



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:57 PM BST

PDB ID : 1AWE
Title : HUMAN SOS1 PLECKSTRIN HOMOLOGY (PH) DOMAIN, NMR, 20
STRUCTURES
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Deposited on : 1997-10-01

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

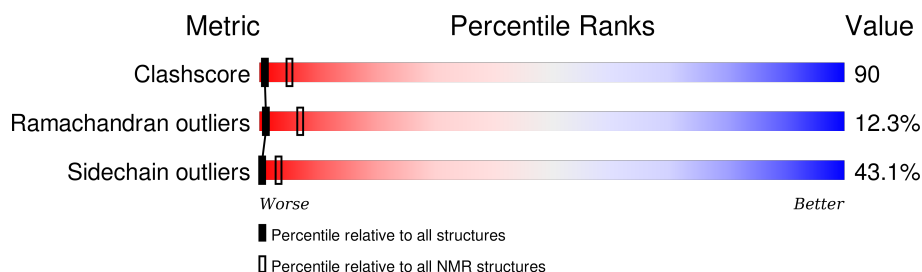
1 Overall quality at a glance

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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 130 | |

2 Ensemble composition and analysis

This entry contains 20 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:26-A:32, A:44-A:74, A:86-A:150 (103) | 0.46 | 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 2 single-model clusters were found.

| Cluster number | Models |
|-----------------------|--|
| 1 | 1, 3, 4, 5, 6, 9, 10, 11, 12, 14, 15, 16, 17, 20 |
| 2 | 2, 8 |
| 3 | 7, 19 |
| Single-model clusters | 13; 18 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1903 atoms, of which 849 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SOS1.

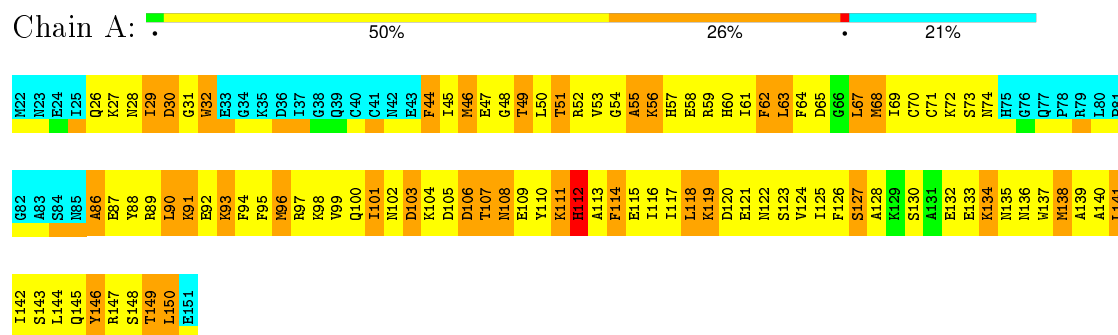
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 130 | Total | C | H | N | O | S | 0 |
| | | | 1903 | 661 | 849 | 185 | 199 | 9 | |

