



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:25 am GMT

PDB ID : 1E2T
Title : ARYLAMINE N-ACETYLTRANSFERASE (NAT) FROM SALMONELLA
TYPHIMURIUM
Authors : Sinclair, J.C.; Sandy, J.; Delgoda, R.; Sim, E.; Noble, M.E.M.
Deposited on : 2000-05-24
Resolution : 2.80 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 : trunk28620
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) : recalc28949

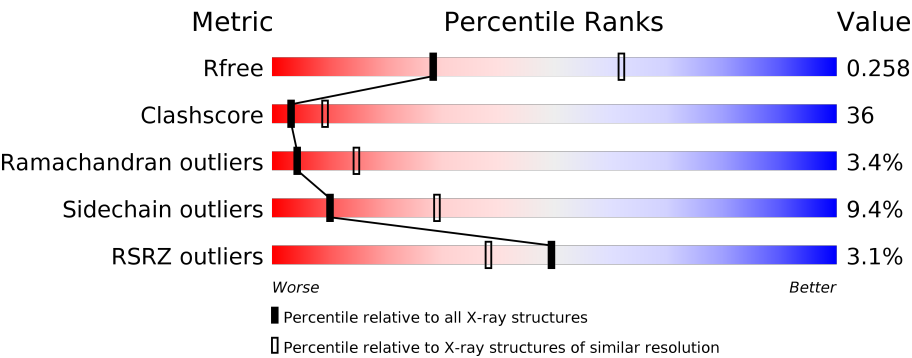
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 | 2583 (2.80-2.80) |
| Clashscore | 112137 | 3033 (2.80-2.80) |
| Ramachandran outliers | 110173 | 2983 (2.80-2.80) |
| Sidechain outliers | 110143 | 2985 (2.80-2.80) |
| RSRZ outliers | 101464 | 2610 (2.80-2.80) |

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 | 284 | <div><div>0%</div><div><div></div><div>43%</div><div>44%</div><div>8%</div><div></div></div><div></div></div> |
| 1 | B | 284 | <div><div>2%</div><div><div></div><div>45%</div><div>40%</div><div>10%</div><div></div></div><div></div></div> |
| 1 | C | 284 | <div><div>5%</div><div><div></div><div>42%</div><div>45%</div><div>10%</div><div></div></div><div></div></div> |
| 1 | D | 284 | <div><div>6%</div><div><div></div><div>43%</div><div>44%</div><div>8%</div><div></div></div><div></div></div> |
| 1 | E | 284 | <div><div></div><div><div></div><div>46%</div><div>41%</div><div>8%</div><div></div></div><div></div></div> |
| 1 | F | 284 | <div><div>4%</div><div><div></div><div>45%</div><div>42%</div><div>8%</div><div></div></div><div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | G | 284 | <div><div>%</div><div><div></div><div>44%</div><div>44%</div><div>8%</div><div></div></div></div> |
| 1 | H | 284 | <div><div>4%</div><div><div></div><div>44%</div><div>45%</div><div>7%</div><div></div></div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18260 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 N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | B | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | C | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | D | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | E | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | F | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | G | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |
| 1 | H | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2224 | 1421 | 403 | 389 | 11 | | | |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 56 | Total | O | 0 | 0 |
| | | | 56 | 56 | | |
| 2 | B | 51 | Total | O | 0 | 0 |
| | | | 51 | 51 | | |
| 2 | C | 79 | Total | O | 0 | 0 |
| | | | 79 | 79 | | |
| 2 | D | 36 | Total | O | 0 | 0 |
| | | | 36 | 36 | | |
| 2 | E | 92 | Total | O | 0 | 0 |
| | | | 92 | 92 | | |
| 2 | F | 48 | Total | O | 0 | 0 |
| | | | 48 | 48 | | |

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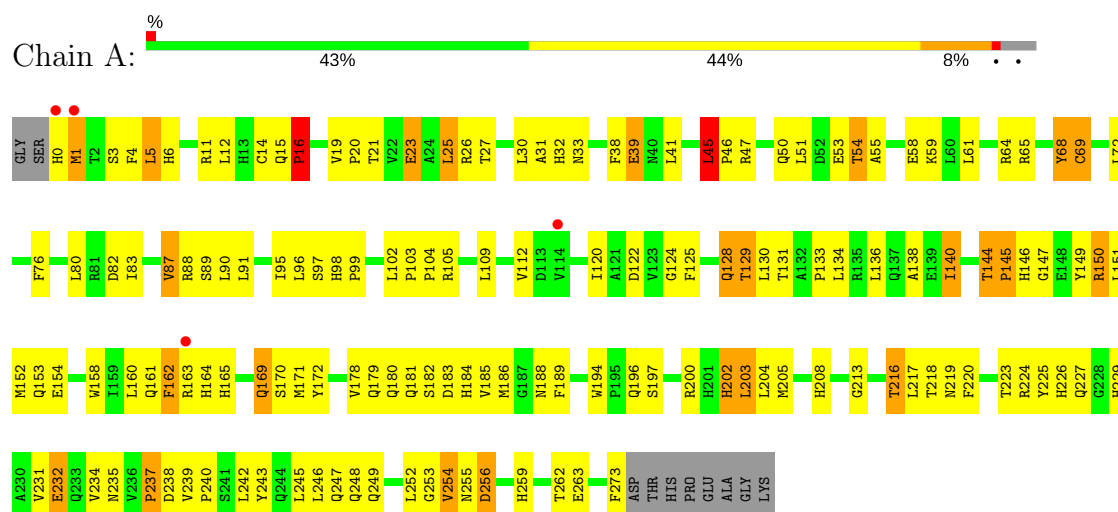
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | G | 56 | Total | O | 0 | 0 |
| | | | 56 | 56 | | |
| 2 | H | 50 | Total | O | 0 | 0 |
| | | | 50 | 50 | | |

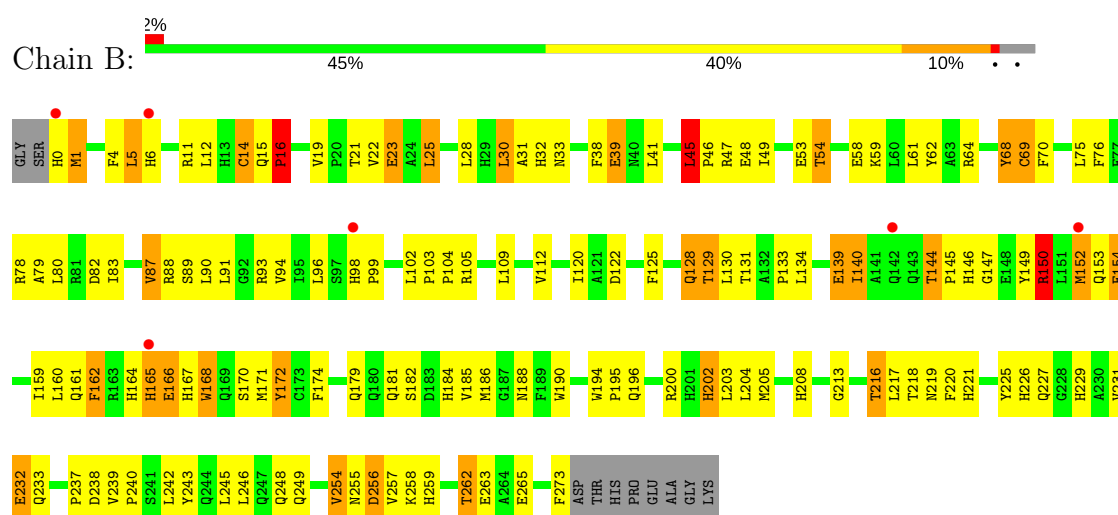
3 Residue-property plots

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: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

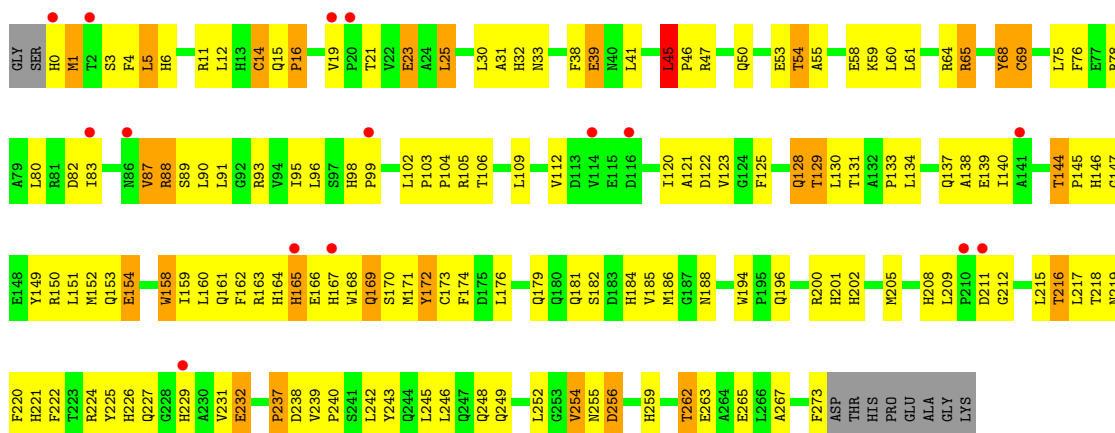


• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

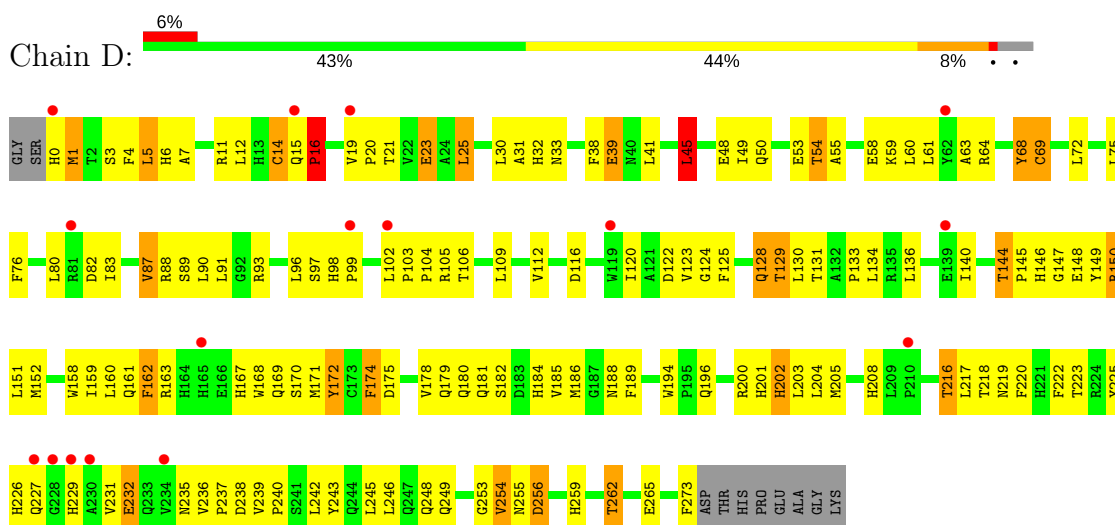


• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE

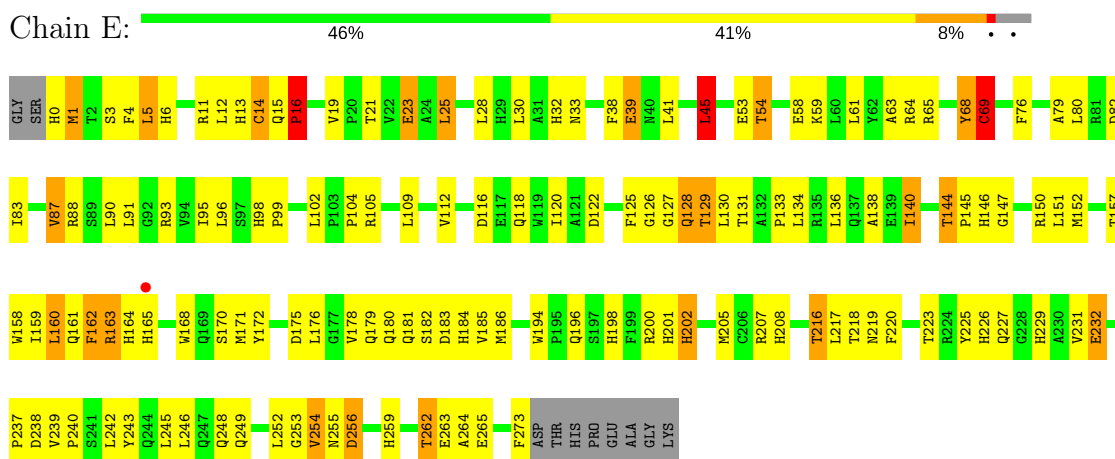




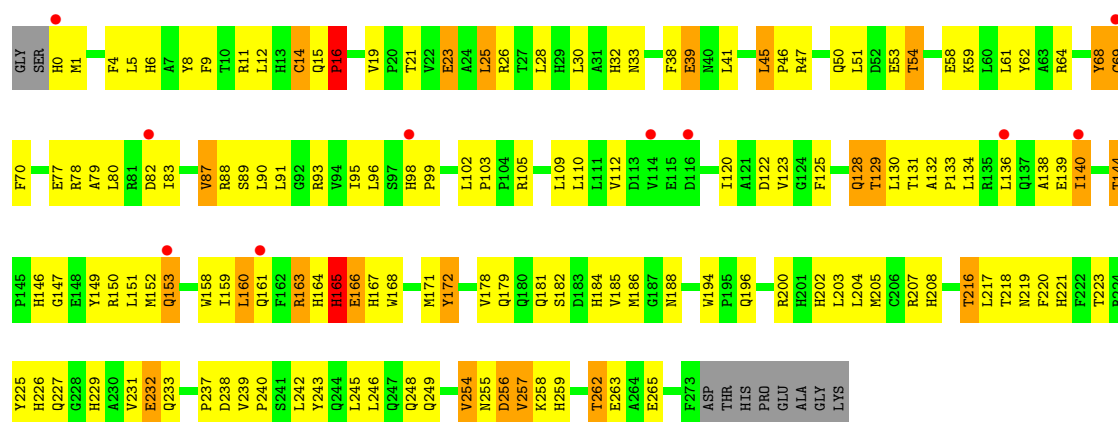
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



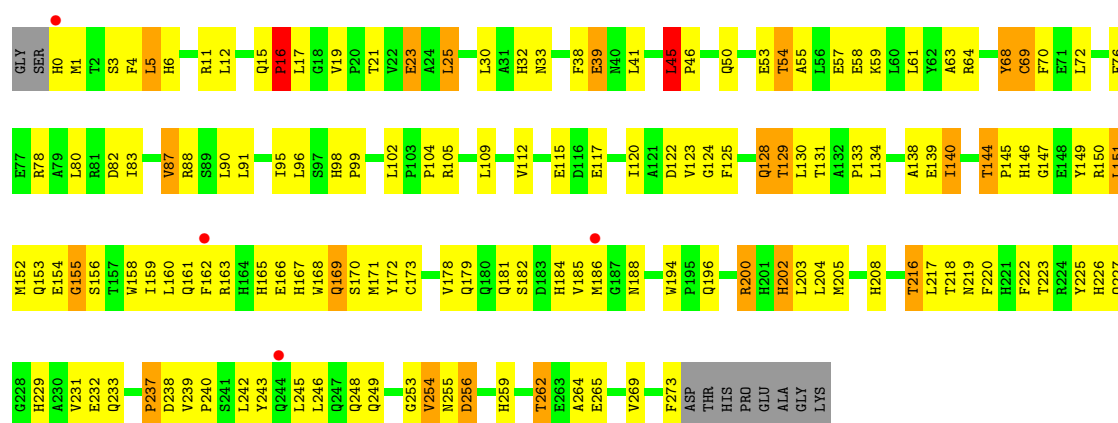
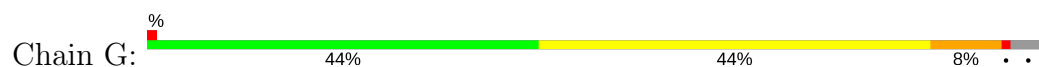
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



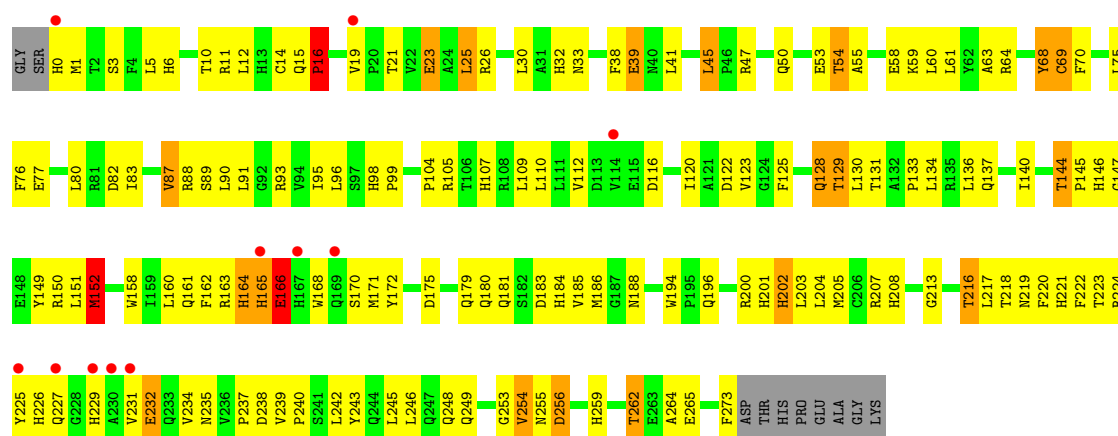
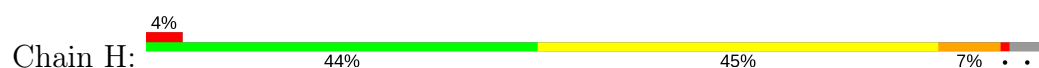
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 2 ₁ 2 ₁ 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 134.53Å 222.42Å 104.66Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.80 40.75 – 2.65 | Depositor EDS |
| % Data completeness (in resolution range) | 94.7 (30.00-2.80) 78.7 (40.75-2.65) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.06 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.93 (at 2.65Å) | Xtriage |
| Refinement program | CNS 0.5 | Depositor |
| R, R_{free} | 0.264 , 0.302 0.267 , 0.258 | Depositor DCC |
| R_{free} test set | 3338 reflections (5.05%) | DCC |
| Wilson B-factor (Å ²) | 59.0 | Xtriage |
| Anisotropy | 0.642 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 66.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 18260 | wwPDB-VP |
| Average B, all atoms (Å ²) | 78.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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 | 0.78 | 0/2290 | 0.87 | 2/3113 (0.1%) |
| 1 | B | 0.82 | 1/2290 (0.0%) | 0.91 | 2/3113 (0.1%) |
| 1 | C | 0.79 | 2/2290 (0.1%) | 0.90 | 2/3113 (0.1%) |
| 1 | D | 0.70 | 1/2290 (0.0%) | 0.85 | 1/3113 (0.0%) |
| 1 | E | 0.92 | 2/2290 (0.1%) | 0.94 | 2/3113 (0.1%) |
| 1 | F | 0.84 | 1/2290 (0.0%) | 0.88 | 2/3113 (0.1%) |
| 1 | G | 0.78 | 1/2290 (0.0%) | 0.88 | 2/3113 (0.1%) |
| 1 | H | 0.78 | 0/2290 | 0.89 | 2/3113 (0.1%) |
| All | All | 0.80 | 8/18320 (0.0%) | 0.89 | 15/24904 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | B | 0 | 1 |
| 1 | F | 0 | 1 |
| All | All | 0 | 2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | B | 14 | CYS | CB-SG | -8.15 | 1.68 | 1.82 |
| 1 | F | 14 | CYS | CB-SG | -7.24 | 1.70 | 1.82 |
| 1 | E | 14 | CYS | CB-SG | -6.82 | 1.70 | 1.82 |
| 1 | G | 173 | CYS | CB-SG | -6.71 | 1.70 | 1.82 |
| 1 | E | 69 | CYS | CB-SG | -5.71 | 1.72 | 1.81 |
| 1 | C | 158 | TRP | CB-CG | -5.54 | 1.40 | 1.50 |
| 1 | D | 14 | CYS | CB-SG | -5.18 | 1.73 | 1.81 |
| 1 | C | 14 | CYS | CB-SG | -5.10 | 1.73 | 1.81 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | E | 45 | LEU | N-CA-C | -8.12 | 89.08 | 111.00 |
| 1 | A | 45 | LEU | N-CA-C | -8.07 | 89.22 | 111.00 |
| 1 | B | 45 | LEU | N-CA-C | -7.72 | 90.14 | 111.00 |
| 1 | C | 45 | LEU | N-CA-C | -7.62 | 90.42 | 111.00 |
| 1 | B | 150 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 1 | G | 45 | LEU | N-CA-C | -7.60 | 90.47 | 111.00 |
| 1 | H | 45 | LEU | N-CA-C | -7.59 | 90.50 | 111.00 |
| 1 | F | 45 | LEU | N-CA-C | -7.55 | 90.61 | 111.00 |
| 1 | D | 45 | LEU | N-CA-C | -7.50 | 90.74 | 111.00 |
| 1 | G | 200 | ARG | NE-CZ-NH1 | -6.51 | 117.04 | 120.30 |
| 1 | F | 45 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 1 | H | 45 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 1 | E | 175 | ASP | CB-CG-OD2 | -5.18 | 113.64 | 118.30 |
| 1 | C | 65 | ARG | NE-CZ-NH1 | -5.09 | 117.76 | 120.30 |
| 1 | A | 203 | LEU | CB-CG-CD2 | -5.08 | 102.36 | 111.00 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 172 | TYR | Sidechain |
| 1 | F | 172 | TYR | Sidechain |

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 | 2224 | 0 | 2149 | 156 | 0 |
| 1 | B | 2224 | 0 | 2149 | 179 | 1 |
| 1 | C | 2224 | 0 | 2149 | 177 | 2 |
| 1 | D | 2224 | 0 | 2149 | 157 | 0 |
| 1 | E | 2224 | 0 | 2149 | 145 | 0 |
| 1 | F | 2224 | 0 | 2149 | 151 | 1 |
| 1 | G | 2224 | 0 | 2149 | 167 | 0 |
| 1 | H | 2224 | 0 | 2149 | 161 | 2 |
| 2 | A | 56 | 0 | 0 | 13 | 0 |
| 2 | B | 51 | 0 | 0 | 26 | 0 |
| 2 | C | 79 | 0 | 0 | 29 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | D | 36 | 0 | 0 | 18 | 0 |
| 2 | E | 92 | 0 | 0 | 19 | 0 |
| 2 | F | 48 | 0 | 0 | 13 | 0 |
| 2 | G | 56 | 0 | 0 | 19 | 0 |
| 2 | H | 50 | 0 | 0 | 13 | 0 |
| All | All | 18260 | 0 | 17192 | 1252 | 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 36.

