



Full wwPDB X-ray Structure Validation Report i

May 22, 2020 – 02:01 pm BST

PDB ID : 5L5N
Title : Plexin A4 full extracellular region, domains 1 to 7 modeled, data to 8.5 angstrom, spacegroup P4(3)22
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kauffman, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 8.50 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 i symbol.

The following versions of software and data (see references ①) were used in the production of this report:

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

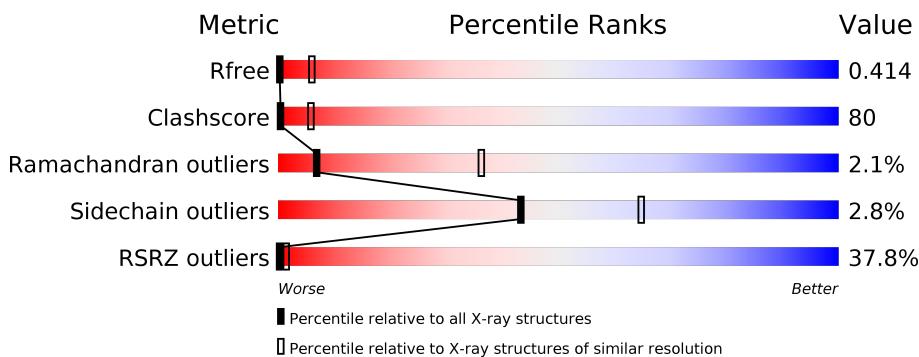
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| R_{free} | 130704 | 1005 (11.50-3.90) |
| Clashscore | 141614 | 1070 (11.50-3.90) |
| Ramachandran outliers | 138981 | 1003 (11.50-3.90) |
| Sidechain outliers | 138945 | 1003 (11.50-3.86) |
| RSRZ outliers | 127900 | 1004 (9.50-3.80) |

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

| Mol | Chain | Length | Quality of chain | | | | |
|-----|-------|--------|---|---|---|--|---|
| 1 | A | 1207 |  29% |  24% |  48% |  • |  24% |

2 Entry composition [\(i\)](#)

There is only 1 type of molecule in this entry. The entry contains 7189 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 Plexin-A4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----------|-----------|-----------|-----------|---------|---------|-------|
| 1 | A | 915 | Total | C 7189 | N 4533 | O 1239 | S 1357 | 60 | 0 | 0 |

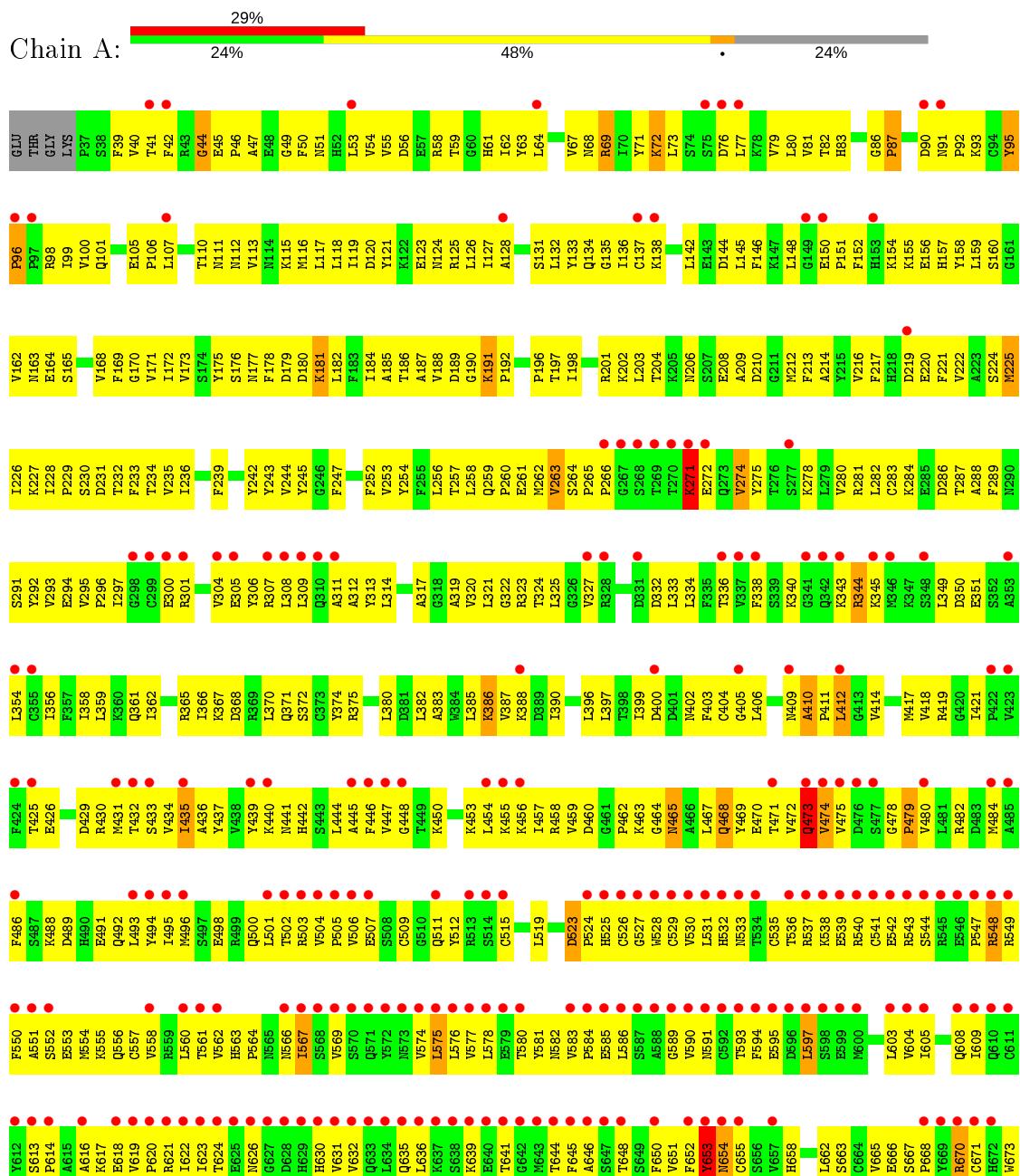
There are 13 discrepancies between the modelled and reference sequences:

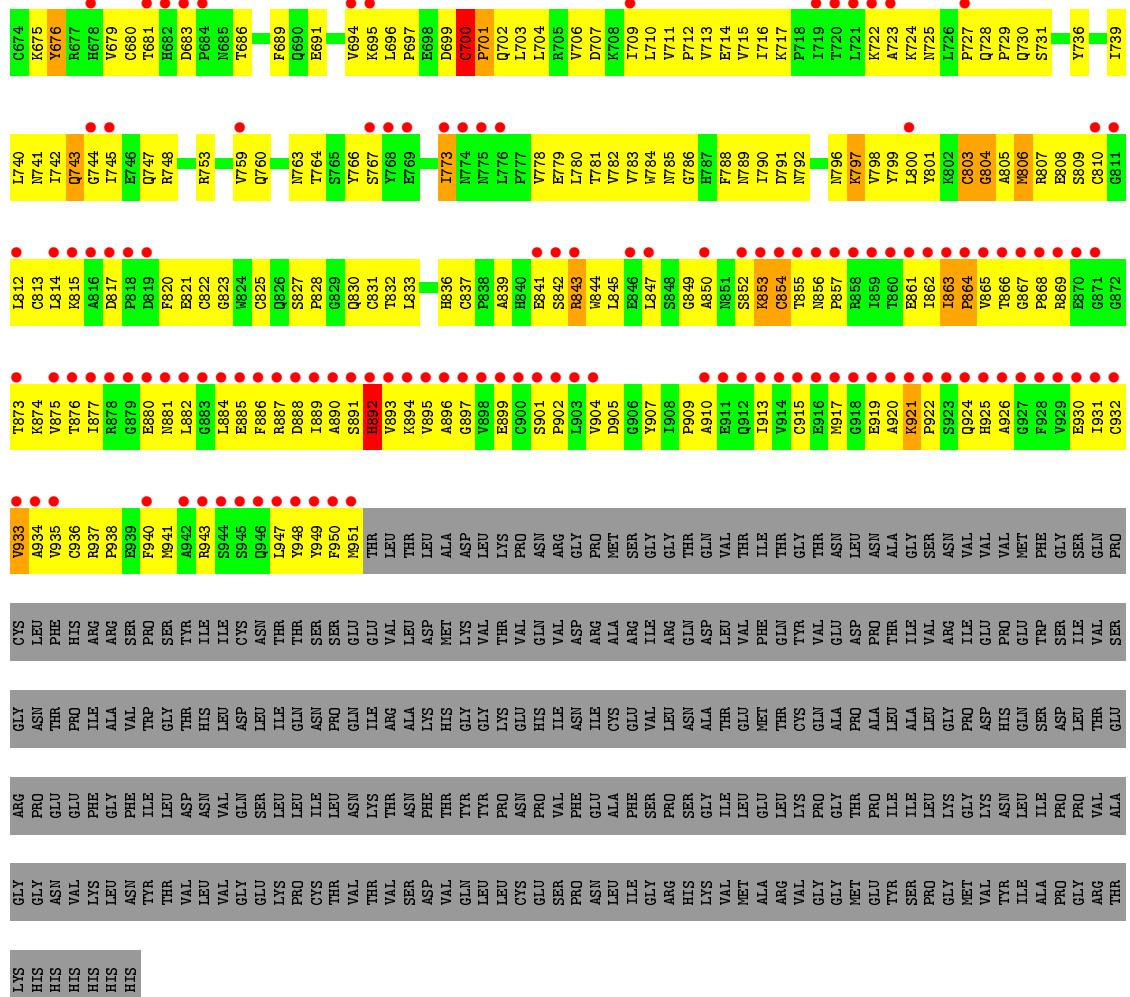
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 33 | GLU | - | expression tag | UNP Q80UG2 |
| A | 34 | THR | - | expression tag | UNP Q80UG2 |
| A | 35 | GLY | - | expression tag | UNP Q80UG2 |
| A | 1230 | GLY | - | expression tag | UNP Q80UG2 |
| A | 1231 | ARG | - | expression tag | UNP Q80UG2 |
| A | 1232 | THR | - | expression tag | UNP Q80UG2 |
| A | 1233 | LYS | - | expression tag | UNP Q80UG2 |
| A | 1234 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1235 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1236 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1237 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1238 | HIS | - | expression tag | UNP Q80UG2 |
| A | 1239 | HIS | - | expression tag | UNP Q80UG2 |

3 Residue-property plots

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

- Molecule 1: Plexin-A4





4 Data and refinement statistics (i)

| Property | Value | Source |
|---|--|------------------|
| Space group | P 43 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 189.48 Å 189.48 Å 252.59 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 70.37 – 8.50 70.37 – 8.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (70.37-8.50) 99.6 (70.37-8.50) | Depositor EDS |
| R_{merge} | 0.33 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle^1$ | 1.94 (at 8.39 Å) | Xtriage |
| Refinement program | PHENIX 1.8.2_1309 | Depositor |
| R , R_{free} | 0.401 , 0.412 0.411 , 0.414 | Depositor DCC |
| R_{free} test set | 203 reflections (4.64%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 502.9 | Xtriage |
| Anisotropy | 0.294 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 149.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.53 | EDS |
| Total number of atoms | 7189 | wwPDB-VP |
| Average B, all atoms (Å ²) | 162.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 1.10 | 4/7343 (0.1%) | 1.26 | 20/9940 (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 | 4 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | A | 653 | TYR | C-N | -36.36 | 0.50 | 1.34 |
| 1 | A | 700 | CYS | C-N | -33.68 | 0.70 | 1.34 |
| 1 | A | 49 | GLY | CA-C | 6.43 | 1.62 | 1.51 |
| 1 | A | 49 | GLY | C-N | 5.09 | 1.45 | 1.34 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 747 | GLN | CG-CD-OE1 | -38.83 | 43.94 | 121.60 |
| 1 | A | 653 | TYR | O-C-N | -20.66 | 89.64 | 122.70 |
| 1 | A | 700 | CYS | C-N-CD | -19.18 | 78.41 | 120.60 |
| 1 | A | 700 | CYS | O-C-N | -10.23 | 101.67 | 121.10 |
| 1 | A | 747 | GLN | CG-CD-NE2 | -9.56 | 93.74 | 116.70 |
| 1 | A | 479 | PRO | N-CA-C | 8.17 | 133.35 | 112.10 |
| 1 | A | 653 | TYR | CA-C-N | -7.88 | 99.87 | 117.20 |
| 1 | A | 843 | ARG | C-N-CA | 7.75 | 141.07 | 121.70 |
| 1 | A | 653 | TYR | C-N-CA | -6.96 | 104.30 | 121.70 |
| 1 | A | 478 | GLY | CA-C-O | -6.89 | 108.19 | 120.60 |
| 1 | A | 747 | GLN | OE1-CD-NE2 | 6.86 | 137.69 | 121.90 |
| 1 | A | 473 | GLN | C-N-CA | -6.68 | 105.00 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 892 | HIS | CA-CB-CG | 6.56 | 124.75 | 113.60 |
| 1 | A | 225 | MET | CG-SD-CE | -5.69 | 91.09 | 100.20 |
| 1 | A | 409 | ASN | C-N-CA | 5.67 | 135.88 | 121.70 |
| 1 | A | 49 | GLY | C-N-CA | 5.58 | 135.66 | 121.70 |
| 1 | A | 274 | VAL | CG1-CB-CG2 | 5.44 | 119.60 | 110.90 |
| 1 | A | 919 | GLU | C-N-CA | 5.27 | 134.88 | 121.70 |
| 1 | A | 803 | CYS | C-N-CA | 5.09 | 132.99 | 122.30 |
| 1 | A | 676 | TYR | CA-CB-CG | -5.08 | 103.75 | 113.40 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 653 | TYR | Mainchain |
| 1 | A | 700 | CYS | Mainchain |
| 1 | A | 863 | ILE | Peptide |
| 1 | A | 95 | TYR | Peptide |

5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 7189 | 0 | 7049 | 1133 | 32 |
| All | All | 7189 | 0 | 7049 | 1133 | 32 |

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 80.