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: SOS1

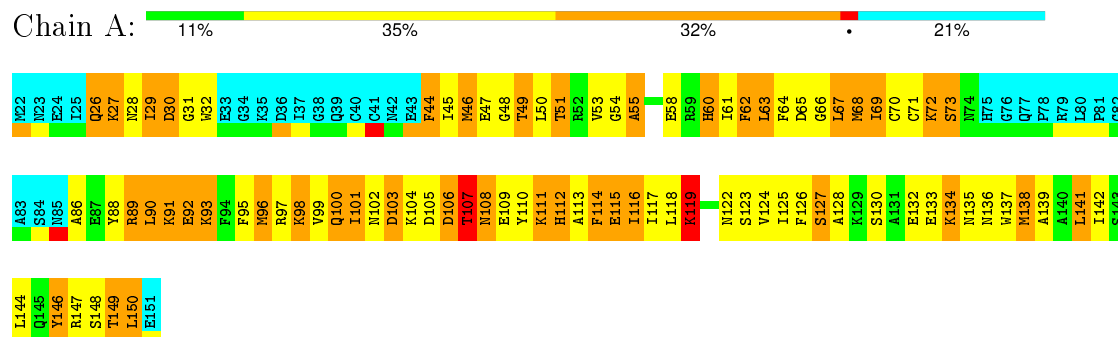


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

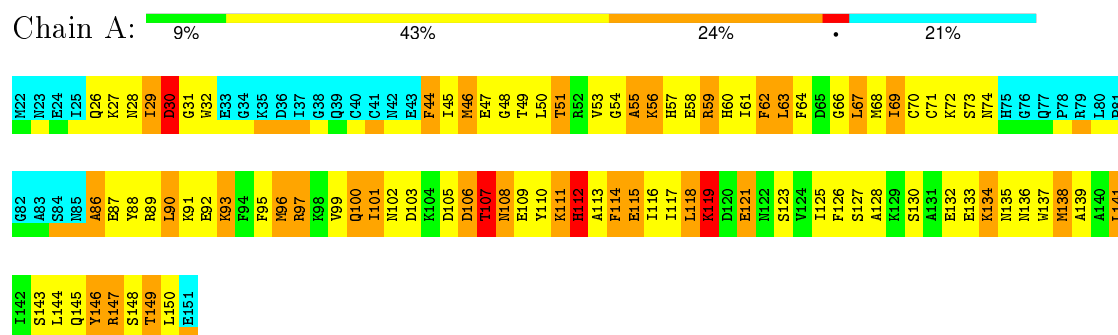
4.2.1 Score per residue for model 1

- Molecule 1: SOS1



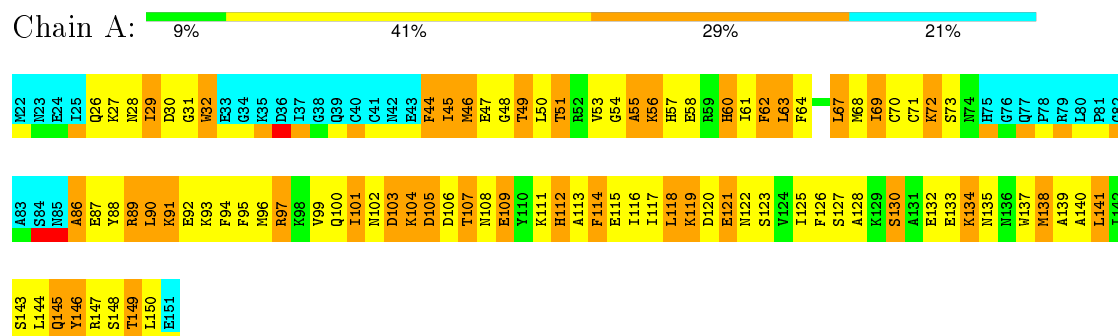
4.2.2 Score per residue for model 2

• Molecule 1: SOS1



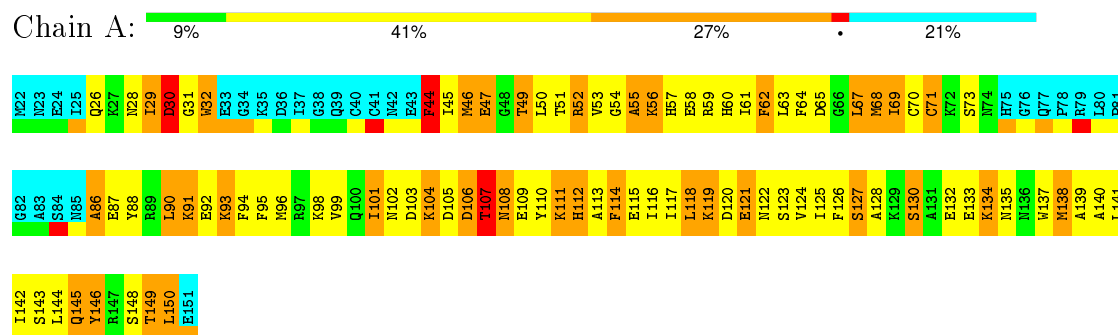
4.2.3 Score per residue for model 3

• Molecule 1: SOS1



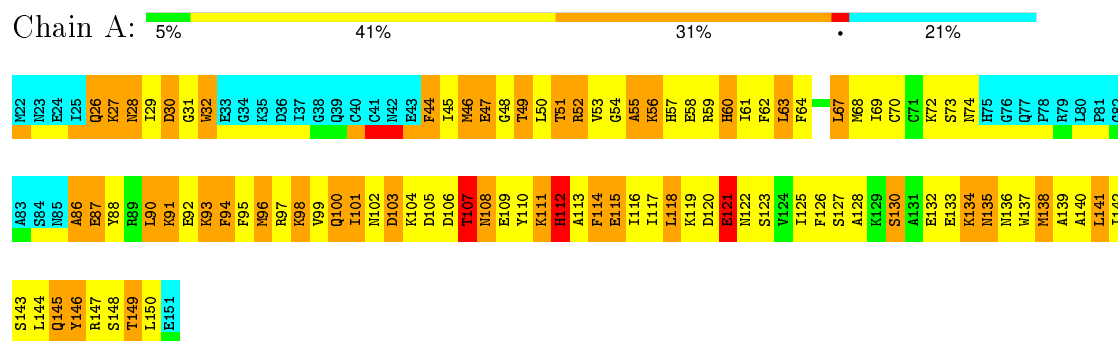
4.2.4 Score per residue for model 4

• Molecule 1: SOS1



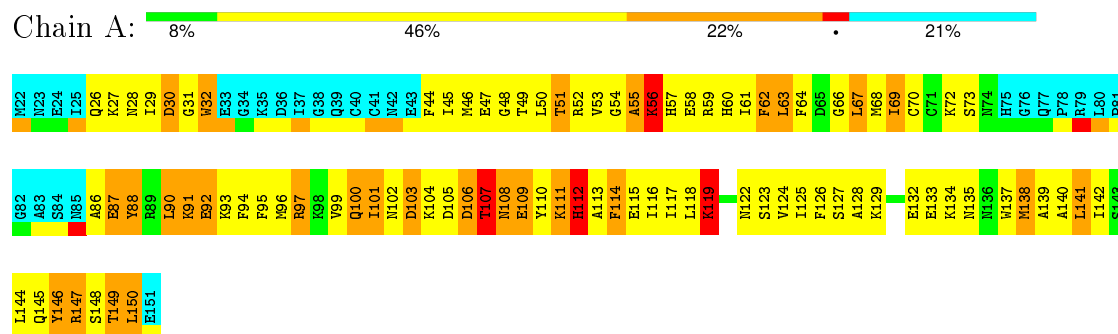
