



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:20 am BST

PDB ID : 3RFU
Title : Crystal structure of a copper-transporting PIB-type ATPase
Authors : Gourdon, P.; Liu, X.; Skjorringe, T.; Morth, J.P.; Birk Moller, L.; Panyella Pedersen, B.; Nissen, P.
Deposited on : 2011-04-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

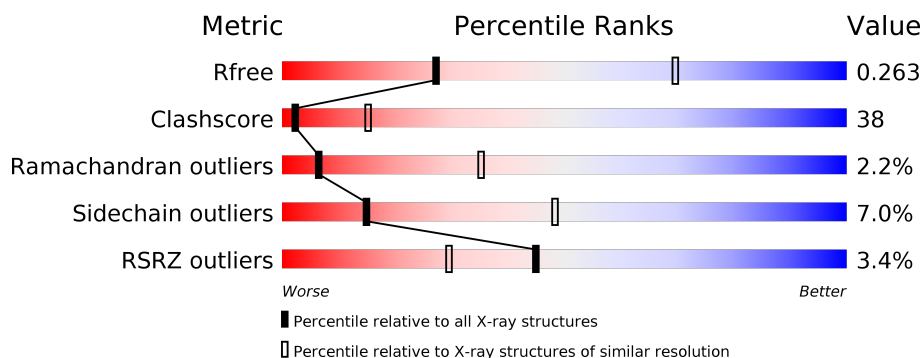
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 736 | |
| 1 | B | 736 | |
| 1 | C | 736 | |
| 1 | D | 736 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | ALF | A | 995 | - | - | X | - |
| 4 | K | A | 997 | - | - | - | X |

2 Entry composition [i](#)

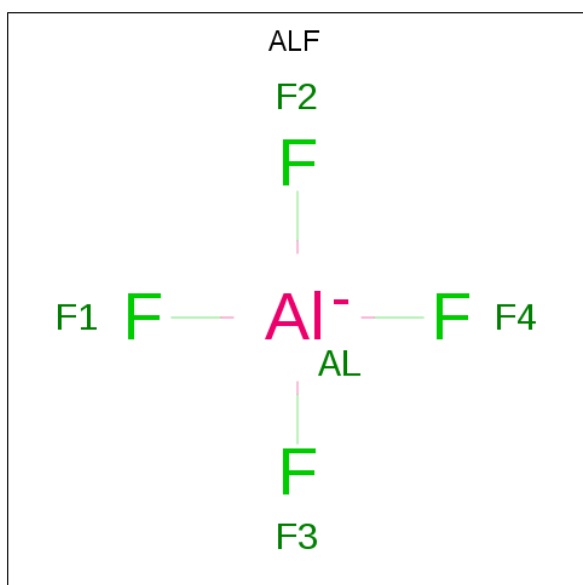
There are 4 unique types of molecules in this entry. The entry contains 19764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper efflux ATPase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 663 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4934 | 3156 | 844 | 909 | 25 | | | |
| 1 | B | 663 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4934 | 3156 | 844 | 909 | 25 | | | |
| 1 | C | 663 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4934 | 3156 | 844 | 909 | 25 | | | |
| 1 | D | 663 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4934 | 3156 | 844 | 909 | 25 | | | |

- Molecule 2 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2 | A | 1 | Total | Al | F | 0 | 0 |
| | | | 5 | 1 | 4 | | |
| 2 | B | 1 | Total | Al | F | 0 | 0 |
| | | | 5 | 1 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2 | C | 1 | Total | Al | F | 0 | 0 |
| | | | 5 | 1 | 4 | | |
| 2 | D | 1 | Total | Al | F | 0 | 0 |
| | | | 5 | 1 | 4 | | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

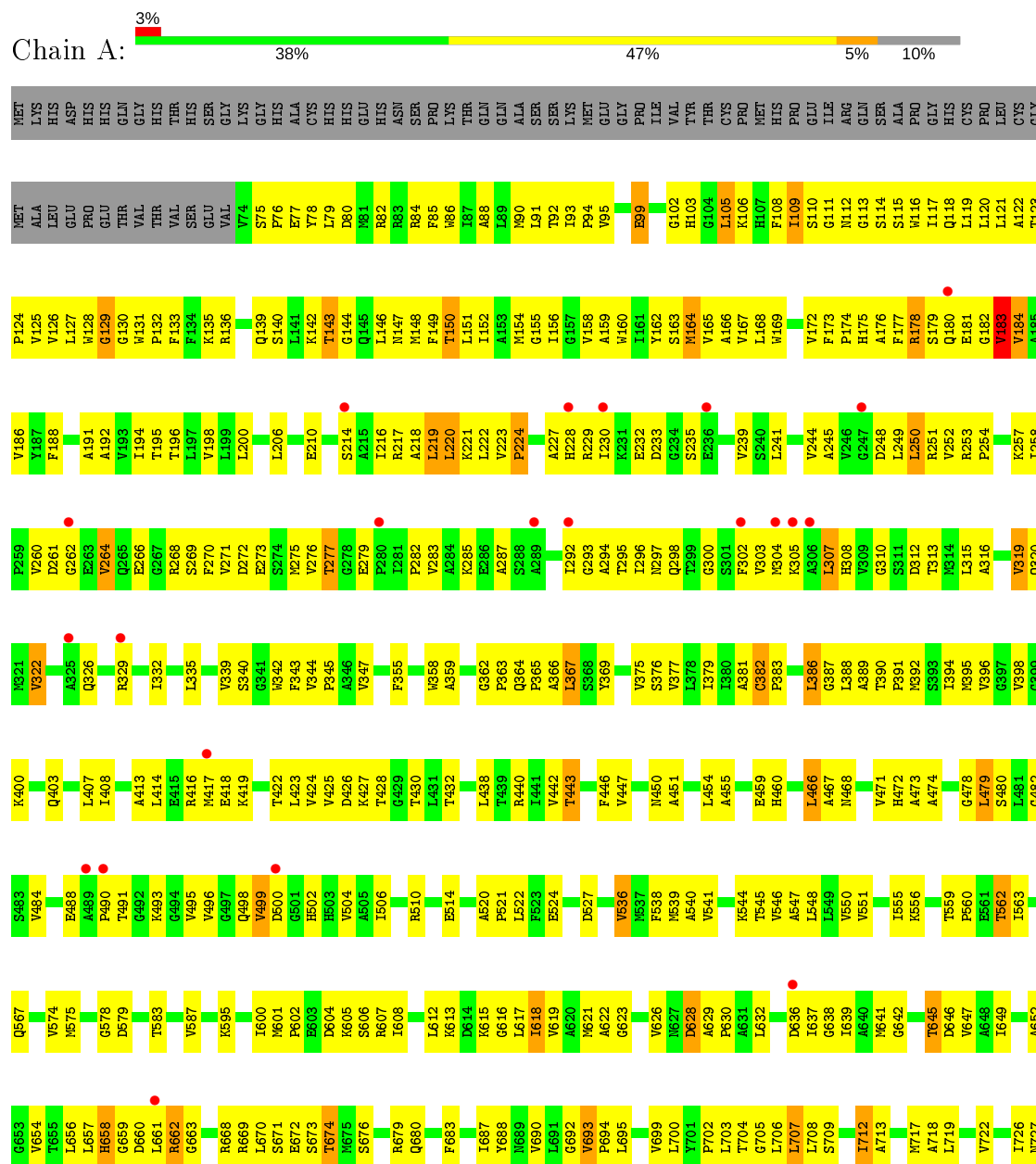
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

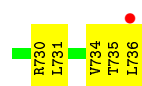
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4 | B | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | A | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | D | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

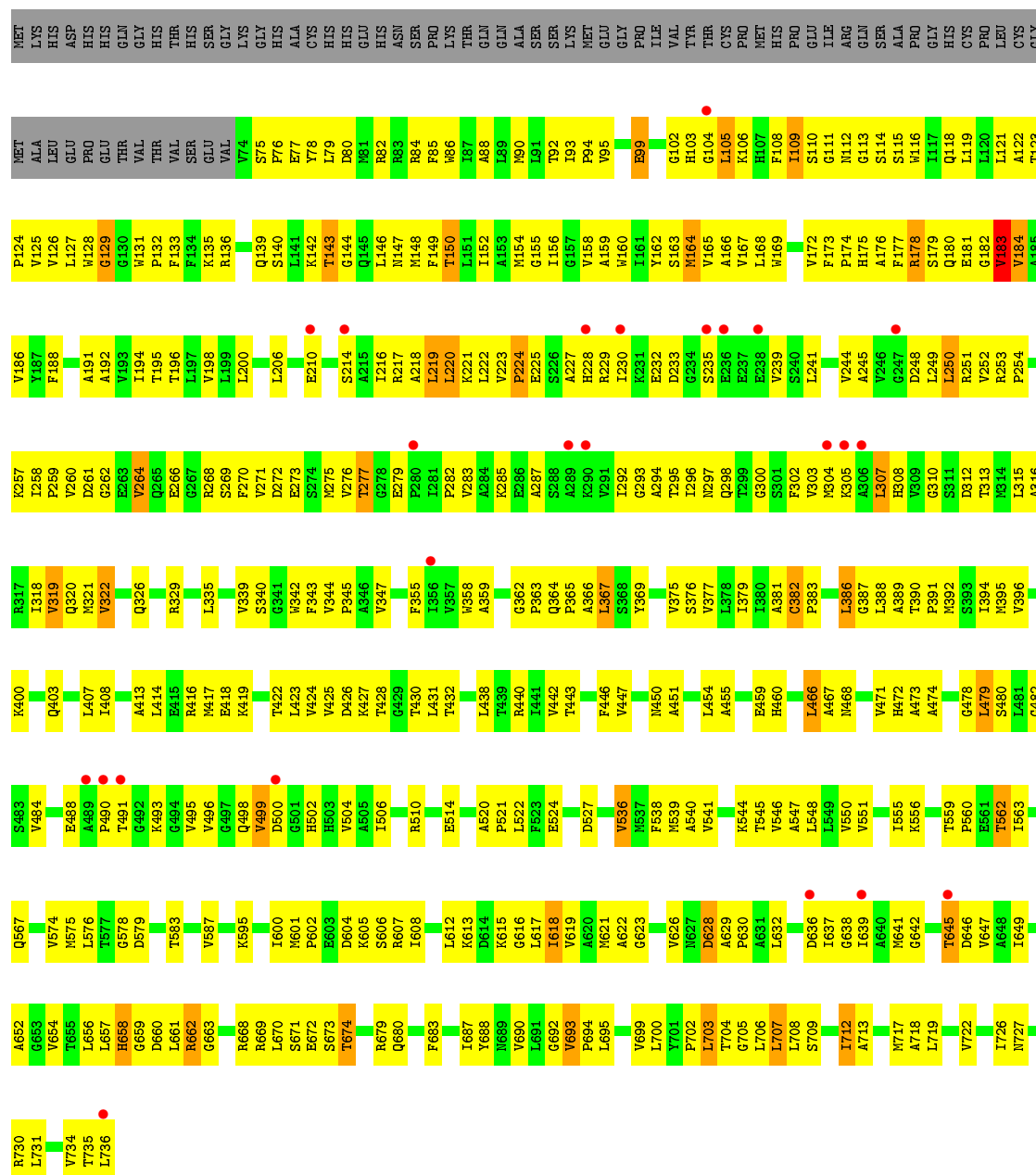
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Copper efflux ATPase





