



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:45 PM UTC

PDB ID : 3ZZI / pdb_00003zzi
Title : Crystal structure of a tetrameric acetylglutamate kinase from *Saccharomyces cerevisiae*
Authors : de Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on : 2011-09-01
Resolution : 3.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

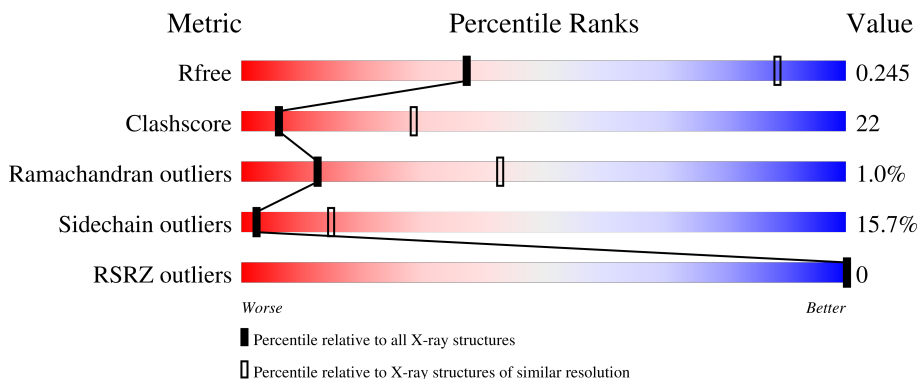
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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






| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 180053 | 1065 (3.96-3.64) |
| Clashscore | 190562 | 1012 (3.94-3.66) |
| Ramachandran outliers | 187476 | 1048 (3.96-3.64) |
| Sidechain outliers | 187428 | 1043 (3.96-3.64) |
| RSRZ outliers | 180081 | 1064 (3.96-3.64) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------|
| 1 | A | 464 | 55% 32% 6% 6% |
| 1 | B | 464 | 55% 32% 7% 6% |
| 1 | C | 464 | 56% 31% 7% 6% |
| 1 | D | 464 | 55% 30% 9% 6% |
| 1 | E | 464 | 52% 34% 8% 6% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | F | 464 |  |
| 1 | G | 464 |  |
| 1 | H | 464 |  |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27248 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 ACETYLGLUTAMATE KINASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 436 | Total 3402 | C 2167 | N 571 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | B | 436 | Total 3402 | C 2167 | N 571 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | C | 436 | Total 3408 | C 2170 | N 574 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | D | 436 | Total 3404 | C 2167 | N 573 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | E | 436 | Total 3408 | C 2170 | N 574 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | F | 436 | Total 3408 | C 2170 | N 574 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | G | 436 | Total 3408 | C 2170 | N 574 | O 655 | S 9 | 0 | 0 | 0 |
| 1 | H | 436 | Total 3408 | C 2170 | N 574 | O 655 | S 9 | 0 | 0 | 0 |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 50 | MET | - | expression tag | UNP Q01217 |
| A | 51 | GLY | - | expression tag | UNP Q01217 |
| A | 52 | HIS | - | expression tag | UNP Q01217 |
| A | 53 | HIS | - | expression tag | UNP Q01217 |
| A | 54 | HIS | - | expression tag | UNP Q01217 |
| A | 55 | HIS | - | expression tag | UNP Q01217 |
| A | 56 | HIS | - | expression tag | UNP Q01217 |
| A | 57 | HIS | - | expression tag | UNP Q01217 |
| B | 50 | MET | - | expression tag | UNP Q01217 |
| B | 51 | GLY | - | expression tag | UNP Q01217 |
| B | 52 | HIS | - | expression tag | UNP Q01217 |
| B | 53 | HIS | - | expression tag | UNP Q01217 |
| B | 54 | HIS | - | expression tag | UNP Q01217 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 55 | HIS | - | expression tag | UNP Q01217 |
| B | 56 | HIS | - | expression tag | UNP Q01217 |
| B | 57 | HIS | - | expression tag | UNP Q01217 |
| C | 50 | MET | - | expression tag | UNP Q01217 |
| C | 51 | GLY | - | expression tag | UNP Q01217 |
| C | 52 | HIS | - | expression tag | UNP Q01217 |
| C | 53 | HIS | - | expression tag | UNP Q01217 |
| C | 54 | HIS | - | expression tag | UNP Q01217 |
| C | 55 | HIS | - | expression tag | UNP Q01217 |
| C | 56 | HIS | - | expression tag | UNP Q01217 |
| C | 57 | HIS | - | expression tag | UNP Q01217 |
| D | 50 | MET | - | expression tag | UNP Q01217 |
| D | 51 | GLY | - | expression tag | UNP Q01217 |
| D | 52 | HIS | - | expression tag | UNP Q01217 |
| D | 53 | HIS | - | expression tag | UNP Q01217 |
| D | 54 | HIS | - | expression tag | UNP Q01217 |
| D | 55 | HIS | - | expression tag | UNP Q01217 |
| D | 56 | HIS | - | expression tag | UNP Q01217 |
| D | 57 | HIS | - | expression tag | UNP Q01217 |
| E | 50 | MET | - | expression tag | UNP Q01217 |
| E | 51 | GLY | - | expression tag | UNP Q01217 |
| E | 52 | HIS | - | expression tag | UNP Q01217 |
| E | 53 | HIS | - | expression tag | UNP Q01217 |
| E | 54 | HIS | - | expression tag | UNP Q01217 |
| E | 55 | HIS | - | expression tag | UNP Q01217 |
| E | 56 | HIS | - | expression tag | UNP Q01217 |
| E | 57 | HIS | - | expression tag | UNP Q01217 |
| F | 50 | MET | - | expression tag | UNP Q01217 |
| F | 51 | GLY | - | expression tag | UNP Q01217 |
| F | 52 | HIS | - | expression tag | UNP Q01217 |
| F | 53 | HIS | - | expression tag | UNP Q01217 |
| F | 54 | HIS | - | expression tag | UNP Q01217 |
| F | 55 | HIS | - | expression tag | UNP Q01217 |
| F | 56 | HIS | - | expression tag | UNP Q01217 |
| F | 57 | HIS | - | expression tag | UNP Q01217 |
| G | 50 | MET | - | expression tag | UNP Q01217 |
| G | 51 | GLY | - | expression tag | UNP Q01217 |
| G | 52 | HIS | - | expression tag | UNP Q01217 |
| G | 53 | HIS | - | expression tag | UNP Q01217 |
| G | 54 | HIS | - | expression tag | UNP Q01217 |
| G | 55 | HIS | - | expression tag | UNP Q01217 |
| G | 56 | HIS | - | expression tag | UNP Q01217 |

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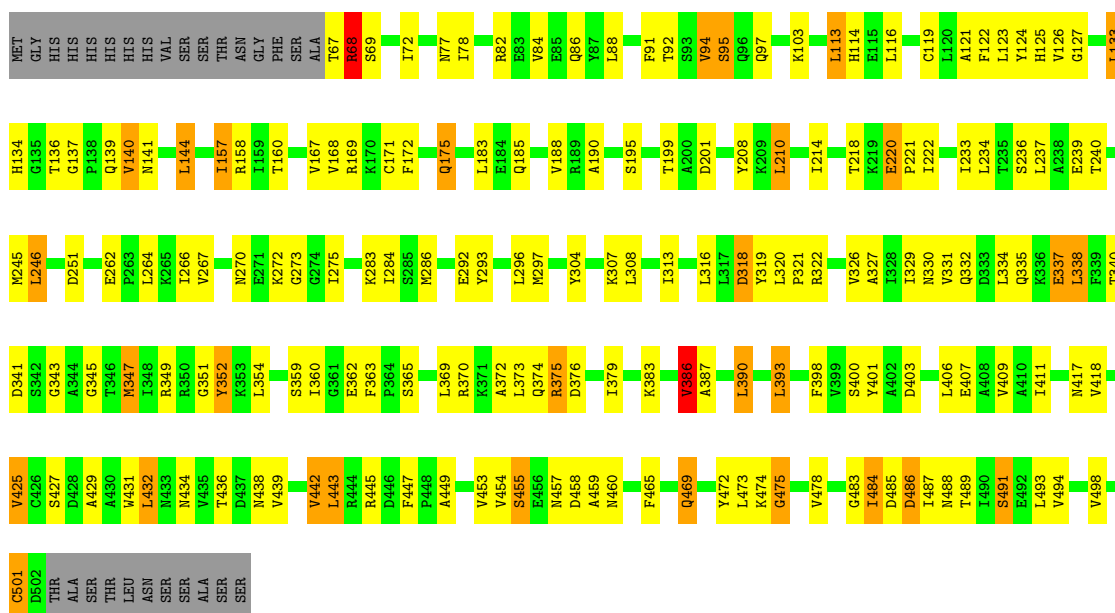
| Chain | Residue | Modelled | Actual | Comment | Reference |
|--------------|----------------|-----------------|---------------|----------------|------------------|
| G | 57 | HIS | - | expression tag | UNP Q01217 |
| H | 50 | MET | - | expression tag | UNP Q01217 |
| H | 51 | GLY | - | expression tag | UNP Q01217 |
| H | 52 | HIS | - | expression tag | UNP Q01217 |
| H | 53 | HIS | - | expression tag | UNP Q01217 |
| H | 54 | HIS | - | expression tag | UNP Q01217 |
| H | 55 | HIS | - | expression tag | UNP Q01217 |
| H | 56 | HIS | - | expression tag | UNP Q01217 |
| H | 57 | HIS | - | expression tag | UNP Q01217 |

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

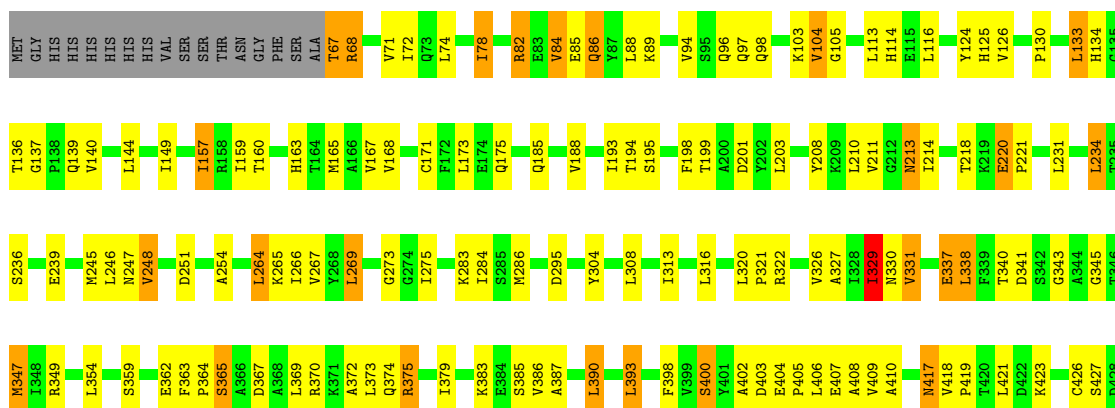
• Molecule 1: ACETYLGLUTAMATE KINASE

Chain A: 



• Molecule 1: ACETYLGLUTAMATE KINASE

Chain B: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 95.24Å 111.29Å 113.14Å 75.77° 89.29° 69.12° | Depositor |
| Resolution (Å) | 109.11 – 3.80 109.11 – 3.80 | Depositor EDS |
| % Data completeness (in resolution range) | 95.3 (109.11-3.80) 96.3 (109.11-3.80) | Depositor EDS |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.35 (at 3.77Å) | Xtrriage |
| Refinement program | REFMAC 5.6.0117 | Depositor |
| R, R_{free} | 0.197 , 0.236 0.200 , 0.245 | Depositor DCC |
| R_{free} test set | 2003 reflections (4.96%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 136.5 | Xtrriage |
| Anisotropy | 0.142 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 128.6 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 27248 | wwPDB-VP |
| Average B, all atoms (Å ²) | 127.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 i

5.1 Standard geometry i

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 | 1.12 | 3/3460 (0.1%) | 1.16 | 11/4686 (0.2%) |
| 1 | B | 1.12 | 8/3460 (0.2%) | 1.13 | 13/4686 (0.3%) |
| 1 | C | 1.03 | 2/3466 (0.1%) | 1.08 | 11/4693 (0.2%) |
| 1 | D | 1.03 | 1/3462 (0.0%) | 1.14 | 9/4689 (0.2%) |
| 1 | E | 1.21 | 2/3466 (0.1%) | 1.19 | 11/4693 (0.2%) |
| 1 | F | 1.11 | 3/3466 (0.1%) | 1.14 | 7/4693 (0.1%) |
| 1 | G | 0.98 | 0/3466 | 1.05 | 5/4693 (0.1%) |
| 1 | H | 1.07 | 6/3466 (0.2%) | 1.18 | 13/4693 (0.3%) |
| All | All | 1.09 | 25/27712 (0.1%) | 1.13 | 80/37526 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | E | 0 | 2 |
| 1 | G | 0 | 2 |
| 1 | H | 0 | 1 |
| All | All | 0 | 7 |

All (25) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 134 | HIS | CG-ND1 | -7.04 | 1.30 | 1.38 |
| 1 | H | 125 | HIS | CG-CD2 | 6.19 | 1.42 | 1.35 |
| 1 | C | 134 | HIS | CG-ND1 | -6.06 | 1.31 | 1.38 |
| 1 | B | 114 | HIS | CG-CD2 | 6.03 | 1.42 | 1.35 |
| 1 | H | 464 | HIS | CG-ND1 | -6.01 | 1.31 | 1.38 |
| 1 | B | 134 | HIS | CD2-NE2 | -5.98 | 1.31 | 1.37 |
| 1 | C | 134 | HIS | CA-C | -5.95 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | H | 399 | VAL | N-CA | -5.93 | 1.39 | 1.46 |
| 1 | H | 114 | HIS | CG-CD2 | 5.79 | 1.42 | 1.35 |
| 1 | F | 134 | HIS | CG-ND1 | -5.56 | 1.32 | 1.38 |
| 1 | B | 269 | LEU | CA-C | -5.48 | 1.46 | 1.52 |
| 1 | B | 134 | HIS | CG-ND1 | -5.44 | 1.32 | 1.38 |
| 1 | E | 391 | ARG | CA-CB | -5.39 | 1.45 | 1.53 |
| 1 | B | 163 | HIS | CG-CD2 | 5.33 | 1.41 | 1.35 |
| 1 | A | 114 | HIS | CG-CD2 | 5.31 | 1.41 | 1.35 |
| 1 | H | 134 | HIS | CG-CD2 | 5.21 | 1.41 | 1.35 |
| 1 | F | 125 | HIS | CG-ND1 | -5.18 | 1.32 | 1.38 |
| 1 | B | 163 | HIS | ND1-CE1 | 5.14 | 1.37 | 1.32 |
| 1 | A | 114 | HIS | CE1-NE2 | 5.13 | 1.37 | 1.32 |
| 1 | D | 239 | GLU | CD-OE1 | 5.11 | 1.35 | 1.25 |
| 1 | B | 114 | HIS | CE1-NE2 | 5.09 | 1.37 | 1.32 |
| 1 | H | 431 | TRP | NE1-CE2 | -5.02 | 1.31 | 1.37 |
| 1 | F | 431 | TRP | NE1-CE2 | -5.02 | 1.31 | 1.37 |
| 1 | A | 318 | ASP | C-O | -5.02 | 1.18 | 1.24 |
| 1 | B | 125 | HIS | ND1-CE1 | 5.01 | 1.37 | 1.32 |

All (80) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 352 | TYR | N-CA-C | 10.72 | 126.06 | 108.26 |
| 1 | A | 352 | TYR | N-CA-C | 10.31 | 125.37 | 108.26 |
| 1 | H | 351 | GLY | O-C-N | 9.42 | 131.72 | 122.77 |
| 1 | H | 352 | TYR | N-CA-C | -9.07 | 98.31 | 110.55 |
| 1 | F | 345 | GLY | N-CA-C | -8.94 | 103.45 | 111.95 |
| 1 | A | 352 | TYR | CB-CA-C | -8.16 | 97.57 | 110.14 |
| 1 | G | 345 | GLY | N-CA-C | -8.03 | 103.30 | 112.29 |
| 1 | B | 345 | GLY | N-CA-C | -7.60 | 103.78 | 112.29 |
| 1 | E | 345 | GLY | N-CA-C | -7.51 | 103.88 | 112.29 |
| 1 | E | 98 | GLN | N-CA-C | 7.46 | 120.49 | 110.35 |
| 1 | B | 442 | VAL | N-CA-C | -7.45 | 103.42 | 110.42 |
| 1 | C | 68 | ARG | CB-CA-C | -7.23 | 95.19 | 110.31 |
| 1 | A | 345 | GLY | N-CA-C | -7.13 | 104.31 | 112.29 |
| 1 | G | 137 | GLY | CA-C-N | 7.06 | 126.31 | 118.97 |
| 1 | G | 137 | GLY | C-N-CA | 7.06 | 126.31 | 118.97 |
| 1 | E | 99 | PHE | N-CA-C | 6.90 | 118.49 | 110.97 |
| 1 | C | 345 | GLY | N-CA-C | -6.87 | 104.59 | 112.29 |
| 1 | H | 435 | VAL | CB-CA-C | -6.72 | 103.36 | 111.97 |
| 1 | H | 324 | SER | N-CA-C | -6.49 | 100.70 | 110.24 |
| 1 | D | 272 | LYS | N-CA-CB | 6.44 | 119.41 | 110.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | D | 98 | GLN | N-CA-C | 6.29 | 118.42 | 110.24 |
| 1 | C | 351 | GLY | CA-C-N | -6.20 | 113.95 | 122.93 |
| 1 | C | 351 | GLY | C-N-CA | -6.20 | 113.95 | 122.93 |
| 1 | A | 386 | VAL | CB-CA-C | -6.15 | 103.96 | 112.02 |
| 1 | E | 352 | TYR | CB-CA-C | -6.12 | 100.71 | 110.14 |
| 1 | B | 137 | GLY | N-CA-C | 6.12 | 124.82 | 112.34 |
| 1 | B | 67 | THR | N-CA-C | -6.11 | 93.89 | 111.00 |
| 1 | E | 98 | GLN | CB-CA-C | -5.98 | 98.91 | 109.62 |
| 1 | E | 68 | ARG | CB-CA-C | -5.94 | 99.27 | 110.67 |
| 1 | F | 217 | VAL | CB-CA-C | -5.93 | 102.85 | 110.98 |
| 1 | A | 214 | ILE | CB-CA-C | -5.93 | 104.89 | 111.35 |
| 1 | C | 98 | GLN | N-CA-C | 5.87 | 118.33 | 110.35 |
| 1 | H | 399 | VAL | CB-CA-C | 5.81 | 119.64 | 110.81 |
| 1 | C | 351 | GLY | O-C-N | -5.74 | 117.32 | 122.77 |
| 1 | H | 345 | GLY | N-CA-C | -5.72 | 106.21 | 112.04 |
| 1 | A | 68 | ARG | CB-CA-C | -5.70 | 99.72 | 110.67 |
| 1 | H | 137 | GLY | CA-C-N | 5.69 | 124.88 | 118.97 |
| 1 | H | 137 | GLY | C-N-CA | 5.69 | 124.88 | 118.97 |
| 1 | B | 88 | LEU | N-CA-C | 5.65 | 117.44 | 111.28 |
| 1 | C | 137 | GLY | N-CA-C | 5.62 | 123.80 | 112.34 |
| 1 | D | 137 | GLY | CA-C-N | 5.61 | 124.80 | 118.97 |
| 1 | D | 137 | GLY | C-N-CA | 5.61 | 124.80 | 118.97 |
| 1 | A | 137 | GLY | N-CA-C | 5.61 | 123.78 | 112.34 |
| 1 | E | 137 | GLY | CA-C-N | 5.55 | 124.74 | 118.97 |
| 1 | E | 137 | GLY | C-N-CA | 5.55 | 124.74 | 118.97 |
| 1 | E | 214 | ILE | CB-CA-C | -5.51 | 105.34 | 111.35 |
| 1 | D | 98 | GLN | CB-CA-C | -5.51 | 99.89 | 109.64 |
| 1 | A | 447 | PHE | CA-C-N | -5.50 | 114.16 | 119.87 |
| 1 | A | 447 | PHE | C-N-CA | -5.50 | 114.16 | 119.87 |
| 1 | A | 442 | VAL | N-CA-C | -5.49 | 105.26 | 110.42 |
| 1 | F | 137 | GLY | CA-C-N | 5.47 | 124.66 | 118.97 |
| 1 | F | 137 | GLY | C-N-CA | 5.47 | 124.66 | 118.97 |
| 1 | F | 191 | ARG | CA-C-N | -5.47 | 114.13 | 119.76 |
| 1 | F | 191 | ARG | C-N-CA | -5.47 | 114.13 | 119.76 |
| 1 | B | 88 | LEU | CB-CA-C | -5.46 | 101.73 | 110.79 |
| 1 | H | 89 | LYS | CB-CG-CD | 5.41 | 123.73 | 111.30 |
| 1 | G | 442 | VAL | N-CA-C | -5.39 | 105.35 | 110.42 |
| 1 | D | 197 | VAL | N-CA-C | -5.38 | 106.45 | 111.45 |
| 1 | B | 331 | VAL | N-CA-CB | 5.35 | 117.16 | 110.47 |
| 1 | H | 90 | TYR | CB-CA-C | -5.33 | 101.78 | 110.85 |
| 1 | D | 68 | ARG | CB-CA-C | -5.32 | 100.45 | 110.67 |
| 1 | B | 104 | VAL | CB-CA-C | -5.31 | 103.20 | 110.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 465 | PHE | N-CA-C | -5.30 | 105.40 | 111.07 |
| 1 | C | 99 | PHE | N-CA-C | 5.27 | 116.89 | 111.03 |
| 1 | C | 197 | VAL | N-CA-C | -5.25 | 106.57 | 111.45 |
| 1 | B | 329 | ILE | CB-CA-C | -5.25 | 101.32 | 110.71 |
| 1 | C | 98 | GLN | CB-CA-C | -5.22 | 100.28 | 109.62 |
| 1 | H | 324 | SER | CB-CA-C | 5.18 | 117.62 | 109.84 |
| 1 | E | 248 | VAL | N-CA-C | 5.17 | 116.11 | 108.45 |
| 1 | C | 353 | LYS | N-CA-C | -5.16 | 102.01 | 109.59 |
| 1 | B | 159 | ILE | N-CA-C | -5.13 | 102.44 | 109.37 |
| 1 | H | 303 | LYS | N-CA-C | 5.12 | 116.71 | 110.41 |
| 1 | B | 484 | ILE | N-CA-C | 5.12 | 116.09 | 108.46 |
| 1 | B | 86 | GLN | N-CA-C | -5.09 | 105.42 | 110.97 |
| 1 | B | 486 | ASP | N-CA-C | -5.09 | 101.83 | 109.15 |
| 1 | D | 239 | GLU | CG-CD-OE2 | -5.08 | 106.72 | 118.40 |
| 1 | H | 140 | VAL | CB-CA-C | -5.06 | 105.49 | 111.97 |
| 1 | F | 90 | TYR | CB-CA-C | -5.05 | 102.26 | 110.85 |
| 1 | D | 180 | VAL | CB-CA-C | 5.03 | 118.41 | 111.97 |
| 1 | G | 439 | VAL | CB-CA-C | -5.01 | 105.48 | 112.04 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 94 | VAL | Peptide |
| 1 | B | 417 | ASN | Peptide |
| 1 | E | 94 | VAL | Peptide |
| 1 | E | 95 | SER | Peptide |
| 1 | G | 501 | CYS | Peptide |
| 1 | G | 95 | SER | Peptide |
| 1 | H | 351 | GLY | Peptide |

5.2 Too-close contacts [i](#)

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 | 3402 | 0 | 3429 | 145 | 0 |
| 1 | B | 3402 | 0 | 3429 | 154 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 3408 | 0 | 3440 | 145 | 0 |
| 1 | D | 3404 | 0 | 3429 | 149 | 0 |
| 1 | E | 3408 | 0 | 3440 | 204 | 0 |
| 1 | F | 3408 | 0 | 3440 | 190 | 0 |
| 1 | G | 3408 | 0 | 3440 | 146 | 1 |
| 1 | H | 3408 | 0 | 3440 | 186 | 0 |
| All | All | 27248 | 0 | 27487 | 1225 | 1 |

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 22.