4.2.5 Score per residue for model 5

• Molecule 1: SOS1



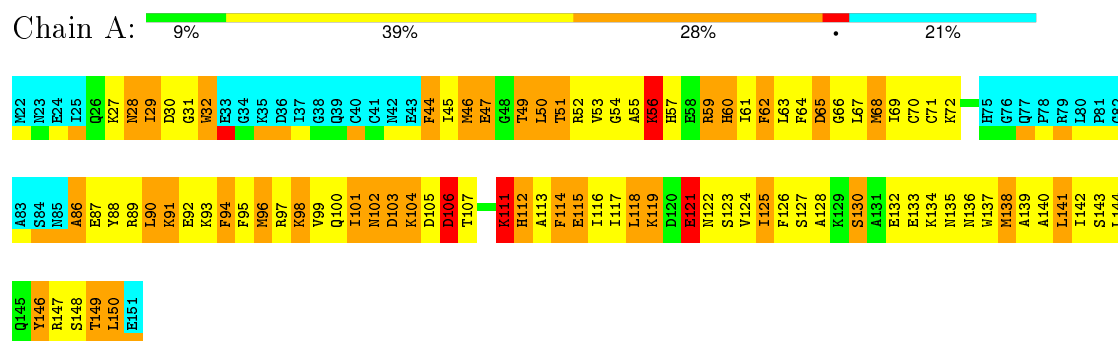
4.2.6 Score per residue for model 6

- Molecule 1: SOS1



4.2.7 Score per residue for model 7

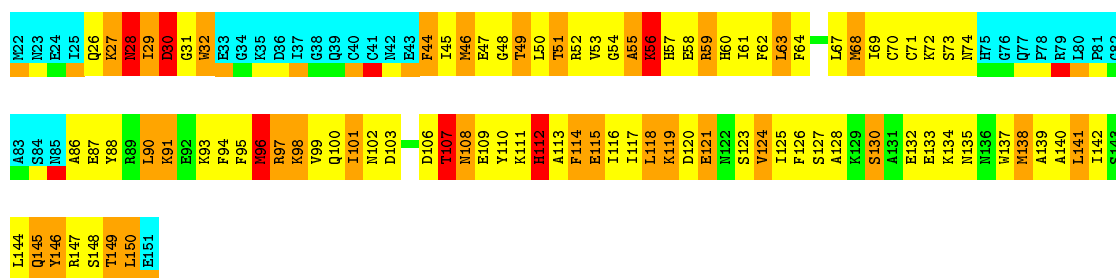
- Molecule 1: SOS1



4.2.8 Score per residue for model 8

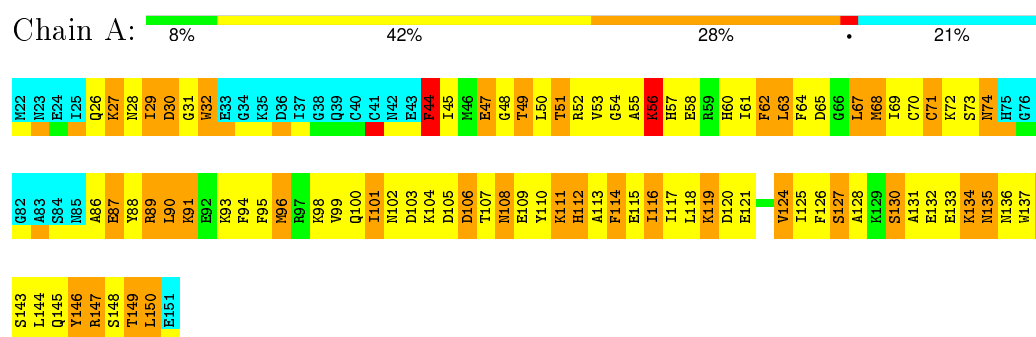
- Molecule 1: SOS1





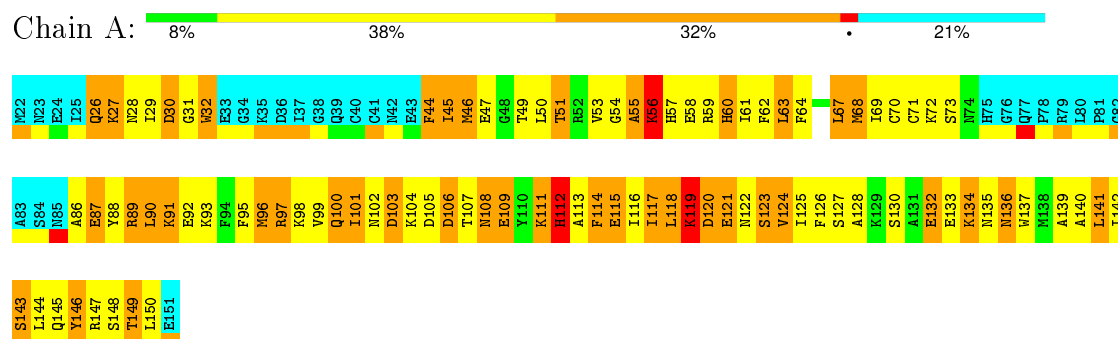
4.2.9 Score per residue for model 9

- Molecule 1: SOS1



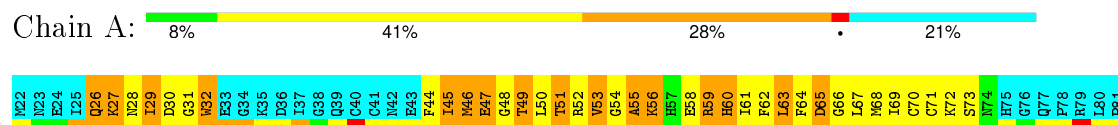
4.2.10 Score per residue for model 10

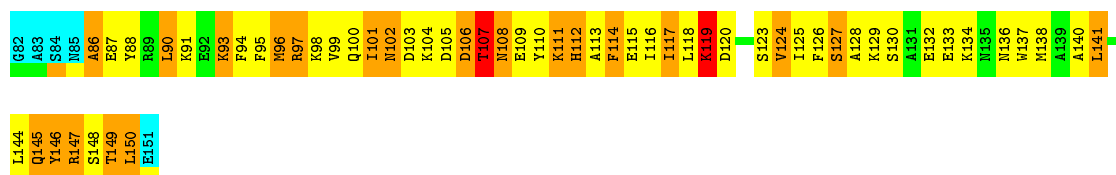
