 58 | ASP |
| 5 | M | 123 | ASP |
| 5 | M | 125 | GLU |
| 5 | M | 133 | ILE |
| 5 | M | 134 | THR |
| 5 | M | 142 | LEU |
| 5 | M | 158 | HIS |
| 5 | M | 160 | GLU |
| 5 | M | 162 | THR |
| 5 | M | 170 | SER |
| 5 | M | 175 | SER |
| 5 | M | 177 | LEU |
| 5 | M | 184 | GLU |
| 5 | M | 187 | ARG |
| 5 | M | 195 | LEU |
| 5 | M | 196 | ILE |
| 5 | M | 197 | HIS |
| 5 | M | 215 | ARG |
| 5 | M | 250 | MET |
| 5 | M | 257 | GLU |
| 5 | M | 267 | LYS |
| 5 | M | 284 | LEU |
| 5 | M | 286 | ILE |
| 5 | M | 291 | ILE |
| 5 | M | 298 | VAL |
| 5 | M | 305 | THR |
| 5 | M | 311 | SER |
| 6 | A | 13 | THR |
| 6 | A | 22 | PHE |
| 6 | A | 23 | SER |
| 6 | A | 37 | PHE |
| 6 | A | 41 | MET |
| 6 | A | 45 | GLN |
| 6 | A | 47 | ARG |
| 6 | A | 49 | LYS |
| 6 | A | 57 | ARG |
| 6 | A | 58 | LEU |
| 6 | A | 61 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | A | 63 | ARG |
| 6 | A | 64 | ASN |
| 6 | A | 68 | GLN |
| 6 | A | 71 | GLN |
| 6 | A | 72 | GLU |
| 6 | A | 84 | ILE |
| 6 | A | 93 | VAL |
| 6 | A | 96 | ILE |
| 6 | A | 110 | CYS |
| 6 | A | 115 | LEU |
| 6 | A | 116 | ASP |
| 6 | A | 117 | GLU |
| 6 | A | 129 | LYS |
| 6 | A | 140 | THR |
| 6 | A | 144 | THR |
| 6 | A | 145 | LYS |
| 6 | A | 147 | VAL |
| 6 | A | 152 | VAL |
| 6 | A | 174 | ILE |
| 6 | A | 175 | ARG |
| 6 | A | 179 | LEU |
| 6 | A | 203 | SER |
| 6 | A | 217 | LYS |
| 6 | A | 219 | PHE |
| 6 | A | 221 | SER |
| 6 | A | 225 | ASN |
| 6 | A | 235 | ILE |
| 6 | A | 236 | LEU |
| 6 | A | 237 | THR |
| 6 | A | 252 | PHE |
| 6 | A | 253 | ASN |
| 6 | A | 254 | GLU |
| 6 | A | 257 | ARG |
| 6 | A | 266 | LEU |
| 6 | A | 269 | ILE |
| 6 | A | 275 | SER |
| 6 | A | 280 | GLU |
| 6 | A | 286 | HIS |
| 6 | A | 299 | HIS |
| 6 | A | 318 | SER |
| 6 | A | 333 | GLU |
| 6 | A | 352 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | A | 354 | SER |
| 6 | A | 359 | LEU |
| 6 | A | 366 | VAL |
| 6 | A | 381 | THR |
| 6 | A | 385 | ILE |
| 6 | A | 389 | THR |
| 6 | A | 398 | GLU |
| 6 | A | 407 | ARG |
| 6 | A | 408 | ASP |
| 6 | A | 411 | ASP |
| 6 | A | 419 | LYS |
| 6 | A | 438 | ASP |
| 6 | A | 440 | ASP |
| 6 | A | 447 | GLN |
| 6 | A | 449 | SER |
| 6 | A | 450 | LEU |
| 6 | A | 469 | ARG |
| 6 | A | 470 | LEU |
| 6 | A | 472 | LEU |
| 6 | A | 476 | SER |
| 6 | A | 486 | GLU |
| 6 | A | 488 | ASN |
| 6 | A | 496 | GLU |
| 6 | A | 497 | THR |
| 6 | A | 502 | SER |
| 6 | A | 524 | VAL |
| 6 | A | 529 | CYS |
| 6 | A | 538 | ASP |
| 6 | A | 546 | VAL |
| 6 | A | 562 | THR |
| 6 | A | 566 | ILE |
| 6 | A | 567 | LYS |
| 6 | A | 573 | SER |
| 6 | A | 579 | SER |
| 6 | A | 589 | GLN |
| 6 | A | 599 | SER |
| 6 | A | 612 | ILE |
| 6 | A | 624 | SER |
| 6 | A | 634 | THR |
| 6 | A | 635 | ARG |
| 6 | A | 644 | LYS |
| 6 | A | 672 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | A | 677 | ARG |
| 6 | A | 678 | GLU |
| 6 | A | 681 | GLU |
| 6 | A | 685 | GLU |
| 6 | A | 716 | ASP |
| 6 | A | 728 | LYS |
| 6 | A | 739 | ASP |
| 6 | A | 740 | LEU |
| 6 | A | 754 | SER |
| 6 | A | 764 | CYS |
| 6 | A | 781 | ASP |
| 6 | A | 783 | THR |
| 6 | A | 788 | SER |
| 6 | A | 790 | ASP |
| 6 | A | 803 | SER |
| 6 | A | 808 | LEU |
| 6 | A | 827 | THR |
| 6 | A | 830 | LYS |
| 6 | A | 853 | ASP |
| 6 | A | 862 | ASN |
| 6 | A | 867 | ILE |
| 6 | A | 879 | GLU |
| 6 | A | 889 | SER |
| 6 | A | 899 | VAL |
| 6 | A | 903 | ASN |
| 6 | A | 905 | ASP |
| 6 | A | 909 | ASP |
| 6 | A | 912 | LEU |
| 6 | A | 914 | GLU |
| 6 | A | 915 | SER |
| 6 | A | 948 | VAL |
| 6 | A | 963 | ILE |
| 6 | A | 965 | GLN |
| 6 | A | 972 | HIS |
| 6 | A | 979 | SER |
| 6 | A | 982 | THR |
| 6 | A | 985 | ASP |
| 6 | A | 998 | LEU |
| 6 | A | 1000 | LEU |
| 6 | A | 1006 | ILE |
| 6 | A | 1015 | VAL |
| 6 | A | 1025 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | A | 1038 | THR |
| 6 | A | 1043 | ASP |
| 6 | A | 1046 | LEU |
| 6 | A | 1056 | SER |
| 6 | A | 1085 | HIS |
| 6 | A | 1089 | VAL |
| 6 | A | 1106 | ASN |