All (1225) 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:E:354:LEU:HD11 | 1:E:438:ASN:ND2 | 1.54 | 1.22 |
| 1:B:327:ALA:HB2 | 1:B:347:MET:CE | 1.75 | 1.14 |
| 1:E:418:VAL:HG21 | 1:E:493:LEU:HD11 | 1.25 | 1.11 |
| 1:D:418:VAL:HG21 | 1:D:493:LEU:HD11 | 1.12 | 1.11 |
| 1:E:267:VAL:HG21 | 1:E:338:LEU:HD11 | 1.25 | 1.10 |
| 1:G:327:ALA:HB2 | 1:G:347:MET:CE | 1.82 | 1.10 |
| 1:F:327:ALA:HB2 | 1:F:347:MET:HE2 | 1.22 | 1.09 |
| 1:A:266:ILE:HD13 | 1:A:316:LEU:HD21 | 1.34 | 1.09 |
| 1:D:334:LEU:HD11 | 1:D:338:LEU:HD12 | 1.32 | 1.09 |
| 1:E:77:ASN:ND2 | 1:E:335:GLN:HE21 | 1.50 | 1.08 |
| 1:B:367:ASP:OD1 | 1:H:323:SER:HB2 | 1.53 | 1.08 |
| 1:D:334:LEU:CD1 | 1:D:338:LEU:HD12 | 1.84 | 1.07 |
| 1:C:327:ALA:HB2 | 1:C:347:MET:HE2 | 1.38 | 1.05 |
| 1:G:267:VAL:HG21 | 1:G:338:LEU:HD11 | 1.31 | 1.04 |
| 1:D:334:LEU:HD11 | 1:D:338:LEU:CD1 | 1.89 | 1.01 |
| 1:B:267:VAL:HG21 | 1:B:338:LEU:HD11 | 1.40 | 1.01 |
| 1:B:327:ALA:HB2 | 1:B:347:MET:HE3 | 1.39 | 1.01 |
| 1:E:267:VAL:CG2 | 1:E:338:LEU:HD11 | 1.89 | 1.01 |
| 1:G:327:ALA:HB2 | 1:G:347:MET:HE2 | 1.42 | 1.01 |
| 1:A:267:VAL:HG21 | 1:A:338:LEU:HD11 | 1.41 | 1.00 |
| 1:A:370:ARG:HG3 | 1:A:386:VAL:HG11 | 1.43 | 0.97 |
| 1:F:73:GLN:NE2 | 1:F:335:GLN:OE1 | 1.97 | 0.95 |
| 1:H:418:VAL:HG21 | 1:H:493:LEU:HD11 | 1.49 | 0.95 |
| 1:D:418:VAL:CG2 | 1:D:493:LEU:HD11 | 1.96 | 0.94 |
| 1:E:84:VAL:HG21 | 1:H:78:ILE:CG2 | 1.98 | 0.94 |
| 1:E:84:VAL:HG21 | 1:H:78:ILE:HG22 | 1.47 | 0.94 |
| 1:F:417:ASN:O | 1:F:418:VAL:HG22 | 1.69 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:418:VAL:HG21 | 1:C:493:LEU:HD11 | 1.52 | 0.92 |
| 1:F:273:GLY:O | 1:F:283:LYS:NZ | 2.01 | 0.92 |
| 1:E:78:ILE:HG22 | 1:H:84:VAL:HG21 | 1.52 | 0.92 |
| 1:F:379:ILE:HG21 | 1:F:386:VAL:HG23 | 1.51 | 0.91 |
| 1:G:418:VAL:HG21 | 1:G:493:LEU:HD11 | 1.52 | 0.91 |
| 1:D:418:VAL:HG21 | 1:D:493:LEU:CD1 | 1.99 | 0.91 |
| 1:E:77:ASN:HD22 | 1:E:335:GLN:HE21 | 1.02 | 0.91 |
| 1:G:313:ILE:HD13 | 1:G:326:VAL:HG11 | 1.53 | 0.91 |
| 1:H:70:THR:HG23 | 1:H:122:PHE:CD1 | 2.05 | 0.90 |
| 1:F:97:GLN:OE1 | 1:F:264:LEU:HD22 | 1.72 | 0.90 |
| 1:E:354:LEU:HD11 | 1:E:438:ASN:HD22 | 1.31 | 0.90 |
| 1:B:387:ALA:HB3 | 1:H:262:GLU:CD | 1.96 | 0.90 |
| 1:B:417:ASN:O | 1:B:418:VAL:HG22 | 1.72 | 0.90 |
| 1:E:354:LEU:CD1 | 1:E:438:ASN:ND2 | 2.36 | 0.89 |
| 1:C:146:ALA:HB1 | 1:F:323:SER:HB2 | 1.55 | 0.88 |
| 1:B:379:ILE:HG21 | 1:B:386:VAL:HG23 | 1.56 | 0.88 |
| 1:B:133:LEU:HD21 | 1:B:236:SER:HB3 | 1.55 | 0.88 |
| 1:C:136:THR:HG23 | 1:C:136:THR:O | 1.72 | 0.88 |
| 1:B:103:LYS:HE3 | 1:B:251:ASP:OD1 | 1.73 | 0.88 |
| 1:A:417:ASN:O | 1:A:418:VAL:HG22 | 1.73 | 0.88 |
| 1:C:327:ALA:HB2 | 1:C:347:MET:CE | 2.04 | 0.88 |
| 1:H:97:GLN:OE1 | 1:H:264:LEU:HD13 | 1.73 | 0.87 |
| 1:E:418:VAL:CG2 | 1:E:493:LEU:HD11 | 2.04 | 0.87 |
| 1:H:313:ILE:HD13 | 1:H:326:VAL:HG11 | 1.56 | 0.87 |
| 1:G:234:LEU:N | 1:G:234:LEU:HD12 | 1.89 | 0.86 |
| 1:E:77:ASN:ND2 | 1:E:335:GLN:NE2 | 2.22 | 0.86 |
| 1:H:370:ARG:HG3 | 1:H:386:VAL:HG11 | 1.58 | 0.86 |
| 1:E:85:GLU:HB3 | 1:E:432:LEU:HD22 | 1.55 | 0.86 |
| 1:B:327:ALA:CB | 1:B:347:MET:HE3 | 2.05 | 0.86 |
| 1:E:88:LEU:HD11 | 1:H:76:ASN:OD1 | 1.76 | 0.85 |
| 1:E:91:PHE:HB3 | 1:H:72:ILE:CD1 | 2.06 | 0.85 |
| 1:C:317:LEU:HD21 | 1:C:326:VAL:HG23 | 1.56 | 0.85 |
| 1:F:97:GLN:OE1 | 1:F:264:LEU:CD2 | 2.24 | 0.85 |
| 1:G:417:ASN:O | 1:G:418:VAL:HG22 | 1.77 | 0.85 |
| 1:H:103:LYS:HE3 | 1:H:251:ASP:OD1 | 1.75 | 0.85 |
| 1:E:91:PHE:HB3 | 1:H:72:ILE:HD13 | 1.59 | 0.84 |
| 1:F:288:ASN:HD22 | 1:F:438:ASN:ND2 | 1.74 | 0.84 |
| 1:H:86:GLN:OE1 | 1:H:340:THR:CB | 2.26 | 0.84 |
| 1:B:157:ILE:HD12 | 1:B:208:TYR:CE1 | 2.13 | 0.84 |
| 1:F:327:ALA:HB2 | 1:F:347:MET:CE | 2.06 | 0.83 |
| 1:B:213:ASN:HD22 | 1:B:213:ASN:C | 1.86 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:387:ALA:HB3 | 1:H:262:GLU:OE2 | 1.78 | 0.83 |
| 1:C:147:GLN:HG3 | 1:F:322:ARG:HB3 | 1.60 | 0.83 |
| 1:B:385:SER:HB3 | 1:H:262:GLU:OE1 | 1.78 | 0.83 |
| 1:E:144:LEU:HD21 | 1:E:164:THR:HG23 | 1.60 | 0.83 |
| 1:E:418:VAL:HG21 | 1:E:493:LEU:CD1 | 2.08 | 0.83 |
| 1:G:103:LYS:HE3 | 1:G:251:ASP:OD1 | 1.77 | 0.83 |
| 1:D:94:VAL:O | 1:D:94:VAL:HG12 | 1.77 | 0.83 |
| 1:F:349:ARG:NH2 | 1:F:433:ASN:O | 2.11 | 0.83 |
| 1:E:273:GLY:O | 1:E:283:LYS:NZ | 2.11 | 0.83 |
| 1:C:146:ALA:CB | 1:F:323:SER:HB2 | 2.08 | 0.82 |
| 1:E:327:ALA:HB2 | 1:E:347:MET:HE2 | 1.58 | 0.82 |
| 1:H:73:GLN:HG2 | 1:H:335:GLN:OE1 | 1.79 | 0.82 |
| 1:C:222:ILE:HD11 | 1:C:234:LEU:HD11 | 1.62 | 0.82 |
| 1:E:136:THR:HA | 1:E:139:GLN:HE22 | 1.45 | 0.82 |
| 1:C:103:LYS:HE3 | 1:C:251:ASP:OD1 | 1.80 | 0.82 |
| 1:B:213:ASN:HD22 | 1:B:214:ILE:N | 1.78 | 0.82 |
| 1:A:157:ILE:HD12 | 1:A:208:TYR:CE1 | 2.15 | 0.81 |
| 1:B:273:GLY:O | 1:B:283:LYS:NZ | 2.14 | 0.81 |
| 1:F:297:MET:HE3 | 1:F:307:LYS:HG2 | 1.62 | 0.81 |
| 1:G:267:VAL:CG2 | 1:G:338:LEU:HD11 | 2.10 | 0.81 |
| 1:B:327:ALA:HB2 | 1:B:347:MET:HE2 | 1.62 | 0.81 |
| 1:B:363:PHE:CG | 1:B:369:LEU:HD12 | 2.16 | 0.81 |
| 1:D:176:ASN:O | 1:D:180:VAL:HG23 | 1.81 | 0.81 |
| 1:G:234:LEU:N | 1:G:234:LEU:CD1 | 2.43 | 0.80 |
| 1:A:474:LYS:NZ | 1:A:501:CYS:SG | 2.54 | 0.80 |
| 1:C:68:ARG:O | 1:C:72:ILE:CD1 | 2.30 | 0.80 |
| 1:G:370:ARG:HG3 | 1:G:386:VAL:HG11 | 1.61 | 0.79 |
| 1:A:327:ALA:HB2 | 1:A:347:MET:HE2 | 1.62 | 0.79 |
| 1:A:487:ILE:HD11 | 1:D:491:SER:HA | 1.63 | 0.79 |
| 1:E:379:ILE:HD11 | 1:E:423:LYS:HZ2 | 1.45 | 0.79 |
| 1:D:327:ALA:HB2 | 1:D:347:MET:HE3 | 1.62 | 0.79 |
| 1:F:379:ILE:HD11 | 1:F:423:LYS:NZ | 1.98 | 0.79 |
| 1:G:169:ARG:HD2 | 1:G:245:MET:HE3 | 1.64 | 0.79 |
| 1:A:103:LYS:HE3 | 1:A:251:ASP:OD1 | 1.82 | 0.79 |
| 1:E:376:ASP:HB2 | 1:E:425:VAL:HG22 | 1.65 | 0.79 |
| 1:D:90:TYR:OH | 1:D:265:LYS:NZ | 2.15 | 0.79 |
| 1:C:68:ARG:O | 1:C:72:ILE:HD12 | 1.83 | 0.79 |
| 1:F:495:GLU:HG3 | 1:G:487:ILE:HD13 | 1.65 | 0.79 |
| 1:G:233:ILE:C | 1:G:234:LEU:HD12 | 2.07 | 0.78 |
| 1:E:82:ARG:HD2 | 1:E:432:LEU:O | 1.83 | 0.78 |
| 1:F:103:LYS:HE3 | 1:F:251:ASP:OD1 | 1.84 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:103:LYS:HE3 | 1:D:251:ASP:OD1 | 1.83 | 0.78 |
| 1:D:193:ILE:HB | 1:D:234:LEU:HD13 | 1.65 | 0.78 |
| 1:E:370:ARG:HG3 | 1:E:386:VAL:HG11 | 1.66 | 0.78 |
| 1:F:120:LEU:HA | 1:F:123:LEU:HD12 | 1.67 | 0.77 |
| 1:H:342:SER:O | 1:H:344:ALA:N | 2.17 | 0.77 |
| 1:F:157:ILE:HD12 | 1:F:208:TYR:CE1 | 2.19 | 0.77 |
| 1:E:136:THR:HA | 1:E:139:GLN:NE2 | 2.00 | 0.76 |
| 1:C:379:ILE:HG21 | 1:C:386:VAL:HG23 | 1.66 | 0.76 |
| 1:H:197:VAL:HG21 | 1:H:234:LEU:HD21 | 1.66 | 0.76 |
| 1:A:313:ILE:HD13 | 1:A:326:VAL:HG11 | 1.68 | 0.76 |
| 1:B:474:LYS:NZ | 1:B:501:CYS:SG | 2.57 | 0.76 |
| 1:E:487:ILE:HD11 | 1:H:491:SER:HB3 | 1.66 | 0.76 |
| 1:F:379:ILE:HD11 | 1:F:423:LYS:HZ2 | 1.51 | 0.76 |
| 1:A:417:ASN:O | 1:A:418:VAL:CG2 | 2.34 | 0.76 |
| 1:F:327:ALA:CB | 1:F:347:MET:HE2 | 2.09 | 0.75 |
| 1:F:491:SER:O | 1:G:487:ILE:HD11 | 1.86 | 0.75 |
| 1:G:417:ASN:O | 1:G:418:VAL:CG2 | 2.34 | 0.75 |
| 1:D:203:LEU:HD22 | 1:D:208:TYR:CE2 | 2.21 | 0.75 |
| 1:H:133:LEU:HD21 | 1:H:236:SER:HB3 | 1.66 | 0.75 |
| 1:G:379:ILE:HD11 | 1:G:423:LYS:HZ2 | 1.52 | 0.75 |
| 1:A:97:GLN:NE2 | 1:A:262:GLU:O | 2.20 | 0.75 |
| 1:D:327:ALA:HB2 | 1:D:347:MET:CE | 2.15 | 0.75 |
| 1:D:379:ILE:HG21 | 1:D:386:VAL:HG23 | 1.68 | 0.75 |
| 1:B:370:ARG:NH2 | 1:H:323:SER:OG | 2.19 | 0.74 |
| 1:F:244:GLN:HE21 | 1:F:245:MET:N | 1.85 | 0.74 |
| 1:G:369:LEU:O | 1:G:369:LEU:HD23 | 1.88 | 0.74 |
| 1:D:342:SER:O | 1:D:344:ALA:N | 2.20 | 0.74 |
| 1:F:140:VAL:CG1 | 1:F:141:ASN:N | 2.50 | 0.74 |
| 1:A:240:THR:CG2 | 1:A:246:LEU:HD11 | 2.18 | 0.74 |
| 1:G:169:ARG:CD | 1:G:245:MET:HE3 | 2.18 | 0.74 |
| 1:C:267:VAL:HG21 | 1:C:338:LEU:HD11 | 1.67 | 0.74 |
| 1:H:140:VAL:CG1 | 1:H:141:ASN:N | 2.50 | 0.74 |
| 1:C:157:ILE:HD12 | 1:C:208:TYR:CE1 | 2.23 | 0.73 |
| 1:F:386:VAL:CG1 | 1:F:390:LEU:HD22 | 2.17 | 0.73 |
| 1:H:327:ALA:HB2 | 1:H:347:MET:HE3 | 1.70 | 0.73 |
| 1:A:273:GLY:O | 1:A:283:LYS:NZ | 2.19 | 0.73 |
| 1:F:119:CYS:SG | 1:F:335:GLN:HB3 | 2.27 | 0.73 |
| 1:F:487:ILE:HD11 | 1:G:491:SER:HA | 1.70 | 0.73 |
| 1:H:136:THR:HG23 | 1:H:136:THR:O | 1.87 | 0.73 |
| 1:H:363:PHE:CG | 1:H:369:LEU:HD12 | 2.24 | 0.73 |
| 1:H:313:ILE:CD1 | 1:H:326:VAL:HG11 | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:490:ILE:O | 1:C:494:VAL:HG23 | 1.88 | 0.72 |
| 1:D:417:ASN:O | 1:D:418:VAL:HG22 | 1.88 | 0.72 |
| 1:E:103:LYS:HE3 | 1:E:251:ASP:OD1 | 1.89 | 0.72 |
| 1:G:267:VAL:HG21 | 1:G:338:LEU:CD1 | 2.15 | 0.72 |
| 1:D:256:GLU:O | 1:D:260:VAL:HG12 | 1.89 | 0.72 |
| 1:F:133:LEU:HD21 | 1:F:236:SER:HB3 | 1.71 | 0.72 |
| 1:D:120:LEU:HD23 | 1:D:123:LEU:HD12 | 1.71 | 0.72 |
| 1:F:297:MET:HE3 | 1:F:307:LYS:CG | 2.20 | 0.72 |
| 1:A:491:SER:HA | 1:D:487:ILE:HD11 | 1.70 | 0.72 |
| 1:G:421:LEU:HD22 | 1:G:443:LEU:HD21 | 1.71 | 0.72 |
| 1:A:270:ASN:ND2 | 1:A:272:LYS:HB2 | 2.04 | 0.71 |
| 1:C:90:TYR:CE2 | 1:C:264:LEU:HD12 | 2.25 | 0.71 |
| 1:F:417:ASN:O | 1:F:418:VAL:CG2 | 2.39 | 0.71 |
| 1:C:133:LEU:HD21 | 1:C:236:SER:HB3 | 1.71 | 0.71 |
| 1:A:418:VAL:HG21 | 1:A:493:LEU:HD11 | 1.70 | 0.71 |
| 1:E:94:VAL:HG12 | 1:E:94:VAL:O | 1.91 | 0.71 |
| 1:E:213:ASN:HD22 | 1:E:214:ILE:N | 1.88 | 0.71 |
| 1:F:140:VAL:HG12 | 1:F:141:ASN:N | 2.05 | 0.71 |
| 1:H:180:VAL:HG13 | 1:H:190:ALA:HB3 | 1.71 | 0.71 |
| 1:H:140:VAL:HG12 | 1:H:141:ASN:N | 2.04 | 0.71 |
| 1:D:474:LYS:NZ | 1:D:501:CYS:SG | 2.63 | 0.70 |
| 1:H:70:THR:HG23 | 1:H:122:PHE:HD1 | 1.54 | 0.70 |
| 1:B:267:VAL:HG21 | 1:B:338:LEU:CD1 | 2.20 | 0.70 |
| 1:B:327:ALA:CB | 1:B:347:MET:CE | 2.62 | 0.70 |
| 1:B:369:LEU:HD23 | 1:B:373:LEU:HD11 | 1.73 | 0.70 |
| 1:H:157:ILE:HD12 | 1:H:208:TYR:CE1 | 2.25 | 0.70 |
| 1:B:418:VAL:HG21 | 1:B:493:LEU:HD11 | 1.74 | 0.70 |
| 1:E:327:ALA:CB | 1:E:347:MET:HE2 | 2.21 | 0.70 |
| 1:A:266:ILE:HD13 | 1:A:316:LEU:CD2 | 2.19 | 0.70 |
| 1:G:82:ARG:O | 1:G:86:GLN:HG2 | 1.92 | 0.70 |
| 1:H:122:PHE:O | 1:H:126:VAL:HG22 | 1.91 | 0.70 |
| 1:E:222:ILE:HD11 | 1:E:234:LEU:HD11 | 1.73 | 0.69 |
| 1:F:354:LEU:HD21 | 1:F:439:VAL:CG2 | 2.22 | 0.69 |
| 1:C:163:HIS:NE2 | 1:F:404:GLU:OE2 | 2.24 | 0.69 |
| 1:A:369:LEU:CD2 | 1:A:373:LEU:HD11 | 2.22 | 0.69 |
| 1:E:74:LEU:CD2 | 1:H:71:VAL:HG13 | 2.23 | 0.69 |
| 1:E:213:ASN:HD22 | 1:E:213:ASN:C | 1.98 | 0.69 |
| 1:G:379:ILE:HG21 | 1:G:386:VAL:HG23 | 1.74 | 0.69 |
| 1:B:417:ASN:O | 1:B:418:VAL:CG2 | 2.39 | 0.69 |
| 1:H:323:SER:O | 1:H:324:SER:C | 2.35 | 0.69 |
| 1:A:266:ILE:CD1 | 1:A:316:LEU:HD21 | 2.19 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:417:ASN:O | 1:D:418:VAL:CG2 | 2.41 | 0.69 |
| 1:A:157:ILE:HD12 | 1:A:208:TYR:CZ | 2.27 | 0.69 |
| 1:D:323:SER:O | 1:D:324:SER:C | 2.36 | 0.69 |
| 1:H:267:VAL:HG21 | 1:H:338:LEU:HD21 | 1.75 | 0.69 |
| 1:A:363:PHE:CD1 | 1:A:369:LEU:HD12 | 2.28 | 0.69 |
| 1:F:286:MET:SD | 1:F:434:ASN:ND2 | 2.65 | 0.68 |
| 1:F:354:LEU:HD21 | 1:F:439:VAL:HG23 | 1.75 | 0.68 |
| 1:A:449:ALA:HB1 | 1:A:484:ILE:HG22 | 1.74 | 0.68 |
| 1:G:327:ALA:CB | 1:G:347:MET:CE | 2.67 | 0.68 |
| 1:H:99:PHE:CZ | 1:H:338:LEU:HD12 | 2.28 | 0.68 |
| 1:F:144:LEU:HD22 | 1:F:167:VAL:HG11 | 1.75 | 0.68 |
| 1:G:169:ARG:HD2 | 1:G:245:MET:CE | 2.23 | 0.68 |
| 1:E:84:VAL:HG11 | 1:H:78:ILE:O | 1.94 | 0.68 |
| 1:D:379:ILE:HG21 | 1:D:386:VAL:CG2 | 2.23 | 0.68 |
| 1:E:376:ASP:HB2 | 1:E:425:VAL:CG2 | 2.24 | 0.68 |
| 1:F:418:VAL:HG11 | 1:F:493:LEU:HD11 | 1.76 | 0.68 |
| 1:G:313:ILE:CD1 | 1:G:326:VAL:HG11 | 2.24 | 0.68 |
| 1:B:385:SER:CB | 1:H:262:GLU:OE1 | 2.42 | 0.67 |
| 1:B:144:LEU:HD22 | 1:B:167:VAL:HG11 | 1.75 | 0.67 |
| 1:B:193:ILE:HB | 1:B:234:LEU:HD22 | 1.75 | 0.67 |
| 1:B:369:LEU:CD2 | 1:B:373:LEU:HD11 | 2.24 | 0.67 |
| 1:G:157:ILE:HD12 | 1:G:208:TYR:CE1 | 2.29 | 0.67 |
| 1:E:157:ILE:HD12 | 1:E:208:TYR:CE1 | 2.29 | 0.67 |
| 1:A:84:VAL:HG21 | 1:D:78:ILE:HG21 | 1.77 | 0.67 |
| 1:C:144:LEU:HD22 | 1:C:167:VAL:HG11 | 1.75 | 0.67 |
| 1:D:82:ARG:O | 1:D:86:GLN:HG2 | 1.94 | 0.67 |
| 1:H:363:PHE:CD1 | 1:H:369:LEU:HD12 | 2.30 | 0.67 |
| 1:A:327:ALA:CB | 1:A:347:MET:HE2 | 2.24 | 0.67 |
| 1:D:473:LEU:HD13 | 1:D:478:VAL:HG22 | 1.77 | 0.67 |
| 1:E:77:ASN:HD22 | 1:E:335:GLN:NE2 | 1.81 | 0.67 |
| 1:E:369:LEU:CD2 | 1:E:373:LEU:HD11 | 2.25 | 0.67 |
| 1:E:78:ILE:CG2 | 1:H:84:VAL:HG21 | 2.23 | 0.67 |
| 1:H:86:GLN:OE1 | 1:H:340:THR:HB | 1.94 | 0.67 |
| 1:H:417:ASN:O | 1:H:418:VAL:CG2 | 2.43 | 0.67 |
| 1:B:213:ASN:C | 1:B:213:ASN:ND2 | 2.53 | 0.66 |
| 1:F:386:VAL:HG12 | 1:F:390:LEU:HD22 | 1.77 | 0.66 |
| 1:G:473:LEU:HD13 | 1:G:478:VAL:HG22 | 1.78 | 0.66 |
| 1:E:417:ASN:O | 1:E:418:VAL:HG22 | 1.94 | 0.66 |
| 1:C:370:ARG:HG3 | 1:C:386:VAL:HG11 | 1.76 | 0.66 |
| 1:F:133:LEU:C | 1:F:133:LEU:HD22 | 2.20 | 0.66 |
| 1:A:267:VAL:CG2 | 1:A:338:LEU:HD11 | 2.21 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:136:THR:HG23 | 1:D:136:THR:O | 1.95 | 0.66 |
| 1:E:88:LEU:CD1 | 1:H:76:ASN:OD1 | 2.42 | 0.66 |
| 1:H:70:THR:CG2 | 1:H:122:PHE:CD1 | 2.77 | 0.66 |
| 1:A:82:ARG:O | 1:A:86:GLN:HG2 | 1.94 | 0.66 |
| 1:D:334:LEU:HD11 | 1:D:338:LEU:HD11 | 1.78 | 0.66 |
| 1:G:136:THR:O | 1:G:136:THR:HG23 | 1.96 | 0.66 |
| 1:A:425:VAL:HG12 | 1:A:425:VAL:O | 1.95 | 0.66 |
| 1:C:418:VAL:HG21 | 1:C:493:LEU:CD1 | 2.25 | 0.66 |
| 1:E:82:ARG:O | 1:E:86:GLN:HG2 | 1.95 | 0.66 |
| 1:E:379:ILE:HG21 | 1:E:386:VAL:HG23 | 1.76 | 0.66 |
| 1:E:457:ASN:ND2 | 1:E:457:ASN:H | 1.94 | 0.65 |
| 1:G:94:VAL:HG12 | 1:G:94:VAL:O | 1.95 | 0.65 |
| 1:G:70:THR:CG2 | 1:G:126:VAL:HG12 | 2.27 | 0.65 |
