



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2017 – 09:11 AM EST

PDB ID : 4EO2
Title : Structure of the bacteriophage C1 tail knob protein, gp12
Authors : Aksyuk, A.A.; Rossmann, M.G.
Deposited on : unknown
Resolution : 3.01 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

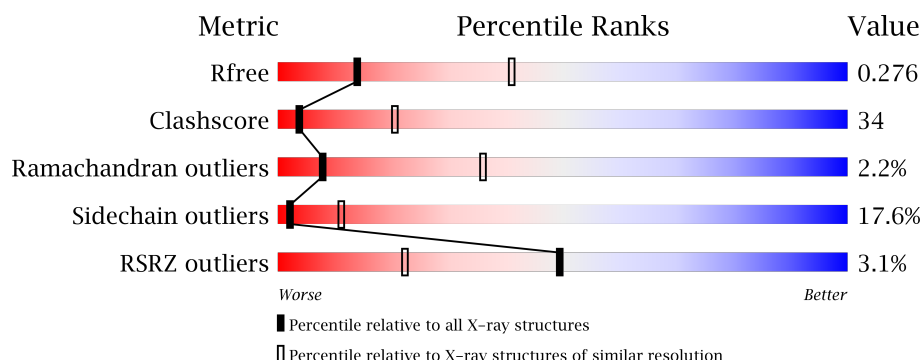
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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} | 100719 | 1692 (3.00-3.00) |
| Clashscore | 112137 | 2037 (3.00-3.00) |
| Ramachandran outliers | 110173 | 1973 (3.00-3.00) |
| Sidechain outliers | 110143 | 1976 (3.00-3.00) |
| RSRZ outliers | 101464 | 1716 (3.00-3.00) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 583 | <div> <div>2%</div> <div> <div></div> <div>42%</div> <div>30%</div> <div>11%</div> <div>16%</div> </div> </div> |
| 1 | B | 583 | <div> <div>0%</div> <div> <div></div> <div>42%</div> <div>31%</div> <div>10%</div> <div>16%</div> </div> </div> |
| 1 | C | 583 | <div> <div>3%</div> <div> <div></div> <div>42%</div> <div>30%</div> <div>11%</div> <div>16%</div> </div> </div> |
| 1 | D | 583 | <div> <div>4%</div> <div> <div></div> <div>39%</div> <div>34%</div> <div>11%</div> <div>16%</div> </div> </div> |
| 1 | E | 583 | <div> <div>3%</div> <div> <div></div> <div>39%</div> <div>33%</div> <div>11%</div> <div>16%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | F | 583 | <div><div></div><div>3%</div><div>39%</div><div>34%</div><div>11%</div><div>16%</div></div> |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23688 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 Major tail protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |
| 1 | B | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |
| 1 | C | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |
| 1 | D | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |
| 1 | E | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |
| 1 | F | 488 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3948 | 2504 | 665 | 761 | 18 | | | |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| A | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| B | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |

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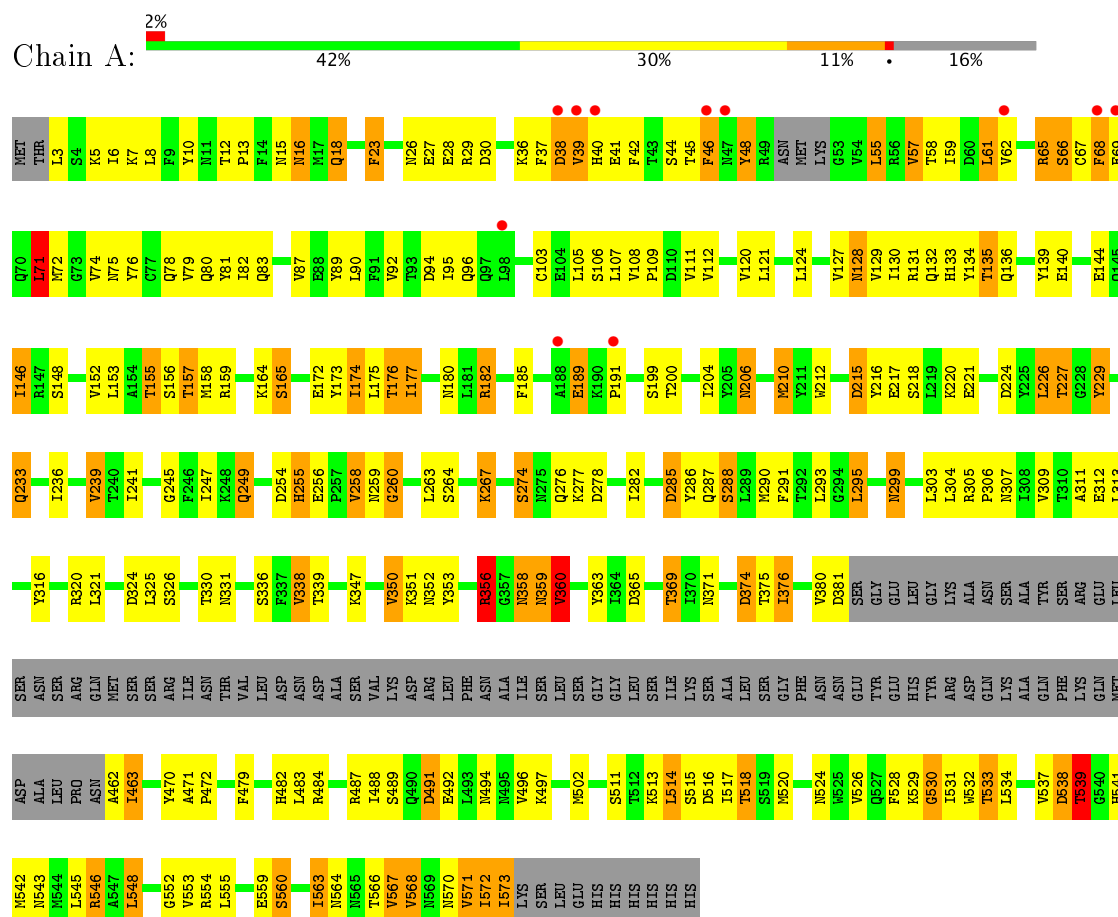
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| C | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| D | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| E | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 575 | SER | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 576 | LEU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 577 | GLU | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 578 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 579 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 580 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 581 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 582 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |
| F | 583 | HIS | - | EXPRESSION TAG | UNP Q7Y3F0 |

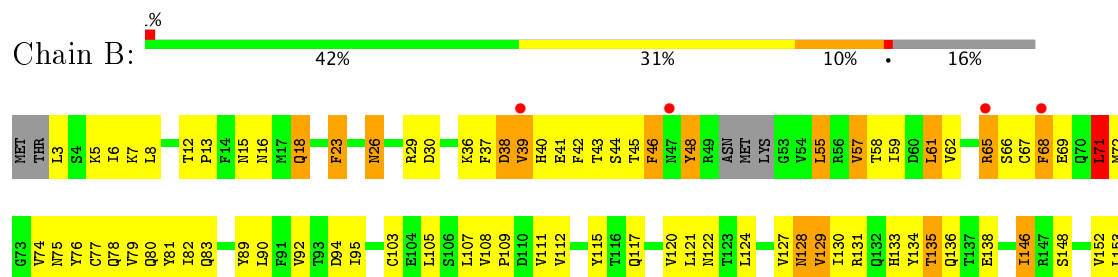
3 Residue-property plots

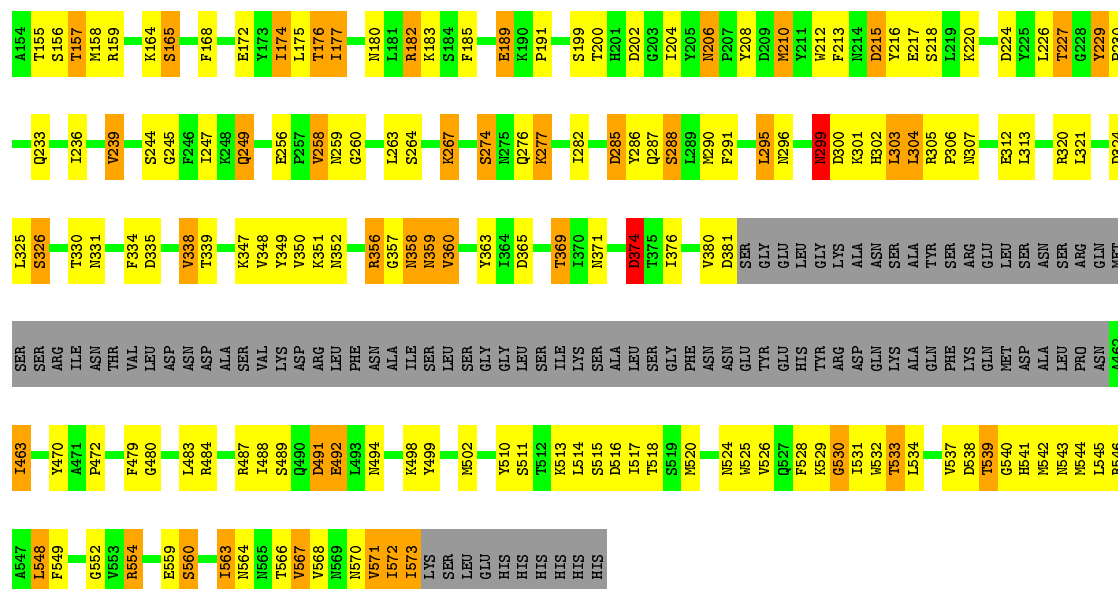
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Major tail protein

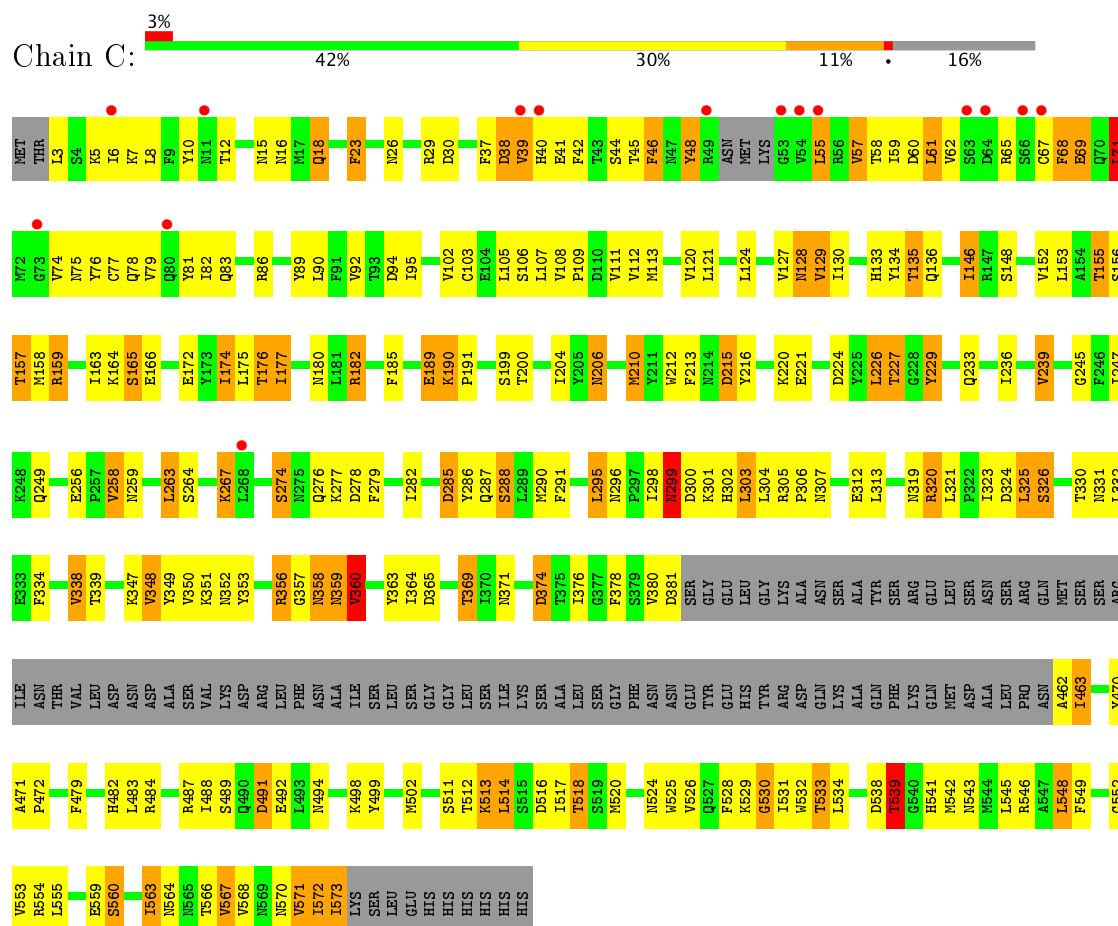


• Molecule 1: Major tail protein



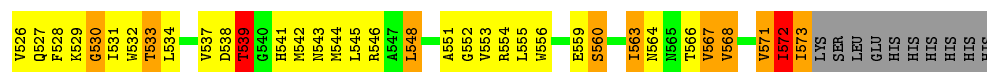


• Molecule 1: Major tail protein

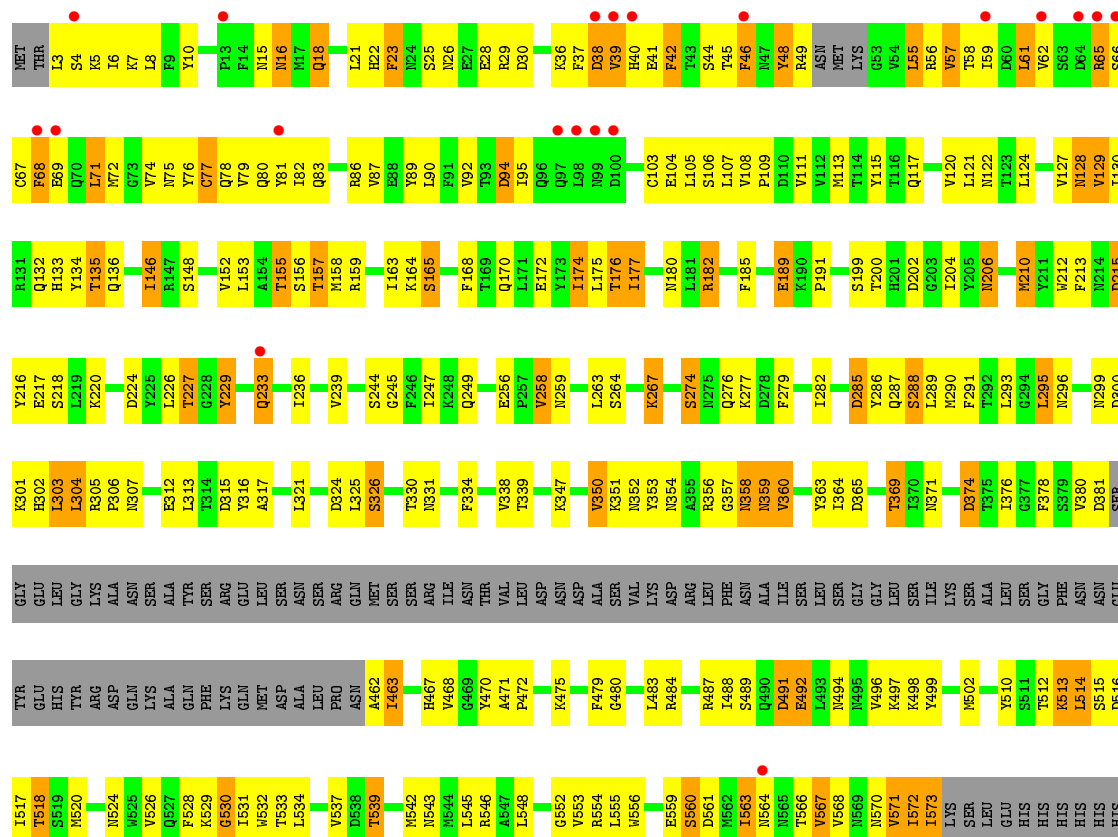


• Molecule 1: Major tail protein





• Molecule 1: Major tail protein



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 205.61Å 209.64Å 102.97Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.01 50.00 – 3.01 | Depositor EDS |
| % Data completeness (in resolution range) | 98.0 (50.00-3.01) 98.1 (50.00-3.01) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | 0.07 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.21 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.238 , 0.282 0.230 , 0.276 | Depositor DCC |
| R_{free} test set | 4386 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 75.3 | Xtriage |
| Anisotropy | 0.837 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 98.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Estimated twinning fraction | 0.000 for k,h,-l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 23688 | wwPDB-VP |
| Average B, all atoms (Å ²) | 108.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 | 0.90 | 0/4030 | 0.97 | 4/5464 (0.1%) |
| 1 | B | 0.89 | 3/4030 (0.1%) | 0.94 | 3/5464 (0.1%) |
| 1 | C | 0.80 | 1/4030 (0.0%) | 0.89 | 2/5464 (0.0%) |
| 1 | D | 0.77 | 0/4030 | 0.88 | 1/5464 (0.0%) |
| 1 | E | 0.81 | 2/4030 (0.0%) | 0.90 | 1/5464 (0.0%) |
| 1 | F | 0.87 | 1/4030 (0.0%) | 0.94 | 1/5464 (0.0%) |
| All | All | 0.84 | 7/24180 (0.0%) | 0.92 | 12/32784 (0.0%) |

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 | 2 |
| 1 | B | 0 | 3 |
| 1 | C | 0 | 2 |
| 1 | D | 0 | 3 |
| 1 | E | 0 | 3 |
| 1 | F | 0 | 2 |
| All | All | 0 | 15 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 299 | ASN | CG-ND2 | -9.03 | 1.10 | 1.32 |
| 1 | B | 299 | ASN | CG-OD1 | -7.23 | 1.08 | 1.24 |
| 1 | C | 299 | ASN | CG-ND2 | -6.63 | 1.16 | 1.32 |
| 1 | F | 492 | GLU | CG-CD | 5.74 | 1.60 | 1.51 |
| 1 | E | 551 | ALA | CA-CB | -5.69 | 1.40 | 1.52 |
| 1 | B | 492 | GLU | CB-CG | 5.43 | 1.62 | 1.52 |
| 1 | E | 492 | GLU | CB-CG | 5.26 | 1.62 | 1.52 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | F | 304 | LEU | CB-CG-CD1 | -8.30 | 96.89 | 111.00 |
| 1 | B | 374 | ASP | CB-CG-OD2 | -6.55 | 112.40 | 118.30 |
| 1 | C | 304 | LEU | CB-CG-CD1 | -5.99 | 100.81 | 111.00 |
| 1 | B | 304 | LEU | CB-CG-CD1 | -5.98 | 100.83 | 111.00 |
| 1 | D | 365 | ASP | CB-CG-OD2 | 5.83 | 123.55 | 118.30 |
| 1 | E | 304 | LEU | CB-CG-CD1 | -5.60 | 101.48 | 111.00 |
| 1 | B | 554 | ARG | NE-CZ-NH1 | -5.56 | 117.52 | 120.30 |
| 1 | A | 356 | ARG | NE-CZ-NH2 | -5.53 | 117.54 | 120.30 |
| 1 | A | 304 | LEU | CB-CG-CD1 | -5.38 | 101.85 | 111.00 |
| 1 | A | 278 | ASP | CB-CG-OD1 | -5.33 | 113.50 | 118.30 |
| 1 | C | 159 | ARG | NE-CZ-NH2 | -5.25 | 117.68 | 120.30 |
| 1 | A | 241 | ILE | CB-CA-C | -5.10 | 101.41 | 111.60 |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 356 | ARG | Peptide |
| 1 | A | 71 | LEU | Peptide |
| 1 | B | 183 | LYS | Peptide |
| 1 | B | 356 | ARG | Peptide |
| 1 | B | 71 | LEU | Peptide |
| 1 | C | 356 | ARG | Peptide |
| 1 | C | 71 | LEU | Peptide |
| 1 | D | 183 | LYS | Peptide |
| 1 | D | 356 | ARG | Peptide |
| 1 | D | 71 | LEU | Peptide |
| 1 | E | 183 | LYS | Peptide |
| 1 | E | 356 | ARG | Peptide |
| 1 | E | 71 | LEU | Peptide |
| 1 | F | 356 | ARG | Peptide |
| 1 | F | 71 | LEU | 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 | 3948 | 0 | 3832 | 264 | 3 |
| 1 | B | 3948 | 0 | 3832 | 264 | 3 |
| 1 | C | 3948 | 0 | 3832 | 282 | 1 |
| 1 | D | 3948 | 0 | 3832 | 284 | 0 |
| 1 | E | 3948 | 0 | 3832 | 271 | 0 |
| 1 | F | 3948 | 0 | 3832 | 279 | 1 |
| All | All | 23688 | 0 | 22992 | 1585 | 4 |

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 34.

