



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B5L
Title : Crystal Structure of DDB1 In Complex with Simian Virus 5 V Protein
Authors : Li, T.; Chen, X.; Garbutt, K.C.; Zhou, P.; Zheng, N.
Deposited on : 2005-09-28
Resolution : 2.85 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

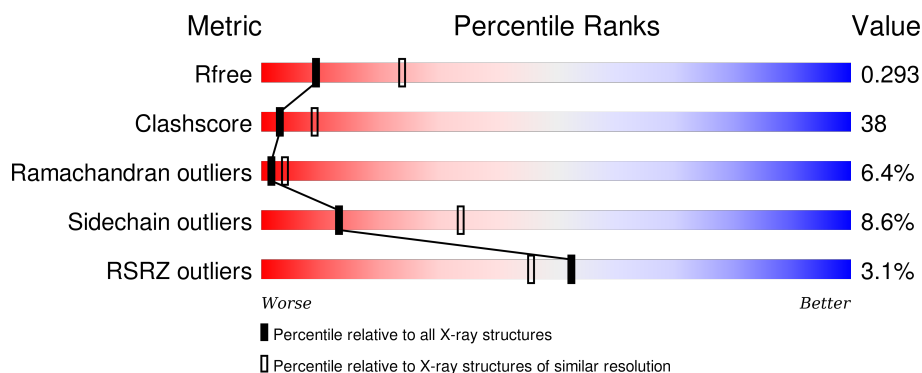
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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} | 91344 | 2228 (2.90-2.82) |
| Clashscore | 102246 | 2499 (2.90-2.82) |
| Ramachandran outliers | 100387 | 2439 (2.90-2.82) |
| Sidechain outliers | 100360 | 2442 (2.90-2.82) |
| RSRZ outliers | 91569 | 2236 (2.90-2.82) |

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. 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 | 1140 | <div> <div>54%</div> <div>37%</div> <div>7%</div> <div>..</div> </div> |
| 1 | B | 1140 | <div> <div>3%</div> <div>41%</div> <div>48%</div> <div>10%</div> <div>..</div> </div> |
| 2 | C | 222 | <div> <div>6%</div> <div>30%</div> <div>37%</div> <div>9%</div> <div>22%</div> </div> |
| 2 | D | 222 | <div> <div>9%</div> <div>25%</div> <div>37%</div> <div>13%</div> <div>21%</div> </div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20399 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 damage-specific DNA binding protein 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8860 | 5610 | 1493 | 1708 | 49 | | | |
| 1 | B | 1134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8876 | 5619 | 1495 | 1713 | 49 | | | |

- Molecule 2 is a protein called Nonstructural protein V.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | C | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1324 | 826 | 229 | 261 | 8 | | | |
| 2 | D | 175 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1335 | 834 | 233 | 260 | 8 | | | |

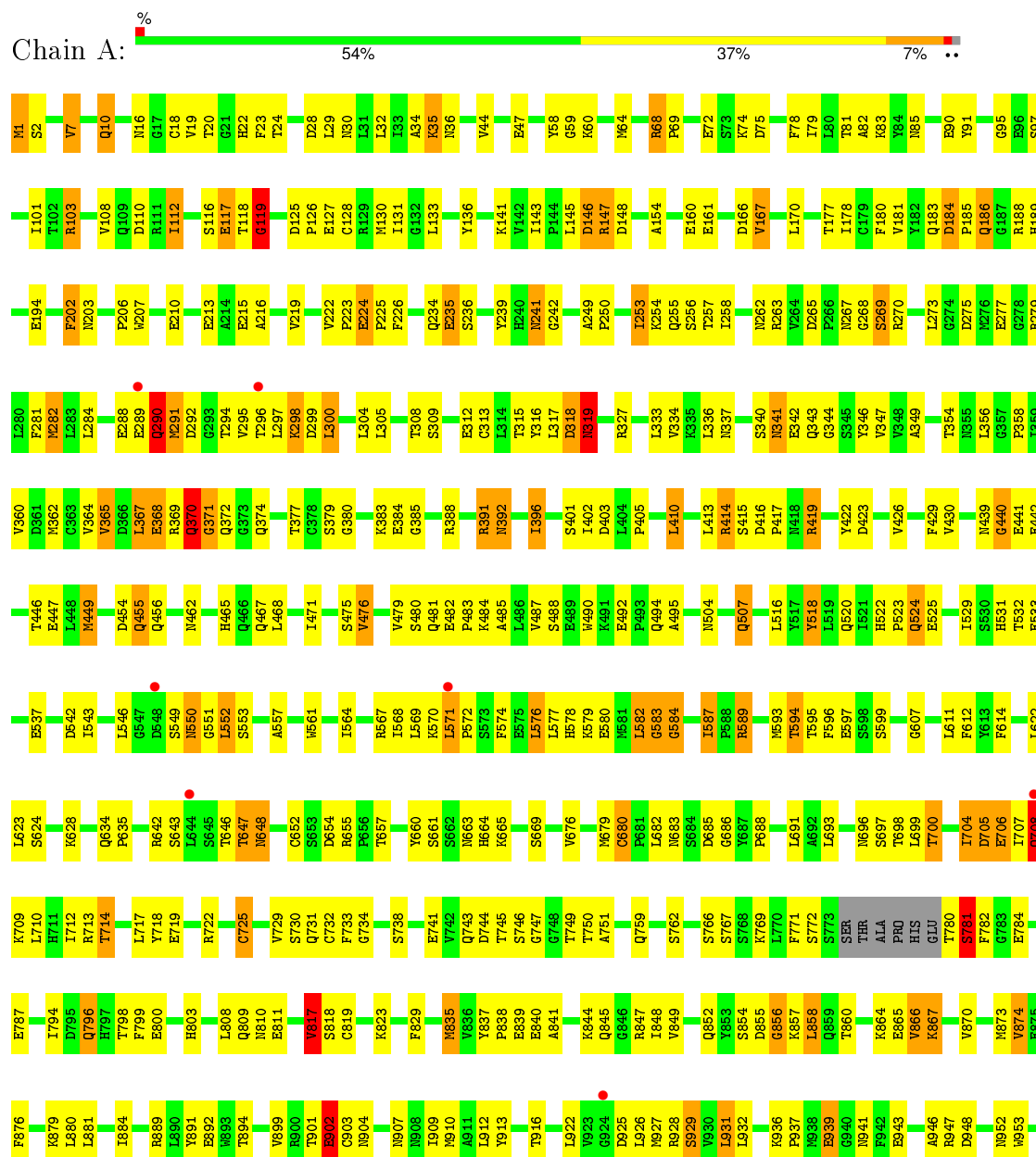
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

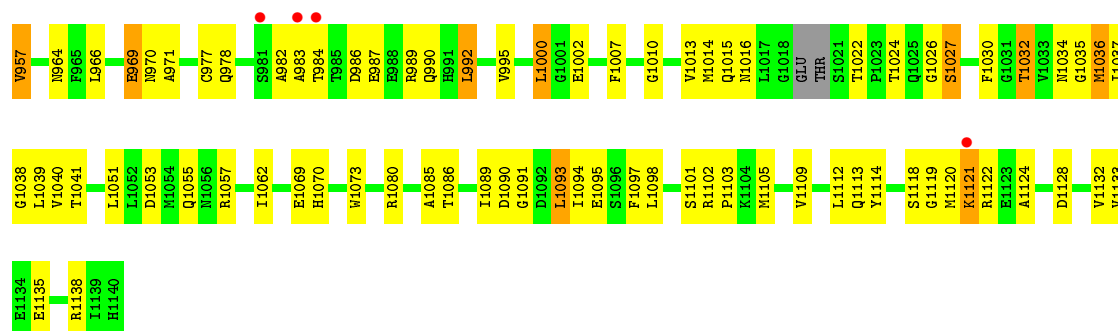
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | D | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | C | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |

3 Residue-property plots

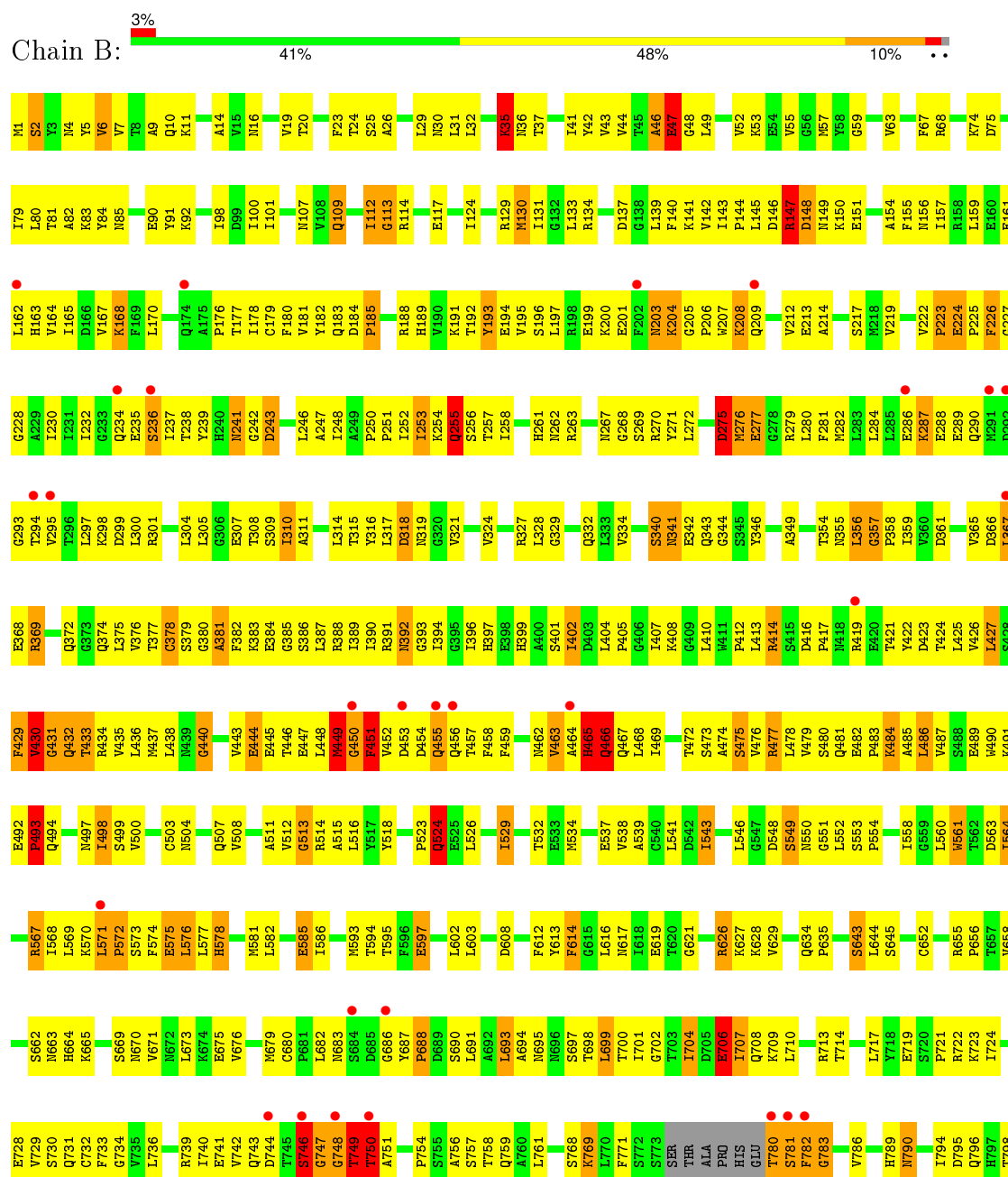
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

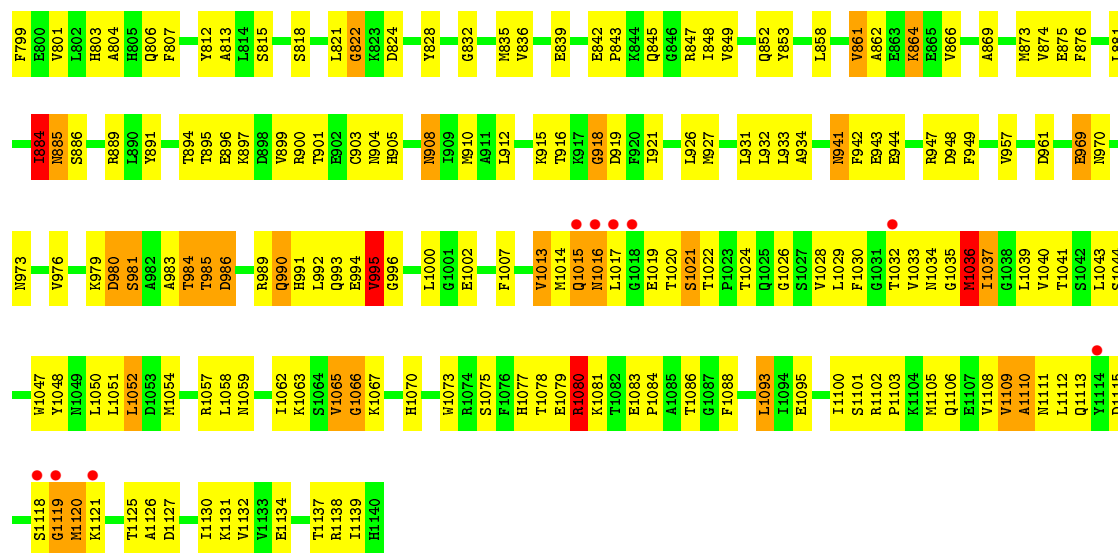
- Molecule 1: damage-specific DNA binding protein 1



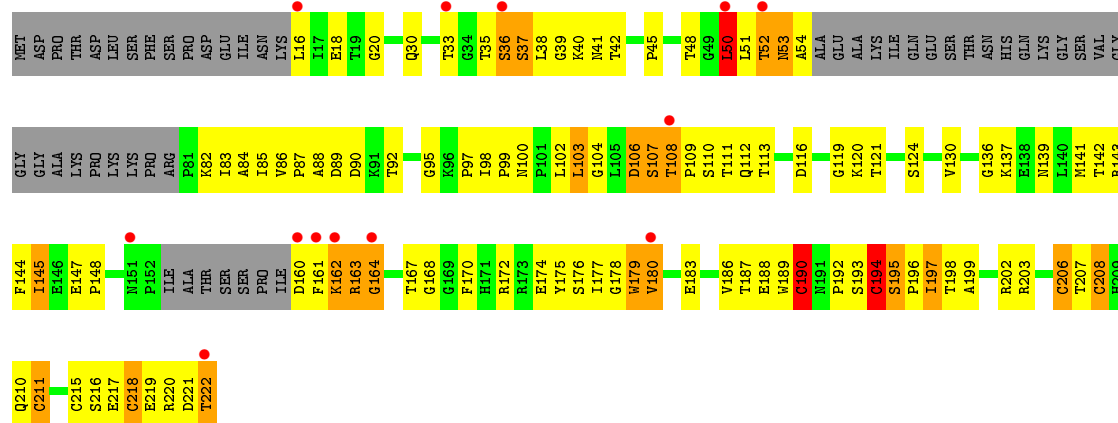


● Molecule 1: damage-specific DNA binding protein 1

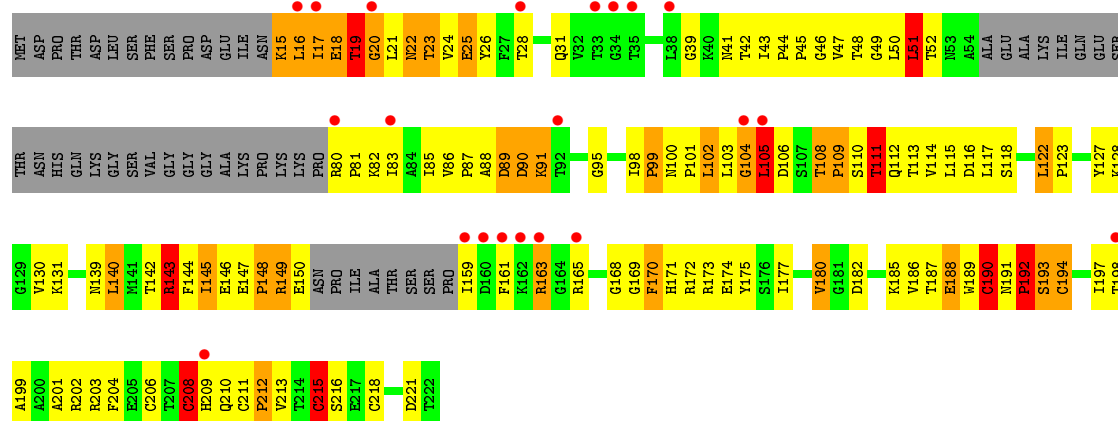
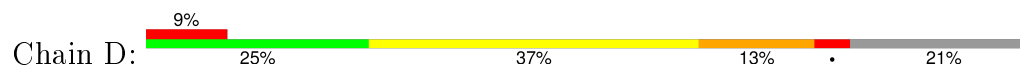




• Molecule 2: Nonstructural protein V



• Molecule 2: Nonstructural protein V



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 62.76Å 240.79Å 117.18Å 90.00° 101.79° 90.00° | Depositor |
| Resolution (Å) | 47.80 – 2.85 47.77 – 2.63 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (47.80-2.85) 86.6 (47.77-2.63) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.84 (at 2.65Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.229 , 0.299 0.226 , 0.293 | Depositor DCC |
| R_{free} test set | 3805 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 46.9 | Xtriage |
| Anisotropy | 0.604 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 62.2 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Outliers | 0 of 92110 reflections | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 20399 | wwPDB-VP |
| Average B, all atoms (Å ²) | 64.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.45 | 1/9022 (0.0%) | 0.77 | 7/12219 (0.1%) |
| 1 | B | 0.45 | 3/9039 (0.0%) | 0.91 | 41/12244 (0.3%) |
| 2 | C | 0.56 | 0/1351 | 0.95 | 9/1832 (0.5%) |
| 2 | D | 0.71 | 2/1361 (0.1%) | 1.24 | 19/1843 (1.0%) |
| All | All | 0.48 | 6/20773 (0.0%) | 0.88 | 76/28138 (0.3%) |

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 | B | 1 | 1 |
| 2 | D | 0 | 1 |
| All | All | 1 | 2 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2 | D | 189 | TRP | C-N | -15.06 | 0.99 | 1.34 |
| 2 | D | 190 | CYS | C-N | 11.09 | 1.59 | 1.34 |
| 1 | B | 748 | GLY | N-CA | -7.48 | 1.34 | 1.46 |
| 1 | B | 431 | GLY | N-CA | -6.93 | 1.35 | 1.46 |
| 1 | A | 725 | CYS | CB-SG | -5.43 | 1.73 | 1.81 |
| 1 | B | 455 | GLN | N-CA | -5.34 | 1.35 | 1.46 |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | B | 749 | THR | N-CA-C | -19.59 | 58.10 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | B | 35 | LYS | CB-CA-C | 18.15 | 146.70 | 110.40 |
| 2 | D | 15 | LYS | N-CA-C | -16.98 | 65.16 | 111.00 |
| 1 | B | 431 | GLY | N-CA-C | -16.54 | 71.75 | 113.10 |
| 1 | B | 749 | THR | N-CA-CB | 14.29 | 137.44 | 110.30 |
| 1 | B | 884 | ILE | CB-CA-C | 13.67 | 138.94 | 111.60 |
| 1 | B | 2 | SER | N-CA-CB | -13.37 | 90.44 | 110.50 |
| 1 | B | 942 | PHE | CB-CA-C | -12.45 | 85.50 | 110.40 |
| 1 | B | 451 | PHE | CB-CG-CD1 | -12.41 | 112.11 | 120.80 |
| 1 | B | 980 | ASP | N-CA-C | -12.21 | 78.02 | 111.00 |
| 1 | B | 981 | SER | N-CA-CB | -11.22 | 93.67 | 110.50 |
| 2 | D | 16 | LEU | CB-CA-C | -10.79 | 89.69 | 110.20 |
| 1 | A | 202 | PHE | CB-CA-C | -10.52 | 89.36 | 110.40 |
| 1 | B | 748 | GLY | N-CA-C | 10.49 | 139.33 | 113.10 |
| 1 | B | 980 | ASP | CB-CA-C | -10.47 | 89.46 | 110.40 |
| 2 | D | 143 | ARG | CB-CA-C | -10.28 | 89.84 | 110.40 |
| 2 | D | 16 | LEU | N-CA-CB | -10.27 | 89.87 | 110.40 |
| 2 | D | 170 | PHE | CB-CG-CD2 | -10.05 | 113.77 | 120.80 |
| 1 | B | 185 | PRO | CA-N-CD | -9.86 | 97.70 | 111.50 |
| 2 | D | 192 | PRO | CA-N-CD | -9.54 | 98.15 | 111.50 |
| 2 | D | 170 | PHE | CB-CG-CD1 | 9.38 | 127.36 | 120.80 |
| 1 | B | 885 | ASN | N-CA-CB | -9.33 | 93.81 | 110.60 |
| 1 | B | 451 | PHE | CB-CG-CD2 | 9.16 | 127.21 | 120.80 |
| 1 | B | 451 | PHE | CB-CA-C | -8.92 | 92.56 | 110.40 |
| 1 | A | 290 | GLN | CB-CA-C | 8.86 | 128.12 | 110.40 |
| 2 | D | 19 | THR | C-N-CA | -8.73 | 103.96 | 122.30 |
| 1 | B | 36 | ASN | N-CA-CB | -8.54 | 95.24 | 110.60 |
| 1 | B | 1 | MET | CB-CA-C | 8.33 | 127.06 | 110.40 |
| 2 | D | 15 | LYS | CB-CA-C | 8.24 | 126.87 | 110.40 |
| 1 | B | 561 | TRP | CB-CA-C | -7.59 | 95.23 | 110.40 |
| 2 | D | 189 | TRP | C-N-CA | 7.55 | 140.58 | 121.70 |
| 2 | C | 194 | CYS | CA-CB-SG | 7.51 | 127.52 | 114.00 |
| 2 | D | 111 | THR | N-CA-C | -7.46 | 90.86 | 111.00 |
| 1 | A | 35 | LYS | CB-CA-C | 7.23 | 124.85 | 110.40 |
| 2 | D | 208 | CYS | CA-CB-SG | 7.18 | 126.93 | 114.00 |
| 1 | B | 429 | PHE | N-CA-C | -7.17 | 91.63 | 111.00 |
| 2 | D | 20 | GLY | N-CA-C | 7.14 | 130.95 | 113.10 |
| 2 | D | 190 | CYS | CA-C-N | -7.13 | 101.51 | 117.20 |
| 1 | B | 455 | GLN | N-CA-C | -7.12 | 91.77 | 111.00 |
| 2 | C | 53 | ASN | CA-C-N | -7.03 | 101.73 | 117.20 |
| 2 | C | 37 | SER | N-CA-C | -6.99 | 92.14 | 111.00 |
| 1 | B | 430 | VAL | C-N-CA | -6.88 | 107.85 | 122.30 |
| 2 | C | 37 | SER | N-CA-CB | 6.77 | 120.66 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | D | 17 | ILE | N-CA-CB | -6.65 | 95.51 | 110.80 |
| 2 | C | 52 | THR | C-N-CA | -6.62 | 105.15 | 121.70 |
| 1 | B | 561 | TRP | N-CA-C | 6.60 | 128.82 | 111.00 |
| 1 | A | 902 | GLU | CA-CB-CG | 6.56 | 127.83 | 113.40 |
| 1 | B | 185 | PRO | N-CA-C | 6.47 | 128.92 | 112.10 |
| 1 | B | 455 | GLN | CB-CA-C | 6.21 | 122.82 | 110.40 |
| 2 | C | 36 | SER | N-CA-C | -6.14 | 94.42 | 111.00 |
| 1 | B | 750 | THR | CB-CA-C | -6.12 | 95.06 | 111.60 |
| 1 | B | 35 | LYS | N-CA-C | -6.12 | 94.47 | 111.00 |
| 2 | C | 190 | CYS | O-C-N | 6.11 | 132.47 | 122.70 |
| 1 | B | 885 | ASN | N-CA-C | -6.03 | 94.72 | 111.00 |
| 2 | C | 53 | ASN | CB-CA-C | 5.97 | 122.35 | 110.40 |
| 1 | B | 747 | GLY | CA-C-N | -5.86 | 104.48 | 116.20 |
| 1 | B | 193 | TYR | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | B | 431 | GLY | C-N-CA | 5.82 | 136.25 | 121.70 |
| 2 | D | 215 | CYS | CA-CB-SG | 5.75 | 124.36 | 114.00 |
| 1 | B | 36 | ASN | N-CA-C | -5.75 | 95.49 | 111.00 |
| 1 | B | 465 | HIS | CB-CA-C | -5.61 | 99.17 | 110.40 |
| 1 | A | 902 | GLU | N-CA-CB | 5.56 | 120.61 | 110.60 |
| 2 | D | 102 | LEU | N-CA-CB | -5.47 | 99.46 | 110.40 |
| 1 | B | 431 | GLY | CA-C-N | -5.42 | 105.28 | 117.20 |
| 1 | B | 780 | THR | CA-C-N | -5.40 | 105.33 | 117.20 |
| 2 | D | 189 | TRP | O-C-N | -5.36 | 114.12 | 122.70 |
| 2 | D | 17 | ILE | N-CA-C | -5.34 | 96.57 | 111.00 |
| 1 | B | 449 | MET | C-N-CA | 5.31 | 133.45 | 122.30 |
| 1 | B | 366 | ASP | CA-C-N | -5.30 | 105.54 | 117.20 |
| 1 | A | 902 | GLU | N-CA-C | -5.26 | 96.79 | 111.00 |
| 1 | B | 378 | CYS | N-CA-C | -5.18 | 97.02 | 111.00 |
| 1 | B | 117 | GLU | N-CA-C | 5.16 | 124.94 | 111.00 |
| 1 | A | 119 | GLY | N-CA-C | 5.16 | 125.99 | 113.10 |
| 1 | B | 746 | SER | CB-CA-C | -5.15 | 100.31 | 110.10 |
| 2 | C | 36 | SER | CB-CA-C | 5.11 | 119.81 | 110.10 |
| 1 | B | 463 | VAL | C-N-CA | 5.08 | 134.41 | 121.70 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | B | 1 | MET | CA |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 430 | VAL | Peptide |
| 2 | D | 190 | CYS | Mainchain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8860 | 0 | 8828 | 466 | 0 |
| 1 | B | 8876 | 0 | 8842 | 793 | 0 |
| 2 | C | 1324 | 0 | 1306 | 128 | 0 |
| 2 | D | 1335 | 0 | 1323 | 177 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| All | All | 20399 | 0 | 20299 | 1549 | 0 |