| 6 | A | 1117 | THR |
| 6 | A | 1135 | ARG |
| 6 | A | 1138 | ILE |
| 6 | A | 1142 | THR |
| 6 | A | 1160 | SER |
| 6 | A | 1172 | LEU |
| 6 | A | 1174 | PHE |
| 6 | A | 1192 | LEU |
| 6 | A | 1196 | GLU |
| 6 | A | 1197 | LEU |
| 6 | A | 1198 | ASP |
| 6 | A | 1204 | ASP |
| 6 | A | 1208 | THR |
| 6 | A | 1211 | GLN |
| 6 | A | 1212 | VAL |
| 6 | A | 1219 | THR |
| 6 | A | 1223 | ASP |
| 6 | A | 1232 | ASN |
| 6 | A | 1237 | ILE |
| 6 | A | 1240 | CYS |
| 6 | A | 1257 | ASP |
| 6 | A | 1261 | LYS |
| 6 | A | 1263 | ILE |
| 6 | A | 1265 | ASN |
| 6 | A | 1274 | ARG |
| 6 | A | 1278 | ASN |
| 6 | A | 1290 | LYS |
| 6 | A | 1291 | VAL |
| 6 | A | 1299 | VAL |
| 6 | A | 1327 | ILE |
| 6 | A | 1329 | THR |
| 6 | A | 1334 | ASP |
| 6 | A | 1358 | SER |
| 6 | A | 1362 | TYR |
| 6 | A | 1368 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | A | 1372 | VAL |
| 6 | A | 1382 | THR |
| 6 | A | 1383 | SER |
| 6 | A | 1386 | ARG |
| 6 | A | 1391 | ARG |
| 6 | A | 1392 | SER |
| 6 | A | 1400 | CYS |
| 6 | A | 1406 | VAL |
| 6 | A | 1407 | GLU |
| 6 | A | 1411 | GLU |
| 6 | A | 1425 | SER |
| 6 | A | 1430 | LEU |
| 6 | A | 1441 | PHE |
| 7 | B | 26 | THR |
| 7 | B | 30 | SER |
| 7 | B | 37 | PHE |
| 7 | B | 46 | GLN |
| 7 | B | 50 | SER |
| 7 | B | 70 | ILE |
| 7 | B | 98 | THR |
| 7 | B | 104 | GLU |
| 7 | B | 135 | ARG |
| 7 | B | 137 | TYR |
| 7 | B | 167 | ILE |
| 7 | B | 183 | GLU |
| 7 | B | 188 | ASP |
| 7 | B | 195 | CYS |
| 7 | B | 199 | MET |
| 7 | B | 208 | SER |
| 7 | B | 209 | GLU |
| 7 | B | 211 | VAL |
| 7 | B | 223 | VAL |
| 7 | B | 234 | ILE |
| 7 | B | 235 | SER |
| 7 | B | 240 | ILE |
| 7 | B | 253 | THR |
| 7 | B | 254 | LEU |
| 7 | B | 294 | ASP |
| 7 | B | 304 | ASP |
| 7 | B | 312 | GLU |
| 7 | B | 333 | PHE |
| 7 | B | 334 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | B | 345 | LYS |
| 7 | B | 347 | LYS |
| 7 | B | 357 | GLN |
| 7 | B | 364 | ILE |
| 7 | B | 365 | THR |
| 7 | B | 376 | PHE |
| 7 | B | 385 | LEU |
| 7 | B | 386 | LEU |
| 7 | B | 393 | LYS |
| 7 | B | 396 | ASP |
| 7 | B | 420 | LEU |
| 7 | B | 428 | ILE |
| 7 | B | 431 | TYR |
| 7 | B | 435 | THR |
| 7 | B | 448 | ILE |
| 7 | B | 455 | SER |
| 7 | B | 457 | LEU |
| 7 | B | 466 | TRP |
| 7 | B | 480 | SER |
| 7 | B | 481 | GLN |
| 7 | B | 487 | THR |
| 7 | B | 493 | SER |
| 7 | B | 513 | GLN |
| 7 | B | 516 | ASN |
| 7 | B | 527 | THR |
| 7 | B | 529 | GLU |
| 7 | B | 531 | GLN |
| 7 | B | 555 | ILE |
| 7 | B | 568 | ASP |
| 7 | B | 574 | SER |
| 7 | B | 583 | ASN |
| 7 | B | 614 | SER |
| 7 | B | 617 | ARG |
| 7 | B | 624 | LEU |
| 7 | B | 625 | LYS |
| 7 | B | 628 | THR |
| 7 | B | 641 | GLU |
| 7 | B | 642 | ASP |
| 7 | B | 649 | LYS |
| 7 | B | 668 | ASP |
| 7 | B | 683 | SER |
| 7 | B | 685 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | B | 690 | VAL |
| 7 | B | 698 | GLU |
| 7 | B | 708 | GLU |
| 7 | B | 722 | ASP |
| 7 | B | 731 | VAL |
| 7 | B | 733 | HIS |
| 7 | B | 736 | THR |
| 7 | B | 737 | THR |
| 7 | B | 764 | SER |
| 7 | B | 771 | SER |
| 7 | B | 783 | THR |
| 7 | B | 789 | MET |
| 7 | B | 812 | LEU |
| 7 | B | 815 | ARG |
| 7 | B | 825 | VAL |
| 7 | B | 836 | GLU |
| 7 | B | 837 | ASP |
| 7 | B | 845 | SER |
| 7 | B | 848 | ARG |
| 7 | B | 852 | ARG |
| 7 | B | 864 | LYS |
| 7 | B | 868 | MET |
| 7 | B | 875 | GLU |
| 7 | B | 879 | ARG |
| 7 | B | 882 | THR |
| 7 | B | 887 | HIS |
| 7 | B | 891 | ASP |
| 7 | B | 893 | LEU |
| 7 | B | 894 | ASP |
| 7 | B | 896 | ASP |
| 7 | B | 908 | GLU |
| 7 | B | 909 | ASP |
| 7 | B | 935 | ARG |
| 7 | B | 944 | THR |
| 7 | B | 951 | GLN |
| 7 | B | 955 | THR |
| 7 | B | 958 | GLN |
| 7 | B | 962 | LYS |
| 7 | B | 963 | PHE |
| 7 | B | 982 | SER |
| 7 | B | 989 | THR |
| 7 | B | 995 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | B | 996 | ARG |
| 7 | B | 1002 | THR |
| 7 | B | 1007 | VAL |
| 7 | B | 1009 | ASP |
| 7 | B | 1022 | THR |
| 7 | B | 1032 | SER |
| 7 | B | 1048 | THR |