All (1585) 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:A:573:ILE:O | 1:A:573:ILE:HG22 | 1.66 | 0.93 |
| 1:F:573:ILE:O | 1:F:573:ILE:HG22 | 1.70 | 0.91 |
| 1:D:158:MET:O | 1:D:159:ARG:HD3 | 1.70 | 0.91 |
| 1:E:573:ILE:HG22 | 1:E:573:ILE:O | 1.71 | 0.91 |
| 1:C:299:ASN:HD22 | 1:C:299:ASN:N | 1.63 | 0.89 |
| 1:B:573:ILE:O | 1:B:573:ILE:HG22 | 1.72 | 0.88 |
| 1:E:285:ASP:OD1 | 1:E:288:SER:OG | 1.90 | 0.88 |
| 1:D:573:ILE:HG22 | 1:D:573:ILE:O | 1.73 | 0.87 |
| 1:A:573:ILE:O | 1:A:573:ILE:CG2 | 2.23 | 0.86 |
| 1:C:285:ASP:OD1 | 1:C:288:SER:OG | 1.93 | 0.86 |
| 1:C:542:MET:HE1 | 1:C:545:LEU:HD23 | 1.58 | 0.86 |
| 1:C:573:ILE:O | 1:C:573:ILE:HG22 | 1.75 | 0.85 |
| 1:D:285:ASP:OD1 | 1:D:288:SER:OG | 1.92 | 0.85 |
| 1:F:215:ASP:OD1 | 1:F:216:TYR:N | 2.10 | 0.85 |
| 1:C:542:MET:CE | 1:C:545:LEU:HD23 | 2.08 | 0.83 |
| 1:B:215:ASP:OD1 | 1:B:216:TYR:N | 2.12 | 0.82 |
| 1:F:285:ASP:OD1 | 1:F:288:SER:OG | 1.97 | 0.82 |
| 1:D:157:THR:O | 1:D:157:THR:HG23 | 1.79 | 0.81 |
| 1:F:573:ILE:O | 1:F:573:ILE:CG2 | 2.27 | 0.81 |
| 1:B:572:ILE:O | 1:B:572:ILE:HG22 | 1.81 | 0.81 |
| 1:D:572:ILE:O | 1:D:572:ILE:HG22 | 1.81 | 0.81 |
| 1:B:26:ASN:OD1 | 1:B:29:ARG:NH2 | 2.15 | 0.80 |
| 1:D:215:ASP:OD1 | 1:D:216:TYR:N | 2.13 | 0.80 |
| 1:C:158:MET:O | 1:C:159:ARG:HD3 | 1.82 | 0.80 |
| 1:D:573:ILE:O | 1:D:573:ILE:CG2 | 2.31 | 0.79 |
| 1:A:3:LEU:HD21 | 1:B:68:PHE:CE2 | 2.18 | 0.79 |
| 1:C:572:ILE:O | 1:C:572:ILE:HG22 | 1.83 | 0.79 |
| 1:F:26:ASN:OD1 | 1:F:29:ARG:NH2 | 2.16 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:572:ILE:O | 1:A:572:ILE:HG22 | 1.81 | 0.78 |
| 1:E:26:ASN:OD1 | 1:E:29:ARG:NH2 | 2.16 | 0.78 |
| 1:A:285:ASP:OD1 | 1:A:288:SER:OG | 2.02 | 0.78 |
| 1:E:572:ILE:HG22 | 1:E:572:ILE:O | 1.84 | 0.77 |
| 1:C:215:ASP:OD1 | 1:C:216:TYR:N | 2.16 | 0.77 |
| 1:C:299:ASN:ND2 | 1:C:299:ASN:N | 2.26 | 0.77 |
| 1:E:215:ASP:OD1 | 1:E:216:TYR:N | 2.17 | 0.77 |
| 1:A:3:LEU:N | 1:A:44:SER:O | 2.18 | 0.77 |
| 1:A:37:PHE:CZ | 1:A:40:HIS:O | 2.39 | 0.76 |
| 1:B:573:ILE:CG2 | 1:B:573:ILE:O | 2.33 | 0.76 |
| 1:A:313:LEU:HB2 | 1:A:321:LEU:HB3 | 1.68 | 0.76 |
| 1:F:572:ILE:HG22 | 1:F:572:ILE:O | 1.86 | 0.76 |
| 1:C:573:ILE:O | 1:C:573:ILE:CG2 | 2.34 | 0.76 |
| 1:B:75:ASN:O | 1:B:92:VAL:N | 2.18 | 0.76 |
| 1:E:516:ASP:OD2 | 1:E:518:THR:N | 2.19 | 0.76 |
| 1:F:78:GLN:HG2 | 1:F:79:VAL:N | 2.00 | 0.76 |
| 1:E:37:PHE:CZ | 1:E:40:HIS:O | 2.39 | 0.75 |
| 1:C:312:GLU:OE2 | 1:C:484:ARG:NH1 | 2.19 | 0.75 |
| 1:D:516:ASP:OD2 | 1:D:518:THR:N | 2.19 | 0.75 |
| 1:F:542:MET:CE | 1:F:545:LEU:HD23 | 2.17 | 0.75 |
| 1:F:158:MET:O | 1:F:159:ARG:HD3 | 1.87 | 0.75 |
| 1:A:233:GLN:NE2 | 1:A:380:VAL:HG13 | 2.02 | 0.75 |
| 1:B:164:LYS:O | 1:B:282:ILE:HD11 | 1.87 | 0.74 |
| 1:A:215:ASP:OD1 | 1:A:216:TYR:N | 2.21 | 0.74 |
| 1:A:158:MET:O | 1:A:159:ARG:HD3 | 1.88 | 0.74 |
| 1:E:158:MET:O | 1:E:159:ARG:HD3 | 1.87 | 0.73 |
| 1:B:115:TYR:CE1 | 1:B:537:VAL:HG13 | 2.24 | 0.73 |
| 1:A:26:ASN:OD1 | 1:A:29:ARG:NH2 | 2.22 | 0.73 |
| 1:A:157:THR:CG2 | 1:A:489:SER:H | 2.01 | 0.73 |
| 1:D:26:ASN:OD1 | 1:D:29:ARG:NH2 | 2.21 | 0.73 |
| 1:B:285:ASP:OD1 | 1:B:288:SER:OG | 2.06 | 0.73 |
| 1:D:157:THR:CG2 | 1:D:489:SER:H | 2.01 | 0.73 |
| 1:B:157:THR:HG23 | 1:B:157:THR:O | 1.88 | 0.73 |
| 1:B:59:ILE:O | 1:B:59:ILE:HG23 | 1.87 | 0.73 |
| 1:D:542:MET:O | 1:D:545:LEU:N | 2.22 | 0.73 |
| 1:A:164:LYS:O | 1:A:282:ILE:HD11 | 1.89 | 0.72 |
| 1:A:290:MET:HE3 | 1:A:295:LEU:HB3 | 1.71 | 0.72 |
| 1:A:75:ASN:O | 1:A:92:VAL:N | 2.23 | 0.72 |
| 1:F:529:LYS:O | 1:F:530:GLY:O | 2.08 | 0.72 |
| 1:C:164:LYS:O | 1:C:282:ILE:HD11 | 1.89 | 0.72 |
| 1:F:146:ILE:O | 1:F:146:ILE:HD12 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:46:PHE:CB | 1:F:57:VAL:HG23 | 2.20 | 0.72 |
| 1:E:573:ILE:CG2 | 1:E:573:ILE:O | 2.38 | 0.72 |
| 1:F:516:ASP:OD2 | 1:F:518:THR:N | 2.20 | 0.72 |
| 1:D:127:VAL:HG21 | 1:D:528:PHE:CD1 | 2.24 | 0.71 |
| 1:D:233:GLN:NE2 | 1:D:380:VAL:HG13 | 2.06 | 0.71 |
| 1:B:37:PHE:CZ | 1:B:40:HIS:O | 2.42 | 0.71 |
| 1:C:146:ILE:HD12 | 1:C:146:ILE:O | 1.89 | 0.71 |
| 1:A:542:MET:O | 1:A:545:LEU:N | 2.23 | 0.71 |
| 1:D:37:PHE:CZ | 1:D:40:HIS:O | 2.43 | 0.71 |
| 1:F:127:VAL:HG21 | 1:F:528:PHE:CD1 | 2.26 | 0.71 |
| 1:B:502:MET:HG2 | 1:B:567:VAL:HG11 | 1.72 | 0.71 |
| 1:E:233:GLN:NE2 | 1:E:380:VAL:HG13 | 2.06 | 0.71 |
| 1:B:516:ASP:OD2 | 1:B:518:THR:N | 2.18 | 0.71 |
| 1:C:26:ASN:OD1 | 1:C:29:ARG:NH2 | 2.24 | 0.71 |
| 1:C:516:ASP:OD2 | 1:C:518:THR:N | 2.20 | 0.70 |
| 1:E:157:THR:O | 1:E:157:THR:HG23 | 1.90 | 0.70 |
| 1:A:59:ILE:HG23 | 1:A:59:ILE:O | 1.91 | 0.70 |
| 1:A:127:VAL:HG21 | 1:A:528:PHE:CD1 | 2.25 | 0.70 |
| 1:B:233:GLN:NE2 | 1:B:380:VAL:HG13 | 2.07 | 0.70 |
| 1:A:516:ASP:OD2 | 1:A:518:THR:N | 2.20 | 0.70 |
| 1:B:29:ARG:HD3 | 1:B:89:TYR:CE2 | 2.27 | 0.70 |
| 1:C:3:LEU:N | 1:C:44:SER:O | 2.24 | 0.70 |
| 1:F:157:THR:O | 1:F:157:THR:HG23 | 1.90 | 0.70 |
| 1:C:298:ILE:C | 1:C:299:ASN:HD22 | 1.94 | 0.70 |
| 1:A:542:MET:CE | 1:A:545:LEU:HD23 | 2.22 | 0.70 |
| 1:D:124:LEU:HD22 | 1:D:532:TRP:HB2 | 1.73 | 0.70 |
| 1:E:347:LYS:HE2 | 1:E:369:THR:CG2 | 2.22 | 0.69 |
| 1:E:189:GLU:C | 1:E:191:PRO:HD3 | 2.13 | 0.69 |
| 1:E:164:LYS:O | 1:E:282:ILE:HD11 | 1.92 | 0.69 |
| 1:E:189:GLU:O | 1:E:191:PRO:HD3 | 1.92 | 0.69 |
| 1:C:189:GLU:O | 1:C:191:PRO:HD3 | 1.91 | 0.69 |
| 1:D:164:LYS:O | 1:D:282:ILE:HD11 | 1.93 | 0.69 |
| 1:A:542:MET:HE2 | 1:A:542:MET:HA | 1.74 | 0.69 |
| 1:A:78:GLN:HG2 | 1:A:79:VAL:N | 2.07 | 0.69 |
| 1:F:542:MET:HE1 | 1:F:545:LEU:HD23 | 1.74 | 0.69 |
| 1:A:146:ILE:O | 1:A:146:ILE:HD12 | 1.92 | 0.69 |
| 1:B:146:ILE:HD12 | 1:B:146:ILE:O | 1.92 | 0.69 |
| 1:E:542:MET:CE | 1:E:545:LEU:HD23 | 2.23 | 0.69 |
| 1:F:157:THR:CG2 | 1:F:489:SER:H | 2.06 | 0.69 |
| 1:F:37:PHE:CZ | 1:F:40:HIS:O | 2.46 | 0.69 |
| 1:D:224:ASP:O | 1:D:227:THR:OG1 | 2.10 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:157:THR:CG2 | 1:E:489:SER:H | 2.06 | 0.68 |
| 1:B:26:ASN:HB3 | 1:B:29:ARG:CZ | 2.24 | 0.68 |
| 1:E:127:VAL:HG21 | 1:E:528:PHE:CD1 | 2.28 | 0.68 |
| 1:B:42:PHE:CE1 | 1:B:59:ILE:HD12 | 2.27 | 0.68 |
| 1:C:233:GLN:NE2 | 1:C:380:VAL:HG13 | 2.09 | 0.68 |
| 1:C:42:PHE:CE1 | 1:C:59:ILE:HD12 | 2.28 | 0.68 |
| 1:F:542:MET:O | 1:F:545:LEU:N | 2.27 | 0.68 |
| 1:C:347:LYS:HE2 | 1:C:369:THR:HG22 | 1.73 | 0.68 |
| 1:F:542:MET:HE2 | 1:F:542:MET:HA | 1.75 | 0.68 |
| 1:C:189:GLU:C | 1:C:191:PRO:HD3 | 2.14 | 0.68 |
| 1:B:542:MET:HE2 | 1:B:542:MET:HA | 1.76 | 0.68 |
| 1:C:374:ASP:N | 1:C:374:ASP:OD1 | 2.25 | 0.68 |
| 1:A:563:ILE:N | 1:A:563:ILE:HD13 | 2.09 | 0.68 |
| 1:B:127:VAL:HG21 | 1:B:528:PHE:CD1 | 2.28 | 0.67 |
| 1:F:124:LEU:HD22 | 1:F:532:TRP:HB2 | 1.76 | 0.67 |
| 1:E:347:LYS:HE2 | 1:E:369:THR:HG22 | 1.77 | 0.67 |
| 1:A:470:TYR:CG | 1:A:479:PHE:CE1 | 2.82 | 0.67 |
| 1:B:158:MET:O | 1:B:159:ARG:HD3 | 1.94 | 0.67 |
| 1:D:120:VAL:HG23 | 1:D:121:LEU:N | 2.08 | 0.67 |
| 1:D:180:ASN:OD1 | 1:D:182:ARG:HG2 | 1.95 | 0.67 |
| 1:D:290:MET:HE3 | 1:D:295:LEU:CB | 2.25 | 0.67 |
| 1:A:180:ASN:OD1 | 1:A:182:ARG:HG2 | 1.94 | 0.67 |
| 1:B:111:VAL:HB | 1:B:545:LEU:HD13 | 1.77 | 0.67 |
| 1:C:127:VAL:HG21 | 1:C:528:PHE:CD1 | 2.30 | 0.67 |
| 1:D:312:GLU:OE2 | 1:D:484:ARG:NH1 | 2.28 | 0.67 |
| 1:F:92:VAL:HG23 | 1:F:92:VAL:O | 1.94 | 0.67 |
| 1:A:177:ILE:HD13 | 1:A:177:ILE:O | 1.95 | 0.66 |
| 1:A:286:TYR:N | 1:A:331:ASN:OD1 | 2.28 | 0.66 |
| 1:B:177:ILE:HG22 | 1:B:236:ILE:HG23 | 1.78 | 0.66 |
| 1:C:30:ASP:OD2 | 1:C:89:TYR:OH | 2.11 | 0.66 |
| 1:B:189:GLU:O | 1:B:191:PRO:HD3 | 1.95 | 0.66 |
| 1:E:312:GLU:OE2 | 1:E:484:ARG:NH1 | 2.29 | 0.66 |
| 1:B:258:VAL:HG13 | 1:B:259:ASN:H | 1.59 | 0.66 |
| 1:B:164:LYS:C | 1:B:282:ILE:CD1 | 2.64 | 0.66 |
| 1:C:180:ASN:OD1 | 1:C:182:ARG:HG2 | 1.96 | 0.66 |
| 1:B:470:TYR:CG | 1:B:479:PHE:CE1 | 2.83 | 0.66 |
| 1:C:37:PHE:CZ | 1:C:40:HIS:O | 2.49 | 0.66 |
| 1:D:78:GLN:HG2 | 1:D:79:VAL:N | 2.11 | 0.66 |
| 1:E:146:ILE:O | 1:E:146:ILE:HD12 | 1.96 | 0.66 |
| 1:B:312:GLU:OE2 | 1:B:484:ARG:NH1 | 2.28 | 0.66 |
| 1:F:189:GLU:C | 1:F:191:PRO:HD3 | 2.16 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:ASP:OD1 | 1:A:374:ASP:N | 2.29 | 0.66 |
| 1:C:347:LYS:HE2 | 1:C:369:THR:CG2 | 2.25 | 0.66 |
| 1:B:133:HIS:HB3 | 1:B:520:MET:HE3 | 1.77 | 0.65 |
| 1:E:470:TYR:CG | 1:E:479:PHE:CE1 | 2.83 | 0.65 |
| 1:C:124:LEU:HD22 | 1:C:532:TRP:HB2 | 1.78 | 0.65 |
| 1:C:542:MET:HE2 | 1:C:542:MET:HA | 1.76 | 0.65 |
| 1:A:42:PHE:CE1 | 1:A:59:ILE:HD12 | 2.32 | 0.65 |
| 1:D:542:MET:CE | 1:D:545:LEU:HD23 | 2.27 | 0.65 |
| 1:A:174:ILE:HG12 | 1:A:176:THR:HG22 | 1.77 | 0.65 |
| 1:C:29:ARG:HD3 | 1:C:89:TYR:CE2 | 2.32 | 0.65 |
| 1:E:75:ASN:O | 1:E:92:VAL:N | 2.30 | 0.65 |
| 1:B:542:MET:O | 1:B:545:LEU:N | 2.29 | 0.65 |
| 1:E:542:MET:HA | 1:E:542:MET:HE2 | 1.77 | 0.65 |
| 1:A:258:VAL:HG13 | 1:A:259:ASN:H | 1.62 | 0.65 |
| 1:B:133:HIS:HB3 | 1:B:520:MET:CE | 2.27 | 0.65 |
| 1:D:146:ILE:HD12 | 1:D:146:ILE:O | 1.97 | 0.65 |
| 1:F:180:ASN:OD1 | 1:F:182:ARG:HG2 | 1.96 | 0.65 |
| 1:C:463:ILE:CD1 | 1:C:463:ILE:O | 2.45 | 0.64 |
| 1:A:133:HIS:HB3 | 1:A:520:MET:HE3 | 1.79 | 0.64 |
| 1:C:224:ASP:O | 1:C:227:THR:OG1 | 2.14 | 0.64 |
| 1:E:59:ILE:O | 1:E:59:ILE:HG23 | 1.98 | 0.64 |
| 1:F:233:GLN:NE2 | 1:F:380:VAL:HG13 | 2.13 | 0.64 |
| 1:A:57:VAL:CG1 | 1:A:57:VAL:O | 2.45 | 0.64 |
| 1:A:124:LEU:HD22 | 1:A:532:TRP:HB2 | 1.79 | 0.64 |
| 1:E:78:GLN:HG2 | 1:E:79:VAL:N | 2.13 | 0.64 |
| 1:B:463:ILE:CD1 | 1:B:463:ILE:O | 2.46 | 0.64 |
| 1:E:172:GLU:OE1 | 1:E:212:TRP:HH2 | 1.80 | 0.64 |
| 1:A:157:THR:HG23 | 1:A:157:THR:O | 1.98 | 0.64 |
| 1:C:40:HIS:CE1 | 1:C:42:PHE:HB3 | 2.33 | 0.64 |
| 1:D:563:ILE:HD13 | 1:D:563:ILE:N | 2.13 | 0.64 |
| 1:C:563:ILE:HD13 | 1:C:563:ILE:N | 2.13 | 0.64 |
| 1:B:78:GLN:HG2 | 1:B:79:VAL:N | 2.12 | 0.64 |
| 1:C:542:MET:O | 1:C:545:LEU:N | 2.31 | 0.64 |
| 1:F:206:ASN:OD1 | 1:F:210:MET:CE | 2.46 | 0.64 |
| 1:C:172:GLU:OE1 | 1:C:212:TRP:HH2 | 1.80 | 0.63 |
| 1:C:164:LYS:C | 1:C:282:ILE:CD1 | 2.67 | 0.63 |
| 1:E:124:LEU:HD22 | 1:E:532:TRP:HB2 | 1.79 | 0.63 |
| 1:F:290:MET:HE3 | 1:F:295:LEU:HB2 | 1.80 | 0.63 |
| 1:B:120:VAL:HG23 | 1:B:121:LEU:N | 2.13 | 0.63 |
| 1:F:172:GLU:OE1 | 1:F:212:TRP:HH2 | 1.80 | 0.63 |
| 1:E:29:ARG:HD2 | 1:E:30:ASP:OD2 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:PHE:CD1 | 1:B:38:ASP:N | 2.65 | 0.63 |
| 1:D:172:GLU:OE1 | 1:D:212:TRP:HH2 | 1.80 | 0.63 |
| 1:B:174:ILE:HG12 | 1:B:176:THR:HG22 | 1.78 | 0.63 |
| 1:C:78:GLN:HG2 | 1:C:79:VAL:N | 2.14 | 0.63 |
| 1:F:120:VAL:HG23 | 1:F:121:LEU:N | 2.13 | 0.63 |
| 1:A:106:SER:O | 1:A:107:LEU:HD12 | 1.99 | 0.63 |
| 1:B:172:GLU:OE1 | 1:B:212:TRP:HH2 | 1.82 | 0.63 |
| 1:D:42:PHE:CE1 | 1:D:59:ILE:HD12 | 2.33 | 0.63 |
| 1:F:312:GLU:OE2 | 1:F:484:ARG:NH1 | 2.32 | 0.63 |
| 1:B:189:GLU:C | 1:B:191:PRO:HD3 | 2.18 | 0.63 |
| 1:D:157:THR:O | 1:D:157:THR:CG2 | 2.47 | 0.63 |
| 1:D:380:VAL:HG12 | 1:D:381:ASP:N | 2.14 | 0.63 |
| 1:D:46:PHE:CB | 1:D:57:VAL:HG23 | 2.29 | 0.62 |
| 1:B:18:GLN:NE2 | 1:B:552:GLY:O | 2.32 | 0.62 |
| 1:F:258:VAL:HG13 | 1:F:259:ASN:H | 1.64 | 0.62 |
| 1:F:233:GLN:O | 1:F:236:ILE:HG13 | 2.00 | 0.62 |
| 1:A:135:THR:O | 1:A:136:GLN:C | 2.38 | 0.62 |
| 1:E:563:ILE:N | 1:E:563:ILE:HD13 | 2.14 | 0.62 |
| 1:E:534:LEU:HB2 | 1:E:542:MET:CE | 2.30 | 0.62 |
| 1:E:542:MET:HE2 | 1:E:545:LEU:HD23 | 1.79 | 0.62 |
| 1:B:224:ASP:O | 1:B:227:THR:OG1 | 2.17 | 0.62 |
| 1:B:46:PHE:O | 1:B:46:PHE:CD2 | 2.53 | 0.62 |
| 1:F:313:LEU:HB2 | 1:F:321:LEU:HB3 | 1.82 | 0.62 |
| 1:B:347:LYS:HE2 | 1:B:369:THR:CG2 | 2.29 | 0.62 |
| 1:C:157:THR:CG2 | 1:C:489:SER:H | 2.12 | 0.62 |
| 1:F:189:GLU:O | 1:F:191:PRO:HD3 | 2.00 | 0.62 |
| 1:C:286:TYR:N | 1:C:331:ASN:OD1 | 2.33 | 0.62 |
| 1:D:75:ASN:O | 1:D:92:VAL:N | 2.31 | 0.62 |
| 1:F:46:PHE:HB3 | 1:F:57:VAL:HG23 | 1.82 | 0.62 |
| 1:E:356:ARG:NH2 | 1:F:487:ARG:O | 2.32 | 0.62 |
| 1:B:40:HIS:CE1 | 1:B:42:PHE:HB3 | 2.35 | 0.62 |
| 1:F:75:ASN:O | 1:F:92:VAL:N | 2.33 | 0.62 |
| 1:A:120:VAL:HG23 | 1:A:121:LEU:N | 2.15 | 0.62 |
| 1:E:380:VAL:HG12 | 1:E:381:ASP:N | 2.15 | 0.62 |
| 1:F:177:ILE:HD13 | 1:F:177:ILE:O | 1.99 | 0.62 |
| 1:F:351:LYS:O | 1:F:352:ASN:HB2 | 1.99 | 0.62 |
| 1:E:40:HIS:CE1 | 1:E:42:PHE:HB3 | 2.34 | 0.61 |
| 1:E:29:ARG:HD3 | 1:E:89:TYR:CE2 | 2.34 | 0.61 |
| 1:D:134:TYR:O | 1:D:572:ILE:HD13 | 1.99 | 0.61 |
| 1:C:5:LYS:NZ | 1:C:41:GLU:OE2 | 2.33 | 0.61 |
| 1:A:312:GLU:OE2 | 1:A:484:ARG:NH1 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:182:ARG:CZ | 1:B:267:LYS:HE2 | 2.30 | 0.61 |
| 1:B:26:ASN:HB3 | 1:B:29:ARG:NH2 | 2.14 | 0.61 |
| 1:E:42:PHE:CE1 | 1:E:59:ILE:HD12 | 2.36 | 0.61 |
| 1:A:224:ASP:O | 1:A:227:THR:OG1 | 2.18 | 0.61 |
| 1:A:29:ARG:HD3 | 1:A:89:TYR:CE2 | 2.36 | 0.61 |
| 1:A:40:HIS:CE1 | 1:A:42:PHE:HB3 | 2.35 | 0.61 |
| 1:B:124:LEU:HD22 | 1:B:532:TRP:HB2 | 1.81 | 0.61 |
| 1:F:290:MET:HE3 | 1:F:295:LEU:CB | 2.30 | 0.61 |
| 1:B:180:ASN:OD1 | 1:B:182:ARG:HG2 | 2.00 | 0.61 |
| 1:B:37:PHE:HZ | 1:B:40:HIS:O | 1.82 | 0.61 |
| 1:E:164:LYS:C | 1:E:282:ILE:CD1 | 2.69 | 0.61 |
| 1:E:463:ILE:O | 1:E:463:ILE:CD1 | 2.49 | 0.61 |
| 1:E:8:LEU:O | 1:E:37:PHE:CZ | 2.54 | 0.61 |
| 1:F:164:LYS:O | 1:F:282:ILE:HD11 | 2.01 | 0.61 |
| 1:F:3:LEU:N | 1:F:44:SER:O | 2.33 | 0.61 |
| 1:A:174:ILE:HD13 | 1:A:174:ILE:O | 2.01 | 0.61 |
| 1:E:120:VAL:HG23 | 1:E:121:LEU:N | 2.15 | 0.61 |
| 1:F:217:GLU:O | 1:F:220:LYS:N | 2.33 | 0.61 |
| 1:F:224:ASP:O | 1:F:227:THR:OG1 | 2.19 | 0.61 |
| 1:A:542:MET:HE1 | 1:A:545:LEU:HD23 | 1.83 | 0.60 |
| 1:D:566:THR:O | 1:D:567:VAL:C | 2.39 | 0.60 |
| 1:D:542:MET:HE2 | 1:D:542:MET:HA | 1.83 | 0.60 |
| 1:F:135:THR:O | 1:F:136:GLN:C | 2.39 | 0.60 |
| 1:A:182:ARG:CZ | 1:A:267:LYS:HE2 | 2.31 | 0.60 |
| 1:B:313:LEU:HB2 | 1:B:321:LEU:HB3 | 1.82 | 0.60 |
| 1:B:75:ASN:N | 1:B:75:ASN:OD1 | 2.34 | 0.60 |
| 1:A:164:LYS:C | 1:A:282:ILE:CD1 | 2.70 | 0.60 |
| 1:B:380:VAL:HG12 | 1:B:381:ASP:N | 2.16 | 0.60 |
| 1:C:470:TYR:CG | 1:C:479:PHE:CE1 | 2.89 | 0.60 |
| 1:C:37:PHE:CD1 | 1:C:38:ASP:N | 2.68 | 0.60 |
| 1:C:566:THR:O | 1:C:567:VAL:C | 2.40 | 0.60 |
| 1:D:542:MET:HE2 | 1:D:545:LEU:HD23 | 1.81 | 0.60 |
| 1:E:206:ASN:OD1 | 1:E:210:MET:CE | 2.48 | 0.60 |
| 1:E:46:PHE:CB | 1:E:57:VAL:HG23 | 2.31 | 0.60 |
| 1:B:290:MET:HE3 | 1:B:295:LEU:CB | 2.31 | 0.60 |
| 1:D:374:ASP:N | 1:D:374:ASP:OD1 | 2.35 | 0.60 |
| 1:F:90:LEU:HD22 | 1:F:107:LEU:HD23 | 1.83 | 0.60 |
| 1:A:8:LEU:O | 1:A:37:PHE:CZ | 2.54 | 0.60 |
| 1:B:157:THR:CG2 | 1:B:489:SER:H | 2.13 | 0.60 |
| 1:D:174:ILE:HG12 | 1:D:176:THR:HG22 | 1.82 | 0.60 |
| 1:B:128:ASN:ND2 | 1:B:128:ASN:C | 2.54 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:542:MET:CE | 1:B:545:LEU:HD23 | 2.32 | 0.60 |
| 1:A:15:ASN:CG | 1:F:546:ARG:NH2 | 2.56 | 0.60 |
| 1:A:463:ILE:O | 1:A:463:ILE:CD1 | 2.50 | 0.60 |
| 1:F:347:LYS:HE2 | 1:F:369:THR:CG2 | 2.32 | 0.60 |
| 1:A:111:VAL:HB | 1:A:545:LEU:HD13 | 1.83 | 0.59 |
| 1:D:233:GLN:O | 1:D:236:ILE:HG13 | 2.02 | 0.59 |
| 1:D:40:HIS:CE1 | 1:D:42:PHE:HB3 | 2.37 | 0.59 |
| 1:D:560:SER:O | 1:D:564:ASN:ND2 | 2.34 | 0.59 |
| 1:C:546:ARG:NH2 | 1:D:15:ASN:OD1 | 2.35 | 0.59 |
| 1:E:174:ILE:HG12 | 1:E:176:THR:HG22 | 1.83 | 0.59 |
| 1:E:182:ARG:NH2 | 1:E:267:LYS:HE2 | 2.17 | 0.59 |
| 1:F:563:ILE:N | 1:F:563:ILE:HD13 | 2.17 | 0.59 |
| 1:B:79:VAL:HG11 | 1:B:81:TYR:CE2 | 2.37 | 0.59 |
| 1:E:79:VAL:HG11 | 1:E:81:TYR:CE2 | 2.37 | 0.59 |
| 1:F:470:TYR:CG | 1:F:479:PHE:CE1 | 2.91 | 0.59 |
| 1:D:133:HIS:HB3 | 1:D:520:MET:HE3 | 1.84 | 0.59 |
| 1:F:347:LYS:HE2 | 1:F:369:THR:HG22 | 1.85 | 0.59 |
| 1:B:563:ILE:N | 1:B:563:ILE:HD13 | 2.17 | 0.59 |
| 1:D:189:GLU:O | 1:D:191:PRO:HD3 | 2.03 | 0.59 |
| 1:E:182:ARG:CZ | 1:E:267:LYS:HE2 | 2.31 | 0.59 |
| 1:F:463:ILE:O | 1:F:463:ILE:CD1 | 2.51 | 0.59 |
| 1:F:566:THR:O | 1:F:567:VAL:C | 2.41 | 0.59 |
| 1:A:128:ASN:C | 1:A:128:ASN:ND2 | 2.55 | 0.59 |
| 1:C:206:ASN:OD1 | 1:C:210:MET:CE | 2.50 | 0.59 |
| 1:D:215:ASP:OD1 | 1:D:215:ASP:C | 2.41 | 0.59 |
| 1:A:359:ASN:O | 1:A:360:VAL:C | 2.41 | 0.59 |
| 1:B:6:ILE:CG2 | 1:B:7:LYS:N | 2.65 | 0.59 |
| 1:A:177:ILE:CG2 | 1:A:236:ILE:HG12 | 2.32 | 0.59 |
| 1:B:566:THR:O | 1:B:567:VAL:C | 2.39 | 0.59 |
| 1:E:502:MET:HG2 | 1:E:567:VAL:HG11 | 1.84 | 0.59 |
| 1:C:135:THR:O | 1:C:136:GLN:C | 2.38 | 0.59 |
| 1:D:258:VAL:HG13 | 1:D:259:ASN:H | 1.68 | 0.59 |
| 1:D:3:LEU:N | 1:D:44:SER:O | 2.36 | 0.59 |
| 1:D:470:TYR:CG | 1:D:479:PHE:CE1 | 2.91 | 0.59 |
| 1:E:282:ILE:HG23 | 1:E:334:PHE:CD2 | 2.37 | 0.59 |
| 1:F:164:LYS:C | 1:F:282:ILE:CD1 | 2.71 | 0.59 |
| 1:B:174:ILE:O | 1:B:174:ILE:HD13 | 2.02 | 0.59 |
| 1:B:347:LYS:HE2 | 1:B:369:THR:HG22 | 1.84 | 0.59 |
| 1:C:258:VAL:HG13 | 1:C:259:ASN:H | 1.68 | 0.59 |
| 1:C:18:GLN:NE2 | 1:C:552:GLY:O | 2.34 | 0.59 |
| 1:E:5:LYS:NZ | 1:E:41:GLU:OE2 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:44:SER:OG | 1:B:45:THR:N | 2.36 | 0.58 |
| 1:B:67:CYS:O | 1:B:68:PHE:HB2 | 2.03 | 0.58 |
| 1:F:380:VAL:HG12 | 1:F:381:ASP:N | 2.18 | 0.58 |
| 1:F:563:ILE:O | 1:F:564:ASN:ND2 | 2.36 | 0.58 |
| 1:A:18:GLN:NE2 | 1:A:552:GLY:O | 2.34 | 0.58 |
| 1:C:120:VAL:HG23 | 1:C:121:LEU:N | 2.17 | 0.58 |
| 1:D:256:GLU:O | 1:D:264:SER:HA | 2.04 | 0.58 |
| 1:D:290:MET:HE3 | 1:D:295:LEU:HB2 | 1.85 | 0.58 |
| 1:E:290:MET:HE3 | 1:E:295:LEU:CB | 2.33 | 0.58 |
| 1:E:75:ASN:HA | 1:E:92:VAL:HG22 | 1.85 | 0.58 |
| 1:D:164:LYS:C | 1:D:282:ILE:CD1 | 2.72 | 0.58 |
| 1:D:59:ILE:O | 1:D:59:ILE:HG23 | 2.03 | 0.58 |
| 1:F:40:HIS:CE1 | 1:F:42:PHE:HB3 | 2.38 | 0.58 |
| 1:F:566:THR:O | 1:F:568:VAL:N | 2.35 | 0.58 |
| 1:C:29:ARG:HD2 | 1:C:30:ASP:OD2 | 2.03 | 0.58 |
| 1:C:380:VAL:HG12 | 1:C:381:ASP:N | 2.19 | 0.58 |
| 1:E:258:VAL:HG13 | 1:E:259:ASN:H | 1.67 | 0.58 |
| 1:F:286:TYR:N | 1:F:331:ASN:OD1 | 2.36 | 0.58 |
| 1:F:302:HIS:CD2 | 1:F:303:LEU:HD13 | 2.38 | 0.58 |
| 1:F:41:GLU:HG2 | 1:F:41:GLU:O | 2.03 | 0.58 |
| 1:C:174:ILE:HG12 | 1:C:176:THR:HG22 | 1.85 | 0.58 |
| 1:F:215:ASP:OD1 | 1:F:215:ASP:C | 2.42 | 0.58 |
| 1:C:67:CYS:O | 1:C:68:PHE:HB2 | 2.04 | 0.58 |
| 1:D:299:ASN:N | 1:D:299:ASN:ND2 | 2.51 | 0.58 |
| 1:D:5:LYS:NZ | 1:D:41:GLU:OE2 | 2.36 | 0.58 |
| 1:D:546:ARG:NH2 | 1:E:15:ASN:CG | 2.57 | 0.58 |
| 1:E:172:GLU:HB3 | 1:E:212:TRP:CH2 | 2.38 | 0.58 |
| 1:B:5:LYS:NZ | 1:B:41:GLU:OE2 | 2.37 | 0.58 |
| 1:D:174:ILE:HD13 | 1:D:174:ILE:O | 2.04 | 0.58 |
| 1:E:529:LYS:O | 1:E:530:GLY:O | 2.22 | 0.58 |
| 1:F:29:ARG:HD3 | 1:F:89:TYR:CE2 | 2.39 | 0.58 |
| 1:C:313:LEU:HB2 | 1:C:321:LEU:HB3 | 1.86 | 0.58 |
| 1:D:57:VAL:CG1 | 1:D:57:VAL:O | 2.51 | 0.58 |
| 1:E:229:TYR:N | 1:E:229:TYR:CD2 | 2.71 | 0.58 |
| 1:B:529:LYS:O | 1:B:530:GLY:O | 2.21 | 0.58 |
| 1:F:30:ASP:OD2 | 1:F:89:TYR:OH | 2.20 | 0.58 |
| 1:F:516:ASP:OD2 | 1:F:518:THR:HG22 | 2.03 | 0.58 |
| 1:D:90:LEU:HA | 1:D:109:PRO:HA | 1.84 | 0.57 |
| 1:F:306:PRO:HD3 | 1:F:326:SER:HB3 | 1.85 | 0.57 |
| 1:B:563:ILE:O | 1:B:564:ASN:ND2 | 2.37 | 0.57 |
| 1:C:157:THR:O | 1:C:157:THR:HG23 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:133:HIS:HB3 | 1:F:520:MET:HE3 | 1.86 | 0.57 |
| 1:A:177:ILE:HG22 | 1:A:236:ILE:HG23 | 1.86 | 0.57 |
| 1:E:258:VAL:HG22 | 1:E:259:ASN:N | 2.18 | 0.57 |
| 1:D:463:ILE:O | 1:D:463:ILE:CD1 | 2.53 | 0.57 |
| 1:E:286:TYR:N | 1:E:331:ASN:OD1 | 2.37 | 0.57 |
| 1:C:298:ILE:HB | 1:C:299:ASN:ND2 | 2.19 | 0.57 |
| 1:D:8:LEU:O | 1:D:37:PHE:CZ | 2.58 | 0.57 |
| 1:A:380:VAL:HG12 | 1:A:381:ASP:N | 2.19 | 0.57 |
| 1:A:67:CYS:O | 1:A:68:PHE:HB2 | 2.05 | 0.57 |
| 1:E:542:MET:O | 1:E:545:LEU:N | 2.35 | 0.57 |
| 1:F:177:ILE:HG22 | 1:F:236:ILE:HG23 | 1.87 | 0.57 |
| 1:F:42:PHE:CE1 | 1:F:59:ILE:HD12 | 2.40 | 0.57 |
| 1:F:59:ILE:HG23 | 1:F:59:ILE:O | 2.05 | 0.57 |
| 1:A:215:ASP:C | 1:A:215:ASP:OD1 | 2.43 | 0.57 |
| 1:B:491:ASP:O | 1:B:492:GLU:C | 2.39 | 0.57 |
| 1:F:182:ARG:CZ | 1:F:267:LYS:HE2 | 2.35 | 0.57 |
| 1:C:215:ASP:OD1 | 1:C:215:ASP:C | 2.44 | 0.57 |
| 1:C:305:ARG:HB2 | 1:C:306:PRO:HD2 | 1.86 | 0.57 |
| 1:D:502:MET:HG2 | 1:D:567:VAL:HG11 | 1.87 | 0.57 |
| 1:B:374:ASP:OD1 | 1:B:374:ASP:N | 2.38 | 0.57 |
| 1:D:46:PHE:HB3 | 1:D:57:VAL:HG23 | 1.87 | 0.57 |
| 1:D:67:CYS:O | 1:D:68:PHE:HB2 | 2.05 | 0.57 |
| 1:E:233:GLN:O | 1:E:236:ILE:HG13 | 2.05 | 0.57 |
| 1:F:67:CYS:O | 1:F:68:PHE:HB2 | 2.04 | 0.57 |
| 1:E:539:THR:CG2 | 1:F:94:ASP:HA | 2.34 | 0.57 |
| 1:A:37:PHE:HZ | 1:A:40:HIS:O | 1.88 | 0.57 |
| 1:C:152:VAL:HG21 | 1:C:307:ASN:HD21 | 1.70 | 0.57 |
| 1:D:37:PHE:CD1 | 1:D:38:ASP:N | 2.73 | 0.57 |
| 1:A:290:MET:CE | 1:A:295:LEU:HB3 | 2.34 | 0.56 |
| 1:B:59:ILE:O | 1:B:59:ILE:CG2 | 2.51 | 0.56 |
| 1:B:356:ARG:NH2 | 1:C:487:ARG:O | 2.38 | 0.56 |
| 1:D:135:THR:O | 1:D:136:GLN:C | 2.42 | 0.56 |
| 1:D:339:THR:HG21 | 1:E:472:PRO:HB3 | 1.87 | 0.56 |
| 1:E:553:VAL:HG12 | 1:E:555:LEU:HD12 | 1.87 | 0.56 |
| 1:A:46:PHE:CB | 1:A:57:VAL:HG23 | 2.36 | 0.56 |
| 1:D:18:GLN:NE2 | 1:D:552:GLY:O | 2.39 | 0.56 |
| 1:D:471:ALA:HB3 | 1:D:472:PRO:HD3 | 1.86 | 0.56 |
| 1:E:224:ASP:O | 1:E:227:THR:OG1 | 2.21 | 0.56 |
| 1:E:111:VAL:HB | 1:E:545:LEU:HD13 | 1.87 | 0.56 |
| 1:B:229:TYR:N | 1:B:229:TYR:CD2 | 2.73 | 0.56 |
| 1:B:134:TYR:O | 1:B:572:ILE:HD13 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:313:LEU:HB2 | 1:D:321:LEU:HB3 | 1.87 | 0.56 |
