



Full wwPDB NMR Structure Validation Report ⓘ

Nov 23, 2017 – 05:35 AM EST

PDB ID : 2PRF
Title : THREE DIMENSIONAL SOLUTION STRUCTURE OF ACANTHAMOEBA PROFILIN I
Authors : Archer, S.J.; Vinson, V.K.; Pollard, T.D.; Lattman, E.E.; Torchia, D.A.
Deposited on : unknown

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

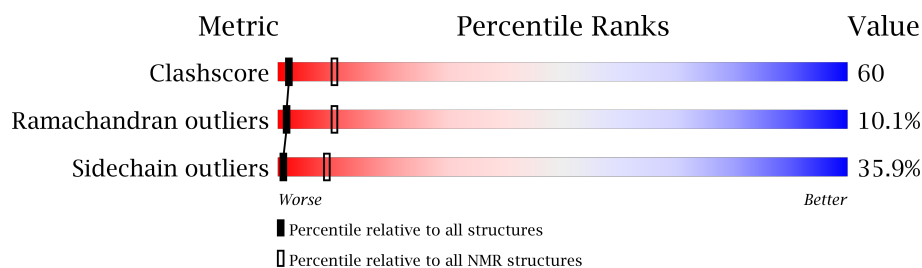
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 125131 | 11601 |
| Ramachandran outliers | 121729 | 10391 |
| Sidechain outliers | 121581 | 10367 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 | 125 |  |

2 Ensemble composition and analysis

This entry contains 19 models. Model 15 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:2-A:125 (124) | 1.01 | 15 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

| Cluster number | Models |
|-----------------------|--------------------------------|
| 1 | 2, 5, 6, 7, 13, 14, 15, 17, 18 |
| 2 | 1, 3, 4, 11, 12, 19 |
| 3 | 9, 10, 16 |
| Single-model clusters | 8 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1826 atoms, of which 910 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROFILIN IA.

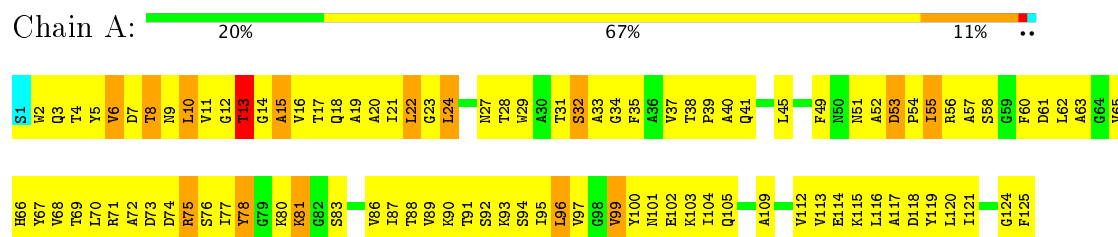
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|
| 1 | A | 125 | Total | C | H | N | O | 0 |
| | | | 1826 | 579 | 910 | 156 | 181 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: PROFILIN IA

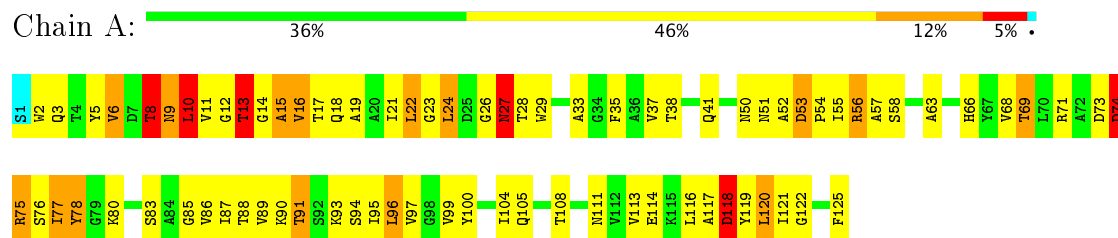


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

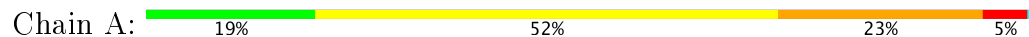
4.2.1 Score per residue for model 1

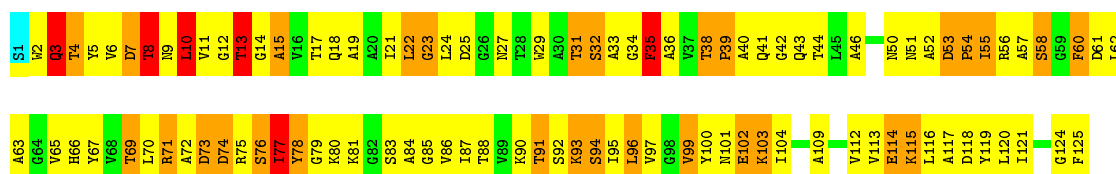
- Molecule 1: PROFILIN IA



4.2.2 Score per residue for model 2

- Molecule 1: PROFILIN IA

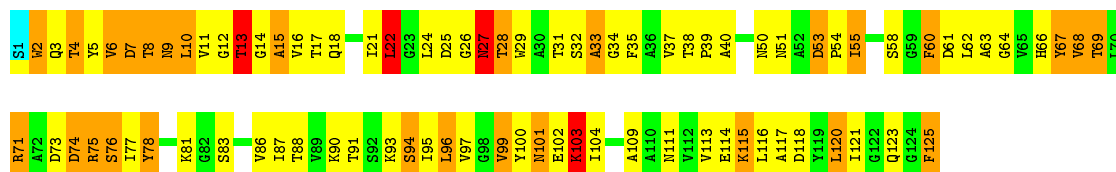




4.2.3 Score per residue for model 3

- Molecule 1: PROFILIN IA

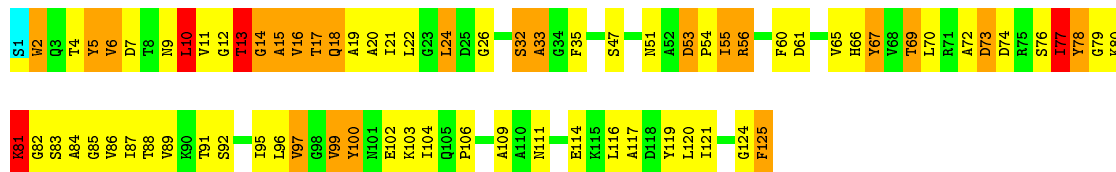
Chain A: 30% 43% 22%



4.2.4 Score per residue for model 4

- Molecule 1: PROFILIN IA

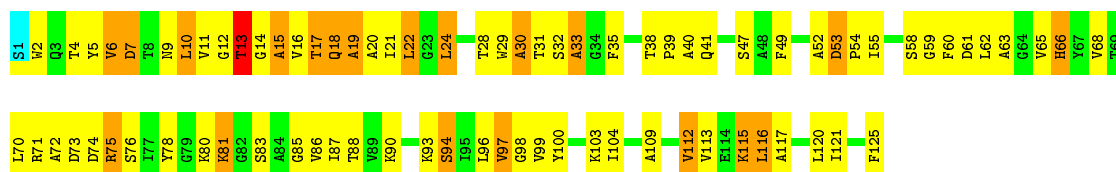
Chain A: 39% 39% 18%



4.2.5 Score per residue for model 5

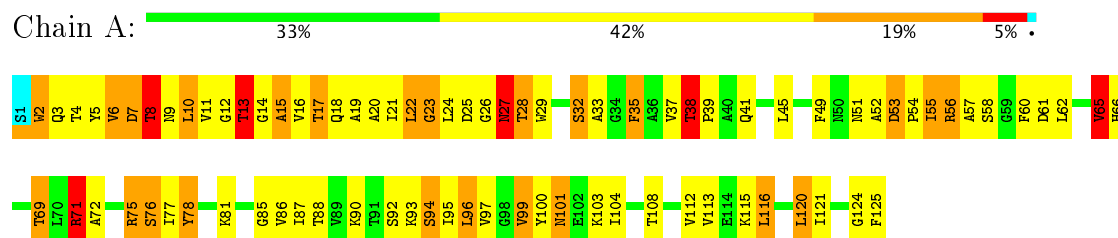
- Molecule 1: PROFILIN IA

Chain A: 35% 47% 16%



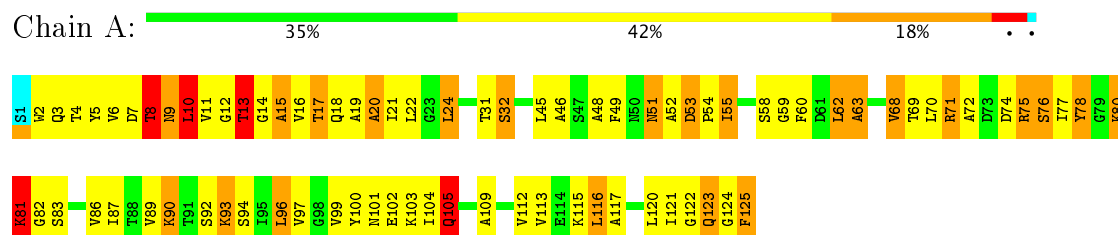
4.2.6 Score per residue for model 6

- Molecule 1: PROFILIN IA



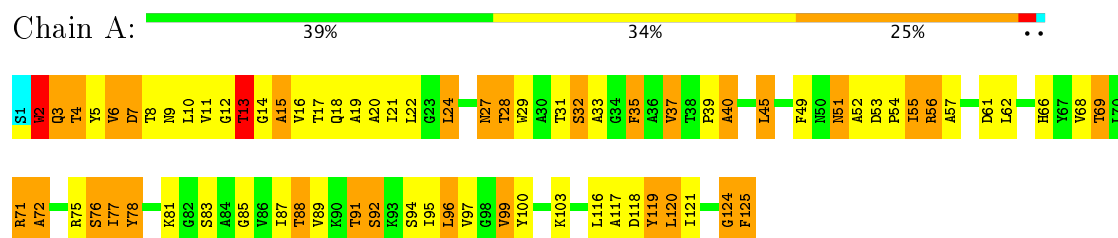
4.2.7 Score per residue for model 7

- Molecule 1: PROFILIN 1A



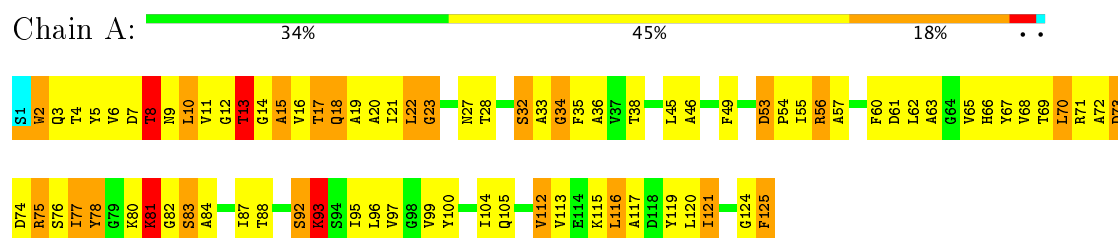
4.2.8 Score per residue for model 8

- Molecule 1: PROFILIN 1A



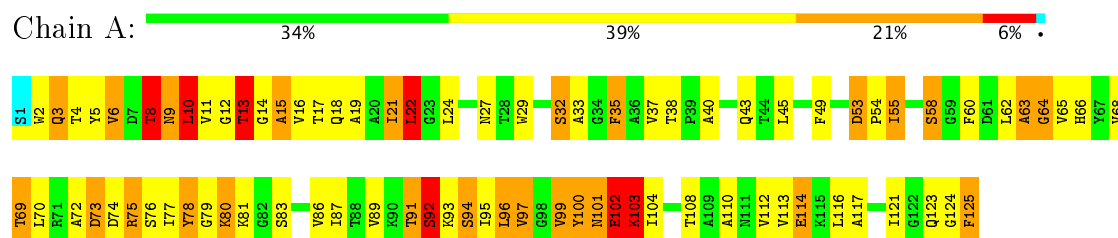
4.2.9 Score per residue for model 9

- Molecule 1: PROFILIN 1A



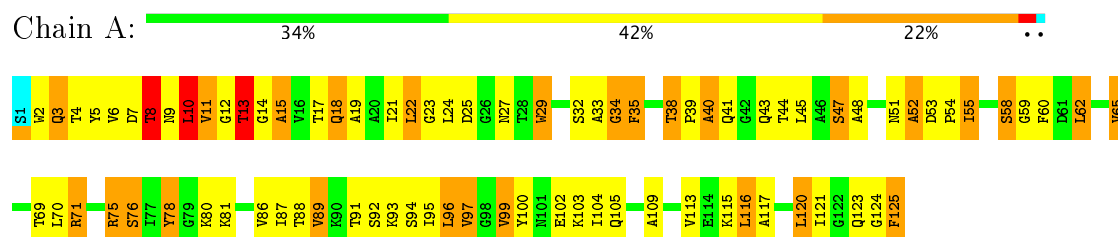
4.2.10 Score per residue for model 10

- Molecule 1: PROFILIN IA



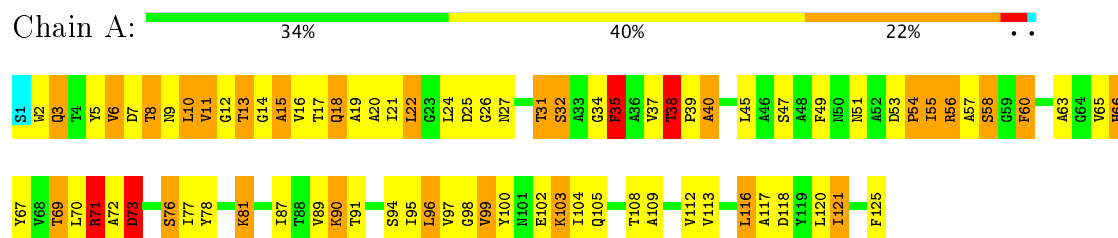
4.2.11 Score per residue for model 11

- Molecule 1: PROFILIN IA



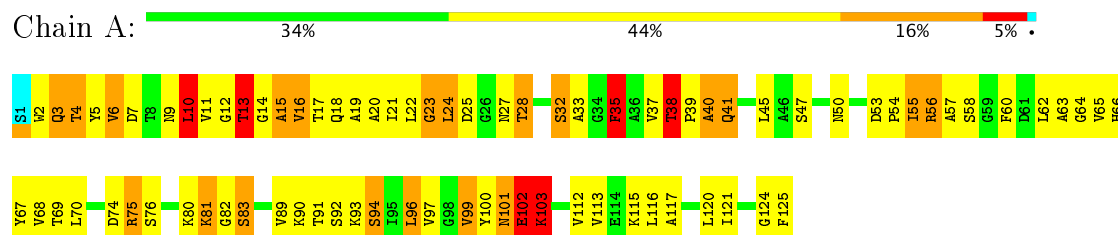
4.2.12 Score per residue for model 12

- Molecule 1: PROFILIN IA



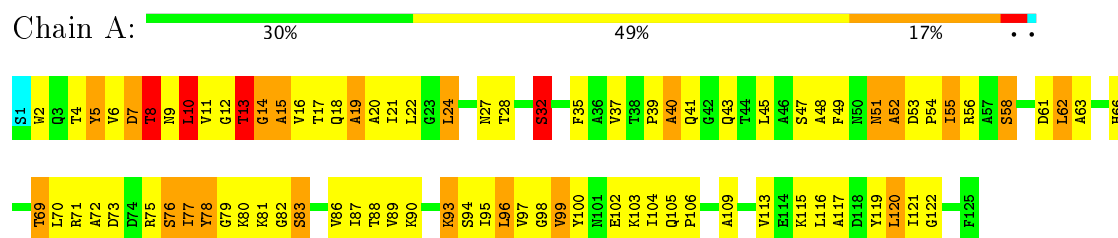
4.2.13 Score per residue for model 13

- Molecule 1: PROFILIN IA



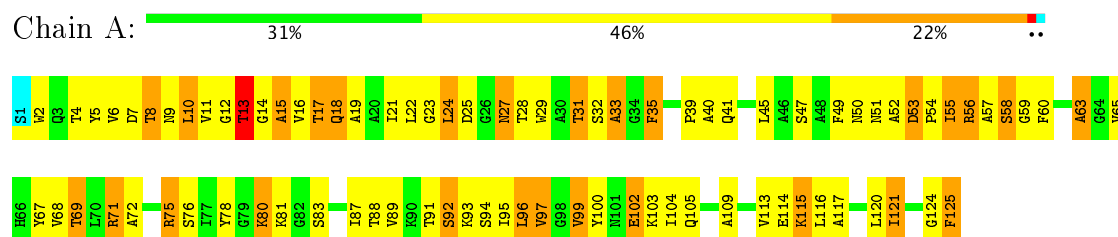
4.2.14 Score per residue for model 14

- Molecule 1: PROFILIN IA



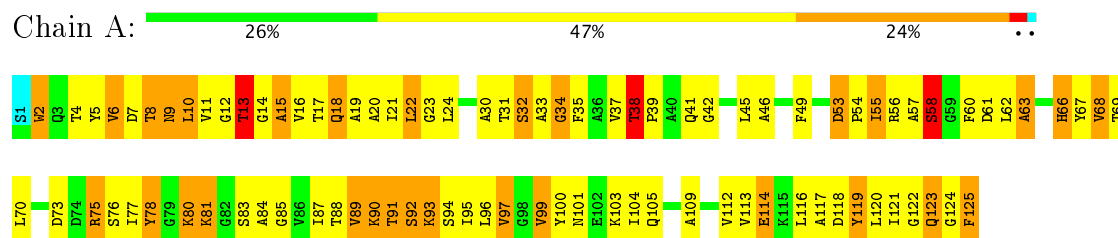
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: PROFILIN IA



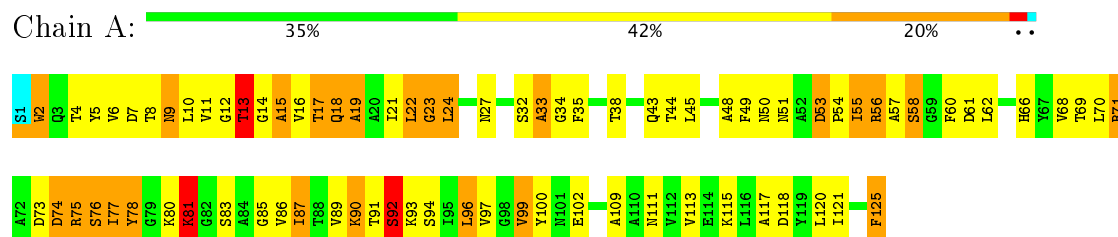
4.2.16 Score per residue for model 16

- Molecule 1: PROFILIN IA



4.2.17 Score per residue for model 17

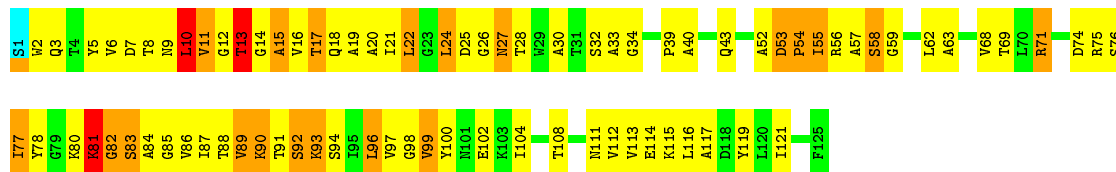
- Molecule 1: PROFILIN IA



4.2.18 Score per residue for model 18

• Molecule 1: PROFILIN IA

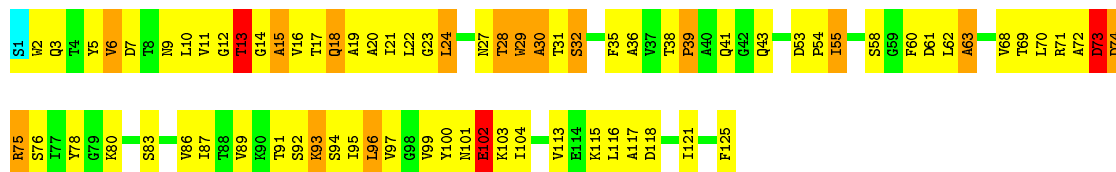
Chain A: 