| 1:E:180:VAL:HG13 | 1:E:190:ALA:HB3 | 1.78 | 0.65 |
| 1:E:379:ILE:HD11 | 1:E:423:LYS:NZ | 2.12 | 0.65 |
| 1:F:99:PHE:HE2 | 1:F:123:LEU:HD22 | 1.60 | 0.65 |
| 1:G:124:TYR:CG | 1:G:188:VAL:HG13 | 2.32 | 0.65 |
| 1:H:393:LEU:HD22 | 1:H:398:PHE:CD1 | 2.32 | 0.65 |
| 1:E:484:ILE:HD11 | 1:E:493:LEU:HD22 | 1.80 | 0.64 |
| 1:H:176:ASN:ND2 | 1:H:233:ILE:HG22 | 2.12 | 0.64 |
| 1:C:82:ARG:O | 1:C:86:GLN:HG2 | 1.96 | 0.64 |
| 1:F:94:VAL:CG1 | 1:F:96:GLN:NE2 | 2.60 | 0.64 |
| 1:E:81:LYS:HG3 | 1:H:79:SER:O | 1.98 | 0.64 |
| 1:A:386:VAL:HG12 | 1:A:387:ALA:N | 2.11 | 0.64 |
| 1:B:354:LEU:HD21 | 1:B:439:VAL:HG23 | 1.79 | 0.64 |
| 1:C:469:GLN:HE21 | 1:C:483:GLY:H | 1.44 | 0.64 |
| 1:D:488:ASN:HD22 | 1:D:489:THR:N | 1.96 | 0.64 |
| 1:E:88:LEU:HD22 | 1:E:92:THR:HG23 | 1.80 | 0.64 |
| 1:F:136:THR:HG23 | 1:F:136:THR:O | 1.97 | 0.64 |
| 1:G:424:PHE:HE1 | 1:G:439:VAL:HG11 | 1.63 | 0.64 |
| 1:C:266:ILE:HD13 | 1:C:316:LEU:HD21 | 1.80 | 0.64 |
| 1:A:124:TYR:CD2 | 1:A:188:VAL:HG22 | 2.32 | 0.63 |
| 1:B:82:ARG:O | 1:B:86:GLN:HG2 | 1.98 | 0.63 |
| 1:E:304:TYR:CE1 | 1:E:308:LEU:HD13 | 2.33 | 0.63 |
| 1:A:133:LEU:HD11 | 1:A:236:SER:HB3 | 1.79 | 0.63 |
| 1:E:474:LYS:NZ | 1:E:501:CYS:SG | 2.67 | 0.63 |
| 1:F:203:LEU:C | 1:F:203:LEU:HD13 | 2.24 | 0.63 |
| 1:D:252:VAL:HG22 | 1:D:312:GLU:CD | 2.23 | 0.63 |
| 1:F:449:ALA:HB1 | 1:F:484:ILE:HG22 | 1.81 | 0.63 |
| 1:E:136:THR:HG23 | 1:E:136:THR:O | 1.99 | 0.62 |
| 1:F:487:ILE:HD11 | 1:G:491:SER:CA | 2.28 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:88:LEU:HD22 | 1:E:92:THR:CG2 | 2.29 | 0.62 |
| 1:F:340:THR:HG23 | 1:F:343:GLY:H | 1.63 | 0.62 |
| 1:H:474:LYS:NZ | 1:H:501:CYS:SG | 2.69 | 0.62 |
| 1:C:473:LEU:HD13 | 1:C:478:VAL:HG22 | 1.81 | 0.62 |
| 1:H:386:VAL:CG1 | 1:H:390:LEU:HD22 | 2.30 | 0.62 |
| 1:C:90:TYR:HE2 | 1:C:264:LEU:HD12 | 1.63 | 0.62 |
| 1:E:68:ARG:O | 1:E:72:ILE:HD12 | 2.00 | 0.62 |
| 1:C:68:ARG:O | 1:C:72:ILE:HD13 | 1.99 | 0.61 |
| 1:C:473:LEU:HD13 | 1:C:478:VAL:CG2 | 2.30 | 0.61 |
| 1:G:266:ILE:HD13 | 1:G:316:LEU:HD21 | 1.81 | 0.61 |
| 1:B:68:ARG:O | 1:B:72:ILE:HD12 | 2.00 | 0.61 |
| 1:B:369:LEU:HD23 | 1:B:373:LEU:CD1 | 2.30 | 0.61 |
| 1:B:393:LEU:HD22 | 1:B:398:PHE:CD1 | 2.36 | 0.61 |
| 1:F:222:ILE:HD11 | 1:F:234:LEU:HD11 | 1.80 | 0.61 |
| 1:F:418:VAL:HG21 | 1:F:493:LEU:HD11 | 1.83 | 0.61 |
| 1:H:417:ASN:O | 1:H:418:VAL:HG22 | 2.00 | 0.61 |
| 1:C:474:LYS:NZ | 1:C:501:CYS:SG | 2.73 | 0.61 |
| 1:A:304:TYR:CE1 | 1:A:308:LEU:HD13 | 2.35 | 0.61 |
| 1:D:133:LEU:HD11 | 1:D:236:SER:HB3 | 1.82 | 0.61 |
| 1:F:393:LEU:HD22 | 1:F:398:PHE:CD1 | 2.35 | 0.61 |
| 1:A:240:THR:HG22 | 1:A:246:LEU:HD11 | 1.81 | 0.61 |
| 1:B:406:LEU:HD12 | 1:B:409:VAL:CG2 | 2.30 | 0.61 |
| 1:D:449:ALA:HB1 | 1:D:484:ILE:HG22 | 1.83 | 0.61 |
| 1:G:140:VAL:CG1 | 1:G:141:ASN:N | 2.63 | 0.61 |
| 1:G:173:LEU:N | 1:G:173:LEU:HD23 | 2.15 | 0.61 |
| 1:G:473:LEU:HD13 | 1:G:478:VAL:CG2 | 2.30 | 0.61 |
| 1:H:472:TYR:CD2 | 1:H:494:VAL:HG13 | 2.36 | 0.61 |
| 1:F:193:ILE:CG2 | 1:F:234:LEU:HD22 | 2.31 | 0.60 |
| 1:H:297:MET:HE3 | 1:H:307:LYS:HD3 | 1.81 | 0.60 |
| 1:A:122:PHE:O | 1:A:126:VAL:HG22 | 2.01 | 0.60 |
| 1:B:313:ILE:HD13 | 1:B:326:VAL:HG11 | 1.83 | 0.60 |
| 1:A:136:THR:HG23 | 1:A:136:THR:O | 2.01 | 0.60 |
| 1:C:116:LEU:HD11 | 1:C:120:LEU:HD11 | 1.83 | 0.60 |
| 1:D:369:LEU:HD23 | 1:D:369:LEU:O | 2.01 | 0.60 |
| 1:H:94:VAL:HG12 | 1:H:96:GLN:NE2 | 2.16 | 0.60 |
| 1:B:157:ILE:HD12 | 1:B:208:TYR:CZ | 2.35 | 0.60 |
| 1:G:240:THR:CG2 | 1:G:246:LEU:HD11 | 2.32 | 0.60 |
| 1:F:160:THR:O | 1:F:160:THR:HG22 | 2.01 | 0.60 |
| 1:B:363:PHE:CD1 | 1:B:369:LEU:CD1 | 2.85 | 0.60 |
| 1:H:87:TYR:OH | 1:H:335:GLN:O | 2.19 | 0.60 |
| 1:E:124:TYR:CD2 | 1:E:188:VAL:HG22 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:442:VAL:HG12 | 1:E:443:LEU:N | 2.16 | 0.60 |
| 1:G:222:ILE:HD11 | 1:G:234:LEU:HD21 | 1.83 | 0.60 |
| 1:A:113:LEU:HD23 | 1:A:113:LEU:O | 2.01 | 0.60 |
| 1:A:297:MET:HE3 | 1:A:307:LYS:HG2 | 1.83 | 0.60 |
| 1:B:136:THR:O | 1:B:136:THR:HG23 | 2.01 | 0.60 |
| 1:C:240:THR:CG2 | 1:C:246:LEU:HD11 | 2.31 | 0.60 |
| 1:E:393:LEU:HD11 | 1:E:411:ILE:HD13 | 1.84 | 0.60 |
| 1:A:487:ILE:HD11 | 1:D:491:SER:CA | 2.32 | 0.60 |
| 1:B:387:ALA:HB3 | 1:H:262:GLU:OE1 | 2.00 | 0.60 |
| 1:D:286:MET:HE2 | 1:D:347:MET:CG | 2.32 | 0.60 |
| 1:F:94:VAL:HG11 | 1:F:96:GLN:NE2 | 2.17 | 0.60 |
| 1:H:369:LEU:CD2 | 1:H:373:LEU:HD11 | 2.31 | 0.60 |
| 1:E:304:TYR:CZ | 1:E:308:LEU:HD13 | 2.37 | 0.60 |
| 1:E:407:GLU:OE2 | 1:E:429:ALA:HB3 | 2.00 | 0.59 |
| 1:C:267:VAL:HG21 | 1:C:338:LEU:CD1 | 2.32 | 0.59 |
| 1:E:74:LEU:HD21 | 1:H:71:VAL:HG13 | 1.84 | 0.59 |
| 1:F:370:ARG:HG3 | 1:F:386:VAL:HG11 | 1.84 | 0.59 |
| 1:C:363:PHE:CD1 | 1:C:369:LEU:HD12 | 2.36 | 0.59 |
| 1:D:479:LEU:HD12 | 1:D:480:PHE:H | 1.67 | 0.59 |
| 1:A:262:GLU:HA | 1:A:320:LEU:HD22 | 1.84 | 0.59 |
| 1:E:354:LEU:CD1 | 1:E:438:ASN:HD21 | 2.12 | 0.59 |
| 1:H:86:GLN:OE1 | 1:H:340:THR:HA | 2.02 | 0.59 |
| 1:G:379:ILE:HD11 | 1:G:423:LYS:NZ | 2.17 | 0.59 |
| 1:G:486:ASP:CB | 1:G:489:THR:HG23 | 2.33 | 0.59 |
| 1:G:273:GLY:O | 1:G:283:LYS:NZ | 2.27 | 0.59 |
| 1:A:407:GLU:OE2 | 1:A:429:ALA:HB3 | 2.03 | 0.59 |
| 1:E:77:ASN:HD21 | 1:E:335:GLN:HG3 | 1.68 | 0.58 |
| 1:G:474:LYS:NZ | 1:G:501:CYS:SG | 2.75 | 0.58 |
| 1:F:133:LEU:C | 1:F:133:LEU:CD2 | 2.75 | 0.58 |
| 1:G:386:VAL:CG1 | 1:G:390:LEU:HD22 | 2.34 | 0.58 |
| 1:H:258:ALA:HB3 | 1:H:316:LEU:HD11 | 1.85 | 0.58 |
| 1:C:417:ASN:O | 1:C:418:VAL:CG2 | 2.51 | 0.58 |
| 1:D:370:ARG:HG3 | 1:D:386:VAL:HG11 | 1.86 | 0.58 |
| 1:E:197:VAL:HG21 | 1:E:234:LEU:HD13 | 1.86 | 0.58 |
| 1:E:418:VAL:HG11 | 1:E:493:LEU:HD21 | 1.84 | 0.58 |
| 1:F:76:ASN:OD1 | 1:G:88:LEU:HD11 | 2.04 | 0.58 |
| 1:F:474:LYS:NZ | 1:F:501:CYS:SG | 2.72 | 0.58 |
| 1:G:421:LEU:HD22 | 1:G:443:LEU:CD2 | 2.33 | 0.58 |
| 1:H:140:VAL:HG11 | 1:H:158:ARG:NH2 | 2.18 | 0.58 |
| 1:C:457:ASN:H | 1:C:457:ASN:ND2 | 1.99 | 0.58 |
| 1:F:327:ALA:CB | 1:F:347:MET:CE | 2.76 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:489:THR:O | 1:H:493:LEU:HD13 | 2.03 | 0.58 |
| 1:E:84:VAL:CG2 | 1:H:78:ILE:HG22 | 2.30 | 0.58 |
| 1:C:486:ASP:CB | 1:C:489:THR:HG23 | 2.34 | 0.58 |
| 1:D:479:LEU:HD12 | 1:D:480:PHE:N | 2.19 | 0.58 |
| 1:H:266:ILE:HD13 | 1:H:316:LEU:HD21 | 1.86 | 0.58 |
| 1:B:74:LEU:CD2 | 1:C:71:VAL:HG13 | 2.34 | 0.57 |
| 1:G:140:VAL:HG11 | 1:G:158:ARG:NH2 | 2.19 | 0.57 |
| 1:C:154:ILE:HD12 | 1:F:371:LYS:NZ | 2.19 | 0.57 |
| 1:C:393:LEU:HD22 | 1:C:398:PHE:CD1 | 2.40 | 0.57 |
| 1:B:379:ILE:HG21 | 1:B:386:VAL:CG2 | 2.31 | 0.57 |
| 1:E:363:PHE:CD1 | 1:E:369:LEU:HD12 | 2.39 | 0.57 |
| 1:H:379:ILE:HG21 | 1:H:386:VAL:HG23 | 1.86 | 0.57 |
| 1:D:193:ILE:HG22 | 1:D:193:ILE:O | 2.03 | 0.57 |
| 1:E:417:ASN:O | 1:E:418:VAL:CG2 | 2.53 | 0.57 |
| 1:F:304:TYR:CZ | 1:F:308:LEU:HD13 | 2.39 | 0.57 |
| 1:A:313:ILE:CD1 | 1:A:326:VAL:HG11 | 2.34 | 0.57 |
| 1:D:473:LEU:HD13 | 1:D:478:VAL:CG2 | 2.34 | 0.57 |
| 1:E:363:PHE:CG | 1:E:369:LEU:HD12 | 2.40 | 0.57 |
| 1:G:160:THR:HG22 | 1:G:160:THR:O | 2.04 | 0.57 |
| 1:B:354:LEU:HD22 | 1:B:439:VAL:HG22 | 1.87 | 0.57 |
| 1:B:363:PHE:CD1 | 1:B:369:LEU:HD12 | 2.39 | 0.57 |
| 1:H:124:TYR:CG | 1:H:188:VAL:HG13 | 2.39 | 0.57 |
| 1:E:136:THR:CA | 1:E:139:GLN:NE2 | 2.68 | 0.57 |
| 1:E:457:ASN:ND2 | 1:E:457:ASN:N | 2.51 | 0.57 |
| 1:D:334:LEU:HD12 | 1:D:338:LEU:HD12 | 1.80 | 0.57 |
| 1:D:379:ILE:HD11 | 1:D:423:LYS:NZ | 2.19 | 0.57 |
| 1:E:160:THR:HG22 | 1:E:160:THR:O | 2.03 | 0.56 |
| 1:F:473:LEU:HD12 | 1:F:474:LYS:O | 2.05 | 0.56 |
| 1:D:70:THR:CG2 | 1:D:126:VAL:HG12 | 2.34 | 0.56 |
| 1:D:299:GLN:HB2 | 1:D:302:VAL:HG23 | 1.87 | 0.56 |
| 1:E:74:LEU:HD22 | 1:H:71:VAL:HG13 | 1.88 | 0.56 |
| 1:F:408:ALA:HB1 | 1:F:426:CYS:SG | 2.44 | 0.56 |
| 1:G:140:VAL:HG12 | 1:G:141:ASN:N | 2.21 | 0.56 |
| 1:H:407:GLU:OE2 | 1:H:429:ALA:HB3 | 2.04 | 0.56 |
| 1:B:364:PRO:HB3 | 1:H:407:GLU:OE2 | 2.06 | 0.56 |
| 1:F:94:VAL:HG12 | 1:F:96:GLN:CD | 2.31 | 0.56 |
| 1:A:469:GLN:HE21 | 1:A:483:GLY:H | 1.53 | 0.56 |
| 1:B:133:LEU:HD12 | 1:B:254:ALA:HA | 1.88 | 0.56 |
| 1:C:154:ILE:HD12 | 1:F:371:LYS:HZ3 | 1.70 | 0.56 |
| 1:D:329:ILE:HD12 | 1:D:337:GLU:CG | 2.34 | 0.56 |
| 1:H:198:PHE:CD1 | 1:H:214:ILE:HD13 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:327:ALA:CB | 1:C:347:MET:CE | 2.80 | 0.56 |
| 1:C:363:PHE:CG | 1:C:369:LEU:HD12 | 2.41 | 0.56 |
| 1:C:449:ALA:HB1 | 1:C:484:ILE:HG22 | 1.86 | 0.56 |
| 1:F:260:VAL:HG12 | 1:F:261:PHE:CD1 | 2.41 | 0.56 |
| 1:E:213:ASN:C | 1:E:213:ASN:ND2 | 2.61 | 0.56 |
| 1:B:97:GLN:OE1 | 1:B:264:LEU:HD23 | 2.06 | 0.56 |
| 1:E:449:ALA:HB1 | 1:E:484:ILE:HG22 | 1.87 | 0.56 |
| 1:H:124:TYR:CD1 | 1:H:188:VAL:HG13 | 2.40 | 0.56 |
| 1:A:222:ILE:HD11 | 1:A:234:LEU:HD21 | 1.88 | 0.55 |
| 1:B:340:THR:HG23 | 1:B:343:GLY:H | 1.71 | 0.55 |
| 1:D:168:VAL:HG11 | 1:D:247:ASN:HD22 | 1.71 | 0.55 |
| 1:A:88:LEU:HD22 | 1:A:92:THR:HG23 | 1.88 | 0.55 |
| 1:D:329:ILE:CD1 | 1:D:337:GLU:HB2 | 2.36 | 0.55 |
| 1:E:88:LEU:HD11 | 1:H:76:ASN:HA | 1.88 | 0.55 |
| 1:B:363:PHE:CE1 | 1:B:369:LEU:HD11 | 2.41 | 0.55 |
| 1:C:136:THR:O | 1:C:136:THR:CG2 | 2.45 | 0.55 |
| 1:F:376:ASP:HB2 | 1:F:425:VAL:HG22 | 1.89 | 0.55 |
| 1:A:297:MET:HE3 | 1:A:307:LYS:CG | 2.37 | 0.55 |
| 1:B:104:VAL:HG12 | 1:B:105:GLY:O | 2.07 | 0.55 |
| 1:C:146:ALA:HB3 | 1:F:323:SER:HB2 | 1.89 | 0.55 |
| 1:F:288:ASN:HD22 | 1:F:438:ASN:CG | 2.15 | 0.55 |
| 1:H:363:PHE:CD1 | 1:H:369:LEU:CD1 | 2.90 | 0.55 |
| 1:A:369:LEU:CD2 | 1:A:373:LEU:CD1 | 2.84 | 0.55 |
| 1:B:491:SER:CB | 1:C:487:ILE:HD11 | 2.37 | 0.55 |
| 1:C:145:GLU:OE2 | 1:F:89:LYS:HE3 | 2.07 | 0.55 |
| 1:E:139:GLN:HG3 | 1:E:175:GLN:HE22 | 1.71 | 0.55 |
| 1:H:86:GLN:OE1 | 1:H:340:THR:OG1 | 2.23 | 0.55 |
| 1:A:94:VAL:HG12 | 1:A:94:VAL:O | 2.07 | 0.55 |
| 1:C:139:GLN:HB3 | 1:F:96:GLN:NE2 | 2.21 | 0.55 |
| 1:F:94:VAL:HG12 | 1:F:96:GLN:NE2 | 2.22 | 0.55 |
| 1:D:180:VAL:HG13 | 1:D:190:ALA:CB | 2.37 | 0.55 |
| 1:G:393:LEU:HD22 | 1:G:398:PHE:CE1 | 2.41 | 0.55 |
| 1:B:374:GLN:O | 1:H:96:GLN:HG3 | 2.07 | 0.55 |
| 1:B:491:SER:HA | 1:C:487:ILE:HD11 | 1.87 | 0.55 |
| 1:E:193:ILE:HB | 1:E:234:LEU:HD22 | 1.87 | 0.55 |
| 1:H:449:ALA:HB1 | 1:H:484:ILE:HG22 | 1.89 | 0.55 |
| 1:C:407:GLU:OE2 | 1:C:429:ALA:HB3 | 2.07 | 0.55 |
| 1:F:369:LEU:HD23 | 1:F:369:LEU:O | 2.06 | 0.55 |
| 1:F:267:VAL:HG21 | 1:F:338:LEU:HD11 | 1.88 | 0.54 |
| 1:C:376:ASP:HB2 | 1:C:425:VAL:HG22 | 1.89 | 0.54 |
| 1:F:123:LEU:HD13 | 1:F:130:PRO:HG3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:386:VAL:HG12 | 1:G:390:LEU:HD22 | 1.88 | 0.54 |
| 1:B:487:ILE:HD11 | 1:C:491:SER:O | 2.07 | 0.54 |
| 1:C:133:LEU:HD12 | 1:C:254:ALA:HA | 1.90 | 0.54 |
| 1:C:400:SER:O | 1:C:400:SER:OG | 2.25 | 0.54 |
| 1:G:68:ARG:O | 1:G:71:VAL:N | 2.39 | 0.54 |
| 1:G:369:LEU:HD23 | 1:G:369:LEU:C | 2.31 | 0.54 |
| 1:A:360:ILE:HD11 | 1:A:393:LEU:HD13 | 1.90 | 0.54 |
| 1:B:367:ASP:CG | 1:H:323:SER:HB2 | 2.32 | 0.54 |
| 1:C:160:THR:HG22 | 1:C:160:THR:O | 2.08 | 0.54 |
| 1:C:180:VAL:HG13 | 1:C:190:ALA:HB3 | 1.89 | 0.54 |
| 1:F:240:THR:CG2 | 1:F:246:LEU:HD11 | 2.38 | 0.54 |
| 1:G:140:VAL:HG21 | 1:G:168:VAL:HG22 | 1.90 | 0.54 |
| 1:H:363:PHE:CE1 | 1:H:369:LEU:HD11 | 2.43 | 0.54 |
| 1:A:363:PHE:CG | 1:A:369:LEU:HD12 | 2.43 | 0.54 |
| 1:C:139:GLN:HE21 | 1:C:175:GLN:CD | 2.16 | 0.54 |
| 1:C:486:ASP:HB3 | 1:C:489:THR:HG23 | 1.89 | 0.54 |
| 1:E:84:VAL:CG2 | 1:H:78:ILE:CG2 | 2.81 | 0.54 |
| 1:G:472:TYR:CD2 | 1:G:494:VAL:HG13 | 2.43 | 0.54 |
| 1:D:198:PHE:CD1 | 1:D:214:ILE:HD13 | 2.42 | 0.54 |
| 1:G:393:LEU:CD2 | 1:G:398:PHE:CD1 | 2.91 | 0.54 |
| 1:C:133:LEU:HD22 | 1:C:133:LEU:C | 2.33 | 0.54 |
| 1:G:400:SER:O | 1:G:400:SER:OG | 2.25 | 0.54 |
| 1:C:139:GLN:CB | 1:F:96:GLN:HG3 | 2.38 | 0.53 |
| 1:F:244:GLN:HE21 | 1:F:245:MET:H | 1.56 | 0.53 |
| 1:A:140:VAL:HG12 | 1:A:141:ASN:N | 2.24 | 0.53 |
| 1:B:364:PRO:HB3 | 1:H:407:GLU:CD | 2.33 | 0.53 |
| 1:E:84:VAL:HG21 | 1:H:78:ILE:HG21 | 1.84 | 0.53 |
| 1:C:113:LEU:HD23 | 1:C:113:LEU:O | 2.08 | 0.53 |
| 1:D:94:VAL:HG23 | 1:E:147:GLN:HG3 | 1.89 | 0.53 |
| 1:D:193:ILE:CG2 | 1:D:234:LEU:CD1 | 2.86 | 0.53 |
| 1:A:376:ASP:HB2 | 1:A:425:VAL:CG2 | 2.39 | 0.53 |
| 1:D:68:ARG:O | 1:D:72:ILE:HD12 | 2.09 | 0.53 |
| 1:H:336:LYS:HG2 | 1:H:340:THR:CG2 | 2.39 | 0.53 |
| 1:A:113:LEU:C | 1:A:113:LEU:CD2 | 2.81 | 0.53 |
| 1:A:486:ASP:O | 1:A:487:ILE:C | 2.50 | 0.53 |
| 1:B:379:ILE:HD13 | 1:B:386:VAL:HG22 | 1.90 | 0.53 |
| 1:H:197:VAL:HG21 | 1:H:234:LEU:CD2 | 2.34 | 0.53 |
| 1:E:393:LEU:HD22 | 1:E:398:PHE:CE1 | 2.44 | 0.53 |
| 1:E:473:LEU:HD13 | 1:E:478:VAL:CG2 | 2.39 | 0.53 |
| 1:H:86:GLN:OE1 | 1:H:340:THR:CA | 2.56 | 0.53 |
| 1:A:77:ASN:ND2 | 1:A:335:GLN:NE2 | 2.57 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:370:ARG:HG3 | 1:B:386:VAL:HG11 | 1.90 | 0.53 |
| 1:D:140:VAL:HG12 | 1:D:141:ASN:N | 2.22 | 0.53 |
| 1:E:486:ASP:CB | 1:E:489:THR:HG23 | 2.39 | 0.53 |
| 1:F:136:THR:HA | 1:F:139:GLN:NE2 | 2.24 | 0.53 |
| 1:A:234:LEU:HD12 | 1:A:234:LEU:N | 2.24 | 0.52 |
| 1:A:352:TYR:CD1 | 1:A:352:TYR:N | 2.77 | 0.52 |
| 1:C:157:ILE:HD12 | 1:C:208:TYR:CZ | 2.44 | 0.52 |
| 1:D:486:ASP:CB | 1:D:489:THR:HG23 | 2.39 | 0.52 |
| 1:E:330:ASN:OD1 | 1:E:331:VAL:N | 2.42 | 0.52 |
| 1:F:124:TYR:CG | 1:F:188:VAL:HG13 | 2.44 | 0.52 |
| 1:B:94:VAL:HG12 | 1:B:96:GLN:HE21 | 1.75 | 0.52 |
| 1:C:457:ASN:ND2 | 1:C:457:ASN:N | 2.54 | 0.52 |
| 1:D:124:TYR:CG | 1:D:188:VAL:HG13 | 2.44 | 0.52 |
| 1:H:317:LEU:HD13 | 1:H:349:ARG:HA | 1.91 | 0.52 |