| 7 | B | 1051 | THR |
| 7 | B | 1052 | VAL |
| 7 | B | 1061 | GLU |
| 7 | B | 1101 | ASP |
| 7 | B | 1111 | MET |
| 7 | B | 1115 | THR |
| 7 | B | 1123 | SER |
| 7 | B | 1129 | ARG |
| 7 | B | 1151 | LEU |
| 7 | B | 1162 | ILE |
| 7 | B | 1183 | LYS |
| 7 | B | 1191 | ILE |
| 7 | B | 1218 | THR |
| 7 | B | 1224 | PHE |
| 8 | C | 14 | SER |
| 8 | C | 18 | VAL |
| 8 | C | 21 | ILE |
| 8 | C | 25 | VAL |
| 8 | C | 26 | ASP |
| 8 | C | 35 | ARG |
| 8 | C | 41 | ILE |
| 8 | C | 52 | GLU |
| 8 | C | 54 | ASN |
| 8 | C | 60 | ASP |
| 8 | C | 76 | ASP |
| 8 | C | 87 | PHE |
| 8 | C | 90 | ASP |
| 8 | C | 93 | ASP |
| 8 | C | 107 | SER |
| 8 | C | 115 | SER |
| 8 | C | 119 | VAL |
| 8 | C | 125 | MET |
| 8 | C | 136 | ASP |
| 8 | C | 137 | LYS |
| 8 | C | 138 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | C | 156 | THR |
| 8 | C | 186 | LEU |
| 8 | C | 195 | GLN |
| 8 | C | 196 | ASP |
| 8 | C | 197 | SER |
| 8 | C | 204 | SER |
| 8 | C | 208 | GLU |
| 8 | C | 211 | ASP |
| 8 | C | 215 | GLU |
| 8 | C | 231 | ASN |
| 8 | C | 235 | VAL |
| 8 | C | 240 | VAL |
| 8 | C | 244 | VAL |
| 8 | C | 258 | ILE |
| 8 | C | 268 | ASP |
| 9 | E | 2 | ASP |
| 9 | E | 4 | GLU |
| 9 | E | 5 | ASN |
| 9 | E | 17 | ARG |
| 9 | E | 19 | VAL |
| 9 | E | 31 | THR |
| 9 | E | 37 | LEU |
| 9 | E | 41 | ASP |
| 9 | E | 54 | GLN |
| 9 | E | 61 | GLN |
| 9 | E | 66 | GLU |
| 9 | E | 67 | GLU |
| 9 | E | 68 | SER |
| 9 | E | 84 | ASP |
| 9 | E | 85 | GLU |
| 9 | E | 92 | THR |
| 9 | E | 98 | ILE |
| 9 | E | 101 | GLN |
| 9 | E | 105 | PHE |
| 9 | E | 107 | THR |
| 9 | E | 131 | THR |
| 9 | E | 134 | THR |
| 9 | E | 149 | LEU |
| 9 | E | 155 | ARG |
| 9 | E | 202 | SER |
| 9 | E | 205 | SER |
| 9 | E | 215 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | F | 71 | GLU |
| 10 | F | 93 | ILE |
| 10 | F | 96 | THR |
| 10 | F | 111 | LEU |
| 10 | F | 112 | GLU |
| 10 | F | 122 | MET |
| 10 | F | 128 | LYS |
| 10 | F | 132 | LEU |
| 10 | F | 133 | VAL |
| 10 | F | 134 | ILE |
| 10 | F | 142 | SER |
| 10 | F | 155 | LEU |
| 11 | H | 9 | ILE |
| 11 | H | 15 | VAL |
| 11 | H | 16 | ASP |
| 11 | H | 26 | ILE |
| 11 | H | 27 | GLU |
| 11 | H | 30 | SER |
| 11 | H | 32 | THR |
| 11 | H | 44 | VAL |
| 11 | H | 55 | LEU |
| 11 | H | 58 | THR |
| 11 | H | 88 | SER |
| 11 | H | 92 | ASP |
| 11 | H | 94 | ASP |
| 11 | H | 95 | TYR |
| 11 | H | 105 | GLU |
| 11 | H | 108 | SER |
| 11 | H | 112 | ILE |
| 11 | H | 128 | ASN |
| 11 | H | 130 | ARG |
| 11 | H | 142 | LEU |
| 11 | H | 143 | LEU |
| 11 | H | 145 | ARG |
| 12 | I | 3 | THR |
| 12 | I | 5 | ARG |
| 12 | I | 9 | ASP |
| 12 | I | 10 | CYS |
| 12 | I | 17 | ARG |
| 12 | I | 19 | ASP |
| 12 | I | 22 | ASN |
| 12 | I | 24 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | I | 25 | LEU |
| 12 | I | 28 | GLU |
| 12 | I | 29 | CYS |
| 12 | I | 32 | CYS |
| 12 | I | 37 | GLU |
| 12 | I | 40 | SER |
| 12 | I | 48 | LEU |
| 12 | I | 49 | ILE |
| 12 | I | 51 | ASN |
| 12 | I | 60 | GLN |
| 12 | I | 67 | THR |
| 12 | I | 70 | ARG |
| 12 | I | 71 | SER |
| 12 | I | 77 | LYS |
| 12 | I | 78 | CYS |
| 12 | I | 80 | SER |
| 12 | I | 88 | SER |
| 12 | I | 104 | LEU |
| 12 | I | 111 | THR |
| 12 | I | 118 | ARG |
| 12 | I | 119 | THR |
| 12 | I | 120 | GLN |
| 13 | J | 3 | VAL |
| 13 | J | 5 | VAL |
| 13 | J | 7 | CYS |
| 13 | J | 9 | SER |
| 13 | J | 10 | CYS |
| 13 | J | 20 | SER |
| 13 | J | 38 | ARG |
| 13 | J | 50 | ILE |
| 13 | J | 64 | ASN |
| 14 | K | 6 | ARG |
| 14 | K | 20 | LYS |
| 14 | K | 54 | ARG |
| 14 | K | 77 | THR |
| 14 | K | 82 | ASP |
| 14 | K | 93 | SER |
| 14 | K | 101 | LEU |
| 14 | K | 104 | ASN |
| 14 | K | 106 | GLU |
| 14 | K | 114 | LEU |
| 15 | L | 27 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | L | 31 | CYS |
| 15 | L | 34 | CYS |
| 15 | L | 35 | SER |
| 15 | L | 42 | ARG |
| 15 | L | 43 | THR |
| 15 | L | 44 | ASP |
| 15 | L | 46 | VAL |
| 15 | L | 48 | CYS |
| 15 | L | 50 | ASP |
| 15 | L | 53 | HIS |