All (1252) 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:F:46:PRO:HD2 | 2:F:2011:HOH:O | 1.24 | 1.34 |
| 1:F:186:MET:CE | 1:H:186:MET:HE3 | 1.63 | 1.27 |
| 1:F:186:MET:HE2 | 1:H:186:MET:CE | 1.70 | 1.20 |
| 1:B:186:MET:HE3 | 1:C:186:MET:CE | 1.79 | 1.11 |
| 1:B:186:MET:CE | 1:C:186:MET:HE3 | 1.80 | 1.10 |
| 1:B:166:GLU:HG2 | 1:G:233:GLN:HB2 | 1.40 | 1.04 |
| 1:A:186:MET:HE1 | 2:A:2034:HOH:O | 1.58 | 1.03 |
| 1:B:128:GLN:H | 1:B:128:GLN:HE21 | 1.03 | 1.01 |
| 1:D:128:GLN:HE21 | 1:D:128:GLN:H | 1.03 | 1.00 |
| 1:E:150:ARG:NH1 | 1:E:152:MET:SD | 2.35 | 0.99 |
| 1:A:128:GLN:HE21 | 1:A:128:GLN:H | 0.99 | 0.99 |
| 1:B:152:MET:HG3 | 1:B:153:GLN:H | 1.26 | 0.98 |
| 1:C:128:GLN:HE21 | 1:C:128:GLN:H | 0.97 | 0.96 |
| 1:G:128:GLN:H | 1:G:128:GLN:HE21 | 1.10 | 0.94 |
| 1:F:128:GLN:HE21 | 1:F:128:GLN:H | 1.07 | 0.94 |
| 1:E:128:GLN:H | 1:E:128:GLN:HE21 | 0.95 | 0.94 |
| 1:A:224:ARG:HD3 | 2:A:2044:HOH:O | 1.66 | 0.93 |
| 1:H:128:GLN:N | 1:H:128:GLN:HE21 | 1.69 | 0.91 |
| 1:E:216:THR:HG22 | 2:E:2076:HOH:O | 1.71 | 0.91 |
| 1:B:25:LEU:HD22 | 1:B:133:PRO:HG3 | 1.53 | 0.90 |
| 1:C:104:PRO:HB2 | 2:C:2032:HOH:O | 1.69 | 0.90 |
| 1:F:25:LEU:HD22 | 1:F:133:PRO:HG3 | 1.52 | 0.90 |
| 1:H:128:GLN:HE21 | 1:H:128:GLN:H | 0.95 | 0.89 |
| 1:E:128:GLN:H | 1:E:128:GLN:NE2 | 1.69 | 0.88 |
| 1:B:166:GLU:CG | 1:G:233:GLN:HB2 | 2.04 | 0.88 |
| 1:C:161:GLN:HG2 | 1:C:170:SER:HA | 1.56 | 0.88 |
| 1:H:25:LEU:HD22 | 1:H:133:PRO:HG3 | 1.56 | 0.88 |
| 1:B:161:GLN:HG2 | 1:B:170:SER:HA | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:25:LEU:HD22 | 1:E:133:PRO:HG3 | 1.57 | 0.87 |
| 1:E:128:GLN:HE21 | 1:E:128:GLN:N | 1.71 | 0.87 |
| 1:A:128:GLN:N | 1:A:128:GLN:HE21 | 1.73 | 0.86 |
| 1:C:128:GLN:HE21 | 1:C:128:GLN:N | 1.73 | 0.86 |
| 1:F:144:THR:HG23 | 1:F:146:HIS:H | 1.40 | 0.86 |
| 1:E:165:HIS:HB2 | 2:E:2057:HOH:O | 1.76 | 0.85 |
| 1:F:58:GLU:HB3 | 2:F:2014:HOH:O | 1.75 | 0.85 |
| 1:E:144:THR:HG23 | 1:E:146:HIS:H | 1.42 | 0.85 |
| 1:H:144:THR:HG23 | 1:H:146:HIS:H | 1.39 | 0.84 |
| 1:G:144:THR:HG23 | 1:G:146:HIS:H | 1.43 | 0.84 |
| 1:B:144:THR:HG23 | 1:B:146:HIS:H | 1.42 | 0.84 |
| 1:F:255:ASN:O | 1:F:256:ASP:HB2 | 1.77 | 0.84 |
| 1:C:144:THR:HG23 | 1:C:146:HIS:H | 1.43 | 0.83 |
| 1:H:128:GLN:NE2 | 1:H:128:GLN:H | 1.74 | 0.83 |
| 1:B:164:HIS:O | 1:B:166:GLU:N | 2.11 | 0.82 |
| 1:G:273:PHE:HE2 | 2:G:2044:HOH:O | 1.62 | 0.82 |
| 1:G:239:VAL:HG23 | 2:G:2049:HOH:O | 1.79 | 0.82 |
| 1:D:144:THR:HG23 | 1:D:146:HIS:H | 1.44 | 0.82 |
| 1:B:186:MET:HE3 | 1:C:186:MET:HE3 | 0.90 | 0.81 |
| 1:C:128:GLN:NE2 | 1:C:128:GLN:H | 1.76 | 0.81 |
| 1:H:161:GLN:HG2 | 1:H:170:SER:HA | 1.62 | 0.81 |
| 1:D:128:GLN:HE21 | 1:D:128:GLN:N | 1.78 | 0.81 |
| 1:A:128:GLN:NE2 | 1:A:128:GLN:H | 1.79 | 0.80 |
| 1:C:138:ALA:HA | 1:C:151:LEU:O | 1.80 | 0.80 |
| 1:B:255:ASN:O | 1:B:256:ASP:HB2 | 1.81 | 0.80 |
| 1:A:252:LEU:HD13 | 2:A:2008:HOH:O | 1.80 | 0.80 |
| 1:E:186:MET:HE3 | 1:G:186:MET:HE2 | 1.63 | 0.80 |
| 1:H:144:THR:HG21 | 2:H:2026:HOH:O | 1.82 | 0.80 |
| 1:G:163:ARG:NE | 1:G:166:GLU:O | 2.14 | 0.80 |
| 1:G:150:ARG:HB2 | 1:G:168:TRP:CZ2 | 2.17 | 0.80 |
| 1:A:144:THR:HG23 | 1:A:146:HIS:H | 1.47 | 0.79 |
| 1:E:163:ARG:HG3 | 2:E:2053:HOH:O | 1.80 | 0.79 |
| 1:F:265:GLU:HB3 | 2:F:2046:HOH:O | 1.82 | 0.79 |
| 1:A:25:LEU:HD22 | 1:A:133:PRO:HG3 | 1.64 | 0.79 |
| 1:C:16:PRO:HD3 | 2:C:2004:HOH:O | 1.83 | 0.79 |
| 1:B:165:HIS:O | 1:B:166:GLU:HB2 | 1.81 | 0.79 |
| 1:D:180:GLN:HG2 | 2:D:2022:HOH:O | 1.82 | 0.79 |
| 1:B:128:GLN:HE21 | 1:B:128:GLN:N | 1.79 | 0.79 |
| 1:B:221:HIS:HB2 | 2:B:2040:HOH:O | 1.83 | 0.79 |
| 1:E:160:LEU:HG | 1:E:171:MET:HE3 | 1.63 | 0.79 |
| 1:B:96:LEU:HD23 | 1:B:171:MET:HA | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:255:ASN:O | 1:G:256:ASP:HB2 | 1.82 | 0.78 |
| 1:C:25:LEU:HD22 | 1:C:133:PRO:HG3 | 1.64 | 0.78 |
| 1:B:255:ASN:HB3 | 2:B:2045:HOH:O | 1.83 | 0.78 |
| 1:G:25:LEU:HD22 | 1:G:133:PRO:HG3 | 1.65 | 0.78 |
| 1:C:255:ASN:O | 1:C:256:ASP:HB2 | 1.84 | 0.77 |
| 1:G:150:ARG:NE | 1:G:152:MET:HG2 | 1.99 | 0.77 |
| 1:B:128:GLN:H | 1:B:128:GLN:NE2 | 1.81 | 0.77 |
| 1:G:128:GLN:N | 1:G:128:GLN:HE21 | 1.83 | 0.76 |
| 1:A:196:GLN:HG2 | 2:A:2037:HOH:O | 1.85 | 0.76 |
| 1:F:128:GLN:N | 1:F:128:GLN:HE21 | 1.81 | 0.76 |
| 1:A:95:ILE:HG12 | 1:A:172:TYR:HA | 1.65 | 0.76 |
| 1:E:102:LEU:HG | 2:E:2037:HOH:O | 1.84 | 0.76 |
| 1:C:33:ASN:O | 1:C:208:HIS:HB2 | 1.86 | 0.76 |
| 1:C:186:MET:HE2 | 2:C:2048:HOH:O | 1.87 | 0.75 |
| 1:D:128:GLN:NE2 | 1:D:128:GLN:H | 1.80 | 0.75 |
| 1:E:159:ILE:N | 1:E:159:ILE:HD12 | 2.01 | 0.75 |
| 1:E:161:GLN:HB3 | 1:E:170:SER:HA | 1.66 | 0.75 |
| 1:C:95:ILE:HG12 | 1:C:172:TYR:HA | 1.68 | 0.75 |
| 1:D:25:LEU:HD22 | 1:D:133:PRO:HG3 | 1.67 | 0.74 |
| 1:G:91:LEU:HD21 | 1:G:184:HIS:HD2 | 1.52 | 0.74 |
| 1:F:164:HIS:O | 1:F:165:HIS:HB3 | 1.87 | 0.74 |
| 1:G:226:HIS:CE1 | 1:G:227:GLN:HE21 | 2.05 | 0.74 |
| 1:A:255:ASN:O | 1:A:256:ASP:HB2 | 1.88 | 0.74 |
| 1:H:136:LEU:HD23 | 1:H:151:LEU:HD13 | 1.70 | 0.73 |
| 1:A:231:VAL:O | 1:A:232:GLU:HB3 | 1.88 | 0.73 |
| 1:G:115:GLU:HG3 | 2:G:2029:HOH:O | 1.89 | 0.73 |
| 1:C:194:TRP:CZ3 | 1:C:196:GLN:HB2 | 2.24 | 0.73 |
| 1:G:231:VAL:O | 1:G:232:GLU:HB3 | 1.88 | 0.73 |
| 1:D:158:TRP:HB2 | 1:D:174:PHE:CE1 | 2.23 | 0.73 |
| 1:E:242:LEU:HG | 2:E:2083:HOH:O | 1.89 | 0.73 |
| 1:C:11:ARG:HD2 | 1:C:61:LEU:HA | 1.70 | 0.73 |
| 1:D:109:LEU:HD21 | 1:D:174:PHE:CD2 | 2.23 | 0.73 |
| 1:F:128:GLN:NE2 | 1:F:128:GLN:H | 1.85 | 0.73 |
| 1:B:33:ASN:O | 1:B:208:HIS:HB2 | 1.89 | 0.72 |
| 1:B:46:PRO:HD2 | 2:D:2027:HOH:O | 1.88 | 0.72 |
| 1:C:152:MET:O | 1:C:159:ILE:HG22 | 1.89 | 0.72 |
| 1:B:94:VAL:HG12 | 2:B:2015:HOH:O | 1.88 | 0.72 |
| 1:E:136:LEU:HD22 | 1:E:158:TRP:CZ2 | 2.24 | 0.72 |
| 1:B:194:TRP:CZ3 | 1:B:196:GLN:HB2 | 2.25 | 0.72 |
| 1:E:226:HIS:CE1 | 1:E:227:GLN:HE21 | 2.07 | 0.72 |
| 1:G:217:LEU:HD11 | 1:G:219:ASN:O | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:130:LEU:HD12 | 2:C:2037:HOH:O | 1.89 | 0.71 |
| 1:D:239:VAL:HB | 1:D:240:PRO:HD3 | 1.72 | 0.71 |
| 1:H:255:ASN:O | 1:H:256:ASP:HB2 | 1.90 | 0.71 |
| 1:F:194:TRP:CZ3 | 1:F:196:GLN:HB2 | 2.25 | 0.71 |
| 1:H:63:ALA:HB1 | 2:H:2045:HOH:O | 1.89 | 0.71 |
| 1:A:104:PRO:HD3 | 1:D:182:SER:HB2 | 1.71 | 0.71 |
| 1:E:144:THR:HG22 | 1:E:147:GLY:N | 2.06 | 0.70 |
| 1:H:144:THR:HG22 | 1:H:147:GLY:H | 1.55 | 0.70 |
| 1:A:226:HIS:CE1 | 1:A:227:GLN:HE21 | 2.10 | 0.70 |
| 1:D:162:PHE:CE1 | 1:D:169:GLN:HB2 | 2.27 | 0.70 |
| 1:D:55:ALA:HA | 2:D:2008:HOH:O | 1.90 | 0.70 |
| 1:B:131:THR:HB | 2:B:2027:HOH:O | 1.91 | 0.70 |
| 1:G:163:ARG:NH2 | 1:G:167:HIS:HA | 2.05 | 0.70 |
| 1:C:237:PRO:HA | 2:C:2068:HOH:O | 1.90 | 0.70 |
| 1:A:186:MET:HE3 | 1:D:186:MET:HE2 | 1.74 | 0.70 |
| 1:F:133:PRO:O | 1:F:134:LEU:HD23 | 1.91 | 0.69 |
| 1:D:255:ASN:O | 1:D:256:ASP:HB2 | 1.90 | 0.69 |
| 1:F:45:LEU:CA | 2:F:2011:HOH:O | 2.39 | 0.69 |
| 1:C:122:ASP:N | 2:C:2037:HOH:O | 2.25 | 0.69 |
| 1:D:11:ARG:HD2 | 1:D:61:LEU:HA | 1.73 | 0.69 |
| 1:F:11:ARG:HD2 | 1:F:61:LEU:HA | 1.73 | 0.69 |
| 1:H:11:ARG:HD2 | 1:H:61:LEU:HA | 1.75 | 0.69 |
| 1:C:164:HIS:CG | 1:C:165:HIS:H | 2.09 | 0.69 |
| 1:F:255:ASN:O | 1:F:256:ASP:CB | 2.40 | 0.69 |
| 2:A:2017:HOH:O | 1:C:46:PRO:HG3 | 1.90 | 0.69 |
| 1:G:11:ARG:HD2 | 1:G:61:LEU:HA | 1.74 | 0.69 |
| 2:E:2039:HOH:O | 1:G:186:MET:HE1 | 1.91 | 0.69 |
| 1:G:239:VAL:HB | 1:G:240:PRO:HD3 | 1.75 | 0.69 |
| 1:A:152:MET:HG3 | 1:A:153:GLN:H | 1.58 | 0.69 |
| 1:B:152:MET:CG | 1:B:153:GLN:H | 2.05 | 0.69 |
| 1:F:109:LEU:HD12 | 1:F:109:LEU:C | 2.14 | 0.69 |
| 1:F:25:LEU:HD22 | 1:F:133:PRO:CG | 2.22 | 0.68 |
| 1:D:91:LEU:HD21 | 1:D:184:HIS:HD2 | 1.59 | 0.68 |
| 1:E:194:TRP:CZ3 | 1:E:196:GLN:HB2 | 2.28 | 0.68 |
| 1:H:39:GLU:OE2 | 2:H:2007:HOH:O | 2.10 | 0.68 |
| 1:D:150:ARG:HD3 | 1:D:161:GLN:NE2 | 2.08 | 0.68 |
| 1:D:69:CYS:SG | 2:D:2004:HOH:O | 2.51 | 0.68 |
| 1:G:217:LEU:HD21 | 1:G:242:LEU:HD11 | 1.75 | 0.68 |
| 1:C:239:VAL:HB | 1:C:240:PRO:HD3 | 1.75 | 0.68 |
| 1:F:144:THR:HG22 | 1:F:147:GLY:H | 1.59 | 0.68 |
| 1:H:217:LEU:HD11 | 1:H:219:ASN:O | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:194:TRP:CD2 | 2:B:2036:HOH:O | 2.46 | 0.68 |
| 1:E:144:THR:HG22 | 1:E:147:GLY:H | 1.58 | 0.68 |
| 1:G:128:GLN:H | 1:G:128:GLN:NE2 | 1.86 | 0.68 |
| 1:C:217:LEU:HD11 | 1:C:219:ASN:O | 1.94 | 0.67 |
| 1:C:47:ARG:HD2 | 2:C:2012:HOH:O | 1.93 | 0.67 |
| 1:F:33:ASN:O | 1:F:208:HIS:HB2 | 1.94 | 0.67 |
| 1:F:128:GLN:HB2 | 1:F:171:MET:CE | 2.24 | 0.67 |
| 1:F:216:THR:HG22 | 1:F:216:THR:O | 1.95 | 0.67 |
| 1:A:138:ALA:HA | 1:A:151:LEU:O | 1.95 | 0.67 |
| 1:H:150:ARG:HB2 | 1:H:168:TRP:CH2 | 2.30 | 0.67 |
| 1:B:144:THR:HG22 | 1:B:147:GLY:H | 1.57 | 0.67 |
| 1:E:223:THR:OG1 | 2:E:2077:HOH:O | 2.13 | 0.67 |
| 1:B:39:GLU:HG2 | 1:B:41:LEU:H | 1.59 | 0.67 |
| 1:F:91:LEU:HD21 | 1:F:184:HIS:HD2 | 1.58 | 0.67 |
| 1:D:226:HIS:CE1 | 1:D:227:GLN:HE21 | 2.13 | 0.67 |
| 1:F:122:ASP:O | 1:F:129:THR:HG22 | 1.94 | 0.67 |
| 1:F:159:ILE:HG22 | 1:F:160:LEU:N | 2.10 | 0.67 |
| 1:F:152:MET:HG2 | 1:F:161:GLN:HE22 | 1.60 | 0.67 |
| 1:A:11:ARG:HD2 | 1:A:61:LEU:HA | 1.77 | 0.67 |
| 1:E:181:GLN:O | 1:E:185:VAL:HG23 | 1.95 | 0.66 |
| 1:H:164:HIS:O | 1:H:166:GLU:N | 2.27 | 0.66 |
| 1:D:33:ASN:O | 1:D:208:HIS:HB2 | 1.95 | 0.66 |
| 1:H:175:ASP:N | 1:H:175:ASP:OD1 | 2.28 | 0.66 |
| 1:H:226:HIS:CE1 | 1:H:227:GLN:HE21 | 2.13 | 0.66 |
| 1:H:144:THR:HG22 | 1:H:147:GLY:N | 2.09 | 0.66 |
| 1:A:217:LEU:HD21 | 1:A:242:LEU:HD11 | 1.76 | 0.66 |
| 1:B:152:MET:HG3 | 1:B:153:GLN:N | 2.05 | 0.66 |
| 1:F:19:VAL:HG12 | 1:F:21:THR:HG23 | 1.78 | 0.66 |
| 1:B:159:ILE:HG22 | 1:B:160:LEU:H | 1.60 | 0.66 |
| 1:F:68:TYR:O | 1:F:69:CYS:C | 2.31 | 0.66 |
| 1:C:217:LEU:HD21 | 1:C:242:LEU:HD11 | 1.77 | 0.66 |
| 1:D:231:VAL:O | 1:D:232:GLU:HB3 | 1.96 | 0.66 |
| 1:E:186:MET:HE2 | 1:G:186:MET:HE3 | 1.78 | 0.66 |
| 1:E:231:VAL:O | 1:E:232:GLU:HB3 | 1.94 | 0.66 |
| 1:G:138:ALA:HA | 1:G:151:LEU:O | 1.94 | 0.66 |
| 1:H:162:PHE:HD2 | 1:H:171:MET:SD | 2.18 | 0.66 |
| 1:B:186:MET:CE | 1:C:186:MET:CE | 2.54 | 0.66 |
| 1:C:211:ASP:HB3 | 2:C:2063:HOH:O | 1.94 | 0.66 |
| 1:C:249:GLN:HA | 2:C:2070:HOH:O | 1.95 | 0.66 |
| 1:B:11:ARG:HD2 | 1:B:61:LEU:HA | 1.76 | 0.66 |
| 1:E:255:ASN:O | 1:E:256:ASP:HB2 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:138:ALA:HA | 1:E:151:LEU:O | 1.96 | 0.66 |
| 1:E:217:LEU:HD11 | 1:E:219:ASN:O | 1.96 | 0.66 |
| 1:C:160:LEU:HG | 1:C:171:MET:CE | 2.27 | 0.65 |
| 1:A:194:TRP:CZ3 | 1:A:196:GLN:HB2 | 2.32 | 0.65 |
| 1:C:122:ASP:O | 1:C:129:THR:HG22 | 1.97 | 0.65 |
| 1:B:96:LEU:CD2 | 1:B:171:MET:HA | 2.26 | 0.65 |
| 1:A:136:LEU:HD22 | 1:A:158:TRP:CZ2 | 2.31 | 0.65 |
| 1:C:144:THR:HG22 | 1:C:147:GLY:H | 1.61 | 0.65 |
| 1:D:162:PHE:HE1 | 1:D:169:GLN:HB2 | 1.61 | 0.65 |
| 1:D:216:THR:HG22 | 2:D:2031:HOH:O | 1.96 | 0.65 |
| 1:G:144:THR:HG22 | 1:G:147:GLY:H | 1.61 | 0.65 |
| 1:C:109:LEU:C | 1:C:109:LEU:HD12 | 2.17 | 0.65 |
| 1:H:47:ARG:HG2 | 2:H:2010:HOH:O | 1.97 | 0.65 |
| 1:D:144:THR:HG22 | 1:D:147:GLY:H | 1.62 | 0.65 |
| 1:F:120:ILE:HG13 | 1:F:120:ILE:O | 1.95 | 0.65 |
| 1:F:144:THR:HG22 | 1:F:147:GLY:N | 2.12 | 0.65 |
| 1:B:256:ASP:N | 2:B:2045:HOH:O | 2.30 | 0.65 |
| 1:F:45:LEU:HA | 2:F:2011:HOH:O | 1.97 | 0.65 |
| 1:G:151:LEU:HD22 | 1:G:159:ILE:O | 1.96 | 0.65 |
| 1:B:139:GLU:HA | 1:B:150:ARG:HH21 | 1.63 | 0.64 |
| 1:H:239:VAL:HB | 1:H:240:PRO:HD3 | 1.79 | 0.64 |
| 1:A:239:VAL:HB | 1:A:240:PRO:HD3 | 1.78 | 0.64 |
| 1:B:25:LEU:HD22 | 1:B:133:PRO:CG | 2.25 | 0.64 |
| 1:B:217:LEU:HD21 | 1:B:242:LEU:HD11 | 1.79 | 0.64 |
| 1:E:109:LEU:HD12 | 1:E:109:LEU:C | 2.17 | 0.64 |
| 1:F:231:VAL:O | 1:F:232:GLU:HB3 | 1.95 | 0.64 |
| 1:G:203:LEU:N | 2:G:2044:HOH:O | 2.29 | 0.64 |
| 1:F:128:GLN:HB2 | 1:F:171:MET:HE1 | 1.79 | 0.64 |
| 1:H:216:THR:HG22 | 1:H:216:THR:O | 1.97 | 0.64 |
| 1:A:91:LEU:HB3 | 1:A:105:ARG:HB3 | 1.80 | 0.64 |
| 1:C:226:HIS:CE1 | 1:C:227:GLN:HE21 | 2.15 | 0.64 |
| 1:H:130:LEU:HA | 2:H:2026:HOH:O | 1.98 | 0.64 |
| 1:G:150:ARG:CD | 1:G:152:MET:HG2 | 2.28 | 0.64 |
| 1:B:144:THR:HG22 | 1:B:147:GLY:N | 2.13 | 0.64 |
| 1:C:163:ARG:HH11 | 1:C:167:HIS:HA | 1.63 | 0.64 |
| 1:E:198:HIS:HB2 | 2:E:2067:HOH:O | 1.96 | 0.64 |
| 1:B:109:LEU:HD12 | 1:B:109:LEU:C | 2.17 | 0.64 |
| 1:B:167:HIS:O | 1:B:168:TRP:HB2 | 1.98 | 0.64 |
| 1:G:154:GLU:O | 1:G:155:GLY:C | 2.36 | 0.64 |
| 1:H:150:ARG:NH2 | 1:H:168:TRP:NE1 | 2.45 | 0.64 |
| 1:H:95:ILE:HG12 | 1:H:172:TYR:HA | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:ARG:HD2 | 1:C:168:TRP:CD2 | 2.33 | 0.63 |
| 1:E:11:ARG:HD2 | 1:E:61:LEU:HA | 1.80 | 0.63 |
| 1:G:194:TRP:CZ3 | 1:G:196:GLN:HB2 | 2.33 | 0.63 |
| 1:E:160:LEU:HG | 1:E:171:MET:CE | 2.29 | 0.63 |
| 1:F:0:HIS:ND1 | 1:F:1:MET:N | 2.47 | 0.63 |
| 1:A:109:LEU:C | 1:A:109:LEU:HD12 | 2.18 | 0.63 |
| 1:B:226:HIS:CE1 | 1:B:227:GLN:HE21 | 2.17 | 0.63 |
| 1:D:217:LEU:HD21 | 1:D:242:LEU:HD11 | 1.79 | 0.63 |
| 1:F:186:MET:HE2 | 1:H:186:MET:HE3 | 0.75 | 0.63 |
| 1:F:91:LEU:HD21 | 1:F:184:HIS:CD2 | 2.33 | 0.63 |
| 1:C:122:ASP:HB3 | 2:C:2037:HOH:O | 1.98 | 0.63 |
| 1:C:39:GLU:HG2 | 1:C:41:LEU:H | 1.64 | 0.63 |
| 1:G:144:THR:HG22 | 1:G:147:GLY:N | 2.13 | 0.63 |
| 1:G:91:LEU:HD21 | 1:G:184:HIS:CD2 | 2.32 | 0.63 |
| 1:H:194:TRP:CZ3 | 1:H:196:GLN:HB2 | 2.34 | 0.63 |
| 1:B:54:THR:O | 1:B:58:GLU:HG3 | 1.98 | 0.63 |
| 1:C:91:LEU:HB3 | 1:C:105:ARG:HB3 | 1.80 | 0.63 |
| 1:G:39:GLU:HG2 | 1:G:41:LEU:H | 1.63 | 0.63 |
| 1:A:90:LEU:HD12 | 1:A:109:LEU:HD11 | 1.80 | 0.63 |
| 1:C:144:THR:HG22 | 1:C:147:GLY:N | 2.14 | 0.63 |
| 1:G:0:HIS:ND1 | 1:G:1:MET:N | 2.47 | 0.63 |
| 1:H:25:LEU:HD22 | 1:H:133:PRO:CG | 2.28 | 0.63 |
| 1:B:122:ASP:O | 1:B:129:THR:HG22 | 1.99 | 0.63 |
| 1:H:149:TYR:CD2 | 1:H:162:PHE:HB3 | 2.34 | 0.63 |
| 1:D:181:GLN:O | 1:D:185:VAL:HG23 | 1.99 | 0.62 |
| 1:E:200:ARG:HH12 | 1:H:200:ARG:HH12 | 1.45 | 0.62 |
| 1:D:150:ARG:HB2 | 1:D:168:TRP:CH2 | 2.35 | 0.62 |
| 1:F:226:HIS:CE1 | 1:F:227:GLN:HE21 | 2.17 | 0.62 |
| 1:G:109:LEU:HD12 | 1:G:109:LEU:C | 2.19 | 0.62 |
| 1:G:150:ARG:HB2 | 1:G:168:TRP:CH2 | 2.34 | 0.62 |
| 1:F:39:GLU:HG2 | 1:F:41:LEU:H | 1.62 | 0.62 |
| 1:F:186:MET:CE | 1:H:186:MET:CE | 2.47 | 0.62 |
| 1:G:33:ASN:O | 1:G:208:HIS:HB2 | 1.98 | 0.62 |
| 1:H:231:VAL:O | 1:H:232:GLU:HB3 | 1.98 | 0.62 |
| 1:A:122:ASP:O | 1:A:129:THR:HG22 | 2.00 | 0.62 |
| 1:A:245:LEU:HD12 | 1:A:249:GLN:HB2 | 1.81 | 0.62 |
| 1:B:133:PRO:O | 1:B:134:LEU:HD23 | 1.99 | 0.62 |
| 1:H:125:PHE:H | 1:H:129:THR:HG23 | 1.65 | 0.62 |
| 1:C:125:PHE:H | 1:C:129:THR:HG23 | 1.62 | 0.62 |
| 1:C:153:GLN:O | 1:C:154:GLU:HG3 | 2.00 | 0.62 |
| 1:D:144:THR:HG22 | 1:D:147:GLY:N | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:120:ILE:O | 1:E:120:ILE:HG13 | 1.98 | 0.62 |
| 1:E:239:VAL:HB | 1:E:240:PRO:HD3 | 1.82 | 0.62 |
| 1:E:182:SER:HB2 | 1:G:104:PRO:HD3 | 1.81 | 0.62 |
| 1:A:161:GLN:HA | 1:A:169:GLN:O | 1.99 | 0.61 |
| 1:B:182:SER:HB2 | 1:C:104:PRO:HD3 | 1.81 | 0.61 |
| 1:F:217:LEU:HD11 | 1:F:219:ASN:O | 1.99 | 0.61 |
| 1:F:217:LEU:HD21 | 1:F:242:LEU:HD11 | 1.82 | 0.61 |
| 1:G:153:GLN:HB2 | 1:G:158:TRP:CE3 | 2.35 | 0.61 |
| 1:B:90:LEU:HD12 | 1:B:109:LEU:HD11 | 1.83 | 0.61 |
| 1:A:205:MET:SD | 1:A:246:LEU:HD22 | 2.41 | 0.61 |
| 1:D:87:VAL:CG1 | 1:D:112:VAL:HG22 | 2.30 | 0.61 |
| 1:G:165:HIS:O | 1:G:166:GLU:HB2 | 2.00 | 0.61 |
| 1:C:23:GLU:OE1 | 1:C:23:GLU:HA | 2.00 | 0.61 |
| 1:F:152:MET:HG2 | 1:F:161:GLN:NE2 | 2.15 | 0.61 |
| 1:F:186:MET:HE3 | 2:H:2022:HOH:O | 1.99 | 0.61 |
| 1:G:163:ARG:HH21 | 1:G:167:HIS:HA | 1.63 | 0.61 |
| 1:G:255:ASN:O | 1:G:256:ASP:CB | 2.48 | 0.61 |
| 1:C:138:ALA:CA | 1:C:151:LEU:O | 2.49 | 0.61 |
| 1:E:246:LEU:HD11 | 2:E:2083:HOH:O | 2.01 | 0.61 |
| 1:G:122:ASP:O | 1:G:129:THR:HG22 | 2.01 | 0.61 |
| 1:E:186:MET:CE | 1:G:186:MET:CE | 2.79 | 0.61 |
| 1:H:120:ILE:O | 1:H:120:ILE:HG13 | 2.00 | 0.61 |
| 1:C:128:GLN:NE2 | 1:C:128:GLN:N | 2.44 | 0.61 |
| 1:C:91:LEU:HD21 | 1:C:184:HIS:HD2 | 1.66 | 0.61 |
| 1:E:186:MET:CE | 1:G:186:MET:HE2 | 2.30 | 0.61 |
| 1:H:23:GLU:OE1 | 1:H:23:GLU:HA | 2.01 | 0.61 |
| 1:C:87:VAL:CG1 | 1:C:112:VAL:HG22 | 2.31 | 0.60 |
| 1:C:137:GLN:O | 1:C:151:LEU:HB2 | 2.00 | 0.60 |
| 1:D:109:LEU:HD12 | 1:D:109:LEU:C | 2.21 | 0.60 |
| 1:G:128:GLN:HB2 | 1:G:171:MET:HE1 | 1.83 | 0.60 |
| 1:B:145:PRO:HB2 | 2:B:2027:HOH:O | 2.00 | 0.60 |
| 1:B:161:GLN:HG2 | 1:B:170:SER:CA | 2.30 | 0.60 |
| 1:E:128:GLN:NE2 | 1:E:128:GLN:N | 2.39 | 0.60 |
| 1:A:144:THR:HG22 | 1:A:147:GLY:N | 2.17 | 0.60 |
| 1:D:194:TRP:CZ3 | 1:D:196:GLN:HB2 | 2.36 | 0.60 |
| 1:G:150:ARG:HE | 1:G:161:GLN:NE2 | 1.99 | 0.60 |
| 1:C:87:VAL:HG12 | 1:C:112:VAL:HG22 | 1.82 | 0.60 |
| 1:H:19:VAL:HG12 | 1:H:21:THR:HG23 | 1.82 | 0.60 |
| 1:C:176:LEU:HD13 | 2:C:2043:HOH:O | 1.99 | 0.60 |
| 1:D:91:LEU:HD21 | 1:D:184:HIS:CD2 | 2.37 | 0.60 |