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

All (1549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CG | 1.51 | 1.38 |
| 1:B:367:LEU:CD2 | 1:B:374:GLN:HB2 | 1.53 | 1.37 |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CB | 1.50 | 1.37 |
| 1:B:742:VAL:CG2 | 1:B:750:THR:HG21 | 1.57 | 1.35 |
| 1:B:367:LEU:CD2 | 1:B:374:GLN:CG | 2.06 | 1.34 |
| 2:D:169:GLY:O | 2:D:212:PRO:CD | 1.75 | 1.33 |
| 1:B:367:LEU:CD2 | 1:B:374:GLN:CB | 2.08 | 1.31 |
| 1:B:367:LEU:CD1 | 1:B:374:GLN:OE1 | 1.79 | 1.31 |
| 1:B:432:GLN:OE1 | 1:B:454:ASP:CB | 1.79 | 1.31 |
| 1:B:367:LEU:O | 1:B:368:GLU:HG2 | 1.12 | 1.29 |
| 1:B:367:LEU:HD13 | 1:B:374:GLN:CD | 1.51 | 1.28 |
| 2:D:169:GLY:O | 2:D:212:PRO:HD2 | 1.28 | 1.27 |
| 2:D:190:CYS:SG | 2:D:218:CYS:HB3 | 1.80 | 1.22 |
| 1:B:369:ARG:HB2 | 1:B:655:ARG:HH12 | 1.07 | 1.19 |
| 1:B:750:THR:O | 1:B:750:THR:CG2 | 1.79 | 1.19 |
| 2:D:170:PHE:O | 2:D:193:SER:HB3 | 1.40 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:289:GLU:O | 1:A:290:GLN:O | 1.55 | 1.19 |
| 1:A:660:TYR:OH | 1:A:708:GLN:OE1 | 1.58 | 1.19 |
| 1:A:16:ASN:ND2 | 1:A:35:LYS:O | 1.74 | 1.19 |
| 2:C:35:THR:HG22 | 2:C:36:SER:O | 1.38 | 1.18 |
| 1:B:742:VAL:CG2 | 1:B:750:THR:CG2 | 2.21 | 1.18 |
| 1:B:367:LEU:HD13 | 1:B:374:GLN:OE1 | 1.02 | 1.18 |
| 1:B:367:LEU:CD2 | 1:B:374:GLN:HG3 | 1.72 | 1.17 |
| 1:B:367:LEU:O | 1:B:368:GLU:CG | 1.90 | 1.17 |
| 1:B:367:LEU:CD1 | 1:B:374:GLN:CD | 2.12 | 1.15 |
| 1:B:474:ALA:HB3 | 1:B:477:ARG:HH22 | 1.08 | 1.14 |
| 1:B:432:GLN:OE1 | 1:B:454:ASP:HB3 | 0.97 | 1.12 |
| 1:B:889:ARG:HD3 | 1:B:904:ASN:HD21 | 0.98 | 1.10 |
| 1:B:742:VAL:HG23 | 1:B:750:THR:HG21 | 1.18 | 1.08 |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:HG3 | 1.18 | 1.08 |
| 1:B:456:GLN:NE2 | 1:B:473:SER:OG | 1.86 | 1.07 |
| 1:B:286:GLU:HB2 | 1:B:299:ASP:H | 1.17 | 1.07 |
| 1:A:81:THR:HG22 | 1:A:83:LYS:H | 1.19 | 1.07 |
| 2:C:52:THR:O | 2:C:52:THR:HG22 | 1.52 | 1.07 |
| 1:B:368:GLU:OE1 | 1:B:391:ARG:NH2 | 1.88 | 1.06 |
| 1:B:367:LEU:HD11 | 1:B:374:GLN:HG3 | 1.37 | 1.06 |
| 2:D:111:THR:O | 2:D:188:GLU:OE2 | 1.74 | 1.05 |
| 1:B:742:VAL:HG23 | 1:B:750:THR:CG2 | 1.83 | 1.05 |
| 1:B:456:GLN:NE2 | 1:B:473:SER:CB | 2.20 | 1.05 |
| 1:A:371:GLY:HA3 | 1:A:1016:ASN:HD21 | 1.13 | 1.05 |
| 1:A:889:ARG:HD3 | 1:A:904:ASN:HD21 | 1.16 | 1.04 |
| 1:B:367:LEU:CD1 | 1:B:374:GLN:HG3 | 1.86 | 1.04 |
| 1:B:367:LEU:CD1 | 1:B:374:GLN:CG | 2.35 | 1.03 |
| 1:B:81:THR:HG22 | 1:B:83:LYS:H | 1.22 | 1.03 |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:HB2 | 1.40 | 1.03 |
| 1:B:367:LEU:HD11 | 1:B:374:GLN:CG | 1.89 | 1.03 |
| 1:A:167:VAL:HG13 | 1:A:180:PHE:HB3 | 1.38 | 1.02 |
| 1:B:450:GLY:HA3 | 1:B:479:VAL:HG11 | 1.42 | 1.01 |
| 1:B:367:LEU:HD12 | 1:B:368:GLU:HG2 | 1.44 | 1.00 |
| 1:B:267:ASN:HD21 | 1:B:269:SER:HB2 | 1.26 | 0.98 |
| 1:A:23:PHE:H | 1:A:30:ASN:HD22 | 1.00 | 0.98 |
| 1:B:482:GLU:HB2 | 1:B:483:PRO:HD3 | 1.43 | 0.98 |
| 2:C:112:GLN:HE22 | 2:C:187:THR:HG23 | 1.28 | 0.98 |
| 2:D:143:ARG:CZ | 2:D:143:ARG:HB3 | 1.89 | 0.98 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:HG12 | 1.43 | 0.97 |
| 1:B:178:ILE:HG22 | 1:B:193:TYR:O | 1.65 | 0.97 |
| 1:B:167:VAL:HG12 | 1:B:180:PHE:HB3 | 1.47 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:288:GLU:HB2 | 1:B:298:LYS:HB2 | 1.45 | 0.97 |
| 1:A:706:GLU:O | 1:A:707:ILE:HG13 | 1.63 | 0.96 |
| 1:A:504:ASN:HD21 | 1:A:507:GLN:HE21 | 1.02 | 0.96 |
| 1:B:889:ARG:HD3 | 1:B:904:ASN:ND2 | 1.81 | 0.96 |
| 1:B:23:PHE:H | 1:B:30:ASN:HD22 | 1.03 | 0.96 |
| 1:B:191:LYS:HG2 | 1:B:192:THR:H | 1.30 | 0.96 |
| 1:A:356:LEU:HD21 | 1:A:712:ILE:HD13 | 1.48 | 0.95 |
| 1:B:367:LEU:CG | 1:B:374:GLN:HG3 | 1.97 | 0.95 |
| 1:B:294:THR:HG22 | 1:B:295:VAL:H | 1.30 | 0.94 |
| 1:B:24:THR:H | 1:B:30:ASN:HD21 | 1.12 | 0.94 |
| 1:B:368:GLU:CD | 1:B:391:ARG:NH2 | 2.20 | 0.93 |
| 1:B:368:GLU:OE2 | 1:B:391:ARG:NH2 | 2.01 | 0.93 |
| 1:A:889:ARG:HD3 | 1:A:904:ASN:ND2 | 1.83 | 0.93 |
| 2:D:171:HIS:NE2 | 2:D:212:PRO:HG2 | 1.84 | 0.93 |
| 1:B:478:LEU:HD23 | 1:B:479:VAL:H | 1.31 | 0.92 |
| 2:C:190:CYS:HB2 | 2:C:218:CYS:SG | 2.09 | 0.92 |
| 2:C:208:CYS:SG | 2:C:210:GLN:HG2 | 2.09 | 0.92 |
| 1:B:976:VAL:HG22 | 1:B:996:GLY:HA3 | 1.50 | 0.92 |
| 1:B:474:ALA:HB3 | 1:B:477:ARG:NH2 | 1.85 | 0.91 |
| 1:B:286:GLU:HG3 | 1:B:299:ASP:HB3 | 1.52 | 0.91 |
| 1:B:480:SER:HB3 | 1:B:485:ALA:H | 1.36 | 0.91 |
| 2:C:194:CYS:SG | 2:C:208:CYS:N | 2.42 | 0.91 |
| 2:D:108:THR:O | 2:D:110:SER:N | 2.04 | 0.91 |
| 1:B:450:GLY:O | 1:B:479:VAL:HG21 | 1.70 | 0.91 |
| 2:D:80:ARG:HB2 | 2:D:81:PRO:HD3 | 1.51 | 0.90 |
| 2:C:52:THR:CG2 | 2:C:85:ILE:HG23 | 2.01 | 0.90 |
| 1:B:1125:THR:HG22 | 1:B:1127:ASP:H | 1.34 | 0.90 |
| 1:B:162:LEU:H | 1:B:162:LEU:HD23 | 1.35 | 0.90 |
| 1:B:742:VAL:O | 1:B:750:THR:HB | 1.71 | 0.90 |
| 1:B:478:LEU:HD23 | 1:B:479:VAL:N | 1.87 | 0.90 |
| 1:B:225:PRO:HG2 | 1:B:267:ASN:HB2 | 1.53 | 0.89 |
| 1:B:450:GLY:HA3 | 1:B:479:VAL:CG1 | 2.01 | 0.89 |
| 1:A:422:TYR:HD1 | 1:A:683:ASN:H | 1.11 | 0.89 |
| 1:B:1032:THR:HG22 | 1:B:1034:ASN:H | 1.35 | 0.89 |
| 1:B:256:SER:HB2 | 1:B:276:MET:HB3 | 1.53 | 0.89 |
| 2:C:109:PRO:HG2 | 2:C:203:ARG:CZ | 2.02 | 0.89 |
| 2:D:190:CYS:SG | 2:D:218:CYS:CB | 2.47 | 0.89 |
| 1:A:889:ARG:HH11 | 1:A:904:ASN:ND2 | 1.69 | 0.88 |
| 1:B:594:THR:HG22 | 1:B:595:THR:H | 1.36 | 0.88 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:HG23 | 1.54 | 0.88 |
| 1:B:453:ASP:OD2 | 1:B:472:THR:HG21 | 1.73 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:24:THR:H | 1:B:30:ASN:ND2 | 1.70 | 0.88 |
| 1:A:253:ILE:HD12 | 1:A:258:ILE:HD11 | 1.55 | 0.87 |
| 2:D:169:GLY:O | 2:D:212:PRO:HD3 | 1.71 | 0.87 |
| 1:B:456:GLN:CD | 1:B:473:SER:HB3 | 1.94 | 0.87 |
| 2:C:52:THR:O | 2:C:54:ALA:N | 2.07 | 0.87 |
| 1:B:570:LYS:HG3 | 1:B:572:PRO:HD2 | 1.56 | 0.87 |
| 1:B:178:ILE:CG2 | 1:B:193:TYR:O | 2.22 | 0.87 |
| 1:B:232:ILE:HG21 | 1:B:258:ILE:HD12 | 1.56 | 0.87 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:CG1 | 2.05 | 0.87 |
| 1:B:746:SER:OG | 1:B:746:SER:O | 1.78 | 0.87 |
| 1:A:699:LEU:HD13 | 1:A:700:THR:N | 1.90 | 0.86 |
| 1:B:507:GLN:HE22 | 1:B:553:SER:H | 1.22 | 0.86 |
| 1:A:396:ILE:HD13 | 1:A:396:ILE:H | 1.38 | 0.86 |
| 1:B:430:VAL:HG13 | 1:B:456:GLN:HB3 | 1.55 | 0.86 |
| 1:A:660:TYR:HH | 1:A:708:GLN:CD | 1.79 | 0.85 |
| 1:B:790:ASN:HB3 | 1:B:806:GLN:HA | 1.59 | 0.85 |
| 1:B:404:LEU:O | 1:B:407:ILE:HD11 | 1.75 | 0.85 |
| 2:D:171:HIS:HB2 | 2:D:215:CYS:CB | 2.06 | 0.85 |
| 2:C:194:CYS:SG | 2:C:207:THR:N | 2.49 | 0.85 |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CG | 2.07 | 0.85 |
| 1:B:869:ALA:O | 1:B:884:ILE:O | 1.94 | 0.85 |
| 1:B:436:LEU:HD12 | 1:B:445:GLU:HB3 | 1.59 | 0.85 |
| 1:B:433:THR:HG21 | 1:B:457:THR:OG1 | 1.76 | 0.85 |
| 1:B:329:GLY:HA3 | 1:B:384:GLU:HG2 | 1.59 | 0.84 |
| 1:B:369:ARG:HB2 | 1:B:655:ARG:NH1 | 1.92 | 0.84 |
| 1:B:994:GLU:O | 1:B:995:VAL:HG22 | 1.78 | 0.84 |
| 1:A:743:GLN:HA | 1:A:749:THR:HG22 | 1.59 | 0.84 |
| 1:B:432:GLN:CD | 1:B:454:ASP:HB3 | 1.98 | 0.84 |
| 1:A:23:PHE:H | 1:A:30:ASN:ND2 | 1.74 | 0.83 |
| 1:B:742:VAL:HG21 | 1:B:750:THR:HG21 | 1.60 | 0.83 |
| 1:A:553:SER:O | 1:A:571:LEU:HD12 | 1.79 | 0.83 |
| 2:C:51:LEU:HD22 | 2:C:142:THR:H | 1.43 | 0.83 |
| 1:B:742:VAL:HG22 | 1:B:750:THR:CG2 | 2.09 | 0.83 |
| 1:A:24:THR:H | 1:A:30:ASN:HD21 | 1.25 | 0.83 |
| 1:A:417:PRO:HG3 | 1:A:481:GLN:HB3 | 1.61 | 0.82 |
| 1:B:731:GLN:HA | 1:B:796:GLN:NE2 | 1.94 | 0.82 |
| 1:B:451:PHE:C | 1:B:451:PHE:CD2 | 2.52 | 0.82 |
| 1:B:756:ALA:HB1 | 1:B:801:VAL:HG21 | 1.61 | 0.82 |
| 1:A:873:MET:HE2 | 1:A:880:LEU:HD11 | 1.61 | 0.82 |
| 1:B:255:GLN:HE21 | 1:B:255:GLN:H | 1.28 | 0.82 |
| 1:A:186:GLN:H | 1:A:186:GLN:HE21 | 1.28 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:168:GLY:HA2 | 2:C:193:SER:HB2 | 1.61 | 0.82 |
| 1:B:10:GLN:HB3 | 1:B:1037:ILE:HB | 1.61 | 0.82 |
| 1:A:780:THR:O | 1:A:781:SER:O | 1.96 | 0.81 |
| 1:B:981:SER:HA | 1:B:989:ARG:HG3 | 1.63 | 0.81 |
| 1:A:1032:THR:HG23 | 1:A:1034:ASN:H | 1.44 | 0.81 |
| 1:B:367:LEU:C | 1:B:368:GLU:HG2 | 2.01 | 0.81 |
| 1:B:367:LEU:HD12 | 1:B:367:LEU:O | 1.80 | 0.81 |
| 1:B:437:MET:HB3 | 1:B:444:GLU:O | 1.80 | 0.81 |
| 2:D:114:VAL:HG22 | 2:D:185:LYS:HD3 | 1.62 | 0.81 |
| 1:B:750:THR:O | 1:B:750:THR:HG22 | 1.01 | 0.81 |
| 1:B:803:HIS:HD2 | 1:B:804:ALA:H | 1.29 | 0.81 |
| 2:C:190:CYS:CB | 2:C:218:CYS:SG | 2.69 | 0.81 |
| 1:B:290:GLN:HE21 | 1:B:293:GLY:HA3 | 1.43 | 0.80 |
| 2:D:88:ALA:HA | 2:D:199:ALA:HB3 | 1.61 | 0.80 |
| 1:A:81:THR:HG22 | 1:A:83:LYS:N | 1.96 | 0.80 |
| 1:B:297:LEU:HD21 | 1:B:300:LEU:HD11 | 1.63 | 0.80 |
| 1:B:25:SER:O | 1:B:74:LYS:HB3 | 1.82 | 0.80 |
| 1:B:476:VAL:HG13 | 1:B:490:TRP:HB3 | 1.64 | 0.80 |
| 1:A:705:ASP:OD2 | 1:A:709:LYS:HE2 | 1.82 | 0.80 |
| 2:C:112:GLN:NE2 | 2:C:187:THR:HG23 | 1.96 | 0.80 |
| 1:B:1101:SER:OG | 1:B:1103:PRO:HD2 | 1.80 | 0.80 |
| 2:D:192:PRO:O | 2:D:194:CYS:N | 2.15 | 0.80 |
| 1:B:466:GLN:O | 1:B:481:GLN:HB2 | 1.82 | 0.79 |
| 1:B:1105:MET:HE3 | 1:B:1126:ALA:HB1 | 1.65 | 0.79 |
| 1:B:275:ASP:HB2 | 1:B:279:ARG:H | 1.45 | 0.79 |
| 1:B:139:LEU:HB3 | 1:B:156:ASN:HD22 | 1.45 | 0.79 |
| 2:D:116:ASP:O | 2:D:182:ASP:HB3 | 1.83 | 0.78 |
| 1:A:454:ASP:O | 1:A:455:GLN:HG2 | 1.83 | 0.78 |
| 1:A:889:ARG:HH11 | 1:A:904:ASN:HD21 | 1.27 | 0.78 |
| 1:A:416:ASP:HB3 | 1:A:419:ARG:HG3 | 1.66 | 0.78 |
| 1:B:894:THR:HG22 | 1:B:896:GLU:H | 1.49 | 0.78 |
| 1:B:419:ARG:HH11 | 1:B:423:ASP:HB3 | 1.48 | 0.78 |
| 1:A:112:ILE:HD13 | 1:A:112:ILE:H | 1.46 | 0.78 |
| 1:B:47:GLU:HG2 | 1:B:48:GLY:H | 1.48 | 0.78 |
| 1:A:186:GLN:H | 1:A:186:GLN:NE2 | 1.81 | 0.78 |
| 1:B:432:GLN:OE1 | 1:B:454:ASP:CA | 2.32 | 0.77 |
| 1:A:24:THR:H | 1:A:30:ASN:ND2 | 1.81 | 0.77 |
| 1:A:706:GLU:O | 1:A:707:ILE:CG1 | 2.31 | 0.77 |
| 1:A:429:PHE:O | 1:A:456:GLN:HG3 | 1.84 | 0.77 |
| 1:A:143:ILE:HG12 | 1:A:154:ALA:HB2 | 1.66 | 0.77 |
| 2:C:52:THR:CG2 | 2:C:52:THR:O | 2.24 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:52:THR:HG21 | 2:C:85:ILE:CG2 | 2.15 | 0.77 |
| 1:A:440:GLY:O | 1:A:686:GLY:HA3 | 1.82 | 0.77 |
| 1:A:68:ARG:HD3 | 1:A:75:ASP:OD2 | 1.84 | 0.77 |
| 1:A:504:ASN:HD21 | 1:A:507:GLN:NE2 | 1.81 | 0.77 |
| 1:A:262:ASN:ND2 | 1:A:316:TYR:H | 1.81 | 0.77 |
| 2:C:50:LEU:HD21 | 2:C:197:ILE:HG13 | 1.65 | 0.77 |
| 1:A:504:ASN:ND2 | 1:A:507:GLN:HE21 | 1.81 | 0.77 |
| 1:A:867:LYS:HE2 | 1:A:889:ARG:HH22 | 1.48 | 0.77 |
| 1:B:81:THR:HB | 1:B:85:ASN:H | 1.50 | 0.77 |
| 2:C:208:CYS:SG | 2:C:211:CYS:N | 2.58 | 0.77 |
| 1:B:255:GLN:NE2 | 1:B:255:GLN:H | 1.82 | 0.76 |
| 1:A:909:ILE:HG12 | 1:A:928:ARG:HD2 | 1.67 | 0.76 |
| 2:D:15:LYS:HD2 | 2:D:41:ASN:ND2 | 1.99 | 0.76 |
| 1:B:450:GLY:CA | 1:B:479:VAL:CG1 | 2.64 | 0.76 |
| 1:B:23:PHE:N | 1:B:30:ASN:HD22 | 1.82 | 0.76 |
| 1:A:589:ARG:HG3 | 1:A:635:PRO:HB2 | 1.67 | 0.76 |
| 2:D:15:LYS:HD2 | 2:D:41:ASN:HD22 | 1.48 | 0.76 |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CB | 1.98 | 0.76 |
| 1:A:901:THR:HG22 | 1:A:902:GLU:O | 1.85 | 0.76 |
| 1:A:234:GLN:HE22 | 1:A:257:THR:HA | 1.51 | 0.76 |
| 2:D:170:PHE:O | 2:D:193:SER:CB | 2.30 | 0.76 |
| 1:A:273:LEU:HB2 | 1:A:281:PHE:HB2 | 1.67 | 0.76 |
| 1:B:492:GLU:HG3 | 1:B:512:VAL:HG11 | 1.68 | 0.76 |
| 1:B:466:GLN:H | 1:B:466:GLN:HE21 | 1.34 | 0.76 |
| 1:A:415:SER:HB3 | 1:A:423:ASP:OD1 | 1.86 | 0.76 |
| 1:B:286:GLU:HB2 | 1:B:299:ASP:N | 1.96 | 0.76 |
| 1:A:910:MET:CE | 1:A:912:LEU:HD21 | 2.16 | 0.76 |
| 1:B:478:LEU:HB2 | 1:B:526:LEU:HD21 | 1.68 | 0.75 |
| 2:D:122:LEU:HD12 | 2:D:122:LEU:H | 1.50 | 0.75 |
| 1:B:396:ILE:HD11 | 1:B:673:LEU:HD11 | 1.66 | 0.75 |
| 1:B:742:VAL:HG22 | 1:B:750:THR:HG22 | 1.66 | 0.75 |
| 1:A:371:GLY:HA3 | 1:A:1016:ASN:ND2 | 1.95 | 0.75 |
| 1:B:405:PRO:HA | 1:B:697:SER:HA | 1.68 | 0.75 |
| 1:A:184:ASP:HB2 | 1:A:185:PRO:CD | 2.15 | 0.75 |
| 2:D:98:ILE:HB | 2:D:201:ALA:HB1 | 1.68 | 0.75 |
| 1:B:191:LYS:HG2 | 1:B:192:THR:N | 2.02 | 0.75 |
| 1:B:594:THR:HG22 | 1:B:595:THR:N | 2.02 | 0.75 |
| 2:D:50:LEU:O | 2:D:52:THR:HG23 | 1.86 | 0.74 |
| 1:B:803:HIS:CD2 | 1:B:804:ALA:H | 2.05 | 0.74 |
| 1:B:235:GLU:H | 1:B:253:ILE:HG22 | 1.52 | 0.74 |
| 1:B:367:LEU:HD12 | 1:B:368:GLU:CG | 2.17 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:146:ASP:C | 1:A:148:ASP:H | 1.89 | 0.74 |
| 1:B:159:LEU:HD23 | 1:B:161:GLU:H | 1.52 | 0.74 |
| 1:A:342:GLU:HG2 | 1:A:343:GLN:HG3 | 1.68 | 0.74 |
| 1:A:798:THR:OG1 | 1:A:800:GLU:HG2 | 1.88 | 0.74 |
| 1:B:864:LYS:HE2 | 1:B:891:TYR:HE2 | 1.52 | 0.74 |
| 1:B:663:ASN:HB2 | 1:B:1134:GLU:HG3 | 1.69 | 0.74 |
| 1:A:1032:THR:HG22 | 1:A:1036:MET:H | 1.53 | 0.74 |
| 1:A:931:LEU:HD23 | 1:A:932:LEU:N | 2.03 | 0.74 |
| 1:B:1070:HIS:CE1 | 1:B:1093:LEU:HD12 | 2.23 | 0.73 |
| 2:D:208:CYS:O | 2:D:210:GLN:N | 2.21 | 0.73 |
| 1:A:903:CYS:SG | 1:A:941:ASN:HA | 2.28 | 0.73 |
| 1:A:750:THR:HG22 | 1:A:751:ALA:H | 1.52 | 0.73 |
| 1:B:368:GLU:OE2 | 1:B:391:ARG:CZ | 2.36 | 0.73 |
| 1:A:282:MET:HG2 | 1:A:305:LEU:HD11 | 1.69 | 0.73 |
| 1:A:642:ARG:HG2 | 1:A:647:THR:HB | 1.69 | 0.73 |
| 1:A:855:ASP:O | 1:A:857:LYS:N | 2.21 | 0.73 |
| 1:B:314:LEU:O | 1:B:314:LEU:HD12 | 1.88 | 0.73 |
| 2:D:108:THR:HB | 2:D:109:PRO:HD3 | 1.71 | 0.73 |
| 1:B:267:ASN:ND2 | 1:B:269:SER:HB2 | 2.03 | 0.73 |
| 1:A:803:HIS:CD2 | 1:A:858:LEU:HB2 | 2.24 | 0.73 |
| 1:B:367:LEU:CD2 | 1:B:374:GLN:CD | 2.56 | 0.73 |
| 1:B:407:ILE:HD12 | 1:B:407:ILE:H | 1.52 | 0.73 |
| 2:D:102:LEU:HD11 | 2:D:180:VAL:HG22 | 1.70 | 0.73 |
| 1:A:936:LYS:HE2 | 1:A:943:GLU:OE2 | 1.89 | 0.72 |
| 1:B:707:ILE:CG2 | 1:B:709:LYS:HE3 | 2.20 | 0.72 |
| 1:B:450:GLY:CA | 1:B:479:VAL:HG13 | 2.19 | 0.72 |
| 1:B:368:GLU:OE2 | 1:B:374:GLN:OE1 | 2.07 | 0.72 |
| 2:D:170:PHE:C | 2:D:193:SER:HB3 | 2.09 | 0.72 |
| 2:C:109:PRO:HG2 | 2:C:203:ARG:NH2 | 2.03 | 0.72 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:CB | 2.19 | 0.72 |
| 1:B:597:GLU:HG2 | 1:B:664:HIS:CE1 | 2.24 | 0.72 |
| 1:B:129:ARG:NH1 | 1:B:176:PRO:HD3 | 2.04 | 0.72 |
| 2:D:19:THR:HG22 | 2:D:20:GLY:H | 1.55 | 0.71 |
| 2:C:30:GLN:HE21 | 2:C:36:SER:HA | 1.54 | 0.71 |
| 1:B:451:PHE:O | 1:B:451:PHE:CD2 | 2.43 | 0.71 |
| 1:B:504:ASN:HD21 | 1:B:507:GLN:HB2 | 1.55 | 0.71 |
| 1:B:141:LYS:HD2 | 1:B:156:ASN:OD1 | 1.90 | 0.71 |
| 1:B:147:ARG:HE | 1:B:147:ARG:HA | 1.56 | 0.71 |
| 1:A:564:ILE:HG22 | 1:A:582:LEU:HD12 | 1.72 | 0.71 |
| 1:A:59:GLY:HA2 | 1:A:1073:TRP:CZ3 | 2.25 | 0.71 |
| 1:B:634:GLN:HB3 | 1:B:635:PRO:HD2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:246:LEU:HD13 | 1:B:300:LEU:HD13 | 1.71 | 0.71 |
| 1:A:867:LYS:CE | 1:A:889:ARG:HH22 | 2.04 | 0.71 |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:CD | 2.10 | 0.71 |
| 1:B:456:GLN:HE22 | 1:B:473:SER:CB | 2.04 | 0.71 |
| 1:B:23:PHE:H | 1:B:30:ASN:ND2 | 1.83 | 0.71 |
| 1:A:648:ASN:HD22 | 1:A:660:TYR:HB3 | 1.56 | 0.71 |
| 2:C:50:LEU:HD21 | 2:C:197:ILE:CG1 | 2.21 | 0.70 |
| 1:B:731:GLN:HA | 1:B:796:GLN:HE21 | 1.56 | 0.70 |
| 1:A:750:THR:HG22 | 1:A:751:ALA:N | 2.06 | 0.70 |
| 1:B:124:ILE:HG23 | 1:B:131:ILE:HD13 | 1.71 | 0.70 |
| 1:B:449:MET:CE | 1:B:449:MET:HA | 2.21 | 0.70 |
| 1:A:1032:THR:HG21 | 1:A:1036:MET:HB3 | 1.71 | 0.70 |
| 1:B:643:SER:HB3 | 1:B:706:GLU:HG3 | 1.73 | 0.70 |
| 2:C:52:THR:CG2 | 2:C:85:ILE:HG12 | 2.20 | 0.70 |
| 1:A:879:LYS:HE2 | 1:A:902:GLU:OE2 | 1.91 | 0.70 |
| 1:A:291:MET:HG3 | 1:A:292:ASP:H | 1.57 | 0.70 |
| 1:A:16:ASN:HD22 | 1:A:35:LYS:C | 1.94 | 0.70 |
| 2:C:108:THR:O | 2:C:110:SER:N | 2.24 | 0.70 |
| 2:C:164:GLY:O | 2:C:194:CYS:HA | 1.91 | 0.70 |
| 1:B:665:LYS:HD3 | 1:B:1138:ARG:NH1 | 2.07 | 0.70 |
| 1:B:656:PRO:HB2 | 1:B:671:VAL:HB | 1.74 | 0.70 |
| 2:D:99:PRO:HG2 | 2:D:106:ASP:HA | 1.73 | 0.70 |
| 1:A:289:GLU:C | 1:A:290:GLN:O | 2.30 | 0.70 |
| 1:B:196:SER:OG | 1:B:199:GLU:HG2 | 1.92 | 0.70 |
| 2:D:171:HIS:CD2 | 2:D:212:PRO:HG2 | 2.25 | 0.69 |
| 1:B:63:VAL:HB | 1:B:80:LEU:HB3 | 1.72 | 0.69 |
| 1:B:419:ARG:NH1 | 1:B:423:ASP:HB3 | 2.05 | 0.69 |
| 1:A:369:ARG:O | 1:A:370:GLN:HB3 | 1.92 | 0.69 |
| 2:C:215:CYS:SG | 2:C:218:CYS:N | 2.64 | 0.69 |
| 1:B:1036:MET:O | 1:B:1037:ILE:HB | 1.92 | 0.69 |
| 2:C:52:THR:CB | 2:C:85:ILE:HA | 2.21 | 0.69 |
| 1:A:1022:THR:HG22 | 1:A:1024:THR:H | 1.58 | 0.69 |
| 1:A:298:LYS:HD3 | 1:A:299:ASP:HB2 | 1.74 | 0.69 |
| 1:A:480:SER:HB3 | 1:A:487:VAL:HG11 | 1.74 | 0.69 |
| 1:B:482:GLU:CB | 1:B:483:PRO:HD3 | 2.18 | 0.69 |
| 1:B:107:ASN:OD1 | 1:B:109:GLN:HG2 | 1.91 | 0.69 |
| 2:D:82:LYS:C | 2:D:83:ILE:HD12 | 2.12 | 0.69 |
| 1:A:507:GLN:NE2 | 1:A:553:SER:H | 1.90 | 0.69 |
| 1:A:253:ILE:O | 1:A:255:GLN:N | 2.25 | 0.69 |
| 1:B:130:MET:HG2 | 1:B:197:LEU:HD21 | 1.73 | 0.69 |
| 1:A:482:GLU:HB2 | 1:A:483:PRO:HD3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:369:ARG:HH12 | 1:B:670:ASN:HB3 | 1.58 | 0.69 |
| 1:B:456:GLN:OE1 | 1:B:473:SER:HB3 | 1.93 | 0.69 |
| 1:B:480:SER:HB3 | 1:B:485:ALA:N | 2.08 | 0.69 |
| 2:C:108:THR:O | 2:C:222:THR:HA | 1.93 | 0.69 |
| 1:B:1026:GLY:O | 1:B:1041:THR:HG22 | 1.92 | 0.69 |
| 1:B:464:ALA:O | 1:B:465:HIS:ND1 | 2.27 | 0.68 |
| 1:A:312:GLU:HG3 | 1:A:327:ARG:HB2 | 1.74 | 0.68 |
| 1:B:736:LEU:HD13 | 1:B:813:ALA:HB1 | 1.75 | 0.68 |
| 1:A:81:THR:CG2 | 1:A:83:LYS:H | 2.02 | 0.68 |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:CA | 2.23 | 0.68 |
| 2:C:86:VAL:CG1 | 2:C:198:THR:HA | 2.23 | 0.68 |
| 1:B:910:MET:HB2 | 1:B:926:LEU:HB3 | 1.75 | 0.68 |
| 1:A:844:LYS:HG3 | 1:A:845:GLN:HG3 | 1.76 | 0.68 |
| 1:B:474:ALA:CB | 1:B:477:ARG:HH22 | 1.96 | 0.68 |
| 1:B:167:VAL:O | 1:B:168:LYS:HB2 | 1.92 | 0.68 |
| 1:A:372:GLN:HB3 | 1:A:1014:MET:SD | 2.34 | 0.68 |
| 1:A:977:CYS:HB3 | 1:A:992:LEU:HD13 | 1.75 | 0.68 |
| 1:B:582:LEU:HD12 | 1:B:582:LEU:O | 1.93 | 0.68 |
| 2:C:161:PHE:CE1 | 2:C:163:ARG:HB2 | 2.29 | 0.67 |
| 2:D:163:ARG:HD2 | 2:D:163:ARG:H | 1.58 | 0.67 |
| 1:B:402:ILE:HD12 | 1:B:402:ILE:N | 2.10 | 0.67 |
| 1:B:450:GLY:HA2 | 1:B:479:VAL:HG13 | 1.75 | 0.67 |
| 1:B:475:SER:HA | 1:B:498:ILE:HD11 | 1.74 | 0.67 |
| 1:B:112:ILE:HG22 | 1:B:113:GLY:H | 1.58 | 0.67 |
| 1:B:294:THR:HG22 | 1:B:295:VAL:N | 2.05 | 0.67 |
| 1:A:929:SER:HB3 | 1:A:952:ASN:HB2 | 1.76 | 0.67 |
| 2:C:38:LEU:O | 2:C:40:LYS:N | 2.27 | 0.67 |
| 1:B:1032:THR:HG22 | 1:B:1033:VAL:N | 2.10 | 0.67 |
| 1:A:839:GLU:H | 1:A:839:GLU:CD | 1.99 | 0.67 |
| 2:C:161:PHE:HE1 | 2:C:163:ARG:HB2 | 1.60 | 0.67 |
| 1:A:992:LEU:O | 1:A:992:LEU:HD12 | 1.94 | 0.67 |
| 2:D:171:HIS:HB2 | 2:D:215:CYS:HB2 | 1.76 | 0.67 |
| 1:B:514:ARG:O | 1:B:514:ARG:HG2 | 1.94 | 0.67 |
| 2:C:88:ALA:HA | 2:C:199:ALA:HB3 | 1.76 | 0.67 |
| 1:A:663:ASN:O | 1:A:664:HIS:HB2 | 1.95 | 0.67 |
| 1:B:355:ASN:C | 1:B:357:GLY:H | 1.96 | 0.66 |
| 1:B:704:ILE:HD13 | 1:B:704:ILE:H | 1.60 | 0.66 |
| 2:D:51:LEU:HD12 | 2:D:142:THR:H | 1.60 | 0.66 |
| 1:B:80:LEU:HD22 | 1:B:133:LEU:HD23 | 1.76 | 0.66 |
| 1:A:207:TRP:HB3 | 1:A:242:GLY:HA2 | 1.77 | 0.66 |
| 1:A:275:ASP:HB3 | 1:A:279:ARG:H | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1128:ASP:O | 1:A:1132:VAL:HG23 | 1.94 | 0.66 |
| 1:A:416:ASP:HB3 | 1:A:419:ARG:CG | 2.25 | 0.66 |
| 1:A:388:ARG:HD3 | 1:A:714:THR:HB | 1.76 | 0.66 |
| 1:A:23:PHE:N | 1:A:30:ASN:HD22 | 1.84 | 0.66 |
| 1:B:1017:LEU:HD12 | 1:B:1019:GLU:OE2 | 1.96 | 0.66 |
| 1:B:232:ILE:CG2 | 1:B:258:ILE:HD12 | 2.25 | 0.66 |
| 2:D:113:THR:HB | 2:D:186:VAL:HB | 1.78 | 0.66 |
| 1:B:690:SER:C | 1:B:691:LEU:HD12 | 2.15 | 0.66 |
| 2:D:168:GLY:CA | 2:D:208:CYS:SG | 2.84 | 0.66 |
| 1:B:270:ARG:HG2 | 1:B:284:LEU:HD23 | 1.78 | 0.66 |
| 1:B:743:GLN:HE21 | 1:B:782:PHE:HA | 1.60 | 0.66 |
| 1:B:275:ASP:CG | 1:B:279:ARG:HB2 | 2.16 | 0.66 |
| 1:B:973:ASN:HD21 | 1:B:1077:HIS:H | 1.42 | 0.66 |
| 1:B:1112:LEU:HD23 | 1:B:1113:GLN:N | 2.11 | 0.66 |
| 1:B:742:VAL:HG23 | 1:B:750:THR:CB | 2.25 | 0.65 |
| 1:A:207:TRP:CB | 1:A:242:GLY:HA2 | 2.27 | 0.65 |
| 1:B:707:ILE:HG23 | 1:B:709:LYS:HE3 | 1.78 | 0.65 |
| 1:B:695:ASN:HB2 | 1:B:698:THR:HG22 | 1.77 | 0.65 |
| 1:A:648:ASN:HD22 | 1:A:660:TYR:CB | 2.09 | 0.65 |
| 1:A:396:ILE:H | 1:A:396:ILE:CD1 | 2.09 | 0.65 |
| 1:B:465:HIS:CE1 | 1:B:523:PRO:HD3 | 2.32 | 0.65 |
| 2:D:163:ARG:HD2 | 2:D:197:ILE:HD11 | 1.78 | 0.65 |
| 1:A:611:LEU:C | 1:A:611:LEU:HD23 | 2.17 | 0.65 |
| 2:D:171:HIS:HB2 | 2:D:215:CYS:HB3 | 1.79 | 0.65 |
| 2:D:168:GLY:HA2 | 2:D:208:CYS:SG | 2.37 | 0.65 |
| 2:D:49:GLY:HA3 | 2:D:83:ILE:HG13 | 1.79 | 0.65 |
| 1:A:1113:GLN:HB3 | 1:A:1121:LYS:HD2 | 1.78 | 0.65 |
| 1:A:1085:ALA:O | 1:A:1086:THR:HG23 | 1.96 | 0.65 |
| 1:A:10:GLN:HB2 | 1:A:1037:ILE:HB | 1.78 | 0.65 |
| 1:B:365:VAL:O | 1:B:367:LEU:HD23 | 1.98 | 0.64 |
| 2:D:163:ARG:CD | 2:D:197:ILE:HD11 | 2.26 | 0.64 |
| 1:A:699:LEU:HD13 | 1:A:700:THR:H | 1.58 | 0.64 |
| 1:B:112:ILE:N | 1:B:112:ILE:HD12 | 2.12 | 0.64 |
| 1:B:894:THR:HG22 | 1:B:895:THR:N | 2.11 | 0.64 |
| 1:B:385:GLY:HA3 | 1:B:719:GLU:O | 1.97 | 0.64 |
| 1:B:427:LEU:HD13 | 1:B:429:PHE:HE1 | 1.62 | 0.64 |
| 1:B:1058:LEU:HD23 | 1:B:1093:LEU:HD22 | 1.80 | 0.64 |
| 1:A:564:ILE:HG22 | 1:A:564:ILE:O | 1.97 | 0.64 |
| 1:B:16:ASN:ND2 | 1:B:35:LYS:O | 2.23 | 0.64 |
