



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:39 am BST

PDB ID : 2WLN
Title : POTASSIUM CHANNEL FROM MAGNETOSPIRILLUM MAGNETO-TACTICUM
Authors : Clarke, O.B.; Caputo, A.T.; Smith, B.J.; Gulbis, J.M.
Deposited on : 2009-06-24
Resolution : 3.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

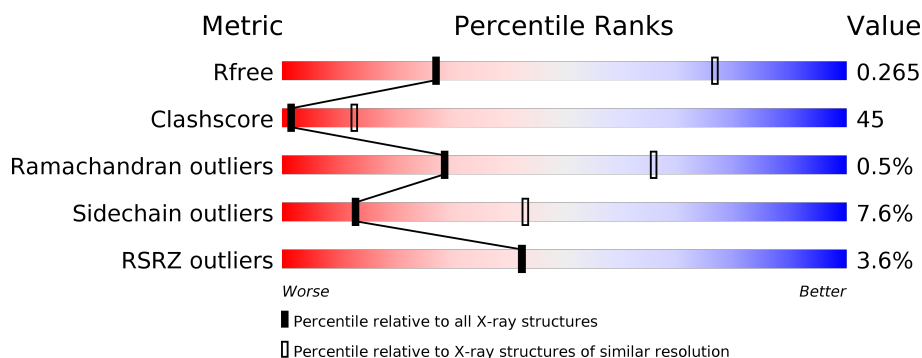
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1278 (3.50-3.38) |
| Clashscore | 141614 | 1361 (3.50-3.38) |
| Ramachandran outliers | 138981 | 1327 (3.50-3.38) |
| Sidechain outliers | 138945 | 1328 (3.50-3.38) |
| RSRZ outliers | 127900 | 1192 (3.50-3.38) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 301 | <div> <div>4%</div> <div> <div></div> <div>39%</div> <div>50%</div> <div>5%</div> <div>6%</div> </div> </div> |
| 1 | B | 301 | <div> <div>3%</div> <div> <div></div> <div>43%</div> <div>46%</div> <div>5%</div> <div>6%</div> </div> </div> |
| 1 | C | 301 | <div> <div>2%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>6%</div> <div>6%</div> </div> </div> |
| 1 | D | 301 | <div> <div>3%</div> <div> <div></div> <div>45%</div> <div>43%</div> <div>6%</div> <div>6%</div> </div> </div> |
| 1 | E | 301 | <div> <div>4%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>7%</div> <div>6%</div> </div> </div> |
| 1 | F | 301 | <div> <div>4%</div> <div> <div></div> <div>43%</div> <div>45%</div> <div>6%</div> <div>6%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | G | 301 | <div><div></div><div>4%</div><div>42%</div><div>47%</div><div>5%</div><div>6%</div></div> |
| 1 | H | 301 | <div><div></div><div>3%</div><div>44%</div><div>44%</div><div>7%</div><div>6%</div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17667 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 POTASSIUM CHANNEL.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2206 | 1417 | 383 | 398 | 8 | | | |
| 1 | B | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2205 | 1418 | 380 | 398 | 9 | | | |
| 1 | C | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2205 | 1418 | 380 | 398 | 9 | | | |
| 1 | D | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2214 | 1426 | 381 | 398 | 9 | | | |
| 1 | E | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2209 | 1421 | 381 | 398 | 9 | | | |
| 1 | F | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2209 | 1419 | 383 | 398 | 9 | | | |
| 1 | G | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2205 | 1418 | 380 | 398 | 9 | | | |
| 1 | H | 283 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2208 | 1419 | 382 | 398 | 9 | | | |

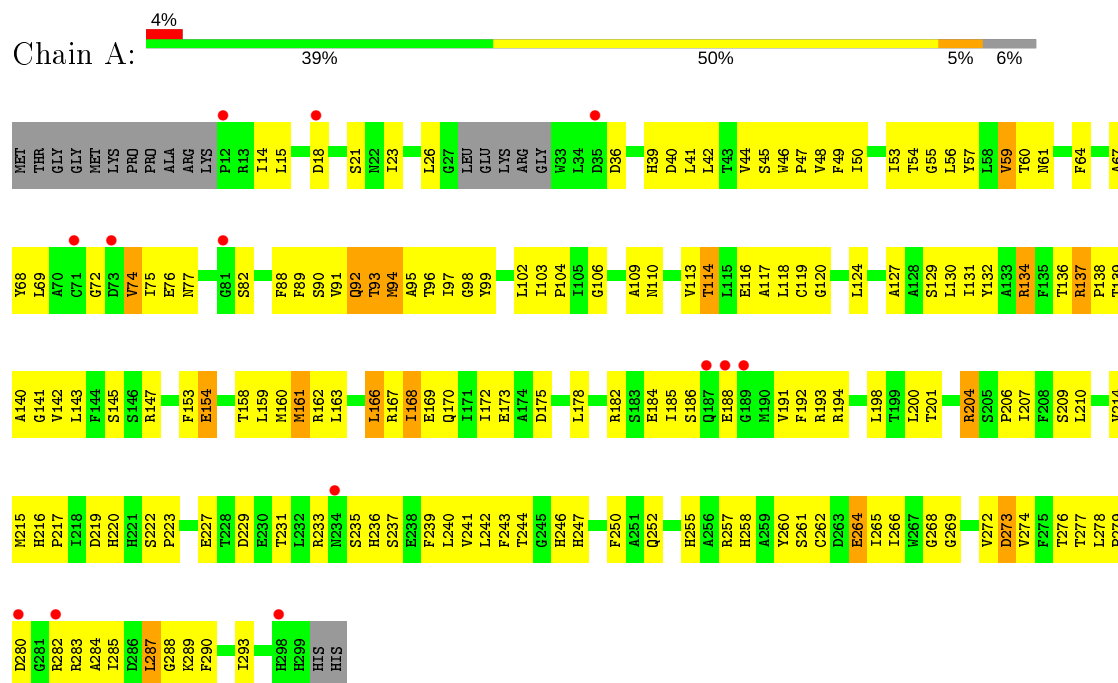
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2 | H | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | A | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |
| 2 | C | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | F | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

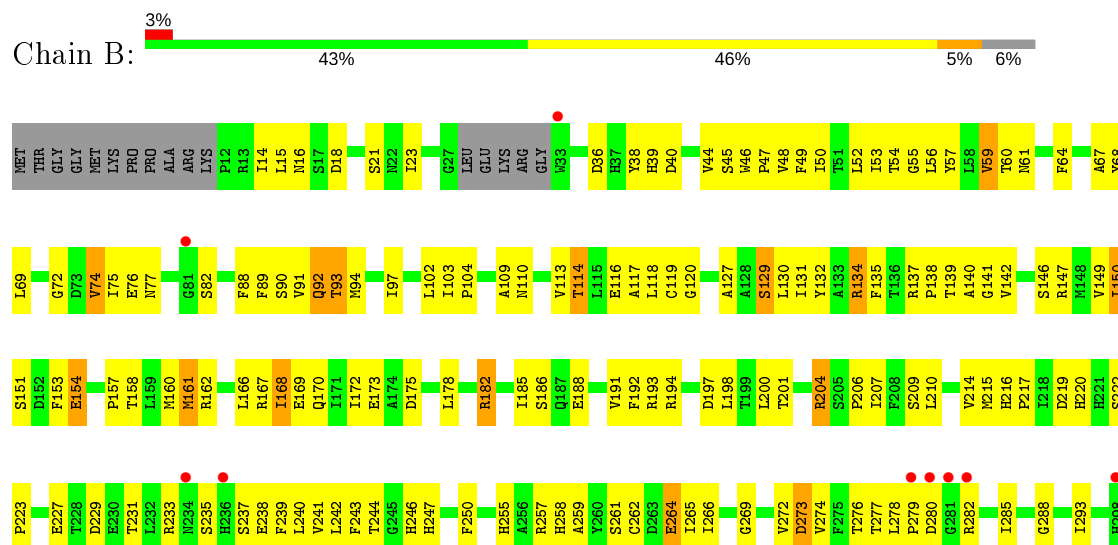
3 Residue-property plots [i](#)

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: POTASSIUM CHANNEL

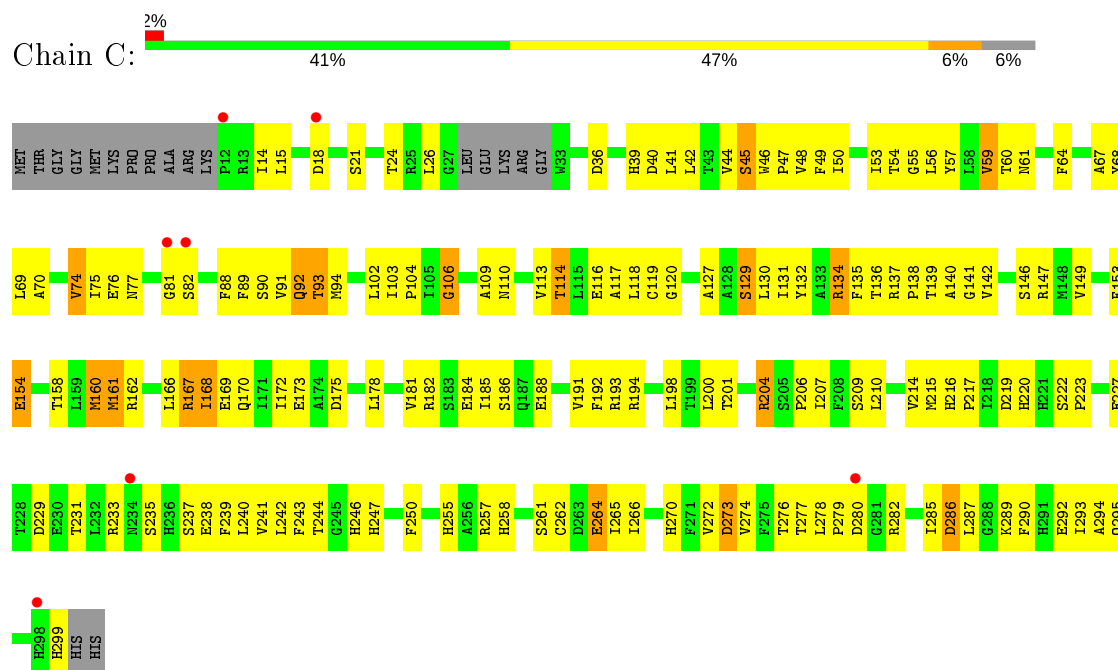


• Molecule 1: POTASSIUM CHANNEL

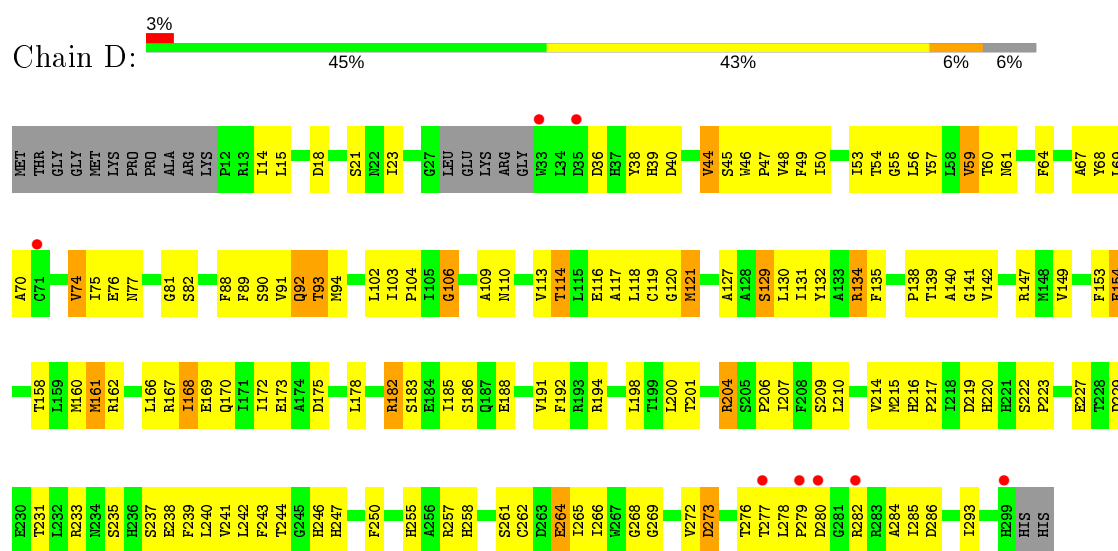




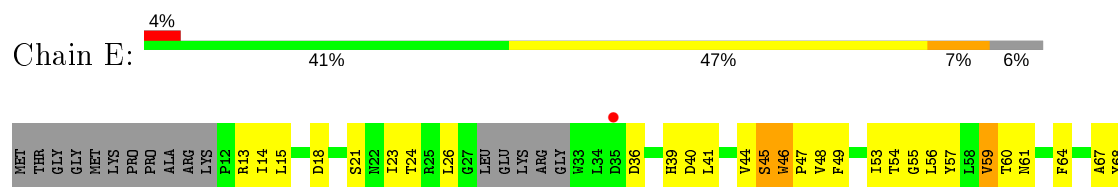
• Molecule 1: POTASSIUM CHANNEL

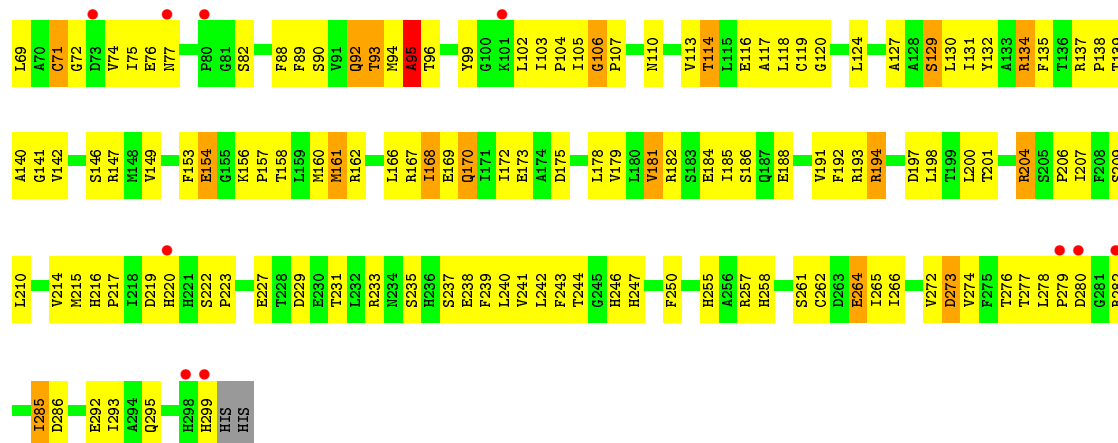


• Molecule 1: POTASSIUM CHANNEL

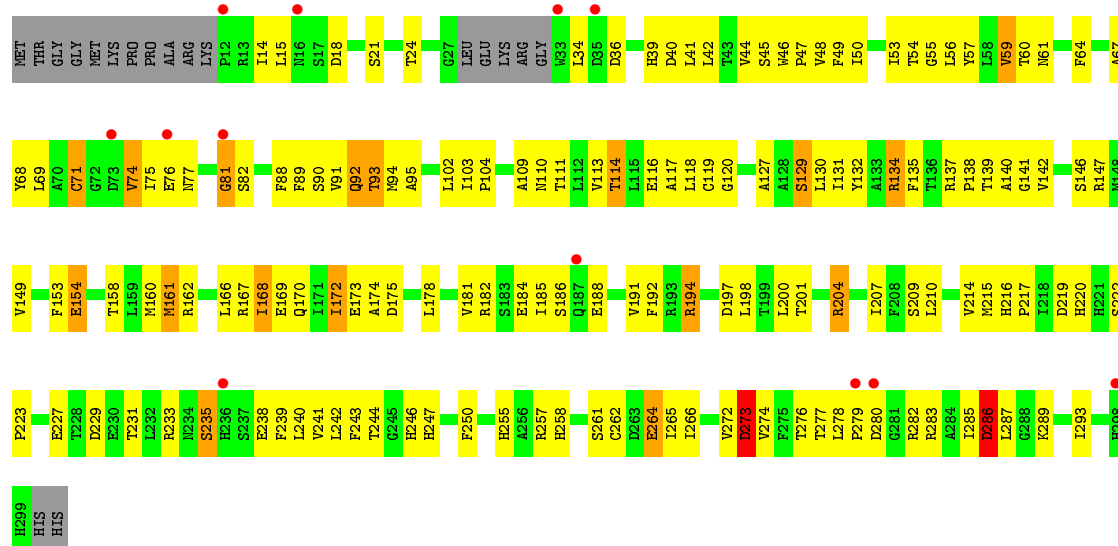
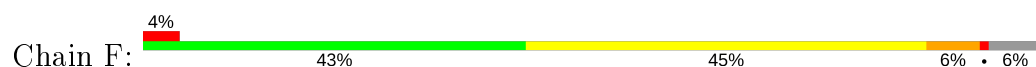


• Molecule 1: POTASSIUM CHANNEL

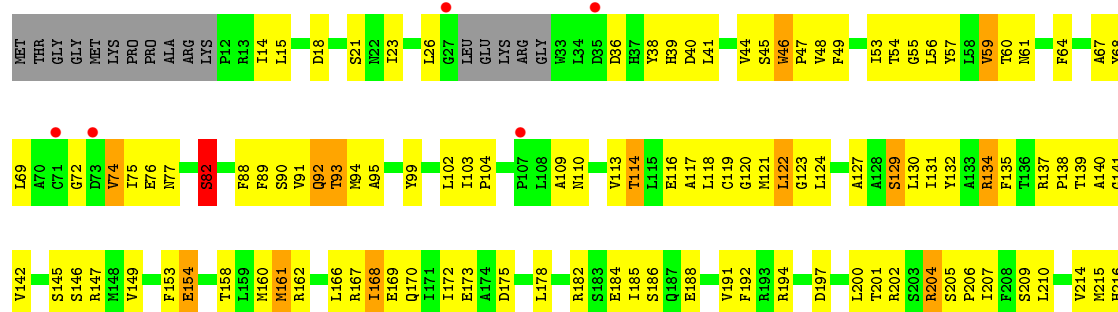


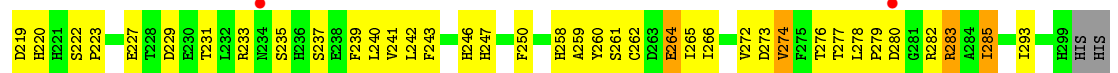


• Molecule 1: POTASSIUM CHANNEL



• Molecule 1: POTASSIUM CHANNEL





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 106.68 Å 109.06 Å 146.39 Å 73.95° 82.30° 89.88° | Depositor |
| Resolution (Å) | 15.00 – 3.44 15.00 – 3.44 | Depositor EDS |
| % Data completeness (in resolution range) | 93.2 (15.00-3.44) 75.7 (15.00-3.44) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.61 (at 3.48 Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, R_{free} | 0.266 , 0.273 0.257 , 0.265 | Depositor DCC |
| R_{free} test set | 3197 reflections (5.13%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 93.9 | Xtriage |
| Anisotropy | 0.020 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 65.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 17667 | wwPDB-VP |
| Average B, all atoms (Å ²) | 121.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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 | 1.13 | 8/2263 (0.4%) | 0.78 | 6/3082 (0.2%) |
| 1 | B | 0.87 | 7/2262 (0.3%) | 0.71 | 1/3080 (0.0%) |
| 1 | C | 0.75 | 4/2262 (0.2%) | 0.81 | 9/3080 (0.3%) |
| 1 | D | 0.85 | 6/2273 (0.3%) | 0.88 | 8/3096 (0.3%) |
| 1 | E | 1.04 | 10/2266 (0.4%) | 0.84 | 11/3084 (0.4%) |
| 1 | F | 0.78 | 6/2266 (0.3%) | 1.00 | 13/3085 (0.4%) |
| 1 | G | 0.95 | 7/2262 (0.3%) | 0.69 | 0/3080 |
| 1 | H | 0.89 | 7/2264 (0.3%) | 0.86 | 11/3081 (0.4%) |
| All | All | 0.92 | 55/18118 (0.3%) | 0.83 | 59/24668 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | B | 0 | 1 |
| 1 | C | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | F | 0 | 4 |
| 1 | G | 0 | 1 |
| All | All | 0 | 8 |

All (55) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | A | 287 | LEU | C-N | -32.15 | 0.75 | 1.33 |
| 1 | E | 71 | CYS | C-N | 20.88 | 1.70 | 1.33 |
| 1 | G | 122 | LEU | C-N | -20.53 | 0.96 | 1.33 |
| 1 | A | 94 | MET | C-N | -20.27 | 0.87 | 1.34 |
| 1 | G | 287 | LEU | C-N | -20.22 | 0.96 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | H | 82 | SER | C-N | -20.21 | 0.87 | 1.34 |
| 1 | E | 106 | GLY | C-N | 19.34 | 1.71 | 1.34 |
| 1 | B | 157 | PRO | C-N | -17.95 | 0.92 | 1.34 |
| 1 | D | 182 | ARG | C-N | 15.61 | 1.70 | 1.34 |
| 1 | H | 274 | VAL | C-N | -14.08 | 1.01 | 1.34 |
| 1 | F | 172 | ILE | C-N | -13.69 | 1.02 | 1.34 |
| 1 | B | 150 | ILE | C-N | 13.65 | 1.65 | 1.34 |
| 1 | E | 95 | ALA | C-N | -13.36 | 1.03 | 1.34 |
| 1 | E | 285 | ILE | C-N | -12.72 | 1.04 | 1.34 |
| 1 | B | 273 | ASP | C-N | 12.62 | 1.63 | 1.34 |
| 1 | D | 273 | ASP | C-N | 12.50 | 1.62 | 1.34 |
| 1 | C | 70 | ALA | C-N | 12.43 | 1.62 | 1.34 |
| 1 | A | 268 | GLY | C-N | 11.73 | 1.54 | 1.33 |
| 1 | E | 137 | ARG | C-N | 10.75 | 1.54 | 1.34 |
| 1 | F | 81 | GLY | C-N | -9.82 | 1.11 | 1.34 |
| 1 | A | 106 | GLY | C-N | -9.70 | 1.15 | 1.34 |
| 1 | A | 159 | LEU | C-N | 9.66 | 1.56 | 1.34 |
| 1 | D | 268 | GLY | C-N | 9.61 | 1.50 | 1.33 |
| 1 | D | 106 | GLY | C-N | -9.47 | 1.16 | 1.34 |
| 1 | G | 95 | ALA | C-N | 9.35 | 1.55 | 1.34 |
| 1 | G | 46 | TRP | C-N | -9.25 | 1.16 | 1.34 |
| 1 | D | 70 | ALA | C-N | 9.10 | 1.54 | 1.34 |
| 1 | A | 166 | LEU | C-N | 8.83 | 1.54 | 1.34 |
| 1 | B | 288 | GLY | C-N | -8.68 | 1.14 | 1.34 |
| 1 | H | 260 | TYR | C-N | 8.65 | 1.53 | 1.34 |
| 1 | H | 195 | PHE | C-N | -8.34 | 1.14 | 1.34 |
| 1 | A | 273 | ASP | C-N | -7.72 | 1.16 | 1.34 |
| 1 | D | 286 | ASP | C-N | -7.68 | 1.16 | 1.34 |
| 1 | G | 137 | ARG | C-N | 7.52 | 1.48 | 1.34 |
| 1 | G | 82 | SER | C-N | -7.48 | 1.16 | 1.34 |
| 1 | C | 81 | GLY | C-N | -7.45 | 1.17 | 1.34 |
| 1 | F | 71 | CYS | C-N | 7.19 | 1.46 | 1.33 |
| 1 | E | 286 | ASP | C-N | -7.02 | 1.17 | 1.34 |
| 1 | E | 273 | ASP | C-N | 6.97 | 1.50 | 1.34 |
| 1 | A | 137 | ARG | C-N | 6.74 | 1.47 | 1.34 |
| 1 | F | 181 | VAL | C-N | 6.68 | 1.49 | 1.34 |
| 1 | E | 181 | VAL | C-N | 6.61 | 1.49 | 1.34 |
| 1 | C | 160 | MET | C-N | 6.57 | 1.49 | 1.34 |
| 1 | H | 44 | VAL | C-N | 6.03 | 1.48 | 1.34 |
| 1 | C | 106 | GLY | C-N | 6.01 | 1.45 | 1.34 |
| 1 | G | 273 | ASP | C-N | -5.85 | 1.20 | 1.34 |
| 1 | F | 95 | ALA | C-N | 5.72 | 1.47 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | E | 274 | VAL | C-N | 5.71 | 1.47 | 1.34 |
| 1 | H | 45 | SER | C-N | 5.48 | 1.46 | 1.34 |
| 1 | F | 194 | ARG | C-N | -5.32 | 1.21 | 1.34 |
| 1 | B | 182 | ARG | C-N | 5.21 | 1.46 | 1.34 |
| 1 | H | 95 | ALA | C-N | -5.20 | 1.22 | 1.34 |
| 1 | B | 193 | ARG | C-N | -5.12 | 1.22 | 1.34 |
| 1 | B | 137 | ARG | C-N | 5.10 | 1.44 | 1.34 |
| 1 | E | 46 | TRP | C-N | -5.06 | 1.24 | 1.34 |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | F | 286 | ASP | O-C-N | -20.18 | 90.41 | 122.70 |
| 1 | D | 286 | ASP | O-C-N | -16.18 | 96.81 | 122.70 |
| 1 | F | 81 | GLY | O-C-N | -14.45 | 99.59 | 122.70 |
| 1 | D | 81 | GLY | O-C-N | -13.70 | 100.78 | 122.70 |
| 1 | F | 273 | ASP | O-C-N | -13.56 | 101.00 | 122.70 |
| 1 | C | 286 | ASP | O-C-N | -13.25 | 101.50 | 122.70 |
| 1 | F | 286 | ASP | CA-C-N | 12.36 | 144.39 | 117.20 |
| 1 | D | 286 | ASP | CA-C-N | 11.47 | 142.44 | 117.20 |
| 1 | H | 95 | ALA | O-C-N | 11.13 | 140.51 | 122.70 |
| 1 | E | 286 | ASP | O-C-N | -11.05 | 105.02 | 122.70 |
| 1 | D | 81 | GLY | CA-C-N | 10.11 | 139.44 | 117.20 |
| 1 | F | 95 | ALA | O-C-N | -10.05 | 106.63 | 122.70 |
| 1 | F | 81 | GLY | CA-C-N | 10.00 | 139.19 | 117.20 |
| 1 | F | 286 | ASP | C-N-CA | 9.05 | 144.33 | 121.70 |
| 1 | H | 95 | ALA | CA-C-N | -8.86 | 97.72 | 117.20 |
| 1 | H | 285 | ILE | CA-C-N | -8.83 | 97.77 | 117.20 |
| 1 | E | 194 | ARG | O-C-N | -8.81 | 108.61 | 122.70 |
| 1 | D | 81 | GLY | C-N-CA | 8.80 | 143.71 | 121.70 |
| 1 | H | 71 | CYS | O-C-N | 8.75 | 138.07 | 123.20 |
| 1 | F | 81 | GLY | C-N-CA | 8.53 | 143.02 | 121.70 |
| 1 | D | 286 | ASP | C-N-CA | 8.44 | 142.79 | 121.70 |
| 1 | C | 273 | ASP | O-C-N | -8.41 | 109.24 | 122.70 |
| 1 | F | 273 | ASP | CA-C-N | 8.38 | 135.64 | 117.20 |
| 1 | A | 94 | MET | O-C-N | 8.35 | 136.07 | 122.70 |
| 1 | H | 71 | CYS | C-N-CA | -8.32 | 104.83 | 122.30 |
| 1 | H | 285 | ILE | O-C-N | 8.14 | 135.73 | 122.70 |
| 1 | H | 71 | CYS | CA-C-N | -7.98 | 100.24 | 116.20 |
| 1 | C | 167 | ARG | O-C-N | -7.88 | 110.09 | 122.70 |
| 1 | A | 287 | LEU | C-N-CA | -7.80 | 105.92 | 122.30 |
| 1 | H | 285 | ILE | C-N-CA | -7.53 | 102.88 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | H | 45 | SER | O-C-N | -7.43 | 110.82 | 122.70 |
| 1 | C | 286 | ASP | CA-C-N | 7.39 | 133.46 | 117.20 |
| 1 | E | 286 | ASP | CA-C-N | 7.34 | 133.36 | 117.20 |
| 1 | F | 273 | ASP | C-N-CA | 7.26 | 139.85 | 121.70 |
| 1 | E | 45 | SER | O-C-N | 7.16 | 134.15 | 122.70 |
| 1 | A | 287 | LEU | O-C-N | 7.14 | 135.34 | 123.20 |
| 1 | E | 46 | TRP | O-C-N | -7.13 | 107.56 | 121.10 |
| 1 | F | 95 | ALA | C-N-CA | 7.06 | 139.34 | 121.70 |
| 1 | D | 273 | ASP | O-C-N | -6.93 | 111.62 | 122.70 |
| 1 | A | 94 | MET | C-N-CA | -6.88 | 104.50 | 121.70 |
| 1 | E | 273 | ASP | O-C-N | -6.84 | 111.76 | 122.70 |
| 1 | A | 94 | MET | CA-C-N | -6.75 | 102.35 | 117.20 |
| 1 | F | 95 | ALA | CA-C-N | 6.59 | 131.69 | 117.20 |
| 1 | A | 287 | LEU | CA-C-N | -6.57 | 103.05 | 116.20 |
| 1 | C | 45 | SER | O-C-N | -6.46 | 112.37 | 122.70 |
| 1 | F | 172 | ILE | O-C-N | -6.32 | 112.59 | 122.70 |
| 1 | H | 95 | ALA | C-N-CA | -6.25 | 106.08 | 121.70 |
| 1 | D | 44 | VAL | O-C-N | -5.67 | 113.63 | 122.70 |
| 1 | C | 273 | ASP | CA-C-N | 5.59 | 129.49 | 117.20 |
| 1 | B | 157 | PRO | O-C-N | 5.56 | 131.60 | 122.70 |
| 1 | C | 167 | ARG | CA-C-N | 5.51 | 129.33 | 117.20 |
| 1 | E | 286 | ASP | C-N-CA | 5.51 | 135.46 | 121.70 |
| 1 | E | 194 | ARG | CA-C-N | 5.48 | 129.25 | 117.20 |
| 1 | E | 45 | SER | CA-C-N | -5.46 | 105.19 | 117.20 |
| 1 | E | 45 | SER | C-N-CA | -5.44 | 108.10 | 121.70 |
| 1 | C | 167 | ARG | C-N-CA | 5.42 | 135.25 | 121.70 |
| 1 | C | 286 | ASP | C-N-CA | 5.13 | 134.53 | 121.70 |
| 1 | H | 45 | SER | CA-C-N | 5.08 | 128.38 | 117.20 |
| 1 | E | 46 | TRP | CA-C-N | 5.08 | 131.32 | 117.10 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 150 | ILE | Mainchain |
| 1 | C | 286 | ASP | Mainchain |
| 1 | E | 95 | ALA | Mainchain |
| 1 | F | 273 | ASP | Mainchain |
| 1 | F | 286 | ASP | Mainchain |
| 1 | F | 71 | CYS | Mainchain |
| 1 | F | 81 | GLY | Mainchain |
| 1 | G | 82 | SER | Mainchain |