4.2.19 Score per residue for model 19

• Molecule 1: PROFILIN IA

Chain A: 



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 19 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR | refinement | |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 910 | 903 | 903 | 109±11 |
| All | All | 17290 | 17157 | 17157 | 2072 |

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 60.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:VAL:HG22 | 1:A:19:ALA:HB3 | 1.12 | 1.19 | 9 | 10 |
| 1:A:22:LEU:HD22 | 1:A:97:VAL:HG21 | 1.04 | 1.26 | 19 | 5 |
| 1:A:55:ILE:HD11 | 1:A:72:ALA:CB | 1.01 | 1.85 | 9 | 2 |
| 1:A:22:LEU:HD22 | 1:A:97:VAL:CG2 | 1.00 | 1.85 | 9 | 3 |
| 1:A:15:ALA:CB | 1:A:112:VAL:HG11 | 1.00 | 1.85 | 12 | 2 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:HD21 | 1.00 | 1.28 | 19 | 2 |
| 1:A:15:ALA:HB1 | 1:A:112:VAL:HG11 | 1.00 | 1.29 | 12 | 2 |
| 1:A:11:VAL:CG2 | 1:A:19:ALA:HB3 | 0.98 | 1.89 | 17 | 12 |
| 1:A:22:LEU:CD2 | 1:A:97:VAL:HG21 | 0.97 | 1.90 | 9 | 5 |
| 1:A:91:THR:CG2 | 1:A:96:LEU:HD21 | 0.97 | 1.89 | 11 | 2 |
| 1:A:2:TRP:CZ3 | 1:A:96:LEU:HD22 | 0.97 | 1.95 | 1 | 6 |
| 1:A:117:ALA:O | 1:A:121:ILE:HD12 | 0.95 | 1.60 | 19 | 14 |
| 1:A:15:ALA:O | 1:A:104:ILE:HG21 | 0.94 | 1.62 | 3 | 6 |
| 1:A:7:ASP:OD2 | 1:A:8:THR:HG22 | 0.93 | 1.63 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:TYR:CB | 1:A:104:ILE:HD12 | 0.93 | 1.94 | 10 | 1 |
| 1:A:22:LEU:HD13 | 1:A:97:VAL:HG21 | 0.92 | 1.41 | 15 | 2 |
| 1:A:100:TYR:HB2 | 1:A:104:ILE:HD12 | 0.92 | 1.38 | 10 | 4 |
| 1:A:89:VAL:HB | 1:A:96:LEU:HD21 | 0.91 | 1.39 | 4 | 2 |
| 1:A:11:VAL:HG21 | 1:A:32:SER:CB | 0.91 | 1.96 | 16 | 2 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:HD13 | 0.90 | 2.01 | 13 | 7 |
| 1:A:5:TYR:CD2 | 1:A:116:LEU:HD21 | 0.90 | 2.01 | 7 | 4 |
| 1:A:2:TRP:N | 1:A:21:ILE:HD11 | 0.90 | 1.81 | 5 | 5 |
| 1:A:2:TRP:CZ2 | 1:A:96:LEU:HD11 | 0.90 | 2.02 | 16 | 1 |
| 1:A:24:LEU:N | 1:A:24:LEU:HD13 | 0.89 | 1.81 | 5 | 1 |
| 1:A:17:THR:HG23 | 1:A:104:ILE:HD11 | 0.89 | 1.40 | 11 | 3 |
| 1:A:6:VAL:HG13 | 1:A:11:VAL:HG21 | 0.89 | 1.45 | 11 | 1 |
| 1:A:4:THR:O | 1:A:8:THR:HG22 | 0.89 | 1.67 | 7 | 5 |
| 1:A:2:TRP:CZ2 | 1:A:96:LEU:HD13 | 0.88 | 2.03 | 1 | 5 |
| 1:A:2:TRP:C | 1:A:21:ILE:HD11 | 0.88 | 1.88 | 8 | 6 |
| 1:A:24:LEU:HD11 | 1:A:93:LYS:O | 0.88 | 1.68 | 7 | 3 |
| 1:A:11:VAL:HG23 | 1:A:19:ALA:HB3 | 0.87 | 1.45 | 12 | 3 |
| 1:A:5:TYR:CB | 1:A:10:LEU:HD12 | 0.87 | 2.00 | 1 | 2 |
| 1:A:11:VAL:HG22 | 1:A:19:ALA:CB | 0.87 | 1.99 | 16 | 9 |
| 1:A:76:SER:OG | 1:A:89:VAL:HG22 | 0.86 | 1.68 | 13 | 1 |
| 1:A:60:PHE:CD2 | 1:A:62:LEU:HD21 | 0.86 | 2.05 | 2 | 1 |
| 1:A:96:LEU:N | 1:A:96:LEU:HD13 | 0.85 | 1.86 | 2 | 3 |
| 1:A:35:PHE:CE1 | 1:A:99:VAL:HG11 | 0.85 | 2.07 | 16 | 2 |
| 1:A:91:THR:HG22 | 1:A:121:ILE:HD11 | 0.85 | 1.46 | 18 | 1 |
| 1:A:91:THR:HG23 | 1:A:96:LEU:HD21 | 0.85 | 1.46 | 11 | 1 |
| 1:A:2:TRP:CZ2 | 1:A:96:LEU:HD22 | 0.84 | 2.06 | 9 | 3 |
| 1:A:96:LEU:HD13 | 1:A:96:LEU:N | 0.84 | 1.87 | 11 | 3 |
| 1:A:10:LEU:HD11 | 1:A:116:LEU:HD13 | 0.84 | 1.50 | 16 | 1 |
| 1:A:55:ILE:HD11 | 1:A:72:ALA:HB1 | 0.82 | 1.51 | 9 | 1 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:HD22 | 0.82 | 2.10 | 9 | 4 |
| 1:A:2:TRP:CD1 | 1:A:10:LEU:HD13 | 0.82 | 2.10 | 1 | 3 |
| 1:A:60:PHE:CE2 | 1:A:62:LEU:HD11 | 0.81 | 2.09 | 13 | 1 |
| 1:A:86:VAL:HG23 | 1:A:97:VAL:HG13 | 0.81 | 1.52 | 6 | 3 |
| 1:A:5:TYR:CD2 | 1:A:10:LEU:HD13 | 0.81 | 2.10 | 4 | 2 |
| 1:A:24:LEU:HD13 | 1:A:93:LYS:O | 0.80 | 1.76 | 1 | 1 |
| 1:A:51:ASN:O | 1:A:55:ILE:HD11 | 0.80 | 1.77 | 4 | 2 |
| 1:A:69:THR:CG2 | 1:A:72:ALA:HB2 | 0.78 | 2.07 | 4 | 4 |
| 1:A:86:VAL:HG22 | 1:A:88:THR:CG2 | 0.78 | 2.07 | 18 | 1 |
| 1:A:40:ALA:HB1 | 1:A:43:GLN:HB3 | 0.78 | 1.56 | 10 | 1 |
| 1:A:11:VAL:HG13 | 1:A:18:GLN:HA | 0.78 | 1.55 | 16 | 3 |
| 1:A:109:ALA:O | 1:A:113:VAL:HG23 | 0.77 | 1.78 | 12 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:VAL:HG12 | 1:A:100:TYR:HB3 | 0.77 | 1.54 | 1 | 8 |
| 1:A:6:VAL:HG13 | 1:A:32:SER:OG | 0.77 | 1.80 | 6 | 5 |
| 1:A:17:THR:HG23 | 1:A:18:GLN:HG3 | 0.77 | 1.53 | 13 | 3 |
| 1:A:22:LEU:HD13 | 1:A:97:VAL:CG2 | 0.77 | 2.10 | 13 | 2 |
| 1:A:22:LEU:N | 1:A:22:LEU:HD23 | 0.76 | 1.95 | 5 | 7 |
| 1:A:16:VAL:HA | 1:A:104:ILE:HD13 | 0.76 | 1.57 | 3 | 4 |
| 1:A:67:TYR:OH | 1:A:86:VAL:HG13 | 0.76 | 1.79 | 4 | 1 |
| 1:A:97:VAL:O | 1:A:99:VAL:HG22 | 0.76 | 1.80 | 18 | 8 |
| 1:A:88:THR:HG22 | 1:A:97:VAL:HG13 | 0.76 | 1.57 | 2 | 2 |
| 1:A:112:VAL:HG22 | 1:A:116:LEU:HD12 | 0.76 | 1.57 | 13 | 1 |
| 1:A:55:ILE:HD13 | 1:A:55:ILE:N | 0.75 | 1.97 | 19 | 3 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:HD12 | 0.75 | 1.57 | 16 | 2 |
| 1:A:38:THR:N | 1:A:39:PRO:CD | 0.75 | 2.50 | 12 | 3 |
| 1:A:78:TYR:CD2 | 1:A:87:ILE:HG23 | 0.75 | 2.17 | 19 | 9 |
| 1:A:78:TYR:CD1 | 1:A:87:ILE:HG23 | 0.75 | 2.17 | 18 | 3 |
| 1:A:96:LEU:N | 1:A:96:LEU:HD22 | 0.74 | 1.96 | 6 | 1 |
| 1:A:2:TRP:NE1 | 1:A:10:LEU:HD23 | 0.74 | 1.96 | 19 | 1 |
| 1:A:120:LEU:HD23 | 1:A:124:GLY:HA3 | 0.74 | 1.59 | 8 | 1 |
| 1:A:36:ALA:O | 1:A:63:ALA:HB2 | 0.74 | 1.83 | 19 | 2 |
| 1:A:2:TRP:HZ2 | 1:A:96:LEU:HD11 | 0.74 | 1.42 | 16 | 1 |
| 1:A:108:THR:O | 1:A:112:VAL:HG23 | 0.73 | 1.81 | 18 | 2 |
| 1:A:45:LEU:HD22 | 1:A:95:ILE:HG21 | 0.73 | 1.60 | 9 | 1 |
| 1:A:15:ALA:HB2 | 1:A:112:VAL:HG11 | 0.73 | 1.58 | 9 | 3 |
| 1:A:70:LEU:HD23 | 1:A:70:LEU:O | 0.73 | 1.82 | 19 | 1 |
| 1:A:6:VAL:HG22 | 1:A:11:VAL:HG21 | 0.73 | 1.59 | 2 | 4 |
| 1:A:16:VAL:HG13 | 1:A:100:TYR:HB3 | 0.73 | 1.60 | 17 | 1 |
| 1:A:6:VAL:HG21 | 1:A:21:ILE:HG13 | 0.73 | 1.61 | 17 | 2 |
| 1:A:2:TRP:HB2 | 1:A:6:VAL:HG23 | 0.73 | 1.61 | 9 | 1 |
| 1:A:22:LEU:HD11 | 1:A:97:VAL:HG21 | 0.72 | 1.60 | 18 | 8 |
| 1:A:55:ILE:N | 1:A:55:ILE:HD13 | 0.72 | 1.98 | 3 | 2 |
| 1:A:97:VAL:HG12 | 1:A:97:VAL:O | 0.72 | 1.84 | 10 | 6 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HD12 | 0.72 | 2.19 | 2 | 1 |
| 1:A:5:TYR:CE1 | 1:A:10:LEU:HD12 | 0.72 | 2.19 | 11 | 1 |
| 1:A:22:LEU:HD22 | 1:A:22:LEU:N | 0.72 | 2.00 | 8 | 1 |
| 1:A:96:LEU:O | 1:A:96:LEU:HD22 | 0.72 | 1.83 | 19 | 1 |
| 1:A:22:LEU:HD23 | 1:A:97:VAL:CG2 | 0.72 | 2.13 | 8 | 1 |
| 1:A:13:THR:O | 1:A:15:ALA:N | 0.72 | 2.21 | 14 | 2 |
| 1:A:2:TRP:CZ3 | 1:A:96:LEU:HD13 | 0.72 | 2.20 | 8 | 3 |
| 1:A:104:ILE:HG22 | 1:A:104:ILE:O | 0.71 | 1.85 | 19 | 1 |
| 1:A:22:LEU:HD23 | 1:A:22:LEU:N | 0.71 | 1.98 | 12 | 4 |
| 1:A:97:VAL:O | 1:A:97:VAL:HG12 | 0.71 | 1.84 | 16 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:2:TRP:CE2 | 1:A:96:LEU:HD22 | 0.71 | 2.19 | 17 | 1 |
| 1:A:11:VAL:HG11 | 1:A:32:SER:HB2 | 0.71 | 1.61 | 2 | 2 |
| 1:A:11:VAL:HG11 | 1:A:32:SER:CB | 0.71 | 2.16 | 2 | 3 |
| 1:A:87:ILE:O | 1:A:87:ILE:HG22 | 0.71 | 1.85 | 7 | 3 |
| 1:A:103:LYS:C | 1:A:104:ILE:HD12 | 0.70 | 2.06 | 2 | 1 |
| 1:A:2:TRP:CZ3 | 1:A:5:TYR:CD2 | 0.70 | 2.79 | 4 | 1 |
| 1:A:89:VAL:HG23 | 1:A:96:LEU:HD21 | 0.70 | 1.63 | 1 | 1 |
| 1:A:12:GLY:C | 1:A:13:THR:HG22 | 0.70 | 2.07 | 18 | 17 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HD22 | 0.70 | 2.22 | 13 | 2 |
| 1:A:2:TRP:NE1 | 1:A:96:LEU:HD22 | 0.70 | 2.02 | 17 | 1 |
| 1:A:5:TYR:HD2 | 1:A:10:LEU:HD13 | 0.70 | 1.45 | 4 | 1 |
| 1:A:24:LEU:HD11 | 1:A:93:LYS:CA | 0.69 | 2.18 | 6 | 4 |
| 1:A:2:TRP:CB | 1:A:21:ILE:HD11 | 0.69 | 2.17 | 11 | 5 |
| 1:A:21:ILE:HG22 | 1:A:29:TRP:CE3 | 0.69 | 2.23 | 1 | 1 |
| 1:A:117:ALA:O | 1:A:121:ILE:HD13 | 0.69 | 1.88 | 10 | 1 |
| 1:A:16:VAL:CA | 1:A:104:ILE:HD13 | 0.69 | 2.17 | 3 | 2 |
| 1:A:96:LEU:HD13 | 1:A:96:LEU:H | 0.68 | 1.47 | 19 | 2 |
| 1:A:69:THR:HG22 | 1:A:72:ALA:HB2 | 0.68 | 1.65 | 15 | 2 |
| 1:A:89:VAL:CG2 | 1:A:96:LEU:HD21 | 0.68 | 2.15 | 19 | 4 |
| 1:A:86:VAL:HG13 | 1:A:86:VAL:O | 0.68 | 1.87 | 3 | 3 |
| 1:A:24:LEU:HD21 | 1:A:94:SER:N | 0.68 | 2.04 | 17 | 5 |
| 1:A:32:SER:O | 1:A:33:ALA:HB3 | 0.68 | 1.89 | 9 | 6 |
| 1:A:14:GLY:O | 1:A:15:ALA:HB3 | 0.68 | 1.88 | 14 | 2 |
| 1:A:11:VAL:HG21 | 1:A:32:SER:HB2 | 0.68 | 1.63 | 16 | 1 |
| 1:A:6:VAL:HA | 1:A:11:VAL:HG23 | 0.68 | 1.66 | 6 | 10 |
| 1:A:39:PRO:O | 1:A:40:ALA:HB3 | 0.68 | 1.89 | 5 | 4 |
| 1:A:24:LEU:HD11 | 1:A:93:LYS:C | 0.68 | 2.09 | 15 | 7 |
| 1:A:21:ILE:C | 1:A:22:LEU:HD23 | 0.67 | 2.10 | 18 | 3 |
| 1:A:11:VAL:HG12 | 1:A:12:GLY:N | 0.67 | 2.04 | 18 | 5 |
| 1:A:38:THR:HG22 | 1:A:39:PRO:HD2 | 0.67 | 1.64 | 11 | 2 |
| 1:A:86:VAL:CG2 | 1:A:97:VAL:HG13 | 0.67 | 2.18 | 7 | 4 |
| 1:A:86:VAL:O | 1:A:86:VAL:HG13 | 0.67 | 1.88 | 1 | 3 |
| 1:A:104:ILE:N | 1:A:104:ILE:HD13 | 0.67 | 2.04 | 4 | 1 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:HD23 | 0.67 | 1.65 | 14 | 1 |
| 1:A:62:LEU:O | 1:A:63:ALA:HB3 | 0.67 | 1.89 | 13 | 5 |
| 1:A:91:THR:HG21 | 1:A:96:LEU:HD21 | 0.67 | 1.67 | 11 | 2 |
| 1:A:6:VAL:HG13 | 1:A:32:SER:HB2 | 0.67 | 1.66 | 8 | 4 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HD11 | 0.67 | 2.24 | 12 | 2 |
| 1:A:2:TRP:CE3 | 1:A:96:LEU:HD11 | 0.67 | 2.25 | 15 | 1 |
| 1:A:6:VAL:HG13 | 1:A:32:SER:CB | 0.67 | 2.19 | 8 | 2 |
| 1:A:2:TRP:CD1 | 1:A:10:LEU:HD23 | 0.67 | 2.25 | 15 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:HD12 | 1:A:94:SER:N | 0.66 | 2.05 | 10 | 1 |
| 1:A:24:LEU:N | 1:A:24:LEU:CD1 | 0.66 | 2.55 | 5 | 1 |
| 1:A:19:ALA:HA | 1:A:99:VAL:HG23 | 0.66 | 1.67 | 14 | 5 |
| 1:A:55:ILE:HG22 | 1:A:59:GLY:O | 0.66 | 1.90 | 18 | 1 |
| 1:A:37:VAL:HG13 | 1:A:41:GLN:CD | 0.66 | 2.11 | 6 | 1 |
| 1:A:117:ALA:C | 1:A:121:ILE:HD12 | 0.66 | 2.10 | 8 | 6 |
| 1:A:78:TYR:HB3 | 1:A:87:ILE:HD13 | 0.66 | 1.67 | 2 | 2 |
| 1:A:2:TRP:CA | 1:A:21:ILE:HD11 | 0.66 | 2.20 | 5 | 6 |
| 1:A:38:THR:HG23 | 1:A:39:PRO:HD3 | 0.66 | 1.67 | 6 | 2 |
| 1:A:60:PHE:HE2 | 1:A:62:LEU:HD11 | 0.66 | 1.48 | 13 | 1 |
| 1:A:14:GLY:O | 1:A:15:ALA:HB2 | 0.66 | 1.91 | 2 | 17 |
| 1:A:120:LEU:C | 1:A:120:LEU:HD12 | 0.66 | 2.10 | 2 | 2 |
| 1:A:22:LEU:CD1 | 1:A:97:VAL:HG21 | 0.66 | 2.19 | 15 | 12 |
| 1:A:77:ILE:O | 1:A:77:ILE:HG22 | 0.66 | 1.91 | 4 | 2 |
| 1:A:15:ALA:HB1 | 1:A:112:VAL:CG1 | 0.66 | 2.17 | 12 | 1 |
| 1:A:60:PHE:CE1 | 1:A:67:TYR:CG | 0.66 | 2.84 | 4 | 1 |
| 1:A:18:GLN:O | 1:A:19:ALA:HB2 | 0.66 | 1.90 | 5 | 7 |
| 1:A:15:ALA:HB1 | 1:A:109:ALA:CB | 0.65 | 2.21 | 3 | 2 |
| 1:A:2:TRP:CE3 | 1:A:96:LEU:HD22 | 0.65 | 2.25 | 1 | 2 |
| 1:A:22:LEU:HG | 1:A:97:VAL:HG21 | 0.65 | 1.67 | 5 | 3 |
| 1:A:2:TRP:CH2 | 1:A:117:ALA:HB2 | 0.65 | 2.26 | 2 | 2 |
| 1:A:11:VAL:HG11 | 1:A:32:SER:OG | 0.65 | 1.91 | 16 | 1 |
| 1:A:7:ASP:C | 1:A:8:THR:HG22 | 0.65 | 2.11 | 14 | 3 |
| 1:A:117:ALA:HB1 | 1:A:121:ILE:HD11 | 0.65 | 1.67 | 1 | 1 |
| 1:A:67:TYR:CE2 | 1:A:86:VAL:CG1 | 0.65 | 2.80 | 4 | 1 |
| 1:A:17:THR:CG2 | 1:A:104:ILE:HD11 | 0.65 | 2.21 | 11 | 1 |
| 1:A:76:SER:CB | 1:A:78:TYR:CZ | 0.65 | 2.80 | 2 | 5 |
| 1:A:2:TRP:HZ2 | 1:A:96:LEU:HD22 | 0.65 | 1.50 | 4 | 1 |
| 1:A:39:PRO:O | 1:A:40:ALA:HB2 | 0.65 | 1.92 | 8 | 4 |
| 1:A:89:VAL:O | 1:A:95:ILE:HG23 | 0.65 | 1.92 | 19 | 3 |
| 1:A:37:VAL:O | 1:A:38:THR:HG22 | 0.65 | 1.92 | 12 | 2 |
| 1:A:90:LYS:HD3 | 1:A:95:ILE:HG23 | 0.65 | 1.68 | 14 | 1 |
| 1:A:65:VAL:CG1 | 1:A:67:TYR:CE1 | 0.64 | 2.80 | 13 | 2 |
| 1:A:77:ILE:HG22 | 1:A:77:ILE:O | 0.64 | 1.92 | 9 | 6 |
| 1:A:60:PHE:CD1 | 1:A:60:PHE:N | 0.64 | 2.66 | 2 | 3 |
| 1:A:21:ILE:HG22 | 1:A:29:TRP:HE3 | 0.64 | 1.52 | 1 | 1 |
| 1:A:38:THR:HG23 | 1:A:39:PRO:CD | 0.64 | 2.22 | 13 | 2 |
| 1:A:91:THR:HG22 | 1:A:121:ILE:HG12 | 0.64 | 1.68 | 13 | 1 |
| 1:A:87:ILE:HG21 | 1:A:113:VAL:HG21 | 0.64 | 1.70 | 12 | 7 |
| 1:A:13:THR:O | 1:A:16:VAL:N | 0.64 | 2.31 | 14 | 2 |
| 1:A:22:LEU:HD23 | 1:A:97:VAL:HG23 | 0.64 | 1.67 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:91:THR:HG22 | 1:A:121:ILE:HG13 | 0.63 | 1.70 | 8 | 1 |
| 1:A:68:VAL:HG12 | 1:A:80:LYS:O | 0.63 | 1.93 | 15 | 2 |
| 1:A:100:TYR:N | 1:A:100:TYR:CD1 | 0.63 | 2.66 | 6 | 8 |
| 1:A:97:VAL:O | 1:A:99:VAL:HG23 | 0.63 | 1.94 | 5 | 2 |
| 1:A:94:SER:CB | 1:A:125:PHE:CG | 0.63 | 2.82 | 6 | 1 |
| 1:A:12:GLY:O | 1:A:13:THR:HG22 | 0.63 | 1.93 | 6 | 16 |
| 1:A:2:TRP:CB | 1:A:21:ILE:CD1 | 0.63 | 2.77 | 12 | 3 |
| 1:A:5:TYR:N | 1:A:5:TYR:CD1 | 0.63 | 2.64 | 2 | 3 |
| 1:A:76:SER:C | 1:A:77:ILE:HD12 | 0.63 | 2.14 | 1 | 3 |
| 1:A:78:TYR:HD2 | 1:A:87:ILE:HG23 | 0.63 | 1.53 | 12 | 9 |
| 1:A:24:LEU:HD11 | 1:A:93:LYS:HA | 0.63 | 1.69 | 6 | 4 |
| 1:A:5:TYR:CD1 | 1:A:5:TYR:N | 0.63 | 2.66 | 3 | 4 |
| 1:A:89:VAL:HB | 1:A:96:LEU:HD23 | 0.62 | 1.71 | 10 | 1 |
| 1:A:24:LEU:HD12 | 1:A:25:ASP:N | 0.62 | 2.10 | 2 | 1 |
| 1:A:2:TRP:CZ2 | 1:A:96:LEU:CD1 | 0.62 | 2.79 | 16 | 1 |
| 1:A:2:TRP:CE2 | 1:A:96:LEU:HD13 | 0.62 | 2.29 | 1 | 1 |
| 1:A:5:TYR:CD2 | 1:A:10:LEU:CD2 | 0.62 | 2.82 | 6 | 1 |
| 1:A:53:ASP:N | 1:A:54:PRO:CD | 0.62 | 2.63 | 19 | 19 |
