



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:20 pm BST

PDB ID : 2ZBE
Title : Calcium pump crystal structure with bound BeF₃ in the absence of calcium and TG
Authors : Toyoshima, C.; Ogawa, H.; Norimatsu, Y.
Deposited on : 2007-10-20
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

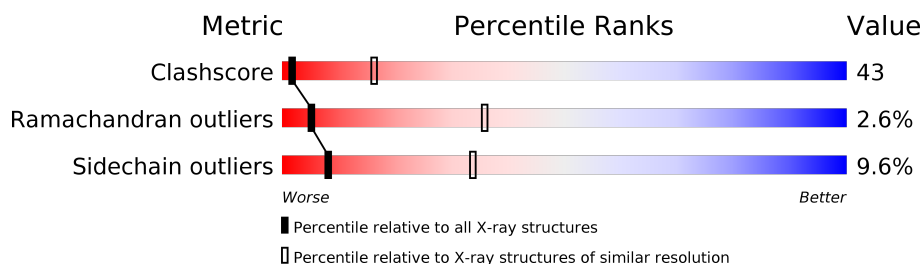
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 1288 (4.00-3.60) |
| Ramachandran outliers | 138981 | 1243 (4.00-3.60) |
| Sidechain outliers | 138945 | 1237 (4.00-3.60) |

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 $\leq 5\%$.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 995 | <div> <div style="width: 49%; background-color: green;"></div> <div style="width: 43%; background-color: yellow;"></div> <div style="width: 8%; background-color: orange;"></div> </div> <div>49% 43% 8%</div> |
| 1 | B | 995 | <div> <div style="width: 49%; background-color: green;"></div> <div style="width: 43%; background-color: yellow;"></div> <div style="width: 8%; background-color: orange;"></div> </div> <div>49% 43% 8%</div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15358 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 995 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 7674 | 4878 | 1287 | 1452 | 57 | | | |
| 1 | B | 995 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 7674 | 4878 | 1287 | 1452 | 57 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 994 | GLY | - | SEE REMARK 999 | UNP P04191 |
| B | 994 | GLY | - | SEE REMARK 999 | UNP P04191 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



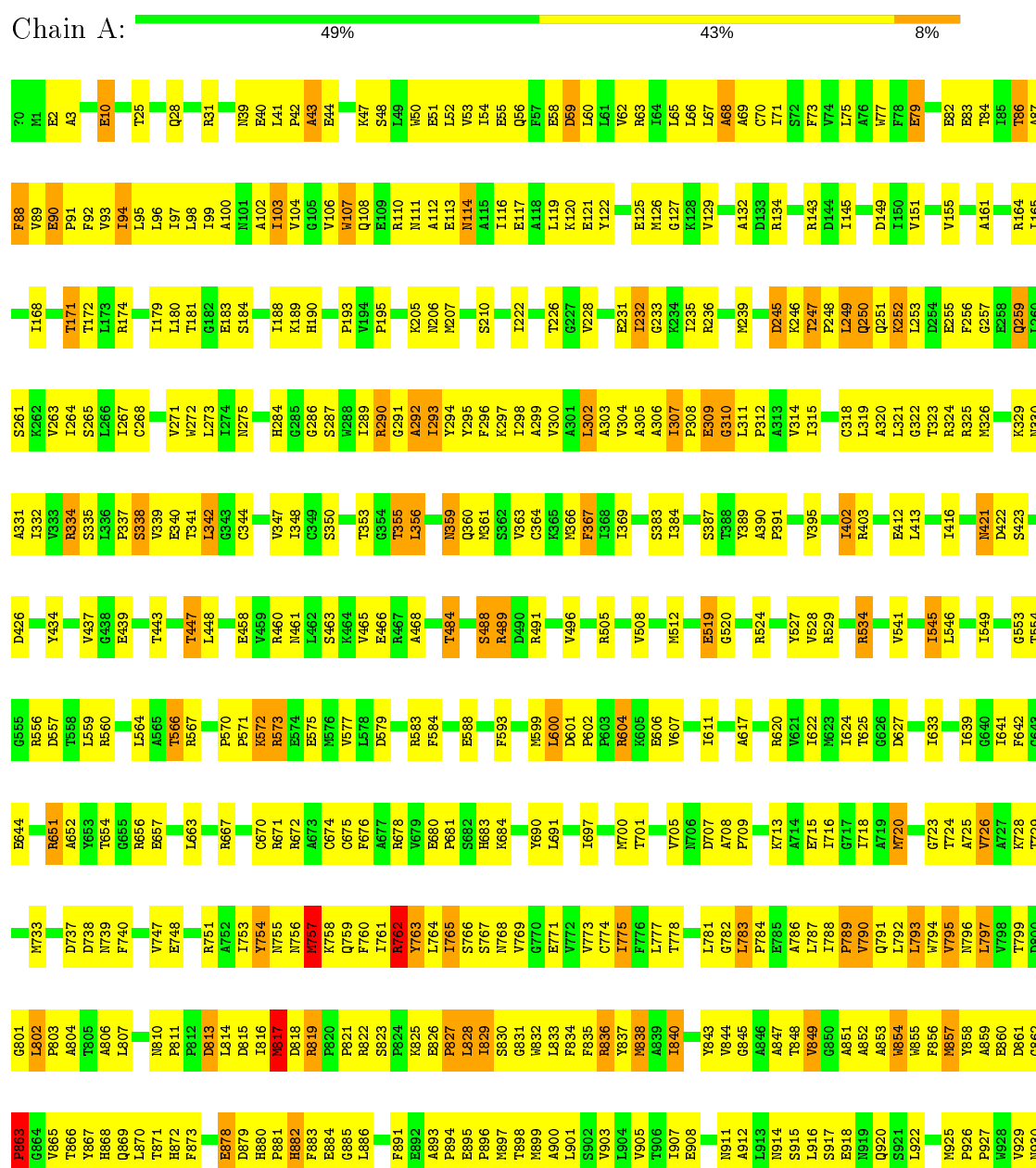
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3 | A | 1 | Total | Be | F | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 3 | B | 1 | Total | Be | F | 0 | 0 |
| | | | 4 | 1 | 3 | | |

3 Residue-property plots

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

Note EDS was not executed.

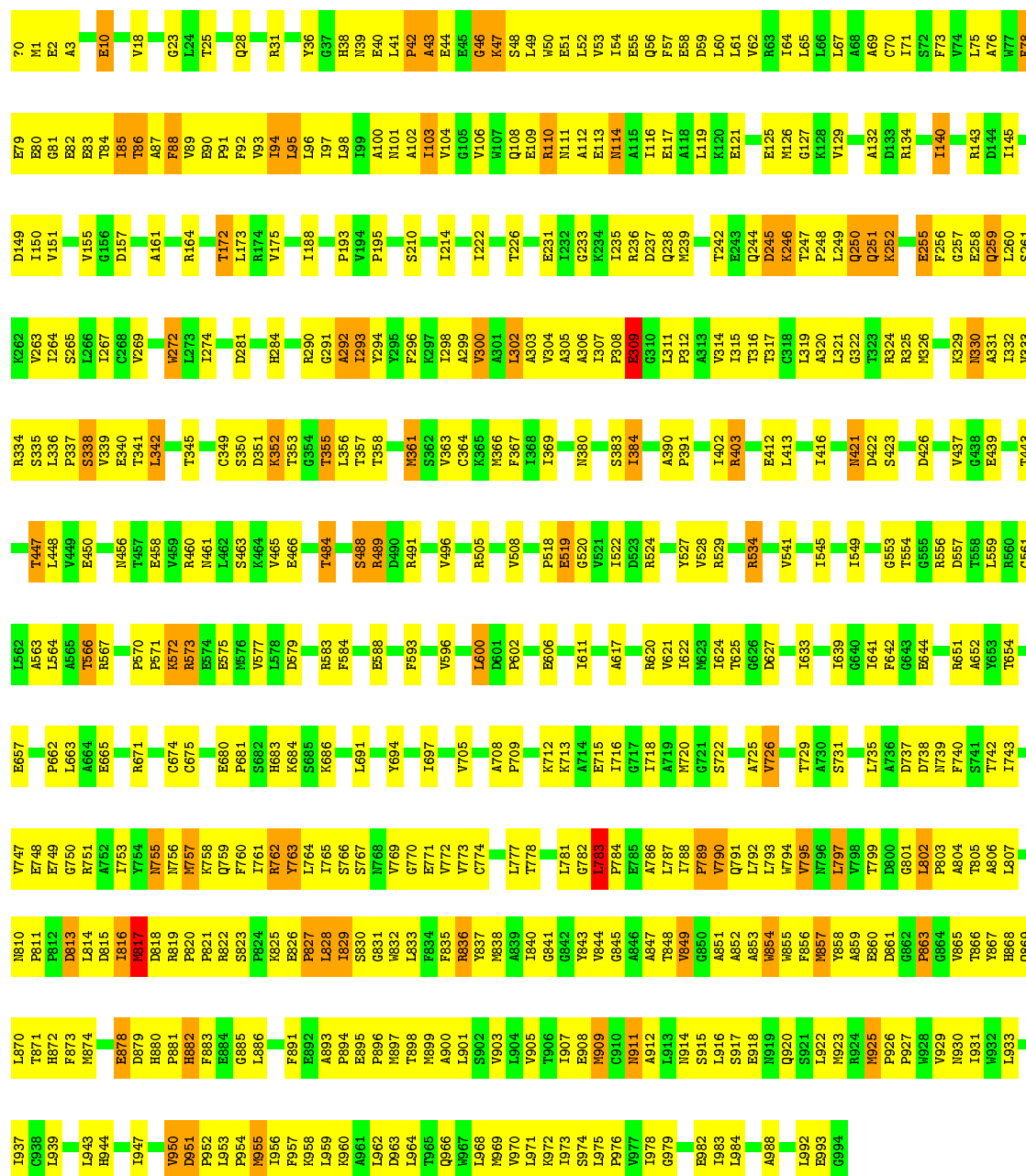
- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B: 49% 43% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 133.87Å 91.59Å 248.46Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 12.00 – 3.80 | Depositor |
| % Data completeness (in resolution range) | 90.3 (12.00-3.80) | Depositor |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.293 , 0.327 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 15358 | wwPDB-VP |
| Average B, all atoms (Å ²) | 163.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.74 | 2/7813 (0.0%) | 0.89 | 25/10594 (0.2%) |
| 1 | B | 0.75 | 1/7813 (0.0%) | 0.86 | 15/10594 (0.1%) |
| All | All | 0.74 | 3/15626 (0.0%) | 0.88 | 40/21188 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 2 |
| All | All | 0 | 4 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 107 | TRP | CB-CG | 5.95 | 1.60 | 1.50 |
| 1 | A | 863 | PRO | C-N | -5.75 | 1.22 | 1.33 |
| 1 | B | 561 | CYS | CB-SG | -5.35 | 1.73 | 1.81 |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | A | 671 | ARG | NE-CZ-NH1 | 9.46 | 125.03 | 120.30 |
| 1 | A | 822 | ARG | NE-CZ-NH2 | 7.72 | 124.16 | 120.30 |
| 1 | A | 651 | ARG | NE-CZ-NH2 | 7.24 | 123.92 | 120.30 |
| 1 | A | 762 | ARG | NE-CZ-NH2 | 7.24 | 123.92 | 120.30 |
| 1 | A | 290 | ARG | NE-CZ-NH2 | 7.05 | 123.82 | 120.30 |
| 1 | A | 560 | ARG | NE-CZ-NH2 | 6.99 | 123.80 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 836 | ARG | NE-CZ-NH2 | 6.97 | 123.79 | 120.30 |
| 1 | A | 751 | ARG | NE-CZ-NH2 | 6.95 | 123.78 | 120.30 |
| 1 | A | 678 | ARG | NE-CZ-NH2 | 6.74 | 123.67 | 120.30 |
| 1 | A | 656 | ARG | NE-CZ-NH2 | 6.67 | 123.63 | 120.30 |
| 1 | A | 819 | ARG | NE-CZ-NH2 | 6.66 | 123.63 | 120.30 |
| 1 | A | 667 | ARG | NE-CZ-NH2 | 6.65 | 123.62 | 120.30 |
| 1 | A | 604 | ARG | NE-CZ-NH2 | 6.47 | 123.53 | 120.30 |
| 1 | B | 822 | ARG | NE-CZ-NH2 | 6.43 | 123.52 | 120.30 |
| 1 | A | 672 | ARG | NE-CZ-NH2 | 6.42 | 123.51 | 120.30 |
| 1 | B | 366 | MET | CG-SD-CE | 6.20 | 110.12 | 100.20 |
| 1 | B | 838 | MET | CG-SD-CE | 6.16 | 110.05 | 100.20 |
| 1 | A | 366 | MET | CG-SD-CE | 6.15 | 110.04 | 100.20 |
| 1 | A | 757 | MET | CG-SD-CE | 6.04 | 109.87 | 100.20 |
| 1 | A | 838 | MET | CG-SD-CE | 6.03 | 109.85 | 100.20 |
| 1 | A | 817 | MET | CG-SD-CE | 5.99 | 109.78 | 100.20 |
| 1 | A | 361 | MET | CG-SD-CE | 5.96 | 109.75 | 100.20 |
| 1 | B | 857 | MET | CG-SD-CE | 5.92 | 109.68 | 100.20 |
| 1 | B | 309 | GLU | O-C-N | -5.92 | 113.14 | 123.20 |
| 1 | B | 126 | MET | CG-SD-CE | 5.91 | 109.65 | 100.20 |
| 1 | A | 599 | MET | CG-SD-CE | 5.79 | 109.46 | 100.20 |
| 1 | B | 361 | MET | CG-SD-CE | 5.75 | 109.39 | 100.20 |
| 1 | A | 720 | MET | CG-SD-CE | 5.73 | 109.37 | 100.20 |
| 1 | A | 857 | MET | CG-SD-CE | 5.65 | 109.25 | 100.20 |
| 1 | B | 836 | ARG | NE-CZ-NH2 | 5.65 | 123.12 | 120.30 |
| 1 | B | 955 | MET | CG-SD-CE | 5.60 | 109.17 | 100.20 |
| 1 | A | 733 | MET | CG-SD-CE | 5.60 | 109.16 | 100.20 |
| 1 | A | 126 | MET | CG-SD-CE | 5.47 | 108.95 | 100.20 |
| 1 | A | 700 | MET | CG-SD-CE | 5.46 | 108.94 | 100.20 |
| 1 | B | 909 | MET | CG-SD-CE | 5.46 | 108.93 | 100.20 |
| 1 | B | 923 | MET | CG-SD-CE | 5.40 | 108.83 | 100.20 |
| 1 | B | 874 | MET | CG-SD-CE | 5.32 | 108.70 | 100.20 |
| 1 | B | 817 | MET | CG-SD-CE | 5.31 | 108.69 | 100.20 |
| 1 | B | 274 | ILE | O-C-N | -5.27 | 114.26 | 122.70 |
| 1 | B | 925 | MET | CG-SD-CE | 5.03 | 108.24 | 100.20 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 310 | GLY | Mainchain |
| 1 | A | 68 | ALA | Mainchain |
| 1 | B | 284 | HIS | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 380 | ASN | Mainchain |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 7674 | 0 | 7765 | 645 | 0 |
| 1 | B | 7674 | 0 | 7765 | 689 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 4 | 0 | 0 | 1 | 0 |
| 3 | B | 4 | 0 | 0 | 0 | 0 |
| All | All | 15358 | 0 | 15530 | 1334 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1334) 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:757:MET:CE | 1:A:761:ILE:HD11 | 1.60 | 1.30 |
| 1:B:762:ARG:HE | 1:B:833:LEU:HD21 | 1.02 | 1.18 |
| 1:B:802:LEU:HD13 | 1:B:939:LEU:CD2 | 1.74 | 1.17 |
| 1:A:247:THR:OG1 | 1:A:250:GLN:HB3 | 1.45 | 1.17 |
| 1:A:802:LEU:HD13 | 1:A:939:LEU:CD2 | 1.76 | 1.15 |
| 1:B:802:LEU:HD13 | 1:B:939:LEU:HD23 | 1.23 | 1.15 |
| 1:B:735:LEU:HD11 | 1:B:743:ILE:HD11 | 1.23 | 1.12 |
| 1:A:762:ARG:HE | 1:A:833:LEU:HD21 | 1.00 | 1.12 |
| 1:A:758:LYS:HA | 1:A:761:ILE:HD12 | 1.32 | 1.11 |
| 1:A:802:LEU:HD13 | 1:A:939:LEU:HD23 | 1.25 | 1.09 |
| 1:A:898:THR:HA | 1:A:959:LEU:HD22 | 1.33 | 1.09 |
| 1:A:248:PRO:HG2 | 1:A:341:THR:CG2 | 1.83 | 1.09 |
| 1:A:248:PRO:HG2 | 1:A:341:THR:HG21 | 1.27 | 1.08 |
| 1:A:757:MET:HE2 | 1:A:761:ILE:HD11 | 1.13 | 1.08 |
| 1:A:803:PRO:O | 1:A:806:ALA:HB3 | 1.52 | 1.08 |
| 1:A:758:LYS:HB2 | 1:A:828:LEU:HD11 | 1.30 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:823:SER:HB3 | 1:A:826:GLU:HB2 | 1.35 | 1.07 |
| 1:B:549:ILE:HD11 | 1:B:596:VAL:HG21 | 1.37 | 1.07 |
| 1:B:803:PRO:O | 1:B:806:ALA:HB3 | 1.55 | 1.06 |
| 1:B:823:SER:HB3 | 1:B:826:GLU:HB2 | 1.37 | 1.06 |
| 1:B:758:LYS:HB2 | 1:B:828:LEU:HD11 | 1.33 | 1.06 |
| 1:B:898:THR:HA | 1:B:959:LEU:HD22 | 1.33 | 1.05 |
| 1:A:762:ARG:NE | 1:A:833:LEU:HD21 | 1.69 | 1.05 |
| 1:B:855:TRP:HA | 1:B:859:ALA:CB | 1.87 | 1.05 |
| 1:A:855:TRP:HA | 1:A:859:ALA:HB2 | 1.06 | 1.04 |
| 1:B:267:ILE:HG12 | 1:B:302:LEU:HD22 | 1.40 | 1.04 |
| 1:B:735:LEU:CD1 | 1:B:743:ILE:HD11 | 1.88 | 1.04 |
| 1:B:762:ARG:NE | 1:B:833:LEU:HD21 | 1.70 | 1.04 |
| 1:A:341:THR:HG22 | 1:A:716:ILE:HD11 | 1.38 | 1.02 |
| 1:A:855:TRP:HA | 1:A:859:ALA:CB | 1.88 | 1.02 |
| 1:B:855:TRP:HA | 1:B:859:ALA:HB2 | 1.05 | 1.02 |
| 1:A:899:MET:HE1 | 1:A:970:VAL:HG23 | 1.42 | 1.01 |
| 1:B:899:MET:HE1 | 1:B:970:VAL:HG23 | 1.41 | 1.00 |
| 1:B:342:LEU:HG | 1:B:716:ILE:HG21 | 1.44 | 0.99 |
| 1:A:760:PHE:HB3 | 1:A:807:LEU:HD12 | 1.44 | 0.99 |
| 1:B:783:LEU:HD12 | 1:B:783:LEU:H | 1.27 | 0.98 |
| 1:B:311:LEU:HD11 | 1:B:761:ILE:CD1 | 1.92 | 0.98 |
| 1:A:849:VAL:O | 1:A:853:ALA:HB3 | 1.63 | 0.97 |
| 1:B:786:ALA:O | 1:B:787:LEU:HG | 1.65 | 0.96 |
| 1:A:120:LYS:HE2 | 1:A:728:LYS:NZ | 1.80 | 0.96 |
| 1:B:963:ASP:HB3 | 1:B:966:GLN:HG3 | 1.48 | 0.96 |
| 1:A:963:ASP:HB3 | 1:A:966:GLN:HG3 | 1.48 | 0.95 |
| 1:B:617:ALA:O | 1:B:821:PRO:HD3 | 1.66 | 0.95 |
| 1:B:311:LEU:HB3 | 1:B:312:PRO:HD3 | 1.46 | 0.95 |
| 1:B:49:LEU:HD13 | 1:B:110:ARG:HE | 1.30 | 0.95 |
| 1:B:573:ARG:HD2 | 1:B:573:ARG:H | 1.32 | 0.95 |
| 1:B:261:SER:HA | 1:B:264:ILE:HD12 | 1.49 | 0.95 |
| 1:B:760:PHE:HB3 | 1:B:807:LEU:HD12 | 1.48 | 0.95 |
| 1:A:866:THR:H | 1:A:869:GLN:HE21 | 1.12 | 0.94 |
| 1:A:622:ILE:HD12 | 1:A:674:CYS:HA | 1.46 | 0.94 |
| 1:A:786:ALA:O | 1:A:787:LEU:HG | 1.67 | 0.94 |
| 1:B:866:THR:H | 1:B:869:GLN:HE21 | 1.14 | 0.93 |
| 1:A:248:PRO:CG | 1:A:341:THR:HG21 | 1.97 | 0.93 |
| 1:B:909:MET:SD | 1:B:937:ILE:HD12 | 2.09 | 0.93 |
| 1:A:783:LEU:H | 1:A:783:LEU:HD12 | 1.32 | 0.92 |
| 1:B:311:LEU:HD11 | 1:B:761:ILE:HD12 | 1.51 | 0.92 |
| 1:A:762:ARG:HE | 1:A:833:LEU:CD2 | 1.82 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:788:ILE:HB | 1:A:789:PRO:HD2 | 1.52 | 0.91 |
| 1:A:757:MET:HE1 | 1:A:761:ILE:HD11 | 1.52 | 0.91 |
| 1:A:573:ARG:H | 1:A:573:ARG:HD2 | 1.36 | 0.91 |
| 1:B:762:ARG:HE | 1:B:833:LEU:CD2 | 1.83 | 0.90 |
| 1:A:59:ASP:OD2 | 1:A:62:VAL:HG23 | 1.72 | 0.90 |
| 1:A:849:VAL:O | 1:A:853:ALA:CB | 2.20 | 0.90 |
| 1:B:50:TRP:CD1 | 1:B:54:ILE:HD11 | 2.07 | 0.90 |
| 1:B:49:LEU:CD1 | 1:B:110:ARG:HE | 1.84 | 0.89 |
| 1:B:844:VAL:HG22 | 1:B:907:ILE:HG21 | 1.52 | 0.89 |
| 1:A:762:ARG:HB3 | 1:A:837:TYR:CZ | 2.07 | 0.89 |
| 1:B:762:ARG:HB3 | 1:B:837:TYR:CZ | 2.07 | 0.89 |
| 1:B:80:GLU:HG2 | 1:B:82:GLU:HG2 | 1.52 | 0.89 |
| 1:A:395:VAL:HG12 | 1:A:402:ILE:HD11 | 1.55 | 0.89 |
| 1:B:622:ILE:HD12 | 1:B:674:CYS:HA | 1.52 | 0.89 |
| 1:B:756:ASN:O | 1:B:759:GLN:HB2 | 1.72 | 0.88 |
| 1:A:757:MET:HG2 | 1:A:760:PHE:CZ | 2.08 | 0.88 |
| 1:A:777:LEU:O | 1:A:781:LEU:HB3 | 1.73 | 0.88 |
| 1:A:899:MET:SD | 1:A:962:LEU:HD13 | 2.13 | 0.88 |
| 1:B:383:SER:C | 1:B:384:ILE:HD12 | 1.94 | 0.87 |
| 1:B:245:ASP:O | 1:B:246:LYS:HG2 | 1.74 | 0.87 |
| 1:B:69:ALA:O | 1:B:73:PHE:HB2 | 1.74 | 0.87 |
| 1:B:57:PHE:CZ | 1:B:102:ALA:HB2 | 2.10 | 0.86 |
| 1:B:899:MET:SD | 1:B:962:LEU:HD13 | 2.16 | 0.86 |
| 1:A:248:PRO:CG | 1:A:341:THR:CG2 | 2.54 | 0.86 |
