



wwPDB EM Map/Model Validation Report ⓘ

Jun 9, 2016 – 05:09 AM EDT

PDB ID : 5JNX
EMDB ID: : EMD8-8169
Title : The 6.6 Å cryo-EM structure of the full-length human NPC1 in complex with the cleaved glycoprotein of Ebola virus
Authors : Gong, X.; Qian, H.W.; Zhou, X.H.; Wu, J.P.; Wan, T.; Shi, Y.; Gao, F.; Zhou, Q.; Yan, N.
Deposited on : 2016-05-01
Resolution : 6.56 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

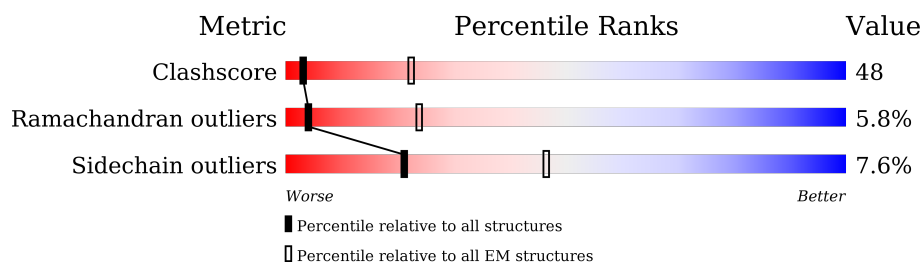
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.56 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1278 | |
| 2 | C | 158 | |
| 2 | E | 158 | |
| 2 | G | 158 | |
| 3 | D | 130 | |
| 3 | F | 130 | |
| 3 | H | 130 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4 | NAG | A | 1306 | - | - | X | - |
| 4 | NAG | A | 1307 | - | - | X | - |
| 4 | NAG | A | 1309 | X | - | - | - |
| 4 | NAG | A | 1312 | - | - | X | - |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Niemann-Pick C1 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 1133 | Total | C | N | O | S | 1 | 0 |
| | | | 7695 | 4862 | 1315 | 1476 | 42 | | |

- Molecule 2 is a protein called Envelope glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | C | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1194 | 757 | 209 | 223 | 5 | | |
| 2 | E | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1194 | 757 | 209 | 223 | 5 | | |
| 2 | G | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1194 | 757 | 209 | 223 | 5 | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| C | 31 | ARG | - | expression tag | UNP P87666 |
| C | 42 | VAL | THR | engineered mutation | UNP P87666 |
| E | 31 | ARG | - | expression tag | UNP P87666 |
| E | 42 | VAL | THR | engineered mutation | UNP P87666 |
| G | 31 | ARG | - | expression tag | UNP P87666 |
| G | 42 | VAL | THR | engineered mutation | UNP P87666 |

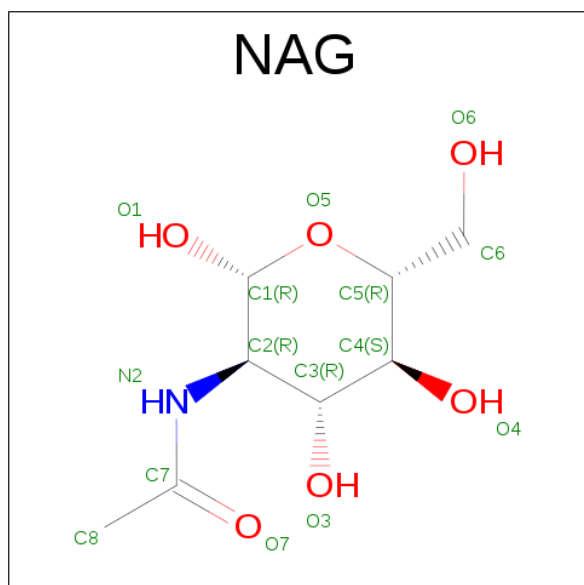
- Molecule 3 is a protein called Envelope glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | D | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 441 | 121 | 122 | 3 | | |
| 3 | F | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 441 | 121 | 122 | 3 | | |
| 3 | H | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 441 | 121 | 122 | 3 | | |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 633 | HIS | - | expression tag | UNP P87666 |
| D | 634 | HIS | - | expression tag | UNP P87666 |
| D | 635 | HIS | - | expression tag | UNP P87666 |
| D | 636 | HIS | - | expression tag | UNP P87666 |
| D | 637 | HIS | - | expression tag | UNP P87666 |
| D | 638 | HIS | - | expression tag | UNP P87666 |
| F | 633 | HIS | - | expression tag | UNP P87666 |
| F | 634 | HIS | - | expression tag | UNP P87666 |
| F | 635 | HIS | - | expression tag | UNP P87666 |
| F | 636 | HIS | - | expression tag | UNP P87666 |
| F | 637 | HIS | - | expression tag | UNP P87666 |
| F | 638 | HIS | - | expression tag | UNP P87666 |
| H | 633 | HIS | - | expression tag | UNP P87666 |
| H | 634 | HIS | - | expression tag | UNP P87666 |
| H | 635 | HIS | - | expression tag | UNP P87666 |
| H | 636 | HIS | - | expression tag | UNP P87666 |
| H | 637 | HIS | - | expression tag | UNP P87666 |
| H | 638 | HIS | - | expression tag | UNP P87666 |

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|-----|----|-----|---------|
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |

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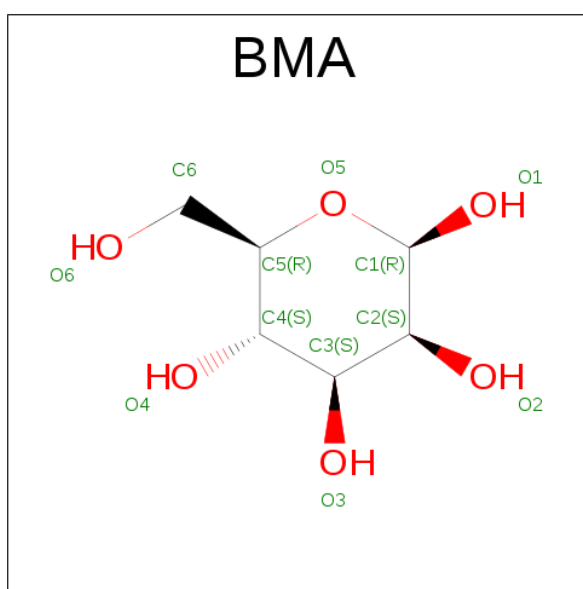
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|-----|----|-----|---------|
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | A | 1 | Total | C | N | O | 0 |
| | | | 294 | 168 | 21 | 105 | |
| 4 | D | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 4 | D | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |

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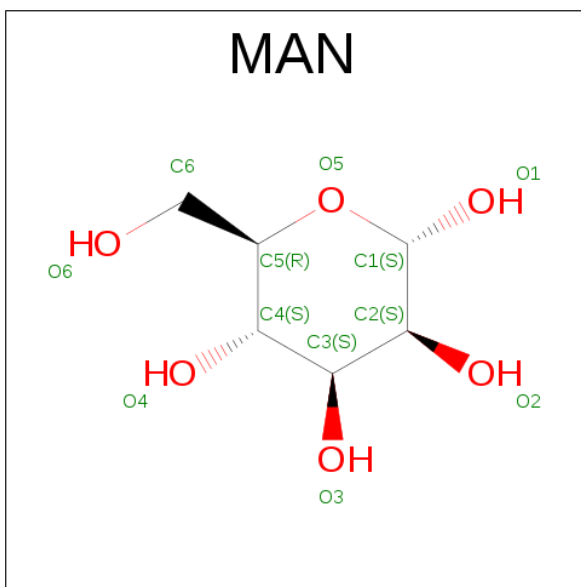
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 4 | F | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 4 | F | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 4 | H | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |
| 4 | H | 1 | Total | C | N | O | 0 |
| | | | 28 | 16 | 2 | 10 | |

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

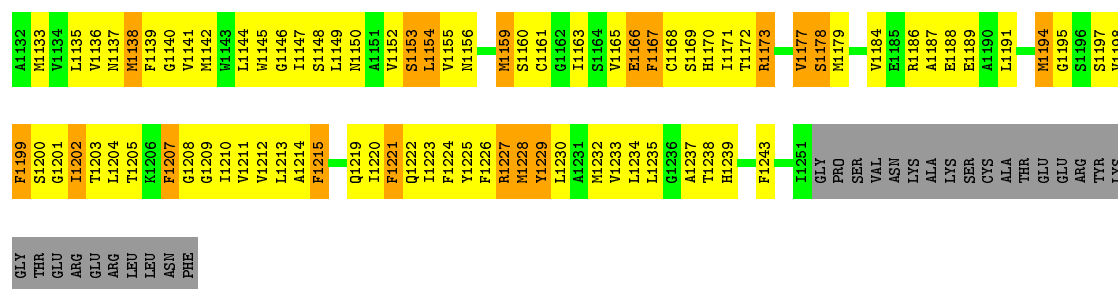


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 5 | A | 1 | Total | C | O | 0 |
| | | | 22 | 12 | 10 | |
| 5 | A | 1 | Total | C | O | 0 |
| | | | 22 | 12 | 10 | |

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 6 | A | 1 | Total | C | O | 0 |
| | | | 11 | 6 | 5 | |



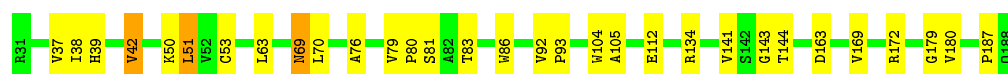
- Molecule 2: Envelope glycoprotein

Chain C: 86% 12% .



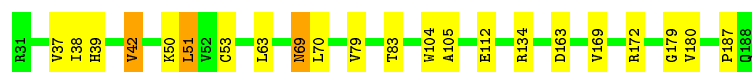
- Molecule 2: Envelope glycoprotein

Chain E: 80% 18% .



- Molecule 2: Envelope glycoprotein

Chain G: 86% 12% .



- Molecule 3: Envelope glycoprotein

Chain D: 52% 14% 33%

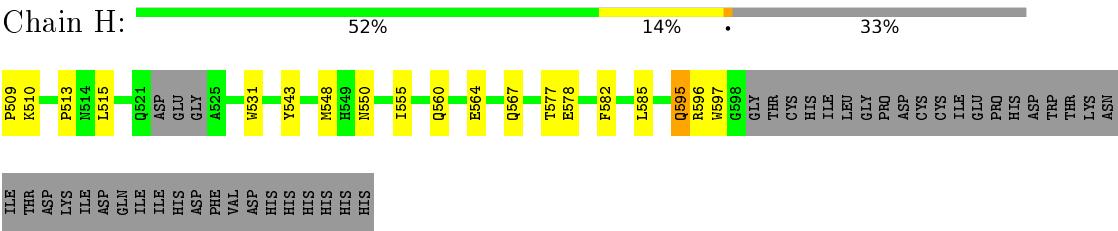


- Molecule 3: Envelope glycoprotein

Chain F: 52% 14% 33%



- Molecule 3: Envelope glycoprotein



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 50223 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1700 | Depositor |
| Maximum defocus (nm) | 2700 | Depositor |
| Magnification | 22500 | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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 >2 | RMSZ | # Z >2 |
| 1 | A | 0.49 | 6/7843 (0.1%) | 0.67 | 29/10748 (0.3%) |
| 2 | C | 0.42 | 0/1223 | 0.59 | 1/1664 (0.1%) |
| 2 | E | 0.44 | 0/1223 | 0.59 | 1/1664 (0.1%) |
| 2 | G | 0.43 | 0/1223 | 0.59 | 1/1664 (0.1%) |
| 3 | D | 0.42 | 0/702 | 0.62 | 0/952 |
| 3 | F | 0.42 | 0/702 | 0.62 | 0/952 |
| 3 | H | 0.42 | 0/702 | 0.62 | 0/952 |
| All | All | 0.47 | 6/13618 (0.0%) | 0.64 | 32/18596 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 2 | C | 0 | 1 |
| 2 | E | 0 | 1 |
| 2 | G | 0 | 1 |
| All | All | 0 | 5 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 429 | VAL | C-N | -5.49 | 1.23 | 1.34 |
| 1 | A | 166 | PRO | N-CD | 5.22 | 1.55 | 1.47 |
| 1 | A | 469 | LEU | C-N | -5.20 | 1.22 | 1.34 |
| 1 | A | 424 | PRO | N-CD | 5.08 | 1.54 | 1.47 |
| 1 | A | 249 | PRO | N-CD | 5.07 | 1.54 | 1.47 |
| 1 | A | 254 | PRO | N-CD | 5.01 | 1.54 | 1.47 |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 602 | SER | CB-CA-C | -9.99 | 91.12 | 110.10 |
| 1 | A | 755 | PRO | CA-N-CD | -8.22 | 99.99 | 111.50 |
| 1 | A | 996 | MET | C-N-CA | -6.63 | 105.12 | 121.70 |
| 1 | A | 887 | PRO | N-CA-CB | 6.58 | 111.20 | 103.30 |
| 1 | A | 836 | PRO | N-CA-CB | 6.46 | 111.06 | 103.30 |
| 1 | A | 256 | PRO | C-N-CD | 6.21 | 141.45 | 128.40 |
| 1 | A | 258 | ALA | C-N-CD | 6.12 | 141.26 | 128.40 |
| 1 | A | 252 | GLN | C-N-CD | 6.08 | 141.17 | 128.40 |
| 1 | A | 253 | PRO | C-N-CD | 6.07 | 141.15 | 128.40 |
| 1 | A | 254 | PRO | C-N-CD | 6.06 | 141.13 | 128.40 |
| 1 | A | 400 | GLY | C-N-CD | 6.06 | 141.13 | 128.40 |
| 1 | A | 383 | ALA | C-N-CD | 6.04 | 141.09 | 128.40 |
| 1 | A | 690 | ILE | C-N-CD | 6.04 | 141.09 | 128.40 |
| 1 | A | 421 | GLN | C-N-CD | 6.02 | 141.03 | 128.40 |
| 1 | A | 1009 | PRO | N-CA-CB | 6.00 | 110.50 | 103.30 |
| 1 | A | 377 | PRO | N-CA-CB | 5.95 | 110.44 | 103.30 |
| 1 | A | 827 | PRO | N-CA-CB | 5.95 | 110.44 | 103.30 |
| 1 | A | 1000 | PRO | N-CA-CB | 5.93 | 110.41 | 103.30 |
| 1 | A | 733 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |
| 1 | A | 867 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |
| 1 | A | 1007 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |
| 1 | A | 888 | PRO | N-CA-CB | 5.90 | 110.38 | 103.30 |
| 1 | A | 350 | PRO | N-CA-CB | 5.88 | 110.35 | 103.30 |
| 1 | A | 165 | ALA | C-N-CD | 5.62 | 140.20 | 128.40 |
| 1 | A | 429 | VAL | O-C-N | -5.32 | 111.00 | 121.10 |
| 2 | C | 42 | VAL | CA-CB-CG2 | 5.25 | 118.78 | 110.90 |
| 1 | A | 1053 | ASP | CB-CG-OD2 | 5.25 | 123.03 | 118.30 |
| 1 | A | 1096 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 2 | G | 42 | VAL | CA-CB-CG2 | 5.23 | 118.74 | 110.90 |
| 2 | E | 42 | VAL | CA-CB-CG2 | 5.20 | 118.70 | 110.90 |
| 1 | A | 248 | GLY | C-N-CD | 5.15 | 139.21 | 128.40 |
| 1 | A | 423 | TYR | C-N-CD | 5.10 | 139.11 | 128.40 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 602 | SER | Peptide |
| 1 | A | 603 | PHE | Peptide |
| 2 | C | 69 | ASN | Sidechain |
| 2 | E | 69 | ASN | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | G | 69 | ASN | Sidechain |

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 | 7695 | 0 | 6476 | 1133 | 0 |
| 2 | C | 1194 | 0 | 1153 | 17 | 0 |
| 2 | E | 1194 | 0 | 1153 | 69 | 0 |
| 2 | G | 1194 | 0 | 1153 | 17 | 0 |
| 3 | D | 687 | 0 | 679 | 19 | 0 |
| 3 | F | 687 | 0 | 679 | 20 | 0 |
| 3 | H | 687 | 0 | 679 | 18 | 0 |
| 4 | A | 294 | 0 | 265 | 42 | 0 |
| 4 | D | 28 | 0 | 25 | 1 | 0 |
| 4 | F | 28 | 0 | 25 | 2 | 0 |
| 4 | H | 28 | 0 | 25 | 1 | 0 |
| 5 | A | 22 | 0 | 19 | 5 | 0 |
| 6 | A | 11 | 0 | 10 | 0 | 0 |
| All | All | 13749 | 0 | 12341 | 1252 | 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 48.