| 1:A:2:TRP:HZ3 | 1:A:91:THR:HG21 | 0.62 | 1.53 | 16 | 2 |
| 1:A:2:TRP:CD1 | 1:A:10:LEU:HD22 | 0.62 | 2.30 | 18 | 2 |
| 1:A:5:TYR:CE1 | 1:A:10:LEU:CD1 | 0.62 | 2.83 | 11 | 1 |
| 1:A:2:TRP:O | 1:A:21:ILE:HD11 | 0.62 | 1.95 | 15 | 4 |
| 1:A:97:VAL:HG12 | 1:A:99:VAL:HG22 | 0.61 | 1.71 | 3 | 4 |
| 1:A:5:TYR:CD1 | 1:A:5:TYR:C | 0.61 | 2.73 | 4 | 1 |
| 1:A:7:ASP:O | 1:A:8:THR:HG23 | 0.61 | 1.96 | 2 | 2 |
| 1:A:16:VAL:HG12 | 1:A:99:VAL:O | 0.61 | 1.96 | 17 | 1 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:HD11 | 0.61 | 1.72 | 1 | 1 |
| 1:A:2:TRP:CD1 | 1:A:5:TYR:CD1 | 0.61 | 2.89 | 11 | 1 |
| 1:A:14:GLY:O | 1:A:15:ALA:CB | 0.61 | 2.48 | 8 | 19 |
| 1:A:96:LEU:N | 1:A:96:LEU:CD1 | 0.61 | 2.60 | 2 | 1 |
| 1:A:125:PHE:CD1 | 1:A:125:PHE:N | 0.61 | 2.69 | 1 | 2 |
| 1:A:37:VAL:C | 1:A:38:THR:HG22 | 0.61 | 2.15 | 6 | 1 |
| 1:A:5:TYR:CG | 1:A:10:LEU:HD13 | 0.61 | 2.31 | 7 | 1 |
| 1:A:2:TRP:CE3 | 1:A:120:LEU:HD12 | 0.61 | 2.30 | 16 | 1 |
| 1:A:17:THR:HG23 | 1:A:104:ILE:CD1 | 0.60 | 2.26 | 1 | 2 |
| 1:A:87:ILE:HG21 | 1:A:113:VAL:HG11 | 0.60 | 1.73 | 11 | 4 |
| 1:A:39:PRO:O | 1:A:41:GLN:N | 0.60 | 2.33 | 13 | 1 |
| 1:A:56:ARG:CZ | 1:A:56:ARG:CB | 0.60 | 2.79 | 6 | 1 |
| 1:A:49:PHE:CD2 | 1:A:77:ILE:HD13 | 0.60 | 2.32 | 8 | 1 |
| 1:A:44:THR:O | 1:A:48:ALA:HB2 | 0.60 | 1.96 | 11 | 2 |
| 1:A:49:PHE:CE1 | 1:A:90:LYS:CE | 0.60 | 2.84 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:53:ASP:N | 1:A:54:PRO:HD2 | 0.60 | 2.12 | 9 | 19 |
| 1:A:112:VAL:HG22 | 1:A:116:LEU:HD13 | 0.60 | 1.71 | 5 | 1 |
| 1:A:96:LEU:H | 1:A:96:LEU:HD22 | 0.60 | 1.53 | 6 | 1 |
| 1:A:35:PHE:CE2 | 1:A:99:VAL:HG21 | 0.60 | 2.31 | 2 | 2 |
| 1:A:2:TRP:HZ2 | 1:A:113:VAL:HG13 | 0.60 | 1.57 | 3 | 3 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:HD13 | 0.60 | 1.72 | 7 | 2 |
| 1:A:91:THR:HG22 | 1:A:121:ILE:CG1 | 0.60 | 2.26 | 13 | 2 |
| 1:A:100:TYR:CD1 | 1:A:100:TYR:N | 0.60 | 2.69 | 10 | 1 |
| 1:A:37:VAL:O | 1:A:38:THR:CB | 0.60 | 2.50 | 12 | 1 |
| 1:A:38:THR:N | 1:A:39:PRO:HD2 | 0.60 | 2.12 | 19 | 3 |
| 1:A:11:VAL:HG21 | 1:A:32:SER:OG | 0.60 | 1.97 | 9 | 3 |
| 1:A:35:PHE:CE2 | 1:A:97:VAL:HG11 | 0.60 | 2.32 | 16 | 1 |
| 1:A:96:LEU:HD22 | 1:A:96:LEU:H | 0.60 | 1.57 | 2 | 2 |
| 1:A:22:LEU:CG | 1:A:97:VAL:HG21 | 0.60 | 2.27 | 5 | 4 |
| 1:A:75:ARG:CB | 1:A:75:ARG:CZ | 0.59 | 2.78 | 3 | 2 |
| 1:A:95:ILE:C | 1:A:96:LEU:HD13 | 0.59 | 2.17 | 6 | 2 |
| 1:A:20:ALA:HB1 | 1:A:31:THR:HG22 | 0.59 | 1.74 | 19 | 1 |
| 1:A:94:SER:HB3 | 1:A:125:PHE:CG | 0.59 | 2.33 | 6 | 1 |
| 1:A:6:VAL:CG2 | 1:A:11:VAL:HG21 | 0.59 | 2.27 | 2 | 1 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HD21 | 0.59 | 2.31 | 7 | 4 |
| 1:A:6:VAL:HG22 | 1:A:11:VAL:CG2 | 0.59 | 2.27 | 13 | 2 |
| 1:A:86:VAL:HG22 | 1:A:88:THR:HG22 | 0.59 | 1.74 | 18 | 1 |
| 1:A:35:PHE:CE2 | 1:A:37:VAL:HG22 | 0.59 | 2.32 | 3 | 2 |
| 1:A:19:ALA:CA | 1:A:99:VAL:HG23 | 0.59 | 2.28 | 14 | 3 |
| 1:A:76:SER:HB2 | 1:A:78:TYR:CZ | 0.59 | 2.32 | 3 | 4 |
| 1:A:91:THR:CG2 | 1:A:96:LEU:CD2 | 0.59 | 2.80 | 3 | 1 |
| 1:A:24:LEU:CB | 1:A:95:ILE:HD11 | 0.59 | 2.28 | 4 | 1 |
| 1:A:2:TRP:CZ2 | 1:A:113:VAL:HG13 | 0.59 | 2.32 | 18 | 5 |
| 1:A:24:LEU:HD22 | 1:A:24:LEU:H | 0.59 | 1.56 | 5 | 1 |
| 1:A:2:TRP:CD1 | 1:A:21:ILE:HD11 | 0.59 | 2.32 | 12 | 3 |
| 1:A:5:TYR:CD2 | 1:A:10:LEU:HD12 | 0.59 | 2.32 | 9 | 1 |
| 1:A:5:TYR:O | 1:A:10:LEU:CB | 0.58 | 2.50 | 11 | 3 |
| 1:A:62:LEU:HD22 | 1:A:62:LEU:N | 0.58 | 2.12 | 2 | 1 |
| 1:A:9:ASN:O | 1:A:14:GLY:N | 0.58 | 2.36 | 5 | 5 |
| 1:A:2:TRP:CG | 1:A:21:ILE:HD11 | 0.58 | 2.32 | 9 | 2 |
| 1:A:60:PHE:CZ | 1:A:67:TYR:CD2 | 0.58 | 2.91 | 4 | 1 |
| 1:A:49:PHE:CE2 | 1:A:90:LYS:CG | 0.58 | 2.86 | 16 | 1 |
| 1:A:100:TYR:CE1 | 1:A:104:ILE:O | 0.58 | 2.56 | 19 | 1 |
| 1:A:91:THR:O | 1:A:125:PHE:CD1 | 0.58 | 2.56 | 1 | 1 |
| 1:A:78:TYR:CD1 | 1:A:78:TYR:N | 0.58 | 2.72 | 10 | 1 |
| 1:A:5:TYR:CE1 | 1:A:10:LEU:CG | 0.58 | 2.87 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:LEU:CD1 | 1:A:96:LEU:N | 0.58 | 2.66 | 19 | 2 |
| 1:A:23:GLY:O | 1:A:29:TRP:CH2 | 0.58 | 2.56 | 1 | 1 |
| 1:A:85:GLY:O | 1:A:100:TYR:CE1 | 0.58 | 2.57 | 6 | 2 |
| 1:A:22:LEU:N | 1:A:22:LEU:CD2 | 0.58 | 2.64 | 5 | 7 |
| 1:A:125:PHE:N | 1:A:125:PHE:CD1 | 0.58 | 2.67 | 17 | 3 |
| 1:A:48:ALA:O | 1:A:55:ILE:HD11 | 0.58 | 1.98 | 17 | 1 |
| 1:A:69:THR:HG21 | 1:A:72:ALA:HB2 | 0.57 | 1.75 | 7 | 5 |
| 1:A:66:HIS:CG | 1:A:66:HIS:O | 0.57 | 2.57 | 17 | 2 |
| 1:A:57:ALA:O | 1:A:58:SER:CB | 0.57 | 2.52 | 13 | 4 |
| 1:A:45:LEU:CD2 | 1:A:95:ILE:HG21 | 0.57 | 2.28 | 9 | 2 |
| 1:A:50:ASN:O | 1:A:51:ASN:CB | 0.57 | 2.53 | 17 | 1 |
| 1:A:12:GLY:O | 1:A:13:THR:CB | 0.57 | 2.50 | 8 | 16 |
| 1:A:2:TRP:HB3 | 1:A:21:ILE:HD13 | 0.57 | 1.77 | 17 | 1 |
| 1:A:5:TYR:HB2 | 1:A:10:LEU:HD12 | 0.57 | 1.73 | 1 | 1 |
| 1:A:2:TRP:HB3 | 1:A:21:ILE:HD11 | 0.57 | 1.76 | 12 | 3 |
| 1:A:28:THR:O | 1:A:29:TRP:CE3 | 0.57 | 2.57 | 19 | 1 |
| 1:A:24:LEU:HB3 | 1:A:95:ILE:HD11 | 0.57 | 1.76 | 4 | 1 |
| 1:A:19:ALA:O | 1:A:32:SER:HA | 0.57 | 1.99 | 18 | 1 |
| 1:A:39:PRO:O | 1:A:40:ALA:CB | 0.57 | 2.53 | 5 | 5 |
| 1:A:17:THR:HG23 | 1:A:18:GLN:HG2 | 0.57 | 1.77 | 14 | 1 |
| 1:A:121:ILE:HD13 | 1:A:121:ILE:N | 0.57 | 2.14 | 1 | 1 |
| 1:A:9:ASN:O | 1:A:11:VAL:N | 0.57 | 2.38 | 7 | 13 |
| 1:A:96:LEU:N | 1:A:96:LEU:CD2 | 0.57 | 2.68 | 6 | 1 |
| 1:A:38:THR:N | 1:A:39:PRO:HD3 | 0.57 | 2.13 | 12 | 1 |
| 1:A:65:VAL:HG12 | 1:A:67:TYR:CE1 | 0.57 | 2.35 | 15 | 1 |
| 1:A:17:THR:O | 1:A:18:GLN:CG | 0.56 | 2.53 | 18 | 12 |
| 1:A:15:ALA:HB1 | 1:A:109:ALA:HB1 | 0.56 | 1.75 | 3 | 1 |
| 1:A:2:TRP:CD2 | 1:A:21:ILE:HD11 | 0.56 | 2.34 | 7 | 1 |
| 1:A:24:LEU:HD23 | 1:A:95:ILE:CG1 | 0.56 | 2.30 | 11 | 2 |
| 1:A:32:SER:O | 1:A:33:ALA:CB | 0.56 | 2.52 | 2 | 6 |
| 1:A:67:TYR:CE1 | 1:A:79:GLY:CA | 0.56 | 2.88 | 4 | 1 |
| 1:A:2:TRP:H | 1:A:21:ILE:HD11 | 0.56 | 1.60 | 5 | 1 |
| 1:A:62:LEU:O | 1:A:63:ALA:CB | 0.56 | 2.53 | 13 | 4 |
| 1:A:2:TRP:CE3 | 1:A:120:LEU:HD21 | 0.56 | 2.35 | 2 | 1 |
| 1:A:35:PHE:CD1 | 1:A:35:PHE:N | 0.56 | 2.72 | 12 | 2 |
| 1:A:22:LEU:CD1 | 1:A:22:LEU:N | 0.56 | 2.69 | 9 | 1 |
| 1:A:78:TYR:CE2 | 1:A:89:VAL:CG2 | 0.56 | 2.89 | 14 | 1 |
| 1:A:61:ASP:O | 1:A:62:LEU:HD23 | 0.56 | 2.00 | 19 | 1 |
| 1:A:87:ILE:HG22 | 1:A:87:ILE:O | 0.56 | 2.00 | 8 | 3 |
| 1:A:35:PHE:CG | 1:A:35:PHE:O | 0.56 | 2.59 | 17 | 2 |
| 1:A:77:ILE:O | 1:A:77:ILE:CG2 | 0.56 | 2.53 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:60:PHE:CE1 | 1:A:62:LEU:HD12 | 0.56 | 2.36 | 5 | 1 |
| 1:A:5:TYR:CD1 | 1:A:10:LEU:HB3 | 0.56 | 2.35 | 11 | 1 |
| 1:A:8:THR:HG22 | 1:A:9:ASN:N | 0.56 | 2.15 | 12 | 4 |
| 1:A:115:LYS:O | 1:A:119:TYR:CD1 | 0.56 | 2.59 | 2 | 1 |
| 1:A:89:VAL:CB | 1:A:96:LEU:HD21 | 0.56 | 2.24 | 4 | 1 |
| 1:A:45:LEU:O | 1:A:49:PHE:CD2 | 0.56 | 2.59 | 6 | 2 |
| 1:A:67:TYR:CE2 | 1:A:86:VAL:HG11 | 0.56 | 2.35 | 4 | 1 |
| 1:A:85:GLY:CA | 1:A:100:TYR:CE2 | 0.56 | 2.89 | 4 | 1 |
| 1:A:2:TRP:O | 1:A:6:VAL:CG2 | 0.56 | 2.54 | 5 | 3 |
| 1:A:85:GLY:N | 1:A:100:TYR:CE1 | 0.56 | 2.74 | 5 | 1 |
| 1:A:68:VAL:HG22 | 1:A:69:THR:N | 0.56 | 2.16 | 9 | 4 |
| 1:A:2:TRP:N | 1:A:21:ILE:CD1 | 0.55 | 2.70 | 13 | 2 |
| 1:A:2:TRP:CZ3 | 1:A:91:THR:HG21 | 0.55 | 2.36 | 16 | 2 |
| 1:A:13:THR:OG1 | 1:A:13:THR:O | 0.55 | 2.24 | 9 | 7 |
| 1:A:27:ASN:O | 1:A:28:THR:C | 0.55 | 2.44 | 3 | 2 |
| 1:A:17:THR:N | 1:A:104:ILE:HD13 | 0.55 | 2.17 | 5 | 1 |
| 1:A:19:ALA:O | 1:A:32:SER:CA | 0.55 | 2.55 | 18 | 1 |
| 1:A:37:VAL:O | 1:A:38:THR:CG2 | 0.55 | 2.54 | 12 | 1 |
| 1:A:16:VAL:HG12 | 1:A:100:TYR:CD1 | 0.55 | 2.36 | 16 | 3 |
| 1:A:29:TRP:CD2 | 1:A:94:SER:OG | 0.55 | 2.59 | 2 | 2 |
| 1:A:11:VAL:HG11 | 1:A:32:SER:HB3 | 0.55 | 1.78 | 9 | 2 |
| 1:A:11:VAL:HG11 | 1:A:32:SER:O | 0.55 | 2.01 | 14 | 1 |
| 1:A:38:THR:CG2 | 1:A:39:PRO:HD3 | 0.55 | 2.32 | 6 | 2 |
| 1:A:69:THR:HG23 | 1:A:72:ALA:HB2 | 0.55 | 1.76 | 4 | 1 |
| 1:A:104:ILE:O | 1:A:104:ILE:HG22 | 0.55 | 2.01 | 7 | 1 |
| 1:A:55:ILE:N | 1:A:55:ILE:CD1 | 0.55 | 2.65 | 19 | 1 |
| 1:A:91:THR:HG21 | 1:A:120:LEU:HD11 | 0.55 | 1.79 | 2 | 1 |
| 1:A:97:VAL:O | 1:A:99:VAL:CG2 | 0.55 | 2.55 | 5 | 3 |
| 1:A:35:PHE:N | 1:A:35:PHE:CD1 | 0.55 | 2.74 | 3 | 3 |
| 1:A:76:SER:HB3 | 1:A:78:TYR:CZ | 0.55 | 2.37 | 18 | 9 |
| 1:A:4:THR:O | 1:A:8:THR:CG2 | 0.55 | 2.55 | 11 | 5 |
| 1:A:113:VAL:O | 1:A:117:ALA:HB3 | 0.55 | 2.02 | 10 | 1 |
| 1:A:5:TYR:CE1 | 1:A:10:LEU:HG | 0.55 | 2.37 | 11 | 1 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:CD2 | 0.54 | 2.91 | 3 | 1 |
| 1:A:67:TYR:CE1 | 1:A:79:GLY:HA3 | 0.54 | 2.37 | 4 | 1 |
| 1:A:18:GLN:O | 1:A:19:ALA:CB | 0.54 | 2.55 | 5 | 2 |
| 1:A:3:GLN:N | 1:A:21:ILE:HD11 | 0.54 | 2.17 | 8 | 1 |
| 1:A:32:SER:O | 1:A:33:ALA:HB2 | 0.54 | 2.02 | 4 | 1 |
| 1:A:55:ILE:HD13 | 1:A:72:ALA:HB3 | 0.54 | 1.79 | 5 | 1 |
| 1:A:91:THR:O | 1:A:92:SER:CB | 0.54 | 2.56 | 16 | 2 |
| 1:A:2:TRP:HB2 | 1:A:21:ILE:CD1 | 0.54 | 2.31 | 11 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:LEU:O | 1:A:96:LEU:CD2 | 0.54 | 2.55 | 19 | 1 |
| 1:A:91:THR:O | 1:A:125:PHE:CB | 0.54 | 2.55 | 19 | 2 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:CD2 | 0.54 | 2.91 | 7 | 1 |
| 1:A:11:VAL:CG1 | 1:A:12:GLY:N | 0.54 | 2.71 | 13 | 3 |
| 1:A:11:VAL:CG1 | 1:A:19:ALA:HB3 | 0.54 | 2.32 | 4 | 1 |
| 1:A:35:PHE:CZ | 1:A:99:VAL:HG21 | 0.54 | 2.37 | 4 | 1 |
| 1:A:86:VAL:CG1 | 1:A:86:VAL:O | 0.54 | 2.56 | 3 | 4 |
| 1:A:55:ILE:CD1 | 1:A:55:ILE:N | 0.54 | 2.65 | 13 | 3 |
| 1:A:2:TRP:CE2 | 1:A:96:LEU:HB3 | 0.54 | 2.37 | 4 | 1 |
| 1:A:96:LEU:H | 1:A:96:LEU:HD23 | 0.54 | 1.61 | 4 | 2 |
| 1:A:70:LEU:H | 1:A:70:LEU:HD23 | 0.54 | 1.61 | 14 | 1 |
| 1:A:84:ALA:HB1 | 1:A:100:TYR:O | 0.54 | 2.03 | 2 | 1 |
| 1:A:16:VAL:CG2 | 1:A:18:GLN:O | 0.54 | 2.56 | 9 | 9 |
| 1:A:122:GLY:O | 1:A:123:GLN:CG | 0.54 | 2.56 | 16 | 1 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:CD2 | 0.54 | 2.19 | 19 | 1 |
| 1:A:12:GLY:O | 1:A:13:THR:CG2 | 0.54 | 2.55 | 8 | 16 |
| 1:A:65:VAL:HG12 | 1:A:66:HIS:N | 0.54 | 2.18 | 2 | 2 |
| 1:A:6:VAL:HG23 | 1:A:21:ILE:HD11 | 0.54 | 1.77 | 4 | 1 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HD13 | 0.54 | 2.38 | 11 | 1 |
| 1:A:113:VAL:O | 1:A:117:ALA:HB2 | 0.54 | 2.03 | 13 | 1 |
| 1:A:92:SER:HB3 | 1:A:125:PHE:CD2 | 0.54 | 2.37 | 10 | 1 |
| 1:A:2:TRP:CE2 | 1:A:96:LEU:HB2 | 0.54 | 2.38 | 12 | 1 |
| 1:A:119:TYR:CD1 | 1:A:119:TYR:C | 0.54 | 2.80 | 16 | 1 |
| 1:A:38:THR:O | 1:A:41:GLN:CG | 0.54 | 2.56 | 1 | 1 |
| 1:A:117:ALA:O | 1:A:121:ILE:CD1 | 0.53 | 2.57 | 12 | 10 |
| 1:A:76:SER:HB2 | 1:A:78:TYR:CE1 | 0.53 | 2.37 | 12 | 2 |
| 1:A:100:TYR:CD1 | 1:A:100:TYR:C | 0.53 | 2.81 | 2 | 1 |
| 1:A:55:ILE:O | 1:A:69:THR:CB | 0.53 | 2.55 | 10 | 2 |
| 1:A:35:PHE:CD1 | 1:A:35:PHE:C | 0.53 | 2.81 | 14 | 3 |
| 1:A:69:THR:HG22 | 1:A:72:ALA:CB | 0.53 | 2.33 | 10 | 1 |
| 1:A:33:ALA:CB | 1:A:35:PHE:CE2 | 0.53 | 2.91 | 5 | 1 |
| 1:A:5:TYR:CB | 1:A:10:LEU:HD13 | 0.53 | 2.33 | 7 | 1 |
| 1:A:5:TYR:CD2 | 1:A:116:LEU:CD2 | 0.53 | 2.87 | 7 | 3 |
| 1:A:89:VAL:HG13 | 1:A:96:LEU:HD12 | 0.53 | 1.80 | 7 | 1 |
| 1:A:37:VAL:HG12 | 1:A:37:VAL:O | 0.53 | 2.03 | 16 | 1 |
| 1:A:61:ASP:C | 1:A:62:LEU:HD22 | 0.53 | 2.24 | 2 | 1 |
| 1:A:2:TRP:HB2 | 1:A:5:TYR:CD2 | 0.53 | 2.39 | 14 | 2 |
| 1:A:2:TRP:CZ3 | 1:A:5:TYR:CE2 | 0.53 | 2.96 | 4 | 1 |
| 1:A:24:LEU:HD23 | 1:A:94:SER:C | 0.53 | 2.24 | 8 | 1 |
| 1:A:117:ALA:C | 1:A:121:ILE:HD13 | 0.53 | 2.22 | 10 | 1 |
| 1:A:2:TRP:HD1 | 1:A:10:LEU:HD23 | 0.53 | 1.60 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:HIS:O | 1:A:66:HIS:CD2 | 0.53 | 2.62 | 17 | 1 |
| 1:A:29:TRP:CH2 | 1:A:94:SER:HA | 0.53 | 2.39 | 1 | 1 |
| 1:A:9:ASN:O | 1:A:10:LEU:C | 0.53 | 2.47 | 12 | 14 |
| 1:A:68:VAL:CG1 | 1:A:80:LYS:O | 0.53 | 2.57 | 10 | 1 |
| 1:A:26:GLY:O | 1:A:28:THR:N | 0.53 | 2.42 | 18 | 2 |
| 1:A:2:TRP:N | 1:A:2:TRP:CE3 | 0.53 | 2.76 | 9 | 1 |
| 1:A:49:PHE:CE2 | 1:A:90:LYS:HG2 | 0.53 | 2.39 | 16 | 2 |
| 1:A:18:GLN:HG2 | 1:A:33:ALA:HB3 | 0.53 | 1.80 | 16 | 1 |
| 1:A:13:THR:O | 1:A:13:THR:OG1 | 0.53 | 2.27 | 13 | 10 |
| 1:A:49:PHE:CE1 | 1:A:90:LYS:HE2 | 0.53 | 2.37 | 14 | 1 |
| 1:A:29:TRP:CZ2 | 1:A:93:LYS:O | 0.53 | 2.62 | 15 | 2 |
| 1:A:49:PHE:N | 1:A:49:PHE:CD1 | 0.53 | 2.73 | 17 | 1 |
| 1:A:53:ASP:CB | 1:A:54:PRO:HD3 | 0.53 | 2.34 | 1 | 12 |
| 1:A:101:ASN:O | 1:A:102:GLU:CG | 0.53 | 2.57 | 13 | 3 |
| 1:A:60:PHE:O | 1:A:67:TYR:CB | 0.53 | 2.57 | 3 | 1 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:HB3 | 0.53 | 2.38 | 7 | 2 |
| 1:A:87:ILE:O | 1:A:87:ILE:CG2 | 0.53 | 2.57 | 7 | 1 |
| 1:A:101:ASN:O | 1:A:102:GLU:CB | 0.53 | 2.55 | 13 | 3 |
| 1:A:89:VAL:HB | 1:A:96:LEU:HD12 | 0.53 | 1.81 | 8 | 1 |