- Molecule 1: SOS1



4.2.11 Score per residue for model 11

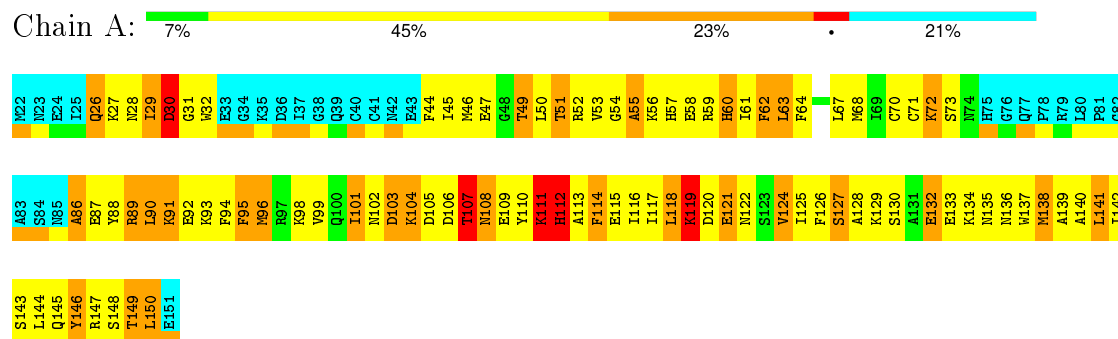
- Molecule 1: SOS1





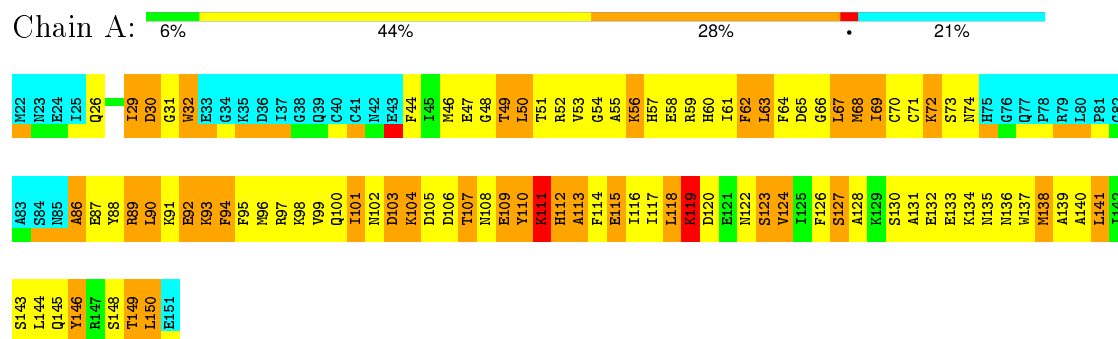
4.2.12 Score per residue for model 12

- Molecule 1: SOS1



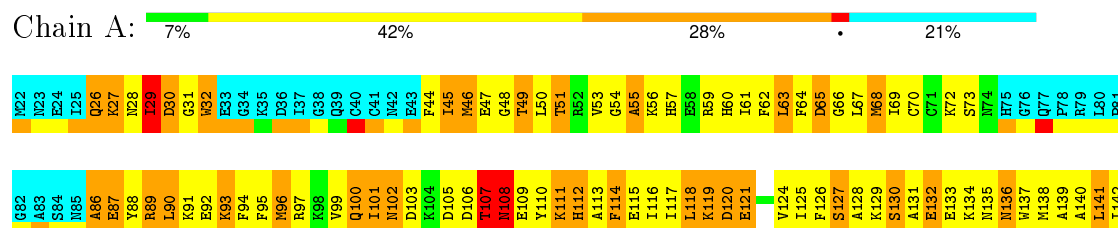
4.2.13 Score per residue for model 13

- Molecule 1: SOS1



4.2.14 Score per residue for model 14

- Molecule 1: SOS1



S143
L144
Q145
Y146
R147
S148
T149
L150
E151

4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: SOS1

Chain A: 9% 39% 27% • 21%