All (1252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:724:LEU:HD22 | 1:A:1170:HIS:CE1 | 1.29 | 1.62 |
| 1:A:656:LEU:CD1 | 1:A:685:ILE:HG13 | 1.17 | 1.60 |
| 1:A:656:LEU:HD11 | 1:A:685:ILE:CG1 | 1.31 | 1.58 |
| 1:A:598:ASN:HD21 | 4:A:1310:NAG:C1 | 0.99 | 1.57 |
| 1:A:693:LEU:HD11 | 1:A:763:PHE:CE2 | 1.41 | 1.53 |
| 1:A:185:ASN:HD21 | 4:A:1319:NAG:C1 | 1.24 | 1.51 |
| 1:A:403:PHE:CE2 | 1:A:566:PRO:HB3 | 1.46 | 1.50 |
| 1:A:503:PHE:CZ | 2:E:86:TRP:HE3 | 1.30 | 1.49 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:HD13 | 1.45 | 1.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:70:ASN:HD21 | 4:A:1317:NAG:C1 | 1.26 | 1.46 |
| 1:A:656:LEU:CD1 | 1:A:685:ILE:CG1 | 1.85 | 1.45 |
| 1:A:659:ALA:HA | 1:A:662:LEU:CD2 | 1.46 | 1.44 |
| 1:A:693:LEU:CD1 | 1:A:763:PHE:HE2 | 1.30 | 1.44 |
| 1:A:503:PHE:CZ | 2:E:86:TRP:CE3 | 2.05 | 1.44 |
| 1:A:631:MET:CE | 1:A:1204:LEU:O | 1.64 | 1.42 |
| 1:A:693:LEU:HD11 | 1:A:763:PHE:CD2 | 1.52 | 1.42 |
| 1:A:1133:MET:HG2 | 1:A:1239:HIS:NE2 | 1.12 | 1.41 |
| 1:A:1138:MET:HE1 | 1:A:1232:MET:CA | 1.44 | 1.41 |
| 1:A:1133:MET:HG2 | 1:A:1239:HIS:CD2 | 1.52 | 1.40 |
| 1:A:693:LEU:CD1 | 1:A:763:PHE:CE2 | 2.03 | 1.39 |
| 1:A:688:GLU:CG | 1:A:724:LEU:HD23 | 1.52 | 1.39 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:HH11 | 1.35 | 1.38 |
| 1:A:503:PHE:CE2 | 2:E:86:TRP:HE3 | 1.41 | 1.36 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:CD1 | 1.51 | 1.36 |
| 1:A:1142:MET:HA | 1:A:1147:ILE:CB | 1.57 | 1.35 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:CD2 | 1.55 | 1.34 |
| 1:A:1133:MET:HE2 | 1:A:1239:HIS:ND1 | 1.07 | 1.34 |
| 1:A:856:VAL:CB | 1:A:1091:TYR:HE2 | 1.41 | 1.32 |
| 1:A:523:LEU:HD11 | 1:A:1016:HIS:CB | 1.58 | 1.31 |
| 1:A:401:PRO:HD3 | 1:A:571:TYR:CE1 | 1.65 | 1.30 |
| 1:A:686:VAL:CG1 | 1:A:690:ILE:HD11 | 1.61 | 1.30 |
| 1:A:724:LEU:CD2 | 1:A:1170:HIS:CE1 | 2.13 | 1.30 |
| 1:A:1084:PHE:CE1 | 1:A:1085:TYR:CD1 | 2.20 | 1.29 |
| 1:A:723:GLN:OE1 | 1:A:1169:SER:HB2 | 1.20 | 1.28 |
| 1:A:751:LEU:O | 1:A:755:PRO:HG3 | 1.29 | 1.28 |
| 1:A:1138:MET:CE | 1:A:1232:MET:HB2 | 1.63 | 1.27 |
| 1:A:452:ASN:HD21 | 4:A:1323:NAG:C1 | 1.45 | 1.27 |
| 1:A:923:ILE:O | 1:A:1042:HIS:CB | 1.83 | 1.27 |
| 1:A:1133:MET:CE | 1:A:1239:HIS:ND1 | 1.96 | 1.26 |
| 1:A:401:PRO:HG3 | 1:A:571:TYR:CD1 | 1.68 | 1.26 |
| 1:A:688:GLU:O | 1:A:691:PRO:HD2 | 1.19 | 1.26 |
| 1:A:648:LEU:HB3 | 1:A:763:PHE:CE1 | 1.70 | 1.26 |
| 1:A:686:VAL:HG12 | 1:A:690:ILE:CD1 | 1.62 | 1.26 |
| 1:A:503:PHE:CE2 | 2:E:86:TRP:CE3 | 2.18 | 1.25 |
| 1:A:1070:GLY:O | 1:A:1071:ILE:CG1 | 1.83 | 1.24 |
| 1:A:162:ASP:OD2 | 1:A:244:SER:CB | 1.86 | 1.24 |
| 1:A:688:GLU:O | 1:A:691:PRO:CD | 1.86 | 1.23 |
| 1:A:1138:MET:CE | 1:A:1232:MET:CB | 2.15 | 1.23 |
| 1:A:688:GLU:HG2 | 1:A:1170:HIS:NE2 | 1.54 | 1.22 |
| 1:A:1055:LEU:HD23 | 1:A:1085:TYR:CZ | 1.73 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:882:TYR:CB | 1:A:1082:SER:HB3 | 1.70 | 1.22 |
| 1:A:1142:MET:HE3 | 1:A:1148:SER:O | 1.11 | 1.22 |
| 1:A:162:ASP:OD2 | 1:A:244:SER:HB3 | 1.04 | 1.22 |
| 1:A:659:ALA:CA | 1:A:662:LEU:HD23 | 1.66 | 1.22 |
| 1:A:915:ASN:CB | 1:A:920:VAL:HA | 1.68 | 1.21 |
| 1:A:478:ASN:HD21 | 4:A:1312:NAG:C1 | 1.52 | 1.21 |
| 1:A:856:VAL:O | 1:A:1048:SER:CB | 1.89 | 1.21 |
| 1:A:406:GLU:OE1 | 1:A:583:TRP:HZ3 | 1.17 | 1.20 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:CG | 1.70 | 1.20 |
| 1:A:926:ALA:O | 1:A:1040:THR:HG22 | 1.34 | 1.20 |
| 1:A:724:LEU:HD22 | 1:A:1170:HIS:NE2 | 1.54 | 1.20 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:CD1 | 2.09 | 1.19 |
| 1:A:1133:MET:CG | 1:A:1239:HIS:CD2 | 2.26 | 1.19 |
| 1:A:503:PHE:CB | 2:E:83:THR:HG21 | 1.48 | 1.19 |
| 1:A:1127:MET:CE | 1:A:1168:CYS:HB3 | 1.74 | 1.18 |
| 1:A:1142:MET:CA | 1:A:1147:ILE:CB | 2.22 | 1.18 |
| 1:A:1108:ALA:O | 1:A:1112:VAL:HG23 | 1.43 | 1.18 |
| 1:A:1084:PHE:CE1 | 1:A:1085:TYR:HD1 | 1.59 | 1.17 |
| 1:A:250:LYS:HB3 | 1:A:251:PRO:CD | 1.70 | 1.17 |
| 1:A:732:ALA:CB | 1:A:749:GLY:HA3 | 1.75 | 1.17 |
| 1:A:1009:PRO:HA | 1:A:1016:HIS:O | 1.44 | 1.17 |
| 1:A:421:GLN:OE1 | 2:E:144:THR:HG22 | 1.45 | 1.17 |
| 1:A:656:LEU:HD13 | 1:A:685:ILE:HG13 | 1.26 | 1.16 |
| 1:A:923:ILE:O | 1:A:1042:HIS:HB2 | 1.33 | 1.16 |
| 1:A:1133:MET:CG | 1:A:1239:HIS:NE2 | 2.08 | 1.16 |
| 1:A:924:PHE:H | 1:A:925:ASN:CB | 1.56 | 1.16 |
| 1:A:730:GLU:CG | 1:A:1108:ALA:HB1 | 1.76 | 1.15 |
| 1:A:1138:MET:CE | 1:A:1232:MET:HA | 1.76 | 1.15 |
| 1:A:755:PRO:HD2 | 1:A:756:ALA:H | 1.06 | 1.15 |
| 1:A:507:ALA:HB1 | 1:A:529:LEU:HG | 1.28 | 1.15 |
| 1:A:1071:ILE:O | 1:A:1072:ASN:O | 1.65 | 1.15 |
| 1:A:1142:MET:CE | 1:A:1148:SER:O | 1.93 | 1.15 |
| 1:A:656:LEU:HD13 | 1:A:685:ILE:CG1 | 1.74 | 1.15 |
| 1:A:1156:ASN:CB | 1:A:1228:MET:HE3 | 1.74 | 1.15 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:CD | 2.25 | 1.15 |
| 1:A:724:LEU:CD1 | 1:A:1166:GLU:HG2 | 1.77 | 1.15 |
| 1:A:676:SER:HB3 | 1:A:1225:TYR:OH | 1.41 | 1.15 |
| 1:A:1133:MET:HG2 | 1:A:1239:HIS:CE1 | 1.81 | 1.15 |
| 1:A:767:ALA:O | 1:A:771:ASP:CB | 1.94 | 1.15 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:HD2 | 1.76 | 1.14 |
| 1:A:959:VAL:CB | 1:A:984:PRO:N | 2.10 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:76:ALA:HB1 | 2:E:81:SER:CB | 1.78 | 1.13 |
| 1:A:1071:ILE:CG2 | 1:A:1072:ASN:H | 1.62 | 1.13 |
| 1:A:1127:MET:HE3 | 1:A:1127:MET:HA | 1.18 | 1.13 |
| 1:A:688:GLU:HG3 | 1:A:724:LEU:HD23 | 1.29 | 1.13 |
| 1:A:631:MET:SD | 1:A:1208:GLY:CA | 2.36 | 1.13 |
| 1:A:856:VAL:O | 1:A:1048:SER:HB3 | 1.44 | 1.13 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:HD22 | 1.79 | 1.12 |
| 1:A:1140:GLY:O | 1:A:1144:LEU:CB | 1.97 | 1.12 |
| 1:A:656:LEU:HD11 | 1:A:685:ILE:CB | 1.77 | 1.12 |
| 1:A:879:ILE:CA | 1:A:1043:THR:HG21 | 1.79 | 1.12 |
| 1:A:1070:GLY:O | 1:A:1071:ILE:HG13 | 0.95 | 1.12 |
| 1:A:135:ASN:HD21 | 4:A:1322:NAG:C1 | 1.50 | 1.12 |
| 1:A:1062:ALA:HB1 | 1:A:1078:VAL:HB | 1.18 | 1.12 |
| 1:A:684:LEU:HD23 | 1:A:728:LEU:HD13 | 1.14 | 1.12 |
| 1:A:1133:MET:HE2 | 1:A:1239:HIS:CG | 1.84 | 1.12 |
| 1:A:752:SER:O | 1:A:755:PRO:HD2 | 1.46 | 1.12 |
| 1:A:656:LEU:CB | 1:A:682:LEU:HD11 | 1.79 | 1.11 |
| 1:A:1098:THR:HG22 | 1:A:1154:LEU:HD21 | 1.22 | 1.11 |
| 1:A:406:GLU:OE1 | 1:A:583:TRP:CZ3 | 2.03 | 1.11 |
| 1:A:915:ASN:CA | 1:A:920:VAL:HA | 1.81 | 1.10 |
| 1:A:1046:GLN:CB | 1:A:1050:ASP:OD2 | 1.98 | 1.10 |
| 1:A:635:ILE:HG23 | 1:A:690:ILE:HD13 | 1.14 | 1.10 |
| 1:A:403:PHE:CD2 | 1:A:566:PRO:HB3 | 1.87 | 1.10 |
| 1:A:752:SER:O | 1:A:755:PRO:CD | 1.99 | 1.10 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:NH1 | 2.15 | 1.09 |
| 1:A:401:PRO:HG3 | 1:A:571:TYR:HD1 | 1.01 | 1.09 |
| 1:A:856:VAL:CB | 1:A:1091:TYR:CE2 | 2.34 | 1.09 |
| 3:F:510:LYS:NZ | 4:F:701:NAG:O6 | 1.86 | 1.09 |
| 1:A:680:LEU:HB3 | 1:A:1229:TYR:OH | 1.51 | 1.09 |
| 1:A:504:PHE:HE2 | 2:E:79:VAL:CG1 | 1.63 | 1.09 |
| 1:A:720:LEU:HD22 | 1:A:1170:HIS:HA | 1.28 | 1.09 |
| 3:D:510:LYS:NZ | 4:D:701:NAG:O6 | 1.86 | 1.08 |
| 1:A:724:LEU:HD11 | 1:A:1166:GLU:CG | 1.81 | 1.08 |
| 4:A:1307:NAG:H62 | 5:A:1308:BMA:C2 | 1.82 | 1.08 |
| 1:A:929:LEU:CB | 1:A:1038:PHE:CD2 | 2.37 | 1.08 |
| 1:A:1138:MET:HE2 | 1:A:1232:MET:CB | 1.78 | 1.07 |
| 1:A:1142:MET:O | 1:A:1147:ILE:CB | 2.02 | 1.07 |
| 1:A:228:ASP:CB | 1:A:246:VAL:HG13 | 1.84 | 1.07 |
| 1:A:659:ALA:HA | 1:A:662:LEU:HD23 | 1.13 | 1.07 |
| 1:A:365:SER:HA | 1:A:662:LEU:HB3 | 1.30 | 1.07 |
| 3:H:510:LYS:NZ | 4:H:701:NAG:O6 | 1.86 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1071:ILE:HG22 | 1:A:1072:ASN:N | 1.61 | 1.07 |
| 1:A:730:GLU:HG3 | 1:A:1108:ALA:CB | 1.82 | 1.07 |
| 1:A:687:ILE:O | 1:A:691:PRO:HD3 | 1.53 | 1.06 |
| 1:A:693:LEU:HD12 | 1:A:763:PHE:HE2 | 1.18 | 1.06 |
| 1:A:1062:ALA:HB1 | 1:A:1078:VAL:CB | 1.86 | 1.06 |
| 1:A:403:PHE:HE2 | 1:A:566:PRO:CB | 1.67 | 1.06 |
| 1:A:915:ASN:HA | 1:A:920:VAL:HA | 1.38 | 1.06 |
| 1:A:503:PHE:HE1 | 2:E:83:THR:O | 1.36 | 1.06 |
| 1:A:1156:ASN:HB3 | 1:A:1228:MET:HE3 | 1.09 | 1.06 |
| 1:A:688:GLU:HG2 | 1:A:724:LEU:HD23 | 1.32 | 1.05 |
| 1:A:879:ILE:N | 1:A:1043:THR:HG21 | 1.71 | 1.05 |
| 1:A:688:GLU:C | 1:A:691:PRO:CD | 2.23 | 1.05 |
| 1:A:196:LYS:HG3 | 1:A:204:THR:OG1 | 1.54 | 1.05 |
| 1:A:685:ILE:O | 1:A:689:VAL:HG23 | 1.56 | 1.05 |
| 1:A:635:ILE:CG2 | 1:A:690:ILE:CD1 | 2.35 | 1.04 |
| 1:A:1127:MET:HE1 | 1:A:1168:CYS:HB3 | 1.33 | 1.04 |
| 1:A:1133:MET:CE | 1:A:1239:HIS:CG | 2.39 | 1.04 |
| 1:A:635:ILE:HG23 | 1:A:690:ILE:CD1 | 1.86 | 1.04 |
| 1:A:503:PHE:CD2 | 2:E:83:THR:HG22 | 1.60 | 1.04 |
| 1:A:1138:MET:HE2 | 1:A:1232:MET:HB2 | 1.34 | 1.04 |
| 1:A:717:GLY:O | 1:A:721:ASP:HB2 | 1.58 | 1.04 |
| 1:A:686:VAL:CG1 | 1:A:690:ILE:CD1 | 2.27 | 1.04 |
| 1:A:1065:VAL:O | 1:A:1068:THR:HG22 | 1.56 | 1.04 |
| 1:A:1194:MET:HE2 | 1:A:1194:MET:HA | 1.37 | 1.04 |
| 1:A:403:PHE:CE2 | 1:A:566:PRO:CB | 2.40 | 1.03 |
| 1:A:1046:GLN:HB3 | 1:A:1050:ASP:OD2 | 1.59 | 1.03 |
| 1:A:1156:ASN:HB3 | 1:A:1228:MET:CE | 1.87 | 1.03 |
| 1:A:688:GLU:HG2 | 1:A:724:LEU:CD2 | 1.87 | 1.03 |
| 1:A:656:LEU:HB2 | 1:A:682:LEU:CD1 | 1.88 | 1.03 |
| 1:A:732:ALA:CB | 1:A:749:GLY:CA | 2.35 | 1.03 |
| 1:A:751:LEU:O | 1:A:755:PRO:CG | 2.05 | 1.03 |
| 1:A:607:ARG:HG2 | 1:A:611:ASP:CG | 1.79 | 1.03 |
| 1:A:659:ALA:C | 1:A:662:LEU:HD23 | 1.77 | 1.03 |
| 1:A:732:ALA:HB3 | 1:A:749:GLY:HA3 | 1.40 | 1.03 |
| 1:A:635:ILE:HG21 | 1:A:690:ILE:HD11 | 1.40 | 1.02 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:CD2 | 2.33 | 1.02 |
| 1:A:250:LYS:HB3 | 1:A:251:PRO:HD3 | 1.38 | 1.02 |
| 1:A:523:LEU:CD1 | 1:A:1016:HIS:CB | 2.36 | 1.02 |
| 4:A:1307:NAG:C6 | 5:A:1308:BMA:H2 | 1.90 | 1.02 |
| 1:A:879:ILE:CA | 1:A:1043:THR:CG2 | 2.38 | 1.02 |
| 1:A:922:GLN:O | 1:A:1042:HIS:ND1 | 1.93 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:924:PHE:N | 1:A:925:ASN:CB | 2.22 | 1.02 |
| 2:E:76:ALA:CB | 2:E:81:SER:HB2 | 1.89 | 1.02 |
| 1:A:631:MET:SD | 1:A:1208:GLY:N | 2.32 | 1.02 |
| 1:A:1084:PHE:CE1 | 1:A:1085:TYR:CE1 | 2.47 | 1.01 |
| 1:A:879:ILE:C | 1:A:1043:THR:CG2 | 2.28 | 1.01 |
| 1:A:659:ALA:CA | 1:A:662:LEU:CD2 | 2.28 | 1.01 |
| 1:A:723:GLN:OE1 | 1:A:1169:SER:CB | 2.08 | 1.01 |
| 1:A:401:PRO:HB2 | 1:A:569:ASN:ND2 | 1.75 | 1.01 |
| 1:A:923:ILE:C | 1:A:1042:HIS:HB3 | 1.80 | 1.01 |
| 1:A:688:GLU:CG | 1:A:724:LEU:CD2 | 2.38 | 1.01 |
| 1:A:879:ILE:C | 1:A:1043:THR:HG22 | 1.81 | 1.00 |
| 3:D:595:GLN:HA | 3:D:595:GLN:HE21 | 1.25 | 1.00 |
| 1:A:337:ARG:HA | 1:A:718:GLU:HG3 | 1.41 | 1.00 |
| 1:A:1138:MET:HE1 | 1:A:1232:MET:CB | 1.84 | 1.00 |
| 1:A:504:PHE:CE2 | 2:E:79:VAL:HG11 | 1.97 | 1.00 |
| 1:A:648:LEU:HD12 | 1:A:763:PHE:CD1 | 1.95 | 1.00 |
| 1:A:401:PRO:CD | 1:A:571:TYR:CE1 | 2.44 | 0.99 |
| 1:A:929:LEU:CB | 1:A:1038:PHE:CE2 | 2.45 | 0.99 |
| 1:A:688:GLU:C | 1:A:691:PRO:HD3 | 1.82 | 0.99 |
| 1:A:503:PHE:HB2 | 2:E:83:THR:HG21 | 1.44 | 0.99 |
| 3:H:595:GLN:HE21 | 3:H:595:GLN:HA | 1.25 | 0.99 |
| 1:A:1062:ALA:HA | 1:A:1078:VAL:HG21 | 1.44 | 0.99 |
| 1:A:1045:LEU:HA | 1:A:1051:PHE:HZ | 1.27 | 0.99 |
| 1:A:676:SER:OG | 1:A:1226:PHE:CE2 | 2.15 | 0.98 |
| 1:A:504:PHE:HE2 | 2:E:79:VAL:HG11 | 1.24 | 0.98 |
| 1:A:724:LEU:HD22 | 1:A:1170:HIS:HE1 | 1.21 | 0.98 |
| 1:A:1209:GLY:HA3 | 1:A:1230:LEU:HD13 | 1.43 | 0.98 |
| 3:F:595:GLN:HE21 | 3:F:595:GLN:HA | 1.25 | 0.98 |
| 4:A:1307:NAG:H62 | 5:A:1308:BMA:H2 | 0.99 | 0.98 |
| 1:A:402:PHE:O | 1:A:403:PHE:HB3 | 1.63 | 0.98 |
| 1:A:631:MET:HE1 | 1:A:1204:LEU:C | 1.81 | 0.98 |
| 1:A:686:VAL:HG12 | 1:A:690:ILE:HD12 | 1.42 | 0.98 |
| 1:A:135:ASN:HD22 | 4:A:1322:NAG:C1 | 1.66 | 0.97 |
| 1:A:684:LEU:CD1 | 1:A:1166:GLU:HG3 | 1.93 | 0.97 |
| 2:E:76:ALA:HB1 | 2:E:81:SER:HB2 | 0.99 | 0.97 |
| 1:A:635:ILE:CG2 | 1:A:690:ILE:HD13 | 1.94 | 0.97 |
| 1:A:1071:ILE:HG22 | 1:A:1072:ASN:H | 0.83 | 0.97 |
| 1:A:656:LEU:HB2 | 1:A:682:LEU:HD11 | 0.98 | 0.97 |
| 1:A:720:LEU:O | 1:A:723:GLN:NE2 | 1.98 | 0.97 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:HB | 1.95 | 0.97 |
| 1:A:459:ASN:HD21 | 4:A:1324:NAG:C1 | 1.66 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:607:ARG:O | 1:A:611:ASP:N | 1.98 | 0.96 |
| 1:A:752:SER:C | 1:A:755:PRO:CD | 2.34 | 0.96 |
| 1:A:680:LEU:CB | 1:A:1229:TYR:OH | 2.13 | 0.96 |
| 1:A:724:LEU:CD2 | 1:A:1170:HIS:NE2 | 2.22 | 0.96 |
| 1:A:677:TYR:O | 1:A:681:PRO:CB | 2.12 | 0.96 |
| 1:A:1045:LEU:HA | 1:A:1051:PHE:CZ | 1.99 | 0.96 |
| 1:A:1062:ALA:CA | 1:A:1078:VAL:HG21 | 1.95 | 0.96 |
| 1:A:1085:TYR:O | 1:A:1087:PHE:N | 1.97 | 0.96 |
| 1:A:1055:LEU:HD23 | 1:A:1085:TYR:OH | 1.66 | 0.96 |
| 1:A:557:ASN:HD22 | 4:A:1306:NAG:C1 | 1.79 | 0.96 |
| 1:A:591:VAL:CG1 | 1:A:603:PHE:CE1 | 2.49 | 0.96 |
| 1:A:506:TYR:CE1 | 2:E:80:PRO:HG3 | 2.00 | 0.96 |
| 1:A:732:ALA:HB1 | 1:A:749:GLY:HA3 | 1.45 | 0.95 |
| 1:A:503:PHE:HB3 | 2:E:83:THR:HG21 | 1.48 | 0.95 |
| 1:A:503:PHE:CE1 | 2:E:83:THR:O | 2.18 | 0.95 |
| 1:A:1127:MET:CE | 1:A:1127:MET:HA | 1.94 | 0.95 |
| 1:A:607:ARG:HG2 | 1:A:611:ASP:OD2 | 1.64 | 0.95 |
| 1:A:686:VAL:O | 1:A:690:ILE:HG13 | 1.65 | 0.95 |
| 1:A:557:ASN:HD21 | 4:A:1306:NAG:C1 | 1.72 | 0.95 |
| 1:A:685:ILE:O | 1:A:689:VAL:CG2 | 2.15 | 0.95 |
| 1:A:718:GLU:O | 1:A:722:GLN:HB2 | 1.67 | 0.95 |
| 1:A:401:PRO:CG | 1:A:571:TYR:CD1 | 2.49 | 0.95 |
| 1:A:659:ALA:O | 1:A:662:LEU:HD23 | 1.66 | 0.95 |
| 1:A:365:SER:HA | 1:A:662:LEU:CB | 1.95 | 0.95 |
| 1:A:653:LYS:O | 1:A:682:LEU:HD21 | 1.65 | 0.95 |
| 1:A:692:PHE:CE1 | 1:A:713:GLU:HA | 2.02 | 0.95 |
| 1:A:241:GLN:NE2 | 1:A:518:ARG:HH22 | 1.64 | 0.94 |
| 1:A:656:LEU:CD1 | 1:A:685:ILE:HG12 | 1.93 | 0.94 |
| 1:A:943:ILE:CB | 1:A:1010:LYS:O | 2.15 | 0.94 |
| 1:A:635:ILE:CG2 | 1:A:690:ILE:HD11 | 1.98 | 0.94 |
| 1:A:879:ILE:O | 1:A:1043:THR:CG2 | 2.14 | 0.94 |
| 1:A:1142:MET:C | 1:A:1147:ILE:CB | 2.35 | 0.94 |
| 1:A:1110:PHE:O | 1:A:1114:MET:HG2 | 1.67 | 0.94 |
| 1:A:398:HIS:HB3 | 1:A:399:PHE:CE1 | 2.02 | 0.94 |
| 1:A:591:VAL:HG11 | 1:A:603:PHE:CE1 | 2.02 | 0.93 |
| 1:A:1046:GLN:CG | 1:A:1050:ASP:OD2 | 2.16 | 0.93 |
| 1:A:688:GLU:HG2 | 1:A:1170:HIS:CE1 | 2.03 | 0.93 |
| 1:A:421:GLN:OE1 | 2:E:144:THR:CG2 | 2.15 | 0.93 |
| 1:A:503:PHE:HZ | 2:E:86:TRP:CE3 | 1.72 | 0.93 |
| 1:A:1135:LEU:HD21 | 1:A:1161:CYS:SG | 2.08 | 0.93 |
| 1:A:729:GLY:O | 1:A:733:PRO:CB | 2.17 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1229:TYR:O | 1:A:1233:VAL:HG23 | 1.69 | 0.93 |
| 1:A:1084:PHE:CZ | 1:A:1085:TYR:HE1 | 1.87 | 0.92 |
| 1:A:507:ALA:HB1 | 1:A:529:LEU:CG | 1.99 | 0.92 |
| 1:A:923:ILE:O | 1:A:1042:HIS:HB3 | 1.63 | 0.92 |
| 1:A:241:GLN:HE22 | 1:A:518:ARG:NH2 | 1.68 | 0.92 |
| 2:E:76:ALA:CB | 2:E:81:SER:CB | 2.46 | 0.92 |
| 1:A:631:MET:HE1 | 1:A:1204:LEU:O | 0.75 | 0.92 |
| 1:A:1084:PHE:CZ | 1:A:1085:TYR:CE1 | 2.57 | 0.92 |
| 1:A:1130:THR:HG21 | 1:A:1168:CYS:SG | 2.08 | 0.92 |
| 1:A:371:VAL:O | 1:A:373:VAL:N | 2.01 | 0.92 |
| 1:A:494:VAL:HA | 1:A:497:HIS:CE1 | 2.06 | 0.91 |
| 1:A:1046:GLN:HG2 | 1:A:1050:ASP:OD2 | 1.71 | 0.91 |
| 1:A:228:ASP:HB3 | 1:A:246:VAL:HG13 | 1.48 | 0.91 |
| 1:A:879:ILE:O | 1:A:1043:THR:HG22 | 1.71 | 0.91 |
| 1:A:1171:ILE:HG23 | 1:A:1191:LEU:CD2 | 2.00 | 0.91 |
| 1:A:1059:ARG:HH11 | 1:A:1059:ARG:HG3 | 1.36 | 0.91 |
| 1:A:885:ALA:O | 1:A:1079:PHE:O | 1.89 | 0.91 |
| 1:A:724:LEU:O | 1:A:728:LEU:HG | 1.70 | 0.91 |
| 1:A:680:LEU:CG | 1:A:1229:TYR:OH | 2.16 | 0.91 |
| 1:A:724:LEU:CD2 | 1:A:1170:HIS:HE1 | 1.74 | 0.90 |
| 1:A:678:ILE:HG12 | 1:A:748:LEU:HD21 | 1.51 | 0.90 |
| 1:A:396:ASP:O | 1:A:400:GLY:N | 2.04 | 0.90 |
| 1:A:656:LEU:HB3 | 1:A:751:LEU:HD21 | 1.54 | 0.90 |
| 1:A:1141:VAL:O | 1:A:1147:ILE:CB | 2.19 | 0.90 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:HD22 | 1.40 | 0.90 |
| 1:A:924:PHE:CB | 1:A:1041:TYR:O | 2.20 | 0.89 |
| 1:A:620:ASP:O | 1:A:623:THR:OG1 | 1.88 | 0.89 |
| 1:A:732:ALA:HB3 | 1:A:749:GLY:CA | 1.98 | 0.89 |
| 1:A:631:MET:HG3 | 1:A:1208:GLY:HA3 | 1.54 | 0.89 |
| 1:A:915:ASN:CB | 1:A:920:VAL:CA | 2.51 | 0.89 |
| 1:A:1082:SER:HB2 | 1:A:1084:PHE:CD1 | 2.08 | 0.89 |
| 1:A:591:VAL:HG12 | 1:A:603:PHE:CZ | 2.08 | 0.89 |
| 1:A:401:PRO:HB2 | 1:A:569:ASN:HD21 | 1.30 | 0.89 |
| 1:A:504:PHE:CE2 | 2:E:79:VAL:CG1 | 2.53 | 0.89 |
| 1:A:641:HIS:O | 1:A:642:MET:O | 1.89 | 0.89 |
| 1:A:1098:THR:HG22 | 1:A:1154:LEU:CD2 | 2.03 | 0.88 |
| 1:A:680:LEU:HG | 1:A:1229:TYR:OH | 1.70 | 0.88 |
| 1:A:506:TYR:OH | 2:E:80:PRO:HA | 1.73 | 0.88 |
| 1:A:755:PRO:HD2 | 1:A:756:ALA:N | 1.84 | 0.88 |
| 1:A:1082:SER:O | 1:A:1084:PHE:N | 2.05 | 0.88 |
| 1:A:228:ASP:HA | 1:A:246:VAL:CG1 | 2.03 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:659:ALA:HA | 1:A:662:LEU:HD22 | 1.54 | 0.88 |
| 1:A:632:PHE:HZ | 1:A:650:VAL:HG23 | 1.39 | 0.88 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:HD3 | 2.04 | 0.88 |
| 1:A:631:MET:SD | 1:A:1208:GLY:HA2 | 2.14 | 0.88 |
| 1:A:752:SER:C | 1:A:755:PRO:HD3 | 1.93 | 0.88 |
| 1:A:1009:PRO:CA | 1:A:1016:HIS:O | 2.22 | 0.87 |
| 1:A:504:PHE:HZ | 2:E:141:VAL:HG21 | 1.39 | 0.87 |
| 1:A:544:TRP:HD1 | 1:A:545:LEU:N | 1.72 | 0.87 |
| 1:A:1127:MET:CE | 1:A:1168:CYS:CB | 2.52 | 0.87 |
| 1:A:929:LEU:CB | 1:A:1038:PHE:HD2 | 1.81 | 0.87 |
| 1:A:507:ALA:CB | 1:A:529:LEU:HG | 2.05 | 0.87 |
| 1:A:879:ILE:HA | 1:A:1043:THR:CG2 | 2.04 | 0.87 |