| 1:A:5:TYR:CZ | 1:A:10:LEU:HG | 0.53 | 2.39 | 11 | 1 |
| 1:A:16:VAL:HG12 | 1:A:100:TYR:CB | 0.53 | 2.31 | 1 | 1 |
| 1:A:120:LEU:HD22 | 1:A:125:PHE:OXT | 0.53 | 2.03 | 7 | 1 |
| 1:A:29:TRP:CE2 | 1:A:94:SER:OG | 0.53 | 2.62 | 8 | 1 |
| 1:A:53:ASP:N | 1:A:53:ASP:OD1 | 0.52 | 2.42 | 2 | 1 |
| 1:A:52:ALA:HA | 1:A:55:ILE:HD11 | 0.52 | 1.81 | 5 | 2 |
| 1:A:17:THR:C | 1:A:18:GLN:CG | 0.52 | 2.77 | 12 | 6 |
| 1:A:29:TRP:O | 1:A:30:ALA:HB2 | 0.52 | 2.04 | 5 | 1 |
| 1:A:83:SER:O | 1:A:102:GLU:N | 0.52 | 2.43 | 15 | 2 |
| 1:A:76:SER:O | 1:A:77:ILE:CG1 | 0.52 | 2.57 | 7 | 5 |
| 1:A:71:ARG:HG3 | 1:A:71:ARG:NH1 | 0.52 | 2.20 | 12 | 2 |
| 1:A:2:TRP:CE3 | 1:A:2:TRP:HA | 0.52 | 2.39 | 4 | 1 |
| 1:A:2:TRP:CA | 1:A:21:ILE:CD1 | 0.52 | 2.87 | 15 | 2 |
| 1:A:37:VAL:C | 1:A:38:THR:CG2 | 0.52 | 2.78 | 6 | 1 |
| 1:A:38:THR:O | 1:A:38:THR:HG23 | 0.52 | 2.03 | 12 | 1 |
| 1:A:15:ALA:HB1 | 1:A:109:ALA:HA | 0.52 | 1.81 | 11 | 2 |
| 1:A:24:LEU:HD21 | 1:A:90:LYS:HB3 | 0.52 | 1.80 | 12 | 1 |
| 1:A:49:PHE:CD1 | 1:A:49:PHE:N | 0.52 | 2.75 | 15 | 1 |
| 1:A:85:GLY:C | 1:A:100:TYR:CZ | 0.52 | 2.83 | 4 | 3 |
| 1:A:23:GLY:HA3 | 1:A:29:TRP:CE3 | 0.52 | 2.40 | 6 | 1 |
| 1:A:55:ILE:CD1 | 1:A:69:THR:HG21 | 0.52 | 2.34 | 6 | 1 |
| 1:A:51:ASN:O | 1:A:53:ASP:N | 0.52 | 2.42 | 11 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:2:TRP:NE1 | 1:A:5:TYR:CE1 | 0.52 | 2.77 | 11 | 1 |
| 1:A:23:GLY:O | 1:A:95:ILE:HD12 | 0.52 | 2.05 | 15 | 2 |
| 1:A:5:TYR:CD2 | 1:A:116:LEU:HD23 | 0.52 | 2.39 | 15 | 1 |
| 1:A:68:VAL:HG12 | 1:A:69:THR:N | 0.52 | 2.20 | 17 | 2 |
| 1:A:62:LEU:O | 1:A:63:ALA:C | 0.52 | 2.48 | 19 | 2 |
| 1:A:11:VAL:O | 1:A:12:GLY:C | 0.52 | 2.49 | 6 | 18 |
| 1:A:24:LEU:CD2 | 1:A:94:SER:N | 0.52 | 2.73 | 2 | 1 |
| 1:A:37:VAL:HG13 | 1:A:41:GLN:NE2 | 0.52 | 2.18 | 6 | 2 |
| 1:A:2:TRP:CD2 | 1:A:96:LEU:HG | 0.52 | 2.40 | 19 | 2 |
| 1:A:117:ALA:HB1 | 1:A:121:ILE:CD1 | 0.52 | 2.35 | 12 | 1 |
| 1:A:12:GLY:O | 1:A:13:THR:HG23 | 0.52 | 2.05 | 12 | 1 |
| 1:A:78:TYR:OH | 1:A:87:ILE:HD11 | 0.52 | 2.05 | 15 | 1 |
| 1:A:24:LEU:HD23 | 1:A:24:LEU:N | 0.52 | 2.20 | 18 | 1 |
| 1:A:86:VAL:HG21 | 1:A:97:VAL:HG13 | 0.51 | 1.82 | 4 | 1 |
| 1:A:23:GLY:HA3 | 1:A:29:TRP:CD2 | 0.51 | 2.40 | 6 | 1 |
| 1:A:2:TRP:CE3 | 1:A:96:LEU:HG | 0.51 | 2.41 | 11 | 3 |
| 1:A:11:VAL:CG2 | 1:A:19:ALA:CB | 0.51 | 2.89 | 4 | 2 |
| 1:A:117:ALA:O | 1:A:121:ILE:HG12 | 0.51 | 2.06 | 1 | 1 |
| 1:A:55:ILE:HG22 | 1:A:60:PHE:HD1 | 0.51 | 1.65 | 3 | 1 |
| 1:A:62:LEU:O | 1:A:64:GLY:N | 0.51 | 2.43 | 3 | 1 |
| 1:A:119:TYR:C | 1:A:119:TYR:CD1 | 0.51 | 2.83 | 4 | 4 |
| 1:A:2:TRP:O | 1:A:6:VAL:HG23 | 0.51 | 2.05 | 8 | 2 |
| 1:A:52:ALA:O | 1:A:56:ARG:CB | 0.51 | 2.58 | 8 | 2 |
| 1:A:16:VAL:CG1 | 1:A:99:VAL:C | 0.51 | 2.78 | 17 | 1 |
| 1:A:2:TRP:CZ3 | 1:A:96:LEU:HG | 0.51 | 2.41 | 11 | 4 |
| 1:A:85:GLY:C | 1:A:100:TYR:CE2 | 0.51 | 2.83 | 4 | 1 |
| 1:A:33:ALA:HB3 | 1:A:35:PHE:CE2 | 0.51 | 2.41 | 5 | 1 |
| 1:A:82:GLY:O | 1:A:83:SER:CB | 0.51 | 2.58 | 13 | 3 |
| 1:A:2:TRP:HA | 1:A:5:TYR:CB | 0.51 | 2.36 | 11 | 1 |
| 1:A:92:SER:O | 1:A:93:LYS:HB2 | 0.51 | 2.05 | 18 | 1 |
| 1:A:67:TYR:CE1 | 1:A:81:LYS:HA | 0.51 | 2.41 | 2 | 1 |
| 1:A:6:VAL:HA | 1:A:11:VAL:CG2 | 0.51 | 2.36 | 3 | 11 |
| 1:A:17:THR:N | 1:A:104:ILE:CD1 | 0.51 | 2.74 | 3 | 2 |
| 1:A:60:PHE:CB | 1:A:68:VAL:O | 0.51 | 2.59 | 3 | 1 |
| 1:A:83:SER:CB | 1:A:102:GLU:OE2 | 0.51 | 2.59 | 3 | 1 |
| 1:A:124:GLY:C | 1:A:125:PHE:CD1 | 0.51 | 2.84 | 10 | 2 |
| 1:A:60:PHE:CE2 | 1:A:62:LEU:HD21 | 0.51 | 2.39 | 2 | 1 |
| 1:A:67:TYR:CZ | 1:A:86:VAL:CG1 | 0.51 | 2.93 | 4 | 1 |
| 1:A:120:LEU:HB3 | 1:A:125:PHE:CE1 | 0.51 | 2.41 | 6 | 1 |
| 1:A:35:PHE:CZ | 1:A:37:VAL:CG2 | 0.51 | 2.94 | 8 | 1 |
| 1:A:86:VAL:CG2 | 1:A:88:THR:CG2 | 0.51 | 2.86 | 18 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:24:LEU:HD11 | 1:A:94:SER:CA | 0.51 | 2.36 | 5 | 1 |
| 1:A:2:TRP:HH2 | 1:A:96:LEU:HD13 | 0.51 | 1.65 | 7 | 1 |
| 1:A:23:GLY:O | 1:A:24:LEU:O | 0.50 | 2.29 | 1 | 1 |
| 1:A:12:GLY:C | 1:A:13:THR:CG2 | 0.50 | 2.78 | 13 | 14 |
| 1:A:62:LEU:CD2 | 1:A:62:LEU:N | 0.50 | 2.75 | 2 | 1 |
| 1:A:75:ARG:HB2 | 1:A:75:ARG:CZ | 0.50 | 2.36 | 6 | 1 |
| 1:A:2:TRP:CD1 | 1:A:21:ILE:HG23 | 0.50 | 2.41 | 4 | 1 |
| 1:A:76:SER:HA | 1:A:89:VAL:HG22 | 0.50 | 1.82 | 4 | 1 |
| 1:A:67:TYR:CE1 | 1:A:79:GLY:N | 0.50 | 2.79 | 4 | 1 |
| 1:A:80:LYS:O | 1:A:81:LYS:CG | 0.50 | 2.60 | 4 | 1 |
| 1:A:16:VAL:CG1 | 1:A:99:VAL:O | 0.50 | 2.59 | 17 | 1 |
| 1:A:5:TYR:CE2 | 1:A:116:LEU:HG | 0.50 | 2.41 | 18 | 1 |
| 1:A:37:VAL:HA | 1:A:63:ALA:HB2 | 0.50 | 1.82 | 14 | 3 |
| 1:A:5:TYR:CG | 1:A:10:LEU:HD23 | 0.50 | 2.40 | 6 | 1 |
| 1:A:6:VAL:CG1 | 1:A:32:SER:OG | 0.50 | 2.56 | 6 | 2 |
| 1:A:55:ILE:HB | 1:A:69:THR:HG21 | 0.50 | 1.83 | 10 | 3 |
| 1:A:96:LEU:HD13 | 1:A:113:VAL:CG1 | 0.50 | 2.37 | 16 | 1 |
| 1:A:11:VAL:HG13 | 1:A:18:GLN:CA | 0.50 | 2.32 | 16 | 1 |
| 1:A:92:SER:O | 1:A:92:SER:OG | 0.50 | 2.29 | 18 | 1 |
| 1:A:76:SER:C | 1:A:77:ILE:CG1 | 0.50 | 2.79 | 2 | 1 |
| 1:A:67:TYR:CE2 | 1:A:81:LYS:HE2 | 0.50 | 2.42 | 2 | 1 |
| 1:A:109:ALA:O | 1:A:112:VAL:HG12 | 0.50 | 2.06 | 5 | 2 |
| 1:A:120:LEU:CB | 1:A:125:PHE:O | 0.50 | 2.60 | 3 | 1 |
| 1:A:11:VAL:O | 1:A:13:THR:N | 0.50 | 2.44 | 7 | 4 |
| 1:A:51:ASN:O | 1:A:52:ALA:C | 0.50 | 2.50 | 11 | 3 |
| 1:A:78:TYR:CE2 | 1:A:89:VAL:HG21 | 0.50 | 2.41 | 12 | 1 |
| 1:A:36:ALA:O | 1:A:63:ALA:CB | 0.50 | 2.60 | 2 | 2 |
| 1:A:24:LEU:CD2 | 1:A:94:SER:C | 0.50 | 2.80 | 8 | 1 |
| 1:A:9:ASN:O | 1:A:12:GLY:N | 0.50 | 2.44 | 12 | 1 |
| 1:A:27:ASN:OD1 | 1:A:27:ASN:N | 0.50 | 2.44 | 14 | 1 |
| 1:A:86:VAL:O | 1:A:86:VAL:CG1 | 0.50 | 2.58 | 1 | 1 |
| 1:A:76:SER:HB3 | 1:A:78:TYR:CE1 | 0.50 | 2.42 | 6 | 3 |
| 1:A:78:TYR:CE2 | 1:A:89:VAL:HG22 | 0.50 | 2.42 | 11 | 1 |
| 1:A:26:GLY:O | 1:A:27:ASN:CB | 0.50 | 2.59 | 1 | 2 |
| 1:A:94:SER:CB | 1:A:125:PHE:CD2 | 0.50 | 2.95 | 6 | 1 |
| 1:A:68:VAL:HG22 | 1:A:69:THR:H | 0.50 | 1.66 | 10 | 4 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:CD1 | 0.50 | 2.90 | 18 | 2 |
| 1:A:87:ILE:O | 1:A:98:GLY:N | 0.50 | 2.45 | 14 | 1 |
| 1:A:80:LYS:O | 1:A:81:LYS:CB | 0.49 | 2.57 | 4 | 1 |
| 1:A:24:LEU:HB3 | 1:A:95:ILE:CG1 | 0.49 | 2.38 | 4 | 2 |
| 1:A:35:PHE:C | 1:A:35:PHE:CD1 | 0.49 | 2.85 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:60:PHE:CE1 | 1:A:69:THR:OG1 | 0.49 | 2.61 | 6 | 1 |
| 1:A:97:VAL:CG1 | 1:A:97:VAL:O | 0.49 | 2.56 | 10 | 2 |
| 1:A:20:ALA:HB2 | 1:A:35:PHE:CD2 | 0.49 | 2.41 | 13 | 1 |
| 1:A:2:TRP:HH2 | 1:A:96:LEU:HD22 | 0.49 | 1.66 | 14 | 1 |
| 1:A:101:ASN:C | 1:A:102:GLU:CG | 0.49 | 2.79 | 10 | 1 |
| 1:A:67:TYR:CE1 | 1:A:81:LYS:HG3 | 0.49 | 2.41 | 12 | 1 |
| 1:A:102:GLU:O | 1:A:104:ILE:N | 0.49 | 2.45 | 3 | 1 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:HB2 | 0.49 | 1.84 | 5 | 3 |
| 1:A:23:GLY:HA3 | 1:A:95:ILE:CD1 | 0.49 | 2.37 | 1 | 1 |
| 1:A:52:ALA:CB | 1:A:72:ALA:O | 0.49 | 2.61 | 6 | 1 |
| 1:A:109:ALA:O | 1:A:113:VAL:CG2 | 0.49 | 2.61 | 11 | 2 |
| 1:A:17:THR:O | 1:A:18:GLN:HG2 | 0.49 | 2.07 | 7 | 6 |
| 1:A:20:ALA:CB | 1:A:31:THR:OG1 | 0.49 | 2.61 | 5 | 1 |
| 1:A:65:VAL:HG11 | 1:A:67:TYR:CE2 | 0.49 | 2.42 | 9 | 1 |
| 1:A:92:SER:O | 1:A:93:LYS:CB | 0.49 | 2.60 | 18 | 2 |
| 1:A:63:ALA:O | 1:A:64:GLY:O | 0.49 | 2.31 | 10 | 1 |
| 1:A:23:GLY:HA2 | 1:A:29:TRP:CZ3 | 0.49 | 2.42 | 11 | 1 |
| 1:A:49:PHE:CE2 | 1:A:90:LYS:HG3 | 0.49 | 2.43 | 7 | 1 |
| 1:A:93:LYS:HB2 | 1:A:125:PHE:CD1 | 0.49 | 2.43 | 9 | 1 |
| 1:A:117:ALA:O | 1:A:119:TYR:N | 0.49 | 2.45 | 1 | 1 |
| 1:A:65:VAL:HG12 | 1:A:66:HIS:CD2 | 0.49 | 2.43 | 6 | 1 |
| 1:A:91:THR:CG2 | 1:A:121:ILE:HG12 | 0.49 | 2.37 | 13 | 1 |
| 1:A:119:TYR:CZ | 1:A:120:LEU:HG | 0.49 | 2.42 | 16 | 1 |
| 1:A:62:LEU:HB2 | 1:A:67:TYR:CE2 | 0.49 | 2.43 | 16 | 1 |
| 1:A:2:TRP:O | 1:A:6:VAL:N | 0.49 | 2.46 | 2 | 2 |
| 1:A:5:TYR:HD2 | 1:A:10:LEU:HD12 | 0.49 | 1.66 | 9 | 1 |
| 1:A:60:PHE:N | 1:A:60:PHE:CD1 | 0.49 | 2.81 | 13 | 1 |
| 1:A:115:LYS:O | 1:A:119:TYR:CE1 | 0.49 | 2.66 | 2 | 1 |
| 1:A:85:GLY:HA3 | 1:A:100:TYR:CE2 | 0.49 | 2.43 | 2 | 1 |
| 1:A:50:ASN:OD1 | 1:A:51:ASN:N | 0.49 | 2.46 | 3 | 1 |
| 1:A:26:GLY:O | 1:A:27:ASN:C | 0.49 | 2.50 | 18 | 2 |
| 1:A:2:TRP:O | 1:A:2:TRP:CD1 | 0.49 | 2.65 | 14 | 1 |
| 1:A:57:ALA:O | 1:A:59:GLY:N | 0.49 | 2.45 | 15 | 1 |
| 1:A:5:TYR:O | 1:A:10:LEU:HB2 | 0.48 | 2.08 | 1 | 3 |
| 1:A:104:ILE:O | 1:A:105:GLN:O | 0.48 | 2.30 | 7 | 1 |
| 1:A:26:GLY:O | 1:A:27:ASN:ND2 | 0.48 | 2.45 | 12 | 1 |
| 1:A:10:LEU:HD21 | 1:A:116:LEU:CD2 | 0.48 | 2.38 | 15 | 1 |
| 1:A:6:VAL:CG2 | 1:A:21:ILE:HG13 | 0.48 | 2.37 | 17 | 1 |
| 1:A:35:PHE:CE2 | 1:A:37:VAL:CG2 | 0.48 | 2.96 | 1 | 1 |
| 1:A:2:TRP:CH2 | 1:A:96:LEU:HG | 0.48 | 2.43 | 11 | 3 |
| 1:A:20:ALA:HB2 | 1:A:31:THR:OG1 | 0.48 | 2.07 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:38:THR:OG1 | 1:A:39:PRO:HD3 | 0.48 | 2.08 | 13 | 2 |
| 1:A:46:ALA:HA | 1:A:49:PHE:CD2 | 0.48 | 2.43 | 7 | 2 |
| 1:A:34:GLY:O | 1:A:35:PHE:CB | 0.48 | 2.61 | 16 | 1 |
| 1:A:24:LEU:HD21 | 1:A:93:LYS:C | 0.48 | 2.27 | 17 | 2 |
| 1:A:101:ASN:O | 1:A:103:LYS:N | 0.48 | 2.47 | 19 | 2 |
| 1:A:2:TRP:CE2 | 1:A:91:THR:HG21 | 0.48 | 2.44 | 4 | 1 |
| 1:A:16:VAL:HG23 | 1:A:18:GLN:O | 0.48 | 2.08 | 9 | 4 |
| 1:A:17:THR:O | 1:A:18:GLN:OE1 | 0.48 | 2.32 | 11 | 3 |
| 1:A:5:TYR:CB | 1:A:10:LEU:HD23 | 0.48 | 2.37 | 14 | 1 |
| 1:A:85:GLY:HA3 | 1:A:100:TYR:CZ | 0.48 | 2.43 | 18 | 5 |
| 1:A:89:VAL:CG1 | 1:A:96:LEU:HD12 | 0.48 | 2.38 | 7 | 1 |
| 1:A:76:SER:HB3 | 1:A:78:TYR:CE2 | 0.48 | 2.43 | 17 | 1 |
| 1:A:11:VAL:C | 1:A:13:THR:N | 0.48 | 2.65 | 14 | 4 |
| 1:A:4:THR:HG23 | 1:A:5:TYR:N | 0.48 | 2.23 | 7 | 2 |
| 1:A:92:SER:CB | 1:A:125:PHE:CD2 | 0.48 | 2.96 | 10 | 1 |
| 1:A:27:ASN:O | 1:A:28:THR:O | 0.48 | 2.31 | 13 | 1 |
| 1:A:22:LEU:O | 1:A:23:GLY:O | 0.48 | 2.32 | 13 | 5 |
| 1:A:81:LYS:HE3 | 1:A:82:GLY:N | 0.48 | 2.23 | 7 | 1 |
| 1:A:86:VAL:HG23 | 1:A:97:VAL:CG1 | 0.48 | 2.38 | 17 | 2 |
| 1:A:29:TRP:N | 1:A:29:TRP:CD1 | 0.48 | 2.81 | 8 | 2 |
| 1:A:29:TRP:CH2 | 1:A:93:LYS:O | 0.48 | 2.67 | 15 | 1 |
| 1:A:19:ALA:O | 1:A:32:SER:N | 0.48 | 2.47 | 18 | 1 |
| 1:A:85:GLY:C | 1:A:100:TYR:CE1 | 0.48 | 2.87 | 1 | 1 |
| 1:A:32:SER:O | 1:A:33:ALA:C | 0.48 | 2.52 | 3 | 2 |
| 1:A:49:PHE:CE1 | 1:A:75:ARG:O | 0.48 | 2.67 | 5 | 1 |
| 1:A:22:LEU:CD2 | 1:A:22:LEU:N | 0.48 | 2.67 | 12 | 1 |
| 1:A:72:ALA:O | 1:A:73:ASP:C | 0.48 | 2.52 | 12 | 1 |
| 1:A:112:VAL:CG2 | 1:A:116:LEU:HD12 | 0.48 | 2.35 | 13 | 1 |
| 1:A:5:TYR:CB | 1:A:10:LEU:HB2 | 0.48 | 2.39 | 14 | 1 |
| 1:A:55:ILE:HD13 | 1:A:72:ALA:CB | 0.48 | 2.38 | 5 | 1 |
| 1:A:2:TRP:CE2 | 1:A:96:LEU:HG | 0.48 | 2.44 | 19 | 2 |
| 1:A:2:TRP:O | 1:A:3:GLN:C | 0.48 | 2.52 | 2 | 2 |
| 1:A:102:GLU:O | 1:A:103:LYS:HG2 | 0.48 | 2.09 | 13 | 3 |
| 1:A:46:ALA:HA | 1:A:49:PHE:CE2 | 0.48 | 2.43 | 7 | 1 |
| 1:A:3:GLN:O | 1:A:5:TYR:N | 0.48 | 2.47 | 8 | 1 |
| 1:A:88:THR:HA | 1:A:96:LEU:O | 0.48 | 2.09 | 15 | 8 |
| 1:A:75:ARG:NH1 | 1:A:75:ARG:HG2 | 0.48 | 2.23 | 16 | 2 |
| 1:A:71:ARG:NH1 | 1:A:71:ARG:HG2 | 0.47 | 2.23 | 2 | 1 |
| 1:A:4:THR:O | 1:A:7:ASP:OD1 | 0.47 | 2.32 | 3 | 2 |
| 1:A:81:LYS:O | 1:A:84:ALA:O | 0.47 | 2.32 | 4 | 1 |
| 1:A:16:VAL:HG13 | 1:A:100:TYR:CB | 0.47 | 2.35 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:ILE:HG22 | 1:A:21:ILE:O | 0.47 | 2.09 | 7 | 1 |
| 1:A:75:ARG:HG2 | 1:A:75:ARG:NH1 | 0.47 | 2.22 | 14 | 2 |
| 1:A:85:GLY:HA3 | 1:A:100:TYR:CE1 | 0.47 | 2.44 | 17 | 1 |
| 1:A:78:TYR:HD1 | 1:A:87:ILE:HG23 | 0.47 | 1.60 | 18 | 3 |
| 1:A:29:TRP:CD1 | 1:A:29:TRP:N | 0.47 | 2.82 | 3 | 2 |
| 1:A:76:SER:CB | 1:A:89:VAL:HG22 | 0.47 | 2.39 | 4 | 1 |
| 1:A:93:LYS:HB2 | 1:A:125:PHE:CG | 0.47 | 2.44 | 7 | 1 |
| 1:A:124:GLY:C | 1:A:125:PHE:CG | 0.47 | 2.88 | 15 | 1 |
| 1:A:81:LYS:N | 1:A:84:ALA:O | 0.47 | 2.47 | 18 | 1 |
| 1:A:104:ILE:CG2 | 1:A:104:ILE:O | 0.47 | 2.57 | 19 | 1 |
| 1:A:13:THR:O | 1:A:16:VAL:O | 0.47 | 2.33 | 4 | 2 |
| 1:A:33:ALA:O | 1:A:34:GLY:O | 0.47 | 2.32 | 11 | 3 |
| 1:A:37:VAL:O | 1:A:38:THR:O | 0.47 | 2.33 | 16 | 1 |
| 1:A:72:ALA:HA | 1:A:77:ILE:HG23 | 0.47 | 1.85 | 2 | 1 |
| 1:A:13:THR:O | 1:A:14:GLY:C | 0.47 | 2.53 | 4 | 2 |
| 1:A:20:ALA:O | 1:A:22:LEU:HD22 | 0.47 | 2.09 | 8 | 1 |
| 1:A:66:HIS:N | 1:A:66:HIS:CD2 | 0.47 | 2.83 | 8 | 2 |
| 1:A:15:ALA:O | 1:A:104:ILE:HD13 | 0.47 | 2.10 | 15 | 2 |
| 1:A:78:TYR:CZ | 1:A:114:GLU:CD | 0.47 | 2.88 | 16 | 1 |
| 1:A:38:THR:HG22 | 1:A:39:PRO:HD3 | 0.47 | 1.87 | 19 | 1 |
| 1:A:33:ALA:HB3 | 1:A:35:PHE:CE1 | 0.47 | 2.45 | 1 | 1 |
| 1:A:89:VAL:CG2 | 1:A:96:LEU:HD11 | 0.47 | 2.40 | 1 | 1 |
| 1:A:55:ILE:HG22 | 1:A:60:PHE:CD1 | 0.47 | 2.45 | 3 | 1 |
| 1:A:5:TYR:HE2 | 1:A:116:LEU:HD11 | 0.47 | 1.69 | 12 | 2 |