| 15 | L | 55 | ILE |
| 17 | 0 | 5 | ILE |
| 17 | 0 | 49 | THR |
| 17 | 0 | 109 | THR |
| 17 | 0 | 115 | CYS |
| 17 | 0 | 140 | GLN |
| 17 | 0 | 142 | LYS |
| 17 | 0 | 162 | LEU |
| 17 | 0 | 175 | VAL |
| 17 | 0 | 221 | ARG |
| 17 | 0 | 241 | ASP |
| 17 | 0 | 253 | THR |
| 17 | 0 | 259 | ARG |
| 17 | 0 | 315 | ASP |
| 17 | 0 | 325 | ILE |
| 17 | 0 | 344 | THR |
| 17 | 0 | 349 | LEU |
| 17 | 0 | 388 | LEU |
| 17 | 0 | 393 | VAL |
| 17 | 0 | 395 | ASP |
| 17 | 0 | 414 | GLU |
| 17 | 0 | 419 | ILE |
| 17 | 0 | 421 | GLU |
| 17 | 0 | 511 | GLU |
| 17 | 0 | 532 | ILE |
| 17 | 0 | 572 | GLU |
| 17 | 0 | 584 | GLU |
| 17 | 0 | 585 | THR |
| 17 | 0 | 647 | ARG |
| 17 | 0 | 656 | PHE |
| 18 | 4 | 52 | LYS |
| 18 | 4 | 123 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | 4 | 125 | LEU |
| 18 | 4 | 132 | LEU |
| 18 | 4 | 149 | LEU |
| 18 | 4 | 176 | LEU |
| 18 | 4 | 180 | THR |
| 18 | 4 | 223 | PHE |
| 18 | 4 | 228 | THR |
| 18 | 4 | 252 | MET |
| 18 | 4 | 263 | VAL |
| 18 | 4 | 276 | CYS |
| 18 | 4 | 287 | PHE |
| 19 | 6 | 118 | TYR |
| 19 | 6 | 123 | ILE |
| 19 | 6 | 166 | ILE |
| 19 | 6 | 230 | ARG |
| 19 | 6 | 270 | VAL |
| 19 | 6 | 310 | VAL |
| 19 | 6 | 372 | LEU |
| 19 | 6 | 384 | MET |
| 19 | 6 | 440 | CYS |
| 19 | 6 | 448 | LEU |
| 20 | 1 | 189 | LYS |
| 20 | 1 | 261 | GLU |
| 20 | 1 | 277 | ASN |
| 20 | 1 | 282 | GLU |
| 20 | 1 | 321 | PHE |
| 20 | 1 | 331 | HIS |
| 20 | 1 | 339 | LEU |
| 20 | 1 | 348 | VAL |
| 20 | 1 | 381 | LEU |
| 21 | 7 | 313 | VAL |
| 21 | 7 | 323 | VAL |
| 21 | 7 | 393 | THR |
| 21 | 7 | 408 | ILE |
| 21 | 7 | 431 | GLN |
| 21 | 7 | 435 | CYS |
| 21 | 7 | 437 | VAL |
| 21 | 7 | 447 | GLN |
| 21 | 7 | 453 | VAL |
| 21 | 7 | 478 | THR |
| 21 | 7 | 490 | VAL |
| 21 | 7 | 514 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | 7 | 534 | LYS |
| 21 | 7 | 573 | THR |
| 21 | 7 | 605 | ILE |
| 21 | 7 | 610 | ASP |
| 21 | 7 | 620 | LEU |
| 21 | 7 | 634 | GLN |
| 21 | 7 | 680 | ARG |
| 21 | 7 | 692 | ARG |
| 23 | 2 | 21 | VAL |
| 23 | 2 | 60 | LEU |
| 23 | 2 | 72 | LEU |
| 23 | 2 | 87 | LEU |
| 23 | 2 | 92 | SER |
| 23 | 2 | 385 | ARG |
| 23 | 2 | 410 | ARG |
| 23 | 2 | 484 | LYS |
| 25 | U | 264 | ASP |
| 26 | V | 57 | GLN |
| 26 | V | 76 | TRP |
| 29 | O | 91 | ASN |
| 29 | O | 136 | SER |
| 29 | O | 161 | VAL |
| 29 | O | 181 | THR |
| 29 | O | 182 | PHE |
| 29 | O | 183 | SER |
| 29 | O | 218 | LYS |
| 29 | O | 221 | GLU |
| 30 | W | 15 | PHE |
| 30 | W | 58 | ILE |
| 30 | W | 123 | MET |
| 30 | W | 126 | ILE |
| 30 | W | 133 | GLN |
| 30 | W | 147 | PHE |
| 30 | W | 149 | CYS |
| 30 | W | 151 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 138 | GLN |
| 3 | D | 28 | GLN |
| 3 | D | 40 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 179 | GLN |
| 4 | G | 97 | HIS |
| 4 | G | 131 | GLN |
| 4 | G | 153 | GLN |
| 5 | M | 124 | ASN |
| 6 | A | 68 | GLN |
| 6 | A | 80 | HIS |
| 6 | A | 282 | ASN |
| 6 | A | 339 | ASN |
| 6 | A | 451 | HIS |
| 6 | A | 741 | ASN |
| 6 | A | 935 | GLN |
| 6 | A | 1078 | GLN |
| 6 | A | 1173 | HIS |
| 6 | A | 1188 | GLN |
| 6 | A | 1218 | GLN |
| 6 | A | 1232 | ASN |
| 6 | A | 1278 | ASN |
| 7 | B | 178 | ASN |
| 7 | B | 481 | GLN |
| 7 | B | 686 | ASN |
| 7 | B | 794 | ASN |
| 7 | B | 1177 | HIS |
| 7 | B | 1179 | GLN |
| 8 | C | 231 | ASN |
| 11 | H | 128 | ASN |
| 12 | I | 12 | ASN |
| 12 | I | 89 | GLN |
| 17 | 0 | 60 | GLN |
| 17 | 0 | 224 | ASN |
| 17 | 0 | 283 | GLN |
| 17 | 0 | 521 | ASN |
| 17 | 0 | 726 | GLN |
| 18 | 4 | 225 | GLN |
| 19 | 6 | 351 | ASN |
| 20 | 1 | 331 | HIS |
| 21 | 7 | 331 | GLN |
| 21 | 7 | 611 | ASN |
| 23 | 2 | 90 | ASN |
| 23 | 2 | 99 | ASN |
| 23 | 2 | 356 | GLN |
| 24 | X | 265 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | O | 68 | GLN |
| 29 | O | 158 | GLN |
| 30 | W | 138 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 31 | P | 4/5 (80%) | 1 (25%) | 0 |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | P | 8 | G |