| 1:A:459:ASN:HD22 | 4:A:1324:NAG:C1 | 1.87 | 0.87 |
| 1:A:755:PRO:CD | 1:A:756:ALA:H | 1.88 | 0.87 |
| 1:A:1085:TYR:O | 1:A:1088:TYR:N | 2.06 | 0.86 |
| 1:A:523:LEU:HD11 | 1:A:1016:HIS:CA | 2.04 | 0.86 |
| 1:A:692:PHE:HZ | 1:A:713:GLU:CB | 1.86 | 0.86 |
| 1:A:684:LEU:HD11 | 1:A:728:LEU:CD2 | 2.05 | 0.86 |
| 1:A:692:PHE:CZ | 1:A:713:GLU:HA | 2.10 | 0.86 |
| 1:A:650:VAL:O | 1:A:654:VAL:HG23 | 1.74 | 0.86 |
| 1:A:384:PRO:HA | 1:A:389:ARG:HG3 | 1.58 | 0.85 |
| 1:A:1070:GLY:C | 1:A:1071:ILE:HG13 | 1.97 | 0.85 |
| 1:A:401:PRO:HD3 | 1:A:571:TYR:HE1 | 1.08 | 0.85 |
| 3:D:595:GLN:HA | 3:D:595:GLN:NE2 | 1.92 | 0.85 |
| 1:A:1138:MET:HE1 | 1:A:1232:MET:HA | 0.86 | 0.85 |
| 3:F:595:GLN:NE2 | 3:F:595:GLN:HA | 1.92 | 0.85 |
| 1:A:688:GLU:CG | 1:A:1170:HIS:NE2 | 2.39 | 0.85 |
| 1:A:441:HIS:CE1 | 1:A:495:LEU:HD23 | 2.12 | 0.85 |
| 1:A:894:GLU:CB | 1:A:995:PHE:CB | 2.55 | 0.84 |
| 1:A:1138:MET:CE | 1:A:1232:MET:CA | 2.31 | 0.84 |
| 1:A:402:PHE:O | 1:A:403:PHE:CB | 2.25 | 0.84 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:CB | 2.52 | 0.84 |
| 1:A:720:LEU:HD22 | 1:A:1170:HIS:CA | 2.06 | 0.84 |
| 1:A:656:LEU:CD1 | 1:A:682:LEU:HD12 | 2.07 | 0.84 |
| 1:A:1133:MET:CG | 1:A:1239:HIS:CE1 | 2.53 | 0.84 |
| 1:A:1055:LEU:HD22 | 1:A:1055:LEU:O | 1.78 | 0.84 |
| 1:A:196:LYS:CG | 1:A:204:THR:OG1 | 2.25 | 0.84 |
| 1:A:1084:PHE:HE1 | 1:A:1085:TYR:CD1 | 1.88 | 0.84 |
| 2:C:39:HIS:HB2 | 2:C:42:VAL:HG22 | 1.60 | 0.84 |
| 1:A:167:SER:O | 1:A:168:SER:OG | 1.96 | 0.83 |
| 1:A:228:ASP:CB | 1:A:246:VAL:CG1 | 2.56 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:684:LEU:HG | 1:A:1166:GLU:HG3 | 1.61 | 0.83 |
| 1:A:1167:PHE:CE2 | 1:A:1237:ALA:HA | 2.13 | 0.83 |
| 1:A:693:LEU:CD1 | 1:A:763:PHE:CD2 | 2.48 | 0.83 |
| 1:A:1082:SER:HB2 | 1:A:1084:PHE:CE1 | 2.14 | 0.83 |
| 1:A:1142:MET:HE2 | 1:A:1153:SER:OG | 1.79 | 0.83 |
| 2:G:39:HIS:HB2 | 2:G:42:VAL:HG22 | 1.60 | 0.83 |
| 3:H:595:GLN:NE2 | 3:H:595:GLN:HA | 1.92 | 0.83 |
| 1:A:1068:THR:HG23 | 1:A:1069:MET:H | 1.44 | 0.83 |
| 1:A:732:ALA:HB1 | 1:A:749:GLY:CA | 2.02 | 0.83 |
| 1:A:1133:MET:SD | 1:A:1239:HIS:CE1 | 2.71 | 0.82 |
| 1:A:656:LEU:CB | 1:A:682:LEU:CD1 | 2.53 | 0.82 |
| 1:A:1209:GLY:O | 1:A:1213:LEU:N | 2.11 | 0.82 |
| 1:A:926:ALA:O | 1:A:1040:THR:CG2 | 2.23 | 0.82 |
| 1:A:241:GLN:HE22 | 1:A:518:ARG:HH22 | 0.85 | 0.82 |
| 1:A:631:MET:CG | 1:A:1208:GLY:HA3 | 2.10 | 0.82 |
| 1:A:856:VAL:O | 1:A:1048:SER:HB2 | 1.75 | 0.82 |
| 1:A:591:VAL:CG1 | 1:A:603:PHE:CZ | 2.63 | 0.82 |
| 1:A:1210:ILE:HG13 | 1:A:1214:ALA:HB3 | 1.61 | 0.82 |
| 1:A:686:VAL:HG13 | 1:A:690:ILE:HD11 | 1.62 | 0.82 |
| 1:A:684:LEU:CG | 1:A:1166:GLU:HG3 | 2.10 | 0.81 |
| 2:E:39:HIS:HB2 | 2:E:42:VAL:HG22 | 1.60 | 0.81 |
| 1:A:503:PHE:HE2 | 2:E:86:TRP:CE3 | 1.97 | 0.81 |
| 1:A:228:ASP:HA | 1:A:246:VAL:HG11 | 1.61 | 0.81 |
| 1:A:656:LEU:HD13 | 1:A:685:ILE:HG12 | 1.56 | 0.81 |
| 1:A:396:ASP:HA | 1:A:400:GLY:CA | 2.11 | 0.81 |
| 1:A:1133:MET:HE2 | 1:A:1239:HIS:CE1 | 2.10 | 0.81 |
| 1:A:1202:ILE:HG21 | 1:A:1237:ALA:HB1 | 1.62 | 0.81 |
| 1:A:720:LEU:O | 1:A:723:GLN:HG3 | 1.79 | 0.81 |
| 1:A:676:SER:OG | 1:A:1226:PHE:HE2 | 1.60 | 0.81 |
| 1:A:1135:LEU:O | 1:A:1139:PHE:HD2 | 1.64 | 0.81 |
| 1:A:693:LEU:HD11 | 1:A:763:PHE:HD2 | 1.36 | 0.81 |
| 1:A:421:GLN:HG2 | 2:E:143:GLY:HA2 | 1.60 | 0.81 |
| 1:A:1140:GLY:O | 1:A:1144:LEU:N | 2.13 | 0.80 |
| 1:A:396:ASP:HA | 1:A:400:GLY:HA2 | 1.63 | 0.80 |
| 1:A:1108:ALA:O | 1:A:1112:VAL:CG2 | 2.28 | 0.80 |
| 1:A:1229:TYR:CE1 | 1:A:1233:VAL:HG21 | 2.15 | 0.80 |
| 1:A:678:ILE:CG1 | 1:A:748:LEU:HD21 | 2.11 | 0.80 |
| 1:A:1142:MET:CE | 1:A:1153:SER:OG | 2.30 | 0.80 |
| 1:A:648:LEU:CB | 1:A:763:PHE:CE1 | 2.60 | 0.80 |
| 1:A:985:GLU:CB | 1:A:986:GLY:HA2 | 2.11 | 0.80 |
| 1:A:1171:ILE:CG2 | 1:A:1191:LEU:CD2 | 2.59 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1229:TYR:CD1 | 1:A:1233:VAL:HG21 | 2.15 | 0.80 |
| 1:A:628:TYR:OH | 1:A:653:LYS:HD2 | 1.82 | 0.80 |
| 1:A:1209:GLY:HA3 | 1:A:1230:LEU:CD1 | 2.10 | 0.80 |
| 1:A:503:PHE:CE2 | 2:E:86:TRP:CZ3 | 2.69 | 0.80 |
| 1:A:608:SER:O | 1:A:612:GLU:HB2 | 1.82 | 0.80 |
| 4:A:1306:NAG:H62 | 4:A:1307:NAG:C8 | 2.12 | 0.79 |
| 1:A:503:PHE:CZ | 2:E:86:TRP:HB2 | 2.17 | 0.79 |
| 1:A:633:LEU:O | 1:A:636:SER:OG | 1.99 | 0.79 |
| 1:A:648:LEU:HB3 | 1:A:763:PHE:CZ | 2.17 | 0.79 |
| 1:A:687:ILE:O | 1:A:691:PRO:CD | 2.28 | 0.79 |
| 1:A:503:PHE:CZ | 2:E:83:THR:HA | 2.15 | 0.79 |
| 1:A:504:PHE:HE2 | 2:E:79:VAL:HG12 | 1.46 | 0.79 |
| 1:A:404:ARG:HD2 | 1:A:567:VAL:CG2 | 2.12 | 0.79 |
| 1:A:648:LEU:HD11 | 1:A:763:PHE:HA | 1.64 | 0.79 |
| 1:A:959:VAL:C | 1:A:984:PRO:N | 2.36 | 0.79 |
| 1:A:381:TRP:HD1 | 1:A:382:SER:N | 1.80 | 0.79 |
| 1:A:584:GLU:OE2 | 1:A:606:GLU:HB2 | 1.82 | 0.79 |
| 1:A:580:ALA:O | 1:A:584:GLU:HG3 | 1.83 | 0.79 |
| 1:A:631:MET:CE | 1:A:1204:LEU:C | 2.44 | 0.79 |
| 1:A:401:PRO:CB | 1:A:569:ASN:HD21 | 1.96 | 0.79 |
| 1:A:472:LEU:HD21 | 1:A:1017:ALA:CB | 2.13 | 0.78 |
| 1:A:730:GLU:HG2 | 1:A:1112:VAL:CG2 | 2.13 | 0.78 |
| 1:A:1171:ILE:HG23 | 1:A:1191:LEU:HD23 | 1.63 | 0.78 |
| 1:A:185:ASN:HD22 | 4:A:1319:NAG:C1 | 1.93 | 0.78 |
| 1:A:720:LEU:CD2 | 1:A:1170:HIS:HA | 2.11 | 0.78 |
| 4:A:1312:NAG:H62 | 4:A:1313:NAG:HN2 | 1.47 | 0.78 |
| 1:A:659:ALA:O | 1:A:662:LEU:CD2 | 2.31 | 0.78 |
| 1:A:337:ARG:HA | 1:A:718:GLU:CG | 2.12 | 0.78 |
| 1:A:635:ILE:HG21 | 1:A:690:ILE:CD1 | 2.09 | 0.78 |
| 1:A:1110:PHE:HE2 | 1:A:1124:ALA:HB1 | 1.48 | 0.78 |
| 1:A:409:ILE:HG21 | 1:A:872:MET:CB | 2.14 | 0.78 |
| 1:A:1184:VAL:O | 1:A:1184:VAL:HG12 | 1.84 | 0.78 |
| 1:A:228:ASP:CA | 1:A:246:VAL:HG13 | 2.14 | 0.78 |
| 1:A:856:VAL:C | 1:A:1048:SER:CB | 2.53 | 0.78 |
| 1:A:632:PHE:CZ | 1:A:650:VAL:HG23 | 2.19 | 0.78 |
| 1:A:1051:PHE:HB3 | 1:A:1084:PHE:HD2 | 1.49 | 0.77 |
| 1:A:1127:MET:HE2 | 1:A:1168:CYS:CB | 2.13 | 0.77 |
| 1:A:401:PRO:HB2 | 1:A:569:ASN:CG | 2.03 | 0.77 |
| 1:A:1021:SER:O | 1:A:1022:ALA:CB | 2.31 | 0.77 |
| 1:A:629:ALA:O | 1:A:633:LEU:HG | 1.84 | 0.77 |
| 1:A:1201:GLY:O | 1:A:1205:THR:HG23 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:752:SER:HA | 1:A:755:PRO:CG | 2.15 | 0.77 |
| 1:A:1156:ASN:CG | 1:A:1228:MET:HE3 | 2.06 | 0.76 |
| 1:A:544:TRP:CD1 | 1:A:545:LEU:N | 2.53 | 0.76 |
| 1:A:879:ILE:C | 1:A:1043:THR:HG21 | 2.00 | 0.76 |
| 1:A:688:GLU:OE1 | 1:A:721:ASP:OD1 | 2.02 | 0.76 |
| 1:A:381:TRP:O | 1:A:740:PHE:CB | 2.33 | 0.76 |
| 1:A:959:VAL:C | 1:A:984:PRO:CB | 2.54 | 0.76 |
| 1:A:1135:LEU:O | 1:A:1139:PHE:CD2 | 2.38 | 0.76 |
| 1:A:1138:MET:HE2 | 1:A:1232:MET:HB3 | 1.67 | 0.76 |
| 1:A:684:LEU:CD1 | 1:A:728:LEU:HD22 | 2.15 | 0.76 |
| 1:A:1194:MET:CE | 1:A:1194:MET:HA | 2.15 | 0.76 |
| 1:A:631:MET:CG | 1:A:1208:GLY:CA | 2.64 | 0.76 |
| 1:A:494:VAL:HA | 1:A:497:HIS:ND1 | 2.01 | 0.76 |
| 1:A:630:ILE:O | 1:A:634:TYR:CD2 | 2.39 | 0.76 |
| 1:A:503:PHE:HZ | 2:E:86:TRP:HB2 | 1.48 | 0.76 |
| 1:A:503:PHE:CD2 | 2:E:83:THR:CG2 | 2.28 | 0.75 |
| 1:A:1127:MET:CE | 1:A:1130:THR:HG21 | 2.16 | 0.75 |
| 1:A:1127:MET:HE2 | 1:A:1168:CYS:HB3 | 1.67 | 0.75 |
| 1:A:506:TYR:OH | 2:E:80:PRO:CA | 2.34 | 0.75 |
| 1:A:607:ARG:CG | 1:A:611:ASP:CG | 2.53 | 0.75 |
| 1:A:1138:MET:SD | 1:A:1232:MET:HB2 | 2.27 | 0.75 |
| 1:A:656:LEU:HD11 | 1:A:685:ILE:HG13 | 0.78 | 0.75 |
| 1:A:1199:PHE:O | 1:A:1203:THR:CG2 | 2.34 | 0.75 |
| 1:A:726:ARG:HB3 | 1:A:1112:VAL:CG1 | 2.16 | 0.74 |
| 1:A:396:ASP:CA | 1:A:400:GLY:HA2 | 2.17 | 0.74 |
| 1:A:441:HIS:NE2 | 1:A:496:ASP:OD1 | 2.21 | 0.74 |
| 1:A:250:LYS:HB3 | 1:A:251:PRO:HD2 | 1.68 | 0.74 |
| 1:A:407:GLN:HB3 | 1:A:604:THR:HG21 | 1.67 | 0.74 |
| 1:A:515:TYR:CE1 | 1:A:526:THR:CG2 | 2.70 | 0.74 |
| 1:A:684:LEU:HD11 | 1:A:728:LEU:HD21 | 1.68 | 0.74 |
| 1:A:1045:LEU:CA | 1:A:1051:PHE:CZ | 2.70 | 0.74 |
| 1:A:873:VAL:CB | 1:A:1045:LEU:HD13 | 2.17 | 0.74 |
| 1:A:1084:PHE:CD1 | 1:A:1085:TYR:HD1 | 2.06 | 0.74 |
| 1:A:730:GLU:HG3 | 1:A:1108:ALA:HB1 | 0.87 | 0.74 |
| 1:A:185:ASN:ND2 | 4:A:1319:NAG:O5 | 2.20 | 0.74 |
| 1:A:1045:LEU:CA | 1:A:1051:PHE:HZ | 2.00 | 0.74 |
| 1:A:881:GLN:CB | 1:A:1041:TYR:HB2 | 2.17 | 0.74 |
| 1:A:1055:LEU:HD23 | 1:A:1085:TYR:CE2 | 2.23 | 0.74 |
| 1:A:726:ARG:HB3 | 1:A:1112:VAL:HG11 | 1.68 | 0.74 |
| 4:A:1306:NAG:H82 | 4:A:1306:NAG:C1 | 2.18 | 0.74 |
| 2:E:70:LEU:HD13 | 2:E:179:GLY:HA2 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:503:PHE:CE2 | 2:E:83:THR:HG22 | 2.22 | 0.74 |
| 1:A:1127:MET:HE1 | 1:A:1168:CYS:CB | 2.14 | 0.73 |
| 1:A:1127:MET:O | 1:A:1130:THR:OG1 | 2.06 | 0.73 |
| 1:A:656:LEU:HD11 | 1:A:685:ILE:CG2 | 2.18 | 0.73 |
| 1:A:720:LEU:HB3 | 1:A:1170:HIS:HD2 | 1.52 | 0.73 |
| 1:A:621:VAL:O | 1:A:625:VAL:HG23 | 1.87 | 0.73 |
| 1:A:368:LEU:O | 1:A:665:LEU:CB | 2.36 | 0.73 |
| 1:A:1065:VAL:O | 1:A:1068:THR:CG2 | 2.36 | 0.73 |
| 1:A:676:SER:CB | 1:A:1225:TYR:OH | 2.30 | 0.73 |
| 1:A:1062:ALA:O | 1:A:1066:THR:OG1 | 2.06 | 0.73 |
| 1:A:1203:THR:HG23 | 1:A:1204:LEU:N | 2.03 | 0.73 |
| 1:A:228:ASP:CA | 1:A:246:VAL:CG1 | 2.67 | 0.73 |
| 1:A:401:PRO:CB | 1:A:569:ASN:OD1 | 2.36 | 0.73 |
| 1:A:1156:ASN:CB | 1:A:1228:MET:CE | 2.57 | 0.73 |
| 1:A:504:PHE:CZ | 2:E:141:VAL:HG21 | 2.23 | 0.73 |
| 1:A:1210:ILE:CD1 | 1:A:1214:ALA:HB2 | 2.19 | 0.73 |
| 1:A:984:PRO:O | 1:A:989:ARG:N | 2.21 | 0.73 |
| 1:A:1068:THR:HG23 | 1:A:1069:MET:N | 2.03 | 0.73 |
| 1:A:1122:TRP:O | 1:A:1126:ILE:HG13 | 1.89 | 0.72 |
| 1:A:653:LYS:HE3 | 1:A:653:LYS:C | 2.09 | 0.72 |
| 1:A:915:ASN:HA | 1:A:920:VAL:CA | 2.17 | 0.72 |
| 2:G:70:LEU:HD13 | 2:G:179:GLY:HA2 | 1.70 | 0.72 |
| 1:A:108:PHE:HE1 | 1:A:194:PHE:HE1 | 1.37 | 0.72 |
| 1:A:259:PRO:O | 1:A:260:TRP:CB | 2.37 | 0.72 |
| 1:A:684:LEU:HD23 | 1:A:728:LEU:CD1 | 1.96 | 0.72 |
| 2:C:70:LEU:HD13 | 2:C:179:GLY:HA2 | 1.70 | 0.72 |
| 1:A:1138:MET:O | 1:A:1142:MET:HG2 | 1.89 | 0.72 |
| 4:A:1306:NAG:C6 | 4:A:1307:NAG:C8 | 2.68 | 0.72 |
| 1:A:676:SER:HB3 | 1:A:1225:TYR:CZ | 2.23 | 0.72 |
| 1:A:544:TRP:CZ2 | 1:A:1041:TYR:HE1 | 2.07 | 0.72 |
| 1:A:1142:MET:HE3 | 1:A:1148:SER:C | 2.09 | 0.72 |
| 1:A:684:LEU:HD11 | 1:A:1166:GLU:HG3 | 1.71 | 0.72 |
| 1:A:1062:ALA:HB2 | 1:A:1078:VAL:HG11 | 1.70 | 0.71 |
| 1:A:386:SER:O | 1:A:390:LEU:HD12 | 1.90 | 0.71 |
| 1:A:1133:MET:HE3 | 1:A:1239:HIS:CG | 2.26 | 0.71 |
| 1:A:1131:ILE:O | 1:A:1135:LEU:HG | 1.90 | 0.71 |
| 1:A:1211:VAL:O | 1:A:1215:PHE:CB | 2.38 | 0.71 |
| 1:A:632:PHE:CZ | 1:A:650:VAL:CG2 | 2.72 | 0.71 |
| 1:A:1124:ALA:O | 1:A:1128:CYS:HB2 | 1.91 | 0.71 |
| 1:A:693:LEU:HD12 | 1:A:763:PHE:CE2 | 2.01 | 0.71 |
| 1:A:929:LEU:CB | 1:A:1038:PHE:HE2 | 1.98 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1161:CYS:O | 1:A:1165:VAL:HG23 | 1.91 | 0.71 |
| 1:A:631:MET:SD | 1:A:1208:GLY:HA3 | 2.30 | 0.71 |
| 1:A:1046:GLN:O | 1:A:1047:THR:OG1 | 2.06 | 0.71 |
| 1:A:1228:MET:HG3 | 1:A:1229:TYR:N | 2.04 | 0.71 |
| 1:A:1062:ALA:HB1 | 1:A:1078:VAL:CG2 | 2.20 | 0.71 |
| 1:A:1133:MET:HG3 | 1:A:1239:HIS:CD2 | 2.23 | 0.71 |
| 1:A:692:PHE:HE1 | 1:A:713:GLU:HA | 1.53 | 0.71 |
| 1:A:754:MET:N | 1:A:755:PRO:HD3 | 2.05 | 0.71 |
| 1:A:689:VAL:HG21 | 1:A:759:THR:HG21 | 1.72 | 0.71 |
| 1:A:403:PHE:HE2 | 1:A:566:PRO:HB3 | 0.94 | 0.70 |
| 1:A:1098:THR:CG2 | 1:A:1154:LEU:HD21 | 2.13 | 0.70 |
| 1:A:720:LEU:C | 1:A:723:GLN:HE21 | 1.93 | 0.70 |
| 1:A:1051:PHE:HB3 | 1:A:1084:PHE:CD2 | 2.25 | 0.70 |
| 1:A:404:ARG:HD2 | 1:A:567:VAL:HG23 | 1.72 | 0.70 |
| 1:A:591:VAL:HB | 1:A:603:PHE:HE1 | 1.55 | 0.70 |
| 1:A:856:VAL:C | 1:A:1048:SER:HB3 | 2.11 | 0.70 |
| 1:A:503:PHE:HZ | 2:E:86:TRP:CD2 | 2.10 | 0.70 |
| 4:A:1312:NAG:H62 | 4:A:1313:NAG:N2 | 2.06 | 0.70 |
| 1:A:684:LEU:CD1 | 1:A:728:LEU:CD2 | 2.70 | 0.70 |
| 1:A:824:SER:CB | 1:A:1188:GLU:OE1 | 2.40 | 0.70 |
| 1:A:506:TYR:HB3 | 1:A:528:LEU:HD13 | 1.74 | 0.70 |
| 1:A:1138:MET:CE | 1:A:1138:MET:HA | 2.22 | 0.70 |
| 1:A:228:ASP:HA | 1:A:246:VAL:HG13 | 1.74 | 0.70 |
| 1:A:406:GLU:OE2 | 1:A:567:VAL:CG1 | 2.40 | 0.70 |
| 1:A:688:GLU:C | 1:A:691:PRO:HD2 | 1.97 | 0.70 |
| 1:A:591:VAL:HB | 1:A:603:PHE:CE1 | 2.27 | 0.69 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:HD11 | 1.69 | 0.69 |
| 1:A:722:GLN:HE21 | 1:A:1116:LEU:HD11 | 1.57 | 0.69 |
| 2:E:76:ALA:CB | 2:E:81:SER:HB3 | 2.22 | 0.69 |
| 1:A:506:TYR:CZ | 2:E:80:PRO:HG3 | 2.26 | 0.69 |
| 2:E:39:HIS:HD2 | 2:E:42:VAL:HG21 | 1.58 | 0.69 |
| 1:A:730:GLU:HG2 | 1:A:1112:VAL:HG21 | 1.73 | 0.69 |
| 1:A:1106:LEU:CD2 | 1:A:1131:ILE:HD13 | 2.22 | 0.69 |
| 1:A:704:ILE:HA | 1:A:708:ALA:HB3 | 1.75 | 0.69 |
| 1:A:1130:THR:CG2 | 1:A:1168:CYS:SG | 2.79 | 0.69 |
| 1:A:751:LEU:O | 1:A:755:PRO:CD | 2.41 | 0.69 |
| 2:C:39:HIS:HD2 | 2:C:42:VAL:HG21 | 1.58 | 0.69 |
| 1:A:1203:THR:CG2 | 1:A:1204:LEU:N | 2.55 | 0.69 |
| 1:A:607:ARG:HG2 | 1:A:611:ASP:OD1 | 1.93 | 0.69 |
| 1:A:755:PRO:CD | 1:A:756:ALA:N | 2.51 | 0.69 |
| 1:A:692:PHE:CZ | 1:A:713:GLU:CA | 2.76 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:752:SER:O | 1:A:755:PRO:CG | 2.41 | 0.68 |
| 4:A:1305:NAG:O7 | 4:A:1305:NAG:O3 | 2.11 | 0.68 |
| 4:A:1313:NAG:H4 | 5:A:1314:BMA:O2 | 1.93 | 0.68 |
| 1:A:924:PHE:CA | 1:A:925:ASN:CB | 2.71 | 0.68 |
| 1:A:1047:THR:HG22 | 1:A:1048:SER:N | 2.09 | 0.68 |
| 1:A:1160:SER:HB2 | 1:A:1232:MET:SD | 2.34 | 0.68 |
| 1:A:662:LEU:HG | 1:A:663:ILE:N | 2.07 | 0.68 |
| 1:A:108:PHE:CE1 | 1:A:194:PHE:HE1 | 2.12 | 0.68 |
| 1:A:1009:PRO:O | 1:A:1010:LYS:O | 2.11 | 0.68 |
| 1:A:1133:MET:HE3 | 1:A:1239:HIS:HB2 | 1.74 | 0.68 |
| 1:A:1133:MET:CG | 1:A:1239:HIS:CG | 2.77 | 0.68 |
| 4:A:1306:NAG:C6 | 4:A:1307:NAG:H82 | 2.24 | 0.68 |
| 1:A:630:ILE:HG22 | 1:A:634:TYR:HE2 | 1.59 | 0.68 |
| 1:A:704:ILE:HA | 1:A:708:ALA:CB | 2.24 | 0.68 |
| 1:A:1110:PHE:O | 1:A:1114:MET:CG | 2.39 | 0.68 |
| 1:A:1133:MET:HG2 | 1:A:1239:HIS:HE2 | 1.51 | 0.68 |
| 1:A:648:LEU:CD1 | 1:A:763:PHE:CD1 | 2.74 | 0.68 |
| 1:A:1110:PHE:CE2 | 1:A:1124:ALA:HB1 | 2.29 | 0.67 |
| 1:A:158:ASN:CG | 4:A:1303:NAG:C1 | 2.60 | 0.67 |
| 4:A:1312:NAG:C6 | 4:A:1313:NAG:C1 | 2.73 | 0.67 |
| 1:A:544:TRP:CZ2 | 1:A:1041:TYR:CE1 | 2.82 | 0.67 |
| 1:A:762:LEU:O | 1:A:766:LEU:HG | 1.95 | 0.67 |
| 1:A:878:SER:C | 1:A:1043:THR:HG21 | 2.13 | 0.67 |
| 1:A:653:LYS:HB2 | 1:A:682:LEU:HD23 | 1.75 | 0.67 |
| 2:G:39:HIS:HD2 | 2:G:42:VAL:HG21 | 1.57 | 0.67 |
| 3:H:509:PRO:HB2 | 3:H:510:LYS:HG3 | 1.77 | 0.67 |
| 1:A:1133:MET:HG2 | 1:A:1239:HIS:CG | 2.24 | 0.67 |
| 1:A:656:LEU:CG | 1:A:685:ILE:HG13 | 2.18 | 0.67 |
| 1:A:1062:ALA:HB2 | 1:A:1078:VAL:CG1 | 2.24 | 0.67 |
| 1:A:1059:ARG:NH1 | 1:A:1059:ARG:HG3 | 2.09 | 0.67 |
| 1:A:635:ILE:HG13 | 1:A:1204:LEU:HD13 | 1.77 | 0.67 |
| 1:A:751:LEU:C | 1:A:751:LEU:HD23 | 2.15 | 0.67 |
| 1:A:401:PRO:HG3 | 1:A:571:TYR:CE1 | 2.29 | 0.67 |
| 1:A:656:LEU:HD13 | 1:A:682:LEU:HD12 | 1.75 | 0.67 |
| 1:A:1080:PRO:HG2 | 1:A:1085:TYR:CE2 | 2.30 | 0.67 |
| 1:A:401:PRO:HB2 | 1:A:569:ASN:OD1 | 1.94 | 0.67 |
| 1:A:950:VAL:O | 1:A:951:LYS:CB | 2.43 | 0.67 |
| 1:A:627:SER:OG | 1:A:1212:VAL:CG2 | 2.43 | 0.67 |
| 1:A:399:PHE:HE2 | 1:A:1022:ALA:HA | 1.60 | 0.66 |
| 1:A:703:PHE:C | 1:A:708:ALA:HB2 | 2.15 | 0.66 |
| 1:A:1022:ALA:O | 1:A:1035:ALA:N | 2.27 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:407:GLN:HB3 | 1:A:604:THR:CG2 | 2.24 | 0.66 |
| 1:A:688:GLU:CB | 1:A:724:LEU:HD23 | 2.25 | 0.66 |
| 3:D:509:PRO:HB2 | 3:D:510:LYS:HG3 | 1.77 | 0.66 |
| 1:A:503:PHE:CE1 | 2:E:83:THR:C | 2.51 | 0.66 |
| 1:A:691:PRO:HD2 | 1:A:692:PHE:H | 1.60 | 0.66 |
| 1:A:1135:LEU:HB3 | 1:A:1139:PHE:HE2 | 1.59 | 0.66 |
| 1:A:630:ILE:O | 1:A:634:TYR:HD2 | 1.79 | 0.66 |
| 1:A:690:ILE:O | 1:A:694:VAL:HG23 | 1.96 | 0.66 |
| 3:F:595:GLN:HE21 | 3:F:595:GLN:CA | 2.05 | 0.66 |
| 3:H:595:GLN:HE21 | 3:H:595:GLN:CA | 2.05 | 0.66 |
| 3:D:595:GLN:CA | 3:D:595:GLN:HE21 | 2.05 | 0.66 |
| 1:A:506:TYR:OH | 2:E:80:PRO:CB | 2.44 | 0.66 |
| 1:A:250:LYS:CB | 1:A:251:PRO:CD | 2.60 | 0.66 |
| 1:A:611:ASP:O | 1:A:615:ARG:HB2 | 1.96 | 0.66 |
| 1:A:1229:TYR:O | 1:A:1233:VAL:CG2 | 2.43 | 0.65 |
| 1:A:685:ILE:HD13 | 1:A:685:ILE:N | 2.09 | 0.65 |
| 3:F:509:PRO:HB2 | 3:F:510:LYS:HG3 | 1.77 | 0.65 |
| 1:A:1114:MET:CE | 1:A:1124:ALA:HB2 | 2.27 | 0.65 |
| 1:A:1167:PHE:CE2 | 1:A:1237:ALA:CA | 2.79 | 0.65 |
| 1:A:472:LEU:HD22 | 1:A:538:GLY:HA3 | 1.78 | 0.65 |
| 1:A:692:PHE:HZ | 1:A:713:GLU:CA | 2.08 | 0.65 |
| 1:A:723:GLN:NE2 | 1:A:724:LEU:HB2 | 2.12 | 0.65 |
| 1:A:1082:SER:O | 1:A:1084:PHE:HD1 | 1.79 | 0.65 |
| 1:A:724:LEU:HD11 | 1:A:1166:GLU:HG2 | 0.84 | 0.65 |
| 4:A:1306:NAG:O6 | 4:A:1307:NAG:C8 | 2.45 | 0.65 |
| 1:A:656:LEU:HD12 | 1:A:682:LEU:HD12 | 1.77 | 0.65 |
| 1:A:879:ILE:O | 1:A:1043:THR:HG21 | 1.92 | 0.65 |
| 1:A:591:VAL:CB | 1:A:603:PHE:CE1 | 2.80 | 0.65 |
| 1:A:757:VAL:O | 1:A:760:PHE:HB2 | 1.96 | 0.65 |
| 1:A:640:GLY:O | 1:A:642:MET:N | 2.30 | 0.65 |
| 1:A:423:TYR:CE1 | 1:A:424:PRO:HB3 | 2.32 | 0.64 |
| 1:A:1207:PHE:O | 1:A:1210:ILE:HG22 | 1.97 | 0.64 |
| 1:A:1210:ILE:HG23 | 1:A:1211:VAL:N | 2.11 | 0.64 |
| 1:A:1084:PHE:HZ | 1:A:1085:TYR:HE1 | 1.38 | 0.64 |
| 1:A:627:SER:OG | 1:A:1212:VAL:HG22 | 1.96 | 0.64 |
| 1:A:363:ALA:O | 1:A:367:GLY:N | 2.27 | 0.64 |
| 1:A:474:PRO:O | 1:A:476:ASN:N | 2.30 | 0.64 |
| 1:A:674:VAL:O | 1:A:678:ILE:CD1 | 2.46 | 0.64 |
| 1:A:692:PHE:CZ | 1:A:713:GLU:CB | 2.76 | 0.64 |