| 1:A:52:ALA:O | 1:A:56:ARG:HB3 | 0.47 | 2.10 | 1 | 1 |
| 1:A:120:LEU:CD1 | 1:A:120:LEU:C | 0.47 | 2.83 | 2 | 2 |
| 1:A:86:VAL:HG22 | 1:A:88:THR:HG23 | 0.47 | 1.86 | 18 | 3 |
| 1:A:124:GLY:O | 1:A:125:PHE:C | 0.47 | 2.53 | 10 | 6 |
| 1:A:78:TYR:N | 1:A:78:TYR:CD1 | 0.47 | 2.81 | 6 | 3 |
| 1:A:120:LEU:HB3 | 1:A:125:PHE:CZ | 0.47 | 2.44 | 5 | 1 |
| 1:A:23:GLY:CA | 1:A:29:TRP:CE3 | 0.47 | 2.98 | 6 | 1 |
| 1:A:60:PHE:CD1 | 1:A:69:THR:OG1 | 0.47 | 2.67 | 6 | 1 |
| 1:A:3:GLN:O | 1:A:4:THR:C | 0.47 | 2.53 | 8 | 2 |
| 1:A:71:ARG:O | 1:A:76:SER:O | 0.47 | 2.33 | 9 | 1 |
| 1:A:60:PHE:O | 1:A:66:HIS:CB | 0.47 | 2.63 | 10 | 1 |
| 1:A:100:TYR:HB2 | 1:A:104:ILE:CG1 | 0.47 | 2.38 | 11 | 1 |
| 1:A:43:GLN:O | 1:A:47:SER:OG | 0.47 | 2.33 | 11 | 1 |
| 1:A:87:ILE:N | 1:A:98:GLY:O | 0.47 | 2.48 | 14 | 1 |
| 1:A:88:THR:HG22 | 1:A:97:VAL:HA | 0.47 | 1.86 | 14 | 1 |
| 1:A:11:VAL:CG2 | 1:A:32:SER:CB | 0.47 | 2.83 | 16 | 1 |
| 1:A:70:LEU:HD13 | 1:A:80:LYS:CD | 0.47 | 2.40 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:87:ILE:HB | 1:A:98:GLY:O | 0.47 | 2.10 | 14 | 1 |
| 1:A:15:ALA:HB2 | 1:A:112:VAL:CG1 | 0.47 | 2.40 | 16 | 1 |
| 1:A:21:ILE:CG1 | 1:A:30:ALA:HB3 | 0.47 | 2.40 | 18 | 1 |
| 1:A:42:GLY:O | 1:A:46:ALA:HB2 | 0.47 | 2.10 | 2 | 2 |
| 1:A:7:ASP:CG | 1:A:8:THR:N | 0.47 | 2.68 | 3 | 1 |
| 1:A:7:ASP:O | 1:A:8:THR:CB | 0.47 | 2.62 | 14 | 2 |
| 1:A:22:LEU:N | 1:A:22:LEU:CD1 | 0.47 | 2.77 | 19 | 2 |
| 1:A:91:THR:O | 1:A:92:SER:OG | 0.47 | 2.31 | 16 | 1 |
| 1:A:70:LEU:O | 1:A:71:ARG:CG | 0.47 | 2.63 | 19 | 1 |
| 1:A:24:LEU:HB3 | 1:A:95:ILE:CD1 | 0.47 | 2.40 | 4 | 2 |
| 1:A:115:LYS:HG3 | 1:A:116:LEU:N | 0.47 | 2.25 | 3 | 3 |
| 1:A:68:VAL:CG2 | 1:A:69:THR:N | 0.47 | 2.78 | 9 | 1 |
| 1:A:120:LEU:O | 1:A:120:LEU:HD12 | 0.47 | 2.09 | 11 | 1 |
| 1:A:76:SER:CB | 1:A:78:TYR:OH | 0.46 | 2.63 | 7 | 5 |
| 1:A:51:ASN:O | 1:A:55:ILE:CD1 | 0.46 | 2.59 | 4 | 1 |
| 1:A:110:ALA:O | 1:A:114:GLU:OE1 | 0.46 | 2.33 | 10 | 1 |
| 1:A:10:LEU:HD21 | 1:A:116:LEU:HD22 | 0.46 | 1.86 | 15 | 1 |
| 1:A:11:VAL:CG1 | 1:A:32:SER:CB | 0.46 | 2.90 | 2 | 1 |
| 1:A:11:VAL:O | 1:A:16:VAL:O | 0.46 | 2.33 | 3 | 3 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:CB | 0.46 | 2.39 | 5 | 2 |
| 1:A:85:GLY:O | 1:A:100:TYR:CZ | 0.46 | 2.67 | 5 | 1 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:CG | 0.46 | 2.41 | 17 | 1 |
| 1:A:74:ASP:O | 1:A:75:ARG:CD | 0.46 | 2.63 | 1 | 1 |
| 1:A:75:ARG:NH1 | 1:A:75:ARG:CG | 0.46 | 2.78 | 15 | 8 |
| 1:A:4:THR:O | 1:A:8:THR:OG1 | 0.46 | 2.33 | 2 | 1 |
| 1:A:67:TYR:HE2 | 1:A:86:VAL:HG11 | 0.46 | 1.70 | 4 | 1 |
| 1:A:29:TRP:CZ3 | 1:A:93:LYS:O | 0.46 | 2.68 | 11 | 1 |
| 1:A:2:TRP:CZ2 | 1:A:96:LEU:HG | 0.46 | 2.45 | 11 | 1 |
| 1:A:120:LEU:O | 1:A:125:PHE:O | 0.46 | 2.33 | 12 | 1 |
| 1:A:83:SER:O | 1:A:102:GLU:OE2 | 0.46 | 2.34 | 3 | 1 |
| 1:A:18:GLN:CG | 1:A:33:ALA:HA | 0.46 | 2.40 | 8 | 1 |
| 1:A:2:TRP:HB2 | 1:A:21:ILE:HD11 | 0.46 | 1.86 | 9 | 1 |
| 1:A:17:THR:HG22 | 1:A:100:TYR:HA | 0.46 | 1.87 | 16 | 1 |
| 1:A:53:ASP:CB | 1:A:54:PRO:CD | 0.46 | 2.94 | 1 | 7 |
| 1:A:5:TYR:HB3 | 1:A:10:LEU:CD1 | 0.46 | 2.41 | 7 | 2 |
| 1:A:22:LEU:CD2 | 1:A:97:VAL:CG2 | 0.46 | 2.89 | 8 | 1 |
| 1:A:65:VAL:CG1 | 1:A:67:TYR:CE2 | 0.46 | 2.98 | 9 | 1 |
| 1:A:117:ALA:O | 1:A:118:ASP:C | 0.46 | 2.54 | 1 | 1 |
| 1:A:76:SER:HB2 | 1:A:78:TYR:OH | 0.46 | 2.11 | 7 | 2 |
| 1:A:56:ARG:O | 1:A:56:ARG:CG | 0.46 | 2.63 | 8 | 1 |
| 1:A:22:LEU:HG | 1:A:97:VAL:CG2 | 0.46 | 2.40 | 4 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:77:ILE:O | 1:A:88:THR:OG1 | 0.46 | 2.32 | 3 | 2 |
| 1:A:56:ARG:CG | 1:A:56:ARG:NH1 | 0.46 | 2.79 | 4 | 1 |
| 1:A:24:LEU:CD2 | 1:A:94:SER:HA | 0.46 | 2.40 | 18 | 1 |
| 1:A:17:THR:O | 1:A:18:GLN:HG3 | 0.46 | 2.11 | 8 | 6 |
| 1:A:2:TRP:C | 1:A:21:ILE:CD1 | 0.46 | 2.84 | 5 | 2 |
| 1:A:124:GLY:O | 1:A:125:PHE:OXT | 0.46 | 2.33 | 9 | 2 |
| 1:A:55:ILE:HD11 | 1:A:72:ALA:HB2 | 0.46 | 1.81 | 9 | 1 |
| 1:A:67:TYR:N | 1:A:67:TYR:CD1 | 0.46 | 2.83 | 12 | 1 |
| 1:A:34:GLY:O | 1:A:35:PHE:O | 0.46 | 2.34 | 12 | 2 |
| 1:A:54:PRO:O | 1:A:55:ILE:C | 0.46 | 2.55 | 12 | 2 |
| 1:A:75:ARG:CG | 1:A:75:ARG:NH1 | 0.46 | 2.79 | 7 | 1 |
| 1:A:120:LEU:O | 1:A:124:GLY:N | 0.46 | 2.49 | 13 | 1 |
| 1:A:65:VAL:HG13 | 1:A:67:TYR:CE1 | 0.46 | 2.43 | 13 | 1 |
| 1:A:87:ILE:CB | 1:A:98:GLY:O | 0.46 | 2.64 | 14 | 1 |
| 1:A:5:TYR:CE1 | 1:A:6:VAL:HG23 | 0.46 | 2.46 | 4 | 1 |
| 1:A:72:ALA:O | 1:A:73:ASP:OD1 | 0.46 | 2.34 | 9 | 2 |
| 1:A:33:ALA:CB | 1:A:35:PHE:CE1 | 0.46 | 2.99 | 10 | 1 |
| 1:A:25:ASP:O | 1:A:27:ASN:OD1 | 0.46 | 2.34 | 11 | 1 |
| 1:A:24:LEU:HD13 | 1:A:93:LYS:C | 0.45 | 2.29 | 1 | 1 |
| 1:A:8:THR:OG1 | 1:A:9:ASN:N | 0.45 | 2.48 | 11 | 5 |
| 1:A:112:VAL:O | 1:A:116:LEU:HB2 | 0.45 | 2.12 | 10 | 1 |
| 1:A:24:LEU:CD1 | 1:A:94:SER:N | 0.45 | 2.79 | 10 | 1 |
| 1:A:45:LEU:HG | 1:A:49:PHE:CZ | 0.45 | 2.46 | 15 | 1 |
| 1:A:102:GLU:O | 1:A:103:LYS:C | 0.45 | 2.55 | 3 | 2 |
| 1:A:120:LEU:HB3 | 1:A:125:PHE:O | 0.45 | 2.11 | 3 | 1 |
| 1:A:120:LEU:O | 1:A:121:ILE:C | 0.45 | 2.54 | 5 | 2 |
| 1:A:24:LEU:HD13 | 1:A:24:LEU:H | 0.45 | 1.66 | 5 | 1 |
| 1:A:124:GLY:C | 1:A:125:PHE:CD2 | 0.45 | 2.89 | 9 | 1 |
| 1:A:2:TRP:NE1 | 1:A:5:TYR:CD1 | 0.45 | 2.84 | 11 | 1 |
| 1:A:39:PRO:O | 1:A:40:ALA:C | 0.45 | 2.54 | 13 | 1 |
| 1:A:86:VAL:CG2 | 1:A:97:VAL:CG1 | 0.45 | 2.93 | 17 | 1 |
| 1:A:117:ALA:O | 1:A:121:ILE:CG1 | 0.45 | 2.64 | 8 | 2 |
| 1:A:87:ILE:HD11 | 1:A:100:TYR:OH | 0.45 | 2.11 | 10 | 1 |
| 1:A:114:GLU:OE1 | 1:A:114:GLU:N | 0.45 | 2.49 | 10 | 1 |
| 1:A:78:TYR:CZ | 1:A:87:ILE:CD1 | 0.45 | 3.00 | 15 | 1 |
| 1:A:75:ARG:HG2 | 1:A:76:SER:N | 0.45 | 2.26 | 19 | 1 |
| 1:A:28:THR:HG22 | 1:A:29:TRP:H | 0.45 | 1.72 | 1 | 1 |
| 1:A:21:ILE:O | 1:A:22:LEU:O | 0.45 | 2.34 | 3 | 1 |
| 1:A:16:VAL:HG13 | 1:A:109:ALA:HB1 | 0.45 | 1.87 | 4 | 1 |
| 1:A:120:LEU:HD22 | 1:A:125:PHE:CE1 | 0.45 | 2.46 | 5 | 1 |
| 1:A:52:ALA:HA | 1:A:55:ILE:CG1 | 0.45 | 2.42 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:71:ARG:CG | 1:A:71:ARG:NH1 | 0.45 | 2.79 | 15 | 3 |
| 1:A:28:THR:O | 1:A:29:TRP:CD1 | 0.45 | 2.69 | 1 | 1 |
| 1:A:67:TYR:OH | 1:A:86:VAL:CG1 | 0.45 | 2.61 | 4 | 1 |
| 1:A:63:ALA:O | 1:A:64:GLY:C | 0.45 | 2.55 | 10 | 1 |
| 1:A:44:THR:O | 1:A:48:ALA:CB | 0.45 | 2.65 | 11 | 1 |
| 1:A:75:ARG:NH1 | 1:A:75:ARG:HG3 | 0.45 | 2.24 | 11 | 1 |
| 1:A:56:ARG:NH1 | 1:A:56:ARG:HG2 | 0.45 | 2.26 | 17 | 2 |
| 1:A:35:PHE:CE2 | 1:A:99:VAL:HG11 | 0.45 | 2.47 | 15 | 1 |
| 1:A:78:TYR:CE1 | 1:A:114:GLU:OE1 | 0.45 | 2.69 | 16 | 1 |
| 1:A:69:THR:O | 1:A:70:LEU:HD22 | 0.45 | 2.12 | 9 | 2 |
| 1:A:5:TYR:O | 1:A:10:LEU:HB3 | 0.45 | 2.11 | 11 | 1 |
| 1:A:10:LEU:O | 1:A:16:VAL:HG23 | 0.45 | 2.12 | 12 | 1 |
| 1:A:12:GLY:O | 1:A:13:THR:HB | 0.45 | 2.12 | 8 | 4 |
| 1:A:38:THR:CB | 1:A:39:PRO:CD | 0.45 | 2.95 | 13 | 2 |
| 1:A:20:ALA:O | 1:A:22:LEU:CD2 | 0.45 | 2.65 | 8 | 1 |
| 1:A:60:PHE:O | 1:A:66:HIS:HB2 | 0.45 | 2.12 | 10 | 1 |
| 1:A:44:THR:O | 1:A:48:ALA:N | 0.45 | 2.49 | 11 | 1 |
| 1:A:37:VAL:O | 1:A:38:THR:HB | 0.45 | 2.11 | 12 | 1 |
| 1:A:29:TRP:CZ3 | 1:A:94:SER:OG | 0.45 | 2.70 | 15 | 1 |
| 1:A:60:PHE:CD1 | 1:A:60:PHE:C | 0.45 | 2.90 | 17 | 1 |
| 1:A:65:VAL:HG12 | 1:A:66:HIS:H | 0.45 | 1.72 | 5 | 1 |
| 1:A:97:VAL:O | 1:A:98:GLY:C | 0.45 | 2.53 | 14 | 3 |
| 1:A:96:LEU:C | 1:A:96:LEU:CD2 | 0.45 | 2.85 | 19 | 1 |
| 1:A:18:GLN:HG2 | 1:A:33:ALA:CA | 0.45 | 2.42 | 8 | 1 |
| 1:A:11:VAL:CG1 | 1:A:32:SER:HB3 | 0.45 | 2.42 | 15 | 2 |
| 1:A:77:ILE:CG2 | 1:A:77:ILE:O | 0.45 | 2.63 | 18 | 1 |
| 1:A:66:HIS:ND1 | 1:A:66:HIS:N | 0.45 | 2.65 | 1 | 1 |
| 1:A:18:GLN:HB3 | 1:A:33:ALA:CB | 0.45 | 2.42 | 8 | 1 |
| 1:A:113:VAL:O | 1:A:117:ALA:CB | 0.45 | 2.65 | 10 | 2 |
| 1:A:48:ALA:HB1 | 1:A:55:ILE:HD11 | 0.45 | 1.88 | 14 | 1 |
| 1:A:76:SER:O | 1:A:77:ILE:HG13 | 0.45 | 2.12 | 18 | 1 |
| 1:A:10:LEU:CD1 | 1:A:116:LEU:HG | 0.44 | 2.41 | 2 | 1 |
| 1:A:2:TRP:CB | 1:A:5:TYR:CD2 | 0.44 | 3.00 | 2 | 2 |
| 1:A:91:THR:O | 1:A:125:PHE:HB3 | 0.44 | 2.12 | 11 | 2 |
| 1:A:2:TRP:CD1 | 1:A:2:TRP:N | 0.44 | 2.84 | 7 | 1 |
| 1:A:35:PHE:CD1 | 1:A:99:VAL:HG11 | 0.44 | 2.47 | 11 | 1 |
| 1:A:101:ASN:O | 1:A:102:GLU:HG3 | 0.44 | 2.12 | 13 | 1 |
| 1:A:91:THR:CG2 | 1:A:121:ILE:CG1 | 0.44 | 2.94 | 13 | 1 |
| 1:A:37:VAL:C | 1:A:38:THR:OG1 | 0.44 | 2.55 | 16 | 1 |
| 1:A:18:GLN:HB3 | 1:A:33:ALA:HB2 | 0.44 | 1.89 | 17 | 1 |
| 1:A:6:VAL:O | 1:A:11:VAL:HB | 0.44 | 2.12 | 5 | 12 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:29:TRP:CE3 | 1:A:94:SER:OG | 0.44 | 2.58 | 3 | 1 |
| 1:A:94:SER:OG | 1:A:125:PHE:O | 0.44 | 2.35 | 7 | 1 |
| 1:A:100:TYR:C | 1:A:100:TYR:CD1 | 0.44 | 2.90 | 19 | 1 |
| 1:A:81:LYS:HB2 | 1:A:84:ALA:HB3 | 0.44 | 1.88 | 2 | 1 |
| 1:A:96:LEU:HD22 | 1:A:96:LEU:N | 0.44 | 2.25 | 2 | 1 |
| 1:A:5:TYR:CE1 | 1:A:21:ILE:HD11 | 0.44 | 2.47 | 4 | 1 |
| 1:A:24:LEU:H | 1:A:24:LEU:CD2 | 0.44 | 2.22 | 5 | 1 |
| 1:A:22:LEU:N | 1:A:95:ILE:O | 0.44 | 2.51 | 8 | 1 |
| 1:A:5:TYR:HE2 | 1:A:116:LEU:HD22 | 0.44 | 1.69 | 11 | 1 |
| 1:A:38:THR:CG2 | 1:A:39:PRO:CD | 0.44 | 2.95 | 13 | 1 |
| 1:A:37:VAL:HG13 | 1:A:62:LEU:CD2 | 0.44 | 2.42 | 14 | 2 |
| 1:A:71:ARG:NH2 | 1:A:74:ASP:OD2 | 0.44 | 2.51 | 3 | 1 |
| 1:A:76:SER:HB3 | 1:A:89:VAL:CG2 | 0.44 | 2.42 | 4 | 1 |
| 1:A:9:ASN:O | 1:A:14:GLY:CA | 0.44 | 2.66 | 5 | 1 |
| 1:A:100:TYR:HB2 | 1:A:104:ILE:HG13 | 0.44 | 1.90 | 6 | 1 |
| 1:A:55:ILE:HD11 | 1:A:69:THR:HG21 | 0.44 | 1.88 | 6 | 1 |
| 1:A:81:LYS:CE | 1:A:82:GLY:N | 0.44 | 2.80 | 7 | 1 |
| 1:A:2:TRP:CG | 1:A:21:ILE:CD1 | 0.44 | 3.00 | 12 | 1 |
| 1:A:2:TRP:CH2 | 1:A:116:LEU:HD23 | 0.44 | 2.47 | 19 | 1 |
| 1:A:38:THR:O | 1:A:41:GLN:HG3 | 0.44 | 2.12 | 1 | 1 |
| 1:A:17:THR:C | 1:A:18:GLN:HG3 | 0.44 | 2.33 | 7 | 4 |
| 1:A:5:TYR:CE2 | 1:A:10:LEU:HD22 | 0.44 | 2.47 | 4 | 1 |
| 1:A:65:VAL:CG1 | 1:A:66:HIS:N | 0.44 | 2.81 | 4 | 1 |
| 1:A:17:THR:O | 1:A:18:GLN:CD | 0.44 | 2.56 | 8 | 5 |
| 1:A:54:PRO:O | 1:A:56:ARG:N | 0.44 | 2.50 | 12 | 1 |
| 1:A:93:LYS:HG3 | 1:A:125:PHE:CE2 | 0.44 | 2.48 | 15 | 1 |
| 1:A:2:TRP:CE3 | 1:A:96:LEU:CD1 | 0.44 | 3.00 | 15 | 1 |
| 1:A:91:THR:OG1 | 1:A:94:SER:O | 0.44 | 2.33 | 19 | 1 |
| 1:A:38:THR:CG2 | 1:A:39:PRO:HD2 | 0.44 | 2.42 | 3 | 2 |
| 1:A:4:THR:O | 1:A:5:TYR:C | 0.44 | 2.55 | 7 | 2 |
| 1:A:18:GLN:CG | 1:A:33:ALA:CB | 0.44 | 2.95 | 16 | 1 |
| 1:A:86:VAL:HA | 1:A:98:GLY:O | 0.44 | 2.13 | 18 | 1 |
| 1:A:103:LYS:HB3 | 1:A:104:ILE:HD12 | 0.44 | 1.89 | 2 | 1 |
| 1:A:120:LEU:HD13 | 1:A:125:PHE:CE2 | 0.44 | 2.48 | 2 | 1 |
| 1:A:91:THR:HB | 1:A:120:LEU:HD22 | 0.44 | 1.88 | 3 | 1 |
| 1:A:18:GLN:C | 1:A:99:VAL:O | 0.44 | 2.56 | 5 | 1 |
| 1:A:68:VAL:HG23 | 1:A:81:LYS:HG3 | 0.44 | 1.90 | 7 | 1 |
| 1:A:56:ARG:NH1 | 1:A:56:ARG:CG | 0.44 | 2.79 | 13 | 4 |
| 1:A:16:VAL:CB | 1:A:100:TYR:HB3 | 0.44 | 2.43 | 16 | 1 |
| 1:A:18:GLN:HG2 | 1:A:33:ALA:CB | 0.44 | 2.42 | 16 | 1 |
| 1:A:37:VAL:O | 1:A:38:THR:C | 0.44 | 2.56 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:5:TYR:CZ | 1:A:10:LEU:CD1 | 0.44 | 3.00 | 11 | 1 |
| 1:A:118:ASP:CA | 1:A:121:ILE:HG12 | 0.44 | 2.42 | 1 | 1 |
| 1:A:88:THR:HG22 | 1:A:97:VAL:HG22 | 0.44 | 1.90 | 1 | 1 |
| 1:A:52:ALA:HA | 1:A:55:ILE:CD1 | 0.44 | 2.43 | 5 | 1 |
| 1:A:78:TYR:CE2 | 1:A:87:ILE:HG23 | 0.44 | 2.47 | 19 | 1 |
| 1:A:2:TRP:O | 1:A:6:VAL:HB | 0.43 | 2.13 | 19 | 8 |
| 1:A:86:VAL:HG22 | 1:A:87:ILE:N | 0.43 | 2.28 | 14 | 2 |
| 1:A:101:ASN:N | 1:A:101:ASN:OD1 | 0.43 | 2.51 | 6 | 2 |
| 1:A:3:GLN:O | 1:A:6:VAL:N | 0.43 | 2.51 | 8 | 1 |
| 1:A:112:VAL:HG22 | 1:A:116:LEU:CD1 | 0.43 | 2.36 | 13 | 1 |
| 1:A:2:TRP:HH2 | 1:A:117:ALA:HB2 | 0.43 | 1.72 | 15 | 1 |
| 1:A:30:ALA:O | 1:A:31:THR:CG2 | 0.43 | 2.66 | 16 | 1 |
| 1:A:100:TYR:HB3 | 1:A:104:ILE:HG13 | 0.43 | 1.89 | 4 | 1 |
| 1:A:82:GLY:O | 1:A:83:SER:OG | 0.43 | 2.34 | 7 | 1 |
| 1:A:77:ILE:HB | 1:A:88:THR:O | 0.43 | 2.12 | 16 | 1 |
| 1:A:100:TYR:CZ | 1:A:104:ILE:O | 0.43 | 2.71 | 19 | 1 |
| 1:A:121:ILE:O | 1:A:122:GLY:C | 0.43 | 2.55 | 1 | 2 |
| 1:A:91:THR:HG21 | 1:A:96:LEU:CD2 | 0.43 | 2.40 | 3 | 1 |
| 1:A:115:LYS:O | 1:A:116:LEU:C | 0.43 | 2.57 | 5 | 2 |
| 1:A:18:GLN:CB | 1:A:99:VAL:O | 0.43 | 2.67 | 5 | 1 |
| 1:A:6:VAL:O | 1:A:7:ASP:C | 0.43 | 2.56 | 5 | 1 |
| 1:A:7:ASP:C | 1:A:7:ASP:OD1 | 0.43 | 2.56 | 5 | 1 |
| 1:A:28:THR:O | 1:A:28:THR:HG22 | 0.43 | 2.12 | 8 | 1 |
| 1:A:85:GLY:CA | 1:A:100:TYR:CZ | 0.43 | 3.01 | 8 | 1 |
| 1:A:79:GLY:O | 1:A:86:VAL:O | 0.43 | 2.37 | 14 | 1 |
| 1:A:101:ASN:O | 1:A:102:GLU:C | 0.43 | 2.56 | 19 | 2 |
| 1:A:58:SER:O | 1:A:59:GLY:C | 0.43 | 2.56 | 11 | 2 |
| 1:A:5:TYR:CD1 | 1:A:10:LEU:CB | 0.43 | 3.02 | 11 | 1 |
| 1:A:66:HIS:NE2 | 1:A:81:LYS:HE2 | 0.43 | 2.28 | 17 | 1 |