There are no RNA pucker outliers to report.

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 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 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 | $\# Z > 2$ |
| 34 | SF4 | 0 | 801 | 17 | 0,12,12 | - | - | - | | |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 34 | SF4 | 0 | 801 | 17 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 34 | 0 | 801 | SF4 | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 20 | 1 | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 1 | 355:UNK | C | 368:UNK | N | 14.81 |
| 1 | 1 | 519:UNK | C | 537:GLU | N | 11.86 |

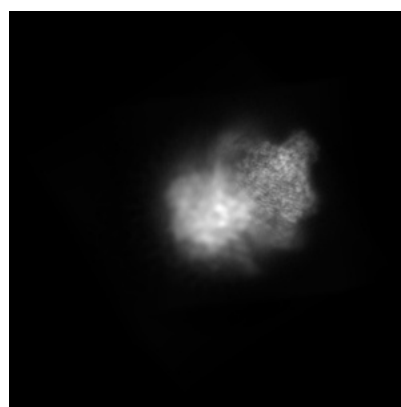
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23908. These allow visual inspection of the internal detail of the map and identification of artifacts.

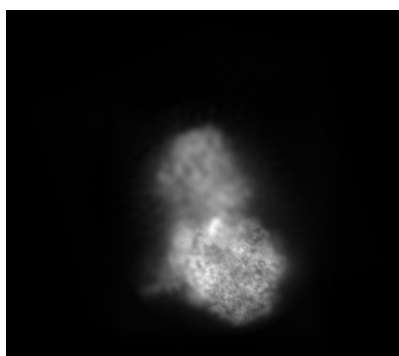
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

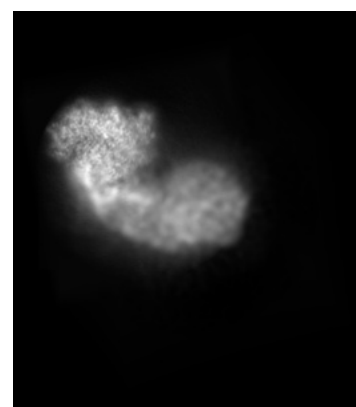
6.1.1 Primary map



X



Y

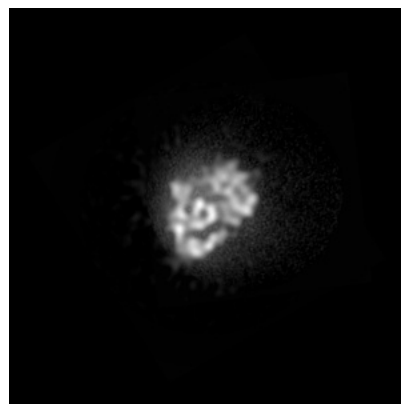


Z

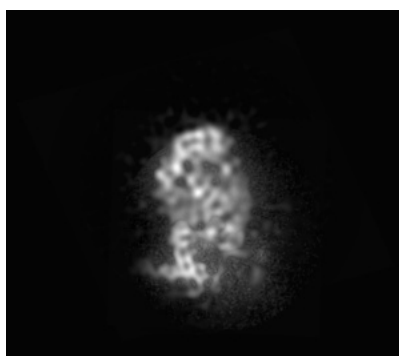
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

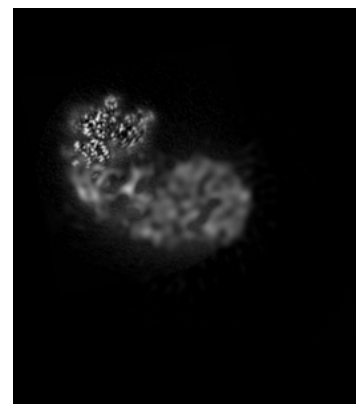
6.2.1 Primary map



X Index: 209



Y Index: 237

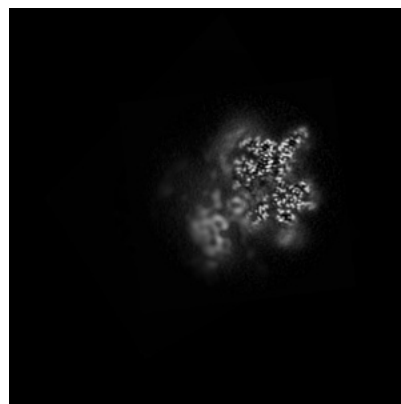


Z Index: 240

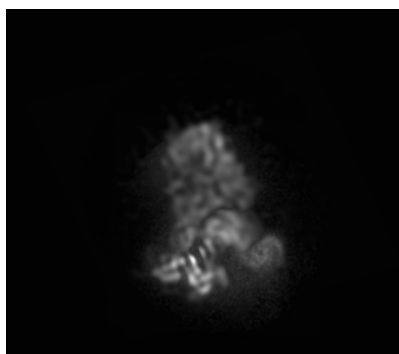
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

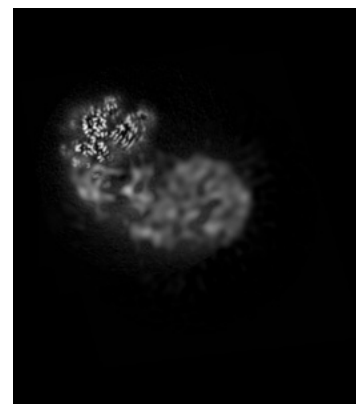
6.3.1 Primary map



X Index: 109



Y Index: 253

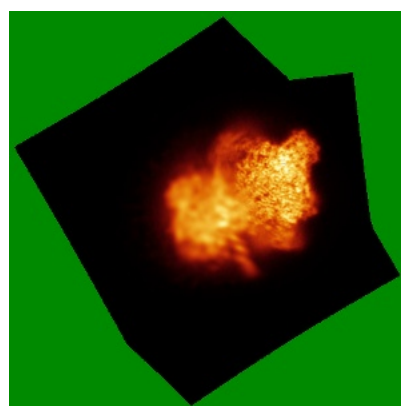


Z Index: 242

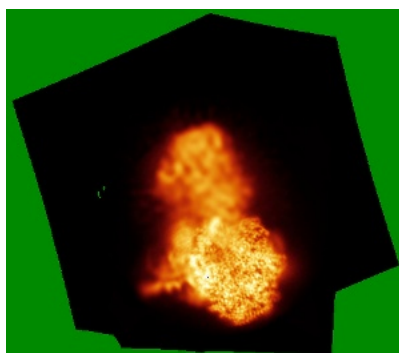
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

