



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 10:11 PM EST

PDB ID : 6BSP
EMDB ID : EMD-7136
Title : High-Resolution Structure Analysis of Antibody V5 and U4 Conformational Epitope on Human Papillomavirus 16
Authors : Guan, J.; Bywaters, S.M.; Brendle, S.A.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Christenson, N.D.; Hafenstein, S.
Deposited on : 2017-12-04
Resolution : 4.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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
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) : 2.39

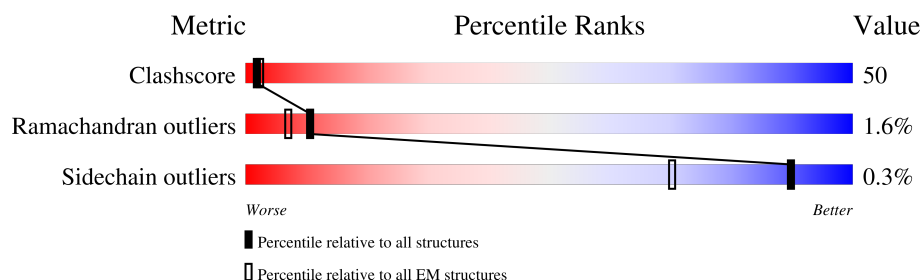
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 |

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 | A | 109 | <div> <div>81%</div> <div>26%</div> <div>73%</div> <div>.</div> </div> |
| 2 | B | 110 | <div> <div>85%</div> <div>26%</div> <div>74%</div> <div>.</div> </div> |
| 3 | C | 469 | <div> <div>17%</div> <div>47%</div> <div>48%</div> <div>..</div> </div> |
| 3 | D | 469 | <div> <div>15%</div> <div>77%</div> <div>6%</div> <div>.</div> </div> |
| 3 | E | 469 | <div> <div>47%</div> <div>50%</div> <div>..</div> </div> |
| 3 | F | 469 | <div> <div>6%</div> <div>46%</div> <div>50%</div> <div>..</div> </div> |
| 3 | G | 469 | <div> <div>47%</div> <div>47%</div> <div>5%</div> <div>.</div> </div> |
| 3 | H | 469 | <div> <div>7%</div> <div>46%</div> <div>50%</div> <div>..</div> </div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23690 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 U4 Heavy chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | A | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 851 | 534 | 145 | 167 | 5 | | |

- Molecule 2 is a protein called U4 Light chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | B | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 541 | 135 | 170 | 4 | | |

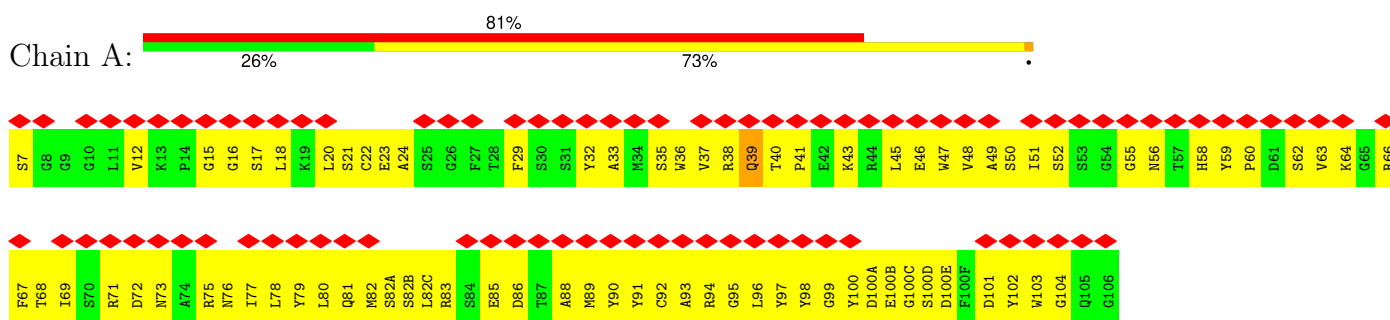
- Molecule 3 is a protein called Major capsid protein L1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 468 | Total | C | N | O | S | 0 | 0 |
| | | | 3675 | 2347 | 617 | 690 | 21 | | |
| 3 | D | 460 | Total | C | N | O | S | 0 | 0 |
| | | | 3614 | 2304 | 609 | 680 | 21 | | |
| 3 | E | 469 | Total | C | N | O | S | 0 | 0 |
| | | | 3686 | 2356 | 618 | 691 | 21 | | |
| 3 | F | 468 | Total | C | N | O | S | 0 | 0 |
| | | | 3675 | 2347 | 617 | 690 | 21 | | |
| 3 | G | 467 | Total | C | N | O | S | 0 | 0 |
| | | | 3666 | 2341 | 615 | 689 | 21 | | |
| 3 | H | 468 | Total | C | N | O | S | 0 | 0 |
| | | | 3673 | 2345 | 617 | 690 | 21 | | |

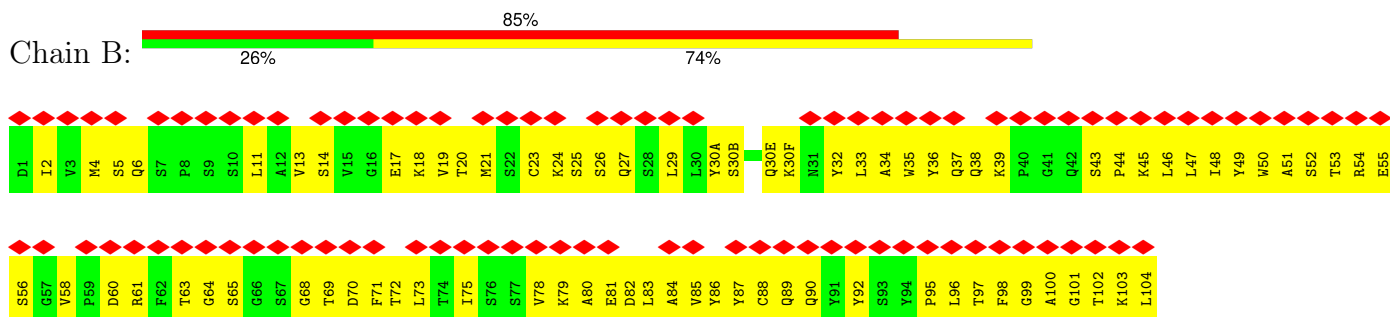
3 Residue-property plots

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.

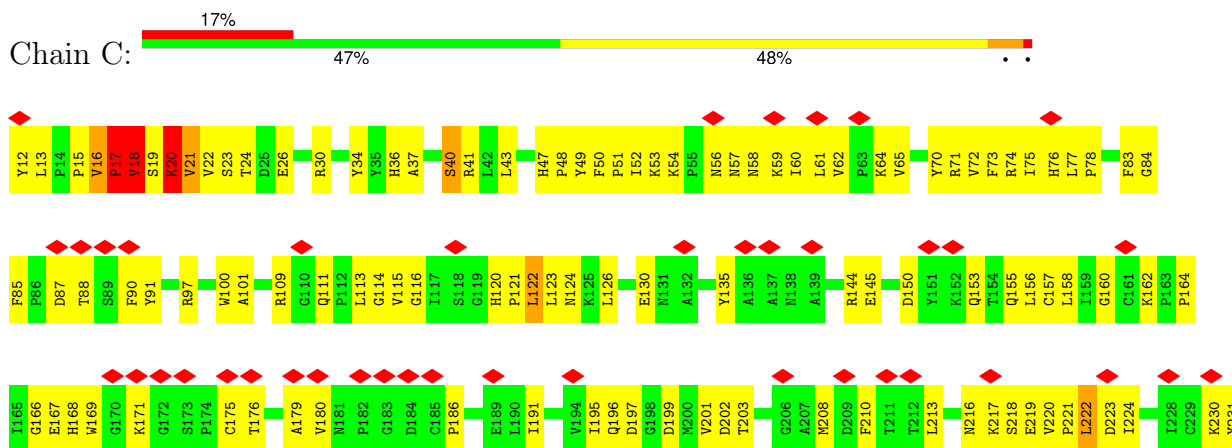
• Molecule 1: U4 Heavy chain

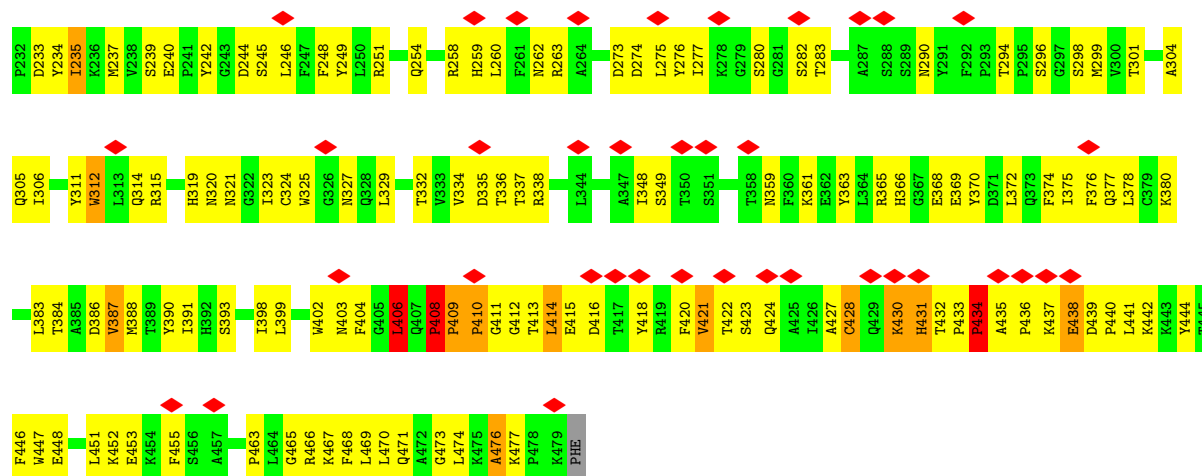


• Molecule 2: U4 Light chain



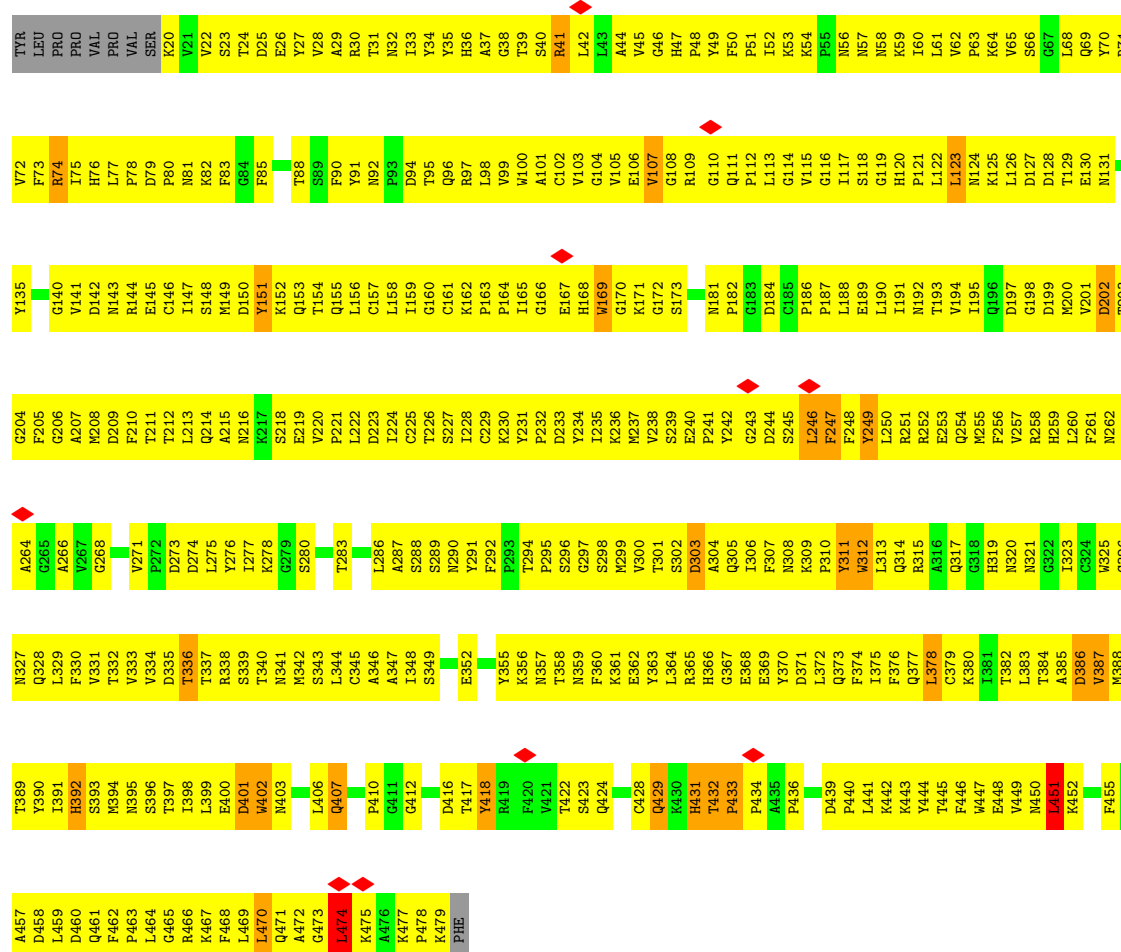
• Molecule 3: Major capsid protein L1





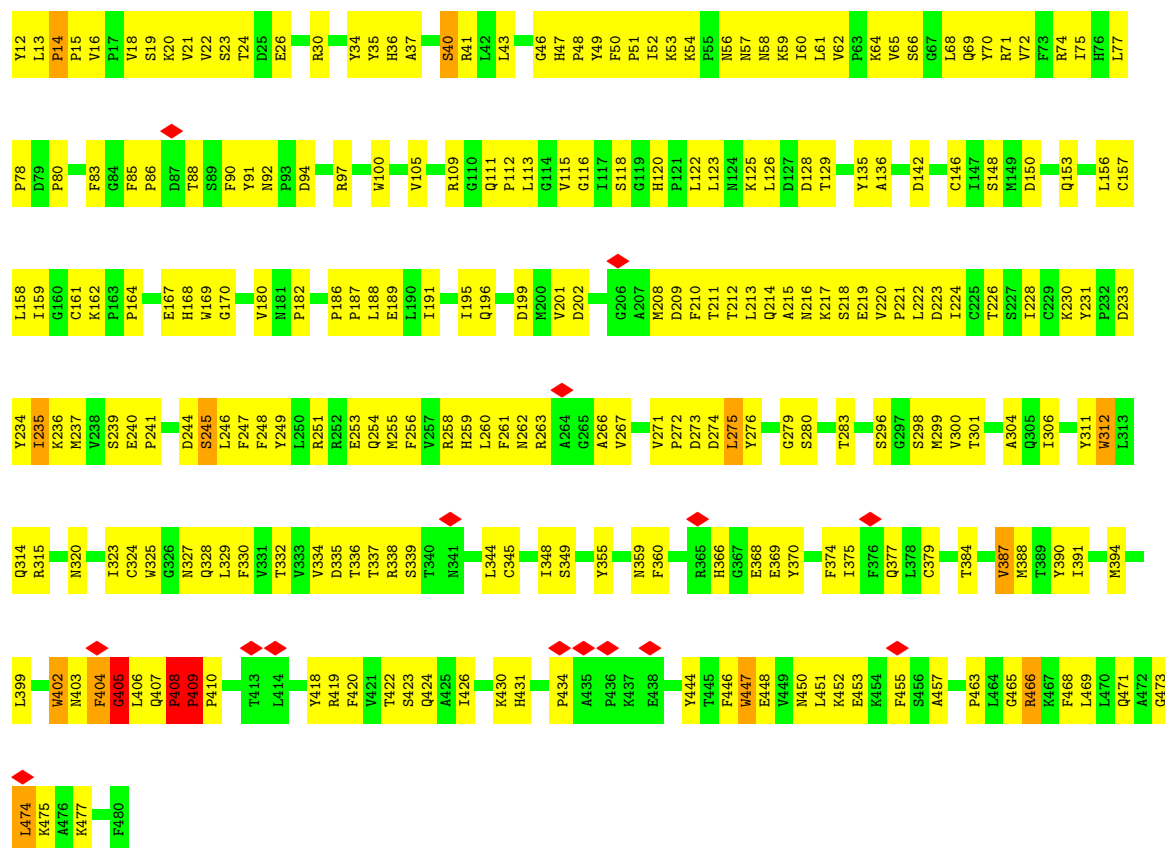
• Molecule 3: Major capsid protein L1

Chain D: 15% 77% 6% .

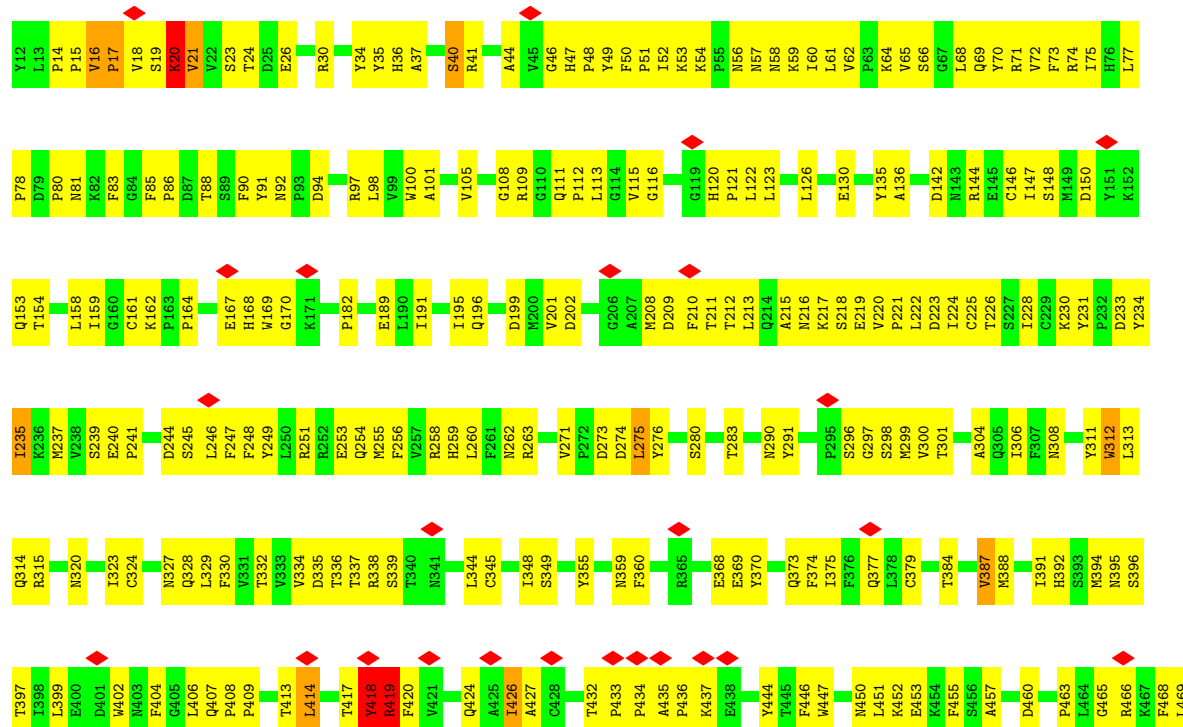


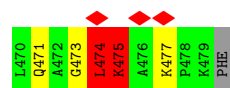
• Molecule 3: Major capsid protein L1

Chain E: 47% 50% . .



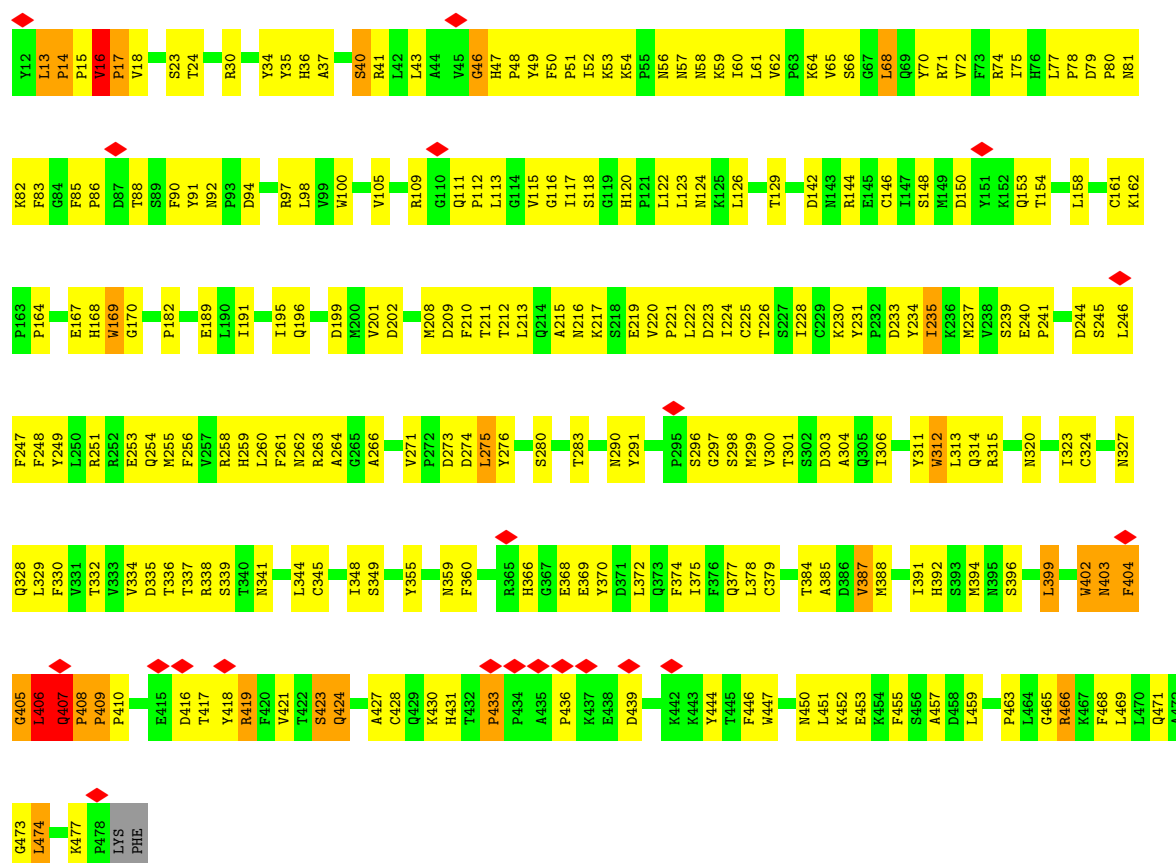
• Molecule 3: Major capsid protein L1





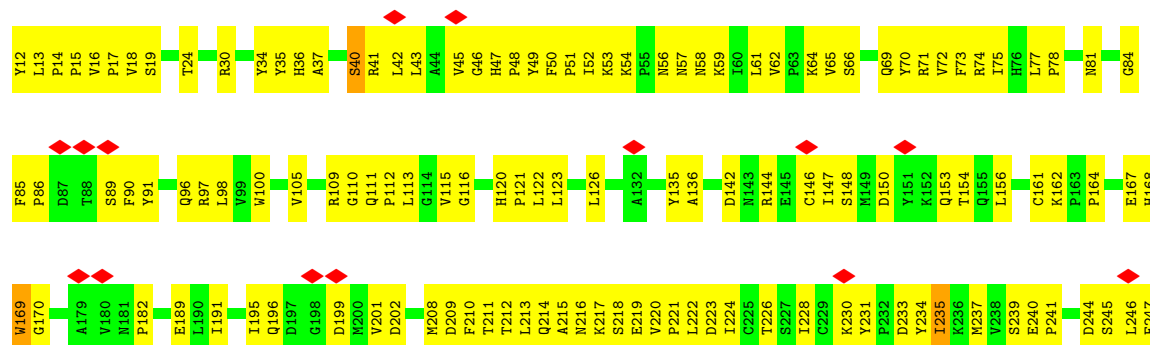
• Molecule 3: Major capsid protein L1

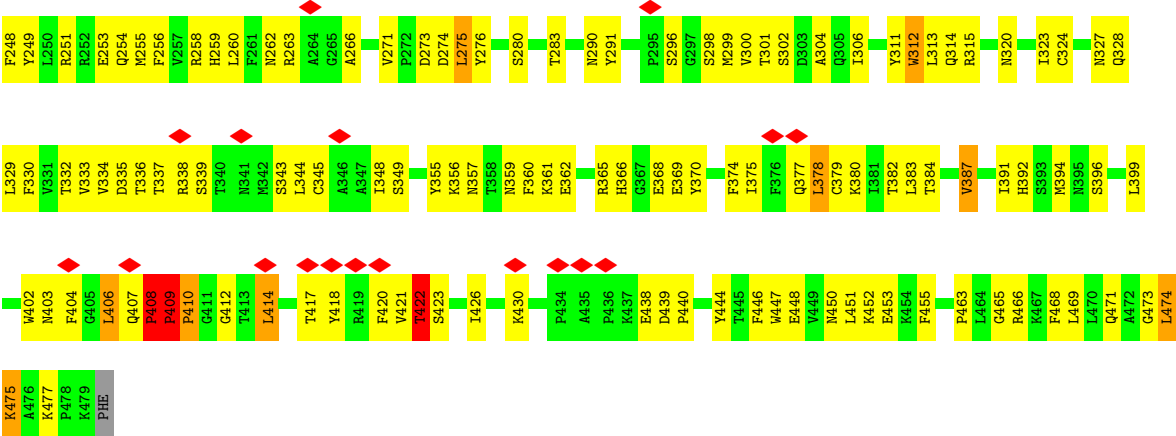
Chain G: 47% 47% 5%



• Molecule 3: Major capsid protein L1

Chain H: 7% 46% 50%





4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 17612 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 7, 7 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 14.058 | Depositor |
| Minimum map value | -8.247 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 2.1 | Depositor |
| Map size (Å) | 779.95996, 779.95996, 779.95996 | wwPDB |
| Map dimensions | 680, 680, 680 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.147, 1.147, 1.147 | Depositor |

5 Model quality

5.1 Standard geometry

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 | A | 0.50 | 1/873 (0.1%) | 0.71 | 1/1177 (0.1%) |
| 2 | B | 0.44 | 0/870 | 0.76 | 0/1181 |
| 3 | C | 0.96 | 10/3776 (0.3%) | 0.93 | 22/5142 (0.4%) |
| 3 | D | 0.82 | 4/3711 (0.1%) | 0.95 | 6/5049 (0.1%) |
| 3 | E | 0.76 | 4/3788 (0.1%) | 0.79 | 7/5158 (0.1%) |
| 3 | F | 0.73 | 1/3776 (0.0%) | 0.79 | 11/5142 (0.2%) |
| 3 | G | 0.75 | 6/3767 (0.2%) | 0.82 | 11/5131 (0.2%) |
| 3 | H | 0.75 | 5/3774 (0.1%) | 0.85 | 13/5139 (0.3%) |
| All | All | 0.78 | 31/24335 (0.1%) | 0.85 | 71/33119 (0.2%) |

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 | A | 0 | 1 |
| 3 | C | 0 | 12 |
| 3 | D | 0 | 21 |
| 3 | E | 0 | 2 |
| 3 | F | 0 | 7 |
| 3 | G | 0 | 9 |
| 3 | H | 0 | 5 |
| All | All | 0 | 57 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3 | C | 18 | VAL | CA-CB | 28.75 | 2.15 | 1.54 |
| 3 | C | 18 | VAL | CB-CG1 | 21.24 | 1.97 | 1.52 |
| 3 | C | 17 | PRO | CA-C | 14.74 | 1.82 | 1.52 |
| 3 | E | 402 | TRP | CB-CG | -10.49 | 1.31 | 1.50 |
| 3 | H | 409 | PRO | N-CA | 9.26 | 1.62 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | C | 17 | PRO | N-CA | 7.90 | 1.60 | 1.47 |
| 3 | D | 312 | TRP | CB-CG | -7.79 | 1.36 | 1.50 |
| 3 | C | 16 | VAL | C-N | 7.79 | 1.49 | 1.34 |
| 3 | D | 169 | TRP | CB-CG | -7.52 | 1.36 | 1.50 |
| 3 | G | 402 | TRP | CB-CG | -7.48 | 1.36 | 1.50 |
| 3 | C | 406 | LEU | CG-CD2 | -7.08 | 1.25 | 1.51 |
| 3 | C | 18 | VAL | CA-C | 7.04 | 1.71 | 1.52 |
| 3 | C | 175 | CYS | CB-SG | -6.90 | 1.70 | 1.82 |
| 3 | C | 18 | VAL | N-CA | 6.79 | 1.59 | 1.46 |
| 3 | C | 409 | PRO | C-N | 6.19 | 1.46 | 1.34 |
| 3 | H | 410 | PRO | CA-C | 6.07 | 1.65 | 1.52 |
| 3 | E | 447 | TRP | CB-CG | -5.84 | 1.39 | 1.50 |
| 3 | G | 13 | LEU | N-CA | 5.69 | 1.57 | 1.46 |
| 3 | H | 402 | TRP | CB-CG | -5.69 | 1.40 | 1.50 |
| 3 | D | 402 | TRP | CB-CG | -5.64 | 1.40 | 1.50 |
| 1 | A | 39 | GLN | C-N | 5.63 | 1.47 | 1.34 |
| 3 | E | 180 | VAL | C-N | -5.55 | 1.21 | 1.34 |
| 3 | G | 408 | PRO | CB-CG | -5.53 | 1.22 | 1.50 |
| 3 | E | 312 | TRP | CB-CG | -5.49 | 1.40 | 1.50 |
| 3 | G | 169 | TRP | CB-CG | -5.37 | 1.40 | 1.50 |
| 3 | G | 46 | GLY | C-N | -5.36 | 1.21 | 1.34 |
| 3 | H | 312 | TRP | CB-CG | -5.26 | 1.40 | 1.50 |
| 3 | H | 169 | TRP | CB-CG | -5.13 | 1.41 | 1.50 |
| 3 | F | 312 | TRP | CB-CG | -5.11 | 1.41 | 1.50 |
| 3 | G | 312 | TRP | CB-CG | -5.10 | 1.41 | 1.50 |
| 3 | D | 151 | TYR | CD1-CE1 | -5.01 | 1.31 | 1.39 |

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3 | H | 409 | PRO | C-N-CD | -20.45 | 75.60 | 120.60 |
| 3 | C | 17 | PRO | C-N-CA | 12.92 | 154.00 | 121.70 |
| 3 | G | 405 | GLY | N-CA-C | -11.90 | 83.35 | 113.10 |
| 3 | G | 16 | VAL | C-N-CD | -11.61 | 95.06 | 120.60 |
| 3 | C | 20 | LYS | CD-CE-NZ | -11.38 | 85.52 | 111.70 |
| 3 | C | 406 | LEU | CA-CB-CG | -10.77 | 90.53 | 115.30 |
| 3 | C | 18 | VAL | CA-CB-CG1 | 10.77 | 127.05 | 110.90 |
| 3 | H | 409 | PRO | CA-N-CD | -10.08 | 97.39 | 111.50 |
| 3 | G | 406 | LEU | CA-CB-CG | 9.86 | 137.98 | 115.30 |
| 3 | C | 18 | VAL | CB-CA-C | 9.66 | 129.75 | 111.40 |
| 3 | C | 406 | LEU | CB-CG-CD2 | -9.29 | 95.21 | 111.00 |
| 3 | C | 18 | VAL | CA-CB-CG2 | 8.93 | 124.30 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | D | 451 | LEU | CA-CB-CG | -8.91 | 94.80 | 115.30 |
| 3 | C | 122 | LEU | CB-CG-CD1 | -8.72 | 96.17 | 111.00 |
| 3 | F | 474 | LEU | CA-CB-CG | 8.21 | 134.18 | 115.30 |
| 3 | C | 406 | LEU | CB-CG-CD1 | -8.09 | 97.25 | 111.00 |
| 3 | H | 409 | PRO | CA-C-N | -7.93 | 94.91 | 117.10 |
| 3 | H | 410 | PRO | C-N-CA | 7.71 | 138.49 | 122.30 |
| 3 | C | 175 | CYS | CA-CB-SG | -7.66 | 100.21 | 114.00 |
| 3 | C | 17 | PRO | N-CA-C | 7.57 | 131.78 | 112.10 |
| 3 | C | 16 | VAL | C-N-CD | -7.38 | 104.36 | 120.60 |
| 3 | H | 409 | PRO | O-C-N | 7.22 | 134.83 | 121.10 |
| 3 | H | 414 | LEU | CA-CB-CG | -7.20 | 98.75 | 115.30 |
| 3 | D | 123 | LEU | CA-CB-CG | -7.19 | 98.75 | 115.30 |
| 3 | H | 412 | GLY | N-CA-C | 7.14 | 130.95 | 113.10 |
| 3 | D | 474 | LEU | CA-CB-CG | 7.04 | 131.49 | 115.30 |
| 3 | F | 414 | LEU | CB-CG-CD2 | -6.79 | 99.46 | 111.00 |
| 3 | C | 19 | SER | C-N-CA | -6.66 | 105.05 | 121.70 |
| 3 | C | 16 | VAL | C-N-CA | 6.53 | 149.41 | 122.00 |
| 3 | E | 474 | LEU | CA-CB-CG | 6.48 | 130.21 | 115.30 |
| 3 | C | 414 | LEU | CA-CB-CG | -6.48 | 100.39 | 115.30 |
| 3 | F | 406 | LEU | CA-CB-CG | 6.42 | 130.06 | 115.30 |
| 3 | H | 406 | LEU | CA-CB-CG | -6.33 | 100.73 | 115.30 |
| 3 | C | 21 | VAL | N-CA-C | -6.31 | 93.97 | 111.00 |
| 3 | C | 20 | LYS | CA-CB-CG | 6.26 | 127.17 | 113.40 |
| 3 | H | 378 | LEU | CB-CG-CD2 | -6.22 | 100.42 | 111.00 |
| 3 | D | 378 | LEU | CA-CB-CG | -6.12 | 101.22 | 115.30 |
| 3 | H | 474 | LEU | CA-CB-CG | 6.11 | 129.34 | 115.30 |
| 3 | C | 18 | VAL | CA-C-N | 6.06 | 130.54 | 117.20 |
| 3 | G | 466 | ARG | NE-CZ-NH1 | -5.96 | 117.32 | 120.30 |
| 3 | F | 419 | ARG | CG-CD-NE | -5.92 | 99.37 | 111.80 |
| 3 | G | 13 | LEU | CB-CG-CD1 | 5.87 | 120.97 | 111.00 |
| 3 | E | 405 | GLY | C-N-CA | -5.78 | 107.26 | 121.70 |
| 1 | A | 99 | GLY | N-CA-C | 5.75 | 127.49 | 113.10 |
| 3 | E | 466 | ARG | NE-CZ-NH1 | -5.66 | 117.47 | 120.30 |
| 3 | F | 275 | LEU | CA-CB-CG | -5.59 | 102.45 | 115.30 |
| 3 | H | 422 | THR | N-CA-CB | 5.59 | 120.91 | 110.30 |
| 3 | G | 407 | GLN | CB-CA-C | 5.57 | 121.55 | 110.40 |
| 3 | E | 405 | GLY | O-C-N | -5.51 | 113.88 | 122.70 |
| 3 | F | 68 | LEU | CA-CB-CG | -5.51 | 102.62 | 115.30 |
| 3 | H | 275 | LEU | CA-CB-CG | -5.50 | 102.65 | 115.30 |
| 3 | C | 19 | SER | O-C-N | -5.47 | 113.95 | 122.70 |
| 3 | H | 409 | PRO | N-CA-C | 5.43 | 126.21 | 112.10 |
| 3 | C | 312 | TRP | CA-CB-CG | -5.41 | 103.42 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | F | 418 | TYR | N-CA-C | -5.41 | 96.39 | 111.00 |
| 3 | G | 68 | LEU | CA-CB-CG | -5.30 | 103.10 | 115.30 |
| 3 | D | 429 | GLN | N-CA-C | 5.30 | 125.31 | 111.00 |
| 3 | F | 414 | LEU | CB-CG-CD1 | -5.28 | 102.02 | 111.00 |
| 3 | E | 434 | PRO | C-N-CA | 5.28 | 134.90 | 121.70 |
| 3 | E | 275 | LEU | CA-CB-CG | -5.22 | 103.28 | 115.30 |
| 3 | D | 470 | LEU | CA-CB-CG | -5.21 | 103.31 | 115.30 |
| 3 | G | 474 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 3 | G | 275 | LEU | CA-CB-CG | -5.18 | 103.38 | 115.30 |
| 3 | E | 312 | TRP | CA-CB-CG | -5.13 | 103.95 | 113.70 |
| 3 | G | 399 | LEU | CA-CB-CG | -5.12 | 103.54 | 115.30 |
| 3 | G | 14 | PRO | C-N-CD | 5.11 | 139.14 | 128.40 |
| 3 | C | 20 | LYS | C-N-CA | 5.08 | 134.40 | 121.70 |
| 3 | F | 435 | ALA | C-N-CD | 5.07 | 139.06 | 128.40 |
| 3 | F | 16 | VAL | C-N-CD | 5.03 | 138.96 | 128.40 |
| 3 | C | 222 | LEU | CB-CG-CD2 | -5.02 | 102.47 | 111.00 |
| 3 | F | 475 | LYS | CB-CA-C | -5.01 | 100.39 | 110.40 |

There are no chirality outliers.

All (57) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 98 | TYR | Peptide |
| 3 | C | 17 | PRO | Peptide |
| 3 | C | 18 | VAL | Peptide |
| 3 | C | 20 | LYS | Peptide |
| 3 | C | 408 | PRO | Mainchain,Peptide |
| 3 | C | 416 | ASP | Peptide |
| 3 | C | 421 | VAL | Peptide |
| 3 | C | 428 | CYS | Peptide |
| 3 | C | 430 | LYS | Peptide |
| 3 | C | 431 | HIS | Peptide |
| 3 | C | 434 | PRO | Peptide |
| 3 | C | 438 | GLU | Peptide |
| 3 | D | 107 | VAL | Peptide |
| 3 | D | 202 | ASP | Peptide |
| 3 | D | 232 | PRO | Peptide |
| 3 | D | 246 | LEU | Peptide |
| 3 | D | 249 | TYR | Peptide |
| 3 | D | 311 | TYR | Peptide |
| 3 | D | 313 | LEU | Peptide |
| 3 | D | 336 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | D | 407 | GLN | Peptide |
| 3 | D | 412 | GLY | Peptide |
| 3 | D | 418 | TYR | Peptide |
| 3 | D | 428 | CYS | Peptide |
| 3 | D | 429 | GLN | Peptide |
| 3 | D | 431 | HIS | Peptide |
| 3 | D | 432 | THR | Peptide |
| 3 | D | 433 | PRO | Peptide |
| 3 | D | 451 | LEU | Peptide |
| 3 | D | 474 | LEU | Peptide |
| 3 | D | 478 | PRO | Peptide |
| 3 | D | 63 | PRO | Peptide |
| 3 | D | 74 | ARG | Peptide |
| 3 | E | 408 | PRO | Peptide |
| 3 | E | 409 | PRO | Peptide |
| 3 | F | 20 | LYS | Peptide |
| 3 | F | 21 | VAL | Peptide |
| 3 | F | 418 | TYR | Peptide |
| 3 | F | 419 | ARG | Peptide |
| 3 | F | 420 | PHE | Peptide |
| 3 | F | 424 | GLN | Peptide |
| 3 | F | 474 | LEU | Peptide |
| 3 | G | 403 | ASN | Peptide |
| 3 | G | 404 | PHE | Peptide |
| 3 | G | 406 | LEU | Peptide |
| 3 | G | 407 | GLN | Peptide |
| 3 | G | 418 | TYR | Peptide |
| 3 | G | 419 | ARG | Peptide |
| 3 | G | 423 | SER | Peptide |
| 3 | G | 433 | PRO | Peptide |
| 3 | G | 439 | ASP | Peptide |
| 3 | H | 408 | PRO | Peptide |
| 3 | H | 409 | PRO | Mainchain |
| 3 | H | 422 | THR | Peptide |
| 3 | H | 438 | GLU | Peptide |
| 3 | H | 475 | LYS | Peptide |

5.2 Too-close contacts

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 | A | 851 | 0 | 792 | 120 | 0 |
| 2 | B | 850 | 0 | 831 | 126 | 0 |
| 3 | C | 3675 | 0 | 3592 | 289 | 0 |
| 3 | D | 3614 | 0 | 3528 | 811 | 0 |
| 3 | E | 3686 | 0 | 3601 | 295 | 0 |
| 3 | F | 3675 | 0 | 3592 | 280 | 0 |
| 3 | G | 3666 | 0 | 3579 | 281 | 0 |
| 3 | H | 3673 | 0 | 3585 | 292 | 0 |
| All | All | 23690 | 0 | 23100 | 2321 | 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 50.

