



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:49 pm BST

PDB ID : 2DU7
Title : Crystal structure of Methanococcus jannacshii O-phosphoseryl-tRNA synthetase
Authors : Fukunaga, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-07-20
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

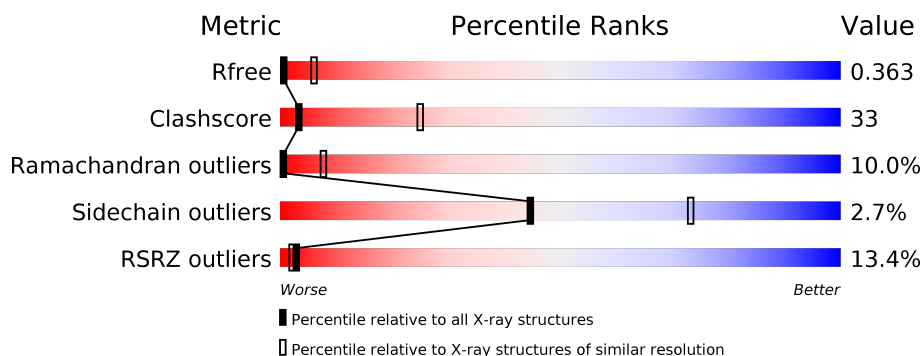
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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 | 1257 (3.70-3.50) |
| Clashscore | 141614 | 1353 (3.70-3.50) |
| Ramachandran outliers | 138981 | 1307 (3.70-3.50) |
| Sidechain outliers | 138945 | 1307 (3.70-3.50) |
| RSRZ outliers | 127900 | 1161 (3.70-3.50) |

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 | 549 | |
| 1 | B | 549 | |
| 1 | C | 549 | |
| 1 | D | 549 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17516 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.

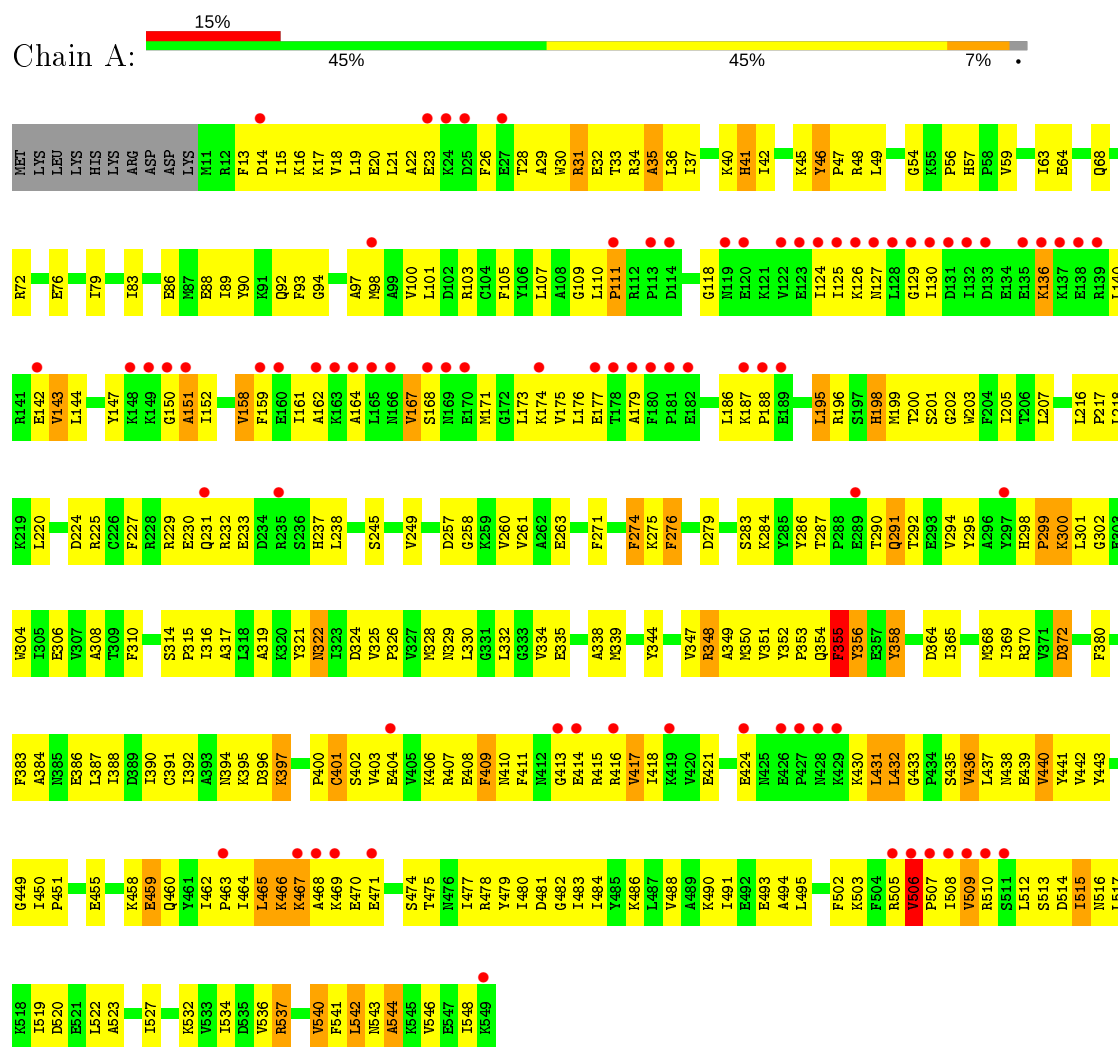
- Molecule 1 is a protein called O-phosphoseryl-tRNA synthetase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 539 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4379 | 2826 | 727 | 807 | 19 | | | |
| 1 | B | 539 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4379 | 2826 | 727 | 807 | 19 | | | |
| 1 | C | 539 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4379 | 2826 | 727 | 807 | 19 | | | |
| 1 | D | 539 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4379 | 2826 | 727 | 807 | 19 | | | |

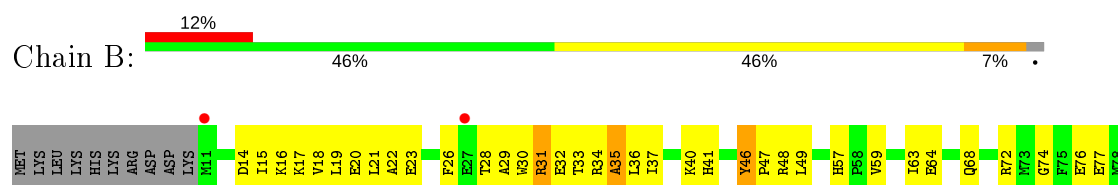
3 Residue-property plots [i](#)

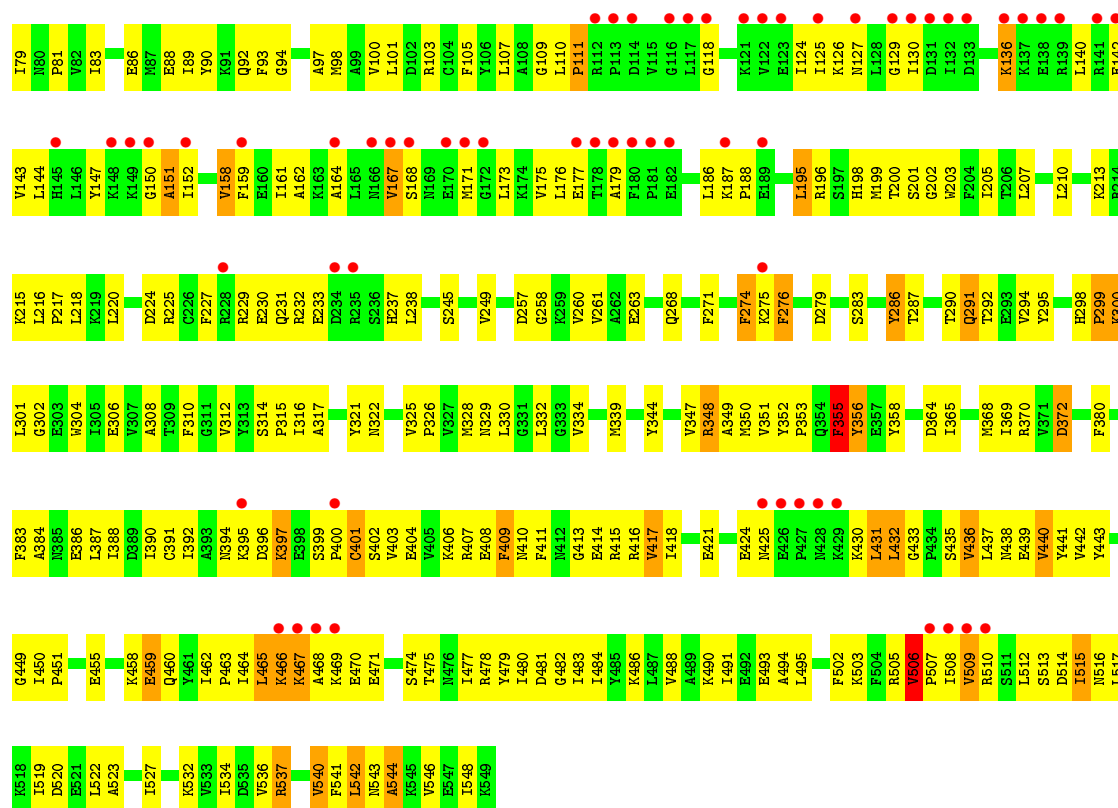
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: O-phosphoseryl-tRNA synthetase

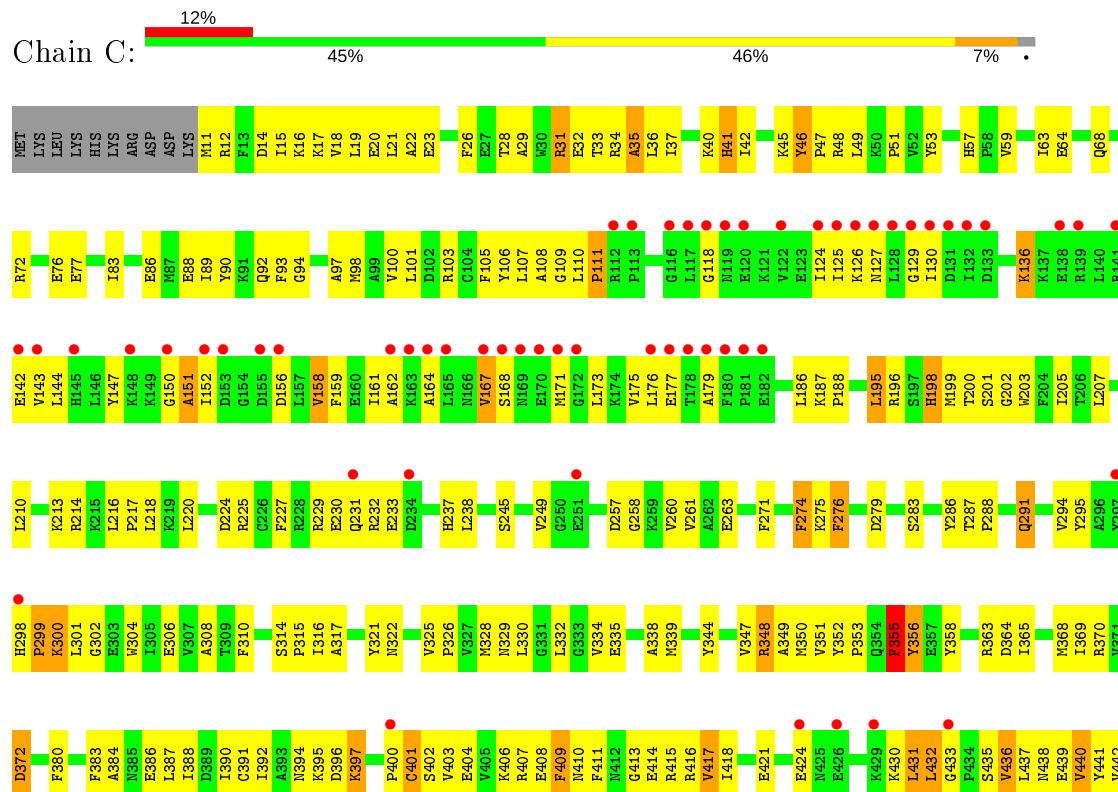


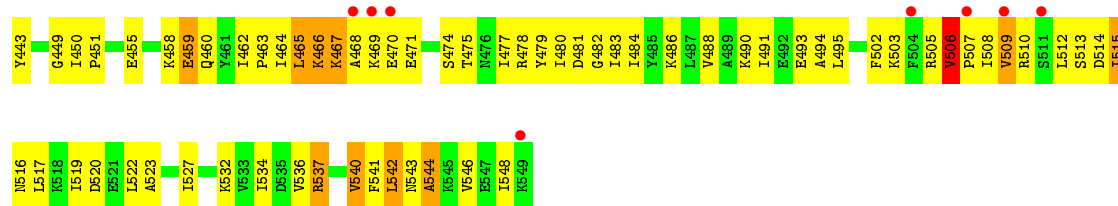
• Molecule 1: O-phosphoseryl-tRNA synthetase



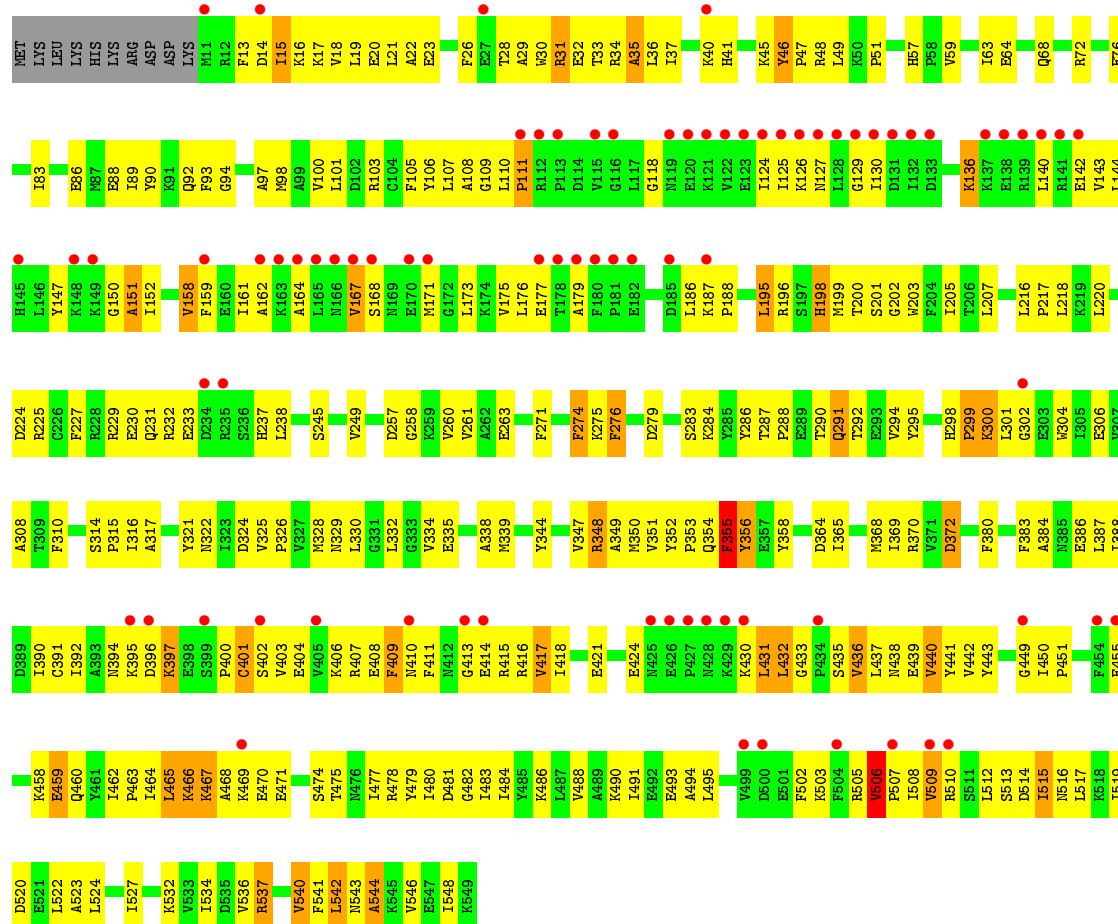


• Molecule 1: O-phosphoseryl-tRNA synthetase





• Molecule 1: O-phosphoseryl-tRNA synthetase



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 196.35Å 299.45Å 125.88Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 19.79 – 3.60 19.79 – 3.60 | Depositor EDS |
| % Data completeness (in resolution range) | 97.5 (19.79-3.60) 97.6 (19.79-3.60) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.48 (at 3.61Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.330 , 0.387 0.314 , 0.363 | Depositor DCC |
| R_{free} test set | 4236 reflections (10.08%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 118.1 | Xtriage |
| Anisotropy | 0.142 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.25 , 101.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.84 | EDS |
| Total number of atoms | 17516 | wwPDB-VP |
| Average B, all atoms (Å ²) | 129.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.26 | 0/4468 | 0.48 | 0/6023 |
| 1 | B | 0.27 | 0/4468 | 0.48 | 0/6023 |
| 1 | C | 0.27 | 0/4468 | 0.48 | 0/6023 |
| 1 | D | 0.26 | 0/4468 | 0.48 | 0/6023 |
| All | All | 0.27 | 0/17872 | 0.48 | 0/24092 |

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 | 4379 | 0 | 4462 | 326 | 2 |
| 1 | B | 4379 | 0 | 4462 | 318 | 0 |
| 1 | C | 4379 | 0 | 4462 | 299 | 0 |
| 1 | D | 4379 | 0 | 4462 | 311 | 0 |
| All | All | 17516 | 0 | 17848 | 1161 | 2 |

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 33.