| 1:A:1046:GLN:HB3 | 1:A:1050:ASP:CG | 2.18 | 0.64 |
| 1:A:384:PRO:O | 1:A:385:SER:OG | 2.14 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:407:GLN:O | 1:A:604:THR:OG1 | 2.16 | 0.64 |
| 1:A:1137:ASN:HB3 | 1:A:1235:LEU:HD13 | 1.80 | 0.64 |
| 1:A:1145:TRP:O | 1:A:1147:ILE:N | 2.31 | 0.64 |
| 1:A:686:VAL:O | 1:A:690:ILE:N | 2.30 | 0.64 |
| 1:A:653:LYS:HA | 1:A:682:LEU:HG | 1.80 | 0.64 |
| 2:E:76:ALA:HB2 | 2:E:81:SER:HB3 | 1.80 | 0.64 |
| 1:A:723:GLN:HG2 | 1:A:1173:ARG:HG3 | 1.79 | 0.64 |
| 1:A:401:PRO:CG | 1:A:571:TYR:CE1 | 2.79 | 0.64 |
| 1:A:618:ASP:O | 1:A:621:VAL:HG23 | 1.96 | 0.64 |
| 1:A:1080:PRO:HG2 | 1:A:1085:TYR:HE2 | 1.62 | 0.63 |
| 1:A:395:PHE:CD2 | 1:A:1081:TYR:HD2 | 2.15 | 0.63 |
| 1:A:664:VAL:CG1 | 1:A:669:ALA:HB3 | 2.28 | 0.63 |
| 1:A:674:VAL:O | 1:A:678:ILE:HG13 | 1.97 | 0.63 |
| 1:A:403:PHE:HE2 | 1:A:566:PRO:CG | 2.11 | 0.63 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:HG11 | 2.29 | 0.63 |
| 1:A:401:PRO:CD | 1:A:571:TYR:HE1 | 1.96 | 0.63 |
| 1:A:630:ILE:CG2 | 1:A:634:TYR:HE2 | 2.12 | 0.63 |
| 1:A:1229:TYR:CD1 | 1:A:1233:VAL:CG2 | 2.82 | 0.63 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:CG1 | 2.77 | 0.62 |
| 1:A:1045:LEU:N | 1:A:1051:PHE:CZ | 2.67 | 0.62 |
| 1:A:252:GLN:O | 1:A:254:PRO:HD3 | 1.99 | 0.62 |
| 1:A:1177:VAL:O | 1:A:1186:ARG:NH1 | 2.32 | 0.62 |
| 1:A:166:PRO:O | 1:A:167:SER:OG | 2.17 | 0.62 |
| 1:A:228:ASP:HB2 | 1:A:246:VAL:CG1 | 2.29 | 0.62 |
| 1:A:250:LYS:CB | 1:A:251:PRO:HD3 | 2.24 | 0.62 |
| 1:A:630:ILE:HA | 1:A:633:LEU:HD12 | 1.81 | 0.62 |
| 1:A:684:LEU:HD22 | 1:A:728:LEU:HD22 | 1.75 | 0.62 |
| 1:A:754:MET:N | 1:A:755:PRO:CD | 2.62 | 0.62 |
| 1:A:1085:TYR:O | 1:A:1086:VAL:C | 2.37 | 0.62 |
| 1:A:607:ARG:O | 1:A:611:ASP:HB2 | 1.99 | 0.62 |
| 1:A:885:ALA:O | 1:A:1079:PHE:HB2 | 1.99 | 0.62 |
| 1:A:680:LEU:O | 1:A:683:THR:HG22 | 2.00 | 0.62 |
| 1:A:1210:ILE:HG13 | 1:A:1214:ALA:CB | 2.30 | 0.62 |
| 1:A:381:TRP:CD1 | 1:A:382:SER:N | 2.64 | 0.62 |
| 1:A:591:VAL:CB | 1:A:603:PHE:HE1 | 2.12 | 0.62 |
| 1:A:678:ILE:HG12 | 1:A:748:LEU:CD2 | 2.27 | 0.62 |
| 1:A:724:LEU:CD1 | 1:A:1166:GLU:HA | 2.29 | 0.61 |
| 1:A:686:VAL:HG11 | 1:A:690:ILE:HD11 | 1.73 | 0.61 |
| 1:A:1171:ILE:HA | 1:A:1194:MET:HG2 | 1.81 | 0.61 |
| 1:A:1199:PHE:O | 1:A:1203:THR:HG22 | 2.00 | 0.61 |
| 1:A:684:LEU:HD21 | 1:A:728:LEU:HD21 | 1.72 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:631:MET:CE | 1:A:1208:GLY:N | 2.63 | 0.61 |
| 1:A:431:PHE:CE2 | 1:A:510:HIS:HD2 | 2.18 | 0.61 |
| 1:A:875:TYR:O | 1:A:876:PHE:O | 2.18 | 0.61 |
| 1:A:659:ALA:HA | 1:A:662:LEU:HD21 | 1.71 | 0.61 |
| 1:A:1092:LEU:HD13 | 1:A:1093:THR:N | 2.15 | 0.61 |
| 1:A:622:PHE:O | 1:A:626:ILE:HG13 | 2.01 | 0.61 |
| 1:A:752:SER:CA | 1:A:755:PRO:CG | 2.78 | 0.61 |
| 1:A:752:SER:HA | 1:A:755:PRO:HG3 | 1.82 | 0.61 |
| 4:A:1306:NAG:H62 | 4:A:1307:NAG:H82 | 1.80 | 0.61 |
| 1:A:1186:ARG:HG3 | 1:A:1187:ALA:N | 2.15 | 0.60 |
| 1:A:1194:MET:O | 1:A:1198:VAL:HG23 | 2.00 | 0.60 |
| 1:A:1213:LEU:C | 1:A:1227:ARG:HH21 | 2.03 | 0.60 |
| 1:A:881:GLN:CB | 1:A:1041:TYR:CB | 2.79 | 0.60 |
| 1:A:337:ARG:CA | 1:A:718:GLU:HG3 | 2.23 | 0.60 |
| 1:A:724:LEU:HD13 | 1:A:1166:GLU:HA | 1.82 | 0.60 |
| 1:A:723:GLN:O | 1:A:727:VAL:HG23 | 2.01 | 0.60 |
| 1:A:1140:GLY:O | 1:A:1144:LEU:CA | 2.49 | 0.60 |
| 1:A:663:ILE:HD13 | 1:A:750:ALA:HB1 | 1.84 | 0.60 |
| 4:A:1306:NAG:O6 | 4:A:1307:NAG:H82 | 2.02 | 0.60 |
| 1:A:732:ALA:HB3 | 1:A:749:GLY:HA2 | 1.81 | 0.60 |
| 1:A:607:ARG:CG | 1:A:611:ASP:OD1 | 2.50 | 0.60 |
| 1:A:656:LEU:HA | 1:A:751:LEU:HG | 1.84 | 0.60 |
| 1:A:1046:GLN:HB3 | 1:A:1050:ASP:CB | 2.32 | 0.60 |
| 1:A:1115:VAL:HG12 | 1:A:1115:VAL:O | 2.02 | 0.60 |
| 1:A:163:VAL:HA | 1:A:242:ASP:O | 2.01 | 0.60 |
| 1:A:386:SER:O | 1:A:390:LEU:HB2 | 2.01 | 0.60 |
| 1:A:764:ALA:O | 1:A:768:VAL:HG23 | 2.02 | 0.60 |
| 1:A:635:ILE:CG1 | 1:A:1204:LEU:HD13 | 2.31 | 0.59 |
| 1:A:648:LEU:HD12 | 1:A:763:PHE:HD1 | 1.65 | 0.59 |
| 1:A:691:PRO:O | 1:A:695:LEU:HG | 2.02 | 0.59 |
| 1:A:1091:TYR:HA | 1:A:1094:ILE:CG1 | 2.31 | 0.59 |
| 1:A:1110:PHE:HD2 | 1:A:1128:CYS:HG | 1.50 | 0.59 |
| 1:A:373:VAL:O | 1:A:375:THR:N | 2.35 | 0.59 |
| 1:A:924:PHE:CB | 1:A:925:ASN:CA | 2.80 | 0.59 |
| 1:A:1046:GLN:CG | 1:A:1050:ASP:CG | 2.70 | 0.59 |
| 1:A:1021:SER:O | 1:A:1022:ALA:HB3 | 2.01 | 0.59 |
| 1:A:1191:LEU:O | 1:A:1195:GLY:N | 2.36 | 0.59 |
| 1:A:1055:LEU:HD13 | 1:A:1056:LYS:N | 2.17 | 0.59 |
| 1:A:406:GLU:OE2 | 1:A:567:VAL:HG13 | 2.01 | 0.59 |
| 1:A:1209:GLY:O | 1:A:1212:VAL:N | 2.35 | 0.59 |
| 1:A:1106:LEU:HD23 | 1:A:1131:ILE:HD13 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1112:VAL:HA | 1:A:1115:VAL:HG23 | 1.85 | 0.59 |
| 1:A:1149:LEU:HA | 1:A:1153:SER:CB | 2.33 | 0.59 |
| 1:A:122:ASN:ND2 | 1:A:217[B]:MET:CE | 2.66 | 0.59 |
| 1:A:395:PHE:CD2 | 1:A:1081:TYR:CD2 | 2.91 | 0.59 |
| 1:A:1229:TYR:HD1 | 1:A:1233:VAL:CG2 | 2.16 | 0.59 |
| 1:A:1239:HIS:CE1 | 1:A:1243:PHE:CB | 2.86 | 0.59 |
| 1:A:1070:GLY:O | 1:A:1071:ILE:CB | 2.50 | 0.58 |
| 1:A:1082:SER:CB | 1:A:1084:PHE:CE1 | 2.86 | 0.58 |
| 1:A:382:SER:HB3 | 1:A:1086:VAL:O | 2.03 | 0.58 |
| 1:A:985:GLU:HA | 1:A:989:ARG:H | 1.68 | 0.58 |
| 2:E:39:HIS:CD2 | 2:E:42:VAL:HG21 | 2.38 | 0.58 |
| 1:A:476:ASN:OD1 | 1:A:478:ASN:HB2 | 2.02 | 0.58 |
| 1:A:504:PHE:CE2 | 2:E:79:VAL:HG12 | 2.29 | 0.58 |
| 1:A:942:TRP:O | 1:A:943:ILE:CB | 2.50 | 0.58 |
| 1:A:1080:PRO:HB2 | 1:A:1085:TYR:CZ | 2.37 | 0.58 |
| 1:A:1142:MET:HE1 | 1:A:1153:SER:OG | 2.04 | 0.58 |
| 1:A:649:LEU:O | 1:A:652:SER:N | 2.35 | 0.58 |
| 1:A:656:LEU:CD1 | 1:A:682:LEU:CD1 | 2.80 | 0.58 |
| 1:A:1055:LEU:C | 1:A:1055:LEU:HD22 | 2.24 | 0.58 |
| 1:A:1142:MET:CE | 1:A:1148:SER:C | 2.71 | 0.58 |
| 1:A:515:TYR:CE1 | 1:A:526:THR:HG23 | 2.38 | 0.58 |
| 1:A:686:VAL:O | 1:A:690:ILE:CG1 | 2.44 | 0.58 |
| 1:A:752:SER:HA | 1:A:755:PRO:HG2 | 1.84 | 0.58 |
| 1:A:1133:MET:CE | 1:A:1239:HIS:CE1 | 2.74 | 0.58 |
| 1:A:598:ASN:HD21 | 4:A:1310:NAG:C2 | 2.04 | 0.58 |
| 1:A:637:LEU:HA | 1:A:641:HIS:HA | 1.84 | 0.58 |
| 1:A:879:ILE:HA | 1:A:1043:THR:HG23 | 1.85 | 0.58 |
| 1:A:1084:PHE:HE1 | 1:A:1085:TYR:CE1 | 2.08 | 0.58 |
| 1:A:1156:ASN:HD22 | 1:A:1228:MET:HE2 | 1.67 | 0.58 |
| 1:A:724:LEU:HD21 | 1:A:1170:HIS:HE1 | 1.66 | 0.58 |
| 1:A:1210:ILE:HD12 | 1:A:1214:ALA:HB2 | 1.84 | 0.58 |
| 1:A:1133:MET:HE3 | 1:A:1239:HIS:CB | 2.34 | 0.58 |
| 1:A:720:LEU:O | 1:A:723:GLN:CG | 2.51 | 0.58 |
| 1:A:402:PHE:O | 1:A:403:PHE:CD1 | 2.57 | 0.57 |
| 1:A:664:VAL:HG13 | 1:A:669:ALA:HB3 | 1.85 | 0.57 |
| 1:A:557:ASN:ND2 | 4:A:1306:NAG:O5 | 2.38 | 0.57 |
| 1:A:503:PHE:CZ | 2:E:86:TRP:CD2 | 2.81 | 0.57 |
| 1:A:1046:GLN:HG2 | 1:A:1050:ASP:CG | 2.25 | 0.57 |
| 1:A:1085:TYR:C | 1:A:1087:PHE:N | 2.57 | 0.57 |
| 1:A:1203:THR:CG2 | 1:A:1204:LEU:H | 2.18 | 0.57 |
| 1:A:1202:ILE:HG21 | 1:A:1237:ALA:CB | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:252:GLN:H | 1:A:253:PRO:HD3 | 1.69 | 0.57 |
| 1:A:656:LEU:HB3 | 1:A:751:LEU:CD2 | 2.31 | 0.57 |
| 1:A:421:GLN:CG | 2:E:143:GLY:HA2 | 2.32 | 0.57 |
| 1:A:1068:THR:CG2 | 1:A:1069:MET:H | 2.17 | 0.57 |
| 4:A:1313:NAG:O3 | 5:A:1314:BMA:H2 | 2.03 | 0.57 |
| 1:A:635:ILE:HG22 | 1:A:649:LEU:HD11 | 1.86 | 0.57 |
| 1:A:686:VAL:HG12 | 1:A:690:ILE:CG1 | 2.34 | 0.57 |
| 1:A:631:MET:SD | 1:A:1207:PHE:C | 2.83 | 0.57 |
| 1:A:1106:LEU:HD22 | 1:A:1131:ILE:HD13 | 1.87 | 0.57 |
| 1:A:396:ASP:HA | 1:A:400:GLY:N | 2.20 | 0.57 |
| 1:A:656:LEU:HD12 | 1:A:682:LEU:CD1 | 2.34 | 0.57 |
| 1:A:723:GLN:CD | 1:A:1169:SER:HB2 | 2.17 | 0.57 |
| 1:A:257:PRO:O | 1:A:258:ALA:HB2 | 2.05 | 0.57 |
| 1:A:241:GLN:NE2 | 1:A:518:ARG:NH2 | 2.38 | 0.57 |
| 1:A:857:ASP:HA | 1:A:1048:SER:HB3 | 1.87 | 0.57 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:HG21 | 2.35 | 0.57 |
| 1:A:655:SER:HB2 | 1:A:758:HIS:CD2 | 2.40 | 0.57 |
| 1:A:479:CYS:O | 1:A:537:PHE:HB3 | 2.05 | 0.56 |
| 1:A:757:VAL:HA | 1:A:760:PHE:HD2 | 1.70 | 0.56 |
| 2:C:39:HIS:CD2 | 2:C:42:VAL:HG21 | 2.38 | 0.56 |
| 1:A:1055:LEU:CD2 | 1:A:1085:TYR:OH | 2.47 | 0.56 |
| 1:A:252:GLN:C | 1:A:254:PRO:HD3 | 2.25 | 0.56 |
| 1:A:751:LEU:C | 1:A:755:PRO:HG3 | 2.20 | 0.56 |
| 1:A:1059:ARG:HH11 | 1:A:1059:ARG:CG | 2.14 | 0.56 |
| 1:A:1156:ASN:ND2 | 1:A:1228:MET:CE | 2.68 | 0.56 |
| 1:A:1055:LEU:C | 1:A:1055:LEU:HD13 | 2.25 | 0.56 |
| 1:A:676:SER:CB | 1:A:1225:TYR:CZ | 2.87 | 0.56 |
| 1:A:688:GLU:O | 1:A:691:PRO:CG | 2.51 | 0.56 |
| 1:A:396:ASP:C | 1:A:400:GLY:H | 2.06 | 0.56 |
| 1:A:403:PHE:CD2 | 1:A:566:PRO:CB | 2.77 | 0.56 |
| 1:A:752:SER:O | 1:A:755:PRO:HG2 | 2.03 | 0.56 |
| 1:A:916:ASN:N | 1:A:919:LEU:O | 2.23 | 0.56 |
| 2:G:39:HIS:CD2 | 2:G:42:VAL:HG21 | 2.38 | 0.56 |
| 1:A:648:LEU:CD1 | 1:A:763:PHE:HA | 2.33 | 0.56 |
| 1:A:1062:ALA:CB | 1:A:1078:VAL:CG2 | 2.82 | 0.56 |
| 1:A:845:VAL:CB | 1:A:1136:VAL:HG12 | 2.36 | 0.56 |
| 1:A:393:GLU:O | 1:A:396:ASP:HB2 | 2.06 | 0.56 |
| 1:A:724:LEU:HD21 | 1:A:1166:GLU:CD | 2.26 | 0.56 |
| 4:A:1306:NAG:C6 | 4:A:1307:NAG:H83 | 2.36 | 0.56 |
| 1:A:724:LEU:HD23 | 1:A:1170:HIS:NE2 | 2.17 | 0.56 |
| 1:A:491:SER:OG | 1:A:494:VAL:HG23 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:656:LEU:HD11 | 1:A:685:ILE:HG21 | 1.87 | 0.56 |
| 1:A:441:HIS:CE1 | 1:A:496:ASP:OD1 | 2.59 | 0.56 |
| 1:A:1048:SER:HA | 1:A:1088:TYR:CE2 | 2.41 | 0.56 |
| 1:A:1117:LEU:CD2 | 1:A:1123:SER:HB3 | 2.36 | 0.56 |
| 1:A:1229:TYR:HE1 | 1:A:1233:VAL:HG21 | 1.70 | 0.56 |
| 4:A:1306:NAG:H62 | 4:A:1307:NAG:N2 | 2.21 | 0.56 |
| 1:A:650:VAL:O | 1:A:654:VAL:CG2 | 2.52 | 0.56 |
| 1:A:409:ILE:CG2 | 1:A:872:MET:CB | 2.83 | 0.55 |
| 2:G:69:ASN:HD21 | 2:G:105:ALA:HB2 | 1.72 | 0.55 |
| 1:A:1159:MET:HE1 | 1:A:1163:ILE:HD11 | 1.87 | 0.55 |
| 1:A:92:GLN:HE22 | 1:A:526:THR:HB | 1.71 | 0.55 |
| 1:A:1200:SER:O | 1:A:1203:THR:HG22 | 2.07 | 0.55 |
| 1:A:627:SER:O | 1:A:631:MET:HG2 | 2.07 | 0.55 |
| 1:A:924:PHE:CB | 1:A:925:ASN:HA | 2.36 | 0.55 |
| 1:A:1184:VAL:O | 1:A:1184:VAL:CG1 | 2.53 | 0.55 |
| 2:G:112:GLU:OE2 | 2:G:172:ARG:HG3 | 2.07 | 0.55 |
| 1:A:1048:SER:O | 1:A:1052:ILE:HD12 | 2.06 | 0.55 |
| 1:A:504:PHE:HZ | 2:E:141:VAL:CG2 | 2.16 | 0.55 |
| 1:A:674:VAL:O | 1:A:678:ILE:HD12 | 2.06 | 0.55 |
| 1:A:252:GLN:N | 1:A:253:PRO:HD3 | 2.22 | 0.55 |
| 1:A:753:VAL:O | 1:A:757:VAL:HG13 | 2.07 | 0.55 |
| 1:A:754:MET:O | 1:A:757:VAL:HG22 | 2.07 | 0.55 |
| 1:A:1167:PHE:HE2 | 1:A:1237:ALA:CA | 2.19 | 0.55 |
| 1:A:1228:MET:HG3 | 1:A:1229:TYR:H | 1.71 | 0.55 |
| 1:A:191:GLU:OE2 | 1:A:195:ASN:ND2 | 2.39 | 0.55 |
| 1:A:407:GLN:O | 1:A:604:THR:N | 2.40 | 0.55 |
| 1:A:398:HIS:HB3 | 1:A:399:PHE:CD1 | 2.42 | 0.55 |
| 2:E:112:GLU:OE2 | 2:E:172:ARG:HG3 | 2.07 | 0.55 |
| 1:A:185:ASN:ND2 | 1:A:188:ASN:ND2 | 2.55 | 0.54 |
| 1:A:431:PHE:CZ | 1:A:510:HIS:HD2 | 2.25 | 0.54 |
| 1:A:444:LEU:HD23 | 1:A:492:HIS:CG | 2.42 | 0.54 |
| 1:A:732:ALA:HB1 | 1:A:749:GLY:N | 2.22 | 0.54 |
| 1:A:1167:PHE:CE2 | 1:A:1237:ALA:HB2 | 2.43 | 0.54 |
| 1:A:164:GLU:OE1 | 1:A:241:GLN:O | 2.26 | 0.54 |
| 1:A:762:LEU:O | 1:A:766:LEU:CG | 2.55 | 0.54 |
| 2:C:69:ASN:HD21 | 2:C:105:ALA:HB2 | 1.71 | 0.54 |
| 1:A:1100:PHE:O | 1:A:1104:VAL:HG23 | 2.07 | 0.54 |
| 2:E:163:ASP:OD1 | 3:F:543:TYR:OH | 2.24 | 0.54 |
| 1:A:1135:LEU:CD2 | 1:A:1161:CYS:SG | 2.92 | 0.54 |
| 1:A:1224:PHE:HA | 1:A:1227:ARG:HB2 | 1.88 | 0.54 |
| 1:A:723:GLN:HE22 | 1:A:724:LEU:HB2 | 1.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1091:TYR:HA | 1:A:1094:ILE:HG13 | 1.90 | 0.54 |
| 1:A:1109:ILE:O | 1:A:1113:THR:HG23 | 2.07 | 0.54 |
| 1:A:1114:MET:HE1 | 1:A:1124:ALA:HB2 | 1.90 | 0.54 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:HD11 | 2.27 | 0.54 |
| 1:A:664:VAL:CG2 | 1:A:747:PHE:CB | 2.85 | 0.54 |
| 2:C:112:GLU:OE2 | 2:C:172:ARG:HG3 | 2.07 | 0.54 |
| 1:A:653:LYS:HG3 | 1:A:654:VAL:N | 2.23 | 0.54 |
| 1:A:704:ILE:CA | 1:A:708:ALA:HB3 | 2.38 | 0.54 |
| 1:A:631:MET:CG | 1:A:1208:GLY:HA2 | 2.37 | 0.54 |
| 1:A:1133:MET:CE | 1:A:1239:HIS:CB | 2.86 | 0.54 |
| 1:A:398:HIS:CB | 1:A:399:PHE:CE1 | 2.86 | 0.54 |
| 1:A:649:LEU:HD22 | 1:A:686:VAL:HG13 | 1.90 | 0.53 |
| 1:A:674:VAL:O | 1:A:678:ILE:CG1 | 2.56 | 0.53 |
| 1:A:733:PRO:C | 1:A:735:MET:H | 2.10 | 0.53 |
| 1:A:523:LEU:CD1 | 1:A:1016:HIS:N | 2.70 | 0.53 |
| 1:A:882:TYR:CB | 1:A:1082:SER:CB | 2.64 | 0.53 |
| 1:A:347:VAL:C | 1:A:349:ASN:H | 2.12 | 0.53 |
| 1:A:758:HIS:ND1 | 1:A:762:LEU:HD12 | 2.23 | 0.53 |
| 2:E:69:ASN:HD21 | 2:E:105:ALA:HB2 | 1.72 | 0.53 |
| 1:A:1167:PHE:CE2 | 1:A:1237:ALA:CB | 2.91 | 0.53 |
| 1:A:824:SER:CB | 1:A:1188:GLU:CD | 2.77 | 0.53 |
| 1:A:1137:ASN:HB3 | 1:A:1235:LEU:CD1 | 2.37 | 0.53 |
| 1:A:503:PHE:HZ | 2:E:86:TRP:CB | 2.19 | 0.53 |
| 1:A:632:PHE:CZ | 1:A:650:VAL:HG22 | 2.44 | 0.53 |
| 1:A:915:ASN:CB | 1:A:919:LEU:C | 2.77 | 0.53 |
| 1:A:406:GLU:OE2 | 1:A:567:VAL:HG11 | 2.08 | 0.53 |
| 1:A:396:ASP:CB | 1:A:400:GLY:HA2 | 2.38 | 0.53 |
| 2:C:39:HIS:CD2 | 2:C:42:VAL:CG2 | 2.92 | 0.53 |
| 1:A:544:TRP:HZ2 | 1:A:1041:TYR:CE1 | 2.26 | 0.53 |
| 1:A:1167:PHE:HE2 | 1:A:1237:ALA:HB2 | 1.74 | 0.53 |
| 1:A:861:ASP:CB | 1:A:1219:GLN:CB | 2.87 | 0.53 |
| 4:A:1312:NAG:H61 | 4:A:1313:NAG:C1 | 2.38 | 0.53 |
| 1:A:474:PRO:C | 1:A:476:ASN:N | 2.62 | 0.53 |
| 1:A:923:ILE:C | 1:A:1042:HIS:CB | 2.50 | 0.53 |
| 1:A:478:ASN:CG | 4:A:1312:NAG:C1 | 2.78 | 0.53 |
| 1:A:635:ILE:HG22 | 1:A:649:LEU:CD1 | 2.39 | 0.53 |
| 1:A:1234:LEU:O | 1:A:1238:THR:HG23 | 2.09 | 0.53 |
| 1:A:344:SER:O | 1:A:348:ARG:N | 2.41 | 0.53 |
| 1:A:684:LEU:CG | 1:A:728:LEU:HD22 | 2.38 | 0.53 |
| 1:A:924:PHE:CB | 1:A:925:ASN:CB | 2.87 | 0.53 |
| 1:A:93:PHE:CE1 | 1:A:175:LEU:HD13 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1127:MET:HE1 | 1:A:1130:THR:HG21 | 1.88 | 0.52 |
| 1:A:688:GLU:HA | 1:A:691:PRO:HG3 | 1.91 | 0.52 |
| 1:A:758:HIS:O | 1:A:762:LEU:HB2 | 2.09 | 0.52 |
| 1:A:381:TRP:HD1 | 1:A:382:SER:H | 1.55 | 0.52 |
| 1:A:1021:SER:O | 1:A:1022:ALA:HB2 | 2.08 | 0.52 |
| 1:A:1171:ILE:HG23 | 1:A:1191:LEU:HD22 | 1.90 | 0.52 |
| 1:A:402:PHE:O | 1:A:403:PHE:CG | 2.63 | 0.52 |
| 1:A:824:SER:HA | 1:A:1188:GLU:CD | 2.30 | 0.52 |
| 1:A:752:SER:C | 1:A:755:PRO:CG | 2.78 | 0.52 |
| 1:A:1084:PHE:CD1 | 1:A:1085:TYR:N | 2.78 | 0.52 |
| 1:A:1138:MET:N | 1:A:1138:MET:SD | 2.83 | 0.52 |
| 1:A:1210:ILE:CG2 | 1:A:1211:VAL:N | 2.73 | 0.52 |
| 1:A:1210:ILE:O | 1:A:1214:ALA:N | 2.43 | 0.52 |
| 2:C:69:ASN:ND2 | 2:C:105:ALA:HB2 | 2.25 | 0.52 |
| 1:A:1068:THR:CG2 | 1:A:1069:MET:N | 2.73 | 0.52 |
| 2:E:39:HIS:CD2 | 2:E:42:VAL:CG2 | 2.92 | 0.52 |
| 1:A:691:PRO:CD | 1:A:692:PHE:H | 2.21 | 0.52 |
| 3:F:595:GLN:HG3 | 3:F:596:ARG:NH1 | 2.25 | 0.52 |
| 1:A:1239:HIS:NE2 | 1:A:1243:PHE:CB | 2.73 | 0.52 |
| 1:A:685:ILE:O | 1:A:689:VAL:CB | 2.58 | 0.52 |
| 1:A:690:ILE:N | 1:A:691:PRO:CD | 2.73 | 0.52 |
| 2:G:39:HIS:CD2 | 2:G:42:VAL:CG2 | 2.92 | 0.52 |
| 1:A:399:PHE:CE2 | 1:A:1022:ALA:HA | 2.45 | 0.52 |
| 1:A:1047:THR:HG22 | 1:A:1048:SER:H | 1.75 | 0.52 |
| 1:A:387:GLN:O | 1:A:391:GLU:HB2 | 2.10 | 0.52 |
| 1:A:656:LEU:HB3 | 1:A:751:LEU:HD11 | 1.91 | 0.52 |
| 2:E:69:ASN:ND2 | 2:E:105:ALA:HB2 | 2.25 | 0.52 |
| 1:A:1239:HIS:O | 1:A:1243:PHE:N | 2.32 | 0.51 |
| 1:A:114:SER:O | 1:A:117:GLN:HG3 | 2.11 | 0.51 |
| 1:A:1234:LEU:HD22 | 1:A:1234:LEU:O | 2.09 | 0.51 |
| 1:A:915:ASN:CB | 1:A:919:LEU:O | 2.59 | 0.51 |
| 1:A:923:ILE:CA | 1:A:1042:HIS:HB3 | 2.41 | 0.51 |
| 1:A:1047:THR:CG2 | 1:A:1048:SER:N | 2.73 | 0.51 |
| 1:A:1080:PRO:HB2 | 1:A:1085:TYR:OH | 2.10 | 0.51 |
| 1:A:627:SER:CB | 1:A:1211:VAL:HB | 2.40 | 0.51 |
| 1:A:751:LEU:HD23 | 1:A:751:LEU:O | 2.11 | 0.51 |
| 3:F:515:LEU:HB3 | 3:F:548:MET:HB2 | 1.93 | 0.51 |
| 3:H:595:GLN:HG3 | 3:H:596:ARG:NH1 | 2.25 | 0.51 |
| 1:A:1133:MET:CE | 1:A:1239:HIS:HB2 | 2.41 | 0.51 |
| 1:A:1121:LEU:O | 1:A:1125:VAL:HB | 2.11 | 0.51 |
| 1:A:515:TYR:CE1 | 1:A:526:THR:HG22 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1117:LEU:HD13 | 1:A:1173:ARG:HD3 | 1.93 | 0.51 |
| 1:A:1223:ILE:O | 1:A:1227:ARG:HG2 | 2.11 | 0.51 |
| 1:A:915:ASN:CB | 1:A:920:VAL:N | 2.73 | 0.51 |
| 3:D:515:LEU:HB3 | 3:D:548:MET:HB2 | 1.93 | 0.51 |
| 1:A:856:VAL:C | 1:A:1048:SER:OG | 2.49 | 0.51 |
| 1:A:135:ASN:ND2 | 4:A:1322:NAG:O5 | 2.21 | 0.51 |
| 3:D:595:GLN:HG3 | 3:D:596:ARG:NH1 | 2.25 | 0.51 |
| 1:A:1044:VAL:HB | 1:A:1051:PHE:CE1 | 2.45 | 0.51 |
| 1:A:1120:GLU:O | 1:A:1124:ALA:HB3 | 2.10 | 0.51 |
| 1:A:377:PRO:CB | 1:A:378:VAL:HA | 2.39 | 0.51 |
| 2:G:69:ASN:ND2 | 2:G:105:ALA:HB2 | 2.25 | 0.51 |
| 1:A:1111:LEU:O | 1:A:1115:VAL:HG23 | 2.11 | 0.51 |
| 1:A:1119:CYS:CB | 1:A:1122:TRP:CB | 2.89 | 0.51 |
| 1:A:371:VAL:C | 1:A:373:VAL:N | 2.64 | 0.51 |
| 1:A:723:GLN:NE2 | 1:A:724:LEU:N | 2.59 | 0.51 |
| 3:H:515:LEU:HB3 | 3:H:548:MET:HB2 | 1.93 | 0.51 |
| 1:A:1138:MET:HA | 1:A:1138:MET:HE2 | 1.92 | 0.50 |
| 1:A:1209:GLY:CA | 1:A:1230:LEU:HD13 | 2.30 | 0.50 |
| 1:A:683:THR:HG23 | 1:A:684:LEU:N | 2.25 | 0.50 |
| 1:A:648:LEU:CB | 1:A:763:PHE:CZ | 2.93 | 0.50 |
| 1:A:524:ASN:HD22 | 4:A:1304:NAG:C1 | 2.02 | 0.50 |
| 1:A:382:SER:O | 1:A:383:ALA:HB3 | 2.12 | 0.50 |
| 1:A:423:TYR:CG | 1:A:424:PRO:HA | 2.47 | 0.50 |
| 1:A:584:GLU:OE2 | 1:A:606:GLU:CB | 2.56 | 0.50 |
| 1:A:1178:SER:CB | 1:A:1186:ARG:CZ | 2.89 | 0.50 |
| 1:A:423:TYR:CZ | 1:A:424:PRO:HB3 | 2.46 | 0.50 |