All (2321) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:17:PRO:C | 3:C:17:PRO:CA | 1.82 | 1.43 |
| 3:C:18:VAL:CB | 3:C:18:VAL:CG1 | 1.97 | 1.39 |
| 3:F:19:SER:O | 3:F:20:LYS:HG2 | 1.15 | 1.33 |
| 3:C:18:VAL:CB | 3:C:18:VAL:CA | 2.15 | 1.25 |
| 3:G:16:VAL:HB | 3:G:17:PRO:CD | 1.67 | 1.25 |
| 3:G:16:VAL:CB | 3:G:17:PRO:HD2 | 1.67 | 1.22 |
| 3:F:19:SER:O | 3:F:20:LYS:CG | 1.87 | 1.20 |
| 3:D:76:HIS:HB2 | 3:D:450:ASN:HA | 1.34 | 1.09 |
| 3:D:160:GLY:HA3 | 3:D:246:LEU:HA | 1.31 | 1.08 |
| 3:C:52:ILE:HB | 3:C:62:VAL:HB | 1.35 | 1.06 |
| 2:B:86:TYR:HB2 | 2:B:102:THR:HB | 1.41 | 1.02 |
| 3:D:109:ARG:HH22 | 3:D:111:GLN:HG2 | 1.21 | 1.02 |
| 3:H:162:LYS:HB2 | 3:H:245:SER:HA | 1.41 | 1.02 |
| 3:D:468:PHE:HA | 3:D:471:GLN:HB3 | 1.40 | 1.01 |
| 3:D:47:HIS:HE1 | 3:D:49:TYR:HB2 | 1.26 | 1.00 |
| 3:D:234:TYR:O | 3:D:238:VAL:N | 1.93 | 1.00 |
| 3:D:459:LEU:HD23 | 3:D:462:PHE:HB2 | 1.39 | 1.00 |
| 3:F:426:ILE:HG22 | 3:F:427:ALA:H | 1.26 | 0.99 |
| 3:D:103:VAL:H | 3:D:376:PHE:HA | 1.24 | 0.98 |
| 3:C:111:GLN:HB2 | 3:C:338:ARG:HD3 | 1.46 | 0.98 |
| 3:D:25:ASP:HA | 3:D:28:VAL:HB | 1.45 | 0.98 |
| 3:F:162:LYS:HB2 | 3:F:245:SER:HA | 1.46 | 0.97 |
| 3:D:168:HIS:O | 3:D:191:ILE:N | 1.97 | 0.97 |
| 3:G:463:PRO:HA | 3:G:466:ARG:HH12 | 1.29 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:162:LYS:HB2 | 3:G:245:SER:HA | 1.47 | 0.96 |
| 3:G:16:VAL:HB | 3:G:17:PRO:HD2 | 0.97 | 0.96 |
| 3:D:24:THR:HG21 | 3:D:323:ILE:HG13 | 1.47 | 0.95 |
| 3:E:463:PRO:HA | 3:E:466:ARG:HH12 | 1.30 | 0.95 |
| 1:A:81:GLN:NE2 | 1:A:82:MET:O | 1.99 | 0.94 |
| 3:C:406:LEU:HD11 | 3:C:411:GLY:N | 1.81 | 0.94 |
| 3:D:207:ALA:HA | 3:D:229:CYS:HB2 | 1.49 | 0.94 |
| 3:G:417:THR:HB | 3:G:419:ARG:HE | 1.31 | 0.94 |
| 2:B:6:GLN:H | 2:B:100:ALA:HB3 | 1.30 | 0.93 |
| 3:D:114:GLY:H | 3:D:338:ARG:HA | 1.31 | 0.93 |
| 3:C:18:VAL:CA | 3:C:18:VAL:HB | 1.96 | 0.93 |
| 3:D:399:LEU:HD23 | 3:D:402:TRP:HB2 | 1.51 | 0.93 |
| 3:D:389:THR:O | 3:D:393:SER:N | 2.00 | 0.92 |
| 3:D:287:ALA:HB3 | 3:H:121:PRO:HB3 | 1.49 | 0.92 |
| 3:G:109:ARG:NH1 | 3:G:369:GLU:O | 2.01 | 0.92 |
| 3:C:62:VAL:HG13 | 3:H:426:ILE:HD11 | 1.48 | 0.92 |
| 3:D:36:HIS:CE1 | 3:D:37:ALA:O | 2.23 | 0.91 |
| 3:F:74:ARG:HB2 | 3:F:446:PHE:HE1 | 1.35 | 0.91 |
| 3:D:38:GLY:HA3 | 3:D:373:GLN:HG2 | 1.50 | 0.91 |
| 3:F:109:ARG:NH1 | 3:F:369:GLU:O | 2.04 | 0.91 |
| 3:H:422:THR:OG1 | 3:H:430:LYS:NZ | 2.04 | 0.91 |
| 2:B:80:ALA:O | 2:B:83:LEU:N | 2.04 | 0.91 |
| 3:G:74:ARG:HB2 | 3:G:446:PHE:HE1 | 1.33 | 0.91 |
| 3:C:109:ARG:NH1 | 3:C:369:GLU:O | 2.03 | 0.91 |
| 3:H:109:ARG:NH1 | 3:H:369:GLU:O | 2.03 | 0.90 |
| 3:D:349:SER:O | 3:D:359:ASN:ND2 | 2.03 | 0.90 |
| 3:H:219:GLU:OE1 | 3:H:263:ARG:NH1 | 2.04 | 0.90 |
| 3:E:162:LYS:HB2 | 3:E:245:SER:HA | 1.52 | 0.90 |
| 3:G:424:GLN:NE2 | 3:G:428:CYS:O | 2.04 | 0.89 |
| 3:E:109:ARG:NH1 | 3:E:369:GLU:O | 2.06 | 0.89 |
| 3:D:113:LEU:HA | 3:D:338:ARG:HG2 | 1.53 | 0.89 |
| 3:D:210:PHE:O | 3:D:214:GLN:N | 2.05 | 0.89 |
| 3:D:115:VAL:N | 3:D:340:THR:OG1 | 2.04 | 0.89 |
| 3:D:240:GLU:HG2 | 3:D:242:TYR:H | 1.37 | 0.88 |
| 1:A:66:ARG:HA | 3:C:176:THR:HB | 1.56 | 0.88 |
| 3:H:74:ARG:HB2 | 3:H:446:PHE:HE1 | 1.36 | 0.88 |
| 3:D:216:ASN:N | 3:H:345:CYS:SG | 2.46 | 0.88 |
| 3:D:301:THR:HG23 | 3:D:304:ALA:H | 1.37 | 0.88 |
| 3:F:463:PRO:HA | 3:F:466:ARG:HH12 | 1.37 | 0.88 |
| 3:D:114:GLY:N | 3:D:338:ARG:HA | 1.88 | 0.87 |
| 3:F:418:TYR:HB2 | 3:F:419:ARG:HH11 | 1.38 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:C:15:PRO:HB2 | 3:C:17:PRO:HD2 | 1.56 | 0.87 |
| 3:D:111:GLN:HB2 | 3:D:338:ARG:HD3 | 1.55 | 0.87 |
| 3:D:355:TYR:OH | 3:D:357:ASN:ND2 | 2.08 | 0.87 |
| 3:G:16:VAL:HG23 | 3:G:17:PRO:N | 1.88 | 0.87 |
| 3:C:74:ARG:NH1 | 3:C:439:ASP:OD2 | 2.07 | 0.87 |
| 3:G:16:VAL:CB | 3:G:17:PRO:CD | 2.27 | 0.87 |
| 3:F:219:GLU:OE1 | 3:F:263:ARG:NH1 | 2.07 | 0.87 |
| 3:H:407:GLN:HB2 | 3:H:408:PRO:HD3 | 1.57 | 0.87 |
| 3:G:219:GLU:OE1 | 3:G:263:ARG:NH1 | 2.07 | 0.86 |
| 3:C:406:LEU:HD11 | 3:C:411:GLY:H | 1.38 | 0.86 |
| 1:A:100(C):GLY:HA3 | 2:B:50:TRP:HB2 | 1.57 | 0.86 |
| 3:F:216:ASN:ND2 | 3:F:219:GLU:OE2 | 2.09 | 0.86 |
| 3:D:314:GLN:HG3 | 3:D:315:ARG:H | 1.38 | 0.86 |
| 3:D:77:LEU:HB2 | 3:D:327:ASN:HB3 | 1.58 | 0.86 |
| 3:H:404:PHE:CE1 | 3:H:409:PRO:HD3 | 2.10 | 0.86 |
| 3:H:463:PRO:HA | 3:H:466:ARG:HH12 | 1.37 | 0.86 |
| 2:B:36:TYR:HB2 | 2:B:87:TYR:HB2 | 1.55 | 0.86 |
| 3:D:70:TYR:OH | 3:D:230:LYS:O | 1.92 | 0.86 |
| 3:D:468:PHE:O | 3:D:472:ALA:N | 2.08 | 0.86 |
| 3:D:310:PRO:HB2 | 3:D:312:TRP:HE1 | 1.41 | 0.86 |
| 3:C:420:PHE:HA | 3:H:41:ARG:HD3 | 1.58 | 0.85 |
| 3:D:257:VAL:HA | 3:D:295:PRO:HA | 1.58 | 0.85 |
| 3:D:119:GLY:HA3 | 3:D:148:SER:HA | 1.57 | 0.85 |
| 3:D:39:THR:OG1 | 3:D:371:ASP:OD1 | 1.92 | 0.85 |
| 3:D:46:GLY:O | 3:D:366:HIS:N | 2.09 | 0.84 |
| 3:D:118:SER:N | 3:D:151:TYR:OH | 2.10 | 0.84 |
| 3:D:259:HIS:O | 3:D:294:THR:N | 2.11 | 0.84 |
| 3:E:74:ARG:HB2 | 3:E:446:PHE:HE1 | 1.42 | 0.84 |
| 3:C:415:GLU:HA | 3:D:241:PRO:HG3 | 1.58 | 0.84 |
| 3:F:19:SER:O | 3:F:20:LYS:CD | 2.25 | 0.84 |
| 3:D:47:HIS:CE1 | 3:D:49:TYR:HB2 | 2.12 | 0.84 |
| 3:D:360:PHE:HE1 | 3:E:215:ALA:HB3 | 1.42 | 0.84 |
| 3:D:240:GLU:OE1 | 3:D:244:ASP:N | 2.08 | 0.84 |
| 3:D:385:ALA:O | 3:D:389:THR:N | 2.09 | 0.84 |
| 3:E:463:PRO:HA | 3:E:466:ARG:NH1 | 1.91 | 0.84 |
| 3:C:97:ARG:NH2 | 3:C:402:TRP:HB3 | 1.93 | 0.84 |
| 3:D:126:LEU:N | 3:D:262:ASN:O | 2.10 | 0.84 |
| 3:D:262:ASN:ND2 | 3:D:290:ASN:O | 2.09 | 0.84 |
| 3:G:116:GLY:N | 3:G:339:SER:OG | 2.11 | 0.84 |
| 2:B:86:TYR:N | 2:B:102:THR:O | 2.09 | 0.84 |
| 3:D:273:ASP:HA | 3:D:276:TYR:CZ | 2.12 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:411:GLY:O | 3:D:20:LYS:N | 2.10 | 0.83 |
| 3:D:202:ASP:HB2 | 3:D:204:GLY:H | 1.43 | 0.83 |
| 3:G:453:GLU:O | 3:H:12:TYR:N | 2.10 | 0.83 |
| 3:C:162:LYS:HB2 | 3:C:245:SER:HA | 1.59 | 0.83 |
| 3:D:44:ALA:HB3 | 3:D:368:GLU:HB2 | 1.61 | 0.83 |
| 3:D:382:THR:HG22 | 3:D:383:LEU:H | 1.43 | 0.83 |
| 3:D:386:ASP:O | 3:D:390:TYR:N | 2.11 | 0.83 |
| 3:D:263:ARG:HB2 | 3:D:290:ASN:HB3 | 1.61 | 0.83 |
| 3:G:463:PRO:HA | 3:G:466:ARG:NH1 | 1.91 | 0.83 |
| 3:D:209:ASP:O | 3:D:212:THR:OG1 | 1.94 | 0.83 |
| 3:D:459:LEU:O | 3:D:466:ARG:NE | 2.10 | 0.83 |
| 3:H:216:ASN:ND2 | 3:H:219:GLU:OE2 | 2.11 | 0.83 |
| 3:H:52:ILE:HG22 | 3:H:61:LEU:HB3 | 1.61 | 0.82 |
| 3:D:210:PHE:HB3 | 3:D:214:GLN:HB2 | 1.59 | 0.82 |
| 3:E:219:GLU:OE1 | 3:E:263:ARG:NH1 | 2.12 | 0.82 |
| 3:D:287:ALA:HB1 | 3:H:146:CYS:HB2 | 1.60 | 0.82 |
| 3:G:16:VAL:CG2 | 3:G:17:PRO:HD2 | 2.08 | 0.82 |
| 3:D:150:ASP:OD2 | 3:D:258:ARG:NH2 | 2.12 | 0.82 |
| 3:D:135:TYR:OH | 3:D:286:LEU:O | 1.97 | 0.82 |
| 3:F:111:GLN:HB2 | 3:F:338:ARG:HD3 | 1.62 | 0.82 |
| 3:H:54:LYS:HB3 | 3:H:57:ASN:HB3 | 1.60 | 0.82 |
| 3:D:96:GLN:NE2 | 3:D:382:THR:OG1 | 2.12 | 0.82 |
| 3:D:188:LEU:HD22 | 3:H:45:VAL:HG11 | 1.61 | 0.82 |
| 3:E:422:THR:HA | 3:E:426:ILE:HD12 | 1.60 | 0.82 |
| 3:G:216:ASN:ND2 | 3:G:219:GLU:OE2 | 2.13 | 0.81 |
| 2:B:2:ILE:O | 2:B:97:THR:OG1 | 1.98 | 0.81 |
| 3:G:52:ILE:HG22 | 3:G:61:LEU:HB3 | 1.62 | 0.81 |
| 1:A:59:TYR:HB2 | 1:A:64:LYS:HD2 | 1.62 | 0.81 |
| 3:C:74:ARG:HB2 | 3:C:446:PHE:HE1 | 1.45 | 0.81 |
| 3:F:116:GLY:N | 3:F:339:SER:OG | 2.11 | 0.81 |
| 3:D:169:TRP:N | 3:D:207:ALA:O | 2.13 | 0.81 |
| 3:F:54:LYS:HB3 | 3:F:57:ASN:HB3 | 1.63 | 0.81 |
| 1:A:94:ARG:NH2 | 1:A:101:ASP:OD2 | 2.14 | 0.80 |
| 3:F:19:SER:C | 3:F:20:LYS:HG2 | 2.01 | 0.80 |
| 3:D:69:GLN:HB3 | 3:D:198:GLY:HA2 | 1.62 | 0.80 |
| 3:D:108:GLY:N | 3:D:371:ASP:O | 2.14 | 0.80 |
| 3:D:397:THR:HA | 3:D:400:GLU:CD | 2.01 | 0.80 |
| 3:D:117:ILE:HG13 | 3:D:149:MET:O | 1.82 | 0.80 |
| 3:F:463:PRO:HA | 3:F:466:ARG:NH1 | 1.95 | 0.80 |
| 3:F:70:TYR:OH | 3:F:230:LYS:O | 2.00 | 0.80 |
| 3:H:463:PRO:HA | 3:H:466:ARG:NH1 | 1.96 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:H:116:GLY:N | 3:H:339:SER:OG | 2.12 | 0.80 |
| 3:D:109:ARG:O | 3:D:308:ASN:ND2 | 2.14 | 0.80 |
| 3:C:126:LEU:HB3 | 3:C:262:ASN:HB2 | 1.63 | 0.80 |
| 3:E:54:LYS:HB3 | 3:E:57:ASN:HB3 | 1.62 | 0.79 |
| 3:F:83:PHE:HD1 | 3:G:13:LEU:HD12 | 1.48 | 0.79 |
| 1:A:59:TYR:CG | 1:A:64:LYS:HA | 2.17 | 0.79 |
| 3:H:312:TRP:CH2 | 3:H:468:PHE:HD1 | 2.01 | 0.79 |
| 3:C:164:PRO:HB2 | 3:C:195:ILE:HD12 | 1.65 | 0.79 |
| 3:G:120:HIS:ND1 | 3:G:122:LEU:O | 2.16 | 0.79 |
| 3:H:469:LEU:O | 3:H:473:GLY:N | 2.16 | 0.78 |
| 3:H:120:HIS:ND1 | 3:H:122:LEU:O | 2.15 | 0.78 |
| 3:D:54:LYS:HB3 | 3:D:57:ASN:HB3 | 1.65 | 0.78 |
| 3:D:155:GLN:OE1 | 3:D:305:GLN:NE2 | 2.17 | 0.78 |
| 1:A:24:ALA:HB3 | 1:A:76:ASN:HB3 | 1.66 | 0.78 |
| 3:D:69:GLN:HB2 | 3:D:71:ARG:NH2 | 1.99 | 0.78 |
| 3:D:165:ILE:HG12 | 3:D:194:VAL:HA | 1.66 | 0.78 |
| 2:B:29:LEU:HB2 | 2:B:68:GLY:HA2 | 1.66 | 0.78 |
| 3:C:428:CYS:HA | 3:C:430:LYS:O | 1.82 | 0.78 |
| 3:D:159:ILE:HD12 | 3:D:248:PHE:CD2 | 2.18 | 0.78 |
| 3:D:166:GLY:N | 3:D:195:ILE:HG13 | 1.99 | 0.78 |
| 3:C:463:PRO:HA | 3:C:466:ARG:HH12 | 1.48 | 0.77 |
| 3:C:54:LYS:HB3 | 3:C:57:ASN:HB3 | 1.65 | 0.77 |
| 3:D:101:ALA:N | 3:D:377:GLN:O | 2.17 | 0.77 |
| 3:D:102:CYS:HA | 3:D:376:PHE:HD1 | 1.49 | 0.77 |
| 3:E:37:ALA:HB2 | 3:E:455:PHE:HA | 1.65 | 0.77 |
| 3:E:18:VAL:H | 3:E:19:SER:HA | 1.49 | 0.77 |
| 3:D:109:ARG:HH11 | 3:D:110:GLY:H | 1.29 | 0.77 |
| 3:D:162:LYS:HB2 | 3:D:245:SER:HA | 1.65 | 0.77 |
| 3:D:366:HIS:ND1 | 3:D:368:GLU:OE2 | 2.17 | 0.77 |
| 3:F:37:ALA:HB2 | 3:F:455:PHE:HA | 1.65 | 0.77 |
| 3:H:37:ALA:HB2 | 3:H:455:PHE:HA | 1.65 | 0.77 |
| 1:A:39:GLN:H | 1:A:88:ALA:HB1 | 1.50 | 0.77 |
| 3:D:72:VAL:N | 3:D:197:ASP:OD1 | 2.18 | 0.77 |
| 3:G:37:ALA:HB2 | 3:G:455:PHE:HA | 1.66 | 0.77 |
| 3:D:44:ALA:O | 3:D:368:GLU:N | 2.18 | 0.77 |
| 3:D:335:ASP:OD2 | 3:D:337:THR:OG1 | 2.03 | 0.77 |
| 2:B:32:TYR:HD2 | 2:B:92:TYR:HB2 | 1.47 | 0.76 |
| 3:D:416:ASP:O | 3:D:417:THR:OG1 | 2.03 | 0.76 |
| 3:F:120:HIS:ND1 | 3:F:122:LEU:O | 2.19 | 0.76 |
| 1:A:29:PHE:CD2 | 1:A:73:ASN:HA | 2.20 | 0.76 |
| 1:A:82(A):SER:HB2 | 3:C:179:ALA:HB2 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:2:ILE:HD13 | 2:B:25:SER:HB2 | 1.65 | 0.76 |
| 3:D:22:VAL:HB | 3:D:26:GLU:HG3 | 1.66 | 0.76 |
| 3:G:74:ARG:HB2 | 3:G:446:PHE:CE1 | 2.18 | 0.76 |
| 1:A:22:CYS:HB3 | 1:A:78:LEU:HB3 | 1.66 | 0.76 |
| 2:B:30(A):TYR:O | 2:B:30(E):GLN:NE2 | 2.19 | 0.76 |
| 3:D:76:HIS:ND1 | 3:D:449:VAL:O | 2.15 | 0.76 |
| 3:D:182:PRO:HB2 | 3:H:348:ILE:HG13 | 1.66 | 0.76 |
| 3:H:52:ILE:O | 3:H:61:LEU:N | 2.18 | 0.76 |
| 3:D:120:HIS:ND1 | 3:D:122:LEU:O | 2.17 | 0.76 |
| 3:E:70:TYR:OH | 3:E:230:LYS:O | 2.02 | 0.76 |
| 3:F:220:VAL:HB | 3:F:224:ILE:HD11 | 1.68 | 0.76 |
| 3:D:302:SER:OG | 3:E:253:GLU:N | 2.19 | 0.76 |
| 3:G:81:ASN:HD21 | 3:G:98:LEU:H | 1.34 | 0.76 |
| 3:H:220:VAL:HB | 3:H:224:ILE:HD11 | 1.67 | 0.76 |
| 3:C:258:ARG:NH2 | 3:C:296:SER:OG | 2.17 | 0.76 |
| 3:F:210:PHE:HE2 | 3:F:224:ILE:HD12 | 1.51 | 0.76 |
| 3:D:96:GLN:HG2 | 3:D:382:THR:HA | 1.65 | 0.76 |
| 3:D:372:LEU:HB3 | 3:D:374:PHE:CZ | 2.21 | 0.76 |
| 3:G:406:LEU:HA | 3:G:408:PRO:HD3 | 1.67 | 0.75 |
| 3:F:418:TYR:HB3 | 3:F:419:ARG:HA | 1.68 | 0.75 |
| 3:F:74:ARG:HB2 | 3:F:446:PHE:CE1 | 2.20 | 0.75 |
| 2:B:13:VAL:HG11 | 2:B:19:VAL:HA | 1.67 | 0.75 |
| 3:C:312:TRP:CH2 | 3:C:468:PHE:HD1 | 2.05 | 0.75 |
| 3:E:52:ILE:HG22 | 3:E:61:LEU:HB3 | 1.67 | 0.75 |
| 3:F:52:ILE:HG22 | 3:F:61:LEU:HB3 | 1.69 | 0.75 |
| 3:C:399:LEU:HB3 | 3:C:404:PHE:CE1 | 2.21 | 0.75 |
| 3:D:47:HIS:HA | 3:D:365:ARG:HA | 1.66 | 0.75 |
| 3:D:99:VAL:O | 3:D:379:CYS:N | 2.17 | 0.75 |
| 3:C:53:LYS:HA | 3:C:61:LEU:H | 1.52 | 0.74 |
| 3:G:421:VAL:HG12 | 3:G:423:SER:H | 1.52 | 0.74 |
| 3:D:109:ARG:NH2 | 3:D:111:GLN:HG2 | 1.99 | 0.74 |
| 3:E:312:TRP:CH2 | 3:E:468:PHE:HD1 | 2.06 | 0.74 |
| 1:A:72:ASP:HB3 | 1:A:79:TYR:HE2 | 1.51 | 0.74 |
| 3:G:46:GLY:HA3 | 3:G:65:VAL:HB | 1.69 | 0.74 |
| 3:D:162:LYS:N | 3:D:244:ASP:O | 2.21 | 0.74 |
| 3:D:299:MET:HA | 3:E:256:PHE:HB3 | 1.70 | 0.74 |
| 3:C:158:LEU:HB2 | 3:C:332:THR:HB | 1.70 | 0.74 |
| 3:E:120:HIS:ND1 | 3:E:122:LEU:O | 2.21 | 0.74 |
| 3:F:312:TRP:CH2 | 3:F:468:PHE:HD1 | 2.06 | 0.74 |
| 3:C:97:ARG:HH22 | 3:C:404:PHE:N | 1.85 | 0.74 |
| 2:B:37:GLN:N | 2:B:45:LYS:O | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:157:CYS:HA | 3:D:333:VAL:HG22 | 1.70 | 0.74 |
| 3:D:461:GLN:OE1 | 3:D:461:GLN:N | 2.20 | 0.74 |
| 3:G:312:TRP:CH2 | 3:G:468:PHE:HD1 | 2.06 | 0.74 |
| 3:H:70:TYR:OH | 3:H:230:LYS:O | 2.06 | 0.74 |
| 3:D:277:ILE:HD11 | 3:H:216:ASN:O | 1.88 | 0.74 |
| 3:F:57:ASN:OD1 | 3:F:58:ASN:N | 2.21 | 0.74 |
| 1:A:93:ALA:HA | 1:A:103:TRP:HB2 | 1.70 | 0.73 |
| 3:D:401:ASP:N | 3:D:401:ASP:OD1 | 2.17 | 0.73 |
| 3:E:220:VAL:HB | 3:E:224:ILE:HD11 | 1.70 | 0.73 |
| 3:G:421:VAL:HB | 3:G:430:LYS:HZ1 | 1.53 | 0.73 |
| 3:D:258:ARG:N | 3:D:294:THR:O | 2.22 | 0.73 |
| 3:E:216:ASN:ND2 | 3:E:219:GLU:OE2 | 2.21 | 0.73 |
| 3:G:421:VAL:HB | 3:G:430:LYS:NZ | 2.02 | 0.73 |
| 3:H:57:ASN:OD1 | 3:H:58:ASN:N | 2.22 | 0.73 |
| 1:A:68:THR:O | 1:A:81:GLN:N | 2.18 | 0.73 |
| 3:D:306:ILE:O | 3:D:311:TYR:OH | 2.05 | 0.73 |
| 3:F:418:TYR:HB2 | 3:F:419:ARG:HD3 | 1.68 | 0.73 |
| 3:D:169:TRP:HB2 | 3:D:208:MET:HB3 | 1.70 | 0.73 |
| 3:G:54:LYS:HB3 | 3:G:57:ASN:HB3 | 1.69 | 0.73 |
| 3:G:70:TYR:OH | 3:G:230:LYS:O | 2.06 | 0.73 |
| 3:C:463:PRO:HA | 3:C:466:ARG:NH1 | 2.03 | 0.73 |
| 3:D:111:GLN:O | 3:D:338:ARG:NE | 2.22 | 0.73 |
| 3:D:391:ILE:O | 3:D:395:ASN:N | 2.22 | 0.73 |
| 3:E:74:ARG:HB2 | 3:E:446:PHE:CE1 | 2.24 | 0.73 |
| 3:E:469:LEU:O | 3:E:473:GLY:N | 2.22 | 0.73 |
| 3:G:220:VAL:HB | 3:G:224:ILE:HD11 | 1.71 | 0.73 |
| 3:G:403:ASN:HB3 | 3:G:405:GLY:HA2 | 1.71 | 0.73 |
| 3:G:469:LEU:O | 3:G:473:GLY:N | 2.21 | 0.73 |
| 3:G:57:ASN:OD1 | 3:G:58:ASN:N | 2.22 | 0.73 |
| 3:C:120:HIS:HB2 | 3:C:221:PRO:HA | 1.71 | 0.72 |
| 3:D:187:PRO:HA | 3:D:188:LEU:HD12 | 1.71 | 0.72 |
| 3:G:97:ARG:NH2 | 3:G:404:PHE:O | 2.22 | 0.72 |
| 3:C:469:LEU:O | 3:C:473:GLY:N | 2.22 | 0.72 |
| 3:E:57:ASN:OD1 | 3:E:58:ASN:N | 2.22 | 0.72 |
| 3:C:427:ALA:HB1 | 3:D:173:SER:H | 1.54 | 0.72 |
| 3:H:384:THR:O | 3:H:387:VAL:HB | 1.89 | 0.72 |
| 3:D:57:ASN:OD1 | 3:D:58:ASN:N | 2.23 | 0.72 |
| 3:D:129:THR:OG1 | 3:D:130:GLU:N | 2.22 | 0.72 |
| 3:C:312:TRP:HH2 | 3:C:468:PHE:HD1 | 1.36 | 0.72 |
| 3:D:240:GLU:CD | 3:D:244:ASP:H | 1.92 | 0.72 |
| 3:D:468:PHE:CZ | 3:D:472:ALA:HB2 | 2.25 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:459:LEU:HB3 | 3:D:466:ARG:HB3 | 1.70 | 0.72 |
| 3:E:406:LEU:HB2 | 3:E:408:PRO:HB3 | 1.72 | 0.72 |
| 1:A:83:ARG:HB3 | 1:A:85:GLU:HG2 | 1.70 | 0.72 |
| 1:A:93:ALA:HA | 1:A:103:TRP:CB | 2.20 | 0.72 |
| 3:D:189:GLU:HG2 | 3:D:190:LEU:N | 2.03 | 0.72 |
| 3:E:46:GLY:HA3 | 3:E:65:VAL:HB | 1.70 | 0.72 |
| 3:G:406:LEU:HA | 3:G:408:PRO:CD | 2.20 | 0.72 |
| 3:H:210:PHE:HE2 | 3:H:224:ILE:HD12 | 1.55 | 0.71 |
| 2:B:38:GLN:OE1 | 2:B:87:TYR:OH | 2.09 | 0.71 |
| 3:D:390:TYR:O | 3:D:394:MET:N | 2.21 | 0.71 |
| 3:E:52:ILE:O | 3:E:61:LEU:N | 2.23 | 0.71 |
| 3:D:188:LEU:HD21 | 3:H:365:ARG:HG3 | 1.73 | 0.71 |
| 3:D:479:LYS:HD2 | 3:E:22:VAL:HG11 | 1.72 | 0.71 |
| 3:H:51:PRO:HD3 | 3:H:64:LYS:HD2 | 1.72 | 0.71 |
| 3:C:50:PHE:HA | 3:C:64:LYS:HD2 | 1.72 | 0.71 |
| 3:C:325:TRP:HZ3 | 3:C:402:TRP:CH2 | 2.08 | 0.71 |
| 3:D:211:THR:OG1 | 3:D:225:CYS:O | 2.08 | 0.71 |
| 3:D:384:THR:H | 3:D:387:VAL:HB | 1.56 | 0.71 |
| 3:C:306:ILE:O | 3:C:311:TYR:OH | 2.09 | 0.71 |
| 3:D:168:HIS:N | 3:D:191:ILE:O | 2.19 | 0.71 |
| 3:G:405:GLY:O | 3:G:408:PRO:HD3 | 1.91 | 0.71 |
| 1:A:17:SER:HA | 1:A:82(A):SER:HA | 1.71 | 0.71 |
| 3:D:255:MET:HG2 | 3:D:256:PHE:N | 2.06 | 0.71 |
| 3:H:126:LEU:HB3 | 3:H:262:ASN:HB2 | 1.71 | 0.71 |
| 3:G:335:ASP:OD1 | 3:G:336:THR:N | 2.24 | 0.71 |
| 3:D:103:VAL:N | 3:D:376:PHE:HA | 2.04 | 0.70 |
| 3:D:170:GLY:N | 3:D:189:GLU:O | 2.18 | 0.70 |
| 3:G:111:GLN:HB2 | 3:G:338:ARG:HD3 | 1.71 | 0.70 |
| 3:H:74:ARG:HB2 | 3:H:446:PHE:CE1 | 2.23 | 0.70 |
| 3:D:459:LEU:HD13 | 3:D:465:GLY:C | 2.11 | 0.70 |
| 3:D:52:ILE:HG21 | 3:D:61:LEU:HD23 | 1.73 | 0.70 |
| 1:A:12:VAL:HG21 | 1:A:18:LEU:HD13 | 1.71 | 0.70 |
| 3:C:301:THR:HG23 | 3:C:304:ALA:H | 1.56 | 0.70 |
| 3:D:383:LEU:HA | 3:D:387:VAL:HG11 | 1.73 | 0.70 |
| 3:D:79:ASP:HA | 3:D:327:ASN:HD21 | 1.57 | 0.70 |
| 3:D:127:ASP:O | 3:D:262:ASN:N | 2.21 | 0.70 |
| 3:D:159:ILE:HD12 | 3:D:248:PHE:HD2 | 1.55 | 0.70 |
| 3:F:301:THR:HG23 | 3:F:304:ALA:H | 1.56 | 0.70 |
| 3:H:312:TRP:HH2 | 3:H:468:PHE:HD1 | 1.38 | 0.70 |
| 3:D:79:ASP:HB3 | 3:D:82:LYS:HG2 | 1.73 | 0.70 |
| 3:D:389:THR:HA | 3:D:392:HIS:HB3 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:G:148:SER:OG | 3:H:260:LEU:HD23 | 1.92 | 0.70 |
| 3:H:56:ASN:OD1 | 3:H:57:ASN:N | 2.25 | 0.69 |
| 3:C:47:HIS:HE1 | 3:C:49:TYR:HB2 | 1.57 | 0.69 |
| 3:D:216:ASN:HA | 3:H:360:PHE:CE2 | 2.27 | 0.69 |
| 3:D:298:SER:OG | 3:D:299:MET:N | 2.25 | 0.69 |
| 3:D:372:LEU:HD22 | 3:D:374:PHE:HZ | 1.56 | 0.69 |
| 3:D:220:VAL:HB | 3:D:224:ILE:HD11 | 1.72 | 0.69 |
| 3:D:106:GLU:N | 3:D:373:GLN:O | 2.25 | 0.69 |
| 3:C:404:PHE:O | 3:C:406:LEU:N | 2.19 | 0.69 |
| 3:D:70:TYR:H | 3:D:199:ASP:N | 1.91 | 0.69 |
| 3:D:172:GLY:H | 3:D:187:PRO:C | 1.95 | 0.69 |
| 3:E:111:GLN:HB2 | 3:E:338:ARG:HD3 | 1.73 | 0.69 |
| 3:E:164:PRO:HB2 | 3:E:195:ILE:HD12 | 1.75 | 0.69 |
| 2:B:65:SER:N | 2:B:72:THR:O | 2.25 | 0.69 |
| 3:E:116:GLY:N | 3:E:339:SER:OG | 2.14 | 0.69 |
| 1:A:67:PHE:HB3 | 1:A:80:LEU:HD11 | 1.75 | 0.69 |
| 1:A:100(E):ASP:HB3 | 2:B:49:TYR:CD2 | 2.28 | 0.69 |
| 3:D:109:ARG:NH1 | 3:D:110:GLY:H | 1.91 | 0.69 |
| 3:D:256:PHE:HB3 | 3:H:299:MET:HA | 1.75 | 0.69 |
| 3:D:464:LEU:O | 3:D:467:LYS:N | 2.21 | 0.69 |
| 3:E:384:THR:O | 3:E:387:VAL:HB | 1.93 | 0.69 |
| 3:F:426:ILE:HG22 | 3:F:427:ALA:N | 2.06 | 0.69 |
| 3:G:16:VAL:CG2 | 3:G:17:PRO:CD | 2.70 | 0.69 |
| 3:H:53:LYS:HA | 3:H:61:LEU:H | 1.58 | 0.69 |
| 1:A:38:ARG:NH1 | 1:A:86:ASP:HA | 2.07 | 0.69 |
| 3:E:43:LEU:HD12 | 3:E:368:GLU:O | 1.93 | 0.69 |
| 3:F:392:HIS:O | 3:F:396:SER:OG | 2.11 | 0.69 |
| 3:G:126:LEU:HB3 | 3:G:262:ASN:HB2 | 1.73 | 0.69 |
| 3:D:148:SER:OG | 3:E:260:LEU:HD23 | 1.92 | 0.68 |
| 3:H:97:ARG:NH2 | 3:H:403:ASN:HB2 | 2.06 | 0.68 |
| 3:D:104:GLY:O | 3:D:375:ILE:N | 2.27 | 0.68 |
| 3:D:106:GLU:OE2 | 3:D:309:LYS:N | 2.25 | 0.68 |
| 3:D:166:GLY:N | 3:D:193:THR:O | 2.26 | 0.68 |
| 3:D:216:ASN:HB3 | 3:D:219:GLU:HG2 | 1.74 | 0.68 |
| 3:E:18:VAL:HB | 3:E:20:LYS:HG3 | 1.74 | 0.68 |
| 2:B:37:GLN:HG3 | 2:B:84:ALA:HB1 | 1.75 | 0.68 |
| 3:C:76:HIS:HB3 | 3:C:452:LYS:HE3 | 1.73 | 0.68 |
| 3:D:118:SER:O | 3:D:149:MET:N | 2.19 | 0.68 |
| 3:D:171:LYS:HG3 | 3:D:186:PRO:HB2 | 1.76 | 0.68 |
| 3:D:254:GLN:OE1 | 3:D:299:MET:O | 2.11 | 0.68 |
| 3:E:407:GLN:HB2 | 3:E:408:PRO:O | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:426:ILE:CG2 | 3:F:427:ALA:H | 2.01 | 0.68 |
| 3:C:49:TYR:HB3 | 3:C:222:LEU:CD2 | 2.23 | 0.68 |
| 3:D:216:ASN:OD1 | 3:D:219:GLU:OE2 | 2.11 | 0.68 |
| 3:D:391:ILE:HA | 3:D:394:MET:HB3 | 1.74 | 0.68 |
| 3:F:18:VAL:HG12 | 3:F:19:SER:N | 2.09 | 0.68 |
| 3:F:335:ASP:OD1 | 3:F:336:THR:N | 2.27 | 0.68 |
| 1:A:37:VAL:N | 1:A:91:TYR:O | 2.26 | 0.68 |
| 3:D:165:ILE:HG23 | 3:D:193:THR:C | 2.14 | 0.68 |
| 3:H:46:GLY:HA3 | 3:H:65:VAL:HB | 1.74 | 0.68 |
| 3:D:360:PHE:CE1 | 3:E:215:ALA:HB3 | 2.29 | 0.68 |
| 3:E:126:LEU:HB3 | 3:E:262:ASN:HB2 | 1.76 | 0.68 |
| 3:D:352:GLU:OE1 | 3:D:352:GLU:N | 2.26 | 0.68 |
| 3:F:56:ASN:OD1 | 3:F:57:ASN:N | 2.26 | 0.68 |
| 3:F:306:ILE:O | 3:F:311:TYR:OH | 2.10 | 0.68 |
| 3:G:306:ILE:O | 3:G:311:TYR:OH | 2.11 | 0.68 |
| 3:E:210:PHE:HE2 | 3:E:224:ILE:HD12 | 1.58 | 0.68 |
| 3:F:384:THR:O | 3:F:387:VAL:HB | 1.94 | 0.68 |
| 3:D:153:GLN:NE2 | 3:D:299:MET:O | 2.22 | 0.67 |
| 3:D:399:LEU:HA | 3:D:402:TRP:HB2 | 1.74 | 0.67 |
| 3:F:254:GLN:NE2 | 3:F:298:SER:HB3 | 2.09 | 0.67 |
| 1:A:35:SER:OG | 1:A:49:ALA:O | 2.10 | 0.67 |
| 3:C:37:ALA:HB2 | 3:C:455:PHE:HA | 1.76 | 0.67 |
| 3:D:468:PHE:CA | 3:D:471:GLN:HB3 | 2.21 | 0.67 |
| 3:E:404:PHE:HB2 | 3:E:405:GLY:O | 1.95 | 0.67 |
| 3:C:97:ARG:CZ | 3:C:402:TRP:HB3 | 2.24 | 0.67 |
| 3:E:312:TRP:HH2 | 3:E:468:PHE:HD1 | 1.42 | 0.67 |
| 1:A:33:ALA:HB3 | 1:A:95:GLY:HA3 | 1.77 | 0.67 |
| 1:A:45:LEU:HB2 | 2:B:98:PHE:CD2 | 2.30 | 0.67 |
| 3:C:40:SER:OG | 3:C:41:ARG:N | 2.28 | 0.67 |
| 3:C:404:PHE:C | 3:C:406:LEU:H | 1.97 | 0.67 |
| 3:G:52:ILE:O | 3:G:61:LEU:N | 2.26 | 0.67 |
| 1:A:83:ARG:HD3 | 1:A:85:GLU:OE2 | 1.95 | 0.67 |
| 1:A:94:ARG:HH21 | 1:A:101:ASP:HB3 | 1.60 | 0.67 |
| 2:B:54:ARG:NH1 | 2:B:63:THR:OG1 | 2.28 | 0.67 |
| 3:D:263:ARG:HG2 | 3:D:292:PHE:CD2 | 2.30 | 0.67 |
| 2:B:61:ARG:NE | 2:B:82:ASP:OD1 | 2.17 | 0.67 |
| 3:C:90:PHE:HD1 | 3:C:380:LYS:HZ1 | 1.42 | 0.67 |
| 3:D:160:GLY:HA2 | 3:D:247:PHE:CZ | 2.29 | 0.67 |
| 3:D:356:LYS:HB3 | 3:D:358:THR:HG23 | 1.76 | 0.67 |
| 3:C:156:LEU:HG | 3:C:334:VAL:HB | 1.77 | 0.67 |
| 3:D:109:ARG:HB3 | 3:D:308:ASN:HD21 | 1.59 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:255:MET:HG2 | 3:D:256:PHE:H | 1.59 | 0.66 |
| 3:F:469:LEU:O | 3:F:473:GLY:N | 2.27 | 0.66 |
| 3:C:196:GLN:HE21 | 3:C:444:TYR:HD1 | 1.44 | 0.66 |
| 3:E:254:GLN:NE2 | 3:E:298:SER:HB3 | 2.10 | 0.66 |
| 3:G:97:ARG:HH21 | 3:G:404:PHE:N | 1.92 | 0.66 |
| 3:G:210:PHE:HE2 | 3:G:224:ILE:HD12 | 1.59 | 0.66 |
| 3:D:268:GLY:HA3 | 3:H:362:GLU:O | 1.94 | 0.66 |
| 1:A:86:ASP:O | 1:A:90:TYR:OH | 2.13 | 0.66 |
| 3:C:49:TYR:HB3 | 3:C:222:LEU:HD22 | 1.77 | 0.66 |
| 3:D:345:CYS:SG | 3:E:216:ASN:N | 2.66 | 0.66 |
| 3:D:107:VAL:HA | 3:D:372:LEU:HD23 | 1.76 | 0.66 |
| 3:D:361:LYS:HA | 3:E:266:ALA:O | 1.95 | 0.66 |
| 3:D:159:ILE:O | 3:D:248:PHE:N | 2.29 | 0.66 |
| 3:D:273:ASP:O | 3:D:276:TYR:N | 2.28 | 0.66 |
| 3:E:41:ARG:HH21 | 3:E:369:GLU:HG3 | 1.59 | 0.66 |
| 3:G:258:ARG:NH2 | 3:G:296:SER:OG | 2.29 | 0.66 |
| 3:H:109:ARG:NH2 | 3:H:338:ARG:HD2 | 2.11 | 0.66 |
| 1:A:69:ILE:HD11 | 1:A:78:LEU:HD11 | 1.78 | 0.66 |
| 3:C:17:PRO:HG2 | 3:C:386:ASP:OD1 | 1.95 | 0.66 |
| 3:D:235:ILE:O | 3:D:239:SER:OG | 2.11 | 0.66 |
| 3:D:247:PHE:O | 3:D:317:GLN:NE2 | 2.29 | 0.66 |
| 3:D:348:ILE:HG13 | 3:E:182:PRO:HB2 | 1.78 | 0.66 |
| 3:E:51:PRO:HD3 | 3:E:64:LYS:HD2 | 1.77 | 0.66 |
| 2:B:38:GLN:HG3 | 2:B:44:PRO:HG3 | 1.78 | 0.66 |
| 3:C:57:ASN:OD1 | 3:C:58:ASN:N | 2.29 | 0.66 |
| 3:C:406:LEU:CD1 | 3:C:411:GLY:H | 2.09 | 0.66 |
| 3:C:258:ARG:HG2 | 3:C:259:HIS:ND1 | 2.10 | 0.65 |
| 3:D:73:PHE:HD1 | 3:D:447:TRP:CD1 | 2.14 | 0.65 |
| 3:E:148:SER:OG | 3:F:260:LEU:HD23 | 1.97 | 0.65 |
| 3:E:407:GLN:HB3 | 3:E:410:PRO:HD2 | 1.78 | 0.65 |
| 3:C:70:TYR:OH | 3:C:230:LYS:O | 2.15 | 0.65 |
| 3:C:72:VAL:HB | 3:C:446:PHE:HB2 | 1.76 | 0.65 |
| 3:D:66:SER:O | 3:D:71:ARG:NH2 | 2.29 | 0.65 |
| 3:D:162:LYS:HB3 | 3:D:163:PRO:HD2 | 1.78 | 0.65 |
| 3:F:47:HIS:HE1 | 3:F:49:TYR:HB2 | 1.61 | 0.65 |
| 2:B:4:MET:O | 2:B:100:ALA:N | 2.28 | 0.65 |
| 3:D:345:CYS:SG | 3:E:215:ALA:N | 2.70 | 0.65 |
| 3:G:421:VAL:HG12 | 3:G:423:SER:N | 2.12 | 0.65 |
| 3:H:258:ARG:HG2 | 3:H:259:HIS:ND1 | 2.11 | 0.65 |
| 3:C:169:TRP:HB2 | 3:C:208:MET:HB3 | 1.78 | 0.65 |
| 3:E:56:ASN:OD1 | 3:E:57:ASN:N | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:H:404:PHE:HE1 | 3:H:409:PRO:CD | 2.09 | 0.65 |
| 3:C:312:TRP:CE2 | 3:C:471:GLN:NE2 | 2.65 | 0.65 |
| 3:G:312:TRP:CE2 | 3:G:471:GLN:NE2 | 2.65 | 0.65 |
| 3:D:42:LEU:N | 3:D:370:TYR:O | 2.30 | 0.65 |
| 3:D:105:VAL:HA | 3:D:374:PHE:HD1 | 1.62 | 0.65 |
| 3:C:219:GLU:OE1 | 3:C:263:ARG:NH1 | 2.29 | 0.65 |
| 3:F:15:PRO:C | 3:F:17:PRO:HD3 | 2.17 | 0.65 |
| 3:G:223:ASP:OD1 | 3:G:224:ILE:N | 2.30 | 0.65 |
| 1:A:100(A):ASP:OD2 | 2:B:53:THR:OG1 | 2.14 | 0.65 |
| 3:D:102:CYS:HA | 3:D:376:PHE:CD1 | 2.31 | 0.65 |
| 3:D:450:ASN:OD1 | 3:D:451:LEU:N | 2.30 | 0.65 |
| 3:H:335:ASP:OD1 | 3:H:336:THR:N | 2.30 | 0.65 |
| 3:D:128:ASP:OD1 | 3:D:129:THR:N | 2.29 | 0.64 |
| 3:F:15:PRO:HB2 | 3:F:17:PRO:HD3 | 1.79 | 0.64 |
| 2:B:35:TRP:CB | 2:B:47:LEU:HB2 | 2.27 | 0.64 |
| 3:C:325:TRP:HZ3 | 3:C:402:TRP:HH2 | 1.43 | 0.64 |
| 3:D:124:ASN:O | 3:D:263:ARG:NH1 | 2.31 | 0.64 |
| 3:F:52:ILE:O | 3:F:61:LEU:N | 2.28 | 0.64 |
| 2:B:5:SER:O | 2:B:23:CYS:HA | 1.98 | 0.64 |
| 3:D:72:VAL:HB | 3:D:197:ASP:HB2 | 1.79 | 0.64 |
| 3:F:258:ARG:NH2 | 3:F:296:SER:OG | 2.31 | 0.64 |
| 1:A:33:ALA:O | 1:A:95:GLY:N | 2.20 | 0.64 |
| 3:D:50:PHE:HA | 3:D:64:LYS:HD2 | 1.80 | 0.64 |
| 3:D:156:LEU:N | 3:D:334:VAL:O | 2.22 | 0.64 |
| 3:D:249:TYR:OH | 3:D:251:ARG:NH1 | 2.30 | 0.64 |
| 3:D:406:LEU:HA | 3:D:407:GLN:HB2 | 1.79 | 0.64 |
| 3:G:120:HIS:HB2 | 3:G:221:PRO:HA | 1.78 | 0.64 |
| 3:G:234:TYR:OH | 3:G:251:ARG:HD3 | 1.98 | 0.64 |
| 3:D:222:LEU:O | 3:D:225:CYS:HB3 | 1.97 | 0.64 |
| 3:G:273:ASP:OD1 | 3:G:274:ASP:N | 2.31 | 0.64 |
| 3:G:301:THR:HG23 | 3:G:304:ALA:H | 1.61 | 0.64 |
| 3:H:47:HIS:HE1 | 3:H:49:TYR:HB2 | 1.62 | 0.64 |
| 3:D:61:LEU:HG | 3:D:62:VAL:HG23 | 1.79 | 0.64 |
| 3:D:246:LEU:HD22 | 3:D:249:TYR:HB3 | 1.79 | 0.64 |
| 3:E:301:THR:HG23 | 3:E:304:ALA:H | 1.62 | 0.64 |
| 3:E:348:ILE:HG13 | 3:F:182:PRO:HB2 | 1.80 | 0.64 |
| 3:G:345:CYS:SG | 3:H:215:ALA:N | 2.71 | 0.64 |