| 1:F:133:HIS:HB3 | 1:F:520:MET:CE | 2.35 | 0.56 |
| 1:E:46:PHE:O | 1:E:46:PHE:CD2 | 2.58 | 0.56 |
| 1:F:18:GLN:NE2 | 1:F:552:GLY:O | 2.38 | 0.56 |
| 1:C:148:SER:CB | 1:D:156:SER:O | 2.54 | 0.56 |
| 1:D:286:TYR:N | 1:D:331:ASN:OD1 | 2.38 | 0.56 |
| 1:A:133:HIS:HB3 | 1:A:520:MET:CE | 2.35 | 0.56 |
| 1:E:305:ARG:HB2 | 1:E:306:PRO:HD2 | 1.86 | 0.56 |
| 1:D:148:SER:CB | 1:E:156:SER:O | 2.53 | 0.56 |
| 1:F:44:SER:OG | 1:F:45:THR:N | 2.37 | 0.56 |
| 1:A:90:LEU:HD22 | 1:A:107:LEU:HD23 | 1.88 | 0.56 |
| 1:B:233:GLN:O | 1:B:236:ILE:HG13 | 2.06 | 0.56 |
| 1:D:90:LEU:HD22 | 1:D:107:LEU:HD23 | 1.86 | 0.56 |
| 1:B:286:TYR:CE1 | 1:B:301:LYS:HE3 | 2.41 | 0.56 |
| 1:E:180:ASN:OD1 | 1:E:182:ARG:HG2 | 2.06 | 0.56 |
| 1:E:46:PHE:HB3 | 1:E:57:VAL:HG23 | 1.87 | 0.56 |
| 1:F:502:MET:HG2 | 1:F:567:VAL:HG11 | 1.88 | 0.56 |
| 1:A:79:VAL:HG11 | 1:A:81:TYR:CE2 | 2.41 | 0.56 |
| 1:B:502:MET:O | 1:B:554:ARG:NH1 | 2.36 | 0.56 |
| 1:C:6:ILE:CG2 | 1:C:7:LYS:N | 2.69 | 0.56 |
| 1:D:175:LEU:CD1 | 1:D:177:ILE:HG23 | 2.36 | 0.56 |
| 1:D:351:LYS:HG2 | 1:D:352:ASN:OD1 | 2.06 | 0.56 |
| 1:E:290:MET:HE3 | 1:E:295:LEU:HB2 | 1.88 | 0.56 |
| 1:E:37:PHE:HZ | 1:E:40:HIS:O | 1.87 | 0.56 |
| 1:F:134:TYR:O | 1:F:572:ILE:HD13 | 2.05 | 0.56 |
| 1:F:5:LYS:NZ | 1:F:41:GLU:OE2 | 2.38 | 0.56 |
| 1:A:172:GLU:OE1 | 1:A:212:TRP:HH2 | 1.89 | 0.56 |
| 1:B:45:THR:HG23 | 1:B:45:THR:O | 2.05 | 0.56 |
| 1:C:8:LEU:O | 1:C:37:PHE:CZ | 2.59 | 0.56 |
| 1:C:42:PHE:CE1 | 1:C:59:ILE:CD1 | 2.89 | 0.56 |
| 1:E:3:LEU:N | 1:E:44:SER:O | 2.39 | 0.56 |
| 1:E:67:CYS:SG | 1:E:68:PHE:N | 2.79 | 0.56 |
| 1:F:305:ARG:HB2 | 1:F:306:PRO:HD2 | 1.87 | 0.56 |
| 1:A:134:TYR:O | 1:A:572:ILE:HD13 | 2.06 | 0.55 |
| 1:A:177:ILE:HG21 | 1:A:236:ILE:HG12 | 1.87 | 0.55 |
| 1:A:290:MET:HE3 | 1:A:295:LEU:CB | 2.35 | 0.55 |
| 1:B:46:PHE:CB | 1:B:57:VAL:HG23 | 2.36 | 0.55 |
| 1:C:258:VAL:HG22 | 1:C:259:ASN:N | 2.20 | 0.55 |
| 1:C:59:ILE:HG23 | 1:C:59:ILE:O | 2.05 | 0.55 |
| 1:A:502:MET:HG2 | 1:A:567:VAL:HG11 | 1.87 | 0.55 |
| 1:D:189:GLU:C | 1:D:191:PRO:HD3 | 2.26 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:566:THR:O | 1:D:568:VAL:N | 2.40 | 0.55 |
| 1:C:133:HIS:HB3 | 1:C:520:MET:CE | 2.36 | 0.55 |
| 1:E:566:THR:O | 1:E:567:VAL:C | 2.43 | 0.55 |
| 1:F:175:LEU:CD1 | 1:F:177:ILE:HG23 | 2.36 | 0.55 |
| 1:E:174:ILE:HD13 | 1:E:174:ILE:O | 2.05 | 0.55 |
| 1:F:374:ASP:N | 1:F:374:ASP:OD1 | 2.32 | 0.55 |
| 1:A:206:ASN:OD1 | 1:A:210:MET:CE | 2.55 | 0.55 |
| 1:B:57:VAL:O | 1:B:57:VAL:CG1 | 2.55 | 0.55 |
| 1:B:8:LEU:O | 1:B:37:PHE:CZ | 2.60 | 0.55 |
| 1:C:174:ILE:O | 1:C:174:ILE:HD13 | 2.06 | 0.55 |
| 1:D:534:LEU:HB2 | 1:D:542:MET:CE | 2.36 | 0.55 |
| 1:E:471:ALA:HB3 | 1:E:472:PRO:HD3 | 1.89 | 0.55 |
| 1:F:75:ASN:HA | 1:F:92:VAL:HG22 | 1.89 | 0.55 |
| 1:A:359:ASN:C | 1:A:360:VAL:O | 2.41 | 0.55 |
| 1:E:128:ASN:ND2 | 1:E:128:ASN:C | 2.58 | 0.55 |
| 1:F:157:THR:CG2 | 1:F:157:THR:O | 2.54 | 0.55 |
| 1:F:177:ILE:CG2 | 1:F:236:ILE:HG12 | 2.36 | 0.55 |
| 1:A:156:SER:O | 1:F:148:SER:CB | 2.55 | 0.55 |
| 1:C:566:THR:O | 1:C:568:VAL:N | 2.40 | 0.55 |
| 1:D:12:THR:HG21 | 1:D:76:TYR:HB2 | 1.89 | 0.55 |
| 1:B:566:THR:O | 1:B:568:VAL:N | 2.39 | 0.55 |
| 1:D:79:VAL:HG11 | 1:D:81:TYR:CE2 | 2.42 | 0.55 |
| 1:E:563:ILE:O | 1:E:564:ASN:ND2 | 2.40 | 0.55 |
| 1:A:175:LEU:CD1 | 1:A:177:ILE:HG23 | 2.37 | 0.55 |
| 1:C:471:ALA:HB3 | 1:C:472:PRO:HD3 | 1.89 | 0.55 |
| 1:F:534:LEU:HB2 | 1:F:542:MET:CE | 2.37 | 0.55 |
| 1:A:305:ARG:HB2 | 1:A:306:PRO:HD2 | 1.88 | 0.54 |
| 1:B:90:LEU:HA | 1:B:109:PRO:HA | 1.88 | 0.54 |
| 1:E:296:ASN:O | 1:E:300:ASP:HB2 | 2.06 | 0.54 |
| 1:A:15:ASN:OD1 | 1:F:546:ARG:NH2 | 2.40 | 0.54 |
| 1:A:189:GLU:O | 1:A:191:PRO:HD3 | 2.08 | 0.54 |
| 1:A:256:GLU:O | 1:A:264:SER:HA | 2.07 | 0.54 |
| 1:A:566:THR:O | 1:A:567:VAL:C | 2.46 | 0.54 |
| 1:C:518:THR:O | 1:C:518:THR:HG23 | 2.06 | 0.54 |
| 1:C:534:LEU:HB2 | 1:C:542:MET:SD | 2.47 | 0.54 |
| 1:C:546:ARG:NH2 | 1:D:15:ASN:CG | 2.60 | 0.54 |
| 1:C:134:TYR:O | 1:C:572:ILE:HD13 | 2.07 | 0.54 |
| 1:E:256:GLU:O | 1:E:264:SER:HA | 2.07 | 0.54 |
| 1:F:26:ASN:O | 1:F:29:ARG:HB3 | 2.06 | 0.54 |
| 1:A:41:GLU:HG2 | 1:A:41:GLU:O | 2.07 | 0.54 |
| 1:B:175:LEU:CD1 | 1:B:177:ILE:HG23 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:177:ILE:O | 1:C:177:ILE:HD13 | 2.08 | 0.54 |
| 1:C:79:VAL:HG11 | 1:C:81:TYR:CE2 | 2.42 | 0.54 |
| 1:E:374:ASP:OD1 | 1:E:374:ASP:N | 2.36 | 0.54 |
| 1:B:546:ARG:NH2 | 1:C:15:ASN:OD1 | 2.41 | 0.54 |
| 1:D:229:TYR:CD2 | 1:D:229:TYR:N | 2.75 | 0.54 |
| 1:E:67:CYS:O | 1:E:68:PHE:HB2 | 2.07 | 0.54 |
| 1:B:30:ASP:OD2 | 1:B:89:TYR:OH | 2.21 | 0.54 |
| 1:C:175:LEU:CD1 | 1:C:177:ILE:HG23 | 2.37 | 0.54 |
| 1:C:190:LYS:HG2 | 1:C:190:LYS:O | 2.06 | 0.54 |
| 1:D:172:GLU:HB3 | 1:D:212:TRP:CH2 | 2.43 | 0.54 |
| 1:D:206:ASN:OD1 | 1:D:210:MET:CE | 2.56 | 0.54 |
| 1:A:471:ALA:HB3 | 1:A:472:PRO:HD3 | 1.90 | 0.54 |
| 1:C:182:ARG:CZ | 1:C:267:LYS:HE2 | 2.37 | 0.54 |
| 1:E:135:THR:O | 1:E:136:GLN:C | 2.46 | 0.54 |
| 1:E:204:ILE:HD13 | 1:F:468:VAL:HG23 | 1.90 | 0.54 |
| 1:F:174:ILE:HG12 | 1:F:176:THR:HG22 | 1.88 | 0.54 |
| 1:A:189:GLU:C | 1:A:191:PRO:HD3 | 2.27 | 0.54 |
| 1:A:57:VAL:O | 1:A:57:VAL:HG12 | 2.07 | 0.54 |
| 1:D:3:LEU:HD21 | 1:E:68:PHE:CE2 | 2.43 | 0.54 |
| 1:F:8:LEU:O | 1:F:37:PHE:CZ | 2.61 | 0.54 |
| 1:B:291:PHE:C | 1:B:291:PHE:CD2 | 2.80 | 0.54 |
| 1:B:360:VAL:HG23 | 1:B:363:TYR:HB2 | 1.88 | 0.54 |
| 1:C:128:ASN:ND2 | 1:C:128:ASN:C | 2.62 | 0.54 |
| 1:D:44:SER:OG | 1:D:45:THR:N | 2.41 | 0.54 |
| 1:E:44:SER:OG | 1:E:45:THR:N | 2.40 | 0.54 |
| 1:F:46:PHE:O | 1:F:46:PHE:CD2 | 2.61 | 0.54 |
| 1:F:46:PHE:HB2 | 1:F:57:VAL:HG23 | 1.88 | 0.54 |
| 1:A:59:ILE:CG2 | 1:A:59:ILE:O | 2.56 | 0.54 |
| 1:C:279:PHE:HB3 | 1:C:282:ILE:HG22 | 1.89 | 0.54 |
| 1:D:305:ARG:HB2 | 1:D:306:PRO:HD2 | 1.90 | 0.54 |
| 1:E:152:VAL:HG22 | 1:E:153:LEU:N | 2.23 | 0.54 |
| 1:D:204:ILE:HD13 | 1:E:468:VAL:HG23 | 1.90 | 0.54 |
| 1:C:46:PHE:CB | 1:C:57:VAL:HG23 | 2.37 | 0.54 |
| 1:D:46:PHE:CE1 | 1:D:55:LEU:CD1 | 2.91 | 0.54 |
| 1:E:532:TRP:CZ2 | 1:E:546:ARG:HA | 2.43 | 0.53 |
| 1:F:174:ILE:HD13 | 1:F:174:ILE:O | 2.08 | 0.53 |
| 1:A:229:TYR:CD2 | 1:A:229:TYR:N | 2.75 | 0.53 |
| 1:B:182:ARG:NH2 | 1:B:267:LYS:HE2 | 2.24 | 0.53 |
| 1:B:23:PHE:CD2 | 1:B:23:PHE:N | 2.75 | 0.53 |
| 1:D:158:MET:O | 1:D:159:ARG:CD | 2.50 | 0.53 |
| 1:F:229:TYR:N | 1:F:229:TYR:CD2 | 2.76 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:12:THR:HG21 | 1:B:76:TYR:HB2 | 1.90 | 0.53 |
| 1:B:534:LEU:HB2 | 1:B:542:MET:CE | 2.37 | 0.53 |
| 1:B:542:MET:HE2 | 1:B:545:LEU:HD23 | 1.90 | 0.53 |
| 1:F:212:TRP:CZ3 | 1:F:247:ILE:HG13 | 2.43 | 0.53 |
| 1:A:172:GLU:HB3 | 1:A:212:TRP:CH2 | 2.44 | 0.53 |
| 1:C:463:ILE:HD12 | 1:C:463:ILE:O | 2.09 | 0.53 |
| 1:D:182:ARG:CZ | 1:D:267:LYS:HE2 | 2.38 | 0.53 |
| 1:A:470:TYR:HB3 | 1:A:479:PHE:CD1 | 2.44 | 0.53 |
| 1:B:286:TYR:N | 1:B:331:ASN:OD1 | 2.41 | 0.53 |
| 1:C:302:HIS:CD2 | 1:C:303:LEU:HD13 | 2.43 | 0.53 |
| 1:E:37:PHE:CD1 | 1:E:38:ASP:N | 2.77 | 0.53 |
| 1:E:470:TYR:HB3 | 1:E:479:PHE:CD1 | 2.44 | 0.53 |
| 1:E:18:GLN:NE2 | 1:E:552:GLY:O | 2.39 | 0.53 |
| 1:A:185:PHE:CE2 | 1:A:259:ASN:HB2 | 2.43 | 0.53 |
| 1:A:44:SER:OG | 1:A:45:THR:N | 2.40 | 0.53 |
| 1:B:339:THR:HG21 | 1:C:472:PRO:HB3 | 1.91 | 0.53 |
| 1:B:463:ILE:HD13 | 1:B:463:ILE:O | 2.09 | 0.53 |
| 1:E:46:PHE:CE1 | 1:E:55:LEU:CD1 | 2.91 | 0.53 |
| 1:F:152:VAL:HG21 | 1:F:307:ASN:HD21 | 1.73 | 0.53 |
| 1:F:534:LEU:HB2 | 1:F:542:MET:HE3 | 1.91 | 0.53 |
| 1:E:175:LEU:CD1 | 1:E:177:ILE:HG23 | 2.39 | 0.53 |
| 1:E:133:HIS:HB3 | 1:E:520:MET:HE3 | 1.91 | 0.53 |
| 1:A:233:GLN:O | 1:A:236:ILE:HG13 | 2.09 | 0.53 |
| 1:A:37:PHE:CD1 | 1:A:38:ASP:N | 2.75 | 0.53 |
| 1:C:60:ASP:HA | 1:C:102:VAL:HG22 | 1.91 | 0.53 |
| 1:C:46:PHE:HB3 | 1:C:57:VAL:HG23 | 1.90 | 0.53 |
| 1:D:148:SER:HB3 | 1:E:156:SER:O | 2.09 | 0.53 |
| 1:E:157:THR:O | 1:E:157:THR:CG2 | 2.55 | 0.53 |
| 1:E:491:ASP:O | 1:E:492:GLU:C | 2.47 | 0.53 |
| 1:F:182:ARG:NH2 | 1:F:267:LYS:HE2 | 2.24 | 0.53 |
| 1:D:152:VAL:HG22 | 1:D:153:LEU:N | 2.23 | 0.53 |
| 1:D:152:VAL:HG21 | 1:D:307:ASN:HD21 | 1.74 | 0.53 |
| 1:F:177:ILE:HG21 | 1:F:236:ILE:HG12 | 1.90 | 0.53 |
| 1:F:471:ALA:HB3 | 1:F:472:PRO:HD3 | 1.90 | 0.53 |
| 1:A:358:ASN:O | 1:A:358:ASN:CG | 2.47 | 0.52 |
| 1:B:259:ASN:O | 1:B:260:GLY:C | 2.46 | 0.52 |
| 1:D:302:HIS:CD2 | 1:D:303:LEU:HD13 | 2.44 | 0.52 |
| 1:D:46:PHE:O | 1:D:46:PHE:CD2 | 2.62 | 0.52 |
| 1:D:572:ILE:CG2 | 1:D:572:ILE:O | 2.50 | 0.52 |
| 1:E:90:LEU:HA | 1:E:109:PRO:HA | 1.91 | 0.52 |
| 1:E:26:ASN:HB3 | 1:E:29:ARG:CZ | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:360:VAL:HG13 | 1:F:163:ILE:HD12 | 1.89 | 0.52 |
| 1:F:286:TYR:CE1 | 1:F:301:LYS:HE3 | 2.44 | 0.52 |
| 1:B:90:LEU:HD22 | 1:B:107:LEU:HD23 | 1.90 | 0.52 |
| 1:E:134:TYR:O | 1:E:572:ILE:HD13 | 2.09 | 0.52 |
| 1:F:124:LEU:HD21 | 1:F:532:TRP:HE3 | 1.73 | 0.52 |
| 1:F:172:GLU:HB3 | 1:F:212:TRP:CH2 | 2.44 | 0.52 |
| 1:C:46:PHE:CD2 | 1:C:46:PHE:O | 2.63 | 0.52 |
| 1:E:215:ASP:C | 1:E:215:ASP:OD1 | 2.46 | 0.52 |
| 1:E:313:LEU:HB2 | 1:E:321:LEU:HB3 | 1.90 | 0.52 |
| 1:F:359:ASN:O | 1:F:360:VAL:C | 2.45 | 0.52 |
| 1:A:491:ASP:O | 1:A:494:ASN:N | 2.41 | 0.52 |
| 1:A:529:LYS:O | 1:A:530:GLY:O | 2.28 | 0.52 |
| 1:A:542:MET:O | 1:A:543:ASN:C | 2.48 | 0.52 |
| 1:B:157:THR:O | 1:B:157:THR:CG2 | 2.56 | 0.52 |
| 1:B:572:ILE:CG2 | 1:B:572:ILE:O | 2.49 | 0.52 |
| 1:C:148:SER:HB3 | 1:D:156:SER:O | 2.09 | 0.52 |
| 1:C:256:GLU:O | 1:C:264:SER:HA | 2.08 | 0.52 |
| 1:C:516:ASP:OD2 | 1:C:517:ILE:N | 2.42 | 0.52 |
| 1:D:177:ILE:HG22 | 1:D:236:ILE:HG23 | 1.92 | 0.52 |
| 1:D:26:ASN:O | 1:D:29:ARG:HB3 | 2.09 | 0.52 |
| 1:D:30:ASP:OD2 | 1:D:89:TYR:OH | 2.21 | 0.52 |
| 1:D:358:ASN:O | 1:D:358:ASN:CG | 2.48 | 0.52 |
| 1:A:217:GLU:O | 1:A:220:LYS:N | 2.42 | 0.52 |
| 1:B:164:LYS:C | 1:B:282:ILE:HD11 | 2.29 | 0.52 |
| 1:C:502:MET:HG2 | 1:C:567:VAL:HG11 | 1.91 | 0.52 |
| 1:C:75:ASN:O | 1:C:92:VAL:N | 2.40 | 0.52 |
| 1:C:539:THR:CG2 | 1:D:94:ASP:HA | 2.39 | 0.52 |
| 1:F:359:ASN:C | 1:F:360:VAL:O | 2.48 | 0.52 |
| 1:A:470:TYR:CB | 1:A:479:PHE:CE1 | 2.93 | 0.52 |
| 1:B:42:PHE:CE2 | 1:B:44:SER:HB2 | 2.44 | 0.52 |
| 1:B:470:TYR:HB3 | 1:B:479:PHE:CD1 | 2.44 | 0.52 |
| 1:E:363:TYR:HD2 | 1:F:316:TYR:CE1 | 2.28 | 0.52 |
| 1:F:256:GLU:O | 1:F:264:SER:HA | 2.09 | 0.52 |
| 1:B:217:GLU:O | 1:B:220:LYS:N | 2.42 | 0.52 |
| 1:B:286:TYR:HE1 | 1:B:301:LYS:HE3 | 1.74 | 0.52 |
| 1:C:45:THR:HG23 | 1:C:45:THR:O | 2.10 | 0.52 |
| 1:A:157:THR:HG22 | 1:A:488:ILE:HB | 1.91 | 0.52 |
| 1:A:520:MET:SD | 1:A:572:ILE:HG12 | 2.50 | 0.52 |
| 1:B:135:THR:O | 1:B:136:GLN:C | 2.44 | 0.52 |
| 1:B:285:ASP:HA | 1:B:331:ASN:OD1 | 2.10 | 0.52 |
| 1:C:172:GLU:CD | 1:C:212:TRP:CZ2 | 2.83 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:111:VAL:HB | 1:C:545:LEU:HD13 | 1.92 | 0.52 |
| 1:D:516:ASP:OD2 | 1:D:518:THR:HG22 | 2.09 | 0.52 |
| 1:D:111:VAL:HB | 1:D:545:LEU:HD13 | 1.91 | 0.52 |
| 1:D:546:ARG:NH2 | 1:E:15:ASN:OD1 | 2.43 | 0.52 |
| 1:E:177:ILE:HG22 | 1:E:236:ILE:HG23 | 1.91 | 0.52 |
| 1:B:3:LEU:N | 1:B:44:SER:O | 2.43 | 0.52 |
| 1:C:175:LEU:HD11 | 1:C:177:ILE:HG23 | 1.92 | 0.52 |
| 1:F:37:PHE:CD1 | 1:F:38:ASP:N | 2.78 | 0.52 |
| 1:F:37:PHE:HZ | 1:F:40:HIS:O | 1.92 | 0.52 |
| 1:A:563:ILE:O | 1:A:564:ASN:ND2 | 2.42 | 0.52 |
| 1:B:560:SER:O | 1:B:564:ASN:ND2 | 2.41 | 0.52 |
| 1:E:175:LEU:HD23 | 1:E:239:VAL:HB | 1.92 | 0.52 |
| 1:E:285:ASP:OD2 | 1:E:287:GLN:N | 2.42 | 0.52 |
| 1:A:5:LYS:NZ | 1:A:41:GLU:OE2 | 2.43 | 0.51 |
| 1:C:48:TYR:OH | 1:C:109:PRO:HG3 | 2.11 | 0.51 |
| 1:D:128:ASN:ND2 | 1:D:128:ASN:C | 2.64 | 0.51 |
| 1:C:539:THR:HG23 | 1:D:93:THR:O | 2.10 | 0.51 |
| 1:A:472:PRO:HB3 | 1:F:339:THR:HG21 | 1.92 | 0.51 |
| 1:A:46:PHE:HB3 | 1:A:57:VAL:HG23 | 1.91 | 0.51 |
| 1:B:324:ASP:C | 1:B:324:ASP:OD1 | 2.48 | 0.51 |
| 1:D:306:PRO:HD3 | 1:D:326:SER:HB3 | 1.92 | 0.51 |
| 1:F:90:LEU:HA | 1:F:109:PRO:HA | 1.93 | 0.51 |
| 1:B:148:SER:CB | 1:C:156:SER:O | 2.58 | 0.51 |
| 1:C:164:LYS:CB | 1:C:282:ILE:HD12 | 2.40 | 0.51 |
| 1:C:41:GLU:O | 1:C:41:GLU:HG2 | 2.11 | 0.51 |
| 1:D:356:ARG:NH2 | 1:E:487:ARG:O | 2.42 | 0.51 |
| 1:C:534:LEU:HB2 | 1:C:542:MET:CE | 2.41 | 0.51 |
| 1:D:347:LYS:HE2 | 1:D:369:THR:CG2 | 2.41 | 0.51 |
| 1:A:182:ARG:NH2 | 1:A:267:LYS:HE2 | 2.25 | 0.51 |
| 1:C:206:ASN:OD1 | 1:C:210:MET:HE1 | 2.09 | 0.51 |
| 1:C:356:ARG:NH2 | 1:D:487:ARG:O | 2.38 | 0.51 |
| 1:D:542:MET:O | 1:D:543:ASN:C | 2.48 | 0.51 |
| 1:E:351:LYS:O | 1:E:352:ASN:HB2 | 2.10 | 0.51 |
| 1:F:6:ILE:CG2 | 1:F:7:LYS:N | 2.73 | 0.51 |
| 1:A:157:THR:HG23 | 1:A:489:SER:H | 1.75 | 0.51 |
| 1:B:75:ASN:HA | 1:B:92:VAL:HG22 | 1.91 | 0.51 |
| 1:D:175:LEU:HD11 | 1:D:177:ILE:HG23 | 1.91 | 0.51 |
| 1:A:48:TYR:OH | 1:A:109:PRO:HG3 | 2.11 | 0.51 |
| 1:A:534:LEU:HB2 | 1:A:542:MET:CE | 2.41 | 0.51 |
| 1:C:351:LYS:HG2 | 1:C:352:ASN:OD1 | 2.10 | 0.51 |
| 1:C:46:PHE:CE1 | 1:C:55:LEU:CD1 | 2.94 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:299:ASN:OD1 | 1:D:571:VAL:HG22 | 2.11 | 0.51 |
| 1:F:206:ASN:OD1 | 1:F:210:MET:HE1 | 2.11 | 0.51 |
| 1:B:164:LYS:CB | 1:B:282:ILE:HD12 | 2.41 | 0.51 |
| 1:C:133:HIS:CD2 | 1:C:525:TRP:H | 2.29 | 0.51 |
| 1:C:290:MET:HE3 | 1:C:295:LEU:HD23 | 1.93 | 0.51 |
| 1:E:566:THR:O | 1:E:568:VAL:N | 2.44 | 0.51 |
| 1:E:6:ILE:CG2 | 1:E:7:LYS:N | 2.74 | 0.51 |
| 1:B:148:SER:HB3 | 1:C:156:SER:O | 2.10 | 0.51 |
| 1:C:177:ILE:HG22 | 1:C:236:ILE:HG23 | 1.93 | 0.51 |
| 1:C:185:PHE:CE2 | 1:C:259:ASN:HB2 | 2.46 | 0.51 |
| 1:D:45:THR:HG23 | 1:D:45:THR:O | 2.11 | 0.51 |
| 1:D:563:ILE:O | 1:D:564:ASN:ND2 | 2.44 | 0.51 |
| 1:E:285:ASP:HA | 1:E:331:ASN:OD1 | 2.11 | 0.51 |
| 1:F:111:VAL:HB | 1:F:545:LEU:HD13 | 1.93 | 0.51 |
| 1:A:45:THR:O | 1:A:45:THR:HG23 | 2.10 | 0.51 |
| 1:A:537:VAL:O | 1:A:538:ASP:C | 2.48 | 0.51 |
| 1:B:215:ASP:OD1 | 1:B:215:ASP:C | 2.48 | 0.51 |
| 1:D:553:VAL:HG12 | 1:D:555:LEU:HD12 | 1.91 | 0.51 |
| 1:E:324:ASP:C | 1:E:324:ASP:OD1 | 2.49 | 0.51 |
| 1:E:79:VAL:CG1 | 1:E:81:TYR:CE2 | 2.93 | 0.51 |
| 1:F:491:ASP:O | 1:F:492:GLU:C | 2.47 | 0.51 |
| 1:F:572:ILE:CG2 | 1:F:572:ILE:O | 2.54 | 0.51 |
| 1:C:172:GLU:HB3 | 1:C:212:TRP:CH2 | 2.46 | 0.50 |
| 1:C:233:GLN:O | 1:C:236:ILE:HG13 | 2.11 | 0.50 |
| 1:D:133:HIS:HB3 | 1:D:520:MET:CE | 2.40 | 0.50 |
| 1:E:57:VAL:O | 1:E:57:VAL:CG1 | 2.58 | 0.50 |
| 1:F:157:THR:HG22 | 1:F:488:ILE:HB | 1.93 | 0.50 |
| 1:B:42:PHE:CE1 | 1:B:59:ILE:CD1 | 2.93 | 0.50 |
| 1:D:360:VAL:HG13 | 1:E:163:ILE:HD12 | 1.93 | 0.50 |
| 1:E:185:PHE:CE2 | 1:E:259:ASN:HB2 | 2.46 | 0.50 |
| 1:E:286:TYR:HE1 | 1:E:301:LYS:HG3 | 1.75 | 0.50 |
| 1:F:175:LEU:HD11 | 1:F:177:ILE:HG23 | 1.93 | 0.50 |
| 1:F:217:GLU:O | 1:F:218:SER:C | 2.48 | 0.50 |
| 1:F:358:ASN:O | 1:F:358:ASN:CG | 2.50 | 0.50 |
| 1:E:208:TYR:CZ | 1:F:463:ILE:HG12 | 2.45 | 0.50 |
| 1:A:177:ILE:CB | 1:A:236:ILE:HA | 2.42 | 0.50 |
| 1:B:46:PHE:CE1 | 1:B:55:LEU:CD1 | 2.94 | 0.50 |
| 1:C:44:SER:OG | 1:C:45:THR:N | 2.42 | 0.50 |
| 1:D:152:VAL:O | 1:D:152:VAL:HG13 | 2.09 | 0.50 |
| 1:F:502:MET:O | 1:F:554:ARG:NH1 | 2.41 | 0.50 |
| 1:A:12:THR:HG21 | 1:A:76:TYR:HB2 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:46:PHE:CD2 | 1:A:46:PHE:O | 2.64 | 0.50 |
| 1:C:553:VAL:HG12 | 1:C:555:LEU:HD12 | 1.92 | 0.50 |
| 1:C:360:VAL:HG13 | 1:D:163:ILE:HD12 | 1.92 | 0.50 |
| 1:E:359:ASN:O | 1:E:360:VAL:C | 2.50 | 0.50 |
| 1:F:172:GLU:CD | 1:F:212:TRP:CH2 | 2.85 | 0.50 |
| 1:F:46:PHE:CE1 | 1:F:55:LEU:CD1 | 2.94 | 0.50 |
| 1:B:79:VAL:CG1 | 1:B:81:TYR:CE2 | 2.94 | 0.50 |
| 1:C:164:LYS:HB2 | 1:C:282:ILE:HD12 | 1.94 | 0.50 |
| 1:C:212:TRP:O | 1:C:213:PHE:CD2 | 2.65 | 0.50 |
| 1:C:229:TYR:N | 1:C:229:TYR:CD2 | 2.79 | 0.50 |
| 1:C:559:GLU:O | 1:C:560:SER:C | 2.50 | 0.50 |
| 1:D:120:VAL:CG2 | 1:D:121:LEU:N | 2.73 | 0.50 |
| 1:D:491:ASP:O | 1:D:494:ASN:N | 2.44 | 0.50 |
| 1:F:164:LYS:CB | 1:F:282:ILE:HD12 | 2.42 | 0.50 |
| 1:A:46:PHE:CE1 | 1:A:55:LEU:CD1 | 2.94 | 0.50 |
| 1:C:212:TRP:CZ3 | 1:C:247:ILE:HG13 | 2.47 | 0.50 |
| 1:C:545:LEU:O | 1:C:546:ARG:C | 2.50 | 0.50 |
| 1:E:164:LYS:C | 1:E:282:ILE:HD11 | 2.31 | 0.50 |
| 1:E:59:ILE:O | 1:E:59:ILE:CG2 | 2.59 | 0.50 |
| 1:A:90:LEU:HA | 1:A:109:PRO:HA | 1.93 | 0.50 |
| 1:B:175:LEU:HD11 | 1:B:177:ILE:HG23 | 1.93 | 0.50 |
| 1:B:306:PRO:HD3 | 1:B:326:SER:HB3 | 1.92 | 0.50 |
| 1:E:95:ILE:HG12 | 1:E:105:LEU:HD22 | 1.94 | 0.50 |
| 1:E:541:HIS:O | 1:E:545:LEU:HB2 | 2.11 | 0.50 |
| 1:F:470:TYR:HB3 | 1:F:479:PHE:CD1 | 2.47 | 0.50 |
| 1:A:542:MET:HE2 | 1:A:545:LEU:HD23 | 1.93 | 0.50 |
| 1:B:152:VAL:HG22 | 1:B:153:LEU:N | 2.27 | 0.50 |
| 1:E:106:SER:O | 1:E:107:LEU:HD12 | 2.11 | 0.50 |
| 1:F:172:GLU:CD | 1:F:212:TRP:CZ2 | 2.85 | 0.50 |
| 1:F:491:ASP:O | 1:F:494:ASN:N | 2.44 | 0.50 |
| 1:F:520:MET:HB3 | 1:F:570:ASN:OD1 | 2.12 | 0.50 |
| 1:F:79:VAL:HG11 | 1:F:81:TYR:CE2 | 2.47 | 0.50 |
| 1:A:226:LEU:HD12 | 1:A:233:GLN:HB3 | 1.94 | 0.50 |
| 1:E:133:HIS:HB3 | 1:E:520:MET:CE | 2.42 | 0.50 |
| 1:E:90:LEU:HD22 | 1:E:107:LEU:HD23 | 1.94 | 0.50 |
| 1:F:78:GLN:CG | 1:F:79:VAL:N | 2.73 | 0.50 |
| 1:A:6:ILE:CG2 | 1:A:7:LYS:N | 2.75 | 0.49 |
| 1:B:360:VAL:CG2 | 1:B:363:TYR:HB2 | 2.42 | 0.49 |
| 1:C:90:LEU:HD22 | 1:C:107:LEU:HD23 | 1.94 | 0.49 |
| 1:C:285:ASP:HA | 1:C:331:ASN:OD1 | 2.12 | 0.49 |
| 1:D:157:THR:HG22 | 1:D:488:ILE:HB | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:351:LYS:O | 1:D:352:ASN:HB2 | 2.13 | 0.49 |
| 1:E:305:ARG:HB2 | 1:E:306:PRO:CD | 2.43 | 0.49 |
| 1:E:157:THR:HG22 | 1:E:488:ILE:HB | 1.93 | 0.49 |
| 1:F:202:ASP:OD2 | 1:F:274:SER:OG | 2.30 | 0.49 |
| 1:F:185:PHE:CE2 | 1:F:259:ASN:HB2 | 2.46 | 0.49 |
| 1:B:172:GLU:HB3 | 1:B:212:TRP:CH2 | 2.47 | 0.49 |
| 1:B:282:ILE:HG23 | 1:B:334:PHE:CD2 | 2.47 | 0.49 |
| 1:B:48:TYR:CE1 | 1:B:55:LEU:HD22 | 2.48 | 0.49 |
| 1:D:29:ARG:HD2 | 1:D:30:ASP:OD2 | 2.11 | 0.49 |
| 1:D:92:VAL:O | 1:D:92:VAL:HG23 | 2.12 | 0.49 |
| 1:E:172:GLU:OE1 | 1:E:212:TRP:CH2 | 2.64 | 0.49 |
| 1:E:172:GLU:CD | 1:E:212:TRP:CH2 | 2.85 | 0.49 |
| 1:F:23:PHE:N | 1:F:23:PHE:CD2 | 2.80 | 0.49 |
| 1:F:351:LYS:HG2 | 1:F:352:ASN:OD1 | 2.12 | 0.49 |
| 1:A:165:SER:HA | 1:A:282:ILE:HD13 | 1.94 | 0.49 |
| 1:B:26:ASN:O | 1:B:29:ARG:HB3 | 2.12 | 0.49 |
| 1:B:67:CYS:SG | 1:B:68:PHE:N | 2.85 | 0.49 |
| 1:C:296:ASN:O | 1:C:300:ASP:HB2 | 2.12 | 0.49 |
| 1:C:306:PRO:HD3 | 1:C:326:SER:HB3 | 1.94 | 0.49 |
| 1:C:339:THR:HG21 | 1:D:472:PRO:HB3 | 1.93 | 0.49 |
| 1:E:172:GLU:CD | 1:E:212:TRP:CZ2 | 2.85 | 0.49 |
| 1:E:130:ILE:CG2 | 1:E:527:GLN:HG2 | 2.43 | 0.49 |
| 1:E:532:TRP:HZ2 | 1:E:546:ARG:HA | 1.76 | 0.49 |
| 1:F:152:VAL:HG13 | 1:F:152:VAL:O | 2.11 | 0.49 |
| 1:F:172:GLU:OE1 | 1:F:212:TRP:CH2 | 2.64 | 0.49 |
| 1:A:339:THR:HG21 | 1:B:472:PRO:HB3 | 1.93 | 0.49 |
| 1:B:202:ASP:OD2 | 1:B:274:SER:OG | 2.30 | 0.49 |
| 1:C:6:ILE:HG23 | 1:C:7:LYS:N | 2.27 | 0.49 |
| 1:F:285:ASP:OD2 | 1:F:287:GLN:N | 2.45 | 0.49 |
| 1:B:542:MET:HB3 | 1:B:546:ARG:NH1 | 2.27 | 0.49 |
| 1:A:156:SER:O | 1:F:148:SER:HB3 | 2.12 | 0.49 |
| 1:A:177:ILE:HG22 | 1:A:236:ILE:HA | 1.94 | 0.49 |
| 1:A:360:VAL:HG23 | 1:A:363:TYR:HB2 | 1.94 | 0.49 |
| 1:B:307:ASN:N | 1:B:307:ASN:OD1 | 2.36 | 0.49 |
| 1:D:244:SER:O | 1:D:245:GLY:C | 2.51 | 0.49 |
| 1:E:128:ASN:HB2 | 1:E:510:TYR:HA | 1.94 | 0.49 |
| 1:F:75:ASN:N | 1:F:75:ASN:OD1 | 2.45 | 0.49 |
| 1:A:75:ASN:HA | 1:A:92:VAL:HG22 | 1.95 | 0.49 |
| 1:B:286:TYR:C | 1:B:286:TYR:CD2 | 2.85 | 0.49 |
| 1:C:106:SER:O | 1:C:107:LEU:HD12 | 2.13 | 0.49 |
| 1:C:291:PHE:CD2 | 1:C:291:PHE:C | 2.86 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:483:LEU:HD12 | 1:D:484:ARG:N | 2.28 | 0.49 |
| 1:A:10:TYR:HB2 | 1:A:38:ASP:HB2 | 1.94 | 0.49 |
| 1:A:144:GLU:OE1 | 1:A:356:ARG:NH1 | 2.46 | 0.49 |
| 1:C:23:PHE:CD2 | 1:C:23:PHE:N | 2.80 | 0.49 |
| 1:C:290:MET:HE2 | 1:C:295:LEU:HB3 | 1.94 | 0.49 |
| 1:F:566:THR:C | 1:F:568:VAL:N | 2.64 | 0.49 |
| 1:B:6:ILE:HG23 | 1:B:7:LYS:N | 2.27 | 0.49 |
| 1:C:324:ASP:C | 1:C:324:ASP:OD1 | 2.51 | 0.49 |
| 1:D:206:ASN:OD1 | 1:D:210:MET:HE1 | 2.13 | 0.49 |
| 1:E:122:ASN:OD1 | 1:E:517:ILE:HG12 | 2.13 | 0.49 |
| 1:B:516:ASP:OD2 | 1:B:518:THR:HG22 | 2.13 | 0.49 |
| 1:B:61:LEU:HD12 | 1:B:61:LEU:N | 2.28 | 0.49 |
| 1:C:360:VAL:HG23 | 1:C:363:TYR:HB2 | 1.95 | 0.49 |
| 1:E:129:VAL:CG2 | 1:E:130:ILE:N | 2.76 | 0.49 |
| 1:A:124:LEU:HD21 | 1:A:532:TRP:HE3 | 1.78 | 0.48 |
| 1:A:282:ILE:HD11 | 1:A:483:LEU:HB3 | 1.95 | 0.48 |
| 1:A:239:VAL:HG22 | 1:A:376:ILE:HG13 | 1.95 | 0.48 |
| 1:B:177:ILE:CG2 | 1:B:236:ILE:HG12 | 2.43 | 0.48 |
| 1:B:299:ASN:ND2 | 1:B:571:VAL:HG22 | 2.27 | 0.48 |
| 1:B:360:VAL:HG13 | 1:C:163:ILE:HD12 | 1.95 | 0.48 |
| 1:D:276:GLN:O | 1:D:277:LYS:C | 2.50 | 0.48 |
| 1:E:26:ASN:HB3 | 1:E:29:ARG:NH2 | 2.28 | 0.48 |
| 1:F:177:ILE:C | 1:F:177:ILE:HD13 | 2.34 | 0.48 |
| 1:F:45:THR:HG23 | 1:F:45:THR:O | 2.12 | 0.48 |
| 1:A:572:ILE:O | 1:A:573:ILE:HB | 2.12 | 0.48 |
| 1:B:185:PHE:CE2 | 1:B:259:ASN:HB2 | 2.48 | 0.48 |
| 1:B:276:GLN:O | 1:B:277:LYS:C | 2.51 | 0.48 |
| 1:D:285:ASP:O | 1:D:286:TYR:C | 2.50 | 0.48 |