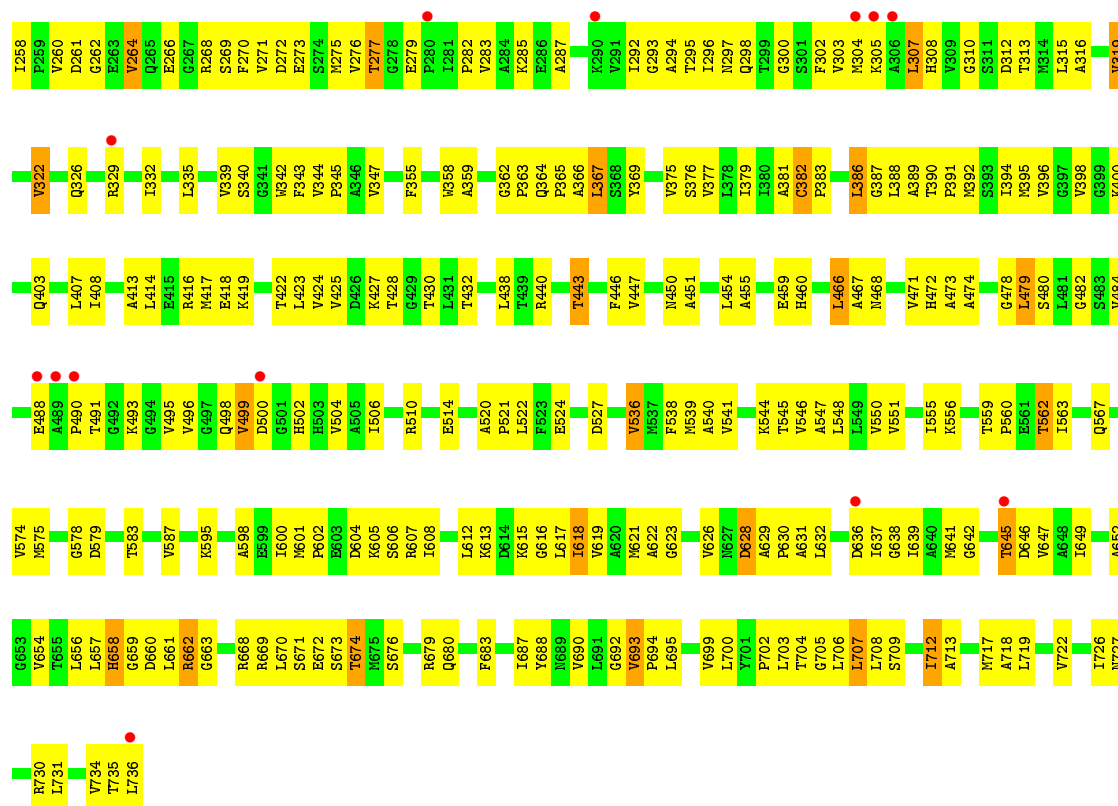
- Molecule 1: Copper efflux ATPase



- Molecule 1: Copper efflux ATPase







4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 44.15Å 72.98Å 329.95Å 89.96° 90.04° 90.22° | Depositor |
| Resolution (Å) | 20.00 – 3.20 71.27 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 96.8 (20.00-3.20) 95.5 (71.27-3.00) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.64 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.4_486) | Depositor |
| R, R_{free} | 0.235 , 0.261 0.243 , 0.263 | Depositor DCC |
| R_{free} test set | 1945 reflections (2.44%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 89.5 | Xtriage |
| Anisotropy | 0.525 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 83.6 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.438 for h,-k,-l 0.428 for -h,k,-l 0.438 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 19764 | wwPDB-VP |
| Average B, all atoms (Å ²) | 128.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.25 | 0/5017 | 0.53 | 0/6812 |
| 1 | B | 0.25 | 0/5017 | 0.53 | 0/6812 |
| 1 | C | 0.25 | 0/5017 | 0.53 | 0/6812 |
| 1 | D | 0.25 | 0/5017 | 0.53 | 0/6812 |
| All | All | 0.25 | 0/20068 | 0.53 | 0/27248 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 | 4934 | 0 | 5125 | 387 | 0 |
| 1 | B | 4934 | 0 | 5125 | 393 | 0 |
| 1 | C | 4934 | 0 | 5125 | 394 | 0 |
| 1 | D | 4934 | 0 | 5125 | 385 | 0 |
| 2 | A | 5 | 0 | 0 | 2 | 0 |
| 2 | B | 5 | 0 | 0 | 0 | 0 |
| 2 | C | 5 | 0 | 0 | 1 | 0 |
| 2 | D | 5 | 0 | 0 | 1 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| All | All | 19764 | 0 | 20500 | 1547 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1547) 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:B:123:THR:HG23 | 1:B:124:PRO:HD3 | 1.31 | 1.12 |
| 1:C:123:THR:HG23 | 1:C:124:PRO:HD3 | 1.31 | 1.12 |
| 1:A:123:THR:HG23 | 1:A:124:PRO:HD3 | 1.31 | 1.12 |
| 1:D:123:THR:HG23 | 1:D:124:PRO:HD3 | 1.31 | 1.12 |
| 1:A:662:ARG:HB2 | 1:A:663:GLY:HA3 | 1.34 | 1.09 |
| 1:D:662:ARG:HB2 | 1:D:663:GLY:HA3 | 1.34 | 1.09 |
| 1:B:662:ARG:HB2 | 1:B:663:GLY:HA3 | 1.34 | 1.09 |
| 1:C:662:ARG:HB2 | 1:C:663:GLY:HA3 | 1.35 | 1.08 |
| 1:D:112:ASN:O | 1:D:116:TRP:HB2 | 1.55 | 1.06 |
| 1:A:112:ASN:O | 1:A:116:TRP:HB2 | 1.55 | 1.06 |
| 1:B:112:ASN:O | 1:B:116:TRP:HB2 | 1.54 | 1.05 |
| 1:C:112:ASN:O | 1:C:116:TRP:HB2 | 1.54 | 1.05 |
| 1:C:264:VAL:HA | 1:C:303:VAL:O | 1.57 | 1.04 |
| 1:B:264:VAL:HA | 1:B:303:VAL:O | 1.57 | 1.04 |
| 1:A:264:VAL:HA | 1:A:303:VAL:O | 1.57 | 1.02 |
| 1:D:264:VAL:HA | 1:D:303:VAL:O | 1.57 | 1.02 |
| 1:C:109:ILE:HG23 | 1:C:110:SER:HB3 | 1.41 | 1.00 |
| 1:B:109:ILE:HG23 | 1:B:110:SER:HB3 | 1.42 | 0.99 |
| 1:D:109:ILE:HG23 | 1:D:110:SER:HB3 | 1.43 | 0.96 |
| 1:A:109:ILE:HG23 | 1:A:110:SER:HB3 | 1.43 | 0.96 |
| 1:D:178:ARG:HB3 | 1:D:179:SER:HA | 1.47 | 0.94 |
| 1:A:178:ARG:HB3 | 1:A:179:SER:HA | 1.46 | 0.94 |
| 1:C:178:ARG:HB3 | 1:C:179:SER:HA | 1.47 | 0.94 |
| 1:B:178:ARG:HB3 | 1:B:179:SER:HA | 1.47 | 0.94 |
| 1:A:102:GLY:HA3 | 1:A:103:HIS:C | 1.92 | 0.89 |
| 1:D:102:GLY:HA3 | 1:D:103:HIS:C | 1.92 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:THR:CG2 | 1:A:124:PRO:HD3 | 2.04 | 0.88 |
| 1:B:102:GLY:HA3 | 1:B:103:HIS:C | 1.93 | 0.88 |
| 1:D:123:THR:CG2 | 1:D:124:PRO:HD3 | 2.04 | 0.88 |
| 1:C:102:GLY:HA3 | 1:C:103:HIS:C | 1.92 | 0.88 |
| 1:C:123:THR:CG2 | 1:C:124:PRO:HD3 | 2.03 | 0.87 |
| 1:B:123:THR:CG2 | 1:B:124:PRO:HD3 | 2.04 | 0.87 |
| 1:B:482:GLY:HA3 | 1:B:499:VAL:HG23 | 1.58 | 0.85 |
| 1:C:482:GLY:HA3 | 1:C:499:VAL:HG23 | 1.59 | 0.85 |
| 1:A:482:GLY:HA3 | 1:A:499:VAL:HG23 | 1.59 | 0.84 |
| 1:D:482:GLY:HA3 | 1:D:499:VAL:HG23 | 1.59 | 0.84 |
| 1:D:229:ARG:HG2 | 1:D:250:LEU:HD21 | 1.60 | 0.83 |
| 1:A:229:ARG:HG2 | 1:A:250:LEU:HD21 | 1.60 | 0.83 |
| 1:A:416:ARG:HB2 | 1:A:637:ILE:HD11 | 1.60 | 0.83 |
| 1:D:416:ARG:HB2 | 1:D:637:ILE:HD11 | 1.59 | 0.83 |
| 1:C:229:ARG:HG2 | 1:C:250:LEU:HD21 | 1.60 | 0.82 |
| 1:B:229:ARG:HG2 | 1:B:250:LEU:HD21 | 1.60 | 0.82 |
| 1:C:416:ARG:HB2 | 1:C:637:ILE:HD11 | 1.59 | 0.82 |
| 1:B:416:ARG:HB2 | 1:B:637:ILE:HD11 | 1.59 | 0.82 |
| 1:B:232:GLU:HG3 | 1:B:233:ASP:H | 1.43 | 0.81 |
| 1:C:232:GLU:HG3 | 1:C:233:ASP:H | 1.43 | 0.81 |
| 1:A:563:ILE:O | 1:A:567:GLN:HG2 | 1.81 | 0.81 |
| 1:B:222:LEU:C | 1:B:224:PRO:HD2 | 2.01 | 0.81 |
| 1:C:222:LEU:C | 1:C:224:PRO:HD2 | 2.02 | 0.81 |
| 1:D:563:ILE:O | 1:D:567:GLN:HG2 | 1.81 | 0.81 |
| 1:D:232:GLU:HG3 | 1:D:233:ASP:H | 1.43 | 0.81 |
| 1:A:222:LEU:C | 1:A:224:PRO:HD2 | 2.02 | 0.80 |
| 1:A:232:GLU:HG3 | 1:A:233:ASP:H | 1.43 | 0.80 |
| 1:B:563:ILE:O | 1:B:567:GLN:HG2 | 1.81 | 0.80 |
| 1:D:222:LEU:C | 1:D:224:PRO:HD2 | 2.02 | 0.80 |
| 1:C:563:ILE:O | 1:C:567:GLN:HG2 | 1.81 | 0.80 |
| 1:D:662:ARG:HB2 | 1:D:663:GLY:CA | 2.11 | 0.80 |
| 1:A:662:ARG:HB2 | 1:A:663:GLY:CA | 2.12 | 0.80 |
| 1:D:254:PRO:HB3 | 1:D:300:GLY:H | 1.47 | 0.80 |
| 1:B:662:ARG:HB2 | 1:B:663:GLY:CA | 2.11 | 0.79 |
| 1:A:254:PRO:HB3 | 1:A:300:GLY:H | 1.48 | 0.79 |
| 1:C:662:ARG:HB2 | 1:C:663:GLY:CA | 2.12 | 0.79 |
| 1:D:708:LEU:HD21 | 1:D:712:ILE:HD11 | 1.63 | 0.79 |
| 1:C:254:PRO:HB3 | 1:C:300:GLY:H | 1.47 | 0.79 |
| 1:A:708:LEU:HD21 | 1:A:712:ILE:HD11 | 1.64 | 0.78 |
| 1:B:254:PRO:HB3 | 1:B:300:GLY:H | 1.48 | 0.78 |
| 1:C:708:LEU:HD21 | 1:C:712:ILE:HD11 | 1.63 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:119:LEU:O | 1:B:123:THR:HG22 | 1.84 | 0.78 |
| 1:B:708:LEU:HD21 | 1:B:712:ILE:HD11 | 1.64 | 0.78 |
| 1:B:430:THR:HG21 | 1:B:623:GLY:HA2 | 1.66 | 0.77 |
| 1:B:604:ASP:O | 1:B:608:ILE:HG12 | 1.84 | 0.77 |
| 1:C:604:ASP:O | 1:C:608:ILE:HG12 | 1.85 | 0.77 |
| 1:C:119:LEU:O | 1:C:123:THR:HG22 | 1.85 | 0.77 |
| 1:C:430:THR:HG21 | 1:C:623:GLY:HA2 | 1.67 | 0.77 |
| 1:A:119:LEU:O | 1:A:123:THR:HG22 | 1.84 | 0.77 |
| 1:D:119:LEU:O | 1:D:123:THR:HG22 | 1.84 | 0.77 |
| 1:D:499:VAL:HG22 | 1:D:500:ASP:H | 1.49 | 0.77 |
| 1:B:499:VAL:HG22 | 1:B:500:ASP:H | 1.49 | 0.77 |
| 1:D:430:THR:HG21 | 1:D:623:GLY:HA2 | 1.66 | 0.76 |
| 1:A:499:VAL:HG22 | 1:A:500:ASP:H | 1.49 | 0.76 |
| 1:C:499:VAL:HG22 | 1:C:500:ASP:H | 1.49 | 0.76 |
| 1:A:430:THR:HG21 | 1:A:623:GLY:HA2 | 1.66 | 0.76 |
| 1:D:604:ASP:O | 1:D:608:ILE:HG12 | 1.84 | 0.76 |
| 1:A:124:PRO:O | 1:A:128:TRP:HB3 | 1.85 | 0.76 |
| 1:A:604:ASP:O | 1:A:608:ILE:HG12 | 1.84 | 0.76 |
| 1:B:662:ARG:CB | 1:B:663:GLY:HA3 | 2.14 | 0.76 |
| 1:C:662:ARG:CB | 1:C:663:GLY:HA3 | 2.14 | 0.76 |
| 1:D:124:PRO:O | 1:D:128:TRP:HB3 | 1.86 | 0.75 |
| 1:A:335:LEU:O | 1:A:339:VAL:HG12 | 1.87 | 0.75 |
| 1:D:335:LEU:O | 1:D:339:VAL:HG12 | 1.87 | 0.75 |
| 1:B:124:PRO:O | 1:B:128:TRP:HB3 | 1.86 | 0.74 |
| 1:C:124:PRO:O | 1:C:128:TRP:HB3 | 1.86 | 0.74 |
| 1:C:232:GLU:CG | 1:C:233:ASP:H | 2.00 | 0.74 |
| 1:B:232:GLU:CG | 1:B:233:ASP:H | 2.00 | 0.74 |
| 1:B:159:ALA:HB2 | 1:B:379:ILE:HD13 | 1.68 | 0.74 |
| 1:D:232:GLU:CG | 1:D:233:ASP:H | 2.00 | 0.74 |
| 1:A:232:GLU:CG | 1:A:233:ASP:H | 2.00 | 0.74 |
| 1:B:78:TYR:HD2 | 1:B:79:LEU:HD12 | 1.53 | 0.74 |
| 1:D:662:ARG:CB | 1:D:663:GLY:HA3 | 2.14 | 0.74 |
| 1:B:335:LEU:O | 1:B:339:VAL:HG12 | 1.87 | 0.74 |
| 1:C:78:TYR:HD2 | 1:C:79:LEU:HD12 | 1.53 | 0.74 |
| 1:A:662:ARG:CB | 1:A:663:GLY:HA3 | 2.14 | 0.73 |
| 1:C:159:ALA:HB2 | 1:C:379:ILE:HD13 | 1.68 | 0.73 |
| 1:C:147:ASN:H | 1:C:150:THR:HG23 | 1.53 | 0.73 |
| 1:D:110:SER:HB2 | 1:D:114:SER:HB3 | 1.69 | 0.73 |
| 1:D:159:ALA:HB2 | 1:D:379:ILE:HD13 | 1.67 | 0.73 |
| 1:A:110:SER:HB2 | 1:A:114:SER:HB3 | 1.69 | 0.73 |
| 1:C:335:LEU:O | 1:C:339:VAL:HG12 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:147:ASN:H | 1:B:150:THR:HG23 | 1.53 | 0.73 |
| 1:C:88:ALA:HB1 | 1:C:196:THR:HG22 | 1.70 | 0.73 |
| 1:C:110:SER:HB2 | 1:C:114:SER:HB3 | 1.69 | 0.73 |
| 1:B:110:SER:HB2 | 1:B:114:SER:HB3 | 1.70 | 0.72 |
| 1:C:152:ILE:HA | 1:C:382:CYS:SG | 2.29 | 0.72 |
| 1:B:88:ALA:HB1 | 1:B:196:THR:HG22 | 1.71 | 0.72 |
| 1:D:615:LYS:HG3 | 1:D:616:GLY:H | 1.54 | 0.72 |
| 1:A:159:ALA:HB2 | 1:A:379:ILE:HD13 | 1.69 | 0.72 |
| 1:B:152:ILE:HA | 1:B:382:CYS:SG | 2.29 | 0.72 |
| 1:A:152:ILE:HA | 1:A:382:CYS:SG | 2.29 | 0.72 |
| 1:A:615:LYS:HG3 | 1:A:616:GLY:H | 1.55 | 0.72 |
| 1:A:147:ASN:H | 1:A:150:THR:HG23 | 1.53 | 0.72 |
| 1:A:78:TYR:HD2 | 1:A:79:LEU:HD12 | 1.53 | 0.72 |
| 1:D:147:ASN:H | 1:D:150:THR:HG23 | 1.53 | 0.72 |
| 1:D:700:LEU:HB3 | 1:D:704:THR:OG1 | 1.88 | 0.72 |
| 1:C:700:LEU:HB3 | 1:C:704:THR:OG1 | 1.88 | 0.72 |
| 1:D:78:TYR:HD2 | 1:D:79:LEU:HD12 | 1.53 | 0.72 |
| 1:C:418:GLU:HG3 | 1:C:672:GLU:HG2 | 1.70 | 0.71 |
| 1:D:418:GLU:HG3 | 1:D:672:GLU:HG2 | 1.70 | 0.71 |
| 1:A:418:GLU:HG3 | 1:A:672:GLU:HG2 | 1.70 | 0.71 |
| 1:B:418:GLU:HG3 | 1:B:672:GLU:HG2 | 1.70 | 0.71 |
| 1:C:615:LYS:HG3 | 1:C:616:GLY:H | 1.54 | 0.71 |
| 1:B:608:ILE:O | 1:B:612:LEU:HD23 | 1.90 | 0.71 |
| 1:B:700:LEU:HB3 | 1:B:704:THR:OG1 | 1.88 | 0.71 |
| 1:A:413:ALA:HA | 1:A:637:ILE:HD12 | 1.72 | 0.71 |
| 1:B:140:SER:OG | 1:B:150:THR:HG22 | 1.89 | 0.71 |
| 1:B:175:HIS:HB2 | 1:B:176:ALA:HA | 1.71 | 0.71 |
| 1:C:175:HIS:HB2 | 1:C:176:ALA:HA | 1.71 | 0.71 |
| 1:D:152:ILE:HA | 1:D:382:CYS:SG | 2.30 | 0.71 |
| 1:A:140:SER:OG | 1:A:150:THR:HG22 | 1.90 | 0.71 |
| 1:B:615:LYS:HG3 | 1:B:616:GLY:H | 1.55 | 0.71 |
| 1:C:608:ILE:O | 1:C:612:LEU:HD23 | 1.90 | 0.71 |
| 1:A:700:LEU:HB3 | 1:A:704:THR:OG1 | 1.89 | 0.71 |
| 1:A:88:ALA:HB1 | 1:A:196:THR:HG22 | 1.71 | 0.71 |
| 1:C:140:SER:OG | 1:C:150:THR:HG22 | 1.90 | 0.71 |
| 1:A:175:HIS:HB2 | 1:A:176:ALA:HA | 1.72 | 0.71 |
| 1:C:160:TRP:O | 1:C:164:MET:HB2 | 1.91 | 0.71 |
| 1:D:140:SER:OG | 1:D:150:THR:HG22 | 1.90 | 0.71 |
| 1:D:175:HIS:HB2 | 1:D:176:ALA:HA | 1.72 | 0.71 |
| 1:D:413:ALA:HA | 1:D:637:ILE:HD12 | 1.72 | 0.71 |
| 1:B:160:TRP:O | 1:B:164:MET:HB2 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:687:ILE:HA | 1:D:690:VAL:HG12 | 1.73 | 0.71 |
| 1:A:688:TYR:CD1 | 1:A:719:LEU:HD23 | 2.26 | 0.71 |
| 1:A:249:LEU:O | 1:A:250:LEU:HD23 | 1.91 | 0.70 |
| 1:D:249:LEU:O | 1:D:250:LEU:HD23 | 1.92 | 0.70 |
| 1:C:688:TYR:CD1 | 1:C:719:LEU:HD23 | 2.26 | 0.70 |
| 1:C:413:ALA:HA | 1:C:637:ILE:HD12 | 1.72 | 0.70 |
| 1:D:608:ILE:O | 1:D:612:LEU:HD23 | 1.90 | 0.70 |
| 1:A:687:ILE:HA | 1:A:690:VAL:HG12 | 1.74 | 0.70 |
| 1:C:556:LYS:HB2 | 1:C:559:THR:OG1 | 1.92 | 0.70 |
| 1:D:254:PRO:HB3 | 1:D:300:GLY:N | 2.07 | 0.70 |
| 1:A:254:PRO:HB3 | 1:A:300:GLY:N | 2.07 | 0.70 |
| 1:B:413:ALA:HA | 1:B:637:ILE:HD12 | 1.72 | 0.70 |
| 1:C:687:ILE:HA | 1:C:690:VAL:HG12 | 1.74 | 0.70 |
| 1:D:121:LEU:O | 1:D:124:PRO:HD2 | 1.92 | 0.70 |
| 1:B:283:VAL:HG23 | 1:B:285:LYS:HE2 | 1.74 | 0.70 |
| 1:B:556:LYS:HB2 | 1:B:559:THR:OG1 | 1.92 | 0.70 |
| 1:B:687:ILE:HA | 1:B:690:VAL:HG12 | 1.74 | 0.70 |
| 1:C:432:THR:HG22 | 1:C:555:ILE:HA | 1.74 | 0.70 |
| 1:A:432:THR:HG22 | 1:A:555:ILE:HA | 1.74 | 0.70 |
| 1:B:194:ILE:O | 1:B:198:VAL:HG12 | 1.92 | 0.70 |
| 1:B:432:THR:HG22 | 1:B:555:ILE:HA | 1.74 | 0.70 |
| 1:C:283:VAL:HG23 | 1:C:285:LYS:HE2 | 1.74 | 0.70 |
| 1:A:608:ILE:O | 1:A:612:LEU:HD23 | 1.91 | 0.69 |
| 1:C:254:PRO:HB3 | 1:C:300:GLY:N | 2.07 | 0.69 |
| 1:D:160:TRP:O | 1:D:164:MET:HB2 | 1.91 | 0.69 |
| 1:D:432:THR:HG22 | 1:D:555:ILE:HA | 1.74 | 0.69 |
| 1:A:160:TRP:O | 1:A:164:MET:HB2 | 1.91 | 0.69 |
| 1:B:254:PRO:HB3 | 1:B:300:GLY:N | 2.07 | 0.69 |
| 1:C:661:LEU:HD23 | 1:C:661:LEU:O | 1.92 | 0.69 |
| 1:D:93:ILE:HG23 | 1:D:94:PRO:HD3 | 1.75 | 0.69 |
| 1:C:121:LEU:O | 1:C:124:PRO:HD2 | 1.92 | 0.69 |
| 1:C:249:LEU:O | 1:C:250:LEU:HD23 | 1.91 | 0.69 |
| 1:D:688:TYR:CD1 | 1:D:719:LEU:HD23 | 2.28 | 0.69 |
| 1:A:93:ILE:HG23 | 1:A:94:PRO:HD3 | 1.75 | 0.69 |
| 1:D:661:LEU:O | 1:D:661:LEU:HD23 | 1.92 | 0.69 |
| 1:B:249:LEU:O | 1:B:250:LEU:HD23 | 1.91 | 0.69 |
| 1:B:688:TYR:CD1 | 1:B:719:LEU:HD23 | 2.27 | 0.69 |
| 1:D:122:ALA:HA | 1:D:125:VAL:HG12 | 1.74 | 0.69 |
| 1:D:88:ALA:HB1 | 1:D:196:THR:HG22 | 1.72 | 0.69 |
| 1:C:194:ILE:O | 1:C:198:VAL:HG12 | 1.92 | 0.69 |
| 1:D:194:ILE:O | 1:D:198:VAL:HG12 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:122:ALA:HA | 1:A:125:VAL:HG12 | 1.74 | 0.69 |
| 1:C:122:ALA:HA | 1:C:125:VAL:HG12 | 1.74 | 0.69 |
| 1:A:556:LYS:HB2 | 1:A:559:THR:OG1 | 1.91 | 0.69 |
| 1:A:661:LEU:HD23 | 1:A:661:LEU:O | 1.92 | 0.69 |
| 1:B:121:LEU:O | 1:B:124:PRO:HD2 | 1.93 | 0.69 |
| 1:A:194:ILE:O | 1:A:198:VAL:HG12 | 1.93 | 0.69 |
| 1:B:122:ALA:HA | 1:B:125:VAL:HG12 | 1.75 | 0.69 |
| 1:B:661:LEU:HD23 | 1:B:661:LEU:O | 1.93 | 0.69 |
| 1:A:121:LEU:O | 1:A:124:PRO:HD2 | 1.93 | 0.68 |
| 1:B:93:ILE:HG23 | 1:B:94:PRO:HD3 | 1.75 | 0.68 |
| 1:A:283:VAL:HG23 | 1:A:285:LYS:HE2 | 1.74 | 0.68 |
| 1:D:283:VAL:HG23 | 1:D:285:LYS:HE2 | 1.74 | 0.68 |
| 1:B:273:GLU:O | 1:B:273:GLU:HG2 | 1.93 | 0.68 |
| 1:C:273:GLU:O | 1:C:273:GLU:HG2 | 1.94 | 0.68 |
| 1:C:377:VAL:HG23 | 1:C:693:VAL:HB | 1.75 | 0.68 |
| 1:C:93:ILE:HG23 | 1:C:94:PRO:HD3 | 1.76 | 0.68 |
| 1:B:520:ALA:HB3 | 1:B:521:PRO:HD3 | 1.76 | 0.68 |
| 1:D:556:LYS:HB2 | 1:D:559:THR:OG1 | 1.92 | 0.68 |
| 1:D:273:GLU:O | 1:D:273:GLU:HG2 | 1.93 | 0.68 |
| 1:A:273:GLU:O | 1:A:273:GLU:HG2 | 1.93 | 0.67 |
| 1:B:541:VAL:HG22 | 1:B:546:VAL:HG11 | 1.77 | 0.67 |
| 1:C:520:ALA:HB3 | 1:C:521:PRO:HD3 | 1.76 | 0.67 |
| 1:A:108:PHE:O | 1:A:109:ILE:HD12 | 1.95 | 0.67 |
| 1:B:377:VAL:HG23 | 1:B:693:VAL:HB | 1.76 | 0.67 |
| 1:A:520:ALA:HB3 | 1:A:521:PRO:HD3 | 1.76 | 0.67 |
| 1:A:377:VAL:HG23 | 1:A:693:VAL:HB | 1.75 | 0.67 |
| 1:C:541:VAL:HG22 | 1:C:546:VAL:HG11 | 1.77 | 0.67 |
| 1:D:108:PHE:O | 1:D:109:ILE:HD12 | 1.95 | 0.67 |
| 1:C:110:SER:HA | 1:C:114:SER:H | 1.60 | 0.67 |
| 1:A:110:SER:HA | 1:A:114:SER:H | 1.60 | 0.67 |
| 1:D:377:VAL:HG23 | 1:D:693:VAL:HB | 1.76 | 0.67 |
| 1:D:520:ALA:HB3 | 1:D:521:PRO:HD3 | 1.77 | 0.66 |
| 1:B:307:LEU:HD13 | 1:B:308:HIS:HD2 | 1.61 | 0.66 |
| 1:B:687:ILE:HD13 | 1:D:120:LEU:HD12 | 1.76 | 0.66 |
| 1:D:541:VAL:HG22 | 1:D:546:VAL:HG11 | 1.77 | 0.66 |
| 1:A:307:LEU:HD13 | 1:A:308:HIS:HD2 | 1.60 | 0.66 |
| 1:C:307:LEU:HD13 | 1:C:308:HIS:HD2 | 1.61 | 0.66 |
| 1:A:541:VAL:HG22 | 1:A:546:VAL:HG11 | 1.77 | 0.66 |
| 1:B:108:PHE:O | 1:B:109:ILE:HD12 | 1.95 | 0.66 |
| 1:D:110:SER:HA | 1:D:114:SER:H | 1.61 | 0.66 |
| 1:B:110:SER:HA | 1:B:114:SER:H | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:PHE:O | 1:C:109:ILE:HD12 | 1.96 | 0.66 |
| 1:A:179:SER:HB2 | 1:A:183:VAL:N | 2.11 | 0.66 |
| 1:D:307:LEU:HD13 | 1:D:308:HIS:HD2 | 1.61 | 0.66 |
| 1:D:179:SER:HB2 | 1:D:183:VAL:N | 2.11 | 0.65 |
| 1:C:179:SER:HB2 | 1:C:183:VAL:N | 2.11 | 0.65 |
| 1:A:605:LYS:HE2 | 1:A:628:ASP:HB3 | 1.79 | 0.65 |
| 1:D:605:LYS:HE2 | 1:D:628:ASP:HB3 | 1.79 | 0.65 |
| 1:A:490:PRO:HB2 | 1:A:493:LYS:HD3 | 1.79 | 0.65 |
| 1:B:179:SER:HB2 | 1:B:183:VAL:N | 2.11 | 0.65 |
| 1:B:605:LYS:HE2 | 1:B:628:ASP:HB3 | 1.78 | 0.65 |
| 1:D:192:ALA:O | 1:D:196:THR:HG23 | 1.96 | 0.65 |
| 1:D:490:PRO:HB2 | 1:D:493:LYS:HD3 | 1.79 | 0.64 |
| 1:A:192:ALA:O | 1:A:196:THR:HG23 | 1.96 | 0.64 |
| 1:B:192:ALA:O | 1:B:196:THR:HG23 | 1.98 | 0.64 |
| 1:C:192:ALA:O | 1:C:196:THR:HG23 | 1.98 | 0.64 |
| 1:C:490:PRO:HB2 | 1:C:493:LYS:HD3 | 1.79 | 0.64 |
| 1:C:605:LYS:HE2 | 1:C:628:ASP:HB3 | 1.78 | 0.64 |
| 1:C:670:LEU:HD23 | 1:C:736:LEU:HD11 | 1.79 | 0.64 |
| 1:A:93:ILE:CG2 | 1:A:94:PRO:HD3 | 2.27 | 0.64 |
| 1:B:112:ASN:O | 1:B:116:TRP:CB | 2.40 | 0.64 |
| 1:B:490:PRO:HB2 | 1:B:493:LYS:HD3 | 1.79 | 0.64 |
| 1:D:93:ILE:CG2 | 1:D:94:PRO:HD3 | 2.27 | 0.64 |
| 1:A:670:LEU:O | 1:A:674:THR:HG23 | 1.98 | 0.64 |
| 1:C:112:ASN:O | 1:C:116:TRP:CB | 2.40 | 0.64 |
| 1:B:223:VAL:O | 1:B:224:PRO:C | 2.37 | 0.64 |
| 1:D:670:LEU:O | 1:D:674:THR:HG23 | 1.98 | 0.64 |
| 1:B:506:ILE:HD12 | 1:B:538:PHE:O | 1.98 | 0.64 |
| 1:C:223:VAL:O | 1:C:224:PRO:C | 2.37 | 0.64 |
| 1:A:111:GLY:O | 1:A:115:SER:HB2 | 1.98 | 0.63 |
| 1:B:111:GLY:O | 1:B:115:SER:HB2 | 1.98 | 0.63 |
| 1:B:670:LEU:HD23 | 1:B:736:LEU:HD11 | 1.80 | 0.63 |
| 1:B:275:MET:HE1 | 1:B:294:ALA:HB3 | 1.79 | 0.63 |
| 1:B:93:ILE:CG2 | 1:B:94:PRO:HD3 | 2.28 | 0.63 |
| 1:C:93:ILE:CG2 | 1:C:94:PRO:HD3 | 2.28 | 0.63 |
| 1:D:111:GLY:O | 1:D:115:SER:HB2 | 1.98 | 0.63 |
| 1:C:109:ILE:CG2 | 1:C:110:SER:HB3 | 2.22 | 0.63 |
| 1:C:275:MET:HE1 | 1:C:294:ALA:HB3 | 1.79 | 0.63 |
| 1:C:506:ILE:HD12 | 1:C:538:PHE:O | 1.99 | 0.63 |
| 1:A:275:MET:HE1 | 1:A:294:ALA:HB3 | 1.80 | 0.63 |
| 1:D:275:MET:HE1 | 1:D:294:ALA:HB3 | 1.80 | 0.63 |
| 1:A:670:LEU:HD23 | 1:A:736:LEU:HD11 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:111:GLY:O | 1:C:115:SER:HB2 | 1.98 | 0.63 |
| 1:A:506:ILE:HD12 | 1:A:538:PHE:O | 1.98 | 0.63 |
| 1:D:506:ILE:HD12 | 1:D:538:PHE:O | 1.98 | 0.63 |
| 1:B:109:ILE:CG2 | 1:B:110:SER:HB3 | 2.23 | 0.63 |
| 1:C:670:LEU:O | 1:C:674:THR:HG23 | 1.98 | 0.63 |
| 1:D:223:VAL:O | 1:D:224:PRO:C | 2.37 | 0.63 |
| 1:D:670:LEU:HD23 | 1:D:736:LEU:HD11 | 1.79 | 0.63 |
| 1:A:223:VAL:O | 1:A:224:PRO:C | 2.37 | 0.62 |
| 1:B:670:LEU:O | 1:B:674:THR:HG23 | 1.98 | 0.62 |
| 1:A:105:LEU:HD12 | 1:A:106:LYS:N | 2.14 | 0.62 |