| 3:H:301:THR:HG23 | 3:H:304:ALA:H | 1.60 | 0.64 |
| 3:D:130:GLU:HA | 3:H:147:ILE:HG23 | 1.79 | 0.64 |
| 3:D:156:LEU:O | 3:D:333:VAL:HG13 | 1.97 | 0.64 |
| 3:D:158:LEU:HD12 | 3:D:332:THR:CG2 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:391:ILE:O | 3:F:394:MET:N | 2.31 | 0.64 |
| 3:G:56:ASN:OD1 | 3:G:57:ASN:N | 2.31 | 0.64 |
| 3:D:71:ARG:O | 3:D:332:THR:HG23 | 1.98 | 0.64 |
| 3:D:222:LEU:H | 3:D:222:LEU:HD12 | 1.62 | 0.64 |
| 3:H:273:ASP:OD1 | 3:H:274:ASP:N | 2.31 | 0.64 |
| 2:B:13:VAL:HG21 | 2:B:19:VAL:HG12 | 1.79 | 0.64 |
| 2:B:34:ALA:HB3 | 2:B:89:GLN:HB3 | 1.78 | 0.64 |
| 3:C:262:ASN:ND2 | 3:C:290:ASN:O | 2.30 | 0.64 |
| 3:D:103:VAL:H | 3:D:376:PHE:CA | 2.06 | 0.64 |
| 3:D:144:ARG:NH2 | 3:E:279:GLY:HA2 | 2.13 | 0.64 |
| 3:G:345:CYS:SG | 3:H:216:ASN:N | 2.63 | 0.64 |
| 2:B:6:GLN:N | 2:B:100:ALA:HB3 | 2.08 | 0.63 |
| 3:F:46:GLY:HA3 | 3:F:65:VAL:HB | 1.80 | 0.63 |
| 3:G:85:PHE:HB2 | 3:G:88:THR:HG22 | 1.80 | 0.63 |
| 3:G:391:ILE:O | 3:G:394:MET:N | 2.31 | 0.63 |
| 3:D:45:VAL:HA | 3:D:367:GLY:HA2 | 1.81 | 0.63 |
| 3:D:76:HIS:HD1 | 3:D:449:VAL:C | 2.01 | 0.63 |
| 3:D:121:PRO:HA | 3:D:146:CYS:SG | 2.37 | 0.63 |
| 3:D:124:ASN:HB3 | 3:D:263:ARG:HH11 | 1.63 | 0.63 |
| 3:D:470:LEU:O | 3:D:473:GLY:N | 2.31 | 0.63 |
| 3:E:335:ASP:OD1 | 3:E:336:THR:N | 2.31 | 0.63 |
| 3:D:109:ARG:HH22 | 3:D:111:GLN:CG | 2.06 | 0.63 |
| 3:D:310:PRO:HB2 | 3:D:312:TRP:NE1 | 2.13 | 0.63 |
| 3:F:97:ARG:HH22 | 3:F:404:PHE:HB2 | 1.64 | 0.63 |
| 3:G:408:PRO:HB2 | 3:G:409:PRO:HD3 | 1.79 | 0.63 |
| 2:B:64:GLY:HA2 | 2:B:73:LEU:HA | 1.81 | 0.63 |
| 3:D:129:THR:O | 3:H:147:ILE:HG12 | 1.98 | 0.63 |
| 3:E:72:VAL:O | 3:E:447:TRP:HB3 | 1.99 | 0.63 |
| 3:F:477:LYS:HZ2 | 3:G:23:SER:HB2 | 1.63 | 0.63 |
| 3:D:208:MET:O | 3:D:228:ILE:HA | 1.99 | 0.63 |
| 3:F:273:ASP:OD1 | 3:F:274:ASP:N | 2.32 | 0.63 |
| 3:G:312:TRP:HH2 | 3:G:468:PHE:HD1 | 1.47 | 0.63 |
| 1:A:52:SER:OG | 1:A:56:ASN:N | 2.30 | 0.63 |
| 3:D:53:LYS:HA | 3:D:61:LEU:H | 1.64 | 0.63 |
| 3:D:70:TYR:OH | 3:D:201:VAL:HA | 1.99 | 0.63 |
| 3:D:240:GLU:HG2 | 3:D:242:TYR:N | 2.08 | 0.63 |
| 3:D:300:VAL:HG22 | 3:E:255:MET:H | 1.64 | 0.63 |
| 3:D:443:LYS:O | 3:D:445:THR:HG23 | 1.99 | 0.63 |
| 3:F:51:PRO:HD3 | 3:F:64:LYS:HD2 | 1.80 | 0.63 |
| 3:F:223:ASP:OD1 | 3:F:224:ILE:N | 2.30 | 0.63 |
| 3:F:234:TYR:OH | 3:F:251:ARG:HD3 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:372:LEU:HB3 | 3:D:374:PHE:CE2 | 2.33 | 0.63 |
| 3:E:234:TYR:OH | 3:E:251:ARG:HD3 | 1.99 | 0.63 |
| 3:G:53:LYS:HA | 3:G:61:LEU:H | 1.63 | 0.63 |
| 3:G:474:LEU:HD12 | 3:G:474:LEU:O | 1.99 | 0.63 |
| 3:H:404:PHE:CE1 | 3:H:409:PRO:CD | 2.81 | 0.63 |
| 3:D:209:ASP:HB2 | 3:D:228:ILE:HG13 | 1.79 | 0.62 |
| 3:D:169:TRP:CD1 | 3:D:207:ALA:N | 2.68 | 0.62 |
| 3:D:235:ILE:O | 3:D:238:VAL:HB | 1.98 | 0.62 |
| 3:D:85:PHE:H | 3:D:88:THR:HG22 | 1.63 | 0.62 |
| 3:D:150:ASP:OD2 | 3:D:297:GLY:N | 2.30 | 0.62 |
| 3:D:344:LEU:HD21 | 3:D:363:TYR:HD2 | 1.64 | 0.62 |
| 3:E:97:ARG:NH2 | 3:E:404:PHE:N | 2.47 | 0.62 |
| 3:E:403:ASN:C | 3:E:405:GLY:O | 2.36 | 0.62 |
| 3:F:299:MET:HA | 3:G:256:PHE:HB3 | 1.80 | 0.62 |
| 3:D:299:MET:HG2 | 3:D:300:VAL:N | 2.15 | 0.62 |
| 3:F:345:CYS:SG | 3:G:215:ALA:N | 2.71 | 0.62 |
| 3:G:384:THR:O | 3:G:387:VAL:HB | 1.99 | 0.62 |
| 3:H:81:ASN:HD21 | 3:H:98:LEU:H | 1.46 | 0.62 |
| 3:D:215:ALA:N | 3:H:345:CYS:SG | 2.72 | 0.62 |
| 3:E:109:ARG:NH2 | 3:E:338:ARG:HD2 | 2.15 | 0.62 |
| 3:C:210:PHE:HE2 | 3:C:224:ILE:HD12 | 1.65 | 0.62 |
| 3:D:77:LEU:HD23 | 3:D:451:LEU:HB2 | 1.82 | 0.62 |
| 3:D:80:PRO:HD3 | 3:D:100:TRP:NE1 | 2.15 | 0.62 |
| 3:E:223:ASP:OD1 | 3:E:224:ILE:N | 2.33 | 0.62 |
| 1:A:66:ARG:HA | 3:C:176:THR:CB | 2.27 | 0.62 |
| 2:B:4:MET:HB2 | 2:B:99:GLY:HA2 | 1.82 | 0.62 |
| 3:C:150:ASP:OD1 | 3:C:296:SER:HA | 1.99 | 0.62 |
| 3:D:46:GLY:CA | 3:D:65:VAL:HB | 2.30 | 0.62 |
| 3:F:348:ILE:HG13 | 3:G:182:PRO:HB2 | 1.80 | 0.62 |
| 1:A:38:ARG:HA | 1:A:90:TYR:HA | 1.81 | 0.62 |
| 3:D:114:GLY:O | 3:D:339:SER:N | 2.33 | 0.62 |
| 3:D:123:LEU:HD11 | 3:D:263:ARG:HH12 | 1.65 | 0.62 |
| 3:G:71:ARG:O | 3:G:332:THR:HG23 | 2.00 | 0.62 |
| 1:A:22:CYS:O | 1:A:78:LEU:N | 2.26 | 0.62 |
| 3:E:280:SER:N | 3:E:283:THR:OG1 | 2.29 | 0.62 |
| 3:E:387:VAL:O | 3:E:391:ILE:HD12 | 2.00 | 0.62 |
| 3:D:125:LYS:NZ | 3:D:127:ASP:HA | 2.15 | 0.61 |
| 3:D:152:LYS:HE3 | 3:D:203:THR:C | 2.21 | 0.61 |
| 3:F:450:ASN:OD1 | 3:F:452:LYS:HG3 | 2.00 | 0.61 |
| 3:H:52:ILE:HB | 3:H:62:VAL:HB | 1.82 | 0.61 |
| 3:C:219:GLU:OE1 | 3:C:263:ARG:CZ | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:142:ASP:OD1 | 3:D:144:ARG:NE | 2.27 | 0.61 |
| 3:D:162:LYS:HB2 | 3:D:245:SER:CA | 2.30 | 0.61 |
| 3:D:397:THR:O | 3:D:400:GLU:HB2 | 2.00 | 0.61 |
| 3:E:299:MET:HA | 3:F:256:PHE:HB3 | 1.80 | 0.61 |
| 3:F:312:TRP:HH2 | 3:F:468:PHE:HD1 | 1.45 | 0.61 |
| 3:H:254:GLN:OE1 | 3:H:298:SER:HB3 | 1.99 | 0.61 |
| 2:B:47:LEU:HD21 | 2:B:86:TYR:CE1 | 2.35 | 0.61 |
| 3:D:113:LEU:HA | 3:D:338:ARG:CG | 2.28 | 0.61 |
| 3:D:335:ASP:OD1 | 3:D:337:THR:HG23 | 2.00 | 0.61 |
| 3:D:384:THR:O | 3:D:388:MET:N | 2.16 | 0.61 |
| 3:E:306:ILE:O | 3:E:311:TYR:OH | 2.17 | 0.61 |
| 2:B:4:MET:HB3 | 2:B:23:CYS:SG | 2.40 | 0.61 |
| 3:C:101:ALA:O | 3:C:377:GLN:N | 2.31 | 0.61 |
| 3:F:126:LEU:HB3 | 3:F:262:ASN:HB2 | 1.81 | 0.61 |
| 3:C:71:ARG:HG3 | 3:C:370:TYR:OH | 1.99 | 0.61 |
| 3:D:57:ASN:CG | 3:D:59:LYS:H | 2.03 | 0.61 |
| 3:D:390:TYR:O | 3:D:393:SER:HB2 | 2.00 | 0.61 |
| 3:E:273:ASP:OD1 | 3:E:274:ASP:N | 2.34 | 0.61 |
| 3:F:15:PRO:CB | 3:F:17:PRO:HD3 | 2.30 | 0.61 |
| 3:F:148:SER:OG | 3:G:260:LEU:HD23 | 1.99 | 0.61 |
| 3:H:223:ASP:OD1 | 3:H:224:ILE:N | 2.33 | 0.61 |
| 3:D:44:ALA:CB | 3:D:368:GLU:HB2 | 2.29 | 0.61 |
| 3:D:233:ASP:CG | 3:D:236:LYS:H | 2.04 | 0.61 |
| 3:G:51:PRO:HD3 | 3:G:64:LYS:HD2 | 1.81 | 0.61 |
| 3:C:47:HIS:CE1 | 3:C:49:TYR:HB2 | 2.35 | 0.61 |
| 3:C:431:HIS:ND1 | 3:C:433:PRO:O | 2.33 | 0.61 |
| 3:D:100:TRP:HA | 3:D:378:LEU:HA | 1.81 | 0.61 |
| 3:G:465:GLY:O | 3:G:468:PHE:N | 2.33 | 0.61 |
| 3:H:40:SER:OG | 3:H:41:ARG:N | 2.34 | 0.61 |
| 1:A:59:TYR:CB | 1:A:64:LYS:HD2 | 2.30 | 0.61 |
| 2:B:14:SER:N | 2:B:17:GLU:OE1 | 2.25 | 0.61 |
| 3:D:69:GLN:OE1 | 3:D:71:ARG:NH2 | 2.34 | 0.61 |
| 3:D:200:MET:HB2 | 3:D:228:ILE:O | 2.01 | 0.61 |
| 3:D:307:PHE:O | 3:D:309:LYS:HG3 | 2.00 | 0.61 |
| 3:D:344:LEU:HD22 | 3:E:186:PRO:HD2 | 1.83 | 0.61 |
| 3:H:30:ARG:HD3 | 3:H:379:CYS:SG | 2.40 | 0.61 |
| 3:C:109:ARG:NH2 | 3:C:338:ARG:HD2 | 2.15 | 0.61 |
| 3:D:32:ASN:H | 3:D:33:ILE:HD12 | 1.65 | 0.61 |
| 3:D:303:ASP:OD1 | 3:D:303:ASP:N | 2.29 | 0.61 |
| 3:C:37:ALA:HB2 | 3:C:455:PHE:HD1 | 1.66 | 0.61 |
| 3:C:90:PHE:HD1 | 3:C:380:LYS:NZ | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:124:ASN:ND2 | 3:C:219:GLU:OE2 | 2.33 | 0.61 |
| 3:D:116:GLY:N | 3:D:339:SER:OG | 2.25 | 0.61 |
| 3:E:258:ARG:NH2 | 3:E:296:SER:OG | 2.34 | 0.61 |
| 3:E:406:LEU:HB2 | 3:E:408:PRO:CB | 2.30 | 0.61 |
| 3:E:418:TYR:HB3 | 3:E:420:PHE:CE2 | 2.36 | 0.61 |
| 3:H:164:PRO:HB2 | 3:H:195:ILE:HD12 | 1.83 | 0.61 |
| 3:E:404:PHE:HB2 | 3:E:405:GLY:CA | 2.31 | 0.60 |
| 3:C:56:ASN:OD1 | 3:C:57:ASN:N | 2.34 | 0.60 |
| 3:C:349:SER:N | 3:C:359:ASN:OD1 | 2.30 | 0.60 |
| 3:D:66:SER:OG | 3:D:68:LEU:N | 2.34 | 0.60 |
| 3:E:345:CYS:SG | 3:F:215:ALA:N | 2.74 | 0.60 |
| 3:G:258:ARG:HB2 | 3:G:296:SER:HB2 | 1.82 | 0.60 |
| 3:G:405:GLY:O | 3:G:408:PRO:CD | 2.48 | 0.60 |
| 3:D:223:ASP:OD1 | 3:D:224:ILE:N | 2.34 | 0.60 |
| 3:F:16:VAL:O | 3:F:16:VAL:HG12 | 2.01 | 0.60 |
| 3:G:258:ARG:HG2 | 3:G:259:HIS:ND1 | 2.16 | 0.60 |
| 3:G:348:ILE:HG13 | 3:H:182:PRO:HB2 | 1.82 | 0.60 |
| 3:G:387:VAL:O | 3:G:391:ILE:HD12 | 2.01 | 0.60 |
| 3:H:70:TYR:HD1 | 3:H:334:VAL:HG21 | 1.65 | 0.60 |
| 2:B:85:VAL:HG22 | 2:B:103:LYS:HG3 | 1.83 | 0.60 |
| 3:D:50:PHE:CE2 | 3:E:271:VAL:HA | 2.37 | 0.60 |
| 3:F:105:VAL:HG13 | 3:F:374:PHE:CE1 | 2.35 | 0.60 |
| 3:D:78:PRO:HD3 | 3:D:452:LYS:HA | 1.82 | 0.60 |
| 3:D:216:ASN:HD21 | 3:D:218:SER:HB2 | 1.67 | 0.60 |
| 3:F:335:ASP:OD2 | 3:F:337:THR:OG1 | 2.19 | 0.60 |
| 3:C:43:LEU:HD23 | 3:H:421:VAL:HG13 | 1.84 | 0.60 |
| 3:C:424:GLN:OE1 | 3:C:430:LYS:HB3 | 2.02 | 0.60 |
| 3:D:24:THR:HA | 3:D:27:TYR:CZ | 2.37 | 0.60 |
| 3:D:99:VAL:N | 3:D:379:CYS:O | 2.28 | 0.60 |
| 3:D:100:TRP:HA | 3:D:378:LEU:HD12 | 1.82 | 0.60 |
| 3:D:459:LEU:HD13 | 3:D:466:ARG:N | 2.16 | 0.60 |
| 3:G:16:VAL:HG23 | 3:G:17:PRO:CD | 2.31 | 0.60 |
| 3:D:170:GLY:O | 3:D:189:GLU:N | 2.34 | 0.60 |
| 3:D:261:PHE:HD2 | 3:D:294:THR:HG1 | 1.46 | 0.60 |
| 3:E:164:PRO:HG2 | 3:E:195:ILE:HB | 1.82 | 0.60 |
| 3:G:235:ILE:O | 3:G:239:SER:N | 2.33 | 0.60 |
| 3:H:306:ILE:O | 3:H:311:TYR:OH | 2.20 | 0.60 |
| 3:D:280:SER:N | 3:D:283:THR:OG1 | 2.28 | 0.60 |
| 3:D:466:ARG:HA | 3:D:469:LEU:HB2 | 1.83 | 0.60 |
| 3:E:335:ASP:OD2 | 3:E:337:THR:OG1 | 2.20 | 0.60 |
| 3:F:263:ARG:HB2 | 3:F:290:ASN:HD22 | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:15:GLY:H | 1:A:82(C):LEU:HB2 | 1.67 | 0.60 |
| 3:D:70:TYR:CE1 | 3:D:201:VAL:HG22 | 2.37 | 0.60 |
| 3:D:101:ALA:O | 3:D:377:GLN:N | 2.32 | 0.60 |
| 3:D:223:ASP:OD1 | 3:D:223:ASP:N | 2.28 | 0.60 |
| 3:D:398:ILE:HA | 3:D:401:ASP:OD2 | 2.02 | 0.60 |
| 3:E:169:TRP:HB2 | 3:E:208:MET:HB3 | 1.83 | 0.60 |
| 3:E:258:ARG:HG2 | 3:E:259:HIS:ND1 | 2.16 | 0.60 |
| 3:G:170:GLY:O | 3:G:189:GLU:N | 2.34 | 0.60 |
| 3:G:399:LEU:HD13 | 3:G:404:PHE:HZ | 1.66 | 0.60 |
| 3:G:408:PRO:HB2 | 3:G:409:PRO:CD | 2.32 | 0.60 |
| 3:D:158:LEU:N | 3:D:332:THR:O | 2.34 | 0.60 |
| 3:D:221:PRO:HD2 | 3:D:224:ILE:HD11 | 1.83 | 0.60 |
| 3:D:441:LEU:HG | 3:D:444:TYR:HE2 | 1.65 | 0.60 |
| 3:F:120:HIS:CD2 | 3:F:222:LEU:HD12 | 2.36 | 0.60 |
| 3:G:280:SER:N | 3:G:283:THR:OG1 | 2.32 | 0.60 |
| 1:A:16:GLY:O | 1:A:82(B):SER:N | 2.35 | 0.59 |
| 3:D:104:GLY:C | 3:D:375:ILE:H | 2.05 | 0.59 |
| 3:D:340:THR:HG22 | 3:D:341:ASN:O | 2.02 | 0.59 |
| 3:F:418:TYR:CB | 3:F:419:ARG:HA | 2.31 | 0.59 |
| 3:H:120:HIS:HB2 | 3:H:221:PRO:HA | 1.83 | 0.59 |
| 2:B:19:VAL:HB | 2:B:104:LEU:HD21 | 1.85 | 0.59 |
| 2:B:29:LEU:HB2 | 2:B:68:GLY:CA | 2.31 | 0.59 |
| 3:C:406:LEU:HD13 | 3:C:409:PRO:O | 2.02 | 0.59 |
| 3:D:77:LEU:HD22 | 3:D:455:PHE:CZ | 2.37 | 0.59 |
| 3:D:141:VAL:HG13 | 3:H:357:ASN:H | 1.67 | 0.59 |
| 3:D:287:ALA:HB3 | 3:H:121:PRO:CB | 2.28 | 0.59 |
| 3:D:123:LEU:H | 3:D:145:GLU:H | 1.50 | 0.59 |
| 3:D:395:ASN:OD1 | 3:D:396:SER:N | 2.35 | 0.59 |
| 3:E:240:GLU:HG3 | 3:E:241:PRO:HD2 | 1.83 | 0.59 |
| 3:E:258:ARG:HB2 | 3:E:296:SER:HB2 | 1.84 | 0.59 |
| 3:C:47:HIS:CE1 | 3:C:49:TYR:H | 2.20 | 0.59 |
| 3:E:120:HIS:CD2 | 3:E:222:LEU:HD12 | 2.37 | 0.59 |
| 3:H:234:TYR:OH | 3:H:251:ARG:HD3 | 2.02 | 0.59 |
| 1:A:68:THR:HB | 1:A:81:GLN:HB3 | 1.83 | 0.59 |
| 2:B:35:TRP:HB3 | 2:B:47:LEU:HB2 | 1.82 | 0.59 |
| 3:C:90:PHE:CE1 | 3:C:91:TYR:HD2 | 2.19 | 0.59 |
| 3:C:404:PHE:C | 3:C:406:LEU:N | 2.54 | 0.59 |
| 3:D:109:ARG:CZ | 3:D:369:GLU:O | 2.50 | 0.59 |
| 3:D:449:VAL:HG12 | 3:D:451:LEU:HD21 | 1.84 | 0.59 |
| 1:A:22:CYS:N | 1:A:78:LEU:O | 2.33 | 0.59 |
| 3:C:23:SER:O | 3:C:26:GLU:HG2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:302:SER:O | 3:D:305:GLN:HB2 | 2.01 | 0.59 |
| 3:D:384:THR:O | 3:D:387:VAL:HB | 2.03 | 0.59 |
| 3:C:72:VAL:O | 3:C:447:TRP:HB3 | 2.01 | 0.59 |
| 3:D:23:SER:HA | 3:D:319:HIS:HB3 | 1.84 | 0.59 |
| 3:G:24:THR:HG21 | 3:G:320:ASN:HA | 1.83 | 0.59 |
| 3:G:211:THR:OG1 | 3:G:226:THR:O | 2.21 | 0.59 |
| 3:H:474:LEU:O | 3:H:474:LEU:HD12 | 2.03 | 0.59 |
| 3:C:84:GLY:HA2 | 3:H:84:GLY:HA3 | 1.85 | 0.59 |
| 3:C:124:ASN:HA | 3:C:144:ARG:HG2 | 1.83 | 0.59 |
| 3:D:25:ASP:HA | 3:D:28:VAL:CB | 2.28 | 0.59 |
| 3:D:53:LYS:HB3 | 3:D:60:ILE:HA | 1.83 | 0.59 |
| 3:D:171:LYS:HB2 | 3:D:213:LEU:HD21 | 1.84 | 0.59 |
| 3:D:274:ASP:N | 3:D:274:ASP:OD1 | 2.30 | 0.59 |
| 3:E:71:ARG:HG3 | 3:E:370:TYR:OH | 2.02 | 0.59 |
| 2:B:2:ILE:HD11 | 2:B:27:GLN:HB2 | 1.84 | 0.59 |
| 3:D:70:TYR:H | 3:D:199:ASP:H | 1.49 | 0.59 |
| 3:D:258:ARG:HG2 | 3:D:259:HIS:NE2 | 2.18 | 0.59 |
| 3:D:335:ASP:OD1 | 3:D:337:THR:N | 2.26 | 0.59 |
| 3:H:71:ARG:O | 3:H:332:THR:HG23 | 2.03 | 0.59 |
| 3:H:391:ILE:O | 3:H:394:MET:N | 2.35 | 0.59 |
| 1:A:38:ARG:HH12 | 1:A:86:ASP:HA | 1.67 | 0.59 |
| 3:D:221:PRO:HB2 | 3:D:224:ILE:HG12 | 1.85 | 0.59 |
| 3:D:345:CYS:HB2 | 3:D:360:PHE:CD1 | 2.38 | 0.59 |
| 3:E:116:GLY:H | 3:E:339:SER:HG | 1.46 | 0.59 |
| 3:F:85:PHE:HB2 | 3:F:88:THR:HG22 | 1.85 | 0.59 |
| 3:G:153:GLN:NE2 | 3:G:300:VAL:HG12 | 2.18 | 0.59 |
| 2:B:11:LEU:HD11 | 2:B:104:LEU:HD22 | 1.85 | 0.58 |
| 3:D:69:GLN:HB2 | 3:D:71:ARG:HH22 | 1.66 | 0.58 |
| 3:E:474:LEU:HD12 | 3:E:474:LEU:O | 2.03 | 0.58 |
| 3:C:115:VAL:HG12 | 3:C:116:GLY:O | 2.03 | 0.58 |
| 3:E:404:PHE:HB2 | 3:E:405:GLY:C | 2.23 | 0.58 |
| 1:A:37:VAL:HB | 1:A:91:TYR:HB2 | 1.84 | 0.58 |
| 3:D:91:TYR:HB3 | 3:D:380:LYS:NZ | 2.18 | 0.58 |
| 3:D:157:CYS:O | 3:D:158:LEU:HD23 | 2.02 | 0.58 |
| 3:D:422:THR:O | 3:D:423:SER:OG | 2.20 | 0.58 |
| 3:F:71:ARG:HG3 | 3:F:370:TYR:OH | 2.03 | 0.58 |
| 3:G:70:TYR:HD1 | 3:G:334:VAL:HG21 | 1.67 | 0.58 |
| 2:B:47:LEU:HB3 | 2:B:48:ILE:HG12 | 1.85 | 0.58 |
| 3:C:16:VAL:CG1 | 3:C:17:PRO:HD3 | 2.33 | 0.58 |
| 3:C:406:LEU:HD13 | 3:C:409:PRO:C | 2.23 | 0.58 |
| 3:C:406:LEU:CD2 | 3:C:408:PRO:C | 2.72 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:31:THR:O | 3:D:377:GLN:OE1 | 2.22 | 0.58 |
| 3:D:259:HIS:N | 3:D:294:THR:O | 2.32 | 0.58 |
| 3:E:53:LYS:HA | 3:E:61:LEU:H | 1.68 | 0.58 |
| 3:F:53:LYS:HA | 3:F:61:LEU:H | 1.69 | 0.58 |
| 3:F:153:GLN:NE2 | 3:F:300:VAL:HG12 | 2.18 | 0.58 |
| 3:D:77:LEU:CD2 | 3:D:451:LEU:HB2 | 2.32 | 0.58 |
| 3:F:150:ASP:OD1 | 3:F:296:SER:HA | 2.04 | 0.58 |
| 3:G:416:ASP:O | 3:G:417:THR:OG1 | 2.21 | 0.58 |
| 3:C:383:LEU:HD23 | 3:C:387:VAL:HG11 | 1.85 | 0.58 |
| 3:D:45:VAL:HA | 3:D:366:HIS:O | 2.04 | 0.58 |
| 3:D:57:ASN:OD1 | 3:D:59:LYS:N | 2.35 | 0.58 |
| 3:D:112:PRO:HB3 | 3:E:231:TYR:CE1 | 2.39 | 0.58 |
| 3:D:248:PHE:CG | 3:D:249:TYR:N | 2.72 | 0.58 |
| 3:D:360:PHE:O | 3:E:266:ALA:N | 2.36 | 0.58 |
| 2:B:35:TRP:CE3 | 2:B:88:CYS:HB3 | 2.38 | 0.58 |
| 3:C:431:HIS:HD1 | 3:C:433:PRO:C | 2.07 | 0.58 |
| 3:D:92:ASN:HB3 | 3:D:95:THR:OG1 | 2.03 | 0.58 |
| 3:D:236:LYS:C | 3:D:239:SER:H | 2.07 | 0.58 |
| 3:D:249:TYR:HE1 | 3:D:251:ARG:HG2 | 1.68 | 0.58 |
| 3:F:120:HIS:HB2 | 3:F:221:PRO:HA | 1.86 | 0.58 |
| 3:H:153:GLN:NE2 | 3:H:300:VAL:HG12 | 2.19 | 0.58 |
| 3:D:274:ASP:OD1 | 3:D:275:LEU:HG | 2.03 | 0.58 |
| 3:D:377:GLN:HG2 | 3:D:378:LEU:N | 2.19 | 0.58 |
| 3:D:459:LEU:HB2 | 3:D:469:LEU:CD1 | 2.33 | 0.58 |
| 3:F:109:ARG:NH2 | 3:F:338:ARG:HD2 | 2.17 | 0.58 |
| 1:A:75:ARG:O | 1:A:77:ILE:HG13 | 2.04 | 0.58 |
| 3:D:24:THR:O | 3:D:28:VAL:HG23 | 2.03 | 0.58 |
| 3:D:70:TYR:HB2 | 3:D:199:ASP:H | 1.69 | 0.58 |
| 3:E:349:SER:O | 3:E:359:ASN:ND2 | 2.34 | 0.58 |
| 3:F:52:ILE:HB | 3:F:62:VAL:HB | 1.85 | 0.58 |
| 3:D:40:SER:OG | 3:D:41:ARG:N | 2.35 | 0.58 |
| 3:D:97:ARG:HG3 | 3:D:402:TRP:CE3 | 2.39 | 0.58 |
| 3:D:106:GLU:H | 3:D:374:PHE:HD1 | 1.51 | 0.58 |
| 3:D:109:ARG:NH1 | 3:D:369:GLU:O | 2.36 | 0.58 |
| 3:D:167:GLU:CD | 3:D:233:ASP:HB2 | 2.24 | 0.58 |
| 3:D:231:TYR:CZ | 3:H:112:PRO:HA | 2.39 | 0.58 |
| 3:E:41:ARG:NH2 | 3:E:369:GLU:HG3 | 2.18 | 0.58 |
| 3:F:164:PRO:HB2 | 3:F:195:ILE:HD12 | 1.84 | 0.58 |
| 3:G:164:PRO:HB2 | 3:G:195:ILE:HD12 | 1.86 | 0.58 |
| 3:H:54:LYS:HD2 | 3:H:57:ASN:HB2 | 1.85 | 0.58 |
| 3:D:77:LEU:HD22 | 3:D:455:PHE:HZ | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:154:THR:HG23 | 3:D:252:ARG:O | 2.04 | 0.57 |
| 3:D:374:PHE:HB2 | 3:D:376:PHE:CZ | 2.38 | 0.57 |
| 3:H:168:HIS:CE1 | 3:H:191:ILE:HB | 2.39 | 0.57 |
| 3:C:57:ASN:OD1 | 3:C:59:LYS:N | 2.31 | 0.57 |
| 3:F:47:HIS:CG | 3:F:48:PRO:HD2 | 2.39 | 0.57 |
| 1:A:92:CYS:O | 1:A:103:TRP:HB2 | 2.02 | 0.57 |
| 2:B:54:ARG:HH22 | 3:D:431:HIS:CE1 | 2.22 | 0.57 |
| 3:C:220:VAL:HB | 3:C:224:ILE:HD11 | 1.86 | 0.57 |
| 3:C:223:ASP:OD1 | 3:C:224:ILE:N | 2.37 | 0.57 |
| 3:D:128:ASP:HA | 3:D:261:PHE:CD1 | 2.39 | 0.57 |
| 3:H:387:VAL:O | 3:H:391:ILE:HD12 | 2.05 | 0.57 |
| 3:C:167:GLU:CD | 3:C:233:ASP:HB2 | 2.24 | 0.57 |
| 3:D:52:ILE:O | 3:D:61:LEU:N | 2.38 | 0.57 |
| 3:D:68:LEU:O | 3:D:201:VAL:HG23 | 2.04 | 0.57 |
| 3:D:91:TYR:HB3 | 3:D:380:LYS:HZ1 | 1.69 | 0.57 |
| 3:D:103:VAL:HB | 3:D:375:ILE:HG22 | 1.86 | 0.57 |
| 3:D:46:GLY:HA2 | 3:D:365:ARG:HD2 | 1.87 | 0.57 |
| 3:D:236:LYS:HA | 3:D:239:SER:HB2 | 1.87 | 0.57 |
| 3:D:314:GLN:HG3 | 3:D:315:ARG:N | 2.14 | 0.57 |
| 3:E:47:HIS:CG | 3:E:48:PRO:HD2 | 2.39 | 0.57 |
| 3:F:90:PHE:CE1 | 3:F:91:TYR:HD2 | 2.22 | 0.57 |
| 3:G:109:ARG:NH2 | 3:G:338:ARG:HD2 | 2.20 | 0.57 |
| 3:H:71:ARG:HG3 | 3:H:370:TYR:OH | 2.05 | 0.57 |
| 3:C:18:VAL:CG1 | 3:C:18:VAL:CG2 | 2.80 | 0.57 |
| 3:D:47:HIS:CE1 | 3:D:49:TYR:H | 2.22 | 0.57 |
| 3:D:126:LEU:HB3 | 3:D:262:ASN:CB | 2.34 | 0.57 |
| 3:D:371:ASP:OD2 | 3:D:372:LEU:N | 2.38 | 0.57 |
| 3:D:465:GLY:O | 3:D:468:PHE:N | 2.38 | 0.57 |
| 3:H:335:ASP:OD2 | 3:H:337:THR:OG1 | 2.22 | 0.57 |
| 3:D:172:GLY:O | 3:D:187:PRO:HG2 | 2.03 | 0.57 |
| 3:D:441:LEU:HG | 3:D:444:TYR:CE2 | 2.40 | 0.57 |
| 3:D:45:VAL:HG12 | 3:D:365:ARG:HB3 | 1.87 | 0.57 |
| 3:D:70:TYR:CE2 | 3:D:200:MET:O | 2.57 | 0.57 |
| 3:D:156:LEU:HG | 3:D:334:VAL:HB | 1.87 | 0.57 |
| 3:D:249:TYR:HE1 | 3:D:251:ARG:CG | 2.18 | 0.57 |
| 3:E:407:GLN:N | 3:E:408:PRO:HA | 2.19 | 0.57 |
| 3:F:35:TYR:CD1 | 3:F:457:ALA:HA | 2.40 | 0.57 |
| 3:G:105:VAL:HG13 | 3:G:374:PHE:CE1 | 2.40 | 0.57 |
| 3:C:17:PRO:C | 3:C:17:PRO:HA | 2.10 | 0.57 |
| 3:C:195:ILE:HA | 3:C:230:LYS:NZ | 2.20 | 0.57 |
| 3:D:96:GLN:OE1 | 3:D:380:LYS:HB2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:122:LEU:HB3 | 3:D:144:ARG:HB3 | 1.86 | 0.57 |
| 3:D:158:LEU:HD12 | 3:D:332:THR:HG22 | 1.87 | 0.57 |
| 3:D:357:ASN:OD1 | 3:E:142:ASP:N | 2.36 | 0.57 |
| 3:G:47:HIS:CG | 3:G:48:PRO:HD2 | 2.40 | 0.57 |
| 3:D:106:GLU:O | 3:D:373:GLN:N | 2.33 | 0.57 |
| 3:D:109:ARG:HH11 | 3:D:110:GLY:N | 2.02 | 0.57 |
| 3:G:40:SER:OG | 3:G:41:ARG:N | 2.38 | 0.57 |
| 3:G:335:ASP:OD2 | 3:G:337:THR:OG1 | 2.21 | 0.57 |
| 3:D:30:ARG:HA | 3:D:379:CYS:SG | 2.45 | 0.56 |
| 3:D:119:GLY:HA2 | 3:D:221:PRO:HG3 | 1.87 | 0.56 |
| 3:F:418:TYR:CB | 3:F:419:ARG:HH11 | 2.15 | 0.56 |
| 3:H:404:PHE:CZ | 3:H:409:PRO:HD3 | 2.39 | 0.56 |
| 1:A:63:VAL:HG11 | 1:A:67:PHE:CE2 | 2.40 | 0.56 |
| 2:B:21:MET:SD | 2:B:102:THR:HG21 | 2.45 | 0.56 |
| 2:B:35:TRP:HB2 | 2:B:48:ILE:H | 1.70 | 0.56 |
| 3:C:428:CYS:O | 3:C:432:THR:HG23 | 2.06 | 0.56 |
| 3:D:162:LYS:CB | 3:D:245:SER:HA | 2.35 | 0.56 |
| 3:E:16:VAL:O | 3:E:18:VAL:HG23 | 2.05 | 0.56 |
| 3:E:153:GLN:NE2 | 3:E:300:VAL:HG12 | 2.19 | 0.56 |
| 2:B:24:LYS:CE | 2:B:70:ASP:HB2 | 2.35 | 0.56 |
| 2:B:85:VAL:HA | 2:B:103:LYS:HA | 1.86 | 0.56 |
| 3:C:164:PRO:HG2 | 3:C:195:ILE:HB | 1.85 | 0.56 |
| 3:C:406:LEU:HD22 | 3:C:409:PRO:HA | 1.86 | 0.56 |
| 3:D:47:HIS:O | 3:D:65:VAL:N | 2.38 | 0.56 |
| 3:D:70:TYR:HE2 | 3:D:230:LYS:HB2 | 1.71 | 0.56 |
| 3:D:266:ALA:HB3 | 3:H:360:PHE:O | 2.06 | 0.56 |
| 3:E:83:PHE:CE1 | 3:F:14:PRO:HD3 | 2.40 | 0.56 |
| 3:F:71:ARG:O | 3:F:332:THR:HG23 | 2.04 | 0.56 |
| 3:F:72:VAL:O | 3:F:447:TRP:HB3 | 2.06 | 0.56 |
| 3:F:280:SER:N | 3:F:283:THR:OG1 | 2.33 | 0.56 |
| 2:B:11:LEU:HD11 | 2:B:20:THR:O | 2.05 | 0.56 |
| 3:C:312:TRP:NE1 | 3:C:471:GLN:NE2 | 2.50 | 0.56 |
| 3:D:56:ASN:OD1 | 3:D:57:ASN:N | 2.39 | 0.56 |
| 3:D:109:ARG:HH12 | 3:D:369:GLU:HB3 | 1.70 | 0.56 |
| 3:D:117:ILE:HA | 3:D:151:TYR:CE2 | 2.40 | 0.56 |
| 3:D:273:ASP:OD1 | 3:D:274:ASP:N | 2.38 | 0.56 |
| 3:D:326:GLY:O | 3:D:328:GLN:HB2 | 2.05 | 0.56 |
| 3:E:35:TYR:HD1 | 3:E:457:ALA:HA | 1.69 | 0.56 |
| 3:C:153:GLN:HG3 | 3:C:336:THR:OG1 | 2.06 | 0.56 |
| 3:D:70:TYR:CZ | 3:D:201:VAL:HA | 2.40 | 0.56 |
| 3:D:155:GLN:HA | 3:D:335:ASP:HA | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:221:PRO:O | 3:D:224:ILE:HG12 | 2.05 | 0.56 |
| 3:D:234:TYR:O | 3:D:237:MET:N | 2.38 | 0.56 |
| 3:G:167:GLU:CD | 3:G:233:ASP:HB2 | 2.25 | 0.56 |
| 1:A:51:ILE:HD13 | 1:A:71:ARG:HG3 | 1.88 | 0.56 |
| 2:B:19:VAL:HG13 | 2:B:78:VAL:HG11 | 1.88 | 0.56 |
| 2:B:24:LYS:HE3 | 2:B:70:ASP:HB2 | 1.87 | 0.56 |
| 3:C:273:ASP:OD1 | 3:C:274:ASP:N | 2.38 | 0.56 |
| 3:C:372:LEU:HB3 | 3:C:374:PHE:CZ | 2.40 | 0.56 |
| 3:C:421:VAL:HA | 3:C:424:GLN:NE2 | 2.21 | 0.56 |
| 3:D:123:LEU:H | 3:D:145:GLU:N | 2.04 | 0.56 |
| 3:C:43:LEU:CD2 | 3:H:421:VAL:HG13 | 2.36 | 0.56 |
| 3:C:324:CYS:SG | 3:C:329:LEU:HD12 | 2.45 | 0.56 |
| 3:D:220:VAL:HB | 3:D:224:ILE:CD1 | 2.36 | 0.56 |
| 3:D:305:GLN:NE2 | 3:D:305:GLN:HA | 2.20 | 0.56 |
| 3:C:421:VAL:O | 3:C:424:GLN:HG3 | 2.05 | 0.56 |
| 3:C:439:ASP:O | 3:C:442:LYS:N | 2.30 | 0.56 |
| 3:D:167:GLU:HA | 3:D:192:ASN:HA | 1.88 | 0.56 |
| 3:D:236:LYS:HA | 3:D:239:SER:CB | 2.35 | 0.56 |
| 3:G:392:HIS:O | 3:G:396:SER:OG | 2.24 | 0.56 |
| 3:H:349:SER:O | 3:H:359:ASN:ND2 | 2.39 | 0.56 |
| 2:B:33:LEU:HG | 2:B:35:TRP:NE1 | 2.21 | 0.56 |
| 2:B:50:TRP:O | 2:B:52:SER:N | 2.32 | 0.56 |
| 3:C:51:PRO:N | 3:C:64:LYS:HB2 | 2.20 | 0.56 |
| 3:C:365:ARG:HH12 | 3:H:426:ILE:HG21 | 1.70 | 0.56 |
| 3:D:128:ASP:HA | 3:D:261:PHE:HD1 | 1.71 | 0.56 |
| 3:D:259:HIS:HB2 | 3:D:294:THR:HB | 1.88 | 0.56 |
| 3:E:233:ASP:N | 3:E:237:MET:HE2 | 2.21 | 0.56 |
| 3:F:258:ARG:HG2 | 3:F:259:HIS:ND1 | 2.20 | 0.56 |
| 3:G:399:LEU:HD22 | 3:G:404:PHE:CE1 | 2.41 | 0.56 |
| 3:G:431:HIS:HB3 | 3:G:433:PRO:HD2 | 1.88 | 0.56 |
| 3:H:150:ASP:OD1 | 3:H:296:SER:HA | 2.05 | 0.56 |
| 3:C:20:LYS:O | 3:C:21:VAL:HG23 | 2.05 | 0.56 |
| 3:C:410:PRO:O | 3:D:20:LYS:HB2 | 2.06 | 0.56 |
| 3:D:126:LEU:HB3 | 3:D:262:ASN:HB3 | 1.88 | 0.56 |
| 3:D:416:ASP:HB3 | 3:D:418:TYR:CE2 | 2.41 | 0.56 |
| 3:F:70:TYR:HD2 | 3:F:199:ASP:HB2 | 1.70 | 0.56 |
| 1:A:50:SER:HB2 | 1:A:58:HIS:HB2 | 1.88 | 0.55 |
| 2:B:37:GLN:HG3 | 2:B:84:ALA:CB | 2.35 | 0.55 |
| 3:D:159:ILE:O | 3:D:246:LEU:HB2 | 2.06 | 0.55 |
| 3:E:325:TRP:HZ3 | 3:E:402:TRP:CH2 | 2.24 | 0.55 |
| 3:H:85:PHE:HB3 | 3:H:86:PRO:HD2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:TRP:HZ2 | 1:A:50:SER:HG | 1.55 | 0.55 |
| 3:C:40:SER:HB3 | 3:H:418:TYR:HB3 | 1.88 | 0.55 |
| 3:D:233:ASP:OD1 | 3:D:236:LYS:N | 2.34 | 0.55 |
| 3:D:256:PHE:O | 3:D:296:SER:N | 2.32 | 0.55 |
| 3:D:263:ARG:HG2 | 3:D:292:PHE:HD2 | 1.72 | 0.55 |
| 3:E:47:HIS:HE1 | 3:E:49:TYR:HB2 | 1.71 | 0.55 |
| 3:E:465:GLY:O | 3:E:468:PHE:N | 2.39 | 0.55 |
| 1:A:17:SER:HB2 | 1:A:81:GLN:HE22 | 1.71 | 0.55 |
| 1:A:32:TYR:CD1 | 1:A:96:LEU:HA | 2.42 | 0.55 |
| 3:C:167:GLU:HG2 | 3:C:231:TYR:O | 2.06 | 0.55 |
| 3:C:418:TYR:HD2 | 3:D:239:SER:HB3 | 1.71 | 0.55 |
| 3:D:209:ASP:OD2 | 3:D:211:THR:HB | 2.06 | 0.55 |
| 3:D:372:LEU:HD22 | 3:D:374:PHE:CZ | 2.38 | 0.55 |
| 3:E:406:LEU:HB2 | 3:E:408:PRO:CA | 2.37 | 0.55 |
| 2:B:2:ILE:HD12 | 2:B:90:GLN:NE2 | 2.22 | 0.55 |
| 3:D:42:LEU:HB2 | 3:D:370:TYR:N | 2.21 | 0.55 |
| 3:D:309:LYS:HB2 | 3:D:311:TYR:CE1 | 2.41 | 0.55 |
| 3:F:47:HIS:CE1 | 3:F:49:TYR:HB2 | 2.40 | 0.55 |
| 3:F:169:TRP:HB2 | 3:F:208:MET:HB3 | 1.88 | 0.55 |
| 3:F:233:ASP:N | 3:F:237:MET:HE2 | 2.21 | 0.55 |
| 3:H:47:HIS:CG | 3:H:48:PRO:HD2 | 2.41 | 0.55 |
| 1:A:60:PRO:HD2 | 1:A:63:VAL:HG22 | 1.89 | 0.55 |
| 3:D:34:TYR:CE1 | 3:D:377:GLN:HG3 | 2.42 | 0.55 |
| 3:D:200:MET:CG | 3:D:227:SER:HB2 | 2.36 | 0.55 |
| 3:D:214:GLN:HG2 | 3:H:344:LEU:HA | 1.89 | 0.55 |
| 3:E:71:ARG:O | 3:E:332:THR:HG23 | 2.06 | 0.55 |
| 3:E:408:PRO:HB2 | 3:E:409:PRO:CD | 2.37 | 0.55 |
| 3:F:168:HIS:CE1 | 3:F:191:ILE:HB | 2.40 | 0.55 |
| 3:G:120:HIS:CD2 | 3:G:222:LEU:HD12 | 2.42 | 0.55 |
| 3:G:169:TRP:HB2 | 3:G:208:MET:HB3 | 1.88 | 0.55 |
| 1:A:59:TYR:CD2 | 1:A:64:LYS:HA | 2.42 | 0.55 |
| 3:C:120:HIS:ND1 | 3:C:122:LEU:O | 2.40 | 0.55 |
| 3:D:277:ILE:HG22 | 3:D:278:LYS:H | 1.72 | 0.55 |
| 3:F:300:VAL:HG22 | 3:G:255:MET:O | 2.06 | 0.55 |
| 3:G:48:PRO:HA | 3:G:66:SER:HB2 | 1.89 | 0.55 |
| 3:G:201:VAL:HG12 | 3:G:202:ASP:O | 2.06 | 0.55 |
| 3:H:244:ASP:OD1 | 3:H:320:ASN:HB2 | 2.07 | 0.55 |
| 3:C:97:ARG:HH22 | 3:C:404:PHE:H | 1.52 | 0.55 |
| 3:C:109:ARG:HB3 | 3:C:338:ARG:CZ | 2.37 | 0.55 |
| 3:D:165:ILE:HA | 3:D:194:VAL:HA | 1.87 | 0.55 |
| 3:D:464:LEU:O | 3:D:466:ARG:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:F:54:LYS:HD2 | 3:F:57:ASN:HB2 | 1.88 | 0.55 |
| 3:F:83:PHE:HD1 | 3:G:13:LEU:CD1 | 2.16 | 0.55 |
| 3:H:169:TRP:HB2 | 3:H:208:MET:HB3 | 1.88 | 0.55 |
| 3:C:22:VAL:O | 3:C:319:HIS:HB3 | 2.07 | 0.55 |
| 3:D:355:TYR:CD2 | 3:E:142:ASP:HB2 | 2.42 | 0.55 |
| 3:E:50:PHE:HA | 3:E:64:LYS:HD2 | 1.89 | 0.55 |
| 3:E:97:ARG:HH21 | 3:E:404:PHE:N | 2.05 | 0.55 |
| 3:E:120:HIS:HB2 | 3:E:221:PRO:HA | 1.87 | 0.55 |
| 1:A:100(E):ASP:HB3 | 2:B:49:TYR:CE2 | 2.42 | 0.55 |
| 3:D:235:ILE:O | 3:D:239:SER:N | 2.39 | 0.55 |
| 3:D:299:MET:HG2 | 3:D:300:VAL:H | 1.71 | 0.55 |
| 3:E:170:GLY:O | 3:E:189:GLU:N | 2.37 | 0.55 |
| 1:A:17:SER:HB2 | 1:A:81:GLN:NE2 | 2.22 | 0.55 |
| 3:D:50:PHE:C | 3:D:64:LYS:HB2 | 2.28 | 0.55 |
| 3:D:140:GLY:O | 3:D:143:ASN:ND2 | 2.40 | 0.55 |
| 3:D:463:PRO:HA | 3:D:466:ARG:HH12 | 1.72 | 0.55 |
| 3:E:14:PRO:HG2 | 3:E:15:PRO:HD2 | 1.89 | 0.55 |