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 | 2206 | 0 | 2144 | 234 | 0 |
| 1 | B | 2205 | 0 | 2145 | 193 | 0 |
| 1 | C | 2205 | 0 | 2145 | 194 | 0 |
| 1 | D | 2214 | 0 | 2154 | 213 | 0 |
| 1 | E | 2209 | 0 | 2154 | 239 | 0 |
| 1 | F | 2209 | 0 | 2153 | 214 | 0 |
| 1 | G | 2205 | 0 | 2143 | 224 | 0 |
| 1 | H | 2208 | 0 | 2158 | 215 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | H | 1 | 0 | 0 | 0 | 0 |
| All | All | 17667 | 0 | 17196 | 1571 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:287:LEU:C | 1:A:288:GLY:CA | 1.81 | 1.48 |
| 1:E:71:CYS:C | 1:E:72:GLY:N | 1.70 | 1.44 |
| 1:A:94:MET:C | 1:A:95:ALA:CA | 1.87 | 1.43 |
| 1:E:106:GLY:C | 1:E:107:PRO:N | 1.71 | 1.41 |
| 1:D:182:ARG:C | 1:D:183:SER:N | 1.70 | 1.40 |
| 1:A:287:LEU:CA | 1:A:288:GLY:N | 1.84 | 1.38 |
| 1:G:202:ARG:NH2 | 1:G:205:SER:HA | 1.42 | 1.34 |
| 1:A:94:MET:CA | 1:A:95:ALA:N | 1.92 | 1.33 |
| 1:H:168:ILE:HD12 | 1:H:168:ILE:H | 1.05 | 1.19 |
| 1:A:283:ARG:HE | 1:D:23:ILE:CD1 | 1.55 | 1.19 |
| 1:F:93:THR:HG21 | 1:F:116:GLU:OE1 | 1.38 | 1.18 |
| 1:C:278:LEU:HD12 | 1:C:282:ARG:HG3 | 1.20 | 1.15 |
| 1:H:278:LEU:HD12 | 1:H:282:ARG:HG3 | 1.20 | 1.15 |
| 1:B:168:ILE:HD12 | 1:B:168:ILE:H | 1.04 | 1.15 |
| 1:G:202:ARG:HH22 | 1:G:205:SER:CA | 1.59 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:168:ILE:H | 1:E:168:ILE:HD12 | 1.05 | 1.14 |
| 1:D:168:ILE:H | 1:D:168:ILE:HD12 | 1.05 | 1.14 |
| 1:A:278:LEU:HD12 | 1:A:282:ARG:HG3 | 1.20 | 1.13 |
| 1:G:202:ARG:NH2 | 1:G:205:SER:CA | 2.11 | 1.13 |
| 1:G:168:ILE:H | 1:G:168:ILE:HD12 | 1.04 | 1.13 |
| 1:B:278:LEU:HD12 | 1:B:282:ARG:HG3 | 1.20 | 1.12 |
| 1:A:168:ILE:H | 1:A:168:ILE:HD12 | 1.06 | 1.12 |
| 1:F:278:LEU:HD12 | 1:F:282:ARG:HG3 | 1.20 | 1.12 |
| 1:A:287:LEU:O | 1:A:288:GLY:N | 1.84 | 1.11 |
| 1:D:278:LEU:HD12 | 1:D:282:ARG:HG3 | 1.20 | 1.11 |
| 1:G:278:LEU:HD12 | 1:G:282:ARG:HG3 | 1.20 | 1.10 |
| 1:E:278:LEU:HD12 | 1:E:282:ARG:HG3 | 1.20 | 1.09 |
| 1:F:168:ILE:H | 1:F:168:ILE:HD12 | 1.05 | 1.09 |
| 1:A:283:ARG:HE | 1:D:23:ILE:HD12 | 1.12 | 1.08 |
| 1:D:75:ILE:HD13 | 1:D:89:PHE:CD2 | 1.91 | 1.06 |
| 1:E:75:ILE:CD1 | 1:E:89:PHE:CD2 | 2.40 | 1.05 |
| 1:H:121:MET:SD | 1:H:121:MET:N | 2.30 | 1.05 |
| 1:G:202:ARG:HH21 | 1:G:205:SER:HB2 | 1.15 | 1.04 |
| 1:D:210:LEU:HD13 | 1:D:285:ILE:HD11 | 1.37 | 1.04 |
| 1:D:75:ILE:CD1 | 1:D:89:PHE:CD2 | 2.42 | 1.03 |
| 1:F:93:THR:CG2 | 1:F:116:GLU:OE1 | 2.07 | 1.01 |
| 1:F:75:ILE:CD1 | 1:F:89:PHE:CD2 | 2.43 | 1.00 |
| 1:A:94:MET:O | 1:A:95:ALA:N | 1.95 | 0.99 |
| 1:H:75:ILE:HD13 | 1:H:89:PHE:CD2 | 1.96 | 0.99 |
| 1:E:23:ILE:CD1 | 1:F:283:ARG:HE | 1.74 | 0.98 |
| 1:F:75:ILE:HD13 | 1:F:89:PHE:CD2 | 1.99 | 0.98 |
| 1:B:75:ILE:HD13 | 1:B:89:PHE:CD2 | 1.98 | 0.97 |
| 1:E:76:GLU:HG2 | 1:E:105:ILE:HD11 | 1.46 | 0.96 |
| 1:E:75:ILE:HD13 | 1:E:89:PHE:CD2 | 2.00 | 0.96 |
| 1:C:280:ASP:OD2 | 1:C:282:ARG:HD3 | 1.66 | 0.96 |
| 1:A:287:LEU:O | 1:A:288:GLY:CA | 2.09 | 0.95 |
| 1:H:280:ASP:OD2 | 1:H:282:ARG:HD3 | 1.66 | 0.95 |
| 1:F:280:ASP:OD2 | 1:F:282:ARG:HD3 | 1.66 | 0.95 |
| 1:D:280:ASP:OD2 | 1:D:282:ARG:HD3 | 1.66 | 0.95 |
| 1:D:93:THR:HG21 | 1:D:116:GLU:OE1 | 1.66 | 0.95 |
| 1:B:280:ASP:OD2 | 1:B:282:ARG:HD3 | 1.66 | 0.94 |
| 1:A:280:ASP:OD2 | 1:A:282:ARG:HD3 | 1.66 | 0.94 |
| 1:E:75:ILE:HD11 | 1:E:89:PHE:CD2 | 2.02 | 0.94 |
| 1:G:280:ASP:OD2 | 1:G:282:ARG:HD3 | 1.66 | 0.94 |
| 1:E:61:ASN:HD21 | 1:E:94:MET:CE | 1.81 | 0.94 |
| 1:C:75:ILE:HD13 | 1:C:89:PHE:CD2 | 2.02 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:61:ASN:HD21 | 1:B:94:MET:CE | 1.80 | 0.94 |
| 1:B:75:ILE:CD1 | 1:B:89:PHE:CD2 | 2.51 | 0.94 |
| 1:G:75:ILE:HD13 | 1:G:89:PHE:CD2 | 2.02 | 0.93 |
| 1:A:283:ARG:HH21 | 1:D:23:ILE:HD11 | 1.34 | 0.93 |
| 1:C:75:ILE:CD1 | 1:C:89:PHE:CD2 | 2.51 | 0.93 |
| 1:E:280:ASP:OD2 | 1:E:282:ARG:HD3 | 1.66 | 0.92 |
| 1:E:23:ILE:HG21 | 1:F:285:ILE:HG13 | 1.50 | 0.92 |
| 1:H:121:MET:O | 1:H:124:LEU:N | 2.03 | 0.92 |
| 1:A:283:ARG:NE | 1:D:23:ILE:CD1 | 2.32 | 0.92 |
| 1:A:94:MET:C | 1:A:95:ALA:N | 0.87 | 0.92 |
| 1:G:61:ASN:HD21 | 1:G:94:MET:CE | 1.83 | 0.92 |
| 1:F:110:ASN:HB3 | 1:G:88:PHE:CD2 | 2.05 | 0.91 |
| 1:A:283:ARG:HH21 | 1:D:23:ILE:CD1 | 1.83 | 0.91 |
| 1:D:61:ASN:HD21 | 1:D:94:MET:CE | 1.84 | 0.91 |
| 1:C:61:ASN:HD21 | 1:C:94:MET:CE | 1.84 | 0.91 |
| 1:A:283:ARG:NE | 1:D:23:ILE:HD12 | 1.87 | 0.90 |
| 1:B:61:ASN:HD21 | 1:B:94:MET:HE1 | 1.36 | 0.90 |
| 1:B:210:LEU:HD13 | 1:B:285:ILE:HD11 | 1.53 | 0.89 |
| 1:G:202:ARG:NH2 | 1:G:205:SER:CB | 2.35 | 0.89 |
| 1:D:61:ASN:HD21 | 1:D:94:MET:HE1 | 1.38 | 0.89 |
| 1:H:168:ILE:CD1 | 1:H:168:ILE:H | 1.81 | 0.89 |
| 1:E:168:ILE:CD1 | 1:E:168:ILE:H | 1.81 | 0.88 |
| 1:F:168:ILE:H | 1:F:168:ILE:CD1 | 1.81 | 0.88 |
| 1:G:210:LEU:HD13 | 1:G:285:ILE:HD11 | 1.53 | 0.88 |
| 1:A:56:LEU:O | 1:A:60:THR:HG23 | 1.74 | 0.88 |
| 1:E:56:LEU:O | 1:E:60:THR:HG23 | 1.74 | 0.88 |
| 1:G:202:ARG:HH21 | 1:G:205:SER:CB | 1.86 | 0.88 |
| 1:A:94:MET:O | 1:A:95:ALA:CA | 2.21 | 0.88 |
| 1:B:56:LEU:O | 1:B:60:THR:HG23 | 1.74 | 0.88 |
| 1:F:75:ILE:HD11 | 1:F:89:PHE:CD2 | 2.09 | 0.88 |
| 1:B:61:ASN:ND2 | 1:B:94:MET:HE1 | 1.88 | 0.88 |
| 1:B:168:ILE:CD1 | 1:B:168:ILE:H | 1.81 | 0.87 |
| 1:G:202:ARG:NH2 | 1:G:205:SER:HB2 | 1.88 | 0.87 |
| 1:G:56:LEU:O | 1:G:60:THR:HG23 | 1.74 | 0.87 |
| 1:E:93:THR:HG21 | 1:E:116:GLU:OE1 | 1.75 | 0.87 |
| 1:A:283:ARG:NH2 | 1:D:23:ILE:HD11 | 1.90 | 0.87 |
| 1:D:56:LEU:O | 1:D:60:THR:HG23 | 1.74 | 0.87 |
| 1:G:202:ARG:CZ | 1:G:204:ARG:O | 2.23 | 0.87 |
| 1:B:23:ILE:HG21 | 1:C:285:ILE:HG13 | 1.57 | 0.87 |
| 1:G:93:THR:HG21 | 1:G:116:GLU:OE1 | 1.75 | 0.87 |
| 1:A:168:ILE:N | 1:A:168:ILE:HD12 | 1.90 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:280:ASP:HB3 | 1:C:282:ARG:HG2 | 1.57 | 0.86 |
| 1:D:44:VAL:CG1 | 1:D:48:VAL:HB | 2.05 | 0.86 |
| 1:H:56:LEU:O | 1:H:60:THR:HG23 | 1.74 | 0.86 |
| 1:A:280:ASP:HB3 | 1:A:282:ARG:HG2 | 1.57 | 0.86 |
| 1:F:280:ASP:HB3 | 1:F:282:ARG:HG2 | 1.57 | 0.86 |
| 1:H:280:ASP:HB3 | 1:H:282:ARG:HG2 | 1.58 | 0.86 |
| 1:D:44:VAL:HG11 | 1:D:48:VAL:HG12 | 1.58 | 0.86 |
| 1:G:278:LEU:CD1 | 1:G:282:ARG:HG3 | 2.06 | 0.86 |
| 1:E:61:ASN:HD21 | 1:E:94:MET:HE1 | 1.40 | 0.86 |
| 1:E:280:ASP:HB3 | 1:E:282:ARG:HG2 | 1.57 | 0.86 |
| 1:C:168:ILE:N | 1:C:168:ILE:HD12 | 1.90 | 0.86 |
| 1:F:56:LEU:O | 1:F:60:THR:HG23 | 1.74 | 0.86 |
| 1:B:280:ASP:HB3 | 1:B:282:ARG:HG2 | 1.58 | 0.86 |
| 1:D:278:LEU:CD1 | 1:D:282:ARG:HG3 | 2.06 | 0.86 |
| 1:G:61:ASN:HD21 | 1:G:94:MET:HE1 | 1.40 | 0.86 |
| 1:H:172:ILE:HG13 | 1:H:246:HIS:HB3 | 1.57 | 0.86 |
| 1:C:56:LEU:O | 1:C:60:THR:HG23 | 1.74 | 0.85 |
| 1:E:168:ILE:N | 1:E:168:ILE:HD12 | 1.90 | 0.85 |
| 1:D:168:ILE:H | 1:D:168:ILE:CD1 | 1.81 | 0.85 |
| 1:A:210:LEU:HD21 | 1:D:21:SER:OG | 1.76 | 0.85 |
| 1:F:168:ILE:HD12 | 1:F:168:ILE:N | 1.91 | 0.85 |
| 1:D:280:ASP:HB3 | 1:D:282:ARG:HG2 | 1.58 | 0.85 |
| 1:H:75:ILE:CD1 | 1:H:89:PHE:CD2 | 2.59 | 0.85 |
| 1:A:172:ILE:HG13 | 1:A:246:HIS:HB3 | 1.57 | 0.85 |
| 1:E:23:ILE:HD12 | 1:F:283:ARG:HE | 1.39 | 0.84 |
| 1:E:172:ILE:HG13 | 1:E:246:HIS:HB3 | 1.57 | 0.84 |
| 1:B:93:THR:HG21 | 1:B:116:GLU:OE1 | 1.76 | 0.84 |
| 1:G:280:ASP:HB3 | 1:G:282:ARG:HG2 | 1.57 | 0.84 |
| 1:A:287:LEU:O | 1:A:288:GLY:HA2 | 1.76 | 0.84 |
| 1:C:61:ASN:HD21 | 1:C:94:MET:HE1 | 1.40 | 0.84 |
| 1:A:61:ASN:HD21 | 1:A:94:MET:HE1 | 1.41 | 0.84 |
| 1:B:172:ILE:HG13 | 1:B:246:HIS:HB3 | 1.57 | 0.84 |
| 1:D:168:ILE:HD12 | 1:D:168:ILE:N | 1.91 | 0.84 |
| 1:G:168:ILE:N | 1:G:168:ILE:HD12 | 1.90 | 0.84 |
| 1:A:168:ILE:H | 1:A:168:ILE:CD1 | 1.83 | 0.84 |
| 1:D:172:ILE:HG13 | 1:D:246:HIS:HB3 | 1.57 | 0.84 |
| 1:E:26:LEU:HB2 | 1:F:286:ASP:HA | 1.58 | 0.84 |
| 1:E:278:LEU:CD1 | 1:E:282:ARG:HG3 | 2.06 | 0.83 |
| 1:G:172:ILE:HG13 | 1:G:246:HIS:HB3 | 1.57 | 0.83 |
| 1:A:75:ILE:HD13 | 1:A:89:PHE:CD2 | 2.14 | 0.83 |
| 1:B:168:ILE:HD12 | 1:B:168:ILE:N | 1.90 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:202:ARG:NH2 | 1:G:204:ARG:O | 2.11 | 0.83 |
| 1:F:172:ILE:HG13 | 1:F:246:HIS:HB3 | 1.57 | 0.83 |
| 1:C:278:LEU:HD12 | 1:C:282:ARG:CG | 2.07 | 0.83 |
| 1:A:61:ASN:HD21 | 1:A:94:MET:CE | 1.90 | 0.83 |
| 1:F:61:ASN:HD21 | 1:F:94:MET:CE | 1.91 | 0.83 |
| 1:A:285:ILE:HG13 | 1:D:23:ILE:HG21 | 1.60 | 0.83 |
| 1:C:172:ILE:HG13 | 1:C:246:HIS:HB3 | 1.58 | 0.82 |
| 1:G:61:ASN:ND2 | 1:G:94:MET:HE1 | 1.94 | 0.82 |
| 1:F:278:LEU:HD12 | 1:F:282:ARG:CG | 2.07 | 0.82 |
| 1:H:278:LEU:CD1 | 1:H:282:ARG:HG3 | 2.06 | 0.82 |
| 1:E:23:ILE:HD11 | 1:F:283:ARG:HH21 | 1.42 | 0.82 |
| 1:A:283:ARG:HE | 1:D:23:ILE:HD11 | 1.45 | 0.82 |
| 1:B:273:ASP:OD1 | 1:B:274:VAL:N | 2.13 | 0.81 |
| 1:F:278:LEU:CD1 | 1:F:282:ARG:HG3 | 2.06 | 0.81 |
| 1:H:61:ASN:HD21 | 1:H:94:MET:CE | 1.93 | 0.81 |
| 1:A:278:LEU:CD1 | 1:A:282:ARG:HG3 | 2.06 | 0.81 |
| 1:D:210:LEU:HB3 | 1:D:285:ILE:HD13 | 1.63 | 0.81 |
| 1:A:283:ARG:HH21 | 1:D:23:ILE:CG1 | 1.93 | 0.81 |
| 1:C:278:LEU:CD1 | 1:C:282:ARG:HG3 | 2.06 | 0.81 |
| 1:E:278:LEU:HD12 | 1:E:282:ARG:CG | 2.07 | 0.81 |
| 1:B:278:LEU:CD1 | 1:B:282:ARG:HG3 | 2.06 | 0.81 |
| 1:H:69:LEU:O | 1:H:72:GLY:N | 2.13 | 0.81 |
| 1:D:61:ASN:ND2 | 1:D:94:MET:HE1 | 1.95 | 0.81 |
| 1:D:75:ILE:HD11 | 1:D:89:PHE:CD2 | 2.14 | 0.80 |
| 1:G:210:LEU:HB3 | 1:G:285:ILE:CD1 | 2.11 | 0.80 |
| 1:G:278:LEU:HD12 | 1:G:282:ARG:CG | 2.07 | 0.80 |
| 1:E:179:VAL:HG22 | 1:E:197:ASP:OD1 | 1.80 | 0.80 |
| 1:H:61:ASN:HD21 | 1:H:94:MET:HE1 | 1.47 | 0.80 |
| 1:H:168:ILE:HD12 | 1:H:168:ILE:N | 1.90 | 0.80 |
| 1:H:278:LEU:HD12 | 1:H:282:ARG:CG | 2.08 | 0.80 |
| 1:H:121:MET:O | 1:H:122:LEU:C | 2.11 | 0.80 |
| 1:A:287:LEU:C | 1:A:288:GLY:N | 0.75 | 0.79 |
| 1:E:75:ILE:HD13 | 1:E:89:PHE:CG | 2.16 | 0.79 |
| 1:E:61:ASN:ND2 | 1:E:94:MET:HE1 | 1.96 | 0.79 |
| 1:B:61:ASN:ND2 | 1:B:94:MET:CE | 2.44 | 0.79 |
| 1:B:201:THR:CG2 | 1:B:217:PRO:HD3 | 2.13 | 0.79 |
| 1:E:201:THR:CG2 | 1:E:217:PRO:HD3 | 2.13 | 0.79 |
| 1:D:201:THR:CG2 | 1:D:217:PRO:HD3 | 2.13 | 0.79 |
| 1:F:266:ILE:HG22 | 1:F:266:ILE:O | 1.82 | 0.79 |
| 1:A:278:LEU:HD12 | 1:A:282:ARG:CG | 2.07 | 0.79 |
| 1:D:278:LEU:HD12 | 1:D:282:ARG:CG | 2.08 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:201:THR:CG2 | 1:C:217:PRO:HD3 | 2.13 | 0.79 |
| 1:E:23:ILE:CD1 | 1:F:283:ARG:HH21 | 1.95 | 0.78 |
| 1:G:201:THR:CG2 | 1:G:217:PRO:HD3 | 2.13 | 0.78 |
| 1:G:23:ILE:HD11 | 1:H:283:ARG:HH11 | 1.46 | 0.78 |
| 1:A:201:THR:CG2 | 1:A:217:PRO:HD3 | 2.13 | 0.78 |
| 1:F:201:THR:CG2 | 1:F:217:PRO:HD3 | 2.13 | 0.78 |
| 1:C:266:ILE:O | 1:C:266:ILE:HG22 | 1.83 | 0.78 |
| 1:B:278:LEU:HD12 | 1:B:282:ARG:CG | 2.08 | 0.78 |
| 1:C:61:ASN:ND2 | 1:C:94:MET:HE1 | 1.99 | 0.78 |
| 1:G:138:PRO:HB3 | 1:G:250:PHE:CD1 | 2.19 | 0.78 |
| 1:A:283:ARG:NE | 1:D:23:ILE:HD11 | 1.99 | 0.78 |
| 1:D:266:ILE:HD12 | 1:D:293:ILE:HD12 | 1.65 | 0.78 |
| 1:D:138:PRO:HB3 | 1:D:250:PHE:CD1 | 2.19 | 0.78 |
| 1:H:266:ILE:HG22 | 1:H:266:ILE:O | 1.83 | 0.78 |
| 1:B:138:PRO:HB3 | 1:B:250:PHE:CD1 | 2.19 | 0.77 |
| 1:G:168:ILE:H | 1:G:168:ILE:CD1 | 1.81 | 0.77 |
| 1:H:201:THR:CG2 | 1:H:217:PRO:HD3 | 2.13 | 0.77 |
| 1:A:266:ILE:O | 1:A:266:ILE:HG22 | 1.83 | 0.77 |
| 1:E:138:PRO:HB3 | 1:E:250:PHE:CD1 | 2.19 | 0.77 |
| 1:B:44:VAL:CG1 | 1:B:48:VAL:HB | 2.14 | 0.77 |
| 1:C:138:PRO:HB3 | 1:C:250:PHE:CD1 | 2.19 | 0.77 |
| 1:E:207:ILE:HD13 | 1:H:240:LEU:HD21 | 1.66 | 0.77 |
| 1:H:138:PRO:HB3 | 1:H:250:PHE:CD1 | 2.19 | 0.77 |
| 1:F:138:PRO:HB3 | 1:F:250:PHE:CD1 | 2.19 | 0.77 |
| 1:D:266:ILE:HG22 | 1:D:266:ILE:O | 1.82 | 0.77 |
| 1:F:207:ILE:HG22 | 1:F:207:ILE:O | 1.84 | 0.77 |
| 1:F:44:VAL:CG1 | 1:F:48:VAL:HB | 2.14 | 0.77 |
| 1:A:138:PRO:HB3 | 1:A:250:PHE:CD1 | 2.19 | 0.77 |
| 1:C:207:ILE:O | 1:C:207:ILE:HG22 | 1.84 | 0.77 |
| 1:D:44:VAL:HG11 | 1:D:48:VAL:CG1 | 2.14 | 0.76 |
| 1:E:266:ILE:HG22 | 1:E:266:ILE:O | 1.82 | 0.76 |
| 1:G:210:LEU:HB3 | 1:G:285:ILE:HD13 | 1.68 | 0.76 |
| 1:G:266:ILE:HG22 | 1:G:266:ILE:O | 1.82 | 0.76 |
| 1:B:207:ILE:O | 1:B:207:ILE:HG22 | 1.84 | 0.76 |
| 1:E:23:ILE:HD11 | 1:F:283:ARG:HE | 1.51 | 0.76 |
| 1:B:266:ILE:HG22 | 1:B:266:ILE:O | 1.83 | 0.76 |
| 1:D:104:PRO:HB2 | 1:D:110:ASN:OD1 | 1.85 | 0.76 |
| 1:F:210:LEU:HD13 | 1:F:285:ILE:HD11 | 1.66 | 0.76 |
| 1:G:23:ILE:HG21 | 1:H:285:ILE:HG13 | 1.67 | 0.76 |
| 1:C:75:ILE:HD11 | 1:C:89:PHE:CD2 | 2.20 | 0.76 |
| 1:F:93:THR:CG2 | 1:F:116:GLU:CD | 2.54 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:207:ILE:O | 1:G:207:ILE:HG22 | 1.84 | 0.76 |
| 1:G:266:ILE:HD12 | 1:G:293:ILE:HD12 | 1.68 | 0.76 |
| 1:A:207:ILE:O | 1:A:207:ILE:HG22 | 1.84 | 0.76 |
| 1:F:75:ILE:HD11 | 1:F:89:PHE:CE2 | 2.19 | 0.75 |
| 1:D:74:VAL:HB | 1:D:109:ALA:HB2 | 1.67 | 0.75 |
| 1:G:202:ARG:HH22 | 1:G:205:SER:HA | 0.69 | 0.75 |
| 1:H:61:ASN:ND2 | 1:H:94:MET:HE1 | 2.01 | 0.75 |
| 1:D:207:ILE:O | 1:D:207:ILE:HG22 | 1.85 | 0.75 |
| 1:D:210:LEU:HB3 | 1:D:285:ILE:CD1 | 2.17 | 0.75 |
| 1:F:266:ILE:HD12 | 1:F:293:ILE:HD12 | 1.68 | 0.75 |
| 1:D:93:THR:CG2 | 1:D:116:GLU:OE1 | 2.35 | 0.75 |
| 1:E:207:ILE:HG22 | 1:E:207:ILE:O | 1.84 | 0.75 |
| 1:E:44:VAL:CG1 | 1:E:48:VAL:HB | 2.17 | 0.74 |
| 1:H:207:ILE:O | 1:H:207:ILE:HG22 | 1.84 | 0.74 |
| 1:A:266:ILE:HD12 | 1:A:293:ILE:HD12 | 1.68 | 0.74 |
| 1:E:272:VAL:CG1 | 1:E:273:ASP:N | 2.51 | 0.74 |
| 1:G:44:VAL:CG1 | 1:G:48:VAL:HB | 2.17 | 0.74 |
| 1:H:266:ILE:HD12 | 1:H:293:ILE:HD12 | 1.68 | 0.74 |
| 1:C:266:ILE:HD12 | 1:C:293:ILE:HD12 | 1.68 | 0.74 |
| 1:G:229:ASP:OD1 | 1:G:233:ARG:NH1 | 2.21 | 0.74 |
| 1:E:229:ASP:OD1 | 1:E:233:ARG:NH1 | 2.21 | 0.74 |
| 1:B:229:ASP:OD1 | 1:B:233:ARG:NH1 | 2.21 | 0.74 |
| 1:B:272:VAL:CG1 | 1:B:273:ASP:N | 2.51 | 0.74 |
| 1:B:266:ILE:HD12 | 1:B:293:ILE:HD12 | 1.68 | 0.74 |
| 1:H:186:SER:OG | 1:H:188:GLU:OE1 | 2.06 | 0.74 |
| 1:G:186:SER:OG | 1:G:188:GLU:OE1 | 2.06 | 0.74 |
| 1:A:229:ASP:OD1 | 1:A:233:ARG:NH1 | 2.21 | 0.74 |
| 1:D:186:SER:OG | 1:D:188:GLU:OE1 | 2.06 | 0.74 |
| 1:D:229:ASP:OD1 | 1:D:233:ARG:NH1 | 2.21 | 0.74 |
| 1:E:266:ILE:HD12 | 1:E:293:ILE:HD12 | 1.68 | 0.74 |
| 1:F:229:ASP:OD1 | 1:F:233:ARG:NH1 | 2.21 | 0.74 |
| 1:F:272:VAL:CG1 | 1:F:273:ASP:N | 2.51 | 0.74 |
| 1:C:229:ASP:OD1 | 1:C:233:ARG:NH1 | 2.21 | 0.74 |
| 1:C:272:VAL:CG1 | 1:C:273:ASP:N | 2.51 | 0.74 |
| 1:E:61:ASN:ND2 | 1:E:94:MET:CE | 2.49 | 0.73 |
| 1:G:272:VAL:CG1 | 1:G:273:ASP:N | 2.51 | 0.73 |
| 1:G:75:ILE:CD1 | 1:G:89:PHE:CD2 | 2.70 | 0.73 |
| 1:H:229:ASP:OD1 | 1:H:233:ARG:NH1 | 2.21 | 0.73 |
| 1:B:186:SER:OG | 1:B:188:GLU:OE1 | 2.06 | 0.73 |
| 1:F:186:SER:OG | 1:F:188:GLU:OE1 | 2.06 | 0.73 |
| 1:A:186:SER:OG | 1:A:188:GLU:OE1 | 2.06 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:61:ASN:ND2 | 1:F:94:MET:HE1 | 2.03 | 0.73 |
| 1:A:44:VAL:CG1 | 1:A:48:VAL:HB | 2.19 | 0.73 |
| 1:C:185:ILE:CD1 | 1:C:191:VAL:HB | 2.18 | 0.73 |
| 1:D:185:ILE:CD1 | 1:D:191:VAL:HB | 2.19 | 0.73 |
| 1:D:61:ASN:ND2 | 1:D:94:MET:CE | 2.51 | 0.73 |
| 1:F:185:ILE:CD1 | 1:F:191:VAL:HB | 2.19 | 0.73 |
| 1:B:185:ILE:CD1 | 1:B:191:VAL:HB | 2.18 | 0.73 |
| 1:D:272:VAL:CG1 | 1:D:273:ASP:N | 2.51 | 0.73 |
| 1:D:44:VAL:HG13 | 1:D:48:VAL:HB | 1.69 | 0.73 |
| 1:G:185:ILE:CD1 | 1:G:191:VAL:HB | 2.18 | 0.73 |
| 1:H:272:VAL:CG1 | 1:H:273:ASP:N | 2.50 | 0.73 |
| 1:A:185:ILE:CD1 | 1:A:191:VAL:HB | 2.18 | 0.73 |
| 1:E:90:SER:O | 1:E:93:THR:HG22 | 1.89 | 0.73 |
| 1:A:90:SER:O | 1:A:93:THR:HG22 | 1.89 | 0.73 |
| 1:B:90:SER:O | 1:B:93:THR:HG22 | 1.89 | 0.73 |
| 1:E:185:ILE:CD1 | 1:E:191:VAL:HB | 2.18 | 0.73 |
| 1:C:186:SER:OG | 1:C:188:GLU:OE1 | 2.06 | 0.73 |
| 1:C:204:ARG:HH11 | 1:C:204:ARG:HG2 | 1.54 | 0.72 |
| 1:H:204:ARG:HH11 | 1:H:204:ARG:HG2 | 1.54 | 0.72 |
| 1:A:272:VAL:CG1 | 1:A:273:ASP:N | 2.51 | 0.72 |
| 1:D:210:LEU:CD1 | 1:D:285:ILE:HD11 | 2.18 | 0.72 |
| 1:F:204:ARG:HH11 | 1:F:204:ARG:HG2 | 1.55 | 0.72 |
| 1:H:185:ILE:CD1 | 1:H:191:VAL:HB | 2.18 | 0.72 |
| 1:A:94:MET:O | 1:A:95:ALA:HA | 1.88 | 0.72 |
| 1:D:75:ILE:HD11 | 1:D:89:PHE:CE2 | 2.24 | 0.72 |
| 1:E:186:SER:OG | 1:E:188:GLU:OE1 | 2.06 | 0.72 |
| 1:A:283:ARG:NH2 | 1:D:23:ILE:CD1 | 2.50 | 0.72 |
| 1:E:23:ILE:CD1 | 1:F:283:ARG:NE | 2.51 | 0.72 |
| 1:A:204:ARG:HH11 | 1:A:204:ARG:HG2 | 1.54 | 0.72 |
| 1:D:204:ARG:HH11 | 1:D:204:ARG:HG2 | 1.54 | 0.72 |
| 1:D:44:VAL:CG1 | 1:D:48:VAL:CG1 | 2.68 | 0.72 |
| 1:E:23:ILE:HD12 | 1:F:283:ARG:NE | 2.05 | 0.72 |
| 1:F:90:SER:O | 1:F:93:THR:HG22 | 1.89 | 0.72 |
| 1:F:61:ASN:ND2 | 1:F:94:MET:CE | 2.52 | 0.72 |
| 1:H:94:MET:HB2 | 1:H:116:GLU:HG2 | 1.71 | 0.72 |
| 1:A:61:ASN:ND2 | 1:A:94:MET:HE1 | 2.03 | 0.72 |
| 1:B:204:ARG:HG2 | 1:B:204:ARG:HH11 | 1.54 | 0.72 |
| 1:G:61:ASN:ND2 | 1:G:94:MET:CE | 2.49 | 0.72 |
| 1:G:204:ARG:HH11 | 1:G:204:ARG:HG2 | 1.55 | 0.71 |
| 1:C:61:ASN:ND2 | 1:C:94:MET:CE | 2.53 | 0.71 |
| 1:D:75:ILE:CD1 | 1:D:89:PHE:CE2 | 2.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:139:THR:O | 1:F:167:ARG:NH1 | 2.22 | 0.71 |
| 1:A:88:PHE:CD2 | 1:D:110:ASN:HB3 | 2.25 | 0.71 |
| 1:E:76:GLU:CG | 1:E:105:ILE:HD11 | 2.20 | 0.71 |
| 1:F:75:ILE:HD13 | 1:F:89:PHE:CG | 2.25 | 0.71 |
| 1:H:227:GLU:HG3 | 1:H:231:THR:OG1 | 1.90 | 0.71 |
| 1:C:90:SER:O | 1:C:93:THR:HG22 | 1.89 | 0.71 |
| 1:D:90:SER:O | 1:D:93:THR:HG22 | 1.89 | 0.71 |