| 1:E:470:TYR:CB | 1:E:479:PHE:CE1 | 2.95 | 0.48 |
| 1:F:128:ASN:HB2 | 1:F:510:TYR:HA | 1.94 | 0.48 |
| 1:F:516:ASP:CG | 1:F:518:THR:HG22 | 2.34 | 0.48 |
| 1:F:572:ILE:O | 1:F:573:ILE:HB | 2.12 | 0.48 |
| 1:A:148:SER:CB | 1:B:156:SER:O | 2.62 | 0.48 |
| 1:A:305:ARG:HB2 | 1:A:306:PRO:CD | 2.42 | 0.48 |
| 1:A:307:ASN:N | 1:A:307:ASN:OD1 | 2.44 | 0.48 |
| 1:A:351:LYS:O | 1:A:352:ASN:HB2 | 2.13 | 0.48 |
| 1:A:37:PHE:CE1 | 1:A:40:HIS:O | 2.66 | 0.48 |
| 1:A:502:MET:O | 1:A:554:ARG:NH1 | 2.41 | 0.48 |
| 1:B:256:GLU:O | 1:B:264:SER:HA | 2.13 | 0.48 |
| 1:B:542:MET:O | 1:B:543:ASN:C | 2.51 | 0.48 |
| 1:C:157:THR:HG22 | 1:C:488:ILE:HB | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:177:ILE:HG22 | 1:C:236:ILE:HA | 1.95 | 0.48 |
| 1:C:177:ILE:CG2 | 1:C:236:ILE:HG12 | 2.43 | 0.48 |
| 1:C:164:LYS:C | 1:C:282:ILE:HD11 | 2.32 | 0.48 |
| 1:D:172:GLU:CD | 1:D:212:TRP:CH2 | 2.86 | 0.48 |
| 1:E:463:ILE:HD13 | 1:E:463:ILE:O | 2.13 | 0.48 |
| 1:E:559:GLU:O | 1:E:560:SER:C | 2.50 | 0.48 |
| 1:F:120:VAL:CG2 | 1:F:121:LEU:N | 2.76 | 0.48 |
| 1:A:121:LEU:O | 1:A:124:LEU:HD12 | 2.13 | 0.48 |
| 1:A:470:TYR:CG | 1:A:479:PHE:HE1 | 2.30 | 0.48 |
| 1:C:12:THR:HG21 | 1:C:76:TYR:HB2 | 1.95 | 0.48 |
| 1:C:172:GLU:CD | 1:C:212:TRP:CH2 | 2.87 | 0.48 |
| 1:E:164:LYS:CB | 1:E:282:ILE:HD12 | 2.43 | 0.48 |
| 1:E:544:MET:O | 1:E:548:LEU:HB2 | 2.13 | 0.48 |
| 1:F:553:VAL:HG12 | 1:F:555:LEU:HD12 | 1.94 | 0.48 |
| 1:B:129:VAL:CG2 | 1:B:130:ILE:N | 2.77 | 0.48 |
| 1:C:8:LEU:CD2 | 1:C:77:CYS:HB2 | 2.44 | 0.48 |
| 1:C:90:LEU:HA | 1:C:109:PRO:HA | 1.95 | 0.48 |
| 1:E:23:PHE:CD2 | 1:E:23:PHE:N | 2.80 | 0.48 |
| 1:E:339:THR:HG21 | 1:F:472:PRO:HB3 | 1.93 | 0.48 |
| 1:F:463:ILE:O | 1:F:463:ILE:HD12 | 2.14 | 0.48 |
| 1:A:516:ASP:OD2 | 1:A:518:THR:HG22 | 2.14 | 0.48 |
| 1:B:158:MET:C | 1:B:159:ARG:HG2 | 2.33 | 0.48 |
| 1:B:177:ILE:O | 1:B:177:ILE:HD13 | 2.13 | 0.48 |
| 1:B:282:ILE:HD11 | 1:B:483:LEU:HB3 | 1.95 | 0.48 |
| 1:D:212:TRP:O | 1:D:213:PHE:CD2 | 2.66 | 0.48 |
| 1:D:559:GLU:O | 1:D:560:SER:C | 2.51 | 0.48 |
| 1:E:48:TYR:OH | 1:E:109:PRO:HG3 | 2.14 | 0.48 |
| 1:E:206:ASN:OD1 | 1:E:210:MET:HE1 | 2.12 | 0.48 |
| 1:D:363:TYR:HD2 | 1:E:316:TYR:CE1 | 2.30 | 0.48 |
| 1:F:26:ASN:HB3 | 1:F:29:ARG:CZ | 2.42 | 0.48 |
| 1:F:496:VAL:O | 1:F:497:LYS:C | 2.52 | 0.48 |
| 1:A:42:PHE:CE2 | 1:A:44:SER:HB2 | 2.49 | 0.48 |
| 1:A:61:LEU:HD12 | 1:A:61:LEU:N | 2.29 | 0.48 |
| 1:C:511:SER:OG | 1:C:511:SER:O | 2.30 | 0.48 |
| 1:D:158:MET:C | 1:D:159:ARG:HG2 | 2.34 | 0.48 |
| 1:E:380:VAL:O | 1:E:462:ALA:N | 2.47 | 0.48 |
| 1:E:498:LYS:O | 1:E:499:TYR:C | 2.52 | 0.48 |
| 1:E:516:ASP:OD2 | 1:E:518:THR:HG22 | 2.14 | 0.48 |
| 1:E:554:ARG:HG2 | 1:E:556:TRP:NE1 | 2.28 | 0.48 |
| 1:F:282:ILE:HD12 | 1:F:282:ILE:HA | 1.71 | 0.48 |
| 1:F:512:THR:HG23 | 1:F:513:LYS:N | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:164:LYS:C | 1:A:282:ILE:HD11 | 2.34 | 0.48 |
| 1:B:285:ASP:OD2 | 1:B:287:GLN:N | 2.46 | 0.48 |
| 1:B:55:LEU:N | 1:B:55:LEU:HD23 | 2.29 | 0.48 |
| 1:C:470:TYR:HB3 | 1:C:479:PHE:CD1 | 2.49 | 0.48 |
| 1:D:115:TYR:CE1 | 1:D:537:VAL:HG13 | 2.49 | 0.48 |
| 1:E:175:LEU:HD11 | 1:E:177:ILE:HG23 | 1.95 | 0.48 |
| 1:E:560:SER:O | 1:E:564:ASN:ND2 | 2.44 | 0.48 |
| 1:F:95:ILE:HG12 | 1:F:105:LEU:HD22 | 1.96 | 0.48 |
| 1:F:78:GLN:HG2 | 1:F:79:VAL:H | 1.79 | 0.48 |
| 1:F:92:VAL:O | 1:F:92:VAL:CG2 | 2.59 | 0.48 |
| 1:A:177:ILE:HD13 | 1:A:177:ILE:C | 2.32 | 0.48 |
| 1:A:212:TRP:CZ3 | 1:A:247:ILE:HG13 | 2.49 | 0.48 |
| 1:B:172:GLU:OE2 | 1:B:245:GLY:N | 2.45 | 0.48 |
| 1:B:511:SER:O | 1:B:511:SER:OG | 2.28 | 0.48 |
| 1:B:559:GLU:O | 1:B:560:SER:C | 2.53 | 0.48 |
| 1:A:3:LEU:HD11 | 1:B:68:PHE:CZ | 2.49 | 0.48 |
| 1:E:12:THR:HG21 | 1:E:76:TYR:HB2 | 1.95 | 0.48 |
| 1:B:212:TRP:HA | 1:B:212:TRP:CE3 | 2.49 | 0.48 |
| 1:B:290:MET:HE3 | 1:B:295:LEU:HB3 | 1.96 | 0.48 |
| 1:B:296:ASN:O | 1:B:300:ASP:HB2 | 2.14 | 0.48 |
| 1:C:258:VAL:HG12 | 1:C:263:LEU:O | 2.12 | 0.48 |
| 1:D:285:ASP:OD2 | 1:D:287:GLN:N | 2.46 | 0.48 |
| 1:E:249:GLN:OE1 | 1:E:249:GLN:HA | 2.13 | 0.48 |
| 1:F:177:ILE:HG22 | 1:F:236:ILE:HA | 1.96 | 0.48 |
| 1:B:172:GLU:OE1 | 1:B:212:TRP:CH2 | 2.65 | 0.47 |
| 1:C:534:LEU:HB2 | 1:C:542:MET:HE3 | 1.94 | 0.47 |
| 1:D:172:GLU:CD | 1:D:212:TRP:CZ2 | 2.87 | 0.47 |
| 1:D:172:GLU:OE1 | 1:D:212:TRP:CH2 | 2.65 | 0.47 |
| 1:E:212:TRP:O | 1:E:213:PHE:CD2 | 2.67 | 0.47 |
| 1:E:45:THR:HG23 | 1:E:45:THR:O | 2.13 | 0.47 |
| 1:F:258:VAL:HG22 | 1:F:259:ASN:N | 2.28 | 0.47 |
| 1:A:172:GLU:CD | 1:A:212:TRP:CZ2 | 2.87 | 0.47 |
| 1:B:463:ILE:HD12 | 1:B:463:ILE:O | 2.15 | 0.47 |
| 1:C:157:THR:HG23 | 1:C:489:SER:H | 1.79 | 0.47 |
| 1:D:48:TYR:OH | 1:D:109:PRO:HG3 | 2.13 | 0.47 |
| 1:B:563:ILE:C | 1:B:564:ASN:ND2 | 2.68 | 0.47 |
| 1:D:258:VAL:HG22 | 1:D:259:ASN:N | 2.30 | 0.47 |
| 1:D:29:ARG:HD3 | 1:D:89:TYR:CE2 | 2.49 | 0.47 |
| 1:D:516:ASP:OD1 | 1:D:518:THR:HG22 | 2.14 | 0.47 |
| 1:D:549:PHE:O | 1:D:552:GLY:N | 2.47 | 0.47 |
| 1:A:380:VAL:O | 1:A:462:ALA:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:305:ARG:HB2 | 1:B:306:PRO:HD2 | 1.95 | 0.47 |
| 1:B:470:TYR:CB | 1:B:479:PHE:CE1 | 2.98 | 0.47 |
| 1:C:463:ILE:O | 1:C:463:ILE:HD13 | 2.13 | 0.47 |
| 1:C:498:LYS:O | 1:C:499:TYR:C | 2.52 | 0.47 |
| 1:C:571:VAL:HG13 | 1:C:572:ILE:N | 2.30 | 0.47 |
| 1:D:177:ILE:HD13 | 1:D:177:ILE:O | 2.14 | 0.47 |
| 1:D:470:TYR:HB3 | 1:D:479:PHE:CD1 | 2.50 | 0.47 |
| 1:E:463:ILE:O | 1:E:463:ILE:HD12 | 2.14 | 0.47 |
| 1:E:470:TYR:CG | 1:E:479:PHE:HE1 | 2.28 | 0.47 |
| 1:E:61:LEU:CD2 | 1:E:67:CYS:SG | 3.02 | 0.47 |
| 1:F:177:ILE:CB | 1:F:236:ILE:HA | 2.44 | 0.47 |
| 1:F:353:TYR:O | 1:F:354:ASN:HB3 | 2.15 | 0.47 |
| 1:B:3:LEU:HB3 | 1:B:45:THR:HB | 1.96 | 0.47 |
| 1:B:3:LEU:CB | 1:B:45:THR:HB | 2.44 | 0.47 |
| 1:B:572:ILE:O | 1:B:573:ILE:HB | 2.14 | 0.47 |
| 1:D:129:VAL:CG2 | 1:D:130:ILE:N | 2.78 | 0.47 |
| 1:D:233:GLN:HG3 | 1:D:380:VAL:HG22 | 1.97 | 0.47 |
| 1:F:164:LYS:C | 1:F:282:ILE:HD11 | 2.35 | 0.47 |
| 1:B:177:ILE:HG21 | 1:B:236:ILE:HG12 | 1.96 | 0.47 |
| 1:D:37:PHE:HZ | 1:D:40:HIS:O | 1.94 | 0.47 |
| 1:F:8:LEU:CD2 | 1:F:77:CYS:HB2 | 2.45 | 0.47 |
| 1:B:335:ASP:OD2 | 1:B:351:LYS:HD2 | 2.15 | 0.47 |
| 1:C:48:TYR:CE1 | 1:C:55:LEU:HD22 | 2.49 | 0.47 |
| 1:D:124:LEU:HD21 | 1:D:532:TRP:HE3 | 1.80 | 0.47 |
| 1:D:155:THR:HG21 | 1:D:307:ASN:O | 2.15 | 0.47 |
| 1:D:177:ILE:CB | 1:D:236:ILE:HA | 2.45 | 0.47 |
| 1:E:42:PHE:CE2 | 1:E:44:SER:HB2 | 2.49 | 0.47 |
| 1:F:212:TRP:O | 1:F:213:PHE:CD2 | 2.67 | 0.47 |
| 1:F:542:MET:O | 1:F:543:ASN:C | 2.52 | 0.47 |
| 1:A:217:GLU:O | 1:A:218:SER:C | 2.52 | 0.47 |
| 1:A:157:THR:HB | 1:A:492:GLU:OE1 | 2.14 | 0.47 |
| 1:B:274:SER:HB2 | 1:B:338:VAL:CG2 | 2.45 | 0.47 |
| 1:C:10:TYR:HB2 | 1:C:38:ASP:HB2 | 1.96 | 0.47 |
| 1:E:357:GLY:HA2 | 1:E:358:ASN:HA | 1.69 | 0.47 |
| 1:E:48:TYR:CE1 | 1:E:55:LEU:HD22 | 2.50 | 0.47 |
| 1:A:173:TYR:CD2 | 1:A:173:TYR:N | 2.83 | 0.47 |
| 1:A:175:LEU:HD13 | 1:A:177:ILE:HG23 | 1.96 | 0.47 |
| 1:B:128:ASN:HB2 | 1:B:510:TYR:HA | 1.97 | 0.47 |
| 1:B:470:TYR:CG | 1:B:479:PHE:HE1 | 2.33 | 0.47 |
| 1:C:172:GLU:OE1 | 1:C:212:TRP:CH2 | 2.63 | 0.47 |
| 1:C:26:ASN:O | 1:C:29:ARG:HB3 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:563:ILE:O | 1:C:564:ASN:ND2 | 2.48 | 0.47 |
| 1:D:286:TYR:CE1 | 1:D:301:LYS:HE3 | 2.50 | 0.47 |
| 1:E:212:TRP:O | 1:E:213:PHE:CG | 2.68 | 0.47 |
| 1:E:572:ILE:CG2 | 1:E:572:ILE:O | 2.51 | 0.47 |
| 1:F:206:ASN:OD1 | 1:F:210:MET:HE3 | 2.15 | 0.47 |
| 1:F:516:ASP:OD1 | 1:F:518:THR:HG22 | 2.14 | 0.47 |
| 1:B:177:ILE:HG22 | 1:B:236:ILE:HA | 1.96 | 0.47 |
| 1:B:177:ILE:CB | 1:B:236:ILE:HA | 2.45 | 0.47 |
| 1:C:155:THR:HG21 | 1:C:307:ASN:O | 2.15 | 0.47 |
| 1:E:537:VAL:O | 1:E:539:THR:N | 2.48 | 0.47 |
| 1:E:21:LEU:HD12 | 1:E:556:TRP:O | 2.15 | 0.47 |
| 1:A:23:PHE:CD2 | 1:A:23:PHE:N | 2.82 | 0.47 |
| 1:B:212:TRP:O | 1:B:213:PHE:CD2 | 2.68 | 0.47 |
| 1:C:285:ASP:O | 1:C:286:TYR:C | 2.53 | 0.47 |
| 1:E:177:ILE:O | 1:E:177:ILE:HD13 | 2.15 | 0.47 |
| 1:F:128:ASN:ND2 | 1:F:128:ASN:C | 2.67 | 0.47 |
| 1:F:571:VAL:HG13 | 1:F:572:ILE:N | 2.30 | 0.47 |
| 1:A:276:GLN:O | 1:A:277:LYS:C | 2.52 | 0.46 |
| 1:A:164:LYS:CB | 1:A:282:ILE:HD12 | 2.45 | 0.46 |
| 1:A:487:ARG:HG2 | 1:A:488:ILE:N | 2.30 | 0.46 |
| 1:B:120:VAL:CG2 | 1:B:121:LEU:N | 2.77 | 0.46 |
| 1:C:282:ILE:HD11 | 1:C:483:LEU:HB3 | 1.95 | 0.46 |
| 1:D:185:PHE:CE2 | 1:D:259:ASN:HB2 | 2.49 | 0.46 |
| 1:D:164:LYS:C | 1:D:282:ILE:HD11 | 2.35 | 0.46 |
| 1:E:37:PHE:CE1 | 1:E:40:HIS:O | 2.68 | 0.46 |
| 1:F:324:ASP:OD1 | 1:F:324:ASP:C | 2.52 | 0.46 |
| 1:F:48:TYR:CE1 | 1:F:55:LEU:HD22 | 2.50 | 0.46 |
| 1:A:286:TYR:C | 1:A:286:TYR:CD2 | 2.88 | 0.46 |
| 1:A:491:ASP:O | 1:A:492:GLU:C | 2.51 | 0.46 |
| 1:A:12:THR:HG22 | 1:A:75:ASN:OD1 | 2.15 | 0.46 |
| 1:C:37:PHE:HZ | 1:C:40:HIS:O | 1.96 | 0.46 |
| 1:D:571:VAL:HG13 | 1:D:572:ILE:N | 2.31 | 0.46 |
| 1:D:572:ILE:O | 1:D:573:ILE:HB | 2.14 | 0.46 |
| 1:E:311:ALA:HB2 | 1:E:325:LEU:HD22 | 1.97 | 0.46 |
| 1:A:120:VAL:CG2 | 1:A:121:LEU:N | 2.77 | 0.46 |
| 1:C:323:ILE:HG23 | 1:C:353:TYR:CE1 | 2.49 | 0.46 |
| 1:C:133:HIS:HB3 | 1:C:520:MET:HE2 | 1.97 | 0.46 |
| 1:D:12:THR:HG21 | 1:D:76:TYR:CB | 2.45 | 0.46 |
| 1:D:463:ILE:O | 1:D:463:ILE:HD12 | 2.14 | 0.46 |
| 1:D:529:LYS:O | 1:D:530:GLY:O | 2.33 | 0.46 |
| 1:F:155:THR:HG21 | 1:F:307:ASN:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:291:PHE:CD2 | 1:F:291:PHE:C | 2.89 | 0.46 |
| 1:A:172:GLU:CD | 1:A:212:TRP:CH2 | 2.88 | 0.46 |
| 1:A:285:ASP:HA | 1:A:331:ASN:OD1 | 2.15 | 0.46 |
| 1:A:285:ASP:O | 1:A:286:TYR:C | 2.53 | 0.46 |
| 1:A:29:ARG:HD2 | 1:A:30:ASP:OD2 | 2.16 | 0.46 |
| 1:B:516:ASP:OD2 | 1:B:517:ILE:N | 2.47 | 0.46 |
| 1:D:75:ASN:HA | 1:D:92:VAL:HG22 | 1.98 | 0.46 |
| 1:E:10:TYR:HB2 | 1:E:38:ASP:HB2 | 1.97 | 0.46 |
| 1:E:41:GLU:HG2 | 1:E:41:GLU:O | 2.15 | 0.46 |
| 1:F:315:ASP:C | 1:F:317:ALA:H | 2.18 | 0.46 |
| 1:A:68:PHE:CE2 | 1:F:3:LEU:HD21 | 2.51 | 0.46 |
| 1:A:152:VAL:HG22 | 1:A:153:LEU:N | 2.31 | 0.46 |
| 1:B:164:LYS:O | 1:B:282:ILE:CD1 | 2.59 | 0.46 |
| 1:C:26:ASN:HB3 | 1:C:29:ARG:CZ | 2.45 | 0.46 |
| 1:C:286:TYR:C | 1:C:286:TYR:CD2 | 2.89 | 0.46 |
| 1:D:541:HIS:O | 1:D:545:LEU:HB2 | 2.16 | 0.46 |
| 1:E:120:VAL:CG2 | 1:E:121:LEU:N | 2.78 | 0.46 |
| 1:E:177:ILE:HG22 | 1:E:236:ILE:HA | 1.96 | 0.46 |
| 1:E:291:PHE:C | 1:E:291:PHE:CD2 | 2.89 | 0.46 |
| 1:E:542:MET:O | 1:E:543:ASN:C | 2.54 | 0.46 |
| 1:A:520:MET:HE1 | 1:A:572:ILE:HG12 | 1.98 | 0.46 |
| 1:B:172:GLU:CD | 1:B:212:TRP:CZ2 | 2.88 | 0.46 |
| 1:B:152:VAL:HG21 | 1:B:307:ASN:HD21 | 1.81 | 0.46 |
| 1:E:212:TRP:CE3 | 1:E:212:TRP:HA | 2.50 | 0.46 |
| 1:F:10:TYR:HB2 | 1:F:38:ASP:HB2 | 1.97 | 0.46 |
| 1:F:285:ASP:O | 1:F:286:TYR:C | 2.54 | 0.46 |
| 1:A:95:ILE:HG12 | 1:A:105:LEU:HD22 | 1.98 | 0.46 |
| 1:A:177:ILE:HB | 1:A:236:ILE:HA | 1.97 | 0.46 |
| 1:A:463:ILE:O | 1:A:463:ILE:HD13 | 2.15 | 0.46 |
| 1:C:79:VAL:CG1 | 1:C:81:TYR:CE2 | 2.99 | 0.46 |
| 1:F:38:ASP:O | 1:F:39:VAL:HG23 | 2.16 | 0.46 |
| 1:B:165:SER:HA | 1:B:282:ILE:HD13 | 1.98 | 0.46 |
| 1:B:212:TRP:CZ3 | 1:B:247:ILE:HG13 | 2.51 | 0.46 |
| 1:C:177:ILE:CB | 1:C:236:ILE:HA | 2.45 | 0.46 |
| 1:C:290:MET:HE2 | 1:C:290:MET:HB3 | 1.89 | 0.46 |
| 1:C:348:VAL:CG2 | 1:C:349:TYR:N | 2.77 | 0.46 |
| 1:C:57:VAL:CG1 | 1:C:57:VAL:O | 2.63 | 0.46 |
| 1:D:217:GLU:O | 1:D:220:LYS:N | 2.49 | 0.46 |
| 1:D:249:GLN:OE1 | 1:D:249:GLN:HA | 2.16 | 0.46 |
| 1:D:307:ASN:N | 1:D:307:ASN:OD1 | 2.45 | 0.46 |
| 1:E:358:ASN:O | 1:E:358:ASN:CG | 2.53 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:310:THR:HG22 | 1:E:486:GLY:HA3 | 1.98 | 0.46 |
| 1:F:177:ILE:HB | 1:F:236:ILE:HA | 1.97 | 0.46 |
| 1:A:546:ARG:NH2 | 1:B:15:ASN:CG | 2.69 | 0.46 |
| 1:B:276:GLN:O | 1:B:277:LYS:O | 2.33 | 0.46 |
| 1:C:380:VAL:O | 1:C:462:ALA:N | 2.48 | 0.46 |
| 1:D:233:GLN:HG3 | 1:D:380:VAL:CG2 | 2.46 | 0.46 |
| 1:D:548:LEU:HD23 | 1:D:548:LEU:HA | 1.84 | 0.46 |
| 1:E:152:VAL:HG21 | 1:E:307:ASN:HD21 | 1.81 | 0.46 |
| 1:E:571:VAL:HG13 | 1:E:572:ILE:N | 2.31 | 0.46 |
| 1:F:48:TYR:OH | 1:F:109:PRO:HG3 | 2.16 | 0.46 |
| 1:B:351:LYS:O | 1:B:352:ASN:HB2 | 2.14 | 0.46 |
| 1:C:371:ASN:C | 1:C:371:ASN:OD1 | 2.55 | 0.46 |
| 1:D:259:ASN:O | 1:D:260:GLY:C | 2.55 | 0.46 |
| 1:D:42:PHE:CE2 | 1:D:44:SER:HB2 | 2.51 | 0.46 |
| 1:D:491:ASP:O | 1:D:492:GLU:C | 2.54 | 0.46 |
| 1:D:498:LYS:O | 1:D:499:TYR:C | 2.54 | 0.46 |
| 1:E:306:PRO:HD3 | 1:E:326:SER:HB3 | 1.98 | 0.46 |
| 1:A:463:ILE:O | 1:A:463:ILE:HD12 | 2.15 | 0.45 |
| 1:A:563:ILE:CD1 | 1:A:563:ILE:N | 2.78 | 0.45 |
| 1:B:549:PHE:O | 1:B:552:GLY:N | 2.49 | 0.45 |
| 1:C:541:HIS:O | 1:C:545:LEU:HB2 | 2.17 | 0.45 |
| 1:D:299:ASN:H | 1:D:299:ASN:ND2 | 2.15 | 0.45 |
| 1:D:157:THR:HB | 1:D:492:GLU:OE1 | 2.17 | 0.45 |
| 1:E:319:ASN:C | 1:E:320:ARG:HG2 | 2.36 | 0.45 |
| 1:F:25:SER:OG | 1:F:28:GLU:HG3 | 2.16 | 0.45 |
| 1:F:380:VAL:O | 1:F:462:ALA:N | 2.49 | 0.45 |
| 1:F:6:ILE:HG23 | 1:F:7:LYS:N | 2.31 | 0.45 |
| 1:A:148:SER:HB3 | 1:B:156:SER:O | 2.16 | 0.45 |
| 1:A:259:ASN:O | 1:A:260:GLY:C | 2.51 | 0.45 |
| 1:B:165:SER:CA | 1:B:282:ILE:HD13 | 2.46 | 0.45 |
| 1:C:120:VAL:CG2 | 1:C:121:LEU:N | 2.79 | 0.45 |
| 1:C:133:HIS:HB3 | 1:C:520:MET:HE3 | 1.97 | 0.45 |
| 1:C:95:ILE:HG12 | 1:C:105:LEU:HD22 | 1.99 | 0.45 |
| 1:E:302:HIS:CD2 | 1:E:303:LEU:HD13 | 2.51 | 0.45 |
| 1:E:8:LEU:CD2 | 1:E:77:CYS:HB2 | 2.46 | 0.45 |
| 1:E:92:VAL:HG23 | 1:E:92:VAL:O | 2.16 | 0.45 |
| 1:F:520:MET:HE1 | 1:F:572:ILE:HG12 | 1.98 | 0.45 |
| 1:F:82:ILE:HA | 1:F:83:GLN:HA | 1.74 | 0.45 |
| 1:A:290:MET:CE | 1:A:295:LEU:CB | 2.93 | 0.45 |
| 1:A:38:ASP:O | 1:A:39:VAL:HG23 | 2.16 | 0.45 |
| 1:A:42:PHE:CE1 | 1:A:59:ILE:CD1 | 2.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:538:ASP:O | 1:B:541:HIS:N | 2.40 | 0.45 |
| 1:C:285:ASP:OD2 | 1:C:285:ASP:C | 2.55 | 0.45 |
| 1:D:177:ILE:HB | 1:D:236:ILE:HA | 1.98 | 0.45 |
| 1:D:212:TRP:CZ3 | 1:D:247:ILE:HG13 | 2.51 | 0.45 |
| 1:D:511:SER:OG | 1:D:511:SER:O | 2.28 | 0.45 |
| 1:E:129:VAL:HG23 | 1:E:130:ILE:H | 1.81 | 0.45 |
| 1:E:217:GLU:O | 1:E:220:LYS:N | 2.49 | 0.45 |
| 1:E:177:ILE:CG2 | 1:E:236:ILE:HG12 | 2.46 | 0.45 |
| 1:C:177:ILE:HG21 | 1:C:236:ILE:HG12 | 1.98 | 0.45 |
| 1:C:351:LYS:O | 1:C:352:ASN:HB2 | 2.17 | 0.45 |
| 1:D:122:ASN:OD1 | 1:D:517:ILE:HG12 | 2.16 | 0.45 |
| 1:E:244:SER:O | 1:E:245:GLY:C | 2.55 | 0.45 |
| 1:F:516:ASP:OD2 | 1:F:517:ILE:N | 2.49 | 0.45 |
| 1:F:559:GLU:O | 1:F:560:SER:C | 2.55 | 0.45 |
| 1:A:172:GLU:CD | 1:A:245:GLY:H | 2.20 | 0.45 |
| 1:A:79:VAL:CG1 | 1:A:81:TYR:CE2 | 3.00 | 0.45 |
| 1:B:8:LEU:CD2 | 1:B:77:CYS:HB2 | 2.46 | 0.45 |
| 1:C:286:TYR:CE1 | 1:C:301:LYS:HE3 | 2.51 | 0.45 |
| 1:C:305:ARG:HB2 | 1:C:306:PRO:CD | 2.46 | 0.45 |
| 1:E:38:ASP:O | 1:E:39:VAL:HG23 | 2.16 | 0.45 |
| 1:F:59:ILE:CG2 | 1:F:59:ILE:O | 2.64 | 0.45 |
| 1:A:559:GLU:O | 1:A:560:SER:C | 2.55 | 0.45 |
| 1:B:41:GLU:O | 1:B:41:GLU:HG2 | 2.16 | 0.45 |
| 1:C:175:LEU:HD23 | 1:C:239:VAL:HB | 1.99 | 0.45 |
| 1:C:282:ILE:HA | 1:C:282:ILE:HD12 | 1.75 | 0.45 |
| 1:C:75:ASN:OD1 | 1:C:75:ASN:N | 2.50 | 0.45 |
| 1:F:26:ASN:HB3 | 1:F:29:ARG:NH2 | 2.31 | 0.45 |
| 1:F:463:ILE:HD13 | 1:F:463:ILE:O | 2.16 | 0.45 |
| 1:A:174:ILE:CG1 | 1:A:176:THR:HG22 | 2.44 | 0.45 |
| 1:A:324:ASP:OD1 | 1:A:324:ASP:C | 2.54 | 0.45 |
| 1:B:46:PHE:HB3 | 1:B:57:VAL:HG23 | 1.98 | 0.45 |
| 1:B:498:LYS:O | 1:B:499:TYR:C | 2.54 | 0.45 |
| 1:B:525:TRP:CZ3 | 1:B:554:ARG:NH1 | 2.84 | 0.45 |
| 1:C:129:VAL:CG2 | 1:C:130:ILE:N | 2.79 | 0.45 |
| 1:C:212:TRP:HA | 1:C:212:TRP:CE3 | 2.51 | 0.45 |
| 1:C:358:ASN:CG | 1:C:358:ASN:O | 2.54 | 0.45 |
| 1:C:560:SER:O | 1:C:564:ASN:ND2 | 2.43 | 0.45 |
| 1:C:75:ASN:HA | 1:C:92:VAL:HG22 | 1.99 | 0.45 |
| 1:D:305:ARG:HB2 | 1:D:306:PRO:CD | 2.47 | 0.45 |
| 1:E:286:TYR:C | 1:E:286:TYR:CD2 | 2.89 | 0.45 |
| 1:F:172:GLU:CD | 1:F:245:GLY:H | 2.20 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:LEU:HD11 | 1:A:177:ILE:HG23 | 1.99 | 0.45 |
| 1:A:306:PRO:HD3 | 1:A:326:SER:HB3 | 1.98 | 0.45 |
| 1:A:48:TYR:CE1 | 1:A:55:LEU:HD22 | 2.51 | 0.45 |
| 1:B:95:ILE:HG12 | 1:B:105:LEU:HD22 | 1.97 | 0.45 |
| 1:B:290:MET:HE3 | 1:B:295:LEU:HB2 | 1.98 | 0.45 |
| 1:C:276:GLN:O | 1:C:277:LYS:C | 2.53 | 0.45 |
| 1:C:483:LEU:HD12 | 1:C:484:ARG:N | 2.32 | 0.45 |
| 1:C:82:ILE:HA | 1:C:83:GLN:HA | 1.70 | 0.45 |
| 1:D:371:ASN:C | 1:D:371:ASN:OD1 | 2.55 | 0.45 |
| 1:E:212:TRP:CZ3 | 1:E:247:ILE:HG13 | 2.52 | 0.45 |
| 1:E:351:LYS:HG2 | 1:E:352:ASN:OD1 | 2.17 | 0.45 |
| 1:F:23:PHE:HD2 | 1:F:117:GLN:OE1 | 2.00 | 0.45 |
| 1:F:3:LEU:O | 1:F:82:ILE:HG13 | 2.17 | 0.45 |
| 1:A:106:SER:C | 1:A:107:LEU:HD12 | 2.36 | 0.45 |
| 1:A:155:THR:HG21 | 1:A:307:ASN:O | 2.16 | 0.45 |
| 1:B:129:VAL:HG23 | 1:B:130:ILE:H | 1.82 | 0.45 |
| 1:B:206:ASN:OD1 | 1:B:210:MET:CE | 2.65 | 0.45 |
| 1:C:531:ILE:HA | 1:C:531:ILE:HD12 | 1.87 | 0.45 |
| 1:C:71:LEU:HD12 | 1:C:71:LEU:O | 2.16 | 0.45 |
| 1:D:148:SER:HB2 | 1:E:156:SER:O | 2.16 | 0.45 |
| 1:E:282:ILE:HD11 | 1:E:483:LEU:HB3 | 1.99 | 0.45 |
| 1:E:371:ASN:OD1 | 1:E:371:ASN:C | 2.55 | 0.45 |
| 1:A:156:SER:O | 1:F:148:SER:HB2 | 2.17 | 0.45 |
| 1:B:157:THR:HB | 1:B:492:GLU:OE1 | 2.17 | 0.45 |
| 1:B:358:ASN:O | 1:B:358:ASN:CG | 2.55 | 0.45 |
| 1:B:124:LEU:HD21 | 1:B:532:TRP:HE3 | 1.81 | 0.45 |
| 1:B:544:MET:O | 1:B:548:LEU:HB2 | 2.17 | 0.45 |
| 1:B:546:ARG:NH2 | 1:C:15:ASN:CG | 2.70 | 0.45 |
| 1:C:319:ASN:C | 1:C:320:ARG:HG2 | 2.37 | 0.45 |
| 1:D:212:TRP:O | 1:D:213:PHE:CG | 2.70 | 0.45 |
| 1:D:182:ARG:NH2 | 1:D:267:LYS:HE2 | 2.32 | 0.45 |
| 1:E:274:SER:HB2 | 1:E:338:VAL:CG2 | 2.47 | 0.45 |
| 1:E:359:ASN:C | 1:E:360:VAL:O | 2.52 | 0.45 |
| 1:B:566:THR:C | 1:B:568:VAL:N | 2.67 | 0.44 |
| 1:D:202:ASP:OD2 | 1:D:274:SER:OG | 2.35 | 0.44 |
| 1:D:133:HIS:CD2 | 1:D:525:TRP:H | 2.36 | 0.44 |
| 1:E:158:MET:C | 1:E:159:ARG:HG2 | 2.37 | 0.44 |
| 1:E:572:ILE:O | 1:E:573:ILE:HB | 2.17 | 0.44 |
| 1:F:531:ILE:HA | 1:F:531:ILE:HD12 | 1.78 | 0.44 |
| 1:F:124:LEU:CD2 | 1:F:532:TRP:HB2 | 2.45 | 0.44 |
| 1:B:122:ASN:OD1 | 1:B:517:ILE:HG12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:525:TRP:CE3 | 1:B:554:ARG:NH1 | 2.85 | 0.44 |
| 1:C:190:LYS:CG | 1:C:190:LYS:O | 2.62 | 0.44 |
| 1:C:542:MET:O | 1:C:543:ASN:C | 2.56 | 0.44 |
| 1:C:566:THR:C | 1:C:568:VAL:N | 2.68 | 0.44 |
| 1:D:286:TYR:CD2 | 1:D:286:TYR:C | 2.90 | 0.44 |
| 1:D:128:ASN:HB2 | 1:D:510:TYR:HA | 1.99 | 0.44 |
| 1:E:276:GLN:O | 1:E:277:LYS:C | 2.56 | 0.44 |
| 1:F:115:TYR:CE1 | 1:F:537:VAL:HG13 | 2.52 | 0.44 |
| 1:F:164:LYS:HB2 | 1:F:282:ILE:HD12 | 1.99 | 0.44 |
| 1:F:360:VAL:HG23 | 1:F:363:TYR:HB2 | 2.00 | 0.44 |
| 1:A:96:GLN:OE1 | 1:F:49:ARG:HA | 2.18 | 0.44 |
| 1:A:177:ILE:H | 1:A:177:ILE:HD13 | 1.82 | 0.44 |
| 1:A:293:LEU:HD22 | 1:A:309:VAL:HG11 | 2.00 | 0.44 |
| 1:A:152:VAL:HG21 | 1:A:307:ASN:HD21 | 1.81 | 0.44 |
| 1:A:347:LYS:HE2 | 1:A:369:THR:CG2 | 2.47 | 0.44 |
| 1:A:566:THR:O | 1:A:568:VAL:N | 2.49 | 0.44 |
| 1:B:172:GLU:CD | 1:B:212:TRP:CH2 | 2.90 | 0.44 |
| 1:B:164:LYS:HB2 | 1:B:282:ILE:HD12 | 2.00 | 0.44 |
| 1:B:65:ARG:HG2 | 1:B:66:SER:N | 2.32 | 0.44 |
| 1:C:166:GLU:OE1 | 1:C:279:PHE:HA | 2.17 | 0.44 |
| 1:C:529:LYS:O | 1:C:530:GLY:O | 2.35 | 0.44 |
| 1:C:572:ILE:O | 1:C:573:ILE:HB | 2.18 | 0.44 |
| 1:C:8:LEU:HD22 | 1:C:77:CYS:HB2 | 1.98 | 0.44 |
| 1:D:82:ILE:HA | 1:D:83:GLN:HA | 1.75 | 0.44 |
| 1:E:220:LYS:O | 1:E:221:GLU:C | 2.54 | 0.44 |
| 1:E:360:VAL:HG23 | 1:E:363:TYR:HB2 | 1.97 | 0.44 |
| 1:F:529:LYS:O | 1:F:530:GLY:C | 2.55 | 0.44 |
| 1:B:302:HIS:CD2 | 1:B:303:LEU:HD13 | 2.52 | 0.44 |
| 1:C:274:SER:HB2 | 1:C:338:VAL:CG2 | 2.48 | 0.44 |
| 1:D:157:THR:HG23 | 1:D:489:SER:H | 1.81 | 0.44 |
| 1:D:534:LEU:HB2 | 1:D:542:MET:HE1 | 1.98 | 0.44 |
| 1:E:61:LEU:N | 1:E:61:LEU:HD12 | 2.33 | 0.44 |
| 1:E:65:ARG:HG2 | 1:E:66:SER:N | 2.32 | 0.44 |
| 1:E:75:ASN:OD1 | 1:E:75:ASN:N | 2.48 | 0.44 |
| 1:F:127:VAL:CG2 | 1:F:528:PHE:CD1 | 2.99 | 0.44 |
| 1:F:81:TYR:HE1 | 1:F:86:ARG:NH2 | 2.15 | 0.44 |
| 1:B:23:PHE:HD2 | 1:B:117:GLN:OE1 | 2.01 | 0.44 |
| 1:C:172:GLU:OE2 | 1:C:245:GLY:N | 2.47 | 0.44 |
| 1:C:38:ASP:O | 1:C:39:VAL:HG23 | 2.17 | 0.44 |
| 1:D:177:ILE:HG22 | 1:D:236:ILE:HA | 1.98 | 0.44 |
| 1:D:502:MET:O | 1:D:554:ARG:NH1 | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:TRP:CE3 | 1:A:212:TRP:HA | 2.53 | 0.44 |
| 1:B:177:ILE:HB | 1:B:236:ILE:HA | 2.00 | 0.44 |
| 1:C:502:MET:O | 1:C:554:ARG:NH1 | 2.44 | 0.44 |
| 1:D:532:TRP:CZ2 | 1:D:546:ARG:HA | 2.53 | 0.44 |
| 1:D:79:VAL:CG1 | 1:D:81:TYR:CE2 | 3.00 | 0.44 |
| 1:A:299:ASN:N | 1:A:299:ASN:ND2 | 2.65 | 0.44 |
| 1:C:124:LEU:HD21 | 1:C:532:TRP:HE3 | 1.82 | 0.44 |
| 1:C:152:VAL:HG22 | 1:C:153:LEU:N | 2.33 | 0.44 |
| 1:D:38:ASP:O | 1:D:39:VAL:HG23 | 2.17 | 0.44 |
| 1:E:133:HIS:CD2 | 1:E:525:TRP:H | 2.36 | 0.44 |
| 1:F:175:LEU:HD13 | 1:F:177:ILE:HG23 | 2.00 | 0.44 |
| 1:F:313:LEU:HA | 1:F:313:LEU:HD23 | 1.79 | 0.44 |
| 1:A:516:ASP:OD2 | 1:A:517:ILE:N | 2.50 | 0.44 |
| 1:A:560:SER:O | 1:A:564:ASN:ND2 | 2.44 | 0.44 |
| 1:A:75:ASN:N | 1:A:75:ASN:OD1 | 2.50 | 0.44 |
| 1:A:82:ILE:HA | 1:A:83:GLN:HA | 1.70 | 0.44 |
| 1:B:487:ARG:HG2 | 1:B:488:ILE:N | 2.33 | 0.44 |