| 1:A:297:MET:HE3 | 1:A:307:LYS:CB | 2.39 | 0.52 |
| 1:D:286:MET:HE2 | 1:D:347:MET:CB | 2.38 | 0.52 |
| 1:D:486:ASP:O | 1:D:487:ILE:C | 2.52 | 0.52 |
| 1:F:203:LEU:HD12 | 1:F:208:TYR:CD2 | 2.44 | 0.52 |
| 1:F:473:LEU:CD1 | 1:F:477:LYS:O | 2.57 | 0.52 |
| 1:F:386:VAL:HG13 | 1:F:390:LEU:HD22 | 1.91 | 0.52 |
| 1:E:87:TYR:HB3 | 1:H:75:LEU:HD13 | 1.90 | 0.52 |
| 1:H:212:GLY:O | 1:H:248:VAL:HG13 | 2.10 | 0.52 |
| 1:B:78:ILE:CG2 | 1:C:84:VAL:HG21 | 2.39 | 0.52 |
| 1:H:211:VAL:HG13 | 1:H:247:ASN:O | 2.10 | 0.52 |
| 1:E:369:LEU:CD2 | 1:E:373:LEU:CD1 | 2.88 | 0.52 |
| 1:E:393:LEU:CD2 | 1:E:398:PHE:CD1 | 2.93 | 0.52 |
| 1:F:157:ILE:HD12 | 1:F:208:TYR:CZ | 2.43 | 0.52 |
| 1:B:160:THR:HG22 | 1:B:160:THR:O | 2.10 | 0.52 |
| 1:D:193:ILE:HB | 1:D:234:LEU:CD1 | 2.37 | 0.52 |
| 1:E:240:THR:HG22 | 1:E:246:LEU:HD11 | 1.91 | 0.52 |
| 1:E:334:LEU:HD11 | 1:E:338:LEU:HD22 | 1.92 | 0.52 |
| 1:F:363:PHE:CD1 | 1:F:369:LEU:HD12 | 2.45 | 0.52 |
| 1:E:401:TYR:CE1 | 1:E:442:VAL:HG11 | 2.45 | 0.52 |
| 1:D:379:ILE:HD11 | 1:D:423:LYS:HZ2 | 1.74 | 0.52 |
| 1:H:479:LEU:HD12 | 1:H:480:PHE:H | 1.75 | 0.52 |
| 1:A:407:GLU:HG3 | 1:A:427:SER:HB3 | 1.92 | 0.51 |
| 1:C:198:PHE:CD1 | 1:C:214:ILE:HD13 | 2.45 | 0.51 |
| 1:D:94:VAL:O | 1:D:94:VAL:CG1 | 2.48 | 0.51 |
| 1:D:220:GLU:N | 1:D:221:PRO:CD | 2.74 | 0.51 |
| 1:E:107:ALA:HB1 | 1:E:271:GLU:OE1 | 2.10 | 0.51 |
| 1:E:222:ILE:CD1 | 1:E:234:LEU:HD11 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:354:LEU:HD21 | 1:E:439:VAL:HG23 | 1.93 | 0.51 |
| 1:F:418:VAL:HG23 | 1:F:418:VAL:O | 2.10 | 0.51 |
| 1:G:68:ARG:O | 1:G:69:SER:C | 2.52 | 0.51 |
| 1:B:201:ASP:OD1 | 1:B:201:ASP:N | 2.43 | 0.51 |
| 1:C:418:VAL:CG1 | 1:C:484:ILE:HG21 | 2.40 | 0.51 |
| 1:G:157:ILE:HD12 | 1:G:208:TYR:CZ | 2.46 | 0.51 |
| 1:E:124:TYR:CD1 | 1:E:188:VAL:HG13 | 2.44 | 0.51 |
| 1:F:486:ASP:O | 1:F:487:ILE:C | 2.52 | 0.51 |
| 1:F:486:ASP:CB | 1:F:489:THR:HG23 | 2.40 | 0.51 |
| 1:H:418:VAL:HG21 | 1:H:493:LEU:CD1 | 2.33 | 0.51 |
| 1:B:68:ARG:O | 1:B:72:ILE:CD1 | 2.58 | 0.51 |
| 1:B:354:LEU:HD21 | 1:B:439:VAL:CG2 | 2.40 | 0.51 |
| 1:H:484:ILE:HD11 | 1:H:493:LEU:HD22 | 1.91 | 0.51 |
| 1:A:133:LEU:HD12 | 1:A:134:HIS:N | 2.25 | 0.51 |
| 1:G:88:LEU:HD22 | 1:G:92:THR:HG23 | 1.91 | 0.51 |
| 1:G:486:ASP:HB3 | 1:G:489:THR:HG23 | 1.91 | 0.51 |
| 1:D:203:LEU:HD22 | 1:D:208:TYR:CD2 | 2.45 | 0.51 |
| 1:E:337:GLU:O | 1:E:347:MET:HE1 | 2.10 | 0.51 |
| 1:F:487:ILE:HG21 | 1:G:495:GLU:OE2 | 2.11 | 0.51 |
| 1:G:197:VAL:HG12 | 1:G:198:PHE:CD2 | 2.46 | 0.51 |
| 1:G:376:ASP:HB2 | 1:G:425:VAL:HG22 | 1.91 | 0.51 |
| 1:A:369:LEU:HD23 | 1:A:373:LEU:CD1 | 2.41 | 0.51 |
| 1:D:240:THR:CG2 | 1:D:246:LEU:HD11 | 2.40 | 0.51 |
| 1:D:393:LEU:HD22 | 1:D:398:PHE:CD1 | 2.45 | 0.51 |
| 1:F:136:THR:HA | 1:F:139:GLN:HE22 | 1.76 | 0.51 |
| 1:H:473:LEU:HD13 | 1:H:478:VAL:HG22 | 1.92 | 0.51 |
| 1:D:103:LYS:CE | 1:D:251:ASP:OD1 | 2.55 | 0.51 |
| 1:F:91:PHE:HE1 | 1:F:126:VAL:HB | 1.74 | 0.51 |
| 1:G:407:GLU:OE2 | 1:G:429:ALA:HB3 | 2.10 | 0.51 |
| 1:C:193:ILE:HB | 1:C:234:LEU:CD2 | 2.40 | 0.51 |
| 1:D:317:LEU:HD13 | 1:D:349:ARG:HA | 1.93 | 0.51 |
| 1:H:327:ALA:HB2 | 1:H:347:MET:CE | 2.38 | 0.51 |
| 1:C:133:LEU:C | 1:C:133:LEU:CD2 | 2.84 | 0.51 |
| 1:G:124:TYR:CD1 | 1:G:188:VAL:HG13 | 2.45 | 0.51 |
| 1:C:235:THR:HB | 1:C:237:LEU:HD22 | 1.93 | 0.50 |
| 1:E:193:ILE:O | 1:E:193:ILE:HG22 | 2.09 | 0.50 |
| 1:F:400:SER:O | 1:F:400:SER:OG | 2.24 | 0.50 |
| 1:G:486:ASP:O | 1:G:487:ILE:C | 2.54 | 0.50 |
| 1:B:78:ILE:HG22 | 1:C:84:VAL:HG21 | 1.93 | 0.50 |
| 1:D:286:MET:HE2 | 1:D:347:MET:SD | 2.51 | 0.50 |
| 1:F:124:TYR:CD2 | 1:F:188:VAL:HG22 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:VAL:HG11 | 1:A:158:ARG:NH2 | 2.27 | 0.50 |
| 1:A:340:THR:HG23 | 1:A:343:GLY:H | 1.75 | 0.50 |
| 1:D:107:ALA:HB1 | 1:D:271:GLU:OE1 | 2.11 | 0.50 |
| 1:E:465:PHE:CD1 | 1:H:465:PHE:CD1 | 2.99 | 0.50 |
| 1:F:197:VAL:HG11 | 1:F:234:LEU:HD13 | 1.92 | 0.50 |
| 1:A:393:LEU:HD22 | 1:A:398:PHE:CE1 | 2.46 | 0.50 |
| 1:B:193:ILE:HB | 1:B:234:LEU:CD2 | 2.41 | 0.50 |
| 1:F:354:LEU:CD2 | 1:F:439:VAL:HG22 | 2.41 | 0.50 |
| 1:D:407:GLU:OE2 | 1:D:429:ALA:HB3 | 2.10 | 0.50 |
| 1:F:203:LEU:HD12 | 1:F:208:TYR:CE2 | 2.46 | 0.50 |
| 1:H:479:LEU:HD12 | 1:H:480:PHE:N | 2.26 | 0.50 |
| 1:A:119:CYS:SG | 1:A:334:LEU:HD23 | 2.51 | 0.50 |
| 1:A:220:GLU:N | 1:A:221:PRO:CD | 2.75 | 0.50 |
| 1:C:273:GLY:O | 1:C:283:LYS:NZ | 2.33 | 0.50 |
| 1:E:157:ILE:HD12 | 1:E:208:TYR:CZ | 2.46 | 0.50 |
| 1:E:487:ILE:HD11 | 1:H:491:SER:CB | 2.37 | 0.50 |
| 1:F:99:PHE:CE2 | 1:F:123:LEU:HD22 | 2.43 | 0.50 |
| 1:B:486:ASP:CB | 1:B:489:THR:HG23 | 2.42 | 0.50 |
| 1:E:193:ILE:HB | 1:E:234:LEU:CD2 | 2.41 | 0.50 |
| 1:F:94:VAL:HG11 | 1:F:96:GLN:HE22 | 1.76 | 0.50 |
| 1:F:471:SER:HG | 1:G:471:SER:CB | 2.25 | 0.50 |
| 1:G:169:ARG:CD | 1:G:245:MET:CE | 2.87 | 0.50 |
| 1:H:267:VAL:HG21 | 1:H:338:LEU:CD2 | 2.40 | 0.50 |
| 1:A:376:ASP:HB2 | 1:A:425:VAL:HG22 | 1.94 | 0.49 |
| 1:B:487:ILE:HD11 | 1:C:491:SER:CA | 2.41 | 0.49 |
| 1:D:211:VAL:HG13 | 1:D:247:ASN:O | 2.11 | 0.49 |
| 1:E:109:ILE:HG21 | 1:E:175:GLN:HG3 | 1.94 | 0.49 |
| 1:F:214:ILE:HG13 | 1:F:248:VAL:HG11 | 1.94 | 0.49 |
| 1:A:240:THR:HG23 | 1:A:246:LEU:HD11 | 1.92 | 0.49 |
| 1:C:163:HIS:CE1 | 1:F:404:GLU:OE2 | 2.66 | 0.49 |
| 1:D:469:GLN:HE21 | 1:D:483:GLY:H | 1.60 | 0.49 |
| 1:H:102:ILE:HD13 | 1:H:334:LEU:HD21 | 1.94 | 0.49 |
| 1:H:157:ILE:HD12 | 1:H:208:TYR:CZ | 2.47 | 0.49 |
| 1:H:201:ASP:N | 1:H:201:ASP:OD1 | 2.44 | 0.49 |
| 1:D:337:GLU:O | 1:D:339:PHE:N | 2.45 | 0.49 |
| 1:E:103:LYS:CE | 1:E:251:ASP:OD1 | 2.58 | 0.49 |
| 1:E:491:SER:HA | 1:H:487:ILE:HD11 | 1.93 | 0.49 |
| 1:F:201:ASP:OD1 | 1:F:201:ASP:N | 2.44 | 0.49 |
| 1:H:407:GLU:HG3 | 1:H:427:SER:HB3 | 1.93 | 0.49 |
| 1:B:354:LEU:CD2 | 1:B:439:VAL:CG2 | 2.91 | 0.49 |
| 1:C:393:LEU:CD2 | 1:C:398:PHE:CD1 | 2.96 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:140:VAL:HG11 | 1:F:158:ARG:NH2 | 2.27 | 0.49 |
| 1:F:269:LEU:HD21 | 1:F:334:LEU:HD13 | 1.94 | 0.49 |
| 1:F:407:GLU:HG3 | 1:F:427:SER:HB3 | 1.95 | 0.49 |
| 1:H:421:LEU:HD22 | 1:H:443:LEU:HD21 | 1.94 | 0.49 |
| 1:B:393:LEU:HD22 | 1:B:398:PHE:CE1 | 2.48 | 0.49 |
| 1:E:139:GLN:HE21 | 1:E:175:GLN:NE2 | 2.10 | 0.49 |
| 1:E:220:GLU:N | 1:E:221:PRO:CD | 2.76 | 0.49 |
| 1:E:330:ASN:ND2 | 1:E:332:GLN:HE21 | 2.11 | 0.49 |
| 1:F:473:LEU:HD12 | 1:F:474:LYS:N | 2.26 | 0.49 |
| 1:F:486:ASP:HB3 | 1:F:489:THR:HG23 | 1.94 | 0.49 |
| 1:B:400:SER:O | 1:B:400:SER:OG | 2.25 | 0.49 |
| 1:D:327:ALA:CB | 1:D:347:MET:HE3 | 2.39 | 0.49 |
| 1:E:424:PHE:HE1 | 1:E:439:VAL:HG11 | 1.76 | 0.49 |
| 1:F:424:PHE:HE1 | 1:F:439:VAL:HG11 | 1.77 | 0.49 |
| 1:A:275:ILE:HG21 | 1:A:284:ILE:HD12 | 1.95 | 0.49 |
| 1:B:374:GLN:CD | 1:H:97:GLN:HB2 | 2.37 | 0.49 |
| 1:C:393:LEU:HD21 | 1:C:398:PHE:CG | 2.47 | 0.49 |
| 1:F:124:TYR:CD1 | 1:F:188:VAL:HG13 | 2.47 | 0.49 |
| 1:G:369:LEU:C | 1:G:369:LEU:CD2 | 2.86 | 0.49 |
| 1:G:370:ARG:HG3 | 1:G:386:VAL:CG1 | 2.38 | 0.49 |
| 1:H:124:TYR:CD2 | 1:H:188:VAL:HG22 | 2.48 | 0.49 |
| 1:B:379:ILE:HD11 | 1:B:423:LYS:NZ | 2.28 | 0.49 |
| 1:D:431:TRP:CE2 | 1:D:436:THR:HG21 | 2.48 | 0.49 |
| 1:E:407:GLU:HG3 | 1:E:427:SER:HB3 | 1.95 | 0.49 |
| 1:G:393:LEU:HD21 | 1:G:398:PHE:CG | 2.48 | 0.49 |
| 1:G:407:GLU:HG3 | 1:G:427:SER:HB3 | 1.95 | 0.49 |
| 1:H:486:ASP:O | 1:H:487:ILE:C | 2.55 | 0.49 |
| 1:D:88:LEU:HD22 | 1:D:92:THR:CG2 | 2.42 | 0.49 |
| 1:E:354:LEU:CD2 | 1:E:439:VAL:CG2 | 2.91 | 0.49 |
| 1:F:266:ILE:HD13 | 1:F:316:LEU:HD21 | 1.94 | 0.49 |
| 1:H:432:LEU:C | 1:H:432:LEU:HD12 | 2.38 | 0.49 |
| 1:E:393:LEU:HD21 | 1:E:398:PHE:CG | 2.47 | 0.49 |
| 1:H:220:GLU:N | 1:H:221:PRO:CD | 2.76 | 0.49 |
| 1:A:393:LEU:HD11 | 1:A:411:ILE:HD13 | 1.95 | 0.48 |
| 1:F:74:LEU:O | 1:F:78:ILE:HD12 | 2.13 | 0.48 |
| 1:A:172:PHE:CE2 | 1:A:237:LEU:HD21 | 2.47 | 0.48 |
| 1:B:393:LEU:CD2 | 1:B:398:PHE:CD1 | 2.96 | 0.48 |
| 1:B:479:LEU:HD22 | 1:B:497:PHE:HB2 | 1.95 | 0.48 |
| 1:C:407:GLU:HG3 | 1:C:427:SER:HB3 | 1.94 | 0.48 |
| 1:E:131:ILE:HD13 | 1:E:222:ILE:HG21 | 1.94 | 0.48 |
| 1:E:198:PHE:CD1 | 1:E:214:ILE:HD13 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:472:TYR:CD2 | 1:B:494:VAL:HG13 | 2.48 | 0.48 |
| 1:C:331:VAL:HG13 | 1:C:332:GLN:N | 2.29 | 0.48 |
| 1:C:469:GLN:HE21 | 1:C:483:GLY:N | 2.11 | 0.48 |
| 1:E:87:TYR:HB3 | 1:H:75:LEU:CD1 | 2.43 | 0.48 |
| 1:F:495:GLU:HG3 | 1:G:487:ILE:CD1 | 2.40 | 0.48 |
| 1:G:327:ALA:HB2 | 1:G:347:MET:HE3 | 1.84 | 0.48 |
| 1:A:95:SER:CB | 1:A:97:GLN:O | 2.61 | 0.48 |
| 1:A:136:THR:HG22 | 1:A:172:PHE:CZ | 2.48 | 0.48 |
| 1:A:473:LEU:HD13 | 1:A:478:VAL:CG2 | 2.43 | 0.48 |
| 1:B:330:ASN:OD1 | 1:B:331:VAL:N | 2.47 | 0.48 |
| 1:B:354:LEU:CD2 | 1:B:439:VAL:HG22 | 2.43 | 0.48 |
| 1:D:180:VAL:HG13 | 1:D:190:ALA:HB3 | 1.95 | 0.48 |
| 1:G:208:TYR:O | 1:G:211:VAL:HG23 | 2.13 | 0.48 |
| 1:G:418:VAL:HG21 | 1:G:493:LEU:CD1 | 2.33 | 0.48 |
| 1:B:386:VAL:HG12 | 1:B:390:LEU:HD22 | 1.96 | 0.48 |
| 1:B:408:ALA:HB1 | 1:B:426:CYS:SG | 2.53 | 0.48 |
| 1:B:491:SER:CA | 1:C:487:ILE:HD11 | 2.43 | 0.48 |
| 1:C:275:ILE:HG21 | 1:C:284:ILE:HD12 | 1.96 | 0.48 |
| 1:C:386:VAL:HG13 | 1:C:390:LEU:HD13 | 1.95 | 0.48 |
| 1:D:400:SER:O | 1:D:400:SER:OG | 2.23 | 0.48 |
| 1:E:136:THR:HG22 | 1:E:172:PHE:CZ | 2.49 | 0.48 |
| 1:E:484:ILE:CD1 | 1:E:493:LEU:HD22 | 2.43 | 0.48 |
| 1:E:486:ASP:O | 1:E:487:ILE:C | 2.55 | 0.48 |
| 1:G:189:ARG:HG2 | 1:H:189:ARG:NH1 | 2.28 | 0.48 |
| 1:A:262:GLU:HA | 1:A:320:LEU:CD2 | 2.43 | 0.48 |
| 1:B:84:VAL:HG12 | 1:B:85:GLU:N | 2.29 | 0.48 |
| 1:B:407:GLU:OE2 | 1:B:429:ALA:HB3 | 2.13 | 0.48 |
| 1:E:210:LEU:N | 1:E:210:LEU:HD12 | 2.29 | 0.48 |
| 1:E:473:LEU:HD13 | 1:E:478:VAL:HG22 | 1.96 | 0.48 |
| 1:G:165:MET:HE3 | 1:G:169:ARG:HB2 | 1.96 | 0.48 |
| 1:G:222:ILE:CD1 | 1:G:234:LEU:HD21 | 2.43 | 0.48 |
| 1:D:82:ARG:HG2 | 1:D:86:GLN:HE21 | 1.77 | 0.48 |
| 1:H:473:LEU:HD12 | 1:H:477:LYS:O | 2.14 | 0.48 |
| 1:A:474:LYS:O | 1:A:475:GLY:C | 2.56 | 0.48 |
| 1:C:417:ASN:O | 1:C:418:VAL:HG22 | 2.14 | 0.48 |
| 1:C:486:ASP:O | 1:C:487:ILE:C | 2.55 | 0.48 |
| 1:D:113:LEU:HD23 | 1:D:113:LEU:O | 2.13 | 0.48 |
| 1:D:486:ASP:HB3 | 1:D:489:THR:HG23 | 1.96 | 0.48 |
| 1:E:393:LEU:HD22 | 1:E:398:PHE:CD1 | 2.49 | 0.48 |
| 1:H:393:LEU:CD2 | 1:H:398:PHE:CG | 2.97 | 0.48 |
| 1:A:77:ASN:ND2 | 1:A:335:GLN:HE21 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:407:GLU:HG3 | 1:B:427:SER:HB3 | 1.95 | 0.48 |
| 1:D:456:GLU:OE2 | 1:D:473:LEU:HD21 | 2.13 | 0.48 |
| 1:E:334:LEU:CD1 | 1:E:338:LEU:HD22 | 2.44 | 0.48 |
| 1:F:297:MET:HE3 | 1:F:307:LYS:CB | 2.44 | 0.48 |
| 1:G:116:LEU:HD13 | 1:G:179:LEU:HD11 | 1.95 | 0.48 |
| 1:G:244:GLN:HE21 | 1:G:245:MET:N | 2.11 | 0.48 |
| 1:G:431:TRP:CE2 | 1:G:436:THR:HG21 | 2.49 | 0.48 |
| 1:B:173:LEU:HD22 | 1:B:194:THR:HG21 | 1.96 | 0.48 |
| 1:C:201:ASP:N | 1:C:201:ASP:OD1 | 2.47 | 0.48 |
| 1:C:244:GLN:HE21 | 1:C:245:MET:N | 2.12 | 0.48 |
| 1:E:262:GLU:HA | 1:E:320:LEU:HD22 | 1.94 | 0.48 |
| 1:F:121:ALA:HA | 1:F:188:VAL:HG21 | 1.95 | 0.48 |
| 1:G:327:ALA:CB | 1:G:347:MET:HE3 | 2.44 | 0.48 |
| 1:H:84:VAL:HG12 | 1:H:85:GLU:N | 2.28 | 0.48 |
| 1:A:331:VAL:HG13 | 1:A:332:GLN:N | 2.29 | 0.47 |
| 1:D:99:PHE:CZ | 1:D:338:LEU:HD22 | 2.48 | 0.47 |
| 1:F:453:VAL:HG12 | 1:F:454:VAL:N | 2.29 | 0.47 |
| 1:H:97:GLN:HB3 | 1:H:264:LEU:HD22 | 1.96 | 0.47 |
| 1:H:266:ILE:CD1 | 1:H:316:LEU:HD21 | 2.43 | 0.47 |
| 1:H:276:ILE:HG23 | 1:H:281:GLY:O | 2.14 | 0.47 |
| 1:A:88:LEU:HD22 | 1:A:92:THR:CG2 | 2.43 | 0.47 |
| 1:A:95:SER:HB2 | 1:A:97:GLN:O | 2.14 | 0.47 |
| 1:G:449:ALA:HB1 | 1:G:484:ILE:HG22 | 1.97 | 0.47 |
| 1:A:275:ILE:CG2 | 1:A:284:ILE:HD12 | 2.44 | 0.47 |
| 1:A:431:TRP:CE2 | 1:A:436:THR:HG21 | 2.49 | 0.47 |
| 1:C:340:THR:HG23 | 1:C:343:GLY:H | 1.79 | 0.47 |
| 1:D:121:ALA:HA | 1:D:188:VAL:HG21 | 1.97 | 0.47 |
| 1:E:431:TRP:CE2 | 1:E:436:THR:HG21 | 2.48 | 0.47 |
| 1:E:442:VAL:HG22 | 1:E:445:ARG:HH12 | 1.79 | 0.47 |
| 1:G:393:LEU:HD22 | 1:G:398:PHE:CD1 | 2.49 | 0.47 |
| 1:E:340:THR:HG23 | 1:E:343:GLY:H | 1.79 | 0.47 |
| 1:C:140:VAL:HG13 | 1:C:144:LEU:HD23 | 1.97 | 0.47 |
| 1:C:456:GLU:OE2 | 1:C:473:LEU:HD21 | 2.14 | 0.47 |
| 1:D:329:ILE:HD13 | 1:D:337:GLU:HB2 | 1.96 | 0.47 |
| 1:A:330:ASN:OD1 | 1:A:331:VAL:N | 2.47 | 0.47 |
| 1:B:449:ALA:HB1 | 1:B:484:ILE:HG22 | 1.97 | 0.47 |
| 1:B:471:SER:HG | 1:C:471:SER:CB | 2.27 | 0.47 |
| 1:G:133:LEU:HD23 | 1:G:254:ALA:HA | 1.96 | 0.47 |
| 1:A:201:ASP:OD1 | 1:A:201:ASP:N | 2.48 | 0.47 |
| 1:A:318:ASP:O | 1:A:319:TYR:HD1 | 1.98 | 0.47 |
| 1:D:303:LYS:O | 1:D:306:THR:OG1 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:337:GLU:C | 1:D:339:PHE:H | 2.23 | 0.47 |
| 1:E:78:ILE:CG2 | 1:H:84:VAL:CG2 | 2.92 | 0.47 |
| 1:E:454:VAL:HG12 | 1:E:455:SER:N | 2.29 | 0.47 |
| 1:H:342:SER:O | 1:H:343:GLY:C | 2.58 | 0.47 |
| 1:H:363:PHE:CE1 | 1:H:369:LEU:CD1 | 2.97 | 0.47 |
| 1:H:457:ASN:H | 1:H:457:ASN:ND2 | 2.12 | 0.47 |
| 1:H:473:LEU:HD12 | 1:H:474:LYS:O | 2.14 | 0.47 |
| 1:H:474:LYS:O | 1:H:475:GLY:C | 2.58 | 0.47 |
| 1:A:297:MET:HE1 | 1:A:307:LYS:O | 2.14 | 0.47 |
| 1:B:126:VAL:O | 1:C:68:ARG:HG2 | 2.15 | 0.47 |
| 1:C:220:GLU:N | 1:C:221:PRO:CD | 2.78 | 0.47 |
| 1:E:121:ALA:HA | 1:E:188:VAL:HG21 | 1.97 | 0.47 |
| 1:E:474:LYS:O | 1:E:475:GLY:C | 2.58 | 0.47 |
| 1:A:140:VAL:CG1 | 1:A:141:ASN:N | 2.77 | 0.47 |
| 1:A:354:LEU:HD21 | 1:A:439:VAL:HG23 | 1.95 | 0.47 |
| 1:A:369:LEU:HD21 | 1:A:373:LEU:HD11 | 1.95 | 0.47 |