| 1:G:227:GLU:HG3 | 1:G:231:THR:OG1 | 1.90 | 0.71 |
| 1:E:204:ARG:HH11 | 1:E:204:ARG:HG2 | 1.54 | 0.71 |
| 1:H:90:SER:O | 1:H:93:THR:HG22 | 1.89 | 0.71 |
| 1:F:75:ILE:CD1 | 1:F:89:PHE:CE2 | 2.73 | 0.71 |
| 1:G:90:SER:O | 1:G:93:THR:HG22 | 1.89 | 0.71 |
| 1:F:61:ASN:HD21 | 1:F:94:MET:HE1 | 1.55 | 0.71 |
| 1:A:227:GLU:HG3 | 1:A:231:THR:OG1 | 1.90 | 0.71 |
| 1:B:75:ILE:HD11 | 1:B:89:PHE:CD2 | 2.25 | 0.71 |
| 1:F:227:GLU:HG3 | 1:F:231:THR:OG1 | 1.90 | 0.71 |
| 1:C:227:GLU:HG3 | 1:C:231:THR:OG1 | 1.90 | 0.70 |
| 1:E:227:GLU:HG3 | 1:E:231:THR:OG1 | 1.90 | 0.70 |
| 1:H:200:LEU:HD13 | 1:H:214:VAL:CG1 | 2.21 | 0.70 |
| 1:A:274:VAL:HG12 | 1:A:289:LYS:HB2 | 1.74 | 0.70 |
| 1:A:200:LEU:HD13 | 1:A:214:VAL:CG1 | 2.22 | 0.70 |
| 1:D:227:GLU:HG3 | 1:D:231:THR:OG1 | 1.90 | 0.70 |
| 1:B:227:GLU:HG3 | 1:B:231:THR:OG1 | 1.90 | 0.70 |
| 1:C:172:ILE:O | 1:C:173:GLU:HB2 | 1.91 | 0.70 |
| 1:D:200:LEU:HD13 | 1:D:214:VAL:CG1 | 2.21 | 0.70 |
| 1:H:127:ALA:O | 1:H:131:ILE:HG12 | 1.92 | 0.70 |
| 1:A:287:LEU:C | 1:A:288:GLY:HA2 | 2.03 | 0.70 |
| 1:A:287:LEU:N | 1:A:288:GLY:N | 2.39 | 0.70 |
| 1:D:75:ILE:HD13 | 1:D:89:PHE:CG | 2.27 | 0.70 |
| 1:E:200:LEU:HD13 | 1:E:214:VAL:CG1 | 2.21 | 0.70 |
| 1:G:23:ILE:HD11 | 1:H:283:ARG:NH1 | 2.07 | 0.70 |
| 1:H:15:LEU:HD23 | 1:H:21:SER:HA | 1.74 | 0.70 |
| 1:C:200:LEU:HD13 | 1:C:214:VAL:CG1 | 2.21 | 0.69 |
| 1:G:200:LEU:HD13 | 1:G:214:VAL:CG1 | 2.22 | 0.69 |
| 1:A:184:GLU:OE1 | 1:A:194:ARG:HD2 | 1.93 | 0.69 |
| 1:D:18:ASP:O | 1:D:257:ARG:NH1 | 2.24 | 0.69 |
| 1:H:121:MET:O | 1:H:123:GLY:N | 2.24 | 0.69 |
| 1:B:200:LEU:HD13 | 1:B:214:VAL:CG1 | 2.22 | 0.69 |
| 1:A:283:ARG:CZ | 1:D:23:ILE:HD11 | 2.22 | 0.69 |
| 1:E:99:TYR:OH | 1:H:93:THR:OG1 | 2.03 | 0.69 |
| 1:A:15:LEU:HD23 | 1:A:21:SER:HA | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:127:ALA:O | 1:D:131:ILE:HG12 | 1.92 | 0.69 |
| 1:F:200:LEU:HD13 | 1:F:214:VAL:CG1 | 2.21 | 0.69 |
| 1:H:261:SER:H | 1:H:264:GLU:HG3 | 1.57 | 0.69 |
| 1:E:69:LEU:O | 1:E:72:GLY:N | 2.26 | 0.69 |
| 1:G:127:ALA:O | 1:G:131:ILE:HG12 | 1.92 | 0.69 |
| 1:C:127:ALA:O | 1:C:131:ILE:HG12 | 1.92 | 0.69 |
| 1:E:15:LEU:HD23 | 1:E:21:SER:HA | 1.74 | 0.69 |
| 1:E:23:ILE:HD11 | 1:F:283:ARG:NH2 | 2.08 | 0.69 |
| 1:H:240:LEU:HD12 | 1:H:258:HIS:O | 1.91 | 0.69 |
| 1:A:127:ALA:O | 1:A:131:ILE:HG12 | 1.92 | 0.69 |
| 1:G:130:LEU:HD21 | 1:H:135:PHE:HE2 | 1.56 | 0.69 |
| 1:B:61:ASN:OD1 | 1:B:94:MET:HE2 | 1.93 | 0.69 |
| 1:F:127:ALA:O | 1:F:131:ILE:HG12 | 1.92 | 0.69 |
| 1:B:139:THR:O | 1:B:167:ARG:NH1 | 2.22 | 0.69 |
| 1:B:15:LEU:HD23 | 1:B:21:SER:HA | 1.74 | 0.68 |
| 1:G:139:THR:O | 1:G:167:ARG:NH1 | 2.22 | 0.68 |
| 1:G:15:LEU:HD23 | 1:G:21:SER:HA | 1.74 | 0.68 |
| 1:H:139:THR:O | 1:H:167:ARG:NH1 | 2.22 | 0.68 |
| 1:A:178:LEU:HD13 | 1:A:241:VAL:HG22 | 1.75 | 0.68 |
| 1:C:15:LEU:HD23 | 1:C:21:SER:HA | 1.74 | 0.68 |
| 1:D:139:THR:O | 1:D:167:ARG:NH1 | 2.22 | 0.68 |
| 1:D:15:LEU:HD23 | 1:D:21:SER:HA | 1.74 | 0.68 |
| 1:G:272:VAL:HG12 | 1:G:273:ASP:N | 2.09 | 0.68 |
| 1:A:132:TYR:HD1 | 1:D:129:SER:HB3 | 1.58 | 0.68 |
| 1:A:272:VAL:HG12 | 1:A:273:ASP:N | 2.08 | 0.68 |
| 1:D:178:LEU:HD13 | 1:D:241:VAL:HG22 | 1.75 | 0.68 |
| 1:E:139:THR:O | 1:E:167:ARG:NH1 | 2.22 | 0.68 |
| 1:B:178:LEU:HD13 | 1:B:241:VAL:HG22 | 1.75 | 0.68 |
| 1:C:210:LEU:HD13 | 1:C:285:ILE:HD11 | 1.75 | 0.68 |
| 1:H:178:LEU:HD13 | 1:H:241:VAL:HG22 | 1.75 | 0.68 |
| 1:H:273:ASP:OD1 | 1:H:274:VAL:N | 2.27 | 0.68 |
| 1:C:178:LEU:HD13 | 1:C:241:VAL:HG22 | 1.75 | 0.68 |
| 1:C:44:VAL:CG1 | 1:C:48:VAL:HB | 2.24 | 0.68 |
| 1:D:104:PRO:CB | 1:D:110:ASN:OD1 | 2.41 | 0.68 |
| 1:D:272:VAL:HG12 | 1:D:273:ASP:N | 2.08 | 0.68 |
| 1:E:127:ALA:O | 1:E:131:ILE:HG12 | 1.92 | 0.68 |
| 1:E:178:LEU:HD13 | 1:E:241:VAL:HG22 | 1.75 | 0.68 |
| 1:B:127:ALA:O | 1:B:131:ILE:HG12 | 1.92 | 0.67 |
| 1:F:272:VAL:HG12 | 1:F:273:ASP:N | 2.08 | 0.67 |
| 1:D:14:ILE:HD13 | 1:D:14:ILE:N | 2.10 | 0.67 |
| 1:E:272:VAL:HG12 | 1:E:273:ASP:N | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:272:VAL:HG12 | 1:H:273:ASP:N | 2.08 | 0.67 |
| 1:A:14:ILE:N | 1:A:14:ILE:HD13 | 2.10 | 0.67 |
| 1:G:178:LEU:HD13 | 1:G:241:VAL:HG22 | 1.75 | 0.67 |
| 1:A:91:VAL:HG21 | 1:D:114:THR:HG22 | 1.76 | 0.67 |
| 1:G:276:THR:HG22 | 1:G:277:THR:N | 2.10 | 0.67 |
| 1:C:14:ILE:HD13 | 1:C:14:ILE:N | 2.10 | 0.67 |
| 1:E:21:SER:OG | 1:F:210:LEU:HD21 | 1.93 | 0.67 |
| 1:F:14:ILE:N | 1:F:14:ILE:HD13 | 2.10 | 0.67 |
| 1:F:15:LEU:HD23 | 1:F:21:SER:HA | 1.74 | 0.67 |
| 1:G:14:ILE:HD13 | 1:G:14:ILE:N | 2.10 | 0.67 |
| 1:E:93:THR:CG2 | 1:E:116:GLU:OE1 | 2.42 | 0.67 |
| 1:B:272:VAL:HG12 | 1:B:273:ASP:N | 2.08 | 0.66 |
| 1:B:276:THR:HG22 | 1:B:277:THR:N | 2.10 | 0.66 |
| 1:C:272:VAL:HG12 | 1:C:273:ASP:N | 2.08 | 0.66 |
| 1:D:276:THR:HG22 | 1:D:277:THR:N | 2.10 | 0.66 |
| 1:F:240:LEU:HD12 | 1:F:258:HIS:O | 1.96 | 0.66 |
| 1:C:240:LEU:HD12 | 1:C:258:HIS:O | 1.95 | 0.66 |
| 1:H:44:VAL:CG1 | 1:H:48:VAL:HB | 2.26 | 0.66 |
| 1:B:44:VAL:HG13 | 1:B:48:VAL:HB | 1.76 | 0.66 |
| 1:C:276:THR:HG22 | 1:C:277:THR:N | 2.10 | 0.66 |
| 1:F:276:THR:HG22 | 1:F:277:THR:N | 2.10 | 0.66 |
| 1:H:276:THR:HG22 | 1:H:277:THR:N | 2.10 | 0.66 |
| 1:A:132:TYR:CD1 | 1:D:129:SER:HB3 | 2.31 | 0.66 |
| 1:D:104:PRO:CG | 1:D:110:ASN:OD1 | 2.44 | 0.66 |
| 1:A:240:LEU:HD12 | 1:A:258:HIS:O | 1.96 | 0.66 |
| 1:B:14:ILE:HD13 | 1:B:14:ILE:N | 2.10 | 0.66 |
| 1:A:276:THR:HG22 | 1:A:277:THR:N | 2.10 | 0.66 |
| 1:H:14:ILE:HD13 | 1:H:14:ILE:N | 2.10 | 0.66 |
| 1:A:210:LEU:HD13 | 1:A:285:ILE:HD11 | 1.78 | 0.66 |
| 1:E:14:ILE:HD13 | 1:E:14:ILE:N | 2.10 | 0.66 |
| 1:E:94:MET:HB2 | 1:E:116:GLU:HG2 | 1.77 | 0.66 |
| 1:B:240:LEU:HD12 | 1:B:258:HIS:O | 1.95 | 0.65 |
| 1:E:276:THR:HG22 | 1:E:277:THR:N | 2.10 | 0.65 |
| 1:G:240:LEU:HD12 | 1:G:258:HIS:O | 1.96 | 0.65 |
| 1:E:240:LEU:HD12 | 1:E:258:HIS:O | 1.96 | 0.65 |
| 1:G:14:ILE:HG23 | 1:H:283:ARG:HH11 | 1.61 | 0.65 |
| 1:H:89:PHE:CD1 | 1:H:102:LEU:HB2 | 2.32 | 0.65 |
| 1:G:242:LEU:HD23 | 1:H:206:PRO:HB3 | 1.79 | 0.65 |
| 1:D:240:LEU:HD12 | 1:D:258:HIS:O | 1.96 | 0.65 |
| 1:D:44:VAL:CG1 | 1:D:48:VAL:CB | 2.74 | 0.65 |
| 1:G:273:ASP:OD1 | 1:G:274:VAL:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:139:THR:O | 1:C:167:ARG:NH1 | 2.23 | 0.65 |
| 1:G:21:SER:OG | 1:H:210:LEU:HD21 | 1.95 | 0.65 |
| 1:A:139:THR:O | 1:A:167:ARG:NH1 | 2.24 | 0.65 |
| 1:C:172:ILE:O | 1:C:173:GLU:CB | 2.43 | 0.65 |
| 1:C:240:LEU:HD21 | 1:D:207:ILE:HD13 | 1.77 | 0.65 |
| 1:E:179:VAL:CG2 | 1:E:197:ASP:OD1 | 2.44 | 0.65 |
| 1:G:41:LEU:O | 1:G:134:ARG:NH1 | 2.30 | 0.65 |
| 1:B:93:THR:CG2 | 1:B:116:GLU:OE1 | 2.44 | 0.65 |
| 1:C:93:THR:HG21 | 1:C:116:GLU:OE1 | 1.96 | 0.65 |
| 1:H:61:ASN:ND2 | 1:H:94:MET:CE | 2.58 | 0.65 |
| 1:B:21:SER:OG | 1:C:210:LEU:HD21 | 1.96 | 0.65 |
| 1:A:75:ILE:CD1 | 1:A:89:PHE:CD2 | 2.80 | 0.65 |
| 1:A:94:MET:N | 1:A:95:ALA:N | 2.45 | 0.65 |
| 1:C:75:ILE:HD13 | 1:C:89:PHE:CG | 2.31 | 0.65 |
| 1:D:141:GLY:O | 1:D:166:LEU:HB2 | 1.97 | 0.65 |
| 1:F:216:HIS:NE2 | 1:F:222:SER:OG | 2.20 | 0.65 |
| 1:F:141:GLY:O | 1:F:166:LEU:HB2 | 1.97 | 0.64 |
| 1:F:18:ASP:O | 1:F:257:ARG:NH1 | 2.30 | 0.64 |
| 1:E:172:ILE:CG1 | 1:E:246:HIS:HB3 | 2.28 | 0.64 |
| 1:F:172:ILE:CG1 | 1:F:246:HIS:HB3 | 2.28 | 0.64 |
| 1:C:172:ILE:CG1 | 1:C:246:HIS:HB3 | 2.28 | 0.64 |
| 1:A:104:PRO:CG | 1:A:110:ASN:OD1 | 2.45 | 0.64 |
| 1:A:61:ASN:OD1 | 1:A:90:SER:OG | 2.15 | 0.64 |
| 1:B:173:GLU:HA | 1:B:206:PRO:HA | 1.80 | 0.64 |
| 1:B:172:ILE:CG1 | 1:B:246:HIS:HB3 | 2.28 | 0.64 |
| 1:G:141:GLY:O | 1:G:166:LEU:HB2 | 1.97 | 0.64 |
| 1:H:141:GLY:O | 1:H:166:LEU:HB2 | 1.97 | 0.64 |
| 1:D:94:MET:HB2 | 1:D:116:GLU:HG2 | 1.79 | 0.64 |
| 1:C:130:LEU:HD21 | 1:D:135:PHE:HE2 | 1.63 | 0.64 |
| 1:D:172:ILE:CG1 | 1:D:246:HIS:HB3 | 2.28 | 0.64 |
| 1:D:173:GLU:HA | 1:D:206:PRO:HA | 1.79 | 0.64 |
| 1:E:173:GLU:HA | 1:E:206:PRO:HA | 1.80 | 0.64 |
| 1:E:210:LEU:HB3 | 1:E:285:ILE:CD1 | 2.28 | 0.64 |
| 1:G:173:GLU:HA | 1:G:206:PRO:HA | 1.80 | 0.64 |
| 1:G:172:ILE:CG1 | 1:G:246:HIS:HB3 | 2.28 | 0.64 |
| 1:G:280:ASP:HB3 | 1:G:282:ARG:CG | 2.28 | 0.64 |
| 1:H:93:THR:HG21 | 1:H:116:GLU:OE1 | 1.97 | 0.64 |
| 1:G:110:ASN:HB3 | 1:H:88:PHE:CD2 | 2.33 | 0.64 |
| 1:B:44:VAL:HG11 | 1:B:48:VAL:HG12 | 1.80 | 0.64 |
| 1:E:36:ASP:OD1 | 1:E:39:HIS:HB3 | 1.98 | 0.64 |
| 1:E:71:CYS:C | 1:E:72:GLY:CA | 2.65 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:89:PHE:CD1 | 1:G:102:LEU:HB2 | 2.32 | 0.64 |
| 1:B:36:ASP:OD1 | 1:B:39:HIS:HB3 | 1.98 | 0.63 |
| 1:F:24:THR:O | 1:G:284:ALA:HA | 1.98 | 0.63 |
| 1:G:46:TRP:N | 1:G:47:PRO:HD2 | 2.13 | 0.63 |
| 1:G:94:MET:HB2 | 1:G:116:GLU:HG2 | 1.79 | 0.63 |
| 1:B:94:MET:HB2 | 1:B:116:GLU:HG2 | 1.80 | 0.63 |
| 1:F:173:GLU:O | 1:F:173:GLU:HG3 | 1.98 | 0.63 |
| 1:B:141:GLY:O | 1:B:166:LEU:HB2 | 1.97 | 0.63 |
| 1:E:141:GLY:O | 1:E:166:LEU:HB2 | 1.97 | 0.63 |
| 1:F:44:VAL:HG11 | 1:F:48:VAL:HG12 | 1.81 | 0.63 |
| 1:F:44:VAL:HG13 | 1:F:48:VAL:HB | 1.79 | 0.63 |
| 1:H:88:PHE:O | 1:H:92:GLN:HG3 | 1.99 | 0.63 |
| 1:B:88:PHE:O | 1:B:92:GLN:HG3 | 1.99 | 0.63 |
| 1:D:280:ASP:HB3 | 1:D:282:ARG:CG | 2.28 | 0.63 |
| 1:F:178:LEU:HD13 | 1:F:241:VAL:HG22 | 1.79 | 0.63 |
| 1:D:88:PHE:O | 1:D:92:GLN:HG3 | 1.99 | 0.63 |
| 1:F:280:ASP:HB3 | 1:F:282:ARG:CG | 2.28 | 0.63 |
| 1:H:36:ASP:OD1 | 1:H:39:HIS:HB3 | 1.98 | 0.63 |
| 1:A:173:GLU:HA | 1:A:206:PRO:HA | 1.79 | 0.63 |
| 1:D:216:HIS:NE2 | 1:D:222:SER:OG | 2.20 | 0.63 |
| 1:E:44:VAL:HG11 | 1:E:48:VAL:HG12 | 1.81 | 0.63 |
| 1:F:36:ASP:OD1 | 1:F:39:HIS:HB3 | 1.98 | 0.63 |
| 1:D:36:ASP:OD1 | 1:D:39:HIS:HB3 | 1.98 | 0.63 |
| 1:F:88:PHE:O | 1:F:92:GLN:HG3 | 1.99 | 0.63 |
| 1:A:261:SER:H | 1:A:264:GLU:HG3 | 1.64 | 0.63 |
| 1:A:280:ASP:HB3 | 1:A:282:ARG:CG | 2.28 | 0.63 |
| 1:A:36:ASP:OD1 | 1:A:39:HIS:HB3 | 1.98 | 0.63 |
| 1:A:89:PHE:CD1 | 1:A:102:LEU:HB2 | 2.32 | 0.63 |
| 1:A:88:PHE:O | 1:A:92:GLN:HG3 | 1.99 | 0.63 |
| 1:C:280:ASP:HB3 | 1:C:282:ARG:CG | 2.28 | 0.63 |
| 1:E:88:PHE:O | 1:E:92:GLN:HG3 | 1.99 | 0.63 |
| 1:B:261:SER:H | 1:B:264:GLU:HG3 | 1.64 | 0.62 |
| 1:C:161:MET:HE2 | 1:C:162:ARG:N | 2.14 | 0.62 |
| 1:E:261:SER:H | 1:E:264:GLU:HG3 | 1.64 | 0.62 |
| 1:D:201:THR:HG22 | 1:D:217:PRO:HD3 | 1.81 | 0.62 |
| 1:G:132:TYR:C | 1:G:132:TYR:CD2 | 2.73 | 0.62 |
| 1:G:36:ASP:OD1 | 1:G:39:HIS:HB3 | 1.98 | 0.62 |
| 1:H:182:ARG:HB3 | 1:H:237:SER:HB3 | 1.81 | 0.62 |
| 1:A:201:THR:HG22 | 1:A:217:PRO:HD3 | 1.81 | 0.62 |
| 1:B:280:ASP:HB3 | 1:B:282:ARG:CG | 2.28 | 0.62 |
| 1:C:216:HIS:NE2 | 1:C:222:SER:OG | 2.20 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:274:VAL:HG12 | 1:C:289:LYS:HB2 | 1.81 | 0.62 |
| 1:D:132:TYR:CD2 | 1:D:132:TYR:C | 2.73 | 0.62 |
| 1:D:161:MET:HE2 | 1:D:162:ARG:N | 2.14 | 0.62 |
| 1:D:173:GLU:HG3 | 1:D:173:GLU:O | 1.98 | 0.62 |
| 1:H:173:GLU:HA | 1:H:206:PRO:HA | 1.80 | 0.62 |
| 1:C:132:TYR:CD2 | 1:C:132:TYR:C | 2.73 | 0.62 |
| 1:C:36:ASP:OD1 | 1:C:39:HIS:HB3 | 1.98 | 0.62 |
| 1:D:261:SER:H | 1:D:264:GLU:HG3 | 1.64 | 0.62 |
| 1:E:132:TYR:C | 1:E:132:TYR:CD2 | 2.73 | 0.62 |
| 1:E:173:GLU:HG3 | 1:E:173:GLU:O | 1.98 | 0.62 |
| 1:F:201:THR:HG22 | 1:F:217:PRO:HD3 | 1.81 | 0.62 |
| 1:H:132:TYR:CD2 | 1:H:132:TYR:C | 2.73 | 0.62 |
| 1:H:173:GLU:O | 1:H:173:GLU:HG3 | 1.98 | 0.62 |
| 1:G:201:THR:HG22 | 1:G:217:PRO:HD3 | 1.81 | 0.62 |
| 1:H:161:MET:HE2 | 1:H:162:ARG:N | 2.15 | 0.62 |
| 1:B:201:THR:HG22 | 1:B:217:PRO:HD3 | 1.81 | 0.62 |
| 1:C:88:PHE:O | 1:C:92:GLN:HG3 | 1.99 | 0.62 |
| 1:E:61:ASN:OD1 | 1:E:90:SER:OG | 2.17 | 0.62 |
| 1:G:93:THR:CG2 | 1:G:116:GLU:OE1 | 2.46 | 0.62 |
| 1:G:261:SER:H | 1:G:264:GLU:HG3 | 1.64 | 0.62 |
| 1:G:14:ILE:HG23 | 1:H:283:ARG:NH1 | 2.14 | 0.62 |
| 1:A:283:ARG:HH21 | 1:D:23:ILE:HG13 | 1.63 | 0.62 |
| 1:C:261:SER:H | 1:C:264:GLU:HG3 | 1.64 | 0.62 |
| 1:G:173:GLU:O | 1:G:173:GLU:HG3 | 1.98 | 0.62 |
| 1:G:216:HIS:NE2 | 1:G:222:SER:OG | 2.20 | 0.62 |
| 1:A:161:MET:HE2 | 1:A:162:ARG:N | 2.15 | 0.62 |
| 1:C:201:THR:HG22 | 1:C:217:PRO:HD3 | 1.81 | 0.62 |
| 1:E:210:LEU:HD13 | 1:E:285:ILE:HD11 | 1.82 | 0.62 |
| 1:F:192:PHE:CE1 | 1:F:194:ARG:HB2 | 2.35 | 0.62 |
| 1:F:261:SER:H | 1:F:264:GLU:HG3 | 1.64 | 0.62 |
| 1:A:94:MET:C | 1:A:95:ALA:HA | 2.07 | 0.61 |
| 1:B:173:GLU:O | 1:B:173:GLU:HG3 | 1.98 | 0.61 |
| 1:E:280:ASP:HB3 | 1:E:282:ARG:CG | 2.28 | 0.61 |
| 1:G:88:PHE:O | 1:G:92:GLN:HG3 | 1.99 | 0.61 |
| 1:E:192:PHE:CE1 | 1:E:194:ARG:HB2 | 2.35 | 0.61 |
| 1:H:201:THR:HG22 | 1:H:217:PRO:HD3 | 1.81 | 0.61 |
| 1:A:182:ARG:HB3 | 1:A:237:SER:HB3 | 1.83 | 0.61 |
| 1:F:114:THR:HG22 | 1:G:91:VAL:HG21 | 1.81 | 0.61 |
| 1:A:132:TYR:CD2 | 1:A:132:TYR:C | 2.73 | 0.61 |
| 1:A:173:GLU:HG3 | 1:A:173:GLU:O | 1.98 | 0.61 |
| 1:D:182:ARG:HB3 | 1:D:237:SER:HB3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:201:THR:HG22 | 1:E:217:PRO:HD3 | 1.81 | 0.61 |
| 1:E:44:VAL:HG11 | 1:E:48:VAL:CG1 | 2.30 | 0.61 |
| 1:G:192:PHE:CE1 | 1:G:194:ARG:HB2 | 2.35 | 0.61 |
| 1:H:280:ASP:HB3 | 1:H:282:ARG:CG | 2.28 | 0.61 |
| 1:B:132:TYR:CD2 | 1:B:132:TYR:C | 2.73 | 0.61 |
| 1:E:23:ILE:CG1 | 1:F:283:ARG:HH21 | 2.14 | 0.61 |
| 1:H:158:THR:HG21 | 1:H:215:MET:HB3 | 1.83 | 0.61 |
| 1:B:182:ARG:HB3 | 1:B:237:SER:HB3 | 1.83 | 0.61 |
| 1:C:182:ARG:HB3 | 1:C:237:SER:HB3 | 1.83 | 0.61 |
| 1:F:132:TYR:CD2 | 1:F:132:TYR:C | 2.73 | 0.61 |
| 1:H:172:ILE:CG1 | 1:H:246:HIS:HB3 | 2.28 | 0.61 |
| 1:A:158:THR:HG21 | 1:A:215:MET:HB3 | 1.83 | 0.61 |
| 1:C:153:PHE:CE2 | 1:C:154:GLU:OE1 | 2.54 | 0.61 |
| 1:C:158:THR:HG21 | 1:C:215:MET:HB3 | 1.83 | 0.61 |
| 1:D:153:PHE:CE2 | 1:D:154:GLU:OE1 | 2.54 | 0.61 |
| 1:B:158:THR:HG21 | 1:B:215:MET:HB3 | 1.83 | 0.60 |
| 1:B:216:HIS:NE2 | 1:B:222:SER:OG | 2.20 | 0.60 |
| 1:A:283:ARG:CZ | 1:D:23:ILE:CD1 | 2.79 | 0.60 |
| 1:D:158:THR:HG21 | 1:D:215:MET:HB3 | 1.83 | 0.60 |
| 1:E:153:PHE:CE2 | 1:E:154:GLU:OE1 | 2.54 | 0.60 |
| 1:E:158:THR:HG21 | 1:E:215:MET:HB3 | 1.83 | 0.60 |
| 1:E:88:PHE:CD2 | 1:H:110:ASN:HB3 | 2.35 | 0.60 |
| 1:F:153:PHE:CE2 | 1:F:154:GLU:OE1 | 2.54 | 0.60 |
| 1:F:158:THR:HG21 | 1:F:215:MET:HB3 | 1.83 | 0.60 |
| 1:H:69:LEU:O | 1:H:72:GLY:CA | 2.49 | 0.60 |
| 1:B:153:PHE:CE2 | 1:B:154:GLU:OE1 | 2.54 | 0.60 |
| 1:B:242:LEU:HD23 | 1:C:206:PRO:HB3 | 1.83 | 0.60 |
| 1:G:153:PHE:CE2 | 1:G:154:GLU:OE1 | 2.54 | 0.60 |
| 1:A:172:ILE:CG1 | 1:A:246:HIS:HB3 | 2.28 | 0.60 |
| 1:E:161:MET:HE2 | 1:E:162:ARG:N | 2.16 | 0.60 |
| 1:F:149:VAL:HG12 | 1:F:293:ILE:HD13 | 1.83 | 0.60 |
| 1:G:161:MET:HE2 | 1:G:162:ARG:N | 2.16 | 0.60 |
| 1:A:153:PHE:CE2 | 1:A:154:GLU:OE1 | 2.54 | 0.60 |
| 1:B:75:ILE:HD13 | 1:B:89:PHE:CG | 2.36 | 0.60 |
| 1:G:46:TRP:O | 1:G:47:PRO:C | 2.39 | 0.60 |
| 1:H:149:VAL:HG12 | 1:H:293:ILE:HD13 | 1.83 | 0.60 |
| 1:A:69:LEU:O | 1:A:72:GLY:N | 2.35 | 0.60 |
| 1:G:158:THR:HG21 | 1:G:215:MET:HB3 | 1.83 | 0.60 |
| 1:A:41:LEU:O | 1:A:134:ARG:NH1 | 2.34 | 0.60 |
| 1:G:149:VAL:HG12 | 1:G:293:ILE:HD13 | 1.83 | 0.60 |
| 1:E:149:VAL:HG12 | 1:E:293:ILE:HD13 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:161:MET:HE2 | 1:B:162:ARG:N | 2.17 | 0.59 |
| 1:H:153:PHE:CE2 | 1:H:154:GLU:OE1 | 2.54 | 0.59 |
| 1:H:69:LEU:O | 1:H:72:GLY:HA2 | 2.02 | 0.59 |
| 1:C:149:VAL:HG12 | 1:C:293:ILE:HD13 | 1.83 | 0.59 |
| 1:F:161:MET:HE2 | 1:F:162:ARG:N | 2.18 | 0.59 |
| 1:B:149:VAL:HG12 | 1:B:293:ILE:HD13 | 1.83 | 0.59 |
| 1:C:295:GLN:C | 1:E:292:GLU:HG2 | 2.22 | 0.59 |
| 1:E:23:ILE:CG2 | 1:F:285:ILE:HG13 | 2.26 | 0.59 |
| 1:C:104:PRO:HB2 | 1:C:110:ASN:OD1 | 2.02 | 0.59 |
| 1:A:216:HIS:NE2 | 1:A:222:SER:OG | 2.20 | 0.59 |
| 1:F:110:ASN:C | 1:G:88:PHE:CE2 | 2.75 | 0.58 |
| 1:F:110:ASN:HB3 | 1:G:88:PHE:CE2 | 2.38 | 0.58 |
| 1:B:192:PHE:CE1 | 1:B:194:ARG:HB2 | 2.38 | 0.58 |
| 1:D:93:THR:CG2 | 1:D:94:MET:N | 2.67 | 0.58 |
| 1:F:110:ASN:CB | 1:G:88:PHE:CE2 | 2.86 | 0.58 |
| 1:F:93:THR:CG2 | 1:F:94:MET:N | 2.67 | 0.58 |
| 1:H:93:THR:CG2 | 1:H:94:MET:N | 2.67 | 0.58 |
| 1:A:61:ASN:ND2 | 1:A:94:MET:CE | 2.63 | 0.58 |
| 1:E:23:ILE:HD11 | 1:F:283:ARG:NE | 2.16 | 0.58 |
| 1:B:44:VAL:HG11 | 1:B:48:VAL:CG1 | 2.33 | 0.58 |
| 1:A:26:LEU:HB2 | 1:B:285:ILE:O | 2.04 | 0.58 |
| 1:E:216:HIS:NE2 | 1:E:222:SER:OG | 2.20 | 0.58 |
| 1:F:44:VAL:HG11 | 1:F:48:VAL:CG1 | 2.33 | 0.58 |
| 1:G:110:ASN:HB3 | 1:H:88:PHE:CE2 | 2.38 | 0.58 |
| 1:F:94:MET:HB2 | 1:F:116:GLU:HG2 | 1.86 | 0.58 |
| 1:E:23:ILE:CD1 | 1:F:283:ARG:NH2 | 2.65 | 0.58 |
| 1:A:93:THR:CG2 | 1:A:94:MET:N | 2.67 | 0.58 |
| 1:G:74:VAL:HB | 1:G:109:ALA:HB2 | 1.86 | 0.58 |
| 1:G:274:VAL:HG12 | 1:G:289:LYS:HB2 | 1.85 | 0.58 |
| 1:E:93:THR:CG2 | 1:E:94:MET:N | 2.67 | 0.57 |
| 1:G:93:THR:CG2 | 1:G:94:MET:N | 2.67 | 0.57 |
| 1:A:110:ASN:O | 1:A:114:THR:HG23 | 2.05 | 0.57 |
| 1:A:182:ARG:CB | 1:A:237:SER:HB3 | 2.34 | 0.57 |
| 1:A:44:VAL:HG13 | 1:A:48:VAL:HB | 1.85 | 0.57 |
| 1:C:110:ASN:O | 1:C:114:THR:HG23 | 2.05 | 0.57 |
| 1:D:182:ARG:CB | 1:D:237:SER:HB3 | 2.34 | 0.57 |
| 1:G:192:PHE:HE1 | 1:G:194:ARG:HB2 | 1.70 | 0.57 |
| 1:G:23:ILE:HD12 | 1:H:283:ARG:HB3 | 1.85 | 0.57 |
| 1:A:192:PHE:CE1 | 1:A:194:ARG:HB2 | 2.40 | 0.57 |
| 1:C:110:ASN:HB3 | 1:D:88:PHE:CD2 | 2.39 | 0.57 |