| 1:C:164:LYS:O | 1:C:282:ILE:CD1 | 2.60 | 0.44 |
| 1:D:359:ASN:O | 1:D:360:VAL:C | 2.56 | 0.44 |
| 1:D:509:ASP:O | 1:D:510:TYR:C | 2.56 | 0.44 |
| 1:F:106:SER:O | 1:F:107:LEU:HD12 | 2.17 | 0.44 |
| 1:A:206:ASN:OD1 | 1:A:210:MET:HE3 | 2.17 | 0.44 |
| 1:A:164:LYS:HB2 | 1:A:282:ILE:HD12 | 1.99 | 0.44 |
| 1:A:285:ASP:OD2 | 1:A:287:GLN:N | 2.50 | 0.44 |
| 1:B:38:ASP:O | 1:B:39:VAL:HG23 | 2.18 | 0.44 |
| 1:C:491:ASP:O | 1:C:494:ASN:N | 2.51 | 0.44 |
| 1:C:520:MET:SD | 1:C:572:ILE:HG12 | 2.58 | 0.44 |
| 1:E:177:ILE:HG21 | 1:E:236:ILE:HG12 | 1.99 | 0.44 |
| 1:F:152:VAL:HG22 | 1:F:153:LEU:N | 2.32 | 0.44 |
| 1:F:279:PHE:HB3 | 1:F:282:ILE:HG22 | 2.00 | 0.44 |
| 1:C:533:THR:HG23 | 1:D:15:ASN:ND2 | 2.33 | 0.43 |
| 1:D:37:PHE:CE1 | 1:D:40:HIS:O | 2.71 | 0.43 |
| 1:D:566:THR:C | 1:D:568:VAL:N | 2.70 | 0.43 |
| 1:F:42:PHE:CE2 | 1:F:44:SER:HB2 | 2.53 | 0.43 |
| 1:F:542:MET:HE2 | 1:F:545:LEU:HD23 | 1.96 | 0.43 |
| 1:B:285:ASP:OD2 | 1:B:285:ASP:C | 2.56 | 0.43 |
| 1:C:165:SER:HA | 1:C:282:ILE:HD13 | 1.99 | 0.43 |
| 1:C:516:ASP:OD2 | 1:C:518:THR:HG22 | 2.18 | 0.43 |
| 1:D:291:PHE:C | 1:D:291:PHE:CD2 | 2.91 | 0.43 |
| 1:D:48:TYR:CE1 | 1:D:55:LEU:HD22 | 2.53 | 0.43 |
| 1:D:6:ILE:CG2 | 1:D:7:LYS:N | 2.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:226:LEU:HD12 | 1:E:233:GLN:HB3 | 2.00 | 0.43 |
| 1:E:537:VAL:O | 1:E:538:ASP:C | 2.55 | 0.43 |
| 1:F:5:LYS:HB3 | 1:F:80:GLN:HG3 | 2.00 | 0.43 |
| 1:A:68:PHE:CZ | 1:F:3:LEU:HD11 | 2.53 | 0.43 |
| 1:C:359:ASN:O | 1:C:360:VAL:C | 2.55 | 0.43 |
| 1:E:175:LEU:HA | 1:E:239:VAL:HB | 2.00 | 0.43 |
| 1:E:217:GLU:O | 1:E:218:SER:C | 2.54 | 0.43 |
| 1:A:206:ASN:OD1 | 1:A:210:MET:HE1 | 2.19 | 0.43 |
| 1:B:258:VAL:HG22 | 1:B:259:ASN:N | 2.33 | 0.43 |
| 1:D:347:LYS:HE2 | 1:D:369:THR:HG22 | 1.99 | 0.43 |
| 1:D:124:LEU:CD2 | 1:D:532:TRP:HB2 | 2.46 | 0.43 |
| 1:D:57:VAL:O | 1:D:57:VAL:HG12 | 2.18 | 0.43 |
| 1:E:165:SER:CA | 1:E:282:ILE:HD13 | 2.48 | 0.43 |
| 1:E:573:ILE:HD13 | 1:E:573:ILE:N | 2.33 | 0.43 |
| 1:F:363:TYR:CD1 | 1:F:364:ILE:HG23 | 2.53 | 0.43 |
| 1:F:514:LEU:HD12 | 1:F:514:LEU:HA | 1.78 | 0.43 |
| 1:A:321:LEU:HA | 1:A:321:LEU:HD12 | 1.77 | 0.43 |
| 1:B:282:ILE:HD12 | 1:B:282:ILE:HA | 1.79 | 0.43 |
| 1:B:299:ASN:OD1 | 1:B:299:ASN:N | 2.48 | 0.43 |
| 1:D:110:ASP:OD1 | 1:D:113:MET:HB2 | 2.18 | 0.43 |
| 1:D:12:THR:HG22 | 1:D:75:ASN:OD1 | 2.18 | 0.43 |
| 1:E:75:ASN:CA | 1:E:92:VAL:HG22 | 2.48 | 0.43 |
| 1:F:21:LEU:HG | 1:F:22:HIS:N | 2.34 | 0.43 |
| 1:F:249:GLN:HA | 1:F:249:GLN:OE1 | 2.19 | 0.43 |
| 1:A:215:ASP:OD1 | 1:A:217:GLU:N | 2.51 | 0.43 |
| 1:C:212:TRP:O | 1:C:213:PHE:CG | 2.71 | 0.43 |
| 1:C:357:GLY:HA2 | 1:C:358:ASN:HA | 1.68 | 0.43 |
| 1:C:542:MET:CE | 1:C:542:MET:HA | 2.48 | 0.43 |
| 1:D:360:VAL:HG23 | 1:D:363:TYR:HB2 | 2.00 | 0.43 |
| 1:D:520:MET:HB3 | 1:D:570:ASN:OD1 | 2.19 | 0.43 |
| 1:E:124:LEU:HD21 | 1:E:532:TRP:HE3 | 1.83 | 0.43 |
| 1:E:169:THR:HG23 | 1:E:170:GLN:HG3 | 2.00 | 0.43 |
| 1:E:512:THR:HG23 | 1:E:513:LYS:N | 2.34 | 0.43 |
| 1:E:115:TYR:CE1 | 1:E:537:VAL:HG13 | 2.53 | 0.43 |
| 1:E:12:THR:HG21 | 1:E:76:TYR:CB | 2.47 | 0.43 |
| 1:F:122:ASN:OD1 | 1:F:517:ILE:HG12 | 2.18 | 0.43 |
| 1:A:157:THR:CG2 | 1:A:157:THR:O | 2.64 | 0.43 |
| 1:B:3:LEU:HB3 | 1:B:45:THR:CB | 2.48 | 0.43 |
| 1:B:520:MET:HB3 | 1:B:570:ASN:OD1 | 2.18 | 0.43 |
| 1:D:23:PHE:N | 1:D:23:PHE:CD2 | 2.86 | 0.43 |
| 1:D:290:MET:HE3 | 1:D:295:LEU:HB3 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:59:ILE:O | 1:D:59:ILE:CG2 | 2.66 | 0.43 |
| 1:E:152:VAL:O | 1:E:152:VAL:HG13 | 2.16 | 0.43 |
| 1:F:498:LYS:O | 1:F:499:TYR:C | 2.55 | 0.43 |
| 1:F:55:LEU:HD23 | 1:F:55:LEU:N | 2.33 | 0.43 |
| 1:A:27:GLU:HG2 | 1:A:28:GLU:N | 2.34 | 0.43 |
| 1:C:152:VAL:O | 1:C:152:VAL:HG13 | 2.19 | 0.43 |
| 1:D:129:VAL:HG23 | 1:D:130:ILE:H | 1.84 | 0.43 |
| 1:D:220:LYS:O | 1:D:221:GLU:C | 2.57 | 0.43 |
| 1:D:310:THR:HG22 | 1:D:486:GLY:HA3 | 2.01 | 0.43 |
| 1:E:293:LEU:HD22 | 1:E:309:VAL:HG11 | 2.00 | 0.43 |
| 1:E:491:ASP:O | 1:E:494:ASN:N | 2.51 | 0.43 |
| 1:F:357:GLY:HA2 | 1:F:358:ASN:HA | 1.77 | 0.43 |
| 1:F:42:PHE:CE1 | 1:F:59:ILE:CD1 | 3.02 | 0.43 |
| 1:A:3:LEU:HD11 | 1:B:68:PHE:HZ | 1.84 | 0.43 |
| 1:A:496:VAL:O | 1:A:497:LYS:C | 2.56 | 0.43 |
| 1:B:48:TYR:OH | 1:B:109:PRO:HG3 | 2.19 | 0.43 |
| 1:C:282:ILE:HG23 | 1:C:334:PHE:CD2 | 2.54 | 0.43 |
| 1:D:212:TRP:HA | 1:D:212:TRP:CE3 | 2.54 | 0.43 |
| 1:E:23:PHE:HD2 | 1:E:117:GLN:OE1 | 2.01 | 0.43 |
| 1:E:177:ILE:CB | 1:E:236:ILE:HA | 2.49 | 0.43 |
| 1:F:168:PHE:CD2 | 1:F:480:GLY:HA2 | 2.54 | 0.43 |
| 1:A:371:ASN:C | 1:A:371:ASN:OD1 | 2.54 | 0.43 |
| 1:A:534:LEU:HD23 | 1:A:534:LEU:HA | 1.83 | 0.43 |
| 1:B:175:LEU:HD13 | 1:B:177:ILE:HG23 | 2.00 | 0.43 |
| 1:B:249:GLN:HA | 1:B:249:GLN:OE1 | 2.18 | 0.43 |
| 1:C:157:THR:HB | 1:C:492:GLU:OE1 | 2.19 | 0.43 |
| 1:C:534:LEU:HA | 1:C:534:LEU:HD23 | 1.90 | 0.43 |
| 1:C:12:THR:HG22 | 1:C:75:ASN:OD1 | 2.19 | 0.43 |
| 1:E:12:THR:HA | 1:E:13:PRO:HD3 | 1.87 | 0.43 |
| 1:E:374:ASP:HB3 | 1:E:467:HIS:O | 2.19 | 0.43 |
| 1:F:29:ARG:HD2 | 1:F:30:ASP:OD2 | 2.18 | 0.43 |
| 1:F:8:LEU:HD22 | 1:F:77:CYS:HB2 | 2.01 | 0.43 |
| 1:A:282:ILE:HD12 | 1:A:282:ILE:HA | 1.73 | 0.42 |
| 1:A:291:PHE:C | 1:A:291:PHE:CD2 | 2.92 | 0.42 |
| 1:A:572:ILE:CG2 | 1:A:572:ILE:O | 2.50 | 0.42 |
| 1:B:189:GLU:CD | 1:B:189:GLU:N | 2.73 | 0.42 |
| 1:D:10:TYR:HB2 | 1:D:38:ASP:HB2 | 2.00 | 0.42 |
| 1:D:177:ILE:CG2 | 1:D:236:ILE:HG12 | 2.48 | 0.42 |
| 1:D:95:ILE:HG12 | 1:D:105:LEU:HD22 | 2.01 | 0.42 |
| 1:E:71:LEU:HD12 | 1:E:71:LEU:O | 2.18 | 0.42 |
| 1:F:286:TYR:CD2 | 1:F:286:TYR:C | 2.92 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:3:LEU:HB3 | 1:F:45:THR:HB | 2.01 | 0.42 |
| 1:A:112:VAL:CG2 | 1:A:548:LEU:CD1 | 2.97 | 0.42 |
| 1:A:274:SER:HB2 | 1:A:338:VAL:CG2 | 2.49 | 0.42 |
| 1:A:563:ILE:H | 1:A:563:ILE:HD13 | 1.80 | 0.42 |
| 1:C:363:TYR:CD1 | 1:C:364:ILE:HG23 | 2.54 | 0.42 |
| 1:D:130:ILE:CG2 | 1:D:527:GLN:HG2 | 2.49 | 0.42 |
| 1:D:164:LYS:CB | 1:D:282:ILE:HD12 | 2.49 | 0.42 |
| 1:C:363:TYR:HD2 | 1:D:316:TYR:CE1 | 2.37 | 0.42 |
| 1:D:516:ASP:CG | 1:D:518:THR:HG22 | 2.38 | 0.42 |
| 1:E:282:ILE:HA | 1:E:282:ILE:HD12 | 1.67 | 0.42 |
| 1:A:16:ASN:HB3 | 1:F:531:ILE:CD1 | 2.49 | 0.42 |
| 1:A:277:LYS:O | 1:A:336:SER:OG | 2.37 | 0.42 |
| 1:A:537:VAL:O | 1:A:539:THR:N | 2.52 | 0.42 |
| 1:A:65:ARG:HG2 | 1:A:66:SER:N | 2.34 | 0.42 |
| 1:B:112:VAL:CG2 | 1:B:548:LEU:CD1 | 2.97 | 0.42 |
| 1:B:491:ASP:O | 1:B:494:ASN:N | 2.52 | 0.42 |
| 1:C:470:TYR:CB | 1:C:479:PHE:CE1 | 3.02 | 0.42 |
| 1:C:514:LEU:HD12 | 1:C:514:LEU:HA | 1.90 | 0.42 |
| 1:C:516:ASP:OD1 | 1:C:518:THR:HG22 | 2.19 | 0.42 |
| 1:A:531:ILE:HD12 | 1:A:531:ILE:HA | 1.84 | 0.42 |
| 1:B:133:HIS:HB3 | 1:B:520:MET:HE2 | 2.00 | 0.42 |
| 1:B:111:VAL:CB | 1:B:545:LEU:HD13 | 2.47 | 0.42 |
| 1:C:165:SER:CA | 1:C:282:ILE:HD13 | 2.49 | 0.42 |
| 1:D:112:VAL:CG2 | 1:D:548:LEU:CD1 | 2.97 | 0.42 |
| 1:E:134:TYR:HH | 1:E:507:CYS:HG | 1.63 | 0.42 |
| 1:E:157:THR:HB | 1:E:492:GLU:OE1 | 2.19 | 0.42 |
| 1:A:553:VAL:HG12 | 1:A:555:LEU:HD12 | 2.00 | 0.42 |
| 1:B:174:ILE:CG1 | 1:B:176:THR:HG22 | 2.48 | 0.42 |
| 1:B:571:VAL:HG13 | 1:B:572:ILE:N | 2.34 | 0.42 |
| 1:C:92:VAL:HG23 | 1:C:92:VAL:O | 2.20 | 0.42 |
| 1:D:172:GLU:OE2 | 1:D:245:GLY:N | 2.49 | 0.42 |
| 1:D:542:MET:HB3 | 1:D:546:ARG:NH1 | 2.34 | 0.42 |
| 1:E:542:MET:HB3 | 1:E:546:ARG:NH1 | 2.34 | 0.42 |
| 1:A:55:LEU:HD23 | 1:A:55:LEU:N | 2.34 | 0.42 |
| 1:C:226:LEU:HD12 | 1:C:233:GLN:HB3 | 2.01 | 0.42 |
| 1:C:249:GLN:OE1 | 1:C:249:GLN:HA | 2.19 | 0.42 |
| 1:C:42:PHE:CE2 | 1:C:44:SER:HB2 | 2.54 | 0.42 |
| 1:C:48:TYR:CD2 | 1:C:55:LEU:HD13 | 2.55 | 0.42 |
| 1:C:491:ASP:O | 1:C:492:GLU:C | 2.58 | 0.42 |
| 1:D:258:VAL:HG12 | 1:D:263:LEU:O | 2.18 | 0.42 |
| 1:D:279:PHE:HB3 | 1:D:282:ILE:HG22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:315:ASP:HB3 | 1:D:370:ILE:HD11 | 2.01 | 0.42 |
| 1:D:41:GLU:O | 1:D:41:GLU:HG2 | 2.20 | 0.42 |
| 1:E:516:ASP:OD1 | 1:E:518:THR:HG22 | 2.20 | 0.42 |
| 1:A:254:ASP:O | 1:A:255:HIS:C | 2.57 | 0.42 |
| 1:B:244:SER:O | 1:B:245:GLY:C | 2.58 | 0.42 |
| 1:B:42:PHE:CG | 1:B:43:THR:N | 2.85 | 0.42 |
| 1:B:539:THR:CG2 | 1:B:540:GLY:N | 2.82 | 0.42 |
| 1:C:177:ILE:HB | 1:C:236:ILE:HA | 2.01 | 0.42 |
| 1:C:263:LEU:HA | 1:C:263:LEU:HD12 | 1.90 | 0.42 |
| 1:D:120:VAL:HG23 | 1:D:121:LEU:H | 1.81 | 0.42 |
| 1:D:124:LEU:HD22 | 1:D:532:TRP:CB | 2.47 | 0.42 |
| 1:D:323:ILE:HG23 | 1:D:353:TYR:CE1 | 2.55 | 0.42 |
| 1:D:470:TYR:CB | 1:D:479:PHE:CE1 | 3.02 | 0.42 |
| 1:E:534:LEU:HB2 | 1:E:542:MET:HE1 | 2.01 | 0.42 |
| 1:F:104:GLU:O | 1:F:105:LEU:HD23 | 2.19 | 0.42 |
| 1:F:165:SER:HA | 1:F:282:ILE:HD13 | 2.01 | 0.42 |
| 1:F:571:VAL:CG1 | 1:F:572:ILE:N | 2.79 | 0.42 |
| 1:F:65:ARG:HG2 | 1:F:66:SER:N | 2.35 | 0.42 |
| 1:B:359:ASN:O | 1:B:360:VAL:C | 2.58 | 0.42 |
| 1:C:531:ILE:CD1 | 1:D:16:ASN:HB3 | 2.49 | 0.42 |
| 1:D:359:ASN:C | 1:D:360:VAL:O | 2.58 | 0.42 |
| 1:F:289:LEU:HD11 | 1:F:293:LEU:HD11 | 2.01 | 0.42 |
| 1:F:236:ILE:HG21 | 1:F:378:PHE:CE2 | 2.55 | 0.42 |
| 1:F:542:MET:O | 1:F:545:LEU:CB | 2.68 | 0.42 |
| 1:C:124:LEU:HD22 | 1:C:532:TRP:CB | 2.46 | 0.42 |
| 1:C:182:ARG:NH2 | 1:C:267:LYS:HE2 | 2.35 | 0.42 |
| 1:C:285:ASP:OD2 | 1:C:287:GLN:N | 2.53 | 0.42 |
| 1:C:124:LEU:CD2 | 1:C:532:TRP:HB2 | 2.46 | 0.42 |
| 1:C:549:PHE:O | 1:C:552:GLY:N | 2.53 | 0.42 |
| 1:D:25:SER:OG | 1:D:28:GLU:HG3 | 2.19 | 0.42 |
| 1:D:476:GLN:O | 1:D:478:LYS:HG2 | 2.20 | 0.42 |
| 1:D:89:TYR:N | 1:D:89:TYR:CD2 | 2.88 | 0.42 |
| 1:F:132:GLN:OE1 | 1:F:515:SER:HB3 | 2.20 | 0.42 |
| 1:F:285:ASP:HA | 1:F:331:ASN:OD1 | 2.19 | 0.42 |
| 1:F:4:SER:HA | 1:F:82:ILE:HG12 | 2.01 | 0.42 |
| 1:A:164:LYS:O | 1:A:282:ILE:CD1 | 2.60 | 0.42 |
| 1:A:165:SER:CA | 1:A:282:ILE:HD13 | 2.49 | 0.42 |
| 1:A:48:TYR:CD2 | 1:A:55:LEU:HD13 | 2.55 | 0.42 |
| 1:A:132:GLN:OE1 | 1:A:515:SER:HB3 | 2.19 | 0.42 |
| 1:A:356:ARG:NH2 | 1:B:487:ARG:O | 2.52 | 0.42 |
| 1:B:533:THR:HG23 | 1:B:546:ARG:NH2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:57:VAL:HG12 | 1:B:57:VAL:O | 2.20 | 0.42 |
| 1:C:290:MET:CE | 1:C:295:LEU:HB3 | 2.50 | 0.42 |
| 1:D:177:ILE:HG21 | 1:D:236:ILE:HG12 | 2.01 | 0.42 |
| 1:D:299:ASN:H | 1:D:299:ASN:HD22 | 1.68 | 0.42 |
| 1:D:380:VAL:O | 1:D:462:ALA:N | 2.53 | 0.42 |
| 1:E:106:SER:C | 1:E:107:LEU:HD12 | 2.41 | 0.42 |
| 1:F:534:LEU:HD23 | 1:F:534:LEU:HA | 1.84 | 0.42 |
| 1:A:12:THR:OG1 | 1:A:13:PRO:HD2 | 2.19 | 0.41 |
| 1:A:255:HIS:O | 1:A:256:GLU:HG3 | 2.20 | 0.41 |
| 1:A:350:VAL:HG22 | 1:A:353:TYR:HB2 | 2.01 | 0.41 |
| 1:B:348:VAL:CG2 | 1:B:349:TYR:N | 2.81 | 0.41 |
| 1:C:325:LEU:HD12 | 1:C:325:LEU:HA | 1.90 | 0.41 |
| 1:C:61:LEU:HD12 | 1:C:61:LEU:N | 2.34 | 0.41 |
| 1:D:46:PHE:CE1 | 1:D:55:LEU:HD12 | 2.55 | 0.41 |
| 1:F:561:ASP:OD2 | 1:F:566:THR:HG21 | 2.19 | 0.41 |
| 1:F:56:ARG:HD3 | 1:F:104:GLU:OE1 | 2.20 | 0.41 |
| 1:A:5:LYS:HB3 | 1:A:80:GLN:HG3 | 2.02 | 0.41 |
| 1:C:332:LEU:HA | 1:C:332:LEU:HD12 | 1.84 | 0.41 |
| 1:D:282:ILE:HD12 | 1:D:282:ILE:HA | 1.67 | 0.41 |
| 1:D:285:ASP:HA | 1:D:331:ASN:OD1 | 2.19 | 0.41 |
| 1:D:544:MET:O | 1:D:548:LEU:HB2 | 2.21 | 0.41 |
| 1:D:561:ASP:O | 1:D:563:ILE:N | 2.53 | 0.41 |
| 1:D:61:LEU:HD12 | 1:D:61:LEU:N | 2.35 | 0.41 |
| 1:F:350:VAL:HG22 | 1:F:353:TYR:HB2 | 2.02 | 0.41 |
| 1:A:130:ILE:O | 1:A:131:ARG:CG | 2.69 | 0.41 |
| 1:A:347:LYS:HE2 | 1:A:369:THR:HG22 | 2.01 | 0.41 |
| 1:A:542:MET:O | 1:A:546:ARG:N | 2.53 | 0.41 |
| 1:A:563:ILE:C | 1:A:564:ASN:ND2 | 2.74 | 0.41 |
| 1:B:189:GLU:H | 1:B:189:GLU:CD | 2.24 | 0.41 |
| 1:C:81:TYR:HE1 | 1:C:86:ARG:NH2 | 2.18 | 0.41 |
| 1:D:304:LEU:HA | 1:D:304:LEU:HD23 | 1.83 | 0.41 |
| 1:D:532:TRP:HZ2 | 1:D:546:ARG:HA | 1.86 | 0.41 |
| 1:E:531:ILE:O | 1:E:531:ILE:CG2 | 2.68 | 0.41 |
| 1:E:566:THR:C | 1:E:568:VAL:N | 2.70 | 0.41 |
| 1:F:212:TRP:CE3 | 1:F:212:TRP:HA | 2.55 | 0.41 |
| 1:F:165:SER:CA | 1:F:282:ILE:HD13 | 2.50 | 0.41 |
| 1:A:299:ASN:H | 1:A:299:ASN:ND2 | 2.18 | 0.41 |
| 1:A:514:LEU:HD21 | 1:A:528:PHE:CE2 | 2.55 | 0.41 |
| 1:B:168:PHE:CD2 | 1:B:480:GLY:HA2 | 2.55 | 0.41 |
| 1:B:37:PHE:C | 1:B:38:ASP:CG | 2.79 | 0.41 |
| 1:B:531:ILE:HD12 | 1:B:531:ILE:HA | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:166:GLU:OE1 | 1:C:279:PHE:CA | 2.68 | 0.41 |
| 1:C:26:ASN:HB3 | 1:C:29:ARG:NH2 | 2.36 | 0.41 |
| 1:C:542:MET:O | 1:C:545:LEU:CB | 2.69 | 0.41 |
| 1:E:258:VAL:HG12 | 1:E:263:LEU:O | 2.19 | 0.41 |
| 1:E:46:PHE:CE1 | 1:E:55:LEU:HD12 | 2.54 | 0.41 |
| 1:E:487:ARG:HG2 | 1:E:488:ILE:N | 2.35 | 0.41 |
| 1:E:531:ILE:HD12 | 1:E:531:ILE:HA | 1.82 | 0.41 |
| 1:F:76:TYR:OH | 1:F:113:MET:HG2 | 2.20 | 0.41 |
| 1:F:282:ILE:HG23 | 1:F:334:PHE:CD2 | 2.55 | 0.41 |
| 1:F:371:ASN:OD1 | 1:F:371:ASN:C | 2.57 | 0.41 |
| 1:F:470:TYR:CB | 1:F:479:PHE:CE1 | 3.03 | 0.41 |
| 1:A:541:HIS:O | 1:A:545:LEU:HB2 | 2.19 | 0.41 |
| 1:B:12:THR:HG21 | 1:B:76:TYR:CB | 2.51 | 0.41 |
| 1:B:133:HIS:CD2 | 1:B:525:TRP:H | 2.39 | 0.41 |
| 1:B:48:TYR:CD2 | 1:B:55:LEU:HD13 | 2.55 | 0.41 |
| 1:C:112:VAL:CG2 | 1:C:548:LEU:CD1 | 2.99 | 0.41 |
| 1:D:293:LEU:HD22 | 1:D:309:VAL:HG11 | 2.02 | 0.41 |
| 1:D:81:TYR:HE1 | 1:D:86:ARG:NH2 | 2.19 | 0.41 |
| 1:E:360:VAL:CG2 | 1:E:363:TYR:HB2 | 2.51 | 0.41 |
| 1:F:121:LEU:O | 1:F:124:LEU:HD12 | 2.19 | 0.41 |
| 1:F:129:VAL:CG2 | 1:F:130:ILE:N | 2.83 | 0.41 |
| 1:A:95:ILE:CD1 | 1:A:105:LEU:HD22 | 2.50 | 0.41 |
| 1:A:313:LEU:HA | 1:A:313:LEU:HD23 | 1.83 | 0.41 |
| 1:A:533:THR:HG23 | 1:A:546:ARG:NH2 | 2.36 | 0.41 |
| 1:D:165:SER:CA | 1:D:282:ILE:HD13 | 2.51 | 0.41 |
| 1:D:286:TYR:HE1 | 1:D:301:LYS:HE3 | 1.85 | 0.41 |
| 1:F:79:VAL:CG1 | 1:F:81:TYR:CE2 | 3.03 | 0.41 |
| 1:A:158:MET:C | 1:A:159:ARG:HG2 | 2.41 | 0.41 |
| 1:A:311:ALA:HB2 | 1:A:325:LEU:HD22 | 2.03 | 0.41 |
| 1:B:291:PHE:HD2 | 1:B:291:PHE:C | 2.24 | 0.41 |
| 1:B:548:LEU:HD23 | 1:B:548:LEU:HA | 1.81 | 0.41 |
| 1:C:177:ILE:C | 1:C:177:ILE:HD13 | 2.41 | 0.41 |
| 1:C:55:LEU:HD23 | 1:C:55:LEU:N | 2.36 | 0.41 |
| 1:D:348:VAL:HG13 | 1:D:368:LEU:HB3 | 2.03 | 0.41 |
| 1:E:483:LEU:HD12 | 1:E:484:ARG:N | 2.36 | 0.41 |
| 1:F:276:GLN:O | 1:F:277:LYS:C | 2.59 | 0.41 |
| 1:B:138:GLU:OE2 | 1:B:515:SER:HB2 | 2.21 | 0.41 |
| 1:B:82:ILE:HA | 1:B:83:GLN:HA | 1.72 | 0.41 |
| 1:C:12:THR:HG21 | 1:C:76:TYR:CB | 2.50 | 0.41 |
| 1:C:487:ARG:HG2 | 1:C:488:ILE:N | 2.35 | 0.41 |
| 1:D:324:ASP:C | 1:D:324:ASP:OD1 | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:127:VAL:CG2 | 1:D:528:PHE:CD1 | 3.00 | 0.41 |
| 1:E:164:LYS:HB2 | 1:E:282:ILE:HD12 | 2.03 | 0.41 |
| 1:E:42:PHE:CE1 | 1:E:59:ILE:CD1 | 3.03 | 0.41 |
| 1:E:55:LEU:HD23 | 1:E:55:LEU:N | 2.36 | 0.41 |
| 1:F:3:LEU:CB | 1:F:45:THR:HB | 2.50 | 0.41 |
| 1:A:360:VAL:CG2 | 1:A:363:TYR:HB2 | 2.50 | 0.41 |
| 1:A:572:ILE:O | 1:A:573:ILE:CB | 2.67 | 0.41 |
| 1:C:189:GLU:N | 1:C:189:GLU:CD | 2.74 | 0.41 |
| 1:D:164:LYS:O | 1:D:282:ILE:CD1 | 2.66 | 0.41 |
| 1:D:27:GLU:HG2 | 1:D:28:GLU:N | 2.36 | 0.41 |
| 1:D:164:LYS:HB2 | 1:D:282:ILE:HD12 | 2.03 | 0.41 |
| 1:D:487:ARG:HG2 | 1:D:488:ILE:N | 2.35 | 0.41 |
| 1:E:224:ASP:C | 1:E:226:LEU:N | 2.73 | 0.41 |
| 1:E:531:ILE:HG13 | 1:F:15:ASN:OD1 | 2.21 | 0.41 |
| 1:B:338:VAL:CG2 | 1:B:338:VAL:O | 2.67 | 0.41 |
| 1:B:371:ASN:OD1 | 1:B:371:ASN:C | 2.59 | 0.41 |
| 1:B:542:MET:HE1 | 1:B:545:LEU:HD23 | 2.02 | 0.41 |
| 1:C:220:LYS:O | 1:C:221:GLU:C | 2.59 | 0.41 |
| 1:C:520:MET:HB3 | 1:C:570:ASN:OD1 | 2.21 | 0.41 |
| 1:D:516:ASP:OD2 | 1:D:517:ILE:N | 2.54 | 0.41 |
| 1:E:210:MET:HB3 | 1:E:210:MET:HE2 | 1.99 | 0.41 |
| 1:E:157:THR:HG23 | 1:E:489:SER:H | 1.82 | 0.41 |
| 1:E:519:SER:O | 1:E:573:ILE:HG12 | 2.21 | 0.41 |
| 1:E:130:ILE:HB | 1:E:527:GLN:HG2 | 2.03 | 0.41 |
| 1:E:533:THR:HG23 | 1:E:546:ARG:NH2 | 2.35 | 0.41 |
| 1:F:305:ARG:HB2 | 1:F:306:PRO:CD | 2.50 | 0.41 |
| 1:F:282:ILE:HD11 | 1:F:483:LEU:HB3 | 2.02 | 0.41 |
| 1:F:572:ILE:O | 1:F:573:ILE:C | 2.59 | 0.41 |
| 1:A:249:GLN:HA | 1:A:249:GLN:OE1 | 2.21 | 0.41 |
| 1:A:316:TYR:CE2 | 1:A:482:HIS:CD2 | 3.09 | 0.41 |
| 1:B:357:GLY:HA2 | 1:B:358:ASN:HA | 1.67 | 0.41 |
| 1:B:516:ASP:OD1 | 1:B:518:THR:HG22 | 2.21 | 0.41 |
| 1:B:545:LEU:O | 1:B:546:ARG:C | 2.57 | 0.41 |
| 1:C:512:THR:HG23 | 1:C:513:LYS:N | 2.34 | 0.41 |
| 1:C:563:ILE:H | 1:C:563:ILE:HD13 | 1.85 | 0.41 |
| 1:C:571:VAL:CG1 | 1:C:572:ILE:N | 2.81 | 0.41 |
| 1:C:42:PHE:CD1 | 1:C:59:ILE:HD11 | 2.56 | 0.41 |
| 1:D:463:ILE:O | 1:D:463:ILE:HD13 | 2.20 | 0.41 |
| 1:E:177:ILE:HB | 1:E:236:ILE:HA | 2.03 | 0.41 |
| 1:E:124:LEU:CD2 | 1:E:532:TRP:HB2 | 2.47 | 0.41 |
| 1:E:8:LEU:CD1 | 1:E:105:LEU:HD11 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:21:LEU:HD12 | 1:F:556:TRP:O | 2.21 | 0.41 |
| 1:F:353:TYR:O | 1:F:354:ASN:CB | 2.67 | 0.41 |
| 1:F:374:ASP:HB3 | 1:F:467:HIS:O | 2.20 | 0.41 |
| 1:F:532:TRP:CZ2 | 1:F:546:ARG:HA | 2.56 | 0.41 |
| 1:A:139:TYR:O | 1:A:140:GLU:C | 2.59 | 0.40 |
| 1:A:220:LYS:O | 1:A:221:GLU:C | 2.57 | 0.40 |
| 1:B:573:ILE:HD13 | 1:B:573:ILE:N | 2.36 | 0.40 |
| 1:C:76:TYR:OH | 1:C:113:MET:HG2 | 2.22 | 0.40 |
| 1:C:236:ILE:HG21 | 1:C:378:PHE:CE2 | 2.55 | 0.40 |
| 1:C:512:THR:HG23 | 1:C:513:LYS:O | 2.21 | 0.40 |
| 1:C:533:THR:HG23 | 1:C:546:ARG:NH2 | 2.36 | 0.40 |
| 1:C:89:TYR:CD2 | 1:C:89:TYR:N | 2.89 | 0.40 |
| 1:D:215:ASP:OD1 | 1:D:217:GLU:N | 2.52 | 0.40 |
| 1:D:282:ILE:HD11 | 1:D:483:LEU:HB3 | 2.03 | 0.40 |
| 1:D:75:ASN:N | 1:D:75:ASN:OD1 | 2.53 | 0.40 |
| 1:E:148:SER:CB | 1:F:156:SER:O | 2.69 | 0.40 |
| 1:E:348:VAL:CG2 | 1:E:349:TYR:N | 2.82 | 0.40 |
| 1:F:210:MET:HB3 | 1:F:210:MET:HE2 | 2.03 | 0.40 |
| 1:F:296:ASN:O | 1:F:300:ASP:HB2 | 2.21 | 0.40 |
| 1:A:128:ASN:C | 1:A:128:ASN:HD22 | 2.25 | 0.40 |
| 1:A:189:GLU:CD | 1:A:189:GLU:N | 2.75 | 0.40 |
| 1:A:570:ASN:O | 1:A:571:VAL:HG23 | 2.21 | 0.40 |
| 1:A:571:VAL:HG13 | 1:A:572:ILE:N | 2.36 | 0.40 |
| 1:A:67:CYS:SG | 1:A:68:PHE:N | 2.94 | 0.40 |
| 1:C:514:LEU:HD21 | 1:C:528:PHE:CE2 | 2.56 | 0.40 |
| 1:D:23:PHE:HD2 | 1:D:117:GLN:OE1 | 2.04 | 0.40 |
| 1:D:129:VAL:HG23 | 1:D:130:ILE:N | 2.36 | 0.40 |
| 1:D:514:LEU:HD21 | 1:D:528:PHE:CE2 | 2.56 | 0.40 |
| 1:D:55:LEU:N | 1:D:55:LEU:HD23 | 2.37 | 0.40 |
| 1:E:138:GLU:OE2 | 1:E:515:SER:HB2 | 2.20 | 0.40 |
| 1:E:6:ILE:HG23 | 1:E:7:LYS:N | 2.37 | 0.40 |
| 1:F:106:SER:C | 1:F:107:LEU:HD12 | 2.42 | 0.40 |
| 1:F:16:ASN:HD21 | 1:F:18:GLN:HG3 | 1.86 | 0.40 |
| 1:F:170:GLN:O | 1:F:244:SER:CB | 2.70 | 0.40 |
| 1:F:37:PHE:CE1 | 1:F:40:HIS:O | 2.74 | 0.40 |
| 1:F:48:TYR:CD2 | 1:F:55:LEU:HD13 | 2.56 | 0.40 |
| 1:F:560:SER:O | 1:F:564:ASN:ND2 | 2.52 | 0.40 |
| 1:F:570:ASN:O | 1:F:571:VAL:HG23 | 2.22 | 0.40 |
| 1:A:542:MET:HB3 | 1:A:546:ARG:NH1 | 2.36 | 0.40 |
| 1:A:7:LYS:HG3 | 1:A:37:PHE:CE2 | 2.57 | 0.40 |
| 1:B:12:THR:HA | 1:B:13:PRO:HD3 | 1.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:511:SER:HB2 | 1:B:567:VAL:HG21 | 2.02 | 0.40 |
| 1:C:295:LEU:HA | 1:C:295:LEU:HD12 | 1.93 | 0.40 |
| 1:C:69:GLU:HG2 | 1:C:69:GLU:O | 2.21 | 0.40 |
| 1:D:12:THR:HA | 1:D:13:PRO:HD3 | 1.89 | 0.40 |
| 1:D:518:THR:O | 1:D:518:THR:HG23 | 2.21 | 0.40 |
| 1:D:8:LEU:CD2 | 1:D:77:CYS:HB2 | 2.51 | 0.40 |
| 1:E:148:SER:HB3 | 1:F:156:SER:O | 2.22 | 0.40 |
| 1:E:202:ASP:OD2 | 1:E:274:SER:OG | 2.40 | 0.40 |
| 1:F:212:TRP:O | 1:F:213:PHE:CG | 2.74 | 0.40 |
| 1:B:130:ILE:O | 1:B:131:ARG:CG | 2.69 | 0.40 |
| 1:B:217:GLU:O | 1:B:218:SER:C | 2.60 | 0.40 |
| 1:B:227:THR:O | 1:B:230:PRO:HD3 | 2.22 | 0.40 |
| 1:B:5:LYS:HB3 | 1:B:80:GLN:HG3 | 2.03 | 0.40 |
| 1:B:71:LEU:O | 1:B:71:LEU:CG | 2.69 | 0.40 |
| 1:C:210:MET:HE2 | 1:C:210:MET:HB3 | 2.03 | 0.40 |
| 1:C:307:ASN:N | 1:C:307:ASN:OD1 | 2.46 | 0.40 |
| 1:C:165:SER:HB3 | 1:C:482:HIS:ND1 | 2.35 | 0.40 |
| 1:D:177:ILE:H | 1:D:177:ILE:HD13 | 1.85 | 0.40 |
| 1:D:46:PHE:CE1 | 1:D:55:LEU:HD11 | 2.57 | 0.40 |
| 1:D:496:VAL:O | 1:D:497:LYS:C | 2.59 | 0.40 |
| 1:E:48:TYR:CD2 | 1:E:55:LEU:HD13 | 2.56 | 0.40 |
| 1:F:61:LEU:N | 1:F:61:LEU:HD12 | 2.36 | 0.40 |
| 1:F:75:ASN:CA | 1:F:92:VAL:HG22 | 2.51 | 0.40 |
| 1:A:239:VAL:O | 1:A:375:THR:HA | 2.21 | 0.40 |
| 1:A:71:LEU:O | 1:A:71:LEU:CG | 2.68 | 0.40 |
| 1:B:175:LEU:HD23 | 1:B:239:VAL:HB | 2.04 | 0.40 |
| 1:B:359:ASN:C | 1:B:360:VAL:O | 2.59 | 0.40 |
| 1:B:538:ASP:O | 1:B:540:GLY:N | 2.54 | 0.40 |
| 1:C:538:ASP:O | 1:C:541:HIS:N | 2.52 | 0.40 |
| 1:C:541:HIS:O | 1:C:545:LEU:N | 2.54 | 0.40 |
| 1:C:572:ILE:O | 1:C:573:ILE:C | 2.58 | 0.40 |
| 1:D:111:VAL:CG2 | 1:D:545:LEU:HD13 | 2.51 | 0.40 |
| 1:D:274:SER:HB2 | 1:D:338:VAL:CG2 | 2.52 | 0.40 |
| 1:D:42:PHE:CE1 | 1:D:59:ILE:CD1 | 3.03 | 0.40 |
| 1:D:475:LYS:HA | 1:D:475:LYS:HD2 | 1.96 | 0.40 |
| 1:D:561:ASP:C | 1:D:563:ILE:N | 2.74 | 0.40 |
| 1:E:174:ILE:CG1 | 1:E:176:THR:HG22 | 2.50 | 0.40 |
| 1:E:563:ILE:C | 1:E:564:ASN:ND2 | 2.74 | 0.40 |
| 1:F:286:TYR:HE1 | 1:F:301:LYS:HE3 | 1.84 | 0.40 |
| 1:F:95:ILE:CD1 | 1:F:105:LEU:HD22 | 2.51 | 0.40 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:A:255:HIS:O | 1:B:291:PHE:CZ[2_665] | 1.96 | 0.24 |
| 1:C:295:LEU:O | 1:F:65:ARG:NH2[1_556] | 2.07 | 0.13 |
| 1:A:255:HIS:O | 1:B:291:PHE:CE2[2_665] | 2.09 | 0.11 |
| 1:A:255:HIS:C | 1:B:291:PHE:CZ[2_665] | 2.19 | 0.01 |