| 1:B:266:ILE:HD11 | 1:B:320:LEU:CD1 | 2.45 | 0.47 |
| 1:C:139:GLN:HB2 | 1:F:96:GLN:HG3 | 1.97 | 0.47 |
| 1:C:197:VAL:HG12 | 1:C:198:PHE:CG | 2.49 | 0.47 |
| 1:D:472:TYR:CD2 | 1:D:494:VAL:HG13 | 2.50 | 0.47 |
| 1:F:426:CYS:SG | 1:F:436:THR:HG22 | 2.55 | 0.47 |
| 1:G:372:ALA:O | 1:G:375:ARG:HG2 | 2.15 | 0.47 |
| 1:C:113:LEU:CD2 | 1:C:113:LEU:C | 2.88 | 0.47 |
| 1:C:372:ALA:O | 1:C:375:ARG:HG2 | 2.15 | 0.47 |
| 1:D:407:GLU:HG3 | 1:D:427:SER:HB3 | 1.97 | 0.47 |
| 1:D:479:LEU:HD22 | 1:D:497:PHE:HB2 | 1.96 | 0.47 |
| 1:E:147:GLN:OE1 | 1:E:167:VAL:HG21 | 2.14 | 0.47 |
| 1:F:473:LEU:HD12 | 1:F:477:LYS:O | 2.15 | 0.47 |
| 1:G:201:ASP:OD1 | 1:G:201:ASP:N | 2.46 | 0.47 |
| 1:B:363:PHE:CD2 | 1:B:369:LEU:HD12 | 2.49 | 0.46 |
| 1:D:334:LEU:HD12 | 1:D:334:LEU:O | 2.15 | 0.46 |
| 1:E:68:ARG:O | 1:E:72:ILE:CD1 | 2.63 | 0.46 |
| 1:F:401:TYR:CE2 | 1:F:443:LEU:CD1 | 2.98 | 0.46 |
| 1:B:193:ILE:CB | 1:B:234:LEU:HD22 | 2.45 | 0.46 |
| 1:C:458:ASP:O | 1:C:459:ALA:C | 2.57 | 0.46 |
| 1:C:473:LEU:HD12 | 1:C:477:LYS:O | 2.16 | 0.46 |
| 1:G:197:VAL:HG12 | 1:G:198:PHE:CG | 2.50 | 0.46 |
| 1:G:376:ASP:HB2 | 1:G:425:VAL:CG2 | 2.45 | 0.46 |
| 1:H:421:LEU:HD22 | 1:H:443:LEU:CD2 | 2.45 | 0.46 |
| 1:C:82:ARG:HG2 | 1:C:86:GLN:HE21 | 1.80 | 0.46 |
| 1:D:140:VAL:CG1 | 1:D:141:ASN:N | 2.77 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:147:GLN:OE1 | 1:E:167:VAL:CG2 | 2.63 | 0.46 |
| 1:E:486:ASP:HB3 | 1:E:489:THR:HG23 | 1.96 | 0.46 |
| 1:H:252:VAL:HG22 | 1:H:312:GLU:CD | 2.40 | 0.46 |
| 1:A:472:TYR:CD2 | 1:A:494:VAL:HG13 | 2.51 | 0.46 |
| 1:E:77:ASN:HD21 | 1:E:335:GLN:NE2 | 2.09 | 0.46 |
| 1:F:244:GLN:NE2 | 1:F:245:MET:N | 2.60 | 0.46 |
| 1:G:197:VAL:HG21 | 1:G:222:ILE:HD11 | 1.95 | 0.46 |
| 1:B:393:LEU:HD21 | 1:B:398:PHE:CG | 2.50 | 0.46 |
| 1:D:379:ILE:CG2 | 1:D:386:VAL:HG23 | 2.40 | 0.46 |
| 1:D:474:LYS:O | 1:D:475:GLY:C | 2.59 | 0.46 |
| 1:F:73:GLN:HG2 | 1:F:335:GLN:OE1 | 2.15 | 0.46 |
| 1:H:193:ILE:HG22 | 1:H:193:ILE:O | 2.15 | 0.46 |
| 1:C:240:THR:HG22 | 1:C:246:LEU:HD11 | 1.98 | 0.46 |
| 1:C:393:LEU:HD22 | 1:C:398:PHE:CE1 | 2.51 | 0.46 |
| 1:F:97:GLN:HB3 | 1:F:264:LEU:HD23 | 1.97 | 0.46 |
| 1:H:372:ALA:O | 1:H:375:ARG:HG2 | 2.16 | 0.46 |
| 1:B:104:VAL:HG21 | 1:B:116:LEU:HD21 | 1.98 | 0.46 |
| 1:B:198:PHE:CD1 | 1:B:214:ILE:HD13 | 2.50 | 0.46 |
| 1:B:465:PHE:CD1 | 1:C:465:PHE:CD1 | 3.04 | 0.46 |
| 1:C:147:GLN:HG3 | 1:F:322:ARG:CB | 2.40 | 0.46 |
| 1:C:379:ILE:HG21 | 1:C:386:VAL:CG2 | 2.40 | 0.46 |
| 1:D:372:ALA:O | 1:D:375:ARG:HG2 | 2.16 | 0.46 |
| 1:F:417:ASN:N | 1:F:417:ASN:OD1 | 2.49 | 0.46 |
| 1:G:266:ILE:HD13 | 1:G:316:LEU:CD2 | 2.43 | 0.46 |
| 1:G:340:THR:HG23 | 1:G:343:GLY:H | 1.81 | 0.46 |
| 1:G:488:ASN:HD22 | 1:G:489:THR:N | 2.13 | 0.46 |
| 1:B:379:ILE:HD11 | 1:B:423:LYS:HZ2 | 1.81 | 0.46 |
| 1:B:402:ALA:HB2 | 1:B:409:VAL:HG22 | 1.98 | 0.46 |
| 1:B:431:TRP:CE2 | 1:B:436:THR:HG21 | 2.51 | 0.46 |
| 1:C:417:ASN:O | 1:C:418:VAL:HG23 | 2.16 | 0.46 |
| 1:F:203:LEU:C | 1:F:203:LEU:CD1 | 2.89 | 0.46 |
| 1:H:140:VAL:HG12 | 1:H:141:ASN:H | 1.77 | 0.46 |
| 1:A:372:ALA:O | 1:A:375:ARG:HG2 | 2.16 | 0.46 |
| 1:D:337:GLU:C | 1:D:339:PHE:N | 2.71 | 0.46 |
| 1:E:352:TYR:CD1 | 1:E:352:TYR:N | 2.83 | 0.46 |
| 1:F:197:VAL:HG11 | 1:F:234:LEU:CD1 | 2.46 | 0.46 |
| 1:H:340:THR:CG2 | 1:H:342:SER:HB3 | 2.46 | 0.46 |
| 1:A:140:VAL:HG13 | 1:A:144:LEU:HD12 | 1.98 | 0.46 |
| 1:A:347:MET:HB2 | 1:A:347:MET:HE3 | 1.63 | 0.46 |
| 1:A:474:LYS:CE | 1:A:501:CYS:SG | 3.04 | 0.46 |
| 1:B:234:LEU:N | 1:B:234:LEU:HD23 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:267:VAL:HG21 | 1:F:338:LEU:CD1 | 2.46 | 0.46 |
| 1:E:240:THR:CG2 | 1:E:246:LEU:HD11 | 2.47 | 0.45 |
| 1:E:469:GLN:HE21 | 1:E:483:GLY:H | 1.62 | 0.45 |
| 1:F:379:ILE:HD13 | 1:F:386:VAL:HG22 | 1.97 | 0.45 |
| 1:H:299:GLN:HB2 | 1:H:302:VAL:HG23 | 1.97 | 0.45 |
| 1:A:121:ALA:HA | 1:A:188:VAL:HG21 | 1.98 | 0.45 |
| 1:A:458:ASP:O | 1:A:459:ALA:C | 2.58 | 0.45 |
| 1:C:188:VAL:HG11 | 1:C:231:LEU:HD12 | 1.98 | 0.45 |
| 1:C:421:LEU:HD13 | 1:C:443:LEU:HD21 | 1.98 | 0.45 |
| 1:F:372:ALA:O | 1:F:375:ARG:HG2 | 2.16 | 0.45 |
| 1:G:417:ASN:OD1 | 1:G:417:ASN:N | 2.50 | 0.45 |
| 1:B:116:LEU:HD12 | 1:B:116:LEU:O | 2.16 | 0.45 |
| 1:B:329:ILE:HG22 | 1:B:330:ASN:N | 2.31 | 0.45 |
| 1:B:474:LYS:O | 1:B:475:GLY:C | 2.59 | 0.45 |
| 1:D:257:LEU:HA | 1:D:257:LEU:HD23 | 1.62 | 0.45 |
| 1:E:336:LYS:HG2 | 1:E:340:THR:HG21 | 1.99 | 0.45 |
| 1:E:372:ALA:O | 1:E:375:ARG:HG2 | 2.16 | 0.45 |
| 1:G:147:GLN:OE1 | 1:G:167:VAL:HG21 | 2.16 | 0.45 |
| 1:G:197:VAL:HG12 | 1:G:198:PHE:N | 2.30 | 0.45 |
| 1:C:197:VAL:HG12 | 1:C:198:PHE:CD2 | 2.52 | 0.45 |
| 1:C:474:LYS:O | 1:C:475:GLY:C | 2.58 | 0.45 |
| 1:F:73:GLN:OE1 | 1:F:118:SER:O | 2.34 | 0.45 |
| 1:F:193:ILE:HG21 | 1:F:234:LEU:HD22 | 1.99 | 0.45 |
| 1:F:485:ASP:HB3 | 1:G:472:TYR:OH | 2.17 | 0.45 |
| 1:A:68:ARG:O | 1:A:72:ILE:CD1 | 2.65 | 0.45 |
| 1:A:160:THR:O | 1:A:160:THR:HG22 | 2.16 | 0.45 |
| 1:A:234:LEU:N | 1:A:234:LEU:CD1 | 2.80 | 0.45 |
| 1:A:491:SER:CA | 1:D:487:ILE:HD11 | 2.44 | 0.45 |
| 1:G:88:LEU:HA | 1:G:88:LEU:HD23 | 1.67 | 0.45 |
| 1:D:240:THR:HG22 | 1:D:246:LEU:HD11 | 1.98 | 0.45 |
| 1:D:277:ASN:OD1 | 1:D:301:TRP:CE2 | 2.70 | 0.45 |
| 1:D:334:LEU:HD12 | 1:D:334:LEU:C | 2.41 | 0.45 |
| 1:D:417:ASN:OD1 | 1:D:417:ASN:N | 2.49 | 0.45 |
| 1:F:203:LEU:HD13 | 1:F:203:LEU:O | 2.17 | 0.45 |
| 1:F:456:GLU:OE2 | 1:F:473:LEU:HD21 | 2.17 | 0.45 |
| 1:G:173:LEU:N | 1:G:173:LEU:CD2 | 2.79 | 0.45 |
| 1:H:88:LEU:HD12 | 1:H:88:LEU:HA | 1.67 | 0.45 |
| 1:H:386:VAL:HG12 | 1:H:390:LEU:HD22 | 1.98 | 0.45 |
| 1:A:113:LEU:HD23 | 1:A:113:LEU:C | 2.39 | 0.45 |
| 1:B:484:ILE:HD11 | 1:B:493:LEU:HD22 | 1.99 | 0.45 |
| 1:D:120:LEU:HA | 1:D:123:LEU:HD12 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:88:LEU:CD2 | 1:E:92:THR:HG23 | 2.46 | 0.45 |
| 1:E:338:LEU:HD12 | 1:E:338:LEU:HA | 1.76 | 0.45 |
| 1:E:354:LEU:CD2 | 1:E:439:VAL:HG23 | 2.46 | 0.45 |
| 1:E:365:SER:OG | 1:E:368:ALA:HB3 | 2.17 | 0.45 |
| 1:E:412:VAL:HG13 | 1:E:420:THR:O | 2.17 | 0.45 |
| 1:E:454:VAL:HG21 | 1:E:464:HIS:CD2 | 2.51 | 0.45 |
| 1:F:103:LYS:CE | 1:F:251:ASP:OD1 | 2.60 | 0.45 |
| 1:H:303:LYS:O | 1:H:306:THR:OG1 | 2.33 | 0.45 |
| 1:H:330:ASN:OD1 | 1:H:331:VAL:N | 2.50 | 0.45 |
| 1:A:82:ARG:HG2 | 1:A:86:GLN:HE21 | 1.82 | 0.45 |
| 1:A:84:VAL:HG21 | 1:D:78:ILE:CG2 | 2.47 | 0.45 |
| 1:D:201:ASP:OD1 | 1:D:201:ASP:N | 2.49 | 0.45 |
| 1:H:417:ASN:O | 1:H:418:VAL:HG23 | 2.15 | 0.45 |
| 1:H:486:ASP:CB | 1:H:489:THR:HG23 | 2.46 | 0.45 |
| 1:A:473:LEU:HD13 | 1:A:478:VAL:HG22 | 1.97 | 0.45 |
| 1:B:410:ALA:HB1 | 1:B:421:LEU:HD11 | 1.98 | 0.45 |
| 1:B:474:LYS:CE | 1:B:501:CYS:SG | 3.05 | 0.45 |
| 1:G:74:LEU:HD11 | 1:G:87:TYR:CE2 | 2.51 | 0.45 |
| 1:G:240:THR:HG22 | 1:G:246:LEU:HD11 | 1.98 | 0.45 |
| 1:H:369:LEU:HD23 | 1:H:373:LEU:CD1 | 2.47 | 0.45 |
| 1:B:479:LEU:HD12 | 1:B:480:PHE:H | 1.82 | 0.45 |
| 1:C:144:LEU:HD22 | 1:C:167:VAL:CG1 | 2.46 | 0.45 |
| 1:C:330:ASN:OD1 | 1:C:331:VAL:N | 2.50 | 0.45 |
| 1:C:461:ILE:O | 1:C:462:ALA:C | 2.60 | 0.45 |
| 1:D:270:ASN:ND2 | 1:D:272:LYS:HG2 | 2.31 | 0.45 |
| 1:F:193:ILE:HB | 1:F:234:LEU:HD22 | 1.98 | 0.45 |
| 1:H:180:VAL:HG13 | 1:H:190:ALA:CB | 2.41 | 0.45 |
| 1:E:140:VAL:HG23 | 1:E:171:CYS:SG | 2.56 | 0.44 |
| 1:E:267:VAL:CG2 | 1:E:338:LEU:CD1 | 2.79 | 0.44 |
| 1:H:425:VAL:O | 1:H:425:VAL:HG12 | 2.17 | 0.44 |
| 1:B:354:LEU:HD13 | 1:B:442:VAL:HG21 | 1.99 | 0.44 |
| 1:B:426:CYS:SG | 1:B:436:THR:HG22 | 2.57 | 0.44 |
| 1:B:488:ASN:HD22 | 1:B:489:THR:N | 2.16 | 0.44 |
| 1:B:491:SER:HB3 | 1:C:487:ILE:HD11 | 1.99 | 0.44 |
| 1:D:88:LEU:HD22 | 1:D:92:THR:HG23 | 2.00 | 0.44 |
| 1:D:286:MET:CE | 1:D:347:MET:HB3 | 2.47 | 0.44 |
| 1:F:266:ILE:HB | 1:F:326:VAL:HG22 | 1.98 | 0.44 |
| 1:H:411:ILE:O | 1:H:421:LEU:HD12 | 2.17 | 0.44 |
| 1:C:124:TYR:CD2 | 1:C:188:VAL:HG22 | 2.52 | 0.44 |
| 1:C:469:GLN:NE2 | 1:C:483:GLY:H | 2.13 | 0.44 |
| 1:E:417:ASN:OD1 | 1:E:417:ASN:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:133:LEU:HD11 | 1:F:253:ALA:HB3 | 1.99 | 0.44 |
| 1:F:275:ILE:CG2 | 1:F:284:ILE:HD12 | 2.48 | 0.44 |
| 1:A:86:GLN:OE1 | 1:A:432:LEU:HD13 | 2.17 | 0.44 |
| 1:B:337:GLU:HG2 | 1:B:340:THR:O | 2.18 | 0.44 |
| 1:D:140:VAL:HG13 | 1:D:144:LEU:HD12 | 2.00 | 0.44 |
| 1:E:201:ASP:N | 1:E:201:ASP:OD1 | 2.50 | 0.44 |
| 1:F:373:LEU:HA | 1:F:373:LEU:HD23 | 1.75 | 0.44 |
| 1:F:474:LYS:O | 1:F:475:GLY:C | 2.60 | 0.44 |
| 1:H:101:VAL:O | 1:H:101:VAL:HG12 | 2.15 | 0.44 |
| 1:B:417:ASN:OD1 | 1:B:417:ASN:N | 2.50 | 0.44 |
| 1:D:199:THR:HG22 | 1:D:215:LYS:HB3 | 1.99 | 0.44 |
| 1:E:113:LEU:O | 1:E:113:LEU:HD23 | 2.17 | 0.44 |
| 1:G:266:ILE:HB | 1:G:326:VAL:HG22 | 1.99 | 0.44 |
| 1:F:419:PRO:O | 1:F:450:LEU:HD12 | 2.17 | 0.44 |
| 1:H:363:PHE:CD2 | 1:H:369:LEU:HD12 | 2.53 | 0.44 |
| 1:A:338:LEU:HD12 | 1:A:338:LEU:HA | 1.70 | 0.44 |
| 1:G:489:THR:O | 1:G:493:LEU:HD13 | 2.18 | 0.44 |
| 1:B:387:ALA:CB | 1:H:262:GLU:OE1 | 2.66 | 0.44 |
| 1:B:486:ASP:HB3 | 1:B:489:THR:HG23 | 2.00 | 0.44 |
| 1:E:91:PHE:CB | 1:H:72:ILE:HD13 | 2.41 | 0.44 |
| 1:E:347:MET:HB2 | 1:E:347:MET:HE3 | 1.69 | 0.44 |
| 1:E:359:SER:OG | 1:E:362:GLU:HB2 | 2.17 | 0.44 |
| 1:F:74:LEU:HD21 | 1:G:75:LEU:HD11 | 1.99 | 0.44 |
| 1:G:189:ARG:HE | 1:G:189:ARG:HB3 | 1.64 | 0.44 |
| 1:G:474:LYS:O | 1:G:475:GLY:C | 2.60 | 0.44 |
| 1:A:386:VAL:HG13 | 1:A:390:LEU:HD22 | 1.98 | 0.44 |
| 1:A:393:LEU:CD2 | 1:A:398:PHE:CD1 | 3.00 | 0.44 |
| 1:B:139:GLN:OE1 | 1:B:139:GLN:N | 2.49 | 0.44 |
| 1:E:275:ILE:HG21 | 1:E:284:ILE:HD12 | 2.00 | 0.44 |
| 1:E:400:SER:O | 1:E:400:SER:OG | 2.23 | 0.44 |
| 1:F:244:GLN:NE2 | 1:F:245:MET:H | 2.16 | 0.44 |
| 1:G:408:ALA:HB1 | 1:G:426:CYS:SG | 2.57 | 0.44 |
| 1:B:124:TYR:CG | 1:B:188:VAL:HG13 | 2.52 | 0.43 |
| 1:B:359:SER:OG | 1:B:362:GLU:HB2 | 2.18 | 0.43 |
| 1:D:295:ASP:HA | 1:D:298:LYS:HG2 | 2.00 | 0.43 |
| 1:E:113:LEU:C | 1:E:113:LEU:CD2 | 2.91 | 0.43 |
| 1:E:461:ILE:O | 1:E:462:ALA:C | 2.60 | 0.43 |
| 1:A:418:VAL:HG21 | 1:A:493:LEU:CD1 | 2.45 | 0.43 |
| 1:B:479:LEU:HD12 | 1:B:480:PHE:N | 2.33 | 0.43 |
| 1:C:193:ILE:HB | 1:C:234:LEU:HD23 | 2.00 | 0.43 |
| 1:C:258:ALA:O | 1:C:320:LEU:HD21 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:203:LEU:HD22 | 1:G:208:TYR:CE2 | 2.53 | 0.43 |
| 1:G:369:LEU:HD21 | 1:G:373:LEU:HD11 | 1.99 | 0.43 |
| 1:A:68:ARG:O | 1:A:72:ILE:HD12 | 2.18 | 0.43 |
| 1:A:417:ASN:N | 1:A:417:ASN:OD1 | 2.51 | 0.43 |
| 1:C:104:VAL:HG11 | 1:C:116:LEU:CD2 | 2.48 | 0.43 |
| 1:C:352:TYR:CE2 | 1:C:405:PRO:HG3 | 2.53 | 0.43 |
| 1:C:359:SER:OG | 1:C:362:GLU:HB2 | 2.19 | 0.43 |
| 1:D:474:LYS:CE | 1:D:501:CYS:SG | 3.06 | 0.43 |
| 1:D:488:ASN:HA | 1:D:491:SER:OG | 2.19 | 0.43 |
| 1:F:113:LEU:C | 1:F:113:LEU:CD2 | 2.91 | 0.43 |
| 1:F:359:SER:OG | 1:F:362:GLU:HB2 | 2.17 | 0.43 |
| 1:G:74:LEU:CD1 | 1:G:87:TYR:CE2 | 3.02 | 0.43 |
| 1:G:456:GLU:OE2 | 1:G:473:LEU:HD21 | 2.19 | 0.43 |
| 1:G:488:ASN:HA | 1:G:491:SER:OG | 2.19 | 0.43 |
| 1:C:270:ASN:ND2 | 1:C:272:LYS:HB2 | 2.34 | 0.43 |
| 1:D:365:SER:O | 1:D:365:SER:OG | 2.36 | 0.43 |
| 1:D:418:VAL:HG11 | 1:D:484:ILE:HD13 | 1.99 | 0.43 |
| 1:F:474:LYS:HD2 | 1:F:501:CYS:SG | 2.58 | 0.43 |
| 1:H:73:GLN:OE1 | 1:H:118:SER:O | 2.36 | 0.43 |
| 1:D:342:SER:O | 1:D:343:GLY:C | 2.61 | 0.43 |
| 1:E:406:LEU:HD12 | 1:E:409:VAL:CG2 | 2.49 | 0.43 |
| 1:F:114:HIS:C | 1:F:114:HIS:CD2 | 2.97 | 0.43 |
| 1:G:365:SER:O | 1:G:365:SER:OG | 2.36 | 0.43 |
| 1:G:458:ASP:O | 1:G:459:ALA:C | 2.61 | 0.43 |
| 1:H:73:GLN:CG | 1:H:335:GLN:OE1 | 2.60 | 0.43 |
| 1:A:363:PHE:CE1 | 1:A:369:LEU:HD12 | 2.52 | 0.43 |
| 1:B:275:ILE:HG21 | 1:B:284:ILE:HD12 | 2.00 | 0.43 |
| 1:E:330:ASN:HD21 | 1:E:332:GLN:HE21 | 1.65 | 0.43 |
| 1:F:97:GLN:OE1 | 1:F:264:LEU:HD23 | 2.12 | 0.43 |
| 1:F:275:ILE:HG21 | 1:F:284:ILE:HD12 | 2.01 | 0.43 |
| 1:F:277:ASN:ND2 | 1:F:280:THR:OG1 | 2.52 | 0.43 |
| 1:F:338:LEU:HD12 | 1:F:338:LEU:HA | 1.73 | 0.43 |
| 1:G:393:LEU:HD11 | 1:G:411:ILE:HD13 | 2.00 | 0.43 |
| 1:H:408:ALA:HB3 | 1:H:435:VAL:HG11 | 1.99 | 0.43 |
| 1:B:308:LEU:HD23 | 1:B:308:LEU:O | 2.18 | 0.43 |
| 1:D:193:ILE:HG21 | 1:D:234:LEU:CD1 | 2.47 | 0.43 |
| 1:D:376:ASP:HB2 | 1:D:425:VAL:HG22 | 2.00 | 0.43 |
| 1:D:474:LYS:HD2 | 1:D:501:CYS:SG | 2.58 | 0.43 |
| 1:F:401:TYR:CD2 | 1:F:443:LEU:CD1 | 3.01 | 0.43 |
| 1:H:400:SER:O | 1:H:400:SER:OG | 2.23 | 0.43 |
| 1:H:474:LYS:CE | 1:H:501:CYS:SG | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:393:LEU:CD2 | 1:B:398:PHE:CG | 3.01 | 0.43 |
| 1:C:417:ASN:OD1 | 1:C:417:ASN:N | 2.52 | 0.43 |
| 1:D:133:LEU:HD23 | 1:D:254:ALA:HA | 2.01 | 0.43 |
| 1:D:279:SER:HB2 | 1:D:301:TRP:CD1 | 2.54 | 0.43 |
| 1:E:329:ILE:HG21 | 1:E:329:ILE:HD13 | 1.75 | 0.43 |
| 1:F:180:VAL:HG13 | 1:F:190:ALA:HB3 | 2.00 | 0.43 |
| 1:F:379:ILE:CD1 | 1:F:423:LYS:HZ2 | 2.27 | 0.43 |
| 1:G:220:GLU:N | 1:G:221:PRO:CD | 2.82 | 0.43 |
| 1:H:97:GLN:HB3 | 1:H:264:LEU:CD2 | 2.48 | 0.43 |
| 1:A:359:SER:OG | 1:A:362:GLU:HB2 | 2.18 | 0.43 |
| 1:C:139:GLN:CA | 1:F:96:GLN:HE21 | 2.31 | 0.43 |
| 1:C:140:VAL:HG12 | 1:C:141:ASN:N | 2.33 | 0.43 |
| 1:D:488:ASN:HD22 | 1:D:488:ASN:C | 2.25 | 0.43 |
| 1:E:266:ILE:HB | 1:E:326:VAL:HG22 | 2.01 | 0.43 |
| 1:G:133:LEU:CD2 | 1:G:254:ALA:HA | 2.49 | 0.43 |
| 1:G:338:LEU:HD12 | 1:G:338:LEU:HA | 1.75 | 0.43 |
| 1:G:359:SER:OG | 1:G:362:GLU:HB2 | 2.19 | 0.43 |
| 1:G:370:ARG:CG | 1:G:386:VAL:HG11 | 2.43 | 0.43 |
| 1:H:139:GLN:OE1 | 1:H:139:GLN:N | 2.52 | 0.43 |