| 1:C:454:LEU:HD21 | 1:C:500:ASP:OD1 | 1.99 | 0.62 |
| 1:D:105:LEU:HD12 | 1:D:106:LYS:N | 2.15 | 0.62 |
| 1:C:223:VAL:N | 1:C:224:PRO:HD2 | 2.14 | 0.62 |
| 1:C:342:TRP:O | 1:C:345:PRO:HD2 | 2.00 | 0.62 |
| 1:B:216:ILE:O | 1:B:219:LEU:HD13 | 2.00 | 0.62 |
| 1:B:223:VAL:N | 1:B:224:PRO:HD2 | 2.14 | 0.62 |
| 1:A:315:LEU:O | 1:A:319:VAL:HG12 | 2.00 | 0.62 |
| 1:B:454:LEU:HD21 | 1:B:500:ASP:OD1 | 2.00 | 0.62 |
| 1:C:216:ILE:O | 1:C:219:LEU:HD13 | 2.00 | 0.62 |
| 1:C:423:LEU:HG | 1:C:425:VAL:HG13 | 1.81 | 0.62 |
| 1:C:105:LEU:HD12 | 1:C:106:LYS:N | 2.14 | 0.62 |
| 1:C:315:LEU:O | 1:C:319:VAL:HG12 | 1.99 | 0.62 |
| 1:D:109:ILE:CG2 | 1:D:110:SER:HB3 | 2.23 | 0.62 |
| 1:D:315:LEU:O | 1:D:319:VAL:HG12 | 2.00 | 0.62 |
| 1:A:109:ILE:CG2 | 1:A:110:SER:HB3 | 2.23 | 0.61 |
| 1:A:454:LEU:HD21 | 1:A:500:ASP:OD1 | 2.00 | 0.61 |
| 1:B:105:LEU:HD12 | 1:B:106:LYS:N | 2.14 | 0.61 |
| 1:D:216:ILE:O | 1:D:219:LEU:HD13 | 2.00 | 0.61 |
| 1:D:342:TRP:O | 1:D:345:PRO:HD2 | 2.00 | 0.61 |
| 1:A:178:ARG:CB | 1:A:179:SER:HA | 2.24 | 0.61 |
| 1:A:216:ILE:HG23 | 1:A:217:ARG:H | 1.66 | 0.61 |
| 1:A:216:ILE:O | 1:A:219:LEU:HD13 | 2.00 | 0.61 |
| 1:D:216:ILE:HG23 | 1:D:217:ARG:H | 1.66 | 0.61 |
| 1:D:454:LEU:HD21 | 1:D:500:ASP:OD1 | 2.00 | 0.61 |
| 1:B:342:TRP:O | 1:B:345:PRO:HD2 | 2.00 | 0.61 |
| 1:B:418:GLU:HB2 | 1:B:671:SER:OG | 2.00 | 0.61 |
| 1:B:315:LEU:O | 1:B:319:VAL:HG12 | 2.00 | 0.61 |
| 1:B:423:LEU:HG | 1:B:425:VAL:HG13 | 1.81 | 0.61 |
| 1:C:629:ALA:N | 1:C:630:PRO:HD2 | 2.16 | 0.61 |
| 1:D:223:VAL:N | 1:D:224:PRO:HD2 | 2.15 | 0.61 |
| 1:A:142:LYS:HG2 | 1:A:143:THR:HG23 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:223:VAL:N | 1:A:224:PRO:HD2 | 2.14 | 0.61 |
| 1:B:629:ALA:N | 1:B:630:PRO:HD2 | 2.16 | 0.61 |
| 1:D:142:LYS:HG2 | 1:D:143:THR:HG23 | 1.82 | 0.61 |
| 1:A:342:TRP:O | 1:A:345:PRO:HD2 | 2.01 | 0.61 |
| 1:D:178:ARG:CB | 1:D:179:SER:HA | 2.24 | 0.61 |
| 1:A:423:LEU:HG | 1:A:425:VAL:HG13 | 1.81 | 0.61 |
| 1:C:142:LYS:HG2 | 1:C:143:THR:HG23 | 1.82 | 0.61 |
| 1:D:418:GLU:HB2 | 1:D:671:SER:OG | 2.00 | 0.61 |
| 1:D:629:ALA:N | 1:D:630:PRO:HD2 | 2.15 | 0.61 |
| 1:A:629:ALA:N | 1:A:630:PRO:HD2 | 2.16 | 0.61 |
| 1:B:142:LYS:HG2 | 1:B:143:THR:HG23 | 1.82 | 0.61 |
| 1:A:120:LEU:HD12 | 1:C:687:ILE:HD13 | 1.82 | 0.61 |
| 1:B:179:SER:HB3 | 1:B:181:GLU:N | 2.16 | 0.60 |
| 1:C:344:VAL:HG22 | 1:C:345:PRO:HD3 | 1.82 | 0.60 |
| 1:C:418:GLU:HB2 | 1:C:671:SER:OG | 2.01 | 0.60 |
| 1:B:262:GLY:HA2 | 1:B:307:LEU:HB2 | 1.83 | 0.60 |
| 1:B:662:ARG:CB | 1:B:663:GLY:CA | 2.77 | 0.60 |
| 1:C:179:SER:HB3 | 1:C:181:GLU:N | 2.16 | 0.60 |
| 1:D:166:ALA:HA | 1:D:173:PHE:HE2 | 1.66 | 0.60 |
| 1:D:423:LEU:HG | 1:D:425:VAL:HG13 | 1.82 | 0.60 |
| 1:A:166:ALA:HA | 1:A:173:PHE:HE2 | 1.65 | 0.60 |
| 1:C:166:ALA:HA | 1:C:173:PHE:HE2 | 1.65 | 0.60 |
| 1:C:262:GLY:HA2 | 1:C:307:LEU:HB2 | 1.83 | 0.60 |
| 1:C:662:ARG:CB | 1:C:663:GLY:CA | 2.78 | 0.60 |
| 1:C:709:SER:O | 1:C:712:ILE:HG13 | 2.01 | 0.60 |
| 1:B:216:ILE:HG23 | 1:B:217:ARG:H | 1.66 | 0.60 |
| 1:C:216:ILE:HG23 | 1:C:217:ARG:H | 1.66 | 0.60 |
| 1:D:709:SER:O | 1:D:712:ILE:HG13 | 2.02 | 0.60 |
| 1:B:191:ALA:O | 1:B:195:THR:HG23 | 2.02 | 0.60 |
| 1:B:344:VAL:HG22 | 1:B:345:PRO:HD3 | 1.83 | 0.60 |
| 1:B:709:SER:O | 1:B:712:ILE:HG13 | 2.01 | 0.60 |
| 1:A:709:SER:O | 1:A:712:ILE:HG13 | 2.02 | 0.60 |
| 1:B:166:ALA:HA | 1:B:173:PHE:HE2 | 1.66 | 0.60 |
| 1:A:344:VAL:HG22 | 1:A:345:PRO:HD3 | 1.83 | 0.60 |
| 1:A:418:GLU:HB2 | 1:A:671:SER:OG | 2.01 | 0.60 |
| 1:A:179:SER:HB3 | 1:A:181:GLU:N | 2.17 | 0.59 |
| 1:D:262:GLY:HA2 | 1:D:307:LEU:HB2 | 1.83 | 0.59 |
| 1:D:179:SER:HB3 | 1:D:181:GLU:N | 2.17 | 0.59 |
| 1:D:344:VAL:HG22 | 1:D:345:PRO:HD3 | 1.84 | 0.59 |
| 1:A:112:ASN:O | 1:A:116:TRP:CB | 2.40 | 0.59 |
| 1:A:262:GLY:HA2 | 1:A:307:LEU:HB2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:683:PHE:CZ | 1:B:687:ILE:HD12 | 2.37 | 0.59 |
| 1:C:683:PHE:CZ | 1:C:687:ILE:HD12 | 2.37 | 0.59 |
| 1:A:646:ASP:O | 1:A:649:ILE:HG22 | 2.03 | 0.59 |
| 1:B:499:VAL:HG22 | 1:B:500:ASP:N | 2.18 | 0.59 |
| 1:B:466:LEU:HD21 | 1:B:551:VAL:HG21 | 1.85 | 0.59 |
| 1:D:112:ASN:O | 1:D:116:TRP:CB | 2.40 | 0.59 |
| 1:D:191:ALA:O | 1:D:195:THR:HG23 | 2.03 | 0.59 |
| 1:B:268:ARG:HE | 1:B:491:THR:HG21 | 1.68 | 0.59 |
| 1:C:268:ARG:HE | 1:C:491:THR:HG21 | 1.68 | 0.59 |
| 1:C:499:VAL:HG22 | 1:C:500:ASP:N | 2.18 | 0.58 |
| 1:D:646:ASP:O | 1:D:649:ILE:HG22 | 2.03 | 0.58 |
| 1:A:683:PHE:CZ | 1:A:687:ILE:HD12 | 2.37 | 0.58 |
| 1:C:646:ASP:O | 1:C:649:ILE:HG22 | 2.03 | 0.58 |
| 1:D:268:ARG:HE | 1:D:491:THR:HG21 | 1.68 | 0.58 |
| 1:D:400:LYS:O | 1:D:403:GLN:HB3 | 2.04 | 0.58 |
| 1:D:662:ARG:CB | 1:D:663:GLY:CA | 2.77 | 0.58 |
| 1:C:466:LEU:HD21 | 1:C:551:VAL:HG21 | 1.86 | 0.58 |
| 1:D:683:PHE:CZ | 1:D:687:ILE:HD12 | 2.38 | 0.58 |
| 1:A:147:ASN:H | 1:A:150:THR:CG2 | 2.16 | 0.58 |
| 1:A:268:ARG:HE | 1:A:491:THR:HG21 | 1.68 | 0.58 |
| 1:C:191:ALA:O | 1:C:195:THR:HG23 | 2.04 | 0.58 |
| 1:A:191:ALA:O | 1:A:195:THR:HG23 | 2.04 | 0.58 |
| 1:A:400:LYS:O | 1:A:403:GLN:HB3 | 2.04 | 0.58 |
| 1:A:447:VAL:CG2 | 1:A:450:ASN:HB2 | 2.34 | 0.58 |
| 1:A:662:ARG:CB | 1:A:663:GLY:CA | 2.77 | 0.58 |
| 1:B:400:LYS:O | 1:B:403:GLN:HB3 | 2.04 | 0.58 |
| 1:B:499:VAL:O | 1:B:502:HIS:CG | 2.56 | 0.58 |
| 1:C:400:LYS:O | 1:C:403:GLN:HB3 | 2.04 | 0.58 |
| 1:D:447:VAL:CG2 | 1:D:450:ASN:HB2 | 2.34 | 0.58 |
| 1:D:466:LEU:HD21 | 1:D:551:VAL:HG21 | 1.85 | 0.58 |
| 1:C:499:VAL:O | 1:C:502:HIS:CG | 2.56 | 0.58 |
| 1:D:147:ASN:H | 1:D:150:THR:CG2 | 2.16 | 0.58 |
| 1:D:119:LEU:HD12 | 1:D:167:VAL:HG11 | 1.86 | 0.57 |
| 1:D:499:VAL:HG22 | 1:D:500:ASP:N | 2.18 | 0.57 |
| 1:D:499:VAL:O | 1:D:502:HIS:CG | 2.56 | 0.57 |
| 1:D:414:LEU:HD21 | 1:D:670:LEU:HD12 | 1.86 | 0.57 |
| 1:A:414:LEU:HD21 | 1:A:670:LEU:HD12 | 1.86 | 0.57 |
| 1:B:646:ASP:O | 1:B:649:ILE:HG22 | 2.04 | 0.57 |
| 1:C:386:LEU:HD12 | 1:C:387:GLY:N | 2.19 | 0.57 |
| 1:B:455:ALA:O | 1:B:459:GLU:HG2 | 2.04 | 0.57 |
| 1:C:147:ASN:H | 1:C:150:THR:CG2 | 2.17 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:499:VAL:O | 1:A:502:HIS:CG | 2.56 | 0.57 |
| 1:A:499:VAL:HG22 | 1:A:500:ASP:N | 2.18 | 0.57 |
| 1:B:133:PHE:CE1 | 1:B:198:VAL:HG13 | 2.39 | 0.57 |
| 1:C:455:ALA:O | 1:C:459:GLU:HG2 | 2.04 | 0.57 |
| 1:B:147:ASN:H | 1:B:150:THR:CG2 | 2.17 | 0.57 |
| 1:A:119:LEU:HD12 | 1:A:167:VAL:HG11 | 1.86 | 0.57 |
| 1:A:133:PHE:CE1 | 1:A:198:VAL:HG13 | 2.40 | 0.57 |
| 1:A:466:LEU:HD21 | 1:A:551:VAL:HG21 | 1.86 | 0.57 |
| 1:D:455:ALA:O | 1:D:459:GLU:HG2 | 2.04 | 0.57 |
| 1:C:133:PHE:CE1 | 1:C:198:VAL:HG13 | 2.40 | 0.57 |
| 1:D:386:LEU:HD12 | 1:D:387:GLY:N | 2.19 | 0.57 |
| 1:A:386:LEU:HD12 | 1:A:387:GLY:N | 2.19 | 0.57 |
| 1:A:455:ALA:O | 1:A:459:GLU:HG2 | 2.04 | 0.57 |
| 1:C:77:GLU:O | 1:C:80:ASP:HB3 | 2.04 | 0.57 |
| 1:D:578:GLY:O | 1:D:579:ASP:HB2 | 2.04 | 0.57 |
| 1:D:133:PHE:CE1 | 1:D:198:VAL:HG13 | 2.40 | 0.57 |
| 1:D:229:ARG:HD2 | 1:D:248:ASP:HB3 | 1.87 | 0.57 |
| 1:A:229:ARG:HD2 | 1:A:248:ASP:HB3 | 1.87 | 0.56 |
| 1:A:488:GLU:HB3 | 1:A:496:VAL:HG13 | 1.86 | 0.56 |
| 1:B:414:LEU:HD21 | 1:B:670:LEU:HD12 | 1.86 | 0.56 |
| 1:C:447:VAL:CG2 | 1:C:450:ASN:HB2 | 2.34 | 0.56 |
| 1:C:414:LEU:HD21 | 1:C:670:LEU:HD12 | 1.86 | 0.56 |
| 1:D:488:GLU:HB3 | 1:D:496:VAL:HG13 | 1.86 | 0.56 |
| 1:D:99:GLU:HG2 | 1:D:118:GLN:OE1 | 2.05 | 0.56 |
| 1:B:386:LEU:HD12 | 1:B:387:GLY:N | 2.19 | 0.56 |
| 1:B:499:VAL:H | 1:B:502:HIS:HA | 1.70 | 0.56 |
| 1:B:249:LEU:HB3 | 1:B:303:VAL:CG2 | 2.36 | 0.56 |
| 1:C:119:LEU:HD12 | 1:C:167:VAL:HG11 | 1.86 | 0.56 |
| 1:D:499:VAL:H | 1:D:502:HIS:HA | 1.70 | 0.56 |
| 1:A:99:GLU:HG2 | 1:A:118:GLN:OE1 | 2.05 | 0.56 |
| 1:A:499:VAL:H | 1:A:502:HIS:HA | 1.70 | 0.56 |
| 1:B:662:ARG:HA | 1:B:662:ARG:HH11 | 1.70 | 0.56 |
| 1:B:77:GLU:O | 1:B:80:ASP:HB3 | 2.05 | 0.56 |
| 1:C:249:LEU:HB3 | 1:C:303:VAL:CG2 | 2.36 | 0.56 |
| 1:B:390:THR:O | 1:B:394:ILE:HG12 | 2.06 | 0.56 |
| 1:C:99:GLU:HG2 | 1:C:118:GLN:OE1 | 2.06 | 0.56 |
| 1:C:499:VAL:H | 1:C:502:HIS:HA | 1.71 | 0.56 |
| 1:B:119:LEU:HD12 | 1:B:167:VAL:HG11 | 1.86 | 0.56 |
| 1:B:229:ARG:HD2 | 1:B:248:ASP:HB3 | 1.87 | 0.56 |
| 1:C:229:ARG:HD2 | 1:C:248:ASP:HB3 | 1.87 | 0.56 |
| 1:C:78:TYR:HA | 1:C:206:LEU:CD1 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:488:GLU:HB3 | 1:C:496:VAL:HG13 | 1.86 | 0.56 |
| 1:A:578:GLY:O | 1:A:579:ASP:HB2 | 2.05 | 0.56 |
| 1:A:662:ARG:HA | 1:A:662:ARG:HH11 | 1.70 | 0.56 |
| 1:B:488:GLU:HB3 | 1:B:496:VAL:HG13 | 1.86 | 0.56 |
| 1:B:99:GLU:HG2 | 1:B:118:GLN:OE1 | 2.06 | 0.56 |
| 1:C:662:ARG:HH11 | 1:C:662:ARG:HA | 1.70 | 0.56 |
| 1:D:662:ARG:HH11 | 1:D:662:ARG:HA | 1.70 | 0.56 |
| 1:A:262:GLY:HA2 | 1:A:305:LYS:O | 2.06 | 0.56 |
| 1:A:390:THR:O | 1:A:394:ILE:HG12 | 2.05 | 0.56 |
| 1:A:77:GLU:O | 1:A:80:ASP:HB3 | 2.05 | 0.56 |
| 1:B:112:ASN:HA | 1:B:116:TRP:CD1 | 2.41 | 0.56 |
| 1:B:447:VAL:CG2 | 1:B:450:ASN:HB2 | 2.35 | 0.56 |
| 1:C:578:GLY:O | 1:C:579:ASP:HB2 | 2.04 | 0.56 |
| 1:D:657:LEU:O | 1:D:658:HIS:HB3 | 2.06 | 0.56 |
| 1:D:77:GLU:O | 1:D:80:ASP:HB3 | 2.05 | 0.56 |
| 1:A:657:LEU:O | 1:A:658:HIS:HB3 | 2.06 | 0.56 |
| 1:B:78:TYR:HA | 1:B:206:LEU:CD1 | 2.36 | 0.56 |
| 1:D:262:GLY:HA2 | 1:D:305:LYS:O | 2.06 | 0.56 |
| 1:A:102:GLY:HA3 | 1:A:103:HIS:O | 2.06 | 0.55 |
| 1:C:112:ASN:HA | 1:C:116:TRP:CD1 | 2.41 | 0.55 |
| 1:C:638:GLY:O | 1:C:652:ALA:HB1 | 2.06 | 0.55 |
| 1:D:102:GLY:HA3 | 1:D:103:HIS:O | 2.06 | 0.55 |
| 1:A:78:TYR:HA | 1:A:206:LEU:CD1 | 2.35 | 0.55 |
| 1:B:578:GLY:O | 1:B:579:ASP:HB2 | 2.05 | 0.55 |
| 1:D:390:THR:O | 1:D:394:ILE:HG12 | 2.06 | 0.55 |
| 1:A:638:GLY:O | 1:A:652:ALA:HB1 | 2.06 | 0.55 |
| 1:A:125:VAL:O | 1:A:129:GLY:HA2 | 2.07 | 0.55 |
| 1:D:260:VAL:HG12 | 1:D:261:ASP:N | 2.22 | 0.55 |
| 1:A:249:LEU:HB3 | 1:A:303:VAL:CG2 | 2.36 | 0.55 |
| 1:C:154:MET:O | 1:C:158:VAL:HG12 | 2.07 | 0.55 |
| 1:A:154:MET:O | 1:A:158:VAL:HG12 | 2.07 | 0.55 |
| 1:B:154:MET:O | 1:B:158:VAL:HG12 | 2.07 | 0.55 |
| 1:B:262:GLY:HA2 | 1:B:305:LYS:O | 2.06 | 0.55 |
| 1:C:390:THR:O | 1:C:394:ILE:HG12 | 2.07 | 0.55 |
| 1:C:504:VAL:HB | 1:C:541:VAL:HG12 | 1.89 | 0.55 |
| 1:D:249:LEU:HB3 | 1:D:303:VAL:CG2 | 2.36 | 0.55 |
| 1:A:504:VAL:HB | 1:A:541:VAL:HG12 | 1.88 | 0.55 |
| 1:B:657:LEU:O | 1:B:658:HIS:HB3 | 2.06 | 0.55 |
| 1:C:102:GLY:HA3 | 1:C:103:HIS:O | 2.06 | 0.55 |
| 1:C:262:GLY:HA2 | 1:C:305:LYS:O | 2.06 | 0.55 |
| 1:D:229:ARG:HG2 | 1:D:250:LEU:CD2 | 2.34 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:VAL:HG12 | 1:A:261:ASP:N | 2.22 | 0.55 |
| 1:A:559:THR:HA | 1:A:562:THR:HG23 | 1.89 | 0.55 |
| 1:B:102:GLY:HA3 | 1:B:103:HIS:O | 2.06 | 0.55 |
| 1:D:559:THR:HA | 1:D:562:THR:HG23 | 1.89 | 0.55 |
| 1:A:229:ARG:HG2 | 1:A:250:LEU:CD2 | 2.34 | 0.55 |
| 1:B:504:VAL:HB | 1:B:541:VAL:HG12 | 1.89 | 0.55 |
| 1:C:657:LEU:O | 1:C:658:HIS:HB3 | 2.06 | 0.55 |
| 1:D:112:ASN:HA | 1:D:116:TRP:CD1 | 2.42 | 0.55 |
| 1:D:388:LEU:O | 1:D:392:MET:HG3 | 2.07 | 0.55 |
| 1:B:638:GLY:O | 1:B:652:ALA:HB1 | 2.07 | 0.54 |
| 1:D:310:GLY:O | 1:D:313:THR:HG22 | 2.07 | 0.54 |
| 1:D:504:VAL:HB | 1:D:541:VAL:HG12 | 1.89 | 0.54 |
| 1:A:310:GLY:O | 1:A:313:THR:HG22 | 2.07 | 0.54 |
| 1:B:358:TRP:CE3 | 1:B:369:TYR:HB3 | 2.42 | 0.54 |
| 1:C:270:PHE:CD1 | 1:C:282:PRO:HB2 | 2.42 | 0.54 |
| 1:B:270:PHE:CD1 | 1:B:282:PRO:HB2 | 2.42 | 0.54 |
| 1:B:718:ALA:O | 1:B:722:VAL:HG12 | 2.06 | 0.54 |
| 1:D:154:MET:O | 1:D:158:VAL:HG12 | 2.07 | 0.54 |
| 1:B:502:HIS:CE1 | 1:C:520:ALA:HA | 2.42 | 0.54 |
| 1:C:358:TRP:CE3 | 1:C:369:TYR:HB3 | 2.43 | 0.54 |
| 1:D:78:TYR:HA | 1:D:206:LEU:CD1 | 2.37 | 0.54 |
| 1:A:388:LEU:O | 1:A:392:MET:HG3 | 2.08 | 0.54 |
| 1:C:85:PHE:CZ | 1:C:200:LEU:HD13 | 2.43 | 0.54 |
| 1:C:310:GLY:O | 1:C:313:THR:HG22 | 2.07 | 0.54 |
| 1:C:707:LEU:HD22 | 1:C:707:LEU:C | 2.28 | 0.54 |
| 1:D:718:ALA:O | 1:D:722:VAL:HG12 | 2.07 | 0.54 |
| 1:A:112:ASN:HA | 1:A:116:TRP:CD1 | 2.43 | 0.54 |
| 1:C:718:ALA:O | 1:C:722:VAL:HG12 | 2.07 | 0.54 |
| 1:D:125:VAL:O | 1:D:129:GLY:HA2 | 2.08 | 0.54 |
| 1:D:638:GLY:O | 1:D:652:ALA:HB1 | 2.07 | 0.54 |
| 1:A:229:ARG:NH1 | 1:A:239:VAL:HG21 | 2.22 | 0.54 |
| 1:B:310:GLY:O | 1:B:313:THR:HG22 | 2.07 | 0.54 |
| 1:B:707:LEU:HD22 | 1:B:707:LEU:C | 2.28 | 0.54 |
| 1:A:358:TRP:CE3 | 1:A:369:TYR:HB3 | 2.42 | 0.54 |
| 1:A:712:ILE:C | 1:A:712:ILE:HD12 | 2.28 | 0.54 |
| 1:B:388:LEU:O | 1:B:392:MET:HG3 | 2.07 | 0.54 |
| 1:B:693:VAL:HG22 | 1:B:694:PRO:HD3 | 1.90 | 0.54 |
| 1:C:260:VAL:HG12 | 1:C:261:ASP:N | 2.21 | 0.54 |
| 1:D:229:ARG:NH1 | 1:D:239:VAL:HG21 | 2.22 | 0.54 |
| 1:A:504:VAL:HA | 1:A:540:ALA:O | 2.08 | 0.54 |
| 1:C:121:LEU:C | 1:C:124:PRO:HD2 | 2.28 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:606:SER:HB2 | 1:C:630:PRO:HB2 | 1.90 | 0.54 |
| 1:C:214:SER:HB2 | 1:C:217:ARG:HG2 | 1.89 | 0.54 |
| 1:C:709:SER:OG | 1:C:712:ILE:HG23 | 2.08 | 0.54 |
| 1:D:126:VAL:HG21 | 1:D:191:ALA:HB1 | 1.90 | 0.54 |
| 1:D:358:TRP:CE3 | 1:D:369:TYR:HB3 | 2.43 | 0.54 |
| 1:B:121:LEU:C | 1:B:124:PRO:HD2 | 2.29 | 0.53 |
| 1:B:260:VAL:HG12 | 1:B:261:ASP:N | 2.22 | 0.53 |
| 1:B:559:THR:HA | 1:B:562:THR:HG23 | 1.89 | 0.53 |
| 1:C:232:GLU:CG | 1:C:233:ASP:N | 2.70 | 0.53 |
| 1:A:126:VAL:HG21 | 1:A:191:ALA:HB1 | 1.90 | 0.53 |
| 1:A:85:PHE:CZ | 1:A:200:LEU:HD13 | 2.43 | 0.53 |
| 1:A:541:VAL:HG13 | 1:A:546:VAL:HG21 | 1.90 | 0.53 |
| 1:B:214:SER:HB2 | 1:B:217:ARG:HG2 | 1.89 | 0.53 |
| 1:B:232:GLU:CG | 1:B:233:ASP:N | 2.70 | 0.53 |
| 1:B:600:ILE:HB | 1:B:604:ASP:OD1 | 2.09 | 0.53 |
| 1:C:559:THR:HA | 1:C:562:THR:HG23 | 1.89 | 0.53 |
| 1:D:504:VAL:HA | 1:D:540:ALA:O | 2.08 | 0.53 |
| 1:D:541:VAL:HG13 | 1:D:546:VAL:HG21 | 1.90 | 0.53 |
| 1:A:132:PRO:O | 1:A:136:ARG:HG3 | 2.09 | 0.53 |
| 1:A:270:PHE:CD1 | 1:A:282:PRO:HB2 | 2.42 | 0.53 |
| 1:A:613:LYS:HE2 | 1:A:636:ASP:OD1 | 2.09 | 0.53 |
| 1:B:85:PHE:CZ | 1:B:200:LEU:HD13 | 2.43 | 0.53 |
| 1:B:606:SER:HB2 | 1:B:630:PRO:HB2 | 1.91 | 0.53 |
| 1:B:712:ILE:HD12 | 1:B:712:ILE:C | 2.28 | 0.53 |
| 1:C:388:LEU:O | 1:C:392:MET:HG3 | 2.08 | 0.53 |
| 1:C:600:ILE:HB | 1:C:604:ASP:OD1 | 2.09 | 0.53 |
| 1:D:270:PHE:CD1 | 1:D:282:PRO:HB2 | 2.42 | 0.53 |
| 1:A:482:GLY:HA3 | 1:A:499:VAL:CG2 | 2.35 | 0.53 |
| 1:B:229:ARG:NH1 | 1:B:239:VAL:HG21 | 2.22 | 0.53 |
| 1:D:600:ILE:HB | 1:D:604:ASP:OD1 | 2.09 | 0.53 |
| 1:D:712:ILE:HD12 | 1:D:712:ILE:C | 2.28 | 0.53 |
| 1:A:160:TRP:O | 1:A:164:MET:CB | 2.56 | 0.53 |
| 1:A:227:ALA:HB1 | 1:A:250:LEU:HD11 | 1.90 | 0.53 |
| 1:A:707:LEU:HD22 | 1:A:707:LEU:C | 2.28 | 0.53 |
| 1:C:229:ARG:NH1 | 1:C:239:VAL:HG21 | 2.22 | 0.53 |
| 1:D:160:TRP:O | 1:D:164:MET:CB | 2.56 | 0.53 |
| 1:D:227:ALA:HB1 | 1:D:250:LEU:HD11 | 1.90 | 0.53 |
| 1:A:600:ILE:HB | 1:A:604:ASP:OD1 | 2.09 | 0.53 |
| 1:D:214:SER:HB2 | 1:D:217:ARG:HG2 | 1.89 | 0.53 |
| 1:D:707:LEU:HD22 | 1:D:707:LEU:C | 2.28 | 0.53 |
| 1:D:709:SER:OG | 1:D:712:ILE:HG23 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:214:SER:HB2 | 1:A:217:ARG:HG2 | 1.89 | 0.53 |
| 1:A:499:VAL:O | 1:A:502:HIS:HA | 2.08 | 0.53 |
| 1:B:660:ASP:O | 1:B:662:ARG:HG2 | 2.09 | 0.53 |
| 1:C:229:ARG:HG2 | 1:C:250:LEU:CD2 | 2.34 | 0.53 |
| 1:C:712:ILE:HD12 | 1:C:712:ILE:C | 2.29 | 0.53 |
| 1:D:166:ALA:HA | 1:D:173:PHE:CE2 | 2.44 | 0.53 |
| 1:D:499:VAL:O | 1:D:502:HIS:HA | 2.08 | 0.53 |
| 1:A:166:ALA:HA | 1:A:173:PHE:CE2 | 2.44 | 0.53 |
| 1:A:269:SER:O | 1:A:285:LYS:HB2 | 2.09 | 0.53 |
| 1:B:229:ARG:HG2 | 1:B:250:LEU:CD2 | 2.34 | 0.53 |
| 1:C:166:ALA:HA | 1:C:173:PHE:CE2 | 2.44 | 0.53 |
| 1:C:575:MET:HE1 | 1:C:587:VAL:HG13 | 1.90 | 0.53 |
| 1:D:482:GLY:HA3 | 1:D:499:VAL:CG2 | 2.36 | 0.53 |
| 1:D:613:LYS:HE2 | 1:D:636:ASP:OD1 | 2.09 | 0.53 |
| 1:A:555:ILE:O | 1:A:555:ILE:HD12 | 2.09 | 0.53 |
| 1:A:693:VAL:HG22 | 1:A:694:PRO:HD3 | 1.90 | 0.53 |
| 1:B:499:VAL:O | 1:B:502:HIS:HA | 2.09 | 0.53 |
| 1:C:499:VAL:O | 1:C:502:HIS:HA | 2.09 | 0.53 |
| 1:C:693:VAL:HG22 | 1:C:694:PRO:HD3 | 1.91 | 0.53 |
| 1:D:693:VAL:HG22 | 1:D:694:PRO:HD3 | 1.90 | 0.53 |
| 1:B:482:GLY:HA3 | 1:B:499:VAL:CG2 | 2.35 | 0.53 |
| 1:B:504:VAL:HA | 1:B:540:ALA:O | 2.09 | 0.53 |
| 1:B:604:ASP:HB3 | 1:B:607:ARG:NH2 | 2.25 | 0.53 |
| 1:B:709:SER:OG | 1:B:712:ILE:HG23 | 2.09 | 0.53 |
| 1:C:482:GLY:HA3 | 1:C:499:VAL:CG2 | 2.35 | 0.53 |
| 1:D:132:PRO:O | 1:D:136:ARG:HG3 | 2.09 | 0.53 |
| 1:A:660:ASP:O | 1:A:662:ARG:HG2 | 2.09 | 0.52 |
| 1:A:718:ALA:O | 1:A:722:VAL:HG12 | 2.09 | 0.52 |
| 1:B:613:LYS:HE2 | 1:B:636:ASP:OD1 | 2.09 | 0.52 |
| 1:C:613:LYS:HE2 | 1:C:636:ASP:OD1 | 2.09 | 0.52 |
| 1:D:269:SER:O | 1:D:285:LYS:HB2 | 2.09 | 0.52 |
| 1:B:166:ALA:HA | 1:B:173:PHE:CE2 | 2.44 | 0.52 |
| 1:B:541:VAL:HG13 | 1:B:546:VAL:HG21 | 1.90 | 0.52 |
| 1:C:604:ASP:HB3 | 1:C:607:ARG:NH2 | 2.25 | 0.52 |
| 1:D:85:PHE:CZ | 1:D:200:LEU:HD13 | 2.44 | 0.52 |
| 1:D:391:PRO:O | 1:D:395:MET:HG2 | 2.08 | 0.52 |
| 1:D:604:ASP:HB3 | 1:D:607:ARG:NH2 | 2.25 | 0.52 |
| 1:D:660:ASP:O | 1:D:662:ARG:HG2 | 2.09 | 0.52 |
| 1:A:340:SER:O | 1:A:344:VAL:HG13 | 2.09 | 0.52 |
| 1:A:604:ASP:HB3 | 1:A:607:ARG:NH2 | 2.25 | 0.52 |
| 1:A:391:PRO:O | 1:A:395:MET:HG2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:PHE:HE2 | 1:B:451:ALA:HB2 | 1.75 | 0.52 |
| 1:C:504:VAL:HA | 1:C:540:ALA:O | 2.09 | 0.52 |
| 1:D:555:ILE:HD12 | 1:D:555:ILE:O | 2.09 | 0.52 |
| 1:D:606:SER:HB2 | 1:D:630:PRO:HB2 | 1.91 | 0.52 |
| 1:A:105:LEU:HD12 | 1:A:106:LYS:H | 1.73 | 0.52 |
| 1:A:575:MET:HE1 | 1:A:587:VAL:HG13 | 1.92 | 0.52 |
| 1:B:227:ALA:HB1 | 1:B:250:LEU:HD11 | 1.90 | 0.52 |
| 1:C:125:VAL:O | 1:C:129:GLY:HA2 | 2.08 | 0.52 |
| 1:C:541:VAL:HG13 | 1:C:546:VAL:HG21 | 1.90 | 0.52 |
| 1:C:660:ASP:O | 1:C:662:ARG:HG2 | 2.10 | 0.52 |
| 1:D:121:LEU:C | 1:D:124:PRO:HD2 | 2.28 | 0.52 |
| 1:D:340:SER:O | 1:D:344:VAL:HG13 | 2.10 | 0.52 |
| 1:A:474:ALA:O | 1:A:478:GLY:N | 2.42 | 0.52 |
| 1:A:606:SER:HB2 | 1:A:630:PRO:HB2 | 1.91 | 0.52 |
| 1:C:227:ALA:HB1 | 1:C:250:LEU:HD11 | 1.90 | 0.52 |
| 1:D:105:LEU:HD12 | 1:D:106:LYS:H | 1.73 | 0.52 |
| 1:A:266:GLU:N | 1:A:303:VAL:HG12 | 2.25 | 0.52 |
| 1:B:132:PRO:O | 1:B:136:ARG:HG3 | 2.09 | 0.52 |
| 1:D:474:ALA:O | 1:D:478:GLY:N | 2.42 | 0.52 |
| 1:A:705:GLY:O | 1:A:706:LEU:HG | 2.09 | 0.52 |
| 1:B:266:GLU:N | 1:B:303:VAL:HG12 | 2.25 | 0.52 |
| 1:C:266:GLU:N | 1:C:303:VAL:HG12 | 2.25 | 0.52 |
| 1:C:340:SER:O | 1:C:344:VAL:HG13 | 2.10 | 0.52 |
| 1:D:266:GLU:N | 1:D:303:VAL:HG12 | 2.25 | 0.52 |
| 1:D:451:ALA:HB1 | 1:D:539:MET:HE1 | 1.92 | 0.52 |
| 1:A:121:LEU:C | 1:A:124:PRO:HD2 | 2.29 | 0.52 |
| 1:A:78:TYR:HA | 1:A:206:LEU:HD12 | 1.92 | 0.52 |
| 1:B:125:VAL:O | 1:B:129:GLY:HA2 | 2.09 | 0.52 |
| 1:B:555:ILE:O | 1:B:555:ILE:HD12 | 2.09 | 0.52 |
| 1:B:575:MET:HE1 | 1:B:587:VAL:HG13 | 1.91 | 0.52 |
| 1:B:82:ARG:O | 1:B:86:TRP:HD1 | 1.93 | 0.52 |
| 1:C:269:SER:O | 1:C:285:LYS:HB2 | 2.09 | 0.52 |
| 1:C:446:PHE:HE2 | 1:C:451:ALA:HB2 | 1.75 | 0.52 |
| 1:A:510:ARG:HG3 | 1:A:514:GLU:OE1 | 2.10 | 0.52 |
| 1:B:105:LEU:HD12 | 1:B:106:LYS:H | 1.73 | 0.52 |
| 1:B:450:ASN:HD22 | 1:C:513:GLN:HG3 | 1.75 | 0.52 |
| 1:B:510:ARG:HG3 | 1:B:514:GLU:OE1 | 2.10 | 0.52 |
| 1:C:160:TRP:O | 1:C:164:MET:CB | 2.57 | 0.52 |
| 1:C:82:ARG:O | 1:C:86:TRP:HD1 | 1.93 | 0.52 |
| 1:D:705:GLY:O | 1:D:706:LEU:HG | 2.09 | 0.52 |
| 1:D:78:TYR:HA | 1:D:206:LEU:HD12 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:709:SER:OG | 1:A:712:ILE:HG23 | 2.10 | 0.51 |
| 1:B:269:SER:O | 1:B:285:LYS:HB2 | 2.09 | 0.51 |
| 1:B:340:SER:O | 1:B:344:VAL:HG13 | 2.10 | 0.51 |
| 1:B:391:PRO:O | 1:B:395:MET:HG2 | 2.09 | 0.51 |
| 1:B:440:ARG:HB3 | 1:B:550:VAL:CG2 | 2.40 | 0.51 |
| 1:C:391:PRO:O | 1:C:395:MET:HG2 | 2.08 | 0.51 |
| 1:C:440:ARG:HB3 | 1:C:550:VAL:CG2 | 2.40 | 0.51 |
| 1:C:474:ALA:O | 1:C:478:GLY:N | 2.42 | 0.51 |
| 1:C:555:ILE:HD12 | 1:C:555:ILE:O | 2.09 | 0.51 |
| 1:B:474:ALA:O | 1:B:478:GLY:N | 2.42 | 0.51 |
| 1:D:131:TRP:HB3 | 1:D:132:PRO:HD3 | 1.92 | 0.51 |
| 1:D:510:ARG:HG3 | 1:D:514:GLU:OE1 | 2.10 | 0.51 |
| 1:A:446:PHE:HE2 | 1:A:451:ALA:HB2 | 1.74 | 0.51 |
| 1:B:363:PRO:HB2 | 1:B:364:GLN:NE2 | 2.26 | 0.51 |
| 1:C:105:LEU:HD12 | 1:C:106:LYS:H | 1.73 | 0.51 |
| 1:C:132:PRO:O | 1:C:136:ARG:HG3 | 2.09 | 0.51 |
| 1:C:363:PRO:HB2 | 1:C:364:GLN:NE2 | 2.26 | 0.51 |
| 1:A:376:SER:HA | 1:A:379:ILE:HG22 | 1.93 | 0.51 |
| 1:B:160:TRP:O | 1:B:164:MET:CB | 2.57 | 0.51 |
| 1:D:363:PRO:HB2 | 1:D:364:GLN:NE2 | 2.26 | 0.51 |
| 1:A:363:PRO:HB2 | 1:A:364:GLN:NE2 | 2.26 | 0.51 |
| 1:C:216:ILE:HG21 | 1:C:326:GLN:NE2 | 2.26 | 0.51 |
| 1:C:510:ARG:HG3 | 1:C:514:GLU:OE1 | 2.10 | 0.51 |
| 1:D:261:ASP:CG | 1:D:293:GLY:H | 2.14 | 0.51 |
| 1:A:261:ASP:CG | 1:A:293:GLY:H | 2.14 | 0.51 |
| 1:B:705:GLY:O | 1:B:706:LEU:HG | 2.10 | 0.51 |
| 1:C:376:SER:HA | 1:C:379:ILE:HG22 | 1.93 | 0.51 |
| 1:C:705:GLY:O | 1:C:706:LEU:HG | 2.10 | 0.51 |
| 1:D:446:PHE:HE2 | 1:D:451:ALA:HB2 | 1.75 | 0.51 |
| 1:D:575:MET:HE1 | 1:D:587:VAL:HG13 | 1.93 | 0.51 |
| 1:A:440:ARG:HB3 | 1:A:550:VAL:CG2 | 2.40 | 0.51 |
| 1:B:216:ILE:HG21 | 1:B:326:GLN:NE2 | 2.26 | 0.51 |
| 1:B:376:SER:HA | 1:B:379:ILE:HG22 | 1.93 | 0.51 |
| 1:B:425:VAL:HG12 | 1:B:622:ALA:HB3 | 1.93 | 0.51 |
| 1:C:425:VAL:HG12 | 1:C:622:ALA:HB3 | 1.93 | 0.51 |
| 1:D:440:ARG:HB3 | 1:D:550:VAL:CG2 | 2.40 | 0.51 |
| 1:D:82:ARG:O | 1:D:86:TRP:HD1 | 1.93 | 0.51 |
| 1:A:82:ARG:O | 1:A:86:TRP:HD1 | 1.93 | 0.51 |
| 1:D:376:SER:HA | 1:D:379:ILE:HG22 | 1.93 | 0.51 |
| 1:D:417:MET:HG3 | 1:D:668:ARG:HA | 1.93 | 0.51 |
| 1:A:536:VAL:HG13 | 1:A:550:VAL:HG12 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:MET:HG3 | 1:A:668:ARG:HA | 1.93 | 0.50 |
| 1:A:131:TRP:HB3 | 1:A:132:PRO:HD3 | 1.93 | 0.50 |
| 1:A:163:SER:OG | 1:A:186:VAL:HG23 | 2.11 | 0.50 |
| 1:A:75:SER:HB3 | 1:A:78:TYR:HB3 | 1.93 | 0.50 |
| 1:C:126:VAL:HG21 | 1:C:191:ALA:HB1 | 1.91 | 0.50 |
| 1:B:447:VAL:HG13 | 1:C:510:ARG:HH12 | 1.76 | 0.50 |
| 1:A:428:THR:O | 2:A:995:ALF:F2 | 2.19 | 0.50 |
| 1:B:616:GLY:O | 1:B:617:LEU:HD12 | 2.12 | 0.50 |
| 1:C:358:TRP:O | 1:C:362:GLY:HA3 | 2.11 | 0.50 |
| 1:A:216:ILE:HG21 | 1:A:326:GLN:NE2 | 2.26 | 0.50 |
| 1:B:163:SER:OG | 1:B:186:VAL:HG23 | 2.12 | 0.50 |
| 1:C:179:SER:N | 1:C:180:GLN:HA | 2.27 | 0.50 |
| 1:C:308:HIS:HB3 | 1:C:312:ASP:OD1 | 2.12 | 0.50 |
| 1:C:616:GLY:O | 1:C:617:LEU:HD12 | 2.12 | 0.50 |
| 1:D:216:ILE:HG21 | 1:D:326:GLN:NE2 | 2.26 | 0.50 |
| 1:D:616:GLY:O | 1:D:617:LEU:HD12 | 2.12 | 0.50 |
| 1:A:219:LEU:CD2 | 1:A:647:VAL:HG12 | 2.42 | 0.50 |
| 1:B:358:TRP:O | 1:B:362:GLY:HA3 | 2.12 | 0.50 |
| 1:B:605:LYS:HD3 | 1:B:628:ASP:HB3 | 1.93 | 0.50 |
| 1:D:605:LYS:HD3 | 1:D:628:ASP:HB3 | 1.93 | 0.50 |
| 1:D:219:LEU:CD2 | 1:D:647:VAL:HG12 | 2.42 | 0.50 |
| 1:A:616:GLY:O | 1:A:617:LEU:HD12 | 2.12 | 0.50 |
| 1:B:308:HIS:HB3 | 1:B:312:ASP:OD1 | 2.12 | 0.50 |
| 1:B:75:SER:HB3 | 1:B:78:TYR:HB3 | 1.93 | 0.50 |
| 1:C:131:TRP:HB3 | 1:C:132:PRO:HD3 | 1.93 | 0.50 |
| 1:C:414:LEU:HD21 | 1:C:670:LEU:CD1 | 2.42 | 0.50 |
| 1:C:417:MET:HG3 | 1:C:668:ARG:HA | 1.93 | 0.50 |
| 1:A:358:TRP:O | 1:A:362:GLY:HA3 | 2.11 | 0.50 |
| 1:B:131:TRP:HB3 | 1:B:132:PRO:HD3 | 1.93 | 0.50 |
| 1:B:179:SER:N | 1:B:180:GLN:HA | 2.27 | 0.50 |
| 1:C:163:SER:OG | 1:C:186:VAL:HG23 | 2.12 | 0.50 |
| 1:D:75:SER:HB3 | 1:D:78:TYR:HB3 | 1.93 | 0.50 |
| 1:B:417:MET:HG3 | 1:B:668:ARG:HA | 1.93 | 0.50 |
| 1:C:258:ILE:HD12 | 1:C:295:THR:CG2 | 2.42 | 0.50 |
| 1:C:75:SER:HB3 | 1:C:78:TYR:HB3 | 1.93 | 0.50 |
| 1:D:163:SER:OG | 1:D:186:VAL:HG23 | 2.12 | 0.50 |
| 1:D:358:TRP:O | 1:D:362:GLY:HA3 | 2.11 | 0.50 |
| 1:A:367:LEU:H | 1:A:367:LEU:CD1 | 2.25 | 0.50 |
| 1:B:266:GLU:H | 1:B:303:VAL:HG12 | 1.77 | 0.50 |
| 1:B:414:LEU:HD21 | 1:B:670:LEU:CD1 | 2.42 | 0.50 |
| 1:D:232:GLU:CG | 1:D:233:ASP:N | 2.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:425:VAL:HG12 | 1:D:622:ALA:HB3 | 1.93 | 0.50 |
| 1:A:232:GLU:CG | 1:A:233:ASP:N | 2.70 | 0.49 |
| 1:A:657:LEU:HG | 1:A:658:HIS:N | 2.27 | 0.49 |
| 1:B:261:ASP:CG | 1:B:293:GLY:H | 2.14 | 0.49 |
| 1:B:90:MET:O | 1:B:94:PRO:HD3 | 2.12 | 0.49 |
| 1:B:78:TYR:HA | 1:B:206:LEU:HD12 | 1.93 | 0.49 |
| 1:C:266:GLU:H | 1:C:303:VAL:HG12 | 1.77 | 0.49 |
| 1:C:688:TYR:CE1 | 1:C:719:LEU:HD23 | 2.47 | 0.49 |
| 1:D:615:LYS:HG3 | 1:D:616:GLY:N | 2.25 | 0.49 |
| 1:A:605:LYS:HD3 | 1:A:628:ASP:HB3 | 1.94 | 0.49 |
| 1:A:615:LYS:HG3 | 1:A:616:GLY:N | 2.26 | 0.49 |
| 1:B:110:SER:O | 1:B:111:GLY:C | 2.51 | 0.49 |
| 1:B:126:VAL:HG21 | 1:B:191:ALA:HB1 | 1.93 | 0.49 |
| 1:B:260:VAL:CG1 | 1:B:261:ASP:N | 2.75 | 0.49 |
| 1:B:680:GLN:O | 1:B:683:PHE:HB3 | 2.12 | 0.49 |
| 1:B:735:THR:O | 1:B:736:LEU:C | 2.51 | 0.49 |
| 1:C:260:VAL:CG1 | 1:C:261:ASP:N | 2.75 | 0.49 |
| 1:C:261:ASP:CG | 1:C:293:GLY:H | 2.14 | 0.49 |
| 1:C:276:VAL:HG13 | 1:C:602:PRO:HD3 | 1.94 | 0.49 |
| 1:A:86:TRP:HB2 | 1:C:703:LEU:HD21 | 1.93 | 0.49 |
| 1:C:735:THR:O | 1:C:736:LEU:C | 2.51 | 0.49 |
| 1:C:78:TYR:HA | 1:C:206:LEU:HD12 | 1.93 | 0.49 |
| 1:D:258:ILE:HD12 | 1:D:295:THR:CG2 | 2.42 | 0.49 |
| 1:D:367:LEU:H | 1:D:367:LEU:CD1 | 2.26 | 0.49 |
| 1:D:687:ILE:HA | 1:D:690:VAL:CG1 | 2.41 | 0.49 |
| 1:A:276:VAL:HG13 | 1:A:602:PRO:HD3 | 1.94 | 0.49 |
| 1:A:468:ASN:HA | 1:A:471:VAL:HG22 | 1.94 | 0.49 |
| 1:A:425:VAL:HG12 | 1:A:622:ALA:HB3 | 1.94 | 0.49 |
| 1:C:605:LYS:HD3 | 1:C:628:ASP:HB3 | 1.94 | 0.49 |
| 1:D:260:VAL:CG1 | 1:D:261:ASP:N | 2.75 | 0.49 |
| 1:D:468:ASN:HA | 1:D:471:VAL:HG22 | 1.94 | 0.49 |
| 1:D:536:VAL:HG13 | 1:D:550:VAL:HG12 | 1.95 | 0.49 |
| 1:D:657:LEU:HG | 1:D:658:HIS:N | 2.27 | 0.49 |
| 1:A:260:VAL:CG1 | 1:A:261:ASP:N | 2.75 | 0.49 |
| 1:C:258:ILE:HD12 | 1:C:295:THR:HG23 | 1.95 | 0.49 |
| 1:C:90:MET:O | 1:C:94:PRO:HD3 | 2.13 | 0.49 |
| 1:D:276:VAL:HG13 | 1:D:602:PRO:HD3 | 1.94 | 0.49 |
| 1:A:308:HIS:HB3 | 1:A:312:ASP:OD1 | 2.12 | 0.49 |
| 1:B:162:TYR:HB2 | 1:B:375:VAL:HG11 | 1.94 | 0.49 |
| 1:B:258:ILE:HD12 | 1:B:295:THR:CG2 | 2.43 | 0.49 |
| 1:B:219:LEU:CD2 | 1:B:647:VAL:HG12 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:110:SER:O | 1:C:111:GLY:C | 2.51 | 0.49 |
| 1:D:159:ALA:CB | 1:D:379:ILE:HD13 | 2.41 | 0.49 |
| 1:D:414:LEU:HD21 | 1:D:670:LEU:CD1 | 2.42 | 0.49 |
| 1:A:179:SER:N | 1:A:180:GLN:HA | 2.27 | 0.49 |
| 1:A:258:ILE:HD12 | 1:A:295:THR:CG2 | 2.43 | 0.49 |
| 1:A:266:GLU:H | 1:A:303:VAL:HG12 | 1.77 | 0.49 |
| 1:A:414:LEU:HD21 | 1:A:670:LEU:CD1 | 2.42 | 0.49 |
| 1:B:276:VAL:HG13 | 1:B:602:PRO:HD3 | 1.94 | 0.49 |
| 1:B:687:ILE:HA | 1:B:690:VAL:CG1 | 2.42 | 0.49 |
| 1:C:219:LEU:CD2 | 1:C:647:VAL:HG12 | 2.42 | 0.49 |
| 1:C:693:VAL:N | 1:C:694:PRO:HD2 | 2.28 | 0.49 |
| 1:D:308:HIS:HB3 | 1:D:312:ASP:OD1 | 2.12 | 0.49 |
| 1:D:680:GLN:O | 1:D:683:PHE:HB3 | 2.12 | 0.49 |
| 1:B:152:ILE:O | 1:B:156:ILE:HG12 | 2.13 | 0.49 |
| 1:B:163:SER:O | 1:B:167:VAL:HG12 | 2.13 | 0.49 |
| 1:B:468:ASN:HA | 1:B:471:VAL:HG22 | 1.94 | 0.49 |
| 1:D:179:SER:N | 1:D:180:GLN:HA | 2.27 | 0.49 |
| 1:D:342:TRP:C | 1:D:345:PRO:HD2 | 2.33 | 0.49 |
| 1:B:703:LEU:HD21 | 1:D:86:TRP:HB2 | 1.95 | 0.49 |
| 1:A:152:ILE:O | 1:A:156:ILE:HG12 | 2.13 | 0.49 |
| 1:A:735:THR:O | 1:A:736:LEU:C | 2.51 | 0.49 |
| 1:A:78:TYR:CD2 | 1:A:79:LEU:HD12 | 2.42 | 0.49 |
| 1:B:367:LEU:CD1 | 1:B:367:LEU:H | 2.25 | 0.49 |
| 1:B:693:VAL:N | 1:B:694:PRO:HD2 | 2.28 | 0.49 |
| 1:C:468:ASN:HA | 1:C:471:VAL:HG22 | 1.94 | 0.49 |
| 1:D:152:ILE:O | 1:D:156:ILE:HG12 | 2.13 | 0.49 |
| 1:D:266:GLU:H | 1:D:303:VAL:HG12 | 1.77 | 0.49 |
| 1:D:735:THR:O | 1:D:736:LEU:C | 2.51 | 0.49 |
| 1:B:605:LYS:CD | 1:B:628:ASP:HB3 | 2.43 | 0.49 |
| 1:B:657:LEU:HG | 1:B:658:HIS:N | 2.27 | 0.49 |
| 1:C:152:ILE:O | 1:C:156:ILE:HG12 | 2.13 | 0.49 |
| 1:C:657:LEU:HG | 1:C:658:HIS:N | 2.27 | 0.49 |
| 1:A:342:TRP:C | 1:A:345:PRO:HD2 | 2.34 | 0.48 |
| 1:A:220:LEU:HG | 1:A:647:VAL:HG11 | 1.96 | 0.48 |
| 1:A:680:GLN:O | 1:A:683:PHE:HB3 | 2.13 | 0.48 |
| 1:B:447:VAL:HG22 | 1:C:513:GLN:OE1 | 2.12 | 0.48 |
| 1:C:367:LEU:H | 1:C:367:LEU:CD1 | 2.25 | 0.48 |
| 1:C:536:VAL:HG13 | 1:C:550:VAL:HG12 | 1.95 | 0.48 |
| 1:C:687:ILE:HA | 1:C:690:VAL:CG1 | 2.42 | 0.48 |
| 1:A:687:ILE:HA | 1:A:690:VAL:CG1 | 2.42 | 0.48 |
| 1:A:688:TYR:CE1 | 1:A:719:LEU:HD23 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:MET:O | 1:A:94:PRO:HD3 | 2.13 | 0.48 |
| 1:D:605:LYS:CD | 1:D:628:ASP:HB3 | 2.43 | 0.48 |
| 1:D:430:THR:HG22 | 1:D:641:MET:HG3 | 1.94 | 0.48 |
| 1:A:426:ASP:OD2 | 2:A:995:ALF:F2 | 2.20 | 0.48 |
| 1:B:258:ILE:HD12 | 1:B:295:THR:HG23 | 1.95 | 0.48 |
| 1:B:639:ILE:CG2 | 1:B:656:LEU:HD13 | 2.43 | 0.48 |
| 1:C:342:TRP:C | 1:C:345:PRO:HD2 | 2.33 | 0.48 |
| 1:D:162:TYR:HB2 | 1:D:375:VAL:HG11 | 1.95 | 0.48 |
| 1:D:220:LEU:HG | 1:D:647:VAL:HG11 | 1.96 | 0.48 |
| 1:D:90:MET:O | 1:D:94:PRO:HD3 | 2.13 | 0.48 |
| 1:A:269:SER:HB3 | 1:A:300:GLY:HA3 | 1.96 | 0.48 |
| 1:B:143:THR:OG1 | 1:B:144:GLY:N | 2.47 | 0.48 |
| 1:C:639:ILE:CG2 | 1:C:656:LEU:HD13 | 2.43 | 0.48 |
| 1:C:680:GLN:O | 1:C:683:PHE:HB3 | 2.13 | 0.48 |
| 1:D:110:SER:O | 1:D:111:GLY:C | 2.50 | 0.48 |
| 1:D:78:TYR:CD2 | 1:D:79:LEU:HD12 | 2.43 | 0.48 |
| 1:A:162:TYR:HB2 | 1:A:375:VAL:HG11 | 1.95 | 0.48 |
| 1:A:163:SER:O | 1:A:167:VAL:HG12 | 2.13 | 0.48 |
| 1:A:510:ARG:O | 1:A:514:GLU:HG3 | 2.13 | 0.48 |
| 1:A:143:THR:OG1 | 1:A:144:GLY:N | 2.47 | 0.48 |
| 1:A:605:LYS:CD | 1:A:628:ASP:HB3 | 2.44 | 0.48 |
| 1:B:220:LEU:HG | 1:B:647:VAL:HG11 | 1.95 | 0.48 |
| 1:B:224:PRO:O | 1:B:241:LEU:HD22 | 2.14 | 0.48 |
| 1:B:510:ARG:O | 1:B:514:GLU:HG3 | 2.13 | 0.48 |
| 1:C:143:THR:OG1 | 1:C:144:GLY:N | 2.47 | 0.48 |
| 1:C:162:TYR:HB2 | 1:C:375:VAL:HG11 | 1.95 | 0.48 |
| 1:C:224:PRO:O | 1:C:241:LEU:HD22 | 2.14 | 0.48 |
| 1:D:143:THR:OG1 | 1:D:144:GLY:N | 2.47 | 0.48 |
| 1:D:269:SER:HB3 | 1:D:300:GLY:HA3 | 1.96 | 0.48 |
| 1:D:510:ARG:O | 1:D:514:GLU:HG3 | 2.13 | 0.48 |
| 1:B:536:VAL:HG13 | 1:B:550:VAL:HG12 | 1.96 | 0.48 |
| 1:C:220:LEU:HG | 1:C:647:VAL:HG11 | 1.96 | 0.48 |
| 1:C:636:ASP:O | 1:C:637:ILE:HD13 | 2.14 | 0.48 |
| 1:C:657:LEU:O | 1:C:658:HIS:CB | 2.61 | 0.48 |
| 1:D:390:THR:N | 1:D:391:PRO:HD2 | 2.29 | 0.48 |
| 1:D:693:VAL:N | 1:D:694:PRO:HD2 | 2.29 | 0.48 |
| 1:A:224:PRO:O | 1:A:241:LEU:HD22 | 2.14 | 0.48 |
| 1:B:342:TRP:C | 1:B:345:PRO:HD2 | 2.34 | 0.48 |
| 1:B:440:ARG:HB3 | 1:B:550:VAL:HG21 | 1.96 | 0.48 |
| 1:B:544:LYS:O | 1:B:546:VAL:HG13 | 2.14 | 0.48 |
| 1:B:657:LEU:O | 1:B:658:HIS:CB | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:163:SER:O | 1:C:167:VAL:HG12 | 2.14 | 0.48 |
| 1:D:163:SER:O | 1:D:167:VAL:HG12 | 2.14 | 0.48 |
| 1:D:692:GLY:O | 1:D:695:LEU:HG | 2.14 | 0.48 |
| 1:C:605:LYS:CD | 1:C:628:ASP:HB3 | 2.44 | 0.48 |
| 1:D:136:ARG:HD2 | 1:D:149:PHE:CE2 | 2.49 | 0.48 |
| 1:A:110:SER:O | 1:A:111:GLY:C | 2.51 | 0.48 |
| 1:A:159:ALA:CB | 1:A:379:ILE:HD13 | 2.42 | 0.48 |
| 1:A:390:THR:N | 1:A:391:PRO:HD2 | 2.29 | 0.48 |
| 1:B:636:ASP:O | 1:B:637:ILE:HD13 | 2.14 | 0.48 |
| 1:B:702:PRO:O | 1:B:703:LEU:C | 2.52 | 0.48 |
| 1:C:510:ARG:O | 1:C:514:GLU:HG3 | 2.13 | 0.48 |
| 1:A:657:LEU:O | 1:A:658:HIS:CB | 2.61 | 0.47 |
| 1:A:693:VAL:N | 1:A:694:PRO:HD2 | 2.29 | 0.47 |
| 1:C:269:SER:HB3 | 1:C:300:GLY:HA3 | 1.96 | 0.47 |
| 1:D:657:LEU:O | 1:D:658:HIS:CB | 2.61 | 0.47 |
| 1:A:636:ASP:O | 1:A:637:ILE:HD13 | 2.14 | 0.47 |
| 1:B:269:SER:HB3 | 1:B:300:GLY:HA3 | 1.96 | 0.47 |
| 1:B:688:TYR:CE1 | 1:B:719:LEU:HD23 | 2.49 | 0.47 |
| 1:C:430:THR:HG22 | 1:C:641:MET:HG3 | 1.95 | 0.47 |
| 1:C:440:ARG:HB3 | 1:C:550:VAL:HG21 | 1.97 | 0.47 |
| 1:D:224:PRO:O | 1:D:241:LEU:HD22 | 2.14 | 0.47 |
| 1:D:440:ARG:HB3 | 1:D:550:VAL:HG21 | 1.96 | 0.47 |
| 1:A:136:ARG:HD2 | 1:A:149:PHE:CE2 | 2.50 | 0.47 |
| 1:A:440:ARG:HB3 | 1:A:550:VAL:HG21 | 1.96 | 0.47 |
| 1:A:692:GLY:O | 1:A:695:LEU:HG | 2.14 | 0.47 |
| 1:C:297:ASN:O | 1:C:298:GLN:HG3 | 2.14 | 0.47 |
| 1:C:146:LEU:HD13 | 1:C:344:VAL:HG22 | 1.97 | 0.47 |
| 1:C:692:GLY:O | 1:C:695:LEU:HG | 2.14 | 0.47 |
| 1:C:702:PRO:O | 1:C:703:LEU:C | 2.52 | 0.47 |
| 1:D:258:ILE:HD12 | 1:D:295:THR:HG23 | 1.96 | 0.47 |
| 1:D:92:THR:O | 1:D:95:VAL:HB | 2.15 | 0.47 |
| 1:A:258:ILE:HD12 | 1:A:295:THR:HG23 | 1.96 | 0.47 |
| 1:A:216:ILE:HG21 | 1:A:326:GLN:HE22 | 1.79 | 0.47 |
| 1:A:146:LEU:HD13 | 1:A:344:VAL:HG22 | 1.97 | 0.47 |
| 1:A:430:THR:HG22 | 1:A:641:MET:HG3 | 1.95 | 0.47 |
| 1:B:297:ASN:O | 1:B:298:GLN:HG3 | 2.14 | 0.47 |
| 1:B:692:GLY:O | 1:B:695:LEU:HG | 2.15 | 0.47 |
| 1:C:164:MET:HE2 | 1:C:164:MET:HA | 1.97 | 0.47 |
| 1:C:216:ILE:HD11 | 1:C:322:VAL:HG21 | 1.97 | 0.47 |
| 1:D:224:PRO:HD3 | 1:D:257:LYS:HD2 | 1.97 | 0.47 |
| 1:A:224:PRO:HD3 | 1:A:257:LYS:HD2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:419:LYS:C | 1:A:618:ILE:HD12 | 2.34 | 0.47 |
| 1:B:224:PRO:HD3 | 1:B:257:LYS:HD2 | 1.97 | 0.47 |
| 1:B:159:ALA:CB | 1:B:379:ILE:HD13 | 2.41 | 0.47 |
| 1:B:708:LEU:HD13 | 1:B:709:SER:N | 2.30 | 0.47 |
| 1:C:224:PRO:HD3 | 1:C:257:LYS:HD2 | 1.97 | 0.47 |
| 1:D:616:GLY:C | 1:D:617:LEU:HD12 | 2.35 | 0.47 |
| 1:A:430:THR:HA | 1:A:641:MET:HE2 | 1.95 | 0.47 |
| 1:A:539:MET:CE | 1:A:547:ALA:HB3 | 2.45 | 0.47 |
| 1:A:616:GLY:C | 1:A:617:LEU:HD12 | 2.35 | 0.47 |
| 1:B:216:ILE:HD11 | 1:B:322:VAL:HG21 | 1.97 | 0.47 |
| 1:B:430:THR:HG22 | 1:B:641:MET:HG3 | 1.95 | 0.47 |
| 1:B:657:LEU:O | 1:B:659:GLY:HA2 | 2.14 | 0.47 |
| 1:B:641:MET:HE1 | 1:B:659:GLY:O | 2.15 | 0.47 |
| 1:C:615:LYS:HG3 | 1:C:616:GLY:N | 2.25 | 0.47 |
| 1:C:641:MET:HE1 | 1:C:659:GLY:O | 2.15 | 0.47 |
| 1:C:708:LEU:HD13 | 1:C:709:SER:N | 2.30 | 0.47 |
| 1:D:131:TRP:N | 1:D:132:PRO:CD | 2.77 | 0.47 |
| 1:D:216:ILE:HG21 | 1:D:326:GLN:HE22 | 1.79 | 0.47 |
| 1:D:636:ASP:O | 1:D:637:ILE:HD13 | 2.15 | 0.47 |
| 1:B:615:LYS:HG3 | 1:B:616:GLY:N | 2.25 | 0.47 |
| 1:B:616:GLY:C | 1:B:617:LEU:HD12 | 2.35 | 0.47 |
| 1:D:179:SER:HB3 | 1:D:181:GLU:C | 2.34 | 0.47 |
| 1:A:297:ASN:O | 1:A:298:GLN:HG3 | 2.14 | 0.47 |
| 1:A:92:THR:O | 1:A:95:VAL:HB | 2.15 | 0.47 |
| 1:C:616:GLY:C | 1:C:617:LEU:HD12 | 2.35 | 0.47 |
| 1:C:657:LEU:O | 1:C:659:GLY:HA2 | 2.14 | 0.47 |
| 1:D:297:ASN:O | 1:D:298:GLN:HG3 | 2.14 | 0.47 |