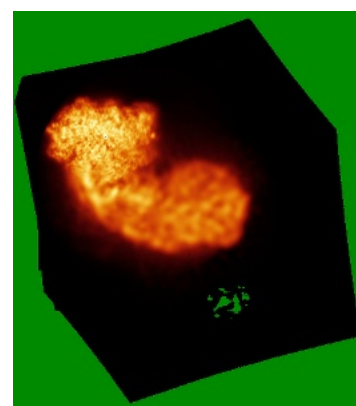
6.4.1 Primary map



X



Y

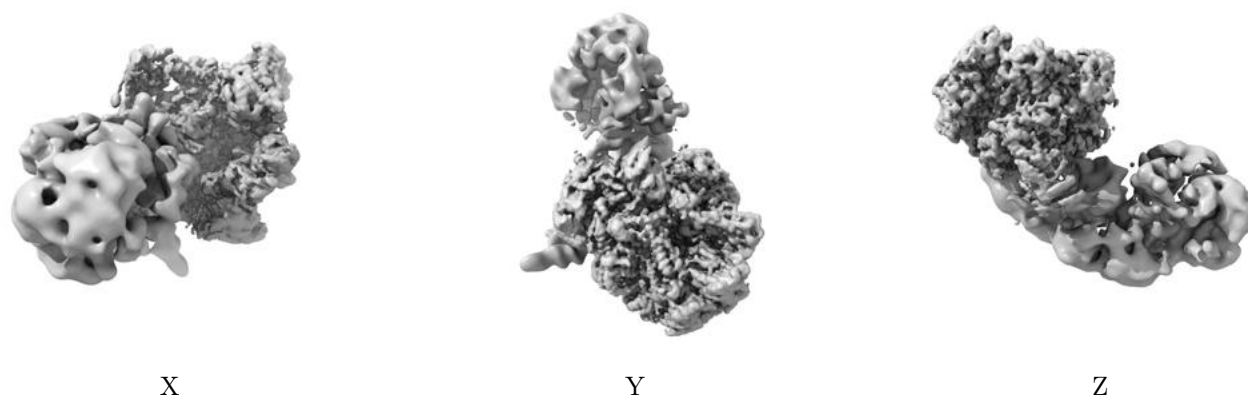


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

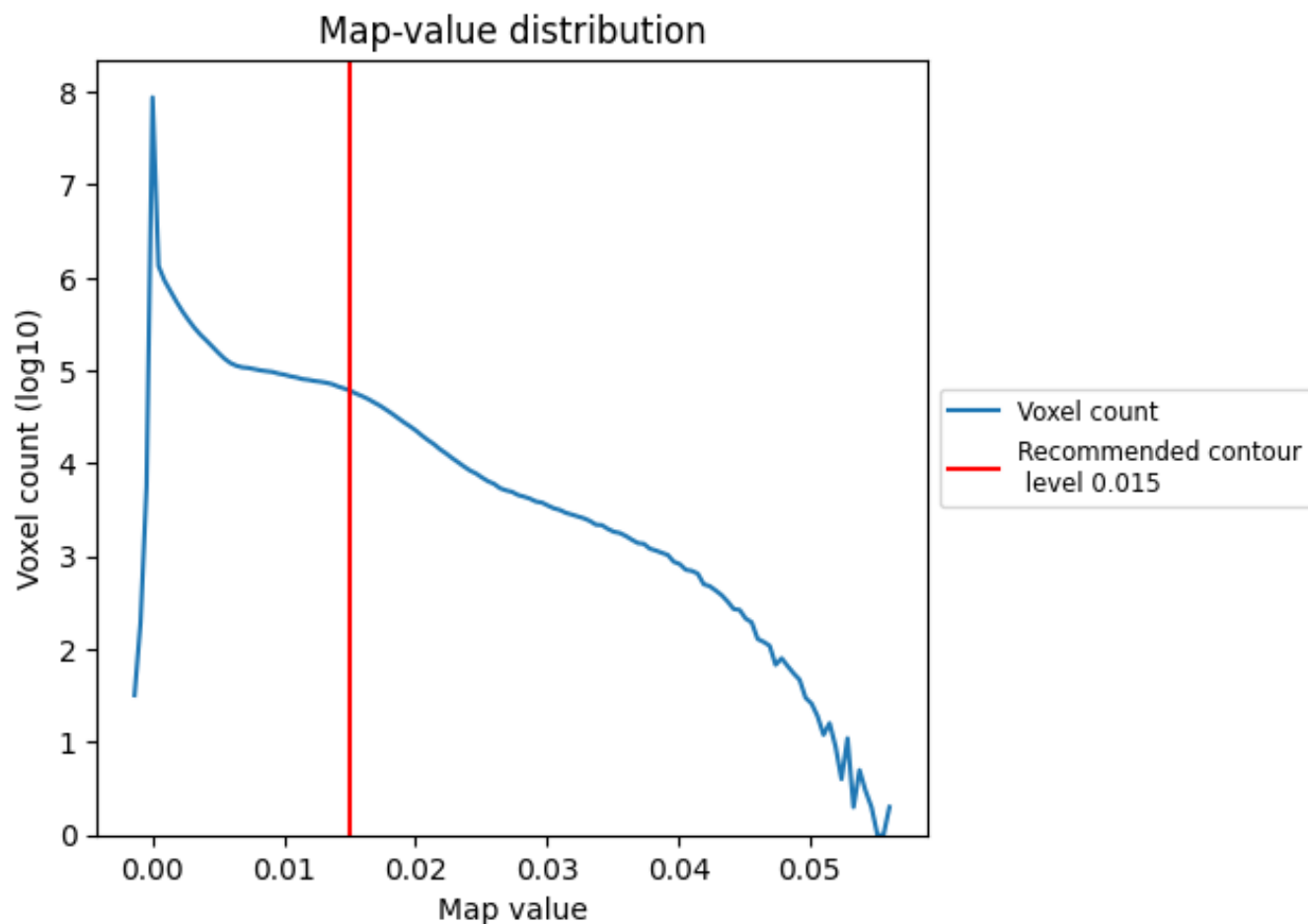
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