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 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 | 482/583 (83%) | 386 (80%) | 82 (17%) | 14 (3%) | 5 | 28 |
| 1 | B | 482/583 (83%) | 390 (81%) | 82 (17%) | 10 (2%) | 8 | 38 |
| 1 | C | 482/583 (83%) | 387 (80%) | 86 (18%) | 9 (2%) | 9 | 41 |
| 1 | D | 482/583 (83%) | 388 (80%) | 81 (17%) | 13 (3%) | 6 | 30 |
| 1 | E | 482/583 (83%) | 390 (81%) | 85 (18%) | 7 (2%) | 12 | 48 |
| 1 | F | 482/583 (83%) | 387 (80%) | 85 (18%) | 10 (2%) | 8 | 38 |
| All | All | 2892/3498 (83%) | 2328 (80%) | 501 (17%) | 63 (2%) | 8 | 36 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 258 | VAL |
| 1 | A | 530 | GLY |
| 1 | A | 539 | THR |
| 1 | B | 258 | VAL |
| 1 | B | 530 | GLY |
| 1 | C | 258 | VAL |
| 1 | C | 530 | GLY |
| 1 | D | 258 | VAL |
| 1 | D | 530 | GLY |
| 1 | D | 539 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 258 | VAL |
| 1 | E | 530 | GLY |
| 1 | E | 539 | THR |
| 1 | F | 258 | VAL |
| 1 | F | 530 | GLY |
| 1 | F | 539 | THR |
| 1 | A | 68 | PHE |
| 1 | A | 233 | GLN |
| 1 | A | 255 | HIS |
| 1 | B | 68 | PHE |
| 1 | B | 539 | THR |
| 1 | C | 68 | PHE |
| 1 | C | 539 | THR |
| 1 | D | 68 | PHE |
| 1 | E | 68 | PHE |
| 1 | F | 68 | PHE |
| 1 | A | 36 | LYS |
| 1 | D | 550 | GLU |
| 1 | F | 567 | VAL |
| 1 | A | 546 | ARG |
| 1 | A | 567 | VAL |
| 1 | B | 304 | LEU |
| 1 | A | 39 | VAL |
| 1 | A | 360 | VAL |
| 1 | A | 538 | ASP |
| 1 | B | 39 | VAL |
| 1 | B | 277 | LYS |
| 1 | B | 567 | VAL |
| 1 | C | 567 | VAL |
| 1 | D | 250 | GLU |
| 1 | D | 567 | VAL |
| 1 | F | 233 | GLN |
| 1 | F | 304 | LEU |
| 1 | A | 260 | GLY |
| 1 | B | 36 | LYS |
| 1 | C | 39 | VAL |
| 1 | D | 39 | VAL |
| 1 | D | 371 | ASN |
| 1 | D | 542 | MET |
| 1 | E | 39 | VAL |
| 1 | F | 36 | LYS |
| 1 | F | 39 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 572 | ILE |
| 1 | D | 245 | GLY |
| 1 | E | 567 | VAL |
| 1 | C | 190 | LYS |
| 1 | D | 260 | GLY |
| 1 | A | 572 | ILE |
| 1 | C | 360 | VAL |
| 1 | C | 572 | ILE |
| 1 | D | 572 | ILE |
| 1 | E | 572 | ILE |
| 1 | F | 572 | 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 | 446/529 (84%) | 368 (82%) | 78 (18%) | 2 | 11 |
| 1 | B | 446/529 (84%) | 369 (83%) | 77 (17%) | 2 | 12 |
| 1 | C | 446/529 (84%) | 369 (83%) | 77 (17%) | 2 | 12 |
| 1 | D | 446/529 (84%) | 367 (82%) | 79 (18%) | 2 | 11 |
| 1 | E | 446/529 (84%) | 365 (82%) | 81 (18%) | 2 | 10 |
| 1 | F | 446/529 (84%) | 367 (82%) | 79 (18%) | 2 | 11 |
| All | All | 2676/3174 (84%) | 2205 (82%) | 471 (18%) | 2 | 11 |