| 1:D:407:LEU:HD23 | 1:D:407:LEU:N | 2.28 | 0.47 |
| 1:D:479:LEU:HD22 | 1:D:479:LEU:C | 2.35 | 0.47 |
| 1:D:605:LYS:CE | 1:D:628:ASP:HB3 | 2.44 | 0.47 |
| 1:D:713:ALA:O | 1:D:717:MET:HG3 | 2.15 | 0.47 |
| 1:A:690:VAL:HA | 1:A:693:VAL:HG13 | 1.97 | 0.47 |
| 1:B:179:SER:HB3 | 1:B:181:GLU:C | 2.35 | 0.47 |
| 1:B:479:LEU:HD22 | 1:B:479:LEU:C | 2.35 | 0.47 |
| 1:C:92:THR:O | 1:C:95:VAL:HB | 2.15 | 0.47 |
| 1:D:216:ILE:HD11 | 1:D:322:VAL:HG21 | 1.97 | 0.47 |
| 1:D:539:MET:CE | 1:D:547:ALA:HB3 | 2.45 | 0.47 |
| 1:D:540:ALA:HB2 | 1:D:545:THR:HA | 1.97 | 0.47 |
| 1:A:414:LEU:HD23 | 1:A:414:LEU:HA | 1.74 | 0.47 |
| 1:A:605:LYS:CE | 1:A:628:ASP:HB3 | 2.44 | 0.47 |
| 1:B:146:LEU:HD13 | 1:B:344:VAL:HG22 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:179:SER:CB | 1:B:183:VAL:HG22 | 2.45 | 0.47 |
| 1:B:562:THR:OG1 | 1:B:661:LEU:HD22 | 2.15 | 0.47 |
| 1:C:136:ARG:HD2 | 1:C:149:PHE:CE2 | 2.49 | 0.47 |
| 1:C:419:LYS:C | 1:C:618:ILE:HD12 | 2.35 | 0.47 |
| 1:C:479:LEU:HD22 | 1:C:479:LEU:C | 2.35 | 0.47 |
| 1:D:639:ILE:CG2 | 1:D:656:LEU:HD13 | 2.44 | 0.47 |
| 1:D:657:LEU:O | 1:D:659:GLY:HA2 | 2.14 | 0.47 |
| 1:D:690:VAL:HA | 1:D:693:VAL:HG13 | 1.97 | 0.47 |
| 1:A:131:TRP:N | 1:A:132:PRO:CD | 2.78 | 0.46 |
| 1:A:407:LEU:HD23 | 1:A:407:LEU:N | 2.29 | 0.46 |
| 1:A:479:LEU:HD22 | 1:A:479:LEU:C | 2.35 | 0.46 |
| 1:A:540:ALA:HB2 | 1:A:545:THR:HA | 1.97 | 0.46 |
| 1:A:639:ILE:CG2 | 1:A:656:LEU:HD13 | 2.44 | 0.46 |
| 1:B:186:VAL:HG22 | 1:B:188:PHE:H | 1.80 | 0.46 |
| 1:B:261:ASP:HB3 | 1:B:307:LEU:HB3 | 1.97 | 0.46 |
| 1:C:109:ILE:HG23 | 1:C:110:SER:CB | 2.29 | 0.46 |
| 1:C:179:SER:HB3 | 1:C:181:GLU:C | 2.35 | 0.46 |
| 1:C:544:LYS:O | 1:C:546:VAL:HG13 | 2.15 | 0.46 |
| 1:D:119:LEU:HD12 | 1:D:167:VAL:CG1 | 2.45 | 0.46 |
| 1:A:216:ILE:HD11 | 1:A:322:VAL:HG21 | 1.97 | 0.46 |
| 1:A:657:LEU:O | 1:A:659:GLY:HA2 | 2.14 | 0.46 |
| 1:A:702:PRO:O | 1:A:703:LEU:C | 2.52 | 0.46 |
| 1:B:605:LYS:CE | 1:B:628:ASP:HB3 | 2.43 | 0.46 |
| 1:C:216:ILE:HG21 | 1:C:326:GLN:HE22 | 1.79 | 0.46 |
| 1:C:539:MET:CE | 1:C:547:ALA:HB3 | 2.45 | 0.46 |
| 1:D:146:LEU:HD13 | 1:D:344:VAL:HG22 | 1.97 | 0.46 |
| 1:D:702:PRO:O | 1:D:703:LEU:C | 2.52 | 0.46 |
| 1:A:119:LEU:HD12 | 1:A:167:VAL:CG1 | 2.46 | 0.46 |
| 1:B:131:TRP:N | 1:B:132:PRO:CD | 2.78 | 0.46 |
| 1:B:390:THR:N | 1:B:391:PRO:HD2 | 2.30 | 0.46 |
| 1:B:460:HIS:HA | 1:B:471:VAL:HG11 | 1.97 | 0.46 |
| 1:C:261:ASP:HB3 | 1:C:307:LEU:HB3 | 1.98 | 0.46 |
| 1:C:159:ALA:CB | 1:C:379:ILE:HD13 | 2.42 | 0.46 |
| 1:C:540:ALA:HB2 | 1:C:545:THR:HA | 1.97 | 0.46 |
| 1:C:562:THR:OG1 | 1:C:661:LEU:HD22 | 2.16 | 0.46 |
| 1:D:414:LEU:HA | 1:D:414:LEU:HD23 | 1.73 | 0.46 |
| 1:A:88:ALA:CB | 1:A:125:VAL:HG23 | 2.46 | 0.46 |
| 1:B:136:ARG:HD2 | 1:B:149:PHE:CE2 | 2.50 | 0.46 |
| 1:B:419:LYS:C | 1:B:618:ILE:HD12 | 2.35 | 0.46 |
| 1:C:390:THR:N | 1:C:391:PRO:HD2 | 2.30 | 0.46 |
| 1:C:574:VAL:HG22 | 1:C:595:LYS:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:490:PRO:HB2 | 1:D:493:LYS:HB2 | 1.98 | 0.46 |
| 1:D:544:LYS:O | 1:D:546:VAL:HG13 | 2.15 | 0.46 |
| 1:A:179:SER:HB3 | 1:A:181:GLU:C | 2.36 | 0.46 |
| 1:A:713:ALA:O | 1:A:717:MET:HG3 | 2.16 | 0.46 |
| 1:B:621:MET:CE | 1:B:628:ASP:HB2 | 2.46 | 0.46 |
| 1:C:119:LEU:HD12 | 1:C:167:VAL:CG1 | 2.45 | 0.46 |
| 1:C:88:ALA:CB | 1:C:125:VAL:HG23 | 2.46 | 0.46 |
| 1:D:109:ILE:HG23 | 1:D:110:SER:CB | 2.30 | 0.46 |
| 1:D:455:ALA:HB2 | 1:D:539:MET:SD | 2.55 | 0.46 |
| 1:D:708:LEU:HD13 | 1:D:709:SER:N | 2.30 | 0.46 |
| 1:A:574:VAL:HG22 | 1:A:595:LYS:HB2 | 1.98 | 0.46 |
| 1:C:186:VAL:HG22 | 1:C:188:PHE:H | 1.81 | 0.46 |
| 1:C:460:HIS:HA | 1:C:471:VAL:HG11 | 1.97 | 0.46 |
| 1:C:621:MET:CE | 1:C:628:ASP:HB2 | 2.46 | 0.46 |
| 1:A:109:ILE:HG23 | 1:A:110:SER:CB | 2.30 | 0.46 |
| 1:A:186:VAL:HG22 | 1:A:188:PHE:H | 1.80 | 0.46 |
| 1:A:490:PRO:HB2 | 1:A:493:LYS:HB2 | 1.98 | 0.46 |
| 1:A:708:LEU:HD13 | 1:A:709:SER:N | 2.30 | 0.46 |
| 1:B:216:ILE:HG21 | 1:B:326:GLN:HE22 | 1.79 | 0.46 |
| 1:B:540:ALA:HB2 | 1:B:545:THR:HA | 1.97 | 0.46 |
| 1:C:131:TRP:N | 1:C:132:PRO:CD | 2.78 | 0.46 |
| 1:C:605:LYS:CE | 1:C:628:ASP:HB3 | 2.44 | 0.46 |
| 1:C:713:ALA:O | 1:C:717:MET:HG3 | 2.16 | 0.46 |
| 1:D:419:LYS:C | 1:D:618:ILE:HD12 | 2.35 | 0.46 |
| 1:B:109:ILE:HG23 | 1:B:110:SER:CB | 2.30 | 0.46 |
| 1:B:164:MET:HE2 | 1:B:164:MET:HA | 1.98 | 0.46 |
| 1:B:381:ALA:O | 1:B:383:PRO:HD3 | 2.15 | 0.46 |
| 1:B:446:PHE:CE2 | 1:B:451:ALA:HB2 | 2.51 | 0.46 |
| 1:B:727:ASN:O | 1:B:730:ARG:HB3 | 2.16 | 0.46 |
| 1:C:179:SER:CB | 1:C:183:VAL:HG22 | 2.46 | 0.46 |
| 1:C:559:THR:N | 1:C:560:PRO:HD2 | 2.31 | 0.46 |
| 1:D:178:ARG:HB2 | 1:D:184:VAL:HA | 1.98 | 0.46 |
| 1:D:186:VAL:HG22 | 1:D:188:PHE:H | 1.80 | 0.46 |
| 1:A:178:ARG:HB2 | 1:A:184:VAL:HA | 1.98 | 0.46 |
| 1:A:688:TYR:CD2 | 1:A:719:LEU:HB3 | 2.51 | 0.46 |
| 1:B:490:PRO:HB2 | 1:B:493:LYS:HB2 | 1.98 | 0.46 |
| 1:B:574:VAL:HG22 | 1:B:595:LYS:HB2 | 1.98 | 0.46 |
| 1:C:381:ALA:O | 1:C:383:PRO:HD3 | 2.16 | 0.46 |
| 1:C:490:PRO:HB2 | 1:C:493:LYS:HB2 | 1.98 | 0.46 |
| 1:D:430:THR:HA | 1:D:641:MET:HE2 | 1.96 | 0.46 |
| 1:D:601:MET:HB3 | 1:D:602:PRO:HD2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:422:THR:HG23 | 1:A:619:VAL:HG23 | 1.98 | 0.46 |
| 1:A:621:MET:CE | 1:A:628:ASP:HB2 | 2.46 | 0.46 |
| 1:B:119:LEU:HD12 | 1:B:167:VAL:CG1 | 2.46 | 0.46 |
| 1:B:670:LEU:O | 1:B:673:SER:HB3 | 2.16 | 0.46 |
| 1:B:92:THR:O | 1:B:95:VAL:HB | 2.16 | 0.46 |
| 1:C:164:MET:CE | 1:C:164:MET:HA | 2.46 | 0.46 |
| 1:C:427:LYS:HG3 | 1:C:428:THR:N | 2.31 | 0.46 |
| 1:B:447:VAL:HG13 | 1:C:510:ARG:NH1 | 2.31 | 0.46 |
| 1:C:626:VAL:HA | 1:C:647:VAL:HG22 | 1.98 | 0.46 |
| 1:C:695:LEU:C | 1:C:695:LEU:HD12 | 2.37 | 0.46 |
| 1:D:88:ALA:CB | 1:D:125:VAL:HG23 | 2.46 | 0.46 |
| 1:D:574:VAL:HG22 | 1:D:595:LYS:HB2 | 1.98 | 0.46 |
| 1:D:621:MET:CE | 1:D:628:ASP:HB2 | 2.46 | 0.46 |
| 1:D:688:TYR:CD2 | 1:D:719:LEU:HB3 | 2.51 | 0.46 |
| 1:D:688:TYR:CE1 | 1:D:719:LEU:HD23 | 2.50 | 0.46 |
| 1:A:446:PHE:CE2 | 1:A:451:ALA:HB2 | 2.51 | 0.45 |
| 1:A:544:LYS:O | 1:A:546:VAL:HG13 | 2.15 | 0.45 |
| 1:A:629:ALA:HA | 1:A:632:LEU:HD23 | 1.98 | 0.45 |
| 1:B:135:LYS:HG2 | 1:B:139:GLN:NE2 | 2.31 | 0.45 |
| 1:B:695:LEU:C | 1:B:695:LEU:HD12 | 2.37 | 0.45 |
| 1:B:713:ALA:O | 1:B:717:MET:HG3 | 2.16 | 0.45 |
| 1:C:178:ARG:HB2 | 1:C:184:VAL:HA | 1.98 | 0.45 |
| 1:C:414:LEU:HD23 | 1:C:414:LEU:HA | 1.73 | 0.45 |
| 1:D:179:SER:CB | 1:D:183:VAL:HG22 | 2.45 | 0.45 |
| 1:A:261:ASP:HB3 | 1:A:307:LEU:HB3 | 1.97 | 0.45 |
| 1:A:427:LYS:HG3 | 1:A:428:THR:N | 2.30 | 0.45 |
| 1:A:601:MET:HB3 | 1:A:602:PRO:HD2 | 1.98 | 0.45 |
| 1:B:539:MET:CE | 1:B:547:ALA:HB3 | 2.46 | 0.45 |
| 1:B:626:VAL:HA | 1:B:647:VAL:HG22 | 1.98 | 0.45 |
| 1:B:690:VAL:HA | 1:B:693:VAL:HG13 | 1.97 | 0.45 |
| 1:C:135:LYS:HG2 | 1:C:139:GLN:NE2 | 2.31 | 0.45 |
| 1:D:261:ASP:HB3 | 1:D:307:LEU:HB3 | 1.97 | 0.45 |
| 1:D:446:PHE:CE2 | 1:D:451:ALA:HB2 | 2.51 | 0.45 |
| 1:D:422:THR:HG23 | 1:D:619:VAL:HG23 | 1.98 | 0.45 |
| 1:A:219:LEU:HD22 | 1:A:219:LEU:C | 2.36 | 0.45 |
| 1:A:440:ARG:O | 1:A:550:VAL:HG22 | 2.16 | 0.45 |
| 1:B:164:MET:CE | 1:B:164:MET:HA | 2.46 | 0.45 |
| 1:B:178:ARG:HB2 | 1:B:184:VAL:HA | 1.98 | 0.45 |
| 1:B:219:LEU:HD22 | 1:B:219:LEU:C | 2.36 | 0.45 |
| 1:B:427:LYS:HG3 | 1:B:428:THR:N | 2.31 | 0.45 |
| 1:B:690:VAL:O | 1:B:694:PRO:HD3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:219:LEU:HD22 | 1:D:219:LEU:C | 2.36 | 0.45 |
| 1:D:670:LEU:O | 1:D:673:SER:HB3 | 2.16 | 0.45 |
| 1:A:479:LEU:HD13 | 1:A:480:SER:H | 1.81 | 0.45 |
| 1:B:440:ARG:O | 1:B:550:VAL:HG22 | 2.16 | 0.45 |
| 1:C:178:ARG:HA | 1:C:178:ARG:HD3 | 1.73 | 0.45 |
| 1:C:218:ALA:O | 1:C:221:LYS:HB2 | 2.17 | 0.45 |
| 1:C:446:PHE:CE2 | 1:C:451:ALA:HB2 | 2.51 | 0.45 |
| 1:C:600:ILE:HD12 | 1:C:600:ILE:O | 2.16 | 0.45 |
| 1:C:629:ALA:HA | 1:C:632:LEU:HD23 | 1.99 | 0.45 |
| 1:D:440:ARG:O | 1:D:550:VAL:HG22 | 2.16 | 0.45 |
| 1:D:727:ASN:O | 1:D:730:ARG:HB3 | 2.16 | 0.45 |
| 1:A:460:HIS:HA | 1:A:471:VAL:HG11 | 1.97 | 0.45 |
| 1:A:548:LEU:HD12 | 1:A:548:LEU:HA | 1.77 | 0.45 |
| 1:A:562:THR:OG1 | 1:A:661:LEU:HD22 | 2.16 | 0.45 |
| 1:B:218:ALA:O | 1:B:221:LYS:HB2 | 2.17 | 0.45 |
| 1:B:292:ILE:O | 1:B:295:THR:HG22 | 2.16 | 0.45 |
| 1:C:219:LEU:C | 1:C:219:LEU:HD22 | 2.36 | 0.45 |
| 1:C:292:ILE:O | 1:C:295:THR:HG22 | 2.16 | 0.45 |
| 1:C:407:LEU:HD23 | 1:C:407:LEU:N | 2.29 | 0.45 |
| 1:D:460:HIS:HA | 1:D:471:VAL:HG11 | 1.97 | 0.45 |
| 1:D:657:LEU:C | 1:D:659:GLY:HA2 | 2.37 | 0.45 |
| 1:D:562:THR:OG1 | 1:D:661:LEU:HD22 | 2.16 | 0.45 |
| 1:A:179:SER:CB | 1:A:183:VAL:HG22 | 2.46 | 0.45 |
| 1:A:559:THR:N | 1:A:560:PRO:HD2 | 2.32 | 0.45 |
| 1:B:559:THR:N | 1:B:560:PRO:HD2 | 2.32 | 0.45 |
| 1:C:392:MET:O | 1:C:396:VAL:HG12 | 2.16 | 0.45 |
| 1:C:656:LEU:HD22 | 1:C:661:LEU:HA | 1.98 | 0.45 |
| 1:D:135:LYS:HG2 | 1:D:139:GLN:NE2 | 2.31 | 0.45 |
| 1:D:629:ALA:HA | 1:D:632:LEU:HD23 | 1.99 | 0.45 |
| 1:A:626:VAL:HA | 1:A:647:VAL:HG22 | 1.97 | 0.45 |
| 1:A:657:LEU:C | 1:A:659:GLY:HA2 | 2.37 | 0.45 |
| 1:B:178:ARG:HD3 | 1:B:178:ARG:HA | 1.73 | 0.45 |
| 1:B:479:LEU:HD13 | 1:B:480:SER:H | 1.82 | 0.45 |
| 1:B:455:ALA:HB2 | 1:B:539:MET:SD | 2.57 | 0.45 |
| 1:B:600:ILE:O | 1:B:600:ILE:HD12 | 2.17 | 0.45 |
| 1:B:629:ALA:HA | 1:B:632:LEU:HD23 | 1.99 | 0.45 |
| 1:B:706:LEU:HB3 | 1:B:707:LEU:H | 1.42 | 0.45 |
| 1:C:690:VAL:O | 1:C:694:PRO:HD3 | 2.17 | 0.45 |
| 1:C:706:LEU:HB3 | 1:C:707:LEU:H | 1.42 | 0.45 |
| 1:D:427:LYS:HG3 | 1:D:428:THR:N | 2.31 | 0.45 |
| 1:D:695:LEU:C | 1:D:695:LEU:HD12 | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:MET:HE1 | 1:A:637:ILE:HG21 | 1.98 | 0.45 |
| 1:A:600:ILE:HD12 | 1:A:600:ILE:O | 2.16 | 0.45 |
| 1:A:690:VAL:O | 1:A:694:PRO:HD3 | 2.17 | 0.45 |
| 1:C:498:GLN:HG2 | 1:C:502:HIS:O | 2.17 | 0.45 |
| 1:C:670:LEU:O | 1:C:673:SER:HB3 | 2.17 | 0.45 |
| 1:C:688:TYR:CD2 | 1:C:719:LEU:HB3 | 2.51 | 0.45 |
| 1:D:343:PHE:O | 1:D:347:VAL:HG23 | 2.17 | 0.45 |
| 1:D:539:MET:HE2 | 1:D:547:ALA:HB3 | 1.99 | 0.45 |
| 1:D:626:VAL:HA | 1:D:647:VAL:HG22 | 1.98 | 0.45 |
| 1:A:135:LYS:HG2 | 1:A:139:GLN:NE2 | 2.31 | 0.45 |
| 1:A:670:LEU:O | 1:A:673:SER:HB3 | 2.17 | 0.45 |
| 1:A:695:LEU:HD12 | 1:A:695:LEU:C | 2.37 | 0.45 |
| 1:C:140:SER:HG | 1:C:150:THR:HG22 | 1.82 | 0.45 |
| 1:C:440:ARG:O | 1:C:550:VAL:HG22 | 2.16 | 0.45 |
| 1:D:479:LEU:HD13 | 1:D:480:SER:H | 1.82 | 0.45 |
| 1:A:343:PHE:O | 1:A:347:VAL:HG23 | 2.17 | 0.45 |
| 1:A:365:PRO:HA | 1:A:366:ALA:C | 2.37 | 0.45 |
| 1:B:656:LEU:HD22 | 1:B:661:LEU:HA | 1.98 | 0.45 |
| 1:C:343:PHE:O | 1:C:347:VAL:HG23 | 2.16 | 0.45 |
| 1:C:479:LEU:HD13 | 1:C:480:SER:H | 1.82 | 0.45 |
| 1:C:524:GLU:HA | 1:C:527:ASP:OD2 | 2.17 | 0.45 |
| 1:C:690:VAL:HA | 1:C:693:VAL:HG13 | 1.98 | 0.45 |
| 1:D:548:LEU:HD12 | 1:D:548:LEU:HA | 1.77 | 0.45 |
| 1:A:451:ALA:HB1 | 1:A:539:MET:HE1 | 1.98 | 0.44 |
| 1:A:656:LEU:HD22 | 1:A:661:LEU:HA | 1.98 | 0.44 |
| 1:B:122:ALA:O | 1:B:125:VAL:HG12 | 2.17 | 0.44 |
| 1:B:407:LEU:HD23 | 1:B:407:LEU:N | 2.30 | 0.44 |
| 1:B:657:LEU:C | 1:B:659:GLY:HA2 | 2.37 | 0.44 |
| 1:B:688:TYR:CD2 | 1:B:719:LEU:HB3 | 2.51 | 0.44 |
| 1:C:727:ASN:O | 1:C:730:ARG:HB3 | 2.17 | 0.44 |
| 1:D:261:ASP:HA | 1:D:293:GLY:N | 2.33 | 0.44 |
| 1:D:392:MET:O | 1:D:396:VAL:HG12 | 2.17 | 0.44 |
| 1:D:559:THR:N | 1:D:560:PRO:HD2 | 2.32 | 0.44 |
| 1:D:600:ILE:HD12 | 1:D:600:ILE:O | 2.17 | 0.44 |
| 1:A:261:ASP:HA | 1:A:293:GLY:N | 2.33 | 0.44 |
| 1:B:479:LEU:HD13 | 1:B:480:SER:N | 2.33 | 0.44 |
| 1:B:601:MET:HB3 | 1:B:602:PRO:HD2 | 1.98 | 0.44 |
| 1:C:230:ILE:HG12 | 1:C:235:SER:O | 2.17 | 0.44 |
| 1:C:576:LEU:HB3 | 1:C:605:LYS:HZ2 | 1.83 | 0.44 |
| 1:C:601:MET:HB3 | 1:C:602:PRO:HD2 | 1.98 | 0.44 |
| 1:C:657:LEU:C | 1:C:659:GLY:HA2 | 2.37 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:430:THR:HG21 | 1:D:623:GLY:CA | 2.43 | 0.44 |
| 1:A:727:ASN:O | 1:A:730:ARG:HB3 | 2.17 | 0.44 |
| 1:B:230:ILE:HG12 | 1:B:235:SER:O | 2.17 | 0.44 |
| 1:B:365:PRO:HA | 1:B:366:ALA:C | 2.37 | 0.44 |
| 1:B:498:GLN:HG2 | 1:B:502:HIS:O | 2.17 | 0.44 |
| 1:B:422:THR:HG23 | 1:B:619:VAL:HG23 | 1.98 | 0.44 |
| 1:B:88:ALA:CB | 1:B:125:VAL:HG23 | 2.47 | 0.44 |
| 1:C:450:ASN:O | 1:C:454:LEU:HG | 2.17 | 0.44 |
| 1:D:365:PRO:HA | 1:D:366:ALA:C | 2.37 | 0.44 |
| 1:D:690:VAL:O | 1:D:694:PRO:HD3 | 2.17 | 0.44 |
| 1:A:218:ALA:O | 1:A:221:LYS:HB2 | 2.17 | 0.44 |
| 1:A:292:ILE:O | 1:A:295:THR:HG22 | 2.17 | 0.44 |
| 1:A:450:ASN:O | 1:A:454:LEU:HG | 2.18 | 0.44 |
| 1:A:498:GLN:HG2 | 1:A:502:HIS:O | 2.17 | 0.44 |
| 1:B:392:MET:O | 1:B:396:VAL:HG12 | 2.17 | 0.44 |
| 1:B:450:ASN:O | 1:B:454:LEU:HG | 2.17 | 0.44 |
| 1:C:365:PRO:HA | 1:C:366:ALA:C | 2.37 | 0.44 |
| 1:D:218:ALA:O | 1:D:221:LYS:HB2 | 2.17 | 0.44 |
| 1:D:381:ALA:O | 1:D:383:PRO:HD3 | 2.16 | 0.44 |
| 1:D:468:ASN:O | 1:D:472:HIS:HB2 | 2.18 | 0.44 |
| 1:D:498:GLN:HG2 | 1:D:502:HIS:O | 2.17 | 0.44 |
| 1:D:413:ALA:HB1 | 1:D:654:VAL:HG23 | 1.99 | 0.44 |
| 1:D:656:LEU:HD22 | 1:D:661:LEU:HA | 1.98 | 0.44 |
| 1:A:122:ALA:O | 1:A:125:VAL:HG12 | 2.17 | 0.44 |
| 1:A:392:MET:O | 1:A:396:VAL:HG12 | 2.17 | 0.44 |
| 1:A:468:ASN:O | 1:A:472:HIS:HB2 | 2.18 | 0.44 |
| 1:B:343:PHE:O | 1:B:347:VAL:HG23 | 2.17 | 0.44 |
| 1:D:450:ASN:O | 1:D:454:LEU:HG | 2.18 | 0.44 |
| 1:A:430:THR:HG21 | 1:A:623:GLY:CA | 2.44 | 0.44 |
| 1:B:219:LEU:HD22 | 1:B:647:VAL:HG12 | 2.00 | 0.44 |
| 1:C:122:ALA:O | 1:C:125:VAL:HG12 | 2.18 | 0.44 |
| 1:C:479:LEU:HD13 | 1:C:480:SER:N | 2.33 | 0.44 |
| 1:D:292:ILE:O | 1:D:295:THR:HG22 | 2.17 | 0.44 |
| 1:A:156:ILE:HD11 | 1:A:194:ILE:CG2 | 2.48 | 0.44 |
| 1:A:230:ILE:HG12 | 1:A:235:SER:O | 2.17 | 0.44 |
| 1:A:381:ALA:O | 1:A:383:PRO:HD3 | 2.17 | 0.44 |
| 1:A:699:VAL:HG23 | 1:A:700:LEU:HD23 | 1.99 | 0.44 |
| 1:B:168:LEU:HA | 1:B:168:LEU:HD12 | 1.86 | 0.44 |
| 1:B:277:THR:CG2 | 1:B:578:GLY:O | 2.66 | 0.44 |
| 1:B:430:THR:HG21 | 1:B:623:GLY:CA | 2.43 | 0.44 |
| 1:B:524:GLU:HA | 1:B:527:ASP:OD2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:413:ALA:HB1 | 1:B:654:VAL:HG23 | 1.99 | 0.44 |
| 1:C:417:MET:HE1 | 1:C:637:ILE:HG21 | 2.00 | 0.44 |
| 1:D:164:MET:CE | 1:D:164:MET:HA | 2.48 | 0.44 |
| 1:D:156:ILE:HD11 | 1:D:194:ILE:CG2 | 2.48 | 0.44 |
| 1:A:179:SER:N | 1:A:180:GLN:CA | 2.81 | 0.44 |
| 1:A:313:THR:HG22 | 1:A:316:ALA:HB3 | 1.98 | 0.44 |
| 1:A:277:THR:CG2 | 1:A:578:GLY:O | 2.66 | 0.44 |
| 1:B:261:ASP:HA | 1:B:293:GLY:N | 2.33 | 0.44 |
| 1:B:490:PRO:HD2 | 1:B:495:VAL:HA | 1.99 | 0.44 |
| 1:B:78:TYR:CD2 | 1:B:79:LEU:HD12 | 2.42 | 0.44 |
| 1:C:119:LEU:C | 1:C:119:LEU:HD23 | 2.38 | 0.44 |
| 1:C:178:ARG:CB | 1:C:179:SER:HA | 2.24 | 0.44 |
| 1:C:219:LEU:HD22 | 1:C:647:VAL:HG12 | 2.00 | 0.44 |
| 1:C:261:ASP:HA | 1:C:293:GLY:N | 2.33 | 0.44 |
| 1:C:313:THR:HG22 | 1:C:316:ALA:HB3 | 1.98 | 0.44 |
| 1:D:179:SER:N | 1:D:180:GLN:CA | 2.81 | 0.44 |
| 1:D:230:ILE:HG12 | 1:D:235:SER:O | 2.17 | 0.44 |
| 1:D:498:GLN:HA | 1:D:502:HIS:O | 2.18 | 0.44 |
| 1:B:103:HIS:HA | 1:B:104:GLY:HA3 | 1.78 | 0.44 |
| 1:B:140:SER:HG | 1:B:150:THR:HG22 | 1.83 | 0.44 |
| 1:B:178:ARG:CB | 1:B:179:SER:HA | 2.24 | 0.44 |
| 1:B:313:THR:HG22 | 1:B:316:ALA:HB3 | 1.98 | 0.44 |
| 1:B:498:GLN:HA | 1:B:502:HIS:O | 2.18 | 0.44 |
| 1:B:703:LEU:CD2 | 1:D:86:TRP:HB2 | 2.48 | 0.44 |
| 1:C:413:ALA:HB1 | 1:C:654:VAL:HG23 | 1.99 | 0.44 |
| 1:C:78:TYR:CD2 | 1:C:79:LEU:HD12 | 2.42 | 0.44 |
| 1:D:326:GLN:O | 1:D:329:ARG:HG3 | 2.18 | 0.44 |
| 1:A:228:HIS:O | 1:A:250:LEU:HD22 | 2.18 | 0.43 |
| 1:A:326:GLN:O | 1:A:329:ARG:HG3 | 2.18 | 0.43 |
| 1:A:455:ALA:HB2 | 1:A:539:MET:SD | 2.58 | 0.43 |
| 1:C:103:HIS:HA | 1:C:104:GLY:HA3 | 1.78 | 0.43 |
| 1:C:422:THR:HG23 | 1:C:619:VAL:HG23 | 1.99 | 0.43 |
| 1:C:455:ALA:HB2 | 1:C:539:MET:SD | 2.58 | 0.43 |
| 1:D:122:ALA:O | 1:D:125:VAL:HG12 | 2.18 | 0.43 |
| 1:D:277:THR:CG2 | 1:D:578:GLY:O | 2.66 | 0.43 |
| 1:D:699:VAL:HG23 | 1:D:700:LEU:HD23 | 2.00 | 0.43 |
| 1:A:313:THR:HG23 | 1:A:316:ALA:H | 1.83 | 0.43 |
| 1:B:122:ALA:HA | 1:B:125:VAL:CG1 | 2.47 | 0.43 |
| 1:B:414:LEU:HA | 1:B:414:LEU:HD23 | 1.73 | 0.43 |
| 1:B:416:ARG:HG2 | 1:B:416:ARG:HH11 | 1.82 | 0.43 |
| 1:B:468:ASN:O | 1:B:472:HIS:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:LEU:HD12 | 1:C:168:LEU:HA | 1.86 | 0.43 |
| 1:C:430:THR:HG21 | 1:C:623:GLY:CA | 2.43 | 0.43 |
| 1:C:490:PRO:HD2 | 1:C:495:VAL:HA | 2.00 | 0.43 |
| 1:D:228:HIS:O | 1:D:250:LEU:HD22 | 2.18 | 0.43 |
| 1:D:313:THR:HG22 | 1:D:316:ALA:HB3 | 1.98 | 0.43 |
| 1:D:313:THR:HG23 | 1:D:316:ALA:H | 1.83 | 0.43 |
| 1:D:417:MET:HE1 | 1:D:637:ILE:HG21 | 1.99 | 0.43 |
| 1:A:498:GLN:HA | 1:A:502:HIS:O | 2.18 | 0.43 |
| 1:A:524:GLU:HA | 1:A:527:ASP:OD2 | 2.17 | 0.43 |
| 1:C:122:ALA:HA | 1:C:125:VAL:CG1 | 2.47 | 0.43 |
| 1:D:206:LEU:O | 1:D:210:GLU:HB2 | 2.19 | 0.43 |
| 1:D:276:VAL:O | 1:D:277:THR:CB | 2.67 | 0.43 |
| 1:A:164:MET:CE | 1:A:164:MET:HA | 2.48 | 0.43 |
| 1:A:416:ARG:HH11 | 1:A:416:ARG:HG2 | 1.82 | 0.43 |
| 1:A:479:LEU:HD13 | 1:A:480:SER:N | 2.33 | 0.43 |