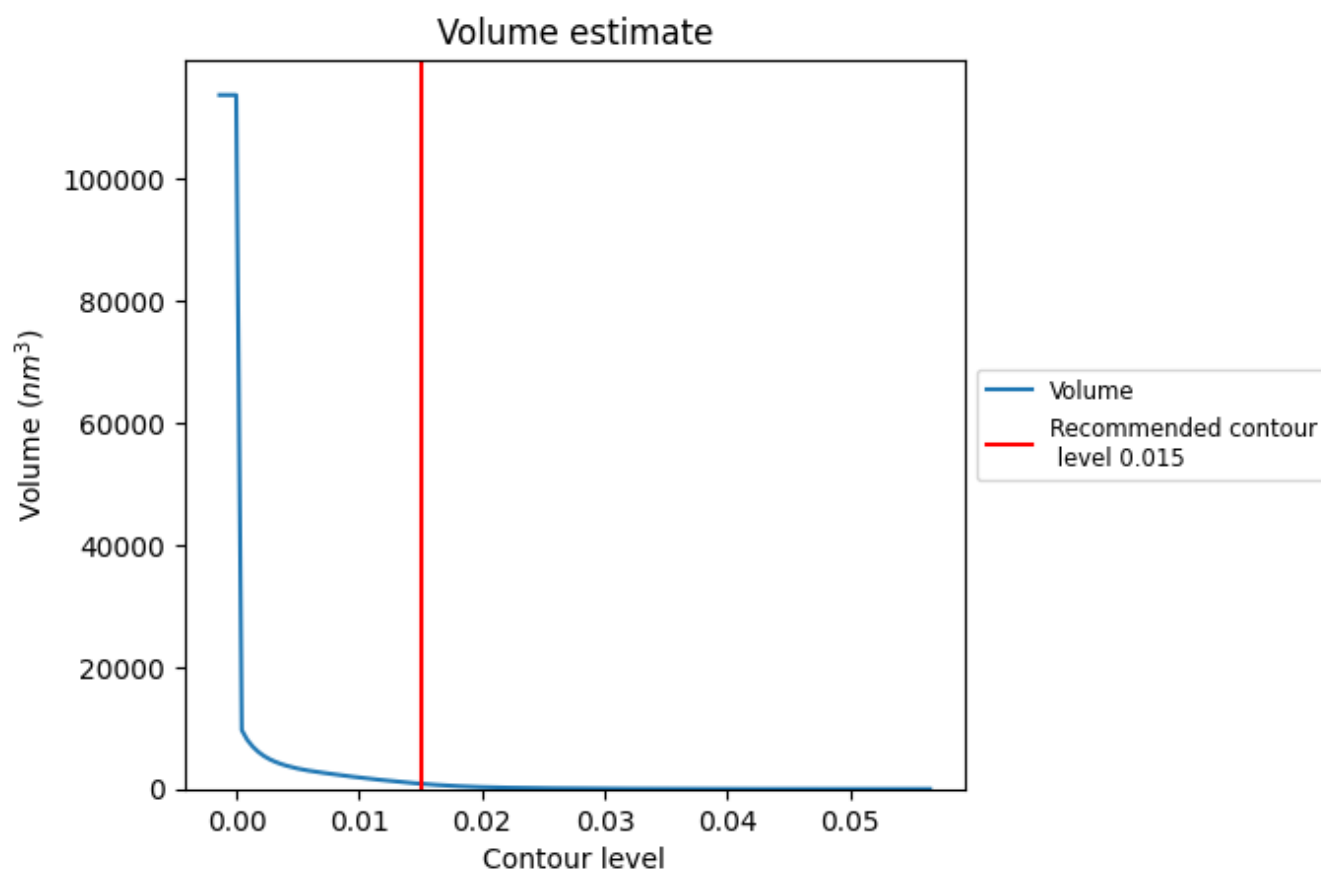
This section contains the results of statistical analysis of the map.

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 863 nm³; this corresponds to an approximate mass of 779 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

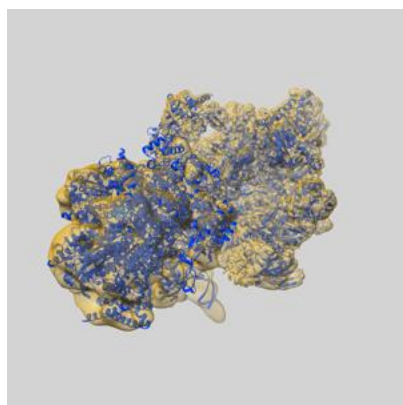
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

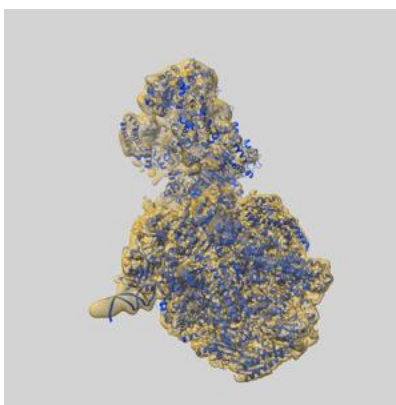
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23908 and PDB model 7ML4. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

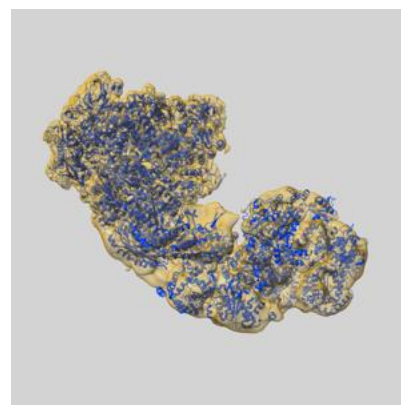
9.1 Map-model overlay [i](#)