| 1:A:363:PHE:CE1 | 1:A:369:LEU:CD1 | 3.01 | 0.43 |
| 1:A:474:LYS:HD2 | 1:A:501:CYS:SG | 2.59 | 0.43 |
| 1:A:486:ASP:CB | 1:A:489:THR:HG23 | 2.48 | 0.43 |
| 1:D:180:VAL:HG13 | 1:D:190:ALA:HB1 | 2.01 | 0.43 |
| 1:D:259:ARG:HG3 | 1:D:316:LEU:CD1 | 2.49 | 0.43 |
| 1:D:452:TRP:O | 1:D:479:LEU:HD12 | 2.19 | 0.43 |
| 1:E:337:GLU:HG2 | 1:E:340:THR:O | 2.19 | 0.43 |
| 1:G:474:LYS:CE | 1:G:501:CYS:SG | 3.07 | 0.43 |
| 1:G:474:LYS:HD2 | 1:G:501:CYS:SG | 2.59 | 0.43 |
| 1:H:482:TYR:CD1 | 1:H:482:TYR:C | 2.97 | 0.43 |
| 1:B:193:ILE:CG2 | 1:B:234:LEU:HD22 | 2.49 | 0.42 |
| 1:D:359:SER:OG | 1:D:362:GLU:HB2 | 2.19 | 0.42 |
| 1:E:491:SER:HB3 | 1:H:487:ILE:HD11 | 2.00 | 0.42 |
| 1:F:136:THR:HG22 | 1:F:172:PHE:CZ | 2.53 | 0.42 |
| 1:F:184:GLU:HA | 1:F:188:VAL:O | 2.19 | 0.42 |
| 1:G:418:VAL:CG2 | 1:G:493:LEU:HD11 | 2.37 | 0.42 |
| 1:H:173:LEU:N | 1:H:173:LEU:HD23 | 2.33 | 0.42 |
| 1:A:354:LEU:HD12 | 1:A:438:ASN:ND2 | 2.34 | 0.42 |
| 1:B:372:ALA:O | 1:B:375:ARG:HG2 | 2.18 | 0.42 |
| 1:B:474:LYS:HD2 | 1:B:501:CYS:SG | 2.59 | 0.42 |
| 1:B:487:ILE:HD11 | 1:C:491:SER:HA | 2.01 | 0.42 |
| 1:D:109:ILE:HG21 | 1:D:175:GLN:HG3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:276:ILE:HG23 | 1:D:281:GLY:O | 2.18 | 0.42 |
| 1:E:124:TYR:CG | 1:E:188:VAL:HG13 | 2.54 | 0.42 |
| 1:E:275:ILE:CG2 | 1:E:284:ILE:HD12 | 2.49 | 0.42 |
| 1:E:365:SER:OG | 1:E:365:SER:O | 2.36 | 0.42 |
| 1:F:122:PHE:O | 1:F:123:LEU:C | 2.62 | 0.42 |
| 1:F:488:ASN:HD22 | 1:F:489:THR:N | 2.17 | 0.42 |
| 1:G:203:LEU:HD22 | 1:G:208:TYR:CD2 | 2.54 | 0.42 |
| 1:H:365:SER:O | 1:H:365:SER:OG | 2.37 | 0.42 |
| 1:H:417:ASN:N | 1:H:417:ASN:OD1 | 2.52 | 0.42 |
| 1:A:169:ARG:NE | 1:A:245:MET:HE3 | 2.34 | 0.42 |
| 1:A:210:LEU:N | 1:A:210:LEU:HD12 | 2.34 | 0.42 |
| 1:A:308:LEU:HA | 1:A:308:LEU:HD12 | 1.78 | 0.42 |
| 1:B:365:SER:O | 1:B:365:SER:OG | 2.35 | 0.42 |
| 1:C:365:SER:O | 1:C:365:SER:OG | 2.36 | 0.42 |
| 1:F:390:LEU:HD12 | 1:F:390:LEU:HA | 1.69 | 0.42 |
| 1:A:91:PHE:HE1 | 1:A:126:VAL:O | 2.02 | 0.42 |
| 1:A:432:LEU:C | 1:A:432:LEU:HD12 | 2.44 | 0.42 |
| 1:A:454:VAL:HG12 | 1:A:455:SER:N | 2.34 | 0.42 |
| 1:E:390:LEU:HD12 | 1:E:390:LEU:HA | 1.89 | 0.42 |
| 1:F:70:THR:HG23 | 1:F:122:PHE:CD1 | 2.53 | 0.42 |
| 1:F:123:LEU:HD21 | 1:F:338:LEU:HD23 | 2.00 | 0.42 |
| 1:F:473:LEU:HD12 | 1:F:473:LEU:C | 2.43 | 0.42 |
| 1:H:139:GLN:HE21 | 1:H:175:GLN:CD | 2.27 | 0.42 |
| 1:H:431:TRP:CE2 | 1:H:436:THR:HG21 | 2.54 | 0.42 |
| 1:A:403:ASP:OD1 | 1:A:403:ASP:N | 2.52 | 0.42 |
| 1:C:474:LYS:CE | 1:C:501:CYS:SG | 3.08 | 0.42 |
| 1:E:91:PHE:HB3 | 1:H:72:ILE:HD11 | 1.95 | 0.42 |
| 1:E:197:VAL:HG21 | 1:E:234:LEU:CD1 | 2.49 | 0.42 |
| 1:E:206:ASP:N | 1:E:206:ASP:OD1 | 2.53 | 0.42 |
| 1:E:318:ASP:O | 1:E:319:TYR:HD1 | 2.02 | 0.42 |
| 1:E:458:ASP:O | 1:E:459:ALA:C | 2.63 | 0.42 |
| 1:F:84:VAL:HG21 | 1:G:78:ILE:HG22 | 2.02 | 0.42 |
| 1:H:376:ASP:HB2 | 1:H:425:VAL:HG22 | 2.00 | 0.42 |
| 1:A:401:TYR:CE1 | 1:A:442:VAL:HG11 | 2.55 | 0.42 |
| 1:B:461:ILE:O | 1:B:462:ALA:C | 2.61 | 0.42 |
| 1:B:470:GLY:HA3 | 1:B:481:TRP:CZ2 | 2.54 | 0.42 |
| 1:E:100:ALA:HA | 1:E:265:LYS:O | 2.19 | 0.42 |
| 1:E:336:LYS:C | 1:E:340:THR:HG22 | 2.45 | 0.42 |
| 1:E:474:LYS:CE | 1:E:501:CYS:SG | 3.07 | 0.42 |
| 1:F:386:VAL:CG1 | 1:F:390:LEU:CD2 | 2.95 | 0.42 |
| 1:F:431:TRP:CE2 | 1:F:436:THR:HG21 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:457:ASN:ND2 | 1:H:457:ASN:N | 2.66 | 0.42 |
| 1:B:220:GLU:N | 1:B:221:PRO:CD | 2.83 | 0.42 |
| 1:C:104:VAL:HG11 | 1:C:116:LEU:HD21 | 2.02 | 0.42 |
| 1:C:234:LEU:HD12 | 1:C:257:LEU:HD11 | 2.02 | 0.42 |
| 1:D:113:LEU:C | 1:D:113:LEU:CD2 | 2.93 | 0.42 |
| 1:G:184:GLU:HA | 1:G:188:VAL:O | 2.20 | 0.42 |
| 1:A:122:PHE:O | 1:A:123:LEU:C | 2.62 | 0.42 |
| 1:A:484:ILE:HG21 | 1:A:484:ILE:HD13 | 1.78 | 0.42 |
| 1:B:338:LEU:HD12 | 1:B:338:LEU:HA | 1.88 | 0.42 |
| 1:C:269:LEU:HD23 | 1:C:269:LEU:HA | 1.81 | 0.42 |
| 1:C:337:GLU:HG2 | 1:C:340:THR:O | 2.20 | 0.42 |
| 1:D:189:ARG:HE | 1:D:189:ARG:HB3 | 1.67 | 0.42 |
| 1:D:330:ASN:OD1 | 1:D:331:VAL:N | 2.52 | 0.42 |
| 1:E:386:VAL:CG1 | 1:E:390:LEU:HD22 | 2.49 | 0.42 |
| 1:F:140:VAL:HG12 | 1:F:141:ASN:H | 1.79 | 0.42 |
| 1:G:208:TYR:HB3 | 1:G:211:VAL:CG2 | 2.50 | 0.42 |
| 1:C:421:LEU:HB3 | 1:C:452:TRP:HB3 | 2.02 | 0.42 |
| 1:E:207:LYS:HB3 | 1:E:208:TYR:CD2 | 2.55 | 0.42 |
| 1:H:474:LYS:HD2 | 1:H:501:CYS:SG | 2.59 | 0.42 |
| 1:H:479:LEU:HD22 | 1:H:497:PHE:HB2 | 2.02 | 0.42 |
| 1:A:406:LEU:HD12 | 1:A:409:VAL:CG2 | 2.50 | 0.42 |
| 1:B:316:LEU:HA | 1:B:316:LEU:HD12 | 1.76 | 0.42 |
| 1:C:150:GLU:N | 1:F:407:GLU:OE2 | 2.48 | 0.42 |
| 1:C:373:LEU:HD23 | 1:C:373:LEU:HA | 1.83 | 0.42 |
| 1:C:474:LYS:HD2 | 1:C:501:CYS:SG | 2.60 | 0.42 |
| 1:D:139:GLN:HE21 | 1:D:175:GLN:CD | 2.28 | 0.42 |
| 1:E:234:LEU:HD12 | 1:E:257:LEU:HD11 | 2.02 | 0.42 |
| 1:E:454:VAL:HG21 | 1:E:464:HIS:CG | 2.54 | 0.42 |
| 1:F:139:GLN:HG3 | 1:F:175:GLN:HE22 | 1.85 | 0.42 |
| 1:F:393:LEU:HD21 | 1:F:398:PHE:CG | 2.55 | 0.42 |
| 1:H:197:VAL:HG12 | 1:H:198:PHE:CD2 | 2.55 | 0.42 |
| 1:H:458:ASP:O | 1:H:459:ALA:C | 2.63 | 0.42 |
| 1:B:418:VAL:O | 1:B:419:PRO:C | 2.61 | 0.41 |
| 1:D:86:GLN:O | 1:D:89:LYS:HB2 | 2.20 | 0.41 |
| 1:D:498:VAL:CG1 | 1:D:499:LYS:N | 2.79 | 0.41 |
| 1:E:354:LEU:CD2 | 1:E:439:VAL:HG22 | 2.50 | 0.41 |
| 1:F:458:ASP:O | 1:F:459:ALA:C | 2.62 | 0.41 |
| 1:G:113:LEU:O | 1:G:113:LEU:HD23 | 2.20 | 0.41 |
| 1:H:354:LEU:HD21 | 1:H:439:VAL:HG22 | 2.02 | 0.41 |
| 1:H:486:ASP:HB3 | 1:H:489:THR:HG23 | 2.02 | 0.41 |
| 1:C:431:TRP:CE2 | 1:C:436:THR:HG21 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:184:GLU:HA | 1:E:188:VAL:O | 2.19 | 0.41 |
| 1:F:474:LYS:CE | 1:F:501:CYS:SG | 3.08 | 0.41 |
| 1:A:297:MET:HE3 | 1:A:307:LYS:HB3 | 2.02 | 0.41 |
| 1:A:469:GLN:NE2 | 1:A:483:GLY:H | 2.17 | 0.41 |
| 1:B:130:PRO:HG2 | 1:B:231:LEU:HD22 | 2.02 | 0.41 |
| 1:G:116:LEU:CD1 | 1:G:179:LEU:HD11 | 2.49 | 0.41 |
| 1:H:386:VAL:HG13 | 1:H:390:LEU:HD22 | 2.00 | 0.41 |
| 1:B:211:VAL:HG13 | 1:B:247:ASN:O | 2.20 | 0.41 |
| 1:C:379:ILE:HD11 | 1:C:423:LYS:NZ | 2.35 | 0.41 |
| 1:E:133:LEU:HD23 | 1:E:254:ALA:HA | 2.02 | 0.41 |
| 1:F:421:LEU:HB3 | 1:F:452:TRP:HB3 | 2.02 | 0.41 |
| 1:F:425:VAL:O | 1:F:425:VAL:HG12 | 2.16 | 0.41 |
| 1:G:122:PHE:O | 1:G:123:LEU:C | 2.62 | 0.41 |
| 1:G:337:GLU:HG2 | 1:G:340:THR:O | 2.20 | 0.41 |
| 1:H:225:SER:O | 1:H:226:ILE:C | 2.62 | 0.41 |
| 1:H:488:ASN:HD22 | 1:H:489:THR:N | 2.18 | 0.41 |
| 1:A:88:LEU:HD23 | 1:A:88:LEU:HA | 1.70 | 0.41 |
| 1:A:139:GLN:HE21 | 1:A:175:GLN:CD | 2.29 | 0.41 |
| 1:B:443:LEU:HA | 1:B:443:LEU:HD12 | 1.66 | 0.41 |
| 1:C:121:ALA:HA | 1:C:188:VAL:HG21 | 2.01 | 0.41 |
| 1:D:113:LEU:HD23 | 1:D:113:LEU:C | 2.45 | 0.41 |
| 1:D:393:LEU:HA | 1:D:393:LEU:HD23 | 1.67 | 0.41 |
| 1:F:113:LEU:HD23 | 1:F:113:LEU:O | 2.20 | 0.41 |
| 1:G:136:THR:HG22 | 1:G:172:PHE:CZ | 2.56 | 0.41 |
| 1:G:470:GLY:HA3 | 1:G:481:TRP:CZ2 | 2.56 | 0.41 |
| 1:H:403:ASP:OD1 | 1:H:403:ASP:N | 2.53 | 0.41 |
| 1:H:456:GLU:OE2 | 1:H:473:LEU:HD21 | 2.20 | 0.41 |
| 1:B:86:GLN:O | 1:B:89:LYS:HB2 | 2.20 | 0.41 |
| 1:B:370:ARG:NH1 | 1:H:323:SER:OG | 2.52 | 0.41 |
| 1:B:485:ASP:HB3 | 1:C:472:TYR:HH | 1.85 | 0.41 |
| 1:E:375:ARG:HA | 1:E:375:ARG:HD2 | 1.96 | 0.41 |
| 1:F:337:GLU:O | 1:F:347:MET:HE1 | 2.20 | 0.41 |
| 1:G:297:MET:HE3 | 1:G:307:LYS:HG2 | 2.02 | 0.41 |
| 1:G:372:ALA:O | 1:G:425:VAL:HG11 | 2.20 | 0.41 |
| 1:H:379:ILE:HD11 | 1:H:423:LYS:NZ | 2.36 | 0.41 |
| 1:A:354:LEU:HD21 | 1:A:439:VAL:CG2 | 2.50 | 0.41 |
| 1:D:244:GLN:HE21 | 1:D:245:MET:N | 2.18 | 0.41 |
| 1:F:144:LEU:CD2 | 1:F:167:VAL:HG11 | 2.49 | 0.41 |
| 1:F:189:ARG:HE | 1:F:189:ARG:HB3 | 1.65 | 0.41 |
| 1:G:100:ALA:HA | 1:G:265:LYS:O | 2.21 | 0.41 |
| 1:A:337:GLU:HG2 | 1:A:340:THR:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:VAL:CG1 | 1:A:390:LEU:HD22 | 2.51 | 0.41 |
| 1:B:488:ASN:HA | 1:B:491:SER:OG | 2.21 | 0.41 |
| 1:E:369:LEU:HD21 | 1:E:373:LEU:HD11 | 2.00 | 0.41 |
| 1:E:401:TYR:CD1 | 1:E:442:VAL:HG11 | 2.56 | 0.41 |
| 1:F:70:THR:HG23 | 1:F:122:PHE:HD1 | 1.86 | 0.41 |
| 1:F:407:GLU:HG3 | 1:F:430:ALA:HB2 | 2.03 | 0.41 |
| 1:F:443:LEU:HA | 1:F:443:LEU:HD12 | 1.80 | 0.41 |
| 1:A:91:PHE:O | 1:D:68:ARG:NH1 | 2.53 | 0.41 |
| 1:A:133:LEU:HD12 | 1:A:133:LEU:C | 2.46 | 0.41 |
| 1:A:292:GLU:O | 1:A:293:TYR:C | 2.64 | 0.41 |
| 1:A:351:GLY:C | 1:A:352:TYR:CD1 | 2.99 | 0.41 |
| 1:A:442:VAL:O | 1:A:443:LEU:C | 2.63 | 0.41 |
| 1:B:124:TYR:CD1 | 1:B:188:VAL:HG13 | 2.56 | 0.41 |
| 1:B:165:MET:HE1 | 1:B:246:LEU:CA | 2.51 | 0.41 |
| 1:B:269:LEU:HD23 | 1:B:269:LEU:HA | 1.90 | 0.41 |
| 1:B:404:GLU:N | 1:B:405:PRO:CD | 2.84 | 0.41 |
| 1:B:473:LEU:HD13 | 1:B:478:VAL:HG23 | 2.03 | 0.41 |
| 1:B:486:ASP:O | 1:B:487:ILE:C | 2.62 | 0.41 |
| 1:C:322:ARG:HD3 | 1:C:352:TYR:CZ | 2.56 | 0.41 |
| 1:D:120:LEU:HD23 | 1:D:120:LEU:HA | 1.66 | 0.41 |
| 1:D:289:LEU:HD23 | 1:D:289:LEU:HA | 1.94 | 0.41 |
| 1:D:404:GLU:N | 1:D:405:PRO:CD | 2.83 | 0.41 |
| 1:E:84:VAL:CG2 | 1:H:78:ILE:HG21 | 2.47 | 0.41 |
| 1:F:329:ILE:HG22 | 1:F:330:ASN:N | 2.36 | 0.41 |
| 1:F:365:SER:O | 1:F:365:SER:OG | 2.35 | 0.41 |
| 1:F:472:TYR:CD2 | 1:F:494:VAL:HG13 | 2.56 | 0.41 |
| 1:G:330:ASN:OD1 | 1:G:331:VAL:N | 2.54 | 0.41 |
| 1:G:393:LEU:CD2 | 1:G:398:PHE:CG | 3.04 | 0.41 |
| 1:H:99:PHE:CE2 | 1:H:123:LEU:HD22 | 2.56 | 0.41 |
| 1:H:121:ALA:HA | 1:H:188:VAL:HG21 | 2.01 | 0.41 |
| 1:H:369:LEU:CD2 | 1:H:373:LEU:CD1 | 2.97 | 0.41 |
| 1:A:125:HIS:C | 1:A:127:GLY:H | 2.29 | 0.41 |
| 1:A:183:LEU:HD13 | 1:A:190:ALA:HB2 | 2.03 | 0.41 |
| 1:A:379:ILE:HD13 | 1:A:379:ILE:HG21 | 1.85 | 0.41 |
| 1:B:214:ILE:HG13 | 1:B:248:VAL:HG11 | 2.01 | 0.41 |
| 1:E:470:GLY:HA3 | 1:E:481:TRP:CZ2 | 2.56 | 0.41 |
| 1:F:491:SER:C | 1:G:487:ILE:HD11 | 2.46 | 0.41 |
| 1:H:133:LEU:HD12 | 1:H:254:ALA:HA | 2.02 | 0.41 |
| 1:B:144:LEU:HD12 | 1:B:149:ILE:CG2 | 2.51 | 0.40 |
| 1:B:265:LYS:HE3 | 1:B:347:MET:HE1 | 2.02 | 0.40 |
| 1:E:71:VAL:HG13 | 1:H:74:LEU:CD2 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:ILE:HG21 | 1:E:102:ILE:HD13 | 1.76 | 0.40 |
| 1:E:184:GLU:OE1 | 1:F:228:ALA:HB1 | 2.21 | 0.40 |
| 1:E:257:LEU:HD23 | 1:E:257:LEU:HA | 1.79 | 0.40 |
| 1:E:316:LEU:HD12 | 1:E:316:LEU:HA | 1.66 | 0.40 |
| 1:H:337:GLU:C | 1:H:339:PHE:N | 2.77 | 0.40 |
| 1:H:404:GLU:N | 1:H:405:PRO:CD | 2.83 | 0.40 |
| 1:B:313:ILE:CD1 | 1:B:326:VAL:HG11 | 2.49 | 0.40 |
| 1:B:379:ILE:O | 1:B:379:ILE:HG22 | 2.21 | 0.40 |
| 1:C:286:MET:HA | 1:C:347:MET:O | 2.21 | 0.40 |
| 1:C:360:ILE:HD11 | 1:C:393:LEU:HD13 | 2.03 | 0.40 |
| 1:D:286:MET:HG3 | 1:D:347:MET:HB3 | 2.03 | 0.40 |
| 1:E:191:ARG:HD2 | 1:E:225:SER:HB2 | 2.03 | 0.40 |
| 1:E:289:LEU:HD13 | 1:E:314:LYS:HA | 2.02 | 0.40 |
| 1:E:328:ILE:HG21 | 1:E:328:ILE:HD13 | 1.64 | 0.40 |
| 1:E:374:GLN:HE21 | 1:E:374:GLN:HB3 | 1.76 | 0.40 |
| 1:F:193:ILE:HB | 1:F:234:LEU:CD2 | 2.51 | 0.40 |
| 1:F:461:ILE:O | 1:F:462:ALA:C | 2.62 | 0.40 |
| 1:H:408:ALA:HB1 | 1:H:426:CYS:SG | 2.61 | 0.40 |
| 1:A:172:PHE:CD2 | 1:A:237:LEU:HD21 | 2.56 | 0.40 |
| 1:B:403:ASP:OD1 | 1:B:403:ASP:N | 2.54 | 0.40 |
| 1:C:169:ARG:NE | 1:C:245:MET:HE3 | 2.36 | 0.40 |
| 1:D:104:VAL:HG22 | 1:D:269:LEU:HD12 | 2.03 | 0.40 |
| 1:D:303:LYS:HA | 1:D:303:LYS:HD2 | 1.93 | 0.40 |
| 1:E:289:LEU:O | 1:E:290:ASP:C | 2.64 | 0.40 |
| 1:E:474:LYS:HD2 | 1:E:501:CYS:SG | 2.61 | 0.40 |
| 1:F:379:ILE:HG21 | 1:F:386:VAL:CG2 | 2.37 | 0.40 |
| 1:F:418:VAL:HG21 | 1:F:493:LEU:CD1 | 2.49 | 0.40 |
| 1:H:336:LYS:O | 1:H:337:GLU:C | 2.64 | 0.40 |
| 1:H:359:SER:OG | 1:H:362:GLU:HB2 | 2.21 | 0.40 |
| 1:B:165:MET:CE | 1:B:245:MET:O | 2.70 | 0.40 |
| 1:B:458:ASP:O | 1:B:459:ALA:C | 2.64 | 0.40 |
| 1:C:473:LEU:HD13 | 1:C:478:VAL:HG23 | 2.01 | 0.40 |
| 1:C:479:LEU:HD22 | 1:C:497:PHE:HB2 | 2.03 | 0.40 |
| 1:D:206:ASP:OD1 | 1:D:206:ASP:N | 2.54 | 0.40 |
| 1:E:180:VAL:HG13 | 1:E:190:ALA:CB | 2.47 | 0.40 |
| 1:G:375:ARG:HA | 1:G:375:ARG:HD2 | 1.97 | 0.40 |
| 1:H:94:VAL:CG1 | 1:H:96:GLN:NE2 | 2.85 | 0.40 |
| 1:H:131:ILE:HD13 | 1:H:222:ILE:HG21 | 2.04 | 0.40 |
| 1:A:68:ARG:O | 1:A:69:SER:C | 2.65 | 0.40 |
| 1:A:233:ILE:C | 1:A:234:LEU:HD12 | 2.46 | 0.40 |
| 1:D:175:GLN:HE21 | 1:D:175:GLN:HB2 | 1.67 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:SER:O | 1:D:226:ILE:C | 2.64 | 0.40 |
| 1:D:288:ASN:OD1 | 1:D:438:ASN:ND2 | 2.55 | 0.40 |
| 1:E:289:LEU:HD23 | 1:E:289:LEU:HA | 1.73 | 0.40 |
| 1:E:352:TYR:HE1 | 1:E:433:ASN:HD22 | 1.69 | 0.40 |
| 1:E:403:ASP:OD1 | 1:E:403:ASP:N | 2.54 | 0.40 |
| 1:E:488:ASN:HA | 1:E:491:SER:OG | 2.21 | 0.40 |
| 1:F:288:ASN:ND2 | 1:F:438:ASN:ND2 | 2.55 | 0.40 |
| 1:G:72:ILE:HD12 | 1:G:72:ILE:N | 2.35 | 0.40 |
| 1:G:206:ASP:OD1 | 1:G:206:ASP:N | 2.55 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:B:304:TYR:OH | 1:G:495:GLU:OE2[1_546] | 2.15 | 0.05 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 434/464 (94%) | 386 (89%) | 44 (10%) | 4 (1%) | 14 | 45 |
| 1 | B | 434/464 (94%) | 386 (89%) | 44 (10%) | 4 (1%) | 14 | 45 |
| 1 | C | 434/464 (94%) | 385 (89%) | 45 (10%) | 4 (1%) | 14 | 45 |
| 1 | D | 434/464 (94%) | 386 (89%) | 44 (10%) | 4 (1%) | 14 | 45 |
| 1 | E | 434/464 (94%) | 387 (89%) | 43 (10%) | 4 (1%) | 14 | 45 |
| 1 | F | 434/464 (94%) | 387 (89%) | 43 (10%) | 4 (1%) | 14 | 45 |
| 1 | G | 434/464 (94%) | 388 (89%) | 42 (10%) | 4 (1%) | 14 | 45 |
| 1 | H | 434/464 (94%) | 381 (88%) | 46 (11%) | 7 (2%) | 7 | 35 |
| All | All | 3472/3712 (94%) | 3086 (89%) | 351 (10%) | 35 (1%) | 12 | 43 |