| 1:B:407:ILE:HD12 | 1:B:407:ILE:N | 2.11 | 0.64 |
| 1:A:368:GLU:HB3 | 1:A:370:GLN:HE22 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:275:ASP:HB2 | 1:A:279:ARG:HB2 | 1.79 | 0.64 |
| 1:B:238:THR:HA | 1:B:247:ALA:HA | 1.79 | 0.64 |
| 2:D:46:GLY:O | 2:D:146:GLU:HG3 | 1.97 | 0.64 |
| 1:B:208:LYS:HG3 | 1:B:209:GLN:H | 1.62 | 0.64 |
| 1:B:432:GLN:OE1 | 1:B:454:ASP:O | 2.16 | 0.64 |
| 1:B:451:PHE:HD2 | 1:B:451:PHE:O | 1.81 | 0.64 |
| 2:C:145:ILE:HD11 | 2:C:174:GLU:CD | 2.18 | 0.64 |
| 1:B:419:ARG:HD3 | 1:B:421:THR:O | 1.97 | 0.64 |
| 1:B:317:LEU:O | 1:B:318:ASP:HB2 | 1.96 | 0.64 |
| 2:D:170:PHE:CD1 | 2:D:170:PHE:N | 2.66 | 0.64 |
| 1:A:1051:LEU:HD22 | 1:A:1094:ILE:HG12 | 1.79 | 0.63 |
| 1:B:19:VAL:HG22 | 1:B:20:THR:H | 1.63 | 0.63 |
| 1:B:682:LEU:HD13 | 1:B:683:ASN:N | 2.13 | 0.63 |
| 1:B:367:LEU:HD22 | 1:B:374:GLN:NE2 | 2.13 | 0.63 |
| 2:D:218:CYS:HB2 | 2:D:221:ASP:OD1 | 1.98 | 0.63 |
| 1:B:272:LEU:HD22 | 1:B:280:LEU:HD11 | 1.80 | 0.63 |
| 1:A:767:SER:O | 1:A:769:LYS:HE3 | 1.98 | 0.63 |
| 1:B:1130:ILE:O | 1:B:1134:GLU:HB2 | 1.97 | 0.63 |
| 1:B:394:ILE:HD12 | 1:B:658:VAL:HB | 1.81 | 0.63 |
| 1:B:1022:THR:HG22 | 1:B:1024:THR:OG1 | 1.99 | 0.63 |
| 1:B:866:VAL:HG12 | 1:B:884:ILE:HG21 | 1.80 | 0.63 |
| 1:B:432:GLN:O | 1:B:433:THR:OG1 | 2.17 | 0.63 |
| 1:B:481:GLN:NE2 | 1:B:484:LYS:NZ | 2.47 | 0.63 |
| 1:B:129:ARG:HD3 | 1:B:176:PRO:HG3 | 1.81 | 0.63 |
| 1:B:742:VAL:CG2 | 1:B:750:THR:HG22 | 2.19 | 0.62 |
| 1:A:706:GLU:C | 1:A:707:ILE:HG13 | 2.19 | 0.62 |
| 1:A:580:GLU:HG2 | 1:A:614:PHE:CZ | 2.33 | 0.62 |
| 1:A:780:THR:HB | 1:A:784:GLU:HB2 | 1.81 | 0.62 |
| 1:A:268:GLY:O | 1:A:270:ARG:N | 2.32 | 0.62 |
| 1:B:507:GLN:NE2 | 1:B:553:SER:H | 1.96 | 0.62 |
| 2:D:128:LYS:HE2 | 2:D:146:GLU:OE1 | 2.00 | 0.62 |
| 1:B:513:GLY:O | 1:B:514:ARG:HB3 | 1.99 | 0.62 |
| 1:B:926:LEU:HG | 1:B:927:MET:HG3 | 1.81 | 0.62 |
| 2:D:102:LEU:HD23 | 2:D:102:LEU:O | 1.99 | 0.62 |
| 1:B:803:HIS:CD2 | 1:B:804:ALA:N | 2.67 | 0.62 |
| 1:A:1114:TYR:HB2 | 1:A:1124:ALA:HB2 | 1.82 | 0.62 |
| 1:A:986:ASP:HB2 | 1:B:1118:SER:HB3 | 1.81 | 0.62 |
| 1:B:474:ALA:O | 1:B:475:SER:HB3 | 2.00 | 0.62 |
| 1:B:1051:LEU:HA | 1:B:1054:MET:HB2 | 1.80 | 0.62 |
| 1:B:456:GLN:NE2 | 1:B:473:SER:HB3 | 2.00 | 0.62 |
| 2:C:164:GLY:HA2 | 2:C:194:CYS:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:910:MET:HE3 | 1:A:912:LEU:HD21 | 1.81 | 0.62 |
| 1:B:414:ARG:HB2 | 1:B:462:ASN:ND2 | 2.13 | 0.62 |
| 2:D:173:ARG:NH1 | 2:D:218:CYS:HB3 | 2.14 | 0.62 |
| 1:B:739:ARG:NH1 | 1:B:758:THR:HG23 | 2.15 | 0.61 |
| 1:B:918:GLY:O | 1:B:919:ASP:HB2 | 1.99 | 0.61 |
| 1:A:414:ARG:HG2 | 1:A:414:ARG:HH11 | 1.64 | 0.61 |
| 2:D:47:VAL:HG12 | 2:D:48:THR:N | 2.15 | 0.61 |
| 1:B:629:VAL:HA | 1:B:1017:LEU:O | 1.99 | 0.61 |
| 1:B:769:LYS:H | 1:B:769:LYS:HD2 | 1.65 | 0.61 |
| 1:B:440:GLY:O | 1:B:686:GLY:HA3 | 2.00 | 0.61 |
| 1:B:386:SER:HA | 1:B:717:LEU:HG | 1.81 | 0.61 |
| 1:A:986:ASP:H | 1:B:1118:SER:HB3 | 1.65 | 0.61 |
| 1:B:414:ARG:HB2 | 1:B:462:ASN:HD21 | 1.64 | 0.61 |
| 1:B:14:ALA:HB1 | 1:B:327:ARG:HG3 | 1.82 | 0.61 |
| 2:C:52:THR:HG22 | 2:C:85:ILE:HG23 | 1.82 | 0.61 |
| 2:C:119:GLY:O | 2:C:120:LYS:HB2 | 1.99 | 0.61 |
| 1:B:286:GLU:O | 1:B:297:LEU:HD12 | 2.00 | 0.61 |
| 1:A:358:PRO:O | 1:A:379:SER:HA | 2.01 | 0.61 |
| 1:A:234:GLN:NE2 | 1:A:257:THR:HA | 2.14 | 0.61 |
| 1:B:644:LEU:HD23 | 1:B:644:LEU:H | 1.66 | 0.61 |
| 1:B:740:ILE:HD12 | 1:B:740:ILE:N | 2.16 | 0.61 |
| 2:C:160:ASP:CG | 2:C:161:PHE:H | 2.04 | 0.60 |
| 1:A:564:ILE:HG22 | 1:A:582:LEU:CD1 | 2.29 | 0.60 |
| 1:B:1105:MET:CE | 1:B:1126:ALA:HB1 | 2.31 | 0.60 |
| 1:A:722:ARG:HH11 | 1:A:722:ARG:HG3 | 1.65 | 0.60 |
| 1:B:1013:VAL:O | 1:B:1014:MET:HB3 | 2.01 | 0.60 |
| 1:A:889:ARG:HD2 | 1:A:901:THR:HG23 | 1.84 | 0.60 |
| 1:B:594:THR:CG2 | 1:B:595:THR:H | 2.12 | 0.60 |
| 1:A:184:ASP:HB2 | 1:A:185:PRO:HD2 | 1.83 | 0.60 |
| 1:B:432:GLN:OE1 | 1:B:454:ASP:C | 2.39 | 0.60 |
| 2:D:111:THR:C | 2:D:188:GLU:OE2 | 2.38 | 0.60 |
| 1:B:994:GLU:HG3 | 1:B:995:VAL:H | 1.66 | 0.60 |
| 1:B:232:ILE:HG12 | 1:B:237:ILE:HG23 | 1.82 | 0.60 |
| 1:B:43:VAL:HG23 | 1:B:52:VAL:HG11 | 1.83 | 0.60 |
| 1:B:693:LEU:HD23 | 1:B:693:LEU:N | 2.16 | 0.60 |
| 1:B:367:LEU:HD21 | 1:B:374:GLN:N | 2.16 | 0.60 |
| 1:A:660:TYR:CZ | 1:A:708:GLN:OE1 | 2.50 | 0.60 |
| 1:B:498:ILE:CG2 | 1:B:512:VAL:HG22 | 2.31 | 0.60 |
| 1:B:162:LEU:H | 1:B:162:LEU:CD2 | 2.10 | 0.60 |
| 1:A:564:ILE:N | 1:A:564:ILE:HD12 | 2.16 | 0.60 |
| 2:C:180:VAL:O | 2:C:180:VAL:HG12 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:570:LYS:HG2 | 1:B:575:GLU:OE1 | 2.02 | 0.60 |
| 2:D:147:GLU:O | 2:D:149:ARG:N | 2.34 | 0.60 |
| 1:B:1118:SER:O | 1:B:1120:MET:HG3 | 2.02 | 0.60 |
| 1:A:848:ILE:HD11 | 1:A:870:VAL:HG11 | 1.83 | 0.60 |
| 1:A:543:ILE:HG13 | 1:A:543:ILE:O | 2.02 | 0.60 |
| 1:B:985:THR:O | 1:B:989:ARG:HB3 | 2.02 | 0.59 |
| 1:B:356:LEU:HD23 | 1:B:388:ARG:HG3 | 1.83 | 0.59 |
| 1:B:1108:VAL:O | 1:B:1109:VAL:HB | 2.02 | 0.59 |
| 2:D:143:ARG:HA | 2:D:175:TYR:O | 2.01 | 0.59 |
| 1:A:160:GLU:HB3 | 1:A:161:GLU:OE2 | 2.02 | 0.59 |
| 1:B:5:TYR:CE2 | 1:B:7:VAL:CG2 | 2.85 | 0.59 |
| 1:A:300:LEU:N | 1:A:300:LEU:HD23 | 2.17 | 0.59 |
| 1:B:167:VAL:HG12 | 1:B:180:PHE:CB | 2.26 | 0.59 |
| 2:D:174:GLU:O | 2:D:188:GLU:HA | 2.03 | 0.59 |
| 1:A:867:LYS:CD | 1:A:867:LYS:H | 2.15 | 0.59 |
| 2:D:192:PRO:C | 2:D:194:CYS:H | 2.05 | 0.59 |
| 1:A:589:ARG:HG2 | 1:A:589:ARG:HH11 | 1.66 | 0.59 |
| 1:B:472:THR:OG1 | 1:B:477:ARG:NH2 | 2.33 | 0.59 |
| 1:A:492:GLU:CD | 1:A:494:GLN:H | 2.05 | 0.59 |
| 1:A:743:GLN:HB3 | 1:A:782:PHE:O | 2.03 | 0.59 |
| 2:D:112:GLN:HE22 | 2:D:187:THR:HG23 | 1.67 | 0.59 |
| 2:D:22:ASN:O | 2:D:24:VAL:N | 2.36 | 0.59 |
| 1:B:449:MET:O | 1:B:451:PHE:N | 2.35 | 0.59 |
| 1:B:1032:THR:CG2 | 1:B:1033:VAL:N | 2.66 | 0.59 |
| 1:A:20:THR:HB | 1:A:315:THR:HG21 | 1.84 | 0.59 |
| 2:C:208:CYS:SG | 2:C:210:GLN:CG | 2.88 | 0.59 |
| 1:B:192:THR:OG1 | 1:B:205:GLY:HA3 | 2.02 | 0.59 |
| 1:A:186:GLN:N | 1:A:186:GLN:NE2 | 2.50 | 0.59 |
| 2:D:208:CYS:C | 2:D:210:GLN:H | 2.03 | 0.59 |
| 1:B:1062:ILE:HD13 | 1:B:1100:ILE:HD11 | 1.85 | 0.59 |
| 1:A:532:THR:HG22 | 1:A:533:GLU:N | 2.17 | 0.59 |
| 1:A:36:ASN:OD1 | 1:A:60:LYS:HD2 | 2.02 | 0.59 |
| 1:A:1070:HIS:CE1 | 1:A:1093:LEU:HD12 | 2.38 | 0.59 |
| 1:B:417:PRO:HG3 | 1:B:481:GLN:OE1 | 2.03 | 0.58 |
| 1:A:507:GLN:HE22 | 1:A:553:SER:HB3 | 1.68 | 0.58 |
| 1:A:780:THR:HG22 | 1:A:781:SER:H | 1.68 | 0.58 |
| 2:D:112:GLN:NE2 | 2:D:187:THR:HG23 | 2.18 | 0.58 |
| 1:A:188:ARG:NH1 | 1:A:216:ALA:O | 2.36 | 0.58 |
| 1:B:466:GLN:HE21 | 1:B:466:GLN:N | 1.99 | 0.58 |
| 1:B:866:VAL:HG11 | 1:B:884:ILE:HD12 | 1.86 | 0.58 |
| 1:B:706:GLU:O | 1:B:707:ILE:HB | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:795:ASP:HB3 | 1:B:798:THR:OG1 | 2.03 | 0.58 |
| 1:A:288:GLU:HB3 | 1:A:296:THR:HG23 | 1.86 | 0.58 |
| 1:A:1118:SER:C | 1:A:1120:MET:H | 2.07 | 0.58 |
| 1:B:369:ARG:HH21 | 1:B:372:GLN:CD | 2.06 | 0.58 |
| 1:B:577:LEU:O | 1:B:578:HIS:HB2 | 2.02 | 0.58 |
| 1:B:199:GLU:HG3 | 1:B:201:GLU:HG2 | 1.84 | 0.58 |
| 1:B:1014:MET:HG3 | 1:B:1015:GLN:N | 2.17 | 0.58 |
| 2:C:51:LEU:HD23 | 2:C:141:MET:HA | 1.86 | 0.58 |
| 1:B:129:ARG:HD3 | 1:B:176:PRO:CG | 2.33 | 0.58 |
| 1:A:298:LYS:C | 1:A:298:LYS:HD3 | 2.24 | 0.58 |
| 1:B:341:ASN:ND2 | 1:B:342:GLU:HG2 | 2.19 | 0.58 |
| 1:A:146:ASP:C | 1:A:148:ASP:N | 2.56 | 0.58 |
| 1:B:1070:HIS:NE2 | 1:B:1093:LEU:HD12 | 2.19 | 0.58 |
| 1:B:356:LEU:O | 1:B:357:GLY:O | 2.21 | 0.58 |
| 1:B:53:LYS:HE3 | 1:B:98:ILE:HB | 1.85 | 0.58 |
| 1:B:368:GLU:HG3 | 1:B:369:ARG:HG2 | 1.86 | 0.58 |
| 1:B:367:LEU:HD11 | 1:B:374:GLN:OE1 | 1.95 | 0.58 |
| 2:D:172:ARG:HH21 | 2:D:191:ASN:HD22 | 1.50 | 0.58 |
| 1:A:1032:THR:HB | 1:A:1036:MET:O | 2.03 | 0.58 |
| 1:A:910:MET:HE2 | 1:A:912:LEU:HD21 | 1.84 | 0.58 |
| 1:B:864:LYS:HE2 | 1:B:891:TYR:CE2 | 2.35 | 0.58 |
| 1:A:771:PHE:CE2 | 1:A:845:GLN:HB3 | 2.39 | 0.58 |
| 1:B:1065:VAL:C | 1:B:1067:LYS:H | 2.07 | 0.58 |
| 1:A:766:SER:HB3 | 1:A:808:LEU:HD23 | 1.85 | 0.58 |
| 1:B:310:ILE:HG21 | 1:B:328:LEU:HD12 | 1.86 | 0.58 |
| 1:B:368:GLU:CD | 1:B:391:ARG:HH21 | 2.06 | 0.58 |
| 1:B:842:GLU:HG2 | 2:D:128:LYS:NZ | 2.18 | 0.58 |
| 1:B:437:MET:HB2 | 1:B:446:THR:HG23 | 1.85 | 0.58 |
| 1:B:143:ILE:HG12 | 1:B:154:ALA:HB2 | 1.85 | 0.58 |
| 1:A:864:LYS:HE2 | 1:A:891:TYR:HE2 | 1.68 | 0.58 |
| 1:A:578:HIS:CD2 | 1:A:623:LEU:H | 2.22 | 0.58 |
| 2:D:108:THR:HG22 | 2:D:109:PRO:N | 2.17 | 0.57 |
| 1:B:294:THR:CG2 | 1:B:295:VAL:H | 2.11 | 0.57 |
| 1:A:262:ASN:HD21 | 1:A:316:TYR:H | 1.48 | 0.57 |
| 2:D:173:ARG:HH12 | 2:D:218:CYS:HB3 | 1.69 | 0.57 |
| 1:B:1039:LEU:HD12 | 1:B:1040:VAL:H | 1.69 | 0.57 |
| 2:D:108:THR:CB | 2:D:109:PRO:HD3 | 2.34 | 0.57 |
| 1:B:486:LEU:O | 1:B:486:LEU:HG | 2.05 | 0.57 |
| 1:B:1108:VAL:HG12 | 1:B:1109:VAL:N | 2.19 | 0.57 |
| 1:B:1028:VAL:O | 1:B:1039:LEU:HD12 | 2.05 | 0.57 |
| 1:B:433:THR:O | 1:B:433:THR:HG22 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:450:GLY:O | 1:B:479:VAL:CG2 | 2.49 | 0.57 |
| 1:B:465:HIS:O | 1:B:467:GLN:HG3 | 2.04 | 0.57 |
| 1:B:256:SER:HB3 | 1:B:277:GLU:OE2 | 2.04 | 0.57 |
| 1:B:550:ASN:O | 1:B:552:LEU:N | 2.38 | 0.57 |
| 1:B:769:LYS:N | 1:B:769:LYS:HD2 | 2.18 | 0.57 |
| 1:B:500:VAL:HB | 1:B:511:ALA:HB3 | 1.85 | 0.57 |
| 1:A:117:GLU:O | 1:A:119:GLY:N | 2.37 | 0.57 |
| 1:B:365:VAL:O | 1:B:367:LEU:CD2 | 2.52 | 0.57 |
| 1:B:24:THR:N | 1:B:30:ASN:HD21 | 1.92 | 0.57 |
| 1:B:504:ASN:OD1 | 1:B:507:GLN:N | 2.31 | 0.57 |
| 1:A:1032:THR:CG2 | 1:A:1036:MET:H | 2.17 | 0.57 |
| 1:A:507:GLN:HE22 | 1:A:553:SER:H | 1.51 | 0.57 |
| 1:B:743:GLN:NE2 | 1:B:781:SER:OG | 2.30 | 0.57 |
| 1:B:1039:LEU:HD21 | 1:B:1139:ILE:HG22 | 1.87 | 0.57 |
| 1:B:876:PHE:CE1 | 1:B:921:ILE:HD11 | 2.40 | 0.57 |
| 1:B:433:THR:HG21 | 1:B:457:THR:CB | 2.35 | 0.57 |
| 1:A:894:THR:HG22 | 1:B:585:GLU:OE1 | 2.04 | 0.57 |
| 1:B:731:GLN:CA | 1:B:796:GLN:HE21 | 2.17 | 0.56 |
| 1:B:1057:ARG:CZ | 1:B:1112:LEU:HB2 | 2.35 | 0.56 |
| 2:D:202:ARG:HD2 | 2:D:204:PHE:CZ | 2.39 | 0.56 |
| 1:A:1101:SER:HB2 | 1:A:1103:PRO:HD2 | 1.87 | 0.56 |
| 1:B:744:ASP:OD2 | 1:B:747:GLY:N | 2.37 | 0.56 |
| 1:B:731:GLN:O | 1:B:796:GLN:HG2 | 2.05 | 0.56 |
| 1:A:722:ARG:HG3 | 1:A:722:ARG:NH1 | 2.19 | 0.56 |
| 1:B:1014:MET:CG | 1:B:1015:GLN:N | 2.68 | 0.56 |
| 1:B:503:CYS:SG | 1:B:508:VAL:HG22 | 2.46 | 0.56 |
| 1:B:159:LEU:CD2 | 1:B:161:GLU:HB2 | 2.36 | 0.56 |
| 2:C:97:PRO:HA | 2:C:202:ARG:HA | 1.86 | 0.56 |
| 1:B:334:VAL:HG12 | 1:B:349:ALA:HA | 1.88 | 0.56 |
| 1:B:1075:SER:HB2 | 1:B:1084:PRO:HA | 1.88 | 0.56 |
| 1:A:225:PRO:HG2 | 1:A:267:ASN:HB2 | 1.87 | 0.56 |
| 2:C:52:THR:HB | 2:C:86:VAL:H | 1.71 | 0.56 |
| 1:B:275:ASP:OD1 | 1:B:279:ARG:HB2 | 2.04 | 0.56 |
| 1:A:417:PRO:CG | 1:A:481:GLN:HB3 | 2.33 | 0.56 |
| 1:B:255:GLN:NE2 | 1:B:255:GLN:N | 2.52 | 0.56 |
| 1:B:261:HIS:HA | 1:B:272:LEU:O | 2.06 | 0.56 |
| 1:A:476:VAL:HG13 | 1:A:490:TRP:HB3 | 1.86 | 0.56 |
| 2:C:215:CYS:H | 2:C:218:CYS:HB2 | 1.70 | 0.56 |
| 1:B:1125:THR:HG22 | 1:B:1127:ASP:N | 2.15 | 0.56 |
| 1:A:564:ILE:HD12 | 1:A:564:ILE:H | 1.71 | 0.56 |
| 1:A:19:VAL:HG22 | 1:A:20:THR:N | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:334:VAL:HG11 | 1:A:347:VAL:HG13 | 1.88 | 0.56 |
| 1:A:108:VAL:O | 1:A:141:LYS:HE2 | 2.05 | 0.56 |
| 1:B:178:ILE:HG23 | 1:B:193:TYR:O | 2.03 | 0.56 |
| 1:A:224:GLU:HB2 | 1:A:225:PRO:HD3 | 1.87 | 0.56 |
| 2:C:99:PRO:HG3 | 2:C:106:ASP:O | 2.05 | 0.56 |
| 2:D:169:GLY:HA2 | 2:D:211:CYS:HA | 1.87 | 0.56 |
| 2:D:102:LEU:CD1 | 2:D:180:VAL:HG22 | 2.36 | 0.56 |
| 1:B:1022:THR:C | 1:B:1024:THR:H | 2.09 | 0.56 |
| 1:B:308:THR:OG1 | 1:B:309:SER:N | 2.38 | 0.56 |
| 1:B:560:LEU:HD12 | 1:B:567:ARG:HH11 | 1.71 | 0.56 |
| 1:B:429:PHE:O | 1:B:432:GLN:N | 2.28 | 0.56 |
| 1:A:707:ILE:HG23 | 1:A:708:GLN:HG2 | 1.87 | 0.56 |
| 1:B:511:ALA:HB2 | 1:B:541:LEU:HD11 | 1.87 | 0.56 |
| 1:B:367:LEU:CG | 1:B:374:GLN:CG | 2.66 | 0.56 |
| 2:C:163:ARG:HB3 | 2:C:195:SER:O | 2.04 | 0.56 |
| 1:B:159:LEU:HD21 | 1:B:161:GLU:HB2 | 1.87 | 0.56 |
| 1:A:589:ARG:HG3 | 1:A:635:PRO:CB | 2.34 | 0.56 |
| 1:A:852:GLN:HG2 | 1:A:854:SER:H | 1.71 | 0.56 |
| 1:B:262:ASN:ND2 | 1:B:316:TYR:H | 2.03 | 0.56 |
| 1:B:662:SER:CB | 1:B:1138:ARG:HH21 | 2.19 | 0.55 |
| 1:B:223:PRO:HD3 | 1:B:271:TYR:OH | 2.05 | 0.55 |
| 1:A:161:GLU:CD | 1:A:161:GLU:H | 2.09 | 0.55 |
| 2:C:90:ASP:OD1 | 2:C:92:THR:HB | 2.07 | 0.55 |
| 1:B:573:SER:O | 1:B:574:PHE:HB2 | 2.05 | 0.55 |
| 2:C:100:ASN:HB3 | 2:C:103:LEU:HG | 1.87 | 0.55 |
| 1:A:838:PRO:HD2 | 1:A:839:GLU:OE2 | 2.05 | 0.55 |
| 1:B:626:ARG:HG2 | 1:B:626:ARG:O | 2.06 | 0.55 |
| 2:D:159:ILE:HG22 | 2:D:159:ILE:O | 2.07 | 0.55 |
| 1:B:206:PRO:HB2 | 1:B:207:TRP:CE3 | 2.41 | 0.55 |
| 1:A:340:SER:HB3 | 1:A:346:TYR:CE1 | 2.41 | 0.55 |
| 1:A:537:GLU:HB3 | 1:A:561:TRP:HB2 | 1.87 | 0.55 |
| 1:B:498:ILE:HG22 | 1:B:512:VAL:HG22 | 1.88 | 0.55 |
| 2:D:113:THR:HG22 | 2:D:114:VAL:N | 2.21 | 0.55 |
| 2:D:51:LEU:HD12 | 2:D:142:THR:N | 2.21 | 0.55 |
| 1:B:235:GLU:H | 1:B:253:ILE:CG2 | 2.19 | 0.55 |
| 1:B:1120:MET:O | 1:B:1121:LYS:HB3 | 2.06 | 0.55 |
| 2:D:87:PRO:HG3 | 2:D:91:LYS:NZ | 2.22 | 0.55 |
| 1:B:1002:GLU:HB3 | 1:B:1032:THR:HG21 | 1.88 | 0.55 |
| 1:A:250:PRO:HG2 | 1:A:253:ILE:HG12 | 1.89 | 0.55 |
| 1:B:235:GLU:O | 1:B:236:SER:HB2 | 2.07 | 0.55 |
| 1:A:634:GLN:HG2 | 1:A:654:ASP:OD1 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:19:THR:HG22 | 2:D:20:GLY:N | 2.19 | 0.55 |
| 1:B:389:ILE:N | 1:B:389:ILE:HD12 | 2.22 | 0.55 |
| 2:C:52:THR:OG1 | 2:C:85:ILE:HA | 2.07 | 0.55 |
| 2:D:143:ARG:HB3 | 2:D:143:ARG:NH1 | 2.22 | 0.55 |
| 1:B:329:GLY:HA3 | 1:B:384:GLU:CG | 2.34 | 0.55 |
| 1:A:811:GLU:HB2 | 1:A:835:MET:SD | 2.47 | 0.55 |
| 1:A:1119:GLY:HA3 | 1:B:984:THR:HG23 | 1.89 | 0.55 |
| 1:B:427:LEU:H | 1:B:427:LEU:HD12 | 1.72 | 0.55 |
| 1:A:369:ARG:O | 1:A:370:GLN:CB | 2.54 | 0.55 |
| 1:B:1065:VAL:O | 1:B:1067:LYS:N | 2.40 | 0.55 |
| 1:A:341:ASN:CG | 1:A:342:GLU:N | 2.57 | 0.54 |
| 1:A:931:LEU:HD23 | 1:A:931:LEU:C | 2.27 | 0.54 |
| 2:D:82:LYS:HZ3 | 2:D:161:PHE:HZ | 1.55 | 0.54 |
| 1:B:494:GLN:HG2 | 1:B:494:GLN:O | 2.05 | 0.54 |
| 1:B:976:VAL:O | 1:B:994:GLU:O | 2.24 | 0.54 |
| 1:B:1102:ARG:HB2 | 1:B:1103:PRO:HD3 | 1.88 | 0.54 |
| 1:B:396:ILE:HD11 | 1:B:673:LEU:CD1 | 2.37 | 0.54 |
| 1:A:117:GLU:C | 1:A:119:GLY:H | 2.10 | 0.54 |
| 1:B:475:SER:HB2 | 1:B:490:TRP:O | 2.08 | 0.54 |
| 1:B:57:MET:HE3 | 1:B:1066:GLY:H | 1.72 | 0.54 |
| 1:B:1095:GLU:HG2 | 1:B:1137:THR:HG22 | 1.89 | 0.54 |
| 2:C:161:PHE:HZ | 2:C:196:PRO:HA | 1.73 | 0.54 |
| 1:A:146:ASP:O | 1:A:148:ASP:N | 2.41 | 0.54 |
| 1:B:242:GLY:O | 1:B:243:ASP:CB | 2.56 | 0.54 |
| 1:B:1050:LEU:C | 1:B:1050:LEU:HD23 | 2.28 | 0.54 |
| 1:A:969:GLU:HG2 | 1:A:970:ASN:N | 2.23 | 0.54 |
| 1:B:477:ARG:HD2 | 1:B:489:GLU:HG3 | 1.90 | 0.54 |
| 2:D:18:GLU:HA | 2:D:18:GLU:OE1 | 2.06 | 0.54 |
| 1:B:1065:VAL:HG12 | 1:B:1066:GLY:N | 2.23 | 0.54 |
| 1:B:881:LEU:HD22 | 1:B:921:ILE:HD12 | 1.88 | 0.54 |
| 2:C:95:GLY:O | 2:C:202:ARG:HD2 | 2.07 | 0.54 |
| 1:B:560:LEU:HD12 | 1:B:567:ARG:NH1 | 2.22 | 0.54 |
| 1:A:982:ALA:C | 1:A:984:THR:H | 2.11 | 0.54 |
| 1:B:165:ILE:HG21 | 1:B:217:SER:HA | 1.90 | 0.54 |
| 2:D:170:PHE:HD1 | 2:D:170:PHE:H | 1.56 | 0.54 |
| 2:C:50:LEU:CD2 | 2:C:86:VAL:HG21 | 2.37 | 0.54 |
| 1:B:401:SER:HA | 1:B:700:THR:HG22 | 1.89 | 0.54 |
| 1:B:430:VAL:HG13 | 1:B:456:GLN:CB | 2.34 | 0.54 |
| 1:A:396:ILE:N | 1:A:396:ILE:CD1 | 2.69 | 0.54 |
| 1:A:416:ASP:CB | 1:A:419:ARG:HG3 | 2.35 | 0.54 |
| 2:D:102:LEU:CD1 | 2:D:180:VAL:CG2 | 2.86 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:665:LYS:HD3 | 1:A:1138:ARG:CZ | 2.37 | 0.54 |
| 1:B:228:GLY:HA2 | 1:B:241:ASN:HA | 1.90 | 0.54 |
| 1:B:182:TYR:CZ | 1:B:189:HIS:HB2 | 2.43 | 0.54 |
| 1:B:1102:ARG:O | 1:B:1106:GLN:HG3 | 2.08 | 0.54 |
| 1:B:504:ASN:ND2 | 1:B:507:GLN:HB2 | 2.22 | 0.54 |
| 1:B:1036:MET:O | 1:B:1037:ILE:CB | 2.56 | 0.54 |
| 1:B:717:LEU:HD12 | 1:B:721:PRO:HG3 | 1.90 | 0.54 |
| 1:A:612:PHE:CE2 | 1:A:628:LYS:HD2 | 2.43 | 0.54 |
| 1:A:189:HIS:HB3 | 1:A:210:GLU:HA | 1.90 | 0.54 |
| 1:B:516:LEU:HD13 | 1:B:534:MET:HG2 | 1.90 | 0.54 |
| 2:C:206:CYS:SG | 2:C:211:CYS:HB3 | 2.48 | 0.54 |
| 1:B:866:VAL:CG1 | 1:B:884:ILE:HG21 | 2.38 | 0.54 |
| 1:B:1075:SER:HB2 | 1:B:1083:GLU:O | 2.08 | 0.54 |
| 1:A:130:MET:HA | 1:A:145:LEU:HD13 | 1.90 | 0.54 |
| 1:B:616:LEU:HD12 | 1:B:617:ASN:N | 2.22 | 0.54 |
| 2:D:17:ILE:HD11 | 2:D:139:ASN:ND2 | 2.23 | 0.54 |
| 1:B:450:GLY:O | 1:B:451:PHE:C | 2.44 | 0.53 |
| 1:A:889:ARG:NH1 | 1:A:904:ASN:ND2 | 2.49 | 0.53 |
| 1:B:949:PHE:HA | 2:D:122:LEU:HD21 | 1.89 | 0.53 |
| 2:D:98:ILE:HB | 2:D:201:ALA:CB | 2.36 | 0.53 |
| 1:B:652:CYS:HB3 | 1:B:676:VAL:O | 2.09 | 0.53 |
| 2:C:215:CYS:O | 2:C:219:GLU:OE1 | 2.25 | 0.53 |
| 2:D:90:ASP:O | 2:D:91:LYS:HG3 | 2.07 | 0.53 |
| 2:D:171:HIS:ND1 | 2:D:215:CYS:HB3 | 2.23 | 0.53 |
| 1:B:248:ILE:C | 1:B:250:PRO:HD3 | 2.29 | 0.53 |
| 1:B:511:ALA:HA | 1:B:515:ALA:O | 2.09 | 0.53 |
| 1:B:771:PHE:CE2 | 1:B:845:GLN:HB2 | 2.43 | 0.53 |
| 2:C:144:PHE:HB2 | 2:C:175:TYR:HB2 | 1.91 | 0.53 |
| 1:B:451:PHE:C | 1:B:451:PHE:HD2 | 2.05 | 0.53 |
| 1:A:867:LYS:HD2 | 1:A:867:LYS:H | 1.73 | 0.53 |
| 1:B:564:ILE:HG22 | 1:B:582:LEU:HD12 | 1.91 | 0.53 |
| 1:A:354:THR:HG21 | 1:A:712:ILE:HD12 | 1.91 | 0.53 |
| 1:B:414:ARG:HH21 | 1:B:462:ASN:HB2 | 1.74 | 0.53 |
| 2:D:169:GLY:O | 2:D:212:PRO:CG | 2.51 | 0.53 |
| 2:C:143:ARG:NH2 | 2:C:174:GLU:OE1 | 2.42 | 0.53 |
| 1:B:731:GLN:CA | 1:B:796:GLN:NE2 | 2.71 | 0.53 |
| 1:B:19:VAL:O | 1:B:31:LEU:HD12 | 2.08 | 0.53 |
| 1:B:644:LEU:HG | 1:B:645:SER:N | 2.24 | 0.53 |
| 1:A:183:GLN:HB2 | 1:A:188:ARG:HG2 | 1.90 | 0.53 |
| 1:B:413:LEU:HD22 | 1:B:424:THR:HB | 1.90 | 0.53 |
| 1:B:170:LEU:HD12 | 1:B:177:THR:HG22 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:707:ILE:CG2 | 1:A:708:GLN:HG2 | 2.39 | 0.53 |
| 1:A:487:VAL:HG23 | 1:A:524:GLN:HA | 1.91 | 0.53 |
| 1:B:586:ILE:HG21 | 1:B:608:ASP:H | 1.72 | 0.53 |
| 1:A:725:CYS:O | 1:A:733:PHE:HD2 | 1.92 | 0.53 |
| 1:B:1020:THR:O | 1:B:1021:SER:HB2 | 2.08 | 0.53 |
| 1:B:90:GLU:HB3 | 1:B:101:ILE:HG12 | 1.91 | 0.53 |
| 1:B:1118:SER:O | 1:B:1119:GLY:C | 2.47 | 0.53 |
| 2:D:108:THR:O | 2:D:109:PRO:C | 2.46 | 0.53 |
| 1:A:23:PHE:N | 1:A:30:ASN:ND2 | 2.48 | 0.53 |
| 1:B:159:LEU:HD23 | 1:B:161:GLU:N | 2.22 | 0.53 |
| 1:B:340:SER:HB3 | 1:B:346:TYR:CD1 | 2.43 | 0.53 |
| 1:B:432:GLN:CD | 1:B:454:ASP:O | 2.47 | 0.52 |
| 1:A:686:GLY:C | 1:A:688:PRO:HD3 | 2.29 | 0.52 |
| 1:B:369:ARG:CG | 1:B:369:ARG:O | 2.56 | 0.52 |
| 2:C:35:THR:C | 2:C:36:SER:O | 2.42 | 0.52 |
| 2:C:179:TRP:O | 2:C:180:VAL:HB | 2.09 | 0.52 |
| 1:B:1079:GLU:HA | 1:B:1079:GLU:OE2 | 2.09 | 0.52 |
| 1:B:369:ARG:NH1 | 1:B:670:ASN:HB3 | 2.22 | 0.52 |
| 2:D:169:GLY:N | 2:D:211:CYS:SG | 2.69 | 0.52 |
| 2:D:110:SER:O | 2:D:221:ASP:HA | 2.10 | 0.52 |
| 2:D:87:PRO:HG3 | 2:D:91:LYS:CE | 2.39 | 0.52 |
| 1:B:134:ARG:NH1 | 1:B:164:VAL:HB | 2.25 | 0.52 |
| 1:B:355:ASN:C | 1:B:357:GLY:N | 2.62 | 0.52 |
| 1:A:275:ASP:CB | 1:A:279:ARG:HB2 | 2.38 | 0.52 |
| 1:B:1015:GLN:O | 1:B:1015:GLN:HG3 | 2.09 | 0.52 |
| 2:D:202:ARG:HB3 | 2:D:204:PHE:CE1 | 2.44 | 0.52 |
| 1:A:334:VAL:CG1 | 1:A:347:VAL:HG13 | 2.39 | 0.52 |
| 2:D:143:ARG:NH2 | 2:D:174:GLU:OE1 | 2.42 | 0.52 |
| 1:B:162:LEU:HG | 1:B:163:HIS:H | 1.74 | 0.52 |
| 1:A:1030:PHE:CZ | 1:A:1038:GLY:HA3 | 2.44 | 0.52 |
| 1:B:29:LEU:HB3 | 1:B:44:VAL:HB | 1.91 | 0.52 |
| 1:B:475:SER:OG | 1:B:477:ARG:NH1 | 2.42 | 0.52 |
| 1:B:180:PHE:CE1 | 1:B:182:TYR:HB3 | 2.45 | 0.52 |
| 2:D:18:GLU:O | 2:D:42:THR:HG23 | 2.09 | 0.52 |
| 1:B:973:ASN:ND2 | 1:B:1077:HIS:H | 2.06 | 0.52 |
| 1:B:741:GLU:OE1 | 1:B:749:THR:HB | 2.09 | 0.52 |
| 2:C:86:VAL:HG13 | 2:C:87:PRO:HD2 | 1.92 | 0.52 |
| 1:A:848:ILE:CD1 | 1:A:870:VAL:HG11 | 2.40 | 0.52 |
| 1:A:476:VAL:CG1 | 1:A:490:TRP:HB3 | 2.40 | 0.52 |
| 2:D:115:LEU:HD23 | 2:D:123:PRO:HB3 | 1.90 | 0.52 |
| 2:C:161:PHE:O | 2:C:162:LYS:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:10:GLN:O | 1:B:1036:MET:O | 2.28 | 0.52 |
| 1:A:112:ILE:HD13 | 1:A:112:ILE:N | 2.22 | 0.52 |
| 1:A:922:LEU:HD23 | 1:A:957:VAL:HG13 | 1.91 | 0.52 |
| 1:A:655:ARG:HH11 | 1:A:655:ARG:HG3 | 1.74 | 0.52 |
| 1:B:489:GLU:OE2 | 1:B:491:LYS:HE3 | 2.10 | 0.52 |
| 1:A:780:THR:HB | 1:A:784:GLU:CB | 2.39 | 0.52 |
| 2:D:171:HIS:CB | 2:D:215:CYS:HB3 | 2.40 | 0.51 |
| 1:B:228:GLY:CA | 1:B:241:ASN:HA | 2.40 | 0.51 |
| 2:C:109:PRO:HG2 | 2:C:203:ARG:NH1 | 2.24 | 0.51 |
| 1:B:237:ILE:O | 1:B:248:ILE:HG12 | 2.09 | 0.51 |
| 1:B:383:LYS:HG3 | 1:B:384:GLU:OE2 | 2.10 | 0.51 |
| 1:B:57:MET:CE | 1:B:1066:GLY:H | 2.23 | 0.51 |
| 1:A:309:SER:HA | 1:A:384:GLU:OE2 | 2.10 | 0.51 |
| 2:D:192:PRO:C | 2:D:194:CYS:N | 2.62 | 0.51 |
| 1:A:837:TYR:HB3 | 1:A:839:GLU:OE2 | 2.10 | 0.51 |
| 1:B:769:LYS:HG2 | 1:B:769:LYS:O | 2.11 | 0.51 |
| 2:D:86:VAL:HG13 | 2:D:87:PRO:HD2 | 1.92 | 0.51 |
| 2:D:104:GLY:O | 2:D:105:LEU:HB3 | 2.11 | 0.51 |
| 1:B:281:PHE:CD2 | 1:B:304:LEU:HA | 2.46 | 0.51 |