All (1161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:28:THR:HA | 1:A:31:ARG:HE | 1.06 | 1.17 |
| 1:B:28:THR:HA | 1:B:31:ARG:HE | 1.06 | 1.11 |
| 1:C:28:THR:HA | 1:C:31:ARG:HE | 1.06 | 1.10 |
| 1:D:28:THR:HA | 1:D:31:ARG:HE | 1.06 | 1.07 |
| 1:D:31:ARG:H | 1:D:31:ARG:HD3 | 1.18 | 1.07 |
| 1:D:506:VAL:HG23 | 1:D:507:PRO:HD3 | 1.38 | 1.06 |
| 1:C:31:ARG:H | 1:C:31:ARG:HD3 | 1.18 | 1.05 |
| 1:A:506:VAL:HG23 | 1:A:507:PRO:HD3 | 1.39 | 1.04 |
| 1:B:31:ARG:H | 1:B:31:ARG:HD3 | 1.19 | 1.03 |
| 1:A:31:ARG:H | 1:A:31:ARG:HD3 | 1.18 | 1.02 |
| 1:C:506:VAL:HG23 | 1:C:507:PRO:HD3 | 1.40 | 1.01 |
| 1:B:506:VAL:HG23 | 1:B:507:PRO:HD3 | 1.39 | 0.98 |
| 1:A:283:SER:H | 1:A:291:GLN:HE22 | 1.11 | 0.95 |
| 1:A:158:VAL:HG13 | 1:A:159:PHE:H | 1.33 | 0.94 |
| 1:C:283:SER:H | 1:C:291:GLN:HE22 | 1.12 | 0.93 |
| 1:D:28:THR:HA | 1:D:31:ARG:NE | 1.85 | 0.92 |
| 1:B:68:GLN:HE22 | 1:D:72:ARG:HH11 | 1.16 | 0.92 |
| 1:A:28:THR:HA | 1:A:31:ARG:NE | 1.85 | 0.92 |
| 1:C:28:THR:HA | 1:C:31:ARG:NE | 1.85 | 0.92 |
| 1:D:158:VAL:HG13 | 1:D:159:PHE:H | 1.33 | 0.92 |
| 1:A:354:GLN:HB3 | 1:B:210:LEU:HD13 | 1.50 | 0.91 |
| 1:B:28:THR:HA | 1:B:31:ARG:NE | 1.85 | 0.91 |
| 1:C:158:VAL:HG13 | 1:C:159:PHE:H | 1.33 | 0.91 |
| 1:B:283:SER:H | 1:B:291:GLN:HE22 | 1.12 | 0.90 |
| 1:B:158:VAL:HG13 | 1:B:159:PHE:H | 1.33 | 0.90 |
| 1:A:161:ILE:HG12 | 1:A:167:VAL:HG11 | 1.55 | 0.89 |
| 1:B:161:ILE:HG12 | 1:B:167:VAL:HG11 | 1.55 | 0.89 |
| 1:D:283:SER:H | 1:D:291:GLN:HE22 | 1.12 | 0.89 |
| 1:B:274:PHE:HD1 | 1:B:275:LYS:H | 1.22 | 0.88 |
| 1:C:161:ILE:HG12 | 1:C:167:VAL:HG11 | 1.56 | 0.88 |
| 1:D:161:ILE:HG12 | 1:D:167:VAL:HG11 | 1.56 | 0.87 |
| 1:C:210:LEU:HD13 | 1:D:354:GLN:HB3 | 1.56 | 0.87 |
| 1:C:274:PHE:HD1 | 1:C:275:LYS:H | 1.22 | 0.86 |
| 1:C:395:LYS:HG2 | 1:C:396:ASP:H | 1.41 | 0.86 |
| 1:A:395:LYS:HG2 | 1:A:396:ASP:H | 1.40 | 0.86 |
| 1:B:395:LYS:HG2 | 1:B:396:ASP:H | 1.40 | 0.85 |
| 1:A:30:TRP:CZ2 | 1:D:288:PRO:HG3 | 2.11 | 0.85 |
| 1:A:274:PHE:HD1 | 1:A:275:LYS:H | 1.23 | 0.84 |
| 1:D:436:VAL:HB | 1:D:480:ILE:HG23 | 1.59 | 0.84 |
| 1:C:436:VAL:HB | 1:C:480:ILE:HG23 | 1.60 | 0.84 |
| 1:D:395:LYS:HG2 | 1:D:396:ASP:H | 1.40 | 0.84 |
| 1:B:436:VAL:HB | 1:B:480:ILE:HG23 | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:274:PHE:HD1 | 1:D:275:LYS:H | 1.23 | 0.83 |
| 1:A:97:ALA:HA | 1:A:100:VAL:HG12 | 1.60 | 0.83 |
| 1:D:89:ILE:HG21 | 1:D:101:LEU:HD21 | 1.61 | 0.83 |
| 1:B:97:ALA:HA | 1:B:100:VAL:HG12 | 1.61 | 0.83 |
| 1:A:436:VAL:HB | 1:A:480:ILE:HG23 | 1.59 | 0.82 |
| 1:C:89:ILE:HG21 | 1:C:101:LEU:HD21 | 1.61 | 0.82 |
| 1:D:97:ALA:HA | 1:D:100:VAL:HG12 | 1.60 | 0.82 |
| 1:B:300:LYS:HG2 | 1:B:301:LEU:H | 1.45 | 0.81 |
| 1:C:97:ALA:HA | 1:C:100:VAL:HG12 | 1.61 | 0.81 |
| 1:A:89:ILE:HG21 | 1:A:101:LEU:HD21 | 1.62 | 0.81 |
| 1:C:503:LYS:HB3 | 1:C:543:ASN:HB3 | 1.63 | 0.81 |
| 1:A:300:LYS:HG2 | 1:A:301:LEU:H | 1.45 | 0.81 |
| 1:B:89:ILE:HG21 | 1:B:101:LEU:HD21 | 1.62 | 0.81 |
| 1:D:111:PRO:HD3 | 1:D:188:PRO:HA | 1.63 | 0.80 |
| 1:C:111:PRO:HD3 | 1:C:188:PRO:HA | 1.63 | 0.80 |
| 1:A:503:LYS:HB3 | 1:A:543:ASN:HB3 | 1.64 | 0.80 |
| 1:C:283:SER:H | 1:C:291:GLN:NE2 | 1.80 | 0.80 |
| 1:C:300:LYS:HG2 | 1:C:301:LEU:H | 1.45 | 0.80 |
| 1:D:283:SER:H | 1:D:291:GLN:NE2 | 1.80 | 0.80 |
| 1:D:300:LYS:HG2 | 1:D:301:LEU:H | 1.45 | 0.79 |
| 1:B:72:ARG:HH11 | 1:D:68:GLN:HE22 | 1.27 | 0.79 |
| 1:B:111:PRO:HD3 | 1:B:188:PRO:HA | 1.63 | 0.79 |
| 1:A:111:PRO:HD3 | 1:A:188:PRO:HA | 1.63 | 0.79 |
| 1:A:68:GLN:HE22 | 1:C:72:ARG:HH11 | 1.27 | 0.79 |
| 1:A:22:ALA:HA | 1:A:26:PHE:HD1 | 1.48 | 0.79 |
| 1:B:418:ILE:HG12 | 1:B:548:ILE:HG23 | 1.65 | 0.79 |
| 1:B:503:LYS:HB3 | 1:B:543:ASN:HB3 | 1.64 | 0.78 |
| 1:D:503:LYS:HB3 | 1:D:543:ASN:HB3 | 1.64 | 0.78 |
| 1:A:418:ILE:HG12 | 1:A:548:ILE:HG23 | 1.64 | 0.78 |
| 1:A:326:PRO:HB3 | 1:D:37:ILE:HG21 | 1.64 | 0.78 |
| 1:B:22:ALA:HA | 1:B:26:PHE:HD1 | 1.48 | 0.78 |
| 1:B:283:SER:H | 1:B:291:GLN:NE2 | 1.81 | 0.78 |
| 1:A:283:SER:H | 1:A:291:GLN:NE2 | 1.80 | 0.78 |
| 1:A:72:ARG:HH11 | 1:C:68:GLN:HE22 | 1.28 | 0.78 |
| 1:B:30:TRP:CE2 | 1:C:288:PRO:HG3 | 2.19 | 0.78 |
| 1:C:22:ALA:HA | 1:C:26:PHE:HD1 | 1.48 | 0.77 |
| 1:C:418:ILE:HG12 | 1:C:548:ILE:HG23 | 1.65 | 0.77 |
| 1:D:22:ALA:HA | 1:D:26:PHE:HD1 | 1.48 | 0.77 |
| 1:D:418:ILE:HG12 | 1:D:548:ILE:HG23 | 1.65 | 0.77 |
| 1:A:404:GLU:O | 1:A:406:LYS:HG2 | 1.85 | 0.76 |
| 1:B:404:GLU:O | 1:B:406:LYS:HG2 | 1.84 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:LEU:HB3 | 1:B:249:VAL:HB | 1.68 | 0.76 |
| 1:C:404:GLU:O | 1:C:406:LYS:HG2 | 1.85 | 0.76 |
| 1:D:404:GLU:O | 1:D:406:LYS:HG2 | 1.85 | 0.76 |
| 1:A:98:MET:SD | 1:B:176:LEU:HD12 | 2.25 | 0.75 |
| 1:C:370:ARG:O | 1:C:517:LEU:HA | 1.86 | 0.75 |
| 1:D:218:LEU:HB3 | 1:D:249:VAL:HB | 1.68 | 0.75 |
| 1:D:86:GLU:O | 1:D:89:ILE:HG22 | 1.87 | 0.75 |
| 1:A:86:GLU:O | 1:A:89:ILE:HG22 | 1.86 | 0.75 |
| 1:C:86:GLU:O | 1:C:89:ILE:HG22 | 1.86 | 0.74 |
| 1:A:218:LEU:HB3 | 1:A:249:VAL:HB | 1.68 | 0.74 |
| 1:D:370:ARG:O | 1:D:517:LEU:HA | 1.87 | 0.74 |
| 1:A:523:ALA:O | 1:A:527:ILE:HG12 | 1.88 | 0.74 |
| 1:B:86:GLU:O | 1:B:89:ILE:HG22 | 1.87 | 0.74 |
| 1:C:218:LEU:HB3 | 1:C:249:VAL:HB | 1.68 | 0.74 |
| 1:C:439:GLU:HB2 | 1:C:441:TYR:CE1 | 2.23 | 0.74 |
| 1:C:76:GLU:HB3 | 1:C:220:LEU:HD23 | 1.70 | 0.73 |
| 1:B:370:ARG:O | 1:B:517:LEU:HA | 1.87 | 0.73 |
| 1:C:31:ARG:H | 1:C:31:ARG:CD | 1.96 | 0.73 |
| 1:B:523:ALA:O | 1:B:527:ILE:HG12 | 1.88 | 0.73 |
| 1:D:523:ALA:O | 1:D:527:ILE:HG12 | 1.88 | 0.73 |
| 1:A:370:ARG:O | 1:A:517:LEU:HA | 1.87 | 0.73 |
| 1:A:76:GLU:HB3 | 1:A:220:LEU:HD23 | 1.71 | 0.73 |
| 1:D:439:GLU:HB2 | 1:D:441:TYR:CE1 | 2.24 | 0.73 |
| 1:A:439:GLU:HB2 | 1:A:441:TYR:CE1 | 2.24 | 0.72 |
| 1:B:439:GLU:HB2 | 1:B:441:TYR:CE1 | 2.25 | 0.72 |
| 1:C:462:ILE:HB | 1:C:463:PRO:HD3 | 1.72 | 0.72 |
| 1:C:348:ARG:HH11 | 1:C:349:ALA:HA | 1.55 | 0.71 |
| 1:C:523:ALA:O | 1:C:527:ILE:HG12 | 1.89 | 0.71 |
| 1:D:462:ILE:HB | 1:D:463:PRO:HD3 | 1.72 | 0.71 |
| 1:A:46:TYR:HA | 1:A:49:LEU:H | 1.55 | 0.71 |
| 1:B:46:TYR:HA | 1:B:49:LEU:H | 1.55 | 0.71 |
| 1:D:46:TYR:HA | 1:D:49:LEU:H | 1.55 | 0.71 |
| 1:D:76:GLU:HB3 | 1:D:220:LEU:HD23 | 1.71 | 0.70 |
| 1:B:76:GLU:HB3 | 1:B:220:LEU:HD23 | 1.71 | 0.70 |
| 1:B:462:ILE:HB | 1:B:463:PRO:HD3 | 1.72 | 0.70 |
| 1:C:205:ILE:HD13 | 1:C:321:TYR:HE2 | 1.56 | 0.70 |
| 1:A:205:ILE:HD13 | 1:A:321:TYR:HE2 | 1.57 | 0.70 |
| 1:A:462:ILE:HB | 1:A:463:PRO:HD3 | 1.72 | 0.70 |
| 1:C:46:TYR:HA | 1:C:49:LEU:H | 1.56 | 0.70 |
| 1:A:326:PRO:HB3 | 1:D:37:ILE:CG2 | 2.22 | 0.70 |
| 1:A:348:ARG:HH11 | 1:A:349:ALA:HA | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:83:ILE:HD13 | 1:B:107:LEU:HD21 | 1.74 | 0.69 |
| 1:D:348:ARG:HH11 | 1:D:349:ALA:HA | 1.56 | 0.69 |
| 1:A:354:GLN:CB | 1:B:210:LEU:HD13 | 2.22 | 0.69 |
| 1:B:31:ARG:H | 1:B:31:ARG:CD | 1.97 | 0.69 |
| 1:D:205:ILE:HD13 | 1:D:321:TYR:HE2 | 1.56 | 0.69 |
| 1:B:348:ARG:HH11 | 1:B:349:ALA:HA | 1.56 | 0.69 |
| 1:C:348:ARG:HH22 | 1:C:356:TYR:HB2 | 1.58 | 0.69 |
| 1:A:229:ARG:NE | 1:B:109:GLY:HA3 | 2.07 | 0.69 |
| 1:B:536:VAL:HG23 | 1:B:537:ARG:H | 1.58 | 0.68 |
| 1:B:205:ILE:HD13 | 1:B:321:TYR:HE2 | 1.56 | 0.68 |
| 1:A:348:ARG:HH22 | 1:A:356:TYR:HB2 | 1.58 | 0.68 |
| 1:A:64:GLU:HG3 | 1:B:64:GLU:OE1 | 1.94 | 0.68 |
| 1:C:83:ILE:HD13 | 1:C:107:LEU:HD21 | 1.74 | 0.68 |
| 1:D:83:ILE:HD13 | 1:D:107:LEU:HD21 | 1.74 | 0.68 |
| 1:B:372:ASP:HB3 | 1:B:516:ASN:OD1 | 1.94 | 0.68 |
| 1:B:348:ARG:HH22 | 1:B:356:TYR:HB2 | 1.59 | 0.68 |
| 1:A:507:PRO:HG2 | 1:A:514:ASP:HB2 | 1.74 | 0.68 |
| 1:A:372:ASP:HB3 | 1:A:516:ASN:OD1 | 1.94 | 0.68 |
| 1:A:438:ASN:ND2 | 1:A:451:PRO:HD3 | 2.09 | 0.68 |
| 1:A:83:ILE:HD13 | 1:A:107:LEU:HD21 | 1.74 | 0.68 |
| 1:B:507:PRO:HG2 | 1:B:514:ASP:HB2 | 1.75 | 0.68 |
| 1:A:536:VAL:HG23 | 1:A:537:ARG:H | 1.59 | 0.67 |
| 1:C:507:PRO:HG2 | 1:C:514:ASP:HB2 | 1.75 | 0.67 |
| 1:B:68:GLN:HE22 | 1:D:72:ARG:NH1 | 1.90 | 0.67 |
| 1:D:348:ARG:HH22 | 1:D:356:TYR:HB2 | 1.58 | 0.67 |
| 1:D:507:PRO:HG2 | 1:D:514:ASP:HB2 | 1.74 | 0.67 |
| 1:B:369:ILE:HD12 | 1:B:475:THR:HG21 | 1.77 | 0.67 |
| 1:A:64:GLU:OE1 | 1:B:64:GLU:HG3 | 1.95 | 0.67 |
| 1:C:438:ASN:ND2 | 1:C:451:PRO:HD3 | 2.10 | 0.67 |
| 1:C:369:ILE:HD12 | 1:C:475:THR:HG21 | 1.77 | 0.67 |
| 1:A:57:HIS:CE1 | 1:B:79:ILE:HD12 | 2.30 | 0.66 |
| 1:D:536:VAL:HG23 | 1:D:537:ARG:H | 1.59 | 0.66 |
| 1:C:536:VAL:HG23 | 1:C:537:ARG:H | 1.58 | 0.66 |
| 1:D:438:ASN:ND2 | 1:D:451:PRO:HD3 | 2.10 | 0.66 |
| 1:D:512:LEU:HA | 1:D:536:VAL:HG21 | 1.77 | 0.66 |
| 1:C:512:LEU:HA | 1:C:536:VAL:HG21 | 1.78 | 0.66 |
| 1:C:372:ASP:HB3 | 1:C:516:ASN:OD1 | 1.96 | 0.66 |
| 1:A:339:MET:SD | 1:A:347:VAL:HG22 | 2.35 | 0.66 |
| 1:B:158:VAL:HG13 | 1:B:159:PHE:N | 2.10 | 0.66 |
| 1:C:158:VAL:HG13 | 1:C:159:PHE:N | 2.10 | 0.66 |
| 1:D:372:ASP:HB3 | 1:D:516:ASN:OD1 | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:512:LEU:HA | 1:A:536:VAL:HG21 | 1.77 | 0.65 |
| 1:B:438:ASN:ND2 | 1:B:451:PRO:HD3 | 2.10 | 0.65 |
| 1:D:287:THR:HG22 | 1:D:314:SER:HA | 1.77 | 0.65 |
| 1:A:260:VAL:HG22 | 1:D:51:PRO:HB3 | 1.76 | 0.65 |
| 1:D:369:ILE:HD12 | 1:D:475:THR:HG21 | 1.78 | 0.65 |
| 1:A:435:SER:HB2 | 1:A:438:ASN:OD1 | 1.97 | 0.65 |
| 1:A:287:THR:HG22 | 1:A:314:SER:HA | 1.78 | 0.65 |
| 1:C:108:ALA:HB3 | 1:D:106:TYR:HB2 | 1.79 | 0.65 |
| 1:C:287:THR:HG22 | 1:C:314:SER:HA | 1.77 | 0.65 |
| 1:D:158:VAL:HG13 | 1:D:159:PHE:N | 2.10 | 0.65 |
| 1:B:287:THR:HG22 | 1:B:314:SER:HA | 1.79 | 0.65 |
| 1:A:506:VAL:CG2 | 1:A:507:PRO:HD3 | 2.23 | 0.64 |
| 1:D:339:MET:SD | 1:D:347:VAL:HG22 | 2.36 | 0.64 |
| 1:B:512:LEU:HA | 1:B:536:VAL:HG21 | 1.78 | 0.64 |
| 1:B:506:VAL:CG2 | 1:B:507:PRO:HD3 | 2.23 | 0.64 |
| 1:A:158:VAL:HG13 | 1:A:159:PHE:N | 2.09 | 0.64 |
| 1:A:369:ILE:HD12 | 1:A:475:THR:HG21 | 1.78 | 0.64 |
| 1:C:339:MET:SD | 1:C:347:VAL:HG22 | 2.38 | 0.64 |
| 1:A:344:TYR:CD2 | 1:A:350:MET:HB2 | 2.33 | 0.64 |
| 1:B:344:TYR:CD2 | 1:B:350:MET:HB2 | 2.33 | 0.64 |
| 1:A:31:ARG:H | 1:A:31:ARG:CD | 1.96 | 0.63 |
| 1:D:435:SER:HB2 | 1:D:438:ASN:OD1 | 1.98 | 0.63 |
| 1:B:435:SER:HB2 | 1:B:438:ASN:OD1 | 1.98 | 0.63 |
| 1:A:477:ILE:HG21 | 1:A:517:LEU:HD21 | 1.81 | 0.63 |
| 1:C:435:SER:HB2 | 1:C:438:ASN:OD1 | 1.98 | 0.63 |
| 1:B:339:MET:SD | 1:B:347:VAL:HG22 | 2.38 | 0.63 |
| 1:B:536:VAL:HG23 | 1:B:537:ARG:N | 2.14 | 0.63 |
| 1:C:344:TYR:CD2 | 1:C:350:MET:HB2 | 2.34 | 0.63 |
| 1:C:395:LYS:HG3 | 1:C:430:LYS:HG2 | 1.81 | 0.63 |
| 1:C:430:LYS:HD2 | 1:C:433:GLY:O | 1.99 | 0.63 |
| 1:D:31:ARG:CD | 1:D:31:ARG:H | 1.96 | 0.62 |
| 1:C:477:ILE:HG21 | 1:C:517:LEU:HD21 | 1.80 | 0.62 |
| 1:C:98:MET:SD | 1:D:176:LEU:HD12 | 2.38 | 0.62 |
| 1:D:536:VAL:HG23 | 1:D:537:ARG:N | 2.15 | 0.62 |
| 1:A:395:LYS:HG3 | 1:A:430:LYS:HG2 | 1.81 | 0.62 |
| 1:B:430:LYS:HD2 | 1:B:433:GLY:O | 1.99 | 0.62 |
| 1:B:477:ILE:HG21 | 1:B:517:LEU:HD21 | 1.81 | 0.62 |
| 1:A:352:TYR:HE2 | 1:B:81:PRO:N | 1.97 | 0.62 |
| 1:D:430:LYS:HD2 | 1:D:433:GLY:O | 2.00 | 0.62 |
| 1:D:477:ILE:HG21 | 1:D:517:LEU:HD21 | 1.81 | 0.62 |
| 1:C:536:VAL:HG23 | 1:C:537:ARG:N | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:508:ILE:O | 1:D:510:ARG:HG3 | 1.99 | 0.62 |
| 1:C:508:ILE:O | 1:C:510:ARG:HG3 | 2.00 | 0.62 |
| 1:B:195:LEU:HD13 | 1:B:227:PHE:CG | 2.35 | 0.61 |
| 1:C:506:VAL:CG2 | 1:C:507:PRO:HD3 | 2.24 | 0.61 |
| 1:D:344:TYR:CD2 | 1:D:350:MET:HB2 | 2.34 | 0.61 |
| 1:A:230:GLU:HB3 | 1:A:233:GLU:HG3 | 1.82 | 0.61 |
| 1:A:287:THR:CG2 | 1:A:314:SER:HA | 2.30 | 0.61 |
| 1:C:432:LEU:HD12 | 1:C:432:LEU:N | 2.16 | 0.61 |
| 1:B:230:GLU:HB3 | 1:B:233:GLU:HG3 | 1.82 | 0.61 |
| 1:B:395:LYS:HG3 | 1:B:430:LYS:HG2 | 1.81 | 0.61 |
| 1:C:287:THR:CG2 | 1:C:314:SER:HA | 2.31 | 0.61 |
| 1:A:322:ASN:ND2 | 1:D:15:ILE:HD11 | 2.16 | 0.61 |
| 1:D:195:LEU:HD13 | 1:D:227:PHE:CG | 2.35 | 0.61 |
| 1:C:230:GLU:HB3 | 1:C:233:GLU:HG3 | 1.82 | 0.61 |
| 1:A:322:ASN:HD21 | 1:D:15:ILE:HD11 | 1.66 | 0.61 |
| 1:A:430:LYS:HD2 | 1:A:433:GLY:O | 2.00 | 0.61 |
| 1:C:186:LEU:HD23 | 1:C:187:LYS:N | 2.16 | 0.61 |
| 1:A:195:LEU:HD13 | 1:A:227:PHE:CG | 2.36 | 0.61 |
| 1:A:508:ILE:O | 1:A:510:ARG:HG3 | 2.00 | 0.60 |
| 1:B:287:THR:CG2 | 1:B:314:SER:HA | 2.31 | 0.60 |
| 1:C:283:SER:N | 1:C:291:GLN:HE22 | 1.93 | 0.60 |
| 1:D:287:THR:CG2 | 1:D:314:SER:HA | 2.31 | 0.60 |
| 1:C:109:GLY:O | 1:C:111:PRO:HD3 | 2.01 | 0.60 |
| 1:D:230:GLU:HB3 | 1:D:233:GLU:HG3 | 1.82 | 0.60 |