| 1:A:732:ALA:CB | 1:A:749:GLY:HA2 | 2.31 | 0.50 |
| 1:A:382:SER:HA | 1:A:1090:GLN:HG3 | 1.93 | 0.50 |
| 1:A:680:LEU:HB3 | 1:A:1229:TYR:HH | 1.73 | 0.50 |
| 1:A:1229:TYR:HD1 | 1:A:1233:VAL:HG21 | 1.69 | 0.50 |
| 1:A:523:LEU:HD11 | 1:A:1016:HIS:N | 2.25 | 0.50 |
| 1:A:1062:ALA:C | 1:A:1078:VAL:HG21 | 2.32 | 0.49 |
| 1:A:1115:VAL:O | 1:A:1116:LEU:HG | 2.12 | 0.49 |
| 1:A:719:THR:O | 1:A:723:GLN:HG3 | 2.12 | 0.49 |
| 1:A:688:GLU:CB | 1:A:724:LEU:CD2 | 2.89 | 0.49 |
| 1:A:749:GLY:O | 1:A:752:SER:CB | 2.60 | 0.49 |
| 1:A:1063:SER:O | 1:A:1067:GLU:HB2 | 2.10 | 0.49 |
| 1:A:676:SER:OG | 1:A:1225:TYR:CE1 | 2.65 | 0.49 |
| 1:A:381:TRP:CD1 | 1:A:381:TRP:C | 2.85 | 0.49 |
| 1:A:656:LEU:CA | 1:A:751:LEU:HG | 2.42 | 0.49 |
| 1:A:659:ALA:O | 1:A:663:ILE:HG13 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1071:ILE:CG2 | 1:A:1072:ASN:N | 2.34 | 0.49 |
| 1:A:108:PHE:HE1 | 1:A:194:PHE:CE1 | 2.26 | 0.49 |
| 1:A:686:VAL:CG1 | 1:A:690:ILE:CG1 | 2.90 | 0.49 |
| 1:A:729:GLY:O | 1:A:733:PRO:N | 2.45 | 0.49 |
| 1:A:1092:LEU:C | 1:A:1094:ILE:H | 2.16 | 0.49 |
| 1:A:1167:PHE:CD2 | 1:A:1237:ALA:HA | 2.47 | 0.49 |
| 1:A:402:PHE:C | 1:A:403:PHE:HD1 | 2.15 | 0.49 |
| 1:A:431:PHE:CZ | 1:A:510:HIS:CD2 | 3.00 | 0.49 |
| 1:A:506:TYR:OH | 2:E:80:PRO:HB3 | 2.12 | 0.49 |
| 1:A:337:ARG:HA | 1:A:718:GLU:CD | 2.32 | 0.49 |
| 1:A:663:ILE:HD11 | 1:A:754:MET:HG3 | 1.93 | 0.49 |
| 1:A:653:LYS:C | 1:A:682:LEU:HD21 | 2.30 | 0.49 |
| 2:E:38:ILE:HG13 | 2:E:187:PRO:HD3 | 1.95 | 0.49 |
| 1:A:1152:VAL:HG11 | 1:A:1225:TYR:HD2 | 1.77 | 0.49 |
| 1:A:1091:TYR:HA | 1:A:1094:ILE:HG12 | 1.94 | 0.49 |
| 1:A:1093:THR:HG22 | 1:A:1093:THR:O | 2.13 | 0.49 |
| 1:A:1153:SER:HA | 1:A:1156:ASN:HB2 | 1.94 | 0.49 |
| 1:A:631:MET:CE | 1:A:1208:GLY:H | 2.26 | 0.49 |
| 4:A:1306:NAG:O6 | 4:A:1307:NAG:H83 | 2.12 | 0.49 |
| 1:A:506:TYR:CZ | 2:E:80:PRO:HB3 | 2.48 | 0.49 |
| 1:A:611:ASP:O | 1:A:615:ARG:CB | 2.60 | 0.49 |
| 3:F:510:LYS:NZ | 4:F:701:NAG:HO6 | 2.08 | 0.49 |
| 1:A:1223:ILE:O | 1:A:1227:ARG:CG | 2.61 | 0.49 |
| 1:A:885:ALA:O | 1:A:1079:PHE:CA | 2.61 | 0.49 |
| 1:A:398:HIS:C | 1:A:399:PHE:CG | 2.86 | 0.49 |
| 1:A:726:ARG:HB3 | 1:A:1112:VAL:HG13 | 1.94 | 0.49 |
| 2:C:39:HIS:CB | 2:C:42:VAL:HG22 | 2.40 | 0.49 |
| 1:A:627:SER:HB3 | 1:A:1211:VAL:HB | 1.93 | 0.48 |
| 1:A:959:VAL:CA | 1:A:984:PRO:N | 2.74 | 0.48 |
| 2:C:51:LEU:HA | 2:C:51:LEU:HD12 | 1.68 | 0.48 |
| 1:A:1210:ILE:HG23 | 1:A:1211:VAL:H | 1.76 | 0.48 |
| 1:A:724:LEU:O | 1:A:728:LEU:CG | 2.53 | 0.48 |
| 1:A:404:ARG:HG3 | 1:A:567:VAL:O | 2.13 | 0.48 |
| 1:A:1059:ARG:NH1 | 1:A:1059:ARG:CG | 2.73 | 0.48 |
| 1:A:1156:ASN:ND2 | 1:A:1228:MET:HE2 | 2.27 | 0.48 |
| 1:A:618:ASP:O | 1:A:621:VAL:CG2 | 2.60 | 0.48 |
| 1:A:1138:MET:CE | 1:A:1138:MET:CA | 2.91 | 0.48 |
| 1:A:1167:PHE:HE2 | 1:A:1237:ALA:CB | 2.27 | 0.48 |
| 1:A:720:LEU:HD21 | 1:A:1170:HIS:O | 2.13 | 0.48 |
| 1:A:985:GLU:CB | 1:A:989:ARG:CB | 2.91 | 0.48 |
| 2:C:163:ASP:OD1 | 3:D:543:TYR:OH | 2.24 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1156:ASN:ND2 | 1:A:1228:MET:HE3 | 2.28 | 0.48 |
| 1:A:35:TYR:CZ | 1:A:38:LYS:HD2 | 2.48 | 0.48 |
| 1:A:402:PHE:C | 1:A:403:PHE:CD1 | 2.87 | 0.48 |
| 1:A:684:LEU:HG | 1:A:1166:GLU:CG | 2.38 | 0.48 |
| 1:A:1063:SER:O | 1:A:1067:GLU:CB | 2.62 | 0.48 |
| 1:A:544:TRP:O | 1:A:879:ILE:CB | 2.62 | 0.48 |
| 1:A:472:LEU:HB3 | 1:A:476:ASN:HB3 | 1.96 | 0.48 |
| 1:A:1063:SER:O | 1:A:1067:GLU:HG3 | 2.14 | 0.48 |
| 1:A:444:LEU:HD23 | 1:A:492:HIS:CE1 | 2.49 | 0.48 |
| 1:A:653:LYS:HE3 | 1:A:653:LYS:O | 2.13 | 0.48 |
| 2:G:163:ASP:OD1 | 3:H:543:TYR:OH | 2.24 | 0.48 |
| 1:A:1045:LEU:HD23 | 1:A:1051:PHE:HZ | 1.79 | 0.47 |
| 1:A:656:LEU:CB | 1:A:751:LEU:HD11 | 2.44 | 0.47 |
| 1:A:1114:MET:HE2 | 1:A:1124:ALA:HB2 | 1.95 | 0.47 |
| 1:A:915:ASN:HA | 1:A:921:GLN:N | 2.29 | 0.47 |
| 2:G:38:ILE:HG13 | 2:G:187:PRO:HD3 | 1.95 | 0.47 |
| 1:A:704:ILE:CA | 1:A:708:ALA:CB | 2.92 | 0.47 |
| 1:A:688:GLU:HB2 | 1:A:724:LEU:CD2 | 2.44 | 0.47 |
| 1:A:1081:TYR:C | 1:A:1081:TYR:CD1 | 2.86 | 0.47 |
| 1:A:1130:THR:HA | 1:A:1133:MET:HB3 | 1.95 | 0.47 |
| 1:A:1210:ILE:CD1 | 1:A:1214:ALA:CB | 2.91 | 0.47 |
| 1:A:690:ILE:HG22 | 1:A:690:ILE:O | 2.14 | 0.47 |
| 1:A:704:ILE:N | 1:A:708:ALA:HB2 | 2.29 | 0.47 |
| 1:A:252:GLN:N | 1:A:253:PRO:CD | 2.78 | 0.47 |
| 2:E:104:TRP:CZ2 | 2:E:134:ARG:HD2 | 2.50 | 0.47 |
| 1:A:1127:MET:CE | 1:A:1130:THR:CG2 | 2.92 | 0.47 |
| 1:A:523:LEU:CD1 | 1:A:1015:GLY:C | 2.83 | 0.47 |
| 1:A:684:LEU:CD2 | 1:A:728:LEU:CG | 2.57 | 0.47 |
| 2:C:104:TRP:CZ2 | 2:C:134:ARG:HD2 | 2.50 | 0.47 |
| 1:A:437:ILE:HD13 | 1:A:509:TYR:CD1 | 2.50 | 0.47 |
| 2:G:104:TRP:CZ2 | 2:G:134:ARG:HD2 | 2.50 | 0.47 |
| 1:A:1232:MET:HG3 | 1:A:1233:VAL:N | 2.29 | 0.47 |
| 2:C:38:ILE:HG13 | 2:C:187:PRO:HD3 | 1.95 | 0.47 |
| 3:F:595:GLN:NE2 | 3:F:595:GLN:CA | 2.72 | 0.47 |
| 1:A:421:GLN:HB3 | 1:A:426:GLY:HA2 | 1.96 | 0.47 |
| 1:A:758:HIS:C | 1:A:760:PHE:H | 2.18 | 0.47 |
| 1:A:1048:SER:O | 1:A:1052:ILE:CD1 | 2.63 | 0.46 |
| 1:A:474:PRO:C | 1:A:476:ASN:H | 2.18 | 0.46 |
| 1:A:656:LEU:CD1 | 1:A:685:ILE:CB | 2.62 | 0.46 |
| 1:A:616:GLU:O | 1:A:618:ASP:N | 2.48 | 0.46 |
| 1:A:688:GLU:HA | 1:A:691:PRO:CG | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:E:37:VAL:HG21 | 2:E:51:LEU:HD11 | 1.97 | 0.46 |
| 1:A:648:LEU:CG | 1:A:763:PHE:CD1 | 2.98 | 0.46 |
| 2:G:37:VAL:HG21 | 2:G:51:LEU:HD11 | 1.97 | 0.46 |
| 1:A:635:ILE:HG12 | 1:A:1204:LEU:CD1 | 2.45 | 0.46 |
| 1:A:507:ALA:CB | 1:A:529:LEU:CG | 2.80 | 0.46 |
| 1:A:632:PHE:HE1 | 1:A:649:LEU:CB | 2.28 | 0.46 |
| 1:A:880:SER:O | 1:A:1043:THR:HG22 | 2.15 | 0.46 |
| 1:A:1210:ILE:CG2 | 1:A:1211:VAL:H | 2.29 | 0.46 |
| 1:A:503:PHE:HZ | 2:E:86:TRP:CG | 2.33 | 0.46 |
| 1:A:1127:MET:HE3 | 1:A:1130:THR:CG2 | 2.45 | 0.46 |
| 1:A:824:SER:HA | 1:A:1188:GLU:OE2 | 2.16 | 0.46 |
| 1:A:381:TRP:C | 1:A:383:ALA:H | 2.19 | 0.46 |
| 1:A:656:LEU:CD2 | 1:A:685:ILE:HG13 | 2.45 | 0.46 |
| 1:A:736:PHE:O | 1:A:737:LEU:O | 2.34 | 0.46 |
| 1:A:1084:PHE:CZ | 1:A:1085:TYR:CD1 | 2.84 | 0.46 |
| 1:A:1090:GLN:C | 1:A:1092:LEU:H | 2.19 | 0.46 |
| 1:A:162:ASP:OD2 | 1:A:244:SER:OG | 2.33 | 0.46 |
| 1:A:598:ASN:ND2 | 4:A:1310:NAG:C2 | 2.70 | 0.46 |
| 1:A:1131:ILE:O | 1:A:1135:LEU:CG | 2.63 | 0.46 |
| 1:A:656:LEU:HD22 | 1:A:751:LEU:CD2 | 2.46 | 0.46 |
| 1:A:656:LEU:HB3 | 1:A:682:LEU:CD1 | 2.42 | 0.46 |
| 1:A:688:GLU:CA | 1:A:691:PRO:HD3 | 2.45 | 0.46 |
| 2:C:37:VAL:HG21 | 2:C:51:LEU:HD11 | 1.97 | 0.46 |
| 3:H:560:GLN:O | 3:H:564:GLU:HG3 | 2.16 | 0.46 |
| 1:A:1062:ALA:O | 1:A:1078:VAL:HG21 | 2.15 | 0.45 |
| 1:A:168:SER:C | 1:A:170:ASP:H | 2.20 | 0.45 |
| 1:A:476:ASN:HA | 4:A:1312:NAG:H82 | 1.98 | 0.45 |
| 1:A:985:GLU:HA | 1:A:989:ARG:CB | 2.46 | 0.45 |
| 1:A:1115:VAL:C | 1:A:1116:LEU:HG | 2.36 | 0.45 |
| 1:A:635:ILE:HG21 | 1:A:686:VAL:CG1 | 2.46 | 0.45 |
| 1:A:676:SER:CB | 1:A:1225:TYR:CE1 | 2.99 | 0.45 |
| 1:A:484:VAL:HG11 | 1:A:547:LEU:HD21 | 1.98 | 0.45 |
| 1:A:635:ILE:HG21 | 1:A:686:VAL:HG11 | 1.97 | 0.45 |
| 1:A:1202:ILE:O | 1:A:1205:THR:OG1 | 2.21 | 0.45 |
| 1:A:122:ASN:ND2 | 1:A:217[B]:MET:HE1 | 2.31 | 0.45 |
| 1:A:165:ALA:O | 1:A:167:SER:N | 2.50 | 0.45 |
| 1:A:38:LYS:HB3 | 1:A:202:PRO:HB3 | 1.97 | 0.45 |
| 1:A:122:ASN:CG | 1:A:217[B]:MET:CE | 2.85 | 0.45 |
| 1:A:401:PRO:CG | 1:A:569:ASN:OD1 | 2.64 | 0.45 |
| 1:A:1149:LEU:HA | 1:A:1153:SER:HB2 | 1.97 | 0.45 |
| 1:A:506:TYR:CZ | 2:E:80:PRO:CG | 2.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:753:VAL:C | 1:A:755:PRO:CD | 2.85 | 0.45 |
| 1:A:885:ALA:O | 1:A:1079:PHE:C | 2.53 | 0.45 |
| 3:D:560:GLN:O | 3:D:564:GLU:HG3 | 2.16 | 0.45 |
| 1:A:1034:GLY:HA2 | 1:A:1035:ALA:HA | 1.69 | 0.45 |
| 1:A:396:ASP:CA | 1:A:400:GLY:H | 2.30 | 0.45 |
| 1:A:401:PRO:CB | 1:A:569:ASN:ND2 | 2.58 | 0.45 |
| 1:A:1044:VAL:O | 1:A:1045:LEU:C | 2.56 | 0.45 |
| 1:A:1047:THR:CG2 | 1:A:1048:SER:H | 2.30 | 0.45 |
| 1:A:1127:MET:HE3 | 1:A:1130:THR:HG21 | 1.99 | 0.45 |
| 1:A:723:GLN:HG2 | 1:A:1173:ARG:CG | 2.46 | 0.45 |
| 3:F:560:GLN:O | 3:F:564:GLU:HG3 | 2.16 | 0.45 |
| 1:A:732:ALA:O | 1:A:746:PHE:HA | 2.17 | 0.45 |
| 1:A:238:CYS:O | 1:A:246:VAL:HG21 | 2.17 | 0.44 |
| 1:A:713:GLU:C | 1:A:715:LEU:H | 2.21 | 0.44 |
| 1:A:1053:ASP:O | 1:A:1057:LYS:HD2 | 2.18 | 0.44 |
| 1:A:1225:TYR:HD1 | 1:A:1226:PHE:CG | 2.35 | 0.44 |
| 1:A:627:SER:CB | 1:A:1212:VAL:HG23 | 2.47 | 0.44 |
| 1:A:653:LYS:HG3 | 1:A:654:VAL:H | 1.82 | 0.44 |
| 1:A:751:LEU:O | 1:A:755:PRO:HD3 | 2.17 | 0.44 |
| 2:G:39:HIS:CB | 2:G:42:VAL:HG22 | 2.39 | 0.44 |
| 1:A:91:LEU:HD13 | 1:A:101:PHE:CZ | 2.52 | 0.44 |
| 1:A:382:SER:OG | 1:A:1086:VAL:HG13 | 2.17 | 0.44 |
| 1:A:246:VAL:O | 1:A:246:VAL:HG23 | 2.18 | 0.44 |
| 1:A:472:LEU:HD21 | 1:A:1017:ALA:HB1 | 1.96 | 0.44 |
| 2:E:51:LEU:HA | 2:E:51:LEU:HD12 | 1.68 | 0.44 |
| 1:A:1080:PRO:O | 1:A:1085:TYR:CE2 | 2.71 | 0.44 |
| 1:A:384:PRO:HA | 1:A:389:ARG:CG | 2.38 | 0.44 |
| 1:A:688:GLU:HB2 | 1:A:724:LEU:HD21 | 1.98 | 0.44 |
| 2:C:79:VAL:O | 2:C:83:THR:HG23 | 2.17 | 0.44 |
| 1:A:682:LEU:HA | 1:A:682:LEU:HD12 | 1.77 | 0.44 |
| 1:A:683:THR:CG2 | 1:A:684:LEU:N | 2.80 | 0.44 |
| 1:A:930:ASP:O | 1:A:933:THR:N | 2.50 | 0.44 |
| 1:A:649:LEU:CD2 | 1:A:686:VAL:HG13 | 2.47 | 0.44 |
| 1:A:653:LYS:HA | 1:A:682:LEU:CG | 2.47 | 0.44 |
| 1:A:122:ASN:CG | 1:A:217[B]:MET:HE3 | 2.38 | 0.44 |
| 1:A:396:ASP:HA | 1:A:400:GLY:H | 1.80 | 0.44 |
| 1:A:404:ARG:HH11 | 1:A:404:ARG:CG | 2.30 | 0.44 |
| 1:A:632:PHE:HE1 | 1:A:649:LEU:HB3 | 1.83 | 0.44 |
| 1:A:690:ILE:N | 1:A:691:PRO:HD3 | 2.32 | 0.43 |
| 1:A:893:LEU:O | 1:A:894:GLU:C | 2.55 | 0.43 |
| 1:A:1090:GLN:O | 1:A:1094:ILE:HG12 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:352:CYS:O | 1:A:353:VAL:C | 2.56 | 0.43 |
| 1:A:421:GLN:OE1 | 1:A:421:GLN:N | 2.39 | 0.43 |
| 1:A:444:LEU:HD23 | 1:A:492:HIS:CD2 | 2.53 | 0.43 |
| 1:A:690:ILE:O | 1:A:694:VAL:CG2 | 2.64 | 0.43 |
| 1:A:691:PRO:HB3 | 1:A:1197:SER:HB2 | 2.00 | 0.43 |
| 1:A:228:ASP:CG | 1:A:245:ILE:HG21 | 2.39 | 0.43 |
| 1:A:723:GLN:OE1 | 1:A:1169:SER:CA | 2.63 | 0.43 |
| 2:E:79:VAL:O | 2:E:83:THR:HG23 | 2.17 | 0.43 |
| 2:G:70:LEU:HD11 | 2:G:180:VAL:HG22 | 2.00 | 0.43 |
| 1:A:1117:LEU:HD23 | 1:A:1123:SER:HB3 | 2.00 | 0.43 |
| 1:A:627:SER:CB | 1:A:1212:VAL:CG2 | 2.96 | 0.43 |
| 1:A:66:PHE:HB3 | 1:A:73:LEU:HD21 | 2.00 | 0.43 |
| 1:A:676:SER:HB3 | 1:A:1225:TYR:HH | 1.71 | 0.43 |
| 1:A:876:PHE:O | 1:A:877:LYS:CB | 2.67 | 0.43 |
| 2:G:79:VAL:O | 2:G:83:THR:HG23 | 2.17 | 0.43 |
| 1:A:885:ALA:O | 1:A:1079:PHE:CB | 2.65 | 0.43 |
| 1:A:1045:LEU:HD23 | 1:A:1051:PHE:CZ | 2.54 | 0.43 |
| 1:A:1117:LEU:HD11 | 1:A:1173:ARG:HH11 | 1.84 | 0.43 |
| 1:A:684:LEU:HD12 | 1:A:1166:GLU:HG3 | 1.94 | 0.43 |
| 1:A:1213:LEU:O | 1:A:1227:ARG:NH2 | 2.41 | 0.43 |
| 1:A:1094:ILE:O | 1:A:1098:THR:HG23 | 2.18 | 0.43 |
| 1:A:122:ASN:ND2 | 1:A:217[B]:MET:HE3 | 2.34 | 0.43 |
| 1:A:911:GLY:C | 1:A:913:GLY:H | 2.22 | 0.43 |
| 1:A:1048:SER:O | 1:A:1052:ILE:HG13 | 2.18 | 0.43 |
| 1:A:1059:ARG:HD3 | 1:A:1059:ARG:HA | 1.75 | 0.43 |
| 1:A:364:CYS:O | 1:A:662:LEU:HB2 | 2.18 | 0.43 |
| 1:A:404:ARG:HH11 | 1:A:404:ARG:CB | 2.32 | 0.43 |
| 2:C:70:LEU:HD11 | 2:C:180:VAL:HG22 | 2.00 | 0.43 |
| 2:E:70:LEU:HD11 | 2:E:180:VAL:HG22 | 2.00 | 0.43 |
| 1:A:1159:MET:HB3 | 1:A:1159:MET:HE2 | 1.91 | 0.42 |
| 1:A:116:ARG:HB3 | 1:A:116:ARG:HE | 1.32 | 0.42 |
| 1:A:196:LYS:HG3 | 1:A:196:LYS:H | 1.53 | 0.42 |
| 2:G:63:LEU:HB3 | 3:H:585:LEU:HD22 | 2.01 | 0.42 |
| 1:A:523:LEU:CG | 1:A:1016:HIS:CB | 2.96 | 0.42 |
| 1:A:726:ARG:CB | 1:A:1112:VAL:HG11 | 2.45 | 0.42 |
| 1:A:1117:LEU:HB3 | 1:A:1118:GLY:H | 1.70 | 0.42 |
| 1:A:1198:VAL:O | 1:A:1202:ILE:HB | 2.18 | 0.42 |
| 1:A:239:SER:O | 1:A:243:CYS:HB3 | 2.20 | 0.42 |
| 1:A:622:PHE:O | 1:A:626:ILE:CG1 | 2.67 | 0.42 |
| 1:A:635:ILE:CG1 | 1:A:1204:LEU:CD1 | 2.98 | 0.42 |
| 1:A:653:LYS:C | 1:A:653:LYS:CE | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:582:PHE:HE2 | 3:H:577:THR:HG23 | 1.85 | 0.42 |
| 1:A:1046:GLN:CB | 1:A:1050:ASP:CG | 2.80 | 0.42 |
| 1:A:1222:GLN:C | 1:A:1224:PHE:N | 2.72 | 0.42 |
| 1:A:726:ARG:NE | 1:A:726:ARG:HA | 2.35 | 0.42 |
| 1:A:684:LEU:CG | 1:A:728:LEU:CD2 | 2.95 | 0.42 |
| 1:A:656:LEU:HD22 | 1:A:751:LEU:O | 2.19 | 0.42 |
| 1:A:1100:PHE:CE1 | 1:A:1104:VAL:CG2 | 3.02 | 0.42 |
| 1:A:637:LEU:O | 1:A:638:ALA:C | 2.57 | 0.42 |
| 1:A:730:GLU:HG2 | 1:A:1112:VAL:HG23 | 1.99 | 0.42 |
| 3:D:577:THR:HG23 | 3:H:582:PHE:HE2 | 1.85 | 0.42 |
| 1:A:1199:PHE:O | 1:A:1203:THR:HB | 2.20 | 0.42 |
| 1:A:1160:SER:HB2 | 1:A:1232:MET:CE | 2.50 | 0.42 |
| 4:A:1306:NAG:C1 | 4:A:1306:NAG:C8 | 2.86 | 0.42 |
| 1:A:370:PHE:O | 1:A:371:VAL:CB | 2.67 | 0.42 |
| 3:D:582:PHE:HE2 | 3:F:577:THR:HG23 | 1.85 | 0.42 |
| 2:E:63:LEU:HB3 | 3:F:585:LEU:HD22 | 2.01 | 0.42 |
| 1:A:1093:THR:HG22 | 1:A:1096:ASP:HB2 | 2.01 | 0.42 |
| 1:A:507:ALA:CB | 1:A:529:LEU:CD2 | 2.98 | 0.42 |
| 1:A:1229:TYR:C | 1:A:1229:TYR:CD1 | 2.93 | 0.42 |
| 1:A:659:ALA:CA | 1:A:662:LEU:HD21 | 2.36 | 0.42 |
| 1:A:685:ILE:O | 1:A:689:VAL:HB | 2.19 | 0.42 |
| 1:A:749:GLY:O | 1:A:752:SER:HB2 | 2.18 | 0.42 |
| 1:A:656:LEU:CD2 | 1:A:751:LEU:O | 2.67 | 0.42 |
| 1:A:1063:SER:O | 1:A:1067:GLU:CG | 2.67 | 0.42 |
| 1:A:1085:TYR:C | 1:A:1087:PHE:H | 2.22 | 0.42 |
| 1:A:1202:ILE:CG2 | 1:A:1237:ALA:CB | 2.98 | 0.42 |
| 1:A:637:LEU:O | 1:A:638:ALA:O | 2.37 | 0.42 |
| 1:A:668:VAL:O | 1:A:669:ALA:HB2 | 2.20 | 0.42 |
| 1:A:1058:ALA:HA | 1:A:1061:ILE:HD12 | 2.02 | 0.41 |
| 1:A:1227:ARG:HD3 | 1:A:1227:ARG:HA | 1.78 | 0.41 |
| 1:A:396:ASP:O | 1:A:399:PHE:N | 2.50 | 0.41 |
| 1:A:733:PRO:C | 1:A:735:MET:N | 2.73 | 0.41 |
| 1:A:908:VAL:HG13 | 1:A:926:ALA:HA | 2.02 | 0.41 |
| 2:E:39:HIS:CB | 2:E:42:VAL:HG22 | 2.40 | 0.41 |
| 1:A:1060:LEU:O | 1:A:1063:SER:OG | 2.25 | 0.41 |
| 1:A:1210:ILE:HD11 | 1:A:1214:ALA:HB2 | 2.01 | 0.41 |
| 1:A:506:TYR:CZ | 2:E:80:PRO:CB | 3.03 | 0.41 |
| 1:A:649:LEU:O | 1:A:650:VAL:C | 2.57 | 0.41 |
| 1:A:653:LYS:HA | 1:A:682:LEU:CD2 | 2.50 | 0.41 |
| 1:A:691:PRO:CD | 1:A:692:PHE:N | 2.83 | 0.41 |
| 2:G:51:LEU:HD12 | 2:G:51:LEU:HA | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:372:ARG:C | 1:A:374:THR:H | 2.23 | 0.41 |
| 1:A:544:TRP:C | 1:A:544:TRP:CD1 | 2.92 | 0.41 |
| 1:A:842:PHE:O | 1:A:1136:VAL:HG11 | 2.21 | 0.41 |
| 1:A:381:TRP:C | 1:A:383:ALA:N | 2.74 | 0.41 |
| 1:A:509:TYR:CZ | 1:A:510:HIS:CE1 | 3.08 | 0.41 |
| 1:A:878:SER:C | 1:A:1043:THR:CG2 | 2.86 | 0.41 |
| 1:A:1141:VAL:C | 1:A:1147:ILE:CB | 2.89 | 0.41 |
| 1:A:399:PHE:CD1 | 1:A:399:PHE:N | 2.88 | 0.41 |
| 1:A:758:HIS:C | 1:A:760:PHE:N | 2.74 | 0.41 |
| 3:D:582:PHE:CE2 | 3:F:578:GLU:HB3 | 2.56 | 0.41 |
| 1:A:1220:ILE:O | 1:A:1221:PHE:C | 2.59 | 0.41 |
| 1:A:1225:TYR:HD1 | 1:A:1226:PHE:CD1 | 2.39 | 0.41 |
| 1:A:1229:TYR:C | 1:A:1229:TYR:HD1 | 2.24 | 0.41 |
| 3:D:567:GLN:HG3 | 3:H:531:TRP:CG | 2.56 | 0.41 |
| 1:A:885:ALA:O | 1:A:1079:PHE:N | 2.54 | 0.41 |
| 1:A:1112:VAL:HA | 1:A:1115:VAL:CG2 | 2.49 | 0.41 |
| 1:A:131:ASP:HA | 1:A:132:PRO:HD2 | 1.93 | 0.41 |
| 1:A:673:GLY:C | 1:A:675:PHE:H | 2.23 | 0.41 |
| 3:D:513:PRO:O | 3:D:555:ILE:HD13 | 2.21 | 0.41 |
| 3:D:578:GLU:HB3 | 3:H:582:PHE:CZ | 2.56 | 0.41 |
| 2:C:63:LEU:HB3 | 3:D:585:LEU:HD22 | 2.01 | 0.41 |
| 1:A:1048:SER:O | 1:A:1052:ILE:CG1 | 2.69 | 0.41 |
| 1:A:635:ILE:HG12 | 1:A:1204:LEU:HD12 | 2.02 | 0.41 |
| 1:A:648:LEU:CG | 1:A:763:PHE:CE1 | 3.03 | 0.41 |
| 1:A:767:ALA:O | 1:A:771:ASP:N | 2.52 | 0.41 |
| 3:D:578:GLU:HB3 | 3:H:582:PHE:CE2 | 2.56 | 0.41 |
| 1:A:1152:VAL:O | 1:A:1155:VAL:N | 2.54 | 0.41 |
| 3:D:582:PHE:CZ | 3:F:578:GLU:HB3 | 2.56 | 0.41 |
| 3:F:582:PHE:CE2 | 3:H:578:GLU:HB3 | 2.56 | 0.41 |
| 1:A:1228:MET:O | 1:A:1229:TYR:C | 2.58 | 0.41 |
| 1:A:398:HIS:C | 1:A:399:PHE:CD1 | 2.95 | 0.41 |
| 1:A:684:LEU:HD11 | 1:A:1166:GLU:CG | 2.47 | 0.41 |
| 3:F:531:TRP:CG | 3:H:567:GLN:HG3 | 2.56 | 0.41 |
| 3:H:513:PRO:O | 3:H:555:ILE:HD13 | 2.21 | 0.41 |
| 1:A:1154:LEU:HA | 1:A:1154:LEU:HD23 | 1.78 | 0.40 |
| 1:A:1220:ILE:HA | 1:A:1223:ILE:CB | 2.51 | 0.40 |
| 1:A:202:PRO:HG2 | 1:A:203:PHE:CE2 | 2.55 | 0.40 |
| 1:A:515:TYR:HE1 | 1:A:526:THR:CG2 | 2.28 | 0.40 |
| 1:A:893:LEU:O | 1:A:895:GLU:N | 2.54 | 0.40 |
| 2:E:92:VAL:HA | 2:E:93:PRO:HD3 | 1.92 | 0.40 |
| 1:A:1127:MET:HE2 | 1:A:1168:CYS:HB2 | 2.01 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-------------------|--------------------------|-------------------|
| 1:A:885:ALA:N | 1:A:1079:PHE:O | 2.51 | 0.40 |
| 1:A:1222:GLN:O | 1:A:1224:PHE:N | 2.54 | 0.40 |
| 1:A:474:PRO:O | 1:A:475:TYR:C | 2.60 | 0.40 |
| 3:F:513:PRO:O | 3:F:555:ILE:HD13 | 2.21 | 0.40 |
| 3:D:531:TRP:CG | 3:F:567:GLN:HG3 | 2.56 | 0.40 |
| 1:A:1199:PHE:O | 1:A:1203:THR:HG21 | 2.19 | 0.40 |
| 1:A:689:VAL:N | 1:A:691:PRO:HD3 | 2.35 | 0.40 |
| 1:A:720:LEU:C | 1:A:723:GLN:HG3 | 2.38 | 0.40 |
| 1:A:915:ASN:HA | 1:A:921:GLN:H | 1.87 | 0.40 |
| 1:A:923:ILE:CB | 1:A:925:ASN:CB | 2.99 | 0.40 |
| 1:A:1009:PRO:C | 1:A:1010:LYS:O | 2.59 | 0.40 |
| 1:A:1043:THR:C | 1:A:1044:VAL:HG23 | 2.42 | 0.40 |
| 1:A:421:GLN:CD | 1:A:421:GLN:H | 2.20 | 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 PDB entries followed by that with respect to all EM entries.