| 1:A:413:ALA:HB1 | 1:A:654:VAL:HG23 | 2.00 | 0.43 |
| 1:B:307:LEU:HD13 | 1:B:308:HIS:CD2 | 2.49 | 0.43 |
| 1:C:307:LEU:HD13 | 1:C:308:HIS:CD2 | 2.49 | 0.43 |
| 1:D:490:PRO:HD2 | 1:D:495:VAL:HA | 1.99 | 0.43 |
| 1:A:206:LEU:O | 1:A:210:GLU:HB2 | 2.19 | 0.43 |
| 1:A:490:PRO:HD2 | 1:A:495:VAL:HA | 2.00 | 0.43 |
| 1:B:447:VAL:HG23 | 1:B:450:ASN:H | 1.83 | 0.43 |
| 1:C:468:ASN:O | 1:C:472:HIS:HB2 | 2.18 | 0.43 |
| 1:C:699:VAL:HG23 | 1:C:700:LEU:HD23 | 1.99 | 0.43 |
| 1:C:86:TRP:O | 1:C:90:MET:HG3 | 2.18 | 0.43 |
| 1:D:416:ARG:HG2 | 1:D:416:ARG:HH11 | 1.82 | 0.43 |
| 1:A:183:VAL:HG23 | 1:A:184:VAL:N | 2.33 | 0.43 |
| 1:A:276:VAL:O | 1:A:277:THR:CB | 2.67 | 0.43 |
| 1:C:156:ILE:HD11 | 1:C:194:ILE:CG2 | 2.48 | 0.43 |
| 1:C:326:GLN:O | 1:C:329:ARG:HG3 | 2.18 | 0.43 |
| 1:D:119:LEU:C | 1:D:119:LEU:HD23 | 2.39 | 0.43 |
| 1:D:179:SER:HB3 | 1:D:182:GLY:N | 2.34 | 0.43 |
| 1:D:86:TRP:O | 1:D:90:MET:HG3 | 2.18 | 0.43 |
| 1:A:447:VAL:HG23 | 1:A:450:ASN:H | 1.84 | 0.43 |
| 1:B:119:LEU:C | 1:B:119:LEU:HD23 | 2.39 | 0.43 |
| 1:B:156:ILE:HD11 | 1:B:194:ILE:CG2 | 2.48 | 0.43 |
| 1:B:326:GLN:O | 1:B:329:ARG:HG3 | 2.18 | 0.43 |
| 1:C:168:LEU:HD23 | 1:C:169:TRP:CZ3 | 2.54 | 0.43 |
| 1:C:166:ALA:HB1 | 1:C:184:VAL:CG2 | 2.49 | 0.43 |
| 1:C:447:VAL:HG23 | 1:C:450:ASN:H | 1.84 | 0.43 |
| 1:D:447:VAL:HG23 | 1:D:450:ASN:H | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:479:LEU:HD13 | 1:D:480:SER:N | 2.33 | 0.43 |
| 1:D:524:GLU:HA | 1:D:527:ASP:OD2 | 2.17 | 0.43 |
| 1:A:671:SER:O | 1:A:672:GLU:C | 2.57 | 0.43 |
| 1:A:669:ARG:CZ | 1:A:736:LEU:O | 2.67 | 0.43 |
| 1:A:86:TRP:O | 1:A:90:MET:HG3 | 2.18 | 0.43 |
| 1:B:249:LEU:HA | 1:B:304:MET:O | 2.19 | 0.43 |
| 1:B:417:MET:HE1 | 1:B:637:ILE:HG21 | 2.01 | 0.43 |
| 1:B:699:VAL:HG23 | 1:B:700:LEU:HD23 | 2.00 | 0.43 |
| 1:C:179:SER:N | 1:C:180:GLN:CA | 2.80 | 0.43 |
| 1:D:249:LEU:HA | 1:D:304:MET:O | 2.19 | 0.43 |
| 1:D:277:THR:HG23 | 1:D:578:GLY:O | 2.19 | 0.43 |
| 1:D:669:ARG:CZ | 1:D:736:LEU:O | 2.67 | 0.43 |
| 1:A:277:THR:HG23 | 1:A:578:GLY:O | 2.19 | 0.43 |
| 1:B:168:LEU:HD23 | 1:B:169:TRP:CZ3 | 2.54 | 0.43 |
| 1:C:249:LEU:HA | 1:C:304:MET:O | 2.19 | 0.43 |
| 1:D:671:SER:O | 1:D:672:GLU:C | 2.57 | 0.43 |
| 1:A:122:ALA:HA | 1:A:125:VAL:CG1 | 2.46 | 0.43 |
| 1:A:168:LEU:HD23 | 1:A:169:TRP:CZ3 | 2.54 | 0.43 |
| 1:A:249:LEU:HA | 1:A:304:MET:O | 2.19 | 0.43 |
| 1:C:416:ARG:HH11 | 1:C:416:ARG:HG2 | 1.83 | 0.43 |
| 1:C:498:GLN:HA | 1:C:502:HIS:O | 2.19 | 0.43 |
| 1:C:277:THR:CG2 | 1:C:578:GLY:O | 2.67 | 0.43 |
| 1:D:233:ASP:C | 1:D:235:SER:H | 2.23 | 0.43 |
| 1:A:119:LEU:C | 1:A:119:LEU:HD23 | 2.40 | 0.42 |
| 1:A:262:GLY:CA | 1:A:305:LYS:O | 2.67 | 0.42 |
| 1:A:539:MET:HE2 | 1:A:547:ALA:HB3 | 2.01 | 0.42 |
| 1:B:179:SER:N | 1:B:180:GLN:CA | 2.81 | 0.42 |
| 1:B:228:HIS:O | 1:B:250:LEU:HD22 | 2.18 | 0.42 |
| 1:B:277:THR:HG23 | 1:B:578:GLY:O | 2.19 | 0.42 |
| 1:B:262:GLY:CA | 1:B:307:LEU:HB2 | 2.49 | 0.42 |
| 1:B:559:THR:O | 1:B:563:ILE:HG12 | 2.19 | 0.42 |
| 1:B:86:TRP:O | 1:B:90:MET:HG3 | 2.19 | 0.42 |
| 1:C:228:HIS:O | 1:C:250:LEU:HD22 | 2.18 | 0.42 |
| 1:D:122:ALA:HA | 1:D:125:VAL:CG1 | 2.46 | 0.42 |
| 1:D:168:LEU:HD23 | 1:D:169:TRP:CZ3 | 2.54 | 0.42 |
| 1:D:183:VAL:HG23 | 1:D:184:VAL:N | 2.34 | 0.42 |
| 1:A:233:ASP:C | 1:A:235:SER:H | 2.23 | 0.42 |
| 1:B:148:MET:SD | 1:B:386:LEU:HD13 | 2.59 | 0.42 |
| 1:C:179:SER:HB3 | 1:C:182:GLY:N | 2.34 | 0.42 |
| 1:C:559:THR:O | 1:C:563:ILE:HG12 | 2.19 | 0.42 |
| 1:D:262:GLY:CA | 1:D:305:LYS:O | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:559:THR:O | 1:D:563:ILE:HG12 | 2.19 | 0.42 |
| 1:D:219:LEU:HD22 | 1:D:647:VAL:HG12 | 2.00 | 0.42 |
| 1:A:179:SER:HB3 | 1:A:182:GLY:N | 2.35 | 0.42 |
| 1:C:183:VAL:HG23 | 1:C:184:VAL:N | 2.33 | 0.42 |
| 1:C:244:VAL:HG12 | 1:C:245:ALA:N | 2.35 | 0.42 |
| 1:C:313:THR:HG23 | 1:C:316:ALA:H | 1.83 | 0.42 |
| 1:C:148:MET:SD | 1:C:386:LEU:HD13 | 2.59 | 0.42 |
| 1:C:731:LEU:O | 1:C:731:LEU:HD13 | 2.20 | 0.42 |
| 1:D:148:MET:SD | 1:D:386:LEU:HD13 | 2.59 | 0.42 |
| 1:D:272:ASP:HB3 | 1:D:296:ILE:HG23 | 2.01 | 0.42 |
| 1:A:219:LEU:HD22 | 1:A:647:VAL:HG12 | 2.00 | 0.42 |
| 1:B:179:SER:HB3 | 1:B:182:GLY:N | 2.35 | 0.42 |
| 1:B:244:VAL:HG12 | 1:B:245:ALA:N | 2.35 | 0.42 |
| 1:B:313:THR:HG23 | 1:B:316:ALA:H | 1.83 | 0.42 |
| 1:C:122:ALA:CA | 1:C:125:VAL:HG12 | 2.47 | 0.42 |
| 1:C:730:ARG:HG3 | 1:C:730:ARG:HH11 | 1.84 | 0.42 |
| 1:A:168:LEU:HD12 | 1:A:168:LEU:HA | 1.86 | 0.42 |
| 1:A:244:VAL:HG12 | 1:A:245:ALA:N | 2.35 | 0.42 |
| 1:B:166:ALA:HB1 | 1:B:184:VAL:CG2 | 2.50 | 0.42 |
| 1:B:264:VAL:HG22 | 1:B:287:ALA:HA | 2.01 | 0.42 |
| 1:C:264:VAL:HG22 | 1:C:287:ALA:HA | 2.01 | 0.42 |
| 1:D:262:GLY:CA | 1:D:307:LEU:HB2 | 2.49 | 0.42 |
| 1:A:332:ILE:HA | 1:A:332:ILE:HD12 | 1.93 | 0.42 |
| 1:A:641:MET:HE1 | 1:A:659:GLY:O | 2.18 | 0.42 |
| 1:B:122:ALA:CA | 1:B:125:VAL:HG12 | 2.48 | 0.42 |
| 1:B:367:LEU:C | 1:B:367:LEU:HD22 | 2.40 | 0.42 |
| 1:C:276:VAL:O | 1:C:277:THR:CB | 2.66 | 0.42 |
| 1:D:244:VAL:HG12 | 1:D:245:ALA:N | 2.35 | 0.42 |
| 1:D:277:THR:HG22 | 1:D:279:GLU:HG2 | 2.02 | 0.42 |
| 1:A:262:GLY:CA | 1:A:307:LEU:HB2 | 2.50 | 0.42 |
| 1:B:206:LEU:O | 1:B:210:GLU:HB2 | 2.19 | 0.42 |
| 1:B:233:ASP:C | 1:B:235:SER:H | 2.23 | 0.42 |
| 1:B:271:VAL:HA | 1:B:297:ASN:HA | 2.02 | 0.42 |
| 1:B:605:LYS:HD3 | 1:B:628:ASP:CB | 2.50 | 0.42 |
| 1:B:418:GLU:CG | 1:B:672:GLU:HG2 | 2.47 | 0.42 |
| 1:B:730:ARG:HH11 | 1:B:730:ARG:HG3 | 1.85 | 0.42 |
| 1:B:669:ARG:CZ | 1:B:736:LEU:O | 2.67 | 0.42 |
| 1:C:454:LEU:HD22 | 1:C:499:VAL:CG1 | 2.50 | 0.42 |
| 1:C:418:GLU:CG | 1:C:672:GLU:HG2 | 2.47 | 0.42 |
| 1:D:119:LEU:HA | 1:D:188:PHE:CE2 | 2.55 | 0.42 |
| 1:D:642:GLY:O | 1:D:645:THR:HG22 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:418:GLU:CG | 1:D:672:GLU:HG2 | 2.47 | 0.42 |
| 1:D:428:THR:O | 2:D:995:ALF:F2 | 2.28 | 0.42 |
| 1:A:272:ASP:HB3 | 1:A:296:ILE:HG23 | 2.02 | 0.42 |
| 1:A:559:THR:O | 1:A:563:ILE:HG12 | 2.19 | 0.42 |
| 1:B:308:HIS:HB3 | 1:B:312:ASP:CG | 2.40 | 0.42 |
| 1:B:430:THR:HA | 1:B:641:MET:HE2 | 2.02 | 0.42 |
| 1:B:467:ALA:O | 1:B:471:VAL:HG13 | 2.20 | 0.42 |
| 1:B:451:ALA:HB1 | 1:B:539:MET:CE | 2.50 | 0.42 |
| 1:C:88:ALA:HB1 | 1:C:125:VAL:HG23 | 2.02 | 0.42 |
| 1:C:233:ASP:C | 1:C:235:SER:H | 2.23 | 0.42 |
| 1:C:308:HIS:HB3 | 1:C:312:ASP:CG | 2.40 | 0.42 |
| 1:C:367:LEU:C | 1:C:367:LEU:HD22 | 2.40 | 0.42 |
| 1:C:734:VAL:HG22 | 1:C:734:VAL:O | 2.20 | 0.42 |
| 1:C:669:ARG:CZ | 1:C:736:LEU:O | 2.67 | 0.42 |
| 1:C:91:LEU:O | 1:C:95:VAL:HG23 | 2.20 | 0.42 |
| 1:D:332:ILE:HA | 1:D:332:ILE:HD12 | 1.93 | 0.42 |
| 1:D:451:ALA:HB1 | 1:D:539:MET:CE | 2.49 | 0.42 |
| 1:A:148:MET:SD | 1:A:386:LEU:HD13 | 2.60 | 0.42 |
| 1:A:642:GLY:O | 1:A:645:THR:HG22 | 2.20 | 0.42 |
| 1:A:734:VAL:HG22 | 1:A:734:VAL:O | 2.20 | 0.42 |
| 1:B:454:LEU:HD22 | 1:B:499:VAL:CG1 | 2.50 | 0.42 |
| 1:B:731:LEU:HD13 | 1:B:731:LEU:O | 2.20 | 0.42 |
| 1:C:127:LEU:O | 1:C:131:TRP:HB2 | 2.19 | 0.42 |
| 1:C:271:VAL:HA | 1:C:297:ASN:HA | 2.02 | 0.42 |
| 1:C:642:GLY:O | 1:C:645:THR:HG22 | 2.20 | 0.42 |
| 1:D:676:SER:O | 1:D:680:GLN:HG3 | 2.20 | 0.42 |
| 1:A:271:VAL:HA | 1:A:297:ASN:HA | 2.02 | 0.42 |
| 1:A:443:THR:HG21 | 1:A:446:PHE:O | 2.20 | 0.42 |
| 1:A:422:THR:O | 1:A:619:VAL:HG23 | 2.20 | 0.42 |
| 1:A:730:ARG:HH11 | 1:A:730:ARG:HG3 | 1.85 | 0.42 |
| 1:A:86:TRP:HB2 | 1:C:703:LEU:CD2 | 2.50 | 0.42 |
| 1:B:173:PHE:HA | 1:B:174:PRO:HD3 | 1.87 | 0.42 |
| 1:B:183:VAL:HG23 | 1:B:184:VAL:N | 2.34 | 0.42 |
| 1:B:224:PRO:HG3 | 1:B:257:LYS:HD2 | 2.01 | 0.42 |
| 1:B:355:PHE:O | 1:B:359:ALA:HB2 | 2.20 | 0.42 |
| 1:B:499:VAL:O | 1:B:502:HIS:ND1 | 2.53 | 0.42 |
| 1:C:224:PRO:HG3 | 1:C:257:LYS:HD2 | 2.01 | 0.42 |
| 1:D:499:VAL:O | 1:D:502:HIS:ND1 | 2.53 | 0.42 |
| 1:A:119:LEU:HA | 1:A:188:PHE:CE2 | 2.55 | 0.41 |
| 1:A:127:LEU:O | 1:A:131:TRP:HB2 | 2.19 | 0.41 |
| 1:A:84:ARG:NH1 | 1:A:132:PRO:HD3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:264:VAL:HG22 | 1:A:287:ALA:HA | 2.01 | 0.41 |
| 1:A:355:PHE:O | 1:A:359:ALA:HB2 | 2.20 | 0.41 |
| 1:B:642:GLY:O | 1:B:645:THR:HG22 | 2.20 | 0.41 |
| 1:C:173:PHE:HA | 1:C:174:PRO:HD3 | 1.87 | 0.41 |
| 1:C:671:SER:O | 1:C:672:GLU:C | 2.57 | 0.41 |
| 1:D:264:VAL:HG22 | 1:D:287:ALA:HA | 2.01 | 0.41 |
| 1:D:271:VAL:HA | 1:D:297:ASN:HA | 2.02 | 0.41 |
| 1:D:500:ASP:C | 1:D:502:HIS:H | 2.23 | 0.41 |
| 1:D:731:LEU:HD13 | 1:D:731:LEU:O | 2.20 | 0.41 |
| 1:A:129:GLY:HA3 | 1:A:130:GLY:HA3 | 1.70 | 0.41 |
| 1:A:151:LEU:HD13 | 1:A:344:VAL:HG12 | 2.02 | 0.41 |
| 1:A:308:HIS:HB3 | 1:A:312:ASP:CG | 2.40 | 0.41 |
| 1:A:500:ASP:C | 1:A:502:HIS:H | 2.23 | 0.41 |
| 1:C:442:VAL:HG23 | 1:C:548:LEU:HB3 | 2.02 | 0.41 |
| 1:C:605:LYS:HD3 | 1:C:628:ASP:CB | 2.51 | 0.41 |
| 1:D:84:ARG:NH1 | 1:D:132:PRO:HD3 | 2.36 | 0.41 |
| 1:D:355:PHE:O | 1:D:359:ALA:HB2 | 2.20 | 0.41 |
| 1:D:641:MET:HE1 | 1:D:659:GLY:O | 2.19 | 0.41 |
| 1:A:166:ALA:HB1 | 1:A:184:VAL:CG2 | 2.50 | 0.41 |
| 1:A:224:PRO:HG3 | 1:A:257:LYS:HD2 | 2.01 | 0.41 |
| 1:A:467:ALA:O | 1:A:471:VAL:HG13 | 2.21 | 0.41 |
| 1:A:454:LEU:HD22 | 1:A:499:VAL:CG1 | 2.50 | 0.41 |
| 1:B:127:LEU:O | 1:B:131:TRP:HB2 | 2.20 | 0.41 |
| 1:B:262:GLY:CA | 1:B:305:LYS:O | 2.67 | 0.41 |
| 1:B:500:ASP:C | 1:B:502:HIS:H | 2.23 | 0.41 |
| 1:B:695:LEU:O | 1:B:707:LEU:HG | 2.20 | 0.41 |
| 1:B:734:VAL:HG22 | 1:B:734:VAL:O | 2.20 | 0.41 |
| 1:C:355:PHE:O | 1:C:359:ALA:HB2 | 2.21 | 0.41 |
| 1:C:499:VAL:O | 1:C:502:HIS:ND1 | 2.53 | 0.41 |
| 1:D:151:LEU:HD13 | 1:D:344:VAL:HG12 | 2.02 | 0.41 |
| 1:D:224:PRO:HG3 | 1:D:257:LYS:HD2 | 2.01 | 0.41 |
| 1:D:734:VAL:HG22 | 1:D:734:VAL:O | 2.20 | 0.41 |
| 1:A:253:ARG:HD2 | 1:A:254:PRO:O | 2.21 | 0.41 |
| 1:A:499:VAL:O | 1:A:502:HIS:CA | 2.69 | 0.41 |
| 1:B:276:VAL:O | 1:B:277:THR:CB | 2.67 | 0.41 |
| 1:B:318:ILE:HA | 1:B:321:MET:HE2 | 2.02 | 0.41 |
| 1:C:262:GLY:CA | 1:C:305:LYS:O | 2.67 | 0.41 |
| 1:C:277:THR:HG23 | 1:C:578:GLY:O | 2.20 | 0.41 |
| 1:C:430:THR:HA | 1:C:641:MET:HE2 | 2.02 | 0.41 |
| 1:D:168:LEU:HA | 1:D:168:LEU:HD12 | 1.87 | 0.41 |
| 1:D:308:HIS:HB3 | 1:D:312:ASP:CG | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:499:VAL:O | 1:D:502:HIS:CA | 2.69 | 0.41 |
| 1:A:277:THR:HG22 | 1:A:279:GLU:HG2 | 2.03 | 0.41 |
| 1:A:408:ILE:HD12 | 1:A:408:ILE:N | 2.35 | 0.41 |
| 1:A:731:LEU:HD13 | 1:A:731:LEU:O | 2.20 | 0.41 |
| 1:B:272:ASP:HB3 | 1:B:296:ILE:HG23 | 2.01 | 0.41 |
| 1:B:499:VAL:O | 1:B:502:HIS:CA | 2.69 | 0.41 |
| 1:B:442:VAL:HG23 | 1:B:548:LEU:HB3 | 2.03 | 0.41 |
| 1:C:408:ILE:HD12 | 1:C:408:ILE:N | 2.36 | 0.41 |
| 1:D:605:LYS:HD3 | 1:D:628:ASP:CB | 2.50 | 0.41 |
| 1:A:249:LEU:N | 1:A:249:LEU:HD12 | 2.36 | 0.41 |
| 1:A:499:VAL:O | 1:A:502:HIS:ND1 | 2.53 | 0.41 |
| 1:B:253:ARG:HD2 | 1:B:254:PRO:O | 2.20 | 0.41 |
| 1:B:363:PRO:HB2 | 1:B:364:GLN:CD | 2.41 | 0.41 |
| 1:C:318:ILE:HA | 1:C:321:MET:HE2 | 2.02 | 0.41 |
| 1:C:467:ALA:O | 1:C:471:VAL:HG13 | 2.21 | 0.41 |
| 1:C:500:ASP:C | 1:C:502:HIS:H | 2.23 | 0.41 |
| 1:D:127:LEU:O | 1:D:131:TRP:HB2 | 2.20 | 0.41 |
| 1:D:249:LEU:HD12 | 1:D:249:LEU:N | 2.36 | 0.41 |
| 1:D:443:THR:HG21 | 1:D:446:PHE:O | 2.20 | 0.41 |
| 1:D:467:ALA:O | 1:D:471:VAL:HG13 | 2.21 | 0.41 |
| 1:D:629:ALA:N | 1:D:630:PRO:CD | 2.82 | 0.41 |
| 1:D:695:LEU:O | 1:D:707:LEU:HG | 2.21 | 0.41 |
| 1:D:730:ARG:HH11 | 1:D:730:ARG:HG3 | 1.86 | 0.41 |
| 1:A:605:LYS:HD3 | 1:A:628:ASP:CB | 2.51 | 0.41 |
| 1:A:629:ALA:N | 1:A:630:PRO:CD | 2.82 | 0.41 |
| 1:B:671:SER:O | 1:B:672:GLU:C | 2.57 | 0.41 |
| 1:B:84:ARG:NH1 | 1:B:132:PRO:HD3 | 2.35 | 0.41 |
| 1:C:206:LEU:O | 1:C:210:GLU:HB2 | 2.20 | 0.41 |
| 1:C:277:THR:HG22 | 1:C:279:GLU:HG2 | 2.03 | 0.41 |
| 1:C:363:PRO:HB2 | 1:C:364:GLN:CD | 2.41 | 0.41 |
| 1:C:490:PRO:CB | 1:C:493:LYS:HD3 | 2.49 | 0.41 |
| 1:C:499:VAL:O | 1:C:502:HIS:CA | 2.69 | 0.41 |
| 1:D:253:ARG:HD2 | 1:D:254:PRO:O | 2.21 | 0.41 |
| 1:D:367:LEU:C | 1:D:367:LEU:HD22 | 2.40 | 0.41 |
| 1:B:119:LEU:HA | 1:B:188:PHE:CE2 | 2.55 | 0.41 |
| 1:B:312:ASP:OD2 | 1:B:312:ASP:N | 2.53 | 0.41 |
| 1:B:431:LEU:HA | 1:B:431:LEU:HD12 | 1.93 | 0.41 |
| 1:B:490:PRO:CB | 1:B:493:LYS:HD3 | 2.49 | 0.41 |
| 1:B:219:LEU:HD21 | 1:B:647:VAL:HA | 2.02 | 0.41 |
| 1:C:253:ARG:HD2 | 1:C:254:PRO:O | 2.21 | 0.41 |
| 1:C:422:THR:O | 1:C:619:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:454:LEU:HD22 | 1:D:499:VAL:CG1 | 2.51 | 0.41 |
| 1:D:93:ILE:HG23 | 1:D:94:PRO:CD | 2.48 | 0.41 |
| 1:A:173:PHE:HA | 1:A:174:PRO:HD3 | 1.87 | 0.41 |
| 1:A:307:LEU:HD13 | 1:A:308:HIS:CD2 | 2.48 | 0.41 |
| 1:B:408:ILE:N | 1:B:408:ILE:HD12 | 2.36 | 0.41 |
| 1:B:438:LEU:HD12 | 1:B:473:ALA:CB | 2.51 | 0.41 |
| 1:D:129:GLY:HA3 | 1:D:130:GLY:HA3 | 1.70 | 0.41 |
| 1:D:574:VAL:HG12 | 1:D:574:VAL:O | 2.21 | 0.41 |
| 1:A:127:LEU:C | 1:A:129:GLY:N | 2.73 | 0.41 |
| 1:A:695:LEU:O | 1:A:707:LEU:HG | 2.21 | 0.41 |
| 1:A:93:ILE:HG23 | 1:A:94:PRO:CD | 2.49 | 0.41 |
| 1:B:426:ASP:HA | 1:B:576:LEU:O | 2.21 | 0.41 |
| 1:B:451:ALA:HB1 | 1:B:539:MET:HE1 | 2.03 | 0.41 |
| 1:C:219:LEU:HD21 | 1:C:647:VAL:HA | 2.02 | 0.41 |
| 1:C:312:ASP:N | 1:C:312:ASP:OD2 | 2.53 | 0.41 |
| 1:C:431:LEU:HD12 | 1:C:431:LEU:HA | 1.93 | 0.41 |
| 1:C:628:ASP:O | 1:C:631:ALA:HB3 | 2.20 | 0.41 |
| 1:C:695:LEU:O | 1:C:707:LEU:HG | 2.21 | 0.41 |
| 1:C:84:ARG:NH1 | 1:C:132:PRO:HD3 | 2.36 | 0.41 |
| 1:D:173:PHE:HA | 1:D:174:PRO:HD3 | 1.87 | 0.41 |
| 1:D:166:ALA:HB1 | 1:D:184:VAL:CG2 | 2.51 | 0.41 |
| 1:D:297:ASN:C | 1:D:298:GLN:HG3 | 2.41 | 0.41 |
| 1:D:307:LEU:HD13 | 1:D:308:HIS:CD2 | 2.49 | 0.41 |
| 1:A:155:GLY:O | 1:A:159:ALA:HB2 | 2.21 | 0.41 |
| 1:A:297:ASN:C | 1:A:298:GLN:HG3 | 2.41 | 0.41 |
| 1:B:277:THR:HG22 | 1:B:279:GLU:HG2 | 2.03 | 0.41 |
| 1:B:297:ASN:C | 1:B:298:GLN:HG3 | 2.41 | 0.41 |
| 1:B:574:VAL:O | 1:B:574:VAL:HG12 | 2.21 | 0.41 |
| 1:C:119:LEU:HA | 1:C:188:PHE:CE2 | 2.56 | 0.41 |
| 1:C:127:LEU:C | 1:C:129:GLY:N | 2.72 | 0.41 |
| 1:C:272:ASP:HB3 | 1:C:296:ILE:HG23 | 2.02 | 0.41 |
| 1:C:451:ALA:HB1 | 1:C:539:MET:CE | 2.51 | 0.41 |
| 1:A:117:ILE:HG12 | 1:C:687:ILE:HD11 | 2.03 | 0.41 |
| 1:D:127:LEU:C | 1:D:129:GLY:N | 2.73 | 0.41 |
| 1:A:85:PHE:CE1 | 1:A:200:LEU:HB2 | 2.56 | 0.40 |
| 1:A:251:ARG:HA | 1:A:302:PHE:O | 2.21 | 0.40 |
| 1:A:442:VAL:HG23 | 1:A:548:LEU:HB3 | 2.03 | 0.40 |
| 1:A:676:SER:O | 1:A:680:GLN:HG3 | 2.21 | 0.40 |
| 1:B:223:VAL:HG12 | 1:B:225:GLU:HB3 | 2.03 | 0.40 |
| 1:B:249:LEU:HD12 | 1:B:249:LEU:N | 2.36 | 0.40 |
| 1:B:251:ARG:HA | 1:B:302:PHE:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:223:VAL:HG12 | 1:C:225:GLU:HB3 | 2.03 | 0.40 |
| 1:C:249:LEU:HD12 | 1:C:249:LEU:N | 2.36 | 0.40 |
| 1:C:297:ASN:C | 1:C:298:GLN:HG3 | 2.41 | 0.40 |
| 1:C:426:ASP:OD2 | 2:C:995:ALF:F2 | 2.29 | 0.40 |
| 1:C:443:THR:HG21 | 1:C:446:PHE:O | 2.20 | 0.40 |
| 1:C:576:LEU:HB3 | 1:C:605:LYS:NZ | 2.36 | 0.40 |
| 1:D:85:PHE:CE1 | 1:D:200:LEU:HB2 | 2.56 | 0.40 |
| 1:D:363:PRO:HB2 | 1:D:364:GLN:CD | 2.41 | 0.40 |
| 1:D:408:ILE:N | 1:D:408:ILE:HD12 | 2.36 | 0.40 |
| 1:D:219:LEU:HD21 | 1:D:647:VAL:HA | 2.02 | 0.40 |
| 1:A:367:LEU:C | 1:A:367:LEU:HD22 | 2.40 | 0.40 |
| 1:B:131:TRP:N | 1:B:132:PRO:HD2 | 2.36 | 0.40 |
| 1:B:155:GLY:O | 1:B:159:ALA:HB2 | 2.21 | 0.40 |
| 1:B:422:THR:O | 1:B:619:VAL:HG23 | 2.22 | 0.40 |
| 1:B:576:LEU:HB3 | 1:B:605:LYS:NZ | 2.36 | 0.40 |
| 1:C:251:ARG:HA | 1:C:302:PHE:O | 2.21 | 0.40 |
| 1:C:438:LEU:HD12 | 1:C:473:ALA:CB | 2.51 | 0.40 |
| 1:C:522:LEU:HD12 | 1:C:545:THR:HG22 | 2.03 | 0.40 |
| 1:D:131:TRP:N | 1:D:132:PRO:HD2 | 2.35 | 0.40 |
| 1:D:522:LEU:HD12 | 1:D:545:THR:HG22 | 2.03 | 0.40 |
| 1:A:451:ALA:HB1 | 1:A:539:MET:CE | 2.51 | 0.40 |
| 1:A:522:LEU:HD12 | 1:A:545:THR:HG22 | 2.03 | 0.40 |
| 1:B:85:PHE:CE1 | 1:B:200:LEU:HB2 | 2.57 | 0.40 |
| 1:C:131:TRP:N | 1:C:132:PRO:HD2 | 2.36 | 0.40 |
| 1:C:426:ASP:HA | 1:C:576:LEU:O | 2.21 | 0.40 |
| 1:D:251:ARG:HA | 1:D:302:PHE:O | 2.22 | 0.40 |
| 1:D:422:THR:O | 1:D:619:VAL:HG23 | 2.22 | 0.40 |
| 1:A:394:ILE:O | 1:A:398:VAL:HG13 | 2.22 | 0.40 |
| 1:A:219:LEU:HD21 | 1:A:647:VAL:HA | 2.03 | 0.40 |
| 1:A:91:LEU:O | 1:A:95:VAL:HG23 | 2.21 | 0.40 |
| 1:B:127:LEU:C | 1:B:129:GLY:N | 2.73 | 0.40 |
| 1:B:522:LEU:HD12 | 1:B:545:THR:HG22 | 2.04 | 0.40 |
| 1:C:574:VAL:O | 1:C:574:VAL:HG12 | 2.21 | 0.40 |
| 1:D:438:LEU:HD12 | 1:D:473:ALA:CB | 2.51 | 0.40 |
| 1:A:88:ALA:HB1 | 1:A:125:VAL:HG23 | 2.02 | 0.40 |
| 1:A:131:TRP:N | 1:A:132:PRO:HD2 | 2.36 | 0.40 |
| 1:A:258:ILE:HD11 | 1:A:297:ASN:HB3 | 2.03 | 0.40 |
| 1:A:363:PRO:HB2 | 1:A:364:GLN:CD | 2.41 | 0.40 |
| 1:A:438:LEU:HD12 | 1:A:473:ALA:CB | 2.51 | 0.40 |
| 1:B:88:ALA:HB1 | 1:B:125:VAL:HG23 | 2.04 | 0.40 |
| 1:B:258:ILE:HA | 1:B:259:PRO:HD3 | 1.82 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:130:GLY:HA2 | 1:D:133:PHE:CD1 | 2.57 | 0.40 |
| 1:D:394:ILE:O | 1:D:398:VAL:HG13 | 2.22 | 0.40 |
| 1:D:598:ALA:O | 1:D:600:ILE:HG23 | 2.22 | 0.40 |
| 1:D:628:ASP:O | 1:D:631:ALA:HB3 | 2.21 | 0.40 |