| 1:B:855:TRP:CA | 1:B:859:ALA:HB2 | 2.00 | 0.86 |
| 1:A:899:MET:CE | 1:A:970:VAL:HG23 | 2.06 | 0.86 |
| 1:A:556:ARG:HG2 | 1:A:644:GLU:HG3 | 1.56 | 0.86 |
| 1:A:120:LYS:HE2 | 1:A:728:LYS:HZ2 | 1.40 | 0.86 |
| 1:A:765:ILE:HD13 | 1:A:765:ILE:O | 1.76 | 0.86 |
| 1:A:844:VAL:HG22 | 1:A:907:ILE:HG21 | 1.56 | 0.86 |
| 1:A:895:GLU:HG3 | 1:A:960:LYS:HD3 | 1.56 | 0.86 |
| 1:B:898:THR:CA | 1:B:959:LEU:HD22 | 2.06 | 0.85 |
| 1:B:518:PRO:O | 1:B:522:ILE:HD13 | 1.75 | 0.85 |
| 1:A:898:THR:CA | 1:A:959:LEU:HD22 | 2.06 | 0.85 |
| 1:B:757:MET:HG2 | 1:B:760:PHE:CZ | 2.12 | 0.84 |
| 1:A:39:ASN:OD1 | 1:A:226:THR:HB | 1.75 | 0.84 |
| 1:B:895:GLU:HG3 | 1:B:960:LYS:HD3 | 1.57 | 0.84 |
| 1:A:567:ARG:HH11 | 1:A:570:PRO:HA | 1.42 | 0.84 |
| 1:B:787:LEU:HD11 | 1:B:900:ALA:HB1 | 1.59 | 0.84 |
| 1:A:843:TYR:OH | 1:A:976:PRO:HG2 | 1.78 | 0.84 |
| 1:A:865:VAL:HG13 | 1:A:869:GLN:HG3 | 1.59 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:342:LEU:HD11 | 1:B:718:ILE:HD11 | 1.60 | 0.84 |
| 1:A:950:VAL:HG12 | 1:A:952:PRO:HD2 | 1.58 | 0.84 |
| 1:B:816:ILE:HA | 1:B:819:ARG:HH21 | 1.39 | 0.84 |
| 1:B:899:MET:CE | 1:B:970:VAL:HG23 | 2.07 | 0.84 |
| 1:A:833:LEU:HA | 1:A:836:ARG:HB2 | 1.60 | 0.84 |
| 1:A:52:LEU:HD12 | 1:A:106:VAL:HG13 | 1.60 | 0.83 |
| 1:B:857:MET:HB2 | 1:B:858:TYR:CD1 | 2.13 | 0.83 |
| 1:B:421:ASN:ND2 | 1:B:423:SER:H | 1.77 | 0.83 |
| 1:B:567:ARG:HH11 | 1:B:570:PRO:HA | 1.43 | 0.83 |
| 1:B:740:PHE:O | 1:B:743:ILE:HD13 | 1.79 | 0.83 |
| 1:B:843:TYR:OH | 1:B:976:PRO:HG2 | 1.78 | 0.83 |
| 1:A:857:MET:HB2 | 1:A:858:TYR:CD1 | 2.14 | 0.83 |
| 1:A:421:ASN:ND2 | 1:A:423:SER:H | 1.77 | 0.83 |
| 1:A:95:LEU:O | 1:A:99:ILE:HD12 | 1.77 | 0.83 |
| 1:A:245:ASP:O | 1:A:246:LYS:HG3 | 1.77 | 0.83 |
| 1:B:157:ASP:HB2 | 1:B:214:ILE:HD13 | 1.61 | 0.83 |
| 1:B:833:LEU:HA | 1:B:836:ARG:HB2 | 1.61 | 0.82 |
| 1:A:541:VAL:O | 1:A:545:ILE:HD13 | 1.79 | 0.82 |
| 1:B:777:LEU:O | 1:B:781:LEU:HB3 | 1.79 | 0.82 |
| 1:A:802:LEU:CD1 | 1:A:939:LEU:HG | 2.10 | 0.82 |
| 1:A:519:GLU:H | 1:A:519:GLU:CD | 1.83 | 0.82 |
| 1:B:788:ILE:HB | 1:B:789:PRO:HD2 | 1.58 | 0.82 |
| 1:B:802:LEU:CD1 | 1:B:939:LEU:HG | 2.09 | 0.82 |
| 1:A:757:MET:HE2 | 1:A:761:ILE:CD1 | 2.04 | 0.81 |
| 1:A:878:GLU:HG3 | 1:A:879:ASP:H | 1.45 | 0.81 |
| 1:A:773:VAL:O | 1:A:777:LEU:HG | 1.80 | 0.81 |
| 1:B:248:PRO:HG2 | 1:B:341:THR:CG2 | 2.11 | 0.81 |
| 1:B:773:VAL:O | 1:B:777:LEU:HG | 1.81 | 0.81 |
| 1:A:757:MET:CE | 1:A:761:ILE:CD1 | 2.54 | 0.81 |
| 1:B:849:VAL:O | 1:B:853:ALA:HB3 | 1.80 | 0.81 |
| 1:A:758:LYS:CB | 1:A:828:LEU:HD11 | 2.10 | 0.81 |
| 1:B:245:ASP:O | 1:B:246:LYS:CG | 2.29 | 0.81 |
| 1:A:865:VAL:HG13 | 1:A:869:GLN:CG | 2.11 | 0.80 |
| 1:B:363:VAL:HG11 | 1:B:448:LEU:HD22 | 1.64 | 0.79 |
| 1:A:899:MET:HE1 | 1:A:966:GLN:O | 1.81 | 0.79 |
| 1:B:878:GLU:HG3 | 1:B:879:ASP:H | 1.45 | 0.79 |
| 1:B:802:LEU:HD13 | 1:B:939:LEU:CG | 2.12 | 0.79 |
| 1:A:50:TRP:CD1 | 1:A:54:ILE:HD11 | 2.17 | 0.79 |
| 1:A:802:LEU:HD13 | 1:A:939:LEU:CG | 2.13 | 0.79 |
| 1:A:350:SER:OG | 1:A:356:LEU:HD13 | 1.82 | 0.79 |
| 1:B:311:LEU:HD11 | 1:B:761:ILE:HD13 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:899:MET:HA | 1:B:962:LEU:HD11 | 1.64 | 0.79 |
| 1:A:832:TRP:O | 1:A:836:ARG:HG3 | 1.83 | 0.79 |
| 1:B:898:THR:OG1 | 1:B:959:LEU:HB3 | 1.83 | 0.79 |
| 1:A:898:THR:OG1 | 1:A:959:LEU:HB3 | 1.83 | 0.79 |
| 1:A:855:TRP:CA | 1:A:859:ALA:HB2 | 2.01 | 0.78 |
| 1:B:787:LEU:HD21 | 1:B:901:LEU:N | 1.97 | 0.78 |
| 1:B:899:MET:HE1 | 1:B:966:GLN:O | 1.83 | 0.78 |
| 1:B:484:THR:HB | 1:B:496:VAL:HG12 | 1.64 | 0.78 |
| 1:A:484:THR:HB | 1:A:496:VAL:HG12 | 1.64 | 0.78 |
| 1:A:899:MET:HA | 1:A:962:LEU:HD11 | 1.64 | 0.78 |
| 1:B:248:PRO:HG2 | 1:B:341:THR:HG23 | 1.64 | 0.78 |
| 1:A:771:GLU:O | 1:A:775:ILE:HD13 | 1.83 | 0.78 |
| 1:A:852:ALA:HB1 | 1:A:896:PRO:O | 1.84 | 0.78 |
| 1:A:488:SER:HB3 | 1:A:491:ARG:HH21 | 1.49 | 0.78 |
| 1:A:787:LEU:HD11 | 1:A:900:ALA:HB1 | 1.66 | 0.77 |
| 1:B:39:ASN:OD1 | 1:B:226:THR:HB | 1.83 | 0.77 |
| 1:B:926:PRO:O | 1:B:929:VAL:HG23 | 1.85 | 0.77 |
| 1:B:140:ILE:HD13 | 1:B:140:ILE:H | 1.50 | 0.77 |
| 1:B:23:GLY:HA2 | 1:B:150:ILE:HD13 | 1.65 | 0.77 |
| 1:B:519:GLU:CD | 1:B:519:GLU:H | 1.84 | 0.77 |
| 1:B:897:MET:HE1 | 1:B:958:LYS:HB3 | 1.67 | 0.77 |
| 1:B:786:ALA:O | 1:B:897:MET:HA | 1.84 | 0.77 |
| 1:A:851:ALA:HB2 | 1:A:973:ILE:HG13 | 1.67 | 0.77 |
| 1:B:832:TRP:O | 1:B:836:ARG:HG3 | 1.84 | 0.77 |
| 1:A:249:LEU:HD11 | 1:A:253:LEU:HD21 | 1.64 | 0.76 |
| 1:B:855:TRP:O | 1:B:859:ALA:HB3 | 1.85 | 0.76 |
| 1:B:852:ALA:HB1 | 1:B:896:PRO:O | 1.86 | 0.76 |
| 1:A:421:ASN:HD22 | 1:A:423:SER:H | 1.33 | 0.76 |
| 1:A:112:ALA:O | 1:A:116:ILE:HG12 | 1.85 | 0.76 |
| 1:A:807:LEU:O | 1:A:810:ASN:HB2 | 1.84 | 0.76 |
| 1:A:99:ILE:O | 1:A:103:ILE:HG22 | 1.86 | 0.75 |
| 1:A:95:LEU:HA | 1:A:98:LEU:HD12 | 1.66 | 0.75 |
| 1:B:245:ASP:C | 1:B:246:LYS:HG3 | 2.05 | 0.75 |
| 1:A:787:LEU:HD21 | 1:A:901:LEU:N | 2.01 | 0.75 |
| 1:A:866:THR:H | 1:A:869:GLN:NE2 | 1.85 | 0.75 |
| 1:A:903:VAL:HG22 | 1:A:970:VAL:HG13 | 1.68 | 0.75 |
| 1:B:851:ALA:HB2 | 1:B:973:ILE:HG13 | 1.68 | 0.75 |
| 1:B:54:ILE:O | 1:B:58:GLU:HG3 | 1.87 | 0.74 |
| 1:B:807:LEU:O | 1:B:810:ASN:HB2 | 1.86 | 0.74 |
| 1:A:326:MET:HB3 | 1:A:331:ALA:HB3 | 1.67 | 0.74 |
| 1:A:708:ALA:HB3 | 1:A:709:PRO:HD3 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:488:SER:HB3 | 1:B:491:ARG:HH21 | 1.51 | 0.74 |
| 1:B:75:LEU:HD11 | 1:B:300:VAL:HB | 1.68 | 0.74 |
| 1:A:914:ASN:ND2 | 1:A:922:LEU:HD11 | 2.03 | 0.74 |
| 1:A:65:LEU:HD13 | 1:A:307:ILE:HG21 | 1.70 | 0.74 |
| 1:B:950:VAL:HG12 | 1:B:952:PRO:HD2 | 1.70 | 0.74 |
| 1:A:786:ALA:O | 1:A:897:MET:HA | 1.88 | 0.74 |
| 1:A:897:MET:HE1 | 1:A:958:LYS:HB3 | 1.70 | 0.74 |
| 1:B:573:ARG:H | 1:B:573:ARG:CD | 2.01 | 0.74 |
| 1:B:308:PRO:HG3 | 1:B:765:ILE:HG22 | 1.70 | 0.74 |
| 1:B:421:ASN:HD22 | 1:B:423:SER:H | 1.33 | 0.73 |
| 1:B:40:GLU:OE1 | 1:B:143:ARG:HB2 | 1.88 | 0.73 |
| 1:A:171:THR:HG22 | 1:A:172:THR:HG23 | 1.71 | 0.73 |
| 1:A:852:ALA:HA | 1:A:899:MET:CG | 2.19 | 0.73 |
| 1:B:788:ILE:HG13 | 1:B:791:GLN:HB2 | 1.70 | 0.73 |
| 1:B:758:LYS:CB | 1:B:828:LEU:HD11 | 2.15 | 0.73 |
| 1:A:102:ALA:O | 1:A:106:VAL:HG23 | 1.89 | 0.73 |
| 1:B:749:GLU:O | 1:B:753:ILE:HD13 | 1.89 | 0.73 |
| 1:B:914:ASN:ND2 | 1:B:922:LEU:HD11 | 2.02 | 0.73 |
| 1:B:245:ASP:C | 1:B:246:LYS:CG | 2.57 | 0.72 |
| 1:B:611:ILE:HD12 | 1:B:621:VAL:HG11 | 1.70 | 0.72 |
| 1:A:100:ALA:O | 1:A:104:VAL:HG23 | 1.89 | 0.72 |
| 1:A:866:THR:N | 1:A:869:GLN:HE21 | 1.85 | 0.72 |
| 1:B:899:MET:CE | 1:B:966:GLN:O | 2.36 | 0.72 |
| 1:B:903:VAL:HG22 | 1:B:970:VAL:HG13 | 1.71 | 0.72 |
| 1:A:51:GLU:HA | 1:A:54:ILE:HD12 | 1.70 | 0.72 |
| 1:A:790:VAL:HG12 | 1:A:790:VAL:O | 1.89 | 0.72 |
| 1:A:364:CYS:O | 1:A:384:ILE:N | 2.21 | 0.72 |
| 1:A:899:MET:CE | 1:A:966:GLN:O | 2.38 | 0.72 |
| 1:B:866:THR:H | 1:B:869:GLN:NE2 | 1.86 | 0.72 |
| 1:B:76:ALA:HB1 | 1:B:88:PHE:HA | 1.72 | 0.71 |
| 1:B:852:ALA:HA | 1:B:899:MET:CG | 2.19 | 0.71 |
| 1:B:311:LEU:CB | 1:B:312:PRO:HD3 | 2.21 | 0.71 |
| 1:A:855:TRP:O | 1:A:859:ALA:HB3 | 1.89 | 0.71 |
| 1:A:926:PRO:O | 1:A:929:VAL:HG23 | 1.89 | 0.71 |
| 1:B:57:PHE:CZ | 1:B:102:ALA:CB | 2.73 | 0.71 |
| 1:B:802:LEU:N | 1:B:803:PRO:HD2 | 2.06 | 0.71 |
| 1:B:326:MET:HB3 | 1:B:331:ALA:HB3 | 1.71 | 0.71 |
| 1:B:51:GLU:HA | 1:B:54:ILE:HD12 | 1.70 | 0.71 |
| 1:B:611:ILE:HD12 | 1:B:621:VAL:HG21 | 1.72 | 0.71 |
| 1:B:349:CYS:HB3 | 1:B:624:ILE:CD1 | 2.20 | 0.70 |
| 1:A:112:ALA:HB1 | 1:A:334:ARG:HG2 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:PHE:O | 1:A:91:PRO:HD2 | 1.92 | 0.70 |
| 1:B:790:VAL:HG12 | 1:B:790:VAL:O | 1.92 | 0.70 |
| 1:A:573:ARG:CD | 1:A:573:ARG:H | 2.05 | 0.70 |
| 1:B:127:GLY:O | 1:B:140:ILE:HD13 | 1.90 | 0.70 |
| 1:A:40:GLU:OE1 | 1:A:143:ARG:HB2 | 1.91 | 0.70 |
| 1:B:844:VAL:CG2 | 1:B:907:ILE:HG21 | 2.21 | 0.70 |
| 1:A:817:MET:O | 1:A:819:ARG:N | 2.24 | 0.70 |
| 1:B:829:ILE:HD12 | 1:B:829:ILE:H | 1.56 | 0.70 |
| 1:B:866:THR:N | 1:B:869:GLN:HE21 | 1.88 | 0.70 |
| 1:A:181:THR:HB | 1:A:183:GLU:HG3 | 1.74 | 0.69 |
| 1:B:311:LEU:HB3 | 1:B:312:PRO:CD | 2.20 | 0.69 |
| 1:B:349:CYS:HB3 | 1:B:624:ILE:HD13 | 1.74 | 0.69 |
| 1:A:42:PRO:O | 1:A:43:ALA:C | 2.31 | 0.69 |
| 1:B:355:THR:HG23 | 1:B:720:MET:HG2 | 1.74 | 0.69 |
| 1:A:792:LEU:HA | 1:A:795:VAL:CG2 | 2.23 | 0.69 |
| 1:A:802:LEU:CD1 | 1:A:939:LEU:CG | 2.70 | 0.69 |
| 1:B:129:VAL:HG22 | 1:B:140:ILE:HD12 | 1.72 | 0.69 |
| 1:B:342:LEU:CG | 1:B:716:ILE:HG21 | 2.21 | 0.69 |
| 1:B:817:MET:O | 1:B:819:ARG:N | 2.24 | 0.69 |
| 1:B:852:ALA:HA | 1:B:899:MET:HB3 | 1.75 | 0.69 |
| 1:A:784:PRO:CD | 1:A:870:LEU:HD11 | 2.22 | 0.69 |
| 1:A:788:ILE:HB | 1:A:789:PRO:CD | 2.22 | 0.69 |
| 1:B:802:LEU:CD1 | 1:B:939:LEU:CG | 2.69 | 0.69 |
| 1:B:895:GLU:CG | 1:B:960:LYS:HD3 | 2.22 | 0.69 |
| 1:A:75:LEU:HD12 | 1:A:300:VAL:HB | 1.74 | 0.69 |
| 1:A:828:LEU:HG | 1:A:829:ILE:HG13 | 1.75 | 0.69 |
| 1:B:157:ASP:O | 1:B:214:ILE:HD12 | 1.93 | 0.69 |
| 1:B:762:ARG:NH2 | 1:B:918:GLU:HG3 | 2.08 | 0.69 |
| 1:B:412:GLU:OE1 | 1:B:529:ARG:HD2 | 1.93 | 0.69 |
| 1:B:61:LEU:CD1 | 1:B:311:LEU:HD23 | 2.23 | 0.69 |
| 1:B:757:MET:O | 1:B:761:ILE:HG12 | 1.92 | 0.69 |
| 1:B:853:ALA:O | 1:B:856:PHE:HB2 | 1.93 | 0.69 |
| 1:A:844:VAL:CG2 | 1:A:907:ILE:HG21 | 2.22 | 0.68 |
| 1:B:299:ALA:HA | 1:B:302:LEU:HD11 | 1.73 | 0.68 |
| 1:B:56:GLN:HG3 | 1:B:106:VAL:HG23 | 1.75 | 0.68 |
| 1:A:944:HIS:O | 1:A:947:ILE:HG22 | 1.93 | 0.68 |
| 1:B:802:LEU:CD1 | 1:B:939:LEU:CD2 | 2.65 | 0.68 |
| 1:A:489:ARG:H | 1:A:489:ARG:CD | 2.07 | 0.68 |
| 1:A:895:GLU:CG | 1:A:960:LYS:HD3 | 2.23 | 0.68 |
| 1:A:931:ILE:HD12 | 1:A:931:ILE:H | 1.59 | 0.68 |
| 1:B:308:PRO:CG | 1:B:765:ILE:HG22 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:792:LEU:HA | 1:B:795:VAL:CG2 | 2.23 | 0.68 |
| 1:B:129:VAL:HG11 | 1:B:145:ILE:HD12 | 1.76 | 0.68 |
| 1:A:111:ASN:O | 1:A:114:ASN:HB2 | 1.92 | 0.68 |
| 1:B:49:LEU:CD1 | 1:B:110:ARG:HG3 | 2.23 | 0.68 |
| 1:B:67:LEU:O | 1:B:71:ILE:HG12 | 1.94 | 0.68 |
| 1:B:849:VAL:O | 1:B:853:ALA:CB | 2.41 | 0.68 |
| 1:A:311:LEU:HG | 1:A:315:ILE:HD13 | 1.75 | 0.68 |
| 1:A:963:ASP:H | 1:A:966:GLN:HE21 | 1.42 | 0.68 |
| 1:B:61:LEU:HD11 | 1:B:311:LEU:HD23 | 1.74 | 0.68 |
| 1:B:767:SER:O | 1:B:771:GLU:HG3 | 1.93 | 0.68 |
| 1:B:898:THR:OG1 | 1:B:959:LEU:CB | 2.42 | 0.68 |
| 1:A:412:GLU:OE1 | 1:A:529:ARG:HD2 | 1.93 | 0.68 |
| 1:A:899:MET:SD | 1:A:962:LEU:CD1 | 2.82 | 0.68 |
| 1:A:802:LEU:N | 1:A:803:PRO:HD2 | 2.09 | 0.67 |
| 1:A:600:LEU:HD13 | 1:A:600:LEU:O | 1.94 | 0.67 |
| 1:B:489:ARG:CD | 1:B:489:ARG:H | 2.07 | 0.67 |