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 | 1126/1278 (88%) | 897 (80%) | 135 (12%) | 94 (8%) | 1 | 18 |
| 2 | C | 156/158 (99%) | 142 (91%) | 12 (8%) | 2 (1%) | 15 | 60 |
| 2 | E | 156/158 (99%) | 141 (90%) | 13 (8%) | 2 (1%) | 15 | 60 |
| 2 | G | 156/158 (99%) | 142 (91%) | 12 (8%) | 2 (1%) | 15 | 60 |
| 3 | D | 83/130 (64%) | 77 (93%) | 4 (5%) | 2 (2%) | 7 | 47 |
| 3 | F | 83/130 (64%) | 77 (93%) | 4 (5%) | 2 (2%) | 7 | 47 |
| 3 | H | 83/130 (64%) | 77 (93%) | 4 (5%) | 2 (2%) | 7 | 47 |
| All | All | 1843/2142 (86%) | 1553 (84%) | 184 (10%) | 106 (6%) | 4 | 27 |

All (106) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 250 | LYS |
| 1 | A | 256 | PRO |
| 1 | A | 350 | PRO |
| 1 | A | 372 | ARG |
| 1 | A | 374 | THR |
| 1 | A | 376 | ASN |
| 1 | A | 403 | PHE |
| 1 | A | 638 | ALA |
| 1 | A | 639 | LEU |
| 1 | A | 642 | MET |
| 1 | A | 700 | ASP |
| 1 | A | 706 | VAL |
| 1 | A | 737 | LEU |
| 1 | A | 739 | SER |
| 1 | A | 829 | LEU |
| 1 | A | 856 | VAL |
| 1 | A | 864 | LEU |
| 1 | A | 876 | PHE |
| 1 | A | 922 | GLN |
| 1 | A | 929 | LEU |
| 1 | A | 930 | ASP |
| 1 | A | 943 | ILE |
| 1 | A | 951 | LYS |
| 1 | A | 957 | CYS |
| 1 | A | 958 | ARG |
| 1 | A | 1007 | PRO |
| 1 | A | 1008 | ASN |
| 1 | A | 1009 | PRO |
| 1 | A | 1010 | LYS |
| 1 | A | 1044 | VAL |
| 1 | A | 1071 | ILE |
| 1 | A | 1072 | ASN |
| 1 | A | 1083 | VAL |
| 1 | A | 1085 | TYR |
| 1 | A | 1086 | VAL |
| 1 | A | 1122 | TRP |
| 1 | A | 1146 | GLY |
| 1 | A | 260 | TRP |
| 1 | A | 475 | TYR |
| 1 | A | 605 | ALA |
| 1 | A | 606 | GLU |
| 1 | A | 617 | SER |
| 1 | A | 641 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 760 | PHE |
| 1 | A | 830 | LEU |
| 1 | A | 888 | PRO |
| 1 | A | 923 | ILE |
| 1 | A | 1022 | ALA |
| 1 | A | 1073 | GLY |
| 1 | A | 1075 | ALA |
| 1 | A | 1177 | VAL |
| 1 | A | 1179 | MET |
| 1 | A | 1215 | PHE |
| 2 | C | 50 | LYS |
| 2 | C | 51 | LEU |
| 3 | D | 597 | TRP |
| 2 | E | 50 | LYS |
| 2 | E | 51 | LEU |
| 3 | F | 597 | TRP |
| 2 | G | 50 | LYS |
| 2 | G | 51 | LEU |
| 3 | H | 597 | TRP |
| 1 | A | 168 | SER |
| 1 | A | 498 | LYS |
| 1 | A | 668 | VAL |
| 1 | A | 861 | ASP |
| 1 | A | 877 | LYS |
| 1 | A | 890 | TYR |
| 1 | A | 894 | GLU |
| 1 | A | 1178 | SER |
| 1 | A | 1221 | PHE |
| 1 | A | 252 | GLN |
| 1 | A | 348 | ARG |
| 1 | A | 691 | PRO |
| 1 | A | 734 | SER |
| 1 | A | 745 | ALA |
| 1 | A | 891 | PHE |
| 1 | A | 917 | ASP |
| 1 | A | 926 | ALA |
| 1 | A | 1084 | PHE |
| 1 | A | 1093 | THR |
| 1 | A | 1120 | GLU |
| 1 | A | 1150 | ASN |
| 1 | A | 1167 | PHE |
| 3 | D | 550 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | F | 550 | ASN |
| 3 | H | 550 | ASN |
| 1 | A | 258 | ALA |
| 1 | A | 353 | VAL |
| 1 | A | 371 | VAL |
| 1 | A | 384 | PRO |
| 1 | A | 703 | PHE |
| 1 | A | 733 | PRO |
| 1 | A | 925 | ASN |
| 1 | A | 1117 | LEU |
| 1 | A | 253 | PRO |
| 1 | A | 259 | PRO |
| 1 | A | 401 | PRO |
| 1 | A | 880 | SER |
| 1 | A | 887 | PRO |
| 1 | A | 1080 | PRO |
| 1 | A | 166 | PRO |
| 1 | A | 892 | VAL |
| 1 | A | 1202 | ILE |
| 1 | A | 349 | ASN |
| 1 | A | 257 | PRO |

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 PDB entries followed by that with respect to all EM entries.

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 | 643/1109 (58%) | 558 (87%) | 85 (13%) | 5 | 28 |
| 2 | C | 126/130 (97%) | 124 (98%) | 2 (2%) | 70 | 88 |
| 2 | E | 126/130 (97%) | 124 (98%) | 2 (2%) | 70 | 88 |
| 2 | G | 126/130 (97%) | 124 (98%) | 2 (2%) | 70 | 88 |
| 3 | D | 70/111 (63%) | 69 (99%) | 1 (1%) | 74 | 89 |
| 3 | F | 70/111 (63%) | 69 (99%) | 1 (1%) | 74 | 89 |
| 3 | H | 70/111 (63%) | 69 (99%) | 1 (1%) | 74 | 89 |
| All | All | 1231/1832 (67%) | 1137 (92%) | 94 (8%) | 21 | 53 |

All (94) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 27 | TRP |
| 1 | A | 60 | GLN |
| 1 | A | 87 | LEU |
| 1 | A | 91 | LEU |
| 1 | A | 105 | LEU |
| 1 | A | 116 | ARG |
| 1 | A | 122 | ASN |
| 1 | A | 146 | TYR |
| 1 | A | 185 | ASN |
| 1 | A | 195 | ASN |
| 1 | A | 196 | LYS |
| 1 | A | 250 | LYS |
| 1 | A | 252 | GLN |
| 1 | A | 381 | TRP |
| 1 | A | 389 | ARG |
| 1 | A | 394 | TYR |
| 1 | A | 399 | PHE |
| 1 | A | 403 | PHE |
| 1 | A | 404 | ARG |
| 1 | A | 406 | GLU |
| 1 | A | 439 | ILE |
| 1 | A | 472 | LEU |
| 1 | A | 495 | LEU |
| 1 | A | 518 | ARG |
| 1 | A | 526 | THR |
| 1 | A | 544 | TRP |
| 1 | A | 602 | SER |
| 1 | A | 607 | ARG |
| 1 | A | 612 | GLU |
| 1 | A | 614 | ASN |
| 1 | A | 615 | ARG |
| 1 | A | 653 | LYS |
| 1 | A | 662 | LEU |
| 1 | A | 676 | SER |
| 1 | A | 680 | LEU |
| 1 | A | 682 | LEU |
| 1 | A | 684 | LEU |
| 1 | A | 688 | GLU |
| 1 | A | 719 | THR |
| 1 | A | 721 | ASP |
| 1 | A | 722 | GLN |
| 1 | A | 726 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 730 | GLU |
| 1 | A | 751 | LEU |
| 1 | A | 752 | SER |
| 1 | A | 758 | HIS |
| 1 | A | 760 | PHE |
| 1 | A | 763 | PHE |
| 1 | A | 1036 | THR |
| 1 | A | 1037 | TYR |
| 1 | A | 1038 | PHE |
| 1 | A | 1039 | MET |
| 1 | A | 1041 | TYR |
| 1 | A | 1042 | HIS |
| 1 | A | 1050 | ASP |
| 1 | A | 1055 | LEU |
| 1 | A | 1056 | LYS |
| 1 | A | 1057 | LYS |
| 1 | A | 1059 | ARG |
| 1 | A | 1066 | THR |
| 1 | A | 1069 | MET |
| 1 | A | 1072 | ASN |
| 1 | A | 1074 | SER |
| 1 | A | 1077 | ARG |
| 1 | A | 1081 | TYR |
| 1 | A | 1082 | SER |
| 1 | A | 1084 | PHE |
| 1 | A | 1090 | GLN |
| 1 | A | 1117 | LEU |
| 1 | A | 1127 | MET |
| 1 | A | 1128 | CYS |
| 1 | A | 1138 | MET |
| 1 | A | 1153 | SER |
| 1 | A | 1154 | LEU |
| 1 | A | 1159 | MET |
| 1 | A | 1166 | GLU |
| 1 | A | 1172 | THR |
| 1 | A | 1173 | ARG |
| 1 | A | 1189 | GLU |
| 1 | A | 1194 | MET |
| 1 | A | 1199 | PHE |
| 1 | A | 1207 | PHE |
| 1 | A | 1227 | ARG |
| 1 | A | 1228 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1229 | TYR |
| 2 | C | 53 | CYS |
| 2 | C | 169 | VAL |
| 3 | D | 595 | GLN |
| 2 | E | 53 | CYS |
| 2 | E | 169 | VAL |
| 3 | F | 595 | GLN |
| 2 | G | 53 | CYS |
| 2 | G | 169 | VAL |
| 3 | H | 595 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 70 | ASN |
| 1 | A | 86 | ASN |
| 1 | A | 92 | GLN |
| 1 | A | 135 | ASN |
| 1 | A | 154 | ASN |
| 1 | A | 185 | ASN |
| 1 | A | 200 | GLN |
| 1 | A | 241 | GLN |
| 1 | A | 447 | GLN |
| 1 | A | 452 | ASN |
| 1 | A | 459 | ASN |
| 1 | A | 478 | ASN |
| 1 | A | 490 | ASN |
| 1 | A | 510 | HIS |
| 1 | A | 554 | ASN |
| 1 | A | 598 | ASN |
| 1 | A | 722 | GLN |
| 1 | A | 1046 | GLN |
| 1 | A | 1072 | ASN |
| 1 | A | 1156 | ASN |
| 2 | C | 39 | HIS |
| 2 | C | 69 | ASN |
| 3 | D | 595 | GLN |
| 2 | E | 39 | HIS |
| 2 | E | 69 | ASN |
| 3 | F | 595 | GLN |
| 2 | G | 39 | HIS |
| 2 | G | 69 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | H | 595 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