| 1:A:229:ARG:HE | 1:B:109:GLY:HA3 | 1.65 | 0.60 |
| 1:B:508:ILE:O | 1:B:510:ARG:HG3 | 2.01 | 0.60 |
| 1:A:57:HIS:CD2 | 1:B:79:ILE:HG13 | 2.36 | 0.60 |
| 1:A:284:LYS:HA | 1:D:30:TRP:CZ2 | 2.36 | 0.60 |
| 1:D:46:TYR:CD1 | 1:D:47:PRO:HA | 2.37 | 0.60 |
| 1:B:72:ARG:NH1 | 1:D:68:GLN:HE22 | 1.98 | 0.60 |
| 1:C:195:LEU:HD13 | 1:C:227:PHE:CG | 2.36 | 0.60 |
| 1:D:186:LEU:HD23 | 1:D:187:LYS:N | 2.16 | 0.60 |
| 1:A:536:VAL:HG23 | 1:A:537:ARG:N | 2.15 | 0.60 |
| 1:D:395:LYS:HG3 | 1:D:430:LYS:HG2 | 1.82 | 0.60 |
| 1:A:196:ARG:NH1 | 1:A:199:MET:HE1 | 2.17 | 0.60 |
| 1:A:109:GLY:O | 1:A:111:PRO:HD3 | 2.01 | 0.59 |
| 1:A:440:VAL:HA | 1:A:449:GLY:HA3 | 1.84 | 0.59 |
| 1:B:440:VAL:HA | 1:B:449:GLY:HA3 | 1.84 | 0.59 |
| 1:A:46:TYR:CD1 | 1:A:47:PRO:HA | 2.37 | 0.59 |
| 1:B:432:LEU:N | 1:B:432:LEU:HD12 | 2.17 | 0.59 |
| 1:B:186:LEU:HD23 | 1:B:187:LYS:N | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:387:LEU:O | 1:B:387:LEU:HD13 | 2.03 | 0.59 |
| 1:C:401:CYS:SG | 1:C:402:SER:N | 2.74 | 0.59 |
| 1:D:506:VAL:CG2 | 1:D:507:PRO:HD3 | 2.23 | 0.59 |
| 1:B:46:TYR:CD1 | 1:B:47:PRO:HA | 2.37 | 0.59 |
| 1:D:109:GLY:O | 1:D:111:PRO:HD3 | 2.01 | 0.59 |
| 1:B:68:GLN:NE2 | 1:D:72:ARG:HH11 | 1.95 | 0.59 |
| 1:B:196:ARG:NH1 | 1:B:199:MET:HE1 | 2.18 | 0.59 |
| 1:C:46:TYR:CD1 | 1:C:47:PRO:HA | 2.38 | 0.59 |
| 1:A:186:LEU:HD23 | 1:A:187:LYS:N | 2.16 | 0.59 |
| 1:A:432:LEU:HD12 | 1:A:432:LEU:N | 2.18 | 0.59 |
| 1:D:325:VAL:HG23 | 1:D:326:PRO:HD2 | 1.85 | 0.59 |
| 1:C:440:VAL:HA | 1:C:449:GLY:HA3 | 1.85 | 0.59 |
| 1:C:522:LEU:O | 1:C:523:ALA:HB3 | 2.03 | 0.59 |
| 1:B:109:GLY:O | 1:B:111:PRO:HD3 | 2.01 | 0.59 |
| 1:C:210:LEU:HD13 | 1:D:354:GLN:CB | 2.31 | 0.59 |
| 1:C:325:VAL:HG23 | 1:C:326:PRO:HD2 | 1.85 | 0.59 |
| 1:D:432:LEU:N | 1:D:432:LEU:HD12 | 2.17 | 0.59 |
| 1:D:440:VAL:HA | 1:D:449:GLY:HA3 | 1.84 | 0.59 |
| 1:A:294:VAL:HB | 1:A:308:ALA:HB3 | 1.85 | 0.59 |
| 1:C:271:PHE:CZ | 1:C:298:HIS:HB2 | 2.38 | 0.59 |
| 1:A:30:TRP:CH2 | 1:D:288:PRO:HG3 | 2.38 | 0.59 |
| 1:B:502:PHE:HD2 | 1:B:546:VAL:HG13 | 1.68 | 0.58 |
| 1:D:271:PHE:CZ | 1:D:298:HIS:HB2 | 2.38 | 0.58 |
| 1:B:294:VAL:HB | 1:B:308:ALA:HB3 | 1.85 | 0.58 |
| 1:A:271:PHE:CZ | 1:A:298:HIS:HB2 | 2.38 | 0.58 |
| 1:B:401:CYS:SG | 1:B:402:SER:N | 2.76 | 0.58 |
| 1:C:502:PHE:HD2 | 1:C:546:VAL:HG13 | 1.68 | 0.58 |
| 1:A:322:ASN:ND2 | 1:D:15:ILE:CD1 | 2.67 | 0.58 |
| 1:D:508:ILE:HD12 | 1:D:508:ILE:O | 2.04 | 0.58 |
| 1:B:271:PHE:CZ | 1:B:298:HIS:HB2 | 2.39 | 0.58 |
| 1:D:384:ALA:HA | 1:D:488:VAL:HG21 | 1.86 | 0.58 |
| 1:C:294:VAL:HB | 1:C:308:ALA:HB3 | 1.85 | 0.58 |
| 1:A:401:CYS:SG | 1:A:402:SER:N | 2.77 | 0.57 |
| 1:B:93:PHE:HB2 | 1:B:97:ALA:HB2 | 1.86 | 0.57 |
| 1:D:387:LEU:HD13 | 1:D:387:LEU:O | 2.03 | 0.57 |
| 1:D:502:PHE:HD2 | 1:D:546:VAL:HG13 | 1.69 | 0.57 |
| 1:C:93:PHE:HB2 | 1:C:97:ALA:HB2 | 1.87 | 0.57 |
| 1:D:37:ILE:HG13 | 1:D:37:ILE:O | 2.04 | 0.57 |
| 1:A:161:ILE:HG12 | 1:A:167:VAL:CG1 | 2.33 | 0.57 |
| 1:B:275:LYS:HG3 | 1:C:363:ARG:HH12 | 1.70 | 0.57 |
| 1:C:37:ILE:HG13 | 1:C:37:ILE:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:387:LEU:HD12 | 1:D:484:ILE:HG23 | 1.86 | 0.57 |
| 1:D:93:PHE:HB2 | 1:D:97:ALA:HB2 | 1.86 | 0.57 |
| 1:A:37:ILE:O | 1:A:37:ILE:HG13 | 2.05 | 0.57 |
| 1:A:384:ALA:HA | 1:A:488:VAL:HG21 | 1.86 | 0.57 |
| 1:B:527:ILE:O | 1:B:532:LYS:HB2 | 2.04 | 0.57 |
| 1:A:64:GLU:CD | 1:B:64:GLU:HG3 | 2.24 | 0.57 |
| 1:C:387:LEU:HD12 | 1:C:484:ILE:HG23 | 1.87 | 0.57 |
| 1:A:325:VAL:HG23 | 1:A:326:PRO:HD2 | 1.86 | 0.57 |
| 1:A:387:LEU:O | 1:A:387:LEU:HD13 | 2.04 | 0.57 |
| 1:A:527:ILE:O | 1:A:532:LYS:HB2 | 2.04 | 0.57 |
| 1:B:414:GLU:O | 1:B:416:ARG:HG2 | 2.05 | 0.57 |
| 1:D:103:ARG:HA | 1:D:229:ARG:HB3 | 1.87 | 0.57 |
| 1:D:514:ASP:C | 1:D:516:ASN:N | 2.58 | 0.57 |
| 1:A:527:ILE:HG21 | 1:A:534:ILE:HD11 | 1.86 | 0.57 |
| 1:B:527:ILE:HG21 | 1:B:534:ILE:HD11 | 1.86 | 0.57 |
| 1:A:395:LYS:HG2 | 1:A:396:ASP:N | 2.17 | 0.56 |
| 1:B:37:ILE:O | 1:B:37:ILE:HG13 | 2.05 | 0.56 |
| 1:C:384:ALA:HA | 1:C:488:VAL:HG21 | 1.86 | 0.56 |
| 1:C:527:ILE:O | 1:C:532:LYS:HB2 | 2.05 | 0.56 |
| 1:A:37:ILE:HG21 | 1:D:326:PRO:HB3 | 1.88 | 0.56 |
| 1:A:387:LEU:HD12 | 1:A:484:ILE:HG23 | 1.86 | 0.56 |
| 1:B:387:LEU:HD12 | 1:B:484:ILE:HG23 | 1.87 | 0.56 |
| 1:C:161:ILE:HG12 | 1:C:167:VAL:CG1 | 2.34 | 0.56 |
| 1:C:31:ARG:N | 1:C:31:ARG:HD3 | 2.04 | 0.56 |
| 1:C:64:GLU:OE1 | 1:D:64:GLU:HG3 | 2.04 | 0.56 |
| 1:B:325:VAL:HG23 | 1:B:326:PRO:HD2 | 1.86 | 0.56 |
| 1:D:294:VAL:HB | 1:D:308:ALA:HB3 | 1.86 | 0.56 |
| 1:C:64:GLU:HG3 | 1:D:64:GLU:OE1 | 2.04 | 0.56 |
| 1:D:527:ILE:O | 1:D:532:LYS:HB2 | 2.05 | 0.56 |
| 1:A:502:PHE:HD2 | 1:A:546:VAL:HG13 | 1.69 | 0.56 |
| 1:A:512:LEU:HB3 | 1:A:536:VAL:HG11 | 1.87 | 0.56 |
| 1:C:387:LEU:HD13 | 1:C:387:LEU:O | 2.05 | 0.56 |
| 1:D:196:ARG:NH1 | 1:D:199:MET:HE1 | 2.21 | 0.56 |
| 1:D:512:LEU:HB3 | 1:D:536:VAL:HG11 | 1.87 | 0.56 |
| 1:A:414:GLU:O | 1:A:416:ARG:HG2 | 2.06 | 0.56 |
| 1:A:522:LEU:O | 1:A:523:ALA:HB3 | 2.06 | 0.56 |
| 1:A:540:VAL:O | 1:A:541:PHE:HB2 | 2.05 | 0.56 |
| 1:D:31:ARG:N | 1:D:31:ARG:HD3 | 2.04 | 0.56 |
| 1:D:522:LEU:O | 1:D:523:ALA:HB3 | 2.06 | 0.56 |
| 1:A:103:ARG:HA | 1:A:229:ARG:HB3 | 1.87 | 0.56 |
| 1:A:93:PHE:HB2 | 1:A:97:ALA:HB2 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:514:ASP:C | 1:B:516:ASN:N | 2.59 | 0.56 |
| 1:C:103:ARG:HA | 1:C:229:ARG:HB3 | 1.88 | 0.56 |
| 1:D:395:LYS:HG2 | 1:D:396:ASP:N | 2.17 | 0.56 |
| 1:D:527:ILE:HG21 | 1:D:534:ILE:HD11 | 1.87 | 0.56 |
| 1:A:30:TRP:CE2 | 1:D:288:PRO:HG3 | 2.41 | 0.56 |
| 1:B:384:ALA:HA | 1:B:488:VAL:HG21 | 1.87 | 0.56 |
| 1:B:508:ILE:O | 1:B:508:ILE:HD12 | 2.06 | 0.56 |
| 1:D:401:CYS:SG | 1:D:402:SER:N | 2.78 | 0.56 |
| 1:D:414:GLU:O | 1:D:416:ARG:HG2 | 2.06 | 0.56 |
| 1:B:283:SER:N | 1:B:291:GLN:HE22 | 1.94 | 0.56 |
| 1:A:260:VAL:CG2 | 1:D:51:PRO:HB3 | 2.35 | 0.55 |
| 1:B:103:ARG:HA | 1:B:229:ARG:HB3 | 1.87 | 0.55 |
| 1:B:540:VAL:O | 1:B:541:PHE:HB2 | 2.05 | 0.55 |
| 1:C:508:ILE:HD12 | 1:C:510:ARG:HG3 | 1.88 | 0.55 |
| 1:C:527:ILE:HG21 | 1:C:534:ILE:HD11 | 1.87 | 0.55 |
| 1:D:508:ILE:HD12 | 1:D:510:ARG:HG3 | 1.88 | 0.55 |
| 1:C:540:VAL:O | 1:C:541:PHE:HB2 | 2.05 | 0.55 |
| 1:D:540:VAL:O | 1:D:541:PHE:HB2 | 2.05 | 0.55 |
| 1:A:227:PHE:HZ | 1:B:227:PHE:HZ | 1.55 | 0.55 |
| 1:C:508:ILE:O | 1:C:508:ILE:HD12 | 2.06 | 0.55 |
| 1:D:161:ILE:HG12 | 1:D:167:VAL:CG1 | 2.33 | 0.55 |
| 1:D:396:ASP:O | 1:D:397:LYS:HB2 | 2.07 | 0.55 |
| 1:A:372:ASP:H | 1:A:517:LEU:H | 1.55 | 0.55 |
| 1:C:409:PHE:HD1 | 1:C:409:PHE:H | 1.54 | 0.55 |
| 1:B:258:GLY:HA3 | 1:B:310:PHE:CD2 | 2.42 | 0.55 |
| 1:C:396:ASP:O | 1:C:397:LYS:HB2 | 2.06 | 0.55 |
| 1:A:409:PHE:HD1 | 1:A:409:PHE:H | 1.53 | 0.55 |
| 1:C:258:GLY:HA3 | 1:C:310:PHE:CD2 | 2.41 | 0.55 |
| 1:A:109:GLY:HA3 | 1:B:229:ARG:NH1 | 2.21 | 0.55 |
| 1:B:508:ILE:HD12 | 1:B:510:ARG:HG3 | 1.88 | 0.55 |
| 1:C:512:LEU:HB3 | 1:C:536:VAL:HG11 | 1.88 | 0.55 |
| 1:A:298:HIS:O | 1:A:300:LYS:N | 2.40 | 0.55 |
| 1:A:316:ILE:HG23 | 1:A:317:ALA:H | 1.72 | 0.55 |
| 1:B:466:LYS:HD3 | 1:B:470:GLU:OE2 | 2.07 | 0.55 |
| 1:D:35:ALA:C | 1:D:37:ILE:H | 2.10 | 0.55 |
| 1:A:508:ILE:HD12 | 1:A:508:ILE:O | 2.07 | 0.54 |
| 1:B:372:ASP:H | 1:B:517:LEU:H | 1.56 | 0.54 |
| 1:C:298:HIS:O | 1:C:300:LYS:N | 2.40 | 0.54 |
| 1:C:35:ALA:C | 1:C:37:ILE:H | 2.09 | 0.54 |
| 1:C:414:GLU:O | 1:C:416:ARG:HG2 | 2.06 | 0.54 |
| 1:A:396:ASP:O | 1:A:397:LYS:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:512:LEU:HB3 | 1:B:536:VAL:HG11 | 1.87 | 0.54 |
| 1:C:156:ASP:OD2 | 1:D:284:LYS:HE3 | 2.07 | 0.54 |
| 1:D:283:SER:N | 1:D:291:GLN:HE22 | 1.93 | 0.54 |
| 1:B:505:ARG:O | 1:B:506:VAL:HG13 | 2.07 | 0.54 |
| 1:C:395:LYS:HG2 | 1:C:396:ASP:N | 2.17 | 0.54 |
| 1:A:35:ALA:C | 1:A:37:ILE:H | 2.09 | 0.54 |
| 1:B:522:LEU:O | 1:B:523:ALA:HB3 | 2.07 | 0.54 |
| 1:C:466:LYS:HD3 | 1:C:470:GLU:OE2 | 2.07 | 0.54 |
| 1:B:386:GLU:O | 1:B:390:ILE:HG13 | 2.08 | 0.54 |
| 1:C:505:ARG:O | 1:C:506:VAL:HG13 | 2.08 | 0.54 |
| 1:D:258:GLY:HA3 | 1:D:310:PHE:CD2 | 2.42 | 0.54 |
| 1:D:466:LYS:HD3 | 1:D:470:GLU:OE2 | 2.07 | 0.54 |
| 1:A:283:SER:N | 1:A:291:GLN:HE22 | 1.93 | 0.54 |
| 1:A:258:GLY:HA3 | 1:A:310:PHE:CD2 | 2.41 | 0.54 |
| 1:B:257:ASP:O | 1:B:261:VAL:HG23 | 2.07 | 0.54 |
| 1:B:35:ALA:C | 1:B:37:ILE:H | 2.10 | 0.54 |
| 1:B:396:ASP:O | 1:B:397:LYS:HB2 | 2.06 | 0.54 |
| 1:C:513:SER:O | 1:C:514:ASP:HB3 | 2.08 | 0.54 |
| 1:A:466:LYS:HD3 | 1:A:470:GLU:OE2 | 2.08 | 0.54 |
| 1:A:508:ILE:HD12 | 1:A:510:ARG:HG3 | 1.88 | 0.54 |
| 1:B:395:LYS:HG2 | 1:B:396:ASP:N | 2.16 | 0.54 |
| 1:D:505:ARG:O | 1:D:506:VAL:HG13 | 2.08 | 0.54 |
| 1:B:161:ILE:HG12 | 1:B:167:VAL:CG1 | 2.33 | 0.54 |
| 1:C:372:ASP:H | 1:C:517:LEU:H | 1.56 | 0.54 |
| 1:D:386:GLU:O | 1:D:390:ILE:HG13 | 2.08 | 0.54 |
| 1:A:386:GLU:O | 1:A:390:ILE:HG13 | 2.08 | 0.54 |
| 1:D:494:ALA:HB2 | 1:D:502:PHE:HZ | 1.73 | 0.54 |
| 1:A:257:ASP:O | 1:A:261:VAL:HG23 | 2.08 | 0.53 |
| 1:C:16:LYS:HA | 1:C:19:LEU:HB3 | 1.90 | 0.53 |
| 1:D:92:GLN:HE22 | 1:D:201:SER:HA | 1.73 | 0.53 |
| 1:D:372:ASP:H | 1:D:517:LEU:H | 1.55 | 0.53 |
| 1:A:505:ARG:O | 1:A:506:VAL:HG13 | 2.08 | 0.53 |
| 1:B:16:LYS:HA | 1:B:19:LEU:HB3 | 1.90 | 0.53 |
| 1:A:494:ALA:HB2 | 1:A:502:PHE:HZ | 1.73 | 0.53 |
| 1:B:92:GLN:HE22 | 1:B:201:SER:HA | 1.73 | 0.53 |
| 1:D:513:SER:O | 1:D:514:ASP:HB3 | 2.09 | 0.53 |
| 1:A:514:ASP:C | 1:A:516:ASN:N | 2.58 | 0.53 |
| 1:D:316:ILE:HG23 | 1:D:317:ALA:H | 1.74 | 0.53 |
| 1:D:105:PHE:CE1 | 1:D:229:ARG:HG3 | 2.44 | 0.53 |
| 1:A:158:VAL:CG1 | 1:A:159:PHE:H | 2.16 | 0.53 |
| 1:A:92:GLN:HE22 | 1:A:201:SER:HA | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:298:HIS:O | 1:B:300:LYS:N | 2.41 | 0.53 |
| 1:B:494:ALA:HB2 | 1:B:502:PHE:HZ | 1.74 | 0.53 |
| 1:C:386:GLU:O | 1:C:390:ILE:HG13 | 2.09 | 0.53 |
| 1:C:494:ALA:HB2 | 1:C:502:PHE:HZ | 1.74 | 0.53 |
| 1:A:72:ARG:NH1 | 1:C:68:GLN:HE22 | 2.02 | 0.53 |
| 1:B:105:PHE:CE1 | 1:B:229:ARG:HG3 | 2.44 | 0.53 |
| 1:C:106:TYR:HB2 | 1:D:108:ALA:HB3 | 1.88 | 0.53 |
| 1:D:298:HIS:O | 1:D:300:LYS:N | 2.41 | 0.53 |
| 1:C:105:PHE:CE1 | 1:C:229:ARG:HG3 | 2.44 | 0.53 |
| 1:C:92:GLN:HE22 | 1:C:201:SER:HA | 1.73 | 0.53 |
| 1:D:150:GLY:O | 1:D:152:ILE:HG13 | 2.09 | 0.53 |
| 1:D:16:LYS:HA | 1:D:19:LEU:HB3 | 1.91 | 0.53 |
| 1:D:310:PHE:HB3 | 1:D:330:LEU:HD13 | 1.91 | 0.53 |
| 1:D:502:PHE:CD2 | 1:D:546:VAL:HG13 | 2.44 | 0.53 |
| 1:C:316:ILE:HG23 | 1:C:317:ALA:H | 1.73 | 0.52 |
| 1:C:514:ASP:O | 1:C:515:ILE:HB | 2.09 | 0.52 |
| 1:A:105:PHE:CE1 | 1:A:229:ARG:HG3 | 2.44 | 0.52 |
| 1:A:16:LYS:HA | 1:A:19:LEU:HB3 | 1.90 | 0.52 |
| 1:B:513:SER:O | 1:B:514:ASP:HB3 | 2.09 | 0.52 |
| 1:C:502:PHE:CD2 | 1:C:546:VAL:HG13 | 2.44 | 0.52 |
| 1:A:503:LYS:CB | 1:A:543:ASN:HB3 | 2.38 | 0.52 |
| 1:B:150:GLY:O | 1:B:152:ILE:HG13 | 2.09 | 0.52 |
| 1:B:502:PHE:CD2 | 1:B:546:VAL:HG13 | 2.44 | 0.52 |
| 1:C:229:ARG:HG2 | 1:C:229:ARG:HH21 | 1.74 | 0.52 |
| 1:C:48:ARG:HG3 | 1:C:48:ARG:HH21 | 1.73 | 0.52 |
| 1:D:257:ASP:O | 1:D:261:VAL:HG23 | 2.09 | 0.52 |
| 1:A:109:GLY:HA3 | 1:B:229:ARG:NE | 2.24 | 0.52 |
| 1:A:515:ILE:HG22 | 1:A:515:ILE:O | 2.10 | 0.52 |
| 1:C:150:GLY:O | 1:C:152:ILE:HG13 | 2.09 | 0.52 |
| 1:D:229:ARG:HH21 | 1:D:229:ARG:HG2 | 1.75 | 0.52 |
| 1:A:37:ILE:HG22 | 1:D:326:PRO:HG3 | 1.92 | 0.52 |
| 1:A:310:PHE:HB3 | 1:A:330:LEU:HD13 | 1.91 | 0.52 |
| 1:C:199:MET:HE1 | 1:C:224:ASP:HB3 | 1.92 | 0.52 |
| 1:C:257:ASP:O | 1:C:261:VAL:HG23 | 2.09 | 0.52 |
| 1:D:301:LEU:HG | 1:D:302:GLY:N | 2.25 | 0.52 |
| 1:D:32:GLU:O | 1:D:34:ARG:N | 2.43 | 0.52 |
| 1:D:48:ARG:HG3 | 1:D:48:ARG:HH21 | 1.75 | 0.52 |
| 1:A:111:PRO:CD | 1:A:188:PRO:HA | 2.39 | 0.52 |
| 1:B:332:LEU:C | 1:B:332:LEU:HD23 | 2.31 | 0.52 |
| 1:B:450:ILE:HD11 | 1:B:465:LEU:HD11 | 1.92 | 0.52 |
| 1:B:48:ARG:HG3 | 1:B:48:ARG:HH21 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:515:ILE:HG22 | 1:C:515:ILE:O | 2.10 | 0.52 |
| 1:B:316:ILE:HG23 | 1:B:317:ALA:H | 1.73 | 0.52 |
| 1:A:513:SER:O | 1:A:514:ASP:HB3 | 2.09 | 0.51 |
| 1:B:514:ASP:O | 1:B:515:ILE:HB | 2.11 | 0.51 |
| 1:A:324:ASP:HA | 1:D:13:PHE:CE1 | 2.44 | 0.51 |
| 1:D:310:PHE:HB3 | 1:D:330:LEU:CD1 | 2.40 | 0.51 |
| 1:A:150:GLY:O | 1:A:152:ILE:HG13 | 2.09 | 0.51 |
| 1:A:301:LEU:HG | 1:A:302:GLY:N | 2.26 | 0.51 |
| 1:A:458:LYS:C | 1:A:460:GLN:H | 2.14 | 0.51 |
| 1:C:32:GLU:O | 1:C:34:ARG:N | 2.44 | 0.51 |