All (35) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 343 | GLY |
| 1 | H | 343 | GLY |
| 1 | C | 434 | ASN |
| 1 | D | 434 | ASN |
| 1 | E | 434 | ASN |
| 1 | F | 434 | ASN |
| 1 | F | 501 | CYS |
| 1 | G | 434 | ASN |
| 1 | H | 434 | ASN |
| 1 | A | 501 | CYS |
| 1 | B | 501 | CYS |
| 1 | C | 321 | PRO |
| 1 | C | 501 | CYS |
| 1 | D | 501 | CYS |
| 1 | G | 69 | SER |
| 1 | H | 98 | GLN |
| 1 | H | 501 | CYS |
| 1 | B | 98 | GLN |
| 1 | B | 475 | GLY |
| 1 | E | 501 | CYS |
| 1 | H | 69 | SER |
| 1 | H | 475 | GLY |
| 1 | A | 443 | LEU |
| 1 | A | 475 | GLY |
| 1 | C | 475 | GLY |
| 1 | E | 443 | LEU |
| 1 | F | 475 | GLY |
| 1 | B | 321 | PRO |
| 1 | D | 475 | GLY |
| 1 | E | 475 | GLY |
| 1 | G | 475 | GLY |
| 1 | H | 443 | LEU |
| 1 | F | 321 | PRO |
| 1 | G | 321 | PRO |
| 1 | A | 321 | PRO |