| 3:E:450:ASN:HD21 | 3:E:452:LYS:HD2 | 1.71 | 0.55 |
| 3:D:159:ILE:N | 3:D:248:PHE:O | 2.29 | 0.54 |
| 3:E:48:PRO:HA | 3:E:66:SER:HB2 | 1.89 | 0.54 |
| 3:E:450:ASN:OD1 | 3:E:452:LYS:HG3 | 2.06 | 0.54 |
| 3:F:387:VAL:O | 3:F:391:ILE:HD12 | 2.07 | 0.54 |
| 3:H:85:PHE:CZ | 3:H:378:LEU:HD21 | 2.42 | 0.54 |
| 3:C:109:ARG:HH21 | 3:C:338:ARG:HD2 | 1.71 | 0.54 |
| 3:C:168:HIS:CE1 | 3:C:191:ILE:HB | 2.42 | 0.54 |
| 3:C:171:LYS:HB2 | 3:C:213:LEU:HD11 | 1.88 | 0.54 |
| 3:D:48:PRO:HG3 | 3:D:364:LEU:HD13 | 1.90 | 0.54 |
| 3:D:233:ASP:OD1 | 3:D:235:ILE:N | 2.40 | 0.54 |
| 3:D:395:ASN:OD1 | 3:D:397:THR:N | 2.35 | 0.54 |
| 3:E:54:LYS:HD2 | 3:E:57:ASN:HB2 | 1.89 | 0.54 |
| 3:E:146:CYS:HG | 3:F:291:TYR:HH | 1.55 | 0.54 |
| 3:C:384:THR:O | 3:C:387:VAL:HB | 2.07 | 0.54 |
| 3:C:408:PRO:HD2 | 3:C:412:GLY:H | 1.73 | 0.54 |
| 3:D:142:ASP:OD2 | 3:D:144:ARG:NH2 | 2.38 | 0.54 |
| 3:D:450:ASN:OD1 | 3:D:452:LYS:HG3 | 2.07 | 0.54 |
| 3:E:35:TYR:CD1 | 3:E:457:ALA:HA | 2.43 | 0.54 |
| 3:E:85:PHE:HB2 | 3:E:88:THR:HG22 | 1.88 | 0.54 |
| 3:E:407:GLN:CB | 3:E:410:PRO:HD2 | 2.38 | 0.54 |
| 3:F:70:TYR:HD1 | 3:F:334:VAL:HG21 | 1.73 | 0.54 |
| 3:G:115:VAL:HG12 | 3:G:116:GLY:O | 2.06 | 0.54 |
| 3:H:51:PRO:CA | 3:H:64:LYS:HB2 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:39:LYS:NZ | 2:B:81:GLU:HB3 | 2.22 | 0.54 |
| 2:B:82:ASP:O | 2:B:86:TYR:OH | 2.23 | 0.54 |
| 3:D:23:SER:HB3 | 3:D:26:GLU:OE2 | 2.08 | 0.54 |
| 3:D:36:HIS:CE1 | 3:D:37:ALA:C | 2.80 | 0.54 |
| 3:D:105:VAL:HA | 3:D:374:PHE:CD1 | 2.41 | 0.54 |
| 3:D:120:HIS:CE1 | 3:D:122:LEU:H | 2.25 | 0.54 |
| 3:D:152:LYS:HG2 | 3:D:203:THR:HA | 1.90 | 0.54 |
| 3:D:280:SER:O | 3:D:283:THR:OG1 | 2.17 | 0.54 |
| 3:F:78:PRO:HD2 | 3:F:455:PHE:CZ | 2.43 | 0.54 |
| 3:G:233:ASP:N | 3:G:237:MET:HE2 | 2.22 | 0.54 |
| 3:H:233:ASP:N | 3:H:237:MET:HE2 | 2.22 | 0.54 |
| 3:C:248:PHE:CG | 3:C:249:TYR:N | 2.76 | 0.54 |
| 3:C:365:ARG:NH1 | 3:H:426:ILE:HG21 | 2.23 | 0.54 |
| 3:D:65:VAL:HA | 3:D:69:GLN:HE22 | 1.72 | 0.54 |
| 3:D:161:CYS:SG | 3:D:244:ASP:HB3 | 2.48 | 0.54 |
| 3:D:194:VAL:O | 3:D:230:LYS:NZ | 2.41 | 0.54 |
| 3:D:223:ASP:O | 3:D:226:THR:OG1 | 2.14 | 0.54 |
| 3:E:240:GLU:CG | 3:E:241:PRO:HD2 | 2.38 | 0.54 |
| 3:E:300:VAL:HG22 | 3:F:255:MET:O | 2.06 | 0.54 |
| 3:G:72:VAL:O | 3:G:447:TRP:HB3 | 2.08 | 0.54 |
| 3:G:384:THR:H | 3:G:387:VAL:HB | 1.73 | 0.54 |
| 3:C:17:PRO:C | 3:C:17:PRO:CB | 2.71 | 0.54 |
| 3:D:76:HIS:HB2 | 3:D:450:ASN:CA | 2.24 | 0.54 |
| 3:D:147:ILE:HG12 | 3:E:129:THR:O | 2.07 | 0.54 |
| 3:C:123:LEU:N | 3:C:145:GLU:O | 2.40 | 0.54 |
| 3:D:36:HIS:CG | 3:D:37:ALA:N | 2.75 | 0.54 |
| 3:D:378:LEU:HG | 3:D:379:CYS:N | 2.22 | 0.54 |
| 3:E:211:THR:OG1 | 3:E:226:THR:O | 2.26 | 0.54 |
| 3:E:403:ASN:O | 3:E:405:GLY:N | 2.41 | 0.54 |
| 3:H:384:THR:H | 3:H:387:VAL:HB | 1.73 | 0.54 |
| 1:A:24:ALA:N | 1:A:76:ASN:O | 2.30 | 0.54 |
| 3:C:421:VAL:O | 3:C:423:SER:N | 2.41 | 0.54 |
| 3:D:111:GLN:HB2 | 3:D:338:ARG:CD | 2.32 | 0.54 |
| 3:F:30:ARG:HD3 | 3:F:379:CYS:SG | 2.47 | 0.54 |
| 3:H:15:PRO:HB3 | 3:H:17:PRO:HD3 | 1.90 | 0.54 |
| 3:H:24:THR:HG21 | 3:H:320:ASN:HA | 1.89 | 0.54 |
| 3:H:47:HIS:CE1 | 3:H:49:TYR:HB2 | 2.41 | 0.54 |
| 3:H:258:ARG:HB2 | 3:H:296:SER:HB2 | 1.89 | 0.54 |
| 2:B:36:TYR:O | 2:B:86:TYR:HA | 2.08 | 0.54 |
| 3:D:459:LEU:O | 3:D:466:ARG:CZ | 2.56 | 0.54 |
| 3:E:92:ASN:OD1 | 3:E:94:ASP:N | 2.31 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:150:ASP:OD1 | 3:E:296:SER:HA | 2.08 | 0.54 |
| 3:F:97:ARG:NH2 | 3:F:404:PHE:H | 2.05 | 0.54 |
| 2:B:19:VAL:HG13 | 2:B:78:VAL:HG21 | 1.90 | 0.54 |
| 3:D:344:LEU:HD11 | 3:D:363:TYR:CD2 | 2.43 | 0.54 |
| 3:D:399:LEU:HD23 | 3:D:402:TRP:CB | 2.32 | 0.54 |
| 3:E:167:GLU:CD | 3:E:233:ASP:HB2 | 2.28 | 0.54 |
| 3:F:244:ASP:OD1 | 3:F:320:ASN:HB2 | 2.08 | 0.54 |
| 3:G:360:PHE:CE2 | 3:H:216:ASN:HA | 2.42 | 0.54 |
| 1:A:92:CYS:HB3 | 1:A:104:GLY:HA3 | 1.89 | 0.53 |
| 3:D:79:ASP:OD2 | 3:D:81:ASN:HB2 | 2.09 | 0.53 |
| 3:G:30:ARG:HD3 | 3:G:379:CYS:SG | 2.49 | 0.53 |
| 3:H:314:GLN:HG3 | 3:H:315:ARG:N | 2.22 | 0.53 |
| 2:B:30(A):TYR:HH | 2:B:92:TYR:HH | 1.56 | 0.53 |
| 2:B:38:GLN:HB2 | 2:B:44:PRO:HB3 | 1.91 | 0.53 |
| 3:C:62:VAL:HG22 | 3:H:426:ILE:HG12 | 1.89 | 0.53 |
| 3:D:76:HIS:CE1 | 3:D:449:VAL:H | 2.26 | 0.53 |
| 3:D:273:ASP:HA | 3:D:276:TYR:CE2 | 2.43 | 0.53 |
| 3:D:312:TRP:CH2 | 3:D:468:PHE:HB2 | 2.43 | 0.53 |
| 3:D:389:THR:HG22 | 3:D:393:SER:OG | 2.07 | 0.53 |
| 3:H:258:ARG:NH2 | 3:H:296:SER:OG | 2.41 | 0.53 |
| 1:A:21:SER:C | 1:A:36:TRP:HH2 | 2.12 | 0.53 |
| 3:D:72:VAL:HG13 | 3:D:332:THR:OG1 | 2.08 | 0.53 |
| 3:D:187:PRO:CA | 3:D:188:LEU:HD12 | 2.37 | 0.53 |
| 3:E:61:LEU:HG | 3:E:62:VAL:HG23 | 1.89 | 0.53 |
| 3:F:51:PRO:CA | 3:F:64:LYS:HB2 | 2.39 | 0.53 |
| 3:G:298:SER:OG | 3:G:299:MET:N | 2.40 | 0.53 |
| 1:A:59:TYR:HD1 | 1:A:63:VAL:HG23 | 1.74 | 0.53 |
| 3:C:406:LEU:HD22 | 3:C:409:PRO:CA | 2.37 | 0.53 |
| 3:D:152:LYS:HD2 | 3:D:202:ASP:O | 2.09 | 0.53 |
| 3:D:159:ILE:HG22 | 3:D:247:PHE:CE1 | 2.43 | 0.53 |
| 3:H:120:HIS:CD2 | 3:H:222:LEU:HD12 | 2.44 | 0.53 |
| 1:A:29:PHE:HD2 | 1:A:73:ASN:HA | 1.73 | 0.53 |
| 3:C:273:ASP:HA | 3:C:276:TYR:CE2 | 2.43 | 0.53 |
| 3:E:298:SER:OG | 3:E:299:MET:N | 2.41 | 0.53 |
| 3:G:57:ASN:CG | 3:G:59:LYS:H | 2.12 | 0.53 |
| 1:A:39:GLN:N | 1:A:88:ALA:HB1 | 2.20 | 0.53 |
| 3:C:90:PHE:CE1 | 3:C:91:TYR:CD2 | 2.96 | 0.53 |
| 3:D:46:GLY:HA3 | 3:D:65:VAL:HB | 1.89 | 0.53 |
| 3:D:231:TYR:CD1 | 3:H:112:PRO:HB3 | 2.43 | 0.53 |
| 3:E:406:LEU:HB2 | 3:E:408:PRO:HA | 1.91 | 0.53 |
| 3:E:407:GLN:HB2 | 3:E:408:PRO:C | 2.28 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:170:GLY:O | 3:F:189:GLU:N | 2.39 | 0.53 |
| 3:G:36:HIS:HD2 | 3:G:375:ILE:HD13 | 1.73 | 0.53 |
| 3:H:383:LEU:HD23 | 3:H:387:VAL:HG11 | 1.91 | 0.53 |
| 2:B:79:LYS:O | 2:B:82:ASP:HB2 | 2.09 | 0.53 |
| 3:C:20:LYS:HB2 | 3:C:21:VAL:O | 2.08 | 0.53 |
| 3:C:273:ASP:O | 3:C:276:TYR:N | 2.30 | 0.53 |
| 3:C:418:TYR:CD2 | 3:D:239:SER:HB3 | 2.44 | 0.53 |
| 3:C:420:PHE:HA | 3:H:41:ARG:CD | 2.36 | 0.53 |
| 3:D:157:CYS:SG | 3:D:158:LEU:N | 2.81 | 0.53 |
| 3:D:431:HIS:O | 3:D:433:PRO:HD2 | 2.08 | 0.53 |
| 3:F:47:HIS:CE1 | 3:F:49:TYR:H | 2.26 | 0.53 |
| 3:F:235:ILE:O | 3:F:239:SER:N | 2.39 | 0.53 |
| 3:G:70:TYR:HD2 | 3:G:199:ASP:HB2 | 1.73 | 0.53 |
| 3:C:171:LYS:HG3 | 3:C:186:PRO:HB2 | 1.91 | 0.53 |
| 3:D:153:GLN:HE22 | 3:D:299:MET:C | 2.11 | 0.53 |
| 3:D:440:PRO:HG2 | 3:D:441:LEU:HD13 | 1.90 | 0.53 |
| 3:F:50:PHE:CE2 | 3:G:271:VAL:HG22 | 2.43 | 0.53 |
| 3:G:47:HIS:HE1 | 3:G:49:TYR:HB2 | 1.74 | 0.53 |
| 3:G:71:ARG:HG3 | 3:G:370:TYR:OH | 2.08 | 0.53 |
| 3:G:146:CYS:SG | 3:H:291:TYR:OH | 2.65 | 0.53 |
| 3:H:210:PHE:O | 3:H:214:GLN:N | 2.32 | 0.53 |
| 3:C:441:LEU:O | 3:C:444:TYR:N | 2.42 | 0.53 |
| 3:D:66:SER:HB3 | 3:D:69:GLN:HG3 | 1.90 | 0.53 |
| 3:D:309:LYS:HB3 | 3:D:310:PRO:HD2 | 1.91 | 0.53 |
| 3:E:57:ASN:CG | 3:E:59:LYS:H | 2.12 | 0.53 |
| 3:F:40:SER:OG | 3:F:41:ARG:N | 2.42 | 0.53 |
| 3:F:83:PHE:CD1 | 3:G:13:LEU:HD12 | 2.36 | 0.53 |
| 3:G:150:ASP:OD1 | 3:G:296:SER:HA | 2.09 | 0.53 |
| 3:C:437:LYS:HG2 | 3:C:438:GLU:H | 1.74 | 0.53 |
| 3:D:36:HIS:CE1 | 3:D:373:GLN:HB3 | 2.44 | 0.53 |
| 3:C:431:HIS:HA | 3:C:433:PRO:HD2 | 1.90 | 0.52 |
| 3:D:62:VAL:HG11 | 3:D:365:ARG:HE | 1.74 | 0.52 |
| 3:D:96:GLN:HG2 | 3:D:382:THR:CA | 2.37 | 0.52 |
| 3:D:469:LEU:O | 3:D:472:ALA:HB3 | 2.08 | 0.52 |
| 3:E:70:TYR:HD1 | 3:E:334:VAL:HG21 | 1.74 | 0.52 |
| 3:F:35:TYR:HD1 | 3:F:457:ALA:HA | 1.74 | 0.52 |
| 3:F:320:ASN:ND2 | 3:F:323:ILE:O | 2.30 | 0.52 |
| 3:F:436:PRO:O | 3:F:437:LYS:HB2 | 2.10 | 0.52 |
| 3:H:298:SER:OG | 3:H:299:MET:N | 2.41 | 0.52 |
| 3:C:259:HIS:H | 3:C:294:THR:HB | 1.73 | 0.52 |
| 3:F:97:ARG:HE | 3:F:402:TRP:HB3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:F:335:ASP:OD1 | 3:F:337:THR:HG23 | 2.10 | 0.52 |
| 3:G:299:MET:HA | 3:H:256:PHE:HB3 | 1.90 | 0.52 |
| 1:A:43:LYS:HZ3 | 2:B:103:LYS:HE2 | 1.74 | 0.52 |
| 2:B:35:TRP:CZ3 | 2:B:88:CYS:HB3 | 2.44 | 0.52 |
| 3:C:70:TYR:N | 3:C:199:ASP:O | 2.28 | 0.52 |
| 3:D:108:GLY:H | 3:D:371:ASP:C | 2.11 | 0.52 |
| 3:D:470:LEU:C | 3:D:473:GLY:H | 2.13 | 0.52 |
| 3:F:258:ARG:HB2 | 3:F:296:SER:HB2 | 1.90 | 0.52 |
| 3:G:52:ILE:HB | 3:G:62:VAL:H | 1.74 | 0.52 |
| 3:H:258:ARG:HG2 | 3:H:259:HIS:CE1 | 2.45 | 0.52 |
| 3:C:406:LEU:CG | 3:C:411:GLY:H | 2.21 | 0.52 |
| 3:D:79:ASP:HA | 3:D:327:ASN:ND2 | 2.25 | 0.52 |
| 3:D:187:PRO:C | 3:D:188:LEU:HD12 | 2.30 | 0.52 |
| 3:D:234:TYR:OH | 3:D:251:ARG:HD3 | 2.09 | 0.52 |
| 3:D:439:ASP:HB3 | 3:D:442:LYS:HB2 | 1.92 | 0.52 |
| 3:E:244:ASP:OD1 | 3:E:320:ASN:HB2 | 2.10 | 0.52 |
| 2:B:35:TRP:O | 2:B:46:LEU:HD12 | 2.09 | 0.52 |
| 3:C:97:ARG:NH2 | 3:C:404:PHE:N | 2.56 | 0.52 |
| 3:D:120:HIS:ND1 | 3:D:122:LEU:N | 2.57 | 0.52 |
| 3:D:468:PHE:O | 3:D:471:GLN:N | 2.43 | 0.52 |
| 3:E:408:PRO:HB2 | 3:E:409:PRO:HD2 | 1.92 | 0.52 |
| 3:F:18:VAL:HG12 | 3:F:19:SER:H | 1.74 | 0.52 |
| 3:F:201:VAL:HG12 | 3:F:202:ASP:O | 2.10 | 0.52 |
| 3:F:256:PHE:HE2 | 3:F:298:SER:HB2 | 1.75 | 0.52 |
| 1:A:69:ILE:HG13 | 1:A:79:TYR:O | 2.10 | 0.52 |
| 3:C:201:VAL:HG12 | 3:C:202:ASP:O | 2.10 | 0.52 |
| 3:D:129:THR:HG21 | 3:H:148:SER:OG | 2.10 | 0.52 |
| 3:D:387:VAL:O | 3:D:389:THR:N | 2.42 | 0.52 |
| 3:E:52:ILE:HB | 3:E:62:VAL:HB | 1.91 | 0.52 |
| 3:F:18:VAL:CG1 | 3:F:19:SER:N | 2.73 | 0.52 |
| 3:G:450:ASN:OD1 | 3:G:452:LYS:HG3 | 2.10 | 0.52 |
| 1:A:60:PRO:HB3 | 2:B:95:PRO:HB3 | 1.92 | 0.52 |
| 1:A:94:ARG:HH21 | 1:A:101:ASP:CB | 2.21 | 0.52 |
| 1:A:100:TYR:O | 1:A:100(B):GLU:HG3 | 2.09 | 0.52 |
| 2:B:54:ARG:CZ | 2:B:60:ASP:HA | 2.39 | 0.52 |
| 3:D:123:LEU:O | 3:D:144:ARG:HA | 2.09 | 0.52 |
| 3:D:202:ASP:CB | 3:D:204:GLY:H | 2.20 | 0.52 |
| 3:F:324:CYS:SG | 3:F:329:LEU:HD12 | 2.50 | 0.52 |
| 3:G:273:ASP:HA | 3:G:276:TYR:CE2 | 2.45 | 0.52 |
| 3:G:384:THR:OG1 | 3:G:387:VAL:HG23 | 2.10 | 0.52 |
| 3:H:18:VAL:HG12 | 3:H:19:SER:N | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:H:235:ILE:O | 3:H:239:SER:N | 2.39 | 0.52 |
| 3:D:23:SER:O | 3:D:26:GLU:HG2 | 2.10 | 0.52 |
| 3:D:104:GLY:N | 3:D:375:ILE:O | 2.28 | 0.52 |
| 3:E:30:ARG:HD3 | 3:E:379:CYS:SG | 2.50 | 0.52 |
| 3:E:34:TYR:HE1 | 3:E:377:GLN:HG3 | 1.74 | 0.52 |
| 3:E:51:PRO:CA | 3:E:64:LYS:HB2 | 2.40 | 0.52 |
| 3:G:320:ASN:ND2 | 3:G:323:ILE:O | 2.30 | 0.52 |
| 3:C:387:VAL:O | 3:C:391:ILE:HD12 | 2.09 | 0.52 |
| 3:D:38:GLY:HA2 | 3:D:372:LEU:O | 2.10 | 0.52 |
| 3:D:52:ILE:HB | 3:D:62:VAL:H | 1.75 | 0.52 |
| 3:D:73:PHE:O | 3:D:331:VAL:N | 2.38 | 0.52 |
| 3:F:48:PRO:HA | 3:F:66:SER:HB2 | 1.92 | 0.52 |
| 3:G:70:TYR:HE1 | 3:G:201:VAL:HG22 | 1.75 | 0.52 |
| 3:H:164:PRO:HG2 | 3:H:195:ILE:HB | 1.92 | 0.52 |
| 3:H:201:VAL:HG12 | 3:H:202:ASP:O | 2.09 | 0.52 |
| 3:H:324:CYS:SG | 3:H:329:LEU:HD12 | 2.50 | 0.52 |
| 1:A:100(A):ASP:HB3 | 2:B:50:TRP:CD2 | 2.44 | 0.52 |
| 3:D:72:VAL:HG22 | 3:D:332:THR:CG2 | 2.40 | 0.52 |
| 3:D:123:LEU:HG | 3:D:124:ASN:N | 2.24 | 0.52 |
| 3:D:165:ILE:HA | 3:D:195:ILE:H | 1.75 | 0.52 |
| 3:D:289:SER:HA | 3:D:291:TYR:CE2 | 2.45 | 0.52 |
| 3:F:97:ARG:NH2 | 3:F:404:PHE:N | 2.58 | 0.52 |
| 3:H:465:GLY:O | 3:H:468:PHE:N | 2.43 | 0.52 |
| 2:B:30(E):GLN:O | 2:B:30(F):LYS:HD2 | 2.10 | 0.51 |
| 3:C:101:ALA:N | 3:C:377:GLN:O | 2.40 | 0.51 |
| 3:C:312:TRP:HH2 | 3:C:468:PHE:CD1 | 2.22 | 0.51 |
| 3:D:113:LEU:N | 3:D:113:LEU:HD12 | 2.24 | 0.51 |
| 3:D:122:LEU:HD22 | 3:D:144:ARG:HB2 | 1.91 | 0.51 |
| 3:D:168:HIS:HB2 | 3:D:207:ALA:O | 2.10 | 0.51 |
| 3:D:249:TYR:CE1 | 3:D:251:ARG:HG2 | 2.45 | 0.51 |
| 3:D:255:MET:O | 3:H:300:VAL:HG22 | 2.10 | 0.51 |
| 3:D:346:ALA:O | 3:D:360:PHE:HA | 2.10 | 0.51 |
| 3:D:361:LYS:NZ | 3:E:267:VAL:O | 2.42 | 0.51 |
| 3:E:120:HIS:CE1 | 3:E:122:LEU:H | 2.28 | 0.51 |
| 3:H:245:SER:OG | 3:H:246:LEU:N | 2.44 | 0.51 |
| 3:H:466:ARG:O | 3:H:469:LEU:HB2 | 2.10 | 0.51 |
| 3:G:120:HIS:CE1 | 3:G:122:LEU:H | 2.27 | 0.51 |
| 3:G:314:GLN:HG3 | 3:G:315:ARG:N | 2.24 | 0.51 |
| 3:H:15:PRO:CB | 3:H:16:VAL:HA | 2.40 | 0.51 |
| 3:H:312:TRP:HH2 | 3:H:468:PHE:CD1 | 2.24 | 0.51 |
| 2:B:2:ILE:HG12 | 2:B:26:SER:OG | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:47:HIS:CD2 | 3:D:48:PRO:HD2 | 2.45 | 0.51 |
| 3:D:273:ASP:HA | 3:D:276:TYR:CE1 | 2.46 | 0.51 |
| 3:D:382:THR:HG22 | 3:D:383:LEU:N | 2.20 | 0.51 |
| 3:E:201:VAL:HG12 | 3:E:202:ASP:O | 2.10 | 0.51 |
| 3:E:391:ILE:O | 3:E:394:MET:N | 2.43 | 0.51 |
| 3:H:90:PHE:CE1 | 3:H:91:TYR:HD2 | 2.28 | 0.51 |
| 2:B:35:TRP:HB2 | 2:B:47:LEU:HB2 | 1.92 | 0.51 |
| 3:D:69:GLN:HB2 | 3:D:71:ARG:CZ | 2.41 | 0.51 |
| 3:E:245:SER:OG | 3:E:246:LEU:N | 2.43 | 0.51 |
| 3:F:196:GLN:HE21 | 3:F:444:TYR:HD1 | 1.56 | 0.51 |
| 3:H:167:GLU:CD | 3:H:233:ASP:HB2 | 2.31 | 0.51 |
| 3:H:475:LYS:O | 3:H:477:LYS:HG3 | 2.10 | 0.51 |
| 1:A:63:VAL:HA | 1:A:66:ARG:HB2 | 1.91 | 0.51 |
| 3:C:312:TRP:CH2 | 3:C:468:PHE:CD1 | 2.94 | 0.51 |
| 3:D:460:ASP:HB3 | 3:D:461:GLN:OE1 | 2.11 | 0.51 |
| 3:D:466:ARG:HA | 3:D:469:LEU:CB | 2.40 | 0.51 |
| 3:G:85:PHE:HB3 | 3:G:86:PRO:HD2 | 1.93 | 0.51 |
| 3:H:116:GLY:H | 3:H:339:SER:HG | 1.53 | 0.51 |
| 3:H:450:ASN:OD1 | 3:H:452:LYS:HG3 | 2.11 | 0.51 |
| 3:D:106:GLU:OE1 | 3:D:309:LYS:O | 2.29 | 0.51 |
| 3:D:195:ILE:HA | 3:D:230:LYS:HZ3 | 1.75 | 0.51 |
| 3:E:403:ASN:O | 3:E:404:PHE:C | 2.49 | 0.51 |
| 3:G:34:TYR:HE1 | 3:G:377:GLN:HG3 | 1.74 | 0.51 |
| 3:G:399:LEU:HD22 | 3:G:404:PHE:CZ | 2.45 | 0.51 |
| 2:B:55:GLU:HG3 | 2:B:56:SER:O | 2.11 | 0.51 |
| 3:C:87:ASP:OD1 | 3:H:89:SER:HB3 | 2.11 | 0.51 |
| 3:C:406:LEU:HD23 | 3:C:406:LEU:C | 2.31 | 0.51 |
| 3:D:54:LYS:HB3 | 3:D:57:ASN:CB | 2.36 | 0.51 |
| 3:D:182:PRO:CB | 3:H:348:ILE:HG13 | 2.37 | 0.51 |
| 3:D:200:MET:HG3 | 3:D:227:SER:HB2 | 1.92 | 0.51 |
| 3:D:447:TRP:CD1 | 3:D:448:GLU:N | 2.78 | 0.51 |
| 3:D:461:GLN:HE21 | 3:E:20:LYS:HG2 | 1.75 | 0.51 |
| 3:G:16:VAL:HB | 3:G:17:PRO:HD3 | 1.77 | 0.51 |
| 3:G:97:ARG:NH2 | 3:G:404:PHE:N | 2.59 | 0.51 |
| 2:B:6:GLN:HB2 | 2:B:101:GLY:N | 2.26 | 0.51 |
| 3:C:235:ILE:O | 3:C:239:SER:N | 2.42 | 0.51 |
| 3:C:242:TYR:HE1 | 3:C:390:TYR:HH | 1.59 | 0.51 |
| 3:C:254:GLN:NE2 | 3:C:298:SER:HB3 | 2.26 | 0.51 |
| 3:D:32:ASN:N | 3:D:33:ILE:HD12 | 2.26 | 0.51 |
| 3:D:46:GLY:N | 3:D:366:HIS:O | 2.43 | 0.51 |
| 3:D:222:LEU:H | 3:D:222:LEU:CD1 | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:301:THR:CG2 | 3:G:304:ALA:H | 2.23 | 0.51 |
| 3:H:161:CYS:SG | 3:H:244:ASP:HB3 | 2.50 | 0.51 |
| 2:B:47:LEU:HD11 | 2:B:86:TYR:CD1 | 2.46 | 0.51 |
| 3:C:197:ASP:HB3 | 3:C:446:PHE:HA | 1.92 | 0.51 |
| 3:C:249:TYR:HE1 | 3:C:251:ARG:NH1 | 2.08 | 0.51 |
| 3:D:144:ARG:HH21 | 3:E:279:GLY:HA2 | 1.75 | 0.51 |
| 3:D:466:ARG:HA | 3:D:469:LEU:CG | 2.41 | 0.51 |
| 3:F:413:THR:O | 3:F:414:LEU:HB2 | 2.11 | 0.51 |
| 3:G:83:PHE:HZ | 3:H:13:LEU:HB3 | 1.76 | 0.51 |
| 1:A:89:MET:SD | 1:A:91:TYR:OH | 2.69 | 0.51 |
| 2:B:54:ARG:NH2 | 2:B:60:ASP:OD1 | 2.43 | 0.51 |
| 3:D:168:HIS:CE1 | 3:D:191:ILE:HD12 | 2.46 | 0.51 |
| 3:D:258:ARG:HB3 | 3:D:294:THR:HG22 | 1.93 | 0.51 |
| 3:F:19:SER:O | 3:F:20:LYS:HD3 | 2.08 | 0.51 |
| 3:F:349:SER:O | 3:F:359:ASN:ND2 | 2.41 | 0.51 |
| 3:D:466:ARG:HA | 3:D:469:LEU:HG | 1.93 | 0.50 |
| 3:E:40:SER:OG | 3:E:41:ARG:N | 2.39 | 0.50 |
| 3:F:432:THR:HA | 3:F:434:PRO:HD2 | 1.92 | 0.50 |
| 3:G:90:PHE:CE1 | 3:G:91:TYR:HD2 | 2.29 | 0.50 |
| 3:G:240:GLU:HG3 | 3:G:241:PRO:HD2 | 1.93 | 0.50 |
| 3:G:320:ASN:OD1 | 3:G:323:ILE:N | 2.22 | 0.50 |
| 3:H:263:ARG:HB2 | 3:H:290:ASN:HD22 | 1.77 | 0.50 |
| 3:H:273:ASP:O | 3:H:276:TYR:N | 2.38 | 0.50 |
| 2:B:50:TRP:CZ3 | 2:B:52:SER:HB2 | 2.45 | 0.50 |
| 2:B:61:ARG:O | 2:B:75:ILE:HG12 | 2.12 | 0.50 |
| 3:C:36:HIS:HD2 | 3:C:375:ILE:HD13 | 1.75 | 0.50 |
| 3:C:43:LEU:HD12 | 3:C:368:GLU:O | 2.11 | 0.50 |
| 3:D:141:VAL:HA | 3:H:357:ASN:OD1 | 2.11 | 0.50 |
| 3:D:246:LEU:HD13 | 3:D:248:PHE:N | 2.27 | 0.50 |
| 3:F:41:ARG:HH21 | 3:F:369:GLU:HG3 | 1.76 | 0.50 |
| 3:F:384:THR:OG1 | 3:F:387:VAL:HG23 | 2.11 | 0.50 |
| 3:H:70:TYR:HE1 | 3:H:201:VAL:HG22 | 1.76 | 0.50 |
| 1:A:59:TYR:CD2 | 1:A:64:LYS:HD2 | 2.47 | 0.50 |
| 1:A:60:PRO:HG2 | 1:A:62:SER:OG | 2.11 | 0.50 |
| 3:D:349:SER:H | 3:D:359:ASN:HD21 | 1.57 | 0.50 |
| 3:D:384:THR:H | 3:D:387:VAL:CB | 2.22 | 0.50 |
| 3:E:47:HIS:CE1 | 3:E:49:TYR:HB2 | 2.46 | 0.50 |
| 3:E:90:PHE:CE1 | 3:E:91:TYR:HD2 | 2.29 | 0.50 |
| 3:G:81:ASN:ND2 | 3:G:98:LEU:O | 2.45 | 0.50 |
| 3:G:324:CYS:SG | 3:G:329:LEU:HD12 | 2.51 | 0.50 |
| 3:D:45:VAL:HG12 | 3:D:46:GLY:N | 2.25 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:51:PRO:N | 3:E:64:LYS:HB2 | 2.27 | 0.50 |
| 3:E:57:ASN:OD1 | 3:E:59:LYS:N | 2.41 | 0.50 |
| 3:E:320:ASN:ND2 | 3:E:323:ILE:O | 2.30 | 0.50 |
| 3:F:70:TYR:HE1 | 3:F:201:VAL:HG22 | 1.76 | 0.50 |
| 3:G:254:GLN:OE1 | 3:G:298:SER:HB3 | 2.10 | 0.50 |
| 3:H:53:LYS:HA | 3:H:61:LEU:N | 2.23 | 0.50 |
| 1:A:36:TRP:CZ2 | 1:A:78:LEU:HG | 2.46 | 0.50 |
| 3:D:97:ARG:HH21 | 3:D:403:ASN:H | 1.59 | 0.50 |
| 3:D:114:GLY:N | 3:D:337:THR:O | 2.41 | 0.50 |
| 3:E:235:ILE:O | 3:E:239:SER:N | 2.37 | 0.50 |
| 3:F:465:GLY:O | 3:F:468:PHE:HB3 | 2.12 | 0.50 |
| 3:H:274:ASP:OD1 | 3:H:275:LEU:HG | 2.12 | 0.50 |
| 3:H:421:VAL:O | 3:H:422:THR:HG23 | 2.12 | 0.50 |
| 3:C:85:PHE:CD2 | 3:C:88:THR:HG22 | 2.47 | 0.50 |
| 3:D:70:TYR:N | 3:D:199:ASP:O | 2.44 | 0.50 |
| 3:D:150:ASP:CG | 3:D:297:GLY:H | 2.14 | 0.50 |
| 3:D:344:LEU:O | 3:D:362:GLU:HA | 2.12 | 0.50 |
| 3:D:384:THR:H | 3:D:387:VAL:CG2 | 2.25 | 0.50 |
| 3:E:47:HIS:CE1 | 3:E:49:TYR:H | 2.30 | 0.50 |
| 3:E:159:ILE:HG22 | 3:E:247:PHE:CZ | 2.46 | 0.50 |
| 3:G:16:VAL:CG2 | 3:G:17:PRO:N | 2.59 | 0.50 |
| 3:H:48:PRO:HA | 3:H:66:SER:HB2 | 1.93 | 0.50 |
| 3:D:24:THR:HA | 3:D:27:TYR:OH | 2.12 | 0.50 |
| 3:D:90:PHE:HD1 | 3:D:380:LYS:HZ1 | 1.58 | 0.50 |
| 3:D:90:PHE:CE1 | 3:D:91:TYR:CD2 | 3.00 | 0.50 |
| 3:D:216:ASN:CB | 3:D:219:GLU:HG2 | 2.40 | 0.50 |
| 3:D:320:ASN:CG | 3:D:323:ILE:HB | 2.32 | 0.50 |
| 3:D:374:PHE:CB | 3:D:376:PHE:CZ | 2.94 | 0.50 |
| 3:D:384:THR:O | 3:D:388:MET:HG3 | 2.12 | 0.50 |
| 3:C:169:TRP:HB2 | 3:C:208:MET:CB | 2.41 | 0.50 |
| 3:D:120:HIS:O | 3:D:146:CYS:HA | 2.12 | 0.50 |
| 3:D:271:VAL:HG13 | 3:D:275:LEU:HD12 | 1.94 | 0.50 |
| 3:D:386:ASP:N | 3:D:386:ASP:OD1 | 2.36 | 0.50 |
| 3:E:78:PRO:HD2 | 3:E:455:PHE:CZ | 2.47 | 0.50 |
| 3:F:120:HIS:CE1 | 3:F:122:LEU:H | 2.30 | 0.50 |
| 3:F:146:CYS:SG | 3:G:291:TYR:OH | 2.70 | 0.50 |
| 3:F:466:ARG:O | 3:F:469:LEU:HB2 | 2.11 | 0.50 |
| 3:G:219:GLU:OE1 | 3:G:263:ARG:CZ | 2.58 | 0.50 |
| 3:H:301:THR:CG2 | 3:H:304:ALA:H | 2.25 | 0.50 |
| 1:A:94:ARG:HG2 | 1:A:102:TYR:O | 2.12 | 0.50 |
| 3:C:57:ASN:CG | 3:C:59:LYS:H | 2.15 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:466:ARG:O | 3:C:469:LEU:HB2 | 2.11 | 0.50 |
| 3:D:127:ASP:H | 3:D:262:ASN:HB2 | 1.77 | 0.50 |
| 3:D:287:ALA:CB | 3:H:146:CYS:HB2 | 2.39 | 0.50 |
| 3:F:57:ASN:CG | 3:F:59:LYS:H | 2.15 | 0.50 |
| 1:A:39:GLN:HB2 | 1:A:91:TYR:HE2 | 1.75 | 0.49 |
| 3:C:16:VAL:N | 3:C:17:PRO:CD | 2.75 | 0.49 |
| 3:D:157:CYS:HA | 3:D:333:VAL:HA | 1.92 | 0.49 |
| 3:D:159:ILE:HD12 | 3:D:248:PHE:CE2 | 2.48 | 0.49 |
| 3:E:406:LEU:CB | 3:E:408:PRO:HA | 2.41 | 0.49 |
| 1:A:22:CYS:O | 1:A:77:ILE:HA | 2.12 | 0.49 |
| 3:D:299:MET:CA | 3:E:256:PHE:HB3 | 2.39 | 0.49 |
| 3:D:466:ARG:O | 3:D:470:LEU:N | 2.42 | 0.49 |
| 3:F:240:GLU:HG3 | 3:F:241:PRO:HD2 | 1.93 | 0.49 |
| 1:A:52:SER:OG | 1:A:55:GLY:N | 2.45 | 0.49 |
| 3:D:389:THR:O | 3:D:392:HIS:N | 2.46 | 0.49 |
| 3:E:47:HIS:CD2 | 3:E:48:PRO:HD2 | 2.47 | 0.49 |
| 3:F:360:PHE:CE2 | 3:G:216:ASN:HA | 2.48 | 0.49 |
| 3:G:78:PRO:HD2 | 3:G:455:PHE:CZ | 2.47 | 0.49 |
| 3:G:406:LEU:CA | 3:G:408:PRO:HD3 | 2.40 | 0.49 |
| 3:H:36:HIS:HD2 | 3:H:375:ILE:HD13 | 1.77 | 0.49 |
| 3:H:61:LEU:HG | 3:H:62:VAL:HG23 | 1.94 | 0.49 |
| 3:H:70:TYR:CE1 | 3:H:201:VAL:HG22 | 2.47 | 0.49 |
| 3:H:78:PRO:HD2 | 3:H:455:PHE:CZ | 2.48 | 0.49 |
| 3:H:349:SER:N | 3:H:359:ASN:OD1 | 2.44 | 0.49 |
| 3:D:109:ARG:NH1 | 3:D:110:GLY:N | 2.59 | 0.49 |
| 3:D:167:GLU:HB2 | 3:D:192:ASN:OD1 | 2.13 | 0.49 |
| 3:D:234:TYR:CZ | 3:D:251:ARG:HD3 | 2.47 | 0.49 |
| 3:D:357:ASN:CG | 3:E:142:ASP:H | 2.15 | 0.49 |
| 3:E:97:ARG:HH21 | 3:E:403:ASN:C | 2.15 | 0.49 |
| 3:E:196:GLN:HE21 | 3:E:444:TYR:HD1 | 1.61 | 0.49 |
| 3:E:258:ARG:HG2 | 3:E:259:HIS:CE1 | 2.47 | 0.49 |
| 3:F:450:ASN:HD21 | 3:F:452:LYS:HD2 | 1.76 | 0.49 |
| 3:H:240:GLU:HG3 | 3:H:241:PRO:HD2 | 1.92 | 0.49 |
| 3:D:142:ASP:HA | 3:H:355:TYR:CE2 | 2.48 | 0.49 |
| 3:D:147:ILE:HG23 | 3:E:129:THR:O | 2.11 | 0.49 |
| 3:D:236:LYS:HA | 3:D:239:SER:OG | 2.13 | 0.49 |
| 3:E:18:VAL:CB | 3:E:20:LYS:HG3 | 2.43 | 0.49 |
| 3:F:211:THR:OG1 | 3:F:226:THR:O | 2.28 | 0.49 |
| 3:H:111:GLN:HB2 | 3:H:338:ARG:HD3 | 1.93 | 0.49 |
| 3:H:170:GLY:O | 3:H:189:GLU:N | 2.45 | 0.49 |
| 3:H:314:GLN:HG3 | 3:H:315:ARG:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:LYS:NZ | 2:B:103:LYS:HE2 | 2.27 | 0.49 |
| 3:D:45:VAL:HG22 | 3:E:169:TRP:HH2 | 1.77 | 0.49 |
| 3:E:335:ASP:OD1 | 3:E:337:THR:HG23 | 2.12 | 0.49 |
| 3:F:147:ILE:HG23 | 3:G:129:THR:O | 2.13 | 0.49 |
| 3:F:167:GLU:CD | 3:F:233:ASP:HB2 | 2.32 | 0.49 |
| 3:G:300:VAL:HG22 | 3:H:255:MET:O | 2.12 | 0.49 |
| 3:G:312:TRP:CZ3 | 3:G:468:PHE:HD1 | 2.30 | 0.49 |
| 3:H:51:PRO:N | 3:H:64:LYS:HB2 | 2.28 | 0.49 |
| 1:A:100(A):ASP:O | 2:B:50:TRP:NE1 | 2.46 | 0.49 |
| 2:B:18:LYS:HE2 | 2:B:75:ILE:O | 2.13 | 0.49 |
| 3:C:273:ASP:HA | 3:C:276:TYR:CZ | 2.47 | 0.49 |
| 3:C:384:THR:H | 3:C:387:VAL:HB | 1.77 | 0.49 |
| 3:D:62:VAL:HG11 | 3:D:365:ARG:NE | 2.27 | 0.49 |
| 3:D:307:PHE:HZ | 3:D:335:ASP:HB2 | 1.78 | 0.49 |
| 3:F:164:PRO:HG2 | 3:F:195:ILE:HB | 1.94 | 0.49 |
| 3:H:320:ASN:OD1 | 3:H:323:ILE:N | 2.27 | 0.49 |
| 3:H:384:THR:OG1 | 3:H:387:VAL:HG23 | 2.12 | 0.49 |
| 1:A:23:GLU:HG2 | 1:A:24:ALA:O | 2.13 | 0.49 |
| 1:A:32:TYR:CG | 1:A:96:LEU:HA | 2.47 | 0.49 |
| 2:B:18:LYS:HA | 2:B:78:VAL:CG2 | 2.42 | 0.49 |
| 3:C:348:ILE:N | 3:C:359:ASN:O | 2.30 | 0.49 |
| 3:D:159:ILE:HG22 | 3:D:247:PHE:HE1 | 1.77 | 0.49 |
| 3:F:36:HIS:HD2 | 3:F:375:ILE:HD13 | 1.78 | 0.49 |
| 3:H:167:GLU:OE2 | 3:H:233:ASP:HB2 | 2.13 | 0.49 |
| 3:C:298:SER:OG | 3:C:299:MET:N | 2.44 | 0.49 |
| 3:D:71:ARG:HH12 | 3:D:198:GLY:HA2 | 1.77 | 0.49 |
| 3:D:79:ASP:HB3 | 3:D:82:LYS:CG | 2.40 | 0.49 |
| 3:D:170:GLY:C | 3:D:189:GLU:HB3 | 2.33 | 0.49 |
| 3:D:212:THR:OG1 | 3:D:213:LEU:N | 2.46 | 0.49 |
| 3:D:335:ASP:OD1 | 3:D:336:THR:N | 2.46 | 0.49 |
| 3:D:355:TYR:CE2 | 3:E:142:ASP:HB2 | 2.48 | 0.49 |
| 3:D:402:TRP:N | 3:D:402:TRP:CD1 | 2.77 | 0.49 |
| 3:E:125:LYS:HE2 | 3:E:261:PHE:CG | 2.48 | 0.49 |
| 3:F:418:TYR:N | 3:F:419:ARG:NH1 | 2.61 | 0.49 |
| 3:G:57:ASN:OD1 | 3:G:59:LYS:N | 2.44 | 0.49 |
| 3:H:247:PHE:HE1 | 3:H:313:LEU:HD13 | 1.77 | 0.49 |
| 3:C:47:HIS:CG | 3:C:48:PRO:HD2 | 2.48 | 0.49 |
| 3:D:80:PRO:HD3 | 3:D:100:TRP:HE1 | 1.77 | 0.49 |
| 3:D:209:ASP:O | 3:D:213:LEU:N | 2.31 | 0.49 |
| 3:D:213:LEU:O | 3:H:344:LEU:HB2 | 2.13 | 0.49 |
| 3:D:377:GLN:HG2 | 3:D:378:LEU:O | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:459:LEU:HA | 3:D:462:PHE:HB2 | 1.94 | 0.49 |
| 3:G:258:ARG:HG2 | 3:G:259:HIS:CE1 | 2.48 | 0.49 |
| 3:H:328:GLN:HE21 | 3:H:330:PHE:HE1 | 1.61 | 0.49 |
| 3:C:160:GLY:HA3 | 3:C:246:LEU:HA | 1.95 | 0.48 |
| 3:D:160:GLY:HA2 | 3:D:247:PHE:CE1 | 2.48 | 0.48 |
| 3:D:347:ALA:HB1 | 3:D:359:ASN:ND2 | 2.28 | 0.48 |
| 3:E:335:ASP:OD1 | 3:E:337:THR:N | 2.38 | 0.48 |
| 3:F:298:SER:OG | 3:F:299:MET:N | 2.44 | 0.48 |
| 3:F:460:ASP:OD2 | 3:F:477:LYS:HE2 | 2.12 | 0.48 |
| 3:G:50:PHE:CE2 | 3:H:271:VAL:HG22 | 2.48 | 0.48 |
| 3:G:81:ASN:ND2 | 3:G:98:LEU:H | 2.05 | 0.48 |
| 3:H:35:TYR:HD2 | 3:H:100:TRP:CH2 | 2.30 | 0.48 |
| 2:B:54:ARG:HD3 | 2:B:58:VAL:HG12 | 1.95 | 0.48 |
| 3:C:240:GLU:OE1 | 3:C:245:SER:N | 2.37 | 0.48 |
| 3:C:432:THR:O | 3:C:434:PRO:HD2 | 2.13 | 0.48 |
| 3:D:117:ILE:HA | 3:D:151:TYR:OH | 2.13 | 0.48 |
| 3:D:149:MET:O | 3:D:151:TYR:CZ | 2.65 | 0.48 |
| 3:D:371:ASP:CG | 3:D:372:LEU:N | 2.66 | 0.48 |
| 3:D:398:ILE:O | 3:D:401:ASP:HB2 | 2.13 | 0.48 |
| 3:D:459:LEU:O | 3:D:466:ARG:NH2 | 2.46 | 0.48 |
| 3:E:43:LEU:HA | 3:E:368:GLU:O | 2.12 | 0.48 |
| 3:F:48:PRO:O | 3:F:64:LYS:HE3 | 2.12 | 0.48 |
| 3:F:301:THR:CG2 | 3:F:304:ALA:H | 2.24 | 0.48 |
| 3:G:247:PHE:HE1 | 3:G:313:LEU:HD13 | 1.78 | 0.48 |
| 3:H:109:ARG:HB3 | 3:H:338:ARG:CZ | 2.43 | 0.48 |
| 2:B:55:GLU:O | 2:B:58:VAL:HB | 2.13 | 0.48 |
| 3:C:258:ARG:HG2 | 3:C:259:HIS:CE1 | 2.48 | 0.48 |
| 3:C:366:HIS:CE1 | 3:C:368:GLU:OE2 | 2.66 | 0.48 |
| 3:D:206:GLY:O | 3:D:208:MET:HG2 | 2.13 | 0.48 |
| 3:E:18:VAL:HG12 | 3:E:20:LYS:H | 1.78 | 0.48 |
| 3:E:256:PHE:HE2 | 3:E:298:SER:HB2 | 1.79 | 0.48 |
| 3:G:53:LYS:HA | 3:G:61:LEU:N | 2.28 | 0.48 |
| 3:H:48:PRO:O | 3:H:64:LYS:HE3 | 2.14 | 0.48 |
| 3:H:335:ASP:OD1 | 3:H:337:THR:HG23 | 2.13 | 0.48 |
| 1:A:18:LEU:HB3 | 1:A:82:MET:HB2 | 1.95 | 0.48 |
| 2:B:19:VAL:HB | 2:B:104:LEU:CD2 | 2.43 | 0.48 |
| 2:B:36:TYR:HA | 2:B:46:LEU:HA | 1.95 | 0.48 |
| 2:B:38:GLN:CG | 2:B:44:PRO:HG3 | 2.43 | 0.48 |