| 1:A:780:THR:HG22 | 1:A:781:SER:N | 2.24 | 0.51 |
| 1:B:1121:LYS:O | 1:B:1121:LYS:HG2 | 2.10 | 0.51 |
| 1:B:5:TYR:HB2 | 1:B:1043:LEU:HD11 | 1.93 | 0.51 |
| 1:B:790:ASN:ND2 | 1:B:790:ASN:N | 2.58 | 0.51 |
| 1:B:910:MET:HB2 | 1:B:926:LEU:CB | 2.41 | 0.51 |
| 1:A:1114:TYR:CB | 1:A:1124:ALA:HB2 | 2.41 | 0.51 |
| 2:D:21:LEU:HD22 | 2:D:26:TYR:CD1 | 2.46 | 0.51 |
| 1:B:1126:ALA:O | 1:B:1130:ILE:HG13 | 2.10 | 0.51 |
| 1:A:912:LEU:HB2 | 1:A:913:TYR:CE1 | 2.46 | 0.51 |
| 1:B:355:ASN:OD1 | 1:B:357:GLY:N | 2.43 | 0.51 |
| 2:D:87:PRO:HG3 | 2:D:91:LYS:HE3 | 1.93 | 0.51 |
| 1:B:393:GLY:HA2 | 1:B:708:GLN:HG2 | 1.92 | 0.51 |
| 2:D:110:SER:N | 2:D:221:ASP:HB3 | 2.25 | 0.51 |
| 2:C:216:SER:HA | 2:C:219:GLU:OE2 | 2.10 | 0.51 |
| 1:B:419:ARG:HD2 | 1:B:423:ASP:OD1 | 2.11 | 0.51 |
| 2:D:98:ILE:HG22 | 2:D:99:PRO:O | 2.11 | 0.51 |
| 1:B:388:ARG:NE | 1:B:714:THR:HG23 | 2.26 | 0.51 |
| 2:D:171:HIS:CG | 2:D:215:CYS:HB3 | 2.46 | 0.51 |
| 2:C:215:CYS:SG | 2:C:217:GLU:HB2 | 2.51 | 0.51 |
| 1:B:255:GLN:HE21 | 1:B:255:GLN:N | 2.04 | 0.51 |
| 1:B:290:GLN:NE2 | 1:B:293:GLY:HA3 | 2.19 | 0.51 |
| 1:A:634:GLN:HB3 | 1:A:635:PRO:HD2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:130:MET:HA | 1:B:145:LEU:CB | 2.41 | 0.51 |
| 2:D:109:PRO:HB2 | 2:D:203:ARG:NH2 | 2.25 | 0.51 |
| 2:D:163:ARG:NH1 | 2:D:197:ILE:HD11 | 2.25 | 0.51 |
| 2:C:167:THR:O | 2:C:193:SER:HB3 | 2.10 | 0.51 |
| 2:C:100:ASN:HB3 | 2:C:103:LEU:CD1 | 2.40 | 0.51 |
| 1:B:861:VAL:HG12 | 1:B:862:ALA:N | 2.26 | 0.51 |
| 2:D:218:CYS:O | 2:D:221:ASP:HB2 | 2.11 | 0.51 |
| 1:B:451:PHE:HE2 | 1:B:453:ASP:HB3 | 1.76 | 0.51 |
| 2:D:82:LYS:O | 2:D:83:ILE:HD12 | 2.10 | 0.51 |
| 1:B:41:ILE:O | 1:B:52:VAL:HG22 | 2.11 | 0.51 |
| 1:A:1101:SER:CB | 1:A:1103:PRO:HD2 | 2.41 | 0.51 |
| 1:A:537:GLU:HB3 | 1:A:561:TRP:CB | 2.41 | 0.51 |
| 1:B:986:ASP:O | 1:B:990:GLN:HB2 | 2.10 | 0.51 |
| 1:A:1026:GLY:O | 1:A:1027:SER:HB2 | 2.10 | 0.51 |
| 1:B:480:SER:O | 1:B:484:LYS:HA | 2.11 | 0.51 |
| 2:C:108:THR:O | 2:C:222:THR:CA | 2.58 | 0.51 |
| 1:B:230:ILE:HD13 | 1:B:239:TYR:HD1 | 1.75 | 0.50 |
| 1:B:687:TYR:O | 1:B:688:PRO:O | 2.29 | 0.50 |
| 1:B:161:GLU:HB3 | 1:B:182:TYR:HB2 | 1.93 | 0.50 |
| 1:B:63:VAL:HB | 1:B:80:LEU:CB | 2.40 | 0.50 |
| 1:B:342:GLU:C | 1:B:344:GLY:H | 2.15 | 0.50 |
| 2:C:97:PRO:CD | 2:C:202:ARG:HD3 | 2.42 | 0.50 |
| 1:A:410:LEU:HD23 | 1:A:410:LEU:N | 2.25 | 0.50 |
| 1:A:256:SER:OG | 1:A:277:GLU:HG3 | 2.11 | 0.50 |
| 1:A:117:GLU:C | 1:A:119:GLY:N | 2.64 | 0.50 |
| 2:D:89:ASP:OD1 | 2:D:90:ASP:N | 2.45 | 0.50 |
| 1:B:391:ARG:HG2 | 1:B:392:ASN:N | 2.26 | 0.50 |
| 1:B:769:LYS:N | 1:B:769:LYS:CD | 2.74 | 0.50 |
| 2:C:83:ILE:O | 2:C:84:ALA:HB3 | 2.12 | 0.50 |
| 1:A:34:ALA:HB2 | 1:A:64:MET:CE | 2.41 | 0.50 |
| 1:B:568:ILE:O | 1:B:569:LEU:HD23 | 2.11 | 0.50 |
| 1:B:571:LEU:HB3 | 1:B:572:PRO:HD3 | 1.93 | 0.50 |
| 2:D:114:VAL:HG22 | 2:D:185:LYS:CD | 2.39 | 0.50 |
| 1:A:762:SER:HB2 | 1:A:803:HIS:HA | 1.93 | 0.50 |
| 1:B:84:TYR:CG | 1:B:109:GLN:HB3 | 2.46 | 0.50 |
| 1:A:1080:ARG:HD2 | 2:C:119:GLY:HA3 | 1.93 | 0.50 |
| 1:B:413:LEU:C | 1:B:413:LEU:HD23 | 2.32 | 0.50 |
| 1:B:304:LEU:HD23 | 1:B:304:LEU:C | 2.32 | 0.50 |
| 1:A:794:ILE:HG23 | 1:A:799:PHE:HA | 1.92 | 0.50 |
| 1:A:465:HIS:CE1 | 1:A:523:PRO:HD3 | 2.47 | 0.50 |
| 2:D:165:ARG:HH11 | 2:D:165:ARG:HG2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:432:GLN:NE2 | 1:B:454:ASP:O | 2.44 | 0.50 |
| 2:C:162:LYS:HG3 | 2:C:162:LYS:O | 2.11 | 0.50 |
| 1:B:921:ILE:HB | 1:B:933:LEU:HB2 | 1.94 | 0.50 |
| 1:B:223:PRO:HG2 | 1:B:268:GLY:CA | 2.42 | 0.50 |
| 1:B:212:VAL:HG12 | 1:B:213:GLU:N | 2.27 | 0.50 |
| 1:B:476:VAL:CG1 | 1:B:490:TRP:HB3 | 2.38 | 0.50 |
| 2:C:108:THR:HA | 2:C:222:THR:O | 2.11 | 0.50 |
| 1:B:744:ASP:OD2 | 1:B:746:SER:C | 2.50 | 0.50 |
| 1:A:855:ASP:CG | 1:A:856:GLY:N | 2.65 | 0.50 |
| 1:B:1022:THR:C | 1:B:1024:THR:N | 2.65 | 0.50 |
| 2:C:116:ASP:OD2 | 2:C:119:GLY:O | 2.28 | 0.50 |
| 2:D:95:GLY:O | 2:D:202:ARG:NH1 | 2.38 | 0.50 |
| 1:B:410:LEU:HA | 1:B:426:VAL:O | 2.11 | 0.50 |
| 1:B:724:ILE:HA | 1:B:734:GLY:O | 2.12 | 0.50 |
| 1:B:55:VAL:HG21 | 1:B:100:ILE:HG13 | 1.93 | 0.50 |
| 2:D:171:HIS:NE2 | 2:D:212:PRO:CG | 2.68 | 0.50 |
| 1:B:994:GLU:HG3 | 1:B:995:VAL:N | 2.26 | 0.50 |
| 1:B:553:SER:O | 1:B:571:LEU:HG | 2.11 | 0.50 |
| 1:B:1108:VAL:C | 1:B:1110:ALA:H | 2.16 | 0.50 |
| 1:A:580:GLU:HG2 | 1:A:614:PHE:CE2 | 2.47 | 0.50 |
| 2:C:97:PRO:HD3 | 2:C:202:ARG:HD3 | 1.94 | 0.50 |
| 1:B:969:GLU:HG2 | 1:B:970:ASN:N | 2.26 | 0.50 |
| 1:A:704:ILE:CG2 | 1:A:705:ASP:N | 2.73 | 0.50 |
| 1:B:133:LEU:N | 1:B:133:LEU:HD12 | 2.26 | 0.50 |
| 1:B:468:LEU:HD13 | 1:B:481:GLN:HG2 | 1.94 | 0.49 |
| 1:A:597:GLU:OE2 | 1:A:664:HIS:N | 2.41 | 0.49 |
| 1:B:675:GLU:HG2 | 1:B:676:VAL:N | 2.27 | 0.49 |
| 1:B:377:THR:O | 1:B:387:LEU:HA | 2.12 | 0.49 |
| 1:B:91:TYR:OH | 1:B:98:ILE:HD12 | 2.12 | 0.49 |
| 1:A:1032:THR:HG22 | 1:A:1036:MET:N | 2.25 | 0.49 |
| 1:B:47:GLU:CD | 1:B:47:GLU:H | 2.14 | 0.49 |
| 2:D:48:THR:HB | 2:D:145:ILE:CD1 | 2.42 | 0.49 |
| 1:B:170:LEU:HD12 | 1:B:177:THR:CG2 | 2.40 | 0.49 |
| 1:B:1080:ARG:NE | 1:B:1080:ARG:HA | 2.28 | 0.49 |
| 1:A:356:LEU:O | 1:A:379:SER:HB3 | 2.12 | 0.49 |
| 1:B:548:ASP:O | 1:B:550:ASN:N | 2.45 | 0.49 |
| 1:B:743:GLN:HB2 | 1:B:783:GLY:H | 1.78 | 0.49 |
| 1:B:262:ASN:ND2 | 1:B:315:THR:HA | 2.26 | 0.49 |
| 1:A:1057:ARG:NH1 | 1:A:1112:LEU:HB2 | 2.28 | 0.49 |
| 1:A:125:ASP:OD2 | 1:A:127:GLU:HB2 | 2.12 | 0.49 |
| 1:A:594:THR:HG23 | 1:A:595:THR:N | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:359:ILE:HG13 | 1:B:1035:GLY:HA2 | 1.95 | 0.49 |
| 1:B:896:GLU:O | 1:B:897:LYS:HB2 | 2.12 | 0.49 |
| 1:B:614:PHE:N | 1:B:614:PHE:CD1 | 2.79 | 0.49 |
| 1:B:546:LEU:HD11 | 1:B:593:MET:HB3 | 1.95 | 0.49 |
| 1:B:467:GLN:CD | 1:B:478:LEU:HD21 | 2.33 | 0.49 |
| 1:B:467:GLN:HB3 | 1:B:478:LEU:HD21 | 1.94 | 0.49 |
| 1:A:29:LEU:HG | 1:A:44:VAL:HG21 | 1.94 | 0.49 |
| 1:B:910:MET:CE | 1:B:912:LEU:HD21 | 2.43 | 0.49 |
| 2:D:22:ASN:O | 2:D:23:THR:C | 2.51 | 0.49 |
| 1:A:337:ASN:O | 1:A:346:TYR:HB3 | 2.12 | 0.49 |
| 1:A:794:ILE:CG2 | 1:A:799:PHE:HA | 2.43 | 0.49 |
| 1:B:226:PHE:HD2 | 1:B:297:LEU:HB2 | 1.76 | 0.49 |
| 1:B:224:GLU:O | 1:B:225:PRO:C | 2.50 | 0.49 |
| 2:D:102:LEU:HD23 | 2:D:102:LEU:C | 2.33 | 0.49 |
| 1:A:1113:GLN:HA | 1:A:1113:GLN:OE1 | 2.12 | 0.49 |
| 1:A:576:LEU:HD22 | 1:A:578:HIS:H | 1.77 | 0.49 |
| 2:C:97:PRO:N | 2:C:202:ARG:HD3 | 2.28 | 0.49 |
| 2:D:103:LEU:O | 2:D:105:LEU:HD23 | 2.12 | 0.49 |
| 1:A:2:SER:HB2 | 1:A:995:VAL:CG2 | 2.42 | 0.49 |
| 1:A:365:VAL:CG1 | 1:A:367:LEU:HG | 2.43 | 0.49 |
| 1:B:477:ARG:HB3 | 1:B:489:GLU:HG3 | 1.95 | 0.49 |
| 1:B:485:ALA:O | 1:B:487:VAL:HG13 | 2.13 | 0.49 |
| 1:B:358:PRO:O | 1:B:379:SER:HA | 2.13 | 0.49 |
| 1:B:257:THR:HG22 | 1:B:258:ILE:N | 2.28 | 0.49 |
| 2:D:208:CYS:C | 2:D:210:GLN:N | 2.65 | 0.49 |
| 1:B:876:PHE:HD1 | 1:B:916:THR:HG21 | 1.78 | 0.49 |
| 1:B:114:ARG:HG3 | 1:B:137:ASP:OD2 | 2.12 | 0.49 |
| 1:B:451:PHE:CE2 | 1:B:453:ASP:HB3 | 2.48 | 0.49 |
| 1:B:267:ASN:HD21 | 1:B:269:SER:CB | 2.13 | 0.49 |
| 1:A:903:CYS:CB | 1:A:941:ASN:HA | 2.43 | 0.49 |
| 1:A:564:ILE:N | 1:A:564:ILE:CD1 | 2.75 | 0.49 |
| 1:A:582:LEU:O | 1:A:583:GLY:C | 2.51 | 0.49 |
| 1:B:665:LYS:HD3 | 1:B:1138:ARG:CZ | 2.43 | 0.49 |
| 2:C:179:TRP:O | 2:C:183:GLU:O | 2.30 | 0.49 |
| 1:B:771:PHE:HE2 | 1:B:845:GLN:HB2 | 1.76 | 0.49 |
| 1:A:44:VAL:HG11 | 1:A:317:LEU:HB3 | 1.94 | 0.49 |
| 2:C:40:LYS:HG2 | 2:C:42:THR:HG23 | 1.95 | 0.48 |
| 1:A:446:THR:HG22 | 1:A:447:GLU:N | 2.28 | 0.48 |
| 1:A:926:LEU:O | 1:A:953:TRP:HA | 2.12 | 0.48 |
| 1:A:657:THR:HG23 | 1:A:669:SER:O | 2.12 | 0.48 |
| 2:D:50:LEU:O | 2:D:51:LEU:C | 2.51 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:177:ILE:HG23 | 2:D:186:VAL:HG22 | 1.95 | 0.48 |
| 1:B:165:ILE:CD1 | 1:B:188:ARG:HH12 | 2.25 | 0.48 |
| 2:C:136:GLY:O | 2:C:139:ASN:O | 2.31 | 0.48 |
| 1:A:177:THR:CG2 | 1:A:194:GLU:HG2 | 2.43 | 0.48 |
| 1:A:589:ARG:NH1 | 1:A:589:ARG:HG2 | 2.28 | 0.48 |
| 1:A:1121:LYS:HB2 | 1:A:1121:LYS:HZ3 | 1.78 | 0.48 |
| 1:B:843:PRO:HD3 | 2:D:22:ASN:HD21 | 1.78 | 0.48 |
| 1:A:594:THR:CG2 | 1:A:595:THR:N | 2.75 | 0.48 |
| 1:A:876:PHE:HD1 | 1:A:916:THR:HG21 | 1.78 | 0.48 |
| 1:A:385:GLY:HA3 | 1:A:719:GLU:O | 2.13 | 0.48 |
| 2:C:160:ASP:OD2 | 2:C:161:PHE:N | 2.47 | 0.48 |
| 2:D:163:ARG:NH1 | 2:D:197:ILE:CD1 | 2.76 | 0.48 |
| 2:C:192:PRO:HB3 | 2:C:206:CYS:SG | 2.53 | 0.48 |
| 1:B:437:MET:CB | 1:B:446:THR:HG23 | 2.43 | 0.48 |
| 1:B:423:ASP:O | 1:B:438:LEU:HB2 | 2.12 | 0.48 |
| 1:A:487:VAL:O | 1:A:488:SER:HB2 | 2.13 | 0.48 |
| 1:B:612:PHE:CE2 | 1:B:628:LYS:HD2 | 2.49 | 0.48 |
| 1:A:288:GLU:HB3 | 1:A:296:THR:CG2 | 2.42 | 0.48 |
| 2:C:48:THR:HG23 | 2:C:82:LYS:HG2 | 1.94 | 0.48 |
| 1:B:1047:TRP:HZ3 | 1:B:1132:VAL:HG13 | 1.79 | 0.48 |
| 1:A:95:GLY:C | 1:A:97:SER:H | 2.15 | 0.48 |
| 1:A:413:LEU:HD23 | 1:A:462:ASN:OD1 | 2.14 | 0.48 |
| 1:A:81:THR:CG2 | 1:A:82:ALA:N | 2.75 | 0.48 |
| 1:A:741:GLU:CD | 1:A:750:THR:O | 2.52 | 0.48 |
| 1:B:52:VAL:HG23 | 1:B:53:LYS:N | 2.29 | 0.48 |
| 2:D:89:ASP:CG | 2:D:202:ARG:HH21 | 2.17 | 0.48 |
| 2:D:140:LEU:N | 2:D:140:LEU:HD23 | 2.29 | 0.48 |
| 1:A:239:TYR:CE2 | 1:A:241:ASN:HB2 | 2.48 | 0.48 |
| 2:D:173:ARG:NH1 | 2:D:190:CYS:SG | 2.87 | 0.48 |
| 2:C:50:LEU:HD22 | 2:C:86:VAL:HG21 | 1.95 | 0.48 |
| 1:B:239:TYR:CE2 | 1:B:241:ASN:HB2 | 2.48 | 0.48 |
| 1:B:1102:ARG:HD2 | 1:B:1105:MET:HE1 | 1.96 | 0.48 |
| 1:A:475:SER:HB2 | 1:A:490:TRP:O | 2.13 | 0.48 |
| 1:B:824:ASP:OD2 | 1:B:828:TYR:OH | 2.28 | 0.48 |
| 1:B:655:ARG:HG2 | 1:B:655:ARG:HH11 | 1.77 | 0.48 |
| 1:A:16:ASN:ND2 | 1:A:35:LYS:C | 2.56 | 0.48 |
| 1:B:480:SER:OG | 1:B:483:PRO:HD2 | 2.13 | 0.48 |
| 1:B:80:LEU:CD2 | 1:B:133:LEU:HD23 | 2.43 | 0.48 |
| 2:D:198:THR:HG21 | 2:D:204:PHE:HZ | 1.78 | 0.48 |
| 2:D:19:THR:HA | 2:D:43:ILE:HG23 | 1.96 | 0.48 |
| 1:B:617:ASN:OD1 | 1:B:619:GLU:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:542:ASP:OD1 | 1:A:593:MET:N | 2.45 | 0.48 |
| 1:B:786:VAL:O | 1:B:786:VAL:HG23 | 2.14 | 0.48 |
| 2:D:108:THR:CB | 2:D:109:PRO:CD | 2.92 | 0.48 |
| 1:B:286:GLU:HB3 | 1:B:298:LYS:HD3 | 1.95 | 0.48 |
| 1:B:1007:PHE:CD2 | 1:B:1030:PHE:HB3 | 2.49 | 0.48 |
| 2:C:18:GLU:OE1 | 2:C:40:LYS:HD2 | 2.14 | 0.48 |
| 1:A:537:GLU:O | 1:A:561:TRP:HB2 | 2.14 | 0.48 |
| 1:A:729:VAL:HG23 | 1:A:730:SER:N | 2.28 | 0.48 |
| 1:B:476:VAL:C | 1:B:477:ARG:HD3 | 2.34 | 0.48 |
| 1:B:162:LEU:N | 1:B:162:LEU:HD23 | 2.17 | 0.48 |
| 1:B:1015:GLN:O | 1:B:1016:ASN:C | 2.52 | 0.48 |
| 1:B:459:PHE:CD2 | 1:B:503:CYS:HB3 | 2.48 | 0.48 |
| 1:B:835:MET:HB2 | 1:B:845:GLN:HG3 | 1.95 | 0.48 |
| 2:D:115:LEU:HG | 2:D:130:VAL:HG13 | 1.96 | 0.48 |
| 1:B:456:GLN:O | 1:B:472:THR:HG22 | 2.14 | 0.47 |
| 1:B:81:THR:HG22 | 1:B:83:LYS:N | 2.06 | 0.47 |
| 1:B:731:GLN:C | 1:B:796:GLN:HE21 | 2.17 | 0.47 |
| 1:B:1014:MET:O | 1:B:1015:GLN:HB3 | 2.14 | 0.47 |
| 2:D:103:LEU:O | 2:D:105:LEU:N | 2.47 | 0.47 |
| 1:B:794:ILE:HG22 | 1:B:799:PHE:HA | 1.96 | 0.47 |
| 1:B:32:LEU:HD12 | 1:B:32:LEU:N | 2.28 | 0.47 |
| 1:B:427:LEU:HD13 | 1:B:429:PHE:CE1 | 2.48 | 0.47 |
| 1:A:1051:LEU:HB2 | 1:A:1089:ILE:HD13 | 1.95 | 0.47 |
| 1:A:1102:ARG:N | 1:A:1103:PRO:CD | 2.78 | 0.47 |
| 1:B:532:THR:HB | 1:B:574:PHE:CD1 | 2.49 | 0.47 |
| 2:C:177:ILE:HD12 | 2:C:177:ILE:N | 2.29 | 0.47 |
| 2:C:215:CYS:H | 2:C:218:CYS:CB | 2.27 | 0.47 |
| 1:A:112:ILE:CD1 | 1:A:112:ILE:H | 2.20 | 0.47 |
| 1:B:207:TRP:CZ3 | 1:B:241:ASN:O | 2.68 | 0.47 |
| 1:B:991:HIS:HB3 | 1:B:993:GLN:NE2 | 2.29 | 0.47 |
| 1:B:199:GLU:HG3 | 1:B:201:GLU:CG | 2.45 | 0.47 |
| 1:A:1051:LEU:CB | 1:A:1089:ILE:HD13 | 2.44 | 0.47 |
| 2:D:21:LEU:HD22 | 2:D:26:TYR:HD1 | 1.78 | 0.47 |
| 1:B:847:ARG:NH1 | 1:B:849:VAL:HG22 | 2.29 | 0.47 |
| 1:A:520:GLN:HG3 | 1:A:529:ILE:HD12 | 1.97 | 0.47 |
| 2:C:16:LEU:O | 2:C:41:ASN:HB2 | 2.14 | 0.47 |
| 1:B:458:PHE:CD1 | 1:B:458:PHE:N | 2.82 | 0.47 |
| 1:B:68:ARG:HB2 | 1:B:75:ASP:OD2 | 2.14 | 0.47 |
| 1:B:571:LEU:C | 1:B:571:LEU:HD13 | 2.34 | 0.47 |
| 1:A:59:GLY:HA2 | 1:A:1073:TRP:CE3 | 2.48 | 0.47 |
| 1:A:256:SER:HB3 | 1:A:275:ASP:OD1 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:242:GLY:O | 1:B:243:ASP:HB2 | 2.14 | 0.47 |
| 1:A:570:LYS:HG3 | 1:A:572:PRO:HD2 | 1.97 | 0.47 |
| 1:A:333:LEU:HA | 1:A:333:LEU:HD12 | 1.75 | 0.47 |
| 2:D:16:LEU:O | 2:D:41:ASN:HB3 | 2.14 | 0.47 |
| 1:B:1115:ASP:HB2 | 1:B:1120:MET:CB | 2.45 | 0.47 |
| 1:B:1048:TYR:HE2 | 1:B:1052:LEU:HD12 | 1.79 | 0.47 |
| 1:A:213:GLU:OE1 | 1:A:236:SER:HB3 | 2.14 | 0.47 |
| 1:B:886:SER:O | 1:B:908:ASN:ND2 | 2.48 | 0.47 |
| 1:B:449:MET:HA | 1:B:449:MET:HE2 | 1.97 | 0.47 |
| 1:A:889:ARG:CD | 1:A:901:THR:HG23 | 2.44 | 0.47 |
| 1:A:518:TYR:CD1 | 1:A:571:LEU:HD22 | 2.49 | 0.47 |
| 1:B:289:GLU:OE2 | 1:B:289:GLU:HA | 2.14 | 0.47 |
| 1:B:253:ILE:HG22 | 1:B:253:ILE:O | 2.15 | 0.47 |
| 1:B:147:ARG:NE | 1:B:147:ARG:HA | 2.26 | 0.47 |
| 1:A:771:PHE:CD1 | 1:A:835:MET:HE2 | 2.50 | 0.47 |
| 1:A:597:GLU:HG3 | 1:A:661:SER:HB3 | 1.95 | 0.47 |
| 2:D:90:ASP:CG | 2:D:91:LYS:H | 2.18 | 0.47 |
| 1:A:367:LEU:HD12 | 1:A:374:GLN:NE2 | 2.30 | 0.47 |
| 1:A:1055:GLN:HE22 | 1:A:1090:ASP:H | 1.63 | 0.47 |
| 1:A:364:VAL:HG21 | 1:A:1010:GLY:HA3 | 1.97 | 0.47 |
| 1:B:722:ARG:NH1 | 2:D:28:THR:HG21 | 2.30 | 0.47 |
| 1:B:514:ARG:HB2 | 1:B:537:GLU:HA | 1.96 | 0.47 |
| 1:A:867:LYS:CE | 1:A:889:ARG:NH2 | 2.77 | 0.47 |
| 1:B:976:VAL:HG22 | 1:B:996:GLY:CA | 2.35 | 0.47 |
| 1:B:1125:THR:HG22 | 1:B:1126:ALA:N | 2.30 | 0.47 |
| 1:B:290:GLN:HG3 | 1:B:293:GLY:H | 1.80 | 0.47 |
| 1:B:131:ILE:HB | 1:B:143:ILE:HB | 1.96 | 0.47 |
| 1:B:739:ARG:NH1 | 1:B:757:SER:OG | 2.47 | 0.47 |
| 1:A:969:GLU:OE2 | 1:A:971:ALA:HB3 | 2.14 | 0.47 |
| 1:B:458:PHE:HD1 | 1:B:458:PHE:N | 2.13 | 0.47 |
| 1:A:550:ASN:O | 1:A:552:LEU:N | 2.48 | 0.47 |
| 2:D:108:THR:HB | 2:D:109:PRO:CD | 2.41 | 0.47 |
| 1:B:275:ASP:HB3 | 1:B:277:GLU:H | 1.80 | 0.47 |
| 2:D:116:ASP:O | 2:D:118:SER:N | 2.45 | 0.47 |
| 1:A:235:GLU:O | 1:A:249:ALA:HA | 2.15 | 0.47 |
| 2:D:47:VAL:HG12 | 2:D:48:THR:H | 1.79 | 0.47 |
| 1:A:19:VAL:HG22 | 1:A:20:THR:H | 1.78 | 0.47 |
| 1:A:213:GLU:OE2 | 1:A:215:GLU:HB2 | 2.14 | 0.47 |
| 1:A:479:VAL:HG12 | 1:A:480:SER:O | 2.15 | 0.47 |
| 1:B:832:GLY:N | 1:B:873:MET:HE2 | 2.30 | 0.47 |
| 1:B:498:ILE:HG23 | 1:B:512:VAL:HG22 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:172:ARG:CZ | 2:C:197:ILE:HG22 | 2.44 | 0.46 |
| 1:A:741:GLU:HB3 | 1:A:750:THR:O | 2.14 | 0.46 |
| 1:A:870:VAL:HG22 | 1:A:884:ILE:HG13 | 1.96 | 0.46 |
| 1:A:465:HIS:O | 1:A:467:GLN:HG3 | 2.15 | 0.46 |
| 1:B:1044:SER:HG | 1:B:1047:TRP:HD1 | 1.62 | 0.46 |
| 1:B:390:ILE:HG22 | 1:B:710:LEU:HD22 | 1.96 | 0.46 |
| 1:A:110:ASP:HB2 | 1:A:136:TYR:CE1 | 2.50 | 0.46 |
| 1:B:124:ILE:HG23 | 1:B:131:ILE:CD1 | 2.42 | 0.46 |
| 1:B:1065:VAL:C | 1:B:1067:LYS:N | 2.69 | 0.46 |
| 1:B:309:SER:O | 1:B:310:ILE:C | 2.54 | 0.46 |
| 2:D:90:ASP:CG | 2:D:91:LYS:N | 2.68 | 0.46 |
| 1:A:465:HIS:HB2 | 1:A:467:GLN:HE21 | 1.79 | 0.46 |
| 1:A:717:LEU:O | 1:A:718:TYR:HB2 | 2.15 | 0.46 |
| 1:B:368:GLU:O | 1:B:369:ARG:C | 2.53 | 0.46 |
| 2:C:147:GLU:HG2 | 2:C:172:ARG:HG3 | 1.96 | 0.46 |
| 1:B:408:LYS:CB | 1:B:430:VAL:HG23 | 2.44 | 0.46 |
| 1:B:475:SER:HA | 1:B:498:ILE:CD1 | 2.42 | 0.46 |
| 2:C:161:PHE:CD1 | 2:C:197:ILE:HD12 | 2.51 | 0.46 |
| 1:B:436:LEU:HA | 1:B:445:GLU:HA | 1.97 | 0.46 |
| 1:B:789:HIS:ND1 | 1:B:812:TYR:HA | 2.31 | 0.46 |
| 1:A:927:MET:CE | 2:C:130:VAL:HG11 | 2.46 | 0.46 |
| 1:A:360:VAL:HG12 | 1:A:360:VAL:O | 2.16 | 0.46 |
| 1:B:226:PHE:CD1 | 1:B:226:PHE:N | 2.84 | 0.46 |
| 1:B:466:GLN:H | 1:B:466:GLN:NE2 | 2.07 | 0.46 |
| 1:A:1121:LYS:HD3 | 1:A:1122:ARG:H | 1.81 | 0.46 |
| 1:A:1097:PHE:CZ | 1:A:1105:MET:HG2 | 2.50 | 0.46 |
| 1:B:790:ASN:HA | 1:B:807:PHE:CD1 | 2.51 | 0.46 |
| 1:A:745:THR:HG23 | 1:A:782:PHE:CE1 | 2.51 | 0.46 |
| 1:A:234:GLN:O | 1:A:235:GLU:CG | 2.63 | 0.46 |
| 1:A:750:THR:CG2 | 1:A:751:ALA:H | 2.17 | 0.46 |
| 2:D:43:ILE:O | 2:D:43:ILE:HG23 | 2.15 | 0.46 |
| 1:B:683:ASN:HA | 1:B:688:PRO:O | 2.14 | 0.46 |
| 1:B:1002:GLU:HB3 | 1:B:1032:THR:CG2 | 2.45 | 0.46 |
| 1:B:518:TYR:CZ | 1:B:571:LEU:HD11 | 2.50 | 0.46 |
| 1:B:983:ALA:O | 1:B:985:THR:N | 2.44 | 0.46 |
| 1:B:63:VAL:CB | 1:B:80:LEU:HB3 | 2.43 | 0.46 |
| 1:B:699:LEU:HD13 | 1:B:699:LEU:C | 2.35 | 0.46 |
| 1:A:839:GLU:N | 1:A:839:GLU:CD | 2.69 | 0.46 |
| 2:C:178:GLY:C | 2:C:179:TRP:HE3 | 2.19 | 0.46 |
| 1:B:59:GLY:HA2 | 1:B:1073:TRP:CZ3 | 2.50 | 0.46 |
| 1:B:142:VAL:O | 1:B:154:ALA:HB1 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:881:LEU:CD2 | 1:B:921:ILE:HD12 | 2.46 | 0.46 |
| 1:B:984:THR:HG22 | 1:B:984:THR:O | 2.15 | 0.46 |
| 1:B:134:ARG:HD2 | 1:B:134:ARG:C | 2.36 | 0.46 |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:H | 1.80 | 0.46 |
| 2:D:52:THR:OG1 | 2:D:85:ILE:HA | 2.15 | 0.46 |
| 1:A:342:GLU:C | 1:A:344:GLY:H | 2.20 | 0.46 |
| 1:B:662:SER:HB2 | 1:B:1138:ARG:HH21 | 1.79 | 0.46 |
| 1:B:414:ARG:HH11 | 1:B:414:ARG:HG2 | 1.81 | 0.46 |
| 1:B:1014:MET:CG | 1:B:1015:GLN:H | 2.28 | 0.46 |
| 1:B:311:ALA:HB2 | 1:B:324:VAL:HG13 | 1.98 | 0.46 |
| 1:A:665:LYS:HB3 | 1:A:1138:ARG:NH2 | 2.31 | 0.46 |
| 2:D:17:ILE:HG22 | 2:D:17:ILE:O | 2.16 | 0.46 |
| 2:D:28:THR:HA | 2:D:31:GLN:HE21 | 1.80 | 0.46 |
| 1:A:1098:LEU:HD11 | 1:A:1133:VAL:HG12 | 1.97 | 0.46 |
| 1:B:447:GLU:O | 1:B:448:LEU:HD12 | 2.15 | 0.46 |
| 2:D:171:HIS:HA | 2:D:193:SER:H | 1.81 | 0.46 |
| 2:D:149:ARG:O | 2:D:150:GLU:O | 2.33 | 0.46 |
| 1:B:289:GLU:OE2 | 1:B:295:VAL:HG12 | 2.16 | 0.46 |
| 1:B:250:PRO:C | 1:B:252:ILE:H | 2.18 | 0.46 |
| 2:D:206:CYS:SG | 2:D:208:CYS:O | 2.74 | 0.46 |
| 1:A:234:GLN:O | 1:A:235:GLU:CB | 2.64 | 0.46 |
| 1:B:124:ILE:HG12 | 1:B:131:ILE:CD1 | 2.46 | 0.46 |
| 1:A:594:THR:HG23 | 1:A:595:THR:H | 1.80 | 0.46 |
| 1:B:151:GLU:N | 1:B:151:GLU:CD | 2.70 | 0.46 |
| 1:A:269:SER:O | 1:A:284:LEU:HA | 2.15 | 0.46 |
| 2:D:208:CYS:O | 2:D:208:CYS:SG | 2.75 | 0.45 |
| 1:B:905:HIS:CD2 | 1:B:933:LEU:HD21 | 2.50 | 0.45 |
| 1:B:1048:TYR:CE2 | 1:B:1052:LEU:HD12 | 2.51 | 0.45 |
| 1:A:131:ILE:HG22 | 1:A:133:LEU:HD13 | 1.98 | 0.45 |
| 1:B:367:LEU:CG | 1:B:374:GLN:CD | 2.80 | 0.45 |
| 1:B:994:GLU:CG | 1:B:995:VAL:H | 2.29 | 0.45 |
| 1:B:706:GLU:O | 1:B:707:ILE:CB | 2.64 | 0.45 |
| 1:A:116:SER:C | 1:A:117:GLU:O | 2.51 | 0.45 |
| 1:A:334:VAL:HG22 | 1:A:349:ALA:HA | 1.98 | 0.45 |
| 1:B:426:VAL:HG22 | 1:B:435:VAL:HG13 | 1.99 | 0.45 |
| 1:B:412:PRO:HB2 | 1:B:422:TYR:CD2 | 2.51 | 0.45 |
| 1:B:422:TYR:HD1 | 1:B:422:TYR:H | 1.63 | 0.45 |
| 1:B:23:PHE:N | 1:B:30:ASN:ND2 | 2.53 | 0.45 |
| 1:A:396:ILE:N | 1:A:396:ILE:HD13 | 2.11 | 0.45 |
| 1:B:52:VAL:CG2 | 1:B:53:LYS:N | 2.80 | 0.45 |
| 1:A:576:LEU:HD22 | 1:A:578:HIS:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1029:LEU:HD23 | 1:B:1039:LEU:HD13 | 1.97 | 0.45 |
| 2:C:97:PRO:HA | 2:C:202:ARG:HG2 | 1.97 | 0.45 |
| 2:D:100:ASN:HB3 | 2:D:103:LEU:HD12 | 1.97 | 0.45 |
| 1:A:892:GLU:O | 1:A:899:VAL:HA | 2.16 | 0.45 |
| 1:A:18:CYS:N | 1:A:313:CYS:SG | 2.89 | 0.45 |
| 1:A:809:GLN:O | 1:A:810:ASN:HB2 | 2.16 | 0.45 |
| 1:A:652:CYS:HB3 | 1:A:676:VAL:O | 2.17 | 0.45 |
| 1:B:6:VAL:HG22 | 1:B:1088:PHE:HD2 | 1.80 | 0.45 |
| 1:B:430:VAL:C | 1:B:431:GLY:O | 2.52 | 0.45 |
| 2:D:172:ARG:NH2 | 2:D:191:ASN:HD22 | 2.14 | 0.45 |
| 1:B:250:PRO:O | 1:B:252:ILE:N | 2.49 | 0.45 |
| 2:D:116:ASP:C | 2:D:118:SER:H | 2.19 | 0.45 |
| 1:A:596:PHE:HB3 | 1:A:661:SER:HB2 | 1.98 | 0.45 |
| 1:B:679:MET:HE2 | 1:B:691:LEU:HD23 | 1.98 | 0.45 |
| 1:B:5:TYR:HE2 | 1:B:7:VAL:HG21 | 1.82 | 0.45 |
| 2:C:35:THR:CG2 | 2:C:36:SER:O | 2.33 | 0.45 |
| 1:A:166:ASP:HB3 | 1:A:219:VAL:HG23 | 1.98 | 0.45 |
| 1:B:424:THR:HG22 | 1:B:425:LEU:N | 2.32 | 0.45 |
| 2:C:50:LEU:O | 2:C:143:ARG:HB2 | 2.17 | 0.45 |
| 1:B:690:SER:O | 1:B:691:LEU:HD12 | 2.16 | 0.45 |
| 1:A:864:LYS:HE2 | 1:A:891:TYR:CE2 | 2.49 | 0.45 |
| 1:B:263:ARG:HB2 | 1:B:271:TYR:CE2 | 2.51 | 0.45 |
| 1:A:410:LEU:CD2 | 1:A:410:LEU:N | 2.80 | 0.45 |
| 1:B:539:ALA:HB2 | 1:B:561:TRP:CD1 | 2.51 | 0.45 |
| 1:B:853:TYR:HB2 | 1:B:858:LEU:HD23 | 1.99 | 0.45 |
| 2:D:109:PRO:HB2 | 2:D:203:ARG:HH21 | 1.81 | 0.45 |
| 2:C:161:PHE:CE1 | 2:C:197:ILE:HG23 | 2.51 | 0.45 |
| 2:C:52:THR:O | 2:C:53:ASN:C | 2.45 | 0.45 |
| 1:B:10:GLN:NE2 | 1:B:11:LYS:N | 2.64 | 0.45 |
| 2:D:168:GLY:HA3 | 2:D:208:CYS:SG | 2.55 | 0.45 |
| 1:B:196:SER:O | 1:B:200:LYS:HA | 2.16 | 0.45 |
| 1:B:402:ILE:HD13 | 1:B:699:LEU:HD12 | 1.99 | 0.45 |
| 1:B:317:LEU:HD12 | 1:B:321:VAL:HG12 | 1.99 | 0.45 |
| 2:C:89:ASP:OD1 | 2:C:90:ASP:N | 2.37 | 0.45 |
| 1:A:520:GLN:HG3 | 1:A:529:ILE:CD1 | 2.47 | 0.45 |
| 1:B:728:GLU:C | 1:B:730:SER:H | 2.20 | 0.45 |
| 2:D:169:GLY:C | 2:D:212:PRO:HD2 | 2.24 | 0.45 |
| 1:B:569:LEU:CD2 | 1:B:576:LEU:HA | 2.46 | 0.45 |
| 1:B:1066:GLY:O | 1:B:1067:LYS:HB2 | 2.16 | 0.45 |
| 1:B:29:LEU:HG | 1:B:44:VAL:HG21 | 1.99 | 0.45 |
| 1:B:732:CYS:HB2 | 1:B:794:ILE:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:397:HIS:O | 1:B:702:GLY:HA3 | 2.16 | 0.45 |