X



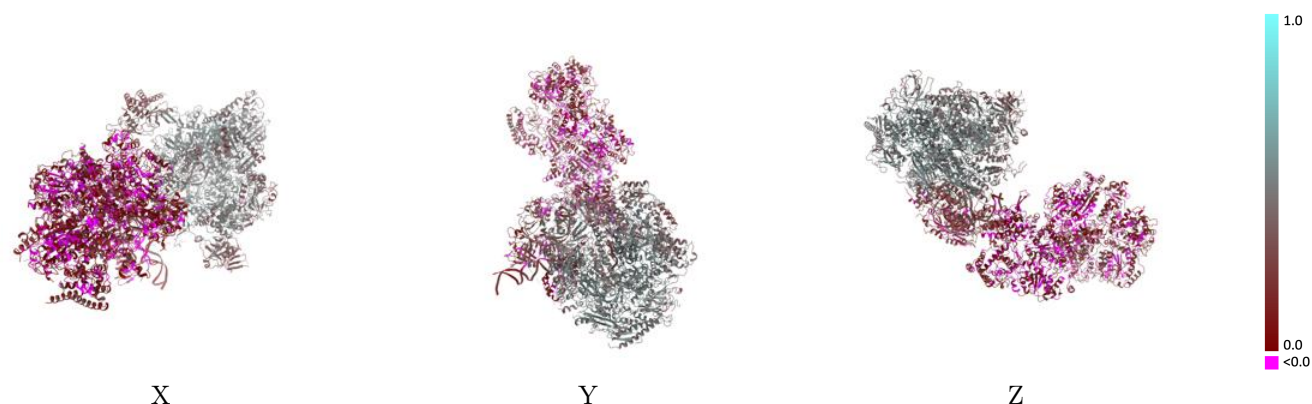
Y



Z

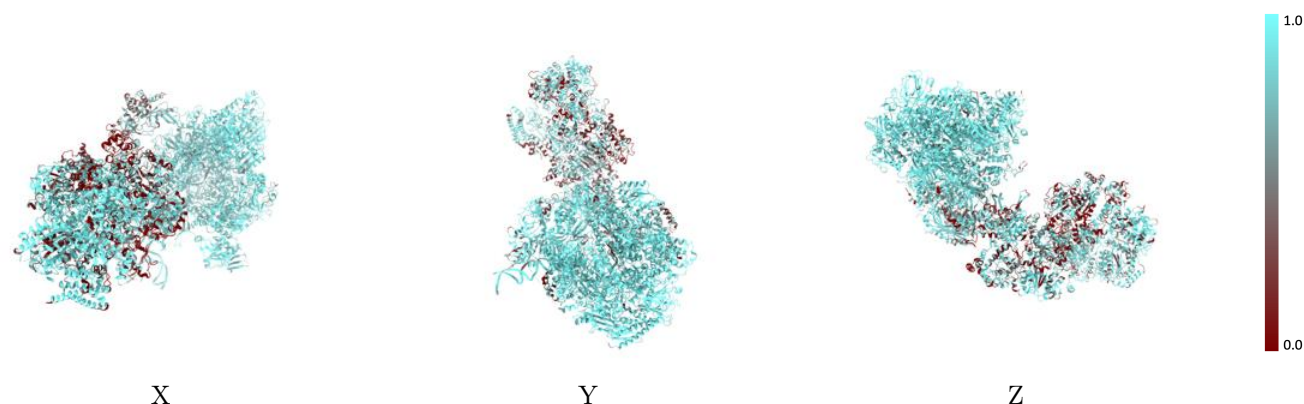
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



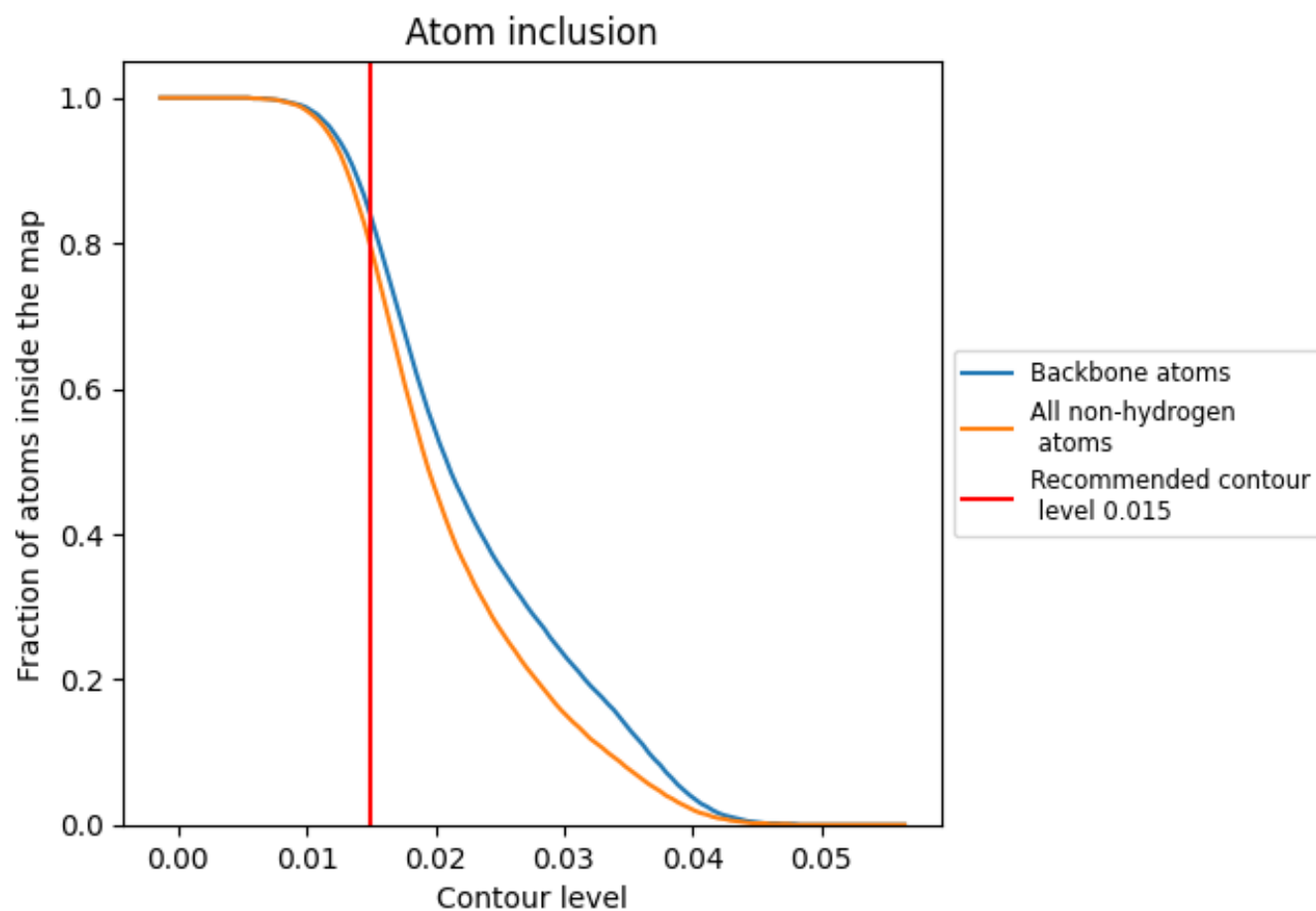
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.015).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7930 |  0.2810 |
| 0 |  0.6660 |  0.0610 |
| 1 |  0.5790 |  0.0820 |
| 2 |  0.6950 |  0.0880 |
| 3 |  0.4380 |  0.1210 |
| 4 |  0.7980 |  0.0710 |
| 5 |  0.4680 |  0.0950 |
| 6 |  0.7830 |  0.0790 |
| 7 |  0.4380 |  0.0470 |
| A |  0.9260 |  0.4730 |
| B |  0.9410 |  0.4960 |
| C |  0.9570 |  0.4930 |
| D |  0.4630 |  0.2750 |
| E |  0.9250 |  0.4610 |
| F |  0.9540 |  0.5000 |
| G |  0.6800 |  0.3600 |
| H |  0.9410 |  0.4440 |
| I |  0.8650 |  0.4200 |
| J |  0.9790 |  0.5080 |
| K |  0.8770 |  0.4750 |
| L |  0.9600 |  0.4430 |
| M |  0.7540 |  0.1890 |
| N |  0.9170 |  0.1710 |
| O |  0.8960 |  0.0690 |
| P |  0.6540 |  0.2610 |
| Q |  0.8950 |  0.3570 |
| R |  0.8490 |  0.2590 |
| T |  0.8460 |  0.1830 |
| U |  0.6490 |  0.0900 |
| V |  0.7880 |  0.1090 |
| W |  0.6690 |  0.1000 |
| X |  0.7940 |  0.0640 |