| 1:F:110:ASN:O | 1:F:114:THR:HG23 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:192:PHE:HE1 | 1:F:194:ARG:HB2 | 1.70 | 0.57 |
| 1:H:185:ILE:CD1 | 1:H:191:VAL:CB | 2.83 | 0.57 |
| 1:A:74:VAL:HB | 1:A:109:ALA:HB2 | 1.86 | 0.57 |
| 1:B:93:THR:CG2 | 1:B:94:MET:N | 2.67 | 0.57 |
| 1:E:185:ILE:CD1 | 1:E:191:VAL:CB | 2.83 | 0.57 |
| 1:E:207:ILE:CD1 | 1:H:240:LEU:HD21 | 2.33 | 0.57 |
| 1:G:140:ALA:HB1 | 1:G:142:VAL:HG23 | 1.87 | 0.57 |
| 1:D:110:ASN:O | 1:D:114:THR:HG23 | 2.05 | 0.57 |
| 1:E:71:CYS:CA | 1:E:72:GLY:N | 2.63 | 0.57 |
| 1:H:110:ASN:O | 1:H:114:THR:HG23 | 2.05 | 0.57 |
| 1:G:110:ASN:O | 1:G:114:THR:HG23 | 2.05 | 0.57 |
| 1:H:71:CYS:HB2 | 1:H:74:VAL:HG21 | 1.86 | 0.57 |
| 1:A:185:ILE:CD1 | 1:A:191:VAL:CB | 2.83 | 0.56 |
| 1:D:140:ALA:HB1 | 1:D:142:VAL:HG23 | 1.87 | 0.56 |
| 1:E:110:ASN:O | 1:E:114:THR:HG23 | 2.05 | 0.56 |
| 1:G:44:VAL:HG11 | 1:G:48:VAL:CG1 | 2.35 | 0.56 |
| 1:F:185:ILE:CD1 | 1:F:191:VAL:CB | 2.83 | 0.56 |
| 1:C:182:ARG:CB | 1:C:237:SER:HB3 | 2.34 | 0.56 |
| 1:D:185:ILE:CD1 | 1:D:191:VAL:CB | 2.83 | 0.56 |
| 1:B:210:LEU:HB3 | 1:B:285:ILE:HD13 | 1.87 | 0.56 |
| 1:A:140:ALA:HB1 | 1:A:142:VAL:HG23 | 1.87 | 0.56 |
| 1:F:274:VAL:HG12 | 1:F:289:LYS:HB2 | 1.87 | 0.56 |
| 1:G:185:ILE:CD1 | 1:G:191:VAL:CB | 2.83 | 0.56 |
| 1:C:93:THR:CG2 | 1:C:94:MET:N | 2.67 | 0.56 |
| 1:B:185:ILE:CD1 | 1:B:191:VAL:CB | 2.83 | 0.56 |
| 1:B:140:ALA:HB1 | 1:B:142:VAL:HG23 | 1.87 | 0.56 |
| 1:A:104:PRO:HB2 | 1:A:110:ASN:OD1 | 2.06 | 0.56 |
| 1:E:192:PHE:HE1 | 1:E:194:ARG:HB2 | 1.70 | 0.56 |
| 1:B:182:ARG:CB | 1:B:237:SER:HB3 | 2.34 | 0.56 |
| 1:H:140:ALA:HB1 | 1:H:142:VAL:HG23 | 1.87 | 0.56 |
| 1:H:216:HIS:NE2 | 1:H:222:SER:OG | 2.20 | 0.56 |
| 1:A:110:ASN:HB3 | 1:B:88:PHE:CD2 | 2.41 | 0.56 |
| 1:B:110:ASN:O | 1:B:114:THR:HG23 | 2.05 | 0.56 |
| 1:E:49:PHE:HE2 | 1:E:131:ILE:HD13 | 1.69 | 0.56 |
| 1:E:95:ALA:C | 1:E:96:THR:HG23 | 2.25 | 0.56 |
| 1:F:140:ALA:HB1 | 1:F:142:VAL:HG23 | 1.87 | 0.56 |
| 1:H:89:PHE:HD1 | 1:H:102:LEU:HB2 | 1.69 | 0.56 |
| 1:E:140:ALA:HB1 | 1:E:142:VAL:HG23 | 1.87 | 0.55 |
| 1:G:130:LEU:O | 1:G:134:ARG:HG2 | 2.06 | 0.55 |
| 1:H:88:PHE:O | 1:H:92:GLN:CG | 2.55 | 0.55 |
| 1:C:94:MET:HB2 | 1:C:116:GLU:HG2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:130:LEU:O | 1:E:134:ARG:HG2 | 2.06 | 0.55 |
| 1:E:26:LEU:HG | 1:F:285:ILE:O | 2.06 | 0.55 |
| 1:A:182:ARG:HA | 1:A:193:ARG:NH1 | 2.20 | 0.55 |
| 1:A:88:PHE:O | 1:A:92:GLN:CG | 2.55 | 0.55 |
| 1:B:116:GLU:O | 1:B:117:ALA:C | 2.45 | 0.55 |
| 1:D:116:GLU:O | 1:D:117:ALA:C | 2.45 | 0.55 |
| 1:F:55:GLY:O | 1:F:59:VAL:HG23 | 2.07 | 0.55 |
| 1:C:129:SER:HB3 | 1:D:132:TYR:CD1 | 2.42 | 0.55 |
| 1:C:130:LEU:O | 1:C:134:ARG:HG2 | 2.06 | 0.55 |
| 1:E:266:ILE:O | 1:E:266:ILE:CG2 | 2.54 | 0.55 |
| 1:F:61:ASN:OD1 | 1:F:94:MET:HE2 | 2.06 | 0.55 |
| 1:G:175:ASP:C | 1:G:175:ASP:OD1 | 2.45 | 0.55 |
| 1:A:130:LEU:O | 1:A:134:ARG:HG2 | 2.06 | 0.55 |
| 1:A:240:LEU:HD21 | 1:B:207:ILE:HD13 | 1.88 | 0.55 |
| 1:B:69:LEU:O | 1:B:72:GLY:N | 2.39 | 0.55 |
| 1:C:140:ALA:HB1 | 1:C:142:VAL:HG23 | 1.87 | 0.55 |
| 1:D:175:ASP:OD1 | 1:D:175:ASP:C | 2.45 | 0.55 |
| 1:G:55:GLY:O | 1:G:59:VAL:HG23 | 2.07 | 0.55 |
| 1:H:175:ASP:OD1 | 1:H:175:ASP:C | 2.45 | 0.55 |
| 1:A:201:THR:HG22 | 1:A:217:PRO:CD | 2.37 | 0.55 |
| 1:B:55:GLY:O | 1:B:59:VAL:HG23 | 2.07 | 0.55 |
| 1:C:55:GLY:O | 1:C:59:VAL:HG23 | 2.07 | 0.55 |
| 1:E:227:GLU:OE2 | 1:E:231:THR:HB | 2.07 | 0.55 |
| 1:F:116:GLU:O | 1:F:117:ALA:C | 2.45 | 0.55 |
| 1:E:132:TYR:CD1 | 1:H:129:SER:HB3 | 2.42 | 0.55 |
| 1:A:175:ASP:C | 1:A:175:ASP:OD1 | 2.45 | 0.55 |
| 1:C:185:ILE:CD1 | 1:C:191:VAL:CB | 2.83 | 0.55 |
| 1:E:88:PHE:O | 1:E:92:GLN:CG | 2.55 | 0.55 |
| 1:C:175:ASP:OD1 | 1:C:175:ASP:C | 2.45 | 0.55 |
| 1:E:44:VAL:HG13 | 1:E:48:VAL:HB | 1.87 | 0.55 |
| 1:F:130:LEU:O | 1:F:134:ARG:HG2 | 2.06 | 0.55 |
| 1:F:175:ASP:C | 1:F:175:ASP:OD1 | 2.45 | 0.55 |
| 1:H:201:THR:HG22 | 1:H:217:PRO:CD | 2.37 | 0.55 |
| 1:A:55:GLY:O | 1:A:59:VAL:HG23 | 2.07 | 0.55 |
| 1:B:88:PHE:O | 1:B:92:GLN:CG | 2.55 | 0.55 |
| 1:D:88:PHE:O | 1:D:92:GLN:CG | 2.55 | 0.55 |
| 1:H:130:LEU:O | 1:H:134:ARG:HG2 | 2.06 | 0.55 |
| 1:A:172:ILE:O | 1:A:173:GLU:HG2 | 2.07 | 0.55 |
| 1:B:201:THR:HG22 | 1:B:217:PRO:CD | 2.37 | 0.55 |
| 1:B:266:ILE:CG2 | 1:B:266:ILE:O | 2.54 | 0.55 |
| 1:D:172:ILE:O | 1:D:173:GLU:HG2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:201:THR:HG22 | 1:D:217:PRO:CD | 2.37 | 0.55 |
| 1:H:116:GLU:O | 1:H:117:ALA:C | 2.45 | 0.55 |
| 1:H:172:ILE:O | 1:H:173:GLU:HG2 | 2.07 | 0.55 |
| 1:B:192:PHE:HE1 | 1:B:194:ARG:HB2 | 1.72 | 0.54 |
| 1:B:227:GLU:OE2 | 1:B:231:THR:HB | 2.07 | 0.54 |
| 1:C:201:THR:HG22 | 1:C:217:PRO:CD | 2.37 | 0.54 |
| 1:D:210:LEU:HD22 | 1:D:285:ILE:CD1 | 2.37 | 0.54 |
| 1:E:88:PHE:CE2 | 1:H:110:ASN:HB3 | 2.42 | 0.54 |
| 1:G:172:ILE:O | 1:G:173:GLU:HG2 | 2.07 | 0.54 |
| 1:G:227:GLU:OE2 | 1:G:231:THR:HB | 2.07 | 0.54 |
| 1:H:138:PRO:HB3 | 1:H:250:PHE:CG | 2.42 | 0.54 |
| 1:B:130:LEU:O | 1:B:134:ARG:HG2 | 2.06 | 0.54 |
| 1:C:116:GLU:O | 1:C:117:ALA:C | 2.45 | 0.54 |
| 1:D:55:GLY:O | 1:D:59:VAL:HG23 | 2.07 | 0.54 |
| 1:E:201:THR:HG22 | 1:E:217:PRO:CD | 2.37 | 0.54 |
| 1:G:89:PHE:HB2 | 1:G:102:LEU:HD13 | 1.88 | 0.54 |
| 1:H:227:GLU:OE2 | 1:H:231:THR:HB | 2.07 | 0.54 |
| 1:H:61:ASN:OD1 | 1:H:94:MET:HE2 | 2.08 | 0.54 |
| 1:A:227:GLU:OE2 | 1:A:231:THR:HB | 2.07 | 0.54 |
| 1:C:49:PHE:HE2 | 1:C:131:ILE:HD13 | 1.72 | 0.54 |
| 1:D:130:LEU:O | 1:D:134:ARG:HG2 | 2.06 | 0.54 |
| 1:E:110:ASN:HB3 | 1:F:88:PHE:CD2 | 2.43 | 0.54 |
| 1:E:26:LEU:HD12 | 1:F:286:ASP:HB2 | 1.90 | 0.54 |
| 1:G:61:ASN:OD1 | 1:G:90:SER:OG | 2.25 | 0.54 |
| 1:G:88:PHE:O | 1:G:92:GLN:CG | 2.55 | 0.54 |
| 1:A:283:ARG:NH2 | 1:D:23:ILE:HG13 | 2.22 | 0.54 |
| 1:C:184:GLU:OE1 | 1:C:194:ARG:HD2 | 2.07 | 0.54 |
| 1:C:88:PHE:O | 1:C:92:GLN:CG | 2.55 | 0.54 |
| 1:E:175:ASP:C | 1:E:175:ASP:OD1 | 2.45 | 0.54 |
| 1:E:210:LEU:HB3 | 1:E:285:ILE:HD11 | 1.89 | 0.54 |
| 1:G:49:PHE:HE2 | 1:G:131:ILE:HD13 | 1.73 | 0.54 |
| 1:B:175:ASP:C | 1:B:175:ASP:OD1 | 2.45 | 0.54 |
| 1:B:209:SER:O | 1:B:210:LEU:HD23 | 2.08 | 0.54 |
| 1:D:46:TRP:O | 1:D:50:ILE:HG13 | 2.08 | 0.54 |
| 1:F:138:PRO:HB3 | 1:F:250:PHE:CG | 2.42 | 0.54 |
| 1:F:201:THR:HG22 | 1:F:217:PRO:CD | 2.37 | 0.54 |
| 1:A:138:PRO:HB3 | 1:A:250:PHE:CG | 2.42 | 0.54 |
| 1:B:172:ILE:O | 1:B:173:GLU:HG2 | 2.07 | 0.54 |
| 1:C:209:SER:O | 1:C:210:LEU:HD23 | 2.08 | 0.54 |
| 1:G:210:LEU:HB3 | 1:G:285:ILE:HD11 | 1.90 | 0.54 |
| 1:H:182:ARG:CB | 1:H:237:SER:HB3 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:55:GLY:O | 1:H:59:VAL:HG23 | 2.07 | 0.54 |
| 1:A:116:GLU:O | 1:A:117:ALA:C | 2.45 | 0.54 |
| 1:D:61:ASN:OD1 | 1:D:94:MET:HE2 | 2.08 | 0.54 |
| 1:E:55:GLY:O | 1:E:59:VAL:HG23 | 2.07 | 0.54 |
| 1:F:88:PHE:O | 1:F:92:GLN:CG | 2.55 | 0.54 |
| 1:G:201:THR:HG22 | 1:G:217:PRO:CD | 2.37 | 0.54 |
| 1:C:276:THR:CG2 | 1:C:277:THR:N | 2.71 | 0.54 |
| 1:D:276:THR:CG2 | 1:D:277:THR:N | 2.71 | 0.54 |
| 1:D:44:VAL:HG13 | 1:D:48:VAL:CB | 2.35 | 0.54 |
| 1:E:116:GLU:O | 1:E:117:ALA:C | 2.45 | 0.54 |
| 1:E:138:PRO:HB3 | 1:E:250:PHE:CG | 2.42 | 0.54 |
| 1:E:209:SER:O | 1:E:210:LEU:HD23 | 2.08 | 0.54 |
| 1:B:149:VAL:CG1 | 1:B:293:ILE:HD13 | 2.38 | 0.54 |
| 1:C:46:TRP:O | 1:C:50:ILE:HG13 | 2.08 | 0.54 |
| 1:E:132:TYR:HD1 | 1:H:129:SER:HB3 | 1.73 | 0.54 |
| 1:F:209:SER:O | 1:F:210:LEU:HD23 | 2.08 | 0.54 |
| 1:A:209:SER:O | 1:A:210:LEU:HD23 | 2.08 | 0.54 |
| 1:A:276:THR:CG2 | 1:A:277:THR:N | 2.71 | 0.54 |
| 1:B:276:THR:CG2 | 1:B:277:THR:N | 2.71 | 0.54 |
| 1:C:172:ILE:O | 1:C:173:GLU:C | 2.41 | 0.54 |
| 1:D:227:GLU:OE2 | 1:D:231:THR:HB | 2.07 | 0.54 |
| 1:C:295:GLN:O | 1:E:292:GLU:HG2 | 2.07 | 0.54 |
| 1:E:49:PHE:CE2 | 1:E:131:ILE:HD13 | 2.43 | 0.54 |
| 1:H:149:VAL:CG1 | 1:H:293:ILE:HD13 | 2.38 | 0.54 |
| 1:B:46:TRP:O | 1:B:50:ILE:HG13 | 2.08 | 0.53 |
| 1:C:138:PRO:HB3 | 1:C:250:PHE:CG | 2.42 | 0.53 |
| 1:E:207:ILE:CG2 | 1:E:207:ILE:O | 2.56 | 0.53 |
| 1:F:276:THR:CG2 | 1:F:277:THR:N | 2.71 | 0.53 |
| 1:A:138:PRO:CG | 1:A:252:GLN:OE1 | 2.56 | 0.53 |
| 1:C:227:GLU:OE2 | 1:C:231:THR:HB | 2.07 | 0.53 |
| 1:E:172:ILE:O | 1:E:173:GLU:HG2 | 2.07 | 0.53 |
| 1:F:227:GLU:OE2 | 1:F:231:THR:HB | 2.07 | 0.53 |
| 1:H:182:ARG:HB3 | 1:H:237:SER:CB | 2.39 | 0.53 |
| 1:H:276:THR:CG2 | 1:H:277:THR:N | 2.71 | 0.53 |
| 1:B:138:PRO:HB3 | 1:B:250:PHE:CG | 2.42 | 0.53 |
| 1:E:149:VAL:CG1 | 1:E:293:ILE:HD13 | 2.38 | 0.53 |
| 1:E:276:THR:CG2 | 1:E:277:THR:N | 2.71 | 0.53 |
| 1:G:276:THR:CG2 | 1:G:277:THR:N | 2.71 | 0.53 |
| 1:G:40:ASP:O | 1:G:44:VAL:HG23 | 2.09 | 0.53 |
| 1:C:240:LEU:HD21 | 1:D:207:ILE:CD1 | 2.38 | 0.53 |
| 1:G:138:PRO:HB3 | 1:G:250:PHE:CG | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:44:VAL:HG13 | 1:G:48:VAL:HB | 1.90 | 0.53 |
| 1:A:207:ILE:CG2 | 1:A:207:ILE:O | 2.56 | 0.53 |
| 1:A:283:ARG:HB3 | 1:D:23:ILE:HD12 | 1.91 | 0.53 |
| 1:A:44:VAL:HG11 | 1:A:48:VAL:HG12 | 1.90 | 0.53 |
| 1:A:46:TRP:O | 1:A:50:ILE:HG13 | 2.08 | 0.53 |
| 1:E:75:ILE:HD11 | 1:E:89:PHE:HD2 | 1.70 | 0.53 |
| 1:F:149:VAL:CG1 | 1:F:293:ILE:HD13 | 2.38 | 0.53 |
| 1:F:40:ASP:O | 1:F:44:VAL:HG23 | 2.09 | 0.53 |
| 1:G:149:VAL:CG1 | 1:G:293:ILE:HD13 | 2.38 | 0.53 |
| 1:H:209:SER:O | 1:H:210:LEU:HD23 | 2.08 | 0.53 |
| 1:H:46:TRP:O | 1:H:50:ILE:HG13 | 2.08 | 0.53 |
| 1:B:207:ILE:O | 1:B:207:ILE:CG2 | 2.56 | 0.53 |
| 1:C:192:PHE:CE1 | 1:C:194:ARG:HB2 | 2.44 | 0.53 |
| 1:D:138:PRO:HB3 | 1:D:250:PHE:CG | 2.42 | 0.53 |
| 1:G:209:SER:O | 1:G:210:LEU:HD23 | 2.08 | 0.53 |
| 1:A:40:ASP:O | 1:A:44:VAL:HG23 | 2.09 | 0.53 |
| 1:C:149:VAL:CG1 | 1:C:293:ILE:HD13 | 2.38 | 0.53 |
| 1:C:41:LEU:O | 1:C:134:ARG:NH1 | 2.38 | 0.53 |
| 1:D:209:SER:O | 1:D:210:LEU:HD23 | 2.08 | 0.53 |
| 1:D:40:ASP:O | 1:D:44:VAL:HG23 | 2.09 | 0.53 |
| 1:E:130:LEU:HD21 | 1:F:135:PHE:HE2 | 1.74 | 0.53 |
| 1:G:116:GLU:O | 1:G:117:ALA:C | 2.45 | 0.53 |
| 1:B:74:VAL:HB | 1:B:109:ALA:HB2 | 1.91 | 0.53 |
| 1:C:40:ASP:O | 1:C:44:VAL:HG23 | 2.09 | 0.53 |
| 1:H:40:ASP:O | 1:H:44:VAL:HG23 | 2.09 | 0.53 |
| 1:A:192:PHE:HE1 | 1:A:194:ARG:HB2 | 1.74 | 0.52 |
| 1:B:210:LEU:HB3 | 1:B:285:ILE:CD1 | 2.39 | 0.52 |
| 1:B:40:ASP:O | 1:B:44:VAL:HG23 | 2.09 | 0.52 |
| 1:C:26:LEU:HB2 | 1:D:285:ILE:O | 2.09 | 0.52 |
| 1:C:299:HIS:HA | 1:E:147:ARG:HH22 | 1.74 | 0.52 |
| 1:F:74:VAL:HB | 1:F:109:ALA:HB2 | 1.91 | 0.52 |
| 1:G:44:VAL:HG11 | 1:G:48:VAL:HG12 | 1.90 | 0.52 |
| 1:E:15:LEU:HB2 | 1:E:238:GLU:OE1 | 2.08 | 0.52 |
| 1:E:75:ILE:HD11 | 1:E:89:PHE:CE2 | 2.44 | 0.52 |
| 1:C:44:VAL:HG13 | 1:C:48:VAL:HB | 1.88 | 0.52 |
| 1:G:61:ASN:OD1 | 1:G:94:MET:HE2 | 2.09 | 0.52 |
| 1:B:15:LEU:HB2 | 1:B:238:GLU:OE1 | 2.09 | 0.52 |
| 1:C:182:ARG:HB3 | 1:C:237:SER:CB | 2.40 | 0.52 |
| 1:B:182:ARG:HB3 | 1:B:237:SER:CB | 2.40 | 0.52 |
| 1:B:185:ILE:HD11 | 1:B:191:VAL:HB | 1.92 | 0.52 |
| 1:D:182:ARG:HB3 | 1:D:237:SER:CB | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:34:LEU:HG | 1:F:34:LEU:O | 2.09 | 0.52 |
| 1:G:56:LEU:HD12 | 1:G:60:THR:HG23 | 1.92 | 0.52 |
| 1:A:182:ARG:HB3 | 1:A:237:SER:CB | 2.40 | 0.52 |
| 1:C:61:ASN:OD1 | 1:C:90:SER:OG | 2.24 | 0.52 |
| 1:G:49:PHE:CE2 | 1:G:131:ILE:HD13 | 2.45 | 0.52 |
| 1:G:129:SER:HB3 | 1:H:132:TYR:HD1 | 1.74 | 0.51 |
| 1:G:129:SER:HB3 | 1:H:132:TYR:CD1 | 2.45 | 0.51 |
| 1:C:56:LEU:HD12 | 1:C:60:THR:HG23 | 1.92 | 0.51 |
| 1:E:158:THR:HG23 | 1:E:216:HIS:C | 2.31 | 0.51 |
| 1:F:110:ASN:CB | 1:G:88:PHE:CD2 | 2.87 | 0.51 |
| 1:B:158:THR:HG23 | 1:B:216:HIS:C | 2.31 | 0.51 |
| 1:E:40:ASP:O | 1:E:44:VAL:HG23 | 2.09 | 0.51 |
| 1:F:44:VAL:CG1 | 1:F:48:VAL:CG1 | 2.88 | 0.51 |
| 1:D:56:LEU:HD12 | 1:D:60:THR:HG23 | 1.92 | 0.51 |
| 1:F:272:VAL:HG13 | 1:F:273:ASP:H | 1.75 | 0.51 |
| 1:C:158:THR:HG23 | 1:C:216:HIS:C | 2.31 | 0.51 |
| 1:B:23:ILE:CG2 | 1:C:285:ILE:HG13 | 2.35 | 0.51 |
| 1:A:44:VAL:HG11 | 1:A:48:VAL:CG1 | 2.40 | 0.51 |
| 1:C:106:GLY:O | 1:C:110:ASN:ND2 | 2.44 | 0.51 |
| 1:F:185:ILE:HD11 | 1:F:191:VAL:HB | 1.92 | 0.51 |
| 1:A:104:PRO:CB | 1:A:110:ASN:OD1 | 2.58 | 0.51 |
| 1:E:219:ASP:OD1 | 1:E:219:ASP:C | 2.49 | 0.51 |
| 1:H:192:PHE:CE1 | 1:H:194:ARG:HB2 | 2.45 | 0.51 |
| 1:A:158:THR:HG23 | 1:A:216:HIS:C | 2.31 | 0.51 |
| 1:C:272:VAL:HG13 | 1:C:273:ASP:H | 1.75 | 0.51 |
| 1:F:158:THR:HG23 | 1:F:216:HIS:C | 2.31 | 0.51 |
| 1:G:18:ASP:O | 1:G:257:ARG:NH1 | 2.43 | 0.51 |
| 1:G:56:LEU:HD12 | 1:G:56:LEU:O | 2.11 | 0.51 |
| 1:A:49:PHE:HE2 | 1:A:131:ILE:HD13 | 1.76 | 0.51 |
| 1:B:104:PRO:HB2 | 1:B:110:ASN:OD1 | 2.11 | 0.51 |
| 1:B:147:ARG:NH1 | 1:B:147:ARG:HG2 | 2.26 | 0.51 |
| 1:B:44:VAL:CG1 | 1:B:48:VAL:CB | 2.88 | 0.51 |
| 1:C:49:PHE:CE2 | 1:C:131:ILE:HD13 | 2.45 | 0.51 |
| 1:D:158:THR:HG23 | 1:D:216:HIS:C | 2.31 | 0.51 |
| 1:E:147:ARG:NH1 | 1:E:147:ARG:HG2 | 2.26 | 0.51 |
| 1:E:44:VAL:CG1 | 1:E:48:VAL:CG1 | 2.89 | 0.51 |
| 1:E:56:LEU:HD12 | 1:E:56:LEU:O | 2.11 | 0.51 |
| 1:F:42:LEU:HB3 | 1:F:137:ARG:NH2 | 2.26 | 0.51 |
| 1:G:200:LEU:HD13 | 1:G:214:VAL:HG12 | 1.92 | 0.51 |
| 1:H:158:THR:HG23 | 1:H:216:HIS:C | 2.31 | 0.51 |
| 1:A:147:ARG:HG2 | 1:A:147:ARG:NH1 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:219:ASP:OD1 | 1:A:219:ASP:C | 2.49 | 0.51 |
| 1:A:114:THR:HG22 | 1:B:91:VAL:HG21 | 1.93 | 0.51 |
| 1:D:56:LEU:HD12 | 1:D:56:LEU:O | 2.11 | 0.51 |
| 1:E:185:ILE:HD11 | 1:E:191:VAL:HB | 1.92 | 0.51 |
| 1:G:158:THR:HG23 | 1:G:216:HIS:C | 2.31 | 0.51 |
| 1:H:56:LEU:HD12 | 1:H:60:THR:HG23 | 1.92 | 0.51 |
| 1:A:18:ASP:O | 1:A:257:ARG:NH1 | 2.44 | 0.50 |
| 1:A:210:LEU:HB3 | 1:A:285:ILE:CD1 | 2.42 | 0.50 |
| 1:B:44:VAL:CG1 | 1:B:48:VAL:CG1 | 2.90 | 0.50 |
| 1:C:56:LEU:O | 1:C:56:LEU:HD12 | 2.11 | 0.50 |
| 1:E:156:LYS:O | 1:E:157:PRO:C | 2.46 | 0.50 |
| 1:F:94:MET:HB2 | 1:F:116:GLU:CG | 2.41 | 0.50 |
| 1:G:184:GLU:OE1 | 1:G:194:ARG:HD2 | 2.11 | 0.50 |
| 1:H:147:ARG:NH1 | 1:H:147:ARG:HG2 | 2.26 | 0.50 |
| 1:D:266:ILE:HG22 | 1:D:269:GLY:HA3 | 1.94 | 0.50 |
| 1:E:170:GLN:HE22 | 1:H:21:SER:H | 1.59 | 0.50 |
| 1:H:272:VAL:HG13 | 1:H:273:ASP:H | 1.75 | 0.50 |
| 1:A:272:VAL:HG13 | 1:A:273:ASP:H | 1.75 | 0.50 |
| 1:B:56:LEU:O | 1:B:56:LEU:HD12 | 2.11 | 0.50 |
| 1:D:147:ARG:HG2 | 1:D:147:ARG:NH1 | 2.26 | 0.50 |
| 1:A:56:LEU:HD12 | 1:A:60:THR:HG23 | 1.92 | 0.50 |
| 1:B:110:ASN:O | 1:B:113:VAL:HB | 2.12 | 0.50 |
| 1:B:219:ASP:OD1 | 1:B:219:ASP:C | 2.49 | 0.50 |
| 1:B:272:VAL:HG13 | 1:B:273:ASP:H | 1.75 | 0.50 |
| 1:C:147:ARG:NH1 | 1:C:147:ARG:HG2 | 2.26 | 0.50 |
| 1:A:89:PHE:HD1 | 1:A:102:LEU:HB2 | 1.77 | 0.50 |
| 1:A:91:VAL:HG21 | 1:D:114:THR:CG2 | 2.42 | 0.50 |
| 1:C:204:ARG:NH1 | 1:C:204:ARG:HG2 | 2.25 | 0.50 |
| 1:D:44:VAL:HG13 | 1:D:48:VAL:CG1 | 2.41 | 0.50 |
| 1:D:61:ASN:OD1 | 1:D:90:SER:OG | 2.25 | 0.50 |
| 1:E:110:ASN:O | 1:E:113:VAL:HB | 2.12 | 0.50 |
| 1:E:272:VAL:HG13 | 1:E:273:ASP:H | 1.75 | 0.50 |
| 1:F:272:VAL:CG1 | 1:F:273:ASP:H | 2.25 | 0.50 |
| 1:G:23:ILE:CD1 | 1:H:283:ARG:HB3 | 2.41 | 0.50 |
| 1:A:204:ARG:NH1 | 1:A:204:ARG:HG2 | 2.25 | 0.50 |
| 1:A:44:VAL:CG1 | 1:A:45:SER:N | 2.75 | 0.50 |
| 1:B:18:ASP:O | 1:B:257:ARG:NH1 | 2.45 | 0.50 |
| 1:B:280:ASP:O | 1:B:280:ASP:OD1 | 2.30 | 0.50 |
| 1:B:56:LEU:HD12 | 1:B:60:THR:HG23 | 1.92 | 0.50 |
| 1:E:184:GLU:OE1 | 1:E:194:ARG:HD2 | 2.11 | 0.50 |
| 1:E:200:LEU:HD13 | 1:E:214:VAL:HG12 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:172:ILE:O | 1:F:173:GLU:HG2 | 2.11 | 0.50 |
| 1:H:185:ILE:HD11 | 1:H:191:VAL:HB | 1.92 | 0.50 |
| 1:H:219:ASP:C | 1:H:219:ASP:OD1 | 2.49 | 0.50 |
| 1:B:116:GLU:O | 1:B:119:CYS:N | 2.45 | 0.50 |
| 1:C:219:ASP:OD1 | 1:C:219:ASP:C | 2.49 | 0.50 |
| 1:E:280:ASP:OD1 | 1:E:280:ASP:O | 2.30 | 0.50 |
| 1:F:110:ASN:O | 1:F:113:VAL:HB | 2.12 | 0.50 |
| 1:F:204:ARG:NH1 | 1:F:204:ARG:HG2 | 2.25 | 0.50 |
| 1:F:219:ASP:OD1 | 1:F:219:ASP:C | 2.49 | 0.50 |
| 1:G:147:ARG:HG2 | 1:G:147:ARG:NH1 | 2.26 | 0.50 |
| 1:G:201:THR:HG23 | 1:G:217:PRO:HD3 | 1.93 | 0.50 |
| 1:H:116:GLU:O | 1:H:119:CYS:N | 2.45 | 0.50 |
| 1:A:116:GLU:O | 1:A:119:CYS:N | 2.45 | 0.50 |
| 1:D:147:ARG:HB2 | 1:D:293:ILE:HD11 | 1.94 | 0.50 |
| 1:E:56:LEU:HD12 | 1:E:60:THR:HG23 | 1.92 | 0.50 |
| 1:F:104:PRO:HB2 | 1:F:110:ASN:OD1 | 2.11 | 0.50 |
| 1:F:184:GLU:OE1 | 1:F:194:ARG:HD2 | 2.11 | 0.50 |
| 1:F:200:LEU:HD13 | 1:F:214:VAL:HG12 | 1.92 | 0.50 |
| 1:C:110:ASN:O | 1:C:113:VAL:HB | 2.12 | 0.50 |
| 1:C:44:VAL:CG1 | 1:C:45:SER:N | 2.75 | 0.50 |
| 1:D:104:PRO:HB2 | 1:D:110:ASN:CG | 2.31 | 0.50 |
| 1:A:88:PHE:CE2 | 1:D:110:ASN:CB | 2.95 | 0.50 |
| 1:D:272:VAL:HG13 | 1:D:273:ASP:H | 1.75 | 0.50 |
| 1:F:129:SER:HB3 | 1:G:132:TYR:CD1 | 2.47 | 0.50 |
| 1:F:56:LEU:HD12 | 1:F:60:THR:HG23 | 1.92 | 0.50 |
| 1:G:272:VAL:HG13 | 1:G:273:ASP:H | 1.75 | 0.50 |
| 1:H:56:LEU:O | 1:H:56:LEU:HD12 | 2.11 | 0.50 |
| 1:A:56:LEU:HD12 | 1:A:56:LEU:O | 2.11 | 0.49 |
| 1:H:44:VAL:CG1 | 1:H:45:SER:N | 2.74 | 0.49 |
| 1:A:110:ASN:O | 1:A:113:VAL:HB | 2.12 | 0.49 |
| 1:B:75:ILE:CD1 | 1:B:89:PHE:CE2 | 2.95 | 0.49 |
| 1:C:272:VAL:CG1 | 1:C:273:ASP:H | 2.25 | 0.49 |
| 1:C:280:ASP:O | 1:C:280:ASP:OD1 | 2.30 | 0.49 |
| 1:E:210:LEU:HB3 | 1:E:285:ILE:HD13 | 1.93 | 0.49 |
| 1:E:46:TRP:N | 1:E:47:PRO:HD2 | 2.27 | 0.49 |
| 1:E:61:ASN:HD21 | 1:E:94:MET:HE2 | 1.72 | 0.49 |