| 1:C:519:ILE:HG22 | 1:C:520:ASP:O | 2.10 | 0.51 |
| 1:A:502:PHE:CD2 | 1:A:546:VAL:HG13 | 2.45 | 0.51 |
| 1:C:396:ASP:N | 1:C:430:LYS:HA | 2.26 | 0.51 |
| 1:C:450:ILE:HD11 | 1:C:465:LEU:HD11 | 1.92 | 0.51 |
| 1:A:229:ARG:HH21 | 1:A:229:ARG:HG2 | 1.75 | 0.51 |
| 1:B:391:CYS:HB3 | 1:B:432:LEU:HD21 | 1.93 | 0.51 |
| 1:D:126:LYS:HG3 | 1:D:127:ASN:ND2 | 2.25 | 0.51 |
| 1:D:515:ILE:HG22 | 1:D:515:ILE:O | 2.10 | 0.51 |
| 1:A:126:LYS:HG3 | 1:A:127:ASN:ND2 | 2.25 | 0.51 |
| 1:A:32:GLU:O | 1:A:34:ARG:N | 2.44 | 0.51 |
| 1:A:332:LEU:HD23 | 1:A:332:LEU:C | 2.31 | 0.51 |
| 1:C:176:LEU:HD12 | 1:D:98:MET:SD | 2.50 | 0.51 |
| 1:C:310:PHE:HB3 | 1:C:330:LEU:HD13 | 1.91 | 0.51 |
| 1:A:198:HIS:CE1 | 1:A:329:ASN:HD21 | 2.29 | 0.51 |
| 1:B:310:PHE:HB3 | 1:B:330:LEU:CD1 | 2.40 | 0.51 |
| 1:B:421:GLU:O | 1:B:544:ALA:HB1 | 2.11 | 0.51 |
| 1:C:276:PHE:HD2 | 1:C:294:VAL:HG22 | 1.76 | 0.51 |
| 1:A:396:ASP:N | 1:A:430:LYS:HA | 2.26 | 0.51 |
| 1:A:450:ILE:HD11 | 1:A:465:LEU:HD11 | 1.93 | 0.51 |
| 1:A:514:ASP:O | 1:A:515:ILE:HB | 2.10 | 0.51 |
| 1:B:310:PHE:HB3 | 1:B:330:LEU:HD13 | 1.92 | 0.51 |
| 1:B:519:ILE:HG22 | 1:B:520:ASP:O | 2.11 | 0.51 |
| 1:C:310:PHE:HB3 | 1:C:330:LEU:CD1 | 2.41 | 0.51 |
| 1:D:450:ILE:HD11 | 1:D:465:LEU:HD11 | 1.92 | 0.51 |
| 1:D:494:ALA:HB2 | 1:D:502:PHE:CZ | 2.46 | 0.51 |
| 1:A:68:GLN:HE22 | 1:C:72:ARG:NH1 | 2.00 | 0.51 |
| 1:B:126:LYS:HG3 | 1:B:127:ASN:ND2 | 2.25 | 0.51 |
| 1:B:458:LYS:C | 1:B:460:GLN:H | 2.13 | 0.51 |
| 1:B:515:ILE:O | 1:B:515:ILE:HG22 | 2.10 | 0.51 |
| 1:C:126:LYS:HG3 | 1:C:127:ASN:ND2 | 2.25 | 0.51 |
| 1:D:409:PHE:HD1 | 1:D:409:PHE:H | 1.53 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:421:GLU:O | 1:D:544:ALA:HB1 | 2.11 | 0.51 |
| 1:A:391:CYS:HB3 | 1:A:432:LEU:HD21 | 1.93 | 0.51 |
| 1:B:540:VAL:HG12 | 1:B:541:PHE:N | 2.25 | 0.51 |
| 1:C:214:ARG:HD3 | 1:D:354:GLN:OE1 | 2.10 | 0.51 |
| 1:C:421:GLU:O | 1:C:544:ALA:HB1 | 2.10 | 0.51 |
| 1:D:519:ILE:HG22 | 1:D:520:ASP:O | 2.11 | 0.51 |
| 1:A:14:ASP:HB2 | 1:A:17:LYS:CB | 2.41 | 0.51 |
| 1:A:310:PHE:HB3 | 1:A:330:LEU:CD1 | 2.41 | 0.51 |
| 1:C:107:LEU:HD23 | 1:D:105:PHE:CG | 2.46 | 0.51 |
| 1:C:299:PRO:O | 1:C:300:LYS:HB2 | 2.11 | 0.51 |
| 1:D:276:PHE:HD2 | 1:D:294:VAL:HG22 | 1.76 | 0.51 |
| 1:D:57:HIS:HE1 | 1:D:59:VAL:HG23 | 1.76 | 0.51 |
| 1:A:494:ALA:HB2 | 1:A:502:PHE:CZ | 2.46 | 0.50 |
| 1:B:14:ASP:HB2 | 1:B:17:LYS:CB | 2.42 | 0.50 |
| 1:B:396:ASP:N | 1:B:430:LYS:HA | 2.26 | 0.50 |
| 1:C:503:LYS:CB | 1:C:543:ASN:HB3 | 2.38 | 0.50 |
| 1:B:224:ASP:CG | 1:B:225:ARG:H | 2.15 | 0.50 |
| 1:B:301:LEU:HG | 1:B:302:GLY:N | 2.25 | 0.50 |
| 1:C:380:PHE:HZ | 1:C:495:LEU:HD12 | 1.76 | 0.50 |
| 1:C:540:VAL:HG12 | 1:C:541:PHE:N | 2.25 | 0.50 |
| 1:D:380:PHE:HZ | 1:D:495:LEU:HD12 | 1.76 | 0.50 |
| 1:D:503:LYS:CB | 1:D:543:ASN:HB3 | 2.38 | 0.50 |
| 1:A:48:ARG:HG3 | 1:A:48:ARG:HH21 | 1.75 | 0.50 |
| 1:B:369:ILE:HD12 | 1:B:475:THR:CG2 | 2.41 | 0.50 |
| 1:A:299:PRO:O | 1:A:300:LYS:HB2 | 2.11 | 0.50 |
| 1:A:486:LYS:HB2 | 1:A:516:ASN:ND2 | 2.27 | 0.50 |
| 1:B:229:ARG:HG2 | 1:B:229:ARG:HH21 | 1.75 | 0.50 |
| 1:C:14:ASP:HB2 | 1:C:17:LYS:CB | 2.42 | 0.50 |
| 1:C:391:CYS:HB3 | 1:C:432:LEU:HD21 | 1.94 | 0.50 |
| 1:C:514:ASP:C | 1:C:516:ASN:N | 2.60 | 0.50 |
| 1:B:260:VAL:HG22 | 1:C:51:PRO:HB3 | 1.93 | 0.50 |
| 1:D:458:LYS:C | 1:D:460:GLN:H | 2.14 | 0.50 |
| 1:D:514:ASP:O | 1:D:515:ILE:HB | 2.12 | 0.50 |
| 1:A:316:ILE:HG23 | 1:A:317:ALA:N | 2.27 | 0.50 |
| 1:A:380:PHE:HZ | 1:A:495:LEU:HD12 | 1.76 | 0.50 |
| 1:B:380:PHE:HZ | 1:B:495:LEU:HD12 | 1.77 | 0.50 |
| 1:C:301:LEU:HG | 1:C:302:GLY:N | 2.25 | 0.50 |
| 1:C:522:LEU:HD12 | 1:C:522:LEU:H | 1.76 | 0.50 |
| 1:C:57:HIS:HE1 | 1:C:59:VAL:HG23 | 1.76 | 0.50 |
| 1:D:14:ASP:HB2 | 1:D:17:LYS:CB | 2.41 | 0.50 |
| 1:D:522:LEU:H | 1:D:522:LEU:HD12 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:ILE:HD12 | 1:A:475:THR:CG2 | 2.42 | 0.50 |
| 1:A:540:VAL:HG12 | 1:A:541:PHE:N | 2.26 | 0.50 |
| 1:B:299:PRO:O | 1:B:300:LYS:HB2 | 2.11 | 0.50 |
| 1:B:32:GLU:O | 1:B:34:ARG:N | 2.44 | 0.50 |
| 1:B:409:PHE:H | 1:B:409:PHE:HD1 | 1.54 | 0.50 |
| 1:C:198:HIS:CE1 | 1:C:329:ASN:HD21 | 2.30 | 0.50 |
| 1:C:216:LEU:HB3 | 1:C:217:PRO:HA | 1.93 | 0.50 |
| 1:C:494:ALA:HB2 | 1:C:502:PHE:CZ | 2.47 | 0.50 |
| 1:D:540:VAL:HG12 | 1:D:541:PHE:N | 2.26 | 0.50 |
| 1:A:514:ASP:C | 1:A:516:ASN:H | 2.15 | 0.50 |
| 1:B:503:LYS:CB | 1:B:543:ASN:HB3 | 2.38 | 0.50 |
| 1:A:56:PRO:HA | 1:B:77:GLU:HB3 | 1.94 | 0.50 |
| 1:D:310:PHE:HB3 | 1:D:330:LEU:HA | 1.94 | 0.50 |
| 1:A:216:LEU:HB3 | 1:A:217:PRO:HA | 1.92 | 0.50 |
| 1:A:519:ILE:HG22 | 1:A:520:ASP:O | 2.11 | 0.50 |
| 1:A:109:GLY:HA3 | 1:B:229:ARG:CZ | 2.42 | 0.50 |
| 1:C:111:PRO:CD | 1:C:188:PRO:HA | 2.39 | 0.50 |
| 1:D:216:LEU:HB3 | 1:D:217:PRO:HA | 1.94 | 0.50 |
| 1:D:486:LYS:HB2 | 1:D:516:ASN:ND2 | 2.27 | 0.50 |
| 1:A:421:GLU:O | 1:A:544:ALA:HB1 | 2.12 | 0.50 |
| 1:B:486:LYS:HB2 | 1:B:516:ASN:ND2 | 2.26 | 0.50 |
| 1:D:332:LEU:C | 1:D:332:LEU:HD23 | 2.31 | 0.50 |
| 1:A:64:GLU:HG3 | 1:B:64:GLU:CD | 2.33 | 0.49 |
| 1:C:196:ARG:NH1 | 1:C:199:MET:HE1 | 2.26 | 0.49 |
| 1:D:416:ARG:HG3 | 1:D:417:VAL:HG23 | 1.94 | 0.49 |
| 1:A:310:PHE:HB3 | 1:A:330:LEU:HA | 1.94 | 0.49 |
| 1:D:316:ILE:HG23 | 1:D:317:ALA:N | 2.27 | 0.49 |
| 1:D:391:CYS:HB3 | 1:D:432:LEU:HD21 | 1.93 | 0.49 |
| 1:A:57:HIS:HE1 | 1:A:59:VAL:HG23 | 1.77 | 0.49 |
| 1:B:47:PRO:HG2 | 1:B:474:SER:O | 2.12 | 0.49 |
| 1:D:410:ASN:HA | 1:D:415:ARG:O | 2.13 | 0.49 |
| 1:B:522:LEU:H | 1:B:522:LEU:HD12 | 1.76 | 0.49 |
| 1:C:369:ILE:HD12 | 1:C:475:THR:CG2 | 2.42 | 0.49 |
| 1:D:14:ASP:HB2 | 1:D:17:LYS:HB3 | 1.95 | 0.49 |
| 1:D:396:ASP:N | 1:D:430:LYS:HA | 2.26 | 0.49 |
| 1:B:198:HIS:CE1 | 1:B:329:ASN:HD21 | 2.31 | 0.49 |
| 1:C:224:ASP:CG | 1:C:225:ARG:H | 2.16 | 0.49 |
| 1:C:310:PHE:HB3 | 1:C:330:LEU:HA | 1.94 | 0.49 |
| 1:D:111:PRO:CD | 1:D:188:PRO:HA | 2.39 | 0.49 |
| 1:A:522:LEU:HD12 | 1:A:522:LEU:H | 1.78 | 0.49 |
| 1:C:332:LEU:C | 1:C:332:LEU:HD23 | 2.32 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:410:ASN:HA | 1:C:415:ARG:O | 2.13 | 0.49 |
| 1:C:458:LYS:C | 1:C:460:GLN:H | 2.14 | 0.49 |
| 1:D:299:PRO:O | 1:D:300:LYS:HB2 | 2.11 | 0.49 |
| 1:D:47:PRO:HG2 | 1:D:474:SER:O | 2.13 | 0.49 |
| 1:A:144:LEU:HG | 1:A:159:PHE:CE1 | 2.48 | 0.49 |
| 1:A:224:ASP:CG | 1:A:225:ARG:H | 2.15 | 0.49 |
| 1:B:14:ASP:HB2 | 1:B:17:LYS:HB3 | 1.94 | 0.49 |
| 1:C:28:THR:O | 1:C:31:ARG:HG2 | 2.12 | 0.49 |
| 1:C:83:ILE:HD13 | 1:C:107:LEU:CD2 | 2.43 | 0.49 |
| 1:D:28:THR:O | 1:D:31:ARG:HG2 | 2.13 | 0.49 |
| 1:A:276:PHE:HD2 | 1:A:294:VAL:HG22 | 1.77 | 0.49 |
| 1:A:28:THR:O | 1:A:31:ARG:HG2 | 2.13 | 0.49 |
| 1:B:216:LEU:HB3 | 1:B:217:PRO:HA | 1.93 | 0.49 |
| 1:B:238:LEU:HD22 | 1:B:238:LEU:N | 2.28 | 0.49 |
| 1:D:175:VAL:O | 1:D:176:LEU:HD23 | 2.13 | 0.49 |
| 1:B:310:PHE:HB3 | 1:B:330:LEU:HA | 1.94 | 0.49 |
| 1:C:350:MET:O | 1:C:353:PRO:HD3 | 2.13 | 0.49 |
| 1:D:198:HIS:CE1 | 1:D:329:ASN:HD21 | 2.30 | 0.49 |
| 1:A:14:ASP:HB2 | 1:A:17:LYS:HB3 | 1.94 | 0.49 |
| 1:A:387:LEU:CD1 | 1:A:484:ILE:HD12 | 2.43 | 0.49 |
| 1:A:410:ASN:HA | 1:A:415:ARG:O | 2.13 | 0.49 |
| 1:A:416:ARG:HG3 | 1:A:417:VAL:HG23 | 1.94 | 0.49 |
| 1:B:199:MET:HB2 | 1:B:245:SER:HB2 | 1.95 | 0.49 |
| 1:B:21:LEU:HD12 | 1:B:21:LEU:N | 2.28 | 0.49 |
| 1:B:416:ARG:HG3 | 1:B:417:VAL:HG23 | 1.95 | 0.49 |
| 1:B:57:HIS:HE1 | 1:B:59:VAL:HG23 | 1.78 | 0.49 |
| 1:B:83:ILE:HD13 | 1:B:107:LEU:CD2 | 2.43 | 0.49 |
| 1:C:295:TYR:HA | 1:C:306:GLU:HA | 1.95 | 0.49 |
| 1:C:486:LYS:HB2 | 1:C:516:ASN:ND2 | 2.28 | 0.49 |
| 1:D:224:ASP:CG | 1:D:225:ARG:H | 2.16 | 0.49 |
| 1:D:514:ASP:C | 1:D:516:ASN:H | 2.15 | 0.49 |
| 1:A:198:HIS:CE1 | 1:A:245:SER:HG | 2.31 | 0.48 |
| 1:A:238:LEU:N | 1:A:238:LEU:HD22 | 2.28 | 0.48 |
| 1:A:356:TYR:N | 1:B:213:LYS:HZ3 | 2.11 | 0.48 |
| 1:D:541:PHE:O | 1:D:542:LEU:C | 2.52 | 0.48 |
| 1:A:175:VAL:O | 1:A:176:LEU:HD23 | 2.13 | 0.48 |
| 1:A:364:ASP:O | 1:A:368:MET:HG3 | 2.13 | 0.48 |
| 1:B:276:PHE:HD2 | 1:B:294:VAL:HG22 | 1.78 | 0.48 |
| 1:B:364:ASP:O | 1:B:368:MET:HG3 | 2.13 | 0.48 |
| 1:B:410:ASN:HA | 1:B:415:ARG:O | 2.13 | 0.48 |
| 1:B:494:ALA:HB2 | 1:B:502:PHE:CZ | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:316:ILE:HG23 | 1:C:317:ALA:N | 2.27 | 0.48 |
| 1:C:401:CYS:SG | 1:C:403:VAL:HG23 | 2.53 | 0.48 |
| 1:C:59:VAL:O | 1:C:63:ILE:HG13 | 2.13 | 0.48 |
| 1:B:316:ILE:HG23 | 1:B:317:ALA:N | 2.27 | 0.48 |
| 1:B:31:ARG:N | 1:B:31:ARG:HD3 | 2.04 | 0.48 |
| 1:B:370:ARG:HH21 | 1:B:370:ARG:HG2 | 1.78 | 0.48 |
| 1:D:350:MET:O | 1:D:353:PRO:HD3 | 2.13 | 0.48 |
| 1:A:111:PRO:HD2 | 1:A:186:LEU:HD21 | 1.95 | 0.48 |
| 1:A:199:MET:HB2 | 1:A:245:SER:HB2 | 1.95 | 0.48 |
| 1:B:175:VAL:O | 1:B:176:LEU:HD23 | 2.14 | 0.48 |
| 1:B:350:MET:O | 1:B:353:PRO:HD3 | 2.13 | 0.48 |
| 1:B:387:LEU:CD1 | 1:B:484:ILE:HD12 | 2.43 | 0.48 |
| 1:C:238:LEU:N | 1:C:238:LEU:HD22 | 2.28 | 0.48 |
| 1:A:68:GLN:NE2 | 1:C:72:ARG:HH11 | 2.06 | 0.48 |
| 1:D:238:LEU:HD22 | 1:D:238:LEU:N | 2.28 | 0.48 |
| 1:D:295:TYR:HA | 1:D:306:GLU:HA | 1.95 | 0.48 |
| 1:D:369:ILE:HD12 | 1:D:475:THR:CG2 | 2.42 | 0.48 |
| 1:D:431:LEU:O | 1:D:431:LEU:HD13 | 2.14 | 0.48 |
| 1:A:431:LEU:HB3 | 1:A:432:LEU:HD12 | 1.95 | 0.48 |
| 1:D:21:LEU:HD12 | 1:D:21:LEU:N | 2.29 | 0.48 |
| 1:D:482:GLY:O | 1:D:516:ASN:ND2 | 2.44 | 0.48 |
| 1:C:541:PHE:O | 1:C:542:LEU:C | 2.52 | 0.48 |
| 1:D:387:LEU:CD1 | 1:D:484:ILE:HD12 | 2.43 | 0.48 |
| 1:A:295:TYR:HA | 1:A:306:GLU:HA | 1.95 | 0.48 |
| 1:B:111:PRO:HD2 | 1:B:186:LEU:HD21 | 1.95 | 0.48 |
| 1:B:195:LEU:HD13 | 1:B:227:PHE:CD1 | 2.49 | 0.48 |
| 1:C:14:ASP:HB2 | 1:C:17:LYS:HB3 | 1.95 | 0.48 |
| 1:C:175:VAL:O | 1:C:176:LEU:HD23 | 2.13 | 0.48 |
| 1:C:47:PRO:HG2 | 1:C:474:SER:O | 2.13 | 0.48 |
| 1:D:508:ILE:O | 1:D:509:VAL:C | 2.52 | 0.48 |
| 1:D:59:VAL:O | 1:D:63:ILE:HG13 | 2.13 | 0.48 |
| 1:A:176:LEU:HD12 | 1:B:98:MET:SD | 2.53 | 0.48 |
| 1:A:431:LEU:HD13 | 1:A:431:LEU:O | 2.14 | 0.48 |
| 1:B:28:THR:O | 1:B:31:ARG:HG2 | 2.13 | 0.48 |
| 1:C:48:ARG:HG3 | 1:C:48:ARG:NH2 | 2.29 | 0.48 |
| 1:D:195:LEU:HD13 | 1:D:227:PHE:CD1 | 2.49 | 0.48 |
| 1:D:380:PHE:CZ | 1:D:495:LEU:HD12 | 2.49 | 0.48 |
| 1:B:431:LEU:HB3 | 1:B:432:LEU:HD12 | 1.96 | 0.48 |
| 1:C:144:LEU:HG | 1:C:159:PHE:CE1 | 2.49 | 0.48 |
| 1:D:364:ASP:O | 1:D:368:MET:HG3 | 2.13 | 0.48 |
| 1:D:507:PRO:CG | 1:D:514:ASP:HB2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:MET:O | 1:A:353:PRO:HD3 | 2.13 | 0.47 |
| 1:B:216:LEU:HD12 | 1:B:216:LEU:N | 2.29 | 0.47 |
| 1:C:199:MET:HB2 | 1:C:245:SER:HB2 | 1.96 | 0.47 |
| 1:C:21:LEU:N | 1:C:21:LEU:HD12 | 2.29 | 0.47 |
| 1:B:30:TRP:CZ2 | 1:C:288:PRO:HG3 | 2.49 | 0.47 |
| 1:C:364:ASP:O | 1:C:368:MET:HG3 | 2.13 | 0.47 |
| 1:C:416:ARG:HG3 | 1:C:417:VAL:HG23 | 1.95 | 0.47 |
| 1:C:508:ILE:O | 1:C:509:VAL:C | 2.52 | 0.47 |
| 1:C:516:ASN:O | 1:C:517:LEU:HB2 | 2.14 | 0.47 |
| 1:B:260:VAL:CG2 | 1:C:51:PRO:HB3 | 2.43 | 0.47 |
| 1:D:136:LYS:HE3 | 1:D:167:VAL:HG23 | 1.96 | 0.47 |
| 1:D:20:GLU:C | 1:D:22:ALA:H | 2.17 | 0.47 |
| 1:A:479:TYR:O | 1:A:483:ILE:HG13 | 2.14 | 0.47 |
| 1:B:59:VAL:O | 1:B:63:ILE:HG13 | 2.14 | 0.47 |
| 1:A:352:TYR:HE2 | 1:B:81:PRO:CA | 2.27 | 0.47 |
| 1:B:144:LEU:HG | 1:B:159:PHE:CE1 | 2.49 | 0.47 |
| 1:D:508:ILE:C | 1:D:508:ILE:HD12 | 2.34 | 0.47 |
| 1:A:21:LEU:N | 1:A:21:LEU:HD12 | 2.29 | 0.47 |
| 1:A:380:PHE:CZ | 1:A:495:LEU:HD12 | 2.48 | 0.47 |
| 1:A:512:LEU:CA | 1:A:536:VAL:HG21 | 2.44 | 0.47 |
| 1:C:352:TYR:HB3 | 1:C:355:PHE:HD2 | 1.79 | 0.47 |
| 1:D:199:MET:HE1 | 1:D:224:ASP:HB3 | 1.95 | 0.47 |
| 1:A:541:PHE:O | 1:A:542:LEU:C | 2.52 | 0.47 |
| 1:A:548:ILE:HG22 | 1:A:548:ILE:O | 2.15 | 0.47 |
| 1:A:83:ILE:HD13 | 1:A:107:LEU:CD2 | 2.43 | 0.47 |
| 1:B:136:LYS:HE3 | 1:B:167:VAL:HG23 | 1.97 | 0.47 |
| 1:C:380:PHE:CZ | 1:C:495:LEU:HD12 | 2.49 | 0.47 |
| 1:A:195:LEU:HD13 | 1:A:227:PHE:CD1 | 2.49 | 0.47 |
| 1:A:436:VAL:HA | 1:A:479:TYR:HB2 | 1.97 | 0.47 |
| 1:A:47:PRO:HG2 | 1:A:474:SER:O | 2.13 | 0.47 |
| 1:A:508:ILE:O | 1:A:509:VAL:C | 2.53 | 0.47 |
| 1:C:136:LYS:HE3 | 1:C:167:VAL:HG23 | 1.97 | 0.47 |
| 1:D:216:LEU:HD12 | 1:D:216:LEU:N | 2.30 | 0.47 |
| 1:B:508:ILE:C | 1:B:508:ILE:HD12 | 2.35 | 0.47 |
| 1:C:548:ILE:HG22 | 1:C:548:ILE:O | 2.15 | 0.47 |
| 1:D:111:PRO:HD2 | 1:D:186:LEU:HD21 | 1.95 | 0.47 |
| 1:D:548:ILE:HG22 | 1:D:548:ILE:O | 2.15 | 0.47 |
| 1:A:260:VAL:HG23 | 1:D:51:PRO:HD3 | 1.95 | 0.47 |