| 1:A:308:THR:O | 1:A:383:LYS:NZ | 2.49 | 0.45 |
| 1:A:860:THR:O | 1:A:860:THR:HG22 | 2.17 | 0.45 |
| 2:D:169:GLY:CA | 2:D:211:CYS:HA | 2.46 | 0.45 |
| 2:D:42:THR:HG22 | 2:D:43:ILE:N | 2.31 | 0.45 |
| 1:B:63:VAL:CG2 | 1:B:80:LEU:HD23 | 2.47 | 0.45 |
| 1:A:837:TYR:HB2 | 1:A:840:GLU:HG3 | 1.98 | 0.45 |
| 1:B:644:LEU:HD23 | 1:B:645:SER:H | 1.81 | 0.45 |
| 2:D:17:ILE:HD11 | 2:D:139:ASN:HD22 | 1.80 | 0.45 |
| 1:A:584:GLY:O | 1:B:900:ARG:NH2 | 2.49 | 0.45 |
| 1:B:529:ILE:N | 1:B:529:ILE:HD13 | 2.32 | 0.45 |
| 1:B:451:PHE:HB2 | 1:B:486:LEU:HD13 | 1.98 | 0.45 |
| 1:B:1127:ASP:HA | 1:B:1130:ILE:HD12 | 1.98 | 0.45 |
| 1:A:1118:SER:C | 1:A:1120:MET:N | 2.70 | 0.45 |
| 1:B:42:TYR:CD2 | 1:B:49:LEU:HB3 | 2.52 | 0.45 |
| 2:C:102:LEU:C | 2:C:104:GLY:H | 2.21 | 0.45 |
| 1:B:449:MET:HE3 | 1:B:449:MET:HA | 1.98 | 0.44 |
| 2:C:147:GLU:CG | 2:C:172:ARG:HG3 | 2.47 | 0.44 |
| 1:B:81:THR:OG1 | 1:B:85:ASN:HB2 | 2.16 | 0.44 |
| 1:B:192:THR:CB | 1:B:206:PRO:HD2 | 2.47 | 0.44 |
| 2:C:109:PRO:CG | 2:C:203:ARG:NH1 | 2.80 | 0.44 |
| 1:A:304:LEU:HD12 | 1:A:305:LEU:H | 1.82 | 0.44 |
| 1:B:63:VAL:HG21 | 1:B:80:LEU:HD23 | 1.98 | 0.44 |
| 1:A:487:VAL:CG2 | 1:A:524:GLN:HA | 2.46 | 0.44 |
| 1:B:37:THR:HG22 | 1:B:59:GLY:O | 2.18 | 0.44 |
| 1:A:587:ILE:CD1 | 1:A:587:ILE:H | 2.30 | 0.44 |
| 2:C:33:THR:HG22 | 2:C:35:THR:H | 1.81 | 0.44 |
| 1:A:865:GLU:HG2 | 1:A:866:VAL:N | 2.32 | 0.44 |
| 1:B:384:GLU:N | 1:B:384:GLU:OE2 | 2.50 | 0.44 |
| 1:B:139:LEU:HD22 | 1:B:156:ASN:HB3 | 1.99 | 0.44 |
| 1:B:894:THR:CG2 | 1:B:895:THR:N | 2.78 | 0.44 |
| 1:A:762:SER:HB3 | 1:A:803:HIS:ND1 | 2.32 | 0.44 |
| 1:A:546:LEU:HD11 | 1:A:593:MET:HB3 | 1.99 | 0.44 |
| 2:C:98:ILE:HG13 | 2:C:189:TRP:CZ2 | 2.53 | 0.44 |
| 1:B:10:GLN:HE21 | 1:B:11:LYS:N | 2.16 | 0.44 |
| 2:D:116:ASP:O | 2:D:182:ASP:CB | 2.62 | 0.44 |
| 1:A:582:LEU:O | 1:A:583:GLY:O | 2.35 | 0.44 |
| 1:B:538:VAL:HG22 | 1:B:558:ILE:HD11 | 1.98 | 0.44 |
| 1:A:282:MET:CG | 1:A:305:LEU:HD11 | 2.44 | 0.44 |
| 1:B:573:SER:O | 1:B:574:PHE:CB | 2.66 | 0.44 |
| 1:A:346:TYR:CD1 | 1:A:346:TYR:N | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:113:THR:HA | 2:C:124:SER:O | 2.17 | 0.44 |
| 1:B:602:LEU:HD13 | 1:B:602:LEU:C | 2.38 | 0.44 |
| 1:B:124:ILE:HG12 | 1:B:131:ILE:HD12 | 1.99 | 0.44 |
| 2:D:47:VAL:CG1 | 2:D:48:THR:N | 2.80 | 0.44 |
| 1:A:1121:LYS:HA | 1:A:1121:LYS:HZ2 | 1.83 | 0.44 |
| 1:A:738:SER:OG | 1:A:787:GLU:HG2 | 2.17 | 0.44 |
| 1:B:704:ILE:CD1 | 1:B:704:ILE:H | 2.29 | 0.44 |
| 1:B:984:THR:O | 1:B:986:ASP:N | 2.51 | 0.44 |
| 2:C:102:LEU:O | 2:C:104:GLY:N | 2.50 | 0.44 |
| 1:A:69:PRO:HD2 | 1:A:72:GLU:HG3 | 1.98 | 0.44 |
| 1:A:7:VAL:HG13 | 1:A:1091:GLY:HA3 | 2.00 | 0.44 |
| 1:A:874:VAL:HG13 | 1:A:881:LEU:HB3 | 2.00 | 0.44 |
| 1:A:704:ILE:HG23 | 1:A:705:ASP:N | 2.32 | 0.44 |
| 2:C:119:GLY:O | 2:C:120:LYS:CB | 2.66 | 0.44 |
| 1:B:342:GLU:O | 1:B:344:GLY:N | 2.51 | 0.44 |
| 1:B:222:VAL:CG1 | 1:B:223:PRO:HD2 | 2.47 | 0.44 |
| 1:B:246:LEU:HD11 | 1:B:299:ASP:HA | 1.99 | 0.44 |
| 1:B:286:GLU:O | 1:B:298:LYS:N | 2.45 | 0.44 |
| 2:C:145:ILE:HD11 | 2:C:174:GLU:OE2 | 2.18 | 0.44 |
| 2:D:147:GLU:HA | 2:D:148:PRO:HD3 | 1.83 | 0.44 |
| 1:B:416:ASP:HA | 1:B:417:PRO:HD3 | 1.86 | 0.44 |
| 1:B:482:GLU:CB | 1:B:483:PRO:CD | 2.92 | 0.44 |
| 1:B:482:GLU:HB2 | 1:B:483:PRO:CD | 2.32 | 0.44 |
| 1:B:47:GLU:HG2 | 1:B:48:GLY:N | 2.25 | 0.44 |
| 1:A:931:LEU:HD12 | 1:A:947:ARG:HH22 | 1.83 | 0.44 |
| 1:A:291:MET:HG3 | 1:A:292:ASP:N | 2.29 | 0.44 |
| 1:B:1017:LEU:C | 1:B:1019:GLU:H | 2.20 | 0.44 |
| 1:A:29:LEU:HG | 1:A:44:VAL:CG2 | 2.47 | 0.44 |
| 2:D:172:ARG:NE | 2:D:174:GLU:OE2 | 2.50 | 0.44 |
| 1:B:140:PHE:CZ | 1:B:178:ILE:HD12 | 2.53 | 0.44 |
| 1:A:745:THR:C | 1:A:747:GLY:H | 2.21 | 0.44 |
| 1:A:663:ASN:O | 1:A:664:HIS:CB | 2.64 | 0.44 |
| 1:B:355:ASN:CG | 1:B:357:GLY:H | 2.21 | 0.44 |
| 1:B:644:LEU:CG | 1:B:645:SER:N | 2.81 | 0.44 |
| 2:D:22:ASN:HD22 | 2:D:22:ASN:C | 2.20 | 0.44 |
| 2:C:89:ASP:OD2 | 2:C:202:ARG:NH2 | 2.51 | 0.44 |
| 1:A:1007:PHE:CD2 | 1:A:1030:PHE:HB3 | 2.53 | 0.44 |
| 1:B:1080:ARG:HG3 | 1:B:1081:LYS:N | 2.32 | 0.44 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:HA | 2.00 | 0.43 |
| 1:B:376:VAL:HA | 1:B:388:ARG:O | 2.18 | 0.43 |
| 1:A:275:ASP:HB3 | 1:A:279:ARG:N | 2.30 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:616:LEU:HD12 | 1:B:617:ASN:H | 1.80 | 0.43 |
| 1:A:95:GLY:C | 1:A:97:SER:N | 2.71 | 0.43 |
| 1:A:587:ILE:HD13 | 1:A:587:ILE:N | 2.32 | 0.43 |
| 1:A:23:PHE:CE2 | 1:A:91:TYR:HB2 | 2.53 | 0.43 |
| 1:B:192:THR:HB | 1:B:206:PRO:HD2 | 2.00 | 0.43 |
| 1:B:358:PRO:HA | 1:B:1033:VAL:O | 2.18 | 0.43 |
| 1:A:705:ASP:OD2 | 1:A:709:LYS:CE | 2.59 | 0.43 |
| 1:A:480:SER:HB3 | 1:A:487:VAL:CG1 | 2.46 | 0.43 |
| 1:B:130:MET:HA | 1:B:145:LEU:HB2 | 2.00 | 0.43 |
| 1:B:1115:ASP:HB2 | 1:B:1120:MET:HB2 | 2.00 | 0.43 |
| 1:A:734:GLY:HA3 | 1:A:829:PHE:CE1 | 2.53 | 0.43 |
| 1:B:821:LEU:O | 1:B:822:GLY:C | 2.57 | 0.43 |
| 1:A:1:MET:CE | 1:A:1:MET:HA | 2.48 | 0.43 |
| 1:A:78:PHE:O | 1:A:79:ILE:HG12 | 2.18 | 0.43 |
| 1:B:456:GLN:CD | 1:B:473:SER:CB | 2.64 | 0.43 |
| 1:B:514:ARG:CG | 1:B:514:ARG:O | 2.63 | 0.43 |
| 1:B:81:THR:HG22 | 1:B:82:ALA:N | 2.34 | 0.43 |
| 1:B:9:ALA:HB3 | 1:B:1037:ILE:HG22 | 2.01 | 0.43 |
| 1:B:843:PRO:HG2 | 2:D:24:VAL:HG21 | 2.00 | 0.43 |
| 1:A:516:LEU:HD23 | 1:A:574:PHE:CE2 | 2.53 | 0.43 |
| 1:A:90:GLU:HB3 | 1:A:101:ILE:HG13 | 2.00 | 0.43 |
| 1:A:405:PRO:HA | 1:A:697:SER:HA | 2.00 | 0.43 |
| 1:B:570:LYS:HE2 | 1:B:577:LEU:HD11 | 2.00 | 0.43 |
| 1:A:744:ASP:HA | 1:A:782:PHE:CE1 | 2.53 | 0.43 |
| 1:A:936:LYS:HB3 | 1:A:939:GLU:HB2 | 2.00 | 0.43 |
| 1:B:112:ILE:N | 1:B:112:ILE:CD1 | 2.78 | 0.43 |
| 1:B:782:PHE:CD2 | 1:B:782:PHE:N | 2.86 | 0.43 |
| 1:B:694:ALA:HA | 1:B:698:THR:O | 2.18 | 0.43 |
| 1:B:1115:ASP:HA | 1:B:1120:MET:HB3 | 2.00 | 0.43 |
| 2:D:115:LEU:CD1 | 2:D:130:VAL:HG13 | 2.48 | 0.43 |
| 1:A:177:THR:HG22 | 1:A:194:GLU:HA | 2.00 | 0.43 |
| 1:B:150:LYS:HB2 | 1:B:151:GLU:OE2 | 2.18 | 0.43 |
| 1:B:941:ASN:HD22 | 1:B:941:ASN:C | 2.22 | 0.43 |
| 2:D:211:CYS:HA | 2:D:212:PRO:HD2 | 1.81 | 0.43 |
| 1:A:1032:THR:CG2 | 1:A:1034:ASN:H | 2.23 | 0.43 |
| 1:B:356:LEU:O | 1:B:357:GLY:C | 2.57 | 0.43 |
| 1:B:263:ARG:HG2 | 1:B:263:ARG:HH11 | 1.83 | 0.43 |
| 1:B:903:CYS:SG | 1:B:941:ASN:HA | 2.59 | 0.43 |
| 1:B:874:VAL:HG22 | 1:B:875:GLU:O | 2.18 | 0.43 |
| 1:B:543:ILE:N | 1:B:543:ILE:HD13 | 2.33 | 0.43 |
| 1:A:401:SER:C | 1:A:402:ILE:HD13 | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1039:LEU:HD12 | 1:A:1040:VAL:H | 1.83 | 0.43 |
| 1:A:679:MET:SD | 1:A:680:CYS:N | 2.92 | 0.43 |
| 1:B:237:ILE:HD11 | 1:B:253:ILE:HD11 | 2.00 | 0.43 |
| 1:A:931:LEU:HD12 | 1:A:947:ARG:NH2 | 2.33 | 0.43 |
| 1:A:762:SER:CB | 1:A:803:HIS:ND1 | 2.82 | 0.43 |
| 1:A:256:SER:HB3 | 1:A:275:ASP:CG | 2.39 | 0.43 |
| 1:B:222:VAL:HA | 1:B:223:PRO:HD3 | 1.82 | 0.43 |
| 2:D:104:GLY:C | 2:D:105:LEU:HD23 | 2.39 | 0.43 |
| 1:A:318:ASP:O | 1:A:319:ASN:C | 2.57 | 0.43 |
| 1:B:248:ILE:O | 1:B:250:PRO:HD3 | 2.19 | 0.43 |
| 1:A:614:PHE:N | 1:A:614:PHE:CD1 | 2.86 | 0.43 |
| 1:B:740:ILE:HD12 | 1:B:740:ILE:H | 1.82 | 0.43 |
| 1:B:832:GLY:N | 1:B:873:MET:CE | 2.82 | 0.43 |
| 1:B:728:GLU:O | 1:B:730:SER:N | 2.51 | 0.43 |
| 2:C:143:ARG:HH11 | 2:C:143:ARG:HG3 | 1.84 | 0.43 |
| 2:D:80:ARG:HB2 | 2:D:81:PRO:CD | 2.36 | 0.43 |
| 1:B:518:TYR:OH | 1:B:571:LEU:HD11 | 2.18 | 0.43 |
| 1:A:58:TYR:HB3 | 1:A:1073:TRP:HB2 | 2.01 | 0.43 |
| 1:A:948:ASP:N | 1:A:992:LEU:HD11 | 2.33 | 0.43 |
| 1:A:532:THR:CG2 | 1:A:533:GLU:N | 2.81 | 0.43 |
| 1:A:522:HIS:HB3 | 1:A:523:PRO:CD | 2.49 | 0.43 |
| 1:B:155:PHE:HE1 | 1:B:157:ILE:HD11 | 1.83 | 0.43 |
| 2:D:218:CYS:CB | 2:D:221:ASP:OD1 | 2.67 | 0.43 |
| 1:B:452:VAL:HG22 | 1:B:453:ASP:N | 2.34 | 0.43 |
| 1:B:463:VAL:HG23 | 1:B:467:GLN:HB2 | 2.01 | 0.43 |
| 1:B:523:PRO:C | 1:B:524:GLN:NE2 | 2.72 | 0.43 |
| 1:B:226:PHE:HB2 | 1:B:227:GLY:H | 1.65 | 0.43 |
| 1:B:191:LYS:HD3 | 1:B:193:TYR:CE2 | 2.54 | 0.43 |
| 1:A:518:TYR:CE1 | 1:A:571:LEU:HD22 | 2.53 | 0.43 |
| 2:D:192:PRO:CG | 2:D:206:CYS:HB2 | 2.48 | 0.43 |
| 1:A:10:GLN:HG2 | 1:A:710:LEU:HD12 | 1.99 | 0.43 |
| 2:D:89:ASP:O | 2:D:90:ASP:O | 2.37 | 0.43 |
| 1:B:170:LEU:HD11 | 1:B:179:CYS:HB2 | 2.00 | 0.43 |
| 1:B:281:PHE:O | 1:B:305:LEU:HD12 | 2.18 | 0.43 |
| 1:B:380:GLY:O | 1:B:381:ALA:HB2 | 2.18 | 0.43 |
| 1:B:375:LEU:HD23 | 1:B:375:LEU:HA | 1.85 | 0.43 |
| 2:D:44:PRO:HA | 2:D:45:PRO:HD3 | 1.94 | 0.43 |
| 1:A:504:ASN:OD1 | 1:A:507:GLN:HG3 | 2.18 | 0.43 |
| 1:A:1032:THR:HG22 | 1:A:1035:GLY:N | 2.34 | 0.43 |
| 1:B:894:THR:HG22 | 1:B:895:THR:H | 1.82 | 0.43 |
| 1:B:46:ALA:HB3 | 1:B:47:GLU:OE1 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1109:VAL:O | 1:B:1110:ALA:O | 2.37 | 0.43 |
| 1:B:919:ASP:O | 1:B:934:ALA:HA | 2.19 | 0.43 |
| 1:A:946:ALA:HB2 | 1:A:989:ARG:O | 2.19 | 0.43 |
| 1:B:948:ASP:N | 1:B:992:LEU:HD12 | 2.33 | 0.43 |
| 1:A:295:VAL:HG23 | 1:A:295:VAL:O | 2.18 | 0.43 |
| 1:B:194:GLU:OE2 | 1:B:204:LYS:O | 2.36 | 0.43 |
| 2:D:173:ARG:HH12 | 2:D:218:CYS:CB | 2.31 | 0.42 |
| 2:D:172:ARG:NH1 | 2:D:197:ILE:HG12 | 2.34 | 0.42 |
| 1:B:275:ASP:HB2 | 1:B:279:ARG:N | 2.25 | 0.42 |
| 1:A:370:GLN:O | 1:A:372:GLN:N | 2.52 | 0.42 |
| 1:B:355:ASN:O | 1:B:357:GLY:N | 2.52 | 0.42 |
| 1:B:1108:VAL:HG12 | 1:B:1109:VAL:H | 1.84 | 0.42 |
| 1:B:843:PRO:HG2 | 2:D:24:VAL:CG2 | 2.49 | 0.42 |
| 2:C:100:ASN:HB3 | 2:C:103:LEU:CG | 2.49 | 0.42 |
| 1:A:1097:PHE:CZ | 1:A:1105:MET:CG | 3.02 | 0.42 |
| 1:B:183:GLN:HG2 | 1:B:184:ASP:N | 2.34 | 0.42 |
| 1:A:391:ARG:HD2 | 1:A:392:ASN:O | 2.19 | 0.42 |
| 1:A:745:THR:O | 1:A:747:GLY:N | 2.50 | 0.42 |
| 1:A:912:LEU:HB2 | 1:A:913:TYR:CD1 | 2.54 | 0.42 |
| 1:B:129:ARG:HH11 | 1:B:176:PRO:HD3 | 1.81 | 0.42 |
| 1:A:576:LEU:HD22 | 1:A:577:LEU:N | 2.34 | 0.42 |
| 1:B:1029:LEU:CD2 | 1:B:1039:LEU:HD13 | 2.49 | 0.42 |
| 1:A:403:ASP:HA | 1:A:698:THR:HG22 | 2.02 | 0.42 |
| 1:B:655:ARG:NH1 | 1:B:655:ARG:HG2 | 2.35 | 0.42 |
| 2:C:145:ILE:HA | 2:C:145:ILE:HD13 | 1.74 | 0.42 |
| 1:B:553:SER:HA | 1:B:554:PRO:HD3 | 1.82 | 0.42 |
| 1:A:780:THR:HB | 1:A:784:GLU:HG3 | 2.01 | 0.42 |
| 1:A:634:GLN:HG2 | 1:A:654:ASP:CG | 2.40 | 0.42 |
| 2:D:22:ASN:ND2 | 2:D:22:ASN:C | 2.72 | 0.42 |
| 1:A:127:GLU:O | 1:A:128:CYS:HB2 | 2.20 | 0.42 |
| 2:D:127:TYR:CE1 | 2:D:131:LYS:HD3 | 2.54 | 0.42 |
| 1:A:731:GLN:HA | 1:A:796:GLN:NE2 | 2.34 | 0.42 |
| 1:B:181:VAL:HG23 | 1:B:219:VAL:CG2 | 2.49 | 0.42 |
| 1:B:961:ASP:C | 1:B:961:ASP:OD2 | 2.58 | 0.42 |
| 1:A:660:TYR:CE2 | 1:A:708:GLN:OE1 | 2.72 | 0.42 |
| 1:A:866:VAL:HA | 1:A:867:LYS:NZ | 2.34 | 0.42 |
| 1:A:68:ARG:HD2 | 1:A:74:LYS:C | 2.40 | 0.42 |
| 1:B:1059:ASN:HD21 | 1:B:1070:HIS:CD2 | 2.36 | 0.42 |
| 1:B:130:MET:HG2 | 1:B:197:LEU:HD11 | 2.01 | 0.42 |
| 1:B:130:MET:HA | 1:B:145:LEU:HB3 | 2.01 | 0.42 |
| 1:B:19:VAL:HG22 | 1:B:20:THR:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:48:THR:HG22 | 2:C:83:ILE:O | 2.18 | 0.42 |
| 1:A:570:LYS:HA | 1:A:570:LYS:HD2 | 1.66 | 0.42 |
| 1:B:407:ILE:HG22 | 1:B:408:LYS:N | 2.35 | 0.42 |
| 1:A:867:LYS:N | 1:A:867:LYS:HD2 | 2.32 | 0.42 |
| 1:B:235:GLU:HB2 | 1:B:254:LYS:HE3 | 2.00 | 0.42 |
| 1:B:1030:PHE:O | 1:B:1037:ILE:HA | 2.19 | 0.42 |
| 1:A:1032:THR:HG23 | 1:A:1034:ASN:N | 2.25 | 0.42 |
| 1:B:662:SER:HB3 | 1:B:1138:ARG:HH21 | 1.85 | 0.42 |
| 1:A:811:GLU:OE2 | 1:A:847:ARG:NE | 2.53 | 0.42 |
| 1:B:414:ARG:NH2 | 1:B:462:ASN:HB2 | 2.34 | 0.42 |
| 1:A:296:THR:OG1 | 1:A:297:LEU:N | 2.53 | 0.42 |
| 1:B:308:THR:OG1 | 1:B:324:VAL:HG11 | 2.19 | 0.42 |
| 1:B:324:VAL:HB | 1:B:332:GLN:HG2 | 2.02 | 0.42 |
| 1:B:516:LEU:HD11 | 1:B:538:VAL:HG21 | 2.01 | 0.42 |
| 1:B:603:LEU:HD23 | 1:B:603:LEU:N | 2.35 | 0.42 |
| 1:B:407:ILE:CD1 | 1:B:407:ILE:H | 2.28 | 0.42 |
| 2:D:177:ILE:HG12 | 2:D:186:VAL:HG22 | 2.02 | 0.42 |
| 1:A:305:LEU:HD13 | 1:A:336:LEU:HD22 | 2.00 | 0.42 |
| 1:B:147:ARG:O | 1:B:148:ASP:C | 2.58 | 0.42 |
| 1:B:130:MET:CE | 1:B:195:VAL:HG11 | 2.50 | 0.42 |
| 1:A:1053:ASP:O | 1:A:1057:ARG:HG3 | 2.20 | 0.42 |
| 1:A:876:PHE:CD1 | 1:A:916:THR:HG21 | 2.55 | 0.42 |
| 1:B:818:SER:HA | 1:B:828:TYR:O | 2.19 | 0.42 |
| 1:B:458:PHE:HE2 | 1:B:499:SER:O | 2.02 | 0.42 |
| 1:A:549:SER:OG | 1:A:550:ASN:N | 2.53 | 0.42 |
| 2:C:113:THR:HB | 2:C:186:VAL:HB | 2.00 | 0.42 |
| 1:B:463:VAL:HG11 | 1:B:469:ILE:HB | 2.01 | 0.42 |
| 1:B:182:TYR:CE1 | 1:B:189:HIS:HD2 | 2.38 | 0.42 |
| 1:B:162:LEU:HG | 1:B:163:HIS:N | 2.34 | 0.42 |
| 1:A:910:MET:HG2 | 1:A:912:LEU:HD21 | 2.01 | 0.42 |
| 1:A:931:LEU:CD2 | 1:A:931:LEU:C | 2.87 | 0.42 |
| 1:B:412:PRO:HD3 | 1:B:680:CYS:HB2 | 2.02 | 0.42 |
| 1:A:1000:LEU:HD13 | 1:A:1002:GLU:HB2 | 2.00 | 0.42 |
| 1:B:575:GLU:O | 1:B:576:LEU:C | 2.58 | 0.42 |
| 1:B:467:GLN:CB | 1:B:478:LEU:HD21 | 2.49 | 0.42 |
| 1:B:512:VAL:O | 1:B:513:GLY:C | 2.57 | 0.42 |
| 1:B:4:ASN:ND2 | 1:B:976:VAL:HG11 | 2.34 | 0.42 |
| 1:A:854:SER:O | 1:A:855:ASP:HB2 | 2.19 | 0.42 |
| 1:A:170:LEU:HD13 | 1:A:207:TRP:CH2 | 2.55 | 0.42 |
| 1:B:394:ILE:HG13 | 1:B:669:SER:HB3 | 2.00 | 0.42 |
| 1:B:43:VAL:HG23 | 1:B:52:VAL:CG1 | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:724:ILE:HD11 | 1:B:733:PHE:CD2 | 2.54 | 0.42 |
| 1:B:451:PHE:HD1 | 1:B:486:LEU:HD22 | 1.85 | 0.42 |
| 2:D:22:ASN:O | 2:D:25:GLU:N | 2.50 | 0.42 |
| 1:A:177:THR:HG22 | 1:A:194:GLU:HG2 | 2.01 | 0.42 |
| 1:A:964:ASN:OD1 | 1:A:978:GLN:HG3 | 2.20 | 0.42 |
| 1:B:915:LYS:HA | 1:B:915:LYS:HD3 | 1.84 | 0.42 |
| 1:B:235:GLU:O | 1:B:236:SER:CB | 2.68 | 0.41 |
| 1:B:437:MET:HB2 | 1:B:446:THR:CG2 | 2.49 | 0.41 |
| 1:A:429:PHE:O | 1:A:430:VAL:C | 2.56 | 0.41 |
| 1:B:503:CYS:HB2 | 1:B:508:VAL:HG22 | 2.02 | 0.41 |
| 1:B:262:ASN:HD21 | 1:B:316:TYR:H | 1.67 | 0.41 |
| 1:B:381:ALA:O | 1:B:382:PHE:HB2 | 2.20 | 0.41 |
| 1:B:613:TYR:CZ | 1:B:627:LYS:HB2 | 2.55 | 0.41 |
| 2:C:221:ASP:O | 2:C:222:THR:HG23 | 2.20 | 0.41 |
| 1:B:396:ILE:CD1 | 1:B:673:LEU:HD11 | 2.42 | 0.41 |
| 1:B:63:VAL:O | 1:B:79:ILE:HA | 2.19 | 0.41 |
| 1:B:130:MET:CG | 1:B:197:LEU:HD11 | 2.51 | 0.41 |
| 1:A:1114:TYR:CE2 | 1:A:1128:ASP:HB3 | 2.56 | 0.41 |
| 1:A:1113:GLN:CB | 1:A:1121:LYS:HD2 | 2.49 | 0.41 |
| 2:D:139:ASN:O | 2:D:140:LEU:C | 2.58 | 0.41 |
| 1:A:410:LEU:HA | 1:A:426:VAL:O | 2.20 | 0.41 |
| 1:A:679:MET:CE | 1:A:691:LEU:HG | 2.50 | 0.41 |
| 1:B:932:LEU:CD2 | 1:B:979:LYS:HD3 | 2.50 | 0.41 |
| 1:B:361:ASP:OD2 | 1:B:723:LYS:HD3 | 2.20 | 0.41 |
| 1:B:1063:LYS:HG3 | 1:B:1063:LYS:O | 2.20 | 0.41 |
| 1:B:167:VAL:O | 1:B:168:LYS:HE2 | 2.20 | 0.41 |
| 1:B:1058:LEU:HD23 | 1:B:1093:LEU:CD2 | 2.48 | 0.41 |
| 1:B:1115:ASP:CB | 1:B:1120:MET:HB2 | 2.50 | 0.41 |
| 1:A:494:GLN:O | 1:A:495:ALA:HB3 | 2.19 | 0.41 |
| 1:A:982:ALA:O | 1:A:984:THR:N | 2.50 | 0.41 |
| 1:B:399:HIS:HB2 | 1:B:701:ILE:O | 2.20 | 0.41 |
| 2:C:112:GLN:HE22 | 2:C:187:THR:CG2 | 2.15 | 0.41 |
| 2:C:170:PHE:HB2 | 2:C:193:SER:OG | 2.20 | 0.41 |
| 2:D:49:GLY:HA2 | 2:D:144:PHE:CD2 | 2.56 | 0.41 |
| 1:A:597:GLU:HG3 | 1:A:661:SER:CB | 2.50 | 0.41 |
| 1:B:342:GLU:C | 1:B:344:GLY:N | 2.73 | 0.41 |
| 1:B:29:LEU:HD23 | 1:B:44:VAL:HG11 | 2.01 | 0.41 |
| 1:A:391:ARG:HH11 | 1:A:391:ARG:HB3 | 1.85 | 0.41 |
| 1:B:754:PRO:HB2 | 1:B:759:GLN:OE1 | 2.20 | 0.41 |
| 1:A:818:SER:O | 1:A:819:CYS:HB3 | 2.20 | 0.41 |
| 2:C:111:THR:HB | 2:C:188:GLU:CG | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:483:PRO:O | 1:B:484:LYS:CB | 2.69 | 0.41 |
| 1:B:314:LEU:C | 1:B:314:LEU:HD12 | 2.40 | 0.41 |
| 1:B:644:LEU:CD2 | 1:B:644:LEU:H | 2.32 | 0.41 |
| 1:B:203:ASN:O | 1:B:204:LYS:HB2 | 2.21 | 0.41 |
| 1:A:222:VAL:HA | 1:A:223:PRO:HD3 | 1.83 | 0.41 |
| 1:B:433:THR:OG1 | 1:B:455:GLN:O | 2.24 | 0.41 |
| 1:B:492:GLU:O | 1:B:493:PRO:C | 2.59 | 0.41 |
| 1:A:81:THR:HG21 | 1:A:85:ASN:OD1 | 2.21 | 0.41 |
| 2:D:147:GLU:OE2 | 2:D:163:ARG:CZ | 2.69 | 0.41 |
| 1:A:1013:VAL:HG12 | 1:A:1014:MET:O | 2.21 | 0.41 |
| 1:B:617:ASN:O | 1:B:621:GLY:N | 2.52 | 0.41 |
| 1:A:90:GLU:OE1 | 1:A:103:ARG:NE | 2.53 | 0.41 |
| 1:A:362:MET:HB3 | 1:A:377:THR:HG22 | 2.03 | 0.41 |
| 2:C:160:ASP:CG | 2:C:161:PHE:N | 2.72 | 0.41 |
| 1:B:548:ASP:O | 1:B:549:SER:C | 2.59 | 0.41 |
| 1:A:372:GLN:NE2 | 1:A:372:GLN:O | 2.53 | 0.41 |
| 2:D:48:THR:HA | 2:D:82:LYS:O | 2.21 | 0.41 |
| 1:A:388:ARG:CD | 1:A:714:THR:HB | 2.46 | 0.41 |
| 1:B:1022:THR:O | 1:B:1024:THR:N | 2.54 | 0.41 |
| 1:B:459:PHE:HE2 | 1:B:503:CYS:SG | 2.44 | 0.41 |
| 1:B:474:ALA:O | 1:B:475:SER:CB | 2.67 | 0.41 |
| 1:B:473:SER:O | 1:B:497:ASN:HA | 2.21 | 0.41 |
| 2:C:215:CYS:SG | 2:C:217:GLU:N | 2.84 | 0.41 |
| 1:B:383:LYS:CG | 1:B:384:GLU:OE2 | 2.69 | 0.41 |
| 1:A:847:ARG:NH1 | 1:A:849:VAL:HG22 | 2.35 | 0.41 |
| 1:A:7:VAL:HG11 | 1:A:1095:GLU:OE2 | 2.20 | 0.41 |
| 1:B:392:ASN:C | 1:B:392:ASN:ND2 | 2.75 | 0.41 |
| 1:A:16:ASN:HB2 | 1:A:35:LYS:O | 2.21 | 0.41 |
| 1:B:408:LYS:HG3 | 1:B:430:VAL:HG23 | 2.03 | 0.41 |
| 2:D:142:THR:O | 2:D:143:ARG:C | 2.59 | 0.41 |
| 1:A:889:ARG:HD2 | 1:A:901:THR:CG2 | 2.51 | 0.41 |
| 1:A:181:VAL:HG23 | 1:A:219:VAL:CG2 | 2.50 | 0.41 |
| 1:A:358:PRO:HD2 | 1:A:380:GLY:HA2 | 2.03 | 0.41 |
| 2:C:110:SER:N | 2:C:221:ASP:HB3 | 2.35 | 0.41 |
| 1:B:277:GLU:HB3 | 1:B:279:ARG:NH1 | 2.35 | 0.41 |
| 1:B:436:LEU:HD11 | 1:B:443:VAL:O | 2.20 | 0.41 |
| 1:B:869:ALA:N | 1:B:885:ASN:OD1 | 2.51 | 0.41 |
| 2:D:82:LYS:HE2 | 2:D:161:PHE:CZ | 2.56 | 0.41 |
| 1:B:318:ASP:O | 1:B:319:ASN:HB2 | 2.20 | 0.41 |
| 1:B:1039:LEU:CD2 | 1:B:1139:ILE:HG22 | 2.50 | 0.41 |
| 1:B:933:LEU:HD23 | 1:B:944:GLU:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:725:CYS:SG | 1:A:817:VAL:HA | 2.60 | 0.41 |
| 1:B:724:ILE:HD11 | 1:B:733:PHE:HD2 | 1.86 | 0.41 |
| 1:A:125:ASP:OD1 | 1:A:126:PRO:HD2 | 2.21 | 0.41 |
| 1:B:947:ARG:C | 1:B:992:LEU:HD12 | 2.41 | 0.41 |
| 1:B:287:LYS:HD3 | 1:B:287:LYS:O | 2.20 | 0.41 |
| 1:A:622:LEU:HD23 | 1:A:622:LEU:H | 1.86 | 0.41 |
| 1:B:450:GLY:CA | 1:B:479:VAL:HG11 | 2.27 | 0.41 |
| 2:C:147:GLU:OE2 | 2:C:163:ARG:HD3 | 2.21 | 0.41 |
| 2:D:142:THR:O | 2:D:143:ARG:O | 2.39 | 0.41 |
| 2:C:219:GLU:O | 2:C:221:ASP:N | 2.53 | 0.41 |
| 1:B:768:SER:C | 1:B:769:LYS:HE2 | 2.41 | 0.41 |
| 1:B:676:VAL:HG22 | 1:B:693:LEU:HD12 | 2.03 | 0.41 |
| 1:B:836:VAL:HG13 | 2:D:22:ASN:OD1 | 2.21 | 0.41 |
| 1:A:537:GLU:HG3 | 1:A:561:TRP:CD1 | 2.56 | 0.41 |
| 1:A:730:SER:HB2 | 1:A:732:CYS:SG | 2.61 | 0.41 |
| 1:A:18:CYS:HA | 1:A:32:LEU:O | 2.21 | 0.41 |
| 1:A:841:ALA:HA | 2:C:45:PRO:HG2 | 2.02 | 0.41 |
| 1:A:226:PHE:N | 1:A:226:PHE:CD1 | 2.89 | 0.41 |
| 1:B:456:GLN:O | 1:B:472:THR:HB | 2.21 | 0.40 |
| 1:B:5:TYR:CE2 | 1:B:7:VAL:HG21 | 2.56 | 0.40 |
| 1:B:213:GLU:OE1 | 1:B:234:GLN:O | 2.38 | 0.40 |
| 1:A:676:VAL:HG11 | 1:A:693:LEU:HD22 | 2.03 | 0.40 |
| 1:A:90:GLU:HB3 | 1:A:101:ILE:CG1 | 2.51 | 0.40 |
| 1:B:994:GLU:O | 1:B:995:VAL:CG2 | 2.60 | 0.40 |
| 2:C:107:SER:O | 2:C:109:PRO:HD2 | 2.21 | 0.40 |
| 1:B:991:HIS:HB3 | 1:B:993:GLN:HE22 | 1.86 | 0.40 |
| 1:B:1110:ALA:C | 1:B:1112:LEU:H | 2.25 | 0.40 |
| 1:A:125:ASP:HA | 1:A:126:PRO:HD3 | 1.97 | 0.40 |
| 1:A:22:HIS:CD2 | 1:A:28:ASP:O | 2.74 | 0.40 |
| 1:A:1109:VAL:HG12 | 1:A:1109:VAL:O | 2.22 | 0.40 |
| 1:B:2:SER:CB | 1:B:995:VAL:HG23 | 2.51 | 0.40 |
| 1:B:554:PRO:C | 1:B:571:LEU:HB3 | 2.42 | 0.40 |
| 1:B:254:LYS:N | 1:B:254:LYS:HD2 | 2.36 | 0.40 |
| 1:B:949:PHE:CE1 | 1:B:991:HIS:CD2 | 3.10 | 0.40 |
| 1:B:628:LYS:HG2 | 1:B:629:VAL:N | 2.36 | 0.40 |
| 1:B:740:ILE:HG22 | 1:B:741:GLU:N | 2.36 | 0.40 |
| 1:A:542:ASP:HB3 | 1:A:557:ALA:HB3 | 2.03 | 0.40 |
| 1:A:439:ASN:O | 1:A:442:GLU:N | 2.47 | 0.40 |
| 1:A:439:ASN:O | 1:A:441:GLU:N | 2.55 | 0.40 |
| 1:A:263:ARG:HD2 | 1:A:265:ASP:O | 2.22 | 0.40 |
| 2:C:52:THR:HG21 | 2:C:85:ILE:CA | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:607:GLY:HA2 | 1:A:635:PRO:HA | 2.04 | 0.40 |
| 1:B:284:LEU:CD1 | 1:B:301:ARG:NH2 | 2.84 | 0.40 |
| 1:A:679:MET:HE2 | 1:A:691:LEU:HG | 2.04 | 0.40 |
| 1:A:568:ILE:O | 1:A:569:LEU:HD23 | 2.20 | 0.40 |
| 1:A:484:LYS:O | 1:A:485:ALA:HB2 | 2.22 | 0.40 |
| 1:A:166:ASP:O | 1:A:180:PHE:HB2 | 2.21 | 0.40 |
| 1:B:507:GLN:NE2 | 1:B:552:LEU:HA | 2.37 | 0.40 |
| 1:B:569:LEU:HD23 | 1:B:576:LEU:HA | 2.03 | 0.40 |
| 1:A:234:GLN:O | 1:A:235:GLU:HG2 | 2.20 | 0.40 |
| 1:A:837:TYR:HA | 1:A:838:PRO:HD3 | 1.95 | 0.40 |
| 1:B:1120:MET:HB2 | 1:B:1121:LYS:H | 1.72 | 0.40 |
| 1:A:492:GLU:OE2 | 1:A:494:GLN:N | 2.54 | 0.40 |
| 1:A:471:ILE:HG23 | 1:A:476:VAL:HB | 2.04 | 0.40 |
| 1:B:281:PHE:HB3 | 1:B:282:MET:H | 1.67 | 0.40 |
| 1:B:378:CYS:SG | 1:B:724:ILE:HB | 2.60 | 0.40 |
| 2:C:102:LEU:C | 2:C:104:GLY:N | 2.75 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 1126/1140 (99%) | 960 (85%) | 128 (11%) | 38 (3%) | 5 | 16 |
| 1 | B | 1130/1140 (99%) | 892 (79%) | 145 (13%) | 93 (8%) | 1 | 2 |
| 2 | C | 168/222 (76%) | 123 (73%) | 33 (20%) | 12 (7%) | 1 | 3 |
| 2 | D | 169/222 (76%) | 115 (68%) | 32 (19%) | 22 (13%) | 0 | 0 |
| All | All | 2593/2724 (95%) | 2090 (81%) | 338 (13%) | 165 (6%) | 2 | 4 |