| 1:G:68:TYR:O | 1:G:69:CYS:C | 2.39 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:150:ARG:NH2 | 1:B:152:MET:SD | 2.66 | 0.60 |
| 1:E:158:TRP:C | 1:E:159:ILE:HD12 | 2.21 | 0.60 |
| 1:E:262:THR:HG23 | 1:E:265:GLU:OE1 | 2.02 | 0.60 |
| 1:G:91:LEU:HB3 | 1:G:105:ARG:HB3 | 1.83 | 0.60 |
| 1:G:245:LEU:HD12 | 1:G:249:GLN:HB2 | 1.83 | 0.60 |
| 1:B:216:THR:O | 1:B:216:THR:HG22 | 2.00 | 0.60 |
| 1:B:22:VAL:HB | 2:B:2022:HOH:O | 2.00 | 0.60 |
| 1:D:128:GLN:HB2 | 1:D:171:MET:CE | 2.31 | 0.60 |
| 1:B:232:GLU:HA | 1:F:233:GLN:O | 2.02 | 0.60 |
| 1:G:237:PRO:HG2 | 1:G:238:ASP:OD1 | 2.02 | 0.60 |
| 1:A:237:PRO:HG2 | 1:A:238:ASP:OD1 | 2.02 | 0.60 |
| 1:D:205:MET:SD | 1:D:246:LEU:HD22 | 2.42 | 0.60 |
| 1:C:160:LEU:HG | 1:C:171:MET:HE1 | 1.84 | 0.60 |
| 1:F:125:PHE:H | 1:F:129:THR:HG23 | 1.66 | 0.60 |
| 1:E:39:GLU:HG2 | 1:E:41:LEU:H | 1.66 | 0.59 |
| 1:A:133:PRO:O | 1:A:134:LEU:HD23 | 2.02 | 0.59 |
| 1:B:239:VAL:HB | 1:B:240:PRO:HD3 | 1.84 | 0.59 |
| 1:D:217:LEU:HD11 | 1:D:219:ASN:O | 2.02 | 0.59 |
| 1:D:19:VAL:HG12 | 1:D:21:THR:HG23 | 1.83 | 0.59 |
| 1:B:5:LEU:HD22 | 1:B:82:ASP:HB3 | 1.84 | 0.59 |
| 1:C:231:VAL:O | 1:C:232:GLU:HB3 | 2.02 | 0.59 |
| 1:D:54:THR:O | 1:D:58:GLU:HG3 | 2.01 | 0.59 |
| 1:D:87:VAL:HG12 | 1:D:112:VAL:HG22 | 1.82 | 0.59 |
| 1:F:159:ILE:HG22 | 1:F:160:LEU:H | 1.68 | 0.59 |
| 1:A:216:THR:HG22 | 1:A:216:THR:O | 2.01 | 0.59 |
| 1:A:14:CYS:SG | 1:A:15:GLN:N | 2.74 | 0.59 |
| 1:B:0:HIS:ND1 | 1:B:1:MET:N | 2.50 | 0.59 |
| 1:H:128:GLN:N | 1:H:128:GLN:NE2 | 2.41 | 0.59 |
| 1:B:91:LEU:HB3 | 1:B:105:ARG:HB3 | 1.85 | 0.59 |
| 1:E:91:LEU:HD21 | 1:E:184:HIS:HD2 | 1.68 | 0.59 |
| 1:A:144:THR:HG22 | 1:A:147:GLY:H | 1.67 | 0.59 |
| 1:B:120:ILE:O | 1:B:120:ILE:HG13 | 2.02 | 0.59 |
| 1:B:91:LEU:HD21 | 1:B:184:HIS:HD2 | 1.68 | 0.59 |
| 1:E:98:HIS:N | 1:E:99:PRO:HD3 | 2.18 | 0.59 |
| 1:H:5:LEU:HD22 | 1:H:82:ASP:HB3 | 1.85 | 0.59 |
| 1:A:162:PHE:CE1 | 1:A:169:GLN:HB3 | 2.38 | 0.59 |
| 1:C:0:HIS:ND1 | 1:C:1:MET:N | 2.51 | 0.59 |
| 1:G:5:LEU:HD22 | 1:G:82:ASP:HB3 | 1.84 | 0.59 |
| 1:B:231:VAL:O | 1:B:232:GLU:HB3 | 2.03 | 0.58 |
| 1:A:217:LEU:HD11 | 1:A:219:ASN:O | 2.01 | 0.58 |
| 1:B:159:ILE:HG22 | 1:B:160:LEU:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:120:ILE:HG13 | 1:C:120:ILE:O | 2.03 | 0.58 |
| 1:E:136:LEU:HD22 | 1:E:158:TRP:CE2 | 2.39 | 0.58 |
| 1:D:23:GLU:OE1 | 1:D:23:GLU:HA | 2.04 | 0.58 |
| 1:D:39:GLU:HG2 | 1:D:41:LEU:H | 1.68 | 0.58 |
| 1:D:5:LEU:HD22 | 1:D:82:ASP:HB3 | 1.85 | 0.58 |
| 1:D:91:LEU:HB3 | 1:D:105:ARG:HB3 | 1.86 | 0.58 |
| 1:F:38:PHE:O | 1:F:205:MET:HA | 2.03 | 0.58 |
| 1:A:5:LEU:HD22 | 1:A:82:ASP:HB3 | 1.85 | 0.58 |
| 1:G:130:LEU:CD2 | 1:G:149:TYR:CD2 | 2.85 | 0.58 |
| 1:A:23:GLU:HA | 1:A:23:GLU:OE1 | 2.03 | 0.58 |
| 1:D:133:PRO:O | 1:D:134:LEU:HD23 | 2.03 | 0.58 |
| 1:G:133:PRO:O | 1:G:134:LEU:HD23 | 2.03 | 0.58 |
| 1:H:96:LEU:HD23 | 1:H:171:MET:HA | 1.86 | 0.58 |
| 1:D:125:PHE:H | 1:D:129:THR:HG23 | 1.67 | 0.58 |
| 1:F:151:LEU:N | 1:F:151:LEU:HD23 | 2.19 | 0.58 |
| 1:G:128:GLN:HB2 | 1:G:171:MET:CE | 2.34 | 0.58 |
| 1:G:169:GLN:HA | 1:G:169:GLN:HE21 | 1.69 | 0.58 |
| 1:H:90:LEU:HD12 | 1:H:109:LEU:HD11 | 1.86 | 0.58 |
| 1:G:90:LEU:HD12 | 1:G:109:LEU:HD11 | 1.85 | 0.58 |
| 1:H:122:ASP:O | 1:H:129:THR:HG22 | 2.03 | 0.58 |
| 1:A:91:LEU:HD21 | 1:A:184:HIS:HD2 | 1.69 | 0.58 |
| 1:E:186:MET:HE3 | 1:G:186:MET:CE | 2.34 | 0.58 |
| 1:F:5:LEU:HD22 | 1:F:82:ASP:HB3 | 1.86 | 0.58 |
| 1:E:68:TYR:O | 1:E:69:CYS:C | 2.41 | 0.57 |
| 1:E:19:VAL:HG12 | 1:E:21:THR:HG23 | 1.86 | 0.57 |
| 1:F:45:LEU:HB2 | 2:F:2011:HOH:O | 2.03 | 0.57 |
| 1:C:237:PRO:HG2 | 1:C:238:ASP:OD1 | 2.03 | 0.57 |
| 1:F:136:LEU:HD22 | 1:F:158:TRP:CZ2 | 2.39 | 0.57 |
| 1:G:19:VAL:HG12 | 1:G:21:THR:HG23 | 1.87 | 0.57 |
| 1:D:160:LEU:HD23 | 1:D:160:LEU:C | 2.24 | 0.57 |
| 1:H:11:ARG:HE | 1:H:64:ARG:HA | 1.69 | 0.57 |
| 1:B:87:VAL:CG1 | 1:B:112:VAL:HG22 | 2.33 | 0.57 |
| 1:C:255:ASN:O | 1:C:256:ASP:CB | 2.53 | 0.57 |
| 1:G:150:ARG:NH2 | 1:G:168:TRP:CD1 | 2.72 | 0.57 |
| 1:G:216:THR:HG22 | 1:G:216:THR:O | 2.03 | 0.57 |
| 1:A:33:ASN:O | 1:A:208:HIS:HB2 | 2.04 | 0.57 |
| 1:A:218:THR:O | 1:A:219:ASN:HB2 | 2.04 | 0.57 |
| 1:A:39:GLU:HG2 | 1:A:41:LEU:H | 1.69 | 0.57 |
| 1:B:68:TYR:O | 1:B:69:CYS:C | 2.42 | 0.57 |
| 1:B:68:TYR:OH | 1:B:188:ASN:ND2 | 2.36 | 0.57 |
| 1:D:0:HIS:ND1 | 1:D:1:MET:N | 2.52 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:122:ASP:O | 1:D:129:THR:HG22 | 2.04 | 0.57 |
| 1:D:93:ARG:HA | 2:D:2015:HOH:O | 2.04 | 0.57 |
| 1:G:25:LEU:HD22 | 1:G:133:PRO:CG | 2.33 | 0.57 |
| 1:A:128:GLN:N | 1:A:128:GLN:NE2 | 2.45 | 0.57 |
| 1:A:15:GLN:NE2 | 1:A:16:PRO:HD2 | 2.19 | 0.57 |
| 1:D:150:ARG:O | 1:D:161:GLN:HG2 | 2.05 | 0.57 |
| 1:E:218:THR:O | 1:E:219:ASN:HB2 | 2.05 | 0.57 |
| 1:G:17:LEU:HB3 | 2:G:2010:HOH:O | 2.04 | 0.57 |
| 1:A:130:LEU:HD13 | 1:A:134:LEU:HG | 1.86 | 0.57 |
| 1:E:91:LEU:HD21 | 1:E:184:HIS:CD2 | 2.40 | 0.57 |
| 1:B:19:VAL:HG12 | 1:B:21:THR:HG23 | 1.87 | 0.57 |
| 1:B:245:LEU:HD12 | 1:B:249:GLN:HB2 | 1.87 | 0.57 |
| 1:D:237:PRO:HG2 | 1:D:238:ASP:OD1 | 2.05 | 0.57 |
| 1:D:53:GLU:O | 1:D:53:GLU:HG3 | 2.04 | 0.57 |
| 1:E:0:HIS:ND1 | 1:E:1:MET:N | 2.52 | 0.57 |
| 1:E:87:VAL:HG12 | 1:E:112:VAL:HG22 | 1.87 | 0.57 |
| 1:H:33:ASN:O | 1:H:208:HIS:HB2 | 2.04 | 0.57 |
| 1:E:226:HIS:HE1 | 1:E:227:GLN:HE21 | 1.49 | 0.57 |
| 1:F:96:LEU:HD23 | 1:F:171:MET:HA | 1.87 | 0.56 |
| 1:G:90:LEU:HB2 | 1:G:109:LEU:CD1 | 2.35 | 0.56 |
| 1:A:120:ILE:HG13 | 1:A:120:ILE:O | 2.04 | 0.56 |
| 1:C:54:THR:O | 1:C:58:GLU:HG3 | 2.04 | 0.56 |
| 1:G:23:GLU:OE1 | 1:G:23:GLU:HA | 2.04 | 0.56 |
| 1:H:91:LEU:HB3 | 1:H:105:ARG:HB3 | 1.86 | 0.56 |
| 1:B:105:ARG:NE | 2:B:2019:HOH:O | 2.38 | 0.56 |
| 1:B:130:LEU:HD13 | 1:B:134:LEU:HG | 1.87 | 0.56 |
| 1:F:91:LEU:HB3 | 1:F:105:ARG:HB3 | 1.86 | 0.56 |
| 1:E:151:LEU:HD23 | 1:E:160:LEU:HA | 1.86 | 0.56 |
| 1:H:137:GLN:HA | 2:H:2027:HOH:O | 2.06 | 0.56 |
| 1:C:245:LEU:HD12 | 1:C:249:GLN:HB2 | 1.87 | 0.56 |
| 1:F:68:TYR:OH | 1:F:188:ASN:ND2 | 2.37 | 0.56 |
| 1:C:68:TYR:O | 1:C:69:CYS:C | 2.43 | 0.56 |
| 1:F:239:VAL:HB | 1:F:240:PRO:HD3 | 1.86 | 0.56 |
| 1:E:136:LEU:HD22 | 1:E:158:TRP:CH2 | 2.40 | 0.56 |
| 1:E:205:MET:SD | 1:E:246:LEU:HD22 | 2.45 | 0.56 |
| 1:B:186:MET:SD | 2:C:2032:HOH:O | 2.58 | 0.56 |
| 1:E:38:PHE:O | 1:E:205:MET:HA | 2.05 | 0.56 |
| 1:G:15:GLN:NE2 | 1:G:16:PRO:HD2 | 2.21 | 0.56 |
| 1:H:218:THR:O | 1:H:219:ASN:HB2 | 2.04 | 0.56 |
| 1:H:68:TYR:O | 1:H:69:CYS:C | 2.44 | 0.56 |
| 1:C:163:ARG:HA | 1:C:167:HIS:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:47:ARG:CD | 2:C:2012:HOH:O | 2.53 | 0.56 |
| 1:F:164:HIS:O | 1:F:165:HIS:CB | 2.53 | 0.56 |
| 1:F:19:VAL:HG12 | 1:F:21:THR:CG2 | 2.36 | 0.56 |
| 1:F:220:PHE:CE1 | 1:F:242:LEU:HD22 | 2.41 | 0.56 |
| 1:G:159:ILE:HG22 | 1:G:160:LEU:N | 2.21 | 0.56 |
| 1:H:50:GLN:HG2 | 2:H:2011:HOH:O | 2.06 | 0.56 |
| 1:H:98:HIS:N | 1:H:99:PRO:HD3 | 2.19 | 0.56 |
| 1:B:255:ASN:O | 1:B:256:ASP:CB | 2.48 | 0.56 |
| 1:E:217:LEU:HD21 | 1:E:242:LEU:HD11 | 1.87 | 0.56 |
| 1:H:150:ARG:NH1 | 1:H:152:MET:CE | 2.69 | 0.56 |
| 1:H:150:ARG:HG2 | 1:H:151:LEU:N | 2.21 | 0.56 |
| 1:H:0:HIS:ND1 | 1:H:1:MET:N | 2.54 | 0.56 |
| 1:D:72:LEU:HD12 | 1:D:124:GLY:HA2 | 1.88 | 0.55 |
| 1:F:123:VAL:HB | 2:F:2025:HOH:O | 2.05 | 0.55 |
| 1:F:130:LEU:HD13 | 1:F:134:LEU:HG | 1.88 | 0.55 |
| 1:A:0:HIS:ND1 | 1:A:1:MET:N | 2.54 | 0.55 |
| 1:F:98:HIS:N | 1:F:99:PRO:HD3 | 2.19 | 0.55 |
| 1:G:98:HIS:N | 1:G:99:PRO:HD3 | 2.21 | 0.55 |
| 1:H:161:GLN:HG2 | 1:H:170:SER:CA | 2.34 | 0.55 |
| 1:A:87:VAL:HG12 | 1:A:112:VAL:HG22 | 1.88 | 0.55 |
| 1:C:252:LEU:HD13 | 2:C:2072:HOH:O | 2.05 | 0.55 |
| 1:D:6:HIS:CD2 | 2:D:2001:HOH:O | 2.60 | 0.55 |
| 1:A:11:ARG:HE | 1:A:64:ARG:HA | 1.71 | 0.55 |
| 1:C:176:LEU:CD1 | 2:C:2043:HOH:O | 2.55 | 0.55 |
| 1:D:48:GLU:N | 2:D:2005:HOH:O | 2.28 | 0.55 |
| 1:B:153:GLN:O | 1:B:154:GLU:HB2 | 2.07 | 0.55 |
| 1:E:220:PHE:CE1 | 1:E:242:LEU:HD22 | 2.41 | 0.55 |
| 1:F:165:HIS:O | 1:F:167:HIS:N | 2.40 | 0.55 |
| 1:C:98:HIS:N | 1:C:99:PRO:HD3 | 2.22 | 0.55 |
| 1:E:122:ASP:O | 1:E:129:THR:HG22 | 2.07 | 0.55 |
| 1:E:90:LEU:HD12 | 1:E:109:LEU:HD11 | 1.88 | 0.55 |
| 1:C:205:MET:SD | 1:C:246:LEU:HD22 | 2.47 | 0.55 |
| 1:E:91:LEU:HB3 | 1:E:105:ARG:HB3 | 1.89 | 0.55 |
| 1:A:151:LEU:HD23 | 1:A:160:LEU:HA | 1.87 | 0.54 |
| 1:B:194:TRP:CG | 2:B:2036:HOH:O | 2.58 | 0.54 |
| 1:B:258:LYS:HG2 | 1:B:259:HIS:CD2 | 2.42 | 0.54 |
| 1:F:139:GLU:HA | 2:F:2029:HOH:O | 2.08 | 0.54 |
| 1:G:120:ILE:HG13 | 1:G:120:ILE:O | 2.07 | 0.54 |
| 1:G:54:THR:O | 1:G:58:GLU:HG3 | 2.07 | 0.54 |
| 1:A:19:VAL:HG12 | 1:A:21:THR:HG23 | 1.88 | 0.54 |
| 1:G:264:ALA:HB3 | 2:G:2053:HOH:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:3:SER:O | 1:G:6:HIS:HB3 | 2.07 | 0.54 |
| 1:A:87:VAL:CG1 | 1:A:112:VAL:HG22 | 2.37 | 0.54 |
| 1:B:150:ARG:HH22 | 1:B:152:MET:CE | 2.20 | 0.54 |
| 1:F:14:CYS:SG | 1:F:15:GLN:N | 2.80 | 0.54 |
| 1:G:160:LEU:CD2 | 1:G:171:MET:SD | 2.95 | 0.54 |
| 1:G:226:HIS:HE1 | 1:G:227:GLN:HE21 | 1.56 | 0.54 |
| 1:H:15:GLN:NE2 | 1:H:16:PRO:HD2 | 2.22 | 0.54 |
| 1:H:83:ILE:HG22 | 1:H:83:ILE:O | 2.05 | 0.54 |
| 1:A:136:LEU:HD22 | 1:A:158:TRP:CE2 | 2.43 | 0.54 |
| 1:A:182:SER:HB2 | 1:D:104:PRO:HD3 | 1.89 | 0.54 |
| 1:A:27:THR:HG23 | 2:A:2006:HOH:O | 2.06 | 0.54 |
| 1:C:121:ALA:C | 2:C:2037:HOH:O | 2.44 | 0.54 |
| 1:D:245:LEU:HD12 | 1:D:249:GLN:HB2 | 1.89 | 0.54 |
| 1:H:205:MET:SD | 1:H:246:LEU:HD22 | 2.47 | 0.54 |
| 1:C:164:HIS:ND1 | 1:C:165:HIS:N | 2.45 | 0.54 |
| 1:E:23:GLU:HA | 1:E:23:GLU:OE1 | 2.07 | 0.54 |
| 1:A:152:MET:HG3 | 1:A:153:GLN:N | 2.22 | 0.54 |
| 1:B:220:PHE:CE1 | 1:B:242:LEU:HD22 | 2.43 | 0.54 |
| 1:C:150:ARG:HD2 | 1:C:168:TRP:CE2 | 2.43 | 0.54 |
| 1:C:90:LEU:HD12 | 1:C:109:LEU:HD11 | 1.88 | 0.54 |
| 1:G:53:GLU:O | 1:G:53:GLU:HG3 | 2.08 | 0.54 |
| 1:A:255:ASN:O | 1:A:256:ASP:CB | 2.56 | 0.54 |
| 1:G:96:LEU:HD23 | 1:G:171:MET:HA | 1.90 | 0.54 |
| 1:E:245:LEU:HD12 | 1:E:249:GLN:HB2 | 1.89 | 0.54 |
| 1:H:245:LEU:HD12 | 1:H:249:GLN:HB2 | 1.90 | 0.54 |
| 1:A:186:MET:HE3 | 1:D:186:MET:CE | 2.37 | 0.54 |
| 1:C:19:VAL:HG12 | 1:C:21:THR:HG23 | 1.89 | 0.54 |
| 1:C:262:THR:HG23 | 1:C:265:GLU:OE1 | 2.07 | 0.54 |
| 1:D:218:THR:O | 1:D:219:ASN:HB2 | 2.06 | 0.54 |
| 1:F:109:LEU:HD23 | 1:F:172:TYR:CE1 | 2.43 | 0.54 |
| 1:D:15:GLN:NE2 | 1:D:16:PRO:HD2 | 2.24 | 0.53 |
| 1:G:4:PHE:O | 1:G:6:HIS:N | 2.41 | 0.53 |
| 1:G:125:PHE:H | 1:G:129:THR:HG23 | 1.73 | 0.53 |
| 1:G:203:LEU:HB2 | 2:G:2044:HOH:O | 2.08 | 0.53 |
| 1:D:150:ARG:HG2 | 1:D:151:LEU:O | 2.09 | 0.53 |
| 1:D:7:ALA:HB2 | 2:D:2001:HOH:O | 2.08 | 0.53 |
| 1:H:237:PRO:HG2 | 1:H:238:ASP:OD1 | 2.09 | 0.53 |
| 1:B:23:GLU:HA | 1:B:23:GLU:OE1 | 2.09 | 0.53 |
| 1:D:98:HIS:N | 1:D:99:PRO:HD3 | 2.24 | 0.53 |
| 1:E:15:GLN:NE2 | 1:E:16:PRO:HD2 | 2.23 | 0.53 |
| 1:F:54:THR:O | 1:F:58:GLU:HG3 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:TYR:O | 1:A:69:CYS:C | 2.46 | 0.53 |
| 1:D:11:ARG:HE | 1:D:64:ARG:HA | 1.72 | 0.53 |
| 1:F:53:GLU:HG3 | 1:F:53:GLU:O | 2.08 | 0.53 |
| 1:A:220:PHE:CE1 | 1:A:242:LEU:HD22 | 2.44 | 0.53 |
| 1:A:89:SER:O | 1:A:90:LEU:HD23 | 2.09 | 0.53 |
| 1:B:254:VAL:O | 1:B:254:VAL:HG13 | 2.09 | 0.53 |
| 1:D:128:GLN:HB2 | 1:D:171:MET:HE3 | 1.90 | 0.53 |
| 1:D:120:ILE:O | 1:D:120:ILE:HG13 | 2.08 | 0.53 |
| 1:F:59:LYS:HG3 | 1:F:259:HIS:ND1 | 2.24 | 0.53 |
| 1:H:54:THR:O | 1:H:58:GLU:HG3 | 2.08 | 0.53 |
| 1:A:11:ARG:HH21 | 1:A:64:ARG:CA | 2.22 | 0.53 |
| 1:B:87:VAL:HG12 | 1:B:112:VAL:HG22 | 1.90 | 0.53 |
| 1:C:25:LEU:HD22 | 1:C:133:PRO:CG | 2.35 | 0.53 |
| 1:C:38:PHE:O | 1:C:205:MET:HA | 2.09 | 0.53 |
| 1:E:133:PRO:O | 1:E:134:LEU:HD23 | 2.07 | 0.53 |
| 1:E:11:ARG:HH21 | 1:E:64:ARG:CA | 2.22 | 0.53 |
| 1:E:11:ARG:HE | 1:E:64:ARG:HA | 1.74 | 0.53 |
| 1:E:96:LEU:HD23 | 1:E:171:MET:HA | 1.90 | 0.53 |
| 1:F:262:THR:HG23 | 1:F:265:GLU:OE1 | 2.08 | 0.53 |
| 1:A:200:ARG:HH12 | 1:C:200:ARG:HH12 | 1.56 | 0.53 |
| 1:B:98:HIS:N | 1:B:99:PRO:HD3 | 2.23 | 0.53 |
| 1:A:91:LEU:HD21 | 1:A:184:HIS:CD2 | 2.44 | 0.53 |
| 1:F:128:GLN:N | 1:F:128:GLN:NE2 | 2.52 | 0.53 |
| 1:G:64:ARG:NH2 | 2:G:2017:HOH:O | 2.42 | 0.53 |
| 1:H:162:PHE:CD2 | 1:H:171:MET:SD | 3.01 | 0.53 |
| 1:H:254:VAL:O | 1:H:254:VAL:HG13 | 2.08 | 0.53 |
| 1:B:238:ASP:OD2 | 1:B:240:PRO:HD2 | 2.09 | 0.52 |
| 1:B:59:LYS:HG3 | 1:B:259:HIS:ND1 | 2.25 | 0.52 |
| 1:E:53:GLU:O | 1:E:53:GLU:HG3 | 2.09 | 0.52 |
| 1:H:39:GLU:HG2 | 1:H:41:LEU:H | 1.74 | 0.52 |
| 1:B:218:THR:O | 1:B:219:ASN:HB2 | 2.09 | 0.52 |
| 1:D:128:GLN:NE2 | 1:D:128:GLN:N | 2.48 | 0.52 |
| 1:D:161:GLN:HB2 | 1:D:169:GLN:O | 2.09 | 0.52 |
| 1:D:91:LEU:HG | 1:D:179:GLN:HG3 | 1.90 | 0.52 |
| 1:F:238:ASP:OD2 | 1:F:240:PRO:HD2 | 2.09 | 0.52 |
| 1:G:128:GLN:N | 1:G:128:GLN:NE2 | 2.52 | 0.52 |
| 1:H:109:LEU:C | 1:H:109:LEU:HD12 | 2.29 | 0.52 |
| 1:C:91:LEU:HD21 | 1:C:184:HIS:CD2 | 2.44 | 0.52 |
| 1:F:26:ARG:NH1 | 2:F:2007:HOH:O | 2.43 | 0.52 |
| 1:G:4:PHE:CE2 | 1:G:78:ARG:HD3 | 2.44 | 0.52 |
| 1:D:120:ILE:HD11 | 1:D:151:LEU:HD21 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:GLN:O | 1:F:232:GLU:HA | 2.10 | 0.52 |
| 1:A:153:GLN:HG3 | 1:A:153:GLN:O | 2.08 | 0.52 |
| 1:A:226:HIS:HE1 | 1:A:227:GLN:HE21 | 1.56 | 0.52 |
| 1:A:247:GLN:HB3 | 2:A:2048:HOH:O | 2.09 | 0.52 |
| 1:H:136:LEU:HD23 | 1:H:151:LEU:CD1 | 2.40 | 0.52 |
| 1:H:161:GLN:CG | 1:H:170:SER:HA | 2.36 | 0.52 |
| 1:C:202:HIS:HA | 1:C:273:PHE:CE2 | 2.45 | 0.52 |
| 1:E:5:LEU:HD22 | 1:E:82:ASP:HB3 | 1.92 | 0.52 |
| 1:F:218:THR:O | 1:F:219:ASN:HB2 | 2.10 | 0.52 |
| 1:B:0:HIS:HA | 2:B:2001:HOH:O | 2.10 | 0.52 |
| 1:H:12:LEU:HD21 | 1:H:32:HIS:HA | 1.90 | 0.52 |
| 1:H:91:LEU:HD21 | 1:H:184:HIS:HD2 | 1.74 | 0.52 |
| 1:E:33:ASN:O | 1:E:208:HIS:HB2 | 2.10 | 0.52 |
| 1:E:237:PRO:HG2 | 1:E:238:ASP:OD1 | 2.08 | 0.52 |
| 1:F:160:LEU:C | 1:F:161:GLN:HG3 | 2.30 | 0.52 |
| 1:E:99:PRO:HA | 2:E:2034:HOH:O | 2.10 | 0.52 |
| 1:F:15:GLN:NE2 | 1:F:16:PRO:HD2 | 2.24 | 0.52 |
| 1:B:11:ARG:HE | 1:B:64:ARG:HA | 1.75 | 0.52 |
| 1:C:181:GLN:O | 1:C:185:VAL:HG23 | 2.09 | 0.52 |
| 1:C:226:HIS:HE1 | 1:C:227:GLN:HE21 | 1.58 | 0.52 |
| 1:C:11:ARG:HH21 | 1:C:64:ARG:CA | 2.23 | 0.52 |
| 1:F:128:GLN:CB | 1:F:171:MET:HE1 | 2.40 | 0.52 |
| 1:C:159:ILE:HD11 | 1:C:170:SER:OG | 2.10 | 0.51 |
| 1:E:104:PRO:HD3 | 1:G:182:SER:HB2 | 1.92 | 0.51 |
| 1:G:262:THR:HG23 | 1:G:265:GLU:OE1 | 2.11 | 0.51 |
| 1:H:181:GLN:O | 1:H:185:VAL:HG23 | 2.10 | 0.51 |
| 1:A:98:HIS:N | 1:A:99:PRO:HD3 | 2.24 | 0.51 |
| 1:D:255:ASN:O | 1:D:256:ASP:CB | 2.56 | 0.51 |
| 1:D:59:LYS:HG3 | 1:D:259:HIS:ND1 | 2.26 | 0.51 |
| 1:E:95:ILE:HG12 | 1:E:172:TYR:HA | 1.92 | 0.51 |
| 1:G:144:THR:HG21 | 1:G:149:TYR:CE2 | 2.45 | 0.51 |
| 1:B:150:ARG:NH2 | 1:B:152:MET:HE1 | 2.26 | 0.51 |
| 1:C:41:LEU:O | 1:C:41:LEU:HD12 | 2.11 | 0.51 |
| 1:A:150:ARG:NH2 | 1:A:152:MET:SD | 2.83 | 0.51 |
| 1:D:38:PHE:O | 1:D:205:MET:HA | 2.09 | 0.51 |
| 1:G:203:LEU:O | 1:G:204:LEU:HD23 | 2.11 | 0.51 |
| 1:B:203:LEU:O | 1:B:204:LEU:HD23 | 2.09 | 0.51 |
| 1:C:150:ARG:HH21 | 1:C:152:MET:CE | 2.23 | 0.51 |
| 1:G:223:THR:HG22 | 1:G:225:TYR:CE1 | 2.45 | 0.51 |
| 1:H:83:ILE:CG2 | 1:H:83:ILE:O | 2.58 | 0.51 |
| 1:B:46:PRO:HD2 | 2:B:2007:HOH:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:130:LEU:HD13 | 1:C:134:LEU:HG | 1.93 | 0.51 |
| 1:C:164:HIS:CG | 1:C:165:HIS:N | 2.76 | 0.51 |
| 1:D:90:LEU:HD12 | 1:D:109:LEU:HD11 | 1.92 | 0.51 |
| 1:D:174:PHE:N | 1:D:174:PHE:CD1 | 2.79 | 0.51 |
| 1:E:216:THR:O | 1:E:216:THR:HG22 | 2.11 | 0.51 |
| 1:E:263:GLU:OE2 | 2:E:2089:HOH:O | 2.18 | 0.51 |
| 1:E:91:LEU:HG | 1:E:179:GLN:HG3 | 1.93 | 0.51 |
| 1:F:12:LEU:HD21 | 1:F:32:HIS:HA | 1.93 | 0.51 |
| 1:H:203:LEU:O | 1:H:204:LEU:HD23 | 2.11 | 0.51 |
| 1:B:83:ILE:HG22 | 1:B:83:ILE:O | 2.09 | 0.51 |
| 1:C:93:ARG:NH2 | 1:C:105:ARG:NH1 | 2.59 | 0.51 |
| 1:D:239:VAL:HG23 | 2:D:2033:HOH:O | 2.09 | 0.51 |
| 1:D:68:TYR:O | 1:D:69:CYS:C | 2.49 | 0.51 |
| 1:E:87:VAL:CG1 | 1:E:112:VAL:HG22 | 2.41 | 0.51 |
| 1:E:125:PHE:H | 1:E:129:THR:HG23 | 1.75 | 0.51 |
| 1:F:149:TYR:N | 1:F:149:TYR:CD1 | 2.78 | 0.51 |
| 1:F:150:ARG:HH21 | 1:F:168:TRP:CB | 2.24 | 0.51 |
| 1:A:162:PHE:O | 1:A:162:PHE:CD1 | 2.63 | 0.51 |
| 1:B:128:GLN:NE2 | 1:B:128:GLN:N | 2.50 | 0.51 |
| 1:B:150:ARG:HH12 | 1:B:152:MET:CE | 2.24 | 0.51 |
| 1:H:163:ARG:NH2 | 1:H:166:GLU:O | 2.44 | 0.51 |
| 1:H:217:LEU:HD21 | 1:H:242:LEU:HD11 | 1.93 | 0.51 |
| 1:G:130:LEU:HD23 | 1:G:149:TYR:CE2 | 2.46 | 0.51 |
| 1:H:150:ARG:NH1 | 1:H:152:MET:HE2 | 2.26 | 0.51 |
| 1:G:218:THR:O | 1:G:219:ASN:HB2 | 2.11 | 0.51 |
| 1:H:255:ASN:O | 1:H:256:ASP:CB | 2.56 | 0.51 |
| 1:H:11:ARG:HH21 | 1:H:64:ARG:CA | 2.24 | 0.51 |
| 1:A:125:PHE:H | 1:A:129:THR:HG23 | 1.75 | 0.50 |
| 1:B:91:LEU:HD21 | 1:B:184:HIS:CD2 | 2.45 | 0.50 |
| 1:B:217:LEU:HD11 | 1:B:219:ASN:O | 2.10 | 0.50 |
| 1:F:160:LEU:HD23 | 1:F:171:MET:SD | 2.51 | 0.50 |
| 1:F:245:LEU:HD12 | 1:F:249:GLN:HB2 | 1.93 | 0.50 |
| 1:G:95:ILE:HG12 | 1:G:172:TYR:HA | 1.92 | 0.50 |
| 1:A:76:PHE:HE1 | 1:A:80:LEU:HD21 | 1.76 | 0.50 |
| 1:F:163:ARG:NH1 | 2:F:2033:HOH:O | 2.43 | 0.50 |
| 1:G:11:ARG:HE | 1:G:64:ARG:HA | 1.76 | 0.50 |
| 1:H:166:GLU:C | 1:H:166:GLU:OE1 | 2.50 | 0.50 |
| 1:H:53:GLU:HG3 | 1:H:53:GLU:O | 2.10 | 0.50 |
| 1:B:202:HIS:HA | 1:B:273:PHE:CE2 | 2.47 | 0.50 |
| 1:D:174:PHE:N | 1:D:174:PHE:HD1 | 2.09 | 0.50 |
| 1:G:254:VAL:O | 1:G:254:VAL:HG13 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:195:PRO:N | 2:B:2036:HOH:O | 2.43 | 0.50 |
| 1:C:216:THR:HG22 | 1:C:216:THR:O | 2.11 | 0.50 |
| 1:H:221:HIS:HD2 | 2:H:2041:HOH:O | 1.93 | 0.50 |
| 1:A:4:PHE:O | 1:A:6:HIS:N | 2.44 | 0.50 |
| 1:B:166:GLU:HG2 | 1:G:233:GLN:O | 2.11 | 0.50 |
| 1:C:125:PHE:H | 1:C:129:THR:CG2 | 2.23 | 0.50 |
| 1:F:91:LEU:HG | 1:F:179:GLN:HG3 | 1.91 | 0.50 |
| 1:G:90:LEU:HB2 | 1:G:109:LEU:HD11 | 1.93 | 0.50 |
| 1:A:53:GLU:HG3 | 1:A:53:GLU:O | 2.12 | 0.50 |
| 1:B:262:THR:HG23 | 1:B:265:GLU:OE1 | 2.11 | 0.50 |
| 1:C:172:TYR:C | 1:C:172:TYR:CD1 | 2.85 | 0.50 |
| 1:F:8:TYR:CZ | 1:F:12:LEU:HD11 | 2.47 | 0.50 |
| 1:G:202:HIS:HA | 1:G:273:PHE:CE2 | 2.46 | 0.50 |
| 1:H:90:LEU:HB2 | 1:H:109:LEU:CD1 | 2.42 | 0.50 |
| 1:H:133:PRO:O | 1:H:134:LEU:HD23 | 2.12 | 0.50 |
| 1:C:212:GLY:N | 2:C:2057:HOH:O | 2.30 | 0.50 |
| 1:D:184:HIS:CE1 | 2:D:2023:HOH:O | 2.65 | 0.50 |
| 1:D:11:ARG:HH21 | 1:D:64:ARG:CA | 2.25 | 0.50 |
| 1:F:23:GLU:HA | 1:F:23:GLU:OE1 | 2.12 | 0.50 |
| 1:A:149:TYR:CD2 | 1:A:162:PHE:HB3 | 2.47 | 0.49 |
| 1:G:38:PHE:O | 1:G:205:MET:HA | 2.11 | 0.49 |
| 1:H:144:THR:CG2 | 1:H:146:HIS:H | 2.20 | 0.49 |
| 1:H:163:ARG:HG2 | 1:H:168:TRP:CE3 | 2.47 | 0.49 |
| 1:H:165:HIS:O | 1:H:166:GLU:CB | 2.60 | 0.49 |
| 1:C:220:PHE:CE1 | 1:C:242:LEU:HD22 | 2.47 | 0.49 |
| 1:C:254:VAL:HG13 | 1:C:254:VAL:O | 2.12 | 0.49 |
| 1:C:11:ARG:HE | 1:C:64:ARG:HA | 1.78 | 0.49 |
| 1:G:130:LEU:HD13 | 1:G:134:LEU:HG | 1.93 | 0.49 |
| 1:H:12:LEU:CD2 | 1:H:32:HIS:HA | 2.43 | 0.49 |
| 1:H:220:PHE:CE1 | 1:H:242:LEU:HD22 | 2.47 | 0.49 |
| 1:H:76:PHE:CE1 | 1:H:80:LEU:HD11 | 2.48 | 0.49 |
| 1:B:243:TYR:CG | 1:B:263:GLU:HG3 | 2.48 | 0.49 |
| 1:B:11:ARG:HH21 | 1:B:64:ARG:CA | 2.26 | 0.49 |
| 1:C:14:CYS:SG | 1:C:15:GLN:N | 2.84 | 0.49 |
| 1:D:163:ARG:NH1 | 1:D:167:HIS:HA | 2.27 | 0.49 |
| 1:E:54:THR:O | 1:E:58:GLU:HG3 | 2.12 | 0.49 |
| 1:F:123:VAL:C | 1:F:129:THR:HG21 | 2.33 | 0.49 |
| 1:G:202:HIS:HD2 | 1:G:202:HIS:O | 1.95 | 0.49 |
| 1:H:41:LEU:HD12 | 1:H:41:LEU:O | 2.12 | 0.49 |
| 1:A:140:ILE:HD13 | 2:A:2030:HOH:O | 2.12 | 0.49 |
| 1:B:125:PHE:H | 1:B:129:THR:HG23 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:38:PHE:O | 1:B:205:MET:HA | 2.11 | 0.49 |
| 1:C:15:GLN:NE2 | 1:C:16:PRO:HD2 | 2.27 | 0.49 |
| 1:D:220:PHE:CE1 | 1:D:242:LEU:HD22 | 2.47 | 0.49 |
| 1:F:205:MET:SD | 1:F:246:LEU:HD22 | 2.53 | 0.49 |
| 1:G:128:GLN:CB | 1:G:171:MET:HE1 | 2.41 | 0.49 |
| 1:G:205:MET:SD | 1:G:246:LEU:HD22 | 2.53 | 0.49 |
| 1:G:68:TYR:OH | 1:G:188:ASN:ND2 | 2.46 | 0.49 |
| 1:A:169:GLN:NE2 | 1:A:170:SER:H | 2.10 | 0.49 |
| 1:E:15:GLN:HE21 | 1:E:16:PRO:HD2 | 1.77 | 0.49 |
| 1:G:4:PHE:C | 1:G:6:HIS:N | 2.65 | 0.49 |
| 1:D:225:TYR:HA | 1:D:229:HIS:O | 2.13 | 0.49 |
| 1:C:59:LYS:HG3 | 1:C:259:HIS:ND1 | 2.27 | 0.49 |
| 1:F:87:VAL:HG12 | 1:F:112:VAL:HG22 | 1.95 | 0.49 |
| 1:G:46:PRO:HD2 | 2:G:2013:HOH:O | 2.13 | 0.49 |
| 1:A:162:PHE:HE1 | 1:A:169:GLN:HB3 | 1.75 | 0.49 |
| 1:C:88:ARG:NH1 | 2:C:2028:HOH:O | 2.46 | 0.49 |
| 1:D:194:TRP:NE1 | 2:D:2025:HOH:O | 2.11 | 0.49 |
| 1:D:216:THR:O | 1:D:216:THR:HG22 | 2.11 | 0.49 |
| 1:G:178:VAL:HG12 | 1:G:179:GLN:N | 2.28 | 0.49 |
| 1:C:160:LEU:HG | 1:C:171:MET:HE2 | 1.95 | 0.49 |
| 1:F:182:SER:HB2 | 1:H:104:PRO:HD3 | 1.94 | 0.49 |
| 1:G:87:VAL:CG1 | 1:G:112:VAL:HG22 | 2.43 | 0.49 |
| 1:H:130:LEU:HD13 | 1:H:134:LEU:HG | 1.95 | 0.49 |
| 1:A:178:VAL:HG12 | 1:A:179:GLN:N | 2.28 | 0.48 |
| 1:D:41:LEU:HD12 | 1:D:41:LEU:O | 2.13 | 0.48 |
| 1:F:90:LEU:HD12 | 1:F:109:LEU:HD11 | 1.95 | 0.48 |
| 1:B:83:ILE:CG2 | 1:B:83:ILE:O | 2.61 | 0.48 |
| 1:C:53:GLU:O | 1:C:53:GLU:HG3 | 2.13 | 0.48 |
| 1:D:96:LEU:HD23 | 1:D:170:SER:O | 2.13 | 0.48 |
| 1:D:25:LEU:HD22 | 1:D:133:PRO:CG | 2.40 | 0.48 |
| 1:D:3:SER:O | 1:D:6:HIS:HB3 | 2.13 | 0.48 |
| 1:H:19:VAL:HG12 | 1:H:21:THR:CG2 | 2.43 | 0.48 |
| 1:D:4:PHE:O | 1:D:6:HIS:N | 2.47 | 0.48 |
| 1:E:11:ARG:HH21 | 1:E:64:ARG:HA | 1.78 | 0.48 |
| 1:F:5:LEU:HD11 | 1:F:83:ILE:HG13 | 1.94 | 0.48 |
| 1:A:253:GLY:HA2 | 2:A:2015:HOH:O | 2.13 | 0.48 |
| 1:B:109:LEU:HD23 | 1:B:172:TYR:CE1 | 2.48 | 0.48 |
| 1:C:211:ASP:HA | 2:C:2057:HOH:O | 2.13 | 0.48 |
| 1:E:225:TYR:HA | 1:E:229:HIS:O | 2.14 | 0.48 |
| 1:H:15:GLN:HE21 | 1:H:16:PRO:HD2 | 1.77 | 0.48 |
| 1:D:184:HIS:HE1 | 2:D:2023:HOH:O | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:15:GLN:HE21 | 1:A:16:PRO:HD2 | 1.79 | 0.48 |
| 1:A:68:TYR:OH | 1:A:188:ASN:ND2 | 2.47 | 0.48 |
| 1:B:104:PRO:HD3 | 1:C:182:SER:HB2 | 1.95 | 0.48 |
| 1:C:133:PRO:O | 1:C:134:LEU:HD23 | 2.13 | 0.48 |
| 1:D:222:PHE:CZ | 1:D:249:GLN:HG2 | 2.49 | 0.48 |
| 1:E:41:LEU:HB3 | 1:E:65:ARG:HH22 | 1.78 | 0.48 |
| 1:B:150:ARG:NH2 | 1:B:152:MET:CE | 2.77 | 0.48 |
| 1:B:30:LEU:HG | 2:B:2027:HOH:O | 2.12 | 0.48 |
| 1:F:178:VAL:HG12 | 1:F:179:GLN:N | 2.29 | 0.48 |
| 1:H:109:LEU:HD23 | 1:H:172:TYR:CE1 | 2.48 | 0.48 |
| 1:B:14:CYS:SG | 1:B:15:GLN:N | 2.87 | 0.48 |
| 1:C:89:SER:O | 1:C:90:LEU:HD23 | 2.14 | 0.48 |
| 1:F:77:GLU:HB2 | 1:F:110:LEU:HD21 | 1.94 | 0.48 |
| 1:A:87:VAL:HG13 | 1:A:112:VAL:HG13 | 1.95 | 0.48 |
| 1:B:93:ARG:NH2 | 1:B:105:ARG:NH1 | 2.62 | 0.48 |
| 1:D:203:LEU:O | 1:D:204:LEU:HD23 | 2.14 | 0.48 |
| 1:E:159:ILE:N | 1:E:159:ILE:CD1 | 2.71 | 0.48 |
| 1:E:273:PHE:C | 2:E:2092:HOH:O | 2.51 | 0.48 |
| 1:H:38:PHE:O | 1:H:205:MET:HA | 2.14 | 0.48 |
| 1:A:181:GLN:O | 1:A:185:VAL:HG23 | 2.13 | 0.48 |
| 1:B:150:ARG:HG2 | 1:B:168:TRP:CE3 | 2.49 | 0.48 |
| 2:A:2040:HOH:O | 1:C:201:HIS:HE1 | 1.97 | 0.48 |
| 1:H:144:THR:HG21 | 1:H:149:TYR:HE1 | 1.79 | 0.48 |
| 1:H:202:HIS:O | 1:H:202:HIS:HD2 | 1.96 | 0.48 |
| 1:H:225:TYR:HA | 1:H:229:HIS:O | 2.13 | 0.47 |
| 1:C:202:HIS:O | 1:C:202:HIS:HD2 | 1.97 | 0.47 |
| 1:F:50:GLN:O | 1:F:51:LEU:HD23 | 2.14 | 0.47 |
| 1:H:226:HIS:HE1 | 1:H:227:GLN:HE21 | 1.61 | 0.47 |
| 1:H:202:HIS:HA | 1:H:273:PHE:CE2 | 2.49 | 0.47 |
| 1:A:3:SER:O | 1:A:6:HIS:HB3 | 2.14 | 0.47 |
| 1:B:225:TYR:HA | 1:B:229:HIS:O | 2.14 | 0.47 |
| 1:B:53:GLU:HG3 | 1:B:53:GLU:O | 2.14 | 0.47 |
| 1:D:262:THR:HG23 | 1:D:265:GLU:OE1 | 2.13 | 0.47 |
| 1:A:163:ARG:HH11 | 1:A:163:ARG:HG3 | 1.80 | 0.47 |
| 1:D:5:LEU:HD11 | 1:D:83:ILE:HG13 | 1.95 | 0.47 |
| 1:E:255:ASN:O | 1:E:256:ASP:CB | 2.62 | 0.47 |
| 1:F:159:ILE:CG2 | 1:F:160:LEU:N | 2.76 | 0.47 |
| 1:G:181:GLN:O | 1:G:185:VAL:HG23 | 2.15 | 0.47 |
| 1:H:201:HIS:O | 1:H:202:HIS:HB3 | 2.14 | 0.47 |
| 1:B:89:SER:O | 1:B:90:LEU:HD23 | 2.14 | 0.47 |
| 1:D:223:THR:HG22 | 1:D:225:TYR:CE1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:254:VAL:HG13 | 1:D:254:VAL:O | 2.14 | 0.47 |
| 1:H:93:ARG:NH2 | 1:H:105:ARG:NH1 | 2.63 | 0.47 |
| 1:B:167:HIS:O | 1:B:168:TRP:CB | 2.61 | 0.47 |
| 1:C:162:PHE:CE1 | 1:C:164:HIS:HB2 | 2.49 | 0.47 |
| 1:C:5:LEU:HD22 | 1:C:82:ASP:HB3 | 1.97 | 0.47 |
| 1:F:203:LEU:O | 1:F:204:LEU:HD23 | 2.13 | 0.47 |
| 1:A:91:LEU:HG | 1:A:179:GLN:HG3 | 1.97 | 0.47 |
| 1:B:239:VAL:HG23 | 2:B:2041:HOH:O | 2.15 | 0.47 |
| 1:C:151:LEU:HD23 | 1:C:160:LEU:HA | 1.97 | 0.47 |
| 1:C:273:PHE:N | 1:C:273:PHE:CD1 | 2.80 | 0.47 |
| 1:E:41:LEU:O | 1:E:41:LEU:HD12 | 2.15 | 0.47 |
| 1:E:45:LEU:HD12 | 1:E:45:LEU:O | 2.15 | 0.47 |
| 1:A:196:GLN:HG3 | 2:C:2078:HOH:O | 2.13 | 0.47 |
| 1:C:139:GLU:N | 1:C:151:LEU:O | 2.46 | 0.47 |
| 1:C:176:LEU:HB3 | 2:C:2028:HOH:O | 2.14 | 0.47 |
| 1:C:83:ILE:O | 1:C:83:ILE:HG22 | 2.15 | 0.47 |
| 1:F:89:SER:O | 1:F:90:LEU:HD23 | 2.15 | 0.47 |
| 1:G:245:LEU:CD1 | 1:G:249:GLN:HB2 | 2.44 | 0.47 |
| 1:D:144:THR:CG2 | 1:D:149:TYR:HE1 | 2.27 | 0.47 |
| 1:D:14:CYS:SG | 1:D:15:GLN:N | 2.88 | 0.47 |
| 1:E:252:LEU:HD13 | 2:E:2014:HOH:O | 2.15 | 0.47 |
| 1:F:87:VAL:CG1 | 1:F:112:VAL:HG22 | 2.45 | 0.47 |
| 1:C:91:LEU:HG | 1:C:179:GLN:HG3 | 1.97 | 0.47 |
| 1:A:186:MET:CE | 1:D:186:MET:CE | 2.93 | 0.47 |
| 1:B:19:VAL:HG12 | 1:B:21:THR:CG2 | 2.45 | 0.46 |
| 1:B:5:LEU:HA | 1:B:5:LEU:HD12 | 1.73 | 0.46 |
| 1:D:200:ARG:HB3 | 2:D:2029:HOH:O | 2.15 | 0.46 |
| 1:E:163:ARG:CG | 2:E:2053:HOH:O | 2.53 | 0.46 |
| 1:A:96:LEU:C | 1:A:98:HIS:H | 2.18 | 0.46 |
| 1:B:45:LEU:HB2 | 2:B:2007:HOH:O | 2.13 | 0.46 |
| 1:F:150:ARG:HH21 | 1:F:168:TRP:HB2 | 1.79 | 0.46 |
| 1:H:11:ARG:HH11 | 1:H:11:ARG:HG2 | 1.79 | 0.46 |
| 1:H:33:ASN:OD1 | 1:H:131:THR:HA | 2.14 | 0.46 |
| 1:C:216:THR:HG21 | 2:C:2062:HOH:O | 2.15 | 0.46 |
| 1:C:245:LEU:CD1 | 1:C:249:GLN:HB2 | 2.45 | 0.46 |
| 1:D:159:ILE:O | 1:D:160:LEU:C | 2.53 | 0.46 |
| 1:D:4:PHE:C | 1:D:6:HIS:N | 2.69 | 0.46 |
| 1:F:12:LEU:CD2 | 1:F:32:HIS:HA | 2.44 | 0.46 |
| 1:F:150:ARG:O | 1:F:151:LEU:HB3 | 2.14 | 0.46 |
| 1:F:243:TYR:CG | 1:F:263:GLU:HG3 | 2.50 | 0.46 |
| 1:H:163:ARG:HG2 | 1:H:163:ARG:HH11 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:160:LEU:HD23 | 1:D:161:GLN:N | 2.31 | 0.46 |
| 1:D:19:VAL:HG12 | 1:D:21:THR:CG2 | 2.44 | 0.46 |
| 1:E:109:LEU:HD23 | 1:E:172:TYR:CE1 | 2.50 | 0.46 |
| 1:F:151:LEU:HB2 | 1:F:159:ILE:O | 2.15 | 0.46 |
| 1:A:38:PHE:O | 1:A:205:MET:HA | 2.16 | 0.46 |
| 1:G:220:PHE:CE1 | 1:G:242:LEU:HD22 | 2.50 | 0.46 |
| 1:G:59:LYS:HG3 | 1:G:259:HIS:ND1 | 2.30 | 0.46 |
| 1:H:91:LEU:HG | 1:H:179:GLN:HG3 | 1.98 | 0.46 |
| 1:H:91:LEU:HD21 | 1:H:184:HIS:CD2 | 2.49 | 0.46 |
| 1:A:164:HIS:O | 1:A:165:HIS:HB2 | 2.16 | 0.46 |
| 1:B:96:LEU:HD21 | 1:B:171:MET:CG | 2.46 | 0.46 |
| 2:B:2019:HOH:O | 1:C:105:ARG:NE | 2.48 | 0.46 |
| 1:D:106:THR:HB | 2:D:2015:HOH:O | 2.15 | 0.46 |
| 1:E:186:MET:HE2 | 1:G:186:MET:CE | 2.41 | 0.46 |
| 1:E:246:LEU:HD21 | 2:E:2083:HOH:O | 2.15 | 0.46 |
| 1:F:254:VAL:O | 1:F:254:VAL:HG13 | 2.16 | 0.46 |
| 1:A:25:LEU:HD22 | 1:A:133:PRO:CG | 2.38 | 0.46 |
| 1:C:76:PHE:CE1 | 1:C:80:LEU:HD11 | 2.51 | 0.46 |
| 1:E:130:LEU:HD13 | 1:E:134:LEU:HG | 1.98 | 0.46 |
| 1:F:181:GLN:O | 1:F:185:VAL:HG23 | 2.15 | 0.46 |
| 1:F:221:HIS:HB2 | 2:F:2016:HOH:O | 2.15 | 0.46 |
| 1:G:154:GLU:O | 1:G:156:SER:N | 2.49 | 0.46 |
| 1:H:76:PHE:HE1 | 1:H:80:LEU:HD21 | 1.80 | 0.46 |
| 1:B:144:THR:HG21 | 1:B:149:TYR:CE1 | 2.51 | 0.46 |
| 1:C:174:PHE:HA | 2:C:2045:HOH:O | 2.15 | 0.46 |
| 1:C:218:THR:O | 1:C:219:ASN:HB2 | 2.15 | 0.46 |
| 1:D:178:VAL:HG12 | 1:D:179:GLN:N | 2.30 | 0.46 |
| 1:H:64:ARG:HD2 | 2:H:2016:HOH:O | 2.15 | 0.46 |
| 1:B:153:GLN:O | 1:B:154:GLU:CB | 2.64 | 0.46 |
| 1:B:194:TRP:C | 2:B:2036:HOH:O | 2.54 | 0.46 |
| 1:B:205:MET:SD | 1:B:246:LEU:HD22 | 2.55 | 0.46 |
| 1:B:48:GLU:HA | 2:B:2008:HOH:O | 2.15 | 0.46 |
| 1:E:12:LEU:CD2 | 1:E:32:HIS:HA | 2.45 | 0.46 |
| 1:F:96:LEU:CD2 | 1:F:171:MET:HA | 2.46 | 0.46 |
| 1:F:93:ARG:NH2 | 1:F:105:ARG:NH1 | 2.64 | 0.46 |
| 1:G:96:LEU:CD2 | 1:G:171:MET:HA | 2.46 | 0.46 |
| 1:G:5:LEU:HD11 | 1:G:83:ILE:HG13 | 1.98 | 0.46 |
| 1:H:224:ARG:NH2 | 2:H:2040:HOH:O | 2.24 | 0.46 |
| 1:H:87:VAL:HG12 | 1:H:112:VAL:HG22 | 1.97 | 0.46 |
| 1:A:161:GLN:CA | 1:A:169:GLN:O | 2.64 | 0.46 |
| 1:B:12:LEU:HD21 | 1:B:32:HIS:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:41:LEU:O | 1:D:45:LEU:HG | 2.16 | 0.46 |
| 1:G:12:LEU:HD21 | 1:G:32:HIS:HA | 1.97 | 0.46 |
| 1:G:130:LEU:HD23 | 1:G:149:TYR:CD2 | 2.51 | 0.46 |
| 1:G:19:VAL:HG12 | 1:G:21:THR:CG2 | 2.46 | 0.46 |
| 1:G:87:VAL:HG12 | 1:G:112:VAL:HG22 | 1.98 | 0.46 |
| 1:H:89:SER:O | 1:H:90:LEU:HD23 | 2.16 | 0.46 |
| 1:A:136:LEU:HD22 | 1:A:158:TRP:CH2 | 2.51 | 0.45 |
| 1:C:45:LEU:O | 1:C:45:LEU:HD12 | 2.16 | 0.45 |
| 1:D:89:SER:O | 1:D:90:LEU:HD23 | 2.16 | 0.45 |
| 1:F:225:TYR:HA | 1:F:229:HIS:O | 2.16 | 0.45 |
| 1:B:79:ALA:O | 1:B:80:LEU:C | 2.54 | 0.45 |
| 1:C:11:ARG:HH21 | 1:C:64:ARG:HA | 1.80 | 0.45 |
| 1:D:202:HIS:HA | 1:D:273:PHE:CE2 | 2.52 | 0.45 |
| 1:E:3:SER:O | 1:E:6:HIS:HB3 | 2.16 | 0.45 |
| 1:H:160:LEU:HD23 | 1:H:171:MET:CE | 2.46 | 0.45 |
| 1:A:138:ALA:O | 1:A:140:ILE:N | 2.46 | 0.45 |
| 1:A:152:MET:HG2 | 1:A:154:GLU:HG3 | 1.99 | 0.45 |
| 1:A:245:LEU:CD1 | 1:A:249:GLN:HB2 | 2.44 | 0.45 |
| 1:C:123:VAL:C | 1:C:129:THR:HG21 | 2.37 | 0.45 |
| 1:C:12:LEU:HD21 | 1:C:32:HIS:HA | 1.97 | 0.45 |
| 1:D:15:GLN:HE21 | 1:D:16:PRO:HD2 | 1.82 | 0.45 |
| 1:E:138:ALA:O | 1:E:140:ILE:N | 2.46 | 0.45 |
| 1:E:178:VAL:HA | 2:E:2027:HOH:O | 2.15 | 0.45 |
| 1:E:178:VAL:HG12 | 1:E:179:GLN:N | 2.30 | 0.45 |
| 1:G:144:THR:HG21 | 1:G:149:TYR:HE2 | 1.78 | 0.45 |
| 1:H:243:TYR:CZ | 1:H:254:VAL:HG21 | 2.52 | 0.45 |
| 1:H:60:LEU:HD12 | 1:H:75:LEU:HD22 | 1.97 | 0.45 |
| 1:A:96:LEU:HD23 | 1:A:171:MET:HA | 1.98 | 0.45 |
| 1:A:202:HIS:HA | 1:A:273:PHE:CE2 | 2.52 | 0.45 |
| 1:B:237:PRO:HG2 | 1:B:238:ASP:OD1 | 2.16 | 0.45 |
| 1:E:186:MET:CE | 1:G:186:MET:HE3 | 2.43 | 0.45 |
| 1:G:262:THR:HG21 | 2:G:2021:HOH:O | 2.16 | 0.45 |
| 1:B:200:ARG:HH12 | 1:D:200:ARG:HH12 | 1.65 | 0.45 |
| 1:B:45:LEU:O | 1:B:45:LEU:HD12 | 2.17 | 0.45 |
| 1:E:96:LEU:CD2 | 1:E:171:MET:HA | 2.47 | 0.45 |
| 1:E:201:HIS:O | 1:E:202:HIS:HB3 | 2.16 | 0.45 |
| 1:G:222:PHE:CZ | 1:G:249:GLN:HG2 | 2.52 | 0.45 |
| 1:G:11:ARG:HH21 | 1:G:64:ARG:CA | 2.29 | 0.45 |
| 1:H:68:TYR:OH | 1:H:188:ASN:ND2 | 2.50 | 0.45 |
| 1:B:33:ASN:OD1 | 1:B:131:THR:HA | 2.16 | 0.45 |
| 1:B:46:PRO:HG3 | 2:D:2011:HOH:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:225:TYR:HA | 1:C:229:HIS:O | 2.17 | 0.45 |
| 1:D:243:TYR:CE1 | 1:D:254:VAL:HG21 | 2.51 | 0.45 |
| 1:E:11:ARG:HH11 | 1:E:11:ARG:HG2 | 1.80 | 0.45 |
| 1:E:150:ARG:HG2 | 1:E:168:TRP:CZ3 | 2.52 | 0.45 |
| 1:F:144:THR:CG2 | 1:F:146:HIS:H | 2.22 | 0.45 |
| 1:F:41:LEU:O | 1:F:41:LEU:HD12 | 2.16 | 0.45 |
| 1:A:12:LEU:HD13 | 1:A:31:ALA:HB3 | 1.98 | 0.45 |
| 1:B:150:ARG:NH1 | 1:B:152:MET:CE | 2.80 | 0.45 |
| 1:B:15:GLN:NE2 | 1:B:16:PRO:HD2 | 2.31 | 0.45 |
| 1:F:163:ARG:HD2 | 1:F:166:GLU:HA | 1.99 | 0.45 |
| 1:F:237:PRO:HG2 | 1:F:238:ASP:OD1 | 2.16 | 0.45 |
| 1:F:69:CYS:HB2 | 1:F:70:PHE:H | 1.61 | 0.45 |
| 1:G:41:LEU:HD12 | 1:G:41:LEU:O | 2.17 | 0.45 |
| 1:H:107:HIS:CE1 | 1:H:125:PHE:HD1 | 2.35 | 0.45 |
| 1:B:220:PHE:CD1 | 1:B:242:LEU:HD22 | 2.52 | 0.45 |
| 1:B:46:PRO:O | 1:B:47:ARG:HB2 | 2.17 | 0.45 |
| 1:C:144:THR:HG21 | 1:C:149:TYR:HE2 | 1.82 | 0.45 |
| 1:E:160:LEU:CG | 1:E:171:MET:HE3 | 2.41 | 0.45 |
| 1:B:262:THR:N | 1:B:265:GLU:OE1 | 2.46 | 0.45 |
| 1:B:91:LEU:HG | 1:B:179:GLN:HG3 | 1.99 | 0.45 |
| 1:C:106:THR:HG21 | 2:C:2018:HOH:O | 2.15 | 0.45 |
| 1:D:125:PHE:H | 1:D:129:THR:CG2 | 2.29 | 0.45 |
| 1:F:11:ARG:HE | 1:F:64:ARG:HA | 1.80 | 0.45 |
| 1:G:152:MET:CG | 1:G:161:GLN:NE2 | 2.80 | 0.45 |
| 1:A:186:MET:HE2 | 1:D:186:MET:HE3 | 1.99 | 0.45 |
| 1:G:45:LEU:O | 1:G:45:LEU:HD12 | 2.17 | 0.45 |
| 1:H:55:ALA:HA | 2:H:2013:HOH:O | 2.17 | 0.45 |
| 1:D:201:HIS:CE1 | 2:D:2030:HOH:O | 2.69 | 0.44 |
| 1:D:96:LEU:C | 1:D:98:HIS:H | 2.20 | 0.44 |
| 1:G:15:GLN:HE21 | 1:G:16:PRO:HD2 | 1.81 | 0.44 |
| 1:H:222:PHE:CZ | 1:H:249:GLN:HG2 | 2.52 | 0.44 |
| 1:A:223:THR:HG22 | 1:A:225:TYR:CE1 | 2.51 | 0.44 |
| 1:F:258:LYS:HG2 | 1:F:259:HIS:CD2 | 2.52 | 0.44 |
| 1:F:4:PHE:CE2 | 1:F:78:ARG:HD3 | 2.53 | 0.44 |
| 1:G:117:GLU:HB2 | 2:G:2029:HOH:O | 2.16 | 0.44 |
| 1:H:96:LEU:CD2 | 1:H:171:MET:HA | 2.46 | 0.44 |
| 1:A:254:VAL:O | 1:A:254:VAL:HG13 | 2.17 | 0.44 |
| 1:B:87:VAL:HG13 | 1:B:112:VAL:HG13 | 1.99 | 0.44 |
| 1:D:102:LEU:HA | 1:D:103:PRO:HD3 | 1.72 | 0.44 |
| 1:D:149:TYR:N | 1:D:149:TYR:CD1 | 2.84 | 0.44 |
| 1:D:245:LEU:CD1 | 1:D:249:GLN:HB2 | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:76:PHE:HE1 | 1:D:80:LEU:HD21 | 1.80 | 0.44 |
| 1:E:105:ARG:HG3 | 2:E:2039:HOH:O | 2.17 | 0.44 |
| 1:E:126:GLY:O | 1:E:127:GLY:C | 2.56 | 0.44 |
| 1:E:176:LEU:HD12 | 1:E:176:LEU:N | 2.33 | 0.44 |
| 1:H:180:GLN:O | 1:H:183:ASP:N | 2.50 | 0.44 |
| 1:H:223:THR:HG22 | 1:H:225:TYR:CE1 | 2.52 | 0.44 |
| 1:H:23:GLU:OE1 | 1:H:26:ARG:HG3 | 2.17 | 0.44 |
| 1:B:144:THR:CG2 | 1:B:149:TYR:HE1 | 2.30 | 0.44 |
| 1:B:181:GLN:O | 1:B:185:VAL:HG23 | 2.17 | 0.44 |
| 1:D:226:HIS:HE1 | 1:D:227:GLN:HE21 | 1.65 | 0.44 |
| 1:F:33:ASN:OD1 | 1:F:131:THR:HA | 2.18 | 0.44 |
| 1:A:11:ARG:HH21 | 1:A:64:ARG:HA | 1.82 | 0.44 |
| 1:B:78:ARG:HD2 | 2:B:2010:HOH:O | 2.16 | 0.44 |
| 1:C:102:LEU:HA | 1:C:103:PRO:HD3 | 1.77 | 0.44 |
| 1:C:11:ARG:HH11 | 1:C:11:ARG:HG2 | 1.83 | 0.44 |
| 1:C:15:GLN:HE21 | 1:C:16:PRO:HD2 | 1.81 | 0.44 |
| 1:F:11:ARG:HH21 | 1:F:64:ARG:CA | 2.31 | 0.44 |
| 1:F:163:ARG:HD3 | 1:F:166:GLU:O | 2.18 | 0.44 |
| 1:G:33:ASN:OD1 | 1:G:131:THR:HA | 2.17 | 0.44 |
| 1:H:5:LEU:HD11 | 1:H:83:ILE:HG13 | 2.00 | 0.44 |
| 1:A:23:GLU:OE1 | 1:A:26:ARG:HG3 | 2.17 | 0.44 |
| 1:A:245:LEU:HD12 | 1:A:245:LEU:O | 2.18 | 0.44 |