| 1:A:6:VAL:HG21 | 1:A:30:ALA:HB1 | 0.43 | 1.90 | 18 | 1 |
| 1:A:31:THR:O | 1:A:32:SER:OG | 0.43 | 2.32 | 3 | 1 |
| 1:A:2:TRP:CE2 | 1:A:10:LEU:HD13 | 0.43 | 2.48 | 9 | 1 |
| 1:A:21:ILE:N | 1:A:21:ILE:HD13 | 0.43 | 2.28 | 12 | 1 |
| 1:A:104:ILE:HG22 | 1:A:105:GLN:N | 0.43 | 2.29 | 15 | 1 |
| 1:A:78:TYR:CE2 | 1:A:87:ILE:HD13 | 0.43 | 2.49 | 15 | 1 |
| 1:A:92:SER:CB | 1:A:125:PHE:HB3 | 0.43 | 2.44 | 16 | 1 |
| 1:A:37:VAL:HB | 1:A:41:GLN:CG | 0.43 | 2.44 | 16 | 1 |
| 1:A:89:VAL:HG13 | 1:A:96:LEU:HB2 | 0.43 | 1.88 | 16 | 1 |
| 1:A:82:GLY:C | 1:A:83:SER:OG | 0.43 | 2.57 | 18 | 1 |
| 1:A:66:HIS:O | 1:A:67:TYR:CD1 | 0.43 | 2.71 | 3 | 2 |
| 1:A:2:TRP:CE3 | 1:A:2:TRP:CA | 0.43 | 3.02 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:62:LEU:CB | 1:A:65:VAL:O | 0.43 | 2.67 | 11 | 1 |
| 1:A:100:TYR:HB2 | 1:A:104:ILE:HG12 | 0.43 | 1.91 | 4 | 1 |
| 1:A:19:ALA:O | 1:A:20:ALA:HB2 | 0.43 | 2.14 | 7 | 1 |
| 1:A:6:VAL:HG12 | 1:A:7:ASP:N | 0.43 | 2.27 | 16 | 3 |
| 1:A:31:THR:C | 1:A:32:SER:OG | 0.43 | 2.56 | 12 | 1 |
| 1:A:51:ASN:O | 1:A:51:ASN:CG | 0.43 | 2.57 | 1 | 1 |
| 1:A:55:ILE:O | 1:A:56:ARG:C | 0.43 | 2.56 | 15 | 2 |
| 1:A:76:SER:CA | 1:A:89:VAL:HG22 | 0.43 | 2.43 | 4 | 1 |
| 1:A:92:SER:HB3 | 1:A:124:GLY:CA | 0.43 | 2.43 | 6 | 1 |
| 1:A:82:GLY:O | 1:A:83:SER:C | 0.43 | 2.57 | 9 | 2 |
| 1:A:24:LEU:HD12 | 1:A:93:LYS:C | 0.43 | 2.33 | 10 | 1 |
| 1:A:49:PHE:CE1 | 1:A:90:LYS:HE3 | 0.43 | 2.49 | 14 | 1 |
| 1:A:90:LYS:HB2 | 1:A:125:PHE:CE1 | 0.43 | 2.49 | 3 | 1 |
| 1:A:55:ILE:O | 1:A:69:THR:HB | 0.43 | 2.12 | 3 | 1 |
| 1:A:20:ALA:O | 1:A:97:VAL:HB | 0.43 | 2.14 | 12 | 5 |
| 1:A:87:ILE:CG2 | 1:A:87:ILE:O | 0.43 | 2.65 | 6 | 1 |
| 1:A:92:SER:O | 1:A:93:LYS:HG3 | 0.43 | 2.14 | 6 | 1 |
| 1:A:2:TRP:N | 1:A:6:VAL:HG23 | 0.43 | 2.29 | 7 | 1 |
| 1:A:93:LYS:O | 1:A:94:SER:CB | 0.43 | 2.67 | 7 | 1 |
| 1:A:24:LEU:HD12 | 1:A:24:LEU:H | 0.43 | 1.74 | 15 | 1 |
| 1:A:57:ALA:C | 1:A:58:SER:OG | 0.43 | 2.55 | 16 | 1 |
| 1:A:48:ALA:O | 1:A:55:ILE:CD1 | 0.43 | 2.67 | 17 | 1 |
| 1:A:21:ILE:HG12 | 1:A:30:ALA:O | 0.43 | 2.14 | 19 | 1 |
| 1:A:68:VAL:O | 1:A:69:THR:HB | 0.43 | 2.14 | 1 | 1 |
| 1:A:5:TYR:CE1 | 1:A:21:ILE:CD1 | 0.43 | 3.02 | 4 | 1 |
| 1:A:65:VAL:HG21 | 1:A:84:ALA:CB | 0.43 | 2.44 | 4 | 1 |
| 1:A:74:ASP:O | 1:A:75:ARG:HD3 | 0.42 | 2.14 | 17 | 2 |
| 1:A:57:ALA:O | 1:A:58:SER:C | 0.42 | 2.57 | 2 | 3 |
| 1:A:2:TRP:CE3 | 1:A:5:TYR:CD2 | 0.42 | 3.06 | 4 | 1 |
| 1:A:85:GLY:CA | 1:A:100:TYR:CE1 | 0.42 | 3.02 | 5 | 1 |
| 1:A:76:SER:HB3 | 1:A:78:TYR:OH | 0.42 | 2.14 | 11 | 1 |
| 1:A:57:ALA:O | 1:A:58:SER:HB2 | 0.42 | 2.14 | 12 | 2 |
| 1:A:87:ILE:HD13 | 1:A:113:VAL:HG21 | 0.42 | 1.89 | 16 | 1 |
| 1:A:49:PHE:CE2 | 1:A:90:LYS:HB2 | 0.42 | 2.48 | 17 | 1 |
| 1:A:87:ILE:O | 1:A:97:VAL:HA | 0.42 | 2.13 | 12 | 2 |
| 1:A:122:GLY:O | 1:A:123:GLN:HG3 | 0.42 | 2.13 | 16 | 2 |
| 1:A:69:THR:CG2 | 1:A:72:ALA:CB | 0.42 | 2.97 | 10 | 1 |
| 1:A:24:LEU:CD2 | 1:A:95:ILE:HG12 | 0.42 | 2.44 | 10 | 1 |
| 1:A:80:LYS:HG2 | 1:A:81:LYS:N | 0.42 | 2.29 | 16 | 1 |
| 1:A:72:ALA:O | 1:A:73:ASP:CB | 0.42 | 2.66 | 19 | 1 |
| 1:A:80:LYS:HD2 | 1:A:106:PRO:CG | 0.42 | 2.44 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:80:LYS:O | 1:A:81:LYS:HB2 | 0.42 | 2.14 | 9 | 2 |
| 1:A:7:ASP:C | 1:A:8:THR:OG1 | 0.42 | 2.57 | 9 | 1 |
| 1:A:62:LEU:HB2 | 1:A:65:VAL:O | 0.42 | 2.14 | 11 | 1 |
| 1:A:11:VAL:CG1 | 1:A:32:SER:HB2 | 0.42 | 2.44 | 12 | 1 |
| 1:A:97:VAL:O | 1:A:97:VAL:CG1 | 0.42 | 2.57 | 16 | 1 |
| 1:A:20:ALA:O | 1:A:21:ILE:HD13 | 0.42 | 2.15 | 18 | 1 |
| 1:A:52:ALA:O | 1:A:56:ARG:HB2 | 0.42 | 2.14 | 2 | 2 |
| 1:A:76:SER:O | 1:A:77:ILE:HD12 | 0.42 | 2.14 | 8 | 1 |
| 1:A:65:VAL:HG12 | 1:A:67:TYR:CD1 | 0.42 | 2.49 | 13 | 2 |
| 1:A:19:ALA:HA | 1:A:99:VAL:CG2 | 0.42 | 2.39 | 14 | 1 |
| 1:A:67:TYR:CZ | 1:A:86:VAL:HG13 | 0.42 | 2.48 | 4 | 1 |
| 1:A:60:PHE:O | 1:A:66:HIS:HA | 0.42 | 2.14 | 10 | 2 |
| 1:A:4:THR:CG2 | 1:A:5:TYR:N | 0.42 | 2.83 | 11 | 1 |
| 1:A:24:LEU:HD23 | 1:A:95:ILE:HG13 | 0.42 | 1.91 | 12 | 1 |
| 1:A:17:THR:C | 1:A:18:GLN:HG2 | 0.42 | 2.35 | 14 | 1 |
| 1:A:101:ASN:O | 1:A:104:ILE:HG13 | 0.42 | 2.15 | 7 | 1 |
| 1:A:68:VAL:HG13 | 1:A:69:THR:N | 0.42 | 2.29 | 10 | 1 |
| 1:A:91:THR:OG1 | 1:A:96:LEU:HD11 | 0.42 | 2.13 | 11 | 1 |
| 1:A:54:PRO:C | 1:A:55:ILE:HD13 | 0.42 | 2.35 | 3 | 2 |
| 1:A:100:TYR:CB | 1:A:104:ILE:CG1 | 0.42 | 2.97 | 4 | 1 |
| 1:A:38:THR:CB | 1:A:39:PRO:HD3 | 0.42 | 2.44 | 6 | 2 |
| 1:A:16:VAL:HA | 1:A:104:ILE:CD1 | 0.42 | 2.44 | 10 | 1 |
| 1:A:24:LEU:HD12 | 1:A:93:LYS:N | 0.42 | 2.30 | 10 | 1 |
| 1:A:76:SER:HA | 1:A:89:VAL:HG12 | 0.42 | 1.91 | 15 | 1 |
| 1:A:117:ALA:O | 1:A:120:LEU:N | 0.42 | 2.53 | 1 | 1 |
| 1:A:83:SER:HB2 | 1:A:102:GLU:OE2 | 0.42 | 2.14 | 3 | 1 |
| 1:A:20:ALA:O | 1:A:22:LEU:HD13 | 0.42 | 2.15 | 9 | 1 |
| 1:A:6:VAL:HG12 | 1:A:32:SER:OG | 0.42 | 2.15 | 11 | 1 |
| 1:A:53:ASP:O | 1:A:56:ARG:HG2 | 0.42 | 2.15 | 16 | 1 |
| 1:A:2:TRP:HA | 1:A:2:TRP:CE3 | 0.42 | 2.49 | 17 | 1 |
| 1:A:2:TRP:HD1 | 1:A:10:LEU:HD22 | 0.42 | 1.72 | 18 | 1 |
| 1:A:96:LEU:HD23 | 1:A:96:LEU:H | 0.42 | 1.74 | 18 | 1 |
| 1:A:114:GLU:O | 1:A:114:GLU:OE1 | 0.42 | 2.38 | 2 | 1 |
| 1:A:2:TRP:CD1 | 1:A:21:ILE:CG2 | 0.42 | 3.03 | 4 | 1 |
| 1:A:45:LEU:HG | 1:A:49:PHE:CE1 | 0.42 | 2.50 | 8 | 1 |
| 1:A:55:ILE:O | 1:A:69:THR:OG1 | 0.42 | 2.35 | 10 | 1 |
| 1:A:87:ILE:HG12 | 1:A:98:GLY:O | 0.42 | 2.15 | 12 | 1 |
| 1:A:96:LEU:N | 1:A:96:LEU:HD23 | 0.42 | 2.30 | 13 | 1 |
| 1:A:91:THR:O | 1:A:92:SER:C | 0.42 | 2.58 | 17 | 1 |
| 1:A:89:VAL:HG23 | 1:A:90:LYS:N | 0.42 | 2.29 | 18 | 1 |
| 1:A:36:ALA:C | 1:A:63:ALA:HB2 | 0.42 | 2.35 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:2:TRP:HD1 | 1:A:10:LEU:HD13 | 0.42 | 1.66 | 2 | 2 |
| 1:A:31:THR:OG1 | 1:A:32:SER:N | 0.42 | 2.53 | 15 | 2 |
| 1:A:71:ARG:O | 1:A:77:ILE:HG23 | 0.42 | 2.15 | 3 | 1 |
| 1:A:124:GLY:O | 1:A:125:PHE:O | 0.42 | 2.38 | 4 | 1 |
| 1:A:6:VAL:CG2 | 1:A:21:ILE:HD11 | 0.42 | 2.45 | 4 | 1 |
| 1:A:18:GLN:HB2 | 1:A:99:VAL:O | 0.42 | 2.15 | 8 | 2 |
| 1:A:120:LEU:O | 1:A:122:GLY:N | 0.42 | 2.53 | 7 | 1 |
| 1:A:2:TRP:CD2 | 1:A:10:LEU:HD13 | 0.42 | 2.50 | 9 | 1 |
| 1:A:53:ASP:HA | 1:A:56:ARG:CD | 0.42 | 2.45 | 16 | 1 |
| 1:A:6:VAL:O | 1:A:11:VAL:CB | 0.41 | 2.68 | 3 | 1 |
| 1:A:7:ASP:CG | 1:A:8:THR:HG22 | 0.41 | 2.33 | 3 | 1 |
| 1:A:60:PHE:O | 1:A:67:TYR:HB2 | 0.41 | 2.14 | 4 | 1 |
| 1:A:89:VAL:C | 1:A:95:ILE:HG23 | 0.41 | 2.34 | 19 | 1 |
| 1:A:120:LEU:HD23 | 1:A:125:PHE:CE1 | 0.41 | 2.50 | 1 | 1 |
| 1:A:26:GLY:O | 1:A:27:ASN:HB2 | 0.41 | 2.14 | 1 | 1 |
| 1:A:87:ILE:CG2 | 1:A:113:VAL:HG11 | 0.41 | 2.45 | 6 | 2 |
| 1:A:115:LYS:O | 1:A:117:ALA:N | 0.41 | 2.54 | 5 | 1 |
| 1:A:104:ILE:O | 1:A:105:GLN:C | 0.41 | 2.58 | 7 | 1 |
| 1:A:68:VAL:HG23 | 1:A:81:LYS:CG | 0.41 | 2.45 | 7 | 1 |
| 1:A:92:SER:HB3 | 1:A:125:PHE:CG | 0.41 | 2.50 | 10 | 1 |
| 1:A:79:GLY:N | 1:A:86:VAL:O | 0.41 | 2.53 | 10 | 1 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:HG | 0.41 | 1.92 | 17 | 1 |
| 1:A:24:LEU:N | 1:A:24:LEU:CD2 | 0.41 | 2.83 | 18 | 1 |
| 1:A:60:PHE:C | 1:A:60:PHE:CD1 | 0.41 | 2.93 | 19 | 1 |
| 1:A:5:TYR:CD2 | 1:A:10:LEU:HD23 | 0.41 | 2.48 | 6 | 1 |
| 1:A:48:ALA:O | 1:A:51:ASN:O | 0.41 | 2.38 | 7 | 1 |
| 1:A:91:THR:HB | 1:A:125:PHE:CB | 0.41 | 2.45 | 10 | 1 |
| 1:A:38:THR:N | 1:A:41:GLN:HG3 | 0.41 | 2.29 | 6 | 1 |
| 1:A:4:THR:HG23 | 1:A:5:TYR:CD1 | 0.41 | 2.50 | 8 | 1 |
| 1:A:2:TRP:HB2 | 1:A:5:TYR:HB2 | 0.41 | 1.91 | 8 | 1 |
| 1:A:19:ALA:N | 1:A:99:VAL:HG23 | 0.41 | 2.30 | 14 | 1 |
| 1:A:27:ASN:O | 1:A:28:THR:OG1 | 0.41 | 2.33 | 15 | 2 |
| 1:A:117:ALA:O | 1:A:121:ILE:N | 0.41 | 2.53 | 2 | 1 |
| 1:A:60:PHE:HE1 | 1:A:62:LEU:HD12 | 0.41 | 1.72 | 5 | 2 |
| 1:A:10:LEU:N | 1:A:14:GLY:HA3 | 0.41 | 2.31 | 7 | 1 |
| 1:A:16:VAL:HA | 1:A:100:TYR:HB3 | 0.41 | 1.91 | 9 | 1 |
| 1:A:63:ALA:O | 1:A:65:VAL:HG23 | 0.41 | 2.15 | 15 | 1 |
| 1:A:34:GLY:O | 1:A:35:PHE:HB3 | 0.41 | 2.15 | 16 | 1 |
| 1:A:20:ALA:CB | 1:A:35:PHE:CD2 | 0.41 | 3.03 | 16 | 1 |
| 1:A:59:GLY:O | 1:A:69:THR:OG1 | 0.41 | 2.38 | 18 | 1 |
| 1:A:89:VAL:HG22 | 1:A:96:LEU:CD1 | 0.41 | 2.42 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:89:VAL:O | 1:A:95:ILE:CG2 | 0.41 | 2.69 | 4 | 1 |
| 1:A:18:GLN:OE1 | 1:A:33:ALA:HB1 | 0.41 | 2.15 | 5 | 1 |
| 1:A:54:PRO:O | 1:A:59:GLY:O | 0.41 | 2.38 | 5 | 1 |
| 1:A:10:LEU:O | 1:A:14:GLY:HA3 | 0.41 | 2.15 | 4 | 1 |
| 1:A:80:LYS:HG3 | 1:A:80:LYS:O | 0.41 | 2.16 | 5 | 1 |
| 1:A:5:TYR:CG | 1:A:10:LEU:CD1 | 0.41 | 3.03 | 7 | 1 |
| 1:A:68:VAL:HG12 | 1:A:69:THR:H | 0.41 | 1.76 | 7 | 1 |
| 1:A:71:ARG:O | 1:A:72:ALA:O | 0.41 | 2.38 | 8 | 1 |
| 1:A:100:TYR:CB | 1:A:104:ILE:HG13 | 0.41 | 2.45 | 11 | 1 |
| 1:A:102:GLU:O | 1:A:103:LYS:CG | 0.41 | 2.69 | 13 | 1 |
| 1:A:10:LEU:CD2 | 1:A:116:LEU:CD2 | 0.41 | 2.99 | 15 | 1 |
| 1:A:88:THR:C | 1:A:89:VAL:CG1 | 0.41 | 2.88 | 18 | 1 |
| 1:A:89:VAL:CG2 | 1:A:91:THR:HG23 | 0.41 | 2.45 | 18 | 1 |
| 1:A:78:TYR:CE2 | 1:A:89:VAL:HG11 | 0.41 | 2.50 | 1 | 1 |
| 1:A:83:SER:O | 1:A:101:ASN:C | 0.41 | 2.59 | 3 | 1 |
| 1:A:88:THR:O | 1:A:88:THR:OG1 | 0.41 | 2.38 | 3 | 1 |
| 1:A:3:GLN:C | 1:A:5:TYR:N | 0.41 | 2.74 | 8 | 1 |
| 1:A:22:LEU:HD13 | 1:A:22:LEU:N | 0.41 | 2.31 | 9 | 1 |
| 1:A:35:PHE:HE2 | 1:A:99:VAL:HG21 | 0.41 | 1.72 | 2 | 1 |
| 1:A:32:SER:O | 1:A:33:ALA:O | 0.41 | 2.38 | 3 | 1 |
| 1:A:29:TRP:O | 1:A:30:ALA:CB | 0.41 | 2.69 | 5 | 1 |
| 1:A:2:TRP:CE3 | 1:A:116:LEU:HD12 | 0.41 | 2.51 | 6 | 1 |
| 1:A:53:ASP:HB2 | 1:A:54:PRO:HD3 | 0.41 | 1.93 | 8 | 1 |
| 1:A:35:PHE:CZ | 1:A:37:VAL:HG21 | 0.41 | 2.51 | 8 | 1 |
| 1:A:56:ARG:O | 1:A:57:ALA:C | 0.41 | 2.58 | 9 | 1 |
| 1:A:84:ALA:HA | 1:A:100:TYR:CE2 | 0.41 | 2.50 | 9 | 1 |
| 1:A:102:GLU:OE2 | 1:A:104:ILE:HG13 | 0.41 | 2.16 | 10 | 1 |
| 1:A:2:TRP:CZ3 | 1:A:96:LEU:CD1 | 0.41 | 3.04 | 15 | 1 |
| 1:A:78:TYR:HB3 | 1:A:87:ILE:CG1 | 0.41 | 2.45 | 17 | 1 |
| 1:A:10:LEU:HA | 1:A:14:GLY:CA | 0.41 | 2.45 | 19 | 1 |
| 1:A:23:GLY:HA3 | 1:A:29:TRP:CZ3 | 0.41 | 2.50 | 19 | 1 |
| 1:A:71:ARG:NH1 | 1:A:71:ARG:CG | 0.41 | 2.81 | 2 | 2 |
| 1:A:82:GLY:O | 1:A:84:ALA:N | 0.41 | 2.54 | 9 | 1 |
| 1:A:70:LEU:HD23 | 1:A:71:ARG:NE | 0.40 | 2.31 | 2 | 1 |
| 1:A:20:ALA:O | 1:A:97:VAL:N | 0.40 | 2.54 | 4 | 1 |
| 1:A:93:LYS:HB2 | 1:A:125:PHE:CB | 0.40 | 2.46 | 7 | 1 |
| 1:A:17:THR:N | 1:A:104:ILE:HD11 | 0.40 | 2.32 | 16 | 1 |
| 1:A:57:ALA:O | 1:A:58:SER:OG | 0.40 | 2.39 | 16 | 1 |
| 1:A:91:THR:HG22 | 1:A:121:ILE:CD1 | 0.40 | 2.33 | 18 | 1 |
| 1:A:2:TRP:CZ3 | 1:A:96:LEU:CD2 | 0.40 | 2.87 | 1 | 1 |
| 1:A:60:PHE:HD2 | 1:A:62:LEU:HD21 | 0.40 | 1.66 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:72:ALA:O | 1:A:73:ASP:HB2 | 0.40 | 2.15 | 2 | 1 |
| 1:A:91:THR:O | 1:A:92:SER:HB2 | 0.40 | 2.16 | 8 | 2 |
| 1:A:53:ASP:HB3 | 1:A:54:PRO:HD3 | 0.40 | 1.93 | 13 | 1 |
| 1:A:66:HIS:CE1 | 1:A:81:LYS:HD2 | 0.40 | 2.51 | 16 | 1 |
| 1:A:2:TRP:O | 1:A:21:ILE:HG13 | 0.40 | 2.16 | 18 | 1 |
| 1:A:41:GLN:OE1 | 1:A:41:GLN:HA | 0.40 | 2.15 | 19 | 1 |
| 1:A:40:ALA:HB3 | 1:A:44:THR:OG1 | 0.40 | 2.16 | 2 | 1 |
| 1:A:61:ASP:O | 1:A:61:ASP:OD1 | 0.40 | 2.39 | 4 | 1 |
| 1:A:23:GLY:HA2 | 1:A:29:TRP:CE3 | 0.40 | 2.51 | 11 | 1 |
| 1:A:19:ALA:C | 1:A:32:SER:CA | 0.40 | 2.89 | 18 | 1 |
| 1:A:101:ASN:C | 1:A:102:GLU:HG2 | 0.40 | 2.37 | 2 | 1 |
| 1:A:79:GLY:C | 1:A:86:VAL:CG1 | 0.40 | 2.90 | 2 | 1 |
| 1:A:82:GLY:C | 1:A:84:ALA:N | 0.40 | 2.75 | 4 | 1 |
| 1:A:2:TRP:O | 1:A:21:ILE:CD1 | 0.40 | 2.70 | 5 | 1 |
| 1:A:71:ARG:O | 1:A:71:ARG:HG2 | 0.40 | 2.17 | 7 | 1 |
| 1:A:76:SER:O | 1:A:77:ILE:CD1 | 0.40 | 2.69 | 8 | 1 |
| 1:A:33:ALA:O | 1:A:34:GLY:C | 0.40 | 2.58 | 9 | 1 |
| 1:A:5:TYR:CD2 | 1:A:116:LEU:HD22 | 0.40 | 2.52 | 11 | 1 |
| 1:A:65:VAL:CG1 | 1:A:67:TYR:CD1 | 0.40 | 3.04 | 13 | 1 |
| 1:A:81:LYS:HB2 | 1:A:84:ALA:O | 0.40 | 2.15 | 16 | 1 |
| 1:A:101:ASN:C | 1:A:103:LYS:N | 0.40 | 2.73 | 19 | 1 |
| 1:A:23:GLY:O | 1:A:24:LEU:HB2 | 0.40 | 2.17 | 1 | 1 |
| 1:A:2:TRP:O | 1:A:6:VAL:CB | 0.40 | 2.70 | 5 | 1 |
| 1:A:100:TYR:C | 1:A:101:ASN:OD1 | 0.40 | 2.60 | 7 | 1 |
| 1:A:24:LEU:HA | 1:A:95:ILE:HD11 | 0.40 | 1.93 | 10 | 1 |
| 1:A:37:VAL:HG12 | 1:A:38:THR:N | 0.40 | 2.32 | 10 | 1 |
| 1:A:2:TRP:CD1 | 1:A:10:LEU:CD2 | 0.40 | 3.05 | 18 | 1 |
| 1:A:20:ALA:N | 1:A:32:SER:HB3 | 0.40 | 2.31 | 18 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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 NMR 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 | 123/125 (98%) | 85±4 (69±3%) | 26±4 (21±3%) | 12±2 (10±2%) | 1 | 10 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-----------|--------------------|
| All | All | 2337/2375 (98%) | 1607 (69%) | 495 (21%) | 235 (10%) | 1 10 |