All (165) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 254 | LYS |
| 1 | A | 269 | SER |
| 1 | A | 290 | GLN |
| 1 | A | 341 | ASN |
| 1 | A | 370 | GLN |
| 1 | A | 371 | GLY |
| 1 | A | 708 | GLN |
| 1 | A | 772 | SER |
| 1 | A | 781 | SER |
| 1 | A | 856 | GLY |
| 1 | A | 929 | SER |
| 1 | B | 46 | ALA |
| 1 | B | 223 | PRO |
| 1 | B | 275 | ASP |
| 1 | B | 310 | ILE |
| 1 | B | 341 | ASN |
| 1 | B | 357 | GLY |
| 1 | B | 430 | VAL |
| 1 | B | 434 | ARG |
| 1 | B | 450 | GLY |
| 1 | B | 466 | GLN |
| 1 | B | 493 | PRO |
| 1 | B | 549 | SER |
| 1 | B | 551 | GLY |
| 1 | B | 576 | LEU |
| 1 | B | 688 | PRO |
| 1 | B | 707 | ILE |
| 1 | B | 751 | ALA |
| 1 | B | 782 | PHE |
| 1 | B | 985 | THR |
| 1 | B | 1015 | GLN |
| 1 | B | 1016 | ASN |
| 1 | B | 1021 | SER |
| 1 | B | 1065 | VAL |
| 1 | B | 1109 | VAL |
| 1 | B | 1110 | ALA |
| 2 | C | 39 | GLY |
| 2 | C | 108 | THR |
| 2 | C | 162 | LYS |
| 2 | D | 23 | THR |
| 2 | D | 51 | LEU |
| 2 | D | 89 | ASP |
| 2 | D | 90 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 104 | GLY |
| 2 | D | 108 | THR |
| 2 | D | 109 | PRO |
| 2 | D | 143 | ARG |
| 2 | D | 193 | SER |
| 2 | D | 209 | HIS |
| 1 | A | 118 | THR |
| 1 | A | 147 | ARG |
| 1 | A | 203 | ASN |
| 1 | A | 294 | THR |
| 1 | A | 449 | MET |
| 1 | A | 524 | GLN |
| 1 | A | 551 | GLY |
| 1 | A | 583 | GLY |
| 1 | A | 643 | SER |
| 1 | A | 646 | THR |
| 1 | A | 706 | GLU |
| 1 | A | 746 | SER |
| 1 | A | 983 | ALA |
| 1 | A | 987 | GLU |
| 1 | B | 26 | ALA |
| 1 | B | 35 | LYS |
| 1 | B | 113 | GLY |
| 1 | B | 146 | ASP |
| 1 | B | 149 | ASN |
| 1 | B | 168 | LYS |
| 1 | B | 214 | ALA |
| 1 | B | 276 | MET |
| 1 | B | 318 | ASP |
| 1 | B | 369 | ARG |
| 1 | B | 451 | PHE |
| 1 | B | 524 | GLN |
| 1 | B | 564 | ILE |
| 1 | B | 626 | ARG |
| 1 | B | 729 | VAL |
| 1 | B | 748 | GLY |
| 1 | B | 986 | ASP |
| 1 | B | 995 | VAL |
| 1 | B | 1037 | ILE |
| 1 | B | 1066 | GLY |
| 1 | B | 1119 | GLY |
| 2 | C | 148 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 180 | VAL |
| 2 | C | 220 | ARG |
| 2 | D | 105 | LEU |
| 2 | D | 148 | PRO |
| 2 | D | 149 | ARG |
| 2 | D | 216 | SER |
| 1 | A | 367 | LEU |
| 1 | A | 368 | GLU |
| 1 | A | 817 | VAL |
| 1 | A | 1015 | GLN |
| 1 | A | 1027 | SER |
| 1 | B | 147 | ARG |
| 1 | B | 148 | ASP |
| 1 | B | 236 | SER |
| 1 | B | 343 | GLN |
| 1 | B | 432 | GLN |
| 1 | B | 433 | THR |
| 1 | B | 440 | GLY |
| 1 | B | 444 | GLU |
| 1 | B | 465 | HIS |
| 1 | B | 475 | SER |
| 1 | B | 484 | LYS |
| 1 | B | 578 | HIS |
| 1 | B | 884 | ILE |
| 1 | B | 1080 | ARG |
| 2 | C | 103 | LEU |
| 2 | C | 107 | SER |
| 2 | D | 39 | GLY |
| 2 | D | 91 | LYS |
| 2 | D | 117 | LEU |
| 1 | A | 319 | ASN |
| 1 | B | 226 | PHE |
| 1 | B | 251 | PRO |
| 1 | B | 253 | ILE |
| 1 | B | 255 | GLN |
| 1 | B | 340 | SER |
| 1 | B | 706 | GLU |
| 1 | B | 761 | LEU |
| 1 | B | 783 | GLY |
| 1 | B | 864 | LYS |
| 1 | B | 918 | GLY |
| 1 | B | 984 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 50 | LEU |
| 2 | D | 19 | THR |
| 2 | D | 99 | PRO |
| 1 | A | 184 | ASP |
| 1 | A | 224 | GLU |
| 1 | A | 440 | GLY |
| 1 | A | 937 | PRO |
| 1 | B | 47 | GLU |
| 1 | B | 203 | ASN |
| 1 | B | 208 | LYS |
| 1 | B | 241 | ASN |
| 1 | B | 243 | ASP |
| 1 | B | 356 | LEU |
| 1 | B | 381 | ALA |
| 1 | B | 572 | PRO |
| 1 | B | 575 | GLU |
| 1 | B | 643 | SER |
| 1 | B | 861 | VAL |
| 1 | B | 1036 | MET |
| 2 | C | 195 | SER |
| 2 | D | 212 | PRO |
| 1 | A | 253 | ILE |
| 1 | B | 204 | LYS |
| 1 | B | 486 | LEU |
| 1 | B | 1111 | ASN |
| 2 | D | 192 | PRO |
| 1 | A | 584 | GLY |
| 1 | B | 513 | GLY |
| 1 | B | 822 | GLY |
| 2 | C | 164 | GLY |
| 2 | D | 180 | VAL |
| 1 | B | 571 | LEU |
| 1 | B | 1013 | VAL |
| 2 | C | 20 | GLY |
| 1 | A | 119 | GLY |
| 1 | B | 144 | PRO |
| 1 | B | 224 | GLU |
| 1 | B | 848 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 992/999 (99%) | 900 (91%) | 92 (9%) | 11 | 29 |
| 1 | B | 994/999 (100%) | 925 (93%) | 69 (7%) | 19 | 45 |
| 2 | C | 151/191 (79%) | 134 (89%) | 17 (11%) | 7 | 19 |
| 2 | D | 151/191 (79%) | 133 (88%) | 18 (12%) | 6 | 17 |
| All | All | 2288/2380 (96%) | 2092 (91%) | 196 (9%) | 13 | 34 |