5.3.2 Protein sidechains [i](#)

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 | 372/397 (94%) | 317 (85%) | 55 (15%) | 3 | 16 |
| 1 | B | 372/397 (94%) | 315 (85%) | 57 (15%) | 3 | 16 |
| 1 | C | 373/397 (94%) | 314 (84%) | 59 (16%) | 2 | 15 |
| 1 | D | 372/397 (94%) | 310 (83%) | 62 (17%) | 2 | 13 |
| 1 | E | 373/397 (94%) | 318 (85%) | 55 (15%) | 3 | 17 |
| 1 | F | 373/397 (94%) | 313 (84%) | 60 (16%) | 2 | 14 |
| 1 | G | 373/397 (94%) | 319 (86%) | 54 (14%) | 3 | 17 |
| 1 | H | 373/397 (94%) | 308 (83%) | 65 (17%) | 2 | 12 |
| All | All | 2981/3176 (94%) | 2514 (84%) | 467 (16%) | 2 | 15 |

All (467) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 67 | THR |
| 1 | A | 68 | ARG |
| 1 | A | 78 | ILE |
| 1 | A | 95 | SER |
| 1 | A | 113 | LEU |
| 1 | A | 116 | LEU |
| 1 | A | 133 | LEU |
| 1 | A | 140 | VAL |
| 1 | A | 144 | LEU |
| 1 | A | 157 | ILE |
| 1 | A | 167 | VAL |
| 1 | A | 168 | VAL |
| 1 | A | 171 | CYS |
| 1 | A | 175 | GLN |
| 1 | A | 185 | GLN |
| 1 | A | 195 | SER |
| 1 | A | 199 | THR |
| 1 | A | 210 | LEU |
| 1 | A | 218 | THR |
| 1 | A | 220 | GLU |
| 1 | A | 239 | GLU |
| 1 | A | 246 | LEU |
| 1 | A | 264 | LEU |
| 1 | A | 286 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 296 | LEU |
| 1 | A | 322 | ARG |
| 1 | A | 329 | ILE |
| 1 | A | 337 | GLU |
| 1 | A | 338 | LEU |
| 1 | A | 341 | ASP |
| 1 | A | 347 | MET |
| 1 | A | 349 | ARG |
| 1 | A | 365 | SER |
| 1 | A | 374 | GLN |
| 1 | A | 375 | ARG |
| 1 | A | 383 | LYS |
| 1 | A | 386 | VAL |
| 1 | A | 390 | LEU |
| 1 | A | 393 | LEU |
| 1 | A | 400 | SER |
| 1 | A | 425 | VAL |
| 1 | A | 432 | LEU |
| 1 | A | 434 | ASN |
| 1 | A | 445 | ARG |
| 1 | A | 453 | VAL |
| 1 | A | 455 | SER |
| 1 | A | 457 | ASN |
| 1 | A | 460 | ASN |
| 1 | A | 469 | GLN |
| 1 | A | 484 | ILE |
| 1 | A | 485 | ASP |
| 1 | A | 486 | ASP |
| 1 | A | 488 | ASN |
| 1 | A | 491 | SER |
| 1 | A | 498 | VAL |
| 1 | B | 67 | THR |
| 1 | B | 68 | ARG |
| 1 | B | 71 | VAL |
| 1 | B | 78 | ILE |
| 1 | B | 82 | ARG |
| 1 | B | 84 | VAL |
| 1 | B | 113 | LEU |
| 1 | B | 133 | LEU |
| 1 | B | 140 | VAL |
| 1 | B | 157 | ILE |
| 1 | B | 168 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 171 | CYS |
| 1 | B | 175 | GLN |
| 1 | B | 185 | GLN |
| 1 | B | 195 | SER |
| 1 | B | 199 | THR |
| 1 | B | 203 | LEU |
| 1 | B | 210 | LEU |
| 1 | B | 213 | ASN |
| 1 | B | 218 | THR |
| 1 | B | 220 | GLU |
| 1 | B | 234 | LEU |
| 1 | B | 239 | GLU |
| 1 | B | 248 | VAL |
| 1 | B | 264 | LEU |
| 1 | B | 286 | MET |
| 1 | B | 295 | ASP |
| 1 | B | 322 | ARG |
| 1 | B | 329 | ILE |
| 1 | B | 337 | GLU |
| 1 | B | 338 | LEU |
| 1 | B | 341 | ASP |
| 1 | B | 347 | MET |
| 1 | B | 349 | ARG |
| 1 | B | 365 | SER |
| 1 | B | 375 | ARG |
| 1 | B | 383 | LYS |
| 1 | B | 390 | LEU |
| 1 | B | 393 | LEU |
| 1 | B | 400 | SER |
| 1 | B | 432 | LEU |
| 1 | B | 434 | ASN |
| 1 | B | 440 | PHE |
| 1 | B | 443 | LEU |
| 1 | B | 445 | ARG |
| 1 | B | 453 | VAL |
| 1 | B | 455 | SER |
| 1 | B | 457 | ASN |
| 1 | B | 460 | ASN |
| 1 | B | 469 | GLN |
| 1 | B | 484 | ILE |
| 1 | B | 485 | ASP |
| 1 | B | 486 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 487 | ILE |
| 1 | B | 488 | ASN |
| 1 | B | 491 | SER |
| 1 | B | 498 | VAL |
| 1 | C | 67 | THR |
| 1 | C | 68 | ARG |
| 1 | C | 69 | SER |
| 1 | C | 78 | ILE |
| 1 | C | 82 | ARG |
| 1 | C | 84 | VAL |
| 1 | C | 113 | LEU |
| 1 | C | 133 | LEU |
| 1 | C | 140 | VAL |
| 1 | C | 144 | LEU |
| 1 | C | 157 | ILE |
| 1 | C | 167 | VAL |
| 1 | C | 168 | VAL |
| 1 | C | 171 | CYS |
| 1 | C | 175 | GLN |
| 1 | C | 185 | GLN |
| 1 | C | 195 | SER |
| 1 | C | 197 | VAL |
| 1 | C | 199 | THR |
| 1 | C | 203 | LEU |
| 1 | C | 210 | LEU |
| 1 | C | 218 | THR |
| 1 | C | 220 | GLU |
| 1 | C | 239 | GLU |
| 1 | C | 245 | MET |
| 1 | C | 264 | LEU |
| 1 | C | 286 | MET |
| 1 | C | 295 | ASP |
| 1 | C | 308 | LEU |
| 1 | C | 322 | ARG |
| 1 | C | 329 | ILE |
| 1 | C | 337 | GLU |
| 1 | C | 338 | LEU |
| 1 | C | 341 | ASP |
| 1 | C | 347 | MET |
| 1 | C | 349 | ARG |
| 1 | C | 365 | SER |
| 1 | C | 375 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 383 | LYS |
| 1 | C | 391 | ARG |
| 1 | C | 393 | LEU |
| 1 | C | 400 | SER |
| 1 | C | 406 | LEU |
| 1 | C | 418 | VAL |
| 1 | C | 432 | LEU |
| 1 | C | 434 | ASN |
| 1 | C | 440 | PHE |
| 1 | C | 453 | VAL |
| 1 | C | 455 | SER |
| 1 | C | 457 | ASN |
| 1 | C | 460 | ASN |
| 1 | C | 469 | GLN |
| 1 | C | 484 | ILE |
| 1 | C | 485 | ASP |
| 1 | C | 486 | ASP |
| 1 | C | 488 | ASN |
| 1 | C | 491 | SER |
| 1 | C | 494 | VAL |
| 1 | C | 498 | VAL |
| 1 | D | 67 | THR |
| 1 | D | 68 | ARG |
| 1 | D | 78 | ILE |
| 1 | D | 82 | ARG |
| 1 | D | 94 | VAL |
| 1 | D | 103 | LYS |
| 1 | D | 113 | LEU |
| 1 | D | 116 | LEU |
| 1 | D | 140 | VAL |
| 1 | D | 144 | LEU |
| 1 | D | 157 | ILE |
| 1 | D | 167 | VAL |
| 1 | D | 168 | VAL |
| 1 | D | 171 | CYS |
| 1 | D | 175 | GLN |
| 1 | D | 185 | GLN |
| 1 | D | 195 | SER |
| 1 | D | 197 | VAL |
| 1 | D | 199 | THR |
| 1 | D | 218 | THR |
| 1 | D | 220 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 246 | LEU |
| 1 | D | 260 | VAL |
| 1 | D | 264 | LEU |
| 1 | D | 282 | GLU |
| 1 | D | 283 | LYS |
| 1 | D | 286 | MET |
| 1 | D | 288 | ASN |
| 1 | D | 296 | LEU |
| 1 | D | 297 | MET |
| 1 | D | 299 | GLN |
| 1 | D | 308 | LEU |
| 1 | D | 323 | SER |
| 1 | D | 324 | SER |
| 1 | D | 337 | GLU |
| 1 | D | 338 | LEU |
| 1 | D | 346 | THR |
| 1 | D | 347 | MET |
| 1 | D | 349 | ARG |
| 1 | D | 350 | ARG |
| 1 | D | 365 | SER |
| 1 | D | 375 | ARG |
| 1 | D | 383 | LYS |
| 1 | D | 391 | ARG |
| 1 | D | 393 | LEU |
| 1 | D | 400 | SER |
| 1 | D | 406 | LEU |
| 1 | D | 417 | ASN |
| 1 | D | 434 | ASN |
| 1 | D | 440 | PHE |
| 1 | D | 443 | LEU |
| 1 | D | 453 | VAL |
| 1 | D | 455 | SER |
| 1 | D | 457 | ASN |
| 1 | D | 460 | ASN |
| 1 | D | 469 | GLN |
| 1 | D | 484 | ILE |
| 1 | D | 485 | ASP |
| 1 | D | 486 | ASP |
| 1 | D | 488 | ASN |
| 1 | D | 491 | SER |
| 1 | D | 498 | VAL |
| 1 | E | 67 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | E | 68 | ARG |
| 1 | E | 78 | ILE |
| 1 | E | 113 | LEU |
| 1 | E | 116 | LEU |
| 1 | E | 140 | VAL |
| 1 | E | 144 | LEU |
| 1 | E | 157 | ILE |
| 1 | E | 167 | VAL |
| 1 | E | 168 | VAL |
| 1 | E | 171 | CYS |
| 1 | E | 175 | GLN |
| 1 | E | 185 | GLN |
| 1 | E | 195 | SER |
| 1 | E | 199 | THR |
| 1 | E | 213 | ASN |
| 1 | E | 218 | THR |
| 1 | E | 220 | GLU |
| 1 | E | 239 | GLU |
| 1 | E | 248 | VAL |
| 1 | E | 260 | VAL |
| 1 | E | 264 | LEU |
| 1 | E | 286 | MET |
| 1 | E | 295 | ASP |
| 1 | E | 308 | LEU |
| 1 | E | 322 | ARG |
| 1 | E | 331 | VAL |
| 1 | E | 337 | GLU |
| 1 | E | 338 | LEU |
| 1 | E | 341 | ASP |
| 1 | E | 347 | MET |
| 1 | E | 349 | ARG |
| 1 | E | 355 | VAL |
| 1 | E | 365 | SER |
| 1 | E | 375 | ARG |
| 1 | E | 383 | LYS |
| 1 | E | 390 | LEU |
| 1 | E | 393 | LEU |
| 1 | E | 400 | SER |
| 1 | E | 417 | ASN |
| 1 | E | 434 | ASN |
| 1 | E | 439 | VAL |
| 1 | E | 440 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | E | 442 | VAL |
| 1 | E | 443 | LEU |
| 1 | E | 453 | VAL |
| 1 | E | 455 | SER |
| 1 | E | 457 | ASN |
| 1 | E | 460 | ASN |
| 1 | E | 469 | GLN |
| 1 | E | 484 | ILE |
| 1 | E | 486 | ASP |
| 1 | E | 488 | ASN |
| 1 | E | 491 | SER |
| 1 | E | 498 | VAL |
| 1 | F | 67 | THR |
| 1 | F | 68 | ARG |
| 1 | F | 72 | ILE |
| 1 | F | 78 | ILE |
| 1 | F | 83 | GLU |
| 1 | F | 95 | SER |
| 1 | F | 98 | GLN |
| 1 | F | 113 | LEU |
| 1 | F | 118 | SER |
| 1 | F | 123 | LEU |
| 1 | F | 128 | LEU |
| 1 | F | 133 | LEU |
| 1 | F | 140 | VAL |
| 1 | F | 144 | LEU |
| 1 | F | 157 | ILE |
| 1 | F | 167 | VAL |
| 1 | F | 168 | VAL |
| 1 | F | 171 | CYS |
| 1 | F | 173 | LEU |
| 1 | F | 175 | GLN |
| 1 | F | 185 | GLN |
| 1 | F | 197 | VAL |
| 1 | F | 199 | THR |
| 1 | F | 217 | VAL |
| 1 | F | 218 | THR |
| 1 | F | 220 | GLU |
| 1 | F | 239 | GLU |
| 1 | F | 260 | VAL |
| 1 | F | 264 | LEU |
| 1 | F | 295 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | F | 296 | LEU |
| 1 | F | 308 | LEU |
| 1 | F | 322 | ARG |
| 1 | F | 337 | GLU |
| 1 | F | 338 | LEU |
| 1 | F | 341 | ASP |
| 1 | F | 347 | MET |
| 1 | F | 349 | ARG |
| 1 | F | 365 | SER |
| 1 | F | 375 | ARG |
| 1 | F | 383 | LYS |
| 1 | F | 390 | LEU |
| 1 | F | 393 | LEU |
| 1 | F | 400 | SER |
| 1 | F | 406 | LEU |
| 1 | F | 432 | LEU |
| 1 | F | 434 | ASN |
| 1 | F | 439 | VAL |
| 1 | F | 440 | PHE |
| 1 | F | 443 | LEU |
| 1 | F | 445 | ARG |
| 1 | F | 455 | SER |
| 1 | F | 457 | ASN |
| 1 | F | 460 | ASN |
| 1 | F | 469 | GLN |
| 1 | F | 484 | ILE |
| 1 | F | 486 | ASP |
| 1 | F | 488 | ASN |
| 1 | F | 491 | SER |
| 1 | F | 498 | VAL |
| 1 | G | 67 | THR |
| 1 | G | 68 | ARG |
| 1 | G | 78 | ILE |
| 1 | G | 113 | LEU |
| 1 | G | 116 | LEU |
| 1 | G | 140 | VAL |
| 1 | G | 144 | LEU |
| 1 | G | 157 | ILE |
| 1 | G | 171 | CYS |
| 1 | G | 173 | LEU |
| 1 | G | 175 | GLN |
| 1 | G | 185 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | G | 195 | SER |
| 1 | G | 197 | VAL |
| 1 | G | 210 | LEU |
| 1 | G | 218 | THR |
| 1 | G | 220 | GLU |
| 1 | G | 234 | LEU |
| 1 | G | 239 | GLU |
| 1 | G | 248 | VAL |
| 1 | G | 264 | LEU |
| 1 | G | 295 | ASP |
| 1 | G | 322 | ARG |
| 1 | G | 326 | VAL |
| 1 | G | 337 | GLU |
| 1 | G | 338 | LEU |
| 1 | G | 341 | ASP |
| 1 | G | 347 | MET |
| 1 | G | 349 | ARG |
| 1 | G | 365 | SER |
| 1 | G | 375 | ARG |
| 1 | G | 383 | LYS |
| 1 | G | 390 | LEU |
| 1 | G | 391 | ARG |
| 1 | G | 393 | LEU |
| 1 | G | 400 | SER |
| 1 | G | 406 | LEU |
| 1 | G | 417 | ASN |
| 1 | G | 432 | LEU |
| 1 | G | 434 | ASN |
| 1 | G | 439 | VAL |
| 1 | G | 440 | PHE |
| 1 | G | 453 | VAL |
| 1 | G | 455 | SER |
| 1 | G | 457 | ASN |
| 1 | G | 460 | ASN |
| 1 | G | 469 | GLN |
| 1 | G | 484 | ILE |
| 1 | G | 485 | ASP |
| 1 | G | 486 | ASP |
| 1 | G | 487 | ILE |
| 1 | G | 488 | ASN |
| 1 | G | 491 | SER |
| 1 | G | 498 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | H | 67 | THR |
| 1 | H | 68 | ARG |
| 1 | H | 72 | ILE |
| 1 | H | 78 | ILE |
| 1 | H | 83 | GLU |
| 1 | H | 84 | VAL |
| 1 | H | 88 | LEU |
| 1 | H | 95 | SER |
| 1 | H | 98 | GLN |
| 1 | H | 101 | VAL |
| 1 | H | 113 | LEU |
| 1 | H | 118 | SER |
| 1 | H | 133 | LEU |
| 1 | H | 140 | VAL |
| 1 | H | 157 | ILE |
| 1 | H | 167 | VAL |
| 1 | H | 168 | VAL |
| 1 | H | 171 | CYS |
| 1 | H | 175 | GLN |
| 1 | H | 185 | GLN |
| 1 | H | 197 | VAL |
| 1 | H | 199 | THR |
| 1 | H | 203 | LEU |
| 1 | H | 218 | THR |
| 1 | H | 220 | GLU |
| 1 | H | 248 | VAL |
| 1 | H | 264 | LEU |
| 1 | H | 283 | LYS |
| 1 | H | 286 | MET |
| 1 | H | 288 | ASN |
| 1 | H | 299 | GLN |
| 1 | H | 308 | LEU |
| 1 | H | 323 | SER |
| 1 | H | 324 | SER |
| 1 | H | 337 | GLU |
| 1 | H | 338 | LEU |
| 1 | H | 347 | MET |
| 1 | H | 349 | ARG |
| 1 | H | 350 | ARG |
| 1 | H | 365 | SER |
| 1 | H | 375 | ARG |
| 1 | H | 383 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | H | 386 | VAL |
| 1 | H | 390 | LEU |
| 1 | H | 391 | ARG |
| 1 | H | 393 | LEU |
| 1 | H | 400 | SER |
| 1 | H | 406 | LEU |
| 1 | H | 416 | THR |
| 1 | H | 432 | LEU |
| 1 | H | 434 | ASN |
| 1 | H | 435 | VAL |
| 1 | H | 440 | PHE |
| 1 | H | 443 | LEU |
| 1 | H | 453 | VAL |
| 1 | H | 455 | SER |
| 1 | H | 457 | ASN |
| 1 | H | 460 | ASN |
| 1 | H | 469 | GLN |
| 1 | H | 484 | ILE |
| 1 | H | 485 | ASP |
| 1 | H | 486 | ASP |
| 1 | H | 488 | ASN |
| 1 | H | 491 | SER |
| 1 | H | 498 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 77 | ASN |
| 1 | A | 114 | HIS |
| 1 | A | 175 | GLN |
| 1 | A | 213 | ASN |
| 1 | A | 335 | GLN |
| 1 | A | 374 | GLN |
| 1 | A | 438 | ASN |
| 1 | A | 457 | ASN |
| 1 | A | 469 | GLN |
| 1 | B | 96 | GLN |
| 1 | B | 213 | ASN |
| 1 | B | 244 | GLN |
| 1 | B | 438 | ASN |
| 1 | B | 488 | ASN |
| 1 | C | 86 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 114 | HIS |
| 1 | C | 175 | GLN |
| 1 | C | 213 | ASN |
| 1 | C | 244 | GLN |
| 1 | C | 374 | GLN |
| 1 | C | 457 | ASN |
| 1 | C | 469 | GLN |
| 1 | D | 86 | GLN |
| 1 | D | 114 | HIS |
| 1 | D | 147 | GLN |
| 1 | D | 175 | GLN |
| 1 | D | 185 | GLN |
| 1 | D | 213 | ASN |
| 1 | D | 247 | ASN |
| 1 | D | 299 | GLN |
| 1 | D | 374 | GLN |
| 1 | D | 433 | ASN |
| 1 | D | 438 | ASN |
| 1 | D | 469 | GLN |
| 1 | D | 488 | ASN |
| 1 | E | 77 | ASN |
| 1 | E | 97 | GLN |
| 1 | E | 114 | HIS |
| 1 | E | 175 | GLN |
| 1 | E | 185 | GLN |
| 1 | E | 213 | ASN |
| 1 | E | 332 | GLN |
| 1 | E | 374 | GLN |
| 1 | E | 433 | ASN |
| 1 | E | 438 | ASN |
| 1 | E | 457 | ASN |
| 1 | E | 469 | GLN |
| 1 | F | 96 | GLN |
| 1 | F | 114 | HIS |
| 1 | F | 175 | GLN |
| 1 | F | 213 | ASN |
| 1 | F | 244 | GLN |
| 1 | F | 277 | ASN |
| 1 | F | 288 | ASN |
| 1 | F | 374 | GLN |
| 1 | F | 433 | ASN |
| 1 | F | 438 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 451 | GLN |
| 1 | F | 469 | GLN |
| 1 | F | 488 | ASN |
| 1 | G | 86 | GLN |
| 1 | G | 114 | HIS |
| 1 | G | 175 | GLN |
| 1 | G | 213 | ASN |
| 1 | G | 244 | GLN |
| 1 | G | 374 | GLN |
| 1 | G | 433 | ASN |
| 1 | G | 469 | GLN |
| 1 | G | 488 | ASN |
| 1 | H | 96 | GLN |
| 1 | H | 114 | HIS |
| 1 | H | 175 | GLN |
| 1 | H | 213 | ASN |
| 1 | H | 288 | ASN |
| 1 | H | 299 | GLN |
| 1 | H | 374 | GLN |
| 1 | H | 438 | ASN |
| 1 | H | 457 | ASN |
| 1 | H | 469 | GLN |
| 1 | H | 488 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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 | 436/464 (93%) | -0.81 | 0 100 100 | 52, 102, 194, 258 | 0 |
| 1 | B | 436/464 (93%) | -0.79 | 0 100 100 | 63, 107, 191, 268 | 0 |
| 1 | C | 436/464 (93%) | -0.76 | 0 100 100 | 76, 126, 279, 425 | 0 |
| 1 | D | 436/464 (93%) | -0.81 | 0 100 100 | 72, 124, 202, 273 | 0 |
| 1 | E | 436/464 (93%) | -0.76 | 0 100 100 | 49, 101, 184, 260 | 0 |
| 1 | F | 436/464 (93%) | -0.79 | 0 100 100 | 54, 117, 194, 296 | 0 |
| 1 | G | 436/464 (93%) | -0.78 | 0 100 100 | 74, 139, 214, 274 | 0 |
| 1 | H | 436/464 (93%) | -0.77 | 0 100 100 | 70, 134, 211, 284 | 0 |
| All | All | 3488/3712 (93%) | -0.78 | 0 100 100 | 49, 118, 210, 425 | 0 |

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.