| 1:B:931:ILE:H | 1:B:931:ILE:HD12 | 1.59 | 0.67 |
| 1:A:69:ALA:O | 1:A:73:PHE:HB2 | 1.94 | 0.67 |
| 1:A:769:VAL:O | 1:A:773:VAL:HG23 | 1.95 | 0.67 |
| 1:A:817:MET:C | 1:A:819:ARG:H | 1.97 | 0.67 |
| 1:A:767:SER:O | 1:A:771:GLU:HG3 | 1.93 | 0.67 |
| 1:A:762:ARG:NH2 | 1:A:918:GLU:HG3 | 2.10 | 0.67 |
| 1:B:784:PRO:CD | 1:B:870:LEU:HD11 | 2.24 | 0.67 |
| 1:B:817:MET:C | 1:B:819:ARG:H | 1.97 | 0.67 |
| 1:A:261:SER:O | 1:A:264:ILE:HG12 | 1.93 | 0.67 |
| 1:A:829:ILE:H | 1:A:829:ILE:HD12 | 1.59 | 0.67 |
| 1:A:120:LYS:NZ | 1:A:723:GLY:O | 2.24 | 0.67 |
| 1:B:786:ALA:HB2 | 1:B:849:VAL:HG13 | 1.77 | 0.67 |
| 1:A:65:LEU:HG | 1:A:94:ILE:HD11 | 1.77 | 0.66 |
| 1:A:788:ILE:CD1 | 1:A:791:GLN:HB2 | 2.24 | 0.66 |
| 1:A:786:ALA:HB2 | 1:A:849:VAL:HG13 | 1.77 | 0.66 |
| 1:A:898:THR:OG1 | 1:A:959:LEU:CB | 2.43 | 0.66 |
| 1:B:252:LYS:HE3 | 1:B:252:LYS:HA | 1.77 | 0.66 |
| 1:B:172:THR:HG23 | 1:B:489:ARG:HD2 | 1.77 | 0.66 |
| 1:A:950:VAL:O | 1:A:954:PRO:HD2 | 1.94 | 0.66 |
| 1:B:651:ARG:HG3 | 1:B:651:ARG:HH11 | 1.59 | 0.66 |
| 1:A:308:PRO:HB2 | 1:A:764:LEU:HD23 | 1.76 | 0.66 |
| 1:A:334:ARG:HB3 | 1:A:334:ARG:HH11 | 1.60 | 0.66 |
| 1:A:774:CYS:SG | 1:A:786:ALA:HB3 | 2.35 | 0.66 |
| 1:A:622:ILE:CD1 | 1:A:674:CYS:HA | 2.23 | 0.66 |
| 1:A:247:THR:HG23 | 1:A:250:GLN:HG2 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:567:ARG:NH1 | 1:A:571:PRO:HD3 | 2.10 | 0.66 |
| 1:B:863:PRO:HB2 | 1:B:865:VAL:HG23 | 1.76 | 0.66 |
| 1:A:639:ILE:HD11 | 1:A:641:ILE:HD12 | 1.77 | 0.66 |
| 1:B:86:THR:HA | 1:B:89:VAL:HG23 | 1.77 | 0.66 |
| 1:B:944:HIS:O | 1:B:947:ILE:HG22 | 1.96 | 0.66 |
| 1:B:893:ALA:HB1 | 1:B:895:GLU:OE1 | 1.95 | 0.66 |
| 1:B:897:MET:CE | 1:B:958:LYS:HB3 | 2.25 | 0.66 |
| 1:B:963:ASP:H | 1:B:966:GLN:HE21 | 1.44 | 0.65 |
| 1:A:54:ILE:O | 1:A:58:GLU:HG3 | 1.96 | 0.65 |
| 1:A:651:ARG:HH11 | 1:A:651:ARG:HG3 | 1.61 | 0.65 |
| 1:A:680:GLU:HB3 | 1:A:681:PRO:HD2 | 1.77 | 0.65 |
| 1:A:852:ALA:HA | 1:A:899:MET:HB3 | 1.78 | 0.65 |
| 1:B:314:VAL:HG11 | 1:B:804:ALA:HB1 | 1.76 | 0.65 |
| 1:A:762:ARG:HH22 | 1:A:918:GLU:HA | 1.61 | 0.65 |
| 1:B:567:ARG:NH1 | 1:B:571:PRO:HD3 | 2.12 | 0.65 |
| 1:B:247:THR:HG21 | 1:B:337:PRO:HB2 | 1.79 | 0.65 |
| 1:B:611:ILE:CD1 | 1:B:621:VAL:HG11 | 2.25 | 0.65 |
| 1:A:25:THR:HA | 1:A:132:ALA:HB3 | 1.77 | 0.65 |
| 1:A:784:PRO:HD2 | 1:A:870:LEU:HD11 | 1.77 | 0.65 |
| 1:B:899:MET:SD | 1:B:962:LEU:CD1 | 2.84 | 0.65 |
| 1:A:232:ILE:HD13 | 1:A:232:ILE:O | 1.97 | 0.65 |
| 1:A:803:PRO:O | 1:A:806:ALA:CB | 2.40 | 0.65 |
| 1:A:259:GLN:O | 1:A:263:VAL:HG23 | 1.96 | 0.65 |
| 1:A:760:PHE:CB | 1:A:807:LEU:HD12 | 2.25 | 0.64 |
| 1:B:832:TRP:CZ3 | 1:B:835:PHE:CD2 | 2.85 | 0.64 |
| 1:A:97:ILE:O | 1:A:100:ALA:HB3 | 1.98 | 0.64 |
| 1:A:113:GLU:O | 1:A:117:GLU:HG2 | 1.97 | 0.64 |
| 1:B:252:LYS:HA | 1:B:252:LYS:CE | 2.28 | 0.64 |
| 1:A:300:VAL:HA | 1:A:303:ALA:HB3 | 1.80 | 0.64 |
| 1:A:600:LEU:O | 1:A:602:PRO:HD3 | 1.97 | 0.64 |
| 1:B:55:GLU:HA | 1:B:58:GLU:OE1 | 1.97 | 0.64 |
| 1:A:795:VAL:HG22 | 1:A:901:LEU:HD11 | 1.80 | 0.64 |
| 1:A:857:MET:HB2 | 1:A:858:TYR:CE1 | 2.32 | 0.64 |
| 1:A:286:GLY:CA | 1:A:290:ARG:HB3 | 2.27 | 0.64 |
| 1:A:342:LEU:HG | 1:A:716:ILE:HG21 | 1.78 | 0.64 |
| 1:A:853:ALA:O | 1:A:856:PHE:HB2 | 1.97 | 0.64 |
| 1:B:303:ALA:O | 1:B:306:ALA:HB3 | 1.98 | 0.64 |
| 1:A:300:VAL:HA | 1:A:303:ALA:CB | 2.28 | 0.64 |
| 1:B:322:GLY:CA | 1:B:325:ARG:HH21 | 2.11 | 0.64 |
| 1:B:857:MET:HB2 | 1:B:858:TYR:CE1 | 2.32 | 0.64 |
| 1:A:600:LEU:HD13 | 1:A:600:LEU:C | 2.19 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:893:ALA:HB1 | 1:A:895:GLU:OE1 | 1.96 | 0.64 |
| 1:B:214:ILE:H | 1:B:214:ILE:HD12 | 1.62 | 0.64 |
| 1:B:329:LYS:O | 1:B:330:ASN:HB2 | 1.97 | 0.63 |
| 1:B:567:ARG:NH1 | 1:B:570:PRO:HA | 2.13 | 0.63 |
| 1:B:715:GLU:O | 1:B:716:ILE:HD13 | 1.97 | 0.63 |
| 1:B:778:THR:HB | 1:B:783:LEU:O | 1.98 | 0.63 |
| 1:A:311:LEU:HG | 1:A:315:ILE:CD1 | 2.28 | 0.63 |
| 1:A:322:GLY:N | 1:A:325:ARG:HH21 | 1.97 | 0.63 |
| 1:B:298:ILE:HD12 | 1:B:299:ALA:N | 2.14 | 0.63 |
| 1:A:783:LEU:HA | 1:A:870:LEU:HG | 1.81 | 0.63 |
| 1:A:832:TRP:CZ3 | 1:A:835:PHE:CD2 | 2.86 | 0.63 |
| 1:B:298:ILE:O | 1:B:302:LEU:HG | 1.98 | 0.63 |
| 1:B:49:LEU:HD13 | 1:B:110:ARG:NE | 2.10 | 0.63 |
| 1:B:781:LEU:HD23 | 1:B:782:GLY:N | 2.13 | 0.63 |
| 1:B:803:PRO:O | 1:B:806:ALA:CB | 2.42 | 0.63 |
| 1:A:577:VAL:HG11 | 1:A:583:ARG:NH1 | 2.14 | 0.63 |
| 1:A:784:PRO:CD | 1:A:870:LEU:CD1 | 2.76 | 0.63 |
| 1:B:49:LEU:HD11 | 1:B:110:ARG:HG3 | 1.80 | 0.63 |
| 1:B:384:ILE:N | 1:B:384:ILE:HD12 | 2.13 | 0.63 |
| 1:B:335:SER:HB3 | 1:B:338:SER:OG | 1.98 | 0.63 |
| 1:B:774:CYS:SG | 1:B:786:ALA:HB3 | 2.38 | 0.63 |
| 1:B:917:SER:OG | 1:B:920:GLN:HB2 | 1.98 | 0.63 |
| 1:A:55:GLU:HA | 1:A:58:GLU:OE1 | 1.99 | 0.63 |
| 1:B:129:VAL:HG22 | 1:B:140:ILE:CD1 | 2.28 | 0.63 |
| 1:B:49:LEU:CD1 | 1:B:110:ARG:NE | 2.60 | 0.63 |
| 1:B:788:ILE:HB | 1:B:789:PRO:CD | 2.29 | 0.63 |
| 1:B:157:ASP:O | 1:B:214:ILE:CD1 | 2.46 | 0.62 |
| 1:A:369:ILE:H | 1:A:369:ILE:HD12 | 1.64 | 0.62 |
| 1:A:395:VAL:O | 1:A:402:ILE:HD13 | 1.99 | 0.62 |
| 1:B:75:LEU:CD1 | 1:B:300:VAL:HB | 2.29 | 0.62 |
| 1:B:795:VAL:HG22 | 1:B:901:LEU:HD11 | 1.80 | 0.62 |
| 1:A:620:ARG:NH2 | 1:A:622:ILE:HD11 | 2.13 | 0.62 |
| 1:B:42:PRO:O | 1:B:43:ALA:C | 2.38 | 0.62 |
| 1:B:577:VAL:HG11 | 1:B:583:ARG:NH1 | 2.14 | 0.62 |
| 1:B:622:ILE:CD1 | 1:B:674:CYS:HA | 2.28 | 0.62 |
| 1:B:150:ILE:HD12 | 1:B:150:ILE:N | 2.14 | 0.62 |
| 1:B:242:THR:O | 1:B:712:LYS:HE2 | 1.99 | 0.62 |
| 1:A:188:ILE:HD12 | 1:A:188:ILE:N | 2.15 | 0.62 |
| 1:A:2:GLU:O | 1:A:3:ALA:HB3 | 2.00 | 0.62 |
| 1:A:527:TYR:HB3 | 1:A:534:ARG:HG3 | 1.82 | 0.62 |
| 1:A:866:THR:HG23 | 1:A:869:GLN:NE2 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:828:LEU:HG | 1:B:829:ILE:HG13 | 1.80 | 0.62 |
| 1:B:969:MET:O | 1:B:973:ILE:HG12 | 1.99 | 0.62 |
| 1:A:606:GLU:H | 1:A:606:GLU:CD | 2.04 | 0.62 |
| 1:B:784:PRO:HD3 | 1:B:870:LEU:CD1 | 2.30 | 0.62 |
| 1:A:121:GLU:O | 1:A:121:GLU:OE2 | 2.16 | 0.61 |
| 1:B:319:LEU:HD21 | 1:B:337:PRO:HA | 1.81 | 0.61 |
| 1:B:783:LEU:H | 1:B:783:LEU:CD1 | 2.07 | 0.61 |
| 1:A:248:PRO:CG | 1:A:341:THR:HG23 | 2.30 | 0.61 |
| 1:A:917:SER:OG | 1:A:920:GLN:HB2 | 1.99 | 0.61 |
| 1:B:762:ARG:HH22 | 1:B:918:GLU:HA | 1.63 | 0.61 |
| 1:B:952:PRO:O | 1:B:956:ILE:HG12 | 2.00 | 0.61 |
| 1:A:120:LYS:HE2 | 1:A:728:LYS:HZ1 | 1.64 | 0.61 |
| 1:A:795:VAL:O | 1:A:799:THR:HB | 2.01 | 0.61 |
| 1:A:897:MET:CE | 1:A:958:LYS:HB3 | 2.30 | 0.61 |
| 1:B:769:VAL:O | 1:B:773:VAL:HG23 | 2.00 | 0.61 |
| 1:B:781:LEU:C | 1:B:781:LEU:HD23 | 2.21 | 0.61 |
| 1:B:83:GLU:O | 1:B:87:ALA:HB2 | 2.00 | 0.61 |
| 1:A:792:LEU:HA | 1:A:795:VAL:HG23 | 1.82 | 0.61 |
| 1:A:969:MET:O | 1:A:973:ILE:HG12 | 2.00 | 0.61 |
| 1:B:527:TYR:HB3 | 1:B:534:ARG:HG3 | 1.83 | 0.61 |
| 1:B:907:ILE:HD11 | 1:B:974:SER:HA | 1.81 | 0.61 |
| 1:A:795:VAL:CG2 | 1:A:901:LEU:HD11 | 2.30 | 0.61 |
| 1:B:518:PRO:O | 1:B:522:ILE:CD1 | 2.46 | 0.61 |
| 1:B:59:ASP:HB3 | 1:B:62:VAL:HG23 | 1.83 | 0.61 |
| 1:B:639:ILE:HD11 | 1:B:641:ILE:HD12 | 1.82 | 0.61 |
| 1:A:572:LYS:N | 1:A:572:LYS:HD2 | 2.16 | 0.61 |
| 1:A:67:LEU:O | 1:A:71:ILE:HG13 | 2.01 | 0.61 |
| 1:A:907:ILE:HD11 | 1:A:974:SER:HA | 1.82 | 0.61 |
| 1:A:275:ASN:HA | 1:A:295:TYR:OH | 2.00 | 0.61 |
| 1:B:311:LEU:CD1 | 1:B:761:ILE:CD1 | 2.74 | 0.61 |
| 1:A:121:GLU:O | 1:A:121:GLU:CD | 2.39 | 0.61 |
| 1:A:412:GLU:OE2 | 1:A:566:THR:HG21 | 2.01 | 0.61 |
| 1:A:775:ILE:N | 1:A:775:ILE:CD1 | 2.63 | 0.61 |
| 1:A:802:LEU:CD1 | 1:A:939:LEU:CD2 | 2.67 | 0.61 |
| 1:B:2:GLU:O | 1:B:3:ALA:HB3 | 2.01 | 0.61 |
| 1:A:802:LEU:N | 1:A:803:PRO:CD | 2.64 | 0.61 |
| 1:A:520:GLY:O | 1:A:524:ARG:HG3 | 2.00 | 0.60 |
| 1:A:528:VAL:HG21 | 1:A:541:VAL:HG11 | 1.82 | 0.60 |
| 1:A:759:GLN:HA | 1:A:762:ARG:HD2 | 1.83 | 0.60 |
| 1:B:792:LEU:HA | 1:B:795:VAL:HG23 | 1.83 | 0.60 |
| 1:A:315:ILE:O | 1:A:319:LEU:HB2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:813:ASP:OD2 | 1:B:813:ASP:N | 2.29 | 0.60 |
| 1:B:867:TYR:O | 1:B:871:THR:HG23 | 2.01 | 0.60 |
| 1:A:755:ASN:O | 1:A:759:GLN:HG2 | 2.01 | 0.60 |
| 1:A:784:PRO:HD3 | 1:A:870:LEU:CD1 | 2.32 | 0.60 |
| 1:B:351:ASP:HB3 | 1:B:355:THR:OG1 | 2.01 | 0.60 |
| 1:B:572:LYS:HD2 | 1:B:572:LYS:N | 2.16 | 0.60 |
| 1:A:310:GLY:O | 1:A:314:VAL:HG23 | 2.02 | 0.60 |
| 1:B:749:GLU:HG3 | 1:B:753:ILE:HD13 | 1.81 | 0.60 |
| 1:B:968:LEU:O | 1:B:972:LYS:HG2 | 2.01 | 0.60 |
| 1:A:778:THR:HB | 1:A:783:LEU:O | 2.01 | 0.60 |
| 1:A:617:ALA:O | 1:A:821:PRO:HD3 | 2.01 | 0.60 |
| 1:B:795:VAL:CG2 | 1:B:901:LEU:HD11 | 2.30 | 0.60 |
| 1:A:781:LEU:HD23 | 1:A:782:GLY:N | 2.17 | 0.60 |
| 1:A:914:ASN:C | 1:A:916:LEU:H | 2.05 | 0.60 |
| 1:B:802:LEU:N | 1:B:803:PRO:CD | 2.63 | 0.60 |
| 1:B:95:LEU:HD23 | 1:B:96:LEU:N | 2.16 | 0.60 |
| 1:A:786:ALA:C | 1:A:787:LEU:HG | 2.21 | 0.60 |
| 1:B:421:ASN:C | 1:B:421:ASN:HD22 | 2.05 | 0.60 |
| 1:B:786:ALA:C | 1:B:787:LEU:HG | 2.21 | 0.60 |
| 1:B:784:PRO:HD2 | 1:B:870:LEU:HD11 | 1.81 | 0.60 |
| 1:A:119:LEU:O | 1:A:122:TYR:HB3 | 2.02 | 0.60 |
| 1:A:326:MET:C | 1:A:331:ALA:HB3 | 2.22 | 0.60 |
| 1:A:567:ARG:NH1 | 1:A:570:PRO:HA | 2.13 | 0.60 |
| 1:B:319:LEU:HD23 | 1:B:336:LEU:HB3 | 1.84 | 0.60 |
| 1:A:489:ARG:H | 1:A:489:ARG:NE | 1.99 | 0.59 |
| 1:B:577:VAL:HG11 | 1:B:583:ARG:HH11 | 1.67 | 0.59 |
| 1:B:760:PHE:CB | 1:B:807:LEU:HD12 | 2.29 | 0.59 |
| 1:B:865:VAL:HG13 | 1:B:869:GLN:HG3 | 1.83 | 0.59 |
| 1:B:852:ALA:HA | 1:B:899:MET:CB | 2.32 | 0.59 |
| 1:A:271:VAL:HG12 | 1:A:275:ASN:HD21 | 1.67 | 0.59 |
| 1:A:577:VAL:HG11 | 1:A:583:ARG:HH11 | 1.67 | 0.59 |
| 1:A:94:ILE:O | 1:A:98:LEU:HG | 2.02 | 0.59 |
| 1:B:489:ARG:NE | 1:B:489:ARG:H | 2.00 | 0.59 |
| 1:A:303:ALA:O | 1:A:306:ALA:HB3 | 2.03 | 0.59 |
| 1:B:57:PHE:CE1 | 1:B:102:ALA:HB2 | 2.36 | 0.59 |
| 1:B:855:TRP:CA | 1:B:859:ALA:CB | 2.73 | 0.59 |
| 1:B:826:GLU:HG2 | 1:B:827:PRO:HD2 | 1.85 | 0.59 |
| 1:A:95:LEU:HA | 1:A:98:LEU:CD1 | 2.32 | 0.59 |
| 1:B:708:ALA:HB3 | 1:B:709:PRO:HD3 | 1.85 | 0.59 |
| 1:B:759:GLN:HA | 1:B:762:ARG:HD2 | 1.84 | 0.59 |
| 1:B:784:PRO:CD | 1:B:870:LEU:CD1 | 2.80 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:ILE:HD12 | 1:A:188:ILE:H | 1.67 | 0.59 |
| 1:A:247:THR:HG23 | 1:A:250:GLN:CG | 2.31 | 0.59 |
| 1:A:762:ARG:HB3 | 1:A:837:TYR:CE2 | 2.38 | 0.59 |
| 1:A:869:GLN:OE1 | 1:A:883:PHE:HB3 | 2.02 | 0.59 |
| 1:B:214:ILE:N | 1:B:214:ILE:HD12 | 2.17 | 0.59 |
| 1:B:317:THR:O | 1:B:321:LEU:HG | 2.03 | 0.59 |
| 1:B:369:ILE:HD12 | 1:B:369:ILE:H | 1.66 | 0.59 |
| 1:A:334:ARG:CB | 1:A:334:ARG:HH11 | 2.16 | 0.59 |
| 1:A:369:ILE:HD13 | 1:A:529:ARG:O | 2.03 | 0.59 |
| 1:A:826:GLU:HG2 | 1:A:827:PRO:HD2 | 1.85 | 0.59 |
| 1:B:18:VAL:HG21 | 1:B:150:ILE:HD11 | 1.85 | 0.59 |
| 1:A:334:ARG:NH1 | 1:A:334:ARG:HB3 | 2.18 | 0.58 |
| 1:A:369:ILE:HG12 | 1:A:528:VAL:CG1 | 2.33 | 0.58 |
| 1:B:322:GLY:HA2 | 1:B:325:ARG:HH21 | 1.68 | 0.58 |
| 1:B:950:VAL:O | 1:B:954:PRO:HD2 | 2.02 | 0.58 |
| 1:A:311:LEU:O | 1:A:315:ILE:HD13 | 2.03 | 0.58 |
| 1:A:413:LEU:HG | 1:A:564:LEU:HD12 | 1.85 | 0.58 |
| 1:A:65:LEU:O | 1:A:68:ALA:HB3 | 2.04 | 0.58 |
| 1:B:421:ASN:HD22 | 1:B:422:ASP:N | 2.01 | 0.58 |
| 1:B:89:VAL:O | 1:B:93:VAL:HG23 | 2.04 | 0.58 |
| 1:A:41:LEU:HD11 | 1:A:233:GLY:HA2 | 1.85 | 0.58 |
| 1:A:120:LYS:CE | 1:A:728:LYS:NZ | 2.63 | 0.58 |
| 1:B:53:VAL:HG22 | 1:B:106:VAL:HG21 | 1.85 | 0.58 |
| 1:B:869:GLN:OE1 | 1:B:883:PHE:HB3 | 2.03 | 0.58 |
| 1:A:247:THR:HG1 | 1:A:250:GLN:HB3 | 1.63 | 0.58 |
| 1:A:90:GLU:HG3 | 1:A:91:PRO:N | 2.18 | 0.58 |
| 1:A:968:LEU:O | 1:A:972:LYS:HG2 | 2.03 | 0.58 |
| 1:A:355:THR:HG23 | 1:A:720:MET:HG2 | 1.85 | 0.58 |
| 1:A:814:LEU:H | 1:A:814:LEU:HD23 | 1.68 | 0.58 |
| 1:A:863:PRO:HB2 | 1:A:865:VAL:HG23 | 1.84 | 0.58 |
| 1:B:121:GLU:O | 1:B:121:GLU:HG2 | 2.02 | 0.58 |
| 1:B:556:ARG:HG2 | 1:B:644:GLU:HG3 | 1.85 | 0.58 |
| 1:A:421:ASN:HD22 | 1:A:422:ASP:N | 2.02 | 0.58 |
| 1:A:725:ALA:O | 1:A:729:THR:HG23 | 2.04 | 0.58 |
| 1:A:963:ASP:N | 1:A:966:GLN:HE21 | 2.01 | 0.58 |
| 1:A:964:LEU:O | 1:A:968:LEU:HG | 2.03 | 0.58 |
| 1:B:113:GLU:O | 1:B:117:GLU:HG2 | 2.03 | 0.58 |
| 1:B:364:CYS:O | 1:B:384:ILE:HD13 | 2.03 | 0.58 |
| 1:B:865:VAL:HG13 | 1:B:869:GLN:CG | 2.33 | 0.58 |
| 1:A:801:GLY:C | 1:A:803:PRO:HD2 | 2.24 | 0.58 |
| 1:B:964:LEU:O | 1:B:968:LEU:HG | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:184:SER:HB3 | 1:A:627:ASP:OD2 | 2.04 | 0.58 |
| 1:A:308:PRO:HG3 | 1:A:765:ILE:HG12 | 1.84 | 0.58 |
| 1:A:783:LEU:N | 1:A:783:LEU:HD12 | 2.12 | 0.58 |
| 1:B:340:GLU:HG2 | 1:B:750:GLY:O | 2.04 | 0.58 |
| 1:B:663:LEU:CD1 | 1:B:663:LEU:H | 2.17 | 0.58 |
| 1:B:783:LEU:HA | 1:B:870:LEU:HG | 1.86 | 0.58 |
| 1:B:833:LEU:HD12 | 1:B:836:ARG:HD3 | 1.86 | 0.58 |
| 1:A:39:ASN:O | 1:A:40:GLU:HB3 | 2.02 | 0.57 |
| 1:B:783:LEU:N | 1:B:783:LEU:HD12 | 2.09 | 0.57 |
| 1:A:338:SER:HA | 1:A:341:THR:HB | 1.86 | 0.57 |
| 1:A:952:PRO:O | 1:A:956:ILE:HG12 | 2.04 | 0.57 |
| 1:B:342:LEU:HG | 1:B:716:ILE:CG2 | 2.29 | 0.57 |
| 1:A:788:ILE:HD12 | 1:A:791:GLN:HB2 | 1.86 | 0.57 |
| 1:A:852:ALA:HA | 1:A:899:MET:HG2 | 1.86 | 0.57 |
| 1:B:898:THR:OG1 | 1:B:959:LEU:CA | 2.52 | 0.57 |
| 1:A:715:GLU:HB3 | 1:A:716:ILE:HD12 | 1.86 | 0.57 |
| 1:A:847:ALA:HB1 | 1:A:903:VAL:HG11 | 1.85 | 0.57 |
| 1:B:364:CYS:C | 1:B:384:ILE:HD13 | 2.25 | 0.57 |
| 1:B:914:ASN:C | 1:B:916:LEU:H | 2.06 | 0.57 |
| 1:A:39:ASN:O | 1:A:143:ARG:HA | 2.05 | 0.57 |
| 1:A:760:PHE:O | 1:A:764:LEU:HB2 | 2.05 | 0.57 |
| 1:B:795:VAL:O | 1:B:799:THR:HB | 2.04 | 0.57 |
| 1:B:91:PRO:O | 1:B:94:ILE:HG22 | 2.04 | 0.57 |
| 1:A:341:THR:CG2 | 1:A:716:ILE:HD11 | 2.24 | 0.57 |
| 1:A:833:LEU:HD12 | 1:A:836:ARG:HD3 | 1.87 | 0.57 |
| 1:B:413:LEU:HG | 1:B:564:LEU:HD12 | 1.86 | 0.57 |
| 1:A:898:THR:HA | 1:A:959:LEU:CD2 | 2.22 | 0.57 |
| 1:B:528:VAL:HG21 | 1:B:541:VAL:HG11 | 1.85 | 0.57 |
| 1:A:867:TYR:O | 1:A:871:THR:HG23 | 2.04 | 0.56 |
| 1:B:384:ILE:N | 1:B:384:ILE:CD1 | 2.67 | 0.56 |
| 1:B:412:GLU:OE2 | 1:B:566:THR:HG21 | 2.04 | 0.56 |
| 1:B:898:THR:HA | 1:B:959:LEU:CD2 | 2.23 | 0.56 |
| 1:A:315:ILE:CD1 | 1:A:760:PHE:HE1 | 2.18 | 0.56 |
| 1:A:782:GLY:HA3 | 1:A:871:THR:HB | 1.88 | 0.56 |
| 1:B:520:GLY:O | 1:B:524:ARG:HG3 | 2.04 | 0.56 |
| 1:A:865:VAL:HG12 | 1:A:866:THR:O | 2.05 | 0.56 |
| 1:A:802:LEU:HD11 | 1:A:939:LEU:HG | 1.87 | 0.56 |
| 1:B:762:ARG:HB3 | 1:B:837:TYR:CE2 | 2.40 | 0.56 |
| 1:A:756:ASN:O | 1:A:759:GLN:HB2 | 2.05 | 0.56 |
| 1:B:749:GLU:HG3 | 1:B:753:ILE:CD1 | 2.34 | 0.56 |
| 1:A:311:LEU:CD2 | 1:A:761:ILE:HG23 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:311:LEU:O | 1:B:315:ILE:HG12 | 2.06 | 0.56 |
| 1:B:606:GLU:CD | 1:B:606:GLU:H | 2.07 | 0.56 |
| 1:B:620:ARG:NH2 | 1:B:622:ILE:HD11 | 2.19 | 0.56 |
| 1:A:402:ILE:HD13 | 1:A:402:ILE:H | 1.70 | 0.56 |
| 1:A:423:SER:HB3 | 1:A:437:VAL:O | 2.05 | 0.56 |
| 1:B:847:ALA:HB1 | 1:B:903:VAL:HG11 | 1.86 | 0.56 |
| 1:B:369:ILE:HD13 | 1:B:529:ARG:O | 2.05 | 0.56 |
| 1:B:41:LEU:HD11 | 1:B:233:GLY:HA2 | 1.87 | 0.56 |
| 1:B:423:SER:HB3 | 1:B:437:VAL:O | 2.04 | 0.56 |
| 1:B:633:ILE:HD11 | 1:B:652:ALA:CB | 2.36 | 0.56 |
| 1:B:866:THR:HG23 | 1:B:869:GLN:NE2 | 2.20 | 0.56 |
| 1:A:360:GLN:HB3 | 1:A:389:TYR:CE2 | 2.40 | 0.56 |
| 1:A:364:CYS:HA | 1:A:384:ILE:HB | 1.87 | 0.56 |
| 1:A:840:ILE:CD1 | 1:A:840:ILE:N | 2.69 | 0.56 |
| 1:A:852:ALA:HA | 1:A:899:MET:CB | 2.34 | 0.56 |
| 1:B:463:SER:OG | 1:B:465:VAL:HG22 | 2.05 | 0.56 |
| 1:B:600:LEU:HD13 | 1:B:600:LEU:C | 2.25 | 0.56 |
| 1:B:651:ARG:HG3 | 1:B:651:ARG:NH1 | 2.21 | 0.56 |
| 1:B:814:LEU:H | 1:B:814:LEU:HD23 | 1.70 | 0.56 |
| 1:A:355:THR:HG21 | 1:A:701:THR:HG22 | 1.88 | 0.56 |
| 1:A:963:ASP:OD2 | 1:A:964:LEU:N | 2.38 | 0.56 |
| 1:B:825:LYS:O | 1:B:826:GLU:C | 2.42 | 0.56 |
| 1:A:421:ASN:C | 1:A:421:ASN:HD22 | 2.07 | 0.56 |
| 1:A:781:LEU:C | 1:A:781:LEU:HD23 | 2.26 | 0.56 |
| 1:A:825:LYS:O | 1:A:826:GLU:C | 2.43 | 0.56 |
| 1:B:157:ASP:CB | 1:B:214:ILE:HD13 | 2.35 | 0.56 |
| 1:B:239:MET:CE | 1:B:708:ALA:HB1 | 2.36 | 0.56 |
| 1:A:318:CYS:O | 1:A:321:LEU:HB2 | 2.06 | 0.56 |
| 1:B:267:ILE:HD13 | 1:B:302:LEU:HD13 | 1.88 | 0.56 |
| 1:B:342:LEU:HD11 | 1:B:718:ILE:CD1 | 2.35 | 0.56 |
| 1:B:792:LEU:HA | 1:B:795:VAL:HG21 | 1.88 | 0.56 |
| 1:B:832:TRP:CZ3 | 1:B:835:PHE:HD2 | 2.23 | 0.56 |
| 1:B:963:ASP:N | 1:B:966:GLN:HE21 | 2.03 | 0.56 |
| 1:A:771:GLU:HG2 | 1:A:792:LEU:HD13 | 1.88 | 0.55 |
| 1:A:309:GLU:OE2 | 1:A:796:ASN:HB2 | 2.06 | 0.55 |
| 1:B:816:ILE:HA | 1:B:819:ARG:NH2 | 2.16 | 0.55 |
| 1:A:355:THR:CG2 | 1:A:701:THR:HG22 | 2.36 | 0.55 |
| 1:A:759:GLN:HE22 | 1:A:762:ARG:HH11 | 1.54 | 0.55 |
| 1:B:121:GLU:O | 1:B:121:GLU:CG | 2.54 | 0.55 |
| 1:B:848:THR:O | 1:B:852:ALA:HB3 | 2.06 | 0.55 |
| 1:A:795:VAL:HA | 1:A:799:THR:OG1 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:832:TRP:CZ3 | 1:A:835:PHE:HD2 | 2.24 | 0.55 |
| 1:B:705:VAL:HG22 | 1:B:726:VAL:HG21 | 1.89 | 0.55 |
| 1:B:311:LEU:CD1 | 1:B:761:ILE:HD12 | 2.30 | 0.55 |
| 1:B:852:ALA:HA | 1:B:899:MET:HG2 | 1.89 | 0.55 |
| 1:A:249:LEU:O | 1:A:252:LYS:HB2 | 2.06 | 0.55 |
| 1:A:600:LEU:CD1 | 1:A:600:LEU:C | 2.75 | 0.55 |
| 1:A:879:ASP:OD1 | 1:A:882:HIS:HB2 | 2.07 | 0.55 |
| 1:B:315:ILE:HD11 | 1:B:757:MET:CE | 2.37 | 0.55 |
| 1:B:557:ASP:HB3 | 1:B:559:LEU:HG | 1.89 | 0.55 |
| 1:A:329:LYS:O | 1:A:330:ASN:HB2 | 2.07 | 0.55 |
| 1:A:757:MET:HG2 | 1:A:760:PHE:HZ | 1.65 | 0.55 |
| 1:A:792:LEU:HA | 1:A:795:VAL:HG21 | 1.87 | 0.55 |
| 1:A:899:MET:SD | 1:A:962:LEU:HD22 | 2.46 | 0.55 |
| 1:B:662:PRO:HG2 | 1:B:665:GLU:HG2 | 1.87 | 0.55 |
| 1:B:771:GLU:HG2 | 1:B:792:LEU:HD13 | 1.89 | 0.55 |
| 1:A:866:THR:HG23 | 1:A:869:GLN:HE21 | 1.72 | 0.55 |
| 1:A:894:PRO:HB2 | 1:A:959:LEU:C | 2.26 | 0.55 |
| 1:B:39:ASN:O | 1:B:143:ARG:HA | 2.07 | 0.55 |
| 1:B:762:ARG:HH22 | 1:B:918:GLU:HG3 | 1.72 | 0.55 |
| 1:A:463:SER:OG | 1:A:465:VAL:HG22 | 2.06 | 0.55 |
| 1:A:41:LEU:HB3 | 1:A:44:GLU:OE2 | 2.07 | 0.54 |
| 1:A:460:ARG:CZ | 1:A:461:ASN:HD21 | 2.21 | 0.54 |
| 1:A:848:THR:O | 1:A:852:ALA:HB3 | 2.07 | 0.54 |
| 1:A:757:MET:O | 1:A:761:ILE:HG13 | 2.07 | 0.54 |
| 1:B:248:PRO:HA | 1:B:251:GLN:HB2 | 1.88 | 0.54 |
| 1:B:333:VAL:HG11 | 1:B:339:VAL:HG22 | 1.89 | 0.54 |
| 1:B:899:MET:SD | 1:B:962:LEU:HD22 | 2.47 | 0.54 |
| 1:A:120:LYS:HE3 | 1:A:728:LYS:HE3 | 1.89 | 0.54 |
| 1:A:355:THR:HG23 | 1:A:720:MET:CG | 2.36 | 0.54 |
| 1:B:239:MET:HE2 | 1:B:708:ALA:HB1 | 1.89 | 0.54 |
| 1:B:248:PRO:O | 1:B:249:LEU:C | 2.43 | 0.54 |
| 1:B:879:ASP:OD1 | 1:B:882:HIS:HB2 | 2.07 | 0.54 |
| 1:B:340:GLU:HA | 1:B:750:GLY:HA2 | 1.88 | 0.54 |
| 1:A:792:LEU:CA | 1:A:795:VAL:HG23 | 2.38 | 0.54 |
| 1:B:759:GLN:HE22 | 1:B:762:ARG:HH11 | 1.55 | 0.54 |
| 1:A:898:THR:OG1 | 1:A:959:LEU:CA | 2.55 | 0.54 |
| 1:B:722:SER:OG | 1:B:738:ASP:OD2 | 2.20 | 0.54 |
| 1:A:315:ILE:HD11 | 1:A:760:PHE:HE1 | 1.71 | 0.54 |
| 1:A:315:ILE:CD1 | 1:A:760:PHE:CE1 | 2.91 | 0.54 |
| 1:A:782:GLY:O | 1:A:783:LEU:O | 2.26 | 0.54 |
| 1:A:914:ASN:HD22 | 1:A:922:LEU:HD11 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:338:SER:HA | 1:B:341:THR:HB | 1.90 | 0.54 |
| 1:B:369:ILE:HG12 | 1:B:528:VAL:CG1 | 2.38 | 0.54 |
| 1:B:815:ASP:O | 1:B:819:ARG:NE | 2.41 | 0.54 |
| 1:B:787:LEU:CD1 | 1:B:900:ALA:HB1 | 2.34 | 0.54 |
| 1:B:912:ALA:HB1 | 1:B:933:LEU:HD11 | 1.90 | 0.54 |
| 1:A:165:ILE:HG21 | 1:A:168:ILE:HD11 | 1.89 | 0.54 |
| 1:A:897:MET:HE1 | 1:A:958:LYS:HE3 | 1.90 | 0.54 |
| 1:B:755:ASN:O | 1:B:759:GLN:HG2 | 2.07 | 0.54 |
| 1:B:857:MET:CE | 1:B:867:TYR:HA | 2.38 | 0.54 |
| 1:A:789:PRO:C | 1:A:791:GLN:H | 2.11 | 0.54 |
| 1:B:112:ALA:O | 1:B:116:ILE:HD12 | 2.07 | 0.54 |
| 1:A:180:LEU:O | 1:A:180:LEU:HD12 | 2.08 | 0.54 |
| 1:B:140:ILE:N | 1:B:140:ILE:HD13 | 2.20 | 0.54 |
| 1:A:546:LEU:HA | 1:A:549:ILE:HD12 | 1.90 | 0.53 |
| 1:A:762:ARG:NH2 | 1:A:833:LEU:CD1 | 2.71 | 0.53 |
| 1:A:840:ILE:HD13 | 1:A:840:ILE:H | 1.74 | 0.53 |
| 1:B:116:ILE:HD11 | 1:B:334:ARG:HG2 | 1.90 | 0.53 |
| 1:B:319:LEU:HD23 | 1:B:336:LEU:C | 2.28 | 0.53 |
| 1:B:979:GLY:O | 1:B:983:ILE:HG12 | 2.08 | 0.53 |
| 1:A:326:MET:HB3 | 1:A:331:ALA:CB | 2.37 | 0.53 |
| 1:B:761:ILE:O | 1:B:765:ILE:HG12 | 2.08 | 0.53 |
| 1:B:795:VAL:HA | 1:B:799:THR:OG1 | 2.08 | 0.53 |
| 1:B:914:ASN:HD22 | 1:B:922:LEU:HD11 | 1.70 | 0.53 |
| 1:A:189:LYS:HE3 | 1:A:207:MET:O | 2.09 | 0.53 |
| 1:A:979:GLY:O | 1:A:983:ILE:HG12 | 2.08 | 0.53 |
| 1:B:460:ARG:CZ | 1:B:461:ASN:HD21 | 2.21 | 0.53 |
| 1:B:792:LEU:CA | 1:B:795:VAL:HG23 | 2.39 | 0.53 |
| 1:A:129:VAL:HG12 | 1:A:151:VAL:HG22 | 1.90 | 0.53 |
| 1:A:161:ALA:HA | 1:A:210:SER:HB2 | 1.91 | 0.53 |
| 1:A:249:LEU:HB2 | 1:A:340:GLU:OE1 | 2.08 | 0.53 |
| 1:A:395:VAL:CG1 | 1:A:402:ILE:HD11 | 2.35 | 0.53 |
| 1:A:86:THR:O | 1:A:89:VAL:HB | 2.08 | 0.53 |
| 1:B:847:ALA:HA | 1:B:973:ILE:HG21 | 1.90 | 0.53 |
| 1:B:62:VAL:CG1 | 1:B:98:LEU:HD22 | 2.39 | 0.53 |
| 1:A:66:LEU:HD13 | 1:A:98:LEU:HD13 | 1.91 | 0.53 |
| 1:A:847:ALA:HA | 1:A:973:ILE:CG2 | 2.38 | 0.53 |
| 1:B:129:VAL:HG12 | 1:B:151:VAL:HG22 | 1.90 | 0.53 |
| 1:B:65:LEU:HB3 | 1:B:98:LEU:HD21 | 1.91 | 0.53 |
| 1:A:718:ILE:HD12 | 1:A:718:ILE:N | 2.23 | 0.53 |
| 1:A:762:ARG:NH2 | 1:A:833:LEU:HD11 | 2.24 | 0.53 |
| 1:B:771:GLU:OE2 | 1:B:792:LEU:HD13 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:894:PRO:HB2 | 1:B:959:LEU:C | 2.29 | 0.53 |
| 1:A:249:LEU:O | 1:A:252:LYS:N | 2.39 | 0.53 |
| 1:B:963:ASP:OD2 | 1:B:964:LEU:N | 2.41 | 0.53 |
| 1:A:306:ALA:O | 1:A:308:PRO:HD3 | 2.08 | 0.53 |
| 1:B:161:ALA:HA | 1:B:210:SER:HB2 | 1.91 | 0.53 |
| 1:B:762:ARG:NH2 | 1:B:833:LEU:CD1 | 2.71 | 0.53 |
| 1:A:315:ILE:HD12 | 1:A:760:PHE:CE1 | 2.44 | 0.53 |
| 1:A:847:ALA:HA | 1:A:973:ILE:HG21 | 1.90 | 0.53 |
| 1:B:735:LEU:HD11 | 1:B:743:ILE:CD1 | 2.17 | 0.53 |
| 1:B:725:ALA:O | 1:B:729:THR:HG23 | 2.09 | 0.52 |
| 1:A:116:ILE:HG13 | 1:A:334:ARG:HD2 | 1.91 | 0.52 |
| 1:A:286:GLY:HA2 | 1:A:290:ARG:HB3 | 1.90 | 0.52 |
| 1:A:782:GLY:CA | 1:A:871:THR:HA | 2.39 | 0.52 |
| 1:B:23:GLY:HA2 | 1:B:150:ILE:CD1 | 2.39 | 0.52 |
| 1:B:248:PRO:HD2 | 1:B:341:THR:HG21 | 1.91 | 0.52 |
| 1:A:633:ILE:HD11 | 1:A:652:ALA:CB | 2.39 | 0.52 |
| 1:B:964:LEU:C | 1:B:964:LEU:HD23 | 2.30 | 0.52 |
| 1:A:311:LEU:HD21 | 1:A:761:ILE:HG23 | 1.90 | 0.52 |
| 1:B:633:ILE:HD11 | 1:B:652:ALA:HB1 | 1.91 | 0.52 |
| 1:B:662:PRO:HG2 | 1:B:665:GLU:CG | 2.40 | 0.52 |
| 1:B:743:ILE:HD12 | 1:B:743:ILE:N | 2.25 | 0.52 |
| 1:B:847:ALA:HA | 1:B:973:ILE:CG2 | 2.39 | 0.52 |
| 1:B:856:PHE:CZ | 1:B:896:PRO:HG3 | 2.45 | 0.52 |
| 1:B:897:MET:HE1 | 1:B:958:LYS:HE3 | 1.90 | 0.52 |
| 1:A:754:TYR:O | 1:A:757:MET:N | 2.37 | 0.52 |
| 1:A:978:ILE:O | 1:A:982:GLU:HB2 | 2.09 | 0.52 |
| 1:B:545:ILE:O | 1:B:549:ILE:HG12 | 2.09 | 0.52 |
| 1:B:96:LEU:C | 1:B:96:LEU:HD23 | 2.30 | 0.52 |
| 1:B:56:GLN:HG3 | 1:B:106:VAL:CG2 | 2.39 | 0.52 |
| 1:B:112:ALA:C | 1:B:116:ILE:HD12 | 2.30 | 0.52 |
| 1:B:789:PRO:C | 1:B:791:GLN:H | 2.13 | 0.52 |
| 1:B:865:VAL:HG12 | 1:B:866:THR:O | 2.08 | 0.52 |
| 1:A:75:LEU:CD1 | 1:A:300:VAL:HB | 2.38 | 0.52 |
| 1:B:600:LEU:HD13 | 1:B:600:LEU:O | 2.09 | 0.52 |
| 1:A:116:ILE:CD1 | 1:A:332:ILE:HG21 | 2.40 | 0.52 |
| 1:A:42:PRO:HD3 | 1:A:228:VAL:HG12 | 1.92 | 0.52 |
| 1:A:248:PRO:CB | 1:A:341:THR:HG23 | 2.40 | 0.52 |
| 1:B:291:GLY:O | 1:B:292:ALA:HB2 | 2.09 | 0.52 |
| 1:B:315:ILE:HD11 | 1:B:757:MET:HE3 | 1.92 | 0.52 |
| 1:A:189:LYS:HD2 | 1:A:205:LYS:O | 2.10 | 0.52 |
| 1:A:489:ARG:H | 1:A:489:ARG:HD3 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:51:GLU:O | 1:A:54:ILE:HB | 2.10 | 0.52 |
| 1:A:611:ILE:CD1 | 1:A:639:ILE:HD12 | 2.40 | 0.52 |
| 1:A:651:ARG:HG3 | 1:A:651:ARG:NH1 | 2.23 | 0.52 |
| 1:A:859:ALA:O | 1:A:861:ASP:N | 2.43 | 0.52 |
| 1:B:847:ALA:HB1 | 1:B:903:VAL:CG1 | 2.39 | 0.52 |
| 1:B:94:ILE:HD13 | 1:B:98:LEU:HG | 1.92 | 0.52 |
| 1:B:988:ALA:HA | 1:B:992:LEU:HB2 | 1.91 | 0.52 |
| 1:A:912:ALA:HB1 | 1:A:933:LEU:HD11 | 1.91 | 0.52 |
| 1:B:249:LEU:O | 1:B:249:LEU:HD12 | 2.10 | 0.52 |
| 1:A:369:ILE:N | 1:A:369:ILE:HD12 | 2.25 | 0.51 |
| 1:A:680:GLU:O | 1:A:683:HIS:HB2 | 2.10 | 0.51 |
| 1:A:737:ASP:O | 1:A:738:ASP:HB2 | 2.10 | 0.51 |
| 1:B:111:ASN:O | 1:B:114:ASN:HB2 | 2.10 | 0.51 |
| 1:B:329:LYS:O | 1:B:330:ASN:CB | 2.59 | 0.51 |
| 1:B:458:GLU:OE2 | 1:B:460:ARG:HG2 | 2.10 | 0.51 |
| 1:B:48:SER:OG | 1:B:51:GLU:HG2 | 2.09 | 0.51 |
| 1:B:735:LEU:HD13 | 1:B:743:ILE:HD11 | 1.86 | 0.51 |
| 1:A:747:VAL:HG12 | 1:A:817:MET:HE1 | 1.91 | 0.51 |
| 1:B:249:LEU:HG | 1:B:250:GLN:N | 2.25 | 0.51 |
| 1:B:792:LEU:C | 1:B:795:VAL:HG23 | 2.31 | 0.51 |
| 1:B:782:GLY:HA3 | 1:B:871:THR:HB | 1.92 | 0.51 |
| 1:A:44:GLU:N | 1:A:44:GLU:CD | 2.64 | 0.51 |
| 1:A:792:LEU:C | 1:A:795:VAL:HG23 | 2.31 | 0.51 |
| 1:A:383:SER:O | 1:A:384:ILE:HD13 | 2.10 | 0.51 |
| 1:A:611:ILE:HD11 | 1:A:639:ILE:HD12 | 1.92 | 0.51 |
| 1:B:341:THR:HB | 1:B:716:ILE:HD11 | 1.91 | 0.51 |
| 1:B:762:ARG:NH2 | 1:B:833:LEU:HD11 | 2.25 | 0.51 |
| 1:B:801:GLY:C | 1:B:803:PRO:HD2 | 2.31 | 0.51 |
| 1:A:94:ILE:HG23 | 1:A:95:LEU:N | 2.26 | 0.51 |
| 1:B:311:LEU:CD1 | 1:B:761:ILE:HD13 | 2.35 | 0.51 |
| 1:A:66:LEU:O | 1:A:69:ALA:HB3 | 2.11 | 0.51 |
| 1:A:94:ILE:HG23 | 1:A:95:LEU:H | 1.76 | 0.51 |
| 1:A:964:LEU:HD23 | 1:A:964:LEU:C | 2.31 | 0.51 |
| 1:B:663:LEU:N | 1:B:663:LEU:CD1 | 2.74 | 0.51 |
| 1:B:866:THR:HG23 | 1:B:869:GLN:HE21 | 1.76 | 0.51 |
| 1:A:60:LEU:HD23 | 1:A:257:GLY:HA3 | 1.93 | 0.51 |
| 1:A:60:LEU:N | 1:A:63:ARG:HH21 | 2.09 | 0.51 |
| 1:B:44:GLU:N | 1:B:44:GLU:CD | 2.63 | 0.51 |
| 1:B:463:SER:OG | 1:B:466:GLU:HG3 | 2.10 | 0.51 |
| 1:A:463:SER:OG | 1:A:466:GLU:HG3 | 2.11 | 0.51 |
| 1:A:600:LEU:N | 1:A:600:LEU:HD12 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:633:ILE:HD11 | 1:A:652:ALA:HB1 | 1.93 | 0.51 |
| 1:A:810:ASN:OD1 | 1:A:930:ASN:ND2 | 2.43 | 0.51 |
| 1:B:369:ILE:HD11 | 1:B:593:PHE:CD1 | 2.46 | 0.51 |
| 1:A:600:LEU:CD1 | 1:A:600:LEU:O | 2.58 | 0.51 |
| 1:B:355:THR:HG23 | 1:B:720:MET:CG | 2.40 | 0.51 |
| 1:B:748:GLU:N | 1:B:817:MET:HE1 | 2.26 | 0.51 |
| 1:B:810:ASN:OD1 | 1:B:930:ASN:ND2 | 2.44 | 0.51 |
| 1:A:65:LEU:HG | 1:A:94:ILE:CD1 | 2.40 | 0.51 |
| 1:A:855:TRP:CA | 1:A:859:ALA:CB | 2.74 | 0.51 |
| 1:A:91:PRO:HA | 1:A:94:ILE:HG22 | 1.91 | 0.50 |
| 1:B:41:LEU:HB3 | 1:B:44:GLU:OE2 | 2.11 | 0.50 |
| 1:A:222:ILE:HG23 | 1:A:222:ILE:O | 2.11 | 0.50 |
| 1:A:907:ILE:HD11 | 1:A:974:SER:CA | 2.41 | 0.50 |
| 1:A:93:VAL:O | 1:A:97:ILE:HG12 | 2.12 | 0.50 |
| 1:A:988:ALA:HA | 1:A:992:LEU:HB2 | 1.92 | 0.50 |
| 1:B:235:ILE:HG21 | 1:B:705:VAL:HG12 | 1.93 | 0.50 |
| 1:B:749:GLU:OE2 | 1:B:753:ILE:HD11 | 2.10 | 0.50 |
| 1:A:104:VAL:O | 1:A:107:TRP:HB3 | 2.12 | 0.50 |
| 1:A:813:ASP:OD2 | 1:A:813:ASP:N | 2.33 | 0.50 |
| 1:A:914:ASN:C | 1:A:916:LEU:N | 2.64 | 0.50 |
| 1:B:238:GLN:O | 1:B:242:THR:HG23 | 2.10 | 0.50 |
| 1:B:369:ILE:HD12 | 1:B:369:ILE:N | 2.26 | 0.50 |
| 1:B:783:LEU:HG | 1:B:870:LEU:HD23 | 1.94 | 0.50 |
| 1:B:939:LEU:O | 1:B:943:LEU:HG | 2.12 | 0.50 |
| 1:A:291:GLY:O | 1:A:292:ALA:HB2 | 2.11 | 0.50 |
| 1:A:116:ILE:HD11 | 1:A:332:ILE:HG21 | 1.92 | 0.50 |
| 1:A:762:ARG:HH22 | 1:A:918:GLU:CA | 2.25 | 0.50 |
| 1:A:963:ASP:H | 1:A:966:GLN:NE2 | 2.08 | 0.50 |
| 1:B:237:ASP:O | 1:B:238:GLN:C | 2.48 | 0.50 |
| 1:B:172:THR:CG2 | 1:B:489:ARG:HD2 | 2.41 | 0.50 |
| 1:B:802:LEU:HD11 | 1:B:939:LEU:HG | 1.89 | 0.50 |
| 1:B:855:TRP:HD1 | 1:B:966:GLN:OE1 | 1.94 | 0.50 |
| 1:A:252:LYS:HA | 1:A:252:LYS:HE2 | 1.94 | 0.50 |
| 1:B:103:ILE:HG23 | 1:B:104:VAL:N | 2.27 | 0.50 |
| 1:B:222:ILE:HG23 | 1:B:222:ILE:O | 2.10 | 0.50 |
| 1:B:60:LEU:CD2 | 1:B:257:GLY:HA3 | 2.42 | 0.50 |
| 1:A:307:ILE:O | 1:A:309:GLU:N | 2.45 | 0.50 |
| 1:A:771:GLU:OE2 | 1:A:792:LEU:HD13 | 2.12 | 0.50 |
| 1:B:116:ILE:HG13 | 1:B:332:ILE:HG21 | 1.93 | 0.50 |
| 1:B:320:ALA:O | 1:B:324:ARG:HG2 | 2.12 | 0.50 |
| 1:A:82:GLU:HG3 | 1:A:83:GLU:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:338:SER:HB2 | 1:B:716:ILE:HD12 | 1.94 | 0.50 |
| 1:B:947:ILE:HD11 | 1:B:957:PHE:CZ | 2.46 | 0.50 |
| 1:A:489:ARG:CD | 1:A:489:ARG:N | 2.75 | 0.50 |
| 1:B:236:ARG:O | 1:B:239:MET:HB3 | 2.11 | 0.50 |
| 1:B:350:SER:OG | 1:B:356:LEU:HD13 | 2.12 | 0.50 |
| 1:B:352:LYS:HE2 | 1:B:627:ASP:HB3 | 1.93 | 0.50 |
| 1:B:893:ALA:O | 1:B:896:PRO:HD2 | 2.12 | 0.50 |
| 1:A:969:MET:HE2 | 1:A:973:ILE:HG12 | 1.94 | 0.50 |
| 1:B:334:ARG:HD3 | 1:B:731:SER:O | 2.12 | 0.50 |
| 1:B:505:ARG:HB3 | 1:B:508:VAL:CG2 | 2.42 | 0.50 |
| 1:B:782:GLY:C | 1:B:871:THR:HA | 2.32 | 0.50 |
| 1:A:762:ARG:HH22 | 1:A:918:GLU:HG3 | 1.77 | 0.49 |
| 1:A:311:LEU:HB3 | 1:A:312:PRO:HD3 | 1.95 | 0.49 |
| 1:A:505:ARG:HB3 | 1:A:508:VAL:CG2 | 2.42 | 0.49 |
| 1:A:624:ILE:CG2 | 1:A:684:LYS:HG2 | 2.42 | 0.49 |
| 1:A:775:ILE:H | 1:A:775:ILE:HD13 | 1.77 | 0.49 |
| 1:B:465:VAL:HG23 | 1:B:466:GLU:N | 2.27 | 0.49 |
| 1:B:757:MET:HG2 | 1:B:760:PHE:HZ | 1.71 | 0.49 |
| 1:A:127:GLY:HA3 | 1:A:145:ILE:HD11 | 1.94 | 0.49 |
| 1:A:261:SER:O | 1:A:264:ILE:HB | 2.11 | 0.49 |
| 1:A:326:MET:O | 1:A:331:ALA:HB3 | 2.12 | 0.49 |
| 1:B:600:LEU:CD1 | 1:B:600:LEU:C | 2.80 | 0.49 |
| 1:B:743:ILE:H | 1:B:743:ILE:HD12 | 1.77 | 0.49 |
| 1:B:787:LEU:HD23 | 1:B:791:GLN:OE1 | 2.12 | 0.49 |
| 1:B:907:ILE:HD11 | 1:B:974:SER:CA | 2.40 | 0.49 |
| 1:A:369:ILE:HD11 | 1:A:593:PHE:CD1 | 2.47 | 0.49 |
| 1:A:947:ILE:HD11 | 1:A:957:PHE:CZ | 2.46 | 0.49 |
| 1:B:25:THR:HA | 1:B:132:ALA:HB3 | 1.94 | 0.49 |
| 1:B:306:ALA:O | 1:B:308:PRO:HD3 | 2.12 | 0.49 |
| 1:B:340:GLU:HA | 1:B:750:GLY:CA | 2.42 | 0.49 |
| 1:B:352:LYS:HE2 | 1:B:627:ASP:CB | 2.42 | 0.49 |
| 1:A:320:ALA:O | 1:A:324:ARG:HG2 | 2.11 | 0.49 |
| 1:A:458:GLU:OE2 | 1:A:460:ARG:HG2 | 2.12 | 0.49 |
| 1:A:342:LEU:HD22 | 1:A:747:VAL:CG2 | 2.42 | 0.49 |
| 1:A:784:PRO:HD3 | 1:A:870:LEU:HD12 | 1.94 | 0.49 |
| 1:B:383:SER:CA | 1:B:384:ILE:HD12 | 2.42 | 0.49 |
| 1:B:518:PRO:C | 1:B:522:ILE:HD13 | 2.33 | 0.49 |
| 1:B:978:ILE:O | 1:B:982:GLU:HB2 | 2.12 | 0.49 |
| 1:A:108:GLN:NE2 | 1:A:108:GLN:HA | 2.26 | 0.49 |
| 1:A:939:LEU:O | 1:A:943:LEU:HG | 2.12 | 0.49 |
| 1:A:957:PHE:O | 1:A:959:LEU:HG | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:402:ILE:HD12 | 1:B:403:ARG:C | 2.32 | 0.49 |
| 1:B:633:ILE:HD12 | 1:B:642:PHE:CE1 | 2.47 | 0.49 |
| 1:B:654:THR:OG1 | 1:B:657:GLU:HG3 | 2.12 | 0.49 |
| 1:B:953:LEU:HB2 | 1:B:954:PRO:HD3 | 1.95 | 0.49 |
| 1:A:847:ALA:HB1 | 1:A:903:VAL:CG1 | 2.42 | 0.49 |
| 1:A:782:GLY:C | 1:A:871:THR:HA | 2.32 | 0.49 |
| 1:B:244:GLN:O | 1:B:246:LYS:N | 2.45 | 0.49 |
| 1:B:489:ARG:H | 1:B:489:ARG:HD3 | 1.75 | 0.49 |
| 1:A:832:TRP:NE1 | 1:A:988:ALA:HB2 | 2.27 | 0.49 |
| 1:B:140:ILE:HD11 | 1:B:145:ILE:HD11 | 1.95 | 0.49 |
| 1:B:782:GLY:CA | 1:B:871:THR:HA | 2.43 | 0.49 |
| 1:B:267:ILE:HG21 | 1:B:302:LEU:CD1 | 2.42 | 0.49 |
| 1:B:749:GLU:C | 1:B:751:ARG:H | 2.16 | 0.49 |
| 1:B:795:VAL:HA | 1:B:799:THR:CB | 2.43 | 0.49 |
| 1:A:179:ILE:HG22 | 1:A:179:ILE:O | 2.13 | 0.49 |
| 1:A:715:GLU:C | 1:A:716:ILE:HD12 | 2.32 | 0.49 |
| 1:A:757:MET:HE1 | 1:A:761:ILE:CD1 | 2.32 | 0.49 |
| 1:A:856:PHE:CZ | 1:A:896:PRO:HG3 | 2.48 | 0.49 |
| 1:B:333:VAL:HG12 | 1:B:335:SER:O | 2.13 | 0.49 |
| 1:B:55:GLU:O | 1:B:58:GLU:HB2 | 2.13 | 0.49 |
| 1:A:179:ILE:HG23 | 1:A:724:THR:CG2 | 2.43 | 0.48 |
| 1:A:320:ALA:O | 1:A:323:THR:HB | 2.13 | 0.48 |
| 1:A:705:VAL:HG22 | 1:A:726:VAL:HG21 | 1.94 | 0.48 |
| 1:A:855:TRP:HD1 | 1:A:966:GLN:OE1 | 1.96 | 0.48 |
| 1:A:787:LEU:CD1 | 1:A:900:ALA:HB1 | 2.40 | 0.48 |
| 1:B:622:ILE:O | 1:B:624:ILE:HD12 | 2.13 | 0.48 |
| 1:B:762:ARG:HH22 | 1:B:918:GLU:CA | 2.26 | 0.48 |
| 1:B:763:TYR:CE1 | 1:B:912:ALA:HB2 | 2.48 | 0.48 |
| 1:A:48:SER:OG | 1:A:51:GLU:HG2 | 2.12 | 0.48 |
| 1:A:758:LYS:O | 1:A:762:ARG:HG3 | 2.13 | 0.48 |
| 1:B:358:THR:OG1 | 1:B:602:PRO:HG2 | 2.13 | 0.48 |
| 1:B:758:LYS:O | 1:B:762:ARG:HG3 | 2.14 | 0.48 |