All (196) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1 | MET |
| 1 | A | 7 | VAL |
| 1 | A | 10 | GLN |
| 1 | A | 47 | GLU |
| 1 | A | 68 | ARG |
| 1 | A | 103 | ARG |
| 1 | A | 112 | ILE |
| 1 | A | 117 | GLU |
| 1 | A | 146 | ASP |
| 1 | A | 147 | ARG |
| 1 | A | 167 | VAL |
| 1 | A | 178 | ILE |
| 1 | A | 186 | GLN |
| 1 | A | 202 | PHE |
| 1 | A | 206 | PRO |
| 1 | A | 235 | GLU |
| 1 | A | 241 | ASN |
| 1 | A | 282 | MET |
| 1 | A | 291 | MET |
| 1 | A | 298 | LYS |
| 1 | A | 300 | LEU |
| 1 | A | 318 | ASP |
| 1 | A | 319 | ASN |
| 1 | A | 365 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 370 | GLN |
| 1 | A | 391 | ARG |
| 1 | A | 392 | ASN |
| 1 | A | 396 | ILE |
| 1 | A | 410 | LEU |
| 1 | A | 414 | ARG |
| 1 | A | 419 | ARG |
| 1 | A | 449 | MET |
| 1 | A | 455 | GLN |
| 1 | A | 468 | LEU |
| 1 | A | 476 | VAL |
| 1 | A | 507 | GLN |
| 1 | A | 518 | TYR |
| 1 | A | 525 | GLU |
| 1 | A | 531 | HIS |
| 1 | A | 550 | ASN |
| 1 | A | 552 | LEU |
| 1 | A | 567 | ARG |
| 1 | A | 571 | LEU |
| 1 | A | 576 | LEU |
| 1 | A | 579 | LYS |
| 1 | A | 582 | LEU |
| 1 | A | 587 | ILE |
| 1 | A | 589 | ARG |
| 1 | A | 594 | THR |
| 1 | A | 599 | SER |
| 1 | A | 624 | SER |
| 1 | A | 647 | THR |
| 1 | A | 648 | ASN |
| 1 | A | 680 | CYS |
| 1 | A | 682 | LEU |
| 1 | A | 685 | ASP |
| 1 | A | 696 | ASN |
| 1 | A | 700 | THR |
| 1 | A | 704 | ILE |
| 1 | A | 705 | ASP |
| 1 | A | 708 | GLN |
| 1 | A | 713 | ARG |
| 1 | A | 714 | THR |
| 1 | A | 759 | GLN |
| 1 | A | 781 | SER |
| 1 | A | 796 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 817 | VAL |
| 1 | A | 823 | LYS |
| 1 | A | 835 | MET |
| 1 | A | 858 | LEU |
| 1 | A | 866 | VAL |
| 1 | A | 867 | LYS |
| 1 | A | 874 | VAL |
| 1 | A | 902 | GLU |
| 1 | A | 907 | ASN |
| 1 | A | 925 | ASP |
| 1 | A | 931 | LEU |
| 1 | A | 939 | GLU |
| 1 | A | 957 | VAL |
| 1 | A | 966 | LEU |
| 1 | A | 969 | GLU |
| 1 | A | 990 | GLN |
| 1 | A | 992 | LEU |
| 1 | A | 1000 | LEU |
| 1 | A | 1032 | THR |
| 1 | A | 1036 | MET |
| 1 | A | 1041 | THR |
| 1 | A | 1062 | ILE |
| 1 | A | 1069 | GLU |
| 1 | A | 1093 | LEU |
| 1 | A | 1121 | LYS |
| 1 | A | 1135 | GLU |
| 1 | B | 6 | VAL |
| 1 | B | 47 | GLU |
| 1 | B | 67 | PHE |
| 1 | B | 92 | LYS |
| 1 | B | 109 | GLN |
| 1 | B | 112 | ILE |
| 1 | B | 130 | MET |
| 1 | B | 147 | ARG |
| 1 | B | 185 | PRO |
| 1 | B | 255 | GLN |
| 1 | B | 275 | ASP |
| 1 | B | 277 | GLU |
| 1 | B | 287 | LYS |
| 1 | B | 307 | GLU |
| 1 | B | 354 | THR |
| 1 | B | 367 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 392 | ASN |
| 1 | B | 402 | ILE |
| 1 | B | 414 | ARG |
| 1 | B | 427 | LEU |
| 1 | B | 449 | MET |
| 1 | B | 466 | GLN |
| 1 | B | 477 | ARG |
| 1 | B | 493 | PRO |
| 1 | B | 498 | ILE |
| 1 | B | 524 | GLN |
| 1 | B | 529 | ILE |
| 1 | B | 543 | ILE |
| 1 | B | 563 | ASP |
| 1 | B | 567 | ARG |
| 1 | B | 581 | MET |
| 1 | B | 585 | GLU |
| 1 | B | 597 | GLU |
| 1 | B | 614 | PHE |
| 1 | B | 693 | LEU |
| 1 | B | 699 | LEU |
| 1 | B | 704 | ILE |
| 1 | B | 706 | GLU |
| 1 | B | 713 | ARG |
| 1 | B | 746 | SER |
| 1 | B | 749 | THR |
| 1 | B | 750 | THR |
| 1 | B | 769 | LYS |
| 1 | B | 780 | THR |
| 1 | B | 781 | SER |
| 1 | B | 790 | ASN |
| 1 | B | 815 | SER |
| 1 | B | 839 | GLU |
| 1 | B | 852 | GLN |
| 1 | B | 899 | VAL |
| 1 | B | 901 | THR |
| 1 | B | 908 | ASN |
| 1 | B | 931 | LEU |
| 1 | B | 941 | ASN |
| 1 | B | 943 | GLU |
| 1 | B | 957 | VAL |
| 1 | B | 969 | GLU |
| 1 | B | 980 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 990 | GLN |
| 1 | B | 995 | VAL |
| 1 | B | 1000 | LEU |
| 1 | B | 1036 | MET |
| 1 | B | 1052 | LEU |
| 1 | B | 1078 | THR |
| 1 | B | 1080 | ARG |
| 1 | B | 1086 | THR |
| 1 | B | 1093 | LEU |
| 1 | B | 1120 | MET |
| 1 | B | 1131 | LYS |
| 2 | C | 37 | SER |
| 2 | C | 50 | LEU |
| 2 | C | 106 | ASP |
| 2 | C | 121 | THR |
| 2 | C | 137 | LYS |
| 2 | C | 145 | ILE |
| 2 | C | 163 | ARG |
| 2 | C | 176 | SER |
| 2 | C | 179 | TRP |
| 2 | C | 190 | CYS |
| 2 | C | 194 | CYS |
| 2 | C | 197 | ILE |
| 2 | C | 206 | CYS |
| 2 | C | 208 | CYS |
| 2 | C | 211 | CYS |
| 2 | C | 218 | CYS |
| 2 | C | 222 | THR |
| 2 | D | 18 | GLU |
| 2 | D | 22 | ASN |
| 2 | D | 25 | GLU |
| 2 | D | 51 | LEU |
| 2 | D | 101 | PRO |
| 2 | D | 105 | LEU |
| 2 | D | 111 | THR |
| 2 | D | 122 | LEU |
| 2 | D | 140 | LEU |
| 2 | D | 143 | ARG |
| 2 | D | 145 | ILE |
| 2 | D | 163 | ARG |
| 2 | D | 188 | GLU |
| 2 | D | 192 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 194 | CYS |
| 2 | D | 208 | CYS |
| 2 | D | 213 | VAL |
| 2 | D | 215 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | ASN |
| 1 | A | 10 | GLN |
| 1 | A | 22 | HIS |
| 1 | A | 30 | ASN |
| 1 | A | 93 | GLN |
| 1 | A | 156 | ASN |
| 1 | A | 186 | GLN |
| 1 | A | 234 | GLN |
| 1 | A | 241 | ASN |
| 1 | A | 262 | ASN |
| 1 | A | 319 | ASN |
| 1 | A | 341 | ASN |
| 1 | A | 343 | GLN |
| 1 | A | 372 | GLN |
| 1 | A | 374 | GLN |
| 1 | A | 455 | GLN |
| 1 | A | 467 | GLN |
| 1 | A | 481 | GLN |
| 1 | A | 507 | GLN |
| 1 | A | 520 | GLN |
| 1 | A | 578 | HIS |
| 1 | A | 634 | GLN |
| 1 | A | 648 | ASN |
| 1 | A | 711 | HIS |
| 1 | A | 743 | GLN |
| 1 | A | 790 | ASN |
| 1 | A | 796 | GLN |
| 1 | A | 809 | GLN |
| 1 | A | 810 | ASN |
| 1 | A | 904 | ASN |
| 1 | A | 907 | ASN |
| 1 | A | 950 | ASN |
| 1 | A | 990 | GLN |
| 1 | A | 991 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1016 | ASN |
| 1 | A | 1034 | ASN |
| 1 | A | 1055 | GLN |
| 1 | A | 1056 | ASN |
| 1 | A | 1070 | HIS |
| 1 | A | 1140 | HIS |
| 1 | B | 4 | ASN |
| 1 | B | 22 | HIS |
| 1 | B | 30 | ASN |
| 1 | B | 109 | GLN |
| 1 | B | 189 | HIS |
| 1 | B | 255 | GLN |
| 1 | B | 262 | ASN |
| 1 | B | 267 | ASN |
| 1 | B | 290 | GLN |
| 1 | B | 343 | GLN |
| 1 | B | 372 | GLN |
| 1 | B | 392 | ASN |
| 1 | B | 399 | HIS |
| 1 | B | 456 | GLN |
| 1 | B | 466 | GLN |
| 1 | B | 481 | GLN |
| 1 | B | 497 | ASN |
| 1 | B | 507 | GLN |
| 1 | B | 524 | GLN |
| 1 | B | 743 | GLN |
| 1 | B | 790 | ASN |
| 1 | B | 796 | GLN |
| 1 | B | 803 | HIS |
| 1 | B | 826 | ASN |
| 1 | B | 904 | ASN |
| 1 | B | 941 | ASN |
| 1 | B | 973 | ASN |
| 1 | B | 991 | HIS |
| 1 | B | 993 | GLN |
| 1 | B | 1015 | GLN |
| 1 | B | 1034 | ASN |
| 1 | B | 1070 | HIS |
| 1 | B | 1140 | HIS |
| 2 | C | 30 | GLN |
| 2 | C | 112 | GLN |
| 2 | C | 210 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 22 | ASN |
| 2 | D | 31 | GLN |
| 2 | D | 41 | ASN |
| 2 | D | 100 | ASN |
| 2 | D | 112 | GLN |
| 2 | D | 191 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1132/1140 (99%) | -0.27 | 11 (0%) 84 81 | 18, 47, 99, 160 | 0 |
| 1 | B | 1134/1140 (99%) | 0.04 | 37 (3%) 50 43 | 29, 68, 122, 173 | 0 |
| 2 | C | 174/222 (78%) | 0.25 | 13 (7%) 17 11 | 32, 62, 118, 183 | 0 |
| 2 | D | 175/222 (78%) | 0.60 | 21 (12%) 6 3 | 39, 81, 138, 168 | 0 |
| All | All | 2615/2724 (95%) | -0.04 | 82 (3%) 52 46 | 18, 59, 117, 183 | 0 |