All (471) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | ASN |
| 1 | A | 18 | GLN |
| 1 | A | 23 | PHE |
| 1 | A | 38 | ASP |
| 1 | A | 46 | PHE |
| 1 | A | 48 | TYR |
| 1 | A | 55 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | VAL |
| 1 | A | 58 | THR |
| 1 | A | 61 | LEU |
| 1 | A | 62 | VAL |
| 1 | A | 65 | ARG |
| 1 | A | 66 | SER |
| 1 | A | 69 | GLU |
| 1 | A | 71 | LEU |
| 1 | A | 72 | MET |
| 1 | A | 74 | VAL |
| 1 | A | 87 | VAL |
| 1 | A | 94 | ASP |
| 1 | A | 103 | CYS |
| 1 | A | 108 | VAL |
| 1 | A | 128 | ASN |
| 1 | A | 129 | VAL |
| 1 | A | 135 | THR |
| 1 | A | 146 | ILE |
| 1 | A | 155 | THR |
| 1 | A | 157 | THR |
| 1 | A | 165 | SER |
| 1 | A | 174 | ILE |
| 1 | A | 176 | THR |
| 1 | A | 177 | ILE |
| 1 | A | 182 | ARG |
| 1 | A | 189 | GLU |
| 1 | A | 199 | SER |
| 1 | A | 200 | THR |
| 1 | A | 204 | ILE |
| 1 | A | 206 | ASN |
| 1 | A | 210 | MET |
| 1 | A | 215 | ASP |
| 1 | A | 226 | LEU |
| 1 | A | 227 | THR |
| 1 | A | 229 | TYR |
| 1 | A | 239 | VAL |
| 1 | A | 249 | GLN |
| 1 | A | 263 | LEU |
| 1 | A | 267 | LYS |
| 1 | A | 274 | SER |
| 1 | A | 285 | ASP |
| 1 | A | 288 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 295 | LEU |
| 1 | A | 299 | ASN |
| 1 | A | 303 | LEU |
| 1 | A | 320 | ARG |
| 1 | A | 330 | THR |
| 1 | A | 338 | VAL |
| 1 | A | 350 | VAL |
| 1 | A | 358 | ASN |
| 1 | A | 359 | ASN |
| 1 | A | 360 | VAL |
| 1 | A | 365 | ASP |
| 1 | A | 369 | THR |
| 1 | A | 374 | ASP |
| 1 | A | 376 | ILE |
| 1 | A | 463 | ILE |
| 1 | A | 491 | ASP |
| 1 | A | 513 | LYS |
| 1 | A | 514 | LEU |
| 1 | A | 518 | THR |
| 1 | A | 524 | ASN |
| 1 | A | 526 | VAL |
| 1 | A | 533 | THR |
| 1 | A | 539 | THR |
| 1 | A | 548 | LEU |
| 1 | A | 560 | SER |
| 1 | A | 563 | ILE |
| 1 | A | 568 | VAL |
| 1 | A | 571 | VAL |
| 1 | A | 573 | ILE |
| 1 | B | 16 | ASN |
| 1 | B | 18 | GLN |
| 1 | B | 23 | PHE |
| 1 | B | 26 | ASN |
| 1 | B | 38 | ASP |
| 1 | B | 46 | PHE |
| 1 | B | 48 | TYR |
| 1 | B | 55 | LEU |
| 1 | B | 57 | VAL |
| 1 | B | 58 | THR |
| 1 | B | 61 | LEU |
| 1 | B | 62 | VAL |
| 1 | B | 65 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 69 | GLU |
| 1 | B | 71 | LEU |
| 1 | B | 72 | MET |
| 1 | B | 74 | VAL |
| 1 | B | 94 | ASP |
| 1 | B | 103 | CYS |
| 1 | B | 108 | VAL |
| 1 | B | 128 | ASN |
| 1 | B | 129 | VAL |
| 1 | B | 135 | THR |
| 1 | B | 146 | ILE |
| 1 | B | 155 | THR |
| 1 | B | 157 | THR |
| 1 | B | 165 | SER |
| 1 | B | 174 | ILE |
| 1 | B | 176 | THR |
| 1 | B | 177 | ILE |
| 1 | B | 182 | ARG |
| 1 | B | 189 | GLU |
| 1 | B | 199 | SER |
| 1 | B | 200 | THR |
| 1 | B | 204 | ILE |
| 1 | B | 206 | ASN |
| 1 | B | 208 | TYR |
| 1 | B | 210 | MET |
| 1 | B | 215 | ASP |
| 1 | B | 226 | LEU |
| 1 | B | 227 | THR |
| 1 | B | 229 | TYR |
| 1 | B | 239 | VAL |
| 1 | B | 249 | GLN |
| 1 | B | 263 | LEU |
| 1 | B | 267 | LYS |
| 1 | B | 274 | SER |
| 1 | B | 285 | ASP |
| 1 | B | 288 | SER |
| 1 | B | 295 | LEU |
| 1 | B | 299 | ASN |
| 1 | B | 303 | LEU |
| 1 | B | 320 | ARG |
| 1 | B | 325 | LEU |
| 1 | B | 326 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 330 | THR |
| 1 | B | 338 | VAL |
| 1 | B | 350 | VAL |
| 1 | B | 358 | ASN |
| 1 | B | 359 | ASN |
| 1 | B | 360 | VAL |
| 1 | B | 365 | ASP |
| 1 | B | 369 | THR |
| 1 | B | 374 | ASP |
| 1 | B | 376 | ILE |
| 1 | B | 463 | ILE |
| 1 | B | 491 | ASP |
| 1 | B | 513 | LYS |
| 1 | B | 514 | LEU |
| 1 | B | 524 | ASN |
| 1 | B | 526 | VAL |
| 1 | B | 533 | THR |
| 1 | B | 548 | LEU |
| 1 | B | 560 | SER |
| 1 | B | 563 | ILE |
| 1 | B | 571 | VAL |
| 1 | B | 573 | ILE |
| 1 | C | 16 | ASN |
| 1 | C | 18 | GLN |
| 1 | C | 23 | PHE |
| 1 | C | 38 | ASP |
| 1 | C | 46 | PHE |
| 1 | C | 48 | TYR |
| 1 | C | 55 | LEU |
| 1 | C | 57 | VAL |
| 1 | C | 58 | THR |
| 1 | C | 61 | LEU |
| 1 | C | 62 | VAL |
| 1 | C | 65 | ARG |
| 1 | C | 69 | GLU |
| 1 | C | 71 | LEU |
| 1 | C | 74 | VAL |
| 1 | C | 94 | ASP |
| 1 | C | 103 | CYS |
| 1 | C | 108 | VAL |
| 1 | C | 128 | ASN |
| 1 | C | 129 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 135 | THR |
| 1 | C | 146 | ILE |
| 1 | C | 155 | THR |
| 1 | C | 157 | THR |
| 1 | C | 165 | SER |
| 1 | C | 174 | ILE |
| 1 | C | 176 | THR |
| 1 | C | 177 | ILE |
| 1 | C | 182 | ARG |
| 1 | C | 189 | GLU |
| 1 | C | 199 | SER |
| 1 | C | 200 | THR |
| 1 | C | 204 | ILE |
| 1 | C | 206 | ASN |
| 1 | C | 210 | MET |
| 1 | C | 215 | ASP |
| 1 | C | 226 | LEU |
| 1 | C | 227 | THR |
| 1 | C | 229 | TYR |
| 1 | C | 239 | VAL |
| 1 | C | 263 | LEU |
| 1 | C | 267 | LYS |
| 1 | C | 274 | SER |
| 1 | C | 278 | ASP |
| 1 | C | 285 | ASP |
| 1 | C | 288 | SER |
| 1 | C | 295 | LEU |
| 1 | C | 299 | ASN |
| 1 | C | 303 | LEU |
| 1 | C | 320 | ARG |
| 1 | C | 325 | LEU |
| 1 | C | 326 | SER |
| 1 | C | 330 | THR |
| 1 | C | 338 | VAL |
| 1 | C | 348 | VAL |
| 1 | C | 350 | VAL |
| 1 | C | 358 | ASN |
| 1 | C | 359 | ASN |
| 1 | C | 360 | VAL |
| 1 | C | 365 | ASP |
| 1 | C | 369 | THR |
| 1 | C | 374 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 376 | ILE |
| 1 | C | 463 | ILE |
| 1 | C | 491 | ASP |
| 1 | C | 513 | LYS |
| 1 | C | 514 | LEU |
| 1 | C | 518 | THR |
| 1 | C | 524 | ASN |
| 1 | C | 526 | VAL |
| 1 | C | 533 | THR |
| 1 | C | 539 | THR |
| 1 | C | 548 | LEU |
| 1 | C | 560 | SER |
| 1 | C | 563 | ILE |
| 1 | C | 571 | VAL |
| 1 | C | 573 | ILE |
| 1 | D | 16 | ASN |
| 1 | D | 18 | GLN |
| 1 | D | 23 | PHE |
| 1 | D | 38 | ASP |
| 1 | D | 42 | PHE |
| 1 | D | 46 | PHE |
| 1 | D | 48 | TYR |
| 1 | D | 55 | LEU |
| 1 | D | 57 | VAL |
| 1 | D | 58 | THR |
| 1 | D | 61 | LEU |
| 1 | D | 62 | VAL |
| 1 | D | 65 | ARG |
| 1 | D | 69 | GLU |
| 1 | D | 71 | LEU |
| 1 | D | 72 | MET |
| 1 | D | 74 | VAL |
| 1 | D | 87 | VAL |
| 1 | D | 94 | ASP |
| 1 | D | 103 | CYS |
| 1 | D | 108 | VAL |
| 1 | D | 128 | ASN |
| 1 | D | 129 | VAL |
| 1 | D | 135 | THR |
| 1 | D | 146 | ILE |
| 1 | D | 155 | THR |
| 1 | D | 157 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 165 | SER |
| 1 | D | 174 | ILE |
| 1 | D | 176 | THR |
| 1 | D | 177 | ILE |
| 1 | D | 182 | ARG |
| 1 | D | 189 | GLU |
| 1 | D | 199 | SER |
| 1 | D | 200 | THR |
| 1 | D | 204 | ILE |
| 1 | D | 206 | ASN |
| 1 | D | 210 | MET |
| 1 | D | 215 | ASP |
| 1 | D | 226 | LEU |
| 1 | D | 227 | THR |
| 1 | D | 229 | TYR |
| 1 | D | 239 | VAL |
| 1 | D | 263 | LEU |
| 1 | D | 267 | LYS |
| 1 | D | 274 | SER |
| 1 | D | 278 | ASP |
| 1 | D | 285 | ASP |
| 1 | D | 288 | SER |
| 1 | D | 295 | LEU |
| 1 | D | 299 | ASN |
| 1 | D | 303 | LEU |
| 1 | D | 320 | ARG |
| 1 | D | 325 | LEU |
| 1 | D | 330 | THR |
| 1 | D | 338 | VAL |
| 1 | D | 350 | VAL |
| 1 | D | 358 | ASN |
| 1 | D | 359 | ASN |
| 1 | D | 360 | VAL |
| 1 | D | 365 | ASP |
| 1 | D | 369 | THR |
| 1 | D | 374 | ASP |
| 1 | D | 376 | ILE |
| 1 | D | 463 | ILE |
| 1 | D | 513 | LYS |
| 1 | D | 514 | LEU |
| 1 | D | 518 | THR |
| 1 | D | 524 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 526 | VAL |
| 1 | D | 533 | THR |
| 1 | D | 539 | THR |
| 1 | D | 548 | LEU |
| 1 | D | 560 | SER |
| 1 | D | 563 | ILE |
| 1 | D | 566 | THR |
| 1 | D | 571 | VAL |
| 1 | D | 572 | ILE |
| 1 | D | 573 | ILE |
| 1 | E | 16 | ASN |
| 1 | E | 18 | GLN |
| 1 | E | 23 | PHE |
| 1 | E | 26 | ASN |
| 1 | E | 38 | ASP |
| 1 | E | 46 | PHE |
| 1 | E | 48 | TYR |
| 1 | E | 55 | LEU |
| 1 | E | 57 | VAL |
| 1 | E | 58 | THR |
| 1 | E | 61 | LEU |
| 1 | E | 62 | VAL |
| 1 | E | 65 | ARG |
| 1 | E | 69 | GLU |
| 1 | E | 71 | LEU |
| 1 | E | 72 | MET |
| 1 | E | 74 | VAL |
| 1 | E | 94 | ASP |
| 1 | E | 103 | CYS |
| 1 | E | 108 | VAL |
| 1 | E | 128 | ASN |
| 1 | E | 129 | VAL |
| 1 | E | 135 | THR |
| 1 | E | 146 | ILE |
| 1 | E | 155 | THR |
| 1 | E | 157 | THR |
| 1 | E | 165 | SER |
| 1 | E | 174 | ILE |
| 1 | E | 176 | THR |
| 1 | E | 177 | ILE |
| 1 | E | 182 | ARG |
| 1 | E | 189 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 199 | SER |
| 1 | E | 200 | THR |
| 1 | E | 204 | ILE |
| 1 | E | 206 | ASN |
| 1 | E | 210 | MET |
| 1 | E | 215 | ASP |
| 1 | E | 226 | LEU |
| 1 | E | 227 | THR |
| 1 | E | 229 | TYR |
| 1 | E | 239 | VAL |
| 1 | E | 249 | GLN |
| 1 | E | 263 | LEU |
| 1 | E | 267 | LYS |
| 1 | E | 274 | SER |
| 1 | E | 278 | ASP |
| 1 | E | 285 | ASP |
| 1 | E | 288 | SER |
| 1 | E | 295 | LEU |
| 1 | E | 299 | ASN |
| 1 | E | 303 | LEU |
| 1 | E | 320 | ARG |
| 1 | E | 325 | LEU |
| 1 | E | 330 | THR |
| 1 | E | 338 | VAL |
| 1 | E | 350 | VAL |
| 1 | E | 358 | ASN |
| 1 | E | 359 | ASN |
| 1 | E | 360 | VAL |
| 1 | E | 365 | ASP |
| 1 | E | 369 | THR |
| 1 | E | 374 | ASP |
| 1 | E | 376 | ILE |
| 1 | E | 463 | ILE |
| 1 | E | 475 | LYS |
| 1 | E | 476 | GLN |
| 1 | E | 513 | LYS |
| 1 | E | 514 | LEU |
| 1 | E | 518 | THR |
| 1 | E | 524 | ASN |
| 1 | E | 526 | VAL |
| 1 | E | 533 | THR |
| 1 | E | 539 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 548 | LEU |
| 1 | E | 560 | SER |
| 1 | E | 563 | ILE |
| 1 | E | 568 | VAL |
| 1 | E | 571 | VAL |
| 1 | E | 572 | ILE |
| 1 | E | 573 | ILE |
| 1 | F | 16 | ASN |
| 1 | F | 18 | GLN |
| 1 | F | 23 | PHE |
| 1 | F | 38 | ASP |
| 1 | F | 42 | PHE |
| 1 | F | 46 | PHE |
| 1 | F | 48 | TYR |
| 1 | F | 55 | LEU |
| 1 | F | 57 | VAL |
| 1 | F | 58 | THR |
| 1 | F | 61 | LEU |
| 1 | F | 62 | VAL |
| 1 | F | 65 | ARG |
| 1 | F | 69 | GLU |
| 1 | F | 71 | LEU |
| 1 | F | 72 | MET |
| 1 | F | 74 | VAL |
| 1 | F | 77 | CYS |
| 1 | F | 87 | VAL |
| 1 | F | 94 | ASP |
| 1 | F | 103 | CYS |
| 1 | F | 108 | VAL |
| 1 | F | 128 | ASN |
| 1 | F | 129 | VAL |
| 1 | F | 135 | THR |
| 1 | F | 146 | ILE |
| 1 | F | 155 | THR |
| 1 | F | 157 | THR |
| 1 | F | 165 | SER |
| 1 | F | 174 | ILE |
| 1 | F | 176 | THR |
| 1 | F | 177 | ILE |
| 1 | F | 182 | ARG |
| 1 | F | 189 | GLU |
| 1 | F | 199 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 200 | THR |
| 1 | F | 204 | ILE |
| 1 | F | 206 | ASN |
| 1 | F | 210 | MET |
| 1 | F | 215 | ASP |
| 1 | F | 226 | LEU |
| 1 | F | 227 | THR |
| 1 | F | 229 | TYR |
| 1 | F | 239 | VAL |
| 1 | F | 263 | LEU |
| 1 | F | 267 | LYS |
| 1 | F | 274 | SER |
| 1 | F | 285 | ASP |
| 1 | F | 288 | SER |
| 1 | F | 295 | LEU |
| 1 | F | 299 | ASN |
| 1 | F | 303 | LEU |
| 1 | F | 325 | LEU |
| 1 | F | 326 | SER |
| 1 | F | 330 | THR |
| 1 | F | 338 | VAL |
| 1 | F | 350 | VAL |
| 1 | F | 358 | ASN |
| 1 | F | 359 | ASN |
| 1 | F | 360 | VAL |
| 1 | F | 365 | ASP |
| 1 | F | 369 | THR |
| 1 | F | 374 | ASP |
| 1 | F | 376 | ILE |
| 1 | F | 463 | ILE |
| 1 | F | 475 | LYS |
| 1 | F | 491 | ASP |
| 1 | F | 513 | LYS |
| 1 | F | 514 | LEU |
| 1 | F | 518 | THR |
| 1 | F | 524 | ASN |
| 1 | F | 526 | VAL |
| 1 | F | 533 | THR |
| 1 | F | 539 | THR |
| 1 | F | 548 | LEU |
| 1 | F | 560 | SER |
| 1 | F | 563 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 571 | VAL |
| 1 | F | 573 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 40 | HIS |
| 1 | A | 233 | GLN |
| 1 | B | 40 | HIS |
| 1 | B | 233 | GLN |
| 1 | B | 564 | ASN |
| 1 | C | 40 | HIS |
| 1 | C | 233 | GLN |
| 1 | C | 299 | ASN |
| 1 | D | 40 | HIS |
| 1 | D | 233 | GLN |
| 1 | E | 40 | HIS |
| 1 | E | 233 | GLN |
| 1 | F | 40 | HIS |
| 1 | F | 233 | GLN |
| 1 | F | 564 | ASN |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 488/583 (83%) | -0.12 | 11 (2%) 61 31 | 48, 91, 189, 275 | 0 |
| 1 | B | 488/583 (83%) | -0.30 | 4 (0%) 86 64 | 50, 92, 180, 276 | 0 |
| 1 | C | 488/583 (83%) | -0.22 | 15 (3%) 49 22 | 58, 102, 192, 278 | 0 |
| 1 | D | 488/583 (83%) | -0.12 | 25 (5%) 29 12 | 65, 104, 205, 279 | 0 |
| 1 | E | 488/583 (83%) | -0.19 | 15 (3%) 49 22 | 58, 103, 198, 275 | 0 |
| 1 | F | 488/583 (83%) | -0.24 | 20 (4%) 38 15 | 52, 94, 194, 281 | 0 |
| All | All | 2928/3498 (83%) | -0.20 | 90 (3%) 49 22 | 48, 99, 194, 281 | 0 |