| 1:B:41:LEU:HD12 | 1:B:41:LEU:O | 2.17 | 0.44 |
| 1:H:3:SER:O | 1:H:6:HIS:HB3 | 2.18 | 0.44 |
| 1:A:4:PHE:C | 1:A:6:HIS:N | 2.68 | 0.44 |
| 1:C:12:LEU:CD2 | 1:C:32:HIS:HA | 2.47 | 0.44 |
| 1:D:262:THR:N | 1:D:265:GLU:OE1 | 2.49 | 0.44 |
| 1:F:140:ILE:O | 1:F:140:ILE:HG22 | 2.17 | 0.44 |
| 1:F:220:PHE:CD1 | 1:F:242:LEU:HD22 | 2.53 | 0.44 |
| 1:F:46:PRO:O | 1:F:47:ARG:HB2 | 2.18 | 0.44 |
| 1:H:123:VAL:C | 1:H:129:THR:HG21 | 2.37 | 0.44 |
| 1:B:15:GLN:NE2 | 2:B:2003:HOH:O | 2.37 | 0.44 |
| 1:C:150:ARG:NH1 | 1:C:168:TRP:CG | 2.86 | 0.44 |
| 1:C:5:LEU:HD11 | 1:C:83:ILE:HG13 | 2.00 | 0.44 |
| 1:C:60:LEU:HB2 | 1:C:75:LEU:HD22 | 2.00 | 0.44 |
| 1:D:130:LEU:HD13 | 1:D:134:LEU:HG | 1.99 | 0.44 |
| 1:D:7:ALA:HB1 | 2:D:2002:HOH:O | 2.17 | 0.44 |
| 1:E:12:LEU:HD21 | 1:E:32:HIS:HA | 2.00 | 0.44 |
| 1:G:163:ARG:NH2 | 1:G:166:GLU:O | 2.51 | 0.44 |
| 1:H:0:HIS:CE1 | 2:H:2004:HOH:O | 2.71 | 0.44 |
| 1:H:11:ARG:HH21 | 1:H:64:ARG:HA | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:THR:CG2 | 1:A:208:HIS:ND1 | 2.80 | 0.44 |
| 1:A:197:SER:HA | 2:A:2039:HOH:O | 2.18 | 0.44 |
| 1:A:243:TYR:CE1 | 1:A:254:VAL:HG21 | 2.53 | 0.44 |
| 1:A:273:PHE:N | 1:A:273:PHE:CD1 | 2.82 | 0.44 |
| 1:B:150:ARG:HH12 | 1:B:152:MET:HE2 | 1.82 | 0.44 |
| 1:D:136:LEU:HD22 | 1:D:158:TRP:CE2 | 2.53 | 0.44 |
| 1:F:159:ILE:CG2 | 1:F:160:LEU:H | 2.30 | 0.44 |
| 1:G:125:PHE:H | 1:G:129:THR:CG2 | 2.31 | 0.44 |
| 1:A:12:LEU:CD2 | 1:A:32:HIS:HA | 2.48 | 0.43 |
| 1:A:1:MET:HE1 | 1:A:6:HIS:ND1 | 2.33 | 0.43 |
| 1:A:50:GLN:O | 1:A:51:LEU:HD23 | 2.18 | 0.43 |
| 1:B:164:HIS:N | 2:B:2030:HOH:O | 2.49 | 0.43 |
| 1:B:69:CYS:HB2 | 1:B:70:PHE:H | 1.62 | 0.43 |
| 1:C:4:PHE:C | 1:C:6:HIS:N | 2.71 | 0.43 |
| 1:C:4:PHE:O | 1:C:6:HIS:N | 2.50 | 0.43 |
| 1:D:160:LEU:CD2 | 1:D:171:MET:SD | 3.06 | 0.43 |
| 1:E:160:LEU:HD21 | 1:E:171:MET:HE1 | 2.00 | 0.43 |
| 1:G:243:TYR:CE1 | 1:G:254:VAL:HG21 | 2.53 | 0.43 |
| 1:G:50:GLN:HB2 | 1:G:55:ALA:CB | 2.48 | 0.43 |
| 1:H:25:LEU:HD13 | 1:H:133:PRO:CG | 2.48 | 0.43 |
| 1:C:3:SER:O | 1:C:6:HIS:HB3 | 2.18 | 0.43 |
| 1:C:83:ILE:CG2 | 1:C:83:ILE:O | 2.67 | 0.43 |
| 1:D:109:LEU:HD21 | 1:D:174:PHE:CE2 | 2.54 | 0.43 |
| 1:E:223:THR:HG22 | 1:E:225:TYR:CE1 | 2.53 | 0.43 |
| 1:F:79:ALA:O | 1:F:80:LEU:C | 2.54 | 0.43 |
| 1:G:202:HIS:O | 1:G:202:HIS:CD2 | 2.72 | 0.43 |
| 1:B:245:LEU:CD1 | 1:B:249:GLN:HB2 | 2.47 | 0.43 |
| 1:E:262:THR:OG1 | 1:E:264:ALA:N | 2.52 | 0.43 |
| 1:G:102:LEU:HB2 | 2:G:2027:HOH:O | 2.17 | 0.43 |
| 1:G:131:THR:CG2 | 1:G:208:HIS:ND1 | 2.82 | 0.43 |
| 1:G:72:LEU:HD12 | 1:G:124:GLY:HA2 | 2.00 | 0.43 |
| 1:G:76:PHE:HE1 | 1:G:80:LEU:HD21 | 1.83 | 0.43 |
| 1:G:91:LEU:HG | 1:G:179:GLN:HG3 | 2.00 | 0.43 |
| 1:B:140:ILE:O | 1:B:140:ILE:HG22 | 2.17 | 0.43 |
| 1:C:25:LEU:HD13 | 1:C:133:PRO:CG | 2.49 | 0.43 |
| 1:E:14:CYS:SG | 1:E:15:GLN:N | 2.92 | 0.43 |
| 1:E:243:TYR:CZ | 1:E:254:VAL:HG21 | 2.53 | 0.43 |
| 1:F:15:GLN:HE21 | 1:F:16:PRO:HD2 | 1.82 | 0.43 |
| 1:F:223:THR:HG22 | 1:F:225:TYR:CE1 | 2.53 | 0.43 |
| 1:H:238:ASP:OD2 | 1:H:240:PRO:HD2 | 2.19 | 0.43 |
| 1:A:103:PRO:HA | 2:A:2024:HOH:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:182:SER:HB2 | 1:C:104:PRO:CD | 2.47 | 0.43 |
| 1:C:4:PHE:CE2 | 1:C:78:ARG:HD3 | 2.54 | 0.43 |
| 1:F:125:PHE:O | 1:F:125:PHE:CD2 | 2.72 | 0.43 |
| 1:H:245:LEU:CD1 | 1:H:249:GLN:HB2 | 2.48 | 0.43 |
| 1:A:172:TYR:O | 1:A:172:TYR:CD1 | 2.71 | 0.43 |
| 1:A:243:TYR:CG | 1:A:263:GLU:HG3 | 2.53 | 0.43 |
| 1:B:28:LEU:O | 1:B:31:ALA:HB3 | 2.19 | 0.43 |
| 1:C:19:VAL:HG12 | 1:C:21:THR:CG2 | 2.49 | 0.43 |
| 1:C:262:THR:N | 1:C:265:GLU:OE1 | 2.49 | 0.43 |
| 1:E:4:PHE:C | 1:E:6:HIS:N | 2.72 | 0.43 |
| 1:F:207:ARG:NH1 | 1:F:249:GLN:O | 2.49 | 0.43 |
| 1:F:153:GLN:HE21 | 1:F:153:GLN:HB3 | 1.51 | 0.43 |
| 1:C:200:ARG:NH1 | 2:C:2052:HOH:O | 2.49 | 0.43 |
| 1:C:221:HIS:HB2 | 2:C:2066:HOH:O | 2.19 | 0.43 |
| 1:E:5:LEU:HA | 1:E:5:LEU:HD12 | 1.79 | 0.43 |
| 1:G:96:LEU:C | 1:G:98:HIS:H | 2.22 | 0.43 |
| 1:H:125:PHE:H | 1:H:129:THR:CG2 | 2.30 | 0.43 |
| 1:A:83:ILE:O | 1:A:83:ILE:HG22 | 2.18 | 0.43 |
| 1:B:165:HIS:ND1 | 1:B:165:HIS:C | 2.72 | 0.43 |
| 1:B:174:PHE:CD1 | 1:B:174:PHE:N | 2.87 | 0.43 |
| 1:C:139:GLU:OE2 | 1:C:152:MET:SD | 2.76 | 0.43 |
| 1:F:11:ARG:CD | 1:F:61:LEU:HA | 2.43 | 0.43 |
| 1:H:77:GLU:HB2 | 1:H:110:LEU:HD21 | 2.01 | 0.43 |
| 1:H:162:PHE:CD2 | 1:H:171:MET:HG3 | 2.53 | 0.43 |
| 1:A:225:TYR:HA | 1:A:229:HIS:O | 2.19 | 0.43 |
| 1:A:54:THR:O | 1:A:58:GLU:HG3 | 2.19 | 0.43 |
| 1:C:93:ARG:N | 1:C:173:CYS:O | 2.48 | 0.43 |
| 1:D:11:ARG:HH21 | 1:D:64:ARG:HA | 1.83 | 0.43 |
| 1:D:96:LEU:HD23 | 1:D:171:MET:HA | 2.01 | 0.43 |
| 1:D:68:TYR:OH | 1:D:188:ASN:ND2 | 2.52 | 0.43 |
| 1:D:76:PHE:CE1 | 1:D:80:LEU:HD21 | 2.54 | 0.43 |
| 1:F:226:HIS:HE1 | 1:F:227:GLN:HE21 | 1.66 | 0.43 |
| 1:G:149:TYR:HD1 | 1:G:162:PHE:CB | 2.32 | 0.43 |
| 1:H:14:CYS:SG | 1:H:15:GLN:N | 2.92 | 0.43 |
| 1:A:180:GLN:O | 1:A:181:GLN:C | 2.57 | 0.42 |
| 1:B:130:LEU:HD23 | 1:B:149:TYR:CE2 | 2.54 | 0.42 |
| 1:D:49:ILE:HG22 | 1:D:49:ILE:O | 2.18 | 0.42 |
| 1:E:33:ASN:OD1 | 1:E:131:THR:HA | 2.18 | 0.42 |
| 1:E:19:VAL:HG12 | 1:E:21:THR:CG2 | 2.48 | 0.42 |
| 1:F:200:ARG:HH12 | 1:G:200:ARG:HH12 | 1.66 | 0.42 |
| 1:A:164:HIS:ND1 | 1:A:165:HIS:CD2 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:76:PHE:CE1 | 1:A:80:LEU:HD21 | 2.54 | 0.42 |
| 1:B:190:TRP:CH2 | 1:B:194:TRP:CE2 | 3.07 | 0.42 |
| 1:B:49:ILE:HG22 | 1:B:49:ILE:O | 2.19 | 0.42 |
| 1:C:68:TYR:OH | 1:C:188:ASN:ND2 | 2.51 | 0.42 |
| 1:E:162:PHE:HD1 | 1:E:162:PHE:H | 1.66 | 0.42 |
| 1:E:207:ARG:NH1 | 1:E:249:GLN:O | 2.51 | 0.42 |
| 1:E:93:ARG:NH2 | 1:E:105:ARG:NH1 | 2.67 | 0.42 |
| 1:B:256:ASP:O | 1:B:257:VAL:C | 2.56 | 0.42 |
| 1:F:125:PHE:H | 1:F:129:THR:CG2 | 2.31 | 0.42 |
| 1:F:256:ASP:O | 1:F:257:VAL:C | 2.56 | 0.42 |
| 1:G:159:ILE:CG2 | 1:G:160:LEU:N | 2.82 | 0.42 |
| 1:H:150:ARG:HD3 | 1:H:152:MET:SD | 2.59 | 0.42 |
| 1:H:87:VAL:CG1 | 1:H:112:VAL:HG22 | 2.48 | 0.42 |
| 1:A:12:LEU:HD21 | 1:A:32:HIS:HA | 2.00 | 0.42 |
| 1:B:144:THR:HG21 | 1:B:149:TYR:HE1 | 1.84 | 0.42 |
| 1:D:231:VAL:O | 1:D:232:GLU:CB | 2.66 | 0.42 |
| 1:E:262:THR:HG23 | 1:E:265:GLU:CD | 2.40 | 0.42 |
| 1:E:200:ARG:NH1 | 1:H:200:ARG:HH12 | 2.15 | 0.42 |
| 1:H:207:ARG:NH1 | 1:H:249:GLN:O | 2.50 | 0.42 |
| 1:A:72:LEU:HD12 | 1:A:124:GLY:HA2 | 2.01 | 0.42 |
| 1:A:125:PHE:H | 1:A:129:THR:CG2 | 2.32 | 0.42 |
| 1:B:202:HIS:HB2 | 1:B:219:ASN:OD1 | 2.20 | 0.42 |
| 1:B:11:ARG:CD | 1:B:61:LEU:HA | 2.48 | 0.42 |
| 1:C:150:ARG:NH1 | 1:C:168:TRP:CB | 2.82 | 0.42 |
| 1:D:160:LEU:HD21 | 1:D:171:MET:SD | 2.60 | 0.42 |
| 1:D:45:LEU:O | 1:D:45:LEU:HD12 | 2.20 | 0.42 |
| 1:D:87:VAL:HG13 | 1:D:112:VAL:HG13 | 2.01 | 0.42 |
| 1:G:5:LEU:HD12 | 1:G:5:LEU:HA | 1.82 | 0.42 |
| 1:A:46:PRO:O | 1:A:47:ARG:HB2 | 2.20 | 0.42 |
| 1:B:109:LEU:CD1 | 1:B:109:LEU:C | 2.87 | 0.42 |
| 1:B:161:GLN:CG | 1:B:170:SER:HA | 2.38 | 0.42 |
| 1:D:60:LEU:HB2 | 1:D:75:LEU:HD22 | 2.01 | 0.42 |
| 1:G:12:LEU:CD2 | 1:G:32:HIS:HA | 2.50 | 0.42 |
| 1:G:178:VAL:HA | 2:G:2020:HOH:O | 2.19 | 0.42 |
| 1:G:225:TYR:HA | 1:G:229:HIS:O | 2.20 | 0.42 |
| 1:H:136:LEU:HD22 | 1:H:158:TRP:CZ2 | 2.54 | 0.42 |
| 1:B:259:HIS:N | 1:B:259:HIS:CD2 | 2.85 | 0.42 |
| 1:C:158:TRP:NE1 | 2:C:2043:HOH:O | 2.32 | 0.42 |
| 1:G:45:LEU:HB2 | 2:G:2013:HOH:O | 2.20 | 0.42 |
| 1:G:87:VAL:HG13 | 1:G:112:VAL:HG13 | 2.01 | 0.42 |
| 1:A:76:PHE:CE1 | 1:A:80:LEU:HD11 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:220:PHE:CD1 | 1:A:242:LEU:HD22 | 2.55 | 0.42 |
| 1:C:150:ARG:HH21 | 1:C:152:MET:HE1 | 1.82 | 0.42 |
| 1:D:33:ASN:OD1 | 1:D:131:THR:HA | 2.20 | 0.42 |
| 1:E:12:LEU:O | 1:E:13:HIS:C | 2.57 | 0.42 |
| 1:E:273:PHE:CD1 | 1:E:273:PHE:N | 2.84 | 0.42 |
| 1:E:4:PHE:O | 1:E:6:HIS:N | 2.53 | 0.42 |
| 1:F:122:ASP:O | 1:F:129:THR:CG2 | 2.66 | 0.42 |
| 1:F:45:LEU:CB | 2:F:2011:HOH:O | 2.61 | 0.42 |
| 1:F:46:PRO:CD | 2:F:2011:HOH:O | 2.11 | 0.42 |
| 1:F:5:LEU:HG | 1:F:9:PHE:CE2 | 2.55 | 0.42 |
| 1:C:130:LEU:HD23 | 1:C:149:TYR:CE2 | 2.55 | 0.42 |
| 1:C:150:ARG:NH2 | 1:C:152:MET:HE2 | 2.35 | 0.42 |
| 1:D:50:GLN:HB2 | 1:D:55:ALA:CB | 2.50 | 0.42 |
| 1:H:163:ARG:NH1 | 1:H:168:TRP:CG | 2.88 | 0.42 |
| 1:A:234:VAL:HG12 | 1:A:235:ASN:N | 2.34 | 0.41 |
| 1:A:59:LYS:HA | 1:A:259:HIS:ND1 | 2.34 | 0.41 |
| 1:A:45:LEU:HD12 | 1:A:45:LEU:O | 2.18 | 0.41 |
| 1:H:262:THR:OG1 | 1:H:264:ALA:N | 2.53 | 0.41 |
| 1:A:33:ASN:OD1 | 1:A:131:THR:HA | 2.20 | 0.41 |
| 1:D:123:VAL:C | 1:D:129:THR:HG21 | 2.40 | 0.41 |
| 1:D:12:LEU:HD21 | 1:D:32:HIS:HA | 2.02 | 0.41 |
| 1:F:132:ALA:O | 1:F:133:PRO:O | 2.38 | 0.41 |
| 1:G:163:ARG:CZ | 1:G:166:GLU:O | 2.65 | 0.41 |
| 1:H:163:ARG:NH1 | 1:H:168:TRP:CD1 | 2.88 | 0.41 |
| 1:A:102:LEU:HA | 1:A:103:PRO:HD3 | 1.74 | 0.41 |
| 1:A:138:ALA:HB2 | 1:A:153:GLN:HB2 | 2.03 | 0.41 |
| 1:A:231:VAL:O | 1:A:232:GLU:CB | 2.60 | 0.41 |
| 1:B:146:HIS:CE1 | 2:B:2027:HOH:O | 2.72 | 0.41 |
| 1:D:12:LEU:CD2 | 1:D:32:HIS:HA | 2.51 | 0.41 |
| 1:D:202:HIS:HD2 | 1:D:202:HIS:O | 2.04 | 0.41 |
| 1:G:53:GLU:HA | 2:G:2016:HOH:O | 2.21 | 0.41 |
| 1:G:76:PHE:CE1 | 1:G:80:LEU:HD21 | 2.56 | 0.41 |
| 1:G:96:LEU:HD23 | 1:G:170:SER:O | 2.20 | 0.41 |
| 1:H:243:TYR:CE1 | 1:H:254:VAL:HG21 | 2.55 | 0.41 |
| 1:H:11:ARG:HH21 | 1:H:64:ARG:C | 2.24 | 0.41 |
| 1:A:19:VAL:HA | 1:A:20:PRO:HD2 | 1.89 | 0.41 |
| 1:A:243:TYR:CZ | 1:A:254:VAL:HG21 | 2.55 | 0.41 |
| 1:A:4:PHE:O | 1:A:5:LEU:C | 2.58 | 0.41 |
| 1:A:5:LEU:HD12 | 1:A:5:LEU:HA | 1.84 | 0.41 |
| 1:B:12:LEU:CD2 | 1:B:32:HIS:HA | 2.51 | 0.41 |
| 1:B:53:GLU:HB3 | 2:B:2010:HOH:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:76:PHE:HE1 | 1:B:80:LEU:HD21 | 1.86 | 0.41 |
| 1:D:172:TYR:HD1 | 1:D:172:TYR:O | 2.03 | 0.41 |
| 1:F:109:LEU:CD1 | 1:F:109:LEU:C | 2.85 | 0.41 |
| 1:H:60:LEU:HB2 | 1:H:75:LEU:HD22 | 2.02 | 0.41 |
| 1:A:180:GLN:O | 1:A:183:ASP:N | 2.53 | 0.41 |
| 1:B:11:ARG:HH21 | 1:B:64:ARG:HA | 1.85 | 0.41 |
| 1:B:5:LEU:HD11 | 1:B:83:ILE:HG13 | 2.02 | 0.41 |
| 1:C:50:GLN:HB2 | 1:C:55:ALA:CB | 2.51 | 0.41 |
| 1:C:60:LEU:CB | 1:C:75:LEU:HD22 | 2.51 | 0.41 |
| 1:D:220:PHE:CD1 | 1:D:242:LEU:HD22 | 2.55 | 0.41 |
| 1:D:5:LEU:HD12 | 1:D:5:LEU:HA | 1.87 | 0.41 |
| 1:E:125:PHE:H | 1:E:129:THR:CG2 | 2.34 | 0.41 |
| 1:E:131:THR:CG2 | 1:E:208:HIS:ND1 | 2.83 | 0.41 |
| 1:G:109:LEU:CD1 | 1:G:109:LEU:C | 2.88 | 0.41 |
| 1:G:59:LYS:HA | 1:G:259:HIS:ND1 | 2.36 | 0.41 |
| 1:H:234:VAL:CG1 | 1:H:235:ASN:N | 2.83 | 0.41 |
| 1:A:19:VAL:HG12 | 1:A:21:THR:CG2 | 2.49 | 0.41 |
| 1:A:213:GLY:HA2 | 1:A:225:TYR:O | 2.21 | 0.41 |
| 1:B:4:PHE:CE2 | 1:B:78:ARG:HD3 | 2.55 | 0.41 |
| 1:C:144:THR:CG2 | 1:C:146:HIS:H | 2.25 | 0.41 |
| 1:C:243:TYR:CZ | 1:C:254:VAL:HG21 | 2.56 | 0.41 |
| 1:C:93:ARG:NH2 | 1:C:105:ARG:HH12 | 2.19 | 0.41 |
| 1:D:63:ALA:O | 1:D:253:GLY:HA3 | 2.20 | 0.41 |
| 1:G:223:THR:CG2 | 1:G:225:TYR:CE1 | 3.04 | 0.41 |
| 1:A:12:LEU:HD13 | 1:A:31:ALA:CB | 2.51 | 0.41 |
| 1:A:96:LEU:C | 1:A:98:HIS:N | 2.74 | 0.41 |
| 1:B:144:THR:CG2 | 1:B:146:HIS:H | 2.22 | 0.41 |
| 1:D:1:MET:HE1 | 1:D:6:HIS:ND1 | 2.34 | 0.41 |
| 1:E:200:ARG:HH12 | 1:H:200:ARG:NH1 | 2.14 | 0.41 |
| 1:E:238:ASP:OD2 | 1:E:240:PRO:HD2 | 2.20 | 0.41 |
| 1:E:63:ALA:O | 1:E:253:GLY:HA3 | 2.20 | 0.41 |
| 1:F:245:LEU:CD1 | 1:F:249:GLN:HB2 | 2.51 | 0.41 |
| 1:H:213:GLY:HA2 | 1:H:225:TYR:O | 2.20 | 0.41 |
| 1:B:162:PHE:N | 1:B:162:PHE:CD1 | 2.88 | 0.41 |
| 1:B:4:PHE:C | 1:B:6:HIS:N | 2.74 | 0.41 |
| 1:C:41:LEU:HB3 | 1:C:65:ARG:HH22 | 1.86 | 0.41 |
| 1:E:59:LYS:HB2 | 1:E:259:HIS:CE1 | 2.55 | 0.41 |
| 1:G:54:THR:N | 2:G:2016:HOH:O | 2.53 | 0.41 |
| 1:H:59:LYS:HG3 | 1:H:259:HIS:ND1 | 2.35 | 0.41 |
| 1:B:102:LEU:HA | 1:B:103:PRO:HD3 | 1.79 | 0.41 |
| 1:C:215:LEU:CD2 | 1:C:224:ARG:HG3 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:118:GLN:N | 2:E:2044:HOH:O | 2.52 | 0.41 |
| 1:E:202:HIS:HA | 1:E:273:PHE:CE2 | 2.56 | 0.41 |
| 1:G:269:VAL:HG13 | 2:G:2054:HOH:O | 2.20 | 0.41 |
| 1:A:172:TYR:C | 1:A:172:TYR:CD1 | 2.93 | 0.41 |
| 1:A:50:GLN:HB2 | 1:A:55:ALA:CB | 2.51 | 0.41 |
| 1:A:5:LEU:HD11 | 1:A:83:ILE:HG13 | 2.02 | 0.41 |
| 1:B:122:ASP:O | 1:B:129:THR:CG2 | 2.67 | 0.41 |
| 1:C:176:LEU:CB | 2:C:2028:HOH:O | 2.69 | 0.41 |
| 1:C:262:THR:HG23 | 1:C:265:GLU:CD | 2.41 | 0.41 |
| 1:C:12:LEU:HD13 | 1:C:31:ALA:CB | 2.51 | 0.41 |
| 1:B:200:ARG:NH1 | 1:D:200:ARG:HH12 | 2.18 | 0.41 |
| 1:D:90:LEU:HB2 | 1:D:109:LEU:CD1 | 2.51 | 0.41 |
| 1:E:180:GLN:O | 1:E:183:ASP:N | 2.53 | 0.41 |
| 1:F:28:LEU:HD23 | 1:F:28:LEU:HA | 1.94 | 0.41 |
| 1:G:57:GLU:N | 2:G:2016:HOH:O | 2.53 | 0.41 |
| 1:G:69:CYS:HB2 | 1:G:70:PHE:H | 1.61 | 0.41 |
| 1:H:63:ALA:O | 1:H:253:GLY:HA3 | 2.21 | 0.41 |
| 1:A:162:PHE:N | 1:A:162:PHE:CD1 | 2.89 | 0.41 |
| 1:C:163:ARG:NH1 | 1:C:167:HIS:HA | 2.32 | 0.41 |
| 1:C:222:PHE:CZ | 1:C:249:GLN:HG2 | 2.56 | 0.41 |
| 1:C:243:TYR:CG | 1:C:263:GLU:HG3 | 2.56 | 0.41 |
| 1:D:150:ARG:HB2 | 1:D:168:TRP:CZ3 | 2.56 | 0.41 |
| 1:H:234:VAL:HG12 | 1:H:235:ASN:N | 2.35 | 0.41 |
| 1:H:69:CYS:HB2 | 1:H:70:PHE:H | 1.70 | 0.41 |
| 1:A:55:ALA:HB1 | 2:A:2052:HOH:O | 2.21 | 0.40 |
| 1:A:41:LEU:HB3 | 1:A:65:ARG:HH22 | 1.86 | 0.40 |
| 1:B:15:GLN:HB3 | 2:B:2002:HOH:O | 2.20 | 0.40 |
| 1:B:195:PRO:HD2 | 2:B:2036:HOH:O | 2.21 | 0.40 |
| 1:B:61:LEU:HD21 | 1:B:75:LEU:HD21 | 2.02 | 0.40 |
| 1:D:148:GLU:HB3 | 1:D:163:ARG:HB2 | 2.03 | 0.40 |
| 1:E:239:VAL:N | 1:E:240:PRO:CD | 2.84 | 0.40 |
| 1:F:95:ILE:HG12 | 1:F:172:TYR:HA | 2.02 | 0.40 |
| 1:H:144:THR:CG2 | 1:H:149:TYR:HE1 | 2.33 | 0.40 |
| 1:H:162:PHE:CE2 | 1:H:171:MET:HG3 | 2.56 | 0.40 |
| 1:B:90:LEU:HB2 | 1:B:109:LEU:CD1 | 2.51 | 0.40 |
| 1:C:239:VAL:HB | 1:C:240:PRO:CD | 2.49 | 0.40 |
| 1:D:162:PHE:CD1 | 1:D:169:GLN:HB2 | 2.55 | 0.40 |
| 1:E:243:TYR:CE1 | 1:E:254:VAL:HG21 | 2.57 | 0.40 |
| 1:F:243:TYR:CE1 | 1:F:254:VAL:HG21 | 2.56 | 0.40 |
| 1:F:87:VAL:HG13 | 1:F:112:VAL:HG13 | 2.02 | 0.40 |
| 1:F:90:LEU:HB2 | 1:F:109:LEU:CD1 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:139:GLU:O | 1:G:140:ILE:C | 2.60 | 0.40 |
| 1:C:232:GLU:HB2 | 2:C:2065:HOH:O | 2.22 | 0.40 |
| 1:C:239:VAL:HG11 | 1:C:267:ALA:HB2 | 2.04 | 0.40 |
| 1:C:12:LEU:HD13 | 1:C:31:ALA:HB3 | 2.03 | 0.40 |
| 1:C:41:LEU:O | 1:C:45:LEU:HG | 2.21 | 0.40 |
| 1:C:96:LEU:C | 1:C:98:HIS:H | 2.23 | 0.40 |
| 1:D:12:LEU:HD13 | 1:D:31:ALA:HB3 | 2.03 | 0.40 |
| 1:D:235:ASN:O | 1:D:236:VAL:C | 2.58 | 0.40 |
| 1:E:79:ALA:O | 1:E:80:LEU:C | 2.59 | 0.40 |
| 1:E:83:ILE:HG22 | 1:E:83:ILE:O | 2.20 | 0.40 |
| 1:G:123:VAL:C | 1:G:129:THR:HG21 | 2.42 | 0.40 |
| 1:G:259:HIS:CD2 | 1:G:259:HIS:N | 2.89 | 0.40 |
| 1:G:63:ALA:HB1 | 2:G:2052:HOH:O | 2.22 | 0.40 |
| 1:H:149:TYR:HD2 | 1:H:162:PHE:HB3 | 1.83 | 0.40 |
| 1:B:166:GLU:HG2 | 1:G:233:GLN:CB | 2.29 | 0.40 |
| 1:B:96:LEU:C | 1:B:98:HIS:H | 2.25 | 0.40 |
| 1:C:125:PHE:CB | 1:C:129:THR:HG23 | 2.52 | 0.40 |
| 1:C:161:GLN:HB3 | 1:C:169:GLN:O | 2.21 | 0.40 |
| 1:A:189:PHE:CE2 | 1:D:189:PHE:CE2 | 3.10 | 0.40 |
| 1:F:102:LEU:HA | 1:F:103:PRO:HD3 | 1.72 | 0.40 |
| 1:F:138:ALA:HA | 1:F:151:LEU:O | 2.22 | 0.40 |
| 1:H:273:PHE:CD1 | 1:H:273:PHE:N | 2.88 | 0.40 |
| 1:A:161:GLN:HB3 | 1:A:169:GLN:O | 2.22 | 0.40 |
| 1:A:203:LEU:O | 1:A:204:LEU:HD23 | 2.22 | 0.40 |
| 1:B:213:GLY:HA2 | 1:B:225:TYR:O | 2.22 | 0.40 |
| 1:C:33:ASN:OD1 | 1:C:131:THR:HA | 2.22 | 0.40 |
| 1:C:243:TYR:CE1 | 1:C:254:VAL:HG21 | 2.56 | 0.40 |
| 1:D:19:VAL:HA | 1:D:20:PRO:HD2 | 1.92 | 0.40 |
| 1:E:205:MET:HG2 | 2:E:2014:HOH:O | 2.20 | 0.40 |
| 1:E:28:LEU:HD23 | 1:E:28:LEU:HA | 1.91 | 0.40 |
| 1:E:59:LYS:HG3 | 1:E:259:HIS:ND1 | 2.37 | 0.40 |
| 1:G:63:ALA:O | 1:G:253:GLY:HA3 | 2.21 | 0.40 |
| 1:H:1:MET:HE1 | 1:H:6:HIS:ND1 | 2.36 | 0.40 |
| 1:H:262:THR:HG23 | 1:H:265:GLU:OE1 | 2.22 | 0.40 |
| 1:H:87:VAL:HG13 | 1:H:112:VAL:HG13 | 2.02 | 0.40 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 1:F:6:HIS:ND1 | 1:F:62:TYR:OH[2_665] | 1.90 | 0.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------------|--------------------------|-------------------|
| 1:C:211:ASP:OD2 | 1:H:10:THR:O[4_556] | 1.92 | 0.28 |
| 1:B:6:HIS:ND1 | 1:B:62:TYR:OH[2_665] | 1.98 | 0.22 |
| 1:C:209:LEU:CD1 | 1:H:6:HIS:NE2[4_556] | 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 | 272/284 (96%) | 225 (83%) | 38 (14%) | 9 (3%) | 4 | 15 |
| 1 | B | 272/284 (96%) | 216 (79%) | 44 (16%) | 12 (4%) | 3 | 9 |
| 1 | C | 272/284 (96%) | 223 (82%) | 41 (15%) | 8 (3%) | 5 | 18 |
| 1 | D | 272/284 (96%) | 217 (80%) | 46 (17%) | 9 (3%) | 4 | 15 |
| 1 | E | 272/284 (96%) | 229 (84%) | 35 (13%) | 8 (3%) | 5 | 18 |
| 1 | F | 272/284 (96%) | 223 (82%) | 40 (15%) | 9 (3%) | 4 | 15 |
| 1 | G | 272/284 (96%) | 221 (81%) | 44 (16%) | 7 (3%) | 6 | 21 |
| 1 | H | 272/284 (96%) | 226 (83%) | 35 (13%) | 11 (4%) | 3 | 11 |
| All | All | 2176/2272 (96%) | 1780 (82%) | 323 (15%) | 73 (3%) | 4 | 15 |

All (73) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 69 | CYS |
| 1 | A | 256 | ASP |
| 1 | B | 69 | CYS |
| 1 | B | 140 | ILE |
| 1 | B | 165 | HIS |
| 1 | B | 166 | GLU |
| 1 | B | 256 | ASP |
| 1 | C | 54 | THR |
| 1 | C | 69 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 140 | ILE |
| 1 | C | 256 | ASP |
| 1 | D | 54 | THR |
| 1 | D | 69 | CYS |
| 1 | D | 140 | ILE |
| 1 | D | 256 | ASP |
| 1 | E | 54 | THR |
| 1 | E | 256 | ASP |
| 1 | F | 69 | CYS |
| 1 | F | 140 | ILE |
| 1 | F | 166 | GLU |
| 1 | F | 256 | ASP |
| 1 | G | 54 | THR |
| 1 | G | 69 | CYS |
| 1 | G | 140 | ILE |
| 1 | G | 256 | ASP |
| 1 | H | 69 | CYS |
| 1 | H | 140 | ILE |
| 1 | H | 164 | HIS |
| 1 | H | 165 | HIS |
| 1 | H | 256 | ASP |
| 1 | A | 54 | THR |
| 1 | A | 140 | ILE |
| 1 | B | 54 | THR |
| 1 | E | 69 | CYS |
| 1 | E | 140 | ILE |
| 1 | F | 54 | THR |
| 1 | G | 5 | LEU |
| 1 | G | 155 | GLY |
| 1 | H | 54 | THR |
| 1 | H | 166 | GLU |
| 1 | B | 154 | GLU |
| 1 | B | 168 | TRP |
| 1 | C | 165 | HIS |
| 1 | D | 5 | LEU |
| 1 | F | 165 | HIS |
| 1 | H | 152 | MET |
| 1 | A | 5 | LEU |
| 1 | C | 5 | LEU |
| 1 | C | 154 | GLU |
| 1 | D | 97 | SER |
| 1 | D | 116 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 16 | PRO |
| 1 | H | 116 | ASP |
| 1 | A | 97 | SER |
| 1 | B | 139 | GLU |
| 1 | B | 232 | GLU |
| 1 | E | 5 | LEU |
| 1 | E | 116 | ASP |
| 1 | E | 232 | GLU |
| 1 | F | 232 | GLU |
| 1 | H | 232 | GLU |
| 1 | A | 232 | GLU |
| 1 | B | 5 | LEU |
| 1 | C | 232 | GLU |
| 1 | D | 16 | PRO |
| 1 | D | 232 | GLU |
| 1 | A | 16 | PRO |
| 1 | E | 16 | PRO |
| 1 | B | 16 | PRO |
| 1 | A | 145 | PRO |
| 1 | F | 16 | PRO |
| 1 | H | 16 | PRO |
| 1 | F | 257 | VAL |