All (82) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1018 | GLY | 6.1 |
| 1 | B | 750 | THR | 5.4 |
| 1 | B | 746 | SER | 5.3 |
| 1 | B | 780 | THR | 5.1 |
| 2 | D | 16 | LEU | 4.9 |
| 1 | B | 744 | ASP | 4.9 |
| 1 | B | 453 | ASP | 4.6 |
| 2 | D | 92 | THR | 4.4 |
| 2 | D | 104 | GLY | 4.2 |
| 1 | A | 548 | ASP | 4.1 |
| 1 | B | 450 | GLY | 4.0 |
| 1 | B | 571 | LEU | 3.9 |
| 1 | B | 1016 | ASN | 3.8 |
| 1 | B | 748 | GLY | 3.6 |
| 1 | A | 984 | THR | 3.6 |
| 1 | B | 294 | THR | 3.4 |
| 2 | C | 162 | LYS | 3.4 |
| 2 | D | 35 | THR | 3.4 |
| 1 | B | 781 | SER | 3.3 |
| 2 | D | 161 | PHE | 3.3 |
| 1 | B | 295 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 782 | PHE | 3.2 |
| 1 | B | 174 | GLN | 3.1 |
| 2 | D | 20 | GLY | 3.1 |
| 2 | D | 17 | ILE | 3.1 |
| 1 | A | 983 | ALA | 3.0 |
| 1 | B | 455 | GLN | 3.0 |
| 2 | D | 83 | ILE | 3.0 |
| 2 | D | 160 | ASP | 2.9 |
| 1 | B | 464 | ALA | 2.9 |
| 1 | B | 1118 | SER | 2.9 |
| 1 | A | 708 | GLN | 2.8 |
| 2 | C | 222 | THR | 2.8 |
| 2 | C | 160 | ASP | 2.8 |
| 2 | C | 164 | GLY | 2.8 |
| 2 | D | 80 | ARG | 2.8 |
| 1 | B | 209 | GLN | 2.7 |
| 1 | B | 419 | ARG | 2.7 |
| 1 | A | 571 | LEU | 2.7 |
| 1 | B | 202 | PHE | 2.6 |
| 2 | D | 159 | ILE | 2.6 |
| 1 | B | 456 | GLN | 2.6 |
| 2 | C | 16 | LEU | 2.6 |
| 2 | C | 180 | VAL | 2.6 |
| 1 | B | 292 | ASP | 2.6 |
| 1 | A | 644 | LEU | 2.6 |
| 1 | B | 367 | LEU | 2.6 |
| 1 | B | 1119 | GLY | 2.6 |
| 1 | B | 684 | SER | 2.5 |
| 1 | B | 234 | GLN | 2.5 |
| 1 | B | 236 | SER | 2.4 |
| 1 | B | 1017 | LEU | 2.4 |
| 2 | D | 198 | THR | 2.4 |
| 1 | B | 1114 | TYR | 2.4 |
| 1 | A | 924 | GLY | 2.3 |
| 2 | C | 52 | THR | 2.3 |
| 1 | B | 286 | GLU | 2.3 |
| 2 | D | 105 | LEU | 2.3 |
| 1 | A | 289 | GLU | 2.3 |
| 1 | B | 1032 | THR | 2.3 |
| 2 | C | 50 | LEU | 2.2 |
| 2 | D | 34 | GLY | 2.2 |
| 2 | C | 36 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | D | 33 | THR | 2.2 |
| 2 | D | 165 | ARG | 2.2 |
| 2 | C | 161 | PHE | 2.2 |
| 2 | C | 33 | THR | 2.2 |
| 2 | D | 209 | HIS | 2.1 |
| 1 | B | 686 | GLY | 2.1 |
| 1 | B | 1015 | GLN | 2.1 |
| 1 | B | 1121 | LYS | 2.1 |
| 1 | B | 291 | MET | 2.1 |
| 2 | D | 38 | LEU | 2.1 |
| 2 | D | 162 | LYS | 2.1 |
| 1 | A | 981 | SER | 2.1 |
| 1 | A | 1121 | LYS | 2.1 |
| 2 | C | 151 | ASN | 2.1 |
| 2 | D | 163 | ARG | 2.1 |
| 2 | D | 28 | THR | 2.0 |
| 1 | A | 296 | THR | 2.0 |
| 1 | B | 162 | LEU | 2.0 |
| 2 | C | 108 | THR | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 3 | ZN | C | 3001 | 1/1 | 0.83 | 0.09 | -1.51 | 35,35,35,35 | 0 |
| 3 | ZN | D | 3003 | 1/1 | 0.96 | 0.05 | -2.08 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3 | ZN | C | 3002 | 1/1 | 0.89 | 0.07 | -2.42 | 35,35,35,35 | 0 |
| 3 | ZN | D | 3004 | 1/1 | 0.96 | 0.08 | -3.98 | 35,35,35,35 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.