| 1:C:514:ASP:C | 1:C:516:ASN:H | 2.17 | 0.47 |
| 1:D:144:LEU:HG | 1:D:159:PHE:CE1 | 2.50 | 0.47 |
| 1:A:161:ILE:HG13 | 1:A:162:ALA:N | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:171:MET:H | 1:B:173:LEU:CD1 | 2.28 | 0.47 |
| 1:C:176:LEU:HD12 | 1:D:98:MET:HE1 | 1.97 | 0.47 |
| 1:C:195:LEU:HD13 | 1:C:227:PHE:CD1 | 2.50 | 0.47 |
| 1:C:436:VAL:HA | 1:C:479:TYR:HB2 | 1.97 | 0.47 |
| 1:D:199:MET:HB2 | 1:D:245:SER:HB2 | 1.95 | 0.47 |
| 1:A:352:TYR:HB3 | 1:A:355:PHE:HD2 | 1.80 | 0.47 |
| 1:A:508:ILE:HD12 | 1:A:508:ILE:C | 2.36 | 0.47 |
| 1:C:161:ILE:HG13 | 1:C:162:ALA:N | 2.30 | 0.47 |
| 1:C:387:LEU:CD1 | 1:C:484:ILE:HD12 | 2.44 | 0.47 |
| 1:A:216:LEU:HD12 | 1:A:216:LEU:N | 2.30 | 0.46 |
| 1:A:20:GLU:C | 1:A:22:ALA:H | 2.18 | 0.46 |
| 1:A:229:ARG:CZ | 1:B:109:GLY:HA3 | 2.45 | 0.46 |
| 1:C:301:LEU:HG | 1:C:302:GLY:H | 1.80 | 0.46 |
| 1:C:508:ILE:HD12 | 1:C:508:ILE:C | 2.36 | 0.46 |
| 1:D:352:TYR:HB3 | 1:D:355:PHE:HD2 | 1.80 | 0.46 |
| 1:B:431:LEU:HD13 | 1:B:431:LEU:O | 2.15 | 0.46 |
| 1:B:436:VAL:HA | 1:B:479:TYR:HB2 | 1.97 | 0.46 |
| 1:B:508:ILE:O | 1:B:509:VAL:C | 2.53 | 0.46 |
| 1:C:370:ARG:HH21 | 1:C:370:ARG:HG2 | 1.80 | 0.46 |
| 1:D:455:GLU:H | 1:D:459:GLU:HG3 | 1.81 | 0.46 |
| 1:D:436:VAL:HA | 1:D:479:TYR:HB2 | 1.97 | 0.46 |
| 1:B:301:LEU:HG | 1:B:302:GLY:H | 1.80 | 0.46 |
| 1:B:502:PHE:HB2 | 1:B:546:VAL:CG1 | 2.45 | 0.46 |
| 1:B:541:PHE:O | 1:B:542:LEU:C | 2.53 | 0.46 |
| 1:B:548:ILE:O | 1:B:548:ILE:HG22 | 2.15 | 0.46 |
| 1:B:72:ARG:HH11 | 1:D:68:GLN:NE2 | 2.04 | 0.46 |
| 1:C:216:LEU:N | 1:C:216:LEU:HD12 | 2.31 | 0.46 |
| 1:C:438:ASN:O | 1:C:478:ARG:HA | 2.15 | 0.46 |
| 1:D:48:ARG:HG3 | 1:D:48:ARG:NH2 | 2.30 | 0.46 |
| 1:A:443:TYR:CG | 1:A:464:ILE:HG23 | 2.50 | 0.46 |
| 1:B:300:LYS:CG | 1:B:301:LEU:H | 2.20 | 0.46 |
| 1:B:295:TYR:HA | 1:B:306:GLU:HA | 1.95 | 0.46 |
| 1:C:171:MET:H | 1:C:173:LEU:CD1 | 2.28 | 0.46 |
| 1:D:502:PHE:HB2 | 1:D:546:VAL:CG1 | 2.45 | 0.46 |
| 1:A:370:ARG:HH21 | 1:A:370:ARG:HG2 | 1.80 | 0.46 |
| 1:A:516:ASN:O | 1:A:517:LEU:HB2 | 2.16 | 0.46 |
| 1:A:59:VAL:O | 1:A:63:ILE:HG13 | 2.14 | 0.46 |
| 1:A:358:TYR:HD2 | 1:B:213:LYS:HD3 | 1.80 | 0.46 |
| 1:C:455:GLU:H | 1:C:459:GLU:HG3 | 1.80 | 0.46 |
| 1:D:370:ARG:HH21 | 1:D:370:ARG:HG2 | 1.79 | 0.46 |
| 1:D:431:LEU:HB3 | 1:D:432:LEU:HD12 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:411:PHE:HB3 | 1:A:415:ARG:HB2 | 1.98 | 0.46 |
| 1:B:443:TYR:CG | 1:B:464:ILE:HG23 | 2.51 | 0.46 |
| 1:A:57:HIS:H | 1:B:77:GLU:HB3 | 1.80 | 0.46 |
| 1:D:301:LEU:HG | 1:D:302:GLY:H | 1.79 | 0.46 |
| 1:A:455:GLU:H | 1:A:459:GLU:HG3 | 1.80 | 0.46 |
| 1:A:387:LEU:HD12 | 1:A:484:ILE:HD12 | 1.98 | 0.46 |
| 1:B:161:ILE:HG13 | 1:B:162:ALA:N | 2.30 | 0.46 |
| 1:B:111:PRO:CD | 1:B:188:PRO:HA | 2.39 | 0.46 |
| 1:B:20:GLU:C | 1:B:22:ALA:H | 2.18 | 0.46 |
| 1:B:283:SER:N | 1:B:291:GLN:NE2 | 2.59 | 0.46 |
| 1:B:380:PHE:CZ | 1:B:495:LEU:HD12 | 2.50 | 0.46 |
| 1:B:514:ASP:C | 1:B:516:ASN:H | 2.16 | 0.46 |
| 1:C:111:PRO:HD2 | 1:C:186:LEU:HD21 | 1.96 | 0.46 |
| 1:C:431:LEU:HB3 | 1:C:432:LEU:HD12 | 1.98 | 0.46 |
| 1:D:161:ILE:HG13 | 1:D:162:ALA:N | 2.30 | 0.46 |
| 1:A:171:MET:H | 1:A:173:LEU:CD1 | 2.28 | 0.46 |
| 1:B:167:VAL:HG13 | 1:B:168:SER:N | 2.31 | 0.46 |
| 1:C:213:LYS:NZ | 1:D:355:PHE:C | 2.69 | 0.46 |
| 1:C:502:PHE:HB2 | 1:C:546:VAL:CG1 | 2.45 | 0.46 |
| 1:A:136:LYS:HE3 | 1:A:167:VAL:HG23 | 1.97 | 0.46 |
| 1:B:411:PHE:HB3 | 1:B:415:ARG:HB2 | 1.98 | 0.46 |
| 1:B:48:ARG:HG3 | 1:B:48:ARG:NH2 | 2.30 | 0.46 |
| 1:A:18:VAL:HA | 1:A:21:LEU:HD13 | 1.98 | 0.46 |
| 1:B:352:TYR:HB3 | 1:B:355:PHE:HD2 | 1.80 | 0.46 |
| 1:A:13:PHE:CE1 | 1:D:324:ASP:HA | 2.51 | 0.45 |
| 1:A:167:VAL:HG13 | 1:A:168:SER:N | 2.31 | 0.45 |
| 1:A:301:LEU:CG | 1:A:302:GLY:H | 2.30 | 0.45 |
| 1:B:401:CYS:SG | 1:B:403:VAL:HG23 | 2.56 | 0.45 |
| 1:D:103:ARG:CA | 1:D:229:ARG:HB3 | 2.46 | 0.45 |
| 1:D:438:ASN:O | 1:D:478:ARG:HA | 2.16 | 0.45 |
| 1:A:348:ARG:HH12 | 1:A:356:TYR:HB3 | 1.81 | 0.45 |
| 1:A:368:MET:CE | 1:B:215:LYS:HD2 | 2.46 | 0.45 |
| 1:B:167:VAL:HG13 | 1:B:168:SER:H | 1.81 | 0.45 |
| 1:A:351:VAL:O | 1:B:79:ILE:HB | 2.16 | 0.45 |
| 1:C:479:TYR:O | 1:C:483:ILE:HG13 | 2.16 | 0.45 |
| 1:D:171:MET:H | 1:D:173:LEU:CD1 | 2.29 | 0.45 |
| 1:D:301:LEU:CG | 1:D:302:GLY:H | 2.29 | 0.45 |
| 1:C:20:GLU:C | 1:C:22:ALA:H | 2.17 | 0.45 |
| 1:C:443:TYR:CG | 1:C:464:ILE:HG23 | 2.52 | 0.45 |
| 1:D:147:TYR:O | 1:D:151:ALA:HB2 | 2.17 | 0.45 |
| 1:D:411:PHE:HB3 | 1:D:415:ARG:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:443:TYR:CG | 1:D:464:ILE:HG23 | 2.51 | 0.45 |
| 1:A:103:ARG:CA | 1:A:229:ARG:HB3 | 2.46 | 0.45 |
| 1:A:167:VAL:HG13 | 1:A:168:SER:H | 1.81 | 0.45 |
| 1:A:424:GLU:OE1 | 1:A:542:LEU:HD23 | 2.17 | 0.45 |
| 1:A:502:PHE:HB2 | 1:A:546:VAL:CG1 | 2.46 | 0.45 |
| 1:A:90:TYR:O | 1:A:94:GLY:HA2 | 2.17 | 0.45 |
| 1:B:103:ARG:CA | 1:B:229:ARG:HB3 | 2.46 | 0.45 |
| 1:D:300:LYS:CG | 1:D:301:LEU:H | 2.20 | 0.45 |
| 1:B:274:PHE:HD1 | 1:B:275:LYS:N | 2.03 | 0.45 |
| 1:B:387:LEU:HD12 | 1:B:484:ILE:HD12 | 1.97 | 0.45 |
| 1:C:167:VAL:HG13 | 1:C:168:SER:N | 2.32 | 0.45 |
| 1:C:431:LEU:O | 1:C:431:LEU:HD13 | 2.16 | 0.45 |
| 1:C:64:GLU:HG3 | 1:D:64:GLU:CD | 2.35 | 0.45 |
| 1:B:348:ARG:HH12 | 1:B:356:TYR:HB3 | 1.82 | 0.45 |
| 1:B:507:PRO:CG | 1:B:514:ASP:HB2 | 2.44 | 0.45 |
| 1:C:301:LEU:CG | 1:C:302:GLY:H | 2.29 | 0.45 |
| 1:C:411:PHE:HB3 | 1:C:415:ARG:HB2 | 1.98 | 0.45 |
| 1:A:90:TYR:HD2 | 1:A:97:ALA:HB3 | 1.82 | 0.45 |
| 1:B:424:GLU:OE1 | 1:B:542:LEU:HD23 | 2.17 | 0.45 |
| 1:C:167:VAL:HG13 | 1:C:168:SER:H | 1.82 | 0.45 |
| 1:C:18:VAL:HA | 1:C:21:LEU:HD13 | 1.99 | 0.45 |
| 1:C:103:ARG:CA | 1:C:229:ARG:HB3 | 2.47 | 0.45 |
| 1:C:325:VAL:CG2 | 1:C:326:PRO:HD2 | 2.47 | 0.45 |
| 1:C:41:HIS:ND1 | 1:C:42:ILE:N | 2.52 | 0.45 |
| 1:D:18:VAL:HA | 1:D:21:LEU:HD13 | 1.98 | 0.45 |
| 1:B:512:LEU:CA | 1:B:536:VAL:HG21 | 2.46 | 0.45 |
| 1:C:424:GLU:OE1 | 1:C:542:LEU:HD23 | 2.16 | 0.45 |
| 1:D:387:LEU:HD12 | 1:D:484:ILE:HD12 | 1.98 | 0.45 |
| 1:A:31:ARG:N | 1:A:31:ARG:HD3 | 2.03 | 0.45 |
| 1:A:48:ARG:HG3 | 1:A:48:ARG:NH2 | 2.31 | 0.45 |
| 1:D:110:LEU:HD13 | 1:D:110:LEU:C | 2.37 | 0.45 |
| 1:D:167:VAL:HG13 | 1:D:168:SER:H | 1.82 | 0.45 |
| 1:D:424:GLU:OE1 | 1:D:542:LEU:HD23 | 2.17 | 0.45 |
| 1:D:516:ASN:O | 1:D:517:LEU:HB2 | 2.16 | 0.45 |
| 1:A:300:LYS:CG | 1:A:301:LEU:H | 2.20 | 0.45 |
| 1:B:455:GLU:H | 1:B:459:GLU:HG3 | 1.81 | 0.45 |
| 1:B:90:TYR:O | 1:B:94:GLY:HA2 | 2.17 | 0.45 |
| 1:B:90:TYR:HD2 | 1:B:97:ALA:HB3 | 1.82 | 0.45 |
| 1:D:167:VAL:HG13 | 1:D:168:SER:N | 2.31 | 0.45 |
| 1:D:401:CYS:SG | 1:D:403:VAL:HG23 | 2.57 | 0.45 |
| 1:A:301:LEU:HG | 1:A:302:GLY:H | 1.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:516:ASN:O | 1:B:517:LEU:HB2 | 2.16 | 0.44 |
| 1:C:387:LEU:HD12 | 1:C:484:ILE:HD12 | 1.99 | 0.44 |
| 1:C:90:TYR:HD2 | 1:C:97:ALA:HB3 | 1.81 | 0.44 |
| 1:D:395:LYS:CG | 1:D:430:LYS:HG2 | 2.47 | 0.44 |
| 1:D:479:TYR:O | 1:D:483:ILE:HG13 | 2.17 | 0.44 |
| 1:A:57:HIS:N | 1:B:77:GLU:HB3 | 2.31 | 0.44 |
| 1:C:512:LEU:CA | 1:C:536:VAL:HG21 | 2.45 | 0.44 |
| 1:C:90:TYR:O | 1:C:94:GLY:HA2 | 2.17 | 0.44 |
| 1:D:512:LEU:CA | 1:D:536:VAL:HG21 | 2.45 | 0.44 |
| 1:A:199:MET:HE1 | 1:A:224:ASP:HB3 | 1.99 | 0.44 |
| 1:A:97:ALA:HA | 1:A:100:VAL:CG1 | 2.41 | 0.44 |
| 1:C:435:SER:O | 1:C:437:LEU:N | 2.51 | 0.44 |
| 1:D:263:GLU:HG3 | 1:D:274:PHE:HZ | 1.83 | 0.44 |
| 1:D:348:ARG:HH12 | 1:D:356:TYR:HB3 | 1.81 | 0.44 |
| 1:D:395:LYS:CG | 1:D:396:ASP:H | 2.14 | 0.44 |
| 1:A:502:PHE:HB3 | 1:A:503:LYS:H | 1.48 | 0.44 |
| 1:B:301:LEU:CG | 1:B:302:GLY:H | 2.30 | 0.44 |
| 1:B:97:ALA:HA | 1:B:100:VAL:CG1 | 2.41 | 0.44 |
| 1:C:348:ARG:HH12 | 1:C:356:TYR:HB3 | 1.82 | 0.44 |
| 1:C:36:LEU:N | 1:C:36:LEU:HD22 | 2.33 | 0.44 |
| 1:A:110:LEU:C | 1:A:110:LEU:HD13 | 2.38 | 0.44 |
| 1:A:158:VAL:HG22 | 1:A:159:PHE:CD2 | 2.52 | 0.44 |
| 1:A:395:LYS:CG | 1:A:430:LYS:HG2 | 2.47 | 0.44 |
| 1:A:507:PRO:CG | 1:A:514:ASP:HB2 | 2.43 | 0.44 |
| 1:B:260:VAL:HG13 | 1:B:261:VAL:N | 2.32 | 0.44 |
| 1:B:438:ASN:O | 1:B:478:ARG:HA | 2.17 | 0.44 |
| 1:C:301:LEU:CG | 1:C:302:GLY:N | 2.81 | 0.44 |
| 1:A:227:PHE:HZ | 1:B:227:PHE:CZ | 2.34 | 0.44 |
| 1:A:438:ASN:O | 1:A:478:ARG:HA | 2.18 | 0.44 |
| 1:B:479:TYR:O | 1:B:483:ILE:HG13 | 2.18 | 0.44 |
| 1:C:110:LEU:HD13 | 1:C:110:LEU:C | 2.38 | 0.44 |
| 1:C:147:TYR:O | 1:C:151:ALA:HB2 | 2.18 | 0.44 |
| 1:C:31:ARG:N | 1:C:31:ARG:CD | 2.74 | 0.44 |
| 1:C:396:ASP:CA | 1:C:430:LYS:HA | 2.48 | 0.44 |
| 1:C:63:ILE:HG12 | 1:C:334:VAL:HG11 | 1.99 | 0.44 |
| 1:D:90:TYR:O | 1:D:94:GLY:HA2 | 2.17 | 0.44 |
| 1:A:401:CYS:SG | 1:A:403:VAL:HG23 | 2.58 | 0.44 |
| 1:B:147:TYR:O | 1:B:151:ALA:HB2 | 2.18 | 0.44 |
| 1:B:482:GLY:HA3 | 1:B:515:ILE:O | 2.18 | 0.44 |
| 1:C:522:LEU:HD12 | 1:C:522:LEU:N | 2.33 | 0.44 |
| 1:D:130:ILE:CD1 | 1:D:179:ALA:HB1 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:63:ILE:HG12 | 1:D:334:VAL:HG11 | 2.00 | 0.44 |
| 1:B:263:GLU:HG3 | 1:B:274:PHE:HZ | 1.83 | 0.44 |
| 1:C:227:PHE:N | 1:C:227:PHE:CD1 | 2.86 | 0.44 |
| 1:C:230:GLU:HB3 | 1:C:233:GLU:CG | 2.48 | 0.44 |
| 1:C:490:LYS:O | 1:C:491:ILE:C | 2.57 | 0.44 |
| 1:D:230:GLU:HB3 | 1:D:233:GLU:CG | 2.48 | 0.44 |
| 1:D:35:ALA:O | 1:D:36:LEU:HB2 | 2.18 | 0.44 |
| 1:A:147:TYR:O | 1:A:151:ALA:HB2 | 2.17 | 0.44 |
| 1:B:199:MET:HE1 | 1:B:224:ASP:HB3 | 1.99 | 0.44 |
| 1:B:230:GLU:HB3 | 1:B:233:GLU:CG | 2.48 | 0.44 |
| 1:B:522:LEU:N | 1:B:522:LEU:HD12 | 2.33 | 0.44 |
| 1:C:507:PRO:CG | 1:C:514:ASP:HB2 | 2.44 | 0.44 |
| 1:D:301:LEU:CG | 1:D:302:GLY:N | 2.81 | 0.44 |
| 1:D:36:LEU:N | 1:D:36:LEU:HD22 | 2.33 | 0.44 |
| 1:D:483:ILE:O | 1:D:486:LYS:HB3 | 2.18 | 0.44 |
| 1:D:90:TYR:HD2 | 1:D:97:ALA:HB3 | 1.82 | 0.44 |
| 1:A:301:LEU:CG | 1:A:302:GLY:N | 2.81 | 0.43 |
| 1:B:325:VAL:CG2 | 1:B:326:PRO:HD2 | 2.48 | 0.43 |
| 1:B:36:LEU:N | 1:B:36:LEU:HD22 | 2.32 | 0.43 |
| 1:B:435:SER:O | 1:B:437:LEU:N | 2.51 | 0.43 |
| 1:B:72:ARG:HE | 1:D:68:GLN:NE2 | 2.15 | 0.43 |
| 1:C:130:ILE:CD1 | 1:C:179:ALA:HB1 | 2.48 | 0.43 |
| 1:C:200:THR:C | 1:C:202:GLY:N | 2.72 | 0.43 |
| 1:C:469:LYS:HG2 | 1:C:469:LYS:O | 2.18 | 0.43 |
| 1:B:388:ILE:HG12 | 1:B:484:ILE:HG13 | 2.00 | 0.43 |
| 1:C:158:VAL:HG22 | 1:C:159:PHE:CD2 | 2.53 | 0.43 |
| 1:C:107:LEU:HD23 | 1:D:105:PHE:CD1 | 2.53 | 0.43 |
| 1:A:130:ILE:CD1 | 1:A:179:ALA:HB1 | 2.49 | 0.43 |
| 1:A:395:LYS:CG | 1:A:396:ASP:N | 2.80 | 0.43 |
| 1:A:41:HIS:ND1 | 1:A:42:ILE:N | 2.53 | 0.43 |
| 1:A:541:PHE:O | 1:A:543:ASN:N | 2.52 | 0.43 |
| 1:B:110:LEU:HD13 | 1:B:110:LEU:C | 2.38 | 0.43 |
| 1:B:18:VAL:HA | 1:B:21:LEU:HD13 | 1.99 | 0.43 |
| 1:B:301:LEU:CG | 1:B:302:GLY:N | 2.81 | 0.43 |
| 1:C:287:THR:HG22 | 1:C:315:PRO:HD3 | 2.01 | 0.43 |
| 1:C:35:ALA:O | 1:C:36:LEU:HB2 | 2.18 | 0.43 |
| 1:C:365:ILE:O | 1:C:369:ILE:HG13 | 2.18 | 0.43 |
| 1:C:380:PHE:O | 1:C:383:PHE:HB3 | 2.18 | 0.43 |
| 1:D:158:VAL:HG22 | 1:D:159:PHE:CD2 | 2.53 | 0.43 |
| 1:D:469:LYS:O | 1:D:469:LYS:HG2 | 2.18 | 0.43 |
| 1:A:35:ALA:O | 1:A:36:LEU:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:158:VAL:HG22 | 1:B:159:PHE:CD2 | 2.54 | 0.43 |
| 1:A:109:GLY:HA3 | 1:B:229:ARG:HH11 | 1.83 | 0.43 |
| 1:B:396:ASP:OD2 | 1:B:397:LYS:N | 2.51 | 0.43 |
| 1:A:54:GLY:N | 1:B:74:GLY:HA2 | 2.33 | 0.43 |
| 1:D:159:PHE:HB3 | 1:D:171:MET:SD | 2.59 | 0.43 |
| 1:D:203:TRP:HA | 1:D:203:TRP:CE3 | 2.54 | 0.43 |
| 1:D:396:ASP:CA | 1:D:430:LYS:HA | 2.49 | 0.43 |
| 1:A:230:GLU:HB3 | 1:A:233:GLU:CG | 2.48 | 0.43 |
| 1:A:335:GLU:O | 1:A:338:ALA:HB3 | 2.19 | 0.43 |
| 1:A:380:PHE:O | 1:A:383:PHE:HB3 | 2.18 | 0.43 |
| 1:A:435:SER:O | 1:A:437:LEU:N | 2.51 | 0.43 |
| 1:A:441:TYR:CG | 1:A:465:LEU:HB2 | 2.54 | 0.43 |
| 1:D:35:ALA:C | 1:D:37:ILE:N | 2.72 | 0.43 |
| 1:D:387:LEU:HD12 | 1:D:484:ILE:CG2 | 2.49 | 0.43 |
| 1:D:83:ILE:HD13 | 1:D:107:LEU:CD2 | 2.43 | 0.43 |
| 1:A:36:LEU:N | 1:A:36:LEU:HD22 | 2.33 | 0.43 |
| 1:A:483:ILE:O | 1:A:486:LYS:HB3 | 2.18 | 0.43 |
| 1:B:130:ILE:CD1 | 1:B:179:ALA:HB1 | 2.48 | 0.43 |
| 1:B:224:ASP:CG | 1:B:225:ARG:N | 2.72 | 0.43 |
| 1:B:35:ALA:O | 1:B:36:LEU:HB2 | 2.18 | 0.43 |
| 1:C:441:TYR:CG | 1:C:465:LEU:HB2 | 2.54 | 0.43 |
| 1:C:541:PHE:O | 1:C:543:ASN:N | 2.51 | 0.43 |
| 1:D:89:ILE:HD13 | 1:D:101:LEU:CD2 | 2.49 | 0.43 |
| 1:A:203:TRP:O | 1:A:207:LEU:N | 2.51 | 0.43 |
| 1:A:287:THR:HG22 | 1:A:315:PRO:HD3 | 2.00 | 0.43 |
| 1:A:325:VAL:CG2 | 1:A:326:PRO:HD2 | 2.48 | 0.43 |
| 1:A:396:ASP:OD2 | 1:A:397:LYS:N | 2.50 | 0.43 |
| 1:B:158:VAL:CG1 | 1:B:159:PHE:H | 2.16 | 0.43 |
| 1:B:35:ALA:C | 1:B:37:ILE:N | 2.72 | 0.43 |
| 1:B:72:ARG:HE | 1:D:68:GLN:HE22 | 1.67 | 0.43 |
| 1:A:205:ILE:HD13 | 1:A:321:TYR:CE2 | 2.46 | 0.43 |
| 1:A:365:ILE:HB | 1:A:442:VAL:HG11 | 2.01 | 0.43 |
| 1:B:380:PHE:O | 1:B:383:PHE:HB3 | 2.18 | 0.43 |
| 1:B:396:ASP:CA | 1:B:430:LYS:HA | 2.49 | 0.43 |
| 1:D:274:PHE:HD1 | 1:D:275:LYS:N | 2.04 | 0.43 |
| 1:D:328:MET:SD | 1:D:328:MET:C | 2.97 | 0.43 |
| 1:D:365:ILE:O | 1:D:369:ILE:HG13 | 2.19 | 0.43 |
| 1:D:435:SER:O | 1:D:437:LEU:N | 2.52 | 0.43 |
| 1:A:396:ASP:CA | 1:A:430:LYS:HA | 2.49 | 0.43 |
| 1:A:88:GLU:OE1 | 1:A:88:GLU:HA | 2.19 | 0.43 |
| 1:B:441:TYR:CG | 1:B:465:LEU:HB2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:513:SER:C | 1:B:514:ASP:O | 2.57 | 0.43 |
| 1:B:543:ASN:O | 1:B:544:ALA:O | 2.37 | 0.43 |
| 1:A:79:ILE:HD12 | 1:B:57:HIS:CE1 | 2.54 | 0.43 |
| 1:C:203:TRP:HA | 1:C:203:TRP:CE3 | 2.54 | 0.43 |
| 1:C:203:TRP:O | 1:C:207:LEU:N | 2.52 | 0.43 |
| 1:C:260:VAL:HG13 | 1:C:261:VAL:N | 2.34 | 0.43 |
| 1:C:516:ASN:HB3 | 1:C:517:LEU:H | 1.68 | 0.43 |
| 1:D:173:LEU:HD12 | 1:D:173:LEU:N | 2.34 | 0.43 |
| 1:D:260:VAL:HG13 | 1:D:261:VAL:N | 2.33 | 0.43 |
| 1:D:325:VAL:CG2 | 1:D:326:PRO:HD2 | 2.47 | 0.43 |
| 1:D:522:LEU:N | 1:D:522:LEU:HD12 | 2.33 | 0.43 |
| 1:D:502:PHE:HB2 | 1:D:546:VAL:HG13 | 2.01 | 0.43 |
| 1:A:260:VAL:HG13 | 1:A:261:VAL:N | 2.34 | 0.43 |
| 1:B:205:ILE:HD13 | 1:B:321:TYR:CE2 | 2.46 | 0.43 |
| 1:B:380:PHE:CE1 | 1:B:409:PHE:HE2 | 2.37 | 0.43 |
| 1:C:213:LYS:HZ2 | 1:D:355:PHE:C | 2.23 | 0.43 |
| 1:D:380:PHE:O | 1:D:383:PHE:HB3 | 2.19 | 0.43 |
| 1:D:97:ALA:HA | 1:D:100:VAL:CG1 | 2.40 | 0.43 |
| 1:A:203:TRP:CE3 | 1:A:203:TRP:HA | 2.54 | 0.42 |
| 1:A:224:ASP:CG | 1:A:225:ARG:N | 2.73 | 0.42 |
| 1:A:469:LYS:HG2 | 1:A:469:LYS:O | 2.18 | 0.42 |
| 1:B:365:ILE:HB | 1:B:442:VAL:HG11 | 2.01 | 0.42 |
| 1:B:63:ILE:HG12 | 1:B:334:VAL:HG11 | 2.00 | 0.42 |
| 1:A:105:PHE:CD1 | 1:B:107:LEU:HB3 | 2.54 | 0.42 |
| 1:A:435:SER:OG | 1:A:436:VAL:N | 2.52 | 0.42 |
| 1:B:203:TRP:HA | 1:B:203:TRP:CE3 | 2.54 | 0.42 |
| 1:B:203:TRP:O | 1:B:207:LEU:N | 2.51 | 0.42 |
| 1:B:387:LEU:HD12 | 1:B:484:ILE:CG2 | 2.49 | 0.42 |
| 1:B:483:ILE:O | 1:B:486:LYS:HB3 | 2.19 | 0.42 |
| 1:B:490:LYS:O | 1:B:491:ILE:C | 2.57 | 0.42 |
| 1:B:541:PHE:O | 1:B:543:ASN:N | 2.52 | 0.42 |
| 1:D:287:THR:HG22 | 1:D:315:PRO:HD3 | 2.01 | 0.42 |
| 1:D:365:ILE:HB | 1:D:442:VAL:HG11 | 2.01 | 0.42 |
| 1:D:482:GLY:HA3 | 1:D:515:ILE:O | 2.19 | 0.42 |
| 1:D:541:PHE:O | 1:D:543:ASN:N | 2.52 | 0.42 |
| 1:A:26:PHE:CE1 | 1:A:29:ALA:HB3 | 2.55 | 0.42 |
| 1:A:35:ALA:C | 1:A:37:ILE:N | 2.71 | 0.42 |
| 1:A:388:ILE:HG12 | 1:A:484:ILE:HG13 | 2.02 | 0.42 |
| 1:A:387:LEU:HD12 | 1:A:484:ILE:CG2 | 2.49 | 0.42 |
| 1:B:365:ILE:O | 1:B:369:ILE:HG13 | 2.19 | 0.42 |
| 1:B:469:LYS:HG2 | 1:B:469:LYS:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:ALA:H | 1:D:106:TYR:H | 1.66 | 0.42 |
| 1:C:205:ILE:HD13 | 1:C:321:TYR:CE2 | 2.45 | 0.42 |
| 1:C:224:ASP:CG | 1:C:225:ARG:N | 2.73 | 0.42 |
| 1:C:482:GLY:O | 1:C:516:ASN:ND2 | 2.46 | 0.42 |
| 1:C:482:GLY:HA3 | 1:C:515:ILE:O | 2.18 | 0.42 |
| 1:D:203:TRP:O | 1:D:207:LEU:N | 2.51 | 0.42 |
| 1:D:388:ILE:HG12 | 1:D:484:ILE:HG13 | 2.01 | 0.42 |
| 1:A:279:ASP:HB3 | 1:A:291:GLN:HG2 | 2.01 | 0.42 |
| 1:B:173:LEU:HD12 | 1:B:173:LEU:N | 2.34 | 0.42 |
| 1:D:490:LYS:O | 1:D:491:ILE:C | 2.58 | 0.42 |
| 1:A:200:THR:C | 1:A:202:GLY:N | 2.72 | 0.42 |
| 1:A:227:PHE:N | 1:A:227:PHE:CD1 | 2.88 | 0.42 |
| 1:C:395:LYS:CG | 1:C:430:LYS:HG2 | 2.47 | 0.42 |
| 1:C:502:PHE:HB2 | 1:C:546:VAL:HG13 | 2.02 | 0.42 |
| 1:D:26:PHE:CE1 | 1:D:29:ALA:HB3 | 2.54 | 0.42 |
| 1:D:395:LYS:CG | 1:D:396:ASP:N | 2.80 | 0.42 |
| 1:D:441:TYR:CG | 1:D:465:LEU:HB2 | 2.54 | 0.42 |
| 1:D:502:PHE:HB3 | 1:D:503:LYS:H | 1.48 | 0.42 |
| 1:A:173:LEU:HD12 | 1:A:173:LEU:N | 2.34 | 0.42 |
| 1:A:46:TYR:HA | 1:A:48:ARG:N | 2.35 | 0.42 |
| 1:C:263:GLU:HG3 | 1:C:274:PHE:HZ | 1.83 | 0.42 |
| 1:C:35:ALA:C | 1:C:37:ILE:N | 2.71 | 0.42 |
| 1:C:543:ASN:O | 1:C:544:ALA:O | 2.38 | 0.42 |
| 1:D:200:THR:C | 1:D:202:GLY:H | 2.23 | 0.42 |
| 1:D:224:ASP:CG | 1:D:225:ARG:N | 2.73 | 0.42 |
| 1:C:77:GLU:HB3 | 1:D:57:HIS:H | 1.84 | 0.42 |
| 1:A:263:GLU:HG3 | 1:A:274:PHE:HZ | 1.84 | 0.42 |
| 1:B:287:THR:HG22 | 1:B:315:PRO:HD3 | 2.01 | 0.42 |
| 1:B:502:PHE:HB2 | 1:B:546:VAL:HG13 | 2.02 | 0.42 |
| 1:C:26:PHE:CE1 | 1:C:29:ALA:HB3 | 2.55 | 0.42 |
| 1:C:396:ASP:OD2 | 1:C:397:LYS:N | 2.51 | 0.42 |
| 1:C:413:GLY:C | 1:C:415:ARG:H | 2.23 | 0.42 |
| 1:D:200:THR:C | 1:D:202:GLY:N | 2.73 | 0.42 |
| 1:D:290:THR:O | 1:D:292:THR:HG23 | 2.20 | 0.42 |
| 1:D:543:ASN:O | 1:D:544:ALA:O | 2.38 | 0.42 |
| 1:A:380:PHE:CE1 | 1:A:409:PHE:HE2 | 2.38 | 0.42 |
| 1:A:490:LYS:O | 1:A:491:ILE:C | 2.58 | 0.42 |
| 1:A:522:LEU:N | 1:A:522:LEU:HD12 | 2.34 | 0.42 |
| 1:C:395:LYS:CG | 1:C:396:ASP:N | 2.80 | 0.42 |
| 1:D:263:GLU:HG3 | 1:D:274:PHE:CZ | 2.55 | 0.42 |
| 1:A:263:GLU:HG3 | 1:A:274:PHE:CZ | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:63:ILE:HG12 | 1:A:334:VAL:HG11 | 2.01 | 0.42 |
| 1:B:227:PHE:CD1 | 1:B:227:PHE:N | 2.88 | 0.42 |
| 1:B:26:PHE:CE1 | 1:B:29:ALA:HB3 | 2.55 | 0.42 |
| 1:D:227:PHE:N | 1:D:227:PHE:CD1 | 2.88 | 0.42 |
| 1:D:279:ASP:HB3 | 1:D:291:GLN:HG2 | 2.02 | 0.42 |
| 1:A:413:GLY:C | 1:A:415:ARG:H | 2.24 | 0.42 |
| 1:A:506:VAL:H | 1:A:507:PRO:CD | 2.33 | 0.42 |
| 1:A:512:LEU:C | 1:A:512:LEU:HD12 | 2.40 | 0.42 |
| 1:B:159:PHE:HB3 | 1:B:171:MET:SD | 2.60 | 0.42 |
| 1:B:328:MET:C | 1:B:328:MET:SD | 2.99 | 0.42 |
| 1:B:88:GLU:OE1 | 1:B:88:GLU:HA | 2.20 | 0.42 |
| 1:C:107:LEU:HD12 | 1:C:107:LEU:N | 2.35 | 0.42 |
| 1:D:392:ILE:HD11 | 1:D:480:ILE:CD1 | 2.50 | 0.42 |
| 1:A:290:THR:O | 1:A:292:THR:HG23 | 2.20 | 0.41 |
| 1:B:263:GLU:HG3 | 1:B:274:PHE:CZ | 2.55 | 0.41 |
| 1:B:370:ARG:NH2 | 1:B:370:ARG:HG2 | 2.35 | 0.41 |
| 1:B:392:ILE:HD11 | 1:B:480:ILE:CD1 | 2.50 | 0.41 |
| 1:C:89:ILE:HD13 | 1:C:101:LEU:CD2 | 2.50 | 0.41 |
| 1:C:173:LEU:HD12 | 1:C:173:LEU:N | 2.34 | 0.41 |
| 1:C:380:PHE:CE1 | 1:C:409:PHE:HE2 | 2.38 | 0.41 |
| 1:C:467:LYS:O | 1:C:468:ALA:HB3 | 2.20 | 0.41 |
| 1:C:388:ILE:HG12 | 1:C:484:ILE:HG13 | 2.01 | 0.41 |
| 1:C:506:VAL:H | 1:C:507:PRO:CD | 2.33 | 0.41 |
| 1:D:380:PHE:CE1 | 1:D:409:PHE:HE2 | 2.38 | 0.41 |
| 1:D:413:GLY:C | 1:D:415:ARG:H | 2.23 | 0.41 |
| 1:D:467:LYS:O | 1:D:468:ALA:HB3 | 2.20 | 0.41 |
| 1:D:512:LEU:C | 1:D:512:LEU:HD12 | 2.41 | 0.41 |
| 1:D:88:GLU:OE1 | 1:D:88:GLU:HA | 2.20 | 0.41 |
| 1:A:328:MET:SD | 1:A:328:MET:C | 2.98 | 0.41 |
| 1:A:467:LYS:O | 1:A:468:ALA:HB3 | 2.20 | 0.41 |
| 1:B:482:GLY:O | 1:B:516:ASN:ND2 | 2.46 | 0.41 |
| 1:C:156:ASP:CG | 1:D:284:LYS:HE3 | 2.40 | 0.41 |
| 1:C:483:ILE:O | 1:C:486:LYS:HB3 | 2.19 | 0.41 |
| 1:D:46:TYR:HA | 1:D:48:ARG:N | 2.35 | 0.41 |
| 1:A:513:SER:C | 1:A:514:ASP:O | 2.57 | 0.41 |
| 1:A:543:ASN:O | 1:A:544:ALA:O | 2.38 | 0.41 |
| 1:A:57:HIS:H | 1:B:77:GLU:CG | 2.33 | 0.41 |
| 1:B:46:TYR:HA | 1:B:48:ARG:N | 2.35 | 0.41 |
| 1:C:200:THR:C | 1:C:202:GLY:H | 2.22 | 0.41 |
| 1:D:516:ASN:HB3 | 1:D:517:LEU:H | 1.67 | 0.41 |
| 1:D:522:LEU:O | 1:D:524:LEU:N | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:482:GLY:O | 1:A:516:ASN:ND2 | 2.44 | 0.41 |
| 1:B:89:ILE:HD13 | 1:B:101:LEU:CD2 | 2.50 | 0.41 |
| 1:B:200:THR:C | 1:B:202:GLY:H | 2.24 | 0.41 |
| 1:B:467:LYS:O | 1:B:468:ALA:HB3 | 2.20 | 0.41 |
| 1:C:159:PHE:HB3 | 1:C:171:MET:SD | 2.61 | 0.41 |
| 1:C:88:GLU:HA | 1:C:88:GLU:OE1 | 2.20 | 0.41 |
| 1:A:109:GLY:HA3 | 1:B:229:ARG:HE | 1.85 | 0.41 |
| 1:A:308:ALA:HB1 | 1:A:330:LEU:HD11 | 2.02 | 0.41 |
| 1:A:352:TYR:CE2 | 1:B:81:PRO:HA | 2.55 | 0.41 |
| 1:A:441:TYR:CE2 | 1:A:474:SER:HB2 | 2.55 | 0.41 |
| 1:A:502:PHE:HB2 | 1:A:546:VAL:HG13 | 2.02 | 0.41 |
| 1:A:482:GLY:HA3 | 1:A:515:ILE:O | 2.20 | 0.41 |
| 1:B:20:GLU:C | 1:B:22:ALA:N | 2.74 | 0.41 |
| 1:B:290:THR:O | 1:B:292:THR:HG23 | 2.21 | 0.41 |
| 1:B:395:LYS:CG | 1:B:396:ASP:N | 2.80 | 0.41 |
| 1:B:502:PHE:O | 1:B:503:LYS:HB2 | 2.20 | 0.41 |
| 1:C:263:GLU:HG3 | 1:C:274:PHE:CZ | 2.55 | 0.41 |
| 1:C:365:ILE:HB | 1:C:442:VAL:HG11 | 2.02 | 0.41 |
| 1:C:395:LYS:CG | 1:C:396:ASP:H | 2.14 | 0.41 |
| 1:D:513:SER:C | 1:D:514:ASP:O | 2.57 | 0.41 |
| 1:B:458:LYS:O | 1:B:460:GLN:N | 2.49 | 0.41 |
| 1:B:512:LEU:C | 1:B:512:LEU:HD12 | 2.41 | 0.41 |
| 1:B:89:ILE:HD11 | 1:B:100:VAL:CG1 | 2.51 | 0.41 |
| 1:C:335:GLU:O | 1:C:338:ALA:HB3 | 2.20 | 0.41 |
| 1:C:441:TYR:CE2 | 1:C:474:SER:HB2 | 2.55 | 0.41 |
| 1:C:513:SER:C | 1:C:514:ASP:O | 2.58 | 0.41 |
| 1:C:522:LEU:O | 1:C:523:ALA:CB | 2.68 | 0.41 |
| 1:D:32:GLU:C | 1:D:34:ARG:N | 2.74 | 0.41 |
| 1:D:506:VAL:H | 1:D:507:PRO:CD | 2.34 | 0.41 |
| 1:C:387:LEU:HD12 | 1:C:484:ILE:CG2 | 2.50 | 0.41 |
| 1:C:502:PHE:O | 1:C:503:LYS:HB2 | 2.20 | 0.41 |
| 1:A:200:THR:C | 1:A:202:GLY:H | 2.23 | 0.41 |
| 1:A:365:ILE:O | 1:A:369:ILE:HG13 | 2.20 | 0.41 |
| 1:A:502:PHE:O | 1:A:503:LYS:HB2 | 2.21 | 0.41 |
| 1:A:57:HIS:HB2 | 1:B:77:GLU:HG2 | 2.01 | 0.41 |
| 1:B:279:ASP:HB3 | 1:B:291:GLN:HG2 | 2.02 | 0.41 |
| 1:B:441:TYR:CE2 | 1:B:474:SER:HB2 | 2.56 | 0.41 |
| 1:C:45:LYS:O | 1:C:46:TYR:HB3 | 2.21 | 0.41 |
| 1:D:107:LEU:HD12 | 1:D:107:LEU:N | 2.36 | 0.41 |
| 1:D:20:GLU:C | 1:D:22:ALA:N | 2.74 | 0.41 |
| 1:D:351:VAL:HB | 1:D:352:TYR:CD1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:441:TYR:CE2 | 1:D:474:SER:HB2 | 2.56 | 0.41 |
| 1:A:20:GLU:C | 1:A:22:ALA:N | 2.74 | 0.41 |
| 1:B:387:LEU:C | 1:B:387:LEU:HD13 | 2.41 | 0.41 |
| 1:C:89:ILE:HD11 | 1:C:100:VAL:CG1 | 2.51 | 0.41 |
| 1:C:88:GLU:OE2 | 1:C:205:ILE:HD12 | 2.21 | 0.41 |
| 1:C:351:VAL:HB | 1:C:352:TYR:CD1 | 2.56 | 0.41 |
| 1:C:392:ILE:HD11 | 1:C:480:ILE:CD1 | 2.51 | 0.41 |
| 1:D:308:ALA:HB1 | 1:D:330:LEU:HD11 | 2.03 | 0.41 |
| 1:D:396:ASP:OD2 | 1:D:397:LYS:N | 2.51 | 0.41 |
| 1:B:399:SER:HB3 | 1:B:425:ASN:HA | 2.03 | 0.41 |
| 1:B:395:LYS:CG | 1:B:430:LYS:HG2 | 2.48 | 0.41 |
| 1:B:506:VAL:H | 1:B:507:PRO:CD | 2.33 | 0.41 |
| 1:C:108:ALA:O | 1:D:105:PHE:HA | 2.21 | 0.41 |
| 1:D:502:PHE:O | 1:D:503:LYS:HB2 | 2.20 | 0.41 |
| 1:A:89:ILE:HD13 | 1:A:101:LEU:CD2 | 2.51 | 0.41 |
| 1:A:370:ARG:NH2 | 1:A:370:ARG:HG2 | 2.36 | 0.41 |
| 1:A:45:LYS:O | 1:A:46:TYR:HB3 | 2.21 | 0.41 |
| 1:C:200:THR:O | 1:C:202:GLY:N | 2.54 | 0.41 |
| 1:C:20:GLU:C | 1:C:22:ALA:N | 2.74 | 0.41 |
| 1:C:279:ASP:HB3 | 1:C:291:GLN:HG2 | 2.03 | 0.41 |
| 1:C:512:LEU:C | 1:C:512:LEU:HD12 | 2.42 | 0.41 |
| 1:D:140:LEU:N | 1:D:140:LEU:HD12 | 2.36 | 0.41 |
| 1:A:89:ILE:HD11 | 1:A:100:VAL:CG1 | 2.50 | 0.40 |
| 1:A:316:ILE:O | 1:A:319:ALA:HB3 | 2.20 | 0.40 |
| 1:C:11:MET:HE3 | 1:C:12:ARG:H | 1.86 | 0.40 |
| 1:A:140:LEU:N | 1:A:140:LEU:HD12 | 2.36 | 0.40 |
| 1:A:159:PHE:HB3 | 1:A:171:MET:SD | 2.61 | 0.40 |
| 1:A:261:VAL:HG12 | 1:A:330:LEU:HD23 | 2.03 | 0.40 |
| 1:A:392:ILE:HD11 | 1:A:480:ILE:CD1 | 2.50 | 0.40 |
| 1:B:32:GLU:C | 1:B:34:ARG:N | 2.75 | 0.40 |
| 1:B:413:GLY:C | 1:B:415:ARG:H | 2.24 | 0.40 |
| 1:A:57:HIS:NE2 | 1:B:79:ILE:HD12 | 2.36 | 0.40 |
| 1:C:301:LEU:HD12 | 1:C:302:GLY:H | 1.86 | 0.40 |
| 1:C:328:MET:SD | 1:C:328:MET:C | 2.99 | 0.40 |
| 1:C:90:TYR:CD2 | 1:C:97:ALA:HB3 | 2.56 | 0.40 |
| 1:D:335:GLU:O | 1:D:338:ALA:HB3 | 2.21 | 0.40 |
| 1:D:45:LYS:O | 1:D:46:TYR:HB3 | 2.22 | 0.40 |
| 1:B:286:TYR:HA | 1:B:312:VAL:O | 2.22 | 0.40 |
| 1:B:301:LEU:HD12 | 1:B:302:GLY:H | 1.86 | 0.40 |
| 1:A:352:TYR:CE2 | 1:B:81:PRO:CA | 3.05 | 0.40 |
| 1:B:268:GLN:HG2 | 1:C:53:TYR:CE2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:298:HIS:ND1 | 1:D:299:PRO:HD2 | 2.37 | 0.40 |
| 1:D:387:LEU:HD13 | 1:D:387:LEU:C | 2.42 | 0.40 |
| 1:A:32:GLU:C | 1:A:34:ARG:N | 2.74 | 0.40 |
| 1:B:107:LEU:N | 1:B:107:LEU:HD12 | 2.36 | 0.40 |
| 1:B:396:ASP:HA | 1:B:430:LYS:HA | 2.04 | 0.40 |
| 1:C:298:HIS:ND1 | 1:C:299:PRO:HD2 | 2.37 | 0.40 |
| 1:C:32:GLU:C | 1:C:34:ARG:N | 2.74 | 0.40 |
| 1:A:396:ASP:HA | 1:A:430:LYS:HA | 2.03 | 0.40 |
| 1:B:140:LEU:N | 1:B:140:LEU:HD12 | 2.36 | 0.40 |
| 1:B:351:VAL:HB | 1:B:352:TYR:CD1 | 2.57 | 0.40 |
| 1:C:513:SER:O | 1:C:514:ASP:CB | 2.69 | 0.40 |
| 1:C:105:PHE:CD1 | 1:D:107:LEU:HD23 | 2.57 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:174:LYS:CB | 1:A:174:LYS:CB[3_655] | 2.14 | 0.06 |
| 1:A:143:VAL:CG1 | 1:A:143:VAL:CG1[3_655] | 2.16 | 0.04 |

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 | 537/549 (98%) | 345 (64%) | 138 (26%) | 54 (10%) | 0 | 7 |
| 1 | B | 537/549 (98%) | 346 (64%) | 138 (26%) | 53 (10%) | 0 | 8 |
| 1 | C | 537/549 (98%) | 344 (64%) | 139 (26%) | 54 (10%) | 0 | 7 |
| 1 | D | 537/549 (98%) | 345 (64%) | 138 (26%) | 54 (10%) | 0 | 7 |
| All | All | 2148/2196 (98%) | 1380 (64%) | 553 (26%) | 215 (10%) | 0 | 8 |

All (215) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | THR |
| 1 | A | 124 | ILE |
| 1 | A | 151 | ALA |
| 1 | A | 167 | VAL |
| 1 | A | 195 | LEU |
| 1 | A | 358 | TYR |
| 1 | A | 397 | LYS |
| 1 | A | 407 | ARG |
| 1 | A | 471 | GLU |
| 1 | A | 506 | VAL |
| 1 | A | 509 | VAL |
| 1 | A | 540 | VAL |
| 1 | A | 544 | ALA |
| 1 | B | 33 | THR |
| 1 | B | 124 | ILE |
| 1 | B | 151 | ALA |
| 1 | B | 167 | VAL |
| 1 | B | 195 | LEU |
| 1 | B | 358 | TYR |
| 1 | B | 397 | LYS |
| 1 | B | 407 | ARG |
| 1 | B | 471 | GLU |
| 1 | B | 506 | VAL |
| 1 | B | 509 | VAL |
| 1 | B | 540 | VAL |
| 1 | B | 544 | ALA |
| 1 | C | 33 | THR |
| 1 | C | 124 | ILE |
| 1 | C | 151 | ALA |
| 1 | C | 167 | VAL |
| 1 | C | 195 | LEU |
| 1 | C | 358 | TYR |
| 1 | C | 397 | LYS |
| 1 | C | 407 | ARG |
| 1 | C | 471 | GLU |
| 1 | C | 506 | VAL |
| 1 | C | 509 | VAL |
| 1 | C | 540 | VAL |
| 1 | C | 544 | ALA |
| 1 | D | 33 | THR |
| 1 | D | 124 | ILE |
| 1 | D | 151 | ALA |
| 1 | D | 167 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 195 | LEU |
| 1 | D | 358 | TYR |
| 1 | D | 397 | LYS |
| 1 | D | 407 | ARG |
| 1 | D | 471 | GLU |
| 1 | D | 506 | VAL |
| 1 | D | 509 | VAL |
| 1 | D | 540 | VAL |
| 1 | D | 544 | ALA |
| 1 | A | 15 | ILE |
| 1 | A | 35 | ALA |
| 1 | A | 40 | LYS |
| 1 | A | 232 | ARG |
| 1 | A | 300 | LYS |
| 1 | A | 394 | ASN |
| 1 | A | 400 | PRO |
| 1 | A | 466 | LYS |
| 1 | A | 542 | LEU |
| 1 | B | 15 | ILE |
| 1 | B | 35 | ALA |
| 1 | B | 158 | VAL |
| 1 | B | 232 | ARG |
| 1 | B | 300 | LYS |
| 1 | B | 394 | ASN |
| 1 | B | 400 | PRO |
| 1 | B | 466 | LYS |
| 1 | B | 542 | LEU |
| 1 | C | 15 | ILE |
| 1 | C | 35 | ALA |
| 1 | C | 40 | LYS |
| 1 | C | 158 | VAL |
| 1 | C | 232 | ARG |
| 1 | C | 300 | LYS |
| 1 | C | 394 | ASN |
| 1 | C | 400 | PRO |
| 1 | C | 466 | LYS |
| 1 | C | 542 | LEU |
| 1 | D | 15 | ILE |
| 1 | D | 35 | ALA |
| 1 | D | 158 | VAL |
| 1 | D | 232 | ARG |
| 1 | D | 300 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 394 | ASN |
| 1 | D | 400 | PRO |
| 1 | D | 466 | LYS |
| 1 | D | 542 | LEU |
| 1 | A | 41 | HIS |
| 1 | A | 136 | LYS |
| 1 | A | 158 | VAL |
| 1 | A | 231 | GLN |
| 1 | A | 299 | PRO |
| 1 | A | 304 | TRP |
| 1 | A | 356 | TYR |
| 1 | A | 372 | ASP |
| 1 | A | 465 | LEU |
| 1 | A | 467 | LYS |
| 1 | A | 537 | ARG |
| 1 | B | 40 | LYS |
| 1 | B | 41 | HIS |
| 1 | B | 136 | LYS |
| 1 | B | 231 | GLN |
| 1 | B | 299 | PRO |
| 1 | B | 304 | TRP |
| 1 | B | 356 | TYR |
| 1 | B | 372 | ASP |
| 1 | B | 465 | LEU |
| 1 | B | 467 | LYS |
| 1 | B | 537 | ARG |
| 1 | C | 41 | HIS |
| 1 | C | 136 | LYS |
| 1 | C | 231 | GLN |
| 1 | C | 299 | PRO |
| 1 | C | 304 | TRP |
| 1 | C | 356 | TYR |
| 1 | C | 372 | ASP |
| 1 | C | 465 | LEU |
| 1 | C | 467 | LYS |
| 1 | C | 537 | ARG |
| 1 | D | 40 | LYS |
| 1 | D | 41 | HIS |
| 1 | D | 136 | LYS |
| 1 | D | 231 | GLN |
| 1 | D | 299 | PRO |
| 1 | D | 304 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 356 | TYR |
| 1 | D | 372 | ASP |
| 1 | D | 465 | LEU |
| 1 | D | 467 | LYS |
| 1 | D | 537 | ARG |
| 1 | A | 142 | GLU |
| 1 | A | 177 | GLU |
| 1 | A | 237 | HIS |
| 1 | A | 291 | GLN |
| 1 | A | 355 | PHE |
| 1 | A | 401 | CYS |
| 1 | A | 459 | GLU |
| 1 | A | 481 | ASP |
| 1 | B | 142 | GLU |
| 1 | B | 177 | GLU |
| 1 | B | 237 | HIS |
| 1 | B | 291 | GLN |
| 1 | B | 355 | PHE |
| 1 | B | 401 | CYS |
| 1 | B | 459 | GLU |
| 1 | C | 142 | GLU |
| 1 | C | 177 | GLU |
| 1 | C | 237 | HIS |
| 1 | C | 291 | GLN |
| 1 | C | 355 | PHE |
| 1 | C | 401 | CYS |
| 1 | C | 459 | GLU |
| 1 | D | 142 | GLU |
| 1 | D | 177 | GLU |
| 1 | D | 237 | HIS |
| 1 | D | 291 | GLN |
| 1 | D | 355 | PHE |
| 1 | D | 401 | CYS |
| 1 | D | 459 | GLU |
| 1 | A | 23 | GLU |
| 1 | A | 46 | TYR |
| 1 | A | 111 | PRO |
| 1 | A | 164 | ALA |
| 1 | B | 23 | GLU |
| 1 | B | 46 | TYR |
| 1 | B | 111 | PRO |
| 1 | B | 164 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 481 | ASP |
| 1 | C | 23 | GLU |
| 1 | C | 46 | TYR |
| 1 | C | 111 | PRO |
| 1 | C | 164 | ALA |
| 1 | C | 481 | ASP |
| 1 | D | 46 | TYR |
| 1 | D | 111 | PRO |
| 1 | D | 164 | ALA |
| 1 | D | 481 | ASP |
| 1 | A | 118 | GLY |
| 1 | A | 198 | HIS |
| 1 | A | 436 | VAL |
| 1 | A | 515 | ILE |
| 1 | B | 118 | GLY |
| 1 | B | 436 | VAL |
| 1 | B | 515 | ILE |
| 1 | C | 118 | GLY |
| 1 | C | 198 | HIS |
| 1 | C | 436 | VAL |
| 1 | C | 515 | ILE |
| 1 | D | 23 | GLU |
| 1 | D | 118 | GLY |
| 1 | D | 198 | HIS |
| 1 | D | 436 | VAL |
| 1 | D | 515 | ILE |
| 1 | A | 417 | VAL |
| 1 | B | 417 | VAL |
| 1 | C | 417 | VAL |
| 1 | D | 417 | VAL |
| 1 | A | 125 | ILE |
| 1 | A | 129 | GLY |
| 1 | A | 440 | VAL |
| 1 | B | 125 | ILE |
| 1 | B | 129 | GLY |
| 1 | B | 440 | VAL |
| 1 | C | 125 | ILE |
| 1 | C | 129 | GLY |
| 1 | C | 440 | VAL |
| 1 | D | 125 | ILE |
| 1 | D | 129 | GLY |
| 1 | D | 440 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 143 | VAL |
| 1 | B | 143 | VAL |
| 1 | C | 143 | VAL |
| 1 | D | 143 | 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 | 481/491 (98%) | 468 (97%) | 13 (3%) | 44 | 73 |
| 1 | B | 481/491 (98%) | 468 (97%) | 13 (3%) | 44 | 73 |
| 1 | C | 481/491 (98%) | 468 (97%) | 13 (3%) | 44 | 73 |
| 1 | D | 481/491 (98%) | 468 (97%) | 13 (3%) | 44 | 73 |
| All | All | 1924/1964 (98%) | 1872 (97%) | 52 (3%) | 44 | 73 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 31 | ARG |
| 1 | A | 274 | PHE |
| 1 | A | 276 | PHE |
| 1 | A | 286 | TYR |
| 1 | A | 322 | ASN |
| 1 | A | 348 | ARG |
| 1 | A | 355 | PHE |
| 1 | A | 408 | GLU |
| 1 | A | 409 | PHE |
| 1 | A | 431 | LEU |
| 1 | A | 432 | LEU |
| 1 | A | 493 | GLU |
| 1 | A | 506 | VAL |
| 1 | B | 31 | ARG |
| 1 | B | 274 | PHE |
| 1 | B | 276 | PHE |
| 1 | B | 286 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 322 | ASN |
| 1 | B | 348 | ARG |
| 1 | B | 355 | PHE |
| 1 | B | 408 | GLU |
| 1 | B | 409 | PHE |
| 1 | B | 431 | LEU |
| 1 | B | 432 | LEU |
| 1 | B | 493 | GLU |
| 1 | B | 506 | VAL |
| 1 | C | 31 | ARG |
| 1 | C | 274 | PHE |
| 1 | C | 276 | PHE |
| 1 | C | 286 | TYR |
| 1 | C | 322 | ASN |
| 1 | C | 348 | ARG |
| 1 | C | 355 | PHE |
| 1 | C | 408 | GLU |
| 1 | C | 409 | PHE |
| 1 | C | 431 | LEU |
| 1 | C | 432 | LEU |
| 1 | C | 493 | GLU |
| 1 | C | 506 | VAL |
| 1 | D | 31 | ARG |
| 1 | D | 274 | PHE |
| 1 | D | 276 | PHE |
| 1 | D | 286 | TYR |
| 1 | D | 322 | ASN |
| 1 | D | 348 | ARG |
| 1 | D | 355 | PHE |
| 1 | D | 408 | GLU |
| 1 | D | 409 | PHE |
| 1 | D | 431 | LEU |
| 1 | D | 432 | LEU |
| 1 | D | 493 | GLU |
| 1 | D | 506 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 68 | GLN |
| 1 | A | 127 | ASN |
| 1 | A | 231 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 242 | HIS |
| 1 | A | 291 | GLN |
| 1 | A | 322 | ASN |
| 1 | A | 329 | ASN |
| 1 | A | 382 | ASN |
| 1 | A | 412 | ASN |
| 1 | A | 476 | ASN |
| 1 | B | 68 | GLN |
| 1 | B | 127 | ASN |
| 1 | B | 231 | GLN |
| 1 | B | 242 | HIS |
| 1 | B | 291 | GLN |
| 1 | B | 322 | ASN |
| 1 | B | 329 | ASN |
| 1 | B | 382 | ASN |
| 1 | B | 412 | ASN |
| 1 | B | 476 | ASN |
| 1 | C | 68 | GLN |
| 1 | C | 127 | ASN |
| 1 | C | 231 | GLN |
| 1 | C | 242 | HIS |
| 1 | C | 291 | GLN |
| 1 | C | 322 | ASN |
| 1 | C | 329 | ASN |
| 1 | C | 382 | ASN |
| 1 | C | 412 | ASN |
| 1 | C | 476 | ASN |
| 1 | D | 68 | GLN |
| 1 | D | 127 | ASN |
| 1 | D | 231 | GLN |
| 1 | D | 242 | HIS |
| 1 | D | 291 | GLN |
| 1 | D | 322 | ASN |
| 1 | D | 329 | ASN |
| 1 | D | 382 | ASN |
| 1 | D | 412 | ASN |
| 1 | D | 476 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [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 | 539/549 (98%) | 0.49 | 80 (14%) 2 1 | 37, 149, 203, 203 | 0 |
| 1 | B | 539/549 (98%) | 0.23 | 64 (11%) 4 3 | 15, 116, 203, 203 | 0 |
| 1 | C | 539/549 (98%) | 0.22 | 65 (12%) 4 3 | 13, 104, 203, 203 | 0 |
| 1 | D | 539/549 (98%) | 0.51 | 79 (14%) 2 1 | 26, 151, 203, 203 | 0 |
| All | All | 2156/2196 (98%) | 0.36 | 288 (13%) 3 2 | 13, 131, 203, 203 | 0 |