| 1:A:305:ALA:C | 1:A:768:ASN:HD22 | 2.17 | 0.48 |
| 1:A:708:ALA:HB3 | 1:A:709:PRO:CD | 2.39 | 0.48 |
| 1:A:79:GLU:HG2 | 1:A:84:THR:HB | 1.94 | 0.48 |
| 1:A:48:SER:H | 1:A:51:GLU:HG2 | 1.79 | 0.48 |
| 1:A:697:ILE:N | 1:A:697:ILE:HD12 | 2.29 | 0.48 |
| 1:A:795:VAL:HA | 1:A:799:THR:CB | 2.43 | 0.48 |
| 1:B:855:TRP:HZ3 | 1:B:856:PHE:CE2 | 2.32 | 0.48 |
| 1:A:314:VAL:HG11 | 1:A:804:ALA:HB1 | 1.96 | 0.48 |
| 1:A:833:LEU:CA | 1:A:836:ARG:HB2 | 2.39 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:931:ILE:HD12 | 1:A:931:ILE:N | 2.28 | 0.48 |
| 1:B:611:ILE:CD1 | 1:B:621:VAL:HG21 | 2.41 | 0.48 |
| 1:A:235:ILE:HG21 | 1:A:705:VAL:HG12 | 1.94 | 0.48 |
| 1:A:878:GLU:HG3 | 1:A:879:ASP:N | 2.23 | 0.48 |
| 1:B:363:VAL:CG1 | 1:B:448:LEU:HD13 | 2.44 | 0.48 |
| 1:B:48:SER:H | 1:B:51:GLU:HG2 | 1.79 | 0.48 |
| 1:B:799:THR:HG21 | 1:B:905:VAL:HG22 | 1.95 | 0.48 |
| 1:B:914:ASN:C | 1:B:916:LEU:N | 2.65 | 0.48 |
| 1:B:832:TRP:NE1 | 1:B:988:ALA:HB2 | 2.28 | 0.48 |
| 1:B:267:ILE:HG21 | 1:B:302:LEU:HD13 | 1.94 | 0.48 |
| 1:B:46:GLY:O | 1:B:47:LYS:C | 2.52 | 0.48 |
| 1:A:42:PRO:O | 1:A:43:ALA:O | 2.31 | 0.48 |
| 1:A:833:LEU:HD11 | 1:A:837:TYR:HE1 | 1.79 | 0.48 |
| 1:A:947:ILE:HD11 | 1:A:957:PHE:CE2 | 2.49 | 0.48 |
| 1:B:787:LEU:HD11 | 1:B:900:ALA:CB | 2.37 | 0.48 |
| 1:B:813:ASP:HB2 | 1:B:815:ASP:OD1 | 2.14 | 0.48 |
| 1:A:359:ASN:O | 1:A:359:ASN:ND2 | 2.46 | 0.48 |
| 1:A:787:LEU:HD23 | 1:A:791:GLN:OE1 | 2.13 | 0.48 |
| 1:B:489:ARG:CD | 1:B:489:ARG:N | 2.75 | 0.48 |
| 1:B:663:LEU:N | 1:B:663:LEU:HD12 | 2.29 | 0.48 |
| 1:B:762:ARG:HH22 | 1:B:918:GLU:CB | 2.27 | 0.48 |
| 1:A:413:LEU:C | 1:A:413:LEU:HD23 | 2.35 | 0.47 |
| 1:A:387:SER:HB2 | 1:A:602:PRO:HB2 | 1.96 | 0.47 |
| 1:A:855:TRP:O | 1:A:862:GLY:HA3 | 2.14 | 0.47 |
| 1:B:756:ASN:O | 1:B:759:GLN:CB | 2.55 | 0.47 |
| 1:B:84:THR:HA | 1:B:87:ALA:HB3 | 1.95 | 0.47 |
| 1:B:852:ALA:O | 1:B:855:TRP:HB3 | 2.14 | 0.47 |
| 1:B:784:PRO:HD3 | 1:B:870:LEU:HD12 | 1.94 | 0.47 |
| 1:B:899:MET:O | 1:B:903:VAL:HG23 | 2.14 | 0.47 |
| 1:A:247:THR:CG2 | 1:A:250:GLN:HB3 | 2.44 | 0.47 |
| 1:A:763:TYR:CE1 | 1:A:912:ALA:HB2 | 2.49 | 0.47 |
| 1:B:150:ILE:CD1 | 1:B:150:ILE:N | 2.78 | 0.47 |
| 1:B:757:MET:HE2 | 1:B:761:ILE:HD11 | 1.95 | 0.47 |
| 1:B:857:MET:HE3 | 1:B:867:TYR:HA | 1.96 | 0.47 |
| 1:B:880:HIS:HB3 | 1:B:881:PRO:HD3 | 1.95 | 0.47 |
| 1:A:356:LEU:CD1 | 1:A:740:PHE:CE1 | 2.97 | 0.47 |
| 1:A:840:ILE:HD13 | 1:A:840:ILE:N | 2.29 | 0.47 |
| 1:B:48:SER:H | 1:B:51:GLU:CG | 2.27 | 0.47 |
| 1:B:633:ILE:HD12 | 1:B:642:PHE:HE1 | 1.79 | 0.47 |
| 1:B:848:THR:O | 1:B:852:ALA:CB | 2.62 | 0.47 |
| 1:B:854:TRP:CE3 | 1:B:855:TRP:N | 2.82 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:783:LEU:HG | 1:B:870:LEU:CD2 | 2.43 | 0.47 |
| 1:B:898:THR:HG1 | 1:B:959:LEU:HA | 1.78 | 0.47 |
| 1:B:899:MET:HE1 | 1:B:970:VAL:CG2 | 2.30 | 0.47 |
| 1:B:947:ILE:HD11 | 1:B:957:PHE:CE2 | 2.49 | 0.47 |
| 1:A:73:PHE:O | 1:A:77:TRP:HB2 | 2.15 | 0.47 |
| 1:B:51:GLU:O | 1:B:54:ILE:HB | 2.14 | 0.47 |
| 1:A:247:THR:CB | 1:A:250:GLN:HB3 | 2.38 | 0.47 |
| 1:A:813:ASP:HB2 | 1:A:815:ASP:OD1 | 2.14 | 0.47 |
| 1:A:84:THR:HA | 1:A:87:ALA:HB3 | 1.97 | 0.47 |
| 1:A:893:ALA:O | 1:A:896:PRO:HD2 | 2.14 | 0.47 |
| 1:B:782:GLY:O | 1:B:783:LEU:O | 2.33 | 0.47 |
| 1:B:917:SER:CB | 1:B:920:GLN:HB2 | 2.44 | 0.47 |
| 1:A:340:GLU:OE2 | 1:A:344:CYS:SG | 2.69 | 0.47 |
| 1:B:639:ILE:HD11 | 1:B:641:ILE:CD1 | 2.43 | 0.47 |
| 1:B:931:ILE:N | 1:B:931:ILE:HD12 | 2.27 | 0.47 |
| 1:A:895:GLU:H | 1:A:895:GLU:CD | 2.17 | 0.47 |
| 1:B:880:HIS:N | 1:B:881:PRO:HD2 | 2.30 | 0.47 |
| 1:B:898:THR:OG1 | 1:B:959:LEU:HA | 2.15 | 0.47 |
| 1:A:545:ILE:CD1 | 1:A:545:ILE:N | 2.77 | 0.47 |
| 1:B:735:LEU:HD22 | 1:B:742:THR:HB | 1.97 | 0.47 |
| 1:A:782:GLY:CA | 1:A:871:THR:HB | 2.45 | 0.47 |
| 1:A:971:LEU:O | 1:A:975:LEU:HD23 | 2.14 | 0.47 |
| 1:B:18:VAL:CG2 | 1:B:150:ILE:HD11 | 2.45 | 0.47 |
| 1:B:315:ILE:CD1 | 1:B:757:MET:CE | 2.93 | 0.47 |
| 1:B:787:LEU:HD21 | 1:B:901:LEU:CA | 2.44 | 0.47 |
| 1:A:465:VAL:HG23 | 1:A:466:GLU:N | 2.29 | 0.47 |
| 1:A:762:ARG:HH22 | 1:A:918:GLU:CB | 2.28 | 0.47 |
| 1:A:783:LEU:H | 1:A:783:LEU:CD1 | 2.12 | 0.47 |
| 1:B:969:MET:O | 1:B:969:MET:HE2 | 2.15 | 0.47 |
| 1:A:367:PHE:C | 1:A:367:PHE:CD2 | 2.88 | 0.47 |
| 1:B:173:LEU:O | 1:B:188:ILE:HA | 2.15 | 0.47 |
| 1:B:71:ILE:N | 1:B:71:ILE:HD13 | 2.29 | 0.47 |
| 1:A:86:THR:HA | 1:A:89:VAL:HG23 | 1.97 | 0.46 |
| 1:A:899:MET:O | 1:A:903:VAL:HG23 | 2.16 | 0.46 |
| 1:B:10:GLU:CD | 1:B:10:GLU:H | 2.13 | 0.46 |
| 1:B:413:LEU:HD23 | 1:B:413:LEU:C | 2.35 | 0.46 |
| 1:B:60:LEU:O | 1:B:64:ILE:HG12 | 2.15 | 0.46 |
| 1:B:737:ASP:C | 1:B:739:ASN:N | 2.69 | 0.46 |
| 1:B:858:TYR:CD1 | 1:B:858:TYR:N | 2.83 | 0.46 |
| 1:B:957:PHE:O | 1:B:959:LEU:HG | 2.15 | 0.46 |
| 1:A:787:LEU:HD21 | 1:A:901:LEU:CA | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:899:MET:CE | 1:A:970:VAL:CG2 | 2.88 | 0.46 |
| 1:B:308:PRO:HB2 | 1:B:764:LEU:HD23 | 1.96 | 0.46 |
| 1:B:553:GLY:O | 1:B:554:THR:HG23 | 2.15 | 0.46 |
| 1:B:878:GLU:HG3 | 1:B:879:ASP:N | 2.23 | 0.46 |
| 1:B:895:GLU:HB2 | 1:B:896:PRO:HD3 | 1.96 | 0.46 |
| 1:B:840:ILE:HD13 | 1:B:911:ASN:HD21 | 1.80 | 0.46 |
| 1:A:10:GLU:CD | 1:A:10:GLU:H | 2.12 | 0.46 |
| 1:A:654:THR:OG1 | 1:A:657:GLU:HG3 | 2.16 | 0.46 |
| 1:B:155:VAL:HG13 | 1:B:155:VAL:O | 2.15 | 0.46 |
| 1:B:249:LEU:HD12 | 1:B:249:LEU:C | 2.36 | 0.46 |
| 1:B:322:GLY:HA2 | 1:B:325:ARG:HE | 1.78 | 0.46 |
| 1:B:747:VAL:HG12 | 1:B:817:MET:HE1 | 1.97 | 0.46 |
| 1:A:715:GLU:CB | 1:A:716:ILE:HD12 | 2.44 | 0.46 |
| 1:A:855:TRP:HZ3 | 1:A:856:PHE:CE2 | 2.33 | 0.46 |
| 1:B:522:ILE:N | 1:B:522:ILE:HD12 | 2.31 | 0.46 |
| 1:B:549:ILE:CD1 | 1:B:596:VAL:HG21 | 2.25 | 0.46 |
| 1:B:315:ILE:HD13 | 1:B:760:PHE:CE1 | 2.50 | 0.46 |
| 1:B:817:MET:C | 1:B:819:ARG:N | 2.66 | 0.46 |
| 1:A:261:SER:O | 1:A:264:ILE:CG1 | 2.62 | 0.46 |
| 1:A:48:SER:H | 1:A:51:GLU:CG | 2.28 | 0.46 |
| 1:A:759:GLN:HE22 | 1:A:762:ARG:NH1 | 2.13 | 0.46 |
| 1:A:783:LEU:HG | 1:A:870:LEU:CD2 | 2.46 | 0.46 |
| 1:B:757:MET:HA | 1:B:760:PHE:CE2 | 2.51 | 0.46 |
| 1:B:878:GLU:C | 1:B:880:HIS:H | 2.19 | 0.46 |
| 1:A:762:ARG:HB3 | 1:A:837:TYR:CE1 | 2.49 | 0.46 |
| 1:B:311:LEU:CB | 1:B:312:PRO:CD | 2.88 | 0.46 |
| 1:B:367:PHE:C | 1:B:367:PHE:CD2 | 2.88 | 0.46 |
| 1:B:751:ARG:O | 1:B:755:ASN:OD1 | 2.34 | 0.46 |
| 1:B:859:ALA:O | 1:B:861:ASP:N | 2.48 | 0.46 |
| 1:A:633:ILE:HD12 | 1:A:642:PHE:CE1 | 2.50 | 0.46 |
| 1:A:716:ILE:N | 1:A:716:ILE:HD12 | 2.30 | 0.46 |
| 1:A:868:HIS:O | 1:A:872:HIS:ND1 | 2.46 | 0.46 |
| 1:B:108:GLN:HE21 | 1:B:108:GLN:HA | 1.80 | 0.46 |
| 1:B:326:MET:HE3 | 1:B:331:ALA:CB | 2.45 | 0.46 |
| 1:B:39:ASN:O | 1:B:40:GLU:HB3 | 2.15 | 0.46 |
| 1:B:633:ILE:CD1 | 1:B:642:PHE:HE1 | 2.27 | 0.46 |
| 1:B:737:ASP:OD2 | 1:B:739:ASN:HB2 | 2.16 | 0.46 |
| 1:A:917:SER:CB | 1:A:920:GLN:HB2 | 2.46 | 0.46 |
| 1:B:249:LEU:HB2 | 1:B:340:GLU:OE1 | 2.16 | 0.46 |
| 1:B:765:ILE:O | 1:B:766:SER:C | 2.53 | 0.46 |
| 1:A:443:THR:O | 1:A:447:THR:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:716:ILE:HG22 | 1:A:718:ILE:HD11 | 1.98 | 0.46 |
| 1:A:854:TRP:CE3 | 1:A:855:TRP:N | 2.84 | 0.46 |
| 1:B:0:ACE:H3 | 1:B:36:TYR:CE2 | 2.51 | 0.46 |
| 1:B:86:THR:HA | 1:B:89:VAL:CG2 | 2.44 | 0.46 |
| 1:A:53:VAL:HG22 | 1:A:106:VAL:HG21 | 1.97 | 0.46 |
| 1:A:75:LEU:CD2 | 1:A:297:LYS:HA | 2.46 | 0.46 |
| 1:A:299:ALA:HA | 1:A:302:LEU:HD11 | 1.98 | 0.46 |
| 1:A:858:TYR:N | 1:A:858:TYR:CD1 | 2.83 | 0.46 |
| 1:B:782:GLY:CA | 1:B:871:THR:HB | 2.46 | 0.46 |
| 1:A:790:VAL:O | 1:A:790:VAL:CG1 | 2.61 | 0.45 |
| 1:A:947:ILE:HD11 | 1:A:957:PHE:CE1 | 2.52 | 0.45 |
| 1:B:491:ARG:HD2 | 1:B:588:GLU:OE2 | 2.15 | 0.45 |
| 1:B:788:ILE:HD11 | 1:B:958:LYS:HB2 | 1.98 | 0.45 |
| 1:B:827:PRO:HB2 | 1:B:828:LEU:H | 1.50 | 0.45 |
| 1:A:304:VAL:CG1 | 1:A:793:LEU:HD21 | 2.45 | 0.45 |
| 1:A:832:TRP:HZ2 | 1:A:984:LEU:O | 1.99 | 0.45 |
| 1:B:757:MET:HA | 1:B:760:PHE:CZ | 2.51 | 0.45 |
| 1:B:762:ARG:HB3 | 1:B:837:TYR:CE1 | 2.50 | 0.45 |
| 1:B:823:SER:HB3 | 1:B:826:GLU:CB | 2.27 | 0.45 |
| 1:B:845:GLY:C | 1:B:847:ALA:H | 2.18 | 0.45 |
| 1:B:868:HIS:O | 1:B:872:HIS:ND1 | 2.47 | 0.45 |
| 1:A:652:ALA:HA | 1:A:675:CYS:O | 2.16 | 0.45 |
| 1:A:852:ALA:O | 1:A:855:TRP:HB3 | 2.16 | 0.45 |
| 1:A:880:HIS:HB3 | 1:A:881:PRO:HD3 | 1.97 | 0.45 |
| 1:B:259:GLN:HE21 | 1:B:259:GLN:HB3 | 1.58 | 0.45 |
| 1:B:898:THR:OG1 | 1:B:960:LYS:N | 2.45 | 0.45 |
| 1:A:91:PRO:HA | 1:A:94:ILE:CG2 | 2.46 | 0.45 |
| 1:B:882:HIS:HB3 | 1:B:883:PHE:CD1 | 2.52 | 0.45 |
| 1:B:97:ILE:O | 1:B:100:ALA:HB3 | 2.17 | 0.45 |
| 1:A:79:GLU:CG | 1:A:84:THR:HB | 2.47 | 0.45 |
| 1:B:62:VAL:HG12 | 1:B:98:LEU:HD22 | 1.99 | 0.45 |
| 1:A:261:SER:HA | 1:A:264:ILE:HG12 | 1.97 | 0.45 |
| 1:A:338:SER:O | 1:A:339:VAL:C | 2.55 | 0.45 |
| 1:B:299:ALA:O | 1:B:302:LEU:HD12 | 2.17 | 0.45 |
| 1:B:349:CYS:HB3 | 1:B:624:ILE:HD11 | 1.95 | 0.45 |
| 1:A:335:SER:OG | 1:A:337:PRO:HD2 | 2.17 | 0.45 |
| 1:A:757:MET:HA | 1:A:760:PHE:CZ | 2.52 | 0.45 |
| 1:B:108:GLN:NE2 | 1:B:108:GLN:HA | 2.32 | 0.45 |
| 1:B:767:SER:O | 1:B:771:GLU:CG | 2.63 | 0.45 |
| 1:B:947:ILE:HD11 | 1:B:957:PHE:CE1 | 2.51 | 0.45 |
| 1:A:639:ILE:HD11 | 1:A:641:ILE:CD1 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:765:ILE:O | 1:A:766:SER:C | 2.55 | 0.45 |
| 1:A:898:THR:CA | 1:A:959:LEU:CD2 | 2.88 | 0.45 |
| 1:A:854:TRP:HH2 | 1:A:966:GLN:HG2 | 1.81 | 0.45 |
| 1:B:342:LEU:O | 1:B:747:VAL:HG22 | 2.17 | 0.45 |
| 1:B:311:LEU:HD11 | 1:B:761:ILE:HG23 | 1.98 | 0.45 |
| 1:B:833:LEU:CA | 1:B:836:ARG:HB2 | 2.41 | 0.45 |
| 1:B:895:GLU:CD | 1:B:895:GLU:H | 2.20 | 0.45 |
| 1:B:971:LEU:O | 1:B:975:LEU:HD23 | 2.16 | 0.45 |
| 1:A:190:HIS:O | 1:A:206:ASN:HA | 2.17 | 0.45 |
| 1:A:39:ASN:O | 1:A:40:GLU:CB | 2.62 | 0.45 |
| 1:A:757:MET:HA | 1:A:760:PHE:CE2 | 2.51 | 0.45 |
| 1:A:817:MET:C | 1:A:819:ARG:N | 2.66 | 0.45 |
| 1:A:849:VAL:O | 1:A:853:ALA:HB2 | 2.12 | 0.45 |
| 1:A:86:THR:HG22 | 1:A:89:VAL:HG21 | 1.99 | 0.45 |
| 1:A:983:ILE:O | 1:A:987:ILE:HG12 | 2.16 | 0.45 |
| 1:B:352:LYS:HB2 | 1:B:625:THR:HB | 1.99 | 0.45 |
| 1:B:885:GLY:O | 1:B:886:LEU:HG | 2.17 | 0.45 |
| 1:B:810:ASN:HA | 1:B:930:ASN:ND2 | 2.32 | 0.45 |
| 1:A:633:ILE:CD1 | 1:A:642:PHE:HE1 | 2.29 | 0.45 |
| 1:A:799:THR:HG21 | 1:A:905:VAL:HG22 | 1.99 | 0.45 |
| 1:A:898:THR:OG1 | 1:A:960:LYS:N | 2.47 | 0.45 |
| 1:A:914:ASN:HD21 | 1:A:922:LEU:HD11 | 1.80 | 0.45 |
| 1:A:975:LEU:H | 1:A:975:LEU:CD2 | 2.30 | 0.45 |
| 1:A:633:ILE:HD12 | 1:A:642:PHE:HE1 | 1.82 | 0.44 |
| 1:A:663:LEU:H | 1:A:663:LEU:CD1 | 2.30 | 0.44 |