| 1:E:75:ILE:O | 1:E:76:GLU:O | 2.28 | 0.49 |
| 1:F:147:ARG:HG2 | 1:F:147:ARG:NH1 | 2.26 | 0.49 |
| 1:F:56:LEU:HD12 | 1:F:56:LEU:O | 2.11 | 0.49 |
| 1:G:110:ASN:O | 1:G:113:VAL:HB | 2.12 | 0.49 |
| 1:G:116:GLU:O | 1:G:119:CYS:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:15:LEU:HB2 | 1:G:238:GLU:OE1 | 2.12 | 0.49 |
| 1:G:169:GLU:HB2 | 1:G:247:HIS:HE1 | 1.77 | 0.49 |
| 1:H:280:ASP:OD1 | 1:H:280:ASP:O | 2.30 | 0.49 |
| 1:H:54:THR:O | 1:H:57:TYR:HB3 | 2.13 | 0.49 |
| 1:A:76:GLU:HG3 | 1:A:77:ASN:ND2 | 2.28 | 0.49 |
| 1:B:169:GLU:HB2 | 1:B:247:HIS:HE1 | 1.77 | 0.49 |
| 1:C:76:GLU:HG3 | 1:C:77:ASN:ND2 | 2.28 | 0.49 |
| 1:D:280:ASP:OD1 | 1:D:280:ASP:O | 2.30 | 0.49 |
| 1:D:54:THR:O | 1:D:57:TYR:HB3 | 2.13 | 0.49 |
| 1:G:44:VAL:CG1 | 1:G:45:SER:N | 2.75 | 0.49 |
| 1:H:76:GLU:HG3 | 1:H:77:ASN:ND2 | 2.28 | 0.49 |
| 1:B:153:PHE:O | 1:B:154:GLU:C | 2.50 | 0.49 |
| 1:B:200:LEU:HD13 | 1:B:214:VAL:HG12 | 1.92 | 0.49 |
| 1:C:54:THR:O | 1:C:57:TYR:HB3 | 2.13 | 0.49 |
| 1:D:116:GLU:O | 1:D:119:CYS:N | 2.45 | 0.49 |
| 1:D:169:GLU:HB2 | 1:D:247:HIS:HE1 | 1.77 | 0.49 |
| 1:D:76:GLU:HG3 | 1:D:77:ASN:ND2 | 2.28 | 0.49 |
| 1:F:169:GLU:HB2 | 1:F:247:HIS:HE1 | 1.77 | 0.49 |
| 1:G:153:PHE:O | 1:G:154:GLU:C | 2.50 | 0.49 |
| 1:G:280:ASP:OD1 | 1:G:280:ASP:O | 2.30 | 0.49 |
| 1:H:168:ILE:CD1 | 1:H:168:ILE:N | 2.61 | 0.49 |
| 1:A:169:GLU:HB2 | 1:A:247:HIS:HE1 | 1.77 | 0.49 |
| 1:A:54:THR:O | 1:A:57:TYR:HB3 | 2.13 | 0.49 |
| 1:B:54:THR:O | 1:B:57:TYR:HB3 | 2.13 | 0.49 |
| 1:B:61:ASN:CG | 1:B:94:MET:HE2 | 2.33 | 0.49 |
| 1:C:129:SER:HB3 | 1:D:132:TYR:HD1 | 1.76 | 0.49 |
| 1:D:219:ASP:C | 1:D:219:ASP:OD1 | 2.49 | 0.49 |
| 1:E:106:GLY:O | 1:E:110:ASN:ND2 | 2.44 | 0.49 |
| 1:F:44:VAL:CG1 | 1:F:48:VAL:CB | 2.88 | 0.49 |
| 1:F:54:THR:O | 1:F:57:TYR:HB3 | 2.13 | 0.49 |
| 1:G:122:LEU:O | 1:G:123:GLY:C | 2.41 | 0.49 |
| 1:G:219:ASP:C | 1:G:219:ASP:OD1 | 2.49 | 0.49 |
| 1:H:204:ARG:NH1 | 1:H:204:ARG:HG2 | 2.25 | 0.49 |
| 1:A:280:ASP:O | 1:A:280:ASP:OD1 | 2.30 | 0.49 |
| 1:C:200:LEU:HD13 | 1:C:214:VAL:HG12 | 1.93 | 0.49 |
| 1:C:162:ARG:O | 1:C:290:PHE:HZ | 1.96 | 0.49 |
| 1:C:61:ASN:OD1 | 1:C:94:MET:HE2 | 2.12 | 0.49 |
| 1:E:169:GLU:HB2 | 1:E:247:HIS:HE1 | 1.77 | 0.49 |
| 1:E:44:VAL:CG1 | 1:E:45:SER:N | 2.75 | 0.49 |
| 1:E:61:ASN:ND2 | 1:E:94:MET:HE2 | 2.26 | 0.49 |
| 1:F:116:GLU:O | 1:F:119:CYS:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:153:PHE:O | 1:F:154:GLU:C | 2.50 | 0.49 |
| 1:F:280:ASP:O | 1:F:280:ASP:OD1 | 2.30 | 0.49 |
| 1:G:76:GLU:HG3 | 1:G:77:ASN:ND2 | 2.28 | 0.49 |
| 1:A:88:PHE:CE2 | 1:D:110:ASN:HB3 | 2.47 | 0.49 |
| 1:B:172:ILE:O | 1:B:173:GLU:CG | 2.61 | 0.49 |
| 1:B:76:GLU:HG3 | 1:B:77:ASN:ND2 | 2.28 | 0.49 |
| 1:C:104:PRO:CB | 1:C:110:ASN:OD1 | 2.61 | 0.49 |
| 1:C:116:GLU:O | 1:C:119:CYS:N | 2.45 | 0.49 |
| 1:C:141:GLY:O | 1:C:166:LEU:HB2 | 2.12 | 0.49 |
| 1:C:169:GLU:HB2 | 1:C:247:HIS:HE1 | 1.77 | 0.49 |
| 1:H:49:PHE:HE2 | 1:H:131:ILE:HD13 | 1.77 | 0.49 |
| 1:H:204:ARG:CG | 1:H:204:ARG:HH11 | 2.23 | 0.49 |
| 1:A:200:LEU:HD13 | 1:A:214:VAL:HG12 | 1.92 | 0.49 |
| 1:B:44:VAL:CG1 | 1:B:45:SER:N | 2.75 | 0.49 |
| 1:D:172:ILE:O | 1:D:173:GLU:CG | 2.61 | 0.49 |
| 1:G:104:PRO:CG | 1:G:110:ASN:OD1 | 2.61 | 0.49 |
| 1:G:54:THR:O | 1:G:57:TYR:HB3 | 2.13 | 0.49 |
| 1:E:154:GLU:CA | 1:H:188:GLU:OE2 | 2.60 | 0.49 |
| 1:H:201:THR:HG23 | 1:H:217:PRO:HD3 | 1.93 | 0.49 |
| 1:A:145:SER:O | 1:A:260:TYR:OH | 2.24 | 0.49 |
| 1:C:185:ILE:HD11 | 1:C:191:VAL:HB | 1.92 | 0.49 |
| 1:D:200:LEU:HD13 | 1:D:214:VAL:HG12 | 1.92 | 0.49 |
| 1:E:54:THR:O | 1:E:57:TYR:HB3 | 2.13 | 0.49 |
| 1:G:182:ARG:CB | 1:G:237:SER:HB3 | 2.43 | 0.49 |
| 1:H:172:ILE:O | 1:H:173:GLU:CG | 2.61 | 0.49 |
| 1:A:141:GLY:O | 1:A:166:LEU:N | 2.43 | 0.49 |
| 1:A:153:PHE:CE2 | 1:A:154:GLU:HB2 | 2.48 | 0.49 |
| 1:A:172:ILE:O | 1:A:173:GLU:CG | 2.61 | 0.49 |
| 1:C:295:GLN:O | 1:E:292:GLU:HA | 2.12 | 0.49 |
| 1:C:74:VAL:HB | 1:C:109:ALA:HB2 | 1.95 | 0.49 |
| 1:E:172:ILE:O | 1:E:173:GLU:CG | 2.61 | 0.49 |
| 1:F:44:VAL:CG1 | 1:F:45:SER:N | 2.75 | 0.49 |
| 1:H:200:LEU:HD13 | 1:H:214:VAL:HG12 | 1.92 | 0.49 |
| 1:D:110:ASN:O | 1:D:113:VAL:HB | 2.12 | 0.48 |
| 1:D:185:ILE:HD11 | 1:D:191:VAL:HB | 1.92 | 0.48 |
| 1:D:266:ILE:CD1 | 1:D:293:ILE:HD12 | 2.39 | 0.48 |
| 1:D:46:TRP:N | 1:D:47:PRO:HD2 | 2.28 | 0.48 |
| 1:E:116:GLU:O | 1:E:119:CYS:N | 2.45 | 0.48 |
| 1:E:153:PHE:CD2 | 1:E:154:GLU:HB2 | 2.48 | 0.48 |
| 1:G:69:LEU:O | 1:G:72:GLY:N | 2.45 | 0.48 |
| 1:H:192:PHE:HE1 | 1:H:194:ARG:HB2 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:266:ILE:CD1 | 1:H:293:ILE:HD12 | 2.42 | 0.48 |
| 1:E:280:ASP:CB | 1:E:282:ARG:HG2 | 2.39 | 0.48 |
| 1:E:23:ILE:HG13 | 1:F:283:ARG:HH21 | 1.78 | 0.48 |
| 1:H:169:GLU:HB2 | 1:H:247:HIS:HE1 | 1.77 | 0.48 |
| 1:C:153:PHE:CE2 | 1:C:154:GLU:HB2 | 2.48 | 0.48 |
| 1:C:182:ARG:HA | 1:C:193:ARG:NH1 | 2.28 | 0.48 |
| 1:D:153:PHE:CE2 | 1:D:154:GLU:HB2 | 2.48 | 0.48 |
| 1:D:153:PHE:O | 1:D:154:GLU:C | 2.51 | 0.48 |
| 1:F:153:PHE:CE2 | 1:F:154:GLU:HB2 | 2.48 | 0.48 |
| 1:G:182:ARG:HB3 | 1:G:237:SER:HB3 | 1.95 | 0.48 |
| 1:A:201:THR:HG23 | 1:A:217:PRO:HD3 | 1.93 | 0.48 |
| 1:C:153:PHE:O | 1:C:154:GLU:C | 2.51 | 0.48 |
| 1:D:149:VAL:HG12 | 1:D:293:ILE:HD13 | 1.96 | 0.48 |
| 1:E:153:PHE:CE2 | 1:E:154:GLU:HB2 | 2.48 | 0.48 |
| 1:G:204:ARG:HG2 | 1:G:204:ARG:NH1 | 2.25 | 0.48 |
| 1:H:153:PHE:CE2 | 1:H:154:GLU:HB2 | 2.48 | 0.48 |
| 1:H:184:GLU:OE1 | 1:H:194:ARG:HD2 | 2.13 | 0.48 |
| 1:H:75:ILE:CD1 | 1:H:89:PHE:HD2 | 2.21 | 0.48 |
| 1:A:153:PHE:CD2 | 1:A:154:GLU:HB2 | 2.48 | 0.48 |
| 1:B:280:ASP:CB | 1:B:282:ARG:HG2 | 2.39 | 0.48 |
| 1:B:46:TRP:N | 1:B:47:PRO:HD2 | 2.28 | 0.48 |
| 1:C:153:PHE:CD2 | 1:C:154:GLU:HB2 | 2.48 | 0.48 |
| 1:E:61:ASN:OD1 | 1:E:94:MET:HE2 | 2.13 | 0.48 |
| 1:A:46:TRP:N | 1:A:47:PRO:HD2 | 2.28 | 0.48 |
| 1:B:153:PHE:CE2 | 1:B:154:GLU:HB2 | 2.48 | 0.48 |
| 1:E:44:VAL:CG1 | 1:E:48:VAL:CB | 2.91 | 0.48 |
| 1:F:172:ILE:O | 1:F:173:GLU:CG | 2.62 | 0.48 |
| 1:F:46:TRP:N | 1:F:47:PRO:HD2 | 2.28 | 0.48 |
| 1:F:76:GLU:HG3 | 1:F:77:ASN:ND2 | 2.28 | 0.48 |
| 1:G:172:ILE:O | 1:G:173:GLU:CG | 2.61 | 0.48 |
| 1:G:201:THR:CG2 | 1:G:217:PRO:CD | 2.90 | 0.48 |
| 1:H:110:ASN:O | 1:H:113:VAL:HB | 2.12 | 0.48 |
| 1:H:153:PHE:CD2 | 1:H:154:GLU:HB2 | 2.48 | 0.48 |
| 1:D:68:TYR:O | 1:D:69:LEU:C | 2.52 | 0.48 |
| 1:A:23:ILE:HG21 | 1:B:285:ILE:HG13 | 1.96 | 0.48 |
| 1:D:153:PHE:CD2 | 1:D:154:GLU:HB2 | 2.48 | 0.48 |
| 1:D:204:ARG:NH1 | 1:D:204:ARG:HG2 | 2.25 | 0.48 |
| 1:E:26:LEU:N | 1:F:285:ILE:O | 2.46 | 0.48 |
| 1:H:93:THR:CG2 | 1:H:116:GLU:OE1 | 2.60 | 0.48 |
| 1:G:14:ILE:CG2 | 1:H:283:ARG:NH1 | 2.77 | 0.48 |
| 1:H:46:TRP:N | 1:H:47:PRO:HD2 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:44:VAL:HG13 | 1:H:48:VAL:HB | 1.94 | 0.48 |
| 1:B:68:TYR:O | 1:B:69:LEU:C | 2.52 | 0.48 |
| 1:C:44:VAL:HG11 | 1:C:48:VAL:HG12 | 1.96 | 0.48 |
| 1:D:201:THR:CG2 | 1:D:217:PRO:CD | 2.90 | 0.48 |
| 1:E:75:ILE:O | 1:E:76:GLU:C | 2.50 | 0.48 |
| 1:F:201:THR:CG2 | 1:F:217:PRO:CD | 2.90 | 0.48 |
| 1:H:153:PHE:O | 1:H:154:GLU:C | 2.51 | 0.48 |
| 1:A:162:ARG:O | 1:A:290:PHE:HZ | 1.96 | 0.48 |
| 1:A:266:ILE:CD1 | 1:A:293:ILE:HD12 | 2.40 | 0.48 |
| 1:C:185:ILE:HD11 | 1:C:191:VAL:CG2 | 2.44 | 0.47 |
| 1:D:64:PHE:O | 1:D:67:ALA:HB3 | 2.14 | 0.47 |
| 1:F:116:GLU:O | 1:F:119:CYS:HB2 | 2.14 | 0.47 |
| 1:F:153:PHE:CD2 | 1:F:154:GLU:HB2 | 2.48 | 0.47 |
| 1:F:172:ILE:O | 1:F:173:GLU:C | 2.47 | 0.47 |
| 1:A:116:GLU:O | 1:A:119:CYS:HB2 | 2.14 | 0.47 |
| 1:B:116:GLU:O | 1:B:119:CYS:HB2 | 2.14 | 0.47 |
| 1:D:185:ILE:HD11 | 1:D:191:VAL:CG2 | 2.44 | 0.47 |
| 1:G:121:MET:O | 1:G:124:LEU:N | 2.47 | 0.47 |
| 1:G:185:ILE:HD11 | 1:G:191:VAL:HB | 1.92 | 0.47 |
| 1:A:130:LEU:HD21 | 1:B:135:PHE:HE2 | 1.79 | 0.47 |
| 1:B:153:PHE:CD2 | 1:B:154:GLU:HB2 | 2.48 | 0.47 |
| 1:C:201:THR:CG2 | 1:C:217:PRO:CD | 2.90 | 0.47 |
| 1:E:201:THR:HG23 | 1:E:217:PRO:HD3 | 1.93 | 0.47 |
| 1:F:185:ILE:HD11 | 1:F:191:VAL:CG2 | 2.44 | 0.47 |
| 1:G:145:SER:O | 1:G:260:TYR:OH | 2.24 | 0.47 |
| 1:G:153:PHE:CD2 | 1:G:154:GLU:HB2 | 2.48 | 0.47 |
| 1:G:153:PHE:CE2 | 1:G:154:GLU:HB2 | 2.48 | 0.47 |
| 1:G:185:ILE:HD11 | 1:G:191:VAL:CG2 | 2.45 | 0.47 |
| 1:G:68:TYR:O | 1:G:69:LEU:C | 2.52 | 0.47 |
| 1:H:64:PHE:O | 1:H:67:ALA:HB3 | 2.14 | 0.47 |
| 1:A:89:PHE:HB2 | 1:A:102:LEU:HD13 | 1.96 | 0.47 |
| 1:B:16:ASN:O | 1:B:259:ALA:HB3 | 2.15 | 0.47 |
| 1:C:46:TRP:N | 1:C:47:PRO:HD2 | 2.28 | 0.47 |
| 1:D:106:GLY:O | 1:D:110:ASN:ND2 | 2.48 | 0.47 |
| 1:D:116:GLU:O | 1:D:119:CYS:HB2 | 2.14 | 0.47 |
| 1:E:116:GLU:O | 1:E:119:CYS:HB2 | 2.14 | 0.47 |
| 1:F:243:PHE:CD2 | 1:F:243:PHE:C | 2.88 | 0.47 |
| 1:F:266:ILE:CD1 | 1:F:293:ILE:HD12 | 2.42 | 0.47 |
| 1:G:210:LEU:CD1 | 1:G:285:ILE:HD11 | 2.34 | 0.47 |
| 1:G:266:ILE:CD1 | 1:G:293:ILE:HD12 | 2.42 | 0.47 |
| 1:A:57:TYR:HE1 | 1:A:94:MET:HE3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:64:PHE:O | 1:F:67:ALA:HB3 | 2.14 | 0.47 |
| 1:G:116:GLU:O | 1:G:119:CYS:HB2 | 2.14 | 0.47 |
| 1:B:56:LEU:HD12 | 1:B:60:THR:CG2 | 2.45 | 0.47 |
| 1:C:266:ILE:CD1 | 1:C:293:ILE:HD12 | 2.42 | 0.47 |
| 1:G:64:PHE:O | 1:G:67:ALA:HB3 | 2.14 | 0.47 |
| 1:A:185:ILE:HD11 | 1:A:191:VAL:CG2 | 2.44 | 0.47 |
| 1:E:124:LEU:CD1 | 1:H:121:MET:HB3 | 2.45 | 0.47 |
| 1:H:185:ILE:HD11 | 1:H:191:VAL:CG2 | 2.44 | 0.47 |
| 1:A:42:LEU:HB3 | 1:A:137:ARG:NH2 | 2.30 | 0.47 |
| 1:A:153:PHE:O | 1:A:154:GLU:C | 2.51 | 0.47 |
| 1:B:175:ASP:OD2 | 1:B:204:ARG:NH1 | 2.48 | 0.47 |
| 1:B:185:ILE:HD11 | 1:B:191:VAL:CG2 | 2.44 | 0.47 |
| 1:C:243:PHE:CD2 | 1:C:243:PHE:C | 2.88 | 0.47 |
| 1:B:64:PHE:O | 1:B:67:ALA:HB3 | 2.14 | 0.47 |
| 1:C:116:GLU:O | 1:C:119:CYS:HB2 | 2.14 | 0.47 |
| 1:E:153:PHE:O | 1:E:154:GLU:C | 2.51 | 0.47 |
| 1:E:166:LEU:HA | 1:E:166:LEU:HD23 | 1.73 | 0.47 |
| 1:F:61:ASN:ND2 | 1:F:94:MET:HE2 | 2.29 | 0.47 |
| 1:G:23:ILE:CG2 | 1:H:285:ILE:HG13 | 2.40 | 0.47 |
| 1:H:56:LEU:HD12 | 1:H:60:THR:CG2 | 2.45 | 0.47 |
| 1:A:49:PHE:CE2 | 1:A:131:ILE:HD13 | 2.50 | 0.47 |
| 1:B:204:ARG:NH1 | 1:B:204:ARG:HG2 | 2.25 | 0.47 |
| 1:E:175:ASP:OD2 | 1:E:204:ARG:NH1 | 2.48 | 0.47 |
| 1:E:185:ILE:HD11 | 1:E:191:VAL:CG2 | 2.45 | 0.47 |
| 1:E:272:VAL:CG1 | 1:E:273:ASP:H | 2.25 | 0.47 |
| 1:F:56:LEU:HD12 | 1:F:60:THR:CG2 | 2.45 | 0.47 |
| 1:H:42:LEU:HB3 | 1:H:137:ARG:NH2 | 2.30 | 0.47 |
| 1:A:124:LEU:CD1 | 1:D:121:MET:HB3 | 2.45 | 0.47 |
| 1:A:185:ILE:HD11 | 1:A:191:VAL:HB | 1.92 | 0.47 |
| 1:A:93:THR:HG21 | 1:A:116:GLU:OE1 | 2.15 | 0.47 |
| 1:E:266:ILE:CD1 | 1:E:293:ILE:HD12 | 2.41 | 0.47 |
| 1:E:68:TYR:O | 1:E:69:LEU:C | 2.52 | 0.47 |
| 1:B:151:SER:HB3 | 1:B:269:GLY:O | 2.15 | 0.46 |
| 1:D:175:ASP:OD2 | 1:D:204:ARG:NH1 | 2.48 | 0.46 |
| 1:E:23:ILE:HD11 | 1:F:283:ARG:CZ | 2.45 | 0.46 |
| 1:E:244:THR:HG22 | 1:E:255:HIS:HB2 | 1.97 | 0.46 |
| 1:G:175:ASP:OD2 | 1:G:204:ARG:NH1 | 2.48 | 0.46 |
| 1:H:116:GLU:O | 1:H:119:CYS:HB2 | 2.14 | 0.46 |
| 1:H:243:PHE:CD2 | 1:H:243:PHE:C | 2.88 | 0.46 |
| 1:H:175:ASP:OD2 | 1:H:204:ARG:NH1 | 2.48 | 0.46 |
| 1:A:175:ASP:OD2 | 1:A:204:ARG:NH1 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:GLN:OE1 | 1:A:99:TYR:HD1 | 1.97 | 0.46 |
| 1:B:201:THR:HG23 | 1:B:217:PRO:HD3 | 1.93 | 0.46 |
| 1:C:166:LEU:HD23 | 1:C:166:LEU:HA | 1.72 | 0.46 |
| 1:C:175:ASP:OD2 | 1:C:204:ARG:NH1 | 2.48 | 0.46 |
| 1:C:56:LEU:HD12 | 1:C:60:THR:CG2 | 2.45 | 0.46 |
| 1:F:166:LEU:HD23 | 1:F:166:LEU:HA | 1.73 | 0.46 |
| 1:F:280:ASP:CB | 1:F:282:ARG:HG2 | 2.39 | 0.46 |
| 1:H:75:ILE:HD11 | 1:H:89:PHE:CD2 | 2.46 | 0.46 |
| 1:A:147:ARG:HB2 | 1:A:293:ILE:HD11 | 1.97 | 0.46 |
| 1:A:284:ALA:HA | 1:D:23:ILE:CG2 | 2.45 | 0.46 |
| 1:B:147:ARG:HG2 | 1:B:147:ARG:HH11 | 1.81 | 0.46 |
| 1:B:266:ILE:CD1 | 1:B:293:ILE:HD12 | 2.42 | 0.46 |
| 1:D:201:THR:HG23 | 1:D:217:PRO:HD3 | 1.93 | 0.46 |
| 1:E:147:ARG:HH11 | 1:E:147:ARG:HG2 | 1.81 | 0.46 |
| 1:E:56:LEU:HD12 | 1:E:60:THR:CG2 | 2.45 | 0.46 |
| 1:G:104:PRO:HB2 | 1:G:110:ASN:OD1 | 2.15 | 0.46 |
| 1:H:272:VAL:CG1 | 1:H:273:ASP:H | 2.25 | 0.46 |
| 1:A:243:PHE:C | 1:A:243:PHE:CD2 | 2.88 | 0.46 |
| 1:C:64:PHE:O | 1:C:67:ALA:HB3 | 2.14 | 0.46 |
| 1:E:243:PHE:CD2 | 1:E:243:PHE:C | 2.88 | 0.46 |
| 1:G:243:PHE:C | 1:G:243:PHE:CD2 | 2.88 | 0.46 |
| 1:G:56:LEU:HD12 | 1:G:60:THR:CG2 | 2.45 | 0.46 |
| 1:A:272:VAL:CG1 | 1:A:273:ASP:H | 2.25 | 0.46 |
| 1:A:64:PHE:O | 1:A:67:ALA:HB3 | 2.14 | 0.46 |
| 1:B:244:THR:HG22 | 1:B:255:HIS:HB2 | 1.97 | 0.46 |
| 1:E:130:LEU:O | 1:E:131:ILE:C | 2.54 | 0.46 |
| 1:E:18:ASP:O | 1:E:257:ARG:NH1 | 2.49 | 0.46 |
| 1:H:104:PRO:CG | 1:H:110:ASN:OD1 | 2.63 | 0.46 |
| 1:H:121:MET:C | 1:H:123:GLY:N | 2.68 | 0.46 |
| 1:A:266:ILE:HG22 | 1:A:269:GLY:HA3 | 1.98 | 0.46 |
| 1:A:94:MET:C | 1:A:95:ALA:C | 2.69 | 0.46 |
| 1:B:204:ARG:NH1 | 1:B:204:ARG:CG | 2.79 | 0.46 |
| 1:B:243:PHE:C | 1:B:243:PHE:CD2 | 2.88 | 0.46 |
| 1:C:114:THR:HG22 | 1:D:91:VAL:HG21 | 1.98 | 0.46 |
| 1:C:147:ARG:HG2 | 1:C:147:ARG:HH11 | 1.81 | 0.46 |
| 1:H:130:LEU:O | 1:H:131:ILE:C | 2.54 | 0.46 |
| 1:C:201:THR:HG23 | 1:C:217:PRO:HD3 | 1.93 | 0.46 |
| 1:E:64:PHE:O | 1:E:67:ALA:HB3 | 2.14 | 0.46 |
| 1:F:244:THR:HG22 | 1:F:255:HIS:HB2 | 1.97 | 0.46 |
| 1:H:147:ARG:HH11 | 1:H:147:ARG:HG2 | 1.81 | 0.46 |
| 1:E:154:GLU:H | 1:H:188:GLU:CD | 2.19 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:141:GLY:O | 1:B:166:LEU:CB | 2.64 | 0.46 |
| 1:C:244:THR:HG22 | 1:C:255:HIS:HB2 | 1.97 | 0.46 |
| 1:E:181:VAL:HG12 | 1:E:193:ARG:CZ | 2.44 | 0.46 |
| 1:F:130:LEU:HD21 | 1:G:135:PHE:HE2 | 1.81 | 0.46 |
| 1:F:210:LEU:HB3 | 1:F:285:ILE:CD1 | 2.45 | 0.46 |
| 1:F:69:LEU:HD23 | 1:F:69:LEU:HA | 1.66 | 0.46 |
| 1:G:166:LEU:HD23 | 1:G:166:LEU:HA | 1.73 | 0.46 |
| 1:F:114:THR:CG2 | 1:G:91:VAL:HG21 | 2.46 | 0.46 |
| 1:A:244:THR:HG22 | 1:A:255:HIS:HB2 | 1.98 | 0.46 |
| 1:A:56:LEU:HD12 | 1:A:60:THR:CG2 | 2.45 | 0.46 |
| 1:D:56:LEU:HD12 | 1:D:60:THR:CG2 | 2.45 | 0.46 |
| 1:G:244:THR:HG22 | 1:G:255:HIS:HB2 | 1.97 | 0.46 |
| 1:G:92:GLN:OE1 | 1:G:99:TYR:HD1 | 1.99 | 0.46 |
| 1:A:204:ARG:NH1 | 1:A:204:ARG:CG | 2.79 | 0.45 |
| 1:B:114:THR:HG22 | 1:C:91:VAL:HG21 | 1.97 | 0.45 |
| 1:G:89:PHE:HD1 | 1:G:102:LEU:HB2 | 1.78 | 0.45 |
| 1:G:38:TYR:OH | 1:H:136:THR:HG22 | 2.16 | 0.45 |
| 1:H:49:PHE:CE2 | 1:H:131:ILE:HD13 | 2.51 | 0.45 |
| 1:G:114:THR:CG2 | 1:H:88:PHE:CE2 | 2.99 | 0.45 |
| 1:D:243:PHE:C | 1:D:243:PHE:CD2 | 2.88 | 0.45 |
| 1:A:201:THR:CG2 | 1:A:217:PRO:CD | 2.90 | 0.45 |
| 1:B:104:PRO:CG | 1:B:110:ASN:OD1 | 2.64 | 0.45 |
| 1:B:38:TYR:OH | 1:C:136:THR:HG22 | 2.17 | 0.45 |
| 1:F:147:ARG:HH11 | 1:F:147:ARG:HG2 | 1.81 | 0.45 |
| 1:F:185:ILE:HD13 | 1:F:191:VAL:HA | 1.99 | 0.45 |
| 1:H:71:CYS:HB2 | 1:H:74:VAL:CG2 | 2.46 | 0.45 |
| 1:A:130:LEU:O | 1:A:131:ILE:C | 2.54 | 0.45 |
| 1:B:272:VAL:CG1 | 1:B:273:ASP:H | 2.25 | 0.45 |
| 1:B:75:ILE:HD11 | 1:B:89:PHE:CE2 | 2.51 | 0.45 |
| 1:C:185:ILE:CD1 | 1:C:191:VAL:HG23 | 2.47 | 0.45 |
| 1:C:68:TYR:O | 1:C:69:LEU:C | 2.52 | 0.45 |
| 1:E:181:VAL:HG12 | 1:E:193:ARG:NH2 | 2.31 | 0.45 |
| 1:E:204:ARG:NH1 | 1:E:204:ARG:HG2 | 2.25 | 0.45 |
| 1:F:130:LEU:O | 1:F:131:ILE:C | 2.54 | 0.45 |
| 1:G:49:PHE:HE2 | 1:G:131:ILE:CD1 | 2.29 | 0.45 |
| 1:H:68:TYR:O | 1:H:69:LEU:C | 2.52 | 0.45 |
| 1:E:95:ALA:O | 1:E:96:THR:OG1 | 2.34 | 0.45 |
| 1:G:185:ILE:CD1 | 1:G:191:VAL:HG23 | 2.47 | 0.45 |
| 1:E:88:PHE:CE2 | 1:H:110:ASN:CB | 2.99 | 0.45 |
| 1:H:141:GLY:O | 1:H:166:LEU:CB | 2.64 | 0.45 |
| 1:H:204:ARG:NH1 | 1:H:204:ARG:CG | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:94:MET:HB2 | 1:H:116:GLU:CG | 2.45 | 0.45 |
| 1:D:244:THR:HG22 | 1:D:255:HIS:HB2 | 1.97 | 0.45 |
| 1:E:154:GLU:N | 1:H:188:GLU:CD | 2.69 | 0.45 |
| 1:F:104:PRO:CG | 1:F:110:ASN:OD1 | 2.64 | 0.45 |
| 1:A:147:ARG:HG2 | 1:A:147:ARG:HH11 | 1.81 | 0.45 |
| 1:A:143:LEU:O | 1:A:163:LEU:HA | 2.17 | 0.45 |
| 1:A:68:TYR:O | 1:A:69:LEU:C | 2.52 | 0.45 |
| 1:C:44:VAL:HG11 | 1:C:48:VAL:CG1 | 2.46 | 0.45 |
| 1:D:185:ILE:CD1 | 1:D:191:VAL:HG23 | 2.47 | 0.45 |
| 1:F:15:LEU:HB2 | 1:F:238:GLU:OE1 | 2.16 | 0.45 |
| 1:A:278:LEU:HG | 1:A:282:ARG:O | 2.17 | 0.45 |
| 1:B:117:ALA:O | 1:B:118:LEU:C | 2.55 | 0.45 |
| 1:D:141:GLY:O | 1:D:166:LEU:CB | 2.64 | 0.45 |
| 1:D:61:ASN:ND2 | 1:D:94:MET:HE2 | 2.31 | 0.45 |
| 1:E:185:ILE:CD1 | 1:E:191:VAL:HG23 | 2.47 | 0.45 |
| 1:F:185:ILE:CD1 | 1:F:191:VAL:HG23 | 2.47 | 0.45 |
| 1:F:41:LEU:O | 1:F:134:ARG:NH1 | 2.49 | 0.45 |
| 1:G:141:GLY:O | 1:G:166:LEU:CB | 2.64 | 0.45 |
| 1:B:185:ILE:CD1 | 1:B:191:VAL:HG23 | 2.47 | 0.45 |
| 1:C:75:ILE:CD1 | 1:C:89:PHE:CE2 | 2.99 | 0.45 |
| 1:D:130:LEU:O | 1:D:131:ILE:C | 2.54 | 0.45 |
| 1:D:204:ARG:CG | 1:D:204:ARG:NH1 | 2.79 | 0.45 |
| 1:E:75:ILE:C | 1:E:76:GLU:O | 2.48 | 0.45 |
| 1:F:201:THR:HG23 | 1:F:217:PRO:HD3 | 1.92 | 0.45 |
| 1:F:68:TYR:O | 1:F:69:LEU:C | 2.52 | 0.45 |
| 1:G:130:LEU:O | 1:G:131:ILE:C | 2.54 | 0.45 |
| 1:A:185:ILE:CD1 | 1:A:191:VAL:HG23 | 2.47 | 0.45 |
| 1:A:284:ALA:HA | 1:D:23:ILE:HG22 | 1.99 | 0.45 |
| 1:B:130:LEU:O | 1:B:131:ILE:C | 2.54 | 0.45 |
| 1:E:185:ILE:HD13 | 1:E:191:VAL:HA | 1.99 | 0.45 |
| 1:E:173:GLU:N | 1:E:206:PRO:O | 2.44 | 0.45 |
| 1:G:278:LEU:HG | 1:G:282:ARG:O | 2.17 | 0.45 |
| 1:H:44:VAL:HG12 | 1:H:45:SER:O | 2.17 | 0.45 |
| 1:A:136:THR:HG22 | 1:D:38:TYR:OH | 2.17 | 0.44 |
| 1:C:117:ALA:O | 1:C:120:GLY:N | 2.50 | 0.44 |
| 1:D:117:ALA:O | 1:D:120:GLY:N | 2.50 | 0.44 |
| 1:D:147:ARG:HG2 | 1:D:147:ARG:HH11 | 1.81 | 0.44 |
| 1:D:278:LEU:HG | 1:D:282:ARG:O | 2.17 | 0.44 |
| 1:C:110:ASN:HB3 | 1:D:88:PHE:CE2 | 2.52 | 0.44 |
| 1:E:114:THR:HG22 | 1:F:91:VAL:HG21 | 1.99 | 0.44 |
| 1:F:174:ALA:HB1 | 1:F:243:PHE:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:185:ILE:HD13 | 1:G:191:VAL:HA | 1.99 | 0.44 |
| 1:A:273:ASP:OD1 | 1:A:274:VAL:N | 2.50 | 0.44 |
| 1:A:93:THR:O | 1:A:96:THR:N | 2.46 | 0.44 |
| 1:C:93:THR:CG2 | 1:C:116:GLU:OE1 | 2.65 | 0.44 |
| 1:C:185:ILE:HD13 | 1:C:191:VAL:HA | 1.99 | 0.44 |
| 1:C:61:ASN:ND2 | 1:C:94:MET:HE2 | 2.30 | 0.44 |
| 1:E:41:LEU:O | 1:E:134:ARG:NH1 | 2.50 | 0.44 |
| 1:F:204:ARG:HH11 | 1:F:204:ARG:CG | 2.24 | 0.44 |
| 1:F:46:TRP:O | 1:F:50:ILE:HG13 | 2.17 | 0.44 |
| 1:G:204:ARG:CG | 1:G:204:ARG:NH1 | 2.79 | 0.44 |
| 1:F:110:ASN:HB2 | 1:G:88:PHE:CZ | 2.52 | 0.44 |
| 1:H:89:PHE:HB2 | 1:H:102:LEU:HD13 | 1.98 | 0.44 |
| 1:B:278:LEU:HG | 1:B:282:ARG:O | 2.17 | 0.44 |
| 1:C:130:LEU:O | 1:C:131:ILE:C | 2.54 | 0.44 |
| 1:C:192:PHE:HE1 | 1:C:194:ARG:HB2 | 1.82 | 0.44 |
| 1:D:242:LEU:HD12 | 1:D:243:PHE:N | 2.33 | 0.44 |
| 1:E:278:LEU:HB3 | 1:E:279:PRO:HD2 | 1.99 | 0.44 |
| 1:F:117:ALA:O | 1:F:120:GLY:N | 2.50 | 0.44 |
| 1:G:147:ARG:HG2 | 1:G:147:ARG:HH11 | 1.81 | 0.44 |
| 1:G:242:LEU:HD12 | 1:G:243:PHE:N | 2.33 | 0.44 |
| 1:G:272:VAL:CG1 | 1:G:273:ASP:H | 2.25 | 0.44 |
| 1:H:117:ALA:O | 1:H:118:LEU:C | 2.55 | 0.44 |
| 1:H:242:LEU:HD12 | 1:H:243:PHE:N | 2.33 | 0.44 |
| 1:A:185:ILE:HD13 | 1:A:191:VAL:HA | 1.99 | 0.44 |
| 1:A:242:LEU:HD12 | 1:A:243:PHE:N | 2.33 | 0.44 |
| 1:A:283:ARG:HB3 | 1:D:23:ILE:CD1 | 2.47 | 0.44 |
| 1:B:278:LEU:HB3 | 1:B:279:PRO:HD2 | 2.00 | 0.44 |
| 1:C:42:LEU:HB3 | 1:C:137:ARG:NH2 | 2.33 | 0.44 |
| 1:E:49:PHE:HE2 | 1:E:131:ILE:CD1 | 2.28 | 0.44 |
| 1:E:124:LEU:HD11 | 1:H:121:MET:HB3 | 1.99 | 0.44 |
| 1:H:278:LEU:HB3 | 1:H:279:PRO:HD2 | 2.00 | 0.44 |
| 1:H:278:LEU:HG | 1:H:282:ARG:O | 2.17 | 0.44 |
| 1:C:278:LEU:HG | 1:C:282:ARG:O | 2.17 | 0.44 |
| 1:C:75:ILE:HD11 | 1:C:89:PHE:CE2 | 2.51 | 0.44 |
| 1:D:185:ILE:HD13 | 1:D:191:VAL:HA | 1.99 | 0.44 |
| 1:E:278:LEU:HG | 1:E:282:ARG:O | 2.17 | 0.44 |
| 1:F:278:LEU:HG | 1:F:282:ARG:O | 2.17 | 0.44 |
| 1:G:110:ASN:CB | 1:H:88:PHE:CE2 | 3.00 | 0.44 |
| 1:H:185:ILE:HD13 | 1:H:191:VAL:HA | 1.99 | 0.44 |
| 1:E:154:GLU:HA | 1:H:188:GLU:OE2 | 2.17 | 0.44 |
| 1:B:185:ILE:HD13 | 1:B:191:VAL:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:147:ARG:HH22 | 1:E:299:HIS:HA | 1.82 | 0.44 |
| 1:C:278:LEU:HB3 | 1:C:279:PRO:HD2 | 2.00 | 0.44 |
| 1:D:93:THR:CG2 | 1:D:116:GLU:CD | 2.86 | 0.44 |
| 1:A:117:ALA:O | 1:A:120:GLY:N | 2.50 | 0.44 |
| 1:B:242:LEU:HD12 | 1:B:243:PHE:N | 2.33 | 0.44 |
| 1:D:166:LEU:HA | 1:D:166:LEU:HD23 | 1.73 | 0.44 |
| 1:E:242:LEU:HD12 | 1:E:243:PHE:N | 2.33 | 0.44 |
| 1:C:104:PRO:CG | 1:C:110:ASN:OD1 | 2.66 | 0.44 |
| 1:D:210:LEU:HD22 | 1:D:285:ILE:HD12 | 1.98 | 0.44 |
| 1:H:185:ILE:CD1 | 1:H:191:VAL:HG23 | 2.47 | 0.44 |
| 1:A:239:PHE:CE1 | 1:A:265:ILE:HD11 | 2.53 | 0.44 |
| 1:B:173:GLU:N | 1:B:206:PRO:O | 2.44 | 0.44 |
| 1:D:278:LEU:HB3 | 1:D:279:PRO:HD2 | 2.00 | 0.44 |
| 1:E:117:ALA:O | 1:E:118:LEU:C | 2.55 | 0.44 |
| 1:E:24:THR:O | 1:F:285:ILE:N | 2.36 | 0.44 |
| 1:E:135:PHE:HE2 | 1:H:130:LEU:HD21 | 1.82 | 0.44 |
| 1:H:210:LEU:HD13 | 1:H:285:ILE:HD11 | 2.00 | 0.44 |
| 1:A:278:LEU:HB3 | 1:A:279:PRO:HD2 | 1.99 | 0.43 |
| 1:C:280:ASP:CB | 1:C:282:ARG:HG2 | 2.39 | 0.43 |
| 1:E:182:ARG:CB | 1:E:237:SER:HB3 | 2.48 | 0.43 |
| 1:F:278:LEU:HB3 | 1:F:279:PRO:HD2 | 1.99 | 0.43 |
| 1:G:278:LEU:HB3 | 1:G:279:PRO:HD2 | 2.00 | 0.43 |
| 1:F:114:THR:CG2 | 1:G:88:PHE:CD2 | 3.00 | 0.43 |
| 1:H:117:ALA:O | 1:H:120:GLY:N | 2.50 | 0.43 |
| 1:H:239:PHE:CE1 | 1:H:265:ILE:HD11 | 2.53 | 0.43 |
| 1:H:92:GLN:NE2 | 1:H:99:TYR:HD1 | 2.16 | 0.43 |
| 1:A:240:LEU:HD21 | 1:B:207:ILE:CD1 | 2.48 | 0.43 |
| 1:B:239:PHE:CE1 | 1:B:265:ILE:HD11 | 2.54 | 0.43 |
| 1:B:69:LEU:HA | 1:B:69:LEU:HD23 | 1.67 | 0.43 |
| 1:G:26:LEU:HB2 | 1:H:285:ILE:O | 2.18 | 0.43 |
| 1:G:61:ASN:ND2 | 1:G:94:MET:HE2 | 2.30 | 0.43 |
| 1:B:117:ALA:O | 1:B:120:GLY:N | 2.50 | 0.43 |
| 1:C:49:PHE:CZ | 1:C:53:ILE:HD11 | 2.54 | 0.43 |
| 1:E:239:PHE:CE1 | 1:E:265:ILE:HD11 | 2.54 | 0.43 |
| 1:E:49:PHE:CZ | 1:E:53:ILE:HD11 | 2.54 | 0.43 |
| 1:H:201:THR:CG2 | 1:H:217:PRO:CD | 2.90 | 0.43 |
| 1:A:39:HIS:HA | 1:B:250:PHE:HE2 | 1.82 | 0.43 |
| 1:A:49:PHE:CZ | 1:A:53:ILE:HD11 | 2.54 | 0.43 |
| 1:C:242:LEU:HD12 | 1:C:243:PHE:N | 2.33 | 0.43 |
| 1:D:49:PHE:CZ | 1:D:53:ILE:HD11 | 2.54 | 0.43 |
| 1:F:242:LEU:HD12 | 1:F:243:PHE:N | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:242:LEU:HD23 | 1:G:206:PRO:HB3 | 1.99 | 0.43 |
| 1:G:114:THR:HG21 | 1:H:88:PHE:CE2 | 2.54 | 0.43 |
| 1:A:117:ALA:O | 1:A:118:LEU:C | 2.55 | 0.43 |
| 1:B:49:PHE:CZ | 1:B:53:ILE:HD11 | 2.54 | 0.43 |
| 1:E:154:GLU:N | 1:H:188:GLU:OE2 | 2.51 | 0.43 |
| 1:E:46:TRP:O | 1:E:47:PRO:C | 2.56 | 0.43 |
| 1:F:239:PHE:CE1 | 1:F:265:ILE:HD11 | 2.53 | 0.43 |
| 1:G:280:ASP:CB | 1:G:282:ARG:HG2 | 2.39 | 0.43 |
| 1:G:49:PHE:CZ | 1:G:53:ILE:HD11 | 2.54 | 0.43 |
| 1:C:239:PHE:CE1 | 1:C:265:ILE:HD11 | 2.54 | 0.43 |
| 1:F:210:LEU:HB3 | 1:F:285:ILE:HD13 | 1.99 | 0.43 |
| 1:G:46:TRP:N | 1:G:47:PRO:CD | 2.78 | 0.43 |
| 1:H:103:ILE:CG2 | 1:H:104:PRO:HD2 | 2.49 | 0.43 |
| 1:B:110:ASN:HB3 | 1:C:88:PHE:CD2 | 2.54 | 0.43 |
| 1:B:191:VAL:HG13 | 1:B:191:VAL:O | 2.19 | 0.43 |
| 1:D:239:PHE:CE1 | 1:D:265:ILE:HD11 | 2.54 | 0.43 |
| 1:E:204:ARG:CG | 1:E:204:ARG:NH1 | 2.79 | 0.43 |
| 1:E:129:SER:HB3 | 1:F:132:TYR:CD1 | 2.53 | 0.43 |
| 1:G:117:ALA:O | 1:G:120:GLY:N | 2.51 | 0.43 |
| 1:G:239:PHE:CE1 | 1:G:265:ILE:HD11 | 2.53 | 0.43 |
| 1:H:49:PHE:CZ | 1:H:53:ILE:HD11 | 2.54 | 0.43 |
| 1:H:75:ILE:CG2 | 1:H:102:LEU:HB3 | 2.49 | 0.43 |
| 1:E:103:ILE:CG2 | 1:E:104:PRO:HD2 | 2.49 | 0.43 |
| 1:E:117:ALA:O | 1:E:120:GLY:N | 2.51 | 0.43 |
| 1:F:49:PHE:CZ | 1:F:53:ILE:HD11 | 2.54 | 0.43 |
| 1:A:210:LEU:HB3 | 1:A:285:ILE:HD13 | 2.01 | 0.43 |
| 1:B:75:ILE:CG2 | 1:B:102:LEU:HB3 | 2.49 | 0.43 |
| 1:C:103:ILE:CG2 | 1:C:104:PRO:HD2 | 2.49 | 0.43 |
| 1:D:49:PHE:HE2 | 1:D:131:ILE:HD13 | 1.84 | 0.43 |
| 1:E:141:GLY:O | 1:E:166:LEU:CB | 2.64 | 0.43 |
| 1:G:103:ILE:CG2 | 1:G:104:PRO:HD2 | 2.49 | 0.43 |
| 1:G:44:VAL:CG1 | 1:G:48:VAL:CG1 | 2.97 | 0.43 |
| 1:B:280:ASP:OD2 | 1:B:282:ARG:CD | 2.54 | 0.43 |
| 1:B:49:PHE:HE2 | 1:B:131:ILE:HD13 | 1.84 | 0.43 |
| 1:B:130:LEU:HD21 | 1:C:135:PHE:HE2 | 1.83 | 0.43 |
| 1:C:18:ASP:O | 1:C:257:ARG:NH1 | 2.51 | 0.43 |
| 1:D:103:ILE:CG2 | 1:D:104:PRO:HD2 | 2.49 | 0.43 |
| 1:E:75:ILE:CD1 | 1:E:89:PHE:CE2 | 2.97 | 0.43 |
| 1:G:94:MET:O | 1:G:94:MET:HG2 | 2.18 | 0.43 |
| 1:H:16:ASN:O | 1:H:259:ALA:HB3 | 2.18 | 0.43 |
| 1:A:103:ILE:CG2 | 1:A:104:PRO:HD2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:129:SER:HB3 | 1:C:132:TYR:HD1 | 1.84 | 0.42 |
| 1:C:49:PHE:HE2 | 1:C:131:ILE:CD1 | 2.31 | 0.42 |
| 1:D:75:ILE:CG2 | 1:D:102:LEU:HB3 | 2.49 | 0.42 |
| 1:D:117:ALA:O | 1:D:118:LEU:C | 2.56 | 0.42 |
| 1:E:75:ILE:CG2 | 1:E:102:LEU:HB3 | 2.49 | 0.42 |
| 1:E:161:MET:HE3 | 1:E:161:MET:HB2 | 1.89 | 0.42 |
| 1:F:75:ILE:CG2 | 1:F:102:LEU:HB3 | 2.49 | 0.42 |
| 1:H:137:ARG:HA | 1:H:138:PRO:HD3 | 1.82 | 0.42 |
| 1:A:145:SER:OG | 1:A:161:MET:HB2 | 2.19 | 0.42 |
| 1:A:166:LEU:HA | 1:A:166:LEU:HD23 | 1.73 | 0.42 |
| 1:A:75:ILE:CG2 | 1:A:102:LEU:HB3 | 2.49 | 0.42 |
| 1:C:75:ILE:CG2 | 1:C:102:LEU:HB3 | 2.49 | 0.42 |
| 1:D:191:VAL:O | 1:D:191:VAL:HG13 | 2.19 | 0.42 |
| 1:C:24:THR:O | 1:D:284:ALA:HA | 2.19 | 0.42 |
| 1:G:75:ILE:CG2 | 1:G:102:LEU:HB3 | 2.49 | 0.42 |
| 1:F:39:HIS:HA | 1:G:250:PHE:HE2 | 1.84 | 0.42 |
| 1:G:44:VAL:HG12 | 1:G:45:SER:N | 2.34 | 0.42 |
| 1:B:61:ASN:ND2 | 1:B:94:MET:HE2 | 2.26 | 0.42 |
| 1:B:94:MET:HG2 | 1:B:94:MET:O | 2.19 | 0.42 |
| 1:G:117:ALA:O | 1:G:118:LEU:C | 2.55 | 0.42 |
| 1:H:69:LEU:C | 1:H:72:GLY:H | 2.21 | 0.42 |
| 1:H:94:MET:HG2 | 1:H:94:MET:O | 2.19 | 0.42 |
| 1:C:191:VAL:O | 1:C:191:VAL:HG13 | 2.19 | 0.42 |
| 1:E:94:MET:HB2 | 1:E:116:GLU:CG | 2.47 | 0.42 |
| 1:F:104:PRO:CB | 1:F:110:ASN:OD1 | 2.67 | 0.42 |
| 1:F:44:VAL:HG12 | 1:F:45:SER:N | 2.34 | 0.42 |
| 1:G:94:MET:HB2 | 1:G:116:GLU:CG | 2.48 | 0.42 |
| 1:A:94:MET:HG2 | 1:A:94:MET:O | 2.19 | 0.42 |
| 1:B:104:PRO:CB | 1:B:110:ASN:OD1 | 2.67 | 0.42 |
| 1:F:191:VAL:O | 1:F:191:VAL:HG13 | 2.19 | 0.42 |
| 1:F:61:ASN:OD1 | 1:F:90:SER:OG | 2.30 | 0.42 |
| 1:F:94:MET:O | 1:F:94:MET:HG2 | 2.19 | 0.42 |
| 1:H:44:VAL:HG11 | 1:H:48:VAL:CG1 | 2.50 | 0.42 |
| 1:B:103:ILE:CG2 | 1:B:104:PRO:HD2 | 2.49 | 0.42 |
| 1:F:141:GLY:O | 1:F:166:LEU:CB | 2.64 | 0.42 |
| 1:F:182:ARG:HB2 | 1:F:235:SER:HB2 | 2.01 | 0.42 |
| 1:G:46:TRP:HB2 | 1:G:47:PRO:HD3 | 2.02 | 0.42 |
| 1:H:41:LEU:O | 1:H:134:ARG:NH1 | 2.51 | 0.42 |
| 1:B:44:VAL:HG12 | 1:B:45:SER:N | 2.34 | 0.42 |
| 1:C:94:MET:HG2 | 1:C:94:MET:O | 2.18 | 0.42 |
| 1:F:117:ALA:O | 1:F:118:LEU:C | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:ILE:HG23 | 1:A:104:PRO:HD2 | 2.02 | 0.42 |
| 1:C:69:LEU:HA | 1:C:69:LEU:HD23 | 1.66 | 0.42 |
| 1:H:191:VAL:HG13 | 1:H:191:VAL:O | 2.19 | 0.42 |
| 1:D:103:ILE:HG23 | 1:D:104:PRO:HD2 | 2.02 | 0.42 |
| 1:D:280:ASP:OD2 | 1:D:282:ARG:CD | 2.54 | 0.42 |
| 1:E:23:ILE:CD1 | 1:F:283:ARG:CZ | 2.98 | 0.42 |
| 1:E:75:ILE:HG22 | 1:E:76:GLU:O | 2.20 | 0.42 |
| 1:F:46:TRP:O | 1:F:47:PRO:C | 2.59 | 0.42 |
| 1:G:191:VAL:HG13 | 1:G:191:VAL:O | 2.19 | 0.42 |
| 1:A:94:MET:C | 1:A:96:THR:N | 2.74 | 0.42 |
| 1:C:44:VAL:HG12 | 1:C:45:SER:O | 2.20 | 0.42 |
| 1:D:272:VAL:CG1 | 1:D:273:ASP:H | 2.25 | 0.42 |
| 1:E:103:ILE:HG23 | 1:E:104:PRO:HD2 | 2.02 | 0.42 |
| 1:E:44:VAL:HG12 | 1:E:45:SER:O | 2.20 | 0.42 |
| 1:F:44:VAL:HG12 | 1:F:45:SER:O | 2.20 | 0.42 |
| 1:A:162:ARG:O | 1:A:290:PHE:CZ | 2.73 | 0.41 |
| 1:A:191:VAL:HG13 | 1:A:191:VAL:O | 2.19 | 0.41 |
| 1:B:46:TRP:O | 1:B:47:PRO:C | 2.59 | 0.41 |
| 1:C:117:ALA:O | 1:C:118:LEU:C | 2.55 | 0.41 |
| 1:C:146:SER:O | 1:C:147:ARG:NH1 | 2.53 | 0.41 |
| 1:F:146:SER:O | 1:F:147:ARG:NH1 | 2.53 | 0.41 |
| 1:H:166:LEU:HA | 1:H:166:LEU:HD23 | 1.72 | 0.41 |
| 1:H:61:ASN:OD1 | 1:H:90:SER:OG | 2.35 | 0.41 |
| 1:B:131:ILE:H | 1:B:131:ILE:HG12 | 1.74 | 0.41 |
| 1:B:44:VAL:HG12 | 1:B:45:SER:O | 2.20 | 0.41 |
| 1:C:46:TRP:O | 1:C:47:PRO:C | 2.59 | 0.41 |
| 1:D:45:SER:O | 1:D:46:TRP:C | 2.58 | 0.41 |
| 1:E:191:VAL:HG13 | 1:E:191:VAL:O | 2.19 | 0.41 |
| 1:E:94:MET:O | 1:E:94:MET:HG2 | 2.19 | 0.41 |
| 1:F:103:ILE:CG2 | 1:F:104:PRO:HD2 | 2.49 | 0.41 |
| 1:E:129:SER:HB3 | 1:F:132:TYR:HD1 | 1.85 | 0.41 |
| 1:F:204:ARG:NH1 | 1:F:204:ARG:CG | 2.79 | 0.41 |
| 1:F:61:ASN:CG | 1:F:94:MET:HE2 | 2.40 | 0.41 |
| 1:H:103:ILE:HG23 | 1:H:104:PRO:HD2 | 2.02 | 0.41 |
| 1:E:44:VAL:HG12 | 1:E:45:SER:N | 2.34 | 0.41 |
| 1:E:39:HIS:HA | 1:F:250:PHE:HE2 | 1.84 | 0.41 |
| 1:H:46:TRP:O | 1:H:47:PRO:C | 2.58 | 0.41 |
| 1:A:44:VAL:HG12 | 1:A:45:SER:N | 2.34 | 0.41 |
| 1:B:94:MET:HB2 | 1:B:116:GLU:CG | 2.48 | 0.41 |
| 1:D:15:LEU:HB2 | 1:D:238:GLU:OE1 | 2.20 | 0.41 |
| 1:D:94:MET:O | 1:D:94:MET:HG2 | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:292:GLU:HG2 | 1:E:295:GLN:O | 2.21 | 0.41 |
| 1:G:44:VAL:HG12 | 1:G:45:SER:O | 2.20 | 0.41 |
| 1:F:111:THR:N | 1:G:88:PHE:CE2 | 2.87 | 0.41 |
| 1:E:88:PHE:CE2 | 1:H:114:THR:CG2 | 3.03 | 0.41 |
| 1:B:198:LEU:HD22 | 1:B:223:PRO:HD2 | 2.03 | 0.41 |
| 1:B:129:SER:HB3 | 1:C:132:TYR:CD1 | 2.55 | 0.41 |
| 1:C:168:ILE:CD1 | 1:C:168:ILE:N | 2.61 | 0.41 |
| 1:D:210:LEU:HB3 | 1:D:285:ILE:HD11 | 1.98 | 0.41 |
| 1:G:75:ILE:CD1 | 1:G:89:PHE:CE2 | 3.03 | 0.41 |
| 1:G:93:THR:HG23 | 1:G:94:MET:N | 2.36 | 0.41 |
| 1:B:146:SER:O | 1:B:147:ARG:NH1 | 2.53 | 0.41 |
| 1:B:93:THR:HG23 | 1:B:94:MET:N | 2.35 | 0.41 |
| 1:C:198:LEU:HD22 | 1:C:223:PRO:HD2 | 2.03 | 0.41 |
| 1:C:44:VAL:HG12 | 1:C:45:SER:N | 2.34 | 0.41 |
| 1:D:185:ILE:HD12 | 1:D:191:VAL:HB | 2.02 | 0.41 |
| 1:D:94:MET:HB2 | 1:D:116:GLU:CG | 2.48 | 0.41 |
| 1:E:198:LEU:HD22 | 1:E:223:PRO:HD2 | 2.03 | 0.41 |
| 1:F:198:LEU:HD22 | 1:F:223:PRO:HD2 | 2.03 | 0.41 |
| 1:A:92:GLN:O | 1:A:97:ILE:N | 2.54 | 0.41 |
| 1:B:44:VAL:HG13 | 1:B:48:VAL:CB | 2.49 | 0.41 |
| 1:A:114:THR:CG2 | 1:B:91:VAL:HG21 | 2.51 | 0.41 |
| 1:E:146:SER:O | 1:E:147:ARG:NH1 | 2.53 | 0.41 |
| 1:F:93:THR:HG23 | 1:F:94:MET:N | 2.36 | 0.41 |
| 1:A:168:ILE:N | 1:A:168:ILE:CD1 | 2.61 | 0.41 |
| 1:A:46:TRP:O | 1:A:47:PRO:C | 2.59 | 0.41 |
| 1:B:103:ILE:HG23 | 1:B:104:PRO:HD2 | 2.02 | 0.41 |
| 1:B:166:LEU:HD23 | 1:B:166:LEU:HA | 1.72 | 0.41 |
| 1:C:103:ILE:HG23 | 1:C:104:PRO:HD2 | 2.02 | 0.41 |
| 1:F:129:SER:HB3 | 1:G:132:TYR:HD1 | 1.84 | 0.41 |
| 1:G:23:ILE:CD1 | 1:H:283:ARG:HD3 | 2.50 | 0.41 |
| 1:C:181:VAL:HG12 | 1:C:193:ARG:CZ | 2.51 | 0.41 |
| 1:D:198:LEU:HD22 | 1:D:223:PRO:HD2 | 2.03 | 0.41 |
| 1:F:114:THR:CG2 | 1:G:88:PHE:CE2 | 3.04 | 0.41 |
| 1:A:44:VAL:CG1 | 1:A:48:VAL:CG1 | 2.99 | 0.41 |
| 1:A:44:VAL:HG12 | 1:A:45:SER:O | 2.20 | 0.41 |
| 1:D:280:ASP:CB | 1:D:282:ARG:HG2 | 2.39 | 0.41 |
| 1:E:13:ARG:H | 1:E:13:ARG:HG2 | 1.74 | 0.41 |
| 1:G:103:ILE:HG23 | 1:G:104:PRO:HD2 | 2.02 | 0.41 |
| 1:G:93:THR:CG2 | 1:G:116:GLU:CD | 2.89 | 0.41 |
| 1:E:69:LEU:HD23 | 1:E:69:LEU:HA | 1.66 | 0.41 |
| 1:A:193:ARG:NH1 | 1:A:236:HIS:O | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:GLN:HA | 1:A:97:ILE:HD12 | 2.03 | 0.40 |
| 1:C:15:LEU:HB2 | 1:C:238:GLU:OE1 | 2.21 | 0.40 |
| 1:D:185:ILE:CD1 | 1:D:191:VAL:CG2 | 2.99 | 0.40 |
| 1:D:91:VAL:CG2 | 1:D:92:GLN:N | 2.85 | 0.40 |
| 1:E:185:ILE:CD1 | 1:E:191:VAL:CG2 | 2.99 | 0.40 |
| 1:H:74:VAL:HB | 1:H:109:ALA:HB2 | 2.02 | 0.40 |
| 1:H:91:VAL:CG2 | 1:H:92:GLN:N | 2.85 | 0.40 |
| 1:H:93:THR:HG23 | 1:H:94:MET:N | 2.35 | 0.40 |
| 1:G:93:THR:OG1 | 1:H:99:TYR:OH | 2.28 | 0.40 |
| 1:A:185:ILE:CD1 | 1:A:191:VAL:CG2 | 2.99 | 0.40 |
| 1:A:266:ILE:CG2 | 1:A:269:GLY:HA3 | 2.52 | 0.40 |
| 1:A:98:GLY:HA3 | 1:B:97:ILE:HG22 | 2.03 | 0.40 |
| 1:B:52:LEU:HA | 1:B:52:LEU:HD23 | 1.91 | 0.40 |
| 1:D:46:TRP:O | 1:D:47:PRO:C | 2.58 | 0.40 |
| 1:D:61:ASN:HD21 | 1:D:94:MET:HE2 | 1.80 | 0.40 |
| 1:C:292:GLU:HG2 | 1:E:295:GLN:C | 2.42 | 0.40 |
| 1:E:23:ILE:HG13 | 1:F:283:ARG:NH2 | 2.36 | 0.40 |
| 1:G:69:LEU:HA | 1:G:69:LEU:HD23 | 1.67 | 0.40 |
| 1:H:44:VAL:HG12 | 1:H:45:SER:N | 2.36 | 0.40 |
| 1:A:104:PRO:HB2 | 1:A:110:ASN:CG | 2.42 | 0.40 |
| 1:A:198:LEU:HD22 | 1:A:223:PRO:HD2 | 2.03 | 0.40 |
| 1:C:110:ASN:CB | 1:D:88:PHE:CE2 | 3.05 | 0.40 |
| 1:C:185:ILE:CD1 | 1:C:191:VAL:CG2 | 2.99 | 0.40 |
| 1:C:91:VAL:CG2 | 1:C:92:GLN:N | 2.85 | 0.40 |
| 1:G:146:SER:O | 1:G:147:ARG:NH1 | 2.53 | 0.40 |
| 1:H:69:LEU:HD23 | 1:H:69:LEU:HA | 1.66 | 0.40 |
| 1:A:69:LEU:HA | 1:A:69:LEU:HD23 | 1.67 | 0.40 |
| 1:A:69:LEU:O | 1:A:72:GLY:HA2 | 2.20 | 0.40 |
| 1:C:204:ARG:NH1 | 1:C:204:ARG:CG | 2.79 | 0.40 |
| 1:F:103:ILE:HG23 | 1:F:104:PRO:HD2 | 2.02 | 0.40 |
| 1:B:185:ILE:CD1 | 1:B:191:VAL:CG2 | 2.99 | 0.40 |
| 1:C:270:HIS:O | 1:C:294:ALA:N | 2.55 | 0.40 |
| 1:D:192:PHE:HE1 | 1:D:194:ARG:HB2 | 1.87 | 0.40 |
| 1:E:93:THR:HG22 | 1:E:94:MET:N | 2.37 | 0.40 |
| 1:F:158:THR:HG23 | 1:F:217:PRO:N | 2.37 | 0.40 |
| 1:G:91:VAL:CG2 | 1:G:92:GLN:N | 2.85 | 0.40 |
| 1:H:105:ILE:H | 1:H:109:ALA:CB | 2.34 | 0.40 |
| 1:H:131:ILE:H | 1:H:131:ILE:HG12 | 1.74 | 0.40 |
| 1:H:198:LEU:HD22 | 1:H:223:PRO:HD2 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 279/301 (93%) | 260 (93%) | 18 (6%) | 1 (0%) | 34 | 70 |
| 1 | B | 279/301 (93%) | 260 (93%) | 18 (6%) | 1 (0%) | 34 | 70 |
| 1 | C | 279/301 (93%) | 259 (93%) | 18 (6%) | 2 (1%) | 22 | 60 |
| 1 | D | 279/301 (93%) | 260 (93%) | 18 (6%) | 1 (0%) | 34 | 70 |
| 1 | E | 279/301 (93%) | 257 (92%) | 20 (7%) | 2 (1%) | 22 | 60 |
| 1 | F | 279/301 (93%) | 257 (92%) | 20 (7%) | 2 (1%) | 22 | 60 |
| 1 | G | 279/301 (93%) | 260 (93%) | 18 (6%) | 1 (0%) | 34 | 70 |
| 1 | H | 279/301 (93%) | 258 (92%) | 20 (7%) | 1 (0%) | 34 | 70 |
| All | All | 2232/2408 (93%) | 2071 (93%) | 150 (7%) | 11 (0%) | 29 | 66 |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 287 | LEU |
| 1 | E | 77 | ASN |
| 1 | A | 59 | VAL |
| 1 | B | 59 | VAL |
| 1 | C | 59 | VAL |
| 1 | C | 287 | LEU |
| 1 | D | 59 | VAL |
| 1 | E | 59 | VAL |
| 1 | F | 59 | VAL |
| 1 | G | 59 | VAL |
| 1 | H | 59 | 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 | 235/256 (92%) | 218 (93%) | 17 (7%) | 14 | 46 |
| 1 | B | 235/256 (92%) | 217 (92%) | 18 (8%) | 13 | 42 |
| 1 | C | 235/256 (92%) | 218 (93%) | 17 (7%) | 14 | 46 |
| 1 | D | 236/256 (92%) | 218 (92%) | 18 (8%) | 13 | 43 |
| 1 | E | 236/256 (92%) | 219 (93%) | 17 (7%) | 14 | 46 |
| 1 | F | 236/256 (92%) | 218 (92%) | 18 (8%) | 13 | 43 |
| 1 | G | 235/256 (92%) | 217 (92%) | 18 (8%) | 13 | 42 |
| 1 | H | 236/256 (92%) | 216 (92%) | 20 (8%) | 10 | 38 |
| All | All | 1884/2048 (92%) | 1741 (92%) | 143 (8%) | 13 | 43 |

All (143) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 74 | VAL |
| 1 | A | 82 | SER |
| 1 | A | 92 | GLN |
| 1 | A | 93 | THR |
| 1 | A | 114 | THR |
| 1 | A | 129 | SER |
| 1 | A | 134 | ARG |
| 1 | A | 154 | GLU |
| 1 | A | 160 | MET |
| 1 | A | 161 | MET |
| 1 | A | 168 | ILE |
| 1 | A | 170 | GLN |
| 1 | A | 204 | ARG |
| 1 | A | 220 | HIS |
| 1 | A | 235 | SER |
| 1 | A | 262 | CYS |
| 1 | A | 264 | GLU |
| 1 | B | 74 | VAL |
| 1 | B | 82 | SER |
| 1 | B | 92 | GLN |
| 1 | B | 93 | THR |
| 1 | B | 114 | THR |
| 1 | B | 129 | SER |
| 1 | B | 134 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 154 | GLU |
| 1 | B | 160 | MET |
| 1 | B | 161 | MET |
| 1 | B | 168 | ILE |
| 1 | B | 170 | GLN |
| 1 | B | 197 | ASP |
| 1 | B | 204 | ARG |
| 1 | B | 220 | HIS |
| 1 | B | 235 | SER |
| 1 | B | 262 | CYS |
| 1 | B | 264 | GLU |
| 1 | C | 74 | VAL |
| 1 | C | 82 | SER |
| 1 | C | 92 | GLN |
| 1 | C | 93 | THR |
| 1 | C | 114 | THR |
| 1 | C | 129 | SER |
| 1 | C | 134 | ARG |
| 1 | C | 154 | GLU |
| 1 | C | 160 | MET |
| 1 | C | 161 | MET |
| 1 | C | 168 | ILE |
| 1 | C | 170 | GLN |
| 1 | C | 204 | ARG |
| 1 | C | 220 | HIS |
| 1 | C | 235 | SER |
| 1 | C | 262 | CYS |
| 1 | C | 264 | GLU |
| 1 | D | 74 | VAL |
| 1 | D | 82 | SER |
| 1 | D | 92 | GLN |
| 1 | D | 93 | THR |
| 1 | D | 114 | THR |
| 1 | D | 121 | MET |
| 1 | D | 129 | SER |
| 1 | D | 134 | ARG |
| 1 | D | 154 | GLU |
| 1 | D | 160 | MET |
| 1 | D | 161 | MET |
| 1 | D | 168 | ILE |
| 1 | D | 170 | GLN |
| 1 | D | 204 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 220 | HIS |
| 1 | D | 235 | SER |
| 1 | D | 262 | CYS |
| 1 | D | 264 | GLU |
| 1 | E | 74 | VAL |
| 1 | E | 82 | SER |
| 1 | E | 92 | GLN |
| 1 | E | 93 | THR |
| 1 | E | 114 | THR |
| 1 | E | 129 | SER |
| 1 | E | 134 | ARG |
| 1 | E | 154 | GLU |
| 1 | E | 160 | MET |
| 1 | E | 161 | MET |
| 1 | E | 168 | ILE |
| 1 | E | 170 | GLN |
| 1 | E | 204 | ARG |
| 1 | E | 220 | HIS |
| 1 | E | 235 | SER |
| 1 | E | 262 | CYS |
| 1 | E | 264 | GLU |
| 1 | F | 74 | VAL |
| 1 | F | 82 | SER |
| 1 | F | 92 | GLN |
| 1 | F | 93 | THR |
| 1 | F | 114 | THR |
| 1 | F | 129 | SER |
| 1 | F | 134 | ARG |
| 1 | F | 154 | GLU |
| 1 | F | 160 | MET |
| 1 | F | 161 | MET |
| 1 | F | 168 | ILE |
| 1 | F | 170 | GLN |
| 1 | F | 197 | ASP |
| 1 | F | 204 | ARG |
| 1 | F | 220 | HIS |
| 1 | F | 235 | SER |
| 1 | F | 262 | CYS |
| 1 | F | 264 | GLU |
| 1 | G | 74 | VAL |
| 1 | G | 82 | SER |
| 1 | G | 92 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 93 | THR |
| 1 | G | 114 | THR |
| 1 | G | 129 | SER |
| 1 | G | 134 | ARG |
| 1 | G | 154 | GLU |
| 1 | G | 160 | MET |
| 1 | G | 161 | MET |
| 1 | G | 168 | ILE |
| 1 | G | 170 | GLN |
| 1 | G | 197 | ASP |
| 1 | G | 204 | ARG |
| 1 | G | 220 | HIS |
| 1 | G | 235 | SER |
| 1 | G | 262 | CYS |
| 1 | G | 264 | GLU |
| 1 | H | 74 | VAL |
| 1 | H | 82 | SER |
| 1 | H | 92 | GLN |
| 1 | H | 93 | THR |
| 1 | H | 114 | THR |
| 1 | H | 121 | MET |
| 1 | H | 129 | SER |
| 1 | H | 134 | ARG |
| 1 | H | 154 | GLU |
| 1 | H | 156 | LYS |
| 1 | H | 160 | MET |
| 1 | H | 161 | MET |
| 1 | H | 168 | ILE |
| 1 | H | 170 | GLN |
| 1 | H | 204 | ARG |
| 1 | H | 220 | HIS |
| 1 | H | 235 | SER |
| 1 | H | 262 | CYS |
| 1 | H | 264 | GLU |
| 1 | H | 283 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 61 | ASN |
| 1 | A | 77 | ASN |
| 1 | A | 170 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 196 | HIS |
| 1 | A | 258 | HIS |
| 1 | B | 61 | ASN |
| 1 | B | 77 | ASN |
| 1 | B | 170 | GLN |
| 1 | B | 258 | HIS |
| 1 | C | 61 | ASN |
| 1 | C | 77 | ASN |
| 1 | C | 196 | HIS |
| 1 | C | 258 | HIS |
| 1 | D | 61 | ASN |
| 1 | D | 77 | ASN |
| 1 | D | 258 | HIS |
| 1 | E | 61 | ASN |
| 1 | E | 170 | GLN |
| 1 | E | 246 | HIS |
| 1 | E | 253 | ASN |
| 1 | E | 258 | HIS |
| 1 | F | 61 | ASN |
| 1 | F | 77 | ASN |
| 1 | F | 170 | GLN |
| 1 | F | 196 | HIS |
| 1 | F | 258 | HIS |
| 1 | G | 61 | ASN |
| 1 | G | 77 | ASN |
| 1 | G | 258 | HIS |
| 1 | H | 61 | ASN |
| 1 | H | 77 | ASN |
| 1 | H | 170 | GLN |
| 1 | H | 196 | HIS |
| 1 | H | 255 | HIS |
| 1 | H | 258 | 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | E | 5 |
| 1 | G | 4 |
| 1 | D | 4 |
| 1 | B | 4 |
| 1 | A | 4 |
| 1 | H | 3 |
| 1 | C | 2 |
| 1 | F | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | E | 106:GLY | C | 107:PRO | N | 1.71 |
| 1 | D | 182:ARG | C | 183:SER | N | 1.70 |
| 1 | E | 71:CYS | C | 72:GLY | N | 1.70 |
| 1 | B | 150:ILE | C | 151:SER | N | 1.65 |
| 1 | B | 273:ASP | C | 274:VAL | N | 1.63 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | C | 70:ALA | C | 71:CYS | N | 1.62 |
| 1 | D | 273:ASP | C | 274:VAL | N | 1.62 |
| 1 | E | 286:ASP | C | 287:LEU | N | 1.17 |
| 1 | A | 273:ASP | C | 274:VAL | N | 1.16 |
| 1 | C | 81:GLY | C | 82:SER | N | 1.16 |
| 1 | D | 106:GLY | C | 107:PRO | N | 1.16 |
| 1 | D | 286:ASP | C | 287:LEU | N | 1.16 |
| 1 | G | 46:TRP | C | 47:PRO | N | 1.16 |
| 1 | G | 82:SER | C | 83:PHE | N | 1.16 |
| 1 | A | 106:GLY | C | 107:PRO | N | 1.15 |
| 1 | B | 288:GLY | C | 289:LYS | N | 1.14 |
| 1 | H | 195:PHE | C | 196:HIS | N | 1.14 |
| 1 | F | 81:GLY | C | 82:SER | N | 1.11 |
| 1 | E | 285:ILE | C | 286:ASP | N | 1.04 |
| 1 | E | 95:ALA | C | 96:THR | N | 1.03 |
| 1 | F | 172:ILE | C | 173:GLU | N | 1.02 |
| 1 | H | 274:VAL | C | 275:PHE | N | 1.01 |
| 1 | G | 122:LEU | C | 123:GLY | N | 0.96 |
| 1 | G | 287:LEU | C | 288:GLY | N | 0.96 |
| 1 | B | 157:PRO | C | 158:THR | N | 0.92 |
| 1 | A | 94:MET | C | 95:ALA | N | 0.87 |
| 1 | H | 82:SER | C | 83:PHE | N | 0.87 |
| 1 | A | 287:LEU | C | 288:GLY | N | 0.75 |

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 | 283/301 (94%) | -0.10 | 13 (4%) 32 32 | 69, 118, 193, 227 | 0 |
| 1 | B | 283/301 (94%) | -0.22 | 9 (3%) 47 46 | 66, 116, 187, 258 | 0 |
| 1 | C | 283/301 (94%) | -0.21 | 7 (2%) 57 55 | 68, 111, 189, 233 | 0 |
| 1 | D | 283/301 (94%) | -0.21 | 8 (2%) 53 51 | 64, 108, 199, 270 | 0 |
| 1 | E | 283/301 (94%) | -0.09 | 11 (3%) 39 38 | 67, 113, 194, 252 | 0 |
| 1 | F | 283/301 (94%) | -0.18 | 12 (4%) 36 35 | 65, 114, 200, 250 | 0 |
| 1 | G | 283/301 (94%) | -0.13 | 13 (4%) 32 32 | 66, 114, 207, 297 | 0 |
| 1 | H | 283/301 (94%) | -0.12 | 9 (3%) 47 46 | 73, 116, 197, 239 | 0 |
| All | All | 2264/2408 (94%) | -0.16 | 82 (3%) 42 42 | 64, 114, 197, 297 | 0 |

All (82) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 280 | ASP | 6.2 |
| 1 | C | 12 | PRO | 4.6 |
| 1 | G | 107 | PRO | 4.5 |
| 1 | A | 35 | ASP | 4.3 |
| 1 | E | 298 | HIS | 4.2 |
| 1 | G | 220 | HIS | 4.0 |
| 1 | D | 280 | ASP | 3.9 |
| 1 | E | 282 | ARG | 3.9 |
| 1 | H | 81 | GLY | 3.9 |
| 1 | G | 282 | ARG | 3.8 |
| 1 | B | 280 | ASP | 3.7 |
| 1 | D | 33 | TRP | 3.6 |
| 1 | G | 281 | GLY | 3.6 |
| 1 | A | 234 | ASN | 3.5 |
| 1 | F | 35 | ASP | 3.5 |
| 1 | B | 282 | ARG | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | H | 35 | ASP | 3.4 |
| 1 | A | 298 | HIS | 3.4 |
| 1 | E | 220 | HIS | 3.3 |
| 1 | E | 280 | ASP | 3.3 |
| 1 | B | 281 | GLY | 3.2 |
| 1 | H | 16 | ASN | 3.2 |
| 1 | D | 299 | HIS | 3.2 |
| 1 | D | 71 | CYS | 3.1 |
| 1 | C | 280 | ASP | 3.1 |
| 1 | F | 12 | PRO | 3.0 |
| 1 | A | 187 | GLN | 3.0 |
| 1 | A | 81 | GLY | 3.0 |
| 1 | C | 298 | HIS | 2.9 |
| 1 | G | 73 | ASP | 2.8 |
| 1 | E | 77 | ASN | 2.8 |
| 1 | E | 299 | HIS | 2.7 |
| 1 | G | 284 | ALA | 2.7 |
| 1 | G | 27 | GLY | 2.7 |
| 1 | F | 187 | GLN | 2.7 |
| 1 | A | 280 | ASP | 2.6 |
| 1 | F | 280 | ASP | 2.6 |
| 1 | A | 188 | GLU | 2.6 |
| 1 | D | 277 | THR | 2.6 |
| 1 | A | 12 | PRO | 2.6 |
| 1 | D | 279 | PRO | 2.5 |
| 1 | F | 76 | GLU | 2.5 |
| 1 | B | 279 | PRO | 2.5 |
| 1 | A | 73 | ASP | 2.5 |
| 1 | F | 73 | ASP | 2.5 |
| 1 | E | 35 | ASP | 2.5 |
| 1 | E | 80 | PRO | 2.5 |
| 1 | E | 101 | LYS | 2.5 |
| 1 | G | 71 | CYS | 2.4 |
| 1 | B | 33 | TRP | 2.4 |
| 1 | G | 35 | ASP | 2.4 |
| 1 | B | 298 | HIS | 2.3 |
| 1 | C | 81 | GLY | 2.3 |
| 1 | H | 234 | ASN | 2.3 |
| 1 | A | 71 | CYS | 2.3 |
| 1 | B | 234 | ASN | 2.3 |
| 1 | C | 234 | ASN | 2.3 |
| 1 | G | 279 | PRO | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 298 | HIS | 2.3 |
| 1 | H | 280 | ASP | 2.3 |
| 1 | D | 282 | ARG | 2.3 |
| 1 | F | 298 | HIS | 2.2 |
| 1 | A | 189 | GLY | 2.2 |
| 1 | C | 18 | ASP | 2.2 |
| 1 | E | 279 | PRO | 2.2 |
| 1 | B | 236 | HIS | 2.2 |
| 1 | A | 18 | ASP | 2.2 |
| 1 | D | 35 | ASP | 2.2 |
| 1 | H | 12 | PRO | 2.2 |
| 1 | E | 73 | ASP | 2.1 |
| 1 | F | 236 | HIS | 2.1 |
| 1 | H | 184 | GLU | 2.1 |
| 1 | H | 80 | PRO | 2.1 |
| 1 | F | 33 | TRP | 2.1 |
| 1 | F | 81 | GLY | 2.1 |
| 1 | H | 71 | CYS | 2.1 |
| 1 | A | 282 | ARG | 2.1 |
| 1 | C | 82 | SER | 2.1 |
| 1 | F | 16 | ASN | 2.0 |
| 1 | G | 236 | HIS | 2.0 |
| 1 | B | 81 | GLY | 2.0 |
| 1 | F | 279 | PRO | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2 | K | C | 1300 | 1/1 | 0.60 | 0.28 | 159,159,159,159 | 0 |
| 2 | K | F | 1300 | 1/1 | 0.78 | 0.09 | 128,128,128,128 | 0 |
| 2 | K | A | 1300 | 1/1 | 0.80 | 0.11 | 149,149,149,149 | 0 |
| 2 | K | A | 1301 | 1/1 | 0.81 | 0.14 | 144,144,144,144 | 0 |
| 2 | K | F | 1301 | 1/1 | 0.87 | 0.19 | 159,159,159,159 | 0 |
| 2 | K | H | 1300 | 1/1 | 0.93 | 0.19 | 145,145,145,145 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.