All (1133) 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:468:GLN:HG3 | 1:A:524:PRO:CD | 1.18 | 1.58 |
| 1:A:530:VAL:HG11 | 1:A:584:PRO:CD | 1.11 | 1.56 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:NZ | 1.78 | 1.51 |
| 1:A:468:GLN:CG | 1:A:524:PRO:HD3 | 1.39 | 1.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:439:TYR:HE2 | 1:A:538:LYS:NZ | 1.11 | 1.44 |
| 1:A:530:VAL:CG1 | 1:A:584:PRO:HD2 | 1.48 | 1.42 |
| 1:A:556:GLN:HA | 1:A:582:ASN:ND2 | 1.33 | 1.36 |
| 1:A:530:VAL:CG1 | 1:A:584:PRO:CD | 2.00 | 1.35 |
| 1:A:815:LYS:CE | 1:A:910:ALA:HB3 | 1.55 | 1.34 |
| 1:A:662:LEU:HD23 | 1:A:791:ASP:OD2 | 1.27 | 1.32 |
| 1:A:557:CYS:O | 1:A:582:ASN:CB | 1.74 | 1.32 |
| 1:A:812:LEU:HD21 | 1:A:880:GLU:O | 1.23 | 1.31 |
| 1:A:699:ASP:HA | 1:A:725:ASN:OD1 | 1.11 | 1.28 |
| 1:A:810:CYS:SG | 1:A:855:THR:HG22 | 1.76 | 1.24 |
| 1:A:557:CYS:C | 1:A:582:ASN:HB2 | 1.58 | 1.24 |
| 1:A:569:VAL:CG2 | 1:A:654:ASN:HB2 | 1.66 | 1.23 |
| 1:A:555:LYS:O | 1:A:582:ASN:OD1 | 1.57 | 1.20 |
| 1:A:569:VAL:HB | 1:A:654:ASN:ND2 | 1.56 | 1.20 |
| 1:A:662:LEU:CD2 | 1:A:791:ASP:OD2 | 1.91 | 1.17 |
| 1:A:469:TYR:CG | 1:A:523:ASP:OD2 | 1.98 | 1.17 |
| 1:A:439:TYR:HE2 | 1:A:538:LYS:CE | 1.59 | 1.16 |
| 1:A:468:GLN:CG | 1:A:524:PRO:CD | 2.08 | 1.15 |
| 1:A:453:LYS:HG2 | 1:A:472:VAL:HG22 | 1.25 | 1.14 |
| 1:A:435:ILE:HG22 | 1:A:446:PHE:HB2 | 1.22 | 1.13 |
| 1:A:468:GLN:HG3 | 1:A:524:PRO:HD2 | 1.27 | 1.13 |
| 1:A:295:VAL:HG12 | 1:A:414:VAL:HG11 | 1.27 | 1.13 |
| 1:A:533:ASN:ND2 | 1:A:644:THR:O | 1.82 | 1.13 |
| 1:A:324:THR:HB | 1:A:462:PRO:HB3 | 1.27 | 1.13 |
| 1:A:533:ASN:HD21 | 1:A:644:THR:C | 1.51 | 1.12 |
| 1:A:533:ASN:ND2 | 1:A:644:THR:C | 2.03 | 1.12 |
| 1:A:469:TYR:CB | 1:A:523:ASP:OD2 | 1.98 | 1.12 |
| 1:A:699:ASP:CA | 1:A:725:ASN:OD1 | 1.98 | 1.11 |
| 1:A:468:GLN:CB | 1:A:524:PRO:HD3 | 1.79 | 1.11 |
| 1:A:595:GLU:HB2 | 1:A:597:LEU:HD23 | 1.32 | 1.11 |
| 1:A:359:LEU:HD12 | 1:A:362:ILE:HD11 | 1.24 | 1.11 |
| 1:A:530:VAL:HB | 1:A:584:PRO:HG3 | 1.21 | 1.09 |
| 1:A:118:LEU:HD12 | 1:A:172:ILE:HD12 | 1.17 | 1.09 |
| 1:A:806:MET:H | 1:A:806:MET:HE3 | 1.14 | 1.08 |
| 1:A:556:GLN:CA | 1:A:582:ASN:ND2 | 2.16 | 1.07 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:HG23 | 1.33 | 1.06 |
| 1:A:662:LEU:HD23 | 1:A:791:ASP:CG | 1.76 | 1.05 |
| 1:A:530:VAL:CG1 | 1:A:584:PRO:CG | 2.33 | 1.05 |
| 1:A:469:TYR:HB2 | 1:A:523:ASP:CG | 1.76 | 1.04 |
| 1:A:469:TYR:HB2 | 1:A:523:ASP:OD2 | 1.55 | 1.04 |
| 1:A:815:LYS:CD | 1:A:910:ALA:HB3 | 1.87 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:815:LYS:HE3 | 1:A:910:ALA:HB3 | 1.31 | 1.04 |
| 1:A:569:VAL:HG23 | 1:A:654:ASN:CB | 1.87 | 1.04 |
| 1:A:812:LEU:CD2 | 1:A:880:GLU:O | 2.05 | 1.03 |
| 1:A:560:LEU:HD23 | 1:A:648:THR:HG23 | 1.37 | 1.03 |
| 1:A:812:LEU:HG | 1:A:881:ASN:OD1 | 1.59 | 1.02 |
| 1:A:620:PRO:HA | 1:A:623:ILE:HG13 | 1.41 | 1.02 |
| 1:A:494:TYR:HB3 | 1:A:501:LEU:HD21 | 1.40 | 1.01 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:CB | 1.89 | 1.01 |
| 1:A:301:ARG:HD2 | 1:A:425:THR:HG21 | 1.37 | 1.01 |
| 1:A:854:CYS:HB3 | 1:A:855:THR:N | 1.75 | 0.99 |
| 1:A:623:ILE:HA | 1:A:626:ASN:HD21 | 1.28 | 0.99 |
| 1:A:444:LEU:HD12 | 1:A:446:PHE:CE1 | 1.98 | 0.98 |
| 1:A:533:ASN:CG | 1:A:645:PHE:HB3 | 1.83 | 0.98 |
| 1:A:117:LEU:HD11 | 1:A:126:LEU:HD21 | 1.45 | 0.98 |
| 1:A:46:PRO:HG2 | 1:A:69:ARG:HG3 | 1.41 | 0.97 |
| 1:A:557:CYS:C | 1:A:558:VAL:HA | 1.85 | 0.97 |
| 1:A:530:VAL:HG11 | 1:A:584:PRO:HD3 | 1.47 | 0.97 |
| 1:A:563:HIS:HB3 | 1:A:564:PRO:HD3 | 1.44 | 0.95 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:CE | 2.40 | 0.95 |
| 1:A:42:PHE:HE1 | 1:A:79:VAL:HG22 | 1.31 | 0.95 |
| 1:A:557:CYS:O | 1:A:582:ASN:HB2 | 0.77 | 0.94 |
| 1:A:72:LYS:HE3 | 1:A:80:LEU:HD13 | 1.49 | 0.94 |
| 1:A:808:GLU:OE2 | 1:A:880:GLU:OE1 | 1.83 | 0.94 |
| 1:A:297:ILE:HG22 | 1:A:418:VAL:CG1 | 1.97 | 0.94 |
| 1:A:530:VAL:HG11 | 1:A:584:PRO:CG | 1.96 | 0.94 |
| 1:A:863:ILE:HG22 | 1:A:876:THR:HB | 1.48 | 0.93 |
| 1:A:862:ILE:HG22 | 1:A:877:ILE:HA | 1.46 | 0.93 |
| 1:A:865:VAL:HG13 | 1:A:866:THR:HG23 | 1.50 | 0.93 |
| 1:A:804:GLY:HA2 | 1:A:806:MET:SD | 2.09 | 0.92 |
| 1:A:39:PHE:CE2 | 1:A:473:GLN:HG3 | 2.04 | 0.92 |
| 1:A:62:ILE:CG1 | 1:A:73:LEU:HB2 | 1.98 | 0.92 |
| 1:A:297:ILE:HG22 | 1:A:418:VAL:HG12 | 1.49 | 0.92 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:HB3 | 1.48 | 0.92 |
| 1:A:530:VAL:CB | 1:A:584:PRO:HG3 | 1.99 | 0.91 |
| 1:A:239:PHE:HA | 1:A:260:PRO:HG2 | 1.51 | 0.91 |
| 1:A:566:ASN:HA | 1:A:651:VAL:HG23 | 1.49 | 0.91 |
| 1:A:435:ILE:HD13 | 1:A:436:ALA:H | 1.34 | 0.91 |
| 1:A:933:VAL:HG23 | 1:A:934:ALA:H | 1.36 | 0.91 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:CZ | 2.04 | 0.91 |
| 1:A:806:MET:SD | 1:A:807:ARG:HG3 | 2.11 | 0.91 |
| 1:A:815:LYS:CE | 1:A:909:PRO:O | 2.19 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:815:LYS:HD2 | 1:A:910:ALA:CB | 2.00 | 0.90 |
| 1:A:569:VAL:HG23 | 1:A:654:ASN:HB2 | 0.91 | 0.90 |
| 1:A:359:LEU:CD1 | 1:A:362:ILE:HD11 | 2.02 | 0.90 |
| 1:A:271:LYS:HG3 | 1:A:272:GLU:H | 1.34 | 0.89 |
| 1:A:447:VAL:HG22 | 1:A:455:LYS:HB2 | 1.53 | 0.89 |
| 1:A:533:ASN:OD1 | 1:A:645:PHE:CB | 2.20 | 0.89 |
| 1:A:446:PHE:HD2 | 1:A:454:LEU:HD21 | 1.38 | 0.88 |
| 1:A:453:LYS:CG | 1:A:472:VAL:HG22 | 2.03 | 0.88 |
| 1:A:486:PHE:CD1 | 1:A:493:LEU:HD13 | 2.09 | 0.88 |
| 1:A:833:LEU:HB2 | 1:A:836:HIS:HD2 | 1.39 | 0.88 |
| 1:A:95:TYR:CD2 | 1:A:96:PRO:HD3 | 2.08 | 0.88 |
| 1:A:532:HIS:HA | 1:A:641:THR:OG1 | 1.72 | 0.88 |
| 1:A:447:VAL:CG2 | 1:A:455:LYS:HB2 | 2.03 | 0.88 |
| 1:A:256:LEU:HB3 | 1:A:309:LEU:HD22 | 1.56 | 0.87 |
| 1:A:892:HIS:HB2 | 1:A:932:CYS:O | 1.74 | 0.87 |
| 1:A:181:LYS:CD | 1:A:202:LYS:HA | 2.04 | 0.87 |
| 1:A:295:VAL:HA | 1:A:414:VAL:CG2 | 2.05 | 0.87 |
| 1:A:468:GLN:HG3 | 1:A:524:PRO:CG | 2.05 | 0.86 |
| 1:A:39:PHE:CE1 | 1:A:505:PRO:HD2 | 2.11 | 0.86 |
| 1:A:439:TYR:CD2 | 1:A:538:LYS:NZ | 2.42 | 0.86 |
| 1:A:110:THR:CG2 | 1:A:132:LEU:HD21 | 2.05 | 0.86 |
| 1:A:473:GLN:CG | 1:A:504:VAL:HG22 | 2.06 | 0.86 |
| 1:A:603:LEU:HD23 | 1:A:604:VAL:N | 1.90 | 0.86 |
| 1:A:863:ILE:HG23 | 1:A:864:PRO:HD2 | 1.56 | 0.86 |
| 1:A:133:TYR:CG | 1:A:136:ILE:HG12 | 2.11 | 0.85 |
| 1:A:847:LEU:HD11 | 1:A:850:ALA:HA | 1.58 | 0.85 |
| 1:A:118:LEU:HD13 | 1:A:119:ILE:N | 1.91 | 0.85 |
| 1:A:370:LEU:CD1 | 1:A:399:ILE:HD12 | 2.05 | 0.85 |
| 1:A:882:LEU:HB2 | 1:A:910:ALA:HA | 1.58 | 0.85 |
| 1:A:854:CYS:O | 1:A:940:PHE:CZ | 2.28 | 0.85 |
| 1:A:118:LEU:HD12 | 1:A:172:ILE:CD1 | 2.05 | 0.85 |
| 1:A:847:LEU:HD12 | 1:A:852:SER:HB3 | 1.58 | 0.85 |
| 1:A:815:LYS:HD2 | 1:A:910:ALA:HB3 | 1.55 | 0.85 |
| 1:A:863:ILE:CG2 | 1:A:876:THR:HB | 2.07 | 0.85 |
| 1:A:706:VAL:HG22 | 1:A:707:ASP:H | 1.42 | 0.84 |
| 1:A:42:PHE:CZ | 1:A:45:GLU:HB2 | 2.12 | 0.84 |
| 1:A:847:LEU:HG | 1:A:850:ALA:H | 1.39 | 0.84 |
| 1:A:295:VAL:CG1 | 1:A:414:VAL:HG11 | 2.07 | 0.84 |
| 1:A:458:ARG:CD | 1:A:524:PRO:HB3 | 2.07 | 0.84 |
| 1:A:50:PHE:HB2 | 1:A:498:GLU:O | 1.78 | 0.83 |
| 1:A:229:PRO:O | 1:A:232:THR:HG22 | 1.79 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:557:CYS:C | 1:A:582:ASN:CB | 2.36 | 0.83 |
| 1:A:569:VAL:CG2 | 1:A:654:ASN:CB | 2.52 | 0.83 |
| 1:A:358:ILE:HG23 | 1:A:361:GLN:H | 1.44 | 0.83 |
| 1:A:295:VAL:HA | 1:A:414:VAL:HG22 | 1.60 | 0.83 |
| 1:A:812:LEU:HD11 | 1:A:880:GLU:HB3 | 1.60 | 0.83 |
| 1:A:100:VAL:HG12 | 1:A:101:GLN:HG3 | 1.58 | 0.82 |
| 1:A:133:TYR:CB | 1:A:136:ILE:HG12 | 2.09 | 0.82 |
| 1:A:356:ILE:CG2 | 1:A:421:ILE:HB | 2.07 | 0.82 |
| 1:A:830:GLN:HG2 | 1:A:831:CYS:H | 1.43 | 0.82 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:CD2 | 2.14 | 0.82 |
| 1:A:809:SER:HB3 | 1:A:856:ASN:HD21 | 1.44 | 0.82 |
| 1:A:53:LEU:HD23 | 1:A:54:VAL:N | 1.94 | 0.82 |
| 1:A:435:ILE:CG2 | 1:A:446:PHE:HB2 | 2.06 | 0.82 |
| 1:A:42:PHE:CE1 | 1:A:79:VAL:HG22 | 2.14 | 0.82 |
| 1:A:40:VAL:CG1 | 1:A:503:ARG:HB3 | 2.08 | 0.82 |
| 1:A:468:GLN:HG3 | 1:A:524:PRO:HD3 | 0.88 | 0.82 |
| 1:A:533:ASN:OD1 | 1:A:645:PHE:HA | 1.78 | 0.82 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CE1 | 2.15 | 0.82 |
| 1:A:336:THR:O | 1:A:354:LEU:HD12 | 1.78 | 0.82 |
| 1:A:44:GLY:HA2 | 1:A:50:PHE:CE2 | 2.15 | 0.82 |
| 1:A:474:VAL:HG22 | 1:A:495:ILE:HG21 | 1.61 | 0.82 |
| 1:A:530:VAL:HB | 1:A:584:PRO:CG | 2.05 | 0.81 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:HD3 | 1.62 | 0.81 |
| 1:A:533:ASN:CG | 1:A:645:PHE:CB | 2.48 | 0.81 |
| 1:A:397:LEU:HD23 | 1:A:399:ILE:HD13 | 1.61 | 0.81 |
| 1:A:926:ALA:HB1 | 1:A:947:LEU:HD12 | 1.63 | 0.81 |
| 1:A:486:PHE:CE1 | 1:A:493:LEU:HD13 | 2.16 | 0.81 |
| 1:A:889:ILE:HG23 | 1:A:892:HIS:CE1 | 2.16 | 0.81 |
| 1:A:359:LEU:HD12 | 1:A:362:ILE:CD1 | 2.09 | 0.81 |
| 1:A:397:LEU:HD23 | 1:A:399:ILE:CD1 | 2.11 | 0.81 |
| 1:A:154:LYS:HD3 | 1:A:210:ASP:OD1 | 1.81 | 0.81 |
| 1:A:533:ASN:ND2 | 1:A:645:PHE:N | 2.28 | 0.80 |
| 1:A:295:VAL:HG12 | 1:A:414:VAL:CG1 | 2.09 | 0.80 |
| 1:A:370:LEU:HD12 | 1:A:399:ILE:HD12 | 1.63 | 0.80 |
| 1:A:62:ILE:HG13 | 1:A:73:LEU:HB2 | 1.62 | 0.80 |
| 1:A:154:LYS:HB2 | 1:A:157:HIS:CD2 | 2.16 | 0.80 |
| 1:A:380:LEU:HD12 | 1:A:386:LYS:HE3 | 1.64 | 0.80 |
| 1:A:356:ILE:HG22 | 1:A:421:ILE:HB | 1.61 | 0.80 |
| 1:A:468:GLN:HB2 | 1:A:523:ASP:HA | 1.64 | 0.80 |
| 1:A:468:GLN:CD | 1:A:524:PRO:HG3 | 2.03 | 0.80 |
| 1:A:314:LEU:HD11 | 1:A:332:ASP:HB3 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:239:PHE:CE1 | 1:A:260:PRO:HD2 | 2.17 | 0.79 |
| 1:A:321:LEU:HD12 | 1:A:462:PRO:HG2 | 1.64 | 0.79 |
| 1:A:244:VAL:HG13 | 1:A:482:ARG:NH1 | 1.98 | 0.79 |
| 1:A:556:GLN:HA | 1:A:582:ASN:HD21 | 1.43 | 0.79 |
| 1:A:192:PRO:HB3 | 1:A:233:PHE:CE1 | 2.17 | 0.79 |
| 1:A:444:LEU:HD13 | 1:A:445:ALA:N | 1.97 | 0.79 |
| 1:A:715:VAL:HG21 | 1:A:717:LYS:HD2 | 1.65 | 0.78 |
| 1:A:56:ASP:OD2 | 1:A:142:LEU:HD11 | 1.83 | 0.78 |
| 1:A:569:VAL:CB | 1:A:654:ASN:ND2 | 2.42 | 0.78 |
| 1:A:317:ALA:HB1 | 1:A:321:LEU:HB3 | 1.64 | 0.78 |
| 1:A:319:ALA:H | 1:A:441:ASN:HD22 | 1.31 | 0.78 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:N | 1.96 | 0.78 |
| 1:A:327:VAL:HG12 | 1:A:358:ILE:HD11 | 1.65 | 0.78 |
| 1:A:700:CYS:CB | 1:A:701:PRO:N | 2.25 | 0.78 |
| 1:A:815:LYS:HE3 | 1:A:910:ALA:CB | 2.13 | 0.78 |
| 1:A:181:LYS:NZ | 1:A:216:VAL:HG23 | 1.99 | 0.78 |
| 1:A:320:VAL:HG21 | 1:A:442:HIS:CD2 | 2.19 | 0.78 |
| 1:A:44:GLY:HA2 | 1:A:50:PHE:HE2 | 1.44 | 0.78 |
| 1:A:742:ILE:HB | 1:A:745:ILE:O | 1.84 | 0.78 |
| 1:A:168:VAL:HG23 | 1:A:185:ALA:O | 1.84 | 0.77 |
| 1:A:324:THR:HB | 1:A:462:PRO:CB | 2.10 | 0.77 |
| 1:A:620:PRO:HA | 1:A:623:ILE:CG1 | 2.12 | 0.77 |
| 1:A:51:ASN:HD21 | 1:A:67:VAL:HG23 | 1.50 | 0.77 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:HD2 | 1.48 | 0.77 |
| 1:A:806:MET:H | 1:A:806:MET:CE | 1.97 | 0.77 |
| 1:A:284:LYS:HD3 | 1:A:284:LYS:O | 1.85 | 0.77 |
| 1:A:439:TYR:CE2 | 1:A:538:LYS:HE3 | 2.19 | 0.77 |
| 1:A:616:ALA:O | 1:A:620:PRO:HD2 | 1.85 | 0.77 |
| 1:A:854:CYS:O | 1:A:940:PHE:HZ | 1.66 | 0.77 |
| 1:A:847:LEU:CG | 1:A:850:ALA:HA | 2.13 | 0.77 |
| 1:A:403:PHE:CE1 | 1:A:406:LEU:HD23 | 2.20 | 0.77 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:CG2 | 2.13 | 0.77 |
| 1:A:327:VAL:CG1 | 1:A:358:ILE:HD11 | 2.14 | 0.77 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:O | 1.84 | 0.77 |
| 1:A:196:PRO:HB3 | 1:A:225:MET:HE1 | 1.67 | 0.77 |
| 1:A:181:LYS:HZ3 | 1:A:216:VAL:HG23 | 1.50 | 0.77 |
| 1:A:231:ASP:O | 1:A:234:THR:HG22 | 1.84 | 0.77 |
| 1:A:591:ASN:OD1 | 1:A:639:LYS:HE2 | 1.83 | 0.76 |
| 1:A:533:ASN:OD1 | 1:A:645:PHE:CA | 2.33 | 0.76 |
| 1:A:595:GLU:CB | 1:A:597:LEU:HD23 | 2.14 | 0.76 |
| 1:A:204:THR:HG21 | 1:A:209:ALA:HB3 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:547:PRO:O | 1:A:548:ARG:HG2 | 1.84 | 0.76 |
| 1:A:64:LEU:HD12 | 1:A:496:MET:CE | 2.16 | 0.76 |
| 1:A:780:LEU:HD12 | 1:A:780:LEU:O | 1.86 | 0.76 |
| 1:A:806:MET:HE3 | 1:A:806:MET:N | 1.98 | 0.76 |
| 1:A:456:LYS:HD3 | 1:A:525:HIS:CE1 | 2.20 | 0.76 |
| 1:A:847:LEU:CD1 | 1:A:850:ALA:HA | 2.16 | 0.76 |
| 1:A:120:ASP:OD2 | 1:A:123:GLU:HG3 | 1.86 | 0.76 |
| 1:A:869:ARG:O | 1:A:920:ALA:HB3 | 1.86 | 0.76 |
| 1:A:278:LYS:HE3 | 1:A:296:PRO:HG3 | 1.67 | 0.75 |
| 1:A:172:ILE:HG12 | 1:A:182:LEU:HD13 | 1.68 | 0.75 |
| 1:A:556:GLN:CA | 1:A:582:ASN:CG | 2.52 | 0.75 |
| 1:A:847:LEU:HD12 | 1:A:852:SER:CB | 2.16 | 0.75 |
| 1:A:448:GLY:HA3 | 1:A:480:VAL:HG21 | 1.68 | 0.75 |
| 1:A:473:GLN:CB | 1:A:504:VAL:HG22 | 2.17 | 0.75 |
| 1:A:42:PHE:HZ | 1:A:45:GLU:HB2 | 1.50 | 0.75 |
| 1:A:323:ARG:HG3 | 1:A:324:THR:N | 2.02 | 0.75 |
| 1:A:676:TYR:HE1 | 1:A:730:GLN:HG2 | 1.52 | 0.75 |
| 1:A:256:LEU:CB | 1:A:309:LEU:HD22 | 2.16 | 0.75 |
| 1:A:188:VAL:HG22 | 1:A:191:LYS:H | 1.52 | 0.74 |
| 1:A:739:ILE:CD1 | 1:A:748:ARG:HG2 | 2.17 | 0.74 |
| 1:A:151:PRO:HB2 | 1:A:157:HIS:ND1 | 2.02 | 0.74 |
| 1:A:460:ASP:HB3 | 1:A:464:GLY:N | 2.00 | 0.74 |
| 1:A:321:LEU:CD1 | 1:A:462:PRO:HG2 | 2.17 | 0.74 |
| 1:A:567:ILE:HD12 | 1:A:650:PHE:CZ | 2.22 | 0.74 |
| 1:A:439:TYR:OH | 1:A:538:LYS:HE3 | 1.88 | 0.74 |
| 1:A:567:ILE:H | 1:A:567:ILE:HD13 | 1.50 | 0.74 |
| 1:A:815:LYS:HE2 | 1:A:910:ALA:HB3 | 1.67 | 0.74 |
| 1:A:569:VAL:HB | 1:A:654:ASN:CG | 2.08 | 0.74 |
| 1:A:822:CYS:HA | 1:A:833:LEU:HD23 | 1.70 | 0.74 |
| 1:A:873:THR:HB | 1:A:917:MET:CE | 2.17 | 0.74 |
| 1:A:202:LYS:HD3 | 1:A:214:ALA:HB3 | 1.69 | 0.74 |
| 1:A:683:ASP:O | 1:A:686:THR:HG22 | 1.87 | 0.74 |
| 1:A:704:LEU:HD11 | 1:A:724:LYS:HE3 | 1.70 | 0.74 |
| 1:A:784:TRP:HD1 | 1:A:790:ILE:HD11 | 1.51 | 0.74 |
| 1:A:533:ASN:CG | 1:A:645:PHE:CA | 2.56 | 0.74 |
| 1:A:530:VAL:CB | 1:A:584:PRO:CG | 2.61 | 0.74 |
| 1:A:154:LYS:H | 1:A:157:HIS:HD2 | 1.36 | 0.74 |
| 1:A:456:LYS:HD3 | 1:A:525:HIS:HE1 | 1.53 | 0.74 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:CD2 | 2.18 | 0.74 |
| 1:A:99:ILE:HD11 | 1:A:152:PHE:HB2 | 1.69 | 0.73 |
| 1:A:278:LYS:HG2 | 1:A:296:PRO:HA | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:468:GLN:HB2 | 1:A:524:PRO:HD3 | 1.71 | 0.73 |
| 1:A:225:MET:CE | 1:A:227:LYS:HG3 | 2.19 | 0.73 |
| 1:A:435:ILE:HD13 | 1:A:436:ALA:N | 2.03 | 0.73 |
| 1:A:446:PHE:HB3 | 1:A:454:LEU:HD11 | 1.69 | 0.73 |
| 1:A:469:TYR:CD1 | 1:A:523:ASP:OD2 | 2.42 | 0.73 |
| 1:A:556:GLN:HA | 1:A:582:ASN:CG | 2.08 | 0.73 |
| 1:A:676:TYR:CE1 | 1:A:730:GLN:CG | 2.72 | 0.73 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CZ | 2.23 | 0.73 |
| 1:A:324:THR:HG21 | 1:A:462:PRO:HA | 1.70 | 0.73 |
| 1:A:458:ARG:HD2 | 1:A:524:PRO:HB2 | 1.71 | 0.73 |
| 1:A:321:LEU:HG | 1:A:325:LEU:HD11 | 1.71 | 0.72 |
| 1:A:623:ILE:HA | 1:A:626:ASN:ND2 | 2.01 | 0.72 |
| 1:A:184:ILE:HD12 | 1:A:184:ILE:O | 1.89 | 0.72 |
| 1:A:225:MET:HE1 | 1:A:227:LYS:HG3 | 1.72 | 0.72 |
| 1:A:704:LEU:HB2 | 1:A:722:LYS:HG3 | 1.71 | 0.72 |
| 1:A:115:LYS:HB3 | 1:A:168:VAL:HG11 | 1.71 | 0.72 |
| 1:A:670:ARG:HA | 1:A:670:ARG:HE | 1.54 | 0.72 |
| 1:A:321:LEU:HG | 1:A:325:LEU:CD1 | 2.20 | 0.72 |
| 1:A:619:VAL:HB | 1:A:620:PRO:HD3 | 1.72 | 0.72 |
| 1:A:814:LEU:HB3 | 1:A:847:LEU:HB2 | 1.70 | 0.72 |
| 1:A:261:GLU:HA | 1:A:264:SER:O | 1.89 | 0.72 |
| 1:A:832:THR:CG2 | 1:A:836:HIS:HB2 | 2.20 | 0.72 |
| 1:A:380:LEU:HB2 | 1:A:386:LYS:CE | 2.20 | 0.72 |
| 1:A:39:PHE:CD2 | 1:A:473:GLN:HG3 | 2.23 | 0.72 |
| 1:A:847:LEU:CD1 | 1:A:852:SER:HB3 | 2.20 | 0.71 |
| 1:A:676:TYR:CE1 | 1:A:730:GLN:HG2 | 2.25 | 0.71 |
| 1:A:700:CYS:HB3 | 1:A:701:PRO:N | 2.04 | 0.71 |
| 1:A:446:PHE:CD2 | 1:A:454:LEU:HD21 | 2.24 | 0.71 |
| 1:A:458:ARG:HG3 | 1:A:468:GLN:OE1 | 1.90 | 0.71 |
| 1:A:46:PRO:HG2 | 1:A:69:ARG:CG | 2.17 | 0.71 |
| 1:A:446:PHE:HZ | 1:A:506:VAL:HG23 | 1.55 | 0.71 |
| 1:A:662:LEU:CD2 | 1:A:791:ASP:CB | 2.69 | 0.71 |
| 1:A:304:VAL:HG11 | 1:A:351:GLU:OE2 | 1.91 | 0.71 |
| 1:A:480:VAL:HB | 1:A:484:MET:CE | 2.21 | 0.71 |
| 1:A:558:VAL:HG11 | 1:A:646:ALA:HB2 | 1.71 | 0.71 |
| 1:A:533:ASN:ND2 | 1:A:645:PHE:CA | 2.54 | 0.71 |
| 1:A:73:LEU:HD22 | 1:A:79:VAL:HA | 1.72 | 0.71 |
| 1:A:847:LEU:HD21 | 1:A:850:ALA:HA | 1.73 | 0.71 |
| 1:A:53:LEU:HB2 | 1:A:496:MET:HE1 | 1.71 | 0.70 |
| 1:A:519:LEU:HD12 | 1:A:552:SER:O | 1.90 | 0.70 |
| 1:A:595:GLU:HG2 | 1:A:632:VAL:HG13 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:937:ARG:CG | 1:A:938:PRO:HD2 | 2.20 | 0.70 |
| 1:A:40:VAL:HG12 | 1:A:503:ARG:HB3 | 1.73 | 0.70 |
| 1:A:530:VAL:CB | 1:A:584:PRO:CD | 2.69 | 0.70 |
| 1:A:812:LEU:HD21 | 1:A:880:GLU:C | 2.09 | 0.70 |
| 1:A:188:VAL:HG13 | 1:A:190:GLY:H | 1.56 | 0.70 |
| 1:A:575:LEU:HD22 | 1:A:575:LEU:H | 1.56 | 0.70 |
| 1:A:533:ASN:CG | 1:A:645:PHE:HA | 2.11 | 0.70 |
| 1:A:380:LEU:HB2 | 1:A:386:LYS:HE3 | 1.74 | 0.70 |
| 1:A:471:THR:HG23 | 1:A:473:GLN:HE22 | 1.55 | 0.70 |
| 1:A:63:TYR:C | 1:A:64:LEU:HD22 | 2.12 | 0.70 |
| 1:A:181:LYS:HD2 | 1:A:202:LYS:HA | 1.71 | 0.70 |
| 1:A:281:ARG:HB3 | 1:A:293:VAL:CG1 | 2.22 | 0.70 |
| 1:A:93:LYS:HD2 | 1:A:105:GLU:OE1 | 1.91 | 0.70 |
| 1:A:551:ALA:HA | 1:A:556:GLN:OE1 | 1.92 | 0.70 |
| 1:A:563:HIS:HB2 | 1:A:577:VAL:CG1 | 2.21 | 0.70 |
| 1:A:450:LYS:HA | 1:A:479:PRO:HB3 | 1.73 | 0.70 |
| 1:A:216:VAL:HG12 | 1:A:224:SER:OG | 1.92 | 0.69 |
| 1:A:367:LYS:HE2 | 1:A:399:ILE:O | 1.91 | 0.69 |
| 1:A:370:LEU:HD21 | 1:A:374:TYR:HE1 | 1.55 | 0.69 |
| 1:A:809:SER:CB | 1:A:856:ASN:HD21 | 2.04 | 0.69 |
| 1:A:533:ASN:ND2 | 1:A:645:PHE:HA | 2.07 | 0.69 |
| 1:A:110:THR:HG22 | 1:A:132:LEU:HD21 | 1.73 | 0.69 |
| 1:A:815:LYS:HE3 | 1:A:909:PRO:O | 1.93 | 0.69 |
| 1:A:474:VAL:HG21 | 1:A:495:ILE:HD13 | 1.72 | 0.69 |
| 1:A:507:GLU:HG3 | 1:A:537:ARG:HG3 | 1.73 | 0.69 |
| 1:A:812:LEU:HG | 1:A:881:ASN:CG | 2.13 | 0.69 |
| 1:A:39:PHE:HE1 | 1:A:505:PRO:HD2 | 1.56 | 0.69 |
| 1:A:689:PHE:CD1 | 1:A:691:GLU:HG2 | 2.28 | 0.69 |
| 1:A:863:ILE:HG23 | 1:A:864:PRO:CD | 2.23 | 0.69 |
| 1:A:473:GLN:OE1 | 1:A:504:VAL:HG13 | 1.93 | 0.69 |
| 1:A:435:ILE:HD12 | 1:A:486:PHE:CD1 | 2.27 | 0.69 |
| 1:A:815:LYS:HE2 | 1:A:909:PRO:O | 1.92 | 0.69 |
| 1:A:474:VAL:CG1 | 1:A:475:VAL:HG23 | 2.18 | 0.68 |
| 1:A:515:CYS:O | 1:A:519:LEU:HD23 | 1.91 | 0.68 |
| 1:A:595:GLU:CG | 1:A:632:VAL:HG13 | 2.22 | 0.68 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:HG21 | 1.73 | 0.68 |
| 1:A:594:PHE:O | 1:A:595:GLU:HG2 | 1.94 | 0.68 |
| 1:A:72:LYS:HE3 | 1:A:80:LEU:CD1 | 2.21 | 0.68 |
| 1:A:62:ILE:HD12 | 1:A:64:LEU:HD21 | 1.76 | 0.68 |
| 1:A:323:ARG:HG3 | 1:A:324:THR:H | 1.58 | 0.68 |
| 1:A:506:VAL:HG13 | 1:A:537:ARG:NH1 | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:LEU:CD2 | 1:A:79:VAL:HA | 2.24 | 0.68 |
| 1:A:773:ILE:HD13 | 1:A:773:ILE:H | 1.59 | 0.68 |
| 1:A:533:ASN:OD1 | 1:A:645:PHE:HB3 | 1.89 | 0.68 |
| 1:A:739:ILE:HD12 | 1:A:748:ARG:HG2 | 1.76 | 0.68 |
| 1:A:739:ILE:HB | 1:A:781:THR:CG2 | 2.22 | 0.68 |
| 1:A:133:TYR:HB2 | 1:A:136:ILE:HG12 | 1.75 | 0.68 |
| 1:A:62:ILE:HD11 | 1:A:73:LEU:HD12 | 1.76 | 0.68 |
| 1:A:532:HIS:O | 1:A:641:THR:HG21 | 1.94 | 0.68 |
| 1:A:98:ARG:HE | 1:A:107:LEU:CD1 | 2.07 | 0.68 |
| 1:A:46:PRO:HG3 | 1:A:69:ARG:HD2 | 1.75 | 0.67 |
| 1:A:190:GLY:HA2 | 1:A:233:PHE:CE2 | 2.29 | 0.67 |
| 1:A:98:ARG:HH21 | 1:A:107:LEU:HD12 | 1.60 | 0.67 |
| 1:A:133:TYR:CD2 | 1:A:136:ILE:HG12 | 2.28 | 0.67 |
| 1:A:847:LEU:HG | 1:A:850:ALA:N | 2.10 | 0.67 |
| 1:A:412:LEU:H | 1:A:412:LEU:HD13 | 1.59 | 0.67 |
| 1:A:62:ILE:HG13 | 1:A:62:ILE:O | 1.94 | 0.67 |
| 1:A:662:LEU:CD2 | 1:A:791:ASP:CG | 2.54 | 0.67 |
| 1:A:555:LYS:HG3 | 1:A:556:GLN:N | 2.09 | 0.67 |
| 1:A:239:PHE:CD1 | 1:A:260:PRO:HD2 | 2.30 | 0.67 |
| 1:A:137:CYS:HB2 | 1:A:213:PHE:CZ | 2.30 | 0.67 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:NE | 2.09 | 0.67 |
| 1:A:620:PRO:CA | 1:A:623:ILE:HG13 | 2.23 | 0.67 |
| 1:A:703:LEU:HD13 | 1:A:723:ALA:HB2 | 1.76 | 0.67 |
| 1:A:98:ARG:HE | 1:A:107:LEU:HD11 | 1.60 | 0.67 |
| 1:A:446:PHE:CZ | 1:A:486:PHE:HZ | 2.13 | 0.66 |
| 1:A:515:CYS:HB2 | 1:A:558:VAL:HG23 | 1.76 | 0.66 |
| 1:A:595:GLU:HG2 | 1:A:632:VAL:CG1 | 2.25 | 0.66 |
| 1:A:560:LEU:CD2 | 1:A:648:THR:HG23 | 2.20 | 0.66 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:CD | 2.25 | 0.66 |
| 1:A:42:PHE:HE1 | 1:A:79:VAL:CG2 | 2.05 | 0.66 |
| 1:A:662:LEU:HD21 | 1:A:791:ASP:CB | 2.25 | 0.66 |
| 1:A:867:GLY:HA3 | 1:A:948:TYR:OH | 1.94 | 0.66 |
| 1:A:410:ALA:HB1 | 1:A:411:PRO:HD2 | 1.78 | 0.66 |
| 1:A:216:VAL:HG12 | 1:A:224:SER:CB | 2.26 | 0.66 |
| 1:A:321:LEU:O | 1:A:325:LEU:HG | 1.95 | 0.66 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:CG2 | 2.21 | 0.66 |
| 1:A:439:TYR:CZ | 1:A:538:LYS:HE3 | 2.31 | 0.66 |
| 1:A:706:VAL:HG13 | 1:A:707:ASP:O | 1.96 | 0.66 |
| 1:A:797:LYS:HD2 | 1:A:797:LYS:N | 2.11 | 0.65 |
| 1:A:460:ASP:HB3 | 1:A:463:LYS:HB3 | 1.77 | 0.65 |
| 1:A:830:GLN:HG2 | 1:A:831:CYS:N | 2.09 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:325:LEU:CD1 | 1:A:333:LEU:HD11 | 2.26 | 0.65 |
| 1:A:892:HIS:NE2 | 1:A:931:ILE:HB | 2.11 | 0.65 |
| 1:A:133:TYR:HB2 | 1:A:136:ILE:H | 1.61 | 0.65 |
| 1:A:296:PRO:HD2 | 1:A:414:VAL:CG2 | 2.27 | 0.65 |
| 1:A:432:THR:OG1 | 1:A:480:VAL:HG23 | 1.96 | 0.65 |
| 1:A:713:VAL:HG12 | 1:A:714:GLU:HG3 | 1.79 | 0.65 |
| 1:A:847:LEU:CD2 | 1:A:850:ALA:HA | 2.27 | 0.65 |
| 1:A:812:LEU:N | 1:A:881:ASN:OD1 | 2.29 | 0.65 |
| 1:A:110:THR:HB | 1:A:132:LEU:CD2 | 2.26 | 0.65 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:C | 2.17 | 0.65 |
| 1:A:261:GLU:HG2 | 1:A:264:SER:C | 2.17 | 0.64 |
| 1:A:368:ASP:O | 1:A:371:GLN:HG2 | 1.97 | 0.64 |
| 1:A:567:ILE:HD13 | 1:A:651:VAL:O | 1.96 | 0.64 |
| 1:A:53:LEU:HG | 1:A:64:LEU:CD1 | 2.28 | 0.64 |
| 1:A:56:ASP:OD1 | 1:A:119:ILE:HD12 | 1.98 | 0.64 |
| 1:A:154:LYS:H | 1:A:157:HIS:CD2 | 2.15 | 0.64 |
| 1:A:181:LYS:HD3 | 1:A:202:LYS:HA | 1.78 | 0.64 |
| 1:A:105:GLU:HB3 | 1:A:106:PRO:HD2 | 1.80 | 0.64 |
| 1:A:566:ASN:HA | 1:A:651:VAL:CG2 | 2.25 | 0.64 |
| 1:A:118:LEU:HG | 1:A:172:ILE:HG13 | 1.80 | 0.64 |
| 1:A:309:LEU:HD11 | 1:A:311:ALA:O | 1.98 | 0.64 |
| 1:A:926:ALA:HB1 | 1:A:947:LEU:CD1 | 2.27 | 0.64 |
| 1:A:295:VAL:HA | 1:A:414:VAL:HG21 | 1.80 | 0.64 |
| 1:A:53:LEU:HB2 | 1:A:496:MET:CE | 2.27 | 0.64 |
| 1:A:933:VAL:HG23 | 1:A:934:ALA:N | 2.10 | 0.64 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CD1 | 2.33 | 0.64 |
| 1:A:782:VAL:HG23 | 1:A:790:ILE:HB | 1.78 | 0.64 |
| 1:A:815:LYS:CE | 1:A:910:ALA:CB | 2.52 | 0.64 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:CG2 | 2.27 | 0.64 |
| 1:A:405:GLY:O | 1:A:406:LEU:HD22 | 1.98 | 0.64 |
| 1:A:440:LYS:HD2 | 1:A:538:LYS:HD2 | 1.79 | 0.63 |
| 1:A:806:MET:HG2 | 1:A:807:ARG:HG3 | 1.80 | 0.63 |
| 1:A:320:VAL:O | 1:A:323:ARG:HG2 | 1.98 | 0.63 |
| 1:A:432:THR:HG1 | 1:A:480:VAL:HG23 | 1.62 | 0.63 |
| 1:A:675:LYS:HE3 | 1:A:694:VAL:HG22 | 1.79 | 0.63 |
| 1:A:706:VAL:HG22 | 1:A:707:ASP:N | 2.12 | 0.63 |
| 1:A:854:CYS:O | 1:A:940:PHE:CE1 | 2.51 | 0.63 |
| 1:A:386:LYS:O | 1:A:386:LYS:HG3 | 1.99 | 0.63 |
| 1:A:474:VAL:CG2 | 1:A:495:ILE:HD13 | 2.29 | 0.63 |
| 1:A:372:SER:O | 1:A:375:ARG:HB2 | 1.99 | 0.63 |
| 1:A:460:ASP:CB | 1:A:463:LYS:HB3 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:446:PHE:CE1 | 1:A:486:PHE:HZ | 2.16 | 0.63 |
| 1:A:186:THR:HG22 | 1:A:187:ALA:N | 2.12 | 0.63 |
| 1:A:480:VAL:HG11 | 1:A:495:ILE:HD11 | 1.81 | 0.63 |
| 1:A:530:VAL:HG12 | 1:A:584:PRO:CG | 2.27 | 0.63 |
| 1:A:855:THR:HG23 | 1:A:856:ASN:OD1 | 1.99 | 0.62 |
| 1:A:405:GLY:C | 1:A:406:LEU:HD22 | 2.19 | 0.62 |
| 1:A:533:ASN:CB | 1:A:645:PHE:HB3 | 2.29 | 0.62 |
| 1:A:180:ASP:O | 1:A:181:LYS:HG2 | 1.99 | 0.62 |
| 1:A:410:ALA:HB1 | 1:A:411:PRO:CD | 2.30 | 0.62 |
| 1:A:448:GLY:CA | 1:A:480:VAL:HG21 | 2.28 | 0.62 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:CZ | 2.29 | 0.62 |
| 1:A:473:GLN:HG2 | 1:A:504:VAL:HG22 | 1.79 | 0.62 |
| 1:A:741:ASN:O | 1:A:778:VAL:HG13 | 1.98 | 0.62 |
| 1:A:555:LYS:O | 1:A:582:ASN:CG | 2.36 | 0.62 |
| 1:A:204:THR:HG22 | 1:A:212:MET:SD | 2.40 | 0.62 |
| 1:A:473:GLN:HB2 | 1:A:504:VAL:HG22 | 1.80 | 0.62 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:CG | 2.29 | 0.62 |
| 1:A:320:VAL:HG21 | 1:A:442:HIS:HD2 | 1.64 | 0.62 |
| 1:A:446:PHE:CZ | 1:A:506:VAL:HG23 | 2.33 | 0.62 |
| 1:A:894:LYS:HD3 | 1:A:899:GLU:HA | 1.80 | 0.62 |
| 1:A:530:VAL:HG21 | 1:A:584:PRO:HD3 | 1.82 | 0.62 |
| 1:A:175:TYR:HD2 | 1:A:179:ASP:HB3 | 1.63 | 0.62 |
| 1:A:181:LYS:HE2 | 1:A:202:LYS:HG2 | 1.80 | 0.61 |
| 1:A:296:PRO:HB2 | 1:A:417:MET:SD | 2.39 | 0.61 |
| 1:A:949:TYR:HE2 | 1:A:951:MET:CE | 2.12 | 0.61 |
| 1:A:333:LEU:CD2 | 1:A:358:ILE:HG13 | 2.31 | 0.61 |
| 1:A:458:ARG:HG3 | 1:A:468:GLN:CD | 2.20 | 0.61 |
| 1:A:506:VAL:CG1 | 1:A:537:ARG:HH12 | 2.14 | 0.61 |
| 1:A:110:THR:HG22 | 1:A:111:ASN:N | 2.14 | 0.61 |
| 1:A:41:THR:HG22 | 1:A:502:THR:HA | 1.81 | 0.61 |
| 1:A:575:LEU:HD22 | 1:A:575:LEU:N | 2.14 | 0.61 |
| 1:A:175:TYR:CD2 | 1:A:179:ASP:HB3 | 2.36 | 0.61 |
| 1:A:676:TYR:CD1 | 1:A:730:GLN:HG3 | 2.36 | 0.61 |
| 1:A:197:THR:HG21 | 1:A:228:ILE:HD11 | 1.82 | 0.61 |
| 1:A:257:THR:C | 1:A:258:LEU:HD12 | 2.21 | 0.61 |
| 1:A:382:LEU:HD23 | 1:A:385:LEU:HB3 | 1.81 | 0.61 |
| 1:A:488:LYS:HG3 | 1:A:489:ASP:N | 2.14 | 0.61 |
| 1:A:566:ASN:HB3 | 1:A:651:VAL:HG21 | 1.80 | 0.61 |
| 1:A:119:ILE:HD13 | 1:A:121:TYR:CZ | 2.36 | 0.61 |
| 1:A:182:LEU:HG | 1:A:184:ILE:HG23 | 1.82 | 0.61 |
| 1:A:474:VAL:HG22 | 1:A:495:ILE:CG2 | 2.29 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:468:GLN:OE1 | 1:A:524:PRO:HG3 | 2.00 | 0.60 |
| 1:A:469:TYR:CE2 | 1:A:471:THR:HB | 2.36 | 0.60 |
| 1:A:712:PRO:HG3 | 1:A:801:TYR:OH | 2.01 | 0.60 |
| 1:A:458:ARG:CD | 1:A:524:PRO:CB | 2.71 | 0.60 |
| 1:A:696:LEU:N | 1:A:696:LEU:HD12 | 2.15 | 0.60 |
| 1:A:662:LEU:HD23 | 1:A:791:ASP:CB | 2.29 | 0.60 |
| 1:A:469:TYR:HE2 | 1:A:471:THR:HB | 1.65 | 0.60 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:CZ | 2.37 | 0.60 |
| 1:A:806:MET:CG | 1:A:807:ARG:HG3 | 2.30 | 0.60 |
| 1:A:440:LYS:CD | 1:A:538:LYS:HD2 | 2.31 | 0.60 |
| 1:A:630:HIS:HD2 | 1:A:632:VAL:CG2 | 2.15 | 0.60 |
| 1:A:403:PHE:CZ | 1:A:406:LEU:HD23 | 2.37 | 0.60 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:CE1 | 2.35 | 0.60 |
| 1:A:323:ARG:HH21 | 1:A:463:LYS:HD2 | 1.67 | 0.60 |
| 1:A:715:VAL:CG2 | 1:A:717:LYS:HD2 | 2.30 | 0.60 |
| 1:A:313:TYR:CE1 | 1:A:435:ILE:HG12 | 2.37 | 0.59 |
| 1:A:314:LEU:HD12 | 1:A:333:LEU:O | 2.01 | 0.59 |
| 1:A:457:ILE:HG12 | 1:A:467:LEU:HD13 | 1.84 | 0.59 |
| 1:A:62:ILE:HD13 | 1:A:77:LEU:CD2 | 2.32 | 0.59 |
| 1:A:95:TYR:CG | 1:A:96:PRO:HD3 | 2.36 | 0.59 |
| 1:A:41:THR:HG22 | 1:A:502:THR:HG23 | 1.83 | 0.59 |
| 1:A:665:VAL:HG12 | 1:A:697:PRO:HG3 | 1.83 | 0.59 |
| 1:A:72:LYS:CD | 1:A:80:LEU:HD12 | 2.30 | 0.59 |
| 1:A:773:ILE:HD13 | 1:A:773:ILE:N | 2.17 | 0.59 |
| 1:A:453:LYS:HG2 | 1:A:472:VAL:CG2 | 2.16 | 0.59 |
| 1:A:566:ASN:CA | 1:A:651:VAL:HG23 | 2.28 | 0.59 |
| 1:A:515:CYS:CB | 1:A:558:VAL:HG23 | 2.31 | 0.59 |
| 1:A:665:VAL:HG11 | 1:A:697:PRO:HD3 | 1.84 | 0.59 |
| 1:A:847:LEU:HD11 | 1:A:850:ALA:CA | 2.29 | 0.59 |
| 1:A:188:VAL:HG22 | 1:A:191:LYS:N | 2.18 | 0.59 |
| 1:A:387:VAL:HG13 | 1:A:388:LYS:HG3 | 1.83 | 0.59 |
| 1:A:387:VAL:HG13 | 1:A:388:LYS:N | 2.18 | 0.59 |
| 1:A:473:GLN:H | 1:A:473:GLN:NE2 | 2.01 | 0.59 |
| 1:A:759:VAL:HG12 | 1:A:760:GLN:N | 2.18 | 0.59 |
| 1:A:495:ILE:CG2 | 1:A:502:THR:HB | 2.32 | 0.59 |
| 1:A:560:LEU:HD23 | 1:A:648:THR:CG2 | 2.25 | 0.59 |
| 1:A:51:ASN:HD21 | 1:A:67:VAL:CG2 | 2.15 | 0.59 |
| 1:A:99:ILE:HG13 | 1:A:100:VAL:N | 2.16 | 0.59 |
| 1:A:243:TYR:CD2 | 1:A:257:THR:HG22 | 2.37 | 0.58 |
| 1:A:350:ASP:HA | 1:A:430:ARG:HB2 | 1.86 | 0.58 |
| 1:A:62:ILE:HD12 | 1:A:501:LEU:CD1 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:931:ILE:O | 1:A:931:ILE:HG13 | 2.02 | 0.58 |
| 1:A:585:GLU:OE1 | 1:A:585:GLU:HA | 2.03 | 0.58 |
| 1:A:873:THR:HB | 1:A:917:MET:HE2 | 1.85 | 0.58 |
| 1:A:110:THR:HB | 1:A:132:LEU:HD23 | 1.85 | 0.58 |
| 1:A:171:VAL:O | 1:A:182:LEU:HD12 | 2.02 | 0.58 |
| 1:A:904:VAL:HG13 | 1:A:905:ASP:N | 2.18 | 0.58 |
| 1:A:814:LEU:HD22 | 1:A:847:LEU:N | 2.18 | 0.58 |
| 1:A:889:ILE:HD12 | 1:A:907:TYR:CZ | 2.38 | 0.58 |
| 1:A:530:VAL:HG11 | 1:A:584:PRO:HD2 | 0.59 | 0.58 |
| 1:A:196:PRO:HB3 | 1:A:225:MET:CE | 2.33 | 0.58 |
| 1:A:263:VAL:O | 1:A:263:VAL:HG12 | 2.04 | 0.58 |
| 1:A:699:ASP:O | 1:A:725:ASN:CB | 2.51 | 0.58 |
| 1:A:40:VAL:HG13 | 1:A:503:ARG:HB3 | 1.85 | 0.58 |
| 1:A:578:LEU:HD13 | 1:A:636:LEU:HD21 | 1.85 | 0.58 |
| 1:A:569:VAL:HB | 1:A:654:ASN:HD22 | 1.63 | 0.57 |
| 1:A:349:LEU:N | 1:A:349:LEU:HD22 | 2.18 | 0.57 |
| 1:A:506:VAL:CG1 | 1:A:537:ARG:NH1 | 2.67 | 0.57 |
| 1:A:832:THR:HG23 | 1:A:836:HIS:HB2 | 1.85 | 0.57 |
| 1:A:892:HIS:CE1 | 1:A:931:ILE:HB | 2.40 | 0.57 |
| 1:A:154:LYS:N | 1:A:157:HIS:HD2 | 2.00 | 0.57 |
| 1:A:198:ILE:HB | 1:A:226:ILE:CG2 | 2.34 | 0.57 |
| 1:A:430:ARG:HH21 | 1:A:432:THR:HG22 | 1.68 | 0.57 |
| 1:A:254:TYR:CZ | 1:A:281:ARG:HD2 | 2.39 | 0.57 |
| 1:A:426:GLU:OE1 | 1:A:426:GLU:HA | 2.04 | 0.57 |
| 1:A:321:LEU:HD12 | 1:A:462:PRO:CG | 2.34 | 0.57 |
| 1:A:434:VAL:HG22 | 1:A:435:ILE:N | 2.20 | 0.57 |
| 1:A:459:VAL:O | 1:A:459:VAL:HG23 | 2.05 | 0.57 |
| 1:A:506:VAL:C | 1:A:507:GLU:N | 2.58 | 0.57 |
| 1:A:42:PHE:CE2 | 1:A:50:PHE:HZ | 2.23 | 0.57 |
| 1:A:833:LEU:HB2 | 1:A:836:HIS:CD2 | 2.29 | 0.57 |
| 1:A:446:PHE:CE1 | 1:A:486:PHE:CZ | 2.93 | 0.56 |
| 1:A:468:GLN:CG | 1:A:524:PRO:CG | 2.75 | 0.56 |
| 1:A:380:LEU:HB2 | 1:A:386:LYS:HE2 | 1.87 | 0.56 |
| 1:A:703:LEU:HD21 | 1:A:782:VAL:HG21 | 1.87 | 0.56 |
| 1:A:239:PHE:CA | 1:A:260:PRO:HG2 | 2.30 | 0.56 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:HG21 | 1.87 | 0.56 |
| 1:A:45:GLU:HB3 | 1:A:46:PRO:CD | 2.35 | 0.56 |
| 1:A:474:VAL:CG2 | 1:A:495:ILE:HG21 | 2.35 | 0.56 |
| 1:A:501:LEU:HD23 | 1:A:502:THR:H | 1.70 | 0.56 |
| 1:A:324:THR:CG2 | 1:A:462:PRO:HA | 2.34 | 0.56 |
| 1:A:456:LYS:O | 1:A:468:GLN:HG2 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:710:LEU:HB2 | 1:A:801:TYR:HE1 | 1.70 | 0.56 |
| 1:A:72:LYS:HD2 | 1:A:80:LEU:HB2 | 1.87 | 0.56 |
| 1:A:885:GLU:HG3 | 1:A:887:ARG:H | 1.70 | 0.56 |
| 1:A:262:MET:O | 1:A:262:MET:HG3 | 2.05 | 0.56 |
| 1:A:433:SER:HB3 | 1:A:484:MET:SD | 2.45 | 0.56 |
| 1:A:41:THR:CG2 | 1:A:502:THR:HG23 | 2.36 | 0.56 |
| 1:A:814:LEU:HD22 | 1:A:847:LEU:H | 1.68 | 0.56 |
| 1:A:865:VAL:HG13 | 1:A:866:THR:N | 2.21 | 0.56 |
| 1:A:370:LEU:HD21 | 1:A:374:TYR:CE1 | 2.39 | 0.56 |
| 1:A:435:ILE:CG2 | 1:A:486:PHE:HE1 | 2.19 | 0.56 |
| 1:A:435:ILE:HD12 | 1:A:486:PHE:HD1 | 1.70 | 0.56 |
| 1:A:785:ASN:ND2 | 1:A:788:PHE:HE2 | 2.03 | 0.56 |
| 1:A:926:ALA:CB | 1:A:947:LEU:HD12 | 2.35 | 0.56 |
| 1:A:271:LYS:HG3 | 1:A:272:GLU:N | 2.13 | 0.56 |
| 1:A:882:LEU:HD12 | 1:A:882:LEU:N | 2.21 | 0.56 |
| 1:A:665:VAL:CG1 | 1:A:697:PRO:HD3 | 2.35 | 0.56 |
| 1:A:305:GLU:O | 1:A:340:LYS:HG3 | 2.06 | 0.56 |
| 1:A:937:ARG:HG2 | 1:A:938:PRO:HD2 | 1.85 | 0.56 |
| 1:A:597:LEU:N | 1:A:597:LEU:HD22 | 2.21 | 0.56 |
| 1:A:785:ASN:HD22 | 1:A:788:PHE:HE2 | 1.54 | 0.56 |
| 1:A:118:LEU:HB3 | 1:A:127:ILE:CG2 | 2.36 | 0.55 |
| 1:A:382:LEU:HD23 | 1:A:385:LEU:CB | 2.36 | 0.55 |
| 1:A:46:PRO:CG | 1:A:69:ARG:HD2 | 2.36 | 0.55 |
| 1:A:526:CYS:HB3 | 1:A:535:CYS:SG | 2.46 | 0.55 |
| 1:A:53:LEU:HG | 1:A:64:LEU:HD13 | 1.87 | 0.55 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:O | 2.07 | 0.55 |
| 1:A:820:PHE:O | 1:A:821:GLU:HB3 | 2.06 | 0.55 |
| 1:A:845:LEU:HD13 | 1:A:845:LEU:C | 2.26 | 0.55 |
| 1:A:116:MET:HG3 | 1:A:117:LEU:N | 2.21 | 0.55 |
| 1:A:190:GLY:O | 1:A:192:PRO:HD3 | 2.07 | 0.55 |
| 1:A:557:CYS:C | 1:A:558:VAL:CA | 2.65 | 0.55 |
| 1:A:861:GLU:HG3 | 1:A:862:ILE:N | 2.21 | 0.55 |
| 1:A:448:GLY:HA3 | 1:A:480:VAL:CG2 | 2.37 | 0.55 |
| 1:A:710:LEU:HB2 | 1:A:801:TYR:CE1 | 2.41 | 0.55 |
| 1:A:676:TYR:CE1 | 1:A:730:GLN:HG3 | 2.42 | 0.55 |
| 1:A:412:LEU:N | 1:A:412:LEU:HD13 | 2.21 | 0.55 |
| 1:A:804:GLY:HA2 | 1:A:806:MET:CE | 2.36 | 0.55 |
| 1:A:370:LEU:HD13 | 1:A:370:LEU:C | 2.27 | 0.55 |
| 1:A:474:VAL:HG12 | 1:A:475:VAL:N | 2.21 | 0.55 |
| 1:A:531:LEU:O | 1:A:641:THR:OG1 | 2.16 | 0.55 |
| 1:A:937:ARG:HG3 | 1:A:938:PRO:HD2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:236:ILE:O | 1:A:236:ILE:HG23 | 2.07 | 0.55 |
| 1:A:563:HIS:HB3 | 1:A:564:PRO:CD | 2.28 | 0.55 |
| 1:A:447:VAL:HG23 | 1:A:447:VAL:O | 2.06 | 0.55 |
| 1:A:62:ILE:HG12 | 1:A:73:LEU:HB2 | 1.84 | 0.55 |
| 1:A:168:VAL:HG22 | 1:A:169:PHE:N | 2.22 | 0.55 |
| 1:A:175:TYR:HB3 | 1:A:179:ASP:HB3 | 1.89 | 0.55 |
| 1:A:370:LEU:HD13 | 1:A:370:LEU:O | 2.07 | 0.55 |
| 1:A:509:CYS:HB3 | 1:A:535:CYS:SG | 2.47 | 0.55 |
| 1:A:460:ASP:OD2 | 1:A:463:LYS:HB3 | 2.06 | 0.54 |
| 1:A:619:VAL:CB | 1:A:620:PRO:HD3 | 2.36 | 0.54 |
| 1:A:780:LEU:HD12 | 1:A:780:LEU:C | 2.27 | 0.54 |
| 1:A:709:ILE:O | 1:A:799:TYR:HD1 | 1.90 | 0.54 |
| 1:A:226:ILE:O | 1:A:226:ILE:HG23 | 2.06 | 0.54 |
| 1:A:242:TYR:CD1 | 1:A:345:LYS:HE2 | 2.41 | 0.54 |
| 1:A:412:LEU:C | 1:A:412:LEU:HD22 | 2.28 | 0.54 |
| 1:A:91:ASN:CG | 1:A:92:PRO:HD2 | 2.27 | 0.54 |
| 1:A:110:THR:HG22 | 1:A:111:ASN:H | 1.72 | 0.54 |
| 1:A:151:PRO:O | 1:A:157:HIS:HB3 | 2.07 | 0.54 |
| 1:A:280:VAL:HG12 | 1:A:281:ARG:N | 2.22 | 0.54 |
| 1:A:495:ILE:O | 1:A:495:ILE:HG23 | 2.08 | 0.54 |
| 1:A:704:LEU:HD11 | 1:A:724:LYS:CE | 2.36 | 0.54 |
| 1:A:713:VAL:HG13 | 1:A:766:TYR:O | 2.06 | 0.54 |
| 1:A:51:ASN:ND2 | 1:A:67:VAL:HG23 | 2.20 | 0.54 |
| 1:A:63:TYR:CE2 | 1:A:72:LYS:HG2 | 2.43 | 0.54 |
| 1:A:930:GLU:OE2 | 1:A:941:MET:HG3 | 2.07 | 0.54 |
| 1:A:921:LYS:N | 1:A:922:PRO:HD2 | 2.23 | 0.54 |
| 1:A:947:LEU:CD2 | 1:A:947:LEU:H | 2.21 | 0.54 |
| 1:A:370:LEU:HD11 | 1:A:399:ILE:HD12 | 1.88 | 0.53 |
| 1:A:630:HIS:HD2 | 1:A:632:VAL:HG23 | 1.73 | 0.53 |
| 1:A:135:GLY:O | 1:A:159:LEU:HD13 | 2.08 | 0.53 |
| 1:A:359:LEU:HA | 1:A:362:ILE:HG12 | 1.89 | 0.53 |
| 1:A:501:LEU:HD23 | 1:A:502:THR:N | 2.22 | 0.53 |
| 1:A:679:VAL:HG12 | 1:A:680:CYS:N | 2.23 | 0.53 |
| 1:A:662:LEU:HD21 | 1:A:791:ASP:HB2 | 1.88 | 0.53 |
| 1:A:429:ASP:OD1 | 1:A:450:LYS:HB3 | 2.08 | 0.53 |
| 1:A:426:GLU:HG2 | 1:A:429:ASP:O | 2.08 | 0.53 |
| 1:A:42:PHE:HE2 | 1:A:50:PHE:HZ | 1.54 | 0.53 |
| 1:A:46:PRO:CG | 1:A:69:ARG:HG3 | 2.27 | 0.53 |
| 1:A:72:LYS:HD2 | 1:A:80:LEU:HD12 | 1.90 | 0.53 |
| 1:A:797:LYS:HD2 | 1:A:797:LYS:H | 1.72 | 0.53 |
| 1:A:807:ARG:HD2 | 1:A:813:CYS:HA | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:321:LEU:CD2 | 1:A:325:LEU:HD11 | 2.39 | 0.53 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:NH2 | 2.24 | 0.53 |
| 1:A:882:LEU:HD13 | 1:A:910:ALA:O | 2.09 | 0.53 |
| 1:A:875:VAL:HG22 | 1:A:915:CYS:O | 2.09 | 0.53 |
| 1:A:119:ILE:O | 1:A:119:ILE:HG23 | 2.08 | 0.53 |
| 1:A:185:ALA:HB3 | 1:A:243:TYR:CG | 2.44 | 0.53 |
| 1:A:947:LEU:O | 1:A:947:LEU:HD23 | 2.09 | 0.53 |
| 1:A:371:GLN:O | 1:A:375:ARG:HG3 | 2.09 | 0.53 |
| 1:A:39:PHE:CD1 | 1:A:505:PRO:HD2 | 2.44 | 0.53 |
| 1:A:716:ILE:HG12 | 1:A:763:ASN:HB3 | 1.90 | 0.53 |
| 1:A:924:GLN:O | 1:A:925:HIS:HB2 | 2.09 | 0.53 |
| 1:A:806:MET:HG2 | 1:A:807:ARG:CG | 2.39 | 0.53 |
| 1:A:847:LEU:HG | 1:A:850:ALA:HA | 1.91 | 0.53 |
| 1:A:42:PHE:HZ | 1:A:45:GLU:CB | 2.22 | 0.53 |
| 1:A:716:ILE:O | 1:A:716:ILE:HG23 | 2.09 | 0.53 |
| 1:A:739:ILE:HB | 1:A:781:THR:HG23 | 1.90 | 0.53 |
| 1:A:783:VAL:HG12 | 1:A:784:TRP:N | 2.24 | 0.53 |
| 1:A:825:CYS:HB3 | 1:A:828:PRO:HG2 | 1.89 | 0.53 |
| 1:A:553:GLU:HG3 | 1:A:554:MET:N | 2.24 | 0.52 |
| 1:A:739:ILE:HB | 1:A:781:THR:HG22 | 1.90 | 0.52 |
| 1:A:578:LEU:HB2 | 1:A:609:ILE:HB | 1.91 | 0.52 |
| 1:A:64:LEU:N | 1:A:64:LEU:HD22 | 2.24 | 0.52 |
| 1:A:949:TYR:HE2 | 1:A:951:MET:HE2 | 1.74 | 0.52 |
| 1:A:589:GLY:HA3 | 1:A:639:LYS:HG3 | 1.90 | 0.52 |
| 1:A:827:SER:HB2 | 1:A:828:PRO:HD3 | 1.91 | 0.52 |
| 1:A:925:HIS:O | 1:A:950:PHE:HD2 | 1.91 | 0.52 |
| 1:A:471:THR:CG2 | 1:A:473:GLN:HE22 | 2.20 | 0.52 |
| 1:A:308:LEU:O | 1:A:338:PHE:HA | 2.09 | 0.52 |
| 1:A:458:ARG:HG3 | 1:A:524:PRO:HG3 | 1.90 | 0.52 |
| 1:A:623:ILE:HD12 | 1:A:623:ILE:C | 2.29 | 0.52 |
| 1:A:396:LEU:C | 1:A:396:LEU:HD13 | 2.30 | 0.52 |
| 1:A:472:VAL:O | 1:A:472:VAL:HG12 | 2.09 | 0.52 |
| 1:A:712:PRO:O | 1:A:715:VAL:HG22 | 2.09 | 0.52 |
| 1:A:181:LYS:CE | 1:A:202:LYS:HG2 | 2.39 | 0.52 |
| 1:A:356:ILE:HG22 | 1:A:421:ILE:O | 2.09 | 0.52 |
| 1:A:580:THR:HG21 | 1:A:583:VAL:HG11 | 1.91 | 0.52 |
| 1:A:458:ARG:HD3 | 1:A:524:PRO:HB3 | 1.90 | 0.52 |
| 1:A:933:VAL:HG22 | 1:A:940:PHE:HB3 | 1.91 | 0.52 |
| 1:A:127:ILE:O | 1:A:127:ILE:HG23 | 2.09 | 0.52 |
| 1:A:228:ILE:HG22 | 1:A:233:PHE:CE1 | 2.45 | 0.52 |
| 1:A:281:ARG:O | 1:A:282:LEU:HD23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:385:LEU:HD13 | 1:A:385:LEU:C | 2.29 | 0.52 |
| 1:A:380:LEU:CD1 | 1:A:386:LYS:HE3 | 2.37 | 0.52 |
| 1:A:716:ILE:CG1 | 1:A:763:ASN:HB3 | 2.40 | 0.52 |
| 1:A:805:ALA:H | 1:A:806:MET:CE | 2.22 | 0.52 |
| 1:A:93:LYS:HD3 | 1:A:105:GLU:OE2 | 2.10 | 0.52 |
| 1:A:198:ILE:HB | 1:A:226:ILE:HG22 | 1.91 | 0.52 |
| 1:A:712:PRO:HG3 | 1:A:801:TYR:CZ | 2.45 | 0.52 |
| 1:A:473:GLN:HB2 | 1:A:504:VAL:CG2 | 2.40 | 0.51 |
| 1:A:64:LEU:HD11 | 1:A:501:LEU:HD12 | 1.92 | 0.51 |
| 1:A:790:ILE:HD12 | 1:A:790:ILE:N | 2.25 | 0.51 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CG | 2.94 | 0.51 |
| 1:A:509:CYS:HB2 | 1:A:536:THR:HA | 1.91 | 0.51 |
| 1:A:321:LEU:CG | 1:A:325:LEU:HD11 | 2.40 | 0.51 |
| 1:A:53:LEU:HD23 | 1:A:53:LEU:C | 2.31 | 0.51 |
| 1:A:560:LEU:HG | 1:A:648:THR:HG21 | 1.92 | 0.51 |
| 1:A:575:LEU:H | 1:A:575:LEU:CD2 | 2.22 | 0.51 |
| 1:A:930:GLU:HG3 | 1:A:941:MET:SD | 2.51 | 0.51 |
| 1:A:59:THR:HB | 1:A:61:HIS:CE1 | 2.45 | 0.51 |
| 1:A:827:SER:HB2 | 1:A:828:PRO:CD | 2.40 | 0.51 |
| 1:A:895:VAL:O | 1:A:896:ALA:HB3 | 2.11 | 0.51 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CD2 | 2.94 | 0.51 |
| 1:A:567:ILE:CD1 | 1:A:650:PHE:CE2 | 2.94 | 0.51 |
| 1:A:798:VAL:O | 1:A:798:VAL:HG13 | 2.10 | 0.51 |
| 1:A:823:GLY:HA3 | 1:A:844:TRP:CZ2 | 2.46 | 0.51 |
| 1:A:204:THR:HG23 | 1:A:206:ASN:O | 2.11 | 0.51 |
| 1:A:216:VAL:HG13 | 1:A:217:PHE:N | 2.26 | 0.51 |
| 1:A:278:LYS:HG2 | 1:A:296:PRO:CA | 2.38 | 0.51 |
| 1:A:519:LEU:N | 1:A:519:LEU:HD22 | 2.26 | 0.51 |
| 1:A:53:LEU:HG | 1:A:64:LEU:HD11 | 1.92 | 0.51 |
| 1:A:541:CYS:SG | 1:A:550:PHE:HD2 | 2.33 | 0.51 |
| 1:A:530:VAL:HG12 | 1:A:584:PRO:HG2 | 1.93 | 0.51 |
| 1:A:889:ILE:CD1 | 1:A:907:TYR:CE1 | 2.94 | 0.51 |
| 1:A:133:TYR:O | 1:A:134:GLN:HB2 | 2.11 | 0.51 |
| 1:A:261:GLU:HG2 | 1:A:265:PRO:N | 2.25 | 0.51 |
| 1:A:593:THR:HG23 | 1:A:593:THR:O | 2.10 | 0.51 |
| 1:A:322:GLY:CA | 1:A:327:VAL:HG22 | 2.40 | 0.51 |
| 1:A:370:LEU:HD13 | 1:A:374:TYR:CD1 | 2.46 | 0.51 |
| 1:A:426:GLU:HG3 | 1:A:429:ASP:H | 1.76 | 0.51 |
| 1:A:444:LEU:HD12 | 1:A:446:PHE:CZ | 2.44 | 0.51 |
| 1:A:76:ASP:O | 1:A:77:LEU:HB2 | 2.11 | 0.51 |
| 1:A:853:LYS:HD2 | 1:A:853:LYS:H | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:VAL:HG12 | 1:A:172:ILE:N | 2.26 | 0.51 |
| 1:A:358:ILE:CG2 | 1:A:361:GLN:HB2 | 2.41 | 0.51 |
| 1:A:531:LEU:HD23 | 1:A:584:PRO:HG2 | 1.93 | 0.51 |
| 1:A:695:LYS:CB | 1:A:696:LEU:HD12 | 2.41 | 0.51 |
| 1:A:785:ASN:HB3 | 1:A:788:PHE:CE2 | 2.46 | 0.51 |
| 1:A:184:ILE:HD12 | 1:A:184:ILE:C | 2.31 | 0.50 |
| 1:A:703:LEU:N | 1:A:703:LEU:HD22 | 2.26 | 0.50 |
| 1:A:81:VAL:HG12 | 1:A:82:THR:N | 2.26 | 0.50 |
| 1:A:892:HIS:HD2 | 1:A:893:VAL:N | 2.10 | 0.50 |
| 1:A:228:ILE:CG2 | 1:A:233:PHE:CE1 | 2.94 | 0.50 |
| 1:A:491:GLU:O | 1:A:506:VAL:HG12 | 2.11 | 0.50 |
| 1:A:567:ILE:N | 1:A:567:ILE:HD13 | 2.20 | 0.50 |
| 1:A:566:ASN:HB3 | 1:A:651:VAL:CG2 | 2.40 | 0.50 |
| 1:A:689:PHE:CE1 | 1:A:691:GLU:CG | 2.94 | 0.50 |
| 1:A:507:GLU:HG3 | 1:A:537:ARG:CG | 2.40 | 0.50 |
| 1:A:533:ASN:HD21 | 1:A:645:PHE:HA | 1.68 | 0.50 |
| 1:A:863:ILE:CG1 | 1:A:864:PRO:HD3 | 2.39 | 0.50 |
| 1:A:727:PRO:O | 1:A:729:PRO:HD3 | 2.11 | 0.50 |
| 1:A:370:LEU:HD11 | 1:A:374:TYR:CE1 | 2.46 | 0.50 |
| 1:A:569:VAL:CB | 1:A:654:ASN:HD22 | 2.21 | 0.50 |
| 1:A:119:ILE:CG2 | 1:A:121:TYR:CE1 | 2.95 | 0.50 |
| 1:A:284:LYS:HD3 | 1:A:284:LYS:C | 2.31 | 0.50 |
| 1:A:296:PRO:HD2 | 1:A:414:VAL:HG22 | 1.92 | 0.50 |
| 1:A:418:VAL:O | 1:A:418:VAL:HG13 | 2.11 | 0.50 |
| 1:A:473:GLN:HB3 | 1:A:502:THR:HG21 | 1.94 | 0.50 |
| 1:A:54:VAL:HG22 | 1:A:55:VAL:N | 2.25 | 0.50 |
| 1:A:699:ASP:C | 1:A:725:ASN:OD1 | 2.50 | 0.50 |
| 1:A:412:LEU:O | 1:A:412:LEU:HD22 | 2.11 | 0.50 |
| 1:A:673:TRP:HB3 | 1:A:694:VAL:HB | 1.94 | 0.50 |
| 1:A:473:GLN:CD | 1:A:504:VAL:HG13 | 2.31 | 0.50 |
| 1:A:506:VAL:HG11 | 1:A:537:ARG:HH12 | 1.77 | 0.50 |
| 1:A:541:CYS:CB | 1:A:544:SER:HB3 | 2.42 | 0.50 |
| 1:A:713:VAL:HG13 | 1:A:767:SER:HA | 1.94 | 0.50 |
| 1:A:782:VAL:CG2 | 1:A:790:ILE:HB | 2.41 | 0.50 |
| 1:A:792:ASN:HD21 | 1:A:796:ASN:N | 2.10 | 0.50 |
| 1:A:807:ARG:HD3 | 1:A:812:LEU:HB3 | 1.93 | 0.50 |
| 1:A:295:VAL:HG23 | 1:A:295:VAL:O | 2.12 | 0.50 |
| 1:A:278:LYS:CE | 1:A:296:PRO:HG3 | 2.41 | 0.50 |
| 1:A:370:LEU:CD1 | 1:A:374:TYR:CD1 | 2.95 | 0.50 |
| 1:A:847:LEU:HG | 1:A:850:ALA:CA | 2.42 | 0.50 |
| 1:A:320:VAL:HG23 | 1:A:441:ASN:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:333:LEU:HD21 | 1:A:358:ILE:HG13 | 1.94 | 0.49 |
| 1:A:882:LEU:HD23 | 1:A:913:ILE:HD11 | 1.94 | 0.49 |
| 1:A:110:THR:CB | 1:A:132:LEU:HD21 | 2.42 | 0.49 |
| 1:A:400:ASP:HB2 | 1:A:402:ASN:OD1 | 2.11 | 0.49 |
| 1:A:39:PHE:CD2 | 1:A:473:GLN:CG | 2.95 | 0.49 |
| 1:A:841:GLU:HG3 | 1:A:842:SER:H | 1.77 | 0.49 |
| 1:A:653:TYR:HE2 | 1:A:655:CYS:SG | 2.35 | 0.49 |
| 1:A:265:PRO:CD | 1:A:274:VAL:HG22 | 2.42 | 0.49 |
| 1:A:312:ALA:HB1 | 1:A:334:LEU:HD11 | 1.94 | 0.49 |
| 1:A:557:CYS:O | 1:A:581:TYR:O | 2.30 | 0.49 |
| 1:A:59:THR:HB | 1:A:61:HIS:ND1 | 2.27 | 0.49 |
| 1:A:185:ALA:HB1 | 1:A:243:TYR:CE2 | 2.47 | 0.49 |
| 1:A:457:ILE:HG12 | 1:A:467:LEU:CD1 | 2.42 | 0.49 |
| 1:A:468:GLN:CD | 1:A:524:PRO:CG | 2.78 | 0.49 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:CA | 2.42 | 0.49 |
| 1:A:254:TYR:CE2 | 1:A:281:ARG:HD2 | 2.48 | 0.49 |
| 1:A:265:PRO:HD3 | 1:A:274:VAL:HG22 | 1.92 | 0.49 |
| 1:A:433:SER:HB3 | 1:A:484:MET:HE3 | 1.95 | 0.49 |
| 1:A:681:THR:HG21 | 1:A:686:THR:HG21 | 1.94 | 0.49 |
| 1:A:40:VAL:HG21 | 1:A:76:ASP:O | 2.12 | 0.49 |
| 1:A:790:ILE:H | 1:A:790:ILE:HD12 | 1.77 | 0.49 |
| 1:A:856:ASN:N | 1:A:857:PRO:HD3 | 2.27 | 0.49 |
| 1:A:863:ILE:HG13 | 1:A:864:PRO:N | 2.28 | 0.49 |
| 1:A:182:LEU:HD21 | 1:A:184:ILE:HG21 | 1.94 | 0.49 |
| 1:A:234:THR:HG23 | 1:A:235:VAL:N | 2.26 | 0.49 |
| 1:A:300:GLU:HG2 | 1:A:305:GLU:HA | 1.93 | 0.49 |
| 1:A:736:TYR:CD2 | 1:A:784:TRP:HB3 | 2.47 | 0.49 |
| 1:A:894:LYS:CD | 1:A:899:GLU:HA | 2.41 | 0.49 |
| 1:A:133:TYR:HB3 | 1:A:136:ILE:HG23 | 1.94 | 0.49 |
| 1:A:190:GLY:C | 1:A:192:PRO:HD3 | 2.33 | 0.49 |
| 1:A:475:VAL:HG22 | 1:A:500:GLN:OE1 | 2.13 | 0.49 |
| 1:A:590:VAL:HG12 | 1:A:591:ASN:N | 2.27 | 0.49 |
| 1:A:781:THR:O | 1:A:781:THR:HG23 | 2.12 | 0.49 |
| 1:A:810:CYS:SG | 1:A:855:THR:CG2 | 2.72 | 0.49 |
| 1:A:132:LEU:HD11 | 1:A:163:ASN:HD22 | 1.77 | 0.49 |
| 1:A:361:GLN:HE21 | 1:A:365:ARG:HH21 | 1.61 | 0.49 |
| 1:A:597:LEU:CD2 | 1:A:597:LEU:H | 2.25 | 0.49 |
| 1:A:809:SER:HB3 | 1:A:856:ASN:ND2 | 2.19 | 0.49 |
| 1:A:190:GLY:HA2 | 1:A:233:PHE:HE2 | 1.73 | 0.48 |
| 1:A:783:VAL:HG13 | 1:A:788:PHE:O | 2.13 | 0.48 |
| 1:A:541:CYS:SG | 1:A:550:PHE:CD2 | 3.06 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:603:LEU:HD23 | 1:A:603:LEU:C | 2.33 | 0.48 |
| 1:A:64:LEU:HB2 | 1:A:71:TYR:HD2 | 1.77 | 0.48 |
| 1:A:716:ILE:HD11 | 1:A:763:ASN:HB3 | 1.95 | 0.48 |
| 1:A:782:VAL:HG23 | 1:A:782:VAL:O | 2.12 | 0.48 |
| 1:A:807:ARG:HB3 | 1:A:812:LEU:HB2 | 1.95 | 0.48 |
| 1:A:185:ALA:HA | 1:A:197:THR:O | 2.12 | 0.48 |
| 1:A:790:ILE:HG22 | 1:A:791:ASP:N | 2.28 | 0.48 |
| 1:A:99:ILE:HD11 | 1:A:152:PHE:CB | 2.41 | 0.48 |
| 1:A:144:ASP:O | 1:A:145:LEU:HB2 | 2.13 | 0.48 |
| 1:A:258:LEU:HD12 | 1:A:258:LEU:N | 2.28 | 0.48 |
| 1:A:597:LEU:HD22 | 1:A:597:LEU:H | 1.77 | 0.48 |
| 1:A:710:LEU:HD13 | 1:A:801:TYR:OH | 2.13 | 0.48 |
| 1:A:715:VAL:HG23 | 1:A:715:VAL:O | 2.13 | 0.48 |
| 1:A:935:VAL:HG12 | 1:A:936:CYS:N | 2.28 | 0.48 |
| 1:A:435:ILE:HG21 | 1:A:486:PHE:CE1 | 2.48 | 0.48 |
| 1:A:626:ASN:ND2 | 1:A:630:HIS:HB2 | 2.29 | 0.48 |
| 1:A:662:LEU:HD22 | 1:A:791:ASP:OD2 | 2.00 | 0.48 |
| 1:A:949:TYR:CE2 | 1:A:951:MET:CE | 2.95 | 0.48 |
| 1:A:265:PRO:HB2 | 1:A:266:PRO:HD2 | 1.94 | 0.48 |
| 1:A:473:GLN:CD | 1:A:504:VAL:HG22 | 2.34 | 0.48 |
| 1:A:907:TYR:CZ | 1:A:909:PRO:HA | 2.48 | 0.48 |
| 1:A:453:LYS:HE3 | 1:A:472:VAL:HG22 | 1.94 | 0.48 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:CE1 | 2.45 | 0.48 |
| 1:A:82:THR:O | 1:A:82:THR:HG23 | 2.14 | 0.48 |
| 1:A:239:PHE:CD1 | 1:A:260:PRO:HG2 | 2.48 | 0.48 |
| 1:A:374:TYR:CE2 | 1:A:397:LEU:HD22 | 2.48 | 0.48 |
| 1:A:862:ILE:CG2 | 1:A:877:ILE:HG23 | 2.44 | 0.48 |
| 1:A:175:TYR:CG | 1:A:176:SER:N | 2.82 | 0.47 |
| 1:A:372:SER:HA | 1:A:375:ARG:NE | 2.30 | 0.47 |
| 1:A:403:PHE:CE1 | 1:A:406:LEU:CD2 | 2.94 | 0.47 |
| 1:A:556:GLN:HA | 1:A:582:ASN:HD22 | 1.59 | 0.47 |
| 1:A:702:GLN:O | 1:A:723:ALA:HB1 | 2.14 | 0.47 |
| 1:A:745:ILE:O | 1:A:745:ILE:HG23 | 2.14 | 0.47 |
| 1:A:154:LYS:HB2 | 1:A:157:HIS:HD2 | 1.70 | 0.47 |
| 1:A:77:LEU:HD22 | 1:A:501:LEU:HD13 | 1.96 | 0.47 |
| 1:A:740:LEU:HD12 | 1:A:740:LEU:N | 2.29 | 0.47 |
| 1:A:814:LEU:HD11 | 1:A:845:LEU:CD1 | 2.44 | 0.47 |
| 1:A:118:LEU:C | 1:A:118:LEU:HD13 | 2.34 | 0.47 |
| 1:A:160:SER:OG | 1:A:162:VAL:HG23 | 2.14 | 0.47 |
| 1:A:440:LYS:HD3 | 1:A:538:LYS:CD | 2.44 | 0.47 |
| 1:A:567:ILE:HD12 | 1:A:650:PHE:CE2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:728:GLN:HA | 1:A:753:ARG:NH2 | 2.30 | 0.47 |
| 1:A:68:ASN:ND2 | 1:A:87:PRO:HD3 | 2.29 | 0.47 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:CG2 | 2.98 | 0.47 |
| 1:A:430:ARG:HG2 | 1:A:431:MET:O | 2.14 | 0.47 |
| 1:A:439:TYR:HE2 | 1:A:538:LYS:HZ1 | 0.83 | 0.47 |
| 1:A:843:ARG:HB2 | 1:A:843:ARG:NH1 | 2.30 | 0.47 |
| 1:A:133:TYR:CG | 1:A:136:ILE:CG1 | 2.94 | 0.47 |
| 1:A:239:PHE:HA | 1:A:260:PRO:CG | 2.32 | 0.47 |
| 1:A:253:VAL:O | 1:A:253:VAL:HG23 | 2.15 | 0.47 |
| 1:A:72:LYS:O | 1:A:80:LEU:HB2 | 2.15 | 0.47 |
| 1:A:530:VAL:CB | 1:A:584:PRO:HD3 | 2.45 | 0.47 |
| 1:A:68:ASN:HB3 | 1:A:86:GLY:HA3 | 1.97 | 0.47 |
| 1:A:262:MET:O | 1:A:263:VAL:HB | 2.15 | 0.47 |
| 1:A:889:ILE:O | 1:A:892:HIS:HB3 | 2.13 | 0.47 |
| 1:A:244:VAL:HB | 1:A:309:LEU:HD23 | 1.97 | 0.47 |
| 1:A:440:LYS:HG2 | 1:A:440:LYS:O | 2.14 | 0.47 |
| 1:A:480:VAL:HB | 1:A:484:MET:HE1 | 1.95 | 0.47 |
| 1:A:561:THR:HG22 | 1:A:562:VAL:N | 2.29 | 0.47 |
| 1:A:124:ASN:OD1 | 1:A:142:LEU:HB3 | 2.14 | 0.47 |
| 1:A:252:PHE:CD1 | 1:A:283:CYS:HA | 2.50 | 0.47 |
| 1:A:296:PRO:CD | 1:A:414:VAL:HG22 | 2.45 | 0.47 |
| 1:A:704:LEU:H | 1:A:723:ALA:HA | 1.79 | 0.47 |
| 1:A:947:LEU:H | 1:A:947:LEU:HD23 | 1.79 | 0.47 |
| 1:A:527:GLY:HA3 | 1:A:550:PHE:HZ | 1.72 | 0.46 |
| 1:A:805:ALA:N | 1:A:806:MET:HE3 | 2.28 | 0.46 |
| 1:A:256:LEU:HD22 | 1:A:256:LEU:N | 2.31 | 0.46 |
| 1:A:333:LEU:CD2 | 1:A:358:ILE:HA | 2.45 | 0.46 |
| 1:A:343:LYS:HG2 | 1:A:344:ARG:HG2 | 1.97 | 0.46 |
| 1:A:495:ILE:HG22 | 1:A:502:THR:HB | 1.96 | 0.46 |
| 1:A:783:VAL:HG11 | 1:A:786:GLY:O | 2.15 | 0.46 |
| 1:A:812:LEU:CG | 1:A:881:ASN:OD1 | 2.47 | 0.46 |
| 1:A:902:PRO:HA | 1:A:915:CYS:HA | 1.97 | 0.46 |
| 1:A:380:LEU:HD12 | 1:A:390:ILE:CG2 | 2.45 | 0.46 |
| 1:A:873:THR:HG22 | 1:A:874:LYS:N | 2.31 | 0.46 |
| 1:A:245:TYR:CE2 | 1:A:247:PHE:HD2 | 2.34 | 0.46 |
| 1:A:62:ILE:HD11 | 1:A:73:LEU:CD1 | 2.45 | 0.46 |
| 1:A:46:PRO:HD2 | 1:A:71:TYR:OH | 2.16 | 0.46 |
| 1:A:695:LYS:HB2 | 1:A:696:LEU:HD12 | 1.97 | 0.46 |
| 1:A:265:PRO:CB | 1:A:266:PRO:HD2 | 2.45 | 0.46 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:HG2 | 1.98 | 0.46 |
| 1:A:676:TYR:CD1 | 1:A:730:GLN:CG | 2.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:VAL:HG11 | 1:A:165:SER:HB3 | 1.96 | 0.46 |
| 1:A:226:ILE:HD11 | 1:A:385:LEU:CD2 | 2.46 | 0.46 |
| 1:A:45:GLU:HB3 | 1:A:46:PRO:HD3 | 1.97 | 0.46 |
| 1:A:530:VAL:CG1 | 1:A:584:PRO:HG2 | 2.38 | 0.46 |
| 1:A:543:ARG:HH11 | 1:A:549:ARG:HH22 | 1.62 | 0.46 |
| 1:A:515:CYS:HB3 | 1:A:558:VAL:N | 2.31 | 0.46 |
| 1:A:569:VAL:CG1 | 1:A:620:PRO:HG3 | 2.45 | 0.46 |
| 1:A:64:LEU:HD12 | 1:A:496:MET:HE3 | 1.98 | 0.46 |
| 1:A:566:ASN:CB | 1:A:651:VAL:CG2 | 2.95 | 0.46 |
| 1:A:695:LYS:C | 1:A:696:LEU:HD12 | 2.37 | 0.46 |
| 1:A:264:SER:HA | 1:A:265:PRO:HA | 1.53 | 0.45 |
| 1:A:286:ASP:OD1 | 1:A:288:ALA:HB3 | 2.16 | 0.45 |
| 1:A:469:TYR:CG | 1:A:470:GLU:N | 2.84 | 0.45 |
| 1:A:503:ARG:O | 1:A:505:PRO:HD3 | 2.15 | 0.45 |
| 1:A:361:GLN:O | 1:A:365:ARG:HG2 | 2.15 | 0.45 |
| 1:A:563:HIS:CB | 1:A:577:VAL:HG12 | 2.46 | 0.45 |
| 1:A:62:ILE:CD1 | 1:A:77:LEU:CD2 | 2.94 | 0.45 |
| 1:A:358:ILE:CG2 | 1:A:361:GLN:CB | 2.95 | 0.45 |
| 1:A:624:THR:O | 1:A:624:THR:HG23 | 2.15 | 0.45 |
| 1:A:863:ILE:HG21 | 1:A:876:THR:HB | 1.97 | 0.45 |
| 1:A:98:ARG:NH2 | 1:A:107:LEU:HD12 | 2.29 | 0.45 |
| 1:A:435:ILE:HG23 | 1:A:486:PHE:HE1 | 1.81 | 0.45 |
| 1:A:586:LEU:HD13 | 1:A:590:VAL:HG21 | 1.99 | 0.45 |
| 1:A:663:SER:O | 1:A:667:SER:HB2 | 2.17 | 0.45 |
| 1:A:828:PRO:HG3 | 1:A:837:CYS:SG | 2.57 | 0.45 |
| 1:A:110:THR:CB | 1:A:132:LEU:CD2 | 2.95 | 0.45 |
| 1:A:159:LEU:HG | 1:A:201:ARG:HH12 | 1.81 | 0.45 |
| 1:A:947:LEU:N | 1:A:947:LEU:HD23 | 2.30 | 0.45 |
| 1:A:182:LEU:HB2 | 1:A:203:LEU:HD11 | 1.99 | 0.45 |
| 1:A:192:PRO:HB3 | 1:A:233:PHE:CZ | 2.51 | 0.45 |
| 1:A:305:GLU:HG2 | 1:A:307:ARG:HG2 | 1.99 | 0.45 |
| 1:A:247:PHE:CD1 | 1:A:314:LEU:HD22 | 2.52 | 0.45 |
| 1:A:40:VAL:HG11 | 1:A:503:ARG:HE | 1.80 | 0.45 |
| 1:A:40:VAL:O | 1:A:40:VAL:HG13 | 2.17 | 0.45 |
| 1:A:442:HIS:CD2 | 1:A:458:ARG:HH21 | 2.35 | 0.45 |
| 1:A:671:CYS:HB3 | 1:A:680:CYS:SG | 2.57 | 0.45 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:HG22 | 2.51 | 0.45 |
| 1:A:118:LEU:HB3 | 1:A:127:ILE:HG22 | 1.98 | 0.45 |
| 1:A:151:PRO:HB2 | 1:A:157:HIS:CE1 | 2.52 | 0.45 |
| 1:A:539:GLU:HG3 | 1:A:540:ARG:N | 2.31 | 0.45 |
| 1:A:541:CYS:HB3 | 1:A:544:SER:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:743:GLN:HG2 | 1:A:744:GLY:N | 2.31 | 0.45 |
| 1:A:815:LYS:CD | 1:A:910:ALA:CB | 2.63 | 0.45 |
| 1:A:91:ASN:OD1 | 1:A:92:PRO:HD2 | 2.16 | 0.45 |
| 1:A:437:TYR:CE2 | 1:A:439:TYR:HB2 | 2.51 | 0.45 |
| 1:A:511:GLN:HG3 | 1:A:512:TYR:CD2 | 2.51 | 0.45 |
| 1:A:653:TYR:CE2 | 1:A:655:CYS:SG | 3.10 | 0.45 |
| 1:A:116:MET:SD | 1:A:169:PHE:HA | 2.57 | 0.45 |
| 1:A:245:TYR:CD2 | 1:A:312:ALA:HB3 | 2.51 | 0.45 |
| 1:A:288:ALA:O | 1:A:289:PHE:HB2 | 2.17 | 0.45 |
| 1:A:306:TYR:HE1 | 1:A:351:GLU:HG2 | 1.82 | 0.45 |
| 1:A:58:ARG:HG2 | 1:A:58:ARG:NH1 | 2.31 | 0.45 |
| 1:A:892:HIS:CD2 | 1:A:893:VAL:N | 2.85 | 0.45 |
| 1:A:118:LEU:O | 1:A:127:ILE:HG22 | 2.17 | 0.45 |
| 1:A:370:LEU:CD2 | 1:A:374:TYR:HE1 | 2.28 | 0.45 |
| 1:A:458:ARG:HG3 | 1:A:468:GLN:NE2 | 2.32 | 0.45 |
| 1:A:574:VAL:HG22 | 1:A:613:SER:OG | 2.17 | 0.45 |
| 1:A:594:PHE:CZ | 1:A:614:PRO:HD3 | 2.51 | 0.45 |
| 1:A:295:VAL:CA | 1:A:414:VAL:HG21 | 2.45 | 0.44 |
| 1:A:435:ILE:HG21 | 1:A:486:PHE:HE1 | 1.81 | 0.44 |
| 1:A:564:PRO:HB2 | 1:A:576:LEU:CD2 | 2.47 | 0.44 |
| 1:A:322:GLY:HA2 | 1:A:327:VAL:HG22 | 1.99 | 0.44 |
| 1:A:42:PHE:CZ | 1:A:45:GLU:CB | 2.95 | 0.44 |
| 1:A:62:ILE:CD1 | 1:A:73:LEU:HB2 | 2.47 | 0.44 |
| 1:A:805:ALA:H | 1:A:806:MET:HE3 | 1.80 | 0.44 |
| 1:A:949:TYR:CE2 | 1:A:951:MET:HE1 | 2.52 | 0.44 |
| 1:A:119:ILE:HG23 | 1:A:121:TYR:CE1 | 2.53 | 0.44 |
| 1:A:162:VAL:HG21 | 1:A:187:ALA:HB3 | 1.99 | 0.44 |
| 1:A:189:ASP:HB3 | 1:A:191:LYS:HD3 | 1.99 | 0.44 |
| 1:A:327:VAL:HG11 | 1:A:358:ILE:HD11 | 1.97 | 0.44 |
| 1:A:567:ILE:HD11 | 1:A:652:PHE:CD1 | 2.53 | 0.44 |
| 1:A:689:PHE:CE1 | 1:A:691:GLU:HG2 | 2.50 | 0.44 |
| 1:A:278:LYS:HD3 | 1:A:294:GLU:HG2 | 1.98 | 0.44 |
| 1:A:301:ARG:CD | 1:A:425:THR:HG21 | 2.26 | 0.44 |
| 1:A:492:GLN:HG2 | 1:A:503:ARG:HD2 | 1.98 | 0.44 |
| 1:A:531:LEU:CD2 | 1:A:584:PRO:HG2 | 2.47 | 0.44 |
| 1:A:274:VAL:HG23 | 1:A:275:TYR:N | 2.30 | 0.44 |
| 1:A:281:ARG:NH1 | 1:A:366:ILE:HG21 | 2.33 | 0.44 |
| 1:A:296:PRO:HB2 | 1:A:417:MET:CE | 2.48 | 0.44 |
| 1:A:446:PHE:CB | 1:A:454:LEU:HD11 | 2.43 | 0.44 |
| 1:A:53:LEU:HD12 | 1:A:501:LEU:HG | 1.99 | 0.44 |
| 1:A:530:VAL:CG2 | 1:A:584:PRO:HD3 | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:217:PHE:CE2 | 1:A:219:ASP:HB2 | 2.53 | 0.44 |
| 1:A:635:GLN:HB3 | 1:A:644:THR:HB | 1.99 | 0.44 |
| 1:A:179:ASP:O | 1:A:180:ASP:HB3 | 2.17 | 0.44 |
| 1:A:471:THR:HG23 | 1:A:473:GLN:NE2 | 2.28 | 0.44 |
| 1:A:778:VAL:O | 1:A:797:LYS:HB2 | 2.17 | 0.44 |
| 1:A:703:LEU:CD2 | 1:A:790:ILE:CG2 | 2.95 | 0.44 |
| 1:A:889:ILE:HA | 1:A:892:HIS:ND1 | 2.33 | 0.44 |
| 1:A:890:ALA:O | 1:A:891:SER:HB2 | 2.17 | 0.44 |
| 1:A:173:VAL:O | 1:A:173:VAL:HG23 | 2.18 | 0.44 |
| 1:A:252:PHE:HD1 | 1:A:283:CYS:HA | 1.82 | 0.44 |
| 1:A:262:MET:SD | 1:A:383:ALA:HB3 | 2.58 | 0.44 |
| 1:A:53:LEU:HD11 | 1:A:501:LEU:HD11 | 2.00 | 0.44 |
| 1:A:863:ILE:HG22 | 1:A:876:THR:CB | 2.35 | 0.44 |
| 1:A:256:LEU:CB | 1:A:309:LEU:CD2 | 2.94 | 0.43 |
| 1:A:291:SER:HB3 | 1:A:404:CYS:O | 2.18 | 0.43 |
| 1:A:358:ILE:HG23 | 1:A:358:ILE:O | 2.18 | 0.43 |
| 1:A:370:LEU:HD12 | 1:A:399:ILE:HG23 | 2.00 | 0.43 |
| 1:A:458:ARG:HB2 | 1:A:468:GLN:HE22 | 1.83 | 0.43 |
| 1:A:567:ILE:HD11 | 1:A:650:PHE:CE2 | 2.53 | 0.43 |
| 1:A:62:ILE:CD1 | 1:A:73:LEU:HD12 | 2.45 | 0.43 |
| 1:A:759:VAL:CG1 | 1:A:760:GLN:N | 2.81 | 0.43 |
| 1:A:889:ILE:CD1 | 1:A:907:TYR:CZ | 3.01 | 0.43 |
| 1:A:123:GLU:HB2 | 1:A:125:ARG:HG2 | 2.00 | 0.43 |
| 1:A:542:GLU:HG2 | 1:A:543:ARG:HG3 | 2.00 | 0.43 |
| 1:A:620:PRO:O | 1:A:623:ILE:HG13 | 2.18 | 0.43 |
| 1:A:711:VAL:HG21 | 1:A:798:VAL:CG2 | 2.48 | 0.43 |
| 1:A:295:VAL:CB | 1:A:414:VAL:HG21 | 2.48 | 0.43 |
| 1:A:336:THR:HG1 | 1:A:338:PHE:HE2 | 1.62 | 0.43 |
| 1:A:528:TRP:HZ2 | 1:A:533:ASN:OD1 | 2.01 | 0.43 |
| 1:A:743:GLN:CD | 1:A:743:GLN:H | 2.22 | 0.43 |
| 1:A:839:ALA:HB1 | 1:A:841:GLU:O | 2.18 | 0.43 |
| 1:A:841:GLU:HG3 | 1:A:842:SER:N | 2.32 | 0.43 |
| 1:A:862:ILE:HG22 | 1:A:877:ILE:CA | 2.32 | 0.43 |
| 1:A:90:ASP:C | 1:A:107:LEU:HD22 | 2.39 | 0.43 |
| 1:A:324:THR:HG22 | 1:A:324:THR:O | 2.18 | 0.43 |
| 1:A:444:LEU:HD12 | 1:A:446:PHE:CD1 | 2.51 | 0.43 |
| 1:A:555:LYS:NZ | 1:A:556:GLN:HG2 | 2.34 | 0.43 |
| 1:A:557:CYS:C | 1:A:582:ASN:HB3 | 2.35 | 0.43 |
| 1:A:464:GLY:O | 1:A:465:ASN:HB3 | 2.17 | 0.43 |
| 1:A:597:LEU:HG | 1:A:622:ILE:HG12 | 1.99 | 0.43 |
| 1:A:53:LEU:CG | 1:A:64:LEU:CD1 | 2.96 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:764:THR:HG23 | 1:A:766:TYR:CZ | 2.54 | 0.43 |
| 1:A:832:THR:CG2 | 1:A:836:HIS:CB | 2.95 | 0.43 |
| 1:A:832:THR:HG21 | 1:A:836:HIS:CB | 2.48 | 0.43 |
| 1:A:117:LEU:HG | 1:A:126:LEU:HD11 | 2.01 | 0.43 |
| 1:A:590:VAL:CG1 | 1:A:591:ASN:N | 2.82 | 0.43 |
| 1:A:574:VAL:CG2 | 1:A:613:SER:HB3 | 2.48 | 0.43 |
| 1:A:699:ASP:O | 1:A:725:ASN:HB3 | 2.18 | 0.43 |
| 1:A:865:VAL:CG1 | 1:A:866:THR:N | 2.82 | 0.43 |
| 1:A:98:ARG:HE | 1:A:107:LEU:HD12 | 1.83 | 0.43 |
| 1:A:55:VAL:HG22 | 1:A:62:ILE:HG22 | 2.00 | 0.43 |
| 1:A:713:VAL:O | 1:A:714:GLU:HB2 | 2.18 | 0.43 |
| 1:A:117:LEU:HD11 | 1:A:126:LEU:CD2 | 2.31 | 0.43 |
| 1:A:332:ASP:O | 1:A:333:LEU:HD23 | 2.18 | 0.43 |
| 1:A:62:ILE:CD1 | 1:A:501:LEU:CD1 | 2.95 | 0.43 |
| 1:A:679:VAL:CG1 | 1:A:680:CYS:N | 2.82 | 0.43 |
| 1:A:764:THR:CG2 | 1:A:766:TYR:CZ | 3.01 | 0.43 |
| 1:A:224:SER:HA | 1:A:289:PHE:CD1 | 2.54 | 0.43 |
| 1:A:460:ASP:CG | 1:A:463:LYS:HB3 | 2.39 | 0.43 |
| 1:A:567:ILE:CD1 | 1:A:567:ILE:N | 2.82 | 0.43 |
| 1:A:716:ILE:CD1 | 1:A:763:ASN:HB3 | 2.48 | 0.43 |
| 1:A:119:ILE:HG21 | 1:A:121:TYR:CE1 | 2.54 | 0.42 |
| 1:A:128:ALA:O | 1:A:138:LYS:HG2 | 2.19 | 0.42 |
| 1:A:178:PHE:O | 1:A:178:PHE:HD1 | 2.02 | 0.42 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CD1 | 3.00 | 0.42 |
| 1:A:380:LEU:CB | 1:A:386:LYS:HE3 | 2.43 | 0.42 |
| 1:A:162:VAL:HG12 | 1:A:164:GLU:H | 1.84 | 0.42 |
| 1:A:185:ALA:CB | 1:A:243:TYR:CE2 | 3.02 | 0.42 |
| 1:A:412:LEU:CD1 | 1:A:412:LEU:N | 2.82 | 0.42 |
| 1:A:435:ILE:CD1 | 1:A:486:PHE:HD1 | 2.31 | 0.42 |
| 1:A:589:GLY:C | 1:A:639:LYS:HG2 | 2.39 | 0.42 |
| 1:A:181:LYS:HZ2 | 1:A:216:VAL:HG23 | 1.81 | 0.42 |
| 1:A:501:LEU:CD2 | 1:A:502:THR:N | 2.82 | 0.42 |
| 1:A:333:LEU:HD23 | 1:A:358:ILE:HA | 2.01 | 0.42 |
| 1:A:471:THR:HG21 | 1:A:473:GLN:OE1 | 2.19 | 0.42 |
| 1:A:617:LYS:HG3 | 1:A:618:GLU:N | 2.34 | 0.42 |
| 1:A:133:TYR:CB | 1:A:136:ILE:HG23 | 2.49 | 0.42 |
| 1:A:541:CYS:HB2 | 1:A:544:SER:HB3 | 2.01 | 0.42 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:HD22 | 1.98 | 0.42 |
| 1:A:68:ASN:CB | 1:A:86:GLY:HA3 | 2.50 | 0.42 |
| 1:A:789:ASN:HD22 | 1:A:790:ILE:N | 2.17 | 0.42 |
| 1:A:805:ALA:N | 1:A:806:MET:CE | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:885:GLU:HG3 | 1:A:886:PHE:N | 2.34 | 0.42 |
| 1:A:380:LEU:CB | 1:A:386:LYS:CE | 2.95 | 0.42 |
| 1:A:543:ARG:HB2 | 1:A:549:ARG:NH1 | 2.34 | 0.42 |
| 1:A:563:HIS:HB2 | 1:A:577:VAL:HG13 | 2.01 | 0.42 |
| 1:A:62:ILE:CD1 | 1:A:501:LEU:HD13 | 2.49 | 0.42 |
| 1:A:100:VAL:HG21 | 1:A:158:TYR:OH | 2.19 | 0.42 |
| 1:A:112:ASN:ND2 | 1:A:133:TYR:HE2 | 2.17 | 0.42 |
| 1:A:169:PHE:CD2 | 1:A:170:GLY:N | 2.84 | 0.42 |
| 1:A:728:GLN:HG3 | 1:A:753:ARG:NH2 | 2.34 | 0.42 |
| 1:A:72:LYS:CD | 1:A:80:LEU:CD1 | 2.97 | 0.42 |
| 1:A:889:ILE:HG23 | 1:A:892:HIS:NE2 | 2.33 | 0.42 |
| 1:A:234:THR:CG2 | 1:A:235:VAL:N | 2.82 | 0.42 |
| 1:A:281:ARG:HB3 | 1:A:293:VAL:HG11 | 1.97 | 0.42 |
| 1:A:403:PHE:CE2 | 1:A:405:GLY:HA2 | 2.55 | 0.42 |
| 1:A:470:GLU:HG2 | 1:A:471:THR:N | 2.34 | 0.42 |
| 1:A:926:ALA:HB2 | 1:A:949:TYR:CD1 | 2.55 | 0.42 |
| 1:A:216:VAL:CG1 | 1:A:217:PHE:N | 2.82 | 0.42 |
| 1:A:44:GLY:O | 1:A:47:ALA:HA | 2.20 | 0.42 |
| 1:A:888:ASP:OD1 | 1:A:889:ILE:HG13 | 2.20 | 0.42 |
| 1:A:947:LEU:CD2 | 1:A:947:LEU:N | 2.83 | 0.42 |
| 1:A:67:VAL:CG1 | 1:A:111:ASN:HB3 | 2.50 | 0.42 |
| 1:A:111:ASN:O | 1:A:132:LEU:HD13 | 2.20 | 0.42 |
| 1:A:380:LEU:HD22 | 1:A:412:LEU:HB3 | 2.02 | 0.42 |
| 1:A:387:VAL:CG1 | 1:A:388:LYS:N | 2.82 | 0.42 |
| 1:A:562:VAL:HG22 | 1:A:578:LEU:HD23 | 1.99 | 0.42 |
| 1:A:662:LEU:O | 1:A:666:GLU:HB3 | 2.20 | 0.42 |
| 1:A:711:VAL:HB | 1:A:800:LEU:HD23 | 2.02 | 0.42 |
| 1:A:773:ILE:CD1 | 1:A:773:ILE:N | 2.82 | 0.42 |
| 1:A:845:LEU:HD11 | 1:A:852:SER:OG | 2.20 | 0.42 |
| 1:A:321:LEU:HD23 | 1:A:333:LEU:CD1 | 2.50 | 0.41 |
| 1:A:528:TRP:CZ2 | 1:A:533:ASN:OD1 | 2.73 | 0.41 |
| 1:A:623:ILE:HD12 | 1:A:624:THR:HA | 2.01 | 0.41 |
| 1:A:563:HIS:CB | 1:A:577:VAL:CG1 | 2.95 | 0.41 |
| 1:A:597:LEU:CD2 | 1:A:597:LEU:N | 2.83 | 0.41 |
| 1:A:630:HIS:CD2 | 1:A:632:VAL:CG2 | 3.00 | 0.41 |
| 1:A:665:VAL:HG11 | 1:A:697:PRO:CD | 2.48 | 0.41 |
| 1:A:225:MET:HE1 | 1:A:227:LYS:CG | 2.46 | 0.41 |
| 1:A:256:LEU:HD12 | 1:A:297:ILE:HD11 | 2.02 | 0.41 |
| 1:A:333:LEU:HD23 | 1:A:358:ILE:HG13 | 2.00 | 0.41 |
| 1:A:44:GLY:CA | 1:A:50:PHE:HE2 | 2.23 | 0.41 |
| 1:A:555:LYS:CG | 1:A:556:GLN:N | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:920:ALA:C | 1:A:922:PRO:HD2 | 2.41 | 0.41 |
| 1:A:137:CYS:SG | 1:A:159:LEU:CD1 | 3.09 | 0.41 |
| 1:A:605:ILE:O | 1:A:608:GLN:HG2 | 2.19 | 0.41 |
| 1:A:696:LEU:N | 1:A:696:LEU:CD1 | 2.83 | 0.41 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:C | 2.40 | 0.41 |
| 1:A:435:ILE:CD1 | 1:A:436:ALA:N | 2.81 | 0.41 |
| 1:A:494:TYR:CB | 1:A:501:LEU:HD21 | 2.30 | 0.41 |
| 1:A:658:HIS:ND1 | 1:A:663:SER:HB3 | 2.36 | 0.41 |
| 1:A:783:VAL:CG1 | 1:A:784:TRP:N | 2.83 | 0.41 |
| 1:A:817:ASP:OD1 | 1:A:820:PHE:CD2 | 2.73 | 0.41 |
| 1:A:847:LEU:HD12 | 1:A:852:SER:HB2 | 2.00 | 0.41 |
| 1:A:904:VAL:CG1 | 1:A:905:ASP:N | 2.82 | 0.41 |
| 1:A:131:SER:O | 1:A:133:TYR:CD2 | 2.74 | 0.41 |
| 1:A:177:ASN:O | 1:A:178:PHE:CG | 2.73 | 0.41 |
| 1:A:226:ILE:HD11 | 1:A:385:LEU:HD23 | 2.03 | 0.41 |
| 1:A:259:GLN:HA | 1:A:260:PRO:HD3 | 1.82 | 0.41 |
| 1:A:370:LEU:CD2 | 1:A:374:TYR:CE1 | 3.03 | 0.41 |
| 1:A:551:ALA:HB1 | 1:A:556:GLN:HB2 | 2.03 | 0.41 |
| 1:A:560:LEU:CG | 1:A:648:THR:CG2 | 2.98 | 0.41 |
| 1:A:282:LEU:HD23 | 1:A:292:TYR:HA | 2.03 | 0.41 |
| 1:A:435:ILE:HD12 | 1:A:486:PHE:CE1 | 2.56 | 0.41 |
| 1:A:843:ARG:CZ | 1:A:843:ARG:CB | 2.99 | 0.41 |
| 1:A:188:VAL:O | 1:A:188:VAL:HG22 | 2.21 | 0.41 |
| 1:A:403:PHE:HE1 | 1:A:406:LEU:HD23 | 1.75 | 0.41 |
| 1:A:39:PHE:CZ | 1:A:473:GLN:HG3 | 2.53 | 0.41 |
| 1:A:492:GLN:HB3 | 1:A:503:ARG:HG3 | 2.02 | 0.41 |
| 1:A:884:LEU:HA | 1:A:884:LEU:HD23 | 1.75 | 0.41 |
| 1:A:225:MET:CE | 1:A:227:LYS:CG | 2.94 | 0.41 |
| 1:A:62:ILE:CD1 | 1:A:64:LEU:HD21 | 2.46 | 0.41 |
| 1:A:862:ILE:HG21 | 1:A:877:ILE:HG12 | 2.03 | 0.41 |
| 1:A:111:ASN:O | 1:A:132:LEU:HD22 | 2.21 | 0.41 |
| 1:A:159:LEU:HG | 1:A:201:ARG:NH1 | 2.36 | 0.41 |
| 1:A:236:ILE:CG2 | 1:A:239:PHE:HB2 | 2.51 | 0.41 |
| 1:A:307:ARG:HA | 1:A:307:ARG:HD3 | 1.88 | 0.41 |
| 1:A:631:VAL:HG13 | 1:A:631:VAL:O | 2.19 | 0.41 |
| 1:A:72:LYS:CE | 1:A:80:LEU:CD1 | 2.95 | 0.41 |
| 1:A:833:LEU:CB | 1:A:836:HIS:HD2 | 2.22 | 0.41 |
| 1:A:188:VAL:CG2 | 1:A:191:LYS:HB2 | 2.51 | 0.41 |
| 1:A:566:ASN:CA | 1:A:651:VAL:CG2 | 2.95 | 0.41 |
| 1:A:703:LEU:HD13 | 1:A:723:ALA:CB | 2.47 | 0.41 |
| 1:A:803:CYS:SG | 1:A:832:THR:HA | 2.61 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:943:ARG:CZ | 1:A:943:ARG:HB2 | 2.51 | 0.41 |
| 1:A:188:VAL:HG13 | 1:A:189:ASP:N | 2.36 | 0.40 |
| 1:A:280:VAL:CG1 | 1:A:281:ARG:N | 2.83 | 0.40 |
| 1:A:419:ARG:HH11 | 1:A:419:ARG:HD3 | 1.72 | 0.40 |
| 1:A:681:THR:OG1 | 1:A:686:THR:HG21 | 2.21 | 0.40 |
| 1:A:867:GLY:HA2 | 1:A:868:PRO:HD3 | 1.91 | 0.40 |
| 1:A:889:ILE:HD12 | 1:A:907:TYR:CE1 | 2.56 | 0.40 |
| 1:A:137:CYS:O | 1:A:150:GLU:HG3 | 2.20 | 0.40 |
| 1:A:689:PHE:HD1 | 1:A:691:GLU:HG2 | 1.80 | 0.40 |
| 1:A:897:GLY:H | 1:A:924:GLN:HE22 | 1.69 | 0.40 |
| 1:A:105:GLU:CB | 1:A:106:PRO:HD2 | 2.42 | 0.40 |
| 1:A:219:ASP:HB3 | 1:A:222:VAL:H | 1.86 | 0.40 |
| 1:A:327:VAL:CG1 | 1:A:358:ILE:CD1 | 2.94 | 0.40 |
| 1:A:667:SER:HB3 | 1:A:668:PRO:CD | 2.51 | 0.40 |
| 1:A:778:VAL:HG12 | 1:A:779:GLU:O | 2.20 | 0.40 |
| 1:A:901:SER:HA | 1:A:902:PRO:HD2 | 1.89 | 0.40 |
| 1:A:252:PHE:HE1 | 1:A:283:CYS:SG | 2.44 | 0.40 |
| 1:A:349:LEU:N | 1:A:349:LEU:CD2 | 2.84 | 0.40 |
| 1:A:469:TYR:CZ | 1:A:470:GLU:O | 2.74 | 0.40 |
| 1:A:492:GLN:CG | 1:A:503:ARG:HD2 | 2.51 | 0.40 |
| 1:A:287:THR:CG2 | 1:A:288:ALA:N | 2.85 | 0.40 |
| 1:A:460:ASP:HB2 | 1:A:465:ASN:N | 2.37 | 0.40 |

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:234:THR:CA | 1:A:234:THR:CA[5_455] | 0.86 | 1.34 |
| 1:A:233:PHE:O | 1:A:234:THR:OG1[5_455] | 0.87 | 1.33 |
| 1:A:146:PHE:CE1 | 1:A:730:GLN:OE1[4_555] | 1.03 | 1.17 |
| 1:A:146:PHE:CE1 | 1:A:730:GLN:CD[4_555] | 1.26 | 0.94 |
| 1:A:146:PHE:CD1 | 1:A:730:GLN:OE1[4_555] | 1.26 | 0.94 |
| 1:A:155:LYS:NZ | 1:A:221:PHE:N[5_455] | 1.34 | 0.86 |
| 1:A:234:THR:O | 1:A:234:THR:O[5_455] | 1.40 | 0.80 |
| 1:A:233:PHE:O | 1:A:234:THR:CB[5_455] | 1.48 | 0.72 |
| 1:A:175:TYR:CE1 | 1:A:842:SER:CB[8_454] | 1.57 | 0.63 |
| 1:A:83:HIS:CE1 | 1:A:731:SER:OG[4_555] | 1.57 | 0.63 |
| 1:A:233:PHE:C | 1:A:234:THR:CB[5_455] | 1.63 | 0.57 |
| 1:A:208:GLU:OE2 | 1:A:728:GLN:NE2[4_555] | 1.77 | 0.43 |
| 1:A:234:THR:N | 1:A:234:THR:CB[5_455] | 1.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:233:PHE:C | 1:A:234:THR:OG1[5_455] | 1.80 | 0.40 |
| 1:A:234:THR:CA | 1:A:234:THR:CB[5_455] | 1.82 | 0.38 |
| 1:A:146:PHE:CZ | 1:A:730:GLN:NE2[4_555] | 1.84 | 0.36 |
| 1:A:155:LYS:NZ | 1:A:221:PHE:CA[5_455] | 1.84 | 0.36 |
| 1:A:234:THR:N | 1:A:234:THR:CA[5_455] | 1.89 | 0.31 |
| 1:A:155:LYS:NZ | 1:A:221:PHE:CG[5_455] | 1.99 | 0.21 |
| 1:A:230:SER:CA | 1:A:230:SER:OG[5_455] | 2.01 | 0.19 |
| 1:A:175:TYR:CD1 | 1:A:842:SER:CB[8_454] | 2.01 | 0.19 |
| 1:A:146:PHE:CZ | 1:A:730:GLN:CD[4_555] | 2.04 | 0.16 |
| 1:A:155:LYS:NZ | 1:A:221:PHE:CD2[5_455] | 2.04 | 0.16 |
| 1:A:146:PHE:CE1 | 1:A:730:GLN:NE2[4_555] | 2.04 | 0.16 |
| 1:A:156:GLU:OE1 | 1:A:220:GLU:OE2[5_455] | 2.05 | 0.15 |
| 1:A:234:THR:CA | 1:A:234:THR:C[5_455] | 2.07 | 0.13 |
| 1:A:175:TYR:OH | 1:A:843:ARG:CG[8_454] | 2.10 | 0.10 |
| 1:A:175:TYR:CD1 | 1:A:842:SER:OG[8_454] | 2.12 | 0.08 |
| 1:A:148:LEU:O | 1:A:728:GLN:NE2[4_555] | 2.16 | 0.04 |
| 1:A:155:LYS:NZ | 1:A:220:GLU:C[5_455] | 2.19 | 0.01 |
| 1:A:234:THR:C | 1:A:234:THR:O[5_455] | 2.19 | 0.01 |
| 1:A:148:LEU:O | 1:A:728:GLN:OE1[4_555] | 2.19 | 0.01 |

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 | 905/1207 (75%) | 842 (93%) | 44 (5%) | 19 (2%) | 7 36 |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 96 | PRO |
| 1 | A | 181 | LYS |
| 1 | A | 191 | LYS |
| 1 | A | 410 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 465 | ASN |
| 1 | A | 654 | ASN |
| 1 | A | 700 | CYS |
| 1 | A | 701 | PRO |
| 1 | A | 804 | GLY |
| 1 | A | 864 | PRO |
| 1 | A | 87 | PRO |
| 1 | A | 271 | LYS |
| 1 | A | 474 | VAL |
| 1 | A | 849 | GLY |
| 1 | A | 263 | VAL |
| 1 | A | 344 | ARG |
| 1 | A | 933 | VAL |
| 1 | A | 44 | GLY |
| 1 | A | 921 | LYS |

5.3.2 Protein sidechains [\(i\)](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| 1 | A | 812/1067 (76%) | 789 (97%) | 23 (3%) | 43 65 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 69 | ARG |
| 1 | A | 72 | LYS |
| 1 | A | 271 | LYS |
| 1 | A | 386 | LYS |
| 1 | A | 412 | LEU |
| 1 | A | 435 | ILE |
| 1 | A | 468 | GLN |
| 1 | A | 473 | GLN |
| 1 | A | 523 | ASP |
| 1 | A | 529 | CYS |
| 1 | A | 548 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 567 | ILE |
| 1 | A | 575 | LEU |
| 1 | A | 597 | LEU |
| 1 | A | 621 | ARG |
| 1 | A | 670 | ARG |
| 1 | A | 743 | GLN |
| 1 | A | 773 | ILE |
| 1 | A | 797 | LYS |
| 1 | A | 806 | MET |
| 1 | A | 853 | LYS |
| 1 | A | 854 | CYS |
| 1 | A | 892 | HIS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 51 | ASN |
| 1 | A | 52 | HIS |
| 1 | A | 101 | GLN |
| 1 | A | 157 | HIS |
| 1 | A | 163 | ASN |
| 1 | A | 273 | GLN |
| 1 | A | 361 | GLN |
| 1 | A | 441 | ASN |
| 1 | A | 442 | HIS |
| 1 | A | 473 | GLN |
| 1 | A | 500 | GLN |
| 1 | A | 582 | ASN |
| 1 | A | 626 | ASN |
| 1 | A | 629 | HIS |
| 1 | A | 630 | HIS |
| 1 | A | 672 | HIS |
| 1 | A | 685 | ASN |
| 1 | A | 690 | GLN |
| 1 | A | 702 | GLN |
| 1 | A | 728 | GLN |
| 1 | A | 747 | GLN |
| 1 | A | 789 | ASN |
| 1 | A | 792 | ASN |
| 1 | A | 826 | GLN |
| 1 | A | 836 | HIS |
| 1 | A | 856 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 892 | HIS |

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 6 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 802:LYS | C | 803:CYS | N | 4.06 |
| 1 | A | 854:CYS | C | 855:THR | N | 3.30 |
| 1 | A | 557:CYS | C | 558:VAL | N | 2.81 |
| 1 | A | 506:VAL | C | 507:GLU | N | 2.58 |
| 1 | A | 700:CYS | C | 701:PRO | N | 0.70 |
| 1 | A | 653:TYR | C | 654:ASN | N | 0.50 |

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---|-----------------------|-------|
| 1 | A | 915/1207 (75%) | 1.97 | 346 (37%) 0 1 | 100, 150, 216, 216 | 0 |

All (346) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 584 | PRO | 11.0 |
| 1 | A | 859 | ILE | 9.9 |
| 1 | A | 585 | GLU | 9.7 |
| 1 | A | 902 | PRO | 9.5 |
| 1 | A | 860 | THR | 9.3 |
| 1 | A | 945 | SER | 8.4 |
| 1 | A | 586 | LEU | 8.4 |
| 1 | A | 587 | SER | 8.3 |
| 1 | A | 924 | GLN | 8.1 |
| 1 | A | 854 | CYS | 8.0 |
| 1 | A | 628 | ASP | 7.9 |
| 1 | A | 946 | GLN | 7.5 |
| 1 | A | 922 | PRO | 7.3 |
| 1 | A | 549 | ARG | 7.3 |
| 1 | A | 640 | GLU | 7.2 |
| 1 | A | 646 | ALA | 7.2 |
| 1 | A | 890 | ALA | 7.2 |
| 1 | A | 531 | LEU | 7.1 |
| 1 | A | 473 | GLN | 7.1 |
| 1 | A | 857 | PRO | 6.9 |
| 1 | A | 530 | VAL | 6.9 |
| 1 | A | 670 | ARG | 6.8 |
| 1 | A | 931 | ILE | 6.5 |
| 1 | A | 893 | VAL | 6.4 |
| 1 | A | 858 | ARG | 6.4 |
| 1 | A | 925 | HIS | 6.3 |
| 1 | A | 569 | VAL | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 636 | LEU | 6.2 |
| 1 | A | 568 | SER | 6.2 |
| 1 | A | 892 | HIS | 6.1 |
| 1 | A | 669 | TYR | 6.1 |
| 1 | A | 622 | ILE | 6.0 |
| 1 | A | 901 | SER | 6.0 |
| 1 | A | 891 | SER | 6.0 |
| 1 | A | 623 | ILE | 5.9 |
| 1 | A | 269 | THR | 5.9 |
| 1 | A | 877 | ILE | 5.8 |
| 1 | A | 495 | ILE | 5.8 |
| 1 | A | 547 | PRO | 5.8 |
| 1 | A | 645 | PHE | 5.8 |
| 1 | A | 882 | LEU | 5.7 |
| 1 | A | 944 | SER | 5.7 |
| 1 | A | 899 | GLU | 5.7 |
| 1 | A | 900 | CYS | 5.6 |
| 1 | A | 548 | ARG | 5.6 |
| 1 | A | 862 | ILE | 5.6 |
| 1 | A | 621 | ARG | 5.5 |
| 1 | A | 654 | ASN | 5.5 |
| 1 | A | 879 | GLY | 5.5 |
| 1 | A | 629 | HIS | 5.4 |
| 1 | A | 641 | THR | 5.4 |
| 1 | A | 915 | CYS | 5.4 |
| 1 | A | 423 | VAL | 5.4 |
| 1 | A | 926 | ALA | 5.4 |
| 1 | A | 529 | CYS | 5.3 |
| 1 | A | 853 | LYS | 5.3 |
| 1 | A | 571 | GLN | 5.2 |
| 1 | A | 588 | ALA | 5.2 |
| 1 | A | 570 | SER | 5.1 |
| 1 | A | 546 | GLU | 5.1 |
| 1 | A | 532 | HIS | 5.1 |
| 1 | A | 635 | GLN | 5.1 |
| 1 | A | 883 | GLY | 5.0 |
| 1 | A | 811 | GLY | 5.0 |
| 1 | A | 644 | THR | 5.0 |
| 1 | A | 880 | GLU | 5.0 |
| 1 | A | 894 | LYS | 5.0 |
| 1 | A | 593 | THR | 5.0 |
| 1 | A | 485 | ALA | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 619 | VAL | 4.9 |
| 1 | A | 942 | ALA | 4.9 |
| 1 | A | 620 | PRO | 4.9 |
| 1 | A | 861 | GLU | 4.8 |
| 1 | A | 551 | ALA | 4.8 |
| 1 | A | 923 | SER | 4.8 |
| 1 | A | 913 | ILE | 4.8 |
| 1 | A | 592 | CYS | 4.8 |
| 1 | A | 270 | THR | 4.7 |
| 1 | A | 589 | GLY | 4.7 |
| 1 | A | 594 | PHE | 4.7 |
| 1 | A | 647 | SER | 4.7 |
| 1 | A | 634 | LEU | 4.7 |
| 1 | A | 624 | THR | 4.6 |
| 1 | A | 424 | PHE | 4.6 |
| 1 | A | 533 | ASN | 4.6 |
| 1 | A | 888 | ASP | 4.6 |
| 1 | A | 637 | LYS | 4.6 |
| 1 | A | 583 | VAL | 4.6 |
| 1 | A | 560 | LEU | 4.6 |
| 1 | A | 552 | SER | 4.6 |
| 1 | A | 929 | VAL | 4.6 |
| 1 | A | 502 | THR | 4.6 |
| 1 | A | 446 | PHE | 4.5 |
| 1 | A | 920 | ALA | 4.5 |
| 1 | A | 652 | PHE | 4.4 |
| 1 | A | 638 | SER | 4.4 |
| 1 | A | 767 | SER | 4.4 |
| 1 | A | 869 | ARG | 4.4 |
| 1 | A | 486 | PHE | 4.3 |
| 1 | A | 930 | GLU | 4.3 |
| 1 | A | 578 | LEU | 4.3 |
| 1 | A | 591 | ASN | 4.3 |
| 1 | A | 653 | TYR | 4.3 |
| 1 | A | 613 | SER | 4.2 |
| 1 | A | 271 | LYS | 4.2 |
| 1 | A | 919 | GLU | 4.2 |
| 1 | A | 474 | VAL | 4.2 |
| 1 | A | 933 | VAL | 4.2 |
| 1 | A | 353 | ALA | 4.2 |
| 1 | A | 543 | ARG | 4.2 |
| 1 | A | 672 | HIS | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 682 | HIS | 4.1 |
| 1 | A | 816 | ALA | 4.1 |
| 1 | A | 875 | VAL | 4.1 |
| 1 | A | 947 | LEU | 4.1 |
| 1 | A | 447 | VAL | 4.1 |
| 1 | A | 775 | ASN | 4.1 |
| 1 | A | 513 | ARG | 4.1 |
| 1 | A | 810 | CYS | 4.1 |
| 1 | A | 493 | LEU | 4.1 |
| 1 | A | 494 | TYR | 4.1 |
| 1 | A | 431 | MET | 4.1 |
| 1 | A | 948 | TYR | 4.0 |
| 1 | A | 815 | LYS | 4.0 |
| 1 | A | 814 | LEU | 4.0 |
| 1 | A | 550 | PHE | 4.0 |
| 1 | A | 544 | SER | 4.0 |
| 1 | A | 504 | VAL | 3.9 |
| 1 | A | 865 | VAL | 3.9 |
| 1 | A | 671 | CYS | 3.9 |
| 1 | A | 889 | ILE | 3.9 |
| 1 | A | 934 | ALA | 3.9 |
| 1 | A | 843 | ARG | 3.8 |
| 1 | A | 881 | ASN | 3.8 |
| 1 | A | 538 | LYS | 3.8 |
| 1 | A | 558 | VAL | 3.8 |
| 1 | A | 895 | VAL | 3.8 |
| 1 | A | 580 | THR | 3.8 |
| 1 | A | 943 | ARG | 3.8 |
| 1 | A | 528 | TRP | 3.8 |
| 1 | A | 721 | LEU | 3.8 |
| 1 | A | 927 | GLY | 3.7 |
| 1 | A | 542 | GLU | 3.7 |
| 1 | A | 422 | PRO | 3.7 |
| 1 | A | 917 | MET | 3.7 |
| 1 | A | 898 | VAL | 3.7 |
| 1 | A | 354 | LEU | 3.7 |
| 1 | A | 886 | PHE | 3.7 |
| 1 | A | 648 | THR | 3.7 |
| 1 | A | 921 | LYS | 3.7 |
| 1 | A | 611 | CYS | 3.6 |
| 1 | A | 695 | LYS | 3.6 |
| 1 | A | 727 | PRO | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 950 | PHE | 3.6 |
| 1 | A | 596 | ASP | 3.6 |
| 1 | A | 639 | LYS | 3.5 |
| 1 | A | 897 | GLY | 3.5 |
| 1 | A | 501 | LEU | 3.5 |
| 1 | A | 299 | CYS | 3.5 |
| 1 | A | 918 | GLY | 3.5 |
| 1 | A | 855 | THR | 3.5 |
| 1 | A | 267 | GLY | 3.5 |
| 1 | A | 614 | PRO | 3.5 |
| 1 | A | 668 | PRO | 3.4 |
| 1 | A | 683 | ASP | 3.4 |
| 1 | A | 64 | LEU | 3.4 |
| 1 | A | 574 | VAL | 3.4 |
| 1 | A | 527 | GLY | 3.4 |
| 1 | A | 590 | VAL | 3.3 |
| 1 | A | 448 | GLY | 3.3 |
| 1 | A | 310 | GLN | 3.3 |
| 1 | A | 505 | PRO | 3.3 |
| 1 | A | 887 | ARG | 3.3 |
| 1 | A | 612 | TYR | 3.3 |
| 1 | A | 630 | HIS | 3.3 |
| 1 | A | 595 | GLU | 3.3 |
| 1 | A | 878 | ARG | 3.2 |
| 1 | A | 435 | ILE | 3.2 |
| 1 | A | 355 | CYS | 3.2 |
| 1 | A | 916 | GLU | 3.2 |
| 1 | A | 744 | GLY | 3.2 |
| 1 | A | 949 | TYR | 3.2 |
| 1 | A | 618 | GLU | 3.2 |
| 1 | A | 884 | LEU | 3.2 |
| 1 | A | 576 | LEU | 3.2 |
| 1 | A | 76 | ASP | 3.2 |
| 1 | A | 847 | LEU | 3.2 |
| 1 | A | 433 | SER | 3.2 |
| 1 | A | 506 | VAL | 3.2 |
| 1 | A | 343 | LYS | 3.1 |
| 1 | A | 633 | GLN | 3.1 |
| 1 | A | 454 | LEU | 3.1 |
| 1 | A | 604 | VAL | 3.1 |
| 1 | A | 514 | SER | 3.1 |
| 1 | A | 642 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 868 | PRO | 3.1 |
| 1 | A | 609 | ILE | 3.1 |
| 1 | A | 432 | THR | 3.1 |
| 1 | A | 867 | GLY | 3.1 |
| 1 | A | 940 | PHE | 3.1 |
| 1 | A | 626 | ASN | 3.1 |
| 1 | A | 610 | GLN | 3.0 |
| 1 | A | 545 | ARG | 3.0 |
| 1 | A | 625 | GLU | 3.0 |
| 1 | A | 541 | CYS | 3.0 |
| 1 | A | 567 | ILE | 3.0 |
| 1 | A | 650 | PHE | 3.0 |
| 1 | A | 904 | VAL | 3.0 |
| 1 | A | 722 | LYS | 3.0 |
| 1 | A | 525 | HIS | 2.9 |
| 1 | A | 914 | VAL | 2.9 |
| 1 | A | 307 | ARG | 2.9 |
| 1 | A | 864 | PRO | 2.9 |
| 1 | A | 598 | SER | 2.9 |
| 1 | A | 842 | SER | 2.9 |
| 1 | A | 852 | SER | 2.9 |
| 1 | A | 643 | MET | 2.9 |
| 1 | A | 932 | CYS | 2.9 |
| 1 | A | 309 | LEU | 2.9 |
| 1 | A | 476 | ASP | 2.9 |
| 1 | A | 896 | ALA | 2.9 |
| 1 | A | 471 | THR | 2.9 |
| 1 | A | 866 | THR | 2.9 |
| 1 | A | 709 | ILE | 2.8 |
| 1 | A | 562 | VAL | 2.8 |
| 1 | A | 484 | MET | 2.8 |
| 1 | A | 561 | THR | 2.8 |
| 1 | A | 627 | GLY | 2.8 |
| 1 | A | 597 | LEU | 2.8 |
| 1 | A | 903 | LEU | 2.8 |
| 1 | A | 137 | CYS | 2.8 |
| 1 | A | 539 | GLU | 2.8 |
| 1 | A | 577 | VAL | 2.8 |
| 1 | A | 425 | THR | 2.8 |
| 1 | A | 540 | ARG | 2.7 |
| 1 | A | 910 | ALA | 2.7 |
| 1 | A | 328 | ARG | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 496 | MET | 2.7 |
| 1 | A | 301 | ARG | 2.7 |
| 1 | A | 475 | VAL | 2.7 |
| 1 | A | 817 | ASP | 2.7 |
| 1 | A | 149 | GLY | 2.7 |
| 1 | A | 575 | LEU | 2.7 |
| 1 | A | 272 | GLU | 2.7 |
| 1 | A | 684 | PRO | 2.7 |
| 1 | A | 599 | GLU | 2.7 |
| 1 | A | 681 | THR | 2.7 |
| 1 | A | 774 | ASN | 2.7 |
| 1 | A | 42 | PHE | 2.7 |
| 1 | A | 515 | CYS | 2.7 |
| 1 | A | 77 | LEU | 2.6 |
| 1 | A | 768 | TYR | 2.6 |
| 1 | A | 573 | ASN | 2.6 |
| 1 | A | 41 | THR | 2.6 |
| 1 | A | 400 | ASP | 2.6 |
| 1 | A | 341 | GLY | 2.6 |
| 1 | A | 150 | GLU | 2.6 |
| 1 | A | 870 | GLU | 2.6 |
| 1 | A | 305 | GLU | 2.6 |
| 1 | A | 678 | HIS | 2.6 |
| 1 | A | 769 | GLU | 2.6 |
| 1 | A | 928 | PHE | 2.6 |
| 1 | A | 300 | GLU | 2.6 |
| 1 | A | 53 | LEU | 2.6 |
| 1 | A | 75 | SER | 2.6 |
| 1 | A | 90 | ASP | 2.5 |
| 1 | A | 759 | VAL | 2.5 |
| 1 | A | 776 | LEU | 2.5 |
| 1 | A | 311 | ALA | 2.5 |
| 1 | A | 819 | ASP | 2.5 |
| 1 | A | 723 | ALA | 2.5 |
| 1 | A | 97 | PRO | 2.5 |
| 1 | A | 526 | CYS | 2.5 |
| 1 | A | 616 | ALA | 2.5 |
| 1 | A | 477 | SER | 2.4 |
| 1 | A | 632 | VAL | 2.4 |
| 1 | A | 337 | VAL | 2.4 |
| 1 | A | 268 | SER | 2.4 |
| 1 | A | 107 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 480 | VAL | 2.4 |
| 1 | A | 511 | GLN | 2.4 |
| 1 | A | 138 | LYS | 2.4 |
| 1 | A | 745 | ILE | 2.4 |
| 1 | A | 600 | MET | 2.4 |
| 1 | A | 336 | THR | 2.4 |
| 1 | A | 876 | THR | 2.4 |
| 1 | A | 657 | VAL | 2.3 |
| 1 | A | 534 | THR | 2.3 |
| 1 | A | 579 | GLU | 2.3 |
| 1 | A | 631 | VAL | 2.3 |
| 1 | A | 440 | LYS | 2.3 |
| 1 | A | 800 | LEU | 2.3 |
| 1 | A | 537 | ARG | 2.3 |
| 1 | A | 655 | CYS | 2.3 |
| 1 | A | 841 | GLU | 2.3 |
| 1 | A | 856 | ASN | 2.3 |
| 1 | A | 96 | PRO | 2.3 |
| 1 | A | 871 | GLY | 2.3 |
| 1 | A | 885 | GLU | 2.3 |
| 1 | A | 850 | ALA | 2.3 |
| 1 | A | 308 | LEU | 2.3 |
| 1 | A | 342 | GLN | 2.3 |
| 1 | A | 507 | GLU | 2.2 |
| 1 | A | 455 | LYS | 2.2 |
| 1 | A | 572 | TYR | 2.2 |
| 1 | A | 409 | ASN | 2.2 |
| 1 | A | 603 | LEU | 2.2 |
| 1 | A | 277 | SER | 2.2 |
| 1 | A | 456 | LYS | 2.2 |
| 1 | A | 719 | ILE | 2.2 |
| 1 | A | 219 | ASP | 2.2 |
| 1 | A | 266 | PRO | 2.2 |
| 1 | A | 327 | VAL | 2.2 |
| 1 | A | 605 | ILE | 2.2 |
| 1 | A | 720 | THR | 2.2 |
| 1 | A | 445 | ALA | 2.2 |
| 1 | A | 346 | MET | 2.2 |
| 1 | A | 536 | THR | 2.2 |
| 1 | A | 405 | GLY | 2.2 |
| 1 | A | 331 | ASP | 2.2 |
| 1 | A | 873 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 694 | VAL | 2.2 |
| 1 | A | 863 | ILE | 2.2 |
| 1 | A | 439 | TYR | 2.2 |
| 1 | A | 812 | LEU | 2.2 |
| 1 | A | 304 | VAL | 2.2 |
| 1 | A | 412 | LEU | 2.2 |
| 1 | A | 935 | VAL | 2.1 |
| 1 | A | 348 | SER | 2.1 |
| 1 | A | 91 | ASN | 2.1 |
| 1 | A | 911 | GLU | 2.1 |
| 1 | A | 128 | ALA | 2.1 |
| 1 | A | 566 | ASN | 2.1 |
| 1 | A | 773 | ILE | 2.1 |
| 1 | A | 338 | PHE | 2.1 |
| 1 | A | 503 | ARG | 2.1 |
| 1 | A | 153 | HIS | 2.1 |
| 1 | A | 912 | GLN | 2.1 |
| 1 | A | 345 | LYS | 2.1 |
| 1 | A | 524 | PRO | 2.1 |
| 1 | A | 298 | GLY | 2.0 |
| 1 | A | 818 | PRO | 2.0 |
| 1 | A | 846 | GLU | 2.0 |
| 1 | A | 388 | LYS | 2.0 |
| 1 | A | 608 | GLN | 2.0 |
| 1 | A | 951 | MET | 2.0 |

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

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

6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.