There are no symmetry-related clashes.

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 | 661/736 (90%) | 578 (87%) | 69 (10%) | 14 (2%) | 7 | 37 |
| 1 | B | 661/736 (90%) | 578 (87%) | 68 (10%) | 15 (2%) | 6 | 34 |
| 1 | C | 661/736 (90%) | 578 (87%) | 69 (10%) | 14 (2%) | 7 | 37 |
| 1 | D | 661/736 (90%) | 579 (88%) | 68 (10%) | 14 (2%) | 7 | 37 |
| All | All | 2644/2944 (90%) | 2313 (88%) | 274 (10%) | 57 (2%) | 6 | 35 |

All (57) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 224 | PRO |
| 1 | A | 662 | ARG |
| 1 | B | 224 | PRO |
| 1 | C | 224 | PRO |
| 1 | C | 662 | ARG |
| 1 | D | 224 | PRO |
| 1 | D | 662 | ARG |
| 1 | A | 129 | GLY |
| 1 | A | 618 | ILE |
| 1 | A | 658 | HIS |
| 1 | B | 129 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 618 | ILE |
| 1 | B | 658 | HIS |
| 1 | B | 662 | ARG |
| 1 | C | 129 | GLY |
| 1 | C | 618 | ILE |
| 1 | C | 658 | HIS |
| 1 | D | 129 | GLY |
| 1 | D | 618 | ILE |
| 1 | D | 658 | HIS |
| 1 | A | 389 | ALA |
| 1 | B | 389 | ALA |
| 1 | C | 389 | ALA |
| 1 | D | 389 | ALA |
| 1 | A | 76 | PRO |
| 1 | A | 499 | VAL |
| 1 | B | 76 | PRO |
| 1 | B | 499 | VAL |
| 1 | B | 628 | ASP |
| 1 | C | 76 | PRO |
| 1 | C | 499 | VAL |
| 1 | D | 76 | PRO |
| 1 | D | 499 | VAL |
| 1 | D | 628 | ASP |
| 1 | A | 143 | THR |
| 1 | A | 628 | ASP |
| 1 | B | 113 | GLY |
| 1 | B | 143 | THR |
| 1 | C | 628 | ASP |
| 1 | D | 143 | THR |
| 1 | A | 113 | GLY |
| 1 | A | 177 | PHE |
| 1 | B | 177 | PHE |
| 1 | B | 703 | LEU |
| 1 | C | 113 | GLY |
| 1 | C | 143 | THR |
| 1 | C | 177 | PHE |
| 1 | D | 113 | GLY |
| 1 | D | 177 | PHE |
| 1 | A | 484 | VAL |
| 1 | B | 183 | VAL |
| 1 | B | 484 | VAL |
| 1 | C | 183 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 484 | VAL |
| 1 | D | 183 | VAL |
| 1 | D | 484 | VAL |
| 1 | A | 183 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 523/586 (89%) | 486 (93%) | 37 (7%) | 14 | 47 |
| 1 | B | 523/586 (89%) | 486 (93%) | 37 (7%) | 14 | 47 |
| 1 | C | 523/586 (89%) | 486 (93%) | 37 (7%) | 14 | 47 |
| 1 | D | 523/586 (89%) | 487 (93%) | 36 (7%) | 15 | 49 |
| All | All | 2092/2344 (89%) | 1945 (93%) | 147 (7%) | 15 | 48 |