| 3:D:39:THR:OG1 | 3:D:41:ARG:N | 2.46 | 0.48 |
| 3:D:106:GLU:O | 3:D:372:LEU:HA | 2.12 | 0.48 |
| 3:D:159:ILE:HB | 3:D:248:PHE:HB3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:377:GLN:HG2 | 3:D:378:LEU:H | 1.78 | 0.48 |
| 3:D:450:ASN:OD1 | 3:D:452:LYS:N | 2.38 | 0.48 |
| 3:D:459:LEU:C | 3:D:462:PHE:H | 2.16 | 0.48 |
| 3:E:161:CYS:SG | 3:E:244:ASP:HB3 | 2.54 | 0.48 |
| 3:G:167:GLU:OE2 | 3:G:233:ASP:HB2 | 2.13 | 0.48 |
| 1:A:23:GLU:HA | 1:A:77:ILE:HA | 1.94 | 0.48 |
| 1:A:63:VAL:O | 1:A:66:ARG:N | 2.38 | 0.48 |
| 1:A:82(B):SER:OG | 3:C:180:VAL:N | 2.47 | 0.48 |
| 3:C:421:VAL:HA | 3:C:424:GLN:HE21 | 1.78 | 0.48 |
| 3:C:432:THR:OG1 | 3:C:433:PRO:HD3 | 2.13 | 0.48 |
| 3:D:31:THR:HG21 | 3:D:378:LEU:HB3 | 1.95 | 0.48 |
| 3:D:389:THR:O | 3:D:390:TYR:C | 2.51 | 0.48 |
| 3:E:301:THR:CG2 | 3:E:304:ALA:H | 2.26 | 0.48 |
| 3:G:51:PRO:CA | 3:G:64:LYS:HB2 | 2.43 | 0.48 |
| 3:D:29:ALA:HB3 | 3:D:380:LYS:O | 2.13 | 0.48 |
| 3:D:53:LYS:HD3 | 3:D:58:ASN:HA | 1.95 | 0.48 |
| 3:D:115:VAL:HA | 3:D:339:SER:OG | 2.14 | 0.48 |
| 3:D:214:GLN:OE1 | 3:H:343:SER:O | 2.32 | 0.48 |
| 3:D:441:LEU:HB3 | 3:D:444:TYR:HD2 | 1.77 | 0.48 |
| 3:E:314:GLN:HG3 | 3:E:315:ARG:N | 2.28 | 0.48 |
| 3:F:90:PHE:CE1 | 3:F:91:TYR:CD2 | 3.00 | 0.48 |
| 3:F:161:CYS:SG | 3:F:244:ASP:HB3 | 2.54 | 0.48 |
| 3:G:161:CYS:SG | 3:G:244:ASP:HB3 | 2.53 | 0.48 |
| 2:B:32:TYR:CD2 | 2:B:92:TYR:HB2 | 2.38 | 0.48 |
| 3:C:348:ILE:HG22 | 3:C:359:ASN:HA | 1.96 | 0.48 |
| 3:D:276:TYR:HE1 | 3:D:278:LYS:NZ | 2.12 | 0.48 |
| 3:D:348:ILE:HG22 | 3:D:359:ASN:OD1 | 2.14 | 0.48 |
| 3:E:70:TYR:HD2 | 3:E:199:ASP:HB2 | 1.79 | 0.48 |
| 3:E:120:HIS:HD2 | 3:E:222:LEU:HD12 | 1.79 | 0.48 |
| 3:E:418:TYR:HB3 | 3:E:420:PHE:CZ | 2.48 | 0.48 |
| 3:G:349:SER:O | 3:G:359:ASN:ND2 | 2.45 | 0.48 |
| 3:H:120:HIS:ND1 | 3:H:122:LEU:N | 2.59 | 0.48 |
| 3:H:120:HIS:CE1 | 3:H:122:LEU:O | 2.67 | 0.48 |
| 3:H:216:ASN:OD1 | 3:H:218:SER:HB2 | 2.13 | 0.48 |
| 3:C:135:TYR:CD2 | 3:C:282:SER:HB2 | 2.49 | 0.48 |
| 3:D:42:LEU:HD12 | 3:D:370:TYR:HB2 | 1.96 | 0.48 |
| 3:D:50:PHE:CE1 | 3:E:272:PRO:HD3 | 2.49 | 0.48 |
| 3:D:75:ILE:HG22 | 3:D:77:LEU:HG | 1.95 | 0.48 |
| 3:D:153:GLN:NE2 | 3:D:300:VAL:HG12 | 2.29 | 0.48 |
| 3:D:156:LEU:HD13 | 3:D:158:LEU:HD21 | 1.96 | 0.48 |
| 3:D:314:GLN:O | 3:D:321:ASN:ND2 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:416:ASP:HB3 | 3:D:418:TYR:CD2 | 2.49 | 0.48 |
| 3:G:122:LEU:HB3 | 3:G:144:ARG:HD2 | 1.96 | 0.48 |
| 3:G:244:ASP:OD1 | 3:G:320:ASN:HB2 | 2.14 | 0.48 |
| 3:D:166:GLY:O | 3:D:193:THR:N | 2.33 | 0.48 |
| 3:D:371:ASP:CG | 3:D:372:LEU:H | 2.17 | 0.48 |
| 3:F:384:THR:H | 3:F:387:VAL:HB | 1.79 | 0.48 |
| 3:G:450:ASN:HD21 | 3:G:452:LYS:HD2 | 1.79 | 0.48 |
| 3:H:35:TYR:HD2 | 3:H:100:TRP:HH2 | 1.60 | 0.48 |
| 3:H:383:LEU:HA | 3:H:387:VAL:HG11 | 1.96 | 0.48 |
| 2:B:13:VAL:HG13 | 2:B:104:LEU:HD11 | 1.96 | 0.48 |
| 3:C:467:LYS:HA | 3:C:470:LEU:HB3 | 1.96 | 0.48 |
| 3:D:259:HIS:C | 3:D:260:LEU:HD12 | 2.34 | 0.48 |
| 3:E:35:TYR:HD2 | 3:E:100:TRP:HH2 | 1.62 | 0.48 |
| 3:E:216:ASN:O | 3:E:217:LYS:HB3 | 2.13 | 0.48 |
| 3:F:245:SER:OG | 3:F:246:LEU:N | 2.46 | 0.48 |
| 3:F:273:ASP:HA | 3:F:276:TYR:CE2 | 2.48 | 0.48 |
| 3:G:335:ASP:OD1 | 3:G:337:THR:HG23 | 2.13 | 0.48 |
| 3:H:105:VAL:HG13 | 3:H:374:PHE:CE1 | 2.49 | 0.48 |
| 3:H:216:ASN:O | 3:H:217:LYS:HB3 | 2.14 | 0.48 |
| 1:A:38:ARG:HD3 | 1:A:46:GLU:HG2 | 1.95 | 0.47 |
| 3:D:156:LEU:CG | 3:D:334:VAL:HB | 2.44 | 0.47 |
| 3:D:170:GLY:H | 3:D:189:GLU:C | 2.14 | 0.47 |
| 3:D:258:ARG:HG2 | 3:D:259:HIS:CD2 | 2.49 | 0.47 |
| 3:D:260:LEU:HD23 | 3:H:148:SER:OG | 2.14 | 0.47 |
| 3:D:349:SER:OG | 3:D:352:GLU:OE1 | 2.30 | 0.47 |
| 3:D:459:LEU:HD22 | 3:D:466:ARG:H | 1.79 | 0.47 |
| 3:G:61:LEU:HG | 3:G:62:VAL:HG23 | 1.96 | 0.47 |
| 3:G:80:PRO:HD3 | 3:G:100:TRP:CD1 | 2.49 | 0.47 |
| 3:G:120:HIS:ND1 | 3:G:122:LEU:N | 2.58 | 0.47 |
| 3:H:47:HIS:CD2 | 3:H:48:PRO:HD2 | 2.49 | 0.47 |
| 1:A:7:SER:HB3 | 1:A:21:SER:O | 2.14 | 0.47 |
| 3:C:70:TYR:HD2 | 3:C:199:ASP:HB2 | 1.79 | 0.47 |
| 3:D:142:ASP:HA | 3:H:355:TYR:HE2 | 1.78 | 0.47 |
| 3:D:169:TRP:HD1 | 3:D:207:ALA:N | 2.13 | 0.47 |
| 3:D:321:ASN:N | 3:D:323:ILE:HG12 | 2.29 | 0.47 |
| 3:E:52:ILE:HB | 3:E:62:VAL:H | 1.80 | 0.47 |
| 3:E:70:TYR:HE1 | 3:E:201:VAL:HG22 | 1.78 | 0.47 |
| 3:E:210:PHE:O | 3:E:214:GLN:N | 2.34 | 0.47 |
| 3:F:314:GLN:HG3 | 3:F:315:ARG:N | 2.29 | 0.47 |
| 3:D:165:ILE:HA | 3:D:195:ILE:N | 2.28 | 0.47 |
| 3:F:47:HIS:CD2 | 3:F:48:PRO:HD2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:57:ASN:OD1 | 3:F:59:LYS:N | 2.46 | 0.47 |
| 3:F:474:LEU:HD12 | 3:F:474:LEU:O | 2.14 | 0.47 |
| 3:H:406:LEU:HD23 | 3:H:406:LEU:HA | 1.63 | 0.47 |
| 1:A:48:VAL:HG13 | 1:A:67:PHE:CE2 | 2.49 | 0.47 |
| 3:C:167:GLU:OE2 | 3:C:233:ASP:HB2 | 2.15 | 0.47 |
| 3:C:280:SER:O | 3:C:283:THR:OG1 | 2.16 | 0.47 |
| 3:D:220:VAL:HB | 3:D:224:ILE:CG1 | 2.44 | 0.47 |
| 3:D:277:ILE:O | 3:D:278:LYS:HD2 | 2.14 | 0.47 |
| 3:D:288:SER:O | 3:D:291:TYR:CZ | 2.68 | 0.47 |
| 3:G:48:PRO:O | 3:G:64:LYS:HE3 | 2.15 | 0.47 |
| 3:D:72:VAL:HB | 3:D:197:ASP:CB | 2.45 | 0.47 |
| 3:D:216:ASN:ND2 | 3:D:218:SER:HB2 | 2.30 | 0.47 |
| 3:E:36:HIS:HD2 | 3:E:375:ILE:HD13 | 1.79 | 0.47 |
| 3:E:85:PHE:HB3 | 3:E:86:PRO:HD2 | 1.96 | 0.47 |
| 3:F:120:HIS:HE1 | 3:F:122:LEU:HB2 | 1.79 | 0.47 |
| 3:H:115:VAL:HG12 | 3:H:116:GLY:O | 2.14 | 0.47 |
| 3:H:120:HIS:CE1 | 3:H:122:LEU:H | 2.32 | 0.47 |
| 2:B:84:ALA:HB3 | 2:B:86:TYR:CE1 | 2.50 | 0.47 |
| 3:D:121:PRO:HA | 3:D:146:CYS:CB | 2.45 | 0.47 |
| 3:G:306:ILE:HG22 | 3:G:311:TYR:OH | 2.15 | 0.47 |
| 2:B:84:ALA:HB3 | 2:B:86:TYR:CZ | 2.49 | 0.47 |
| 3:C:437:LYS:O | 3:C:438:GLU:HG3 | 2.15 | 0.47 |
| 3:D:115:VAL:H | 3:D:340:THR:HG1 | 1.55 | 0.47 |
| 3:D:117:ILE:HA | 3:D:151:TYR:HE2 | 1.80 | 0.47 |
| 3:D:280:SER:O | 3:D:283:THR:N | 2.48 | 0.47 |
| 3:E:74:ARG:O | 3:E:75:ILE:HD13 | 2.15 | 0.47 |
| 3:E:120:HIS:ND1 | 3:E:122:LEU:N | 2.58 | 0.47 |
| 3:E:209:ASP:O | 3:E:213:LEU:HB2 | 2.15 | 0.47 |
| 3:E:219:GLU:OE1 | 3:E:263:ARG:CZ | 2.63 | 0.47 |
| 3:E:466:ARG:O | 3:E:469:LEU:HB2 | 2.15 | 0.47 |
| 3:F:115:VAL:HG12 | 3:F:116:GLY:O | 2.14 | 0.47 |
| 3:F:196:GLN:NE2 | 3:F:444:TYR:HD1 | 2.13 | 0.47 |
| 3:G:79:ASP:HB3 | 3:G:82:LYS:HG2 | 1.97 | 0.47 |
| 3:H:50:PHE:HA | 3:H:64:LYS:HD2 | 1.95 | 0.47 |
| 3:H:57:ASN:CG | 3:H:59:LYS:H | 2.18 | 0.47 |
| 1:A:38:ARG:HB2 | 1:A:88:ALA:CB | 2.44 | 0.47 |
| 3:C:77:LEU:HD22 | 3:C:455:PHE:HZ | 1.80 | 0.47 |
| 3:C:77:LEU:O | 3:C:327:ASN:HB3 | 2.14 | 0.47 |
| 3:D:116:GLY:H | 3:D:339:SER:CB | 2.24 | 0.47 |
| 3:E:50:PHE:CE2 | 3:F:271:VAL:HG22 | 2.50 | 0.47 |
| 3:E:320:ASN:OD1 | 3:E:323:ILE:N | 2.24 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:34:TYR:HE1 | 3:F:377:GLN:HG3 | 1.80 | 0.47 |
| 3:F:248:PHE:CG | 3:F:249:TYR:N | 2.83 | 0.47 |
| 3:H:90:PHE:HD1 | 3:H:380:LYS:HZ1 | 1.63 | 0.47 |
| 3:H:256:PHE:HE2 | 3:H:298:SER:HB2 | 1.80 | 0.47 |
| 3:C:74:ARG:HB2 | 3:C:446:PHE:CE1 | 2.37 | 0.47 |
| 3:C:210:PHE:CE2 | 3:C:220:VAL:HG11 | 2.49 | 0.47 |
| 3:C:447:TRP:CG | 3:C:448:GLU:N | 2.83 | 0.47 |
| 3:C:474:LEU:HD12 | 3:C:476:ALA:N | 2.30 | 0.47 |
| 3:D:70:TYR:CZ | 3:D:200:MET:O | 2.67 | 0.47 |
| 3:D:109:ARG:HD2 | 3:D:109:ARG:HA | 1.54 | 0.47 |
| 3:D:152:LYS:HE3 | 3:D:203:THR:O | 2.13 | 0.47 |
| 3:D:162:LYS:HD3 | 3:D:162:LYS:HA | 1.42 | 0.47 |
| 3:D:249:TYR:CZ | 3:D:251:ARG:NH1 | 2.83 | 0.47 |
| 3:E:13:LEU:N | 3:E:14:PRO:HA | 2.30 | 0.47 |
| 3:F:258:ARG:HG2 | 3:F:259:HIS:CE1 | 2.50 | 0.47 |
| 3:F:355:TYR:HD2 | 3:G:142:ASP:HB2 | 1.79 | 0.47 |
| 3:G:274:ASP:OD1 | 3:G:275:LEU:HG | 2.14 | 0.47 |
| 3:C:474:LEU:C | 3:C:476:ALA:H | 2.18 | 0.47 |
| 3:D:74:ARG:HD3 | 3:D:448:GLU:OE2 | 2.15 | 0.47 |
| 3:D:79:ASP:OD1 | 3:D:81:ASN:N | 2.46 | 0.47 |
| 3:D:168:HIS:C | 3:D:190:LEU:HD12 | 2.35 | 0.47 |
| 3:D:317:GLN:H | 3:D:317:GLN:CD | 2.16 | 0.47 |
| 3:D:391:ILE:HA | 3:D:394:MET:CB | 2.43 | 0.47 |
| 3:E:111:GLN:O | 3:E:113:LEU:HD12 | 2.14 | 0.47 |
| 3:F:109:ARG:HB3 | 3:F:338:ARG:CZ | 2.44 | 0.47 |
| 3:F:312:TRP:CZ3 | 3:F:468:PHE:HD1 | 2.33 | 0.47 |
| 3:G:52:ILE:HB | 3:G:62:VAL:HB | 1.96 | 0.47 |
| 3:H:47:HIS:CE1 | 3:H:49:TYR:H | 2.33 | 0.47 |
| 3:H:167:GLU:HA | 3:H:191:ILE:O | 2.15 | 0.47 |
| 1:A:38:ARG:HG2 | 1:A:48:VAL:HG23 | 1.97 | 0.46 |
| 2:B:13:VAL:HG22 | 2:B:104:LEU:HD11 | 1.98 | 0.46 |
| 3:C:70:TYR:CE1 | 3:C:201:VAL:HG22 | 2.50 | 0.46 |
| 3:C:85:PHE:HB2 | 3:C:88:THR:CG2 | 2.45 | 0.46 |
| 3:D:92:ASN:OD1 | 3:D:94:ASP:N | 2.36 | 0.46 |
| 3:D:391:ILE:O | 3:D:394:MET:N | 2.47 | 0.46 |
| 3:E:360:PHE:CE2 | 3:F:216:ASN:HA | 2.50 | 0.46 |
| 3:F:74:ARG:O | 3:F:75:ILE:HD13 | 2.16 | 0.46 |
| 3:F:146:CYS:HG | 3:G:291:TYR:HH | 1.61 | 0.46 |
| 3:G:407:GLN:O | 3:G:410:PRO:HD3 | 2.15 | 0.46 |
| 3:H:34:TYR:HE1 | 3:H:377:GLN:HG3 | 1.80 | 0.46 |
| 3:H:109:ARG:HH21 | 3:H:338:ARG:HD2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:TYR:CG | 1:A:103:TRP:N | 2.84 | 0.46 |
| 2:B:35:TRP:HB3 | 2:B:47:LEU:HD12 | 1.98 | 0.46 |
| 2:B:54:ARG:NE | 2:B:60:ASP:HA | 2.30 | 0.46 |
| 3:C:22:VAL:HB | 3:C:26:GLU:HG3 | 1.96 | 0.46 |
| 3:C:30:ARG:HB3 | 3:C:377:GLN:OE1 | 2.15 | 0.46 |
| 3:C:155:GLN:OE1 | 3:C:306:ILE:HG12 | 2.16 | 0.46 |
| 3:D:258:ARG:HB2 | 3:D:296:SER:HB2 | 1.98 | 0.46 |
| 3:D:343:SER:HA | 3:D:363:TYR:O | 2.15 | 0.46 |
| 3:F:65:VAL:HA | 3:F:69:GLN:OE1 | 2.16 | 0.46 |
| 3:H:465:GLY:O | 3:H:468:PHE:HB3 | 2.15 | 0.46 |
| 1:A:72:ASP:CB | 1:A:79:TYR:HE2 | 2.24 | 0.46 |
| 1:A:100(D):SER:C | 2:B:49:TYR:HB2 | 2.36 | 0.46 |
| 2:B:32:TYR:HE2 | 2:B:92:TYR:CD1 | 2.34 | 0.46 |
| 3:D:202:ASP:HB3 | 3:D:229:CYS:HB3 | 1.96 | 0.46 |
| 3:D:385:ALA:O | 3:D:388:MET:N | 2.48 | 0.46 |
| 3:E:384:THR:OG1 | 3:E:387:VAL:HG23 | 2.16 | 0.46 |
| 3:F:15:PRO:HG2 | 3:F:17:PRO:HD3 | 1.97 | 0.46 |
| 3:F:120:HIS:ND1 | 3:F:122:LEU:N | 2.59 | 0.46 |
| 3:F:274:ASP:OD1 | 3:F:275:LEU:HG | 2.14 | 0.46 |
| 3:G:344:LEU:HB2 | 3:H:213:LEU:O | 2.15 | 0.46 |
| 3:H:51:PRO:CD | 3:H:64:LYS:HD2 | 2.43 | 0.46 |
| 2:B:50:TRP:C | 2:B:52:SER:H | 2.18 | 0.46 |
| 3:D:79:ASP:HB3 | 3:D:82:LYS:HZ2 | 1.79 | 0.46 |
| 3:D:98:LEU:C | 3:D:378:LEU:HD21 | 2.35 | 0.46 |
| 3:D:115:VAL:O | 3:D:340:THR:HA | 2.16 | 0.46 |
| 3:D:299:MET:HG3 | 3:E:256:PHE:HD2 | 1.80 | 0.46 |
| 3:D:347:ALA:HA | 3:D:359:ASN:O | 2.16 | 0.46 |
| 3:D:373:GLN:OE1 | 3:D:463:PRO:HD2 | 2.15 | 0.46 |
| 3:D:389:THR:CA | 3:D:392:HIS:HB3 | 2.43 | 0.46 |
| 3:F:222:LEU:O | 3:F:225:CYS:N | 2.32 | 0.46 |
| 3:G:168:HIS:CE1 | 3:G:191:ILE:HB | 2.49 | 0.46 |
| 3:G:280:SER:O | 3:G:283:THR:N | 2.47 | 0.46 |
| 3:H:216:ASN:C | 3:H:218:SER:H | 2.18 | 0.46 |
| 3:H:248:PHE:CG | 3:H:249:TYR:N | 2.83 | 0.46 |
| 1:A:51:ILE:HG12 | 1:A:55:GLY:HA2 | 1.97 | 0.46 |
| 1:A:88:ALA:HB3 | 1:A:90:TYR:CE1 | 2.50 | 0.46 |
| 3:D:46:GLY:C | 3:D:366:HIS:H | 2.14 | 0.46 |
| 3:D:459:LEU:HD22 | 3:D:465:GLY:N | 2.30 | 0.46 |
| 3:D:475:LYS:O | 3:D:477:LYS:N | 2.46 | 0.46 |
| 3:E:105:VAL:HG13 | 3:E:374:PHE:CE1 | 2.51 | 0.46 |
| 3:F:51:PRO:CD | 3:F:64:LYS:HD2 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:120:HIS:CE1 | 3:G:122:LEU:O | 2.68 | 0.46 |
| 3:H:70:TYR:HD2 | 3:H:199:ASP:HB2 | 1.80 | 0.46 |
| 3:H:377:GLN:CG | 3:H:378:LEU:H | 2.29 | 0.46 |
| 1:A:94:ARG:NE | 1:A:102:TYR:HB3 | 2.30 | 0.46 |
| 3:C:17:PRO:HG2 | 3:C:386:ASP:CG | 2.34 | 0.46 |
| 3:C:111:GLN:HB2 | 3:C:338:ARG:CD | 2.31 | 0.46 |
| 3:D:50:PHE:CZ | 3:E:272:PRO:HD3 | 2.51 | 0.46 |
| 3:D:274:ASP:OD1 | 3:D:275:LEU:N | 2.49 | 0.46 |
| 3:E:109:ARG:HB3 | 3:E:338:ARG:CZ | 2.46 | 0.46 |
| 3:E:109:ARG:HH21 | 3:E:338:ARG:HD2 | 1.79 | 0.46 |
| 3:G:70:TYR:CE1 | 3:G:201:VAL:HG22 | 2.51 | 0.46 |
| 3:G:120:HIS:HE1 | 3:G:122:LEU:HB2 | 1.80 | 0.46 |
| 2:B:55:GLU:HB3 | 2:B:58:VAL:CG2 | 2.46 | 0.46 |
| 3:C:274:ASP:OD1 | 3:C:275:LEU:N | 2.49 | 0.46 |
| 3:D:236:LYS:O | 3:D:239:SER:N | 2.49 | 0.46 |
| 3:D:242:TYR:N | 3:D:242:TYR:CD2 | 2.84 | 0.46 |
| 3:E:355:TYR:HD2 | 3:F:142:ASP:HB2 | 1.81 | 0.46 |
| 3:H:377:GLN:HG2 | 3:H:378:LEU:N | 2.31 | 0.46 |
| 3:H:417:THR:HG1 | 3:H:418:TYR:HD2 | 1.63 | 0.46 |
| 3:C:16:VAL:HG13 | 3:C:17:PRO:HD3 | 1.97 | 0.46 |
| 3:D:309:LYS:HB3 | 3:D:309:LYS:HE2 | 1.40 | 0.46 |
| 3:G:167:GLU:HA | 3:G:191:ILE:O | 2.15 | 0.46 |
| 3:H:196:GLN:HE21 | 3:H:444:TYR:HD1 | 1.64 | 0.46 |
| 1:A:60:PRO:HD2 | 1:A:63:VAL:CG2 | 2.44 | 0.46 |
| 3:C:16:VAL:N | 3:C:17:PRO:HD2 | 2.31 | 0.46 |
| 3:C:85:PHE:HB2 | 3:C:88:THR:HG23 | 1.98 | 0.46 |
| 3:C:384:THR:H | 3:C:387:VAL:CG2 | 2.29 | 0.46 |
| 3:D:156:LEU:HD11 | 3:D:334:VAL:HG23 | 1.98 | 0.46 |
| 3:D:166:GLY:HA3 | 3:D:230:LYS:CE | 2.46 | 0.46 |
| 3:D:181:ASN:HB2 | 3:D:184:ASP:OD1 | 2.16 | 0.46 |
| 3:D:277:ILE:CG2 | 3:G:355:TYR:HB2 | 2.46 | 0.46 |
| 3:D:338:ARG:O | 3:D:340:THR:N | 2.49 | 0.46 |
| 3:D:474:LEU:HA | 3:D:475:LYS:HZ3 | 1.80 | 0.46 |
| 3:E:23:SER:O | 3:E:26:GLU:HG2 | 2.16 | 0.46 |
| 3:F:77:LEU:O | 3:F:327:ASN:HB3 | 2.16 | 0.46 |
| 3:F:451:LEU:O | 3:F:453:GLU:N | 2.49 | 0.46 |
| 3:G:109:ARG:NH1 | 3:G:370:TYR:CE1 | 2.84 | 0.46 |
| 3:G:222:LEU:O | 3:G:225:CYS:N | 2.39 | 0.46 |
| 3:G:263:ARG:HB2 | 3:G:290:ASN:HD22 | 1.80 | 0.46 |
| 3:G:355:TYR:HD2 | 3:H:142:ASP:HB2 | 1.80 | 0.46 |
| 3:G:407:GLN:N | 3:G:408:PRO:HD3 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:79:ASP:CB | 3:D:82:LYS:HG2 | 2.43 | 0.46 |
| 3:D:97:ARG:HG3 | 3:D:402:TRP:CZ3 | 2.51 | 0.46 |
| 3:D:300:VAL:HG22 | 3:E:255:MET:N | 2.29 | 0.46 |
| 3:E:112:PRO:HB3 | 3:F:231:TYR:CD1 | 2.51 | 0.46 |
| 3:E:366:HIS:CE1 | 3:E:368:GLU:OE2 | 2.69 | 0.46 |
| 3:F:167:GLU:HA | 3:F:191:ILE:O | 2.16 | 0.46 |
| 3:F:450:ASN:HD21 | 3:F:452:LYS:CD | 2.29 | 0.46 |
| 3:G:50:PHE:HA | 3:G:64:LYS:HD2 | 1.98 | 0.46 |
| 3:G:424:GLN:OE1 | 3:G:427:ALA:HB3 | 2.14 | 0.46 |
| 3:H:15:PRO:HB3 | 3:H:16:VAL:HA | 1.97 | 0.46 |
| 3:H:156:LEU:HD12 | 3:H:333:VAL:HA | 1.98 | 0.46 |
| 3:D:70:TYR:N | 3:D:199:ASP:H | 2.14 | 0.45 |
| 3:D:274:ASP:O | 3:H:217:LYS:NZ | 2.38 | 0.45 |
| 3:E:324:CYS:SG | 3:E:329:LEU:HD12 | 2.57 | 0.45 |
| 3:F:216:ASN:O | 3:F:217:LYS:HB3 | 2.16 | 0.45 |
| 3:G:312:TRP:CH2 | 3:G:468:PHE:CD1 | 2.97 | 0.45 |
| 3:H:211:THR:OG1 | 3:H:226:THR:O | 2.34 | 0.45 |
| 3:H:312:TRP:CE2 | 3:H:471:GLN:OE1 | 2.69 | 0.45 |
| 3:D:85:PHE:H | 3:D:88:THR:CG2 | 2.27 | 0.45 |
| 3:D:307:PHE:CZ | 3:D:335:ASP:HB2 | 2.50 | 0.45 |
| 3:D:459:LEU:CB | 3:D:466:ARG:HB3 | 2.43 | 0.45 |
| 3:E:404:PHE:HB2 | 3:E:405:GLY:HA3 | 1.96 | 0.45 |
| 3:F:384:THR:O | 3:F:388:MET:HG3 | 2.16 | 0.45 |
| 3:G:216:ASN:O | 3:G:217:LYS:HB3 | 2.17 | 0.45 |
| 3:G:335:ASP:OD1 | 3:G:337:THR:N | 2.46 | 0.45 |
| 3:H:209:ASP:O | 3:H:213:LEU:HB2 | 2.16 | 0.45 |
| 3:H:209:ASP:OD2 | 3:H:212:THR:HG23 | 2.16 | 0.45 |
| 3:C:47:HIS:O | 3:C:65:VAL:N | 2.44 | 0.45 |
| 3:D:38:GLY:CA | 3:D:373:GLN:HG2 | 2.35 | 0.45 |
| 3:D:65:VAL:HA | 3:D:69:GLN:NE2 | 2.30 | 0.45 |
| 3:D:70:TYR:O | 3:D:198:GLY:N | 2.23 | 0.45 |
| 3:D:189:GLU:OE2 | 3:D:191:ILE:HG12 | 2.16 | 0.45 |
| 3:D:463:PRO:HA | 3:D:466:ARG:NH1 | 2.31 | 0.45 |
| 3:F:24:THR:HG21 | 3:F:320:ASN:HA | 1.97 | 0.45 |
| 3:F:208:MET:O | 3:F:228:ILE:HG23 | 2.16 | 0.45 |
| 3:F:426:ILE:CG2 | 3:F:427:ALA:N | 2.73 | 0.45 |
| 3:F:477:LYS:HZ2 | 3:G:23:SER:CB | 2.28 | 0.45 |
| 3:G:209:ASP:O | 3:G:213:LEU:HB2 | 2.15 | 0.45 |
| 1:A:94:ARG:HH21 | 1:A:101:ASP:CG | 2.20 | 0.45 |
| 3:C:97:ARG:HH12 | 3:C:403:ASN:H | 1.63 | 0.45 |
| 3:F:312:TRP:CE2 | 3:F:471:GLN:OE1 | 2.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:417:THR:O | 3:F:418:TYR:CD1 | 2.70 | 0.45 |
| 3:G:47:HIS:CE1 | 3:G:49:TYR:HB2 | 2.52 | 0.45 |
| 3:H:72:VAL:O | 3:H:447:TRP:HB3 | 2.16 | 0.45 |
| 3:H:384:THR:H | 3:H:387:VAL:CG2 | 2.30 | 0.45 |
| 2:B:35:TRP:O | 2:B:46:LEU:HA | 2.16 | 0.45 |
| 3:C:74:ARG:O | 3:C:75:ILE:HD13 | 2.17 | 0.45 |
| 3:C:90:PHE:CD1 | 3:C:91:TYR:HD2 | 2.34 | 0.45 |
| 3:C:374:PHE:HB3 | 3:C:376:PHE:CE2 | 2.51 | 0.45 |
| 3:C:421:VAL:HG12 | 3:C:422:THR:HA | 1.99 | 0.45 |
| 3:H:123:LEU:HD12 | 3:H:218:SER:O | 2.16 | 0.45 |
| 3:H:384:THR:H | 3:H:387:VAL:CB | 2.30 | 0.45 |
| 1:A:100(A):ASP:O | 2:B:30(F):LYS:HG2 | 2.16 | 0.45 |
| 3:C:325:TRP:CE3 | 3:C:398:ILE:HD13 | 2.51 | 0.45 |
| 3:D:125:LYS:HA | 3:D:263:ARG:HA | 1.98 | 0.45 |
| 3:D:168:HIS:O | 3:D:190:LEU:HD12 | 2.16 | 0.45 |
| 3:E:157:CYS:SG | 3:E:158:LEU:N | 2.89 | 0.45 |
| 3:E:404:PHE:CB | 3:E:405:GLY:CA | 2.94 | 0.45 |
| 3:F:97:ARG:HH12 | 3:F:404:PHE:HD2 | 1.63 | 0.45 |
| 3:F:312:TRP:HH2 | 3:F:468:PHE:CD1 | 2.30 | 0.45 |
| 3:C:431:HIS:CE1 | 3:C:434:PRO:HA | 2.52 | 0.45 |
| 3:C:474:LEU:O | 3:C:476:ALA:O | 2.35 | 0.45 |
| 3:D:71:ARG:HD3 | 3:D:71:ARG:HA | 1.57 | 0.45 |
| 3:F:81:ASN:HD21 | 3:F:98:LEU:N | 2.14 | 0.45 |
| 3:F:408:PRO:N | 3:F:409:PRO:HD2 | 2.32 | 0.45 |
| 3:H:216:ASN:HB3 | 3:H:219:GLU:HG2 | 1.99 | 0.45 |
| 3:H:273:ASP:HA | 3:H:276:TYR:CE2 | 2.52 | 0.45 |
| 3:H:403:ASN:O | 3:H:404:PHE:HB2 | 2.17 | 0.45 |
| 3:D:153:GLN:OE1 | 3:D:254:GLN:OE1 | 2.35 | 0.45 |
| 3:D:164:PRO:HB2 | 3:D:195:ILE:HB | 1.99 | 0.45 |
| 3:D:188:LEU:HD12 | 3:D:188:LEU:N | 2.32 | 0.45 |
| 3:D:395:ASN:OD1 | 3:D:397:THR:HG23 | 2.17 | 0.45 |
| 3:E:109:ARG:HD2 | 3:E:369:GLU:O | 2.17 | 0.45 |
| 3:G:81:ASN:HD21 | 3:G:98:LEU:N | 2.09 | 0.45 |
| 3:G:209:ASP:OD2 | 3:G:212:THR:HG23 | 2.17 | 0.45 |
| 3:H:312:TRP:CZ3 | 3:H:468:PHE:HD1 | 2.32 | 0.45 |
| 3:C:276:TYR:HD1 | 3:C:277:ILE:O | 2.00 | 0.45 |
| 3:D:30:ARG:HD3 | 3:D:379:CYS:SG | 2.57 | 0.45 |
| 3:D:156:LEU:CD2 | 3:D:334:VAL:HB | 2.47 | 0.45 |
| 3:D:201:VAL:HG12 | 3:D:202:ASP:O | 2.17 | 0.45 |
| 3:D:248:PHE:CD2 | 3:D:249:TYR:N | 2.84 | 0.45 |
| 3:D:325:TRP:O | 3:D:328:GLN:HB3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:70:TYR:CE1 | 3:E:201:VAL:HG22 | 2.52 | 0.45 |
| 3:E:236:LYS:O | 3:E:239:SER:HB2 | 2.17 | 0.45 |
| 3:E:275:LEU:HD23 | 3:E:275:LEU:HA | 1.72 | 0.45 |
| 3:E:312:TRP:CE2 | 3:E:471:GLN:OE1 | 2.70 | 0.45 |
| 3:F:216:ASN:HB3 | 3:F:219:GLU:HG2 | 1.98 | 0.45 |
| 3:F:465:GLY:O | 3:F:468:PHE:N | 2.49 | 0.45 |
| 3:C:49:TYR:HB3 | 3:C:222:LEU:HD23 | 1.97 | 0.45 |
| 3:C:465:GLY:O | 3:C:468:PHE:HB3 | 2.17 | 0.45 |
| 3:D:24:THR:CG2 | 3:D:323:ILE:HG13 | 2.34 | 0.45 |
| 3:D:51:PRO:HB3 | 3:D:64:LYS:H | 1.82 | 0.45 |
| 3:D:124:ASN:HB3 | 3:D:263:ARG:NH1 | 2.32 | 0.45 |
| 3:D:291:TYR:OH | 3:H:121:PRO:HG3 | 2.17 | 0.45 |
| 3:D:369:GLU:O | 3:D:370:TYR:CG | 2.70 | 0.45 |
| 3:F:223:ASP:OD1 | 3:F:224:ILE:HG23 | 2.17 | 0.45 |
| 3:F:306:ILE:HG22 | 3:F:311:TYR:OH | 2.17 | 0.45 |
| 3:G:417:THR:HB | 3:G:419:ARG:NE | 2.15 | 0.45 |
| 3:H:280:SER:N | 3:H:283:THR:OG1 | 2.34 | 0.45 |
| 3:C:51:PRO:CD | 3:C:64:LYS:HB2 | 2.47 | 0.44 |
| 3:D:128:ASP:OD2 | 3:D:131:ASN:N | 2.32 | 0.44 |
| 3:D:205:PHE:O | 3:D:210:PHE:HZ | 2.00 | 0.44 |
| 3:D:235:ILE:HA | 3:D:238:VAL:HB | 1.99 | 0.44 |
| 3:D:240:GLU:HB3 | 3:D:243:GLY:HA2 | 1.99 | 0.44 |
| 3:D:257:VAL:HG13 | 3:D:294:THR:O | 2.17 | 0.44 |
| 3:D:310:PRO:HD3 | 3:D:467:LYS:NZ | 2.32 | 0.44 |
| 3:D:371:ASP:O | 3:D:372:LEU:HD23 | 2.16 | 0.44 |
| 3:D:468:PHE:O | 3:D:469:LEU:C | 2.52 | 0.44 |
| 3:E:34:TYR:HE1 | 3:E:377:GLN:CG | 2.29 | 0.44 |
| 3:E:125:LYS:HE2 | 3:E:261:PHE:CD1 | 2.51 | 0.44 |
| 3:F:61:LEU:HG | 3:F:62:VAL:HG23 | 1.98 | 0.44 |
| 3:H:90:PHE:CE1 | 3:H:91:TYR:CD2 | 3.05 | 0.44 |
| 3:H:420:PHE:HB3 | 3:H:430:LYS:CE | 2.47 | 0.44 |
| 2:B:19:VAL:HG22 | 2:B:75:ILE:HD12 | 1.97 | 0.44 |
| 2:B:89:GLN:OE1 | 2:B:96:LEU:HB3 | 2.17 | 0.44 |
| 3:D:42:LEU:HB2 | 3:D:370:TYR:H | 1.81 | 0.44 |
| 3:D:78:PRO:HD2 | 3:D:455:PHE:CZ | 2.53 | 0.44 |
| 3:E:208:MET:O | 3:E:228:ILE:HG23 | 2.17 | 0.44 |
| 3:E:248:PHE:CG | 3:E:249:TYR:N | 2.85 | 0.44 |
| 3:F:120:HIS:HD2 | 3:F:222:LEU:HD12 | 1.79 | 0.44 |
| 3:F:159:ILE:HG22 | 3:F:247:PHE:CZ | 2.52 | 0.44 |
| 3:G:47:HIS:CE1 | 3:G:49:TYR:H | 2.35 | 0.44 |
| 3:G:74:ARG:O | 3:G:75:ILE:HD13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:36:TRP:CE2 | 1:A:78:LEU:HG | 2.53 | 0.44 |
| 2:B:2:ILE:HG23 | 2:B:26:SER:H | 1.81 | 0.44 |
| 3:C:233:ASP:N | 3:C:237:MET:HE2 | 2.32 | 0.44 |
| 3:C:411:GLY:O | 3:C:413:THR:HG23 | 2.17 | 0.44 |
| 3:D:261:PHE:HD2 | 3:D:294:THR:OG1 | 1.99 | 0.44 |
| 3:D:378:LEU:HG | 3:D:379:CYS:H | 1.82 | 0.44 |
| 3:G:248:PHE:CG | 3:G:249:TYR:N | 2.85 | 0.44 |
| 3:G:404:PHE:CD2 | 3:G:409:PRO:HD2 | 2.53 | 0.44 |
| 3:H:335:ASP:OD2 | 3:H:338:ARG:NH1 | 2.50 | 0.44 |
| 3:C:24:THR:HG21 | 3:C:320:ASN:HA | 1.98 | 0.44 |
| 3:C:361:LYS:HB3 | 3:C:363:TYR:CZ | 2.52 | 0.44 |
| 3:C:430:LYS:NZ | 3:D:189:GLU:HG3 | 2.32 | 0.44 |
| 3:D:74:ARG:HH11 | 3:D:446:PHE:HE1 | 1.64 | 0.44 |
| 3:D:125:LYS:HG3 | 3:D:262:ASN:O | 2.17 | 0.44 |
| 3:E:35:TYR:HD2 | 3:E:100:TRP:CH2 | 2.36 | 0.44 |
| 3:E:465:GLY:O | 3:E:468:PHE:HB3 | 2.16 | 0.44 |
| 3:F:18:VAL:CG1 | 3:F:19:SER:H | 2.30 | 0.44 |
| 3:F:30:ARG:HD2 | 3:F:377:GLN:OE1 | 2.18 | 0.44 |
| 3:G:404:PHE:HD2 | 3:G:409:PRO:HD2 | 1.83 | 0.44 |
| 3:H:109:ARG:NH1 | 3:H:370:TYR:CE1 | 2.86 | 0.44 |
| 1:A:38:ARG:CZ | 1:A:86:ASP:HA | 2.47 | 0.44 |
| 1:A:41:PRO:C | 1:A:43:LYS:H | 2.21 | 0.44 |
| 3:C:12:TYR:CD2 | 3:C:13:LEU:HG | 2.53 | 0.44 |
| 3:C:114:GLY:N | 3:C:337:THR:O | 2.47 | 0.44 |
| 3:C:203:THR:HG21 | 3:C:224:ILE:HD13 | 1.98 | 0.44 |
| 3:D:276:TYR:HE1 | 3:D:278:LYS:HZ2 | 1.64 | 0.44 |
| 3:F:70:TYR:CE1 | 3:F:201:VAL:HG22 | 2.53 | 0.44 |
| 3:F:97:ARG:HH22 | 3:F:404:PHE:N | 2.16 | 0.44 |
| 3:G:47:HIS:CD2 | 3:G:48:PRO:HD2 | 2.53 | 0.44 |
| 3:G:109:ARG:HB3 | 3:G:338:ARG:CZ | 2.47 | 0.44 |
| 3:G:123:LEU:N | 3:G:144:ARG:HB3 | 2.33 | 0.44 |
| 3:G:223:ASP:OD1 | 3:G:224:ILE:HG23 | 2.18 | 0.44 |
| 3:H:111:GLN:O | 3:H:113:LEU:HD12 | 2.18 | 0.44 |
| 3:C:40:SER:HG | 3:H:420:PHE:HD2 | 1.64 | 0.44 |
| 3:C:469:LEU:HD21 | 3:C:477:LYS:NZ | 2.32 | 0.44 |
| 3:D:74:ARG:HD3 | 3:D:448:GLU:CD | 2.38 | 0.44 |
| 3:D:162:LYS:HB2 | 3:D:245:SER:N | 2.33 | 0.44 |
| 3:D:287:ALA:HB1 | 3:H:146:CYS:CB | 2.39 | 0.44 |
| 3:E:423:SER:O | 3:E:424:GLN:HB2 | 2.18 | 0.44 |
| 3:F:44:ALA:HB3 | 3:F:368:GLU:HB2 | 1.99 | 0.44 |
| 3:G:78:PRO:HD3 | 3:G:452:LYS:HA | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:G:312:TRP:HH2 | 3:G:468:PHE:CD1 | 2.31 | 0.44 |
| 3:G:372:LEU:HA | 3:G:372:LEU:HD23 | 1.75 | 0.44 |
| 3:C:399:LEU:HB3 | 3:C:404:PHE:CD1 | 2.53 | 0.44 |
| 3:D:91:TYR:CD2 | 3:D:91:TYR:N | 2.85 | 0.44 |
| 3:G:43:LEU:HD12 | 3:G:368:GLU:O | 2.17 | 0.44 |
| 3:G:52:ILE:HB | 3:G:62:VAL:N | 2.32 | 0.44 |
| 3:G:77:LEU:HA | 3:G:77:LEU:HD23 | 1.77 | 0.44 |
| 3:G:245:SER:OG | 3:G:246:LEU:N | 2.49 | 0.44 |
| 3:H:377:GLN:HG2 | 3:H:378:LEU:H | 1.83 | 0.44 |
| 1:A:100(E):ASP:HA | 2:B:46:LEU:HD21 | 1.99 | 0.44 |
| 3:D:123:LEU:CD1 | 3:D:263:ARG:HH12 | 2.29 | 0.44 |
| 3:D:189:GLU:CD | 3:D:191:ILE:HG12 | 2.37 | 0.44 |
| 3:D:342:MET:O | 3:D:364:LEU:HD23 | 2.17 | 0.44 |
| 3:D:391:ILE:O | 3:D:392:HIS:C | 2.56 | 0.44 |
| 3:E:115:VAL:HG12 | 3:E:116:GLY:O | 2.18 | 0.44 |
| 3:E:120:HIS:CE1 | 3:E:122:LEU:O | 2.70 | 0.44 |
| 3:H:219:GLU:OE1 | 3:H:263:ARG:CZ | 2.65 | 0.44 |
| 3:C:84:GLY:HA2 | 3:H:84:GLY:CA | 2.47 | 0.44 |
| 3:C:439:ASP:OD1 | 3:C:440:PRO:HD2 | 2.18 | 0.44 |
| 3:D:92:ASN:ND2 | 3:D:95:THR:HG23 | 2.33 | 0.44 |
| 3:D:109:ARG:N | 3:D:308:ASN:OD1 | 2.50 | 0.44 |
| 3:D:168:HIS:CE1 | 3:D:191:ILE:HB | 2.52 | 0.44 |
| 3:D:170:GLY:CA | 3:D:189:GLU:HB3 | 2.47 | 0.44 |
| 3:D:208:MET:N | 3:D:228:ILE:HG23 | 2.33 | 0.44 |
| 3:E:80:PRO:HD3 | 3:E:100:TRP:CD1 | 2.52 | 0.44 |
| 3:F:50:PHE:HA | 3:F:64:LYS:HD2 | 1.99 | 0.44 |
| 3:F:344:LEU:HB2 | 3:G:213:LEU:O | 2.18 | 0.44 |
| 3:G:196:GLN:HE21 | 3:G:444:TYR:HD1 | 1.66 | 0.44 |
| 1:A:100(C):GLY:O | 2:B:49:TYR:HD1 | 2.01 | 0.43 |
| 3:C:62:VAL:HG13 | 3:H:426:ILE:CD1 | 2.34 | 0.43 |
| 3:C:113:LEU:HD21 | 3:C:305:GLN:NE2 | 2.33 | 0.43 |
| 3:D:124:ASN:OD1 | 3:D:264:ALA:N | 2.31 | 0.43 |
| 3:E:399:LEU:HA | 3:E:399:LEU:HD23 | 1.71 | 0.43 |
| 3:F:111:GLN:OE1 | 3:F:369:GLU:OE1 | 2.36 | 0.43 |
| 3:F:120:HIS:CE1 | 3:F:122:LEU:O | 2.70 | 0.43 |
| 3:G:112:PRO:HB3 | 3:H:231:TYR:CD1 | 2.52 | 0.43 |
| 3:G:341:ASN:OD1 | 3:G:366:HIS:HD2 | 2.01 | 0.43 |
| 1:A:38:ARG:HD3 | 1:A:46:GLU:CG | 2.49 | 0.43 |
| 3:D:47:HIS:HD2 | 3:D:364:LEU:O | 2.00 | 0.43 |
| 3:D:97:ARG:NH2 | 3:D:403:ASN:H | 2.16 | 0.43 |
| 3:D:252:ARG:HD3 | 3:D:252:ARG:HA | 1.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:321:ASN:H | 3:D:323:ILE:HG12 | 1.83 | 0.43 |
| 3:D:321:ASN:C | 3:D:323:ILE:HG12 | 2.38 | 0.43 |
| 3:D:344:LEU:CD2 | 3:D:363:TYR:HB2 | 2.49 | 0.43 |
| 3:E:158:LEU:C | 3:E:159:ILE:HG13 | 2.38 | 0.43 |
| 3:F:23:SER:O | 3:F:26:GLU:HG2 | 2.18 | 0.43 |
| 3:G:54:LYS:HD2 | 3:G:57:ASN:HB2 | 2.00 | 0.43 |
| 3:G:189:GLU:HG2 | 3:G:191:ILE:HG13 | 1.99 | 0.43 |
| 3:G:209:ASP:OD1 | 3:G:211:THR:N | 2.52 | 0.43 |
| 3:G:377:GLN:HG2 | 3:G:378:LEU:N | 2.33 | 0.43 |
| 3:H:366:HIS:CE1 | 3:H:368:GLU:OE2 | 2.71 | 0.43 |
| 1:A:40:THR:HA | 1:A:41:PRO:HD3 | 1.79 | 0.43 |
| 1:A:94:ARG:CZ | 1:A:102:TYR:HB3 | 2.48 | 0.43 |
| 3:F:135:TYR:CG | 3:F:136:ALA:N | 2.86 | 0.43 |
| 3:F:167:GLU:OE2 | 3:F:233:ASP:HB2 | 2.18 | 0.43 |
| 3:F:320:ASN:OD1 | 3:F:323:ILE:N | 2.22 | 0.43 |
| 3:F:407:GLN:HB3 | 3:F:409:PRO:HD2 | 2.01 | 0.43 |
| 3:G:118:SER:O | 3:G:148:SER:HB2 | 2.18 | 0.43 |
| 3:H:208:MET:O | 3:H:228:ILE:HG23 | 2.19 | 0.43 |
| 3:C:144:ARG:NH1 | 3:C:218:SER:OG | 2.51 | 0.43 |
| 3:D:36:HIS:HE1 | 3:D:373:GLN:CB | 2.31 | 0.43 |
| 3:D:39:THR:HG23 | 3:D:372:LEU:H | 1.83 | 0.43 |
| 3:D:277:ILE:HD12 | 3:H:144:ARG:NH1 | 2.33 | 0.43 |
| 3:D:468:PHE:HA | 3:D:471:GLN:OE1 | 2.18 | 0.43 |
| 3:E:123:LEU:HD12 | 3:E:218:SER:O | 2.19 | 0.43 |
| 3:F:109:ARG:NH1 | 3:F:370:TYR:CE1 | 2.86 | 0.43 |
| 3:F:219:GLU:OE1 | 3:F:263:ARG:CZ | 2.63 | 0.43 |
| 3:H:439:ASP:OD1 | 3:H:440:PRO:HD2 | 2.18 | 0.43 |
| 3:D:73:PHE:CD1 | 3:D:447:TRP:CD1 | 3.02 | 0.43 |
| 3:D:462:PHE:O | 3:D:464:LEU:N | 2.51 | 0.43 |
| 3:E:24:THR:HG21 | 3:E:320:ASN:HA | 1.99 | 0.43 |
| 3:E:148:SER:HB3 | 3:F:291:TYR:CE1 | 2.53 | 0.43 |
| 3:E:384:THR:O | 3:E:388:MET:HG3 | 2.19 | 0.43 |
| 3:E:450:ASN:OD1 | 3:E:452:LYS:N | 2.31 | 0.43 |
| 3:F:73:PHE:HZ | 3:F:370:TYR:CD2 | 2.36 | 0.43 |
| 3:F:150:ASP:OD2 | 3:F:297:GLY:N | 2.51 | 0.43 |
| 3:F:154:THR:HG23 | 3:F:253:GLU:HB3 | 1.99 | 0.43 |
| 3:F:275:LEU:HD23 | 3:F:275:LEU:HA | 1.67 | 0.43 |
| 3:H:74:ARG:O | 3:H:75:ILE:HD13 | 2.17 | 0.43 |
| 3:H:120:HIS:HE1 | 3:H:122:LEU:HB2 | 1.82 | 0.43 |
| 2:B:83:LEU:O | 2:B:84:ALA:HB2 | 2.19 | 0.43 |
| 3:C:83:PHE:HD2 | 3:C:85:PHE:CE1 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:113:LEU:N | 3:D:113:LEU:CD1 | 2.82 | 0.43 |
| 3:D:259:HIS:CA | 3:D:294:THR:HB | 2.49 | 0.43 |
| 3:D:275:LEU:C | 3:H:217:LYS:HD3 | 2.39 | 0.43 |
| 3:D:329:LEU:HG | 3:D:330:PHE:H | 1.82 | 0.43 |
| 3:E:65:VAL:HA | 3:E:69:GLN:OE1 | 2.18 | 0.43 |
| 3:G:34:TYR:CE1 | 3:G:377:GLN:HG3 | 2.53 | 0.43 |
| 3:G:399:LEU:HD23 | 3:G:399:LEU:HA | 1.69 | 0.43 |
| 3:G:459:LEU:HD12 | 3:G:477:LYS:HZ3 | 1.83 | 0.43 |
| 1:A:63:VAL:HG12 | 1:A:66:ARG:HH11 | 1.82 | 0.43 |
| 2:B:32:TYR:HE2 | 2:B:92:TYR:HD1 | 1.67 | 0.43 |
| 3:C:248:PHE:CD2 | 3:C:249:TYR:N | 2.87 | 0.43 |
| 3:D:100:TRP:CA | 3:D:378:LEU:HD12 | 2.49 | 0.43 |
| 3:D:150:ASP:C | 3:D:151:TYR:CD1 | 2.92 | 0.43 |
| 3:D:216:ASN:ND2 | 3:D:216:ASN:C | 2.71 | 0.43 |
| 3:D:216:ASN:CG | 3:D:218:SER:H | 2.22 | 0.43 |
| 3:E:384:THR:H | 3:E:387:VAL:CG2 | 2.31 | 0.43 |
| 3:G:92:ASN:OD1 | 3:G:94:ASP:N | 2.41 | 0.43 |
| 3:H:70:TYR:CD1 | 3:H:334:VAL:HG21 | 2.50 | 0.43 |
| 3:H:306:ILE:HG22 | 3:H:311:TYR:OH | 2.19 | 0.43 |
| 2:B:11:LEU:HD13 | 2:B:20:THR:OG1 | 2.19 | 0.43 |
| 3:D:119:GLY:O | 3:D:221:PRO:HA | 2.19 | 0.43 |
| 3:D:250:LEU:HA | 3:D:250:LEU:HD23 | 1.54 | 0.43 |
| 3:D:397:THR:O | 3:D:401:ASP:OD1 | 2.36 | 0.43 |
| 3:D:474:LEU:HD12 | 3:D:474:LEU:O | 2.18 | 0.43 |
| 3:E:116:GLY:HA3 | 3:E:339:SER:O | 2.18 | 0.43 |
| 3:E:209:ASP:OD2 | 3:E:212:THR:HG23 | 2.19 | 0.43 |
| 3:F:80:PRO:HD3 | 3:F:100:TRP:CD1 | 2.53 | 0.43 |
| 3:F:150:ASP:CG | 3:F:297:GLY:H | 2.21 | 0.43 |
| 2:B:21:MET:HB2 | 2:B:102:THR:OG1 | 2.19 | 0.43 |
| 3:C:12:TYR:CE2 | 3:C:13:LEU:HG | 2.54 | 0.43 |
| 3:C:77:LEU:HA | 3:C:77:LEU:HD23 | 1.82 | 0.43 |
| 3:E:46:GLY:CA | 3:E:65:VAL:HB | 2.45 | 0.43 |
| 3:E:52:ILE:HB | 3:E:62:VAL:N | 2.34 | 0.43 |
| 3:E:128:ASP:OD1 | 3:E:129:THR:N | 2.52 | 0.43 |
| 3:E:135:TYR:CG | 3:E:136:ALA:N | 2.87 | 0.43 |
| 3:E:475:LYS:C | 3:E:477:LYS:H | 2.22 | 0.43 |
| 3:F:153:GLN:CD | 3:F:300:VAL:HG12 | 2.39 | 0.43 |
| 3:F:399:LEU:HD23 | 3:F:399:LEU:HA | 1.79 | 0.43 |
| 3:F:433:PRO:HG2 | 3:F:434:PRO:HD3 | 2.01 | 0.43 |
| 3:G:314:GLN:HG3 | 3:G:315:ARG:H | 1.83 | 0.43 |
| 3:G:366:HIS:CE1 | 3:G:368:GLU:OE2 | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:H:12:TYR:C | 3:H:14:PRO:HD2 | 2.39 | 0.43 |
| 3:H:74:ARG:NH2 | 3:H:439:ASP:OD2 | 2.52 | 0.43 |
| 1:A:100(B):GLU:HB2 | 2:B:30(F):LYS:CB | 2.48 | 0.43 |
| 2:B:18:LYS:HA | 2:B:78:VAL:HG23 | 2.01 | 0.43 |
| 3:D:70:TYR:CE2 | 3:D:230:LYS:HB2 | 2.53 | 0.43 |
| 3:D:242:TYR:CZ | 3:D:394:MET:HG3 | 2.53 | 0.43 |
| 3:F:74:ARG:CB | 3:F:446:PHE:HE1 | 2.20 | 0.43 |
| 3:F:108:GLY:HA2 | 3:F:308:ASN:OD1 | 2.19 | 0.43 |
| 3:F:116:GLY:HA3 | 3:F:339:SER:O | 2.19 | 0.43 |
| 3:G:90:PHE:CE1 | 3:G:91:TYR:CD2 | 3.07 | 0.43 |
| 3:D:249:TYR:HE1 | 3:D:251:ARG:CB | 2.31 | 0.42 |
| 3:D:254:GLN:O | 3:D:255:MET:HB2 | 2.19 | 0.42 |
| 3:D:309:LYS:HB2 | 3:D:311:TYR:CZ | 2.54 | 0.42 |
| 3:F:60:ILE:O | 3:F:60:ILE:HG13 | 2.19 | 0.42 |
| 3:G:208:MET:O | 3:G:228:ILE:HG23 | 2.19 | 0.42 |
| 3:H:74:ARG:HB3 | 3:H:448:GLU:OE1 | 2.18 | 0.42 |
| 1:A:100(B):GLU:OE1 | 2:B:30(F):LYS:HB2 | 2.19 | 0.42 |
| 3:C:274:ASP:OD1 | 3:C:275:LEU:HG | 2.18 | 0.42 |
| 3:C:314:GLN:HG3 | 3:C:315:ARG:N | 2.35 | 0.42 |
| 3:C:321:ASN:O | 3:C:323:ILE:HG12 | 2.19 | 0.42 |
| 3:D:126:LEU:HB3 | 3:D:262:ASN:HB2 | 2.01 | 0.42 |
| 3:D:312:TRP:HH2 | 3:D:468:PHE:HB2 | 1.83 | 0.42 |
| 3:D:387:VAL:C | 3:D:389:THR:H | 2.21 | 0.42 |
| 3:F:52:ILE:HB | 3:F:62:VAL:H | 1.84 | 0.42 |
| 3:F:387:VAL:O | 3:F:388:MET:C | 2.57 | 0.42 |
| 3:F:450:ASN:OD1 | 3:F:451:LEU:N | 2.53 | 0.42 |
| 3:F:450:ASN:OD1 | 3:F:452:LYS:N | 2.35 | 0.42 |
| 3:G:68:LEU:HA | 3:G:68:LEU:HD23 | 1.68 | 0.42 |
| 2:B:33:LEU:HD22 | 2:B:71:PHE:CE2 | 2.54 | 0.42 |
| 3:C:34:TYR:HD1 | 3:C:377:GLN:HA | 1.84 | 0.42 |
| 3:C:78:PRO:HD2 | 3:C:455:PHE:CZ | 2.55 | 0.42 |
| 3:C:234:TYR:HA | 3:C:237:MET:HE3 | 2.01 | 0.42 |
| 3:D:42:LEU:HD23 | 3:D:42:LEU:HA | 1.66 | 0.42 |
| 3:D:75:ILE:HG12 | 3:D:329:LEU:O | 2.19 | 0.42 |
| 3:D:450:ASN:OD1 | 3:D:450:ASN:C | 2.56 | 0.42 |
| 3:E:34:TYR:CE1 | 3:E:377:GLN:HG3 | 2.54 | 0.42 |
| 3:E:118:SER:O | 3:E:148:SER:HB2 | 2.18 | 0.42 |
| 3:F:328:GLN:HE21 | 3:F:330:PHE:HE1 | 1.68 | 0.42 |
| 3:G:153:GLN:HE22 | 3:G:300:VAL:HG12 | 1.84 | 0.42 |
| 1:A:38:ARG:NH1 | 1:A:46:GLU:OE2 | 2.53 | 0.42 |
| 3:C:120:HIS:CE1 | 3:C:122:LEU:H | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:130:GLU:HA | 3:C:260:LEU:HD22 | 2.01 | 0.42 |
| 3:C:439:ASP:O | 3:C:441:LEU:N | 2.53 | 0.42 |
| 3:D:159:ILE:HB | 3:D:248:PHE:HD2 | 1.84 | 0.42 |
| 3:D:385:ALA:O | 3:D:386:ASP:C | 2.56 | 0.42 |
| 3:D:459:LEU:HB2 | 3:D:469:LEU:HD11 | 2.00 | 0.42 |
| 3:E:21:VAL:HG13 | 3:E:390:TYR:OH | 2.19 | 0.42 |
| 3:E:109:ARG:NH1 | 3:E:370:TYR:CE1 | 2.88 | 0.42 |
| 3:H:30:ARG:HD2 | 3:H:377:GLN:OE1 | 2.19 | 0.42 |
| 3:D:112:PRO:HB3 | 3:E:231:TYR:CZ | 2.55 | 0.42 |
| 3:D:164:PRO:C | 3:D:195:ILE:HB | 2.40 | 0.42 |
| 3:D:271:VAL:HG12 | 3:D:276:TYR:HE2 | 1.84 | 0.42 |
| 3:D:289:SER:O | 3:D:291:TYR:CD2 | 2.73 | 0.42 |
| 3:D:300:VAL:O | 3:E:254:GLN:HB2 | 2.20 | 0.42 |
| 3:D:344:LEU:HD21 | 3:D:363:TYR:HB2 | 2.01 | 0.42 |
| 3:E:306:ILE:HG22 | 3:E:311:TYR:OH | 2.19 | 0.42 |
| 3:E:450:ASN:OD1 | 3:E:451:LEU:N | 2.52 | 0.42 |
| 3:F:15:PRO:HG2 | 3:F:17:PRO:CD | 2.49 | 0.42 |
| 3:G:35:TYR:HD1 | 3:G:457:ALA:HA | 1.85 | 0.42 |
| 3:G:169:TRP:O | 3:G:208:MET:HA | 2.20 | 0.42 |
| 3:G:451:LEU:O | 3:G:453:GLU:N | 2.52 | 0.42 |
| 2:B:24:LYS:CD | 2:B:70:ASP:HB2 | 2.50 | 0.42 |
| 3:D:107:VAL:HG12 | 3:D:108:GLY:O | 2.19 | 0.42 |
| 3:D:123:LEU:HD12 | 3:D:218:SER:O | 2.20 | 0.42 |
| 3:D:155:GLN:HE22 | 3:D:306:ILE:H | 1.68 | 0.42 |
| 3:D:248:PHE:CZ | 3:D:250:LEU:HG | 2.55 | 0.42 |
| 3:D:323:ILE:HG22 | 3:D:325:TRP:CZ2 | 2.54 | 0.42 |
| 3:D:335:ASP:CG | 3:D:337:THR:H | 2.15 | 0.42 |
| 3:D:391:ILE:HG22 | 3:D:395:ASN:O | 2.20 | 0.42 |
| 3:E:451:LEU:O | 3:E:453:GLU:N | 2.53 | 0.42 |
| 3:F:70:TYR:CD2 | 3:F:199:ASP:HB2 | 2.54 | 0.42 |
| 3:F:121:PRO:HA | 3:F:146:CYS:SG | 2.60 | 0.42 |
| 3:F:158:LEU:C | 3:F:159:ILE:HG13 | 2.40 | 0.42 |
| 3:F:216:ASN:OD1 | 3:F:218:SER:HB2 | 2.19 | 0.42 |
| 3:C:18:VAL:CG1 | 3:C:20:LYS:NZ | 2.82 | 0.42 |
| 3:C:47:HIS:ND1 | 3:C:49:TYR:N | 2.66 | 0.42 |
| 3:C:399:LEU:HA | 3:C:402:TRP:HB2 | 2.02 | 0.42 |
| 3:C:414:LEU:HD23 | 3:C:414:LEU:HA | 1.67 | 0.42 |
| 3:D:53:LYS:CB | 3:D:60:ILE:HA | 2.49 | 0.42 |
| 3:D:71:ARG:HB2 | 3:D:333:VAL:O | 2.19 | 0.42 |
| 3:D:83:PHE:CD2 | 3:D:85:PHE:HD1 | 2.37 | 0.42 |
| 3:D:169:TRP:HA | 3:D:190:LEU:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:169:TRP:HE1 | 3:D:207:ALA:H | 1.68 | 0.42 |
| 3:E:153:GLN:HE22 | 3:E:300:VAL:HG12 | 1.85 | 0.42 |
| 3:E:167:GLU:OE2 | 3:E:233:ASP:HB2 | 2.19 | 0.42 |
| 3:E:246:LEU:HD12 | 3:E:246:LEU:O | 2.20 | 0.42 |
| 3:E:273:ASP:HA | 3:E:276:TYR:CE2 | 2.55 | 0.42 |
| 3:F:85:PHE:HB3 | 3:F:86:PRO:HD2 | 2.02 | 0.42 |
| 3:F:280:SER:O | 3:F:283:THR:N | 2.45 | 0.42 |
| 3:F:474:LEU:O | 3:F:475:LYS:HB2 | 2.20 | 0.42 |
| 3:G:77:LEU:O | 3:G:327:ASN:HB3 | 2.20 | 0.42 |
| 3:G:403:ASN:O | 3:G:404:PHE:HB2 | 2.20 | 0.42 |
| 3:H:273:ASP:O | 3:H:275:LEU:N | 2.53 | 0.42 |
| 2:B:6:GLN:HE21 | 2:B:101:GLY:CA | 2.33 | 0.42 |
| 3:C:77:LEU:HD13 | 3:C:100:TRP:CG | 2.55 | 0.42 |
| 3:C:84:GLY:HA2 | 3:H:84:GLY:N | 2.35 | 0.42 |
| 3:D:432:THR:C | 3:D:434:PRO:HD3 | 2.39 | 0.42 |
| 3:D:468:PHE:HA | 3:D:471:GLN:CB | 2.28 | 0.42 |
| 3:D:475:LYS:HE2 | 3:D:475:LYS:HB2 | 1.81 | 0.42 |
| 3:F:92:ASN:OD1 | 3:F:94:ASP:N | 2.34 | 0.42 |
| 3:G:51:PRO:CD | 3:G:64:LYS:HD2 | 2.48 | 0.42 |
| 3:G:60:ILE:O | 3:G:60:ILE:HG13 | 2.19 | 0.42 |
| 1:A:59:TYR:HB2 | 1:A:64:LYS:CD | 2.43 | 0.42 |
| 3:C:18:VAL:HG13 | 3:C:20:LYS:HZ3 | 1.85 | 0.42 |
| 3:D:120:HIS:CE1 | 3:D:122:LEU:HB2 | 2.55 | 0.42 |
| 3:D:459:LEU:HD12 | 3:D:469:LEU:HG | 2.01 | 0.42 |
| 3:E:49:TYR:C | 3:E:64:LYS:HE3 | 2.40 | 0.42 |
| 3:E:77:LEU:O | 3:E:327:ASN:HB3 | 2.20 | 0.42 |
| 3:E:167:GLU:HA | 3:E:191:ILE:O | 2.19 | 0.42 |
| 3:F:101:ALA:HB3 | 3:F:377:GLN:HB3 | 2.02 | 0.42 |
| 3:H:85:PHE:CE2 | 3:H:378:LEU:HD21 | 2.54 | 0.42 |
| 3:H:153:GLN:C | 3:H:154:THR:HG1 | 2.23 | 0.42 |
| 3:H:414:LEU:HD23 | 3:H:414:LEU:HA | 1.62 | 0.42 |
| 3:C:20:LYS:HB2 | 3:C:21:VAL:H | 1.36 | 0.42 |
| 3:C:157:CYS:SG | 3:C:158:LEU:N | 2.92 | 0.42 |
| 3:C:195:ILE:HA | 3:C:230:LYS:HZ2 | 1.83 | 0.42 |
| 3:C:197:ASP:CB | 3:C:446:PHE:HA | 2.50 | 0.42 |
| 3:D:36:HIS:CE1 | 3:D:373:GLN:CB | 3.03 | 0.42 |
| 3:D:109:ARG:HB3 | 3:D:308:ASN:ND2 | 2.28 | 0.42 |
| 3:D:128:ASP:OD1 | 3:D:130:GLU:N | 2.53 | 0.42 |
| 3:D:158:LEU:HD12 | 3:D:332:THR:HB | 2.02 | 0.42 |
| 3:D:401:ASP:O | 3:D:402:TRP:HD1 | 2.03 | 0.42 |
| 3:D:464:LEU:HD23 | 3:D:465:GLY:HA2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:D:473:GLY:O | 3:D:474:LEU:HG | 2.20 | 0.42 |
| 3:E:68:LEU:HD23 | 3:E:68:LEU:HA | 1.78 | 0.42 |
| 3:E:74:ARG:HB3 | 3:E:448:GLU:OE1 | 2.20 | 0.42 |
| 3:E:126:LEU:CB | 3:E:262:ASN:HB2 | 2.48 | 0.42 |
| 3:E:209:ASP:OD1 | 3:E:211:THR:N | 2.53 | 0.42 |
| 3:E:259:HIS:CE1 | 3:F:130:GLU:OE2 | 2.73 | 0.42 |
| 3:F:101:ALA:N | 3:F:377:GLN:O | 2.49 | 0.42 |
| 3:F:246:LEU:HD12 | 3:F:246:LEU:O | 2.20 | 0.42 |
| 3:C:85:PHE:CZ | 3:C:378:LEU:HD22 | 2.55 | 0.41 |
| 3:E:156:LEU:C | 3:E:156:LEU:HD12 | 2.41 | 0.41 |
| 3:E:168:HIS:CE1 | 3:E:191:ILE:HB | 2.54 | 0.41 |
| 3:G:70:TYR:CD1 | 3:G:334:VAL:HG21 | 2.51 | 0.41 |
| 3:G:261:PHE:O | 3:G:291:TYR:HA | 2.20 | 0.41 |
| 3:H:96:GLN:HG2 | 3:H:382:THR:HA | 2.01 | 0.41 |
| 3:H:223:ASP:OD1 | 3:H:224:ILE:HG23 | 2.20 | 0.41 |
| 3:H:451:LEU:O | 3:H:453:GLU:N | 2.52 | 0.41 |
| 1:A:100(B):GLU:OE1 | 2:B:30(F):LYS:HD3 | 2.20 | 0.41 |
| 2:B:23:CYS:HB3 | 2:B:35:TRP:CH2 | 2.55 | 0.41 |
| 2:B:37:GLN:HA | 2:B:85:VAL:O | 2.20 | 0.41 |
| 3:D:120:HIS:HA | 3:D:121:PRO:HD3 | 1.94 | 0.41 |
| 3:D:202:ASP:HB2 | 3:D:204:GLY:N | 2.23 | 0.41 |
| 3:D:336:THR:O | 3:D:338:ARG:N | 2.53 | 0.41 |
| 3:D:399:LEU:O | 3:D:402:TRP:O | 2.38 | 0.41 |
| 3:E:97:ARG:NH2 | 3:E:403:ASN:C | 2.72 | 0.41 |
| 3:F:94:ASP:HA | 3:F:404:PHE:CE2 | 2.55 | 0.41 |
| 3:G:154:THR:HG23 | 3:G:253:GLU:HB3 | 2.02 | 0.41 |
| 3:G:384:THR:O | 3:G:388:MET:HG3 | 2.20 | 0.41 |
| 3:H:320:ASN:ND2 | 3:H:323:ILE:O | 2.32 | 0.41 |
| 1:A:18:LEU:HD21 | 1:A:90:TYR:HE2 | 1.84 | 0.41 |
| 1:A:39:GLN:HB3 | 1:A:89:MET:H | 1.86 | 0.41 |
| 1:A:96:LEU:HG | 1:A:97:TYR:H | 1.84 | 0.41 |
| 2:B:49:TYR:CZ | 2:B:53:THR:HG22 | 2.54 | 0.41 |
| 3:C:15:PRO:CB | 3:C:17:PRO:HD2 | 2.39 | 0.41 |
| 3:D:141:VAL:CG1 | 3:H:356:LYS:HA | 2.50 | 0.41 |
| 3:D:231:TYR:CE1 | 3:H:112:PRO:HA | 2.55 | 0.41 |
| 3:D:469:LEU:O | 3:D:473:GLY:N | 2.53 | 0.41 |
| 3:D:470:LEU:HD12 | 3:D:470:LEU:HA | 1.62 | 0.41 |
| 3:E:19:SER:O | 3:E:20:LYS:HB2 | 2.21 | 0.41 |
| 3:E:187:PRO:C | 3:E:188:LEU:HD12 | 2.40 | 0.41 |
| 3:E:216:ASN:OD1 | 3:E:218:SER:HB2 | 2.20 | 0.41 |
| 3:E:366:HIS:ND1 | 3:E:368:GLU:OE2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:111:GLN:O | 3:F:113:LEU:HD12 | 2.20 | 0.41 |
| 3:F:216:ASN:C | 3:F:218:SER:H | 2.23 | 0.41 |
| 3:F:360:PHE:O | 3:G:266:ALA:HB3 | 2.20 | 0.41 |
| 3:G:385:ALA:HA | 3:G:388:MET:HE3 | 2.02 | 0.41 |
| 3:H:312:TRP:CH2 | 3:H:468:PHE:CD1 | 2.92 | 0.41 |
| 2:B:6:GLN:HE21 | 2:B:101:GLY:H | 1.68 | 0.41 |
| 2:B:43:SER:HB2 | 2:B:45:LYS:HE3 | 2.03 | 0.41 |
| 3:C:414:LEU:O | 3:C:415:GLU:HB2 | 2.20 | 0.41 |
| 3:C:420:PHE:CD1 | 3:H:41:ARG:NH1 | 2.88 | 0.41 |
| 3:D:51:PRO:N | 3:D:64:LYS:HB2 | 2.35 | 0.41 |
| 3:D:161:CYS:O | 3:D:162:LYS:HD3 | 2.19 | 0.41 |
| 3:E:78:PRO:HD3 | 3:E:452:LYS:HA | 2.01 | 0.41 |
| 3:E:90:PHE:CE1 | 3:E:91:TYR:CD2 | 3.08 | 0.41 |
| 3:E:344:LEU:HB2 | 3:F:213:LEU:O | 2.20 | 0.41 |
| 3:E:387:VAL:O | 3:E:388:MET:C | 2.58 | 0.41 |
| 3:F:97:ARG:HH22 | 3:F:404:PHE:H | 1.69 | 0.41 |
| 3:F:112:PRO:HB3 | 3:G:231:TYR:CD1 | 2.56 | 0.41 |
| 3:G:77:LEU:HD22 | 3:G:455:PHE:HZ | 1.86 | 0.41 |
| 3:G:116:GLY:HA3 | 3:G:339:SER:O | 2.20 | 0.41 |
| 3:H:156:LEU:O | 3:H:333:VAL:HG13 | 2.21 | 0.41 |
| 3:H:256:PHE:CE2 | 3:H:298:SER:HB2 | 2.56 | 0.41 |
| 2:B:11:LEU:HD12 | 2:B:104:LEU:HD13 | 2.02 | 0.41 |
| 3:D:35:TYR:HD1 | 3:D:457:ALA:HA | 1.85 | 0.41 |
| 3:D:53:LYS:HB3 | 3:D:53:LYS:HE2 | 1.72 | 0.41 |
| 3:D:76:HIS:ND1 | 3:D:449:VAL:C | 2.70 | 0.41 |
| 3:D:127:ASP:O | 3:D:261:PHE:HA | 2.20 | 0.41 |
| 3:D:246:LEU:HD13 | 3:D:248:PHE:CA | 2.50 | 0.41 |
| 3:F:16:VAL:N | 3:F:17:PRO:HD3 | 2.36 | 0.41 |
| 3:F:335:ASP:OD1 | 3:F:337:THR:N | 2.48 | 0.41 |
| 3:F:395:ASN:CG | 3:F:397:THR:HG1 | 2.14 | 0.41 |
| 3:H:77:LEU:O | 3:H:327:ASN:HB3 | 2.21 | 0.41 |
| 3:H:154:THR:HG23 | 3:H:253:GLU:HB3 | 2.03 | 0.41 |
| 3:H:156:LEU:HD12 | 3:H:156:LEU:C | 2.40 | 0.41 |
| 3:H:420:PHE:HB3 | 3:H:430:LYS:HE3 | 2.02 | 0.41 |
| 2:B:6:GLN:NE2 | 2:B:101:GLY:CA | 2.83 | 0.41 |
| 3:C:50:PHE:CE1 | 3:C:52:ILE:HD13 | 2.55 | 0.41 |
| 3:C:387:VAL:O | 3:C:388:MET:C | 2.58 | 0.41 |
| 3:D:106:GLU:N | 3:D:374:PHE:HD1 | 2.17 | 0.41 |
| 3:D:123:LEU:HD12 | 3:D:123:LEU:HA | 1.65 | 0.41 |
| 3:D:172:GLY:C | 3:D:187:PRO:HG2 | 2.41 | 0.41 |
| 3:D:253:GLU:HG2 | 3:H:302:SER:OG | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:258:ARG:HB2 | 3:D:295:PRO:O | 2.20 | 0.41 |
| 3:D:387:VAL:C | 3:D:389:THR:N | 2.74 | 0.41 |
| 3:D:416:ASP:O | 3:D:418:TYR:CZ | 2.74 | 0.41 |
| 3:E:60:ILE:O | 3:E:60:ILE:HG13 | 2.21 | 0.41 |
| 3:E:345:CYS:SG | 3:F:216:ASN:N | 2.73 | 0.41 |
| 3:F:51:PRO:N | 3:F:64:LYS:HB2 | 2.36 | 0.41 |
| 3:F:72:VAL:HG12 | 3:F:446:PHE:CD1 | 2.56 | 0.41 |
| 3:H:52:ILE:HB | 3:H:62:VAL:N | 2.36 | 0.41 |
| 3:H:52:ILE:HB | 3:H:62:VAL:H | 1.86 | 0.41 |
| 3:H:73:PHE:HZ | 3:H:370:TYR:CD2 | 2.38 | 0.41 |
| 3:H:135:TYR:CG | 3:H:136:ALA:N | 2.89 | 0.41 |
| 3:H:392:HIS:O | 3:H:396:SER:OG | 2.34 | 0.41 |
| 3:H:406:LEU:O | 3:H:407:GLN:C | 2.59 | 0.41 |
| 2:B:24:LYS:HG3 | 2:B:69:THR:C | 2.41 | 0.41 |
| 3:C:60:ILE:O | 3:C:60:ILE:HG13 | 2.21 | 0.41 |
| 3:C:153:GLN:OE1 | 3:C:337:THR:HG22 | 2.20 | 0.41 |
| 3:D:40:SER:C | 3:D:41:ARG:HG2 | 2.41 | 0.41 |
| 3:D:72:VAL:HG22 | 3:D:332:THR:HG21 | 2.02 | 0.41 |
| 3:D:475:LYS:C | 3:D:477:LYS:H | 2.22 | 0.41 |
| 3:E:48:PRO:O | 3:E:64:LYS:HE3 | 2.21 | 0.41 |
| 3:E:50:PHE:HD1 | 3:E:51:PRO:O | 2.04 | 0.41 |
| 3:E:51:PRO:CD | 3:E:64:LYS:HD2 | 2.47 | 0.41 |
| 3:E:419:ARG:C | 3:E:420:PHE:CD1 | 2.94 | 0.41 |
| 3:F:77:LEU:HA | 3:F:77:LEU:HD23 | 1.83 | 0.41 |
| 3:G:35:TYR:HD2 | 3:G:100:TRP:HH2 | 1.68 | 0.41 |
| 3:G:83:PHE:CZ | 3:H:13:LEU:HB3 | 2.56 | 0.41 |
| 3:G:164:PRO:HG2 | 3:G:195:ILE:HB | 2.01 | 0.41 |
| 3:G:273:ASP:O | 3:G:276:TYR:N | 2.38 | 0.41 |
| 3:G:301:THR:HG23 | 3:G:303:ASP:N | 2.36 | 0.41 |
| 3:G:404:PHE:HE2 | 3:G:409:PRO:CG | 2.34 | 0.41 |
| 3:H:78:PRO:HD3 | 3:H:452:LYS:HA | 2.02 | 0.41 |
| 2:B:88:CYS:SG | 2:B:99:GLY:HA3 | 2.61 | 0.41 |
| 3:C:18:VAL:HG13 | 3:C:20:LYS:NZ | 2.35 | 0.41 |
| 3:C:34:TYR:HE1 | 3:C:377:GLN:CG | 2.34 | 0.41 |
| 3:C:73:PHE:CD1 | 3:C:447:TRP:HD1 | 2.38 | 0.41 |
| 3:C:171:LYS:HB2 | 3:C:213:LEU:CD1 | 2.51 | 0.41 |
| 3:C:335:ASP:OD2 | 3:C:338:ARG:NH1 | 2.53 | 0.41 |
| 3:D:70:TYR:N | 3:D:199:ASP:N | 2.65 | 0.41 |
| 3:D:80:PRO:HD3 | 3:D:100:TRP:CD1 | 2.55 | 0.41 |
| 3:D:103:VAL:N | 3:D:375:ILE:O | 2.53 | 0.41 |
| 3:D:106:GLU:N | 3:D:374:PHE:CD1 | 2.87 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:344:LEU:HD21 | 3:D:363:TYR:CD2 | 2.49 | 0.41 |
| 3:D:382:THR:C | 3:D:383:LEU:HD23 | 2.41 | 0.41 |
| 3:E:223:ASP:OD1 | 3:E:224:ILE:HG23 | 2.20 | 0.41 |
| 3:E:328:GLN:HE21 | 3:E:330:PHE:HE1 | 1.68 | 0.41 |
| 3:F:408:PRO:N | 3:F:409:PRO:CD | 2.84 | 0.41 |
| 3:G:46:GLY:CA | 3:G:65:VAL:HB | 2.44 | 0.41 |
| 3:G:222:LEU:O | 3:G:223:ASP:C | 2.59 | 0.41 |
| 3:G:328:GLN:HE21 | 3:G:330:PHE:HE1 | 1.68 | 0.41 |
| 3:H:123:LEU:N | 3:H:144:ARG:HB3 | 2.35 | 0.41 |
| 1:A:18:LEU:HG | 1:A:20:LEU:HD13 | 2.01 | 0.41 |
| 3:C:78:PRO:HD3 | 3:C:452:LYS:HG2 | 2.02 | 0.41 |
| 3:C:83:PHE:CG | 3:C:84:GLY:N | 2.89 | 0.41 |
| 3:C:156:LEU:C | 3:C:156:LEU:HD12 | 2.41 | 0.41 |
| 3:C:162:LYS:HG2 | 3:C:244:ASP:HB3 | 2.02 | 0.41 |
| 3:C:390:TYR:O | 3:C:393:SER:HB2 | 2.21 | 0.41 |
| 3:D:76:HIS:H | 3:D:451:LEU:HD12 | 1.86 | 0.41 |
| 3:D:112:PRO:HD3 | 3:E:231:TYR:CD2 | 2.56 | 0.41 |
| 3:D:115:VAL:HA | 3:D:339:SER:HG | 1.85 | 0.41 |
| 3:D:189:GLU:HG2 | 3:D:190:LEU:C | 2.41 | 0.41 |
| 3:D:349:SER:H | 3:D:359:ASN:ND2 | 2.18 | 0.41 |
| 3:D:431:HIS:C | 3:D:433:PRO:HD2 | 2.40 | 0.41 |
| 3:D:451:LEU:HD23 | 3:D:451:LEU:HA | 1.76 | 0.41 |
| 3:D:458:ASP:HB2 | 3:D:461:GLN:OE1 | 2.20 | 0.41 |
| 3:D:459:LEU:HB2 | 3:D:469:LEU:HD12 | 2.03 | 0.41 |
| 3:E:12:TYR:CD1 | 3:E:12:TYR:O | 2.74 | 0.41 |
| 3:E:142:ASP:CG | 3:F:283:THR:HG21 | 2.41 | 0.41 |
| 3:E:404:PHE:CB | 3:E:405:GLY:O | 2.67 | 0.41 |
| 3:F:97:ARG:NH1 | 3:F:404:PHE:HD2 | 2.19 | 0.41 |
| 3:F:98:LEU:HD23 | 3:F:98:LEU:HA | 1.83 | 0.41 |
| 3:F:222:LEU:O | 3:F:223:ASP:C | 2.58 | 0.41 |
| 3:F:247:PHE:HE1 | 3:F:313:LEU:HD13 | 1.86 | 0.41 |
| 3:G:111:GLN:O | 3:G:113:LEU:HD12 | 2.21 | 0.41 |
| 3:G:209:ASP:HA | 3:G:228:ILE:HG13 | 2.03 | 0.41 |
| 3:G:377:GLN:CG | 3:G:378:LEU:H | 2.34 | 0.41 |
| 3:H:42:LEU:HD23 | 3:H:42:LEU:HA | 1.92 | 0.41 |
| 3:H:65:VAL:HA | 3:H:69:GLN:OE1 | 2.20 | 0.41 |
| 3:H:450:ASN:HD21 | 3:H:452:LYS:HD2 | 1.86 | 0.41 |
| 1:A:15:GLY:O | 1:A:82(B):SER:HA | 2.21 | 0.41 |
| 3:C:21:VAL:HG12 | 3:C:22:VAL:N | 2.36 | 0.41 |
| 3:C:216:ASN:O | 3:C:217:LYS:HB3 | 2.21 | 0.41 |
| 3:C:424:GLN:HA | 3:H:43:LEU:HD23 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:375:ILE:HG22 | 3:D:376:PHE:N | 2.35 | 0.41 |
| 3:D:433:PRO:O | 3:D:436:PRO:HD3 | 2.21 | 0.41 |
| 3:E:196:GLN:NE2 | 3:E:444:TYR:HD1 | 2.18 | 0.41 |
| 3:F:209:ASP:OD2 | 3:F:212:THR:HG23 | 2.21 | 0.41 |
| 3:G:255:MET:HG2 | 3:G:256:PHE:N | 2.36 | 0.41 |
| 3:G:387:VAL:O | 3:G:388:MET:C | 2.59 | 0.41 |
| 3:G:402:TRP:N | 3:G:402:TRP:CD1 | 2.88 | 0.41 |
| 3:H:46:GLY:CA | 3:H:65:VAL:HB | 2.46 | 0.41 |
| 3:H:280:SER:O | 3:H:283:THR:OG1 | 2.23 | 0.41 |
| 3:H:377:GLN:CG | 3:H:378:LEU:N | 2.84 | 0.41 |
| 1:A:24:ALA:HB2 | 1:A:29:PHE:HD1 | 1.85 | 0.40 |
| 2:B:30(A):TYR:CG | 2:B:30(B):SER:N | 2.89 | 0.40 |
| 3:C:451:LEU:O | 3:C:453:GLU:N | 2.54 | 0.40 |
| 3:D:53:LYS:HB2 | 3:D:59:LYS:O | 2.21 | 0.40 |
| 3:D:266:ALA:HB2 | 3:H:357:ASN:O | 2.21 | 0.40 |
| 3:D:442:LYS:HE3 | 3:D:442:LYS:HB3 | 1.79 | 0.40 |
| 3:D:459:LEU:HA | 3:D:462:PHE:CB | 2.51 | 0.40 |
| 3:E:36:HIS:CE1 | 3:E:37:ALA:O | 2.74 | 0.40 |
| 3:E:113:LEU:HD12 | 3:E:113:LEU:N | 2.36 | 0.40 |
| 3:E:384:THR:H | 3:E:387:VAL:HB | 1.85 | 0.40 |
| 3:F:111:GLN:HB2 | 3:F:338:ARG:CD | 2.43 | 0.40 |
| 3:G:36:HIS:CE1 | 3:G:37:ALA:O | 2.74 | 0.40 |
| 3:G:105:VAL:HG13 | 3:G:374:PHE:CD1 | 2.57 | 0.40 |
| 3:G:150:ASP:CG | 3:G:297:GLY:H | 2.24 | 0.40 |
| 3:H:422:THR:HG23 | 3:H:430:LYS:HG3 | 2.04 | 0.40 |
| 3:C:34:TYR:CE2 | 3:C:468:PHE:HZ | 2.39 | 0.40 |
| 3:C:120:HIS:HA | 3:C:121:PRO:HD3 | 1.94 | 0.40 |
| 3:D:52:ILE:HB | 3:D:62:VAL:N | 2.36 | 0.40 |
| 3:D:70:TYR:HD2 | 3:D:199:ASP:HB2 | 1.85 | 0.40 |
| 3:D:105:VAL:HG13 | 3:D:374:PHE:CE1 | 2.55 | 0.40 |
| 3:D:156:LEU:C | 3:D:156:LEU:HD12 | 2.42 | 0.40 |
| 3:D:161:CYS:HG | 3:D:244:ASP:HB3 | 1.85 | 0.40 |
| 3:D:162:LYS:CA | 3:D:245:SER:HA | 2.51 | 0.40 |
| 3:D:268:GLY:HA2 | 3:H:361:LYS:HB3 | 2.03 | 0.40 |
| 3:D:355:TYR:OH | 3:D:357:ASN:HA | 2.22 | 0.40 |
| 3:D:382:THR:O | 3:D:383:LEU:HD23 | 2.21 | 0.40 |
| 3:E:72:VAL:HG12 | 3:E:446:PHE:CD1 | 2.56 | 0.40 |
| 3:G:35:TYR:HD2 | 3:G:100:TRP:CH2 | 2.39 | 0.40 |
| 3:G:275:LEU:HD23 | 3:G:275:LEU:HA | 1.71 | 0.40 |
| 3:G:335:ASP:CG | 3:G:337:THR:H | 2.23 | 0.40 |
| 3:C:155:GLN:HE22 | 3:C:305:GLN:HA | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:435:ALA:HA | 3:C:436:PRO:HD2 | 1.91 | 0.40 |
| 3:D:119:GLY:HA3 | 3:D:147:ILE:O | 2.21 | 0.40 |
| 3:D:276:TYR:HD1 | 3:D:277:ILE:O | 2.03 | 0.40 |
| 3:D:479:LYS:NZ | 3:E:19:SER:O | 2.47 | 0.40 |
| 3:F:15:PRO:CG | 3:F:17:PRO:HD3 | 2.51 | 0.40 |
| 3:F:373:GLN:O | 3:F:374:PHE:HD1 | 2.04 | 0.40 |
| 3:F:477:LYS:HZ2 | 3:G:23:SER:N | 2.19 | 0.40 |
| 3:G:408:PRO:C | 3:G:410:PRO:HD3 | 2.41 | 0.40 |
| 1:A:47:TRP:HZ2 | 1:A:50:SER:OG | 2.04 | 0.40 |
| 1:A:63:VAL:CA | 1:A:66:ARG:HB2 | 2.51 | 0.40 |
| 3:C:406:LEU:HD11 | 3:C:410:PRO:HA | 2.04 | 0.40 |
| 3:D:123:LEU:N | 3:D:145:GLU:O | 2.53 | 0.40 |
| 3:D:172:GLY:H | 3:D:188:LEU:N | 2.19 | 0.40 |
| 3:D:259:HIS:C | 3:D:294:THR:HB | 2.42 | 0.40 |
| 3:D:386:ASP:O | 3:D:390:TYR:HB3 | 2.21 | 0.40 |
| 3:D:451:LEU:O | 3:D:452:LYS:C | 2.59 | 0.40 |
| 3:D:465:GLY:C | 3:D:467:LYS:N | 2.73 | 0.40 |
| 3:E:312:TRP:CZ3 | 3:E:468:PHE:HD1 | 2.38 | 0.40 |
| 3:F:109:ARG:HH21 | 3:F:338:ARG:HD2 | 1.84 | 0.40 |
| 3:F:255:MET:HG2 | 3:F:256:PHE:N | 2.36 | 0.40 |
| 3:G:117:ILE:HG12 | 3:G:118:SER:N | 2.36 | 0.40 |
| 3:G:158:LEU:HD23 | 3:G:158:LEU:HA | 1.91 | 0.40 |
| 3:G:466:ARG:O | 3:G:469:LEU:HB2 | 2.21 | 0.40 |
| 3:H:57:ASN:OD1 | 3:H:59:LYS:N | 2.49 | 0.40 |
| 1:A:37:VAL:O | 1:A:91:TYR:N | 2.46 | 0.40 |
| 2:B:13:VAL:O | 2:B:13:VAL:HG23 | 2.21 | 0.40 |
| 2:B:30(B):SER:O | 2:B:30(E):GLN:HG2 | 2.21 | 0.40 |
| 3:C:84:GLY:O | 3:C:85:PHE:HD1 | 2.04 | 0.40 |
| 3:C:166:GLY:N | 3:C:195:ILE:HG13 | 2.36 | 0.40 |
| 3:D:157:CYS:CA | 3:D:333:VAL:HG22 | 2.45 | 0.40 |
| 3:E:18:VAL:N | 3:E:19:SER:HA | 2.21 | 0.40 |
| 3:E:216:ASN:HB3 | 3:E:219:GLU:HG2 | 2.04 | 0.40 |
| 3:E:430:LYS:O | 3:E:431:HIS:CG | 2.74 | 0.40 |
| 3:F:123:LEU:O | 3:F:144:ARG:HA | 2.22 | 0.40 |
| 3:F:451:LEU:O | 3:F:452:LYS:C | 2.59 | 0.40 |
| 3:G:124:ASN:OD1 | 3:G:264:ALA:N | 2.52 | 0.40 |
| 3:G:158:LEU:HB2 | 3:G:332:THR:O | 2.21 | 0.40 |
| 3:G:360:PHE:O | 3:H:266:ALA:HB3 | 2.22 | 0.40 |
| 3:H:84:GLY:C | 3:H:85:PHE:CD1 | 2.95 | 0.40 |
| 3:H:110:GLY:HA3 | 3:H:369:GLU:OE2 | 2.20 | 0.40 |
| 3:H:246:LEU:HD12 | 3:H:246:LEU:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 3:H:399:LEU:HA | 3:H:399:LEU:HD23 | 1.89 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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 | A | 107/109 (98%) | 95 (89%) | 12 (11%) | 0 | 100 | 100 |
| 2 | B | 108/110 (98%) | 101 (94%) | 6 (6%) | 1 (1%) | 14 | 51 |
| 3 | C | 466/469 (99%) | 425 (91%) | 33 (7%) | 8 (2%) | 7 | 36 |
| 3 | D | 458/469 (98%) | 401 (88%) | 54 (12%) | 3 (1%) | 19 | 56 |
| 3 | E | 467/469 (100%) | 425 (91%) | 33 (7%) | 9 (2%) | 6 | 32 |
| 3 | F | 466/469 (99%) | 421 (90%) | 36 (8%) | 9 (2%) | 6 | 32 |
| 3 | G | 465/469 (99%) | 425 (91%) | 29 (6%) | 11 (2%) | 5 | 27 |
| 3 | H | 466/469 (99%) | 431 (92%) | 28 (6%) | 7 (2%) | 8 | 39 |
| All | All | 3003/3033 (99%) | 2724 (91%) | 231 (8%) | 48 (2%) | 10 | 38 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | E | 409 | PRO |
| 3 | F | 20 | LYS |
| 3 | G | 16 | VAL |
| 3 | G | 17 | PRO |
| 3 | H | 410 | PRO |
| 3 | C | 410 | PRO |
| 3 | C | 476 | ALA |
| 3 | E | 404 | PHE |
| 3 | E | 408 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | F | 426 | ILE |
| 3 | H | 422 | THR |
| 3 | H | 423 | SER |
| 3 | C | 18 | VAL |
| 3 | C | 408 | PRO |
| 3 | E | 405 | GLY |
| 3 | F | 475 | LYS |
| 3 | G | 409 | PRO |
| 3 | G | 424 | GLN |
| 2 | B | 51 | ALA |
| 3 | E | 14 | PRO |
| 3 | E | 387 | VAL |
| 3 | F | 40 | SER |
| 3 | G | 18 | VAL |
| 3 | G | 387 | VAL |
| 3 | H | 40 | SER |
| 3 | H | 387 | VAL |
| 3 | C | 40 | SER |
| 3 | C | 387 | VAL |
| 3 | C | 434 | PRO |
| 3 | D | 41 | ARG |
| 3 | E | 40 | SER |
| 3 | E | 235 | ILE |
| 3 | F | 387 | VAL |
| 3 | F | 474 | LEU |
| 3 | G | 40 | SER |
| 3 | D | 410 | PRO |
| 3 | E | 245 | SER |
| 3 | F | 17 | PRO |
| 3 | F | 235 | ILE |
| 3 | G | 235 | ILE |
| 3 | G | 436 | PRO |
| 3 | H | 235 | ILE |
| 3 | C | 235 | ILE |
| 3 | D | 387 | VAL |
| 3 | G | 15 | PRO |
| 3 | F | 21 | VAL |
| 3 | H | 408 | PRO |
| 3 | G | 14 | PRO |

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 | A | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 2 | B | 96/96 (100%) | 96 (100%) | 0 | 100 | 100 |
| 3 | C | 407/408 (100%) | 405 (100%) | 2 (0%) | 86 | 90 |
| 3 | D | 399/408 (98%) | 393 (98%) | 6 (2%) | 60 | 75 |
| 3 | E | 408/408 (100%) | 408 (100%) | 0 | 100 | 100 |
| 3 | F | 407/408 (100%) | 407 (100%) | 0 | 100 | 100 |
| 3 | G | 406/408 (100%) | 406 (100%) | 0 | 100 | 100 |
| 3 | H | 406/408 (100%) | 406 (100%) | 0 | 100 | 100 |
| All | All | 2618/2633 (99%) | 2610 (100%) | 8 (0%) | 90 | 92 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 17 | PRO |
| 3 | C | 406 | LEU |
| 3 | D | 247 | PHE |
| 3 | D | 303 | ASP |
| 3 | D | 386 | ASP |
| 3 | D | 392 | HIS |
| 3 | D | 401 | ASP |
| 3 | D | 424 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

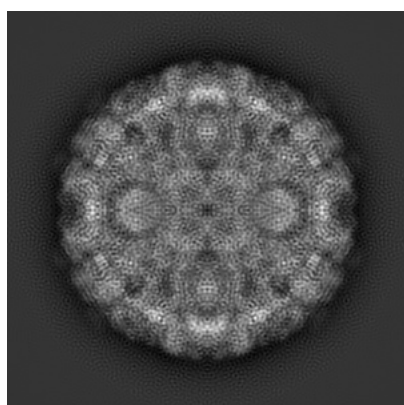
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7136. These allow visual inspection of the internal detail of the map and identification of artifacts.

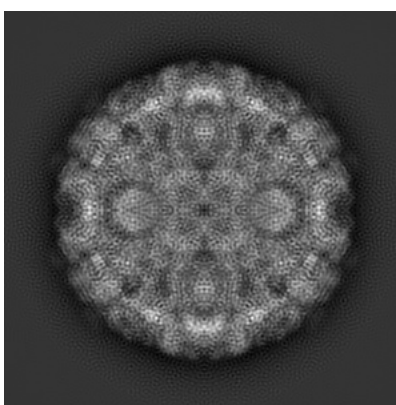
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

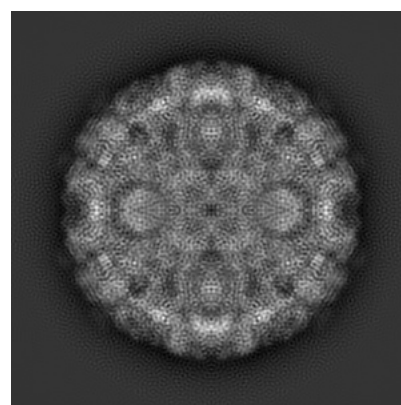
6.1.1 Primary map



X



Y

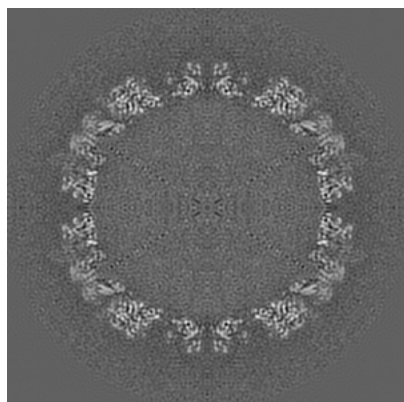


Z

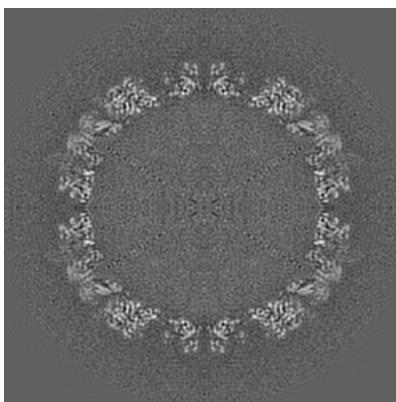
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

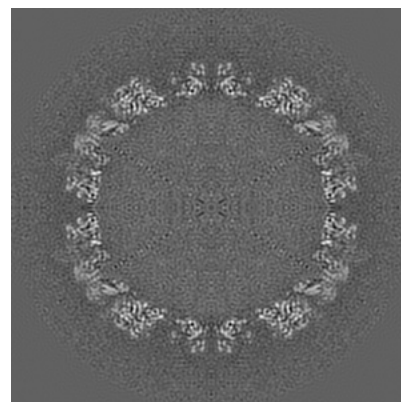
6.2.1 Primary map



X Index: 340



Y Index: 340

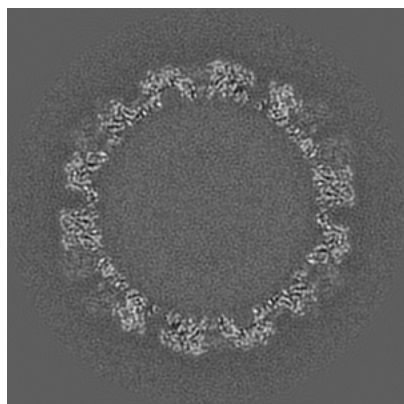


Z Index: 340

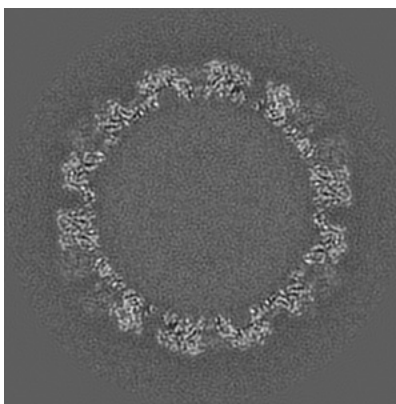
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

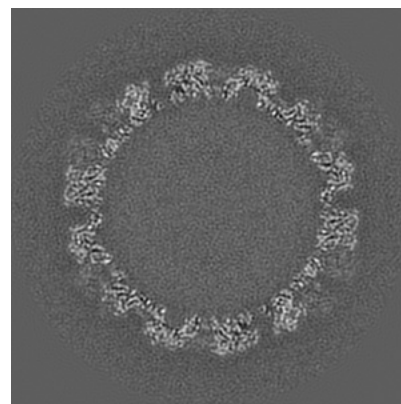
6.3.1 Primary map



X Index: 288



Y Index: 288

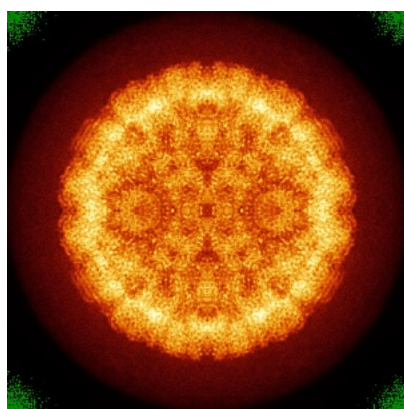


Z Index: 392

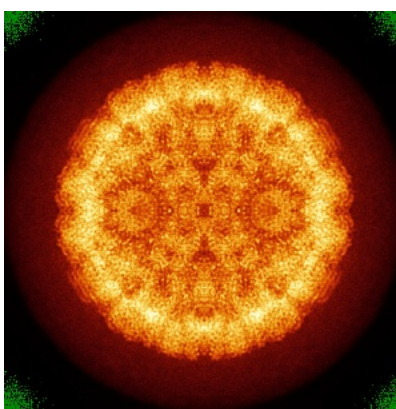
The images above show the largest variance slices of the map in three orthogonal directions.

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

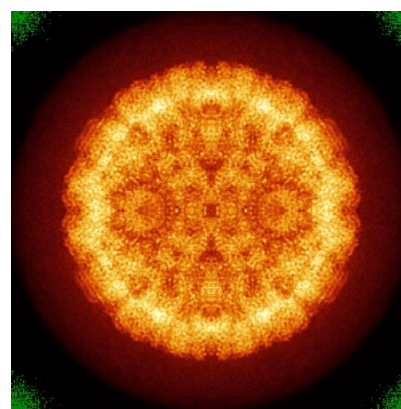
6.4.1 Primary map



X



Y

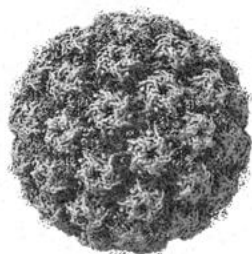


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

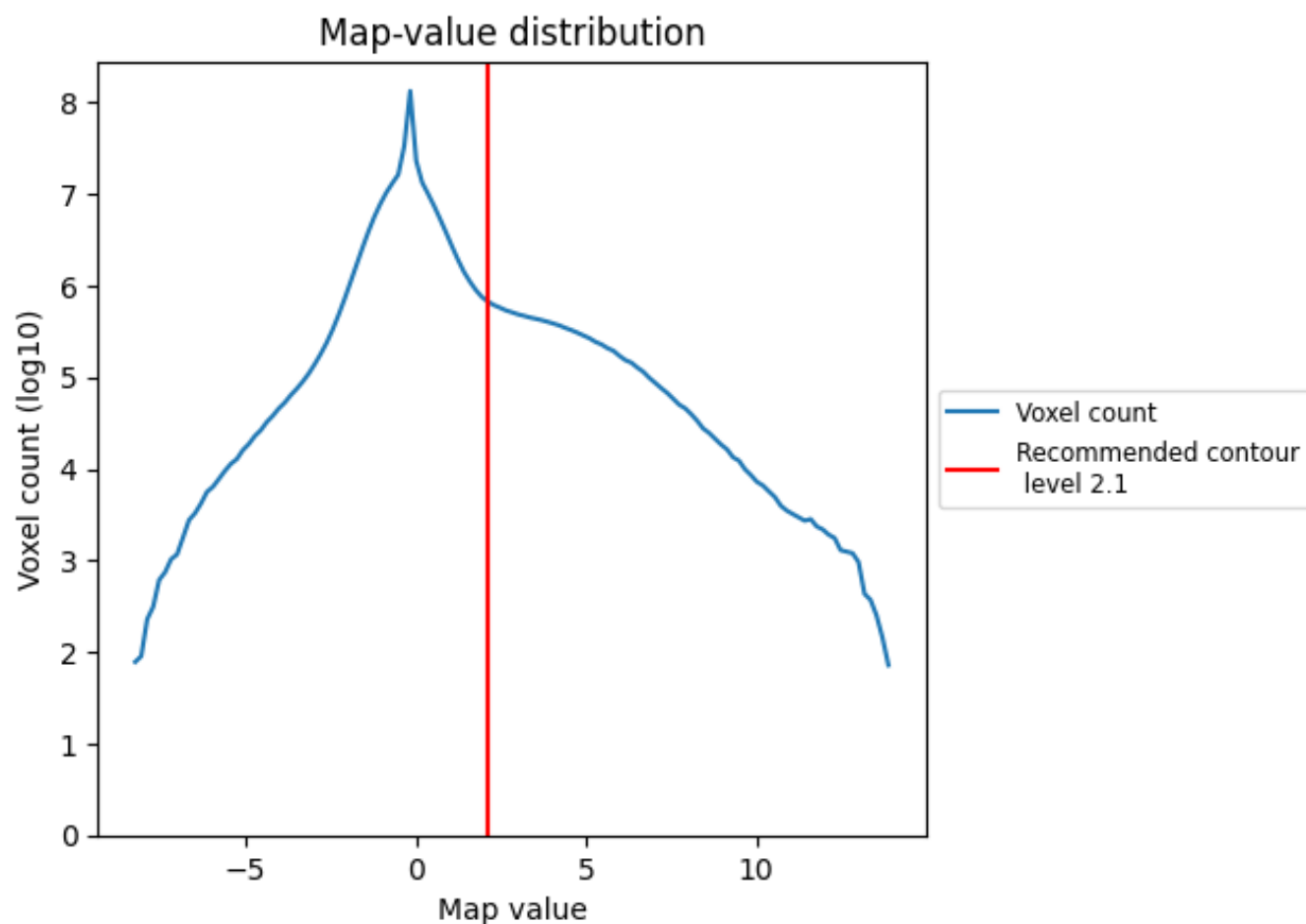
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

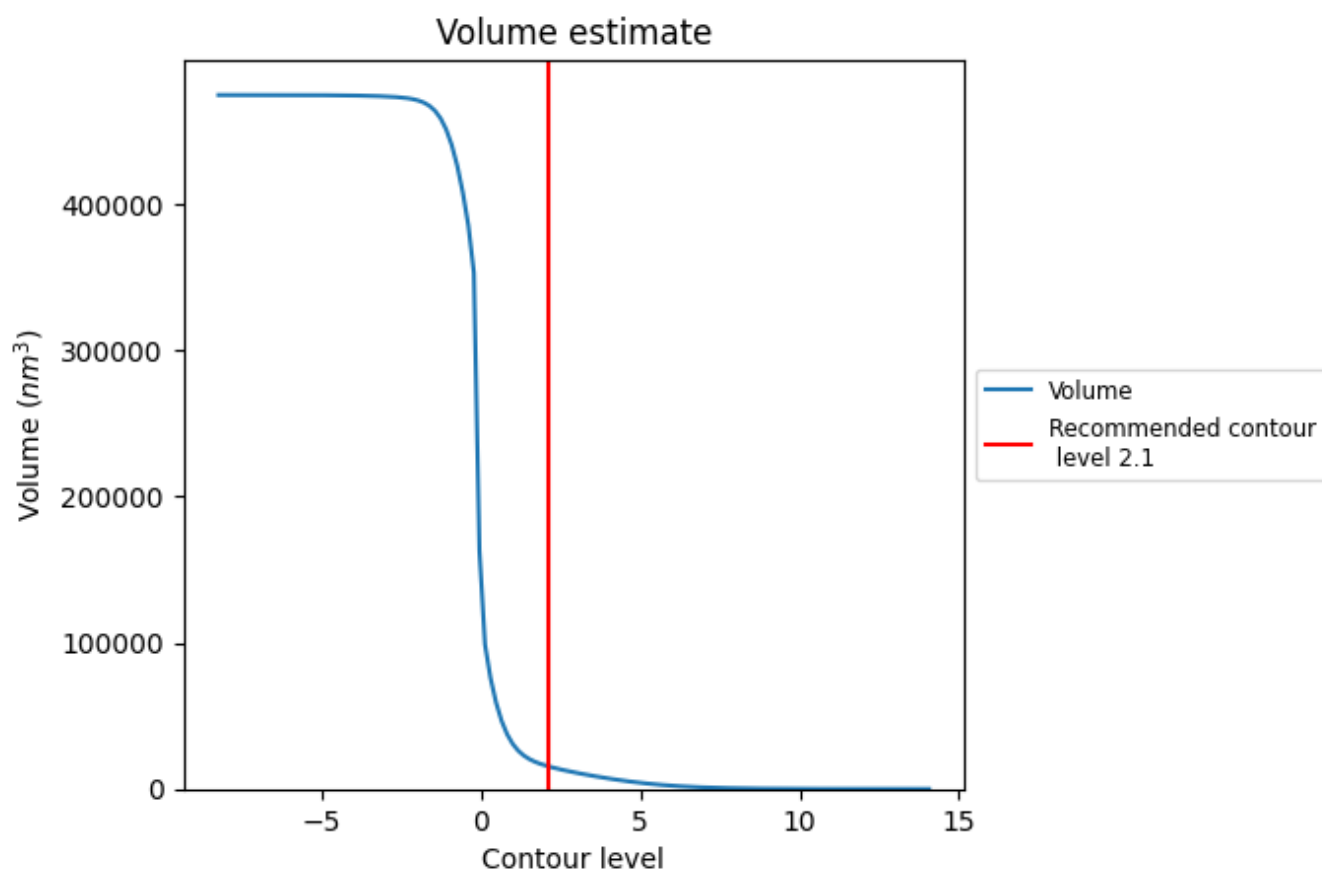
This section contains the results of statistical analysis of the map.

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.

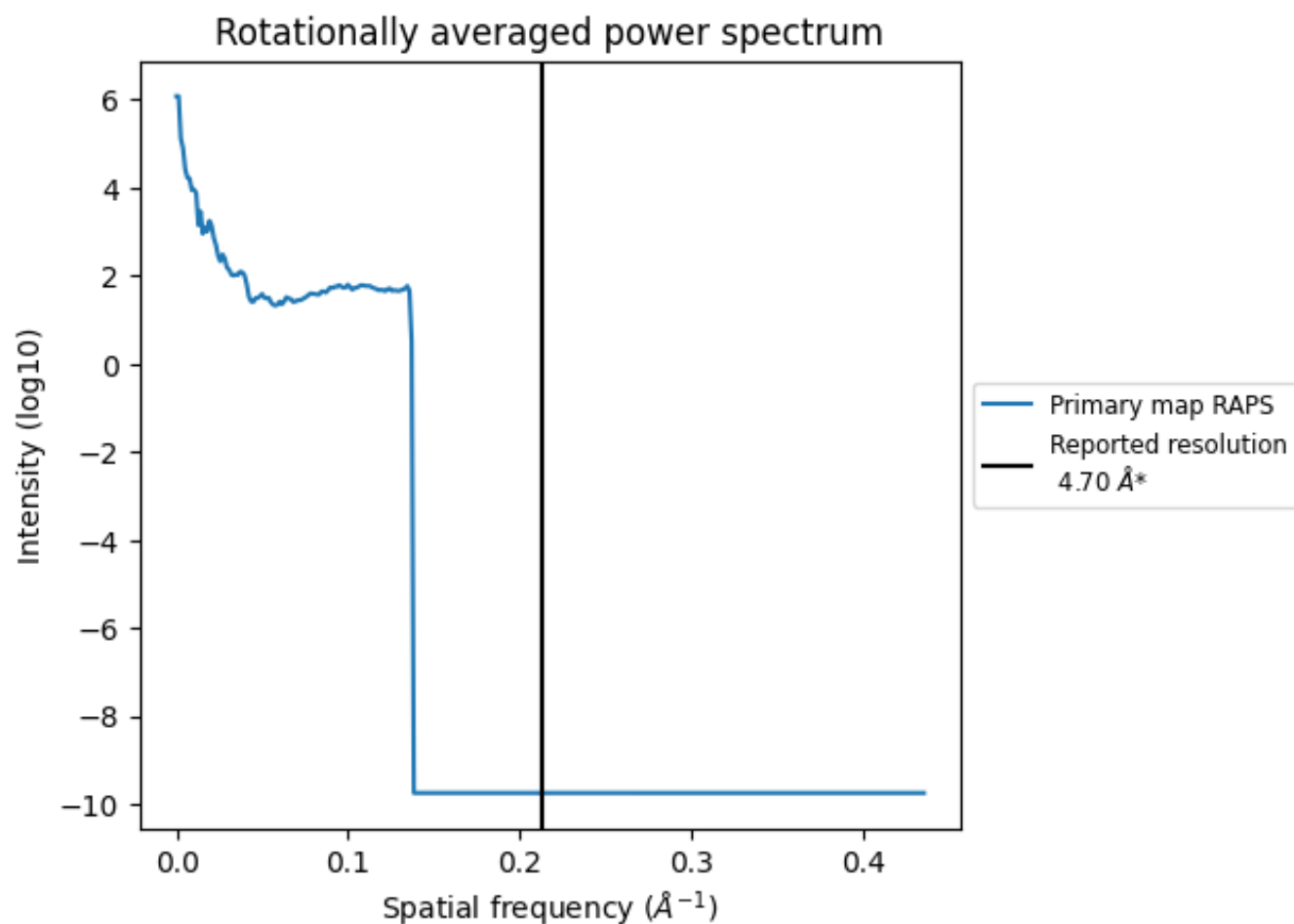
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 15512 nm^3 ; this corresponds to an approximate mass of 14013 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation ⓘ

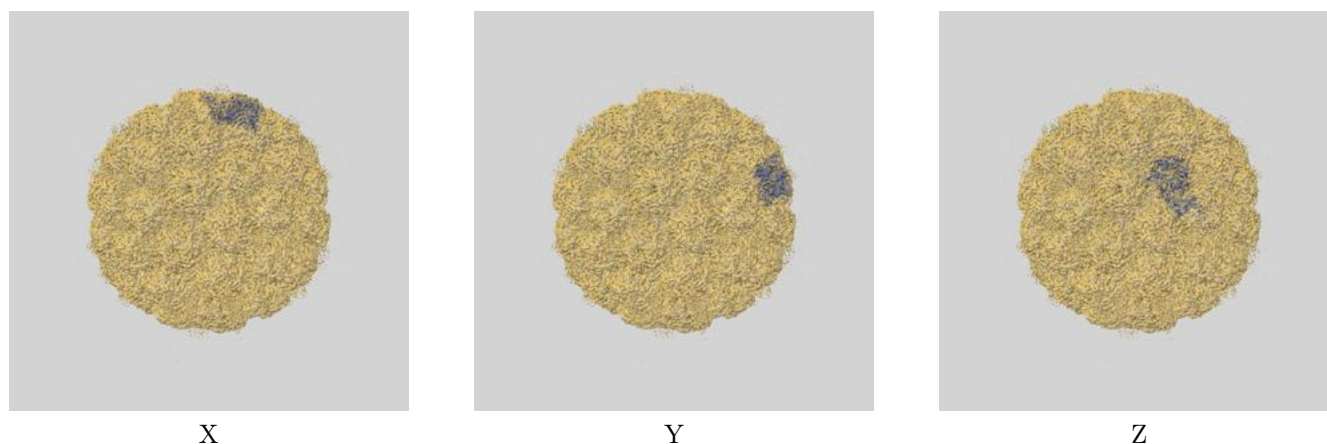
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

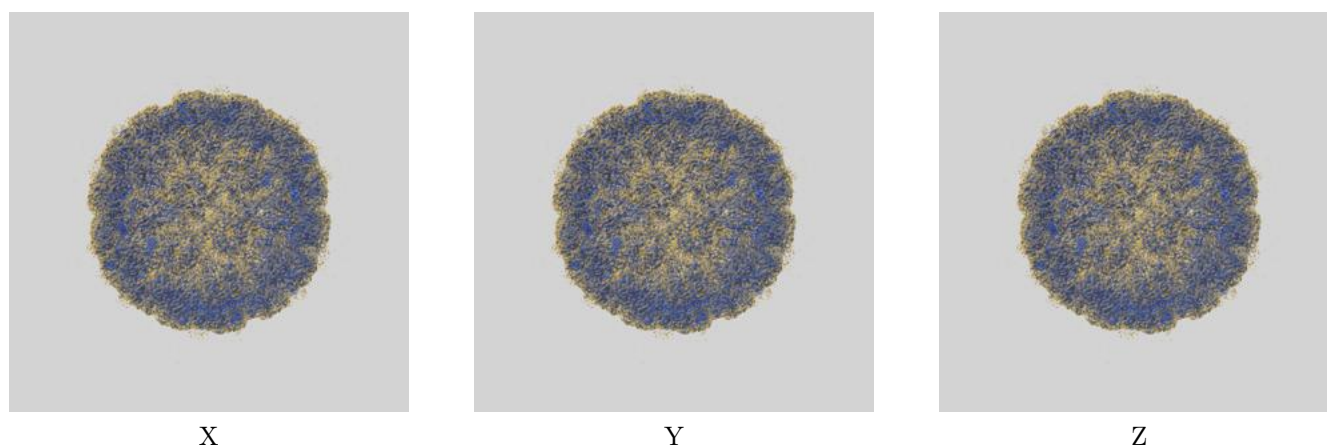
This section contains information regarding the fit between EMDB map EMD-7136 and PDB model 6BSP. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

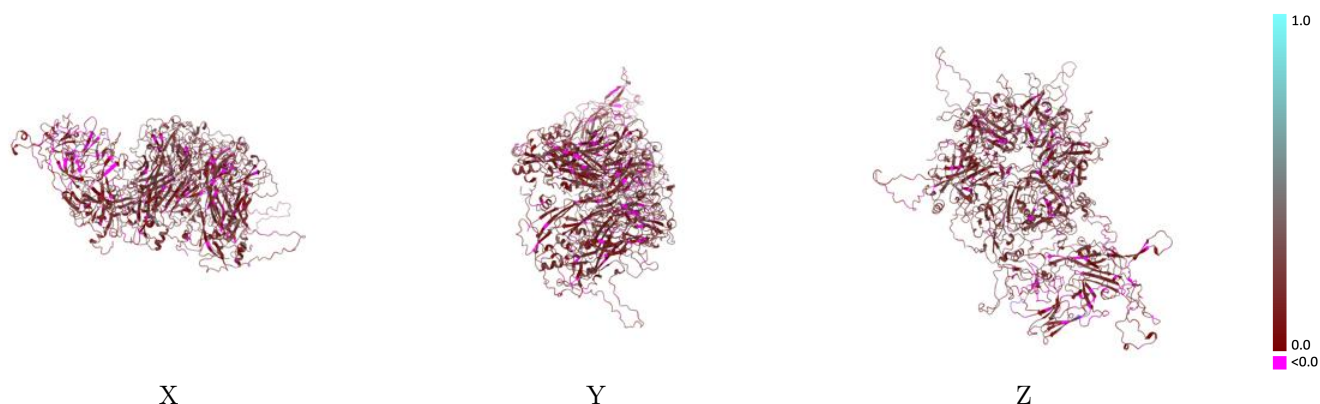


9.1.2 Map-model assembly overlay [i](#)



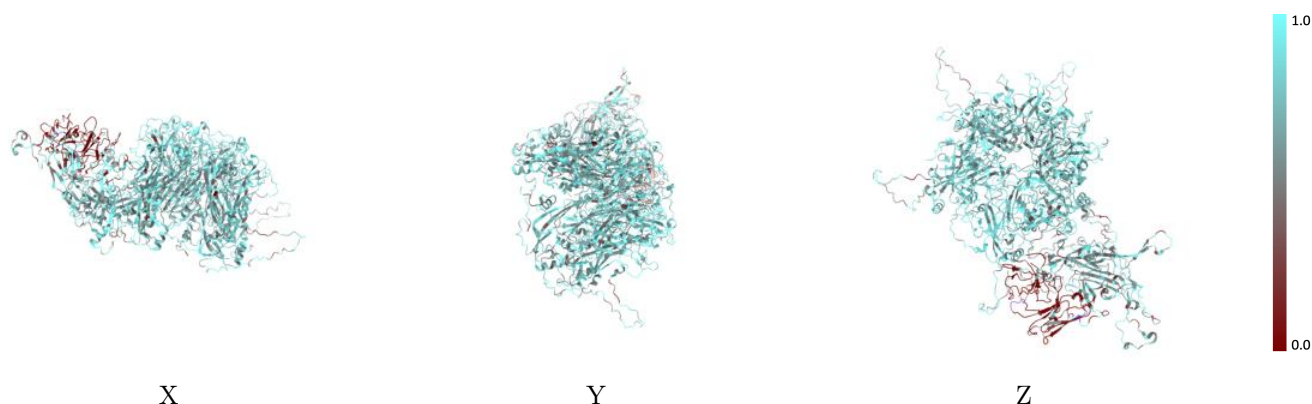
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



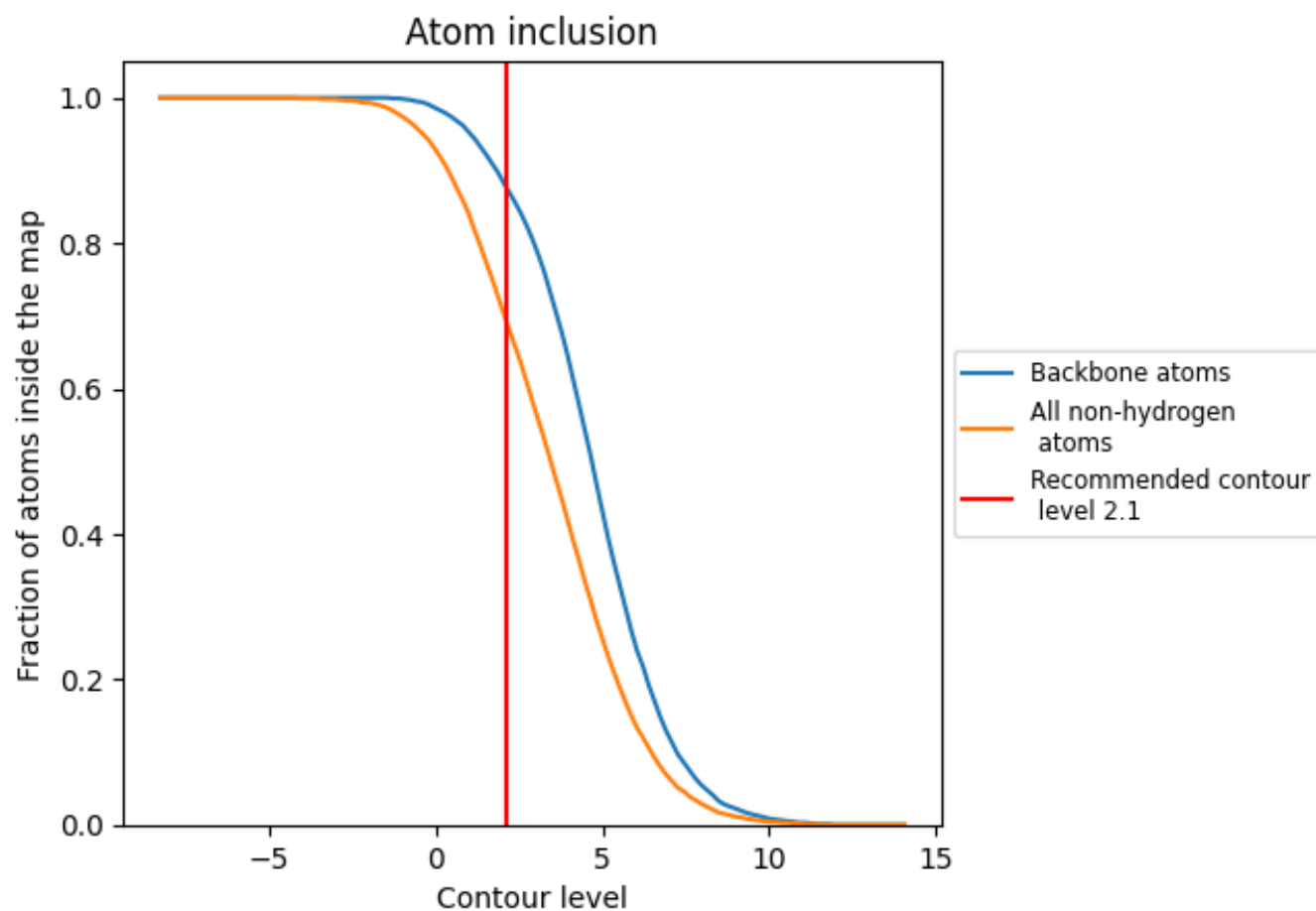
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 70% 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 (2.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.6950 | <div></div> 0.1930 |
| A | <div></div> 0.1210 | <div></div> 0.1620 |
| B | <div></div> 0.1210 | <div></div> 0.1410 |
| C | <div></div> 0.6490 | <div></div> 0.1550 |
| D | <div></div> 0.8420 | <div></div> 0.2590 |
| E | <div></div> 0.7410 | <div></div> 0.1890 |
| F | <div></div> 0.7420 | <div></div> 0.1960 |
| G | <div></div> 0.7350 | <div></div> 0.1910 |
| H | <div></div> 0.7280 | <div></div> 0.1870 |

1.0

0.0

<0.0