| 1:B:193:PRO:O | 1:B:195:PRO:HD3 | 2.18 | 0.44 |
| 1:B:322:GLY:N | 1:B:325:ARG:HH21 | 2.15 | 0.44 |
| 1:B:963:ASP:H | 1:B:966:GLN:NE2 | 2.11 | 0.44 |
| 1:A:308:PRO:CB | 1:A:764:LEU:HD23 | 2.46 | 0.44 |
| 1:A:782:GLY:HA3 | 1:A:871:THR:CB | 2.46 | 0.44 |
| 1:B:671:ARG:HD3 | 1:B:694:TYR:CZ | 2.52 | 0.44 |
| 1:B:794:TRP:O | 1:B:794:TRP:CD1 | 2.70 | 0.44 |
| 1:A:48:SER:O | 1:A:52:LEU:HG | 2.18 | 0.44 |
| 1:A:553:GLY:O | 1:A:554:THR:HG23 | 2.17 | 0.44 |
| 1:A:765:ILE:HD13 | 1:A:765:ILE:C | 2.38 | 0.44 |
| 1:A:857:MET:CE | 1:A:867:TYR:HA | 2.48 | 0.44 |
| 1:B:403:ARG:HH11 | 1:B:456:ASN:HD21 | 1.65 | 0.44 |
| 1:B:680:GLU:O | 1:B:683:HIS:HB2 | 2.16 | 0.44 |
| 1:B:774:CYS:O | 1:B:778:THR:HG23 | 2.17 | 0.44 |
| 1:A:271:VAL:O | 1:A:273:LEU:N | 2.50 | 0.44 |
| 1:A:491:ARG:HD2 | 1:A:588:GLU:OE2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:786:ALA:C | 1:B:897:MET:HG2 | 2.37 | 0.44 |
| 1:B:897:MET:CE | 1:B:958:LYS:HE3 | 2.47 | 0.44 |
| 1:A:300:VAL:HA | 1:A:303:ALA:HB2 | 2.00 | 0.44 |
| 1:A:248:PRO:HB2 | 1:A:341:THR:HG23 | 1.99 | 0.44 |
| 1:A:557:ASP:HB3 | 1:A:559:LEU:HG | 1.98 | 0.44 |
| 1:A:767:SER:O | 1:A:771:GLU:CG | 2.63 | 0.44 |
| 1:B:794:TRP:C | 1:B:794:TRP:CD1 | 2.90 | 0.44 |
| 1:A:155:VAL:HG13 | 1:A:155:VAL:O | 2.17 | 0.44 |
| 1:A:338:SER:HA | 1:A:341:THR:CB | 2.46 | 0.44 |
| 1:A:853:ALA:O | 1:A:856:PHE:N | 2.51 | 0.44 |
| 1:B:443:THR:O | 1:B:447:THR:HG23 | 2.18 | 0.44 |
| 1:B:914:ASN:HD21 | 1:B:922:LEU:HD11 | 1.82 | 0.44 |
| 1:B:899:MET:HE2 | 1:B:966:GLN:O | 2.15 | 0.44 |
| 1:A:624:ILE:CD1 | 1:A:676:PHE:CD1 | 3.01 | 0.44 |
| 1:A:810:ASN:HA | 1:A:930:ASN:ND2 | 2.33 | 0.44 |
| 1:A:762:ARG:CZ | 1:A:833:LEU:HD11 | 2.48 | 0.44 |
| 1:A:878:GLU:C | 1:A:880:HIS:H | 2.20 | 0.44 |
| 1:A:786:ALA:C | 1:A:897:MET:HG2 | 2.38 | 0.44 |
| 1:B:663:LEU:H | 1:B:663:LEU:HD13 | 1.82 | 0.44 |
| 1:B:833:LEU:HD11 | 1:B:837:TYR:HE1 | 1.83 | 0.44 |
| 1:B:85:ILE:HD13 | 1:B:85:ILE:O | 2.17 | 0.44 |
| 1:B:336:LEU:O | 1:B:339:VAL:HG23 | 2.18 | 0.44 |
| 1:B:759:GLN:O | 1:B:760:PHE:C | 2.55 | 0.44 |
| 1:A:307:ILE:N | 1:A:307:ILE:HD13 | 2.33 | 0.43 |
| 1:A:748:GLU:N | 1:A:817:MET:HE1 | 2.33 | 0.43 |
| 1:A:895:GLU:N | 1:A:896:PRO:HD2 | 2.33 | 0.43 |
| 1:B:755:ASN:HD21 | 1:B:816:ILE:HD11 | 1.82 | 0.43 |
| 1:A:261:SER:O | 1:A:264:ILE:CB | 2.66 | 0.43 |
| 1:B:633:ILE:HD13 | 1:B:675:CYS:SG | 2.59 | 0.43 |
| 1:B:81:GLY:HA2 | 1:B:84:THR:HG22 | 2.00 | 0.43 |
| 1:B:873:PHE:HB2 | 1:B:891:PHE:CD2 | 2.53 | 0.43 |
| 1:B:982:GLU:OE1 | 1:B:982:GLU:HA | 2.18 | 0.43 |
| 1:A:293:ILE:H | 1:A:293:ILE:HG13 | 1.59 | 0.43 |
| 1:A:926:PRO:HA | 1:A:927:PRO:HD3 | 1.95 | 0.43 |
| 1:B:524:ARG:HH21 | 1:B:588:GLU:HB2 | 1.83 | 0.43 |
| 1:B:804:ALA:O | 1:B:805:THR:C | 2.56 | 0.43 |
| 1:B:975:LEU:H | 1:B:975:LEU:CD2 | 2.31 | 0.43 |
| 1:A:102:ALA:O | 1:A:106:VAL:CG2 | 2.64 | 0.43 |
| 1:A:342:LEU:O | 1:A:747:VAL:HG22 | 2.18 | 0.43 |
| 1:A:794:TRP:C | 1:A:794:TRP:CD1 | 2.91 | 0.43 |
| 1:A:762:ARG:HH21 | 1:A:833:LEU:HD13 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:895:GLU:HB2 | 1:A:896:PRO:HD3 | 2.00 | 0.43 |
| 1:B:802:LEU:H | 1:B:802:LEU:HG | 1.49 | 0.43 |
| 1:B:907:ILE:CD1 | 1:B:974:SER:HB3 | 2.49 | 0.43 |
| 1:A:873:PHE:HB2 | 1:A:891:PHE:CD2 | 2.53 | 0.43 |
| 1:B:624:ILE:CG2 | 1:B:684:LYS:HG2 | 2.49 | 0.43 |
| 1:B:70:CYS:O | 1:B:73:PHE:HB3 | 2.18 | 0.43 |
| 1:B:759:GLN:HE22 | 1:B:762:ARG:NH1 | 2.15 | 0.43 |
| 1:B:617:ALA:O | 1:B:820:PRO:HA | 2.19 | 0.43 |
| 1:A:299:ALA:O | 1:A:303:ALA:HB2 | 2.18 | 0.43 |
| 1:A:625:THR:HA | 3:A:998:BEF:F1 | 2.08 | 0.43 |
| 1:B:49:LEU:HD12 | 1:B:110:ARG:HG3 | 1.98 | 0.43 |
| 1:B:38:HIS:HD2 | 1:B:143:ARG:NH1 | 2.17 | 0.43 |
| 1:B:522:ILE:HD11 | 1:B:563:ALA:CB | 2.48 | 0.43 |
| 1:B:825:LYS:HA | 1:B:825:LYS:HE2 | 2.00 | 0.43 |
| 1:B:897:MET:HE3 | 1:B:958:LYS:O | 2.18 | 0.43 |
| 1:A:267:ILE:HD12 | 1:A:302:LEU:HD22 | 2.00 | 0.43 |
| 1:A:680:GLU:HB3 | 1:A:681:PRO:CD | 2.48 | 0.43 |
| 1:A:670:CYS:HG | 1:A:690:TYR:HD1 | 1.66 | 0.43 |
| 1:A:898:THR:OG1 | 1:A:959:LEU:HA | 2.18 | 0.43 |
| 1:A:897:MET:HE3 | 1:A:958:LYS:O | 2.19 | 0.43 |
| 1:B:255:GLU:C | 1:B:257:GLY:H | 2.22 | 0.43 |
| 1:B:367:PHE:HE2 | 1:B:545:ILE:HD12 | 1.83 | 0.43 |
| 1:B:48:SER:O | 1:B:52:LEU:HG | 2.19 | 0.43 |
| 1:A:55:GLU:O | 1:A:58:GLU:HB2 | 2.19 | 0.43 |
| 1:A:606:GLU:N | 1:A:606:GLU:CD | 2.71 | 0.43 |
| 1:A:624:ILE:HD13 | 1:A:676:PHE:HD1 | 1.84 | 0.43 |
| 1:A:845:GLY:C | 1:A:847:ALA:H | 2.20 | 0.43 |
| 1:A:783:LEU:HG | 1:A:870:LEU:HD23 | 1.99 | 0.43 |
| 1:A:811:PRO:HG3 | 1:A:929:VAL:O | 2.18 | 0.43 |
| 1:A:975:LEU:N | 1:A:976:PRO:HD2 | 2.34 | 0.43 |
| 1:B:519:GLU:CD | 1:B:519:GLU:N | 2.63 | 0.43 |
| 1:B:895:GLU:N | 1:B:896:PRO:HD2 | 2.33 | 0.43 |
| 1:A:103:ILE:HG23 | 1:A:104:VAL:H | 1.83 | 0.43 |
| 1:A:347:VAL:HG12 | 1:A:348:ILE:N | 2.34 | 0.43 |
| 1:A:524:ARG:HH21 | 1:A:588:GLU:HB2 | 1.84 | 0.43 |
| 1:A:604:ARG:NE | 1:A:720:MET:HE2 | 2.34 | 0.43 |
| 1:A:852:ALA:CA | 1:A:899:MET:HB3 | 2.48 | 0.43 |
| 1:B:214:ILE:H | 1:B:214:ILE:CD1 | 2.31 | 0.43 |
| 1:A:825:LYS:HA | 1:A:825:LYS:HE2 | 2.00 | 0.42 |
| 1:B:119:LEU:HD12 | 1:B:119:LEU:HA | 1.75 | 0.42 |
| 1:B:172:THR:CG2 | 1:B:489:ARG:CD | 2.96 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:342:LEU:HA | 1:B:716:ILE:HG13 | 2.00 | 0.42 |
| 1:A:774:CYS:O | 1:A:778:THR:HG23 | 2.19 | 0.42 |
| 1:A:982:GLU:HA | 1:A:982:GLU:OE1 | 2.19 | 0.42 |
| 1:B:763:TYR:HE1 | 1:B:908:GLU:O | 2.02 | 0.42 |
| 1:B:811:PRO:HG3 | 1:B:929:VAL:O | 2.18 | 0.42 |
| 1:A:314:VAL:CG1 | 1:A:804:ALA:HB1 | 2.49 | 0.42 |
| 1:B:100:ALA:O | 1:B:103:ILE:HG22 | 2.19 | 0.42 |
| 1:B:78:PHE:HE2 | 1:B:293:ILE:HG23 | 1.83 | 0.42 |
| 1:B:894:PRO:HB3 | 1:B:958:LYS:C | 2.39 | 0.42 |
| 1:B:851:ALA:HB3 | 1:B:903:VAL:HG21 | 2.00 | 0.42 |
| 1:A:236:ARG:C | 1:A:236:ARG:HD3 | 2.39 | 0.42 |
| 1:A:823:SER:HB3 | 1:A:826:GLU:CB | 2.26 | 0.42 |
| 1:A:848:THR:O | 1:A:852:ALA:CB | 2.68 | 0.42 |
| 1:B:28:GLN:HG2 | 1:B:31:ARG:HH22 | 1.85 | 0.42 |
| 1:B:62:VAL:HG13 | 1:B:98:LEU:HD22 | 2.00 | 0.42 |
| 1:A:342:LEU:HD22 | 1:A:747:VAL:HG22 | 2.00 | 0.42 |
| 1:A:884:GLU:HG2 | 1:A:884:GLU:H | 1.63 | 0.42 |
| 1:B:60:LEU:HD23 | 1:B:257:GLY:CA | 2.50 | 0.42 |
| 1:B:315:ILE:HD13 | 1:B:760:PHE:HE1 | 1.85 | 0.42 |
| 1:B:391:PRO:HB3 | 1:B:450:GLU:HB3 | 2.01 | 0.42 |
| 1:B:315:ILE:HD11 | 1:B:761:ILE:HD11 | 2.00 | 0.42 |
| 1:B:832:TRP:HZ2 | 1:B:984:LEU:O | 2.03 | 0.42 |
| 1:A:112:ALA:O | 1:A:113:GLU:C | 2.58 | 0.42 |
| 1:A:28:GLN:HG2 | 1:A:31:ARG:HH22 | 1.85 | 0.42 |
| 1:A:624:ILE:HD13 | 1:A:676:PHE:HB2 | 2.01 | 0.42 |
| 1:A:880:HIS:N | 1:A:881:PRO:HD2 | 2.34 | 0.42 |
| 1:A:882:HIS:HB3 | 1:A:883:PHE:CD1 | 2.54 | 0.42 |
| 1:A:975:LEU:HD22 | 1:A:975:LEU:N | 2.35 | 0.42 |
| 1:B:260:LEU:O | 1:B:263:VAL:HB | 2.19 | 0.42 |
| 1:A:103:ILE:HG23 | 1:A:104:VAL:N | 2.35 | 0.42 |
| 1:A:914:ASN:O | 1:A:916:LEU:N | 2.53 | 0.42 |
| 1:A:899:MET:HE2 | 1:A:966:GLN:O | 2.19 | 0.42 |
| 1:B:258:GLU:O | 1:B:259:GLN:C | 2.57 | 0.42 |
| 1:B:402:ILE:HD12 | 1:B:402:ILE:C | 2.40 | 0.42 |
| 1:B:753:ILE:O | 1:B:757:MET:HB2 | 2.19 | 0.42 |
| 1:A:286:GLY:HA3 | 1:A:290:ARG:HB3 | 1.99 | 0.42 |
| 1:A:387:SER:O | 1:A:602:PRO:HG2 | 2.20 | 0.42 |
| 1:A:577:VAL:HG12 | 1:A:579:ASP:OD2 | 2.20 | 0.42 |
| 1:A:120:LYS:CE | 1:A:723:GLY:O | 2.68 | 0.42 |
| 1:A:827:PRO:HB2 | 1:A:828:LEU:H | 1.49 | 0.42 |
| 1:A:834:PHE:O | 1:A:838:MET:HB2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:231:GLU:O | 1:B:235:ILE:HG12 | 2.18 | 0.42 |
| 1:B:311:LEU:HD21 | 1:B:761:ILE:HD12 | 2.01 | 0.42 |
| 1:B:680:GLU:HB3 | 1:B:681:PRO:CD | 2.49 | 0.42 |
| 1:B:795:VAL:HA | 1:B:799:THR:HB | 2.02 | 0.42 |
| 1:B:314:VAL:CG1 | 1:B:804:ALA:HB1 | 2.45 | 0.42 |
| 1:B:899:MET:CE | 1:B:970:VAL:CG2 | 2.89 | 0.42 |
| 1:B:950:VAL:O | 1:B:954:PRO:CD | 2.68 | 0.42 |
| 1:B:962:LEU:HB3 | 1:B:966:GLN:HB2 | 2.01 | 0.42 |
| 1:A:899:MET:SD | 1:A:962:LEU:CD2 | 3.08 | 0.42 |
| 1:B:235:ILE:HD11 | 1:B:681:PRO:HG2 | 2.02 | 0.42 |
| 1:B:338:SER:O | 1:B:339:VAL:C | 2.57 | 0.42 |
| 1:B:577:VAL:HG12 | 1:B:579:ASP:OD2 | 2.19 | 0.42 |
| 1:B:851:ALA:O | 1:B:854:TRP:HB3 | 2.19 | 0.42 |
| 1:A:174:ARG:NH2 | 1:A:188:ILE:HD11 | 2.35 | 0.42 |
| 1:A:181:THR:CB | 1:A:183:GLU:HG3 | 2.48 | 0.42 |
| 1:A:193:PRO:O | 1:A:195:PRO:HD3 | 2.20 | 0.42 |
| 1:A:232:ILE:HD13 | 1:A:232:ILE:C | 2.40 | 0.42 |
| 1:A:265:SER:O | 1:A:268:CYS:HB2 | 2.20 | 0.42 |
| 1:A:624:ILE:HG22 | 1:A:684:LYS:HG2 | 2.00 | 0.42 |
| 1:B:2:GLU:O | 1:B:3:ALA:CB | 2.66 | 0.42 |
| 1:B:59:ASP:OD2 | 1:B:62:VAL:HG23 | 2.19 | 0.42 |
| 1:B:600:LEU:N | 1:B:600:LEU:HD12 | 2.35 | 0.42 |
| 1:B:82:GLU:C | 1:B:83:GLU:HG3 | 2.40 | 0.42 |
| 1:A:624:ILE:HD13 | 1:A:676:PHE:CD1 | 2.55 | 0.41 |
| 1:A:962:LEU:HB3 | 1:A:966:GLN:HB2 | 2.02 | 0.41 |
| 1:B:290:ARG:HE | 1:B:291:GLY:N | 2.18 | 0.41 |
| 1:B:606:GLU:CD | 1:B:606:GLU:N | 2.72 | 0.41 |
| 1:B:606:GLU:HG3 | 1:B:739:ASN:OD1 | 2.20 | 0.41 |
| 1:B:770:GLY:HA2 | 1:B:841:GLY:O | 2.20 | 0.41 |
| 1:B:751:ARG:NH1 | 1:B:819:ARG:O | 2.52 | 0.41 |
| 1:A:2:GLU:O | 1:A:3:ALA:CB | 2.65 | 0.41 |
| 1:B:336:LEU:O | 1:B:339:VAL:CG2 | 2.68 | 0.41 |
| 1:B:549:ILE:CD1 | 1:B:596:VAL:HG11 | 2.50 | 0.41 |
| 1:B:975:LEU:N | 1:B:976:PRO:HD2 | 2.35 | 0.41 |
| 1:A:112:ALA:O | 1:A:114:ASN:N | 2.53 | 0.41 |
| 1:A:290:ARG:HG3 | 1:A:291:GLY:N | 2.34 | 0.41 |
| 1:A:311:LEU:HD11 | 1:A:761:ILE:HG12 | 2.02 | 0.41 |
| 1:A:868:HIS:NE2 | 1:A:883:PHE:HZ | 2.18 | 0.41 |
| 1:A:901:LEU:O | 1:A:905:VAL:HG23 | 2.20 | 0.41 |
| 1:A:931:ILE:CD1 | 1:A:931:ILE:H | 2.31 | 0.41 |
| 1:B:1:MET:O | 1:B:1:MET:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:60:LEU:HD21 | 1:B:257:GLY:HA3 | 2.03 | 0.41 |
| 1:B:336:LEU:HB2 | 1:B:337:PRO:HD3 | 2.02 | 0.41 |
| 1:B:584:PHE:CD2 | 1:B:584:PHE:N | 2.86 | 0.41 |
| 1:A:231:GLU:O | 1:A:235:ILE:HG12 | 2.20 | 0.41 |
| 1:A:434:TYR:HE2 | 1:A:468:ALA:HB2 | 1.85 | 0.41 |
| 1:A:311:LEU:HD22 | 1:A:761:ILE:HG23 | 2.02 | 0.41 |
| 1:B:255:GLU:C | 1:B:257:GLY:N | 2.74 | 0.41 |
| 1:B:749:GLU:C | 1:B:751:ARG:N | 2.74 | 0.41 |
| 1:B:762:ARG:CZ | 1:B:833:LEU:HD11 | 2.51 | 0.41 |
| 1:B:784:PRO:HG2 | 1:B:856:PHE:CE1 | 2.54 | 0.41 |
| 1:B:895:GLU:OE2 | 1:B:960:LYS:HD2 | 2.21 | 0.41 |
| 1:B:854:TRP:HH2 | 1:B:966:GLN:HG2 | 1.84 | 0.41 |
| 1:A:762:ARG:NH2 | 1:A:833:LEU:HD13 | 2.36 | 0.41 |
| 1:A:763:TYR:HE1 | 1:A:908:GLU:O | 2.03 | 0.41 |
| 1:A:762:ARG:O | 1:A:765:ILE:HG22 | 2.20 | 0.41 |
| 1:A:90:GLU:OE1 | 1:A:793:LEU:HD11 | 2.21 | 0.41 |
| 1:A:897:MET:CE | 1:A:958:LYS:HE3 | 2.50 | 0.41 |
| 1:B:42:PRO:O | 1:B:43:ALA:O | 2.37 | 0.41 |
| 1:B:556:ARG:NE | 1:B:644:GLU:CG | 2.83 | 0.41 |
| 1:B:762:ARG:HH21 | 1:B:833:LEU:HD13 | 1.85 | 0.41 |
| 1:A:584:PHE:N | 1:A:584:PHE:CD2 | 2.87 | 0.41 |
| 1:A:697:ILE:H | 1:A:697:ILE:HD12 | 1.85 | 0.41 |
| 1:A:70:CYS:O | 1:A:73:PHE:HB3 | 2.21 | 0.41 |
| 1:A:969:MET:O | 1:A:969:MET:HE2 | 2.20 | 0.41 |
| 1:B:686:LYS:HE3 | 1:B:686:LYS:HB2 | 1.90 | 0.41 |
| 1:B:804:ALA:O | 1:B:807:LEU:N | 2.52 | 0.41 |
| 1:B:868:HIS:NE2 | 1:B:883:PHE:HZ | 2.18 | 0.41 |
| 1:B:975:LEU:N | 1:B:975:LEU:HD22 | 2.36 | 0.41 |
| 1:A:103:ILE:HD13 | 1:A:103:ILE:C | 2.41 | 0.41 |
| 1:A:305:ALA:O | 1:A:768:ASN:HA | 2.20 | 0.41 |
| 1:A:851:ALA:HB3 | 1:A:903:VAL:HG21 | 2.01 | 0.41 |
| 1:A:895:GLU:OE2 | 1:A:960:LYS:CD | 2.69 | 0.41 |
| 1:B:309:GLU:H | 1:B:309:GLU:CD | 2.23 | 0.41 |
| 1:B:352:LYS:HG2 | 1:B:353:THR:N | 2.35 | 0.41 |
| 1:A:663:LEU:CD1 | 1:A:663:LEU:N | 2.83 | 0.41 |
| 1:A:325:ARG:NH2 | 1:A:753:ILE:HD11 | 2.36 | 0.41 |
| 1:A:775:ILE:HD13 | 1:A:775:ILE:N | 2.31 | 0.41 |
| 1:A:794:TRP:O | 1:A:794:TRP:CD1 | 2.73 | 0.41 |
| 1:A:96:LEU:C | 1:A:96:LEU:HD23 | 2.41 | 0.41 |
| 1:B:116:ILE:CD1 | 1:B:334:ARG:HG2 | 2.51 | 0.41 |
| 1:B:390:ALA:HA | 1:B:391:PRO:HD3 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:926:PRO:HA | 1:B:927:PRO:HD3 | 1.95 | 0.41 |
| 1:B:964:LEU:O | 1:B:964:LEU:HD23 | 2.20 | 0.41 |
| 1:A:885:GLY:O | 1:A:886:LEU:HG | 2.21 | 0.41 |
| 1:B:652:ALA:HA | 1:B:675:CYS:O | 2.20 | 0.41 |
| 1:B:740:PHE:HA | 1:B:743:ILE:HD13 | 2.01 | 0.41 |
| 1:B:880:HIS:N | 1:B:881:PRO:CD | 2.83 | 0.41 |
| 1:B:947:ILE:HD11 | 1:B:957:PHE:CD2 | 2.56 | 0.41 |
| 1:A:512:MET:HB2 | 1:A:567:ARG:HB3 | 2.03 | 0.41 |
| 1:A:797:LEU:HA | 1:A:797:LEU:HD23 | 1.64 | 0.41 |
| 1:A:907:ILE:CD1 | 1:A:974:SER:HB3 | 2.51 | 0.41 |
| 1:B:338:SER:HA | 1:B:341:THR:CB | 2.50 | 0.41 |
| 1:B:624:ILE:HG22 | 1:B:684:LYS:HG2 | 2.03 | 0.41 |
| 1:B:853:ALA:O | 1:B:856:PHE:N | 2.54 | 0.41 |
| 1:B:969:MET:HE2 | 1:B:973:ILE:HG12 | 2.03 | 0.41 |
| 1:A:390:ALA:HA | 1:A:391:PRO:HD3 | 1.83 | 0.41 |
| 1:A:416:ILE:HD11 | 1:A:566:THR:HG22 | 2.03 | 0.41 |
| 1:B:261:SER:O | 1:B:264:ILE:HB | 2.20 | 0.41 |
| 1:B:290:ARG:HE | 1:B:291:GLY:CA | 2.34 | 0.41 |
| 1:B:369:ILE:HD11 | 1:B:593:PHE:HD1 | 1.85 | 0.41 |
| 1:B:305:ALA:HB3 | 1:B:772:VAL:HG22 | 2.03 | 0.41 |
| 1:B:895:GLU:OE2 | 1:B:960:LYS:CD | 2.68 | 0.41 |
| 1:A:606:GLU:HG3 | 1:A:739:ASN:OD1 | 2.22 | 0.40 |
| 1:A:895:GLU:OE2 | 1:A:960:LYS:HD2 | 2.21 | 0.40 |
| 1:B:112:ALA:O | 1:B:113:GLU:C | 2.58 | 0.40 |
| 1:B:315:ILE:HG22 | 1:B:316:THR:N | 2.36 | 0.40 |
| 1:B:369:ILE:HG12 | 1:B:528:VAL:HG11 | 2.03 | 0.40 |
| 1:B:345:THR:HG23 | 1:B:697:ILE:O | 2.21 | 0.40 |
| 1:A:363:VAL:HG11 | 1:A:448:LEU:HD22 | 2.03 | 0.40 |
| 1:B:269:VAL:O | 1:B:272:TRP:HE3 | 2.05 | 0.40 |
| 1:B:304:VAL:C | 1:B:306:ALA:H | 2.25 | 0.40 |
| 1:B:556:ARG:NE | 1:B:644:GLU:HG2 | 2.37 | 0.40 |
| 1:B:740:PHE:O | 1:B:743:ILE:CD1 | 2.60 | 0.40 |
| 1:A:843:TYR:HH | 1:A:976:PRO:HG2 | 1.84 | 0.40 |
| 1:B:357:THR:HB | 1:B:602:PRO:O | 2.21 | 0.40 |
| 1:B:914:ASN:O | 1:B:916:LEU:N | 2.55 | 0.40 |
| 1:A:604:ARG:HB2 | 1:A:607:VAL:HG23 | 2.03 | 0.40 |
| 1:A:684:LYS:NZ | 1:A:707:ASP:OD1 | 2.53 | 0.40 |
| 1:A:75:LEU:HD11 | 1:A:300:VAL:HG23 | 2.04 | 0.40 |
| 1:A:795:VAL:HA | 1:A:799:THR:HB | 2.03 | 0.40 |
| 1:A:947:ILE:HD11 | 1:A:957:PHE:CD2 | 2.57 | 0.40 |
| 1:B:236:ARG:HD3 | 1:B:236:ARG:C | 2.41 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:740:PHE:C | 1:B:743:ILE:HD13 | 2.40 | 0.40 |
| 1:B:762:ARG:NH2 | 1:B:833:LEU:HD13 | 2.36 | 0.40 |
| 1:B:797:LEU:HA | 1:B:797:LEU:HD23 | 1.62 | 0.40 |
| 1:B:898:THR:HG21 | 1:B:960:LYS:O | 2.22 | 0.40 |
| 1:B:103:ILE:CG2 | 1:B:104:VAL:N | 2.84 | 0.40 |
| 1:B:416:ILE:HD11 | 1:B:566:THR:HG22 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1 | A | 993/995 (100%) | 883 (89%) | 84 (8%) | 26 (3%) | 5 | 36 |
| 1 | B | 993/995 (100%) | 876 (88%) | 91 (9%) | 26 (3%) | 5 | 36 |
| All | All | 1986/1990 (100%) | 1759 (89%) | 175 (9%) | 52 (3%) | 5 | 36 |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 47 | LYS |
| 1 | A | 245 | ASP |
| 1 | A | 292 | ALA |
| 1 | A | 783 | LEU |
| 1 | A | 818 | ASP |
| 1 | A | 827 | PRO |
| 1 | A | 828 | LEU |
| 1 | B | 47 | LYS |
| 1 | B | 245 | ASP |
| 1 | B | 292 | ALA |
| 1 | B | 783 | LEU |
| 1 | B | 818 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 827 | PRO |
| 1 | B | 828 | LEU |
| 1 | B | 863 | PRO |
| 1 | A | 43 | ALA |
| 1 | A | 293 | ILE |
| 1 | A | 309 | GLU |
| 1 | A | 790 | VAL |
| 1 | A | 860 | GLU |
| 1 | A | 863 | PRO |
| 1 | A | 878 | GLU |
| 1 | B | 43 | ALA |
| 1 | B | 293 | ILE |
| 1 | B | 790 | VAL |
| 1 | B | 860 | GLU |
| 1 | B | 878 | GLU |
| 1 | A | 762 | ARG |
| 1 | A | 830 | SER |
| 1 | B | 309 | GLU |
| 1 | B | 330 | ASN |
| 1 | B | 762 | ARG |
| 1 | B | 830 | SER |
| 1 | A | 272 | TRP |
| 1 | A | 287 | SER |
| 1 | A | 754 | TYR |
| 1 | A | 915 | SER |
| 1 | B | 42 | PRO |
| 1 | B | 831 | GLY |
| 1 | A | 294 | TYR |
| 1 | A | 951 | ASP |
| 1 | B | 294 | TYR |
| 1 | B | 915 | SER |
| 1 | A | 831 | GLY |
| 1 | B | 352 | LYS |
| 1 | B | 951 | ASP |
| 1 | A | 789 | PRO |
| 1 | A | 601 | ASP |
| 1 | B | 46 | GLY |
| 1 | B | 789 | PRO |
| 1 | A | 950 | VAL |
| 1 | B | 950 | 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 | 840/840 (100%) | 757 (90%) | 83 (10%) | 8 | 32 |
| 1 | B | 840/840 (100%) | 761 (91%) | 79 (9%) | 8 | 35 |
| All | All | 1680/1680 (100%) | 1518 (90%) | 162 (10%) | 8 | 34 |

All (162) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | GLU |
| 1 | A | 56 | GLN |
| 1 | A | 59 | ASP |
| 1 | A | 79 | GLU |
| 1 | A | 86 | THR |
| 1 | A | 88 | PHE |
| 1 | A | 90 | GLU |
| 1 | A | 92 | PHE |
| 1 | A | 94 | ILE |
| 1 | A | 103 | ILE |
| 1 | A | 110 | ARG |
| 1 | A | 114 | ASN |
| 1 | A | 125 | GLU |
| 1 | A | 134 | ARG |
| 1 | A | 149 | ASP |
| 1 | A | 164 | ARG |
| 1 | A | 171 | THR |
| 1 | A | 232 | ILE |
| 1 | A | 239 | MET |
| 1 | A | 247 | THR |
| 1 | A | 249 | LEU |
| 1 | A | 250 | GLN |
| 1 | A | 251 | GLN |
| 1 | A | 252 | LYS |
| 1 | A | 255 | GLU |
| 1 | A | 256 | PHE |
| 1 | A | 259 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 284 | HIS |
| 1 | A | 289 | ILE |
| 1 | A | 296 | PHE |
| 1 | A | 298 | ILE |
| 1 | A | 302 | LEU |
| 1 | A | 307 | ILE |
| 1 | A | 334 | ARG |
| 1 | A | 338 | SER |
| 1 | A | 342 | LEU |
| 1 | A | 353 | THR |
| 1 | A | 355 | THR |
| 1 | A | 356 | LEU |
| 1 | A | 359 | ASN |
| 1 | A | 367 | PHE |
| 1 | A | 402 | ILE |
| 1 | A | 403 | ARG |
| 1 | A | 421 | ASN |
| 1 | A | 426 | ASP |
| 1 | A | 439 | GLU |
| 1 | A | 447 | THR |
| 1 | A | 484 | THR |
| 1 | A | 488 | SER |
| 1 | A | 489 | ARG |
| 1 | A | 519 | GLU |
| 1 | A | 534 | ARG |
| 1 | A | 545 | ILE |
| 1 | A | 566 | THR |
| 1 | A | 572 | LYS |
| 1 | A | 573 | ARG |
| 1 | A | 575 | GLU |
| 1 | A | 600 | LEU |
| 1 | A | 691 | LEU |
| 1 | A | 713 | LYS |
| 1 | A | 726 | VAL |
| 1 | A | 757 | MET |
| 1 | A | 763 | TYR |
| 1 | A | 765 | ILE |
| 1 | A | 775 | ILE |
| 1 | A | 793 | LEU |
| 1 | A | 795 | VAL |
| 1 | A | 797 | LEU |
| 1 | A | 802 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 813 | ASP |
| 1 | A | 816 | ILE |
| 1 | A | 817 | MET |
| 1 | A | 829 | ILE |
| 1 | A | 840 | ILE |
| 1 | A | 849 | VAL |
| 1 | A | 854 | TRP |
| 1 | A | 882 | HIS |
| 1 | A | 911 | ASN |
| 1 | A | 925 | MET |
| 1 | A | 951 | ASP |
| 1 | A | 955 | MET |
| 1 | A | 956 | ILE |
| 1 | A | 993 | GLU |
| 1 | B | 10 | GLU |
| 1 | B | 78 | PHE |
| 1 | B | 79 | GLU |
| 1 | B | 85 | ILE |
| 1 | B | 86 | THR |
| 1 | B | 88 | PHE |
| 1 | B | 90 | GLU |
| 1 | B | 92 | PHE |
| 1 | B | 94 | ILE |
| 1 | B | 95 | LEU |
| 1 | B | 101 | ASN |
| 1 | B | 103 | ILE |
| 1 | B | 109 | GLU |
| 1 | B | 110 | ARG |
| 1 | B | 114 | ASN |
| 1 | B | 125 | GLU |
| 1 | B | 134 | ARG |
| 1 | B | 140 | ILE |
| 1 | B | 149 | ASP |
| 1 | B | 164 | ARG |
| 1 | B | 172 | THR |
| 1 | B | 175 | VAL |
| 1 | B | 246 | LYS |
| 1 | B | 250 | GLN |
| 1 | B | 251 | GLN |
| 1 | B | 252 | LYS |
| 1 | B | 255 | GLU |
| 1 | B | 256 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 259 | GLN |
| 1 | B | 265 | SER |
| 1 | B | 272 | TRP |
| 1 | B | 281 | ASP |
| 1 | B | 296 | PHE |
| 1 | B | 300 | VAL |
| 1 | B | 302 | LEU |
| 1 | B | 307 | ILE |
| 1 | B | 338 | SER |
| 1 | B | 342 | LEU |
| 1 | B | 355 | THR |
| 1 | B | 361 | MET |
| 1 | B | 384 | ILE |
| 1 | B | 403 | ARG |
| 1 | B | 421 | ASN |
| 1 | B | 426 | ASP |
| 1 | B | 439 | GLU |
| 1 | B | 447 | THR |
| 1 | B | 484 | THR |
| 1 | B | 488 | SER |
| 1 | B | 489 | ARG |
| 1 | B | 519 | GLU |
| 1 | B | 534 | ARG |
| 1 | B | 566 | THR |
| 1 | B | 572 | LYS |
| 1 | B | 573 | ARG |
| 1 | B | 575 | GLU |
| 1 | B | 600 | LEU |
| 1 | B | 691 | LEU |
| 1 | B | 713 | LYS |
| 1 | B | 726 | VAL |
| 1 | B | 755 | ASN |
| 1 | B | 757 | MET |
| 1 | B | 763 | TYR |
| 1 | B | 783 | LEU |
| 1 | B | 793 | LEU |
| 1 | B | 795 | VAL |
| 1 | B | 797 | LEU |
| 1 | B | 802 | LEU |
| 1 | B | 813 | ASP |
| 1 | B | 816 | ILE |
| 1 | B | 817 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 829 | ILE |
| 1 | B | 849 | VAL |
| 1 | B | 854 | TRP |
| 1 | B | 882 | HIS |
| 1 | B | 911 | ASN |
| 1 | B | 925 | MET |
| 1 | B | 951 | ASP |
| 1 | B | 955 | MET |
| 1 | B | 993 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 108 | GLN |
| 1 | A | 111 | ASN |
| 1 | A | 114 | ASN |
| 1 | A | 177 | GLN |
| 1 | A | 251 | GLN |
| 1 | A | 275 | ASN |
| 1 | A | 359 | ASN |
| 1 | A | 406 | GLN |
| 1 | A | 421 | ASN |
| 1 | A | 461 | ASN |
| 1 | A | 510 | ASN |
| 1 | A | 759 | GLN |
| 1 | A | 869 | GLN |
| 1 | A | 875 | GLN |
| 1 | A | 911 | ASN |
| 1 | A | 914 | ASN |
| 1 | A | 966 | GLN |
| 1 | B | 38 | HIS |
| 1 | B | 108 | GLN |
| 1 | B | 111 | ASN |
| 1 | B | 114 | ASN |
| 1 | B | 250 | GLN |
| 1 | B | 251 | GLN |
| 1 | B | 259 | GLN |
| 1 | B | 359 | ASN |
| 1 | B | 406 | GLN |
| 1 | B | 421 | ASN |
| 1 | B | 456 | ASN |
| 1 | B | 461 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 510 | ASN |
| 1 | B | 759 | GLN |
| 1 | B | 869 | GLN |
| 1 | B | 875 | GLN |
| 1 | B | 911 | ASN |
| 1 | B | 914 | ASN |
| 1 | B | 966 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 3 | BEF | B | 1098 | 1 | 0,3,3 | 0.00 | - | - | | |
| 3 | BEF | A | 998 | 1 | 0,3,3 | 0.00 | - | - | | |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | A | 998 | BEF | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.