All (147) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 99 | GLU |
| 1 | A | 105 | LEU |
| 1 | A | 109 | ILE |
| 1 | A | 150 | THR |
| 1 | A | 164 | MET |
| 1 | A | 165 | VAL |
| 1 | A | 172 | VAL |
| 1 | A | 178 | ARG |
| 1 | A | 183 | VAL |
| 1 | A | 184 | VAL |
| 1 | A | 219 | LEU |
| 1 | A | 220 | LEU |
| 1 | A | 250 | LEU |
| 1 | A | 252 | VAL |
| 1 | A | 264 | VAL |
| 1 | A | 277 | THR |
| 1 | A | 307 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 319 | VAL |
| 1 | A | 320 | GLN |
| 1 | A | 322 | VAL |
| 1 | A | 367 | LEU |
| 1 | A | 382 | CYS |
| 1 | A | 386 | LEU |
| 1 | A | 424 | VAL |
| 1 | A | 443 | THR |
| 1 | A | 466 | LEU |
| 1 | A | 479 | LEU |
| 1 | A | 536 | VAL |
| 1 | A | 562 | THR |
| 1 | A | 583 | THR |
| 1 | A | 645 | THR |
| 1 | A | 674 | THR |
| 1 | A | 679 | ARG |
| 1 | A | 693 | VAL |
| 1 | A | 707 | LEU |
| 1 | A | 712 | ILE |
| 1 | A | 726 | ILE |
| 1 | B | 99 | GLU |
| 1 | B | 105 | LEU |
| 1 | B | 109 | ILE |
| 1 | B | 150 | THR |
| 1 | B | 164 | MET |
| 1 | B | 165 | VAL |
| 1 | B | 172 | VAL |
| 1 | B | 178 | ARG |
| 1 | B | 183 | VAL |
| 1 | B | 184 | VAL |
| 1 | B | 219 | LEU |
| 1 | B | 220 | LEU |
| 1 | B | 250 | LEU |
| 1 | B | 252 | VAL |
| 1 | B | 264 | VAL |
| 1 | B | 277 | THR |
| 1 | B | 307 | LEU |
| 1 | B | 319 | VAL |
| 1 | B | 320 | GLN |
| 1 | B | 322 | VAL |
| 1 | B | 367 | LEU |
| 1 | B | 382 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 386 | LEU |
| 1 | B | 424 | VAL |
| 1 | B | 443 | THR |
| 1 | B | 466 | LEU |
| 1 | B | 479 | LEU |
| 1 | B | 536 | VAL |
| 1 | B | 562 | THR |
| 1 | B | 583 | THR |
| 1 | B | 645 | THR |
| 1 | B | 674 | THR |
| 1 | B | 679 | ARG |
| 1 | B | 693 | VAL |
| 1 | B | 707 | LEU |
| 1 | B | 712 | ILE |
| 1 | B | 726 | ILE |
| 1 | C | 99 | GLU |
| 1 | C | 105 | LEU |
| 1 | C | 109 | ILE |
| 1 | C | 150 | THR |
| 1 | C | 164 | MET |
| 1 | C | 165 | VAL |
| 1 | C | 172 | VAL |
| 1 | C | 178 | ARG |
| 1 | C | 183 | VAL |
| 1 | C | 184 | VAL |
| 1 | C | 219 | LEU |
| 1 | C | 220 | LEU |
| 1 | C | 250 | LEU |
| 1 | C | 252 | VAL |
| 1 | C | 264 | VAL |
| 1 | C | 277 | THR |
| 1 | C | 307 | LEU |
| 1 | C | 319 | VAL |
| 1 | C | 320 | GLN |
| 1 | C | 322 | VAL |
| 1 | C | 367 | LEU |
| 1 | C | 382 | CYS |
| 1 | C | 386 | LEU |
| 1 | C | 424 | VAL |
| 1 | C | 443 | THR |
| 1 | C | 466 | LEU |
| 1 | C | 479 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 536 | VAL |
| 1 | C | 562 | THR |
| 1 | C | 583 | THR |
| 1 | C | 645 | THR |
| 1 | C | 674 | THR |
| 1 | C | 679 | ARG |
| 1 | C | 693 | VAL |
| 1 | C | 707 | LEU |
| 1 | C | 712 | ILE |
| 1 | C | 726 | ILE |
| 1 | D | 99 | GLU |
| 1 | D | 105 | LEU |
| 1 | D | 109 | ILE |
| 1 | D | 150 | THR |
| 1 | D | 164 | MET |
| 1 | D | 165 | VAL |
| 1 | D | 172 | VAL |
| 1 | D | 178 | ARG |
| 1 | D | 183 | VAL |
| 1 | D | 184 | VAL |
| 1 | D | 219 | LEU |
| 1 | D | 220 | LEU |
| 1 | D | 250 | LEU |
| 1 | D | 252 | VAL |
| 1 | D | 264 | VAL |
| 1 | D | 277 | THR |
| 1 | D | 307 | LEU |
| 1 | D | 319 | VAL |
| 1 | D | 322 | VAL |
| 1 | D | 367 | LEU |
| 1 | D | 382 | CYS |
| 1 | D | 386 | LEU |
| 1 | D | 424 | VAL |
| 1 | D | 443 | THR |
| 1 | D | 466 | LEU |
| 1 | D | 479 | LEU |
| 1 | D | 536 | VAL |
| 1 | D | 562 | THR |
| 1 | D | 583 | THR |
| 1 | D | 645 | THR |
| 1 | D | 674 | THR |
| 1 | D | 679 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 693 | VAL |
| 1 | D | 707 | LEU |
| 1 | D | 712 | ILE |
| 1 | D | 726 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 308 | HIS |
| 1 | A | 498 | GLN |
| 1 | A | 727 | ASN |
| 1 | B | 308 | HIS |
| 1 | B | 450 | ASN |
| 1 | B | 498 | GLN |
| 1 | B | 502 | HIS |
| 1 | B | 727 | ASN |
| 1 | C | 308 | HIS |
| 1 | C | 498 | GLN |
| 1 | C | 727 | ASN |
| 1 | D | 308 | HIS |
| 1 | D | 498 | GLN |
| 1 | D | 727 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 2 | ALF | A | 995 | - | 0,4,4 | 0.00 | - | - | | |
| 2 | ALF | B | 995 | - | 0,4,4 | 0.00 | - | - | | |
| 2 | ALF | C | 995 | - | 0,4,4 | 0.00 | - | - | | |
| 2 | ALF | D | 995 | - | 0,4,4 | 0.00 | - | - | | |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 995 | ALF | 2 | 0 |
| 2 | C | 995 | ALF | 1 | 0 |
| 2 | D | 995 | ALF | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-------|-----------------------|-------|
| 1 | A | 663/736 (90%) | 0.02 | 23 (3%) | 44 28 | 56, 106, 243, 371 | 0 |
| 1 | B | 663/736 (90%) | 0.01 | 24 (3%) | 42 27 | 55, 106, 244, 373 | 0 |
| 1 | C | 663/736 (90%) | 0.03 | 23 (3%) | 44 28 | 55, 106, 244, 371 | 0 |
| 1 | D | 663/736 (90%) | -0.05 | 19 (2%) | 51 36 | 56, 106, 244, 369 | 0 |
| All | All | 2652/2944 (90%) | 0.00 | 89 (3%) | 45 29 | 55, 106, 244, 373 | 0 |

All (89) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 500 | ASP | 9.9 |
| 1 | A | 500 | ASP | 8.8 |
| 1 | B | 490 | PRO | 7.8 |
| 1 | B | 214 | SER | 7.5 |
| 1 | D | 489 | ALA | 7.5 |
| 1 | D | 247 | GLY | 7.0 |
| 1 | A | 736 | LEU | 6.8 |
| 1 | B | 489 | ALA | 6.5 |
| 1 | D | 736 | LEU | 6.3 |
| 1 | C | 490 | PRO | 6.1 |
| 1 | B | 500 | ASP | 6.0 |
| 1 | C | 214 | SER | 5.9 |
| 1 | D | 280 | PRO | 5.9 |
| 1 | D | 490 | PRO | 5.6 |
| 1 | B | 290 | LYS | 5.5 |
| 1 | B | 104 | GLY | 5.5 |
| 1 | A | 489 | ALA | 5.4 |
| 1 | D | 500 | ASP | 5.4 |
| 1 | A | 214 | SER | 5.3 |
| 1 | A | 247 | GLY | 5.1 |
| 1 | A | 490 | PRO | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 489 | ALA | 4.9 |
| 1 | A | 305 | LYS | 4.9 |
| 1 | D | 290 | LYS | 4.8 |
| 1 | A | 304 | MET | 4.4 |
| 1 | C | 736 | LEU | 4.4 |
| 1 | C | 236 | GLU | 4.2 |
| 1 | B | 736 | LEU | 4.2 |
| 1 | C | 305 | LYS | 4.0 |
| 1 | B | 236 | GLU | 3.8 |
| 1 | D | 214 | SER | 3.5 |
| 1 | B | 247 | GLY | 3.5 |
| 1 | A | 289 | ALA | 3.4 |
| 1 | B | 238 | GLU | 3.3 |
| 1 | C | 289 | ALA | 3.3 |
| 1 | D | 238 | GLU | 3.2 |
| 1 | B | 304 | MET | 3.2 |
| 1 | A | 280 | PRO | 3.1 |
| 1 | A | 306 | ALA | 3.1 |
| 1 | B | 280 | PRO | 3.1 |
| 1 | D | 306 | ALA | 3.1 |
| 1 | D | 236 | GLU | 3.1 |
| 1 | B | 305 | LYS | 3.1 |
| 1 | B | 235 | SER | 3.1 |
| 1 | D | 645 | THR | 3.0 |
| 1 | D | 636 | ASP | 2.9 |
| 1 | D | 305 | LYS | 2.9 |
| 1 | A | 636 | ASP | 2.9 |
| 1 | C | 302 | PHE | 2.8 |
| 1 | A | 230 | ILE | 2.8 |
| 1 | C | 290 | LYS | 2.8 |
| 1 | C | 304 | MET | 2.7 |
| 1 | A | 180 | GLN | 2.7 |
| 1 | C | 306 | ALA | 2.7 |
| 1 | A | 329 | ARG | 2.6 |
| 1 | A | 325 | ALA | 2.6 |
| 1 | A | 302 | PHE | 2.6 |
| 1 | C | 247 | GLY | 2.6 |
| 1 | A | 236 | GLU | 2.5 |
| 1 | D | 230 | ILE | 2.5 |
| 1 | C | 288 | SER | 2.5 |
| 1 | C | 661 | LEU | 2.5 |
| 1 | B | 230 | ILE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 228 | HIS | 2.5 |
| 1 | C | 211 | GLN | 2.4 |
| 1 | C | 653 | GLY | 2.4 |
| 1 | B | 645 | THR | 2.4 |
| 1 | C | 230 | ILE | 2.4 |
| 1 | C | 213 | GLY | 2.4 |
| 1 | B | 306 | ALA | 2.4 |
| 1 | B | 639 | ILE | 2.4 |
| 1 | D | 329 | ARG | 2.4 |
| 1 | A | 262 | GLY | 2.3 |
| 1 | C | 483 | SER | 2.3 |
| 1 | B | 289 | ALA | 2.3 |
| 1 | C | 104 | GLY | 2.2 |
| 1 | C | 501 | GLY | 2.2 |
| 1 | B | 491 | THR | 2.2 |
| 1 | C | 292 | ILE | 2.2 |
| 1 | A | 417 | MET | 2.2 |
| 1 | B | 356 | ILE | 2.2 |
| 1 | B | 228 | HIS | 2.2 |
| 1 | D | 304 | MET | 2.1 |
| 1 | D | 488 | GLU | 2.1 |
| 1 | A | 292 | ILE | 2.1 |
| 1 | D | 235 | SER | 2.1 |
| 1 | B | 210 | GLU | 2.1 |
| 1 | A | 661 | LEU | 2.1 |
| 1 | B | 636 | ASP | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | K | A | 997 | 1/1 | 0.59 | 0.40 | 141,141,141,141 | 0 |
| 4 | K | C | 997 | 1/1 | 0.72 | 0.38 | 144,144,144,144 | 0 |
| 4 | K | D | 997 | 1/1 | 0.84 | 0.27 | 160,160,160,160 | 0 |
| 4 | K | B | 997 | 1/1 | 0.90 | 0.34 | 154,154,154,154 | 0 |
| 2 | ALF | D | 995 | 5/5 | 0.95 | 0.21 | 57,62,80,127 | 0 |
| 2 | ALF | B | 995 | 5/5 | 0.96 | 0.20 | 48,60,80,130 | 0 |
| 3 | MG | B | 996 | 1/1 | 0.97 | 0.19 | 67,67,67,67 | 0 |
| 2 | ALF | A | 995 | 5/5 | 0.98 | 0.21 | 37,50,60,136 | 0 |
| 3 | MG | A | 996 | 1/1 | 0.98 | 0.17 | 68,68,68,68 | 0 |
| 3 | MG | D | 996 | 1/1 | 0.98 | 0.21 | 77,77,77,77 | 0 |
| 2 | ALF | C | 995 | 5/5 | 0.98 | 0.19 | 45,57,62,117 | 0 |
| 3 | MG | C | 996 | 1/1 | 0.99 | 0.22 | 58,58,58,58 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.