All (90) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 39 | VAL | 9.7 |
| 1 | F | 39 | VAL | 8.7 |
| 1 | B | 39 | VAL | 7.5 |
| 1 | D | 40 | HIS | 7.2 |
| 1 | A | 68 | PHE | 7.1 |
| 1 | A | 39 | VAL | 6.9 |
| 1 | C | 40 | HIS | 6.7 |
| 1 | D | 62 | VAL | 6.4 |
| 1 | D | 58 | THR | 5.8 |
| 1 | D | 47 | ASN | 5.6 |
| 1 | E | 98 | LEU | 5.1 |
| 1 | A | 40 | HIS | 5.1 |
| 1 | A | 62 | VAL | 5.1 |
| 1 | D | 39 | VAL | 4.9 |
| 1 | F | 98 | LEU | 4.8 |
| 1 | D | 46 | PHE | 4.7 |
| 1 | F | 38 | ASP | 4.5 |
| 1 | A | 69 | GLU | 4.4 |
| 1 | E | 58 | THR | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 93 | THR | 4.3 |
| 1 | E | 6 | ILE | 4.0 |
| 1 | C | 53 | GLY | 3.8 |
| 1 | F | 40 | HIS | 3.8 |
| 1 | F | 97 | GLN | 3.8 |
| 1 | E | 62 | VAL | 3.8 |
| 1 | F | 68 | PHE | 3.7 |
| 1 | D | 6 | ILE | 3.7 |
| 1 | D | 77 | CYS | 3.6 |
| 1 | A | 46 | PHE | 3.6 |
| 1 | E | 46 | PHE | 3.5 |
| 1 | B | 68 | PHE | 3.4 |
| 1 | F | 4 | SER | 3.4 |
| 1 | D | 54 | VAL | 3.4 |
| 1 | D | 55 | LEU | 3.4 |
| 1 | B | 47 | ASN | 3.4 |
| 1 | C | 66 | SER | 3.3 |
| 1 | E | 102 | VAL | 3.3 |
| 1 | F | 46 | PHE | 3.3 |
| 1 | D | 68 | PHE | 3.2 |
| 1 | C | 67 | CYS | 3.2 |
| 1 | C | 64 | ASP | 3.1 |
| 1 | D | 98 | LEU | 3.0 |
| 1 | E | 39 | VAL | 3.0 |
| 1 | F | 81 | TYR | 2.9 |
| 1 | F | 62 | VAL | 2.9 |
| 1 | D | 53 | GLY | 2.9 |
| 1 | E | 54 | VAL | 2.9 |
| 1 | F | 99 | ASN | 2.8 |
| 1 | E | 60 | ASP | 2.8 |
| 1 | D | 79 | VAL | 2.8 |
| 1 | D | 104 | GLU | 2.7 |
| 1 | E | 14 | PHE | 2.7 |
| 1 | A | 98 | LEU | 2.7 |
| 1 | C | 63 | SER | 2.7 |
| 1 | F | 66 | SER | 2.7 |
| 1 | C | 55 | LEU | 2.7 |
| 1 | A | 38 | ASP | 2.6 |
| 1 | A | 188 | ALA | 2.6 |
| 1 | D | 80 | GLN | 2.6 |
| 1 | C | 11 | ASN | 2.6 |
| 1 | E | 53 | GLY | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 97 | GLN | 2.5 |
| 1 | D | 60 | ASP | 2.5 |
| 1 | F | 65 | ARG | 2.5 |
| 1 | B | 65 | ARG | 2.4 |
| 1 | D | 8 | LEU | 2.4 |
| 1 | D | 225 | TYR | 2.4 |
| 1 | C | 80 | GLN | 2.4 |
| 1 | D | 48 | TYR | 2.4 |
| 1 | C | 49 | ARG | 2.3 |
| 1 | F | 564 | ASN | 2.3 |
| 1 | C | 6 | ILE | 2.3 |
| 1 | C | 73 | GLY | 2.3 |
| 1 | C | 54 | VAL | 2.3 |
| 1 | F | 59 | ILE | 2.3 |
| 1 | E | 42 | PHE | 2.2 |
| 1 | D | 57 | VAL | 2.2 |
| 1 | F | 100 | ASP | 2.2 |
| 1 | A | 47 | ASN | 2.2 |
| 1 | F | 13 | PRO | 2.2 |
| 1 | E | 59 | ILE | 2.2 |
| 1 | F | 69 | GLU | 2.2 |
| 1 | D | 530 | GLY | 2.2 |
| 1 | A | 191 | PRO | 2.1 |
| 1 | C | 268 | LEU | 2.1 |
| 1 | D | 81 | TYR | 2.1 |
| 1 | D | 49 | ARG | 2.1 |
| 1 | F | 64 | ASP | 2.1 |
| 1 | F | 233 | GLN | 2.1 |
| 1 | D | 56 | ARG | 2.1 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.