All 55 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 15 | ALA | 19 |
| 1 | A | 13 | THR | 18 |
| 1 | A | 10 | LEU | 13 |
| 1 | A | 8 | THR | 12 |
| 1 | A | 27 | ASN | 9 |
| 1 | A | 58 | SER | 9 |
| 1 | A | 74 | ASP | 8 |
| 1 | A | 77 | ILE | 8 |
| 1 | A | 63 | ALA | 7 |
| 1 | A | 73 | ASP | 7 |
| 1 | A | 81 | LYS | 7 |
| 1 | A | 3 | GLN | 7 |
| 1 | A | 33 | ALA | 6 |
| 1 | A | 92 | SER | 6 |
| 1 | A | 34 | GLY | 6 |
| 1 | A | 97 | VAL | 6 |
| 1 | A | 23 | GLY | 5 |
| 1 | A | 32 | SER | 5 |
| 1 | A | 40 | ALA | 5 |
| 1 | A | 71 | ARG | 5 |
| 1 | A | 102 | GLU | 4 |
| 1 | A | 38 | THR | 4 |
| 1 | A | 7 | ASP | 4 |
| 1 | A | 35 | PHE | 4 |
| 1 | A | 103 | LYS | 3 |
| 1 | A | 19 | ALA | 3 |
| 1 | A | 54 | PRO | 3 |
| 1 | A | 28 | THR | 3 |
| 1 | A | 39 | PRO | 2 |
| 1 | A | 65 | VAL | 2 |
| 1 | A | 14 | GLY | 2 |
| 1 | A | 64 | GLY | 2 |
| 1 | A | 22 | LEU | 2 |
| 1 | A | 30 | ALA | 2 |
| 1 | A | 93 | LYS | 2 |
| 1 | A | 69 | THR | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 52 | ALA | 2 |
| 1 | A | 2 | TRP | 2 |
| 1 | A | 57 | ALA | 2 |
| 1 | A | 123 | GLN | 2 |
| 1 | A | 68 | VAL | 1 |
| 1 | A | 4 | THR | 1 |
| 1 | A | 82 | GLY | 1 |
| 1 | A | 72 | ALA | 1 |
| 1 | A | 24 | LEU | 1 |
| 1 | A | 83 | SER | 1 |
| 1 | A | 62 | LEU | 1 |
| 1 | A | 26 | GLY | 1 |
| 1 | A | 118 | ASP | 1 |
| 1 | A | 51 | ASN | 1 |
| 1 | A | 20 | ALA | 1 |
| 1 | A | 106 | PRO | 1 |
| 1 | A | 105 | GLN | 1 |
| 1 | A | 124 | GLY | 1 |
| 1 | A | 9 | ASN | 1 |