30 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | NAG | A | 1301 | 1,4 | 14,14,15 | 0.62 | 0 | 15,19,21 | 0.87 | 0 |
| 4 | NAG | A | 1302 | 4 | 14,14,15 | 0.55 | 0 | 15,19,21 | 0.73 | 1 (6%) |
| 4 | NAG | A | 1303 | 1 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.52 | 0 |
| 4 | NAG | A | 1304 | 1,4 | 14,14,15 | 0.46 | 0 | 15,19,21 | 0.98 | 2 (13%) |
| 4 | NAG | A | 1305 | 4 | 14,14,15 | 0.28 | 0 | 15,19,21 | 0.54 | 0 |
| 4 | NAG | A | 1306 | 1,4 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.52 | 0 |
| 4 | NAG | A | 1307 | 5,4 | 14,14,15 | 0.28 | 0 | 15,19,21 | 0.54 | 0 |
| 5 | BMA | A | 1308 | 4 | 11,11,12 | 0.26 | 0 | 15,15,17 | 0.58 | 0 |
| 4 | NAG | A | 1309 | 1 | 14,14,15 | 0.48 | 0 | 15,19,21 | 0.98 | 0 |
| 4 | NAG | A | 1310 | 1,4 | 14,14,15 | 0.34 | 0 | 15,19,21 | 1.47 | 2 (13%) |
| 4 | NAG | A | 1311 | 4 | 14,14,15 | 0.63 | 0 | 15,19,21 | 1.10 | 2 (13%) |
| 4 | NAG | A | 1312 | 1,4 | 14,14,15 | 0.27 | 0 | 15,19,21 | 0.53 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | A | 1313 | 5,4 | 14,14,15 | 0.26 | 0 | 15,19,21 | 0.85 | 0 |
| 5 | BMA | A | 1314 | 4,6 | 11,11,12 | 0.28 | 0 | 15,15,17 | 0.63 | 0 |
| 6 | MAN | A | 1315 | 5 | 11,11,12 | 0.35 | 0 | 15,15,17 | 1.21 | 1 (6%) |
| 4 | NAG | A | 1316 | 1 | 14,14,15 | 0.40 | 0 | 15,19,21 | 1.16 | 2 (13%) |
| 4 | NAG | A | 1317 | 1 | 14,14,15 | 0.28 | 0 | 15,19,21 | 0.53 | 0 |
| 4 | NAG | A | 1318 | 4 | 14,14,15 | 0.38 | 0 | 15,19,21 | 1.15 | 2 (13%) |
| 4 | NAG | A | 1319 | 1,4 | 14,14,15 | 0.37 | 0 | 15,19,21 | 1.15 | 2 (13%) |
| 4 | NAG | A | 1320 | 1 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.54 | 0 |
| 4 | NAG | A | 1321 | - | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.53 | 0 |
| 4 | NAG | A | 1322 | 1 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.54 | 0 |
| 4 | NAG | A | 1323 | 1 | 14,14,15 | 0.27 | 0 | 15,19,21 | 0.54 | 0 |
| 4 | NAG | A | 1324 | 1 | 14,14,15 | 0.41 | 0 | 15,19,21 | 1.17 | 2 (13%) |
| 4 | NAG | D | 701 | 3,4 | 14,14,15 | 0.68 | 0 | 15,19,21 | 0.70 | 0 |
| 4 | NAG | D | 702 | 4 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.47 | 0 |
| 4 | NAG | F | 701 | 3,4 | 14,14,15 | 0.69 | 0 | 15,19,21 | 0.70 | 0 |
| 4 | NAG | F | 702 | 4 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.47 | 0 |
| 4 | NAG | H | 701 | 3,4 | 14,14,15 | 0.67 | 0 | 15,19,21 | 0.69 | 0 |
| 4 | NAG | H | 702 | 4 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.47 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 4 | NAG | A | 1301 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1302 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1303 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1304 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1305 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1306 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1307 | 5,4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | A | 1308 | 4 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | A | 1309 | 1 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1310 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1311 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1312 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1313 | 5,4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | A | 1314 | 4,6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | MAN | A | 1315 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | A | 1316 | 1 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 4 | NAG | A | 1317 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1318 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1319 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1320 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1321 | - | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1322 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1323 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1324 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | D | 701 | 3,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | D | 702 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | F | 701 | 3,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | F | 702 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | H | 701 | 3,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | H | 702 | 4 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | A | 1310 | NAG | O4-C4-C3 | -3.37 | 102.75 | 110.36 |
| 4 | A | 1324 | NAG | C2-N2-C7 | -2.44 | 119.94 | 123.11 |
| 4 | A | 1318 | NAG | C2-N2-C7 | -2.39 | 119.99 | 123.11 |
| 4 | A | 1316 | NAG | C2-N2-C7 | -2.39 | 120.00 | 123.11 |
| 4 | A | 1319 | NAG | C2-N2-C7 | -2.38 | 120.00 | 123.11 |
| 4 | A | 1311 | NAG | O5-C5-C4 | -2.00 | 106.82 | 110.13 |
| 4 | A | 1316 | NAG | C8-C7-N2 | 2.00 | 119.94 | 116.10 |
| 4 | A | 1324 | NAG | C8-C7-N2 | 2.02 | 119.97 | 116.10 |
| 4 | A | 1318 | NAG | C8-C7-N2 | 2.03 | 119.99 | 116.10 |
| 4 | A | 1302 | NAG | C1-O5-C5 | 2.04 | 115.14 | 112.14 |
| 4 | A | 1319 | NAG | C8-C7-N2 | 2.05 | 120.02 | 116.10 |
| 4 | A | 1304 | NAG | C1-O5-C5 | 2.07 | 115.19 | 112.14 |
| 4 | A | 1304 | NAG | C4-C3-C2 | 2.34 | 114.98 | 111.34 |
| 4 | A | 1311 | NAG | C4-C3-C2 | 2.47 | 115.18 | 111.34 |
| 4 | A | 1310 | NAG | C1-O5-C5 | 3.19 | 116.83 | 112.14 |
| 6 | A | 1315 | MAN | C1-C2-C3 | 3.61 | 113.93 | 109.55 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 4 | A | 1309 | NAG | C1 |

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 4 | A | 1306 | NAG | C8-C7-N2-C2 |
| 4 | A | 1306 | NAG | O7-C7-N2-C2 |

There are no ring outliers.

18 monomers are involved in 46 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | A | 1303 | NAG | 1 | 0 |
| 4 | A | 1304 | NAG | 1 | 0 |
| 4 | A | 1305 | NAG | 1 | 0 |
| 4 | A | 1306 | NAG | 14 | 0 |
| 4 | A | 1307 | NAG | 12 | 0 |
| 5 | A | 1308 | BMA | 3 | 0 |
| 4 | A | 1310 | NAG | 3 | 0 |
| 4 | A | 1312 | NAG | 7 | 0 |
| 4 | A | 1313 | NAG | 6 | 0 |
| 5 | A | 1314 | BMA | 2 | 0 |
| 4 | A | 1317 | NAG | 1 | 0 |
| 4 | A | 1319 | NAG | 3 | 0 |
| 4 | A | 1322 | NAG | 3 | 0 |
| 4 | A | 1323 | NAG | 1 | 0 |
| 4 | A | 1324 | NAG | 2 | 0 |
| 4 | D | 701 | NAG | 1 | 0 |
| 4 | F | 701 | NAG | 2 | 0 |
| 4 | H | 701 | NAG | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.