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 | 236/243 (97%) | 213 (90%) | 23 (10%) | 9 | 27 |
| 1 | B | 236/243 (97%) | 215 (91%) | 21 (9%) | 11 | 32 |
| 1 | C | 236/243 (97%) | 214 (91%) | 22 (9%) | 10 | 30 |
| 1 | D | 236/243 (97%) | 211 (89%) | 25 (11%) | 8 | 23 |
| 1 | E | 236/243 (97%) | 211 (89%) | 25 (11%) | 8 | 23 |
| 1 | F | 236/243 (97%) | 216 (92%) | 20 (8%) | 12 | 35 |
| 1 | G | 236/243 (97%) | 215 (91%) | 21 (9%) | 11 | 32 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | H | 236/243 (97%) | 216 (92%) | 20 (8%) | 12 | 35 |
| All | All | 1888/1944 (97%) | 1711 (91%) | 177 (9%) | 10 | 29 |

All (177) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1 | MET |
| 1 | A | 16 | PRO |
| 1 | A | 23 | GLU |
| 1 | A | 25 | LEU |
| 1 | A | 30 | LEU |
| 1 | A | 39 | GLU |
| 1 | A | 45 | LEU |
| 1 | A | 68 | TYR |
| 1 | A | 87 | VAL |
| 1 | A | 88 | ARG |
| 1 | A | 128 | GLN |
| 1 | A | 129 | THR |
| 1 | A | 144 | THR |
| 1 | A | 145 | PRO |
| 1 | A | 150 | ARG |
| 1 | A | 162 | PHE |
| 1 | A | 169 | GLN |
| 1 | A | 202 | HIS |
| 1 | A | 216 | THR |
| 1 | A | 237 | PRO |
| 1 | A | 248 | GLN |
| 1 | A | 254 | VAL |
| 1 | A | 262 | THR |
| 1 | B | 1 | MET |
| 1 | B | 16 | PRO |
| 1 | B | 23 | GLU |
| 1 | B | 25 | LEU |
| 1 | B | 30 | LEU |
| 1 | B | 39 | GLU |
| 1 | B | 45 | LEU |
| 1 | B | 68 | TYR |
| 1 | B | 87 | VAL |
| 1 | B | 88 | ARG |
| 1 | B | 128 | GLN |
| 1 | B | 129 | THR |
| 1 | B | 144 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 150 | ARG |
| 1 | B | 152 | MET |
| 1 | B | 162 | PHE |
| 1 | B | 202 | HIS |
| 1 | B | 216 | THR |
| 1 | B | 248 | GLN |
| 1 | B | 254 | VAL |
| 1 | B | 262 | THR |
| 1 | C | 1 | MET |
| 1 | C | 16 | PRO |
| 1 | C | 23 | GLU |
| 1 | C | 25 | LEU |
| 1 | C | 30 | LEU |
| 1 | C | 39 | GLU |
| 1 | C | 45 | LEU |
| 1 | C | 68 | TYR |
| 1 | C | 87 | VAL |
| 1 | C | 88 | ARG |
| 1 | C | 128 | GLN |
| 1 | C | 129 | THR |
| 1 | C | 144 | THR |
| 1 | C | 145 | PRO |
| 1 | C | 166 | GLU |
| 1 | C | 169 | GLN |
| 1 | C | 172 | TYR |
| 1 | C | 216 | THR |
| 1 | C | 237 | PRO |
| 1 | C | 248 | GLN |
| 1 | C | 254 | VAL |
| 1 | C | 262 | THR |
| 1 | D | 1 | MET |
| 1 | D | 16 | PRO |
| 1 | D | 23 | GLU |
| 1 | D | 25 | LEU |
| 1 | D | 30 | LEU |
| 1 | D | 39 | GLU |
| 1 | D | 45 | LEU |
| 1 | D | 68 | TYR |
| 1 | D | 87 | VAL |
| 1 | D | 88 | ARG |
| 1 | D | 128 | GLN |
| 1 | D | 129 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 144 | THR |
| 1 | D | 145 | PRO |
| 1 | D | 150 | ARG |
| 1 | D | 152 | MET |
| 1 | D | 162 | PHE |
| 1 | D | 172 | TYR |
| 1 | D | 174 | PHE |
| 1 | D | 175 | ASP |
| 1 | D | 202 | HIS |
| 1 | D | 216 | THR |
| 1 | D | 248 | GLN |
| 1 | D | 254 | VAL |
| 1 | D | 262 | THR |
| 1 | E | 1 | MET |
| 1 | E | 16 | PRO |
| 1 | E | 23 | GLU |
| 1 | E | 25 | LEU |
| 1 | E | 30 | LEU |
| 1 | E | 39 | GLU |
| 1 | E | 45 | LEU |
| 1 | E | 68 | TYR |
| 1 | E | 76 | PHE |
| 1 | E | 87 | VAL |
| 1 | E | 88 | ARG |
| 1 | E | 128 | GLN |
| 1 | E | 129 | THR |
| 1 | E | 144 | THR |
| 1 | E | 145 | PRO |
| 1 | E | 157 | THR |
| 1 | E | 160 | LEU |
| 1 | E | 162 | PHE |
| 1 | E | 163 | ARG |
| 1 | E | 164 | HIS |
| 1 | E | 202 | HIS |
| 1 | E | 216 | THR |
| 1 | E | 248 | GLN |
| 1 | E | 254 | VAL |
| 1 | E | 262 | THR |
| 1 | F | 16 | PRO |
| 1 | F | 23 | GLU |
| 1 | F | 25 | LEU |
| 1 | F | 30 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 39 | GLU |
| 1 | F | 68 | TYR |
| 1 | F | 87 | VAL |
| 1 | F | 88 | ARG |
| 1 | F | 128 | GLN |
| 1 | F | 129 | THR |
| 1 | F | 144 | THR |
| 1 | F | 153 | GLN |
| 1 | F | 160 | LEU |
| 1 | F | 163 | ARG |
| 1 | F | 165 | HIS |
| 1 | F | 202 | HIS |
| 1 | F | 216 | THR |
| 1 | F | 248 | GLN |
| 1 | F | 254 | VAL |
| 1 | F | 262 | THR |
| 1 | G | 16 | PRO |
| 1 | G | 23 | GLU |
| 1 | G | 25 | LEU |
| 1 | G | 30 | LEU |
| 1 | G | 39 | GLU |
| 1 | G | 45 | LEU |
| 1 | G | 68 | TYR |
| 1 | G | 87 | VAL |
| 1 | G | 88 | ARG |
| 1 | G | 128 | GLN |
| 1 | G | 129 | THR |
| 1 | G | 144 | THR |
| 1 | G | 145 | PRO |
| 1 | G | 151 | LEU |
| 1 | G | 169 | GLN |
| 1 | G | 202 | HIS |
| 1 | G | 216 | THR |
| 1 | G | 237 | PRO |
| 1 | G | 248 | GLN |
| 1 | G | 254 | VAL |
| 1 | G | 262 | THR |
| 1 | H | 16 | PRO |
| 1 | H | 23 | GLU |
| 1 | H | 25 | LEU |
| 1 | H | 30 | LEU |
| 1 | H | 39 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 45 | LEU |
| 1 | H | 68 | TYR |
| 1 | H | 87 | VAL |
| 1 | H | 88 | ARG |
| 1 | H | 128 | GLN |
| 1 | H | 129 | THR |
| 1 | H | 144 | THR |
| 1 | H | 145 | PRO |
| 1 | H | 152 | MET |
| 1 | H | 166 | GLU |
| 1 | H | 202 | HIS |
| 1 | H | 216 | THR |
| 1 | H | 248 | GLN |
| 1 | H | 254 | VAL |
| 1 | H | 262 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 15 | GLN |
| 1 | A | 86 | ASN |
| 1 | A | 128 | GLN |
| 1 | A | 153 | GLN |
| 1 | A | 165 | HIS |
| 1 | A | 167 | HIS |
| 1 | A | 169 | GLN |
| 1 | A | 184 | HIS |
| 1 | A | 188 | ASN |
| 1 | A | 198 | HIS |
| 1 | A | 202 | HIS |
| 1 | A | 226 | HIS |
| 1 | A | 244 | GLN |
| 1 | B | 15 | GLN |
| 1 | B | 86 | ASN |
| 1 | B | 128 | GLN |
| 1 | B | 153 | GLN |
| 1 | B | 184 | HIS |
| 1 | B | 188 | ASN |
| 1 | B | 198 | HIS |
| 1 | B | 202 | HIS |
| 1 | B | 221 | HIS |
| 1 | B | 226 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 244 | GLN |
| 1 | C | 15 | GLN |
| 1 | C | 86 | ASN |
| 1 | C | 128 | GLN |
| 1 | C | 169 | GLN |
| 1 | C | 184 | HIS |
| 1 | C | 188 | ASN |
| 1 | C | 198 | HIS |
| 1 | C | 202 | HIS |
| 1 | C | 226 | HIS |
| 1 | C | 244 | GLN |
| 1 | D | 15 | GLN |
| 1 | D | 86 | ASN |
| 1 | D | 128 | GLN |
| 1 | D | 161 | GLN |
| 1 | D | 184 | HIS |
| 1 | D | 188 | ASN |
| 1 | D | 198 | HIS |
| 1 | D | 202 | HIS |
| 1 | D | 226 | HIS |
| 1 | D | 244 | GLN |
| 1 | E | 15 | GLN |
| 1 | E | 86 | ASN |
| 1 | E | 128 | GLN |
| 1 | E | 184 | HIS |
| 1 | E | 188 | ASN |
| 1 | E | 226 | HIS |
| 1 | E | 244 | GLN |
| 1 | F | 15 | GLN |
| 1 | F | 86 | ASN |
| 1 | F | 128 | GLN |
| 1 | F | 153 | GLN |
| 1 | F | 161 | GLN |
| 1 | F | 184 | HIS |
| 1 | F | 188 | ASN |
| 1 | F | 198 | HIS |
| 1 | F | 221 | HIS |
| 1 | F | 226 | HIS |
| 1 | F | 244 | GLN |
| 1 | G | 15 | GLN |
| 1 | G | 86 | ASN |
| 1 | G | 128 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 161 | GLN |
| 1 | G | 169 | GLN |
| 1 | G | 184 | HIS |
| 1 | G | 188 | ASN |
| 1 | G | 198 | HIS |
| 1 | G | 202 | HIS |
| 1 | G | 226 | HIS |
| 1 | G | 244 | GLN |
| 1 | H | 15 | GLN |
| 1 | H | 86 | ASN |
| 1 | H | 128 | GLN |
| 1 | H | 161 | GLN |
| 1 | H | 165 | HIS |
| 1 | H | 184 | HIS |
| 1 | H | 188 | ASN |
| 1 | H | 198 | HIS |
| 1 | H | 202 | HIS |
| 1 | H | 221 | HIS |
| 1 | H | 226 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 | 274/284 (96%) | 0.22 | 4 (1%) 74 67 | 47, 79, 110, 122 | 0 |
| 1 | B | 274/284 (96%) | 0.23 | 6 (2%) 62 52 | 54, 77, 106, 119 | 0 |
| 1 | C | 274/284 (96%) | 0.30 | 15 (5%) 26 17 | 54, 79, 113, 121 | 0 |
| 1 | D | 274/284 (96%) | 0.45 | 16 (5%) 24 15 | 49, 93, 116, 121 | 0 |
| 1 | E | 274/284 (96%) | -0.09 | 1 (0%) 92 90 | 37, 59, 87, 119 | 0 |
| 1 | F | 274/284 (96%) | 0.23 | 10 (3%) 43 32 | 45, 70, 104, 119 | 0 |
| 1 | G | 274/284 (96%) | 0.13 | 4 (1%) 74 67 | 39, 77, 106, 120 | 0 |
| 1 | H | 274/284 (96%) | 0.15 | 11 (4%) 39 28 | 47, 78, 109, 120 | 0 |
| All | All | 2192/2272 (96%) | 0.20 | 67 (3%) 49 38 | 37, 76, 110, 122 | 0 |

All (67) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 2 | THR | 6.5 |
| 1 | A | 0 | HIS | 6.5 |
| 1 | H | 0 | HIS | 5.8 |
| 1 | F | 0 | HIS | 5.3 |
| 1 | G | 0 | HIS | 5.1 |
| 1 | D | 0 | HIS | 5.1 |
| 1 | C | 211 | ASP | 4.9 |
| 1 | B | 0 | HIS | 4.7 |
| 1 | D | 165 | HIS | 4.5 |
| 1 | D | 15 | GLN | 4.4 |
| 1 | D | 19 | VAL | 4.3 |
| 1 | C | 114 | VAL | 4.1 |
| 1 | B | 165 | HIS | 3.9 |
| 1 | H | 19 | VAL | 3.9 |
| 1 | E | 165 | HIS | 3.6 |
| 1 | C | 0 | HIS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 165 | HIS | 3.3 |
| 1 | F | 116 | ASP | 3.2 |
| 1 | D | 230 | ALA | 3.1 |
| 1 | D | 227 | GLN | 3.0 |
| 1 | F | 98 | HIS | 3.0 |
| 1 | D | 119 | TRP | 2.9 |
| 1 | F | 114 | VAL | 2.9 |
| 1 | D | 229 | HIS | 2.8 |
| 1 | F | 136 | LEU | 2.7 |
| 1 | C | 141 | ALA | 2.7 |
| 1 | H | 225 | TYR | 2.7 |
| 1 | B | 152 | MET | 2.7 |
| 1 | C | 86 | ASN | 2.7 |
| 1 | F | 140 | ILE | 2.7 |
| 1 | C | 167 | HIS | 2.7 |
| 1 | H | 165 | HIS | 2.7 |
| 1 | H | 114 | VAL | 2.6 |
| 1 | C | 20 | PRO | 2.6 |
| 1 | H | 169 | GLN | 2.6 |
| 1 | H | 227 | GLN | 2.5 |
| 1 | A | 114 | VAL | 2.5 |
| 1 | F | 69 | CYS | 2.5 |
| 1 | A | 163 | ARG | 2.4 |
| 1 | C | 99 | PRO | 2.4 |
| 1 | C | 210 | PRO | 2.4 |
| 1 | D | 210 | PRO | 2.4 |
| 1 | F | 161 | GLN | 2.4 |
| 1 | D | 99 | PRO | 2.3 |
| 1 | D | 62 | TYR | 2.3 |
| 1 | G | 162 | PHE | 2.3 |
| 1 | H | 167 | HIS | 2.3 |
| 1 | D | 102 | LEU | 2.3 |
| 1 | H | 231 | VAL | 2.2 |
| 1 | B | 142 | GLN | 2.2 |
| 1 | D | 139 | GLU | 2.2 |
| 1 | C | 19 | VAL | 2.2 |
| 1 | C | 83 | ILE | 2.1 |
| 1 | D | 228 | GLY | 2.1 |
| 1 | B | 6 | HIS | 2.1 |
| 1 | C | 229 | HIS | 2.1 |
| 1 | H | 230 | ALA | 2.1 |
| 1 | G | 244 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 116 | ASP | 2.1 |
| 1 | F | 82 | ASP | 2.1 |
| 1 | D | 234 | VAL | 2.1 |
| 1 | F | 153 | GLN | 2.0 |
| 1 | B | 98 | HIS | 2.0 |
| 1 | D | 81 | ARG | 2.0 |
| 1 | H | 229 | HIS | 2.0 |
| 1 | G | 186 | MET | 2.0 |
| 1 | A | 1 | MET | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.