6.3.2 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 NMR 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 | 92/93 (99%) | 59±4 (64±4%) | 33±4 (36±4%) | 1 | 8 |
| All | All | 1748/1767 (99%) | 1120 (64%) | 628 (36%) | 1 | 8 |

All 82 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 13 | THR | 19 |
| 1 | A | 99 | VAL | 18 |
| 1 | A | 55 | ILE | 17 |
| 1 | A | 75 | ARG | 16 |
| 1 | A | 81 | LYS | 16 |
| 1 | A | 96 | LEU | 15 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 103 | LYS | 13 |
| 1 | A | 10 | LEU | 13 |
| 1 | A | 53 | ASP | 13 |
| 1 | A | 78 | TYR | 13 |
| 1 | A | 22 | LEU | 12 |
| 1 | A | 71 | ARG | 12 |
| 1 | A | 80 | LYS | 12 |
| 1 | A | 6 | VAL | 11 |
| 1 | A | 24 | LEU | 11 |
| 1 | A | 32 | SER | 11 |
| 1 | A | 115 | LYS | 11 |
| 1 | A | 83 | SER | 11 |
| 1 | A | 125 | PHE | 11 |
| 1 | A | 56 | ARG | 10 |
| 1 | A | 92 | SER | 10 |
| 1 | A | 7 | ASP | 10 |
| 1 | A | 90 | LYS | 10 |
| 1 | A | 69 | THR | 10 |
| 1 | A | 120 | LEU | 10 |
| 1 | A | 8 | THR | 10 |
| 1 | A | 94 | SER | 10 |
| 1 | A | 4 | THR | 9 |
| 1 | A | 38 | THR | 9 |
| 1 | A | 73 | ASP | 9 |
| 1 | A | 76 | SER | 9 |
| 1 | A | 18 | GLN | 9 |
| 1 | A | 3 | GLN | 9 |
| 1 | A | 61 | ASP | 8 |
| 1 | A | 118 | ASP | 8 |
| 1 | A | 17 | THR | 8 |
| 1 | A | 93 | LYS | 8 |
| 1 | A | 114 | GLU | 8 |
| 1 | A | 35 | PHE | 8 |
| 1 | A | 70 | LEU | 8 |
| 1 | A | 45 | LEU | 7 |
| 1 | A | 91 | THR | 7 |
| 1 | A | 74 | ASP | 7 |
| 1 | A | 62 | LEU | 7 |
| 1 | A | 116 | LEU | 7 |
| 1 | A | 58 | SER | 7 |
| 1 | A | 47 | SER | 7 |
| 1 | A | 105 | GLN | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 102 | GLU | 7 |
| 1 | A | 41 | GLN | 6 |
| 1 | A | 60 | PHE | 6 |
| 1 | A | 25 | ASP | 6 |
| 1 | A | 27 | ASN | 6 |
| 1 | A | 2 | TRP | 6 |
| 1 | A | 68 | VAL | 5 |
| 1 | A | 31 | THR | 5 |
| 1 | A | 51 | ASN | 5 |
| 1 | A | 111 | ASN | 5 |
| 1 | A | 101 | ASN | 5 |
| 1 | A | 43 | GLN | 5 |
| 1 | A | 9 | ASN | 5 |
| 1 | A | 28 | THR | 5 |
| 1 | A | 50 | ASN | 4 |
| 1 | A | 66 | HIS | 4 |
| 1 | A | 121 | ILE | 4 |
| 1 | A | 65 | VAL | 3 |
| 1 | A | 16 | VAL | 3 |
| 1 | A | 77 | ILE | 3 |
| 1 | A | 11 | VAL | 3 |
| 1 | A | 119 | TYR | 3 |
| 1 | A | 89 | VAL | 3 |
| 1 | A | 108 | THR | 3 |
| 1 | A | 123 | GLN | 3 |
| 1 | A | 29 | TRP | 2 |
| 1 | A | 112 | VAL | 2 |
| 1 | A | 5 | TYR | 2 |
| 1 | A | 100 | TYR | 2 |
| 1 | A | 67 | TYR | 2 |
| 1 | A | 37 | VAL | 1 |
| 1 | A | 87 | ILE | 1 |
| 1 | A | 21 | ILE | 1 |
| 1 | A | 88 | THR | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided