



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:57 AM EDT

PDB ID : 6JIV
Title : SspE crystal structure
Authors : Bing, Y.Z.; Yang, H.G.
Deposited on : 2019-02-23
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.37.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1 |

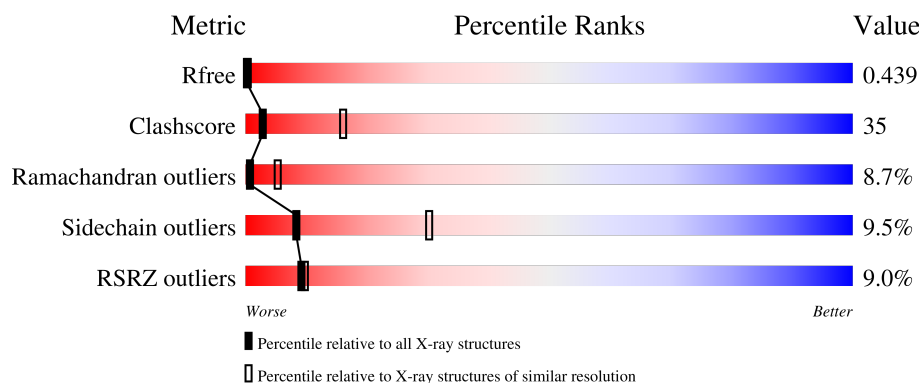
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1089 (3.36-3.28) |
| Clashscore | 141614 | 1137 (3.36-3.28) |
| Ramachandran outliers | 138981 | 1115 (3.36-3.28) |
| Sidechain outliers | 138945 | 1114 (3.36-3.28) |
| RSRZ outliers | 127900 | 1059 (3.36-3.28) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 771 | <div> <div>5%</div> <div>44%</div> <div>23%</div> <div>5%</div> <div>27%</div> </div> |
| 1 | B | 771 | <div> <div>12%</div> <div>46%</div> <div>23%</div> <div>•</div> <div>27%</div> </div> |
| 1 | C | 771 | <div> <div>4%</div> <div>39%</div> <div>27%</div> <div>6%</div> <div>28%</div> </div> |
| 1 | D | 771 | <div> <div>5%</div> <div>43%</div> <div>25%</div> <div>5%</div> <div>27%</div> </div> |

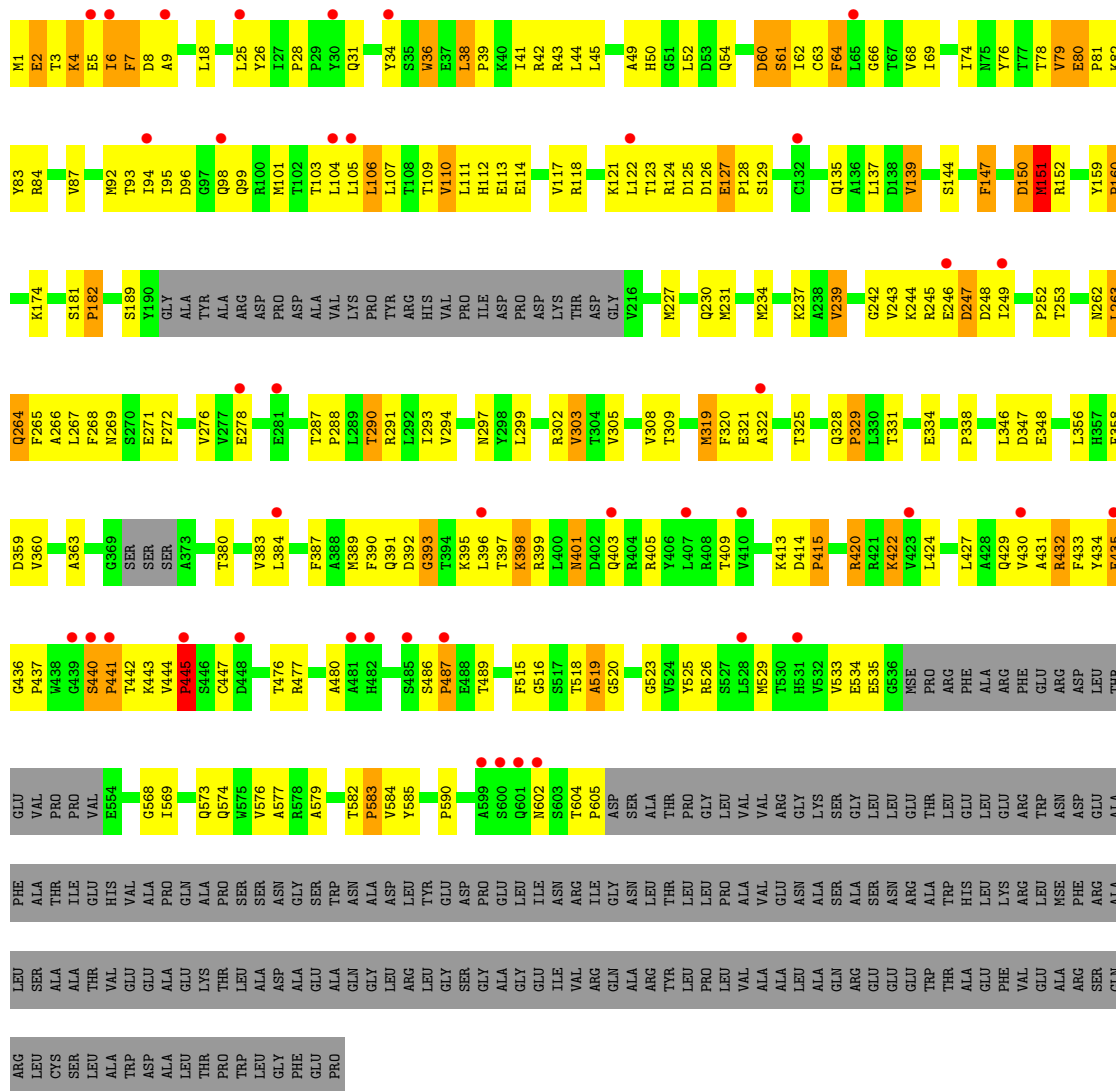
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15028 atoms, of which 0 are hydrogens and 0 are deuteriums.

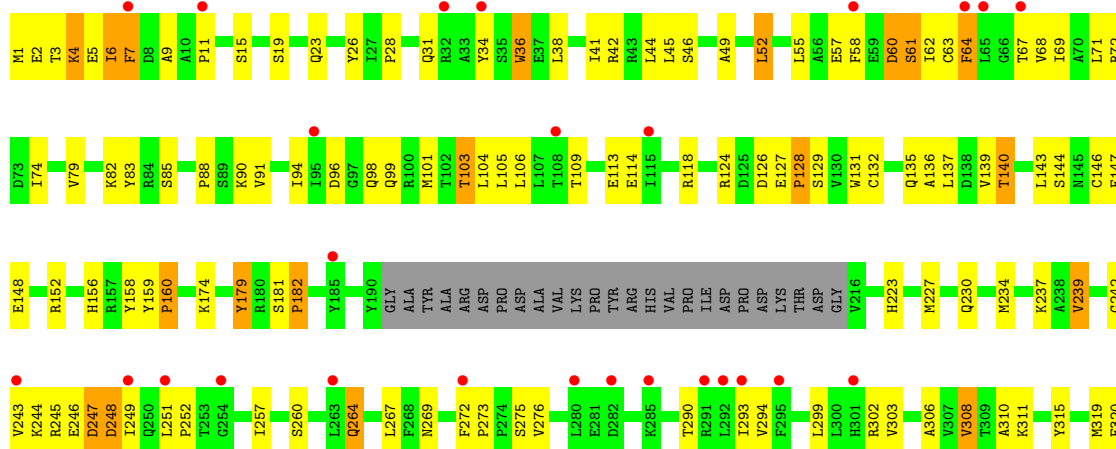
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

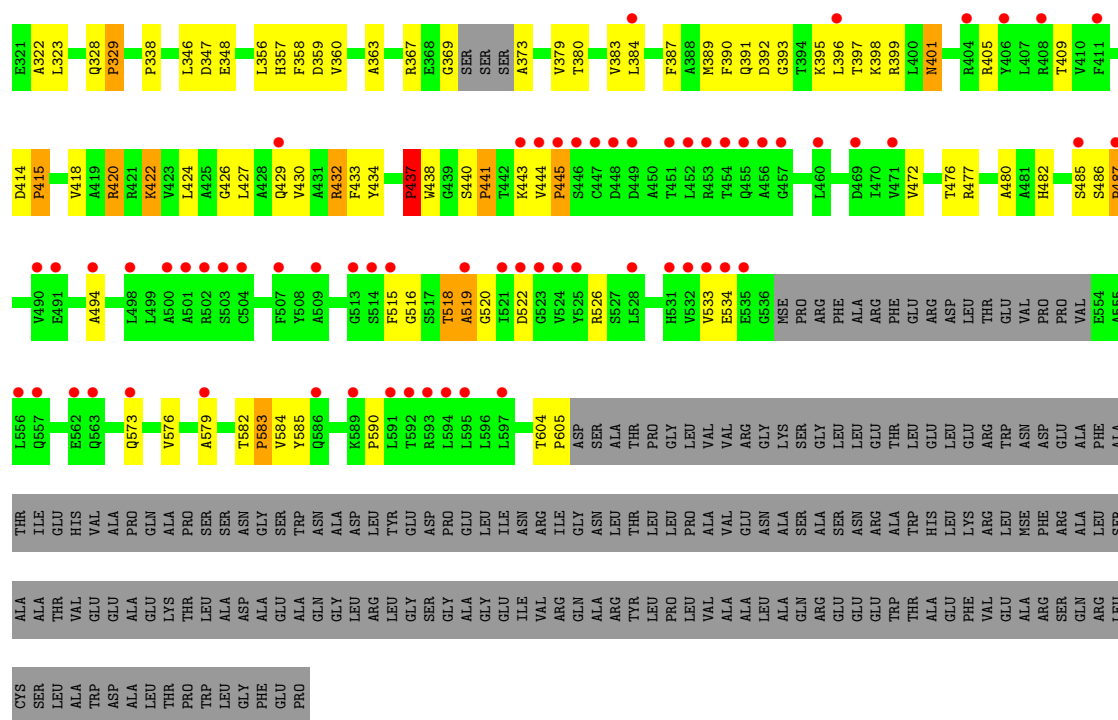
- Molecule 1 is a protein called SspE protein.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1 | D | 560 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3711 | 2310 | 674 | 713 | 3 | 11 | | | |
| 1 | A | 560 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3711 | 2310 | 674 | 713 | 3 | 11 | | | |
| 1 | B | 560 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3711 | 2310 | 674 | 713 | 3 | 11 | | | |
| 1 | C | 557 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3895 | 2439 | 697 | 743 | 4 | 12 | | | |

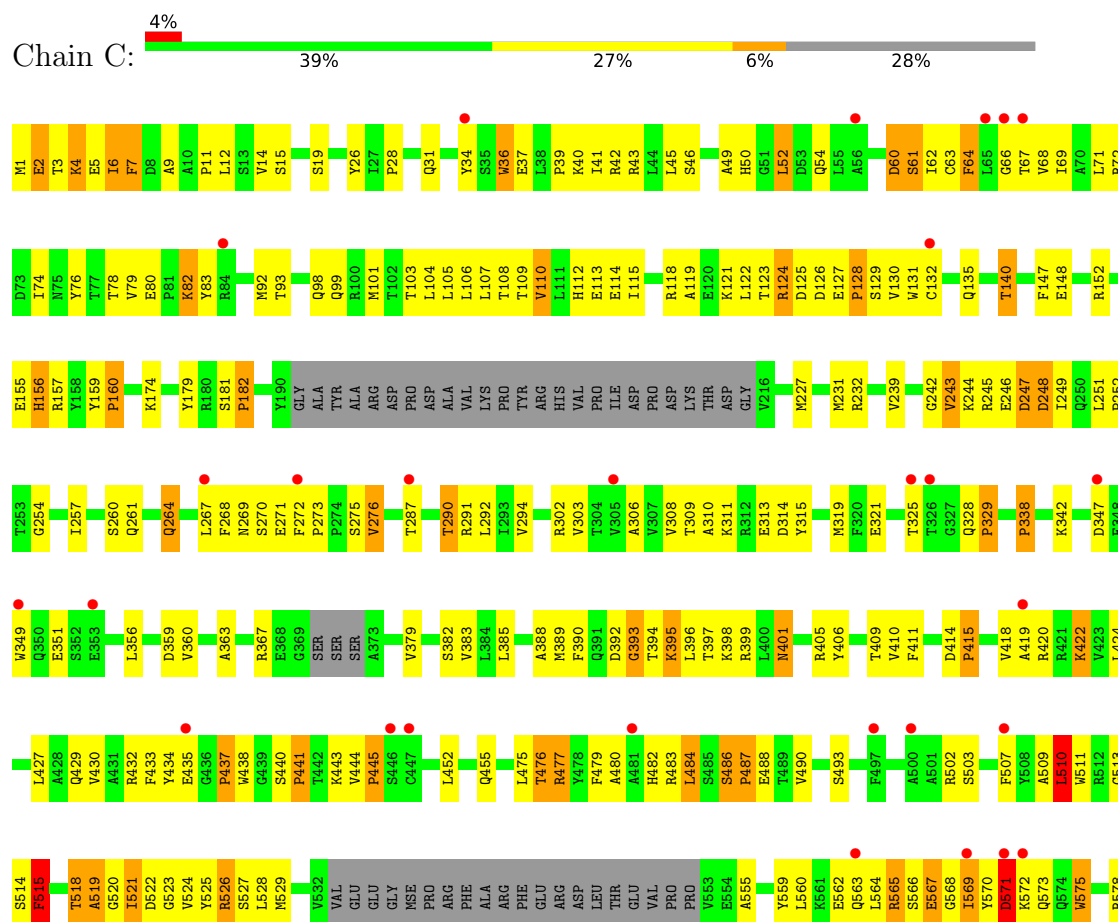


• Molecule 1: SspE protein





● Molecule 1: SspE protein



| | | | |
|-----|-----|-----|------|
| GLU | ALA | SER | A579 |
| ALA | TRP | TRP | |
| GLN | ASN | ASN | T582 |
| GLY | ALA | ALA | P583 |
| LEU | LEU | ASP | V584 |
| ARG | LEU | LEU | Y585 |
| LEU | LEU | TYR | |
| GLY | GLU | GLU | P590 |
| SER | ASP | ASP | |
| GLY | PRO | PRO | A599 |
| ALA | ALA | GLU | S600 |
| GLY | GLY | LEU | Q601 |
| GLU | ILE | ILE | N602 |
| ILE | ASN | ASN | S603 |
| VAL | ARG | ARG | T604 |
| ARG | ILE | ILE | P605 |
| GLN | GLY | GLY | ASP |
| ALA | ALA | SER | SER |
| ARG | LEU | ALA | ALA |
| TYR | THR | THR | THR |
| LEU | LEU | LEU | PRO |
| PRO | LEU | LEU | GLY |
| LEU | PRO | LEU | LEU |
| VAL | VAL | ALA | VAL |
| ALA | VAL | VAL | VAL |
| ALA | GLU | GLU | ARG |
| LEU | ASN | ASN | GLY |
| ALA | ALA | LYS | LYS |
| GLN | SER | SER | SER |
| ARG | ALA | ALA | GLY |
| GLU | GLU | ASN | LEU |
| TRP | TRP | ALA | LEU |
| THR | THR | ALA | THR |
| ALA | ALA | HIS | GLU |
| GLU | GLU | LEU | LEU |
| PHE | PHE | LYS | LEU |
| VAL | ARG | ARG | GLU |
| GLU | LEU | LEU | ARG |
| ALA | ALA | NSE | TRP |
| ALA | ALA | PHE | ASP |
| ARG | ARG | ASP | ASP |
| SER | SER | GLU | GLU |
| GLN | ALA | ALA | ALA |
| ARG | LEU | PHE | PHE |
| LEU | SER | ALA | ALA |
| CYS | ALA | THR | THR |
| SER | SER | ALA | ILE |
| LEU | LEU | THR | GLU |
| ALA | ALA | VAL | HIS |
| TRP | ASP | GLU | VAL |
| ALA | ALA | GLU | ALA |
| ALA | ALA | PRO | PRO |
| LEU | LEU | GLN | ALA |
| THR | THR | LYS | ALA |
| PRO | PRO | THR | PRO |
| TRP | TRP | LEU | SER |
| GLY | GLY | ALA | SER |
| PHE | PHE | ASP | ASN |
| | | ALA | GLY |
| GLU | PRO | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 111.07Å 138.16Å 293.68Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 125.33 – 3.31 125.02 – 3.31 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (125.33-3.31) 99.5 (125.02-3.31) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.77 (at 3.33Å) | Xtriage |
| Refinement program | REFMAC 5.8.0258 | Depositor |
| R, R_{free} | 0.406 , 0.435 0.407 , 0.439 | Depositor DCC |
| R_{free} test set | 3357 reflections (4.96%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 122.6 | Xtriage |
| Anisotropy | 0.299 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 110.6 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.80 | EDS |
| Total number of atoms | 15028 | wwPDB-VP |
| Average B, all atoms (Å ²) | 109.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 | 0.60 | 0/3747 | 0.84 | 17/5100 (0.3%) |
| 1 | B | 0.52 | 0/3747 | 0.75 | 16/5100 (0.3%) |
| 1 | C | 0.57 | 0/3943 | 0.82 | 15/5351 (0.3%) |
| 1 | D | 0.73 | 5/3747 (0.1%) | 0.90 | 16/5100 (0.3%) |
| All | All | 0.61 | 5/15184 (0.0%) | 0.83 | 64/20651 (0.3%) |

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 |
| 1 | C | 0 | 2 |
| All | All | 0 | 3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | D | 146 | CYS | CB-SG | -10.19 | 1.65 | 1.82 |
| 1 | D | 110 | VAL | CB-CG1 | -5.86 | 1.40 | 1.52 |
| 1 | D | 133 | TYR | CE1-CZ | -5.46 | 1.31 | 1.38 |
| 1 | D | 260 | SER | CA-CB | -5.23 | 1.45 | 1.52 |
| 1 | D | 68 | VAL | CB-CG1 | -5.01 | 1.42 | 1.52 |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 484 | LEU | CB-CG-CD1 | -9.98 | 94.03 | 111.00 |
| 1 | D | 160 | PRO | N-CA-CB | 9.37 | 114.54 | 103.30 |
| 1 | A | 160 | PRO | N-CA-CB | 8.07 | 112.98 | 103.30 |
| 1 | A | 329 | PRO | N-CA-CB | 7.82 | 112.69 | 103.30 |
| 1 | B | 329 | PRO | N-CA-CB | 7.54 | 112.35 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 329 | PRO | N-CA-CB | 7.43 | 112.22 | 103.30 |
| 1 | D | 329 | PRO | N-CA-CB | 7.36 | 112.13 | 103.30 |
| 1 | B | 160 | PRO | N-CA-CB | 7.28 | 112.03 | 103.30 |
| 1 | C | 160 | PRO | N-CA-CB | 7.26 | 112.01 | 103.30 |
| 1 | A | 441 | PRO | N-CA-CB | 7.19 | 111.93 | 103.30 |
| 1 | D | 415 | PRO | N-CA-CB | 7.12 | 111.85 | 103.30 |
| 1 | C | 583 | PRO | N-CA-CB | 7.09 | 111.80 | 103.30 |
| 1 | B | 441 | PRO | N-CA-CB | 7.07 | 111.78 | 103.30 |
| 1 | C | 590 | PRO | N-CA-CB | 7.04 | 111.75 | 103.30 |
| 1 | C | 605 | PRO | N-CA-CB | 6.97 | 111.67 | 103.30 |
| 1 | B | 415 | PRO | N-CA-CB | 6.93 | 111.62 | 103.30 |
| 1 | A | 605 | PRO | N-CA-CB | 6.80 | 111.46 | 103.30 |
| 1 | D | 445 | PRO | N-CA-CB | 6.73 | 111.38 | 103.30 |
| 1 | B | 445 | PRO | N-CA-CB | 6.69 | 111.33 | 103.30 |
| 1 | C | 445 | PRO | N-CA-CB | 6.60 | 111.22 | 103.30 |
| 1 | A | 590 | PRO | N-CA-CB | 6.58 | 111.19 | 103.30 |
| 1 | D | 319 | MSE | CB-CG-SE | -6.55 | 93.05 | 112.70 |
| 1 | A | 445 | PRO | N-CA-CB | 6.43 | 111.02 | 103.30 |
| 1 | A | 415 | PRO | N-CA-CB | 6.38 | 110.96 | 103.30 |
| 1 | D | 441 | PRO | N-CA-CB | 6.37 | 110.95 | 103.30 |
| 1 | C | 441 | PRO | N-CA-CB | 6.26 | 110.81 | 103.30 |
| 1 | A | 182 | PRO | N-CA-CB | 6.25 | 110.80 | 103.30 |
| 1 | A | 319 | MSE | CB-CG-SE | -6.20 | 94.09 | 112.70 |
| 1 | A | 583 | PRO | N-CA-CB | 6.20 | 110.73 | 103.30 |
| 1 | B | 605 | PRO | N-CA-CB | 6.19 | 110.73 | 103.30 |
| 1 | B | 182 | PRO | N-CA-CB | 6.16 | 110.69 | 103.30 |
| 1 | C | 510 | LEU | CA-CB-CG | -6.15 | 101.16 | 115.30 |
| 1 | D | 590 | PRO | N-CA-CB | 6.09 | 110.61 | 103.30 |
| 1 | B | 437 | PRO | CA-N-CD | -6.04 | 103.05 | 111.50 |
| 1 | B | 590 | PRO | N-CA-CB | 5.98 | 110.48 | 103.30 |
| 1 | B | 319 | MSE | CB-CG-SE | -5.97 | 94.80 | 112.70 |
| 1 | D | 583 | PRO | N-CA-CB | 5.95 | 110.44 | 103.30 |
| 1 | B | 179 | TYR | CA-CB-CG | 5.93 | 124.68 | 113.40 |
| 1 | C | 182 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |
| 1 | B | 487 | PRO | N-CA-CB | 5.85 | 110.32 | 103.30 |
| 1 | C | 104 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 1 | D | 118 | ARG | NE-CZ-NH1 | 5.77 | 123.19 | 120.30 |
| 1 | C | 338 | PRO | N-CA-CB | 5.75 | 110.20 | 103.30 |
| 1 | D | 182 | PRO | N-CA-CB | 5.68 | 110.12 | 103.30 |
| 1 | B | 583 | PRO | N-CA-CB | 5.66 | 110.09 | 103.30 |
| 1 | D | 487 | PRO | N-CA-CB | 5.62 | 110.04 | 103.30 |
| 1 | D | 605 | PRO | N-CA-CB | 5.59 | 110.01 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 487 | PRO | N-CA-CB | 5.56 | 109.97 | 103.30 |
| 1 | D | 323 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 1 | A | 104 | LEU | CB-CG-CD2 | -5.49 | 101.67 | 111.00 |
| 1 | C | 415 | PRO | N-CA-CB | 5.49 | 109.88 | 103.30 |
| 1 | A | 422 | LYS | CB-CA-C | 5.34 | 121.08 | 110.40 |
| 1 | A | 38 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 1 | D | 256 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | A | 338 | PRO | N-CA-CB | 5.24 | 109.59 | 103.30 |
| 1 | B | 437 | PRO | N-CA-CB | -5.24 | 96.84 | 102.60 |
| 1 | D | 247 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | A | 247 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | C | 247 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | C | 571 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | A | 104 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |
| 1 | B | 247 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | B | 338 | PRO | N-CA-CB | 5.10 | 109.42 | 103.30 |
| 1 | D | 280 | LEU | CB-CG-CD1 | -5.10 | 102.33 | 111.00 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 127 | GLU | Peptide |
| 1 | C | 477 | ARG | Peptide |
| 1 | C | 584 | VAL | 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 | 3711 | 0 | 3036 | 217 | 0 |
| 1 | B | 3711 | 0 | 3038 | 219 | 0 |
| 1 | C | 3895 | 0 | 3376 | 323 | 0 |
| 1 | D | 3711 | 0 | 3038 | 246 | 0 |
| All | All | 15028 | 0 | 12488 | 970 | 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 35.

All (970) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:515:PHE:CZ | 1:C:578:ARG:HD3 | 1.32 | 1.63 |
| 1:D:356:LEU:CA | 1:D:427:LEU:HD11 | 1.17 | 1.59 |
| 1:A:356:LEU:CA | 1:A:427:LEU:HD11 | 1.16 | 1.59 |
| 1:D:356:LEU:HA | 1:D:427:LEU:CD1 | 1.30 | 1.55 |
| 1:D:395:LYS:CE | 1:D:526:ARG:HD3 | 1.37 | 1.55 |
| 1:A:356:LEU:CA | 1:A:427:LEU:CD1 | 1.76 | 1.55 |
| 1:A:356:LEU:HA | 1:A:427:LEU:CD1 | 1.35 | 1.51 |
| 1:D:387:PHE:CA | 1:D:429:GLN:NE2 | 1.71 | 1.51 |
| 1:B:387:PHE:CA | 1:B:429:GLN:HE22 | 1.26 | 1.48 |
| 1:D:356:LEU:CA | 1:D:427:LEU:CD1 | 1.86 | 1.47 |
| 1:D:395:LYS:NZ | 1:D:526:ARG:CD | 1.75 | 1.45 |
| 1:B:391:GLN:NE2 | 1:B:422:LYS:HE3 | 1.14 | 1.44 |
| 1:B:387:PHE:HA | 1:B:429:GLN:NE2 | 1.18 | 1.41 |
| 1:D:359:ASP:CB | 1:D:427:LEU:HD22 | 1.53 | 1.38 |
| 1:B:387:PHE:HB2 | 1:B:429:GLN:OE1 | 1.21 | 1.37 |
| 1:A:356:LEU:C | 1:A:427:LEU:HD11 | 1.09 | 1.37 |
| 1:C:245:ARG:HH12 | 1:C:523:GLY:N | 1.07 | 1.37 |
| 1:C:418:VAL:O | 1:C:422:LYS:CE | 1.72 | 1.37 |
| 1:D:395:LYS:NZ | 1:D:526:ARG:HD2 | 1.04 | 1.36 |
| 1:C:245:ARG:HH22 | 1:C:523:GLY:CA | 1.38 | 1.33 |
| 1:D:356:LEU:C | 1:D:427:LEU:HD11 | 1.09 | 1.32 |
| 1:C:511:TRP:CZ3 | 1:C:567:GLU:HG3 | 1.66 | 1.30 |
| 1:B:395:LYS:NZ | 1:B:526:ARG:HD2 | 1.45 | 1.30 |
| 1:C:418:VAL:O | 1:C:422:LYS:HE3 | 1.26 | 1.30 |
| 1:B:395:LYS:CD | 1:B:526:ARG:HD3 | 1.63 | 1.29 |
| 1:D:395:LYS:CE | 1:D:526:ARG:CD | 2.06 | 1.28 |
| 1:C:432:ARG:HH21 | 1:C:479:PHE:CB | 1.45 | 1.28 |
| 1:D:387:PHE:HA | 1:D:429:GLN:NE2 | 0.96 | 1.27 |
| 1:A:42:ARG:NH2 | 1:A:247:ASP:OD2 | 1.68 | 1.25 |
| 1:C:515:PHE:CZ | 1:C:578:ARG:CD | 2.18 | 1.25 |
| 1:B:391:GLN:NE2 | 1:B:422:LYS:CE | 2.00 | 1.25 |
| 1:A:387:PHE:CB | 1:A:429:GLN:OE1 | 1.80 | 1.25 |
| 1:D:363:ALA:HA | 1:D:434:TYR:OH | 1.37 | 1.24 |
| 1:D:387:PHE:HB2 | 1:D:429:GLN:OE1 | 1.13 | 1.24 |
| 1:D:395:LYS:HD3 | 1:D:526:ARG:CZ | 1.68 | 1.23 |
| 1:B:395:LYS:CE | 1:B:526:ARG:HD3 | 1.69 | 1.22 |
| 1:B:42:ARG:NH2 | 1:B:247:ASP:OD2 | 1.74 | 1.21 |
| 1:D:395:LYS:CD | 1:D:526:ARG:NH1 | 2.06 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:432:ARG:HE | 1:D:476:THR:CB | 1.54 | 1.19 |
| 1:A:433:PHE:CA | 1:A:437:PRO:HG2 | 1.70 | 1.19 |
| 1:C:245:ARG:NH1 | 1:C:523:GLY:N | 1.92 | 1.18 |
| 1:C:356:LEU:CB | 1:C:424:LEU:HD23 | 1.72 | 1.18 |
| 1:C:515:PHE:CE2 | 1:C:578:ARG:HD3 | 1.78 | 1.17 |
| 1:C:524:VAL:HG13 | 1:C:563:GLN:NE2 | 1.59 | 1.17 |
| 1:B:391:GLN:HE22 | 1:B:422:LYS:CE | 1.55 | 1.16 |
| 1:C:524:VAL:CG1 | 1:C:563:GLN:OE1 | 1.93 | 1.16 |
| 1:C:432:ARG:HD3 | 1:C:476:THR:HA | 1.18 | 1.15 |
| 1:C:245:ARG:HH22 | 1:C:523:GLY:HA3 | 0.98 | 1.15 |
| 1:D:387:PHE:CB | 1:D:429:GLN:OE1 | 1.94 | 1.14 |
| 1:D:429:GLN:O | 1:D:433:PHE:CD2 | 2.01 | 1.13 |
| 1:C:430:VAL:CG1 | 1:C:434:TYR:HE2 | 1.61 | 1.13 |
| 1:A:356:LEU:HA | 1:A:427:LEU:HD13 | 1.18 | 1.12 |
| 1:B:356:LEU:CB | 1:B:424:LEU:HD23 | 1.78 | 1.11 |
| 1:B:395:LYS:HZ3 | 1:B:526:ARG:CD | 1.63 | 1.10 |
| 1:C:524:VAL:CG1 | 1:C:563:GLN:CD | 2.19 | 1.10 |
| 1:D:42:ARG:NH2 | 1:D:247:ASP:OD2 | 1.85 | 1.10 |
| 1:B:395:LYS:HD3 | 1:B:526:ARG:CD | 1.82 | 1.10 |
| 1:A:74:ILE:HD11 | 1:B:1:MSE:SE | 2.03 | 1.09 |
| 1:C:528:LEU:CD1 | 1:C:560:LEU:HD23 | 1.81 | 1.09 |
| 1:D:395:LYS:HE2 | 1:D:526:ARG:HD3 | 1.11 | 1.09 |
| 1:C:568:GLY:O | 1:C:578:ARG:NH1 | 1.86 | 1.09 |
| 1:B:387:PHE:CB | 1:B:429:GLN:OE1 | 2.00 | 1.08 |
| 1:C:555:ALA:O | 1:C:559:TYR:HD2 | 1.35 | 1.08 |
| 1:A:356:LEU:CB | 1:A:427:LEU:CD1 | 2.31 | 1.08 |
| 1:A:433:PHE:HA | 1:A:437:PRO:HG2 | 1.15 | 1.08 |
| 1:A:430:VAL:CG1 | 1:A:434:TYR:HE2 | 1.67 | 1.07 |
| 1:C:432:ARG:NH2 | 1:C:479:PHE:CB | 2.17 | 1.07 |
| 1:D:363:ALA:HB2 | 1:D:430:VAL:HG11 | 1.37 | 1.06 |
| 1:A:429:GLN:O | 1:A:433:PHE:CD2 | 2.07 | 1.06 |
| 1:C:245:ARG:NH2 | 1:C:523:GLY:CA | 2.18 | 1.06 |
| 1:D:432:ARG:HD3 | 1:D:476:THR:HA | 1.36 | 1.05 |
| 1:C:575:TRP:CZ3 | 1:C:579:ALA:HB2 | 1.91 | 1.05 |
| 1:D:356:LEU:HA | 1:D:427:LEU:HD13 | 1.38 | 1.05 |
| 1:A:49:ALA:CB | 1:A:249:ILE:CG2 | 2.34 | 1.04 |
| 1:B:395:LYS:CE | 1:B:526:ARG:CD | 2.35 | 1.04 |
| 1:C:432:ARG:CD | 1:C:476:THR:HA | 1.77 | 1.04 |
| 1:D:114:GLU:OE1 | 1:D:118:ARG:NH1 | 1.91 | 1.04 |
| 1:A:430:VAL:HG12 | 1:A:434:TYR:HE2 | 1.18 | 1.03 |
| 1:B:395:LYS:HD3 | 1:B:526:ARG:HD3 | 1.27 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:432:ARG:NE | 1:D:476:THR:CB | 2.21 | 1.03 |
| 1:C:359:ASP:CB | 1:C:427:LEU:HD22 | 1.88 | 1.03 |
| 1:C:430:VAL:HG12 | 1:C:434:TYR:HE2 | 1.18 | 1.03 |
| 1:C:49:ALA:CB | 1:C:249:ILE:CG2 | 2.37 | 1.02 |
| 1:D:363:ALA:HB2 | 1:D:430:VAL:CG1 | 1.90 | 1.02 |
| 1:C:422:LYS:H | 1:C:422:LYS:HE2 | 1.22 | 1.02 |
| 1:A:106:LEU:O | 1:A:109:THR:HB | 1.58 | 1.01 |
| 1:C:432:ARG:NH2 | 1:C:477:ARG:HA | 1.72 | 1.01 |
| 1:D:74:ILE:HD11 | 1:C:1:MSE:SE | 2.11 | 1.01 |
| 1:A:433:PHE:HA | 1:A:437:PRO:CG | 1.90 | 1.01 |
| 1:B:395:LYS:NZ | 1:B:526:ARG:CD | 2.19 | 1.01 |
| 1:D:395:LYS:HD3 | 1:D:526:ARG:NH1 | 1.71 | 1.00 |
| 1:D:74:ILE:CD1 | 1:C:1:MSE:SE | 2.59 | 1.00 |
| 1:D:395:LYS:CD | 1:D:526:ARG:HD3 | 1.90 | 1.00 |
| 1:A:49:ALA:HB2 | 1:A:249:ILE:HG21 | 1.37 | 1.00 |
| 1:C:570:TYR:O | 1:C:571:ASP:CG | 2.00 | 0.99 |
| 1:D:387:PHE:N | 1:D:429:GLN:NE2 | 2.09 | 0.99 |
| 1:C:555:ALA:O | 1:C:559:TYR:CD2 | 2.14 | 0.99 |
| 1:C:515:PHE:CE1 | 1:C:578:ARG:HD3 | 1.96 | 0.99 |
| 1:C:524:VAL:HG13 | 1:C:563:GLN:CD | 1.80 | 0.99 |
| 1:B:395:LYS:HZ3 | 1:B:526:ARG:HD2 | 0.83 | 0.98 |
| 1:C:245:ARG:NH2 | 1:C:523:GLY:HA3 | 1.75 | 0.97 |
| 1:C:432:ARG:CD | 1:C:476:THR:CA | 2.41 | 0.97 |
| 1:C:418:VAL:O | 1:C:422:LYS:HE2 | 1.62 | 0.96 |
| 1:C:245:ARG:HH22 | 1:C:523:GLY:HA2 | 1.30 | 0.96 |
| 1:C:430:VAL:HG12 | 1:C:434:TYR:CE2 | 2.01 | 0.96 |
| 1:A:356:LEU:CB | 1:A:427:LEU:HD12 | 1.93 | 0.96 |
| 1:C:245:ARG:HH12 | 1:C:523:GLY:H | 0.98 | 0.96 |
| 1:D:356:LEU:HA | 1:D:427:LEU:HD12 | 1.48 | 0.96 |
| 1:B:387:PHE:CA | 1:B:429:GLN:NE2 | 2.01 | 0.95 |
| 1:C:422:LYS:HE2 | 1:C:422:LYS:N | 1.80 | 0.95 |
| 1:A:356:LEU:CB | 1:A:427:LEU:HD11 | 1.92 | 0.95 |
| 1:A:430:VAL:HG12 | 1:A:434:TYR:CE2 | 2.01 | 0.94 |
| 1:C:432:ARG:CD | 1:C:476:THR:CB | 2.46 | 0.94 |
| 1:D:42:ARG:CZ | 1:D:247:ASP:CG | 2.36 | 0.94 |
| 1:D:387:PHE:HA | 1:D:429:GLN:CD | 1.88 | 0.93 |
| 1:B:49:ALA:CB | 1:B:249:ILE:CG2 | 2.45 | 0.93 |
| 1:C:429:GLN:O | 1:C:433:PHE:CD2 | 2.22 | 0.93 |
| 1:D:395:LYS:HD2 | 1:D:526:ARG:NH1 | 1.81 | 0.93 |
| 1:C:511:TRP:HZ3 | 1:C:567:GLU:HG3 | 1.28 | 0.93 |
| 1:C:49:ALA:HB2 | 1:C:249:ILE:HG21 | 1.48 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:432:ARG:HD2 | 1:C:476:THR:CB | 1.98 | 0.93 |
| 1:C:515:PHE:HE1 | 1:C:569:ILE:CD1 | 1.81 | 0.93 |
| 1:B:49:ALA:HB2 | 1:B:249:ILE:HG21 | 1.49 | 0.93 |
| 1:B:432:ARG:NE | 1:B:437:PRO:HD2 | 1.83 | 0.93 |
| 1:A:114:GLU:OE1 | 1:A:118:ARG:NH1 | 2.02 | 0.92 |
| 1:C:432:ARG:HD3 | 1:C:476:THR:CA | 2.00 | 0.92 |
| 1:D:395:LYS:NZ | 1:D:526:ARG:HH11 | 1.67 | 0.92 |
| 1:D:41:ILE:HD12 | 1:D:227:MSE:HE3 | 1.51 | 0.92 |
| 1:B:429:GLN:O | 1:B:433:PHE:CD2 | 2.23 | 0.92 |
| 1:B:156:HIS:CE1 | 1:B:179:TYR:OH | 2.23 | 0.92 |
| 1:C:49:ALA:HB2 | 1:C:249:ILE:CG2 | 2.00 | 0.92 |
| 1:B:359:ASP:CB | 1:B:427:LEU:HD22 | 2.00 | 0.91 |
| 1:D:395:LYS:CD | 1:D:526:ARG:HH11 | 1.75 | 0.91 |
| 1:C:515:PHE:HE1 | 1:C:569:ILE:HD11 | 1.36 | 0.91 |
| 1:D:387:PHE:CA | 1:D:429:GLN:CD | 2.39 | 0.91 |
| 1:B:1:MSE:HB2 | 1:B:4:LYS:HG3 | 1.53 | 0.90 |
| 1:B:522:ASP:O | 1:B:526:ARG:HG3 | 1.70 | 0.90 |
| 1:A:356:LEU:CA | 1:A:427:LEU:HD12 | 2.00 | 0.89 |
| 1:D:395:LYS:HD3 | 1:D:526:ARG:NE | 1.87 | 0.89 |
| 1:A:49:ALA:CB | 1:A:249:ILE:HG21 | 2.02 | 0.89 |
| 1:C:528:LEU:CD1 | 1:C:560:LEU:CD2 | 2.50 | 0.89 |
| 1:C:418:VAL:C | 1:C:422:LYS:HE3 | 1.92 | 0.88 |
| 1:C:524:VAL:HG11 | 1:C:563:GLN:OE1 | 1.73 | 0.88 |
| 1:B:49:ALA:CB | 1:B:249:ILE:HG21 | 2.03 | 0.88 |
| 1:A:387:PHE:HB2 | 1:A:429:GLN:OE1 | 1.06 | 0.87 |
| 1:A:433:PHE:C | 1:A:437:PRO:HG2 | 1.94 | 0.87 |
| 1:C:524:VAL:HG12 | 1:C:563:GLN:OE1 | 1.73 | 0.86 |
| 1:C:430:VAL:CG1 | 1:C:434:TYR:CE2 | 2.54 | 0.86 |
| 1:D:430:VAL:HA | 1:D:433:PHE:HD2 | 1.40 | 0.86 |
| 1:B:432:ARG:HD2 | 1:B:437:PRO:HG2 | 1.55 | 0.86 |
| 1:D:60:ASP:OD1 | 1:B:315:TYR:OH | 1.92 | 0.86 |
| 1:D:363:ALA:CA | 1:D:434:TYR:OH | 2.21 | 0.86 |
| 1:D:74:ILE:HD13 | 1:C:1:MSE:SE | 2.26 | 0.86 |
| 1:B:395:LYS:HD3 | 1:B:526:ARG:CZ | 2.06 | 0.85 |
| 1:D:356:LEU:CA | 1:D:427:LEU:HD12 | 2.04 | 0.85 |
| 1:D:389:MSE:HE1 | 1:D:526:ARG:HA | 1.57 | 0.85 |
| 1:C:511:TRP:CH2 | 1:C:567:GLU:HG3 | 2.11 | 0.85 |
| 1:D:363:ALA:CB | 1:D:430:VAL:CG1 | 2.54 | 0.85 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:CD | 1.57 | 0.85 |
| 1:D:432:ARG:HD3 | 1:D:476:THR:CA | 2.06 | 0.85 |
| 1:A:429:GLN:O | 1:A:433:PHE:HD2 | 1.55 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:430:VAL:CG1 | 1:B:434:TYR:HE2 | 1.90 | 0.85 |
| 1:D:430:VAL:CG1 | 1:D:434:TYR:HE2 | 1.89 | 0.84 |
| 1:C:515:PHE:HZ | 1:C:578:ARG:NH1 | 1.75 | 0.84 |
| 1:D:387:PHE:HB2 | 1:D:429:GLN:CD | 1.97 | 0.84 |
| 1:A:363:ALA:CB | 1:A:430:VAL:HG13 | 2.08 | 0.84 |
| 1:C:45:LEU:HD11 | 1:C:231:MSE:HE3 | 1.60 | 0.84 |
| 1:A:359:ASP:CB | 1:A:427:LEU:HD22 | 2.08 | 0.83 |
| 1:A:356:LEU:HA | 1:A:427:LEU:HD12 | 1.60 | 0.83 |
| 1:B:395:LYS:HD3 | 1:B:526:ARG:NE | 1.92 | 0.83 |
| 1:C:432:ARG:NH2 | 1:C:477:ARG:CA | 2.36 | 0.83 |
| 1:A:9:ALA:HB3 | 1:C:9:ALA:HB3 | 1.61 | 0.83 |
| 1:C:565:ARG:HB3 | 1:C:565:ARG:CZ | 2.06 | 0.83 |
| 1:B:395:LYS:CD | 1:B:526:ARG:NH1 | 2.42 | 0.82 |
| 1:C:568:GLY:O | 1:C:578:ARG:CZ | 2.26 | 0.82 |
| 1:B:430:VAL:HG12 | 1:B:434:TYR:HE2 | 1.42 | 0.82 |
| 1:B:432:ARG:CZ | 1:B:437:PRO:CD | 2.58 | 0.82 |
| 1:D:264:GLN:HG2 | 1:D:272:PHE:H | 1.43 | 0.82 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:HD2 | 1.02 | 0.82 |
| 1:A:1:MSE:SE | 1:B:74:ILE:HD13 | 2.30 | 0.82 |
| 1:C:54:GLN:OE1 | 1:C:405:ARG:NH1 | 2.13 | 0.81 |
| 1:C:515:PHE:HZ | 1:C:578:ARG:HH11 | 1.27 | 0.81 |
| 1:C:528:LEU:HD11 | 1:C:560:LEU:HD23 | 1.61 | 0.81 |
| 1:D:429:GLN:O | 1:D:433:PHE:HD2 | 1.64 | 0.81 |
| 1:D:363:ALA:CB | 1:D:430:VAL:HG13 | 2.10 | 0.81 |
| 1:D:395:LYS:CE | 1:D:526:ARG:HH11 | 1.94 | 0.81 |
| 1:D:395:LYS:HZ1 | 1:D:526:ARG:CD | 1.65 | 0.81 |
| 1:C:565:ARG:HG3 | 1:C:570:TYR:CD2 | 2.14 | 0.81 |
| 1:B:391:GLN:HE21 | 1:B:422:LYS:HE3 | 1.40 | 0.81 |
| 1:D:522:ASP:O | 1:D:526:ARG:HG3 | 1.79 | 0.81 |
| 1:A:42:ARG:CZ | 1:A:247:ASP:OD1 | 2.29 | 0.81 |
| 1:C:528:LEU:HD12 | 1:C:560:LEU:CD2 | 2.09 | 0.81 |
| 1:D:9:ALA:HB3 | 1:B:9:ALA:HB3 | 1.63 | 0.81 |
| 1:D:72:ARG:NH2 | 1:C:1:MSE:HE1 | 1.96 | 0.81 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:NH1 | 1.78 | 0.81 |
| 1:B:387:PHE:HA | 1:B:429:GLN:CD | 2.02 | 0.80 |
| 1:D:430:VAL:HA | 1:D:433:PHE:CD2 | 2.17 | 0.80 |
| 1:A:74:ILE:CD1 | 1:B:1:MSE:SE | 2.80 | 0.80 |
| 1:A:363:ALA:CB | 1:A:430:VAL:CG1 | 2.59 | 0.80 |
| 1:A:389:MSE:HE1 | 1:A:526:ARG:HA | 1.64 | 0.80 |
| 1:A:42:ARG:NH2 | 1:A:247:ASP:CG | 2.36 | 0.79 |
| 1:B:156:HIS:HE1 | 1:B:179:TYR:OH | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:ALA:HB2 | 1:A:249:ILE:CG2 | 2.05 | 0.79 |
| 1:A:405:ARG:O | 1:A:409:THR:HG23 | 1.81 | 0.79 |
| 1:C:356:LEU:CB | 1:C:424:LEU:CD2 | 2.59 | 0.79 |
| 1:B:395:LYS:CD | 1:B:526:ARG:HH11 | 1.95 | 0.79 |
| 1:C:42:ARG:CZ | 1:C:247:ASP:OD1 | 2.29 | 0.79 |
| 1:A:363:ALA:HB2 | 1:A:430:VAL:CG1 | 2.12 | 0.79 |
| 1:B:422:LYS:HD2 | 1:B:422:LYS:N | 1.96 | 0.79 |
| 1:C:245:ARG:NH1 | 1:C:523:GLY:H | 1.62 | 0.79 |
| 1:A:432:ARG:CB | 1:A:432:ARG:HH21 | 1.95 | 0.78 |
| 1:B:395:LYS:HE2 | 1:B:526:ARG:HD3 | 1.64 | 0.78 |
| 1:B:405:ARG:O | 1:B:409:THR:HG23 | 1.82 | 0.78 |
| 1:B:391:GLN:HE22 | 1:B:422:LYS:HE3 | 0.96 | 0.78 |
| 1:B:106:LEU:O | 1:B:109:THR:HB | 1.83 | 0.78 |
| 1:B:346:LEU:O | 1:B:348:GLU:N | 2.16 | 0.78 |
| 1:D:363:ALA:HA | 1:D:434:TYR:HH | 1.46 | 0.78 |
| 1:B:387:PHE:N | 1:B:429:GLN:HE22 | 1.82 | 0.78 |
| 1:C:156:HIS:HE1 | 1:C:179:TYR:OH | 1.66 | 0.77 |
| 1:A:45:LEU:HB3 | 1:A:249:ILE:CD1 | 2.14 | 0.77 |
| 1:A:1:MSE:SE | 1:B:74:ILE:CD1 | 2.82 | 0.77 |
| 1:C:524:VAL:CG1 | 1:C:563:GLN:NE2 | 2.40 | 0.77 |
| 1:D:346:LEU:O | 1:D:348:GLU:N | 2.17 | 0.77 |
| 1:A:413:LYS:CB | 1:A:422:LYS:NZ | 2.47 | 0.77 |
| 1:D:260:SER:O | 1:D:264:GLN:NE2 | 2.18 | 0.77 |
| 1:A:431:ALA:O | 1:A:435:GLU:HG2 | 1.83 | 0.77 |
| 1:A:49:ALA:HB1 | 1:A:249:ILE:CG2 | 2.15 | 0.77 |
| 1:C:389:MSE:HE1 | 1:C:526:ARG:HA | 1.67 | 0.76 |
| 1:C:405:ARG:O | 1:C:409:THR:HG23 | 1.84 | 0.76 |
| 1:D:356:LEU:CB | 1:D:427:LEU:CD1 | 2.62 | 0.76 |
| 1:A:245:ARG:NH1 | 1:A:519:ALA:HB1 | 2.01 | 0.76 |
| 1:B:356:LEU:CB | 1:B:424:LEU:CD2 | 2.63 | 0.76 |
| 1:C:5:GLU:O | 1:C:7:PHE:N | 2.19 | 0.76 |
| 1:A:346:LEU:O | 1:A:348:GLU:N | 2.19 | 0.76 |
| 1:C:565:ARG:HA | 1:C:570:TYR:HB3 | 1.68 | 0.76 |
| 1:D:49:ALA:CB | 1:D:249:ILE:CG2 | 2.63 | 0.75 |
| 1:C:45:LEU:C | 1:C:249:ILE:HD13 | 2.07 | 0.75 |
| 1:C:484:LEU:HD13 | 1:C:490:VAL:HA | 1.68 | 0.75 |
| 1:D:42:ARG:CZ | 1:D:247:ASP:OD2 | 2.34 | 0.75 |
| 1:A:432:ARG:HA | 1:A:432:ARG:NH2 | 2.02 | 0.75 |
| 1:A:430:VAL:CG1 | 1:A:434:TYR:CE2 | 2.60 | 0.75 |
| 1:B:360:VAL:H | 1:B:427:LEU:CD2 | 1.99 | 0.74 |
| 1:B:395:LYS:CD | 1:B:526:ARG:CD | 2.43 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:432:ARG:CZ | 1:D:472:VAL:O | 2.35 | 0.74 |
| 1:D:1:MSE:HB2 | 1:D:4:LYS:HG3 | 1.70 | 0.74 |
| 1:C:245:ARG:NH2 | 1:C:523:GLY:HA2 | 1.94 | 0.74 |
| 1:D:395:LYS:CD | 1:D:526:ARG:CD | 2.57 | 0.74 |
| 1:A:432:ARG:O | 1:A:437:PRO:HD3 | 1.87 | 0.74 |
| 1:C:1:MSE:HB2 | 1:C:4:LYS:HG3 | 1.70 | 0.74 |
| 1:A:42:ARG:CZ | 1:A:247:ASP:CG | 2.56 | 0.74 |
| 1:D:99:GLN:O | 1:D:103:THR:HG23 | 1.88 | 0.74 |
| 1:D:232:ARG:O | 1:D:236:ARG:CB | 2.36 | 0.73 |
| 1:B:387:PHE:CA | 1:B:429:GLN:CD | 2.56 | 0.73 |
| 1:C:245:ARG:HH12 | 1:C:522:ASP:C | 1.88 | 0.73 |
| 1:B:15:SER:O | 1:B:19:SER:OG | 2.07 | 0.73 |
| 1:B:395:LYS:HD3 | 1:B:526:ARG:NH1 | 2.02 | 0.73 |
| 1:C:251:LEU:HD23 | 1:C:291:ARG:HB3 | 1.71 | 0.73 |
| 1:D:363:ALA:CB | 1:D:430:VAL:HG11 | 2.16 | 0.73 |
| 1:B:432:ARG:CZ | 1:B:437:PRO:CG | 2.66 | 0.73 |
| 1:C:511:TRP:CD1 | 1:C:521:ILE:HG13 | 2.24 | 0.73 |
| 1:B:430:VAL:HG12 | 1:B:434:TYR:CE2 | 2.23 | 0.73 |
| 1:B:390:PHE:HB2 | 1:B:429:GLN:NE2 | 2.03 | 0.73 |
| 1:B:387:PHE:HB2 | 1:B:429:GLN:CD | 2.09 | 0.72 |
| 1:B:432:ARG:CD | 1:B:437:PRO:HG2 | 2.18 | 0.72 |
| 1:C:46:SER:N | 1:C:249:ILE:HD13 | 2.04 | 0.72 |
| 1:C:452:LEU:HA | 1:C:502:ARG:NH2 | 2.04 | 0.72 |
| 1:D:430:VAL:HG12 | 1:D:434:TYR:HE2 | 1.53 | 0.72 |
| 1:B:5:GLU:O | 1:B:7:PHE:N | 2.23 | 0.72 |
| 1:B:244:LYS:HD2 | 1:B:248:ASP:CB | 2.20 | 0.72 |
| 1:D:237:LYS:O | 1:D:239:VAL:N | 2.21 | 0.72 |
| 1:B:1:MSE:O | 1:B:3:THR:N | 2.22 | 0.72 |
| 1:C:510:LEU:O | 1:C:514:SER:N | 2.23 | 0.72 |
| 1:A:64:PHE:HZ | 1:C:7:PHE:HE1 | 1.37 | 0.71 |
| 1:A:68:VAL:HG11 | 1:A:101:MSE:HE3 | 1.72 | 0.71 |
| 1:C:430:VAL:HG13 | 1:C:434:TYR:HE2 | 1.53 | 0.71 |
| 1:D:395:LYS:HD3 | 1:D:526:ARG:CD | 2.20 | 0.71 |
| 1:A:433:PHE:CA | 1:A:437:PRO:CG | 2.58 | 0.71 |
| 1:B:430:VAL:HA | 1:B:433:PHE:HD2 | 1.56 | 0.71 |
| 1:C:156:HIS:CE1 | 1:C:179:TYR:OH | 2.43 | 0.71 |
| 1:B:389:MSE:HE1 | 1:B:526:ARG:HA | 1.72 | 0.71 |
| 1:D:41:ILE:HG23 | 1:D:231:MSE:HE3 | 1.71 | 0.71 |
| 1:C:114:GLU:OE1 | 1:C:118:ARG:NH1 | 2.20 | 0.71 |
| 1:C:484:LEU:HD11 | 1:C:493:SER:OG | 1.91 | 0.71 |
| 1:B:260:SER:O | 1:B:264:GLN:NE2 | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:49:ALA:HB2 | 1:D:249:ILE:HG21 | 1.73 | 0.70 |
| 1:A:63:CYS:HB3 | 1:A:303:VAL:HB | 1.72 | 0.70 |
| 1:D:1:MSE:O | 1:D:3:THR:N | 2.25 | 0.70 |
| 1:D:106:LEU:O | 1:D:109:THR:HB | 1.91 | 0.70 |
| 1:B:391:GLN:HE22 | 1:B:422:LYS:NZ | 1.88 | 0.70 |
| 1:B:49:ALA:HB2 | 1:B:249:ILE:CG2 | 2.17 | 0.70 |
| 1:B:432:ARG:CZ | 1:B:437:PRO:HD2 | 2.20 | 0.70 |
| 1:D:405:ARG:O | 1:D:409:THR:HG23 | 1.92 | 0.70 |
| 1:D:430:VAL:CA | 1:D:433:PHE:HD2 | 2.05 | 0.70 |
| 1:D:518:THR:O | 1:D:520:GLY:N | 2.25 | 0.70 |
| 1:A:432:ARG:HH21 | 1:A:432:ARG:CG | 2.05 | 0.70 |
| 1:C:49:ALA:CB | 1:C:249:ILE:HG23 | 2.22 | 0.70 |
| 1:C:260:SER:O | 1:C:264:GLN:NE2 | 2.25 | 0.70 |
| 1:B:432:ARG:NE | 1:B:437:PRO:CD | 2.55 | 0.70 |
| 1:A:391:GLN:NE2 | 1:A:422:LYS:HG2 | 2.07 | 0.69 |
| 1:B:390:PHE:HB2 | 1:B:429:GLN:HE21 | 1.57 | 0.69 |
| 1:C:49:ALA:CB | 1:C:249:ILE:HG21 | 2.14 | 0.69 |
| 1:C:524:VAL:HG13 | 1:C:563:GLN:HE22 | 1.57 | 0.69 |
| 1:A:264:GLN:HG2 | 1:A:272:PHE:H | 1.57 | 0.69 |
| 1:C:42:ARG:NE | 1:C:247:ASP:CG | 2.41 | 0.69 |
| 1:C:515:PHE:CE1 | 1:C:569:ILE:HD11 | 2.25 | 0.69 |
| 1:D:74:ILE:HD13 | 1:C:1:MSE:CE | 2.23 | 0.69 |
| 1:D:26:TYR:CE2 | 1:D:79:VAL:HA | 2.27 | 0.69 |
| 1:A:49:ALA:CB | 1:A:249:ILE:HG23 | 2.20 | 0.69 |
| 1:C:429:GLN:O | 1:C:433:PHE:HD2 | 1.75 | 0.69 |
| 1:C:528:LEU:HD12 | 1:C:560:LEU:HD23 | 1.62 | 0.69 |
| 1:D:356:LEU:CB | 1:D:427:LEU:HD12 | 2.22 | 0.69 |
| 1:D:359:ASP:CB | 1:D:427:LEU:CD2 | 2.50 | 0.69 |
| 1:D:356:LEU:CB | 1:D:424:LEU:HD23 | 2.23 | 0.68 |
| 1:A:1:MSE:HB2 | 1:A:4:LYS:HG3 | 1.76 | 0.68 |
| 1:A:265:PHE:CE1 | 1:A:271:GLU:HB2 | 2.27 | 0.68 |
| 1:D:34:TYR:OH | 1:D:103:THR:HG22 | 1.92 | 0.68 |
| 1:A:389:MSE:SE | 1:A:526:ARG:HG2 | 2.43 | 0.68 |
| 1:C:515:PHE:CE2 | 1:C:578:ARG:CD | 2.65 | 0.68 |
| 1:C:563:GLN:O | 1:C:566:SER:OG | 2.07 | 0.68 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:CZ | 2.07 | 0.67 |
| 1:D:430:VAL:HG12 | 1:D:434:TYR:CE2 | 2.29 | 0.67 |
| 1:C:26:TYR:CE2 | 1:C:79:VAL:HA | 2.28 | 0.67 |
| 1:A:391:GLN:NE2 | 1:A:422:LYS:CG | 2.57 | 0.67 |
| 1:C:69:ILE:HA | 1:C:308:VAL:HG23 | 1.75 | 0.67 |
| 1:D:429:GLN:O | 1:D:433:PHE:CE2 | 2.47 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:360:VAL:H | 1:C:427:LEU:CD2 | 2.08 | 0.67 |
| 1:D:5:GLU:O | 1:D:7:PHE:N | 2.27 | 0.67 |
| 1:D:135:GLN:O | 1:D:139:VAL:HG23 | 1.95 | 0.67 |
| 1:B:429:GLN:O | 1:B:433:PHE:HD2 | 1.77 | 0.67 |
| 1:C:515:PHE:CE1 | 1:C:578:ARG:CD | 2.69 | 0.67 |
| 1:C:390:PHE:HB2 | 1:C:429:GLN:HE21 | 1.60 | 0.67 |
| 1:B:395:LYS:HD2 | 1:B:526:ARG:NH1 | 2.10 | 0.67 |
| 1:A:432:ARG:N | 1:A:432:ARG:HD2 | 2.09 | 0.67 |
| 1:D:395:LYS:HE2 | 1:D:526:ARG:CD | 1.95 | 0.67 |
| 1:B:45:LEU:HB3 | 1:B:249:ILE:CD1 | 2.25 | 0.67 |
| 1:B:45:LEU:C | 1:B:249:ILE:HD13 | 2.15 | 0.66 |
| 1:C:245:ARG:HH12 | 1:C:523:GLY:CA | 2.06 | 0.66 |
| 1:D:52:LEU:HD13 | 1:D:252:PRO:HD2 | 1.77 | 0.66 |
| 1:D:105:LEU:O | 1:D:108:THR:OG1 | 2.13 | 0.66 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:HH11 | 1.31 | 0.66 |
| 1:D:264:GLN:HG3 | 1:D:272:PHE:CD1 | 2.30 | 0.66 |
| 1:D:397:THR:O | 1:D:399:ARG:N | 2.28 | 0.66 |
| 1:B:418:VAL:O | 1:B:422:LYS:HD3 | 1.96 | 0.66 |
| 1:D:395:LYS:HZ3 | 1:D:526:ARG:NE | 1.94 | 0.66 |
| 1:A:432:ARG:O | 1:A:437:PRO:CD | 2.44 | 0.66 |
| 1:D:360:VAL:H | 1:D:427:LEU:CD2 | 2.09 | 0.66 |
| 1:D:395:LYS:HZ1 | 1:D:526:ARG:HD2 | 0.84 | 0.66 |
| 1:D:66:GLY:HA2 | 1:B:322:ALA:HB1 | 1.77 | 0.65 |
| 1:D:476:THR:O | 1:D:480:ALA:HB2 | 1.95 | 0.65 |
| 1:A:69:ILE:HA | 1:A:308:VAL:HG23 | 1.78 | 0.65 |
| 1:B:156:HIS:CE1 | 1:B:179:TYR:CZ | 2.84 | 0.65 |
| 1:C:46:SER:N | 1:C:249:ILE:CD1 | 2.59 | 0.65 |
| 1:A:9:ALA:HB2 | 1:A:308:VAL:HG12 | 1.76 | 0.65 |
| 1:B:387:PHE:HA | 1:B:429:GLN:HE22 | 0.52 | 0.65 |
| 1:A:245:ARG:HH11 | 1:A:519:ALA:HB1 | 1.61 | 0.65 |
| 1:C:515:PHE:CE1 | 1:C:569:ILE:CD1 | 2.72 | 0.65 |
| 1:C:15:SER:O | 1:C:19:SER:OG | 2.09 | 0.65 |
| 1:C:486:SER:O | 1:C:488:GLU:N | 2.28 | 0.65 |
| 1:C:564:LEU:O | 1:C:569:ILE:HG22 | 1.96 | 0.65 |
| 1:C:61:SER:HB2 | 1:C:405:ARG:HH12 | 1.62 | 0.65 |
| 1:A:45:LEU:HD11 | 1:A:231:MSE:HE3 | 1.77 | 0.65 |
| 1:B:357:HIS:HA | 1:B:427:LEU:HD21 | 1.79 | 0.65 |
| 1:B:387:PHE:N | 1:B:429:GLN:NE2 | 2.42 | 0.65 |
| 1:B:41:ILE:HD12 | 1:B:227:MSE:HE3 | 1.79 | 0.64 |
| 1:B:26:TYR:CE2 | 1:B:79:VAL:HA | 2.32 | 0.64 |
| 1:D:286:MSE:O | 1:D:290:THR:OG1 | 2.15 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1:MSE:O | 1:A:3:THR:N | 2.30 | 0.64 |
| 1:C:26:TYR:OH | 1:C:80:GLU:HB2 | 1.97 | 0.64 |
| 1:D:139:VAL:HG21 | 1:D:293:ILE:HG23 | 1.78 | 0.64 |
| 1:A:69:ILE:HD13 | 1:A:319:MSE:HE3 | 1.80 | 0.64 |
| 1:C:397:THR:O | 1:C:399:ARG:N | 2.30 | 0.64 |
| 1:C:515:PHE:CZ | 1:C:578:ARG:NH1 | 2.64 | 0.64 |
| 1:C:507:PHE:CD1 | 1:C:564:LEU:HD21 | 2.33 | 0.64 |
| 1:C:524:VAL:HG11 | 1:C:563:GLN:CD | 2.10 | 0.63 |
| 1:B:114:GLU:OE1 | 1:B:118:ARG:NH1 | 2.31 | 0.63 |
| 1:C:34:TYR:OH | 1:C:103:THR:HG22 | 1.99 | 0.63 |
| 1:C:432:ARG:O | 1:C:437:PRO:HD2 | 1.98 | 0.63 |
| 1:D:49:ALA:CB | 1:D:249:ILE:HG21 | 2.29 | 0.63 |
| 1:C:257:ILE:HD13 | 1:C:294:VAL:HG21 | 1.81 | 0.63 |
| 1:C:147:PHE:HB2 | 1:C:148:GLU:HG2 | 1.81 | 0.62 |
| 1:A:253:THR:HA | 1:A:291:ARG:HD2 | 1.81 | 0.62 |
| 1:A:227:MSE:O | 1:A:231:MSE:HG3 | 1.99 | 0.62 |
| 1:D:356:LEU:C | 1:D:427:LEU:CD1 | 2.01 | 0.62 |
| 1:A:476:THR:O | 1:A:480:ALA:HB2 | 1.98 | 0.62 |
| 1:C:486:SER:HA | 1:C:490:VAL:HG23 | 1.81 | 0.62 |
| 1:D:68:VAL:HG11 | 1:D:101:MSE:HE2 | 1.80 | 0.62 |
| 1:D:387:PHE:CA | 1:D:429:GLN:OE1 | 2.46 | 0.62 |
| 1:D:273:PRO:HB2 | 1:D:276:VAL:HB | 1.82 | 0.62 |
| 1:D:363:ALA:HB1 | 1:D:430:VAL:HG13 | 1.80 | 0.62 |
| 1:A:356:LEU:CB | 1:A:424:LEU:HD23 | 2.30 | 0.62 |
| 1:B:387:PHE:CA | 1:B:429:GLN:OE1 | 2.47 | 0.62 |
| 1:C:395:LYS:HD3 | 1:C:526:ARG:NH2 | 2.15 | 0.61 |
| 1:C:486:SER:HB3 | 1:C:487:PRO:HD2 | 1.81 | 0.61 |
| 1:D:90:LYS:HE2 | 1:D:92:MSE:HE2 | 1.80 | 0.61 |
| 1:A:41:ILE:HD12 | 1:A:227:MSE:HE3 | 1.82 | 0.61 |
| 1:A:433:PHE:O | 1:A:437:PRO:HG2 | 2.01 | 0.61 |
| 1:C:570:TYR:O | 1:C:571:ASP:OD1 | 2.18 | 0.61 |
| 1:A:432:ARG:O | 1:A:437:PRO:CG | 2.48 | 0.61 |
| 1:D:42:ARG:CZ | 1:D:247:ASP:OD1 | 2.49 | 0.61 |
| 1:A:237:LYS:O | 1:A:239:VAL:N | 2.34 | 0.61 |
| 1:A:436:GLY:N | 1:A:437:PRO:HD3 | 2.15 | 0.61 |
| 1:B:36:TRP:CE3 | 1:B:103:THR:HG21 | 2.36 | 0.61 |
| 1:C:45:LEU:HB3 | 1:C:249:ILE:CD1 | 2.31 | 0.61 |
| 1:C:76:TYR:HB2 | 1:C:82:LYS:HE3 | 1.83 | 0.61 |
| 1:D:387:PHE:CB | 1:D:429:GLN:CD | 2.56 | 0.61 |
| 1:D:430:VAL:CG1 | 1:D:434:TYR:CE2 | 2.79 | 0.61 |
| 1:B:383:VAL:HA | 1:B:433:PHE:CZ | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:42:ARG:NH1 | 1:C:247:ASP:OD1 | 2.33 | 0.61 |
| 1:C:112:HIS:CE1 | 1:C:140:THR:HG22 | 2.36 | 0.61 |
| 1:B:42:ARG:CZ | 1:B:247:ASP:OD2 | 2.48 | 0.60 |
| 1:C:36:TRP:CE3 | 1:C:103:THR:HG21 | 2.36 | 0.60 |
| 1:C:435:GLU:OE1 | 1:C:482:HIS:CE1 | 2.54 | 0.60 |
| 1:A:34:TYR:OH | 1:A:103:THR:HG22 | 2.01 | 0.60 |
| 1:D:429:GLN:C | 1:D:433:PHE:CD2 | 2.75 | 0.60 |
| 1:C:107:LEU:HD13 | 1:C:231:MSE:HE2 | 1.83 | 0.60 |
| 1:B:363:ALA:CB | 1:B:430:VAL:CG1 | 2.80 | 0.60 |
| 1:A:36:TRP:O | 1:A:227:MSE:HE2 | 2.01 | 0.60 |
| 1:C:565:ARG:HA | 1:C:570:TYR:CB | 2.30 | 0.60 |
| 1:C:569:ILE:O | 1:C:569:ILE:HG23 | 2.01 | 0.60 |
| 1:D:386:PRO:C | 1:D:429:GLN:NE2 | 2.54 | 0.60 |
| 1:D:17:PHE:CE2 | 1:D:101:MSE:HE3 | 2.37 | 0.60 |
| 1:D:287:THR:N | 1:D:288:PRO:HD2 | 2.17 | 0.60 |
| 1:A:356:LEU:C | 1:A:427:LEU:CD1 | 1.97 | 0.60 |
| 1:B:69:ILE:HA | 1:B:308:VAL:HG23 | 1.83 | 0.60 |
| 1:D:360:VAL:N | 1:D:427:LEU:CD2 | 2.65 | 0.59 |
| 1:A:123:THR:O | 1:A:125:ASP:N | 2.34 | 0.59 |
| 1:B:245:ARG:NH1 | 1:B:519:ALA:O | 2.32 | 0.59 |
| 1:D:389:MSE:HA | 1:D:393:GLY:HA2 | 1.83 | 0.59 |
| 1:A:118:ARG:O | 1:A:121:LYS:HG2 | 2.02 | 0.59 |
| 1:B:34:TYR:OH | 1:B:103:THR:HG22 | 2.02 | 0.59 |
| 1:C:28:PRO:HG2 | 1:C:31:GLN:HG2 | 1.84 | 0.59 |
| 1:A:39:PRO:O | 1:A:43:ARG:HG3 | 2.02 | 0.59 |
| 1:B:267:LEU:HD12 | 1:B:294:VAL:HG13 | 1.84 | 0.59 |
| 1:C:1:MSE:O | 1:C:3:THR:N | 2.34 | 0.59 |
| 1:A:5:GLU:O | 1:A:7:PHE:N | 2.36 | 0.59 |
| 1:D:249:ILE:HG22 | 1:D:250:GLN:N | 2.18 | 0.59 |
| 1:C:514:SER:HB3 | 1:C:575:TRP:CE3 | 2.36 | 0.59 |
| 1:D:128:PRO:O | 1:D:276:VAL:HG23 | 2.02 | 0.59 |
| 1:D:432:ARG:CD | 1:D:476:THR:CA | 2.78 | 0.59 |
| 1:C:245:ARG:CZ | 1:C:523:GLY:CA | 2.79 | 0.59 |
| 1:A:440:SER:O | 1:A:442:THR:N | 2.34 | 0.59 |
| 1:D:359:ASP:CA | 1:D:427:LEU:HD22 | 2.30 | 0.59 |
| 1:B:395:LYS:NZ | 1:B:526:ARG:HH11 | 2.01 | 0.59 |
| 1:A:60:ASP:OD1 | 1:A:61:SER:N | 2.34 | 0.59 |
| 1:A:397:THR:O | 1:A:399:ARG:N | 2.36 | 0.59 |
| 1:B:430:VAL:HA | 1:B:433:PHE:CD2 | 2.37 | 0.59 |
| 1:A:126:ASP:OD1 | 1:A:127:GLU:N | 2.36 | 0.58 |
| 1:C:106:LEU:O | 1:C:109:THR:HB | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:26:TYR:CE2 | 1:A:79:VAL:HA | 2.37 | 0.58 |
| 1:A:99:GLN:O | 1:A:103:THR:HG23 | 2.02 | 0.58 |
| 1:B:367:ARG:O | 1:B:379:VAL:HG21 | 2.03 | 0.58 |
| 1:B:432:ARG:NH2 | 1:B:437:PRO:HG3 | 2.18 | 0.58 |
| 1:A:38:LEU:N | 1:A:227:MSE:HE1 | 2.17 | 0.58 |
| 1:A:413:LYS:CB | 1:A:422:LYS:HZ1 | 2.16 | 0.58 |
| 1:B:363:ALA:CB | 1:B:430:VAL:HG13 | 2.34 | 0.58 |
| 1:C:570:TYR:O | 1:C:571:ASP:CB | 2.51 | 0.58 |
| 1:A:1:MSE:SE | 1:B:74:ILE:HD11 | 2.52 | 0.58 |
| 1:C:528:LEU:HD12 | 1:C:560:LEU:HD21 | 1.84 | 0.58 |
| 1:C:52:LEU:HD13 | 1:C:252:PRO:HD2 | 1.85 | 0.58 |
| 1:D:1:MSE:SE | 1:C:74:ILE:HD13 | 2.54 | 0.58 |
| 1:A:267:LEU:HD12 | 1:A:294:VAL:HG13 | 1.86 | 0.58 |
| 1:C:50:HIS:HB2 | 1:C:399:ARG:NH1 | 2.19 | 0.58 |
| 1:D:5:GLU:OE2 | 1:D:311:LYS:HE2 | 2.04 | 0.58 |
| 1:A:383:VAL:HA | 1:A:433:PHE:CZ | 2.38 | 0.58 |
| 1:B:42:ARG:CZ | 1:B:247:ASP:CG | 2.72 | 0.58 |
| 1:A:42:ARG:HG3 | 1:A:234:MSE:SE | 2.54 | 0.57 |
| 1:C:92:MSE:HE1 | 1:C:309:THR:OG1 | 2.04 | 0.57 |
| 1:B:357:HIS:CA | 1:B:427:LEU:HD21 | 2.35 | 0.57 |
| 1:C:575:TRP:CE3 | 1:C:579:ALA:HB2 | 2.38 | 0.57 |
| 1:D:42:ARG:NH2 | 1:D:247:ASP:CG | 2.47 | 0.57 |
| 1:B:237:LYS:O | 1:B:239:VAL:N | 2.37 | 0.57 |
| 1:C:41:ILE:HD12 | 1:C:227:MSE:HE3 | 1.86 | 0.57 |
| 1:C:430:VAL:HG13 | 1:C:434:TYR:CE2 | 2.34 | 0.57 |
| 1:B:34:TYR:CE1 | 1:B:36:TRP:HB2 | 2.38 | 0.57 |
| 1:C:418:VAL:O | 1:C:422:LYS:CD | 2.52 | 0.57 |
| 1:C:430:VAL:HA | 1:C:433:PHE:HD2 | 1.69 | 0.57 |
| 1:D:126:ASP:OD1 | 1:D:127:GLU:N | 2.38 | 0.57 |
| 1:A:41:ILE:CD1 | 1:A:227:MSE:HE3 | 2.34 | 0.57 |
| 1:A:390:PHE:HB2 | 1:A:429:GLN:HE21 | 1.68 | 0.57 |
| 1:C:395:LYS:HB2 | 1:C:526:ARG:HH21 | 1.70 | 0.57 |
| 1:C:518:THR:O | 1:C:520:GLY:N | 2.37 | 0.57 |
| 1:B:397:THR:O | 1:B:399:ARG:N | 2.37 | 0.57 |
| 1:D:36:TRP:CE3 | 1:D:103:THR:HG21 | 2.40 | 0.57 |
| 1:B:42:ARG:CZ | 1:B:247:ASP:OD1 | 2.53 | 0.57 |
| 1:C:245:ARG:NH1 | 1:C:523:GLY:CA | 2.66 | 0.56 |
| 1:D:96:ASP:HB2 | 1:D:320:PHE:CD2 | 2.40 | 0.56 |
| 1:C:11:PRO:O | 1:C:12:LEU:HD23 | 2.05 | 0.56 |
| 1:C:118:ARG:O | 1:C:121:LYS:HG2 | 2.05 | 0.56 |
| 1:B:38:LEU:HA | 1:B:227:MSE:HE1 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:62:ILE:HG23 | 1:B:302:ARG:O | 2.05 | 0.56 |
| 1:C:435:GLU:OE1 | 1:C:482:HIS:HE1 | 1.88 | 0.56 |
| 1:C:565:ARG:HB3 | 1:C:565:ARG:NH2 | 2.20 | 0.56 |
| 1:A:244:LYS:O | 1:A:246:GLU:N | 2.37 | 0.56 |
| 1:B:42:ARG:NH2 | 1:B:247:ASP:CG | 2.56 | 0.56 |
| 1:D:321:GLU:O | 1:D:325:THR:HG22 | 2.05 | 0.56 |
| 1:A:391:GLN:CD | 1:A:422:LYS:HG2 | 2.25 | 0.56 |
| 1:B:264:GLN:HG2 | 1:B:272:PHE:H | 1.70 | 0.56 |
| 1:D:38:LEU:N | 1:D:227:MSE:HE1 | 2.20 | 0.56 |
| 1:B:391:GLN:NE2 | 1:B:422:LYS:NZ | 2.49 | 0.56 |
| 1:D:432:ARG:NH2 | 1:D:472:VAL:O | 2.39 | 0.56 |
| 1:B:223:HIS:O | 1:B:227:MSE:HG2 | 2.05 | 0.56 |
| 1:C:568:GLY:O | 1:C:578:ARG:NH2 | 2.39 | 0.56 |
| 1:C:132:CYS:SG | 1:C:290:THR:HG23 | 2.46 | 0.56 |
| 1:D:249:ILE:CG2 | 1:D:250:GLN:N | 2.69 | 0.56 |
| 1:A:109:THR:O | 1:A:174:LYS:NZ | 2.34 | 0.56 |
| 1:D:49:ALA:HB2 | 1:D:249:ILE:CG2 | 2.33 | 0.55 |
| 1:A:42:ARG:NE | 1:A:247:ASP:OD1 | 2.39 | 0.55 |
| 1:B:113:GLU:HG3 | 1:B:114:GLU:N | 2.21 | 0.55 |
| 1:C:511:TRP:CH2 | 1:C:567:GLU:CG | 2.86 | 0.55 |
| 1:B:136:ALA:O | 1:B:140:THR:OG1 | 2.23 | 0.55 |
| 1:C:411:PHE:CE1 | 1:C:419:ALA:HB1 | 2.41 | 0.55 |
| 1:C:515:PHE:CD1 | 1:C:578:ARG:HB3 | 2.41 | 0.55 |
| 1:B:360:VAL:N | 1:B:427:LEU:CD2 | 2.67 | 0.55 |
| 1:A:45:LEU:HB3 | 1:A:249:ILE:HD11 | 1.88 | 0.55 |
| 1:C:515:PHE:HE1 | 1:C:569:ILE:HD12 | 1.70 | 0.55 |
| 1:B:46:SER:N | 1:B:249:ILE:HD13 | 2.21 | 0.55 |
| 1:C:490:VAL:O | 1:C:493:SER:OG | 2.22 | 0.55 |
| 1:D:287:THR:H | 1:D:288:PRO:HD2 | 1.71 | 0.55 |
| 1:A:389:MSE:HA | 1:A:393:GLY:HA2 | 1.89 | 0.55 |
| 1:B:363:ALA:HB2 | 1:B:430:VAL:CG1 | 2.36 | 0.55 |
| 1:C:511:TRP:CZ3 | 1:C:567:GLU:CG | 2.62 | 0.55 |
| 1:B:128:PRO:HG2 | 1:B:275:SER:CB | 2.37 | 0.54 |
| 1:B:432:ARG:HE | 1:B:437:PRO:HD2 | 1.70 | 0.54 |
| 1:A:331:THR:O | 1:A:334:GLU:N | 2.39 | 0.54 |
| 1:B:126:ASP:OD1 | 1:B:127:GLU:N | 2.39 | 0.54 |
| 1:C:123:THR:O | 1:C:125:ASP:N | 2.41 | 0.54 |
| 1:C:243:VAL:O | 1:C:244:LYS:HG3 | 2.06 | 0.54 |
| 1:A:64:PHE:CZ | 1:C:7:PHE:HE1 | 2.21 | 0.54 |
| 1:A:518:THR:O | 1:A:520:GLY:N | 2.40 | 0.54 |
| 1:C:155:GLU:O | 1:C:157:ARG:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:GLU:O | 1:A:129:SER:N | 2.41 | 0.54 |
| 1:A:432:ARG:HH21 | 1:A:432:ARG:CA | 2.20 | 0.54 |
| 1:B:246:GLU:O | 1:B:247:ASP:OD1 | 2.26 | 0.54 |
| 1:D:42:ARG:NH1 | 1:D:247:ASP:OD1 | 2.41 | 0.54 |
| 1:A:430:VAL:HG13 | 1:A:434:TYR:HE2 | 1.63 | 0.54 |
| 1:A:42:ARG:NE | 1:A:247:ASP:CG | 2.61 | 0.54 |
| 1:B:432:ARG:NH2 | 1:B:437:PRO:CG | 2.71 | 0.54 |
| 1:C:71:LEU:HD22 | 1:C:313:GLU:HB3 | 1.90 | 0.54 |
| 1:C:410:VAL:HG12 | 1:C:422:LYS:HG2 | 1.89 | 0.54 |
| 1:C:515:PHE:CD1 | 1:C:515:PHE:N | 2.76 | 0.53 |
| 1:D:72:ARG:HH21 | 1:C:1:MSE:HE1 | 1.71 | 0.53 |
| 1:D:432:ARG:CD | 1:D:476:THR:CB | 2.86 | 0.53 |
| 1:A:436:GLY:N | 1:A:437:PRO:CD | 2.72 | 0.53 |
| 1:C:49:ALA:HB3 | 1:C:249:ILE:CG2 | 2.36 | 0.53 |
| 1:C:156:HIS:HE1 | 1:C:179:TYR:CZ | 2.27 | 0.53 |
| 1:C:385:LEU:HD22 | 1:C:396:LEU:HB3 | 1.89 | 0.53 |
| 1:D:132:CYS:SG | 1:D:289:LEU:HD23 | 2.48 | 0.53 |
| 1:B:45:LEU:HB3 | 1:B:249:ILE:HD12 | 1.90 | 0.53 |
| 1:B:518:THR:O | 1:B:520:GLY:N | 2.40 | 0.53 |
| 1:C:515:PHE:CE1 | 1:C:569:ILE:HD12 | 2.42 | 0.53 |
| 1:A:299:LEU:HA | 1:A:303:VAL:CG1 | 2.38 | 0.53 |
| 1:B:264:GLN:HG3 | 1:B:272:PHE:CD1 | 2.44 | 0.53 |
| 1:B:299:LEU:HA | 1:B:303:VAL:HG13 | 1.89 | 0.53 |
| 1:D:148:GLU:OE2 | 1:D:179:TYR:CE1 | 2.62 | 0.53 |
| 1:A:432:ARG:HA | 1:A:432:ARG:CZ | 2.38 | 0.53 |
| 1:B:244:LYS:O | 1:B:246:GLU:N | 2.42 | 0.52 |
| 1:D:14:VAL:HG23 | 1:D:303:VAL:HG22 | 1.92 | 0.52 |
| 1:C:124:ARG:O | 1:C:124:ARG:NH1 | 2.43 | 0.52 |
| 1:D:5:GLU:OE1 | 1:D:311:LYS:HB2 | 2.08 | 0.52 |
| 1:B:63:CYS:HB3 | 1:B:303:VAL:HB | 1.90 | 0.52 |
| 1:C:5:GLU:OE2 | 1:C:311:LYS:HE2 | 2.09 | 0.52 |
| 1:C:113:GLU:HG3 | 1:C:114:GLU:N | 2.25 | 0.52 |
| 1:B:44:LEU:HD23 | 1:B:45:LEU:HD12 | 1.92 | 0.52 |
| 1:D:52:LEU:HD12 | 1:D:295:PHE:HD1 | 1.74 | 0.52 |
| 1:B:420:ARG:O | 1:B:424:LEU:HG | 2.10 | 0.52 |
| 1:C:127:GLU:O | 1:C:129:SER:N | 2.42 | 0.52 |
| 1:D:57:GLU:HG3 | 1:D:58:PHE:HD1 | 1.72 | 0.52 |
| 1:A:430:VAL:O | 1:A:434:TYR:CD2 | 2.62 | 0.52 |
| 1:C:565:ARG:NH2 | 1:C:565:ARG:CB | 2.73 | 0.52 |
| 1:B:131:TRP:O | 1:B:135:GLN:HG2 | 2.10 | 0.52 |
| 1:C:515:PHE:N | 1:C:515:PHE:HD1 | 2.07 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:7:PHE:HE1 | 1:B:64:PHE:HZ | 1.57 | 0.52 |
| 1:A:69:ILE:HG12 | 1:A:308:VAL:CG2 | 2.39 | 0.52 |
| 1:C:452:LEU:HA | 1:C:502:ARG:HH22 | 1.74 | 0.52 |
| 1:B:430:VAL:CG1 | 1:B:434:TYR:CE2 | 2.81 | 0.51 |
| 1:C:314:ASP:OD1 | 1:C:315:TYR:N | 2.43 | 0.51 |
| 1:A:28:PRO:HG2 | 1:A:31:GLN:HG2 | 1.92 | 0.51 |
| 1:A:49:ALA:HB1 | 1:A:249:ILE:HG22 | 1.90 | 0.51 |
| 1:B:476:THR:O | 1:B:480:ALA:HB2 | 2.10 | 0.51 |
| 1:C:5:GLU:OE1 | 1:C:311:LYS:HB2 | 2.10 | 0.51 |
| 1:C:360:VAL:N | 1:C:427:LEU:CD2 | 2.73 | 0.51 |
| 1:D:52:LEU:HD22 | 1:D:252:PRO:HG3 | 1.93 | 0.51 |
| 1:B:147:PHE:HB2 | 1:B:148:GLU:HG2 | 1.93 | 0.51 |
| 1:C:49:ALA:HB3 | 1:C:249:ILE:HG23 | 1.89 | 0.51 |
| 1:C:565:ARG:CZ | 1:C:565:ARG:CB | 2.85 | 0.51 |
| 1:C:54:GLN:NE2 | 1:C:405:ARG:HD2 | 2.25 | 0.51 |
| 1:D:181:SER:O | 1:D:183:ILE:N | 2.44 | 0.51 |
| 1:A:432:ARG:HG3 | 1:A:476:THR:HA | 1.91 | 0.51 |
| 1:C:52:LEU:HD21 | 1:C:294:VAL:HG12 | 1.91 | 0.51 |
| 1:D:429:GLN:C | 1:D:433:PHE:CE2 | 2.85 | 0.51 |
| 1:D:432:ARG:HH22 | 1:D:472:VAL:CB | 2.24 | 0.51 |
| 1:A:64:PHE:HZ | 1:C:7:PHE:CE1 | 2.23 | 0.51 |
| 1:B:9:ALA:HB2 | 1:B:308:VAL:HG12 | 1.92 | 0.51 |
| 1:C:68:VAL:HG11 | 1:C:101:MSE:HE2 | 1.92 | 0.51 |
| 1:C:528:LEU:HG | 1:C:563:GLN:NE2 | 2.25 | 0.51 |
| 1:C:49:ALA:CB | 1:C:249:ILE:HG22 | 2.37 | 0.51 |
| 1:B:156:HIS:HE1 | 1:B:179:TYR:CZ | 2.27 | 0.50 |
| 1:C:45:LEU:HD11 | 1:C:231:MSE:CE | 2.39 | 0.50 |
| 1:A:7:PHE:CZ | 1:C:306:ALA:HB2 | 2.46 | 0.50 |
| 1:C:430:VAL:O | 1:C:434:TYR:CD2 | 2.64 | 0.50 |
| 1:D:107:LEU:HA | 1:D:110:VAL:CG1 | 2.41 | 0.50 |
| 1:B:576:VAL:O | 1:B:579:ALA:HB3 | 2.10 | 0.50 |
| 1:D:124:ARG:HG3 | 1:D:125:ASP:OD1 | 2.11 | 0.50 |
| 1:B:23:GLN:HG3 | 1:B:90:LYS:HD3 | 1.93 | 0.50 |
| 1:C:46:SER:CA | 1:C:249:ILE:HD13 | 2.41 | 0.50 |
| 1:C:267:LEU:HD12 | 1:C:294:VAL:HG13 | 1.92 | 0.50 |
| 1:D:244:LYS:O | 1:D:246:GLU:N | 2.45 | 0.50 |
| 1:D:1:MSE:SE | 1:C:74:ILE:CD1 | 3.09 | 0.50 |
| 1:D:63:CYS:SG | 1:D:64:PHE:N | 2.84 | 0.50 |
| 1:D:576:VAL:O | 1:D:579:ALA:HB3 | 2.11 | 0.50 |
| 1:B:49:ALA:CB | 1:B:249:ILE:HG22 | 2.40 | 0.50 |
| 1:B:432:ARG:O | 1:B:432:ARG:HD3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:510:LEU:O | 1:C:514:SER:OG | 2.27 | 0.50 |
| 1:D:42:ARG:HG3 | 1:D:234:MSE:SE | 2.62 | 0.50 |
| 1:D:78:THR:HG21 | 1:D:93:THR:HG21 | 1.93 | 0.50 |
| 1:A:429:GLN:O | 1:A:433:PHE:CE2 | 2.64 | 0.50 |
| 1:B:49:ALA:HB3 | 1:B:249:ILE:CG2 | 2.38 | 0.50 |
| 1:A:395:LYS:NZ | 1:A:523:GLY:HA2 | 2.26 | 0.49 |
| 1:C:45:LEU:HB3 | 1:C:249:ILE:HD12 | 1.94 | 0.49 |
| 1:C:46:SER:CB | 1:C:249:ILE:HG12 | 2.42 | 0.49 |
| 1:C:507:PHE:HD1 | 1:C:564:LEU:HD21 | 1.75 | 0.49 |
| 1:A:321:GLU:O | 1:A:325:THR:HG22 | 2.12 | 0.49 |
| 1:A:363:ALA:HB3 | 1:A:430:VAL:CG1 | 2.41 | 0.49 |
| 1:C:389:MSE:HA | 1:C:393:GLY:HA2 | 1.93 | 0.49 |
| 1:D:118:ARG:O | 1:D:121:LYS:HG2 | 2.12 | 0.49 |
| 1:A:391:GLN:NE2 | 1:A:422:LYS:HG3 | 2.28 | 0.49 |
| 1:B:38:LEU:N | 1:B:227:MSE:HE1 | 2.26 | 0.49 |
| 1:B:99:GLN:O | 1:B:103:THR:HG23 | 2.13 | 0.49 |
| 1:C:424:LEU:HB3 | 1:C:483:ARG:NH2 | 2.28 | 0.49 |
| 1:A:126:ASP:OD1 | 1:A:129:SER:OG | 2.19 | 0.49 |
| 1:B:109:THR:HG23 | 1:B:174:LYS:HG3 | 1.95 | 0.49 |
| 1:C:424:LEU:C | 1:C:483:ARG:HH22 | 2.16 | 0.49 |
| 1:B:128:PRO:HG2 | 1:B:275:SER:HB3 | 1.95 | 0.49 |
| 1:B:430:VAL:CA | 1:B:433:PHE:HD2 | 2.24 | 0.49 |
| 1:D:17:PHE:O | 1:D:23:GLN:NE2 | 2.45 | 0.49 |
| 1:C:245:ARG:NH1 | 1:C:519:ALA:O | 2.46 | 0.49 |
| 1:B:46:SER:N | 1:B:249:ILE:CD1 | 2.76 | 0.49 |
| 1:C:128:PRO:HG2 | 1:C:275:SER:CB | 2.42 | 0.49 |
| 1:C:562:GLU:HG3 | 1:C:565:ARG:HH22 | 1.78 | 0.49 |
| 1:A:390:PHE:HB2 | 1:A:429:GLN:NE2 | 2.28 | 0.49 |
| 1:A:432:ARG:HH21 | 1:A:432:ARG:HA | 1.75 | 0.49 |
| 1:C:62:ILE:HG23 | 1:C:302:ARG:O | 2.13 | 0.49 |
| 1:C:379:VAL:O | 1:C:382:SER:OG | 2.08 | 0.49 |
| 1:C:455:GLN:CB | 1:C:502:ARG:HH21 | 2.24 | 0.49 |
| 1:C:315:TYR:O | 1:C:319:MSE:HB2 | 2.12 | 0.49 |
| 1:D:249:ILE:CG2 | 1:D:250:GLN:H | 2.26 | 0.48 |
| 1:A:44:LEU:HD23 | 1:A:45:LEU:HD12 | 1.95 | 0.48 |
| 1:A:363:ALA:CB | 1:A:430:VAL:HG11 | 2.40 | 0.48 |
| 1:C:243:VAL:O | 1:C:244:LYS:CG | 2.61 | 0.48 |
| 1:C:396:LEU:HD21 | 1:C:406:TYR:CB | 2.42 | 0.48 |
| 1:C:475:LEU:C | 1:C:477:ARG:H | 2.16 | 0.48 |
| 1:C:511:TRP:CG | 1:C:521:ILE:HG13 | 2.48 | 0.48 |
| 1:B:245:ARG:NH1 | 1:B:519:ALA:HA | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:559:TYR:O | 1:C:562:GLU:HB3 | 2.13 | 0.48 |
| 1:D:109:THR:HG22 | 1:D:110:VAL:N | 2.27 | 0.48 |
| 1:D:230:GLN:O | 1:D:234:MSE:HG3 | 2.13 | 0.48 |
| 1:D:257:ILE:HD13 | 1:D:294:VAL:HG21 | 1.95 | 0.48 |
| 1:D:306:ALA:HB2 | 1:B:7:PHE:CE1 | 2.48 | 0.48 |
| 1:A:62:ILE:HG22 | 1:A:63:CYS:O | 2.13 | 0.48 |
| 1:A:230:GLN:O | 1:A:234:MSE:HG3 | 2.12 | 0.48 |
| 1:C:72:ARG:HB2 | 1:C:309:THR:CG2 | 2.43 | 0.48 |
| 1:C:515:PHE:CG | 1:C:578:ARG:HB3 | 2.48 | 0.48 |
| 1:D:360:VAL:HA | 1:D:430:VAL:HG21 | 1.94 | 0.48 |
| 1:B:5:GLU:O | 1:B:6:ILE:C | 2.52 | 0.48 |
| 1:B:401:ASN:N | 1:B:401:ASN:OD1 | 2.46 | 0.48 |
| 1:C:131:TRP:O | 1:C:135:GLN:HG2 | 2.13 | 0.48 |
| 1:B:432:ARG:HH22 | 1:B:472:VAL:HA | 1.79 | 0.48 |
| 1:C:46:SER:HB3 | 1:C:249:ILE:HG12 | 1.96 | 0.48 |
| 1:C:418:VAL:CA | 1:C:422:LYS:HE3 | 2.43 | 0.48 |
| 1:B:104:LEU:HD11 | 1:B:299:LEU:HD11 | 1.96 | 0.48 |
| 1:C:430:VAL:O | 1:C:434:TYR:HD2 | 1.97 | 0.48 |
| 1:D:7:PHE:HB2 | 1:B:11:PRO:HG3 | 1.96 | 0.48 |
| 1:D:279:GLN:HB3 | 1:D:286:MSE:HE2 | 1.95 | 0.48 |
| 1:A:63:CYS:SG | 1:A:64:PHE:N | 2.87 | 0.48 |
| 1:B:69:ILE:HG12 | 1:B:308:VAL:CG2 | 2.44 | 0.48 |
| 1:C:264:GLN:HG3 | 1:C:272:PHE:CG | 2.49 | 0.48 |
| 1:C:480:ALA:O | 1:C:484:LEU:HG | 2.14 | 0.48 |
| 1:A:432:ARG:HH21 | 1:A:432:ARG:HG3 | 1.79 | 0.47 |
| 1:C:37:GLU:N | 1:C:37:GLU:OE1 | 2.46 | 0.47 |
| 1:D:430:VAL:O | 1:D:433:PHE:HB2 | 2.12 | 0.47 |
| 1:A:576:VAL:O | 1:A:579:ALA:HB3 | 2.15 | 0.47 |
| 1:D:268:PHE:HD2 | 1:D:272:PHE:HE1 | 1.61 | 0.47 |
| 1:A:109:THR:HG23 | 1:A:174:LYS:HG3 | 1.97 | 0.47 |
| 1:A:363:ALA:HB2 | 1:A:430:VAL:HG11 | 1.93 | 0.47 |
| 1:B:46:SER:HA | 1:B:249:ILE:HD13 | 1.95 | 0.47 |
| 1:C:395:LYS:HD3 | 1:C:526:ARG:HH22 | 1.79 | 0.47 |
| 1:D:430:VAL:HG13 | 1:D:434:TYR:HE2 | 1.73 | 0.47 |
| 1:A:45:LEU:HB3 | 1:A:249:ILE:HD13 | 1.94 | 0.47 |
| 1:A:322:ALA:HB1 | 1:C:66:GLY:HA2 | 1.97 | 0.47 |
| 1:C:388:ALA:HB1 | 1:C:394:THR:O | 2.14 | 0.47 |
| 1:D:69:ILE:HA | 1:D:308:VAL:HG23 | 1.96 | 0.47 |
| 1:C:60:ASP:OD1 | 1:C:61:SER:N | 2.48 | 0.47 |
| 1:D:45:LEU:HB3 | 1:D:249:ILE:CD1 | 2.45 | 0.47 |
| 1:D:48:VAL:HG23 | 1:D:303:VAL:HG11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:62:ILE:HG23 | 1:D:302:ARG:O | 2.14 | 0.47 |
| 1:D:68:VAL:CG1 | 1:D:101:MSE:HE2 | 2.44 | 0.47 |
| 1:D:253:THR:HG22 | 1:D:256:ASP:OD1 | 2.14 | 0.47 |
| 1:A:430:VAL:HG13 | 1:A:434:TYR:CE2 | 2.44 | 0.47 |
| 1:B:273:PRO:O | 1:B:276:VAL:HG12 | 2.15 | 0.47 |
| 1:D:129:SER:O | 1:D:132:CYS:HB3 | 2.15 | 0.47 |
| 1:A:78:THR:HG21 | 1:A:93:THR:OG1 | 2.14 | 0.47 |
| 1:A:430:VAL:HA | 1:A:433:PHE:HD2 | 1.79 | 0.47 |
| 1:B:127:GLU:O | 1:B:129:SER:N | 2.47 | 0.47 |
| 1:B:380:THR:O | 1:B:384:LEU:HG | 2.14 | 0.47 |
| 1:B:432:ARG:NE | 1:B:437:PRO:CG | 2.77 | 0.47 |
| 1:C:41:ILE:CD1 | 1:C:227:MSE:HE3 | 2.45 | 0.47 |
| 1:C:429:GLN:O | 1:C:433:PHE:CE2 | 2.68 | 0.47 |
| 1:C:486:SER:HA | 1:C:490:VAL:CG2 | 2.45 | 0.47 |
| 1:D:129:SER:H | 1:D:131:TRP:H | 1.62 | 0.46 |
| 1:D:234:MSE:HE2 | 1:D:234:MSE:HB3 | 1.88 | 0.46 |
| 1:D:360:VAL:N | 1:D:427:LEU:HD23 | 2.30 | 0.46 |
| 1:A:80:GLU:HB3 | 1:A:81:PRO:HD3 | 1.97 | 0.46 |
| 1:C:128:PRO:HG2 | 1:C:275:SER:HB2 | 1.97 | 0.46 |
| 1:C:528:LEU:HG | 1:C:563:GLN:HE22 | 1.80 | 0.46 |
| 1:D:299:LEU:HA | 1:D:303:VAL:HG13 | 1.96 | 0.46 |
| 1:B:129:SER:O | 1:B:132:CYS:HB3 | 2.14 | 0.46 |
| 1:D:243:VAL:O | 1:D:244:LYS:HG3 | 2.15 | 0.46 |
| 1:D:476:THR:O | 1:D:480:ALA:CB | 2.62 | 0.46 |
| 1:A:76:TYR:CB | 1:A:82:LYS:HE3 | 2.46 | 0.46 |
| 1:A:389:MSE:HE3 | 1:A:529:MSE:HG3 | 1.98 | 0.46 |
| 1:C:105:LEU:O | 1:C:108:THR:OG1 | 2.24 | 0.46 |
| 1:D:390:PHE:HB2 | 1:D:429:GLN:HE21 | 1.81 | 0.46 |
| 1:A:25:LEU:HD13 | 1:A:94:ILE:HD11 | 1.97 | 0.46 |
| 1:A:401:ASN:OD1 | 1:A:401:ASN:N | 2.49 | 0.46 |
| 1:C:34:TYR:OH | 1:C:41:ILE:HD11 | 2.15 | 0.46 |
| 1:C:514:SER:HB2 | 1:C:515:PHE:HD1 | 1.80 | 0.46 |
| 1:D:7:PHE:CE1 | 1:B:306:ALA:HB2 | 2.51 | 0.46 |
| 1:A:5:GLU:O | 1:A:6:ILE:C | 2.54 | 0.46 |
| 1:A:113:GLU:HG3 | 1:A:114:GLU:N | 2.30 | 0.46 |
| 1:C:156:HIS:CE1 | 1:C:179:TYR:CZ | 3.02 | 0.46 |
| 1:D:109:THR:HG23 | 1:D:174:LYS:HG3 | 1.97 | 0.46 |
| 1:D:150:ASP:O | 1:D:151:MSE:HG2 | 2.16 | 0.46 |
| 1:A:1:MSE:HB2 | 1:A:4:LYS:CG | 2.44 | 0.46 |
| 1:A:389:MSE:HE3 | 1:A:389:MSE:HB3 | 1.91 | 0.46 |
| 1:C:273:PRO:HB2 | 1:C:276:VAL:HB | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:432:ARG:HH21 | 1:C:477:ARG:HA | 1.74 | 0.46 |
| 1:A:18:LEU:HD13 | 1:A:105:LEU:HD13 | 1.98 | 0.46 |
| 1:B:390:PHE:CE2 | 1:B:477:ARG:HA | 2.51 | 0.46 |
| 1:A:262:ASN:O | 1:A:266:ALA:CB | 2.64 | 0.46 |
| 1:A:430:VAL:O | 1:A:434:TYR:HD2 | 1.99 | 0.46 |
| 1:C:71:LEU:HD12 | 1:C:310:ALA:O | 2.16 | 0.46 |
| 1:C:110:VAL:HB | 1:C:232:ARG:HA | 1.97 | 0.46 |
| 1:D:96:ASP:HB2 | 1:D:320:PHE:HD2 | 1.79 | 0.46 |
| 1:D:385:LEU:HD22 | 1:D:396:LEU:HB3 | 1.97 | 0.46 |
| 1:B:38:LEU:CA | 1:B:227:MSE:HE1 | 2.46 | 0.46 |
| 1:B:57:GLU:HG3 | 1:B:58:PHE:N | 2.31 | 0.46 |
| 1:D:155:GLU:O | 1:D:157:ARG:N | 2.49 | 0.46 |
| 1:A:363:ALA:HB3 | 1:A:430:VAL:HG13 | 1.93 | 0.46 |
| 1:C:349:TRP:O | 1:C:351:GLU:N | 2.49 | 0.46 |
| 1:C:430:VAL:HA | 1:C:433:PHE:CD2 | 2.50 | 0.46 |
| 1:C:367:ARG:O | 1:C:379:VAL:HG21 | 2.16 | 0.45 |
| 1:C:599:ALA:O | 1:C:601:GLN:N | 2.50 | 0.45 |
| 1:A:74:ILE:HD13 | 1:B:1:MSE:CE | 2.46 | 0.45 |
| 1:A:398:LYS:O | 1:A:403:GLN:NE2 | 2.49 | 0.45 |
| 1:A:476:THR:O | 1:A:480:ALA:CB | 2.63 | 0.45 |
| 1:A:574:GLN:O | 1:A:577:ALA:HB3 | 2.17 | 0.45 |
| 1:B:7:PHE:HZ | 1:B:323:LEU:HD11 | 1.80 | 0.45 |
| 1:C:49:ALA:HB1 | 1:C:249:ILE:CG2 | 2.38 | 0.45 |
| 1:C:245:ARG:HH11 | 1:C:522:ASP:HB2 | 1.81 | 0.45 |
| 1:B:85:SER:HA | 1:C:270:SER:CB | 2.46 | 0.45 |
| 1:B:88:PRO:HG2 | 1:B:91:VAL:CG2 | 2.45 | 0.45 |
| 1:B:395:LYS:HD2 | 1:B:526:ARG:HH11 | 1.72 | 0.45 |
| 1:C:363:ALA:HB2 | 1:C:430:VAL:CG1 | 2.47 | 0.45 |
| 1:D:260:SER:C | 1:D:264:GLN:NE2 | 2.69 | 0.45 |
| 1:D:264:GLN:HG3 | 1:D:272:PHE:CE1 | 2.52 | 0.45 |
| 1:A:265:PHE:HE1 | 1:A:271:GLU:HB2 | 1.77 | 0.45 |
| 1:B:485:SER:O | 1:B:487:PRO:N | 2.50 | 0.45 |
| 1:D:5:GLU:O | 1:D:6:ILE:C | 2.55 | 0.45 |
| 1:D:388:ALA:O | 1:D:393:GLY:HA2 | 2.17 | 0.45 |
| 1:A:112:HIS:HB3 | 1:A:174:LYS:NZ | 2.31 | 0.45 |
| 1:B:391:GLN:HE21 | 1:B:422:LYS:CE | 2.07 | 0.45 |
| 1:C:36:TRP:O | 1:C:227:MSE:HE2 | 2.17 | 0.45 |
| 1:C:264:GLN:H | 1:C:264:GLN:HE21 | 1.64 | 0.45 |
| 1:D:7:PHE:HB2 | 1:B:11:PRO:CG | 2.47 | 0.45 |
| 1:D:268:PHE:HD2 | 1:D:272:PHE:CE1 | 2.35 | 0.45 |
| 1:A:135:GLN:O | 1:A:139:VAL:HG23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:VAL:HG11 | 1:B:101:MSE:HE3 | 1.98 | 0.45 |
| 1:C:63:CYS:SG | 1:C:64:PHE:N | 2.89 | 0.45 |
| 1:A:84:ARG:HD2 | 1:A:87:VAL:CG1 | 2.47 | 0.45 |
| 1:A:420:ARG:O | 1:A:424:LEU:HG | 2.15 | 0.45 |
| 1:D:148:GLU:OE2 | 1:D:179:TYR:HE1 | 1.99 | 0.45 |
| 1:A:50:HIS:HB2 | 1:A:399:ARG:CZ | 2.47 | 0.45 |
| 1:A:139:VAL:HG21 | 1:A:293:ILE:HG23 | 1.98 | 0.45 |
| 1:C:46:SER:CA | 1:C:249:ILE:CD1 | 2.95 | 0.45 |
| 1:C:383:VAL:HG22 | 1:C:433:PHE:CE2 | 2.51 | 0.45 |
| 1:D:9:ALA:HB2 | 1:D:308:VAL:HG12 | 1.98 | 0.45 |
| 1:D:26:TYR:CZ | 1:D:79:VAL:HA | 2.51 | 0.45 |
| 1:D:390:PHE:CE2 | 1:D:477:ARG:HA | 2.52 | 0.45 |
| 1:A:432:ARG:HH21 | 1:A:432:ARG:HB3 | 1.80 | 0.45 |
| 1:B:68:VAL:HG11 | 1:B:101:MSE:CE | 2.46 | 0.45 |
| 1:B:257:ILE:HD13 | 1:B:294:VAL:HG21 | 1.99 | 0.45 |
| 1:C:321:GLU:O | 1:C:325:THR:HG22 | 2.17 | 0.45 |
| 1:C:486:SER:CB | 1:C:487:PRO:HD2 | 2.47 | 0.45 |
| 1:D:292:LEU:HD12 | 1:D:292:LEU:HA | 1.76 | 0.44 |
| 1:A:92:MSE:HE1 | 1:A:309:THR:OG1 | 2.16 | 0.44 |
| 1:D:38:LEU:HA | 1:D:227:MSE:HE1 | 1.99 | 0.44 |
| 1:A:396:LEU:HD23 | 1:A:396:LEU:HA | 1.67 | 0.44 |
| 1:B:422:LYS:N | 1:B:422:LYS:CD | 2.73 | 0.44 |
| 1:C:389:MSE:HE3 | 1:C:389:MSE:HB3 | 1.83 | 0.44 |
| 1:D:150:ASP:C | 1:D:151:MSE:HG2 | 2.38 | 0.44 |
| 1:A:113:GLU:O | 1:A:117:VAL:HG22 | 2.16 | 0.44 |
| 1:B:245:ARG:HH11 | 1:B:519:ALA:HA | 1.82 | 0.44 |
| 1:C:432:ARG:CZ | 1:C:479:PHE:CB | 2.90 | 0.44 |
| 1:C:515:PHE:CZ | 1:C:578:ARG:NE | 2.82 | 0.44 |
| 1:D:574:GLN:O | 1:D:577:ALA:HB3 | 2.18 | 0.44 |
| 1:C:514:SER:HB2 | 1:C:515:PHE:CD1 | 2.52 | 0.44 |
| 1:D:1:MSE:HB2 | 1:D:4:LYS:CG | 2.43 | 0.44 |
| 1:D:57:GLU:HG3 | 1:D:58:PHE:N | 2.32 | 0.44 |
| 1:A:62:ILE:HG12 | 1:C:315:TYR:OH | 2.17 | 0.44 |
| 1:A:487:PRO:O | 1:A:489:THR:N | 2.50 | 0.44 |
| 1:D:7:PHE:HB2 | 1:B:11:PRO:HD3 | 1.98 | 0.44 |
| 1:B:72:ARG:CZ | 1:B:90:LYS:HG3 | 2.48 | 0.44 |
| 1:A:436:GLY:H | 1:A:437:PRO:HD3 | 1.79 | 0.44 |
| 1:B:49:ALA:HB1 | 1:B:249:ILE:CG2 | 2.40 | 0.44 |
| 1:C:36:TRP:CD1 | 1:C:99:GLN:HB3 | 2.52 | 0.44 |
| 1:C:69:ILE:HG23 | 1:C:319:MSE:CE | 2.46 | 0.44 |
| 1:C:126:ASP:OD1 | 1:C:129:SER:OG | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:406:TYR:CE2 | 1:D:410:VAL:HG21 | 2.52 | 0.44 |
| 1:A:2:GLU:HG2 | 1:A:3:THR:H | 1.82 | 0.44 |
| 1:A:62:ILE:HD13 | 1:A:62:ILE:HA | 1.75 | 0.44 |
| 1:A:109:THR:HG22 | 1:A:110:VAL:N | 2.33 | 0.44 |
| 1:A:360:VAL:H | 1:A:427:LEU:CD2 | 2.31 | 0.44 |
| 1:B:395:LYS:HZ3 | 1:B:526:ARG:HH11 | 1.66 | 0.44 |
| 1:C:76:TYR:O | 1:C:79:VAL:HG12 | 2.17 | 0.44 |
| 1:C:244:LYS:HB2 | 1:C:248:ASP:CB | 2.48 | 0.44 |
| 1:C:528:LEU:CD1 | 1:C:560:LEU:HD21 | 2.43 | 0.44 |
| 1:C:575:TRP:CZ3 | 1:C:579:ALA:CB | 2.81 | 0.44 |
| 1:D:38:LEU:N | 1:D:39:PRO:HD2 | 2.33 | 0.44 |
| 1:A:1:MSE:HB2 | 1:A:4:LYS:CD | 2.48 | 0.44 |
| 1:A:445:PRO:O | 1:A:447:CYS:N | 2.44 | 0.44 |
| 1:A:49:ALA:HB3 | 1:A:249:ILE:HG23 | 1.97 | 0.43 |
| 1:A:319:MSE:HB3 | 1:A:319:MSE:HE2 | 1.43 | 0.43 |
| 1:B:128:PRO:HG2 | 1:B:275:SER:HB2 | 1.99 | 0.43 |
| 1:B:432:ARG:HD3 | 1:B:432:ARG:C | 2.39 | 0.43 |
| 1:C:475:LEU:O | 1:C:477:ARG:N | 2.49 | 0.43 |
| 1:D:11:PRO:O | 1:D:12:LEU:HD23 | 2.17 | 0.43 |
| 1:D:90:LYS:CE | 1:D:92:MSE:HE2 | 2.48 | 0.43 |
| 1:D:487:PRO:O | 1:D:489:THR:N | 2.44 | 0.43 |
| 1:A:391:GLN:HE22 | 1:A:422:LYS:HG3 | 1.82 | 0.43 |
| 1:B:46:SER:CA | 1:B:249:ILE:HD13 | 2.48 | 0.43 |
| 1:C:63:CYS:HB3 | 1:C:303:VAL:HB | 1.99 | 0.43 |
| 1:C:125:ASP:HA | 1:C:130:VAL:CG1 | 2.49 | 0.43 |
| 1:D:113:GLU:O | 1:D:117:VAL:HG22 | 2.18 | 0.43 |
| 1:B:60:ASP:OD1 | 1:B:61:SER:N | 2.51 | 0.43 |
| 1:C:2:GLU:O | 1:C:6:ILE:HD13 | 2.18 | 0.43 |
| 1:C:383:VAL:HA | 1:C:433:PHE:CZ | 2.53 | 0.43 |
| 1:C:477:ARG:C | 1:C:479:PHE:N | 2.72 | 0.43 |
| 1:D:36:TRP:CE2 | 1:D:40:LYS:HD3 | 2.53 | 0.43 |
| 1:D:62:ILE:HD13 | 1:D:62:ILE:HA | 1.83 | 0.43 |
| 1:D:72:ARG:HB3 | 1:D:311:LYS:HG2 | 2.00 | 0.43 |
| 1:A:96:ASP:HB2 | 1:A:320:PHE:CD2 | 2.53 | 0.43 |
| 1:B:28:PRO:HG2 | 1:B:31:GLN:HG2 | 1.99 | 0.43 |
| 1:C:395:LYS:HG3 | 1:C:395:LYS:O | 2.18 | 0.43 |
| 1:C:527:SER:C | 1:C:529:MSE:H | 2.21 | 0.43 |
| 1:D:482:HIS:HA | 1:D:494:ALA:HB1 | 2.00 | 0.43 |
| 1:B:369:GLY:O | 1:B:373:ALA:N | 2.51 | 0.43 |
| 1:C:112:HIS:NE2 | 1:C:140:THR:HG22 | 2.33 | 0.43 |
| 1:A:234:MSE:HB3 | 1:A:234:MSE:HE2 | 1.68 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:252:PRO:O | 1:A:291:ARG:HG2 | 2.17 | 0.43 |
| 1:B:96:ASP:HB2 | 1:B:320:PHE:CD1 | 2.53 | 0.43 |
| 1:C:427:LEU:O | 1:C:430:VAL:HB | 2.18 | 0.43 |
| 1:D:234:MSE:O | 1:D:235:LEU:C | 2.57 | 0.43 |
| 1:A:38:LEU:N | 1:A:39:PRO:HD2 | 2.34 | 0.43 |
| 1:C:115:ILE:HG12 | 1:C:292:LEU:HB3 | 2.01 | 0.43 |
| 1:C:122:LEU:HD23 | 1:C:122:LEU:HA | 1.80 | 0.43 |
| 1:D:64:PHE:CE1 | 1:B:7:PHE:HE1 | 2.37 | 0.43 |
| 1:D:363:ALA:CB | 1:D:434:TYR:OH | 2.66 | 0.43 |
| 1:A:54:GLN:OE1 | 1:A:405:ARG:NH1 | 2.51 | 0.43 |
| 1:C:401:ASN:OD1 | 1:C:401:ASN:N | 2.47 | 0.43 |
| 1:C:515:PHE:CZ | 1:C:578:ARG:CZ | 3.02 | 0.43 |
| 1:D:383:VAL:HA | 1:D:433:PHE:CZ | 2.54 | 0.43 |
| 1:A:62:ILE:HG23 | 1:A:302:ARG:O | 2.19 | 0.43 |
| 1:A:262:ASN:O | 1:A:266:ALA:HB2 | 2.19 | 0.43 |
| 1:D:223:HIS:O | 1:D:227:MSE:HG2 | 2.19 | 0.42 |
| 1:D:252:PRO:O | 1:D:291:ARG:HG2 | 2.19 | 0.42 |
| 1:A:107:LEU:HD13 | 1:A:231:MSE:HE2 | 2.00 | 0.42 |
| 1:A:380:THR:O | 1:A:384:LEU:HG | 2.19 | 0.42 |
| 1:A:432:ARG:NH2 | 1:A:432:ARG:CG | 2.72 | 0.42 |
| 1:B:395:LYS:CE | 1:B:526:ARG:HH11 | 2.31 | 0.42 |
| 1:D:71:LEU:HA | 1:D:310:ALA:O | 2.19 | 0.42 |
| 1:B:267:LEU:CD1 | 1:B:294:VAL:HG13 | 2.46 | 0.42 |
| 1:C:46:SER:HA | 1:C:249:ILE:HD13 | 2.01 | 0.42 |
| 1:C:113:GLU:HB3 | 1:C:174:LYS:NZ | 2.34 | 0.42 |
| 1:D:290:THR:O | 1:D:294:VAL:HG23 | 2.19 | 0.42 |
| 1:A:76:TYR:HB2 | 1:A:82:LYS:HE3 | 2.00 | 0.42 |
| 1:A:139:VAL:HG21 | 1:A:297:ASN:HD21 | 1.85 | 0.42 |
| 1:B:71:LEU:HA | 1:B:310:ALA:O | 2.20 | 0.42 |
| 1:B:94:ILE:CD1 | 1:B:101:MSE:HG3 | 2.49 | 0.42 |
| 1:D:156:HIS:CE1 | 1:D:179:TYR:CE2 | 3.08 | 0.42 |
| 1:B:128:PRO:O | 1:B:276:VAL:HG23 | 2.19 | 0.42 |
| 1:B:482:HIS:HA | 1:B:494:ALA:HB1 | 2.02 | 0.42 |
| 1:C:14:VAL:HG23 | 1:C:303:VAL:HG22 | 2.01 | 0.42 |
| 1:C:46:SER:N | 1:C:249:ILE:HD11 | 2.33 | 0.42 |
| 1:C:61:SER:O | 1:C:62:ILE:HD13 | 2.20 | 0.42 |
| 1:C:396:LEU:HD23 | 1:C:396:LEU:HA | 1.75 | 0.42 |
| 1:B:251:LEU:HA | 1:B:252:PRO:HD2 | 1.87 | 0.42 |
| 1:C:363:ALA:CB | 1:C:430:VAL:HG13 | 2.50 | 0.42 |
| 1:D:7:PHE:CE1 | 1:D:319:MSE:SE | 3.23 | 0.42 |
| 1:D:246:GLU:O | 1:D:247:ASP:OD1 | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:268:PHE:HD2 | 1:C:272:PHE:HE1 | 1.67 | 0.42 |
| 1:D:396:LEU:HD21 | 1:D:406:TYR:HB2 | 2.01 | 0.42 |
| 1:B:396:LEU:HD23 | 1:B:396:LEU:HA | 1.61 | 0.42 |
| 1:C:1:MSE:HB2 | 1:C:4:LYS:CG | 2.45 | 0.42 |
| 1:C:42:ARG:NE | 1:C:247:ASP:OD1 | 2.51 | 0.42 |
| 1:C:418:VAL:CB | 1:C:422:LYS:HE3 | 2.50 | 0.42 |
| 1:A:84:ARG:HD2 | 1:A:87:VAL:HG11 | 2.01 | 0.42 |
| 1:B:139:VAL:HG21 | 1:B:293:ILE:HG23 | 2.02 | 0.42 |
| 1:B:143:LEU:O | 1:B:146:CYS:HB2 | 2.20 | 0.42 |
| 1:C:261:GLN:HG3 | 1:C:271:GLU:OE2 | 2.20 | 0.42 |
| 1:A:263:LEU:HD21 | 1:A:294:VAL:HG11 | 2.01 | 0.41 |
| 1:A:290:THR:O | 1:A:294:VAL:HG23 | 2.19 | 0.41 |
| 1:C:108:THR:O | 1:C:112:HIS:N | 2.46 | 0.41 |
| 1:C:245:ARG:NH1 | 1:C:522:ASP:CB | 2.83 | 0.41 |
| 1:C:338:PRO:O | 1:C:342:LYS:N | 2.53 | 0.41 |
| 1:D:64:PHE:CZ | 1:B:7:PHE:HE1 | 2.38 | 0.41 |
| 1:A:432:ARG:NH2 | 1:A:432:ARG:HG3 | 2.35 | 0.41 |
| 1:B:42:ARG:NE | 1:B:247:ASP:OD1 | 2.52 | 0.41 |
| 1:C:109:THR:HG23 | 1:C:174:LYS:HG3 | 2.02 | 0.41 |
| 1:C:254:GLY:HA3 | 1:C:287:THR:HG23 | 2.02 | 0.41 |
| 1:D:387:PHE:N | 1:D:429:GLN:CD | 2.68 | 0.41 |
| 1:A:66:GLY:O | 1:A:305:VAL:HG23 | 2.20 | 0.41 |
| 1:A:432:ARG:NH2 | 1:A:432:ARG:CA | 2.73 | 0.41 |
| 1:C:119:ALA:O | 1:C:122:LEU:HB2 | 2.20 | 0.41 |
| 1:C:432:ARG:HD3 | 1:C:476:THR:CB | 2.39 | 0.41 |
| 1:A:268:PHE:CD2 | 1:A:272:PHE:HE1 | 2.38 | 0.41 |
| 1:B:88:PRO:HG2 | 1:B:91:VAL:HG22 | 2.01 | 0.41 |
| 1:B:103:THR:HG23 | 1:B:103:THR:H | 1.57 | 0.41 |
| 1:B:430:VAL:O | 1:B:434:TYR:HD2 | 2.03 | 0.41 |
| 1:B:432:ARG:NH1 | 1:B:437:PRO:CD | 2.82 | 0.41 |
| 1:C:105:LEU:HA | 1:C:105:LEU:HD13 | 1.76 | 0.41 |
| 1:C:78:THR:HG21 | 1:C:93:THR:OG1 | 2.20 | 0.41 |
| 1:C:396:LEU:HD21 | 1:C:406:TYR:HB2 | 2.02 | 0.41 |
| 1:C:509:ALA:O | 1:C:513:GLY:HA3 | 2.20 | 0.41 |
| 1:D:3:THR:O | 1:D:4:LYS:O | 2.38 | 0.41 |
| 1:A:111:LEU:HD23 | 1:A:111:LEU:HA | 1.80 | 0.41 |
| 1:C:39:PRO:O | 1:C:43:ARG:HG3 | 2.20 | 0.41 |
| 1:C:264:GLN:HG3 | 1:C:272:PHE:CD1 | 2.55 | 0.41 |
| 1:D:319:MSE:HB3 | 1:D:319:MSE:HE2 | 1.65 | 0.41 |
| 1:A:122:LEU:HD23 | 1:A:122:LEU:HA | 1.82 | 0.41 |
| 1:A:390:PHE:CE2 | 1:A:477:ARG:HA | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:230:GLN:O | 1:B:234:MSE:HG3 | 2.20 | 0.41 |
| 1:B:430:VAL:O | 1:B:434:TYR:CD2 | 2.73 | 0.41 |
| 1:D:113:GLU:HB3 | 1:D:174:LYS:NZ | 2.35 | 0.41 |
| 1:D:253:THR:O | 1:D:257:ILE:N | 2.52 | 0.41 |
| 1:A:429:GLN:HB3 | 1:A:433:PHE:HE2 | 1.86 | 0.41 |
| 1:B:5:GLU:HB3 | 1:B:311:LYS:HD3 | 2.02 | 0.41 |
| 1:B:49:ALA:HB1 | 1:B:249:ILE:HG22 | 2.01 | 0.41 |
| 1:B:52:LEU:O | 1:B:55:LEU:HB3 | 2.21 | 0.41 |
| 1:B:426:GLY:O | 1:B:430:VAL:HG23 | 2.21 | 0.41 |
| 1:D:39:PRO:O | 1:D:43:ARG:HG3 | 2.21 | 0.41 |
| 1:D:122:LEU:HD23 | 1:D:122:LEU:HA | 1.86 | 0.41 |
| 1:C:601:GLN:C | 1:C:603:SER:H | 2.24 | 0.41 |
| 1:A:1:MSE:HE1 | 1:B:72:ARG:NH2 | 2.36 | 0.40 |
| 1:A:144:SER:HA | 1:A:147:PHE:CE2 | 2.57 | 0.40 |
| 1:B:432:ARG:NE | 1:B:437:PRO:HG2 | 2.35 | 0.40 |
| 1:C:244:LYS:O | 1:C:246:GLU:N | 2.53 | 0.40 |
| 1:D:314:ASP:OD1 | 1:D:315:TYR:N | 2.54 | 0.40 |
| 1:A:36:TRP:CE3 | 1:A:103:THR:HG21 | 2.57 | 0.40 |
| 1:A:287:THR:N | 1:A:288:PRO:HD2 | 2.36 | 0.40 |
| 1:A:389:MSE:CE | 1:A:529:MSE:HG3 | 2.51 | 0.40 |
| 1:C:518:THR:OG1 | 1:C:519:ALA:N | 2.54 | 0.40 |
| 1:D:60:ASP:OD1 | 1:B:315:TYR:CZ | 2.71 | 0.40 |
| 1:D:287:THR:N | 1:D:288:PRO:CD | 2.83 | 0.40 |
| 1:A:150:ASP:HB3 | 1:A:151:MSE:H | 1.71 | 0.40 |
| 1:C:107:LEU:HB2 | 1:C:231:MSE:HE1 | 2.03 | 0.40 |
| 1:D:276:VAL:HG22 | 1:D:286:MSE:HE1 | 2.04 | 0.40 |
| 1:A:109:THR:HG23 | 1:A:174:LYS:HE3 | 2.03 | 0.40 |
| 1:B:360:VAL:HA | 1:B:430:VAL:HG21 | 2.02 | 0.40 |
| 1:C:37:GLU:O | 1:C:40:LYS:N | 2.51 | 0.40 |
| 1:C:103:THR:H | 1:C:103:THR:HG23 | 1.59 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | 552/771 (72%) | 429 (78%) | 73 (13%) | 50 (9%) | 1 | 5 |
| 1 | B | 552/771 (72%) | 437 (79%) | 70 (13%) | 45 (8%) | 1 | 6 |
| 1 | C | 549/771 (71%) | 423 (77%) | 80 (15%) | 46 (8%) | 1 | 6 |
| 1 | D | 552/771 (72%) | 427 (77%) | 75 (14%) | 50 (9%) | 1 | 5 |
| All | All | 2205/3084 (72%) | 1716 (78%) | 298 (14%) | 191 (9%) | 1 | 5 |

All (191) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 2 | GLU |
| 1 | D | 4 | LYS |
| 1 | D | 6 | ILE |
| 1 | D | 61 | SER |
| 1 | D | 129 | SER |
| 1 | D | 159 | TYR |
| 1 | D | 160 | PRO |
| 1 | D | 182 | PRO |
| 1 | D | 238 | ALA |
| 1 | D | 243 | VAL |
| 1 | D | 248 | ASP |
| 1 | D | 328 | GLN |
| 1 | D | 329 | PRO |
| 1 | D | 398 | LYS |
| 1 | D | 414 | ASP |
| 1 | D | 415 | PRO |
| 1 | D | 437 | PRO |
| 1 | D | 441 | PRO |
| 1 | D | 443 | LYS |
| 1 | D | 444 | VAL |
| 1 | D | 445 | PRO |
| 1 | D | 518 | THR |
| 1 | D | 519 | ALA |
| 1 | D | 582 | THR |
| 1 | D | 583 | PRO |
| 1 | D | 585 | TYR |
| 1 | A | 2 | GLU |
| 1 | A | 4 | LYS |
| 1 | A | 6 | ILE |
| 1 | A | 159 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 160 | PRO |
| 1 | A | 181 | SER |
| 1 | A | 182 | PRO |
| 1 | A | 243 | VAL |
| 1 | A | 328 | GLN |
| 1 | A | 329 | PRO |
| 1 | A | 347 | ASP |
| 1 | A | 398 | LYS |
| 1 | A | 414 | ASP |
| 1 | A | 415 | PRO |
| 1 | A | 441 | PRO |
| 1 | A | 443 | LYS |
| 1 | A | 444 | VAL |
| 1 | A | 445 | PRO |
| 1 | A | 573 | GLN |
| 1 | A | 582 | THR |
| 1 | A | 583 | PRO |
| 1 | A | 585 | TYR |
| 1 | B | 2 | GLU |
| 1 | B | 4 | LYS |
| 1 | B | 6 | ILE |
| 1 | B | 61 | SER |
| 1 | B | 152 | ARG |
| 1 | B | 159 | TYR |
| 1 | B | 160 | PRO |
| 1 | B | 181 | SER |
| 1 | B | 182 | PRO |
| 1 | B | 243 | VAL |
| 1 | B | 328 | GLN |
| 1 | B | 329 | PRO |
| 1 | B | 347 | ASP |
| 1 | B | 393 | GLY |
| 1 | B | 398 | LYS |
| 1 | B | 414 | ASP |
| 1 | B | 415 | PRO |
| 1 | B | 437 | PRO |
| 1 | B | 441 | PRO |
| 1 | B | 443 | LYS |
| 1 | B | 444 | VAL |
| 1 | B | 445 | PRO |
| 1 | B | 486 | SER |
| 1 | B | 573 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 582 | THR |
| 1 | B | 583 | PRO |
| 1 | B | 585 | TYR |
| 1 | C | 2 | GLU |
| 1 | C | 4 | LYS |
| 1 | C | 6 | ILE |
| 1 | C | 152 | ARG |
| 1 | C | 159 | TYR |
| 1 | C | 160 | PRO |
| 1 | C | 181 | SER |
| 1 | C | 182 | PRO |
| 1 | C | 243 | VAL |
| 1 | C | 328 | GLN |
| 1 | C | 329 | PRO |
| 1 | C | 393 | GLY |
| 1 | C | 398 | LYS |
| 1 | C | 414 | ASP |
| 1 | C | 415 | PRO |
| 1 | C | 441 | PRO |
| 1 | C | 443 | LYS |
| 1 | C | 444 | VAL |
| 1 | C | 445 | PRO |
| 1 | C | 487 | PRO |
| 1 | C | 515 | PHE |
| 1 | C | 571 | ASP |
| 1 | C | 582 | THR |
| 1 | C | 583 | PRO |
| 1 | C | 585 | TYR |
| 1 | D | 234 | MSE |
| 1 | D | 239 | VAL |
| 1 | D | 347 | ASP |
| 1 | D | 534 | GLU |
| 1 | D | 567 | GLU |
| 1 | D | 573 | GLN |
| 1 | A | 124 | ARG |
| 1 | A | 128 | PRO |
| 1 | A | 152 | ARG |
| 1 | A | 189 | SER |
| 1 | A | 393 | GLY |
| 1 | A | 515 | PHE |
| 1 | A | 534 | GLU |
| 1 | A | 535 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 128 | PRO |
| 1 | B | 518 | THR |
| 1 | C | 60 | ASP |
| 1 | C | 61 | SER |
| 1 | C | 128 | PRO |
| 1 | C | 437 | PRO |
| 1 | C | 573 | GLN |
| 1 | D | 516 | GLY |
| 1 | D | 533 | VAL |
| 1 | A | 60 | ASP |
| 1 | A | 61 | SER |
| 1 | A | 80 | GLU |
| 1 | A | 239 | VAL |
| 1 | A | 248 | ASP |
| 1 | A | 486 | SER |
| 1 | A | 516 | GLY |
| 1 | A | 568 | GLY |
| 1 | B | 60 | ASP |
| 1 | B | 248 | ASP |
| 1 | B | 515 | PHE |
| 1 | B | 516 | GLY |
| 1 | C | 242 | GLY |
| 1 | C | 248 | ASP |
| 1 | C | 476 | THR |
| 1 | C | 510 | LEU |
| 1 | C | 519 | ALA |
| 1 | D | 124 | ARG |
| 1 | D | 128 | PRO |
| 1 | D | 152 | ARG |
| 1 | D | 438 | TRP |
| 1 | D | 488 | GLU |
| 1 | A | 151 | MSE |
| 1 | A | 435 | GLU |
| 1 | A | 519 | ALA |
| 1 | A | 602 | ASN |
| 1 | B | 158 | TYR |
| 1 | B | 239 | VAL |
| 1 | B | 519 | ALA |
| 1 | B | 533 | VAL |
| 1 | C | 124 | ARG |
| 1 | C | 347 | ASP |
| 1 | C | 602 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 151 | MSE |
| 1 | D | 181 | SER |
| 1 | D | 393 | GLY |
| 1 | D | 602 | ASN |
| 1 | D | 604 | THR |
| 1 | A | 8 | ASP |
| 1 | A | 242 | GLY |
| 1 | A | 440 | SER |
| 1 | A | 604 | THR |
| 1 | B | 124 | ARG |
| 1 | B | 438 | TRP |
| 1 | B | 440 | SER |
| 1 | B | 534 | GLU |
| 1 | C | 239 | VAL |
| 1 | C | 438 | TRP |
| 1 | C | 440 | SER |
| 1 | C | 584 | VAL |
| 1 | D | 343 | GLU |
| 1 | D | 391 | GLN |
| 1 | A | 95 | ILE |
| 1 | A | 584 | VAL |
| 1 | B | 82 | LYS |
| 1 | B | 584 | VAL |
| 1 | B | 604 | THR |
| 1 | C | 82 | LYS |
| 1 | C | 156 | HIS |
| 1 | C | 572 | LYS |
| 1 | C | 604 | THR |
| 1 | D | 584 | VAL |
| 1 | B | 242 | GLY |
| 1 | D | 436 | GLY |
| 1 | D | 440 | SER |
| 1 | A | 533 | VAL |
| 1 | D | 242 | GLY |
| 1 | A | 569 | ILE |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 268/637 (42%) | 241 (90%) | 27 (10%) | 7 | 28 |
| 1 | B | 268/637 (42%) | 245 (91%) | 23 (9%) | 10 | 36 |
| 1 | C | 322/637 (50%) | 293 (91%) | 29 (9%) | 9 | 33 |
| 1 | D | 268/637 (42%) | 240 (90%) | 28 (10%) | 7 | 26 |
| All | All | 1126/2548 (44%) | 1019 (90%) | 107 (10%) | 8 | 30 |

All (107) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 7 | PHE |
| 1 | D | 36 | TRP |
| 1 | D | 52 | LEU |
| 1 | D | 64 | PHE |
| 1 | D | 83 | TYR |
| 1 | D | 98 | GLN |
| 1 | D | 109 | THR |
| 1 | D | 110 | VAL |
| 1 | D | 137 | LEU |
| 1 | D | 140 | THR |
| 1 | D | 142 | ARG |
| 1 | D | 147 | PHE |
| 1 | D | 231 | MSE |
| 1 | D | 257 | ILE |
| 1 | D | 263 | LEU |
| 1 | D | 264 | GLN |
| 1 | D | 269 | ASN |
| 1 | D | 276 | VAL |
| 1 | D | 286 | MSE |
| 1 | D | 292 | LEU |
| 1 | D | 303 | VAL |
| 1 | D | 308 | VAL |
| 1 | D | 358 | PHE |
| 1 | D | 392 | ASP |
| 1 | D | 401 | ASN |
| 1 | D | 420 | ARG |
| 1 | D | 437 | PRO |
| 1 | D | 525 | TYR |
| 1 | A | 7 | PHE |
| 1 | A | 36 | TRP |
| 1 | A | 52 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | PHE |
| 1 | A | 79 | VAL |
| 1 | A | 83 | TYR |
| 1 | A | 98 | GLN |
| 1 | A | 106 | LEU |
| 1 | A | 110 | VAL |
| 1 | A | 137 | LEU |
| 1 | A | 139 | VAL |
| 1 | A | 147 | PHE |
| 1 | A | 150 | ASP |
| 1 | A | 151 | MSE |
| 1 | A | 263 | LEU |
| 1 | A | 264 | GLN |
| 1 | A | 269 | ASN |
| 1 | A | 276 | VAL |
| 1 | A | 278 | GLU |
| 1 | A | 290 | THR |
| 1 | A | 303 | VAL |
| 1 | A | 358 | PHE |
| 1 | A | 392 | ASP |
| 1 | A | 401 | ASN |
| 1 | A | 420 | ARG |
| 1 | A | 432 | ARG |
| 1 | A | 525 | TYR |
| 1 | B | 7 | PHE |
| 1 | B | 36 | TRP |
| 1 | B | 52 | LEU |
| 1 | B | 64 | PHE |
| 1 | B | 67 | THR |
| 1 | B | 83 | TYR |
| 1 | B | 98 | GLN |
| 1 | B | 103 | THR |
| 1 | B | 105 | LEU |
| 1 | B | 137 | LEU |
| 1 | B | 140 | THR |
| 1 | B | 144 | SER |
| 1 | B | 264 | GLN |
| 1 | B | 269 | ASN |
| 1 | B | 290 | THR |
| 1 | B | 308 | VAL |
| 1 | B | 358 | PHE |
| 1 | B | 392 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 401 | ASN |
| 1 | B | 420 | ARG |
| 1 | B | 422 | LYS |
| 1 | B | 432 | ARG |
| 1 | B | 437 | PRO |
| 1 | C | 7 | PHE |
| 1 | C | 36 | TRP |
| 1 | C | 52 | LEU |
| 1 | C | 64 | PHE |
| 1 | C | 67 | THR |
| 1 | C | 83 | TYR |
| 1 | C | 98 | GLN |
| 1 | C | 110 | VAL |
| 1 | C | 140 | THR |
| 1 | C | 264 | GLN |
| 1 | C | 269 | ASN |
| 1 | C | 276 | VAL |
| 1 | C | 290 | THR |
| 1 | C | 392 | ASP |
| 1 | C | 395 | LYS |
| 1 | C | 401 | ASN |
| 1 | C | 420 | ARG |
| 1 | C | 422 | LYS |
| 1 | C | 486 | SER |
| 1 | C | 503 | SER |
| 1 | C | 515 | PHE |
| 1 | C | 518 | THR |
| 1 | C | 521 | ILE |
| 1 | C | 525 | TYR |
| 1 | C | 526 | ARG |
| 1 | C | 565 | ARG |
| 1 | C | 567 | GLU |
| 1 | C | 569 | ILE |
| 1 | C | 575 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 31 | GLN |
| 1 | D | 264 | GLN |
| 1 | A | 112 | HIS |
| 1 | A | 156 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 391 | GLN |
| 1 | B | 156 | HIS |
| 1 | B | 264 | GLN |
| 1 | B | 391 | GLN |
| 1 | B | 429 | GLN |
| 1 | C | 156 | HIS |
| 1 | C | 482 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 548/771 (71%) | 0.30 | 41 (7%) 14 14 | 53, 109, 176, 219 | 0 |
| 1 | B | 548/771 (71%) | 0.87 | 92 (16%) 1 1 | 62, 120, 274, 329 | 0 |
| 1 | C | 545/771 (70%) | 0.37 | 28 (5%) 28 27 | 30, 104, 136, 171 | 0 |
| 1 | D | 548/771 (71%) | 0.36 | 36 (6%) 18 19 | 37, 91, 169, 223 | 0 |
| All | All | 2189/3084 (70%) | 0.47 | 197 (8%) 9 10 | 30, 106, 216, 329 | 0 |

All (197) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 446 | SER | 14.8 |
| 1 | B | 448 | ASP | 12.9 |
| 1 | B | 533 | VAL | 10.3 |
| 1 | B | 522 | ASP | 9.0 |
| 1 | B | 532 | VAL | 8.3 |
| 1 | D | 605 | PRO | 8.3 |
| 1 | B | 557 | GLN | 8.1 |
| 1 | B | 447 | CYS | 7.9 |
| 1 | B | 471 | VAL | 7.5 |
| 1 | D | 600 | SER | 7.3 |
| 1 | B | 503 | SER | 7.3 |
| 1 | C | 325 | THR | 6.6 |
| 1 | B | 513 | GLY | 6.4 |
| 1 | B | 502 | ARG | 6.3 |
| 1 | B | 591 | LEU | 6.1 |
| 1 | B | 525 | TYR | 5.9 |
| 1 | B | 501 | ALA | 5.9 |
| 1 | D | 599 | ALA | 5.7 |
| 1 | B | 514 | SER | 5.7 |
| 1 | B | 453 | ARG | 5.6 |
| 1 | D | 579 | ALA | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 448 | ASP | 5.4 |
| 1 | B | 443 | LYS | 5.3 |
| 1 | D | 598 | ALA | 5.3 |
| 1 | B | 456 | ALA | 5.3 |
| 1 | B | 449 | ASP | 5.1 |
| 1 | B | 460 | LEU | 5.1 |
| 1 | A | 600 | SER | 5.1 |
| 1 | B | 65 | LEU | 4.9 |
| 1 | A | 439 | GLY | 4.6 |
| 1 | A | 440 | SER | 4.6 |
| 1 | C | 353 | GLU | 4.6 |
| 1 | B | 523 | GLY | 4.5 |
| 1 | D | 602 | ASN | 4.3 |
| 1 | B | 562 | GLU | 4.2 |
| 1 | B | 406 | TYR | 4.2 |
| 1 | B | 500 | ALA | 4.1 |
| 1 | B | 515 | PHE | 4.1 |
| 1 | B | 524 | VAL | 4.1 |
| 1 | B | 58 | PHE | 4.0 |
| 1 | C | 571 | ASP | 4.0 |
| 1 | B | 487 | PRO | 4.0 |
| 1 | A | 25 | LEU | 3.9 |
| 1 | B | 251 | LEU | 3.9 |
| 1 | B | 490 | VAL | 3.9 |
| 1 | A | 485 | SER | 3.9 |
| 1 | C | 67 | THR | 3.8 |
| 1 | C | 419 | ALA | 3.8 |
| 1 | C | 56 | ALA | 3.8 |
| 1 | D | 596 | LEU | 3.8 |
| 1 | B | 491 | GLU | 3.7 |
| 1 | A | 6 | ILE | 3.7 |
| 1 | B | 579 | ALA | 3.7 |
| 1 | C | 65 | LEU | 3.7 |
| 1 | A | 249 | ILE | 3.7 |
| 1 | B | 263 | LEU | 3.7 |
| 1 | C | 497 | PHE | 3.7 |
| 1 | B | 531 | HIS | 3.7 |
| 1 | B | 452 | LEU | 3.7 |
| 1 | A | 396 | LEU | 3.6 |
| 1 | D | 601 | GLN | 3.6 |
| 1 | B | 411 | PHE | 3.6 |
| 1 | A | 407 | LEU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 347 | ASP | 3.6 |
| 1 | B | 254 | GLY | 3.6 |
| 1 | A | 403 | GLN | 3.5 |
| 1 | D | 571 | ASP | 3.5 |
| 1 | B | 451 | THR | 3.5 |
| 1 | D | 416 | ASP | 3.4 |
| 1 | B | 507 | PHE | 3.4 |
| 1 | B | 469 | ASP | 3.4 |
| 1 | B | 521 | ILE | 3.4 |
| 1 | B | 563 | GLN | 3.3 |
| 1 | C | 447 | CYS | 3.3 |
| 1 | A | 122 | LEU | 3.3 |
| 1 | B | 292 | LEU | 3.2 |
| 1 | D | 423 | VAL | 3.2 |
| 1 | A | 481 | ALA | 3.2 |
| 1 | A | 384 | LEU | 3.1 |
| 1 | B | 519 | ALA | 3.1 |
| 1 | D | 460 | LEU | 3.1 |
| 1 | B | 455 | GLN | 3.1 |
| 1 | B | 384 | LEU | 3.1 |
| 1 | A | 430 | VAL | 3.1 |
| 1 | A | 528 | LEU | 3.1 |
| 1 | A | 105 | LEU | 3.0 |
| 1 | B | 528 | LEU | 3.0 |
| 1 | D | 595 | LEU | 3.0 |
| 1 | A | 601 | GLN | 2.9 |
| 1 | B | 594 | LEU | 2.9 |
| 1 | C | 267 | LEU | 2.9 |
| 1 | D | 422 | LYS | 2.9 |
| 1 | B | 597 | LEU | 2.9 |
| 1 | B | 295 | PHE | 2.9 |
| 1 | A | 602 | ASN | 2.8 |
| 1 | D | 578 | ARG | 2.8 |
| 1 | B | 282 | ASP | 2.8 |
| 1 | D | 486 | SER | 2.8 |
| 1 | B | 408 | ARG | 2.8 |
| 1 | A | 30 | TYR | 2.8 |
| 1 | B | 498 | LEU | 2.8 |
| 1 | B | 586 | GLN | 2.7 |
| 1 | A | 435 | GLU | 2.7 |
| 1 | B | 108 | THR | 2.7 |
| 1 | D | 580 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 438 | TRP | 2.7 |
| 1 | B | 185 | TYR | 2.7 |
| 1 | B | 64 | PHE | 2.7 |
| 1 | B | 485 | SER | 2.7 |
| 1 | D | 430 | VAL | 2.7 |
| 1 | C | 326 | THR | 2.6 |
| 1 | A | 441 | PRO | 2.6 |
| 1 | A | 65 | LEU | 2.6 |
| 1 | B | 593 | ARG | 2.6 |
| 1 | D | 577 | ALA | 2.6 |
| 1 | B | 67 | THR | 2.6 |
| 1 | C | 569 | ILE | 2.6 |
| 1 | B | 445 | PRO | 2.5 |
| 1 | D | 396 | LEU | 2.5 |
| 1 | C | 507 | PHE | 2.5 |
| 1 | A | 9 | ALA | 2.5 |
| 1 | B | 592 | THR | 2.5 |
| 1 | C | 500 | ALA | 2.5 |
| 1 | C | 132 | CYS | 2.5 |
| 1 | A | 246 | GLU | 2.5 |
| 1 | D | 93 | THR | 2.5 |
| 1 | A | 281 | GLU | 2.5 |
| 1 | B | 556 | LEU | 2.4 |
| 1 | D | 604 | THR | 2.4 |
| 1 | D | 7 | PHE | 2.4 |
| 1 | A | 94 | ILE | 2.4 |
| 1 | B | 589 | LYS | 2.4 |
| 1 | B | 7 | PHE | 2.4 |
| 1 | B | 11 | PRO | 2.4 |
| 1 | A | 322 | ALA | 2.4 |
| 1 | B | 293 | ILE | 2.4 |
| 1 | B | 32 | ARG | 2.4 |
| 1 | A | 278 | GLU | 2.4 |
| 1 | B | 396 | LEU | 2.4 |
| 1 | C | 84 | ARG | 2.4 |
| 1 | D | 326 | THR | 2.4 |
| 1 | B | 115 | ILE | 2.4 |
| 1 | D | 104 | LEU | 2.4 |
| 1 | D | 6 | ILE | 2.3 |
| 1 | A | 132 | CYS | 2.3 |
| 1 | B | 494 | ALA | 2.3 |
| 1 | D | 433 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 285 | LYS | 2.3 |
| 1 | B | 595 | LEU | 2.3 |
| 1 | A | 445 | PRO | 2.3 |
| 1 | A | 104 | LEU | 2.3 |
| 1 | A | 599 | ALA | 2.3 |
| 1 | C | 481 | ALA | 2.3 |
| 1 | D | 525 | TYR | 2.3 |
| 1 | C | 349 | TRP | 2.3 |
| 1 | B | 301 | HIS | 2.3 |
| 1 | C | 435 | GLU | 2.3 |
| 1 | A | 98 | GLN | 2.2 |
| 1 | B | 573 | GLN | 2.2 |
| 1 | C | 34 | TYR | 2.2 |
| 1 | B | 509 | ALA | 2.2 |
| 1 | B | 34 | TYR | 2.2 |
| 1 | B | 291 | ARG | 2.2 |
| 1 | D | 398 | LYS | 2.2 |
| 1 | A | 487 | PRO | 2.2 |
| 1 | B | 504 | CYS | 2.2 |
| 1 | A | 482 | HIS | 2.2 |
| 1 | B | 404 | ARG | 2.2 |
| 1 | D | 3 | THR | 2.2 |
| 1 | B | 429 | GLN | 2.2 |
| 1 | A | 5 | GLU | 2.2 |
| 1 | C | 287 | THR | 2.2 |
| 1 | C | 446 | SER | 2.2 |
| 1 | C | 272 | PHE | 2.2 |
| 1 | A | 423 | VAL | 2.2 |
| 1 | A | 34 | TYR | 2.1 |
| 1 | D | 247 | ASP | 2.1 |
| 1 | A | 531 | HIS | 2.1 |
| 1 | B | 535 | GLU | 2.1 |
| 1 | D | 447 | CYS | 2.1 |
| 1 | B | 243 | VAL | 2.1 |
| 1 | D | 517 | SER | 2.1 |
| 1 | B | 444 | VAL | 2.1 |
| 1 | B | 249 | ILE | 2.1 |
| 1 | B | 280 | LEU | 2.1 |
| 1 | B | 534 | GLU | 2.1 |
| 1 | B | 95 | ILE | 2.1 |
| 1 | C | 305 | VAL | 2.1 |
| 1 | B | 454 | THR | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 66 | GLY | 2.1 |
| 1 | A | 410 | VAL | 2.0 |
| 1 | C | 563 | GLN | 2.0 |
| 1 | C | 572 | LYS | 2.0 |
| 1 | B | 272 | PHE | 2.0 |
| 1 | D | 429 | GLN | 2.0 |
| 1 | B | 457 | GLY | 2.0 |
| 1 | D | 96 | ASP | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.