All (288) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 133 | ASP | 10.7 |
| 1 | D | 171 | MET | 10.0 |
| 1 | A | 508 | ILE | 9.8 |
| 1 | B | 130 | ILE | 9.7 |
| 1 | D | 179 | ALA | 9.5 |
| 1 | C | 138 | GLU | 9.5 |
| 1 | D | 425 | ASN | 9.3 |
| 1 | D | 128 | LEU | 8.9 |
| 1 | D | 162 | ALA | 8.8 |
| 1 | A | 181 | PRO | 8.5 |
| 1 | A | 179 | ALA | 8.3 |
| 1 | B | 132 | ILE | 8.3 |
| 1 | A | 148 | LYS | 8.3 |
| 1 | A | 180 | PHE | 8.2 |
| 1 | B | 508 | ILE | 8.1 |
| 1 | D | 131 | ASP | 7.7 |
| 1 | D | 500 | ASP | 7.7 |
| 1 | A | 164 | ALA | 7.6 |
| 1 | C | 133 | ASP | 7.5 |
| 1 | C | 118 | GLY | 7.3 |
| 1 | B | 509 | VAL | 7.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 426 | GLU | 7.0 |
| 1 | C | 128 | LEU | 6.9 |
| 1 | C | 125 | ILE | 6.9 |
| 1 | B | 178 | THR | 6.8 |
| 1 | C | 171 | MET | 6.8 |
| 1 | B | 131 | ASP | 6.8 |
| 1 | A | 429 | LYS | 6.7 |
| 1 | D | 138 | GLU | 6.7 |
| 1 | D | 402 | SER | 6.6 |
| 1 | D | 127 | ASN | 6.6 |
| 1 | C | 177 | GLU | 6.3 |
| 1 | A | 163 | LYS | 6.3 |
| 1 | D | 434 | PRO | 6.3 |
| 1 | B | 507 | PRO | 6.3 |
| 1 | D | 177 | GLU | 6.3 |
| 1 | D | 181 | PRO | 6.2 |
| 1 | D | 129 | GLY | 6.1 |
| 1 | B | 127 | ASN | 6.1 |
| 1 | A | 149 | LYS | 6.1 |
| 1 | A | 27 | GLU | 6.0 |
| 1 | A | 426 | GLU | 6.0 |
| 1 | D | 132 | ILE | 5.9 |
| 1 | D | 125 | ILE | 5.7 |
| 1 | D | 413 | GLY | 5.7 |
| 1 | B | 145 | HIS | 5.6 |
| 1 | A | 427 | PRO | 5.6 |
| 1 | A | 177 | GLU | 5.6 |
| 1 | A | 162 | ALA | 5.4 |
| 1 | D | 165 | LEU | 5.4 |
| 1 | A | 165 | LEU | 5.3 |
| 1 | D | 166 | ASN | 5.3 |
| 1 | A | 126 | LYS | 5.3 |
| 1 | C | 168 | SER | 5.3 |
| 1 | B | 133 | ASP | 5.3 |
| 1 | B | 150 | GLY | 5.2 |
| 1 | D | 430 | LYS | 5.2 |
| 1 | C | 127 | ASN | 5.2 |
| 1 | D | 509 | VAL | 5.2 |
| 1 | A | 127 | ASN | 5.2 |
| 1 | D | 145 | HIS | 5.1 |
| 1 | C | 129 | GLY | 5.1 |
| 1 | A | 150 | GLY | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 132 | ILE | 5.1 |
| 1 | A | 133 | ASP | 5.0 |
| 1 | B | 428 | ASN | 5.0 |
| 1 | D | 142 | GLU | 5.0 |
| 1 | D | 302 | GLY | 5.0 |
| 1 | D | 427 | PRO | 4.9 |
| 1 | A | 510 | ARG | 4.9 |
| 1 | B | 429 | LYS | 4.8 |
| 1 | C | 504 | PHE | 4.8 |
| 1 | A | 469 | LYS | 4.8 |
| 1 | A | 187 | LYS | 4.8 |
| 1 | A | 111 | PRO | 4.8 |
| 1 | B | 112 | ARG | 4.8 |
| 1 | C | 507 | PRO | 4.7 |
| 1 | C | 131 | ASP | 4.7 |
| 1 | D | 428 | ASN | 4.7 |
| 1 | D | 170 | GLU | 4.7 |
| 1 | C | 469 | LYS | 4.7 |
| 1 | D | 119 | ASN | 4.6 |
| 1 | A | 178 | THR | 4.6 |
| 1 | B | 467 | LYS | 4.6 |
| 1 | B | 427 | PRO | 4.6 |
| 1 | D | 163 | LYS | 4.5 |
| 1 | C | 234 | ASP | 4.5 |
| 1 | A | 169 | ASN | 4.5 |
| 1 | C | 145 | HIS | 4.4 |
| 1 | B | 234 | ASP | 4.4 |
| 1 | A | 135 | GLU | 4.4 |
| 1 | A | 189 | GLU | 4.4 |
| 1 | C | 164 | ALA | 4.4 |
| 1 | A | 166 | ASN | 4.3 |
| 1 | B | 113 | PRO | 4.3 |
| 1 | C | 116 | GLY | 4.3 |
| 1 | D | 113 | PRO | 4.3 |
| 1 | A | 24 | LYS | 4.3 |
| 1 | C | 509 | VAL | 4.3 |
| 1 | B | 469 | LYS | 4.3 |
| 1 | C | 163 | LYS | 4.3 |
| 1 | B | 179 | ALA | 4.2 |
| 1 | D | 126 | LYS | 4.2 |
| 1 | C | 170 | GLU | 4.2 |
| 1 | C | 176 | LEU | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 112 | ARG | 4.1 |
| 1 | A | 231 | GLN | 4.1 |
| 1 | A | 549 | LYS | 4.1 |
| 1 | B | 172 | GLY | 4.1 |
| 1 | B | 129 | GLY | 4.1 |
| 1 | A | 509 | VAL | 4.1 |
| 1 | D | 168 | SER | 4.0 |
| 1 | D | 137 | LYS | 4.0 |
| 1 | B | 123 | GLU | 4.0 |
| 1 | B | 170 | GLU | 4.0 |
| 1 | B | 166 | ASN | 4.0 |
| 1 | C | 178 | THR | 4.0 |
| 1 | B | 187 | LYS | 4.0 |
| 1 | B | 118 | GLY | 3.9 |
| 1 | D | 182 | GLU | 3.9 |
| 1 | C | 152 | ILE | 3.9 |
| 1 | D | 178 | THR | 3.9 |
| 1 | A | 507 | PRO | 3.9 |
| 1 | C | 120 | GLU | 3.9 |
| 1 | C | 126 | LYS | 3.9 |
| 1 | D | 410 | ASN | 3.9 |
| 1 | B | 167 | VAL | 3.8 |
| 1 | A | 414 | GLU | 3.8 |
| 1 | C | 179 | ALA | 3.8 |
| 1 | C | 180 | PHE | 3.8 |
| 1 | B | 171 | MET | 3.7 |
| 1 | C | 468 | ALA | 3.7 |
| 1 | D | 116 | GLY | 3.7 |
| 1 | D | 124 | ILE | 3.7 |
| 1 | D | 507 | PRO | 3.7 |
| 1 | A | 468 | ALA | 3.7 |
| 1 | D | 449 | GLY | 3.7 |
| 1 | A | 182 | GLU | 3.7 |
| 1 | D | 111 | PRO | 3.7 |
| 1 | C | 117 | LEU | 3.7 |
| 1 | A | 14 | ASP | 3.7 |
| 1 | B | 148 | LYS | 3.7 |
| 1 | C | 298 | HIS | 3.7 |
| 1 | C | 156 | ASP | 3.6 |
| 1 | D | 187 | LYS | 3.6 |
| 1 | B | 466 | LYS | 3.6 |
| 1 | A | 129 | GLY | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 142 | GLU | 3.6 |
| 1 | D | 185 | ASP | 3.6 |
| 1 | C | 297 | TYR | 3.6 |
| 1 | A | 23 | GLU | 3.6 |
| 1 | A | 136 | LYS | 3.6 |
| 1 | A | 404 | GLU | 3.6 |
| 1 | D | 148 | LYS | 3.5 |
| 1 | D | 130 | ILE | 3.5 |
| 1 | D | 455 | GLU | 3.5 |
| 1 | C | 122 | VAL | 3.5 |
| 1 | C | 155 | ASP | 3.5 |
| 1 | D | 121 | LYS | 3.5 |
| 1 | B | 149 | LYS | 3.5 |
| 1 | D | 469 | LYS | 3.4 |
| 1 | C | 424 | GLU | 3.4 |
| 1 | D | 405 | VAL | 3.4 |
| 1 | D | 499 | VAL | 3.4 |
| 1 | C | 181 | PRO | 3.4 |
| 1 | A | 137 | LYS | 3.4 |
| 1 | D | 27 | GLU | 3.4 |
| 1 | A | 235 | ARG | 3.4 |
| 1 | D | 510 | ARG | 3.4 |
| 1 | D | 149 | LYS | 3.3 |
| 1 | A | 511 | SER | 3.3 |
| 1 | B | 177 | GLU | 3.3 |
| 1 | B | 189 | GLU | 3.3 |
| 1 | A | 151 | ALA | 3.3 |
| 1 | C | 124 | ILE | 3.3 |
| 1 | B | 122 | VAL | 3.2 |
| 1 | D | 429 | LYS | 3.2 |
| 1 | C | 130 | ILE | 3.2 |
| 1 | C | 167 | VAL | 3.2 |
| 1 | D | 159 | PHE | 3.2 |
| 1 | A | 289 | GLU | 3.2 |
| 1 | A | 113 | PRO | 3.1 |
| 1 | C | 429 | LYS | 3.1 |
| 1 | D | 140 | LEU | 3.1 |
| 1 | C | 142 | GLU | 3.0 |
| 1 | C | 549 | LYS | 3.0 |
| 1 | D | 123 | GLU | 3.0 |
| 1 | C | 113 | PRO | 3.0 |
| 1 | C | 119 | ASN | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 150 | GLY | 2.9 |
| 1 | A | 505 | ARG | 2.9 |
| 1 | B | 181 | PRO | 2.9 |
| 1 | A | 416 | ARG | 2.9 |
| 1 | C | 148 | LYS | 2.9 |
| 1 | A | 174 | LYS | 2.9 |
| 1 | A | 188 | PRO | 2.8 |
| 1 | B | 168 | SER | 2.8 |
| 1 | B | 426 | GLU | 2.8 |
| 1 | C | 169 | ASN | 2.8 |
| 1 | C | 511 | SER | 2.8 |
| 1 | A | 413 | GLY | 2.8 |
| 1 | B | 400 | PRO | 2.8 |
| 1 | B | 228 | ARG | 2.7 |
| 1 | A | 124 | ILE | 2.7 |
| 1 | A | 125 | ILE | 2.7 |
| 1 | A | 25 | ASP | 2.7 |
| 1 | D | 141 | ARG | 2.7 |
| 1 | C | 433 | GLY | 2.7 |
| 1 | C | 141 | ARG | 2.7 |
| 1 | D | 11 | MET | 2.6 |
| 1 | C | 165 | LEU | 2.6 |
| 1 | A | 119 | ASN | 2.6 |
| 1 | A | 139 | ARG | 2.6 |
| 1 | B | 27 | GLU | 2.6 |
| 1 | D | 112 | ARG | 2.6 |
| 1 | B | 11 | MET | 2.6 |
| 1 | A | 297 | TYR | 2.6 |
| 1 | A | 463 | PRO | 2.5 |
| 1 | D | 164 | ALA | 2.5 |
| 1 | A | 120 | GLU | 2.5 |
| 1 | A | 123 | GLU | 2.5 |
| 1 | D | 120 | GLU | 2.5 |
| 1 | B | 164 | ALA | 2.5 |
| 1 | B | 117 | LEU | 2.5 |
| 1 | A | 122 | VAL | 2.5 |
| 1 | B | 468 | ALA | 2.5 |
| 1 | B | 125 | ILE | 2.4 |
| 1 | B | 141 | ARG | 2.4 |
| 1 | C | 231 | GLN | 2.4 |
| 1 | C | 426 | GLU | 2.4 |
| 1 | D | 414 | GLU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 138 | GLU | 2.4 |
| 1 | A | 419 | LYS | 2.4 |
| 1 | C | 143 | VAL | 2.4 |
| 1 | B | 510 | ARG | 2.3 |
| 1 | C | 470 | GLU | 2.3 |
| 1 | D | 399 | SER | 2.3 |
| 1 | B | 180 | PHE | 2.3 |
| 1 | A | 132 | ILE | 2.3 |
| 1 | C | 251 | GLU | 2.3 |
| 1 | D | 395 | LYS | 2.3 |
| 1 | C | 139 | ARG | 2.3 |
| 1 | A | 98 | MET | 2.3 |
| 1 | B | 121 | LYS | 2.3 |
| 1 | B | 395 | LYS | 2.3 |
| 1 | A | 428 | ASN | 2.3 |
| 1 | A | 128 | LEU | 2.3 |
| 1 | A | 506 | VAL | 2.3 |
| 1 | B | 116 | GLY | 2.3 |
| 1 | A | 467 | LYS | 2.3 |
| 1 | C | 182 | GLU | 2.2 |
| 1 | A | 159 | PHE | 2.2 |
| 1 | C | 400 | PRO | 2.2 |
| 1 | B | 425 | ASN | 2.2 |
| 1 | A | 130 | ILE | 2.2 |
| 1 | D | 167 | VAL | 2.2 |
| 1 | D | 396 | ASP | 2.2 |
| 1 | D | 40 | LYS | 2.2 |
| 1 | D | 504 | PHE | 2.2 |
| 1 | B | 114 | ASP | 2.2 |
| 1 | B | 138 | GLU | 2.2 |
| 1 | A | 170 | GLU | 2.2 |
| 1 | A | 142 | GLU | 2.2 |
| 1 | B | 152 | ILE | 2.2 |
| 1 | D | 454 | PHE | 2.2 |
| 1 | D | 235 | ARG | 2.1 |
| 1 | D | 180 | PHE | 2.1 |
| 1 | B | 182 | GLU | 2.1 |
| 1 | D | 14 | ASP | 2.1 |
| 1 | A | 131 | ASP | 2.1 |
| 1 | A | 114 | ASP | 2.1 |
| 1 | D | 139 | ARG | 2.1 |
| 1 | A | 160 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 137 | LYS | 2.1 |
| 1 | B | 235 | ARG | 2.1 |
| 1 | D | 122 | VAL | 2.1 |
| 1 | D | 234 | ASP | 2.1 |
| 1 | A | 424 | GLU | 2.1 |
| 1 | D | 115 | VAL | 2.1 |
| 1 | C | 162 | ALA | 2.1 |
| 1 | A | 471 | GLU | 2.1 |
| 1 | B | 159 | PHE | 2.0 |
| 1 | C | 153 | ASP | 2.0 |
| 1 | B | 136 | LYS | 2.0 |
| 1 | C | 172 | GLY | 2.0 |
| 1 | A | 168 | SER | 2.0 |
| 1 | B | 139 | ARG | 2.0 |
| 1 | B | 275 | LYS | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.