M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63 M64 M65 M66 M67 M68 M69 M70 M71 M72 M73 M74 M75 M76 M77 M78 M79 M80 M81 M82

A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135 A136 A137 A138 A139 A140 A141 A142 A143

L144
Q145
Y146
R147
S148
T149
L150
E151

4.2.16 Score per residue for model 16

- Molecule 1: SOS1

Chain A: 8% 42% 26% • 21%

M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63 M64 M65 M66 M67 M68 M69 M70 M71 M72 M73 M74 M75 M76 M77 M78 M79 M80 M81

G82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135 A136 A137 A138 A139 A140 A141

I142
S143
L144
Q145
Y146
R147
S148
T149
L150
E151

4.2.17 Score per residue for model 17

- Molecule 1: SOS1

Chain A: 12% 43% 22% • 21%

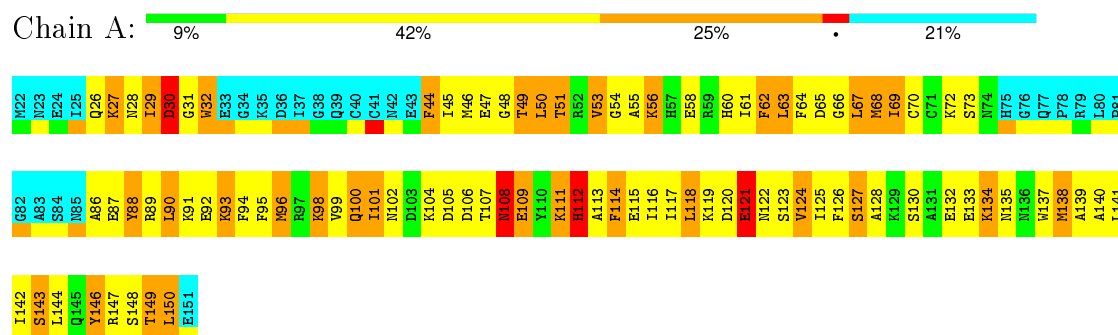
M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63 M64 M65 M66 M67 M68 M69 M70 M71 M72 M73 M74 M75 M76 M77 M78 M79 M80 M81 M82

A83 A84 A85 A86 A87 A88 A89 A90 A91 A92 A93 A94 A95 A96 A97 A98 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109 A110 A111 A112 A113 A114 A115 A116 A117 A118 A119 A120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135 A136 A137 A138 A139 A140 A141 A142 A143 A144 A145 A146

R147
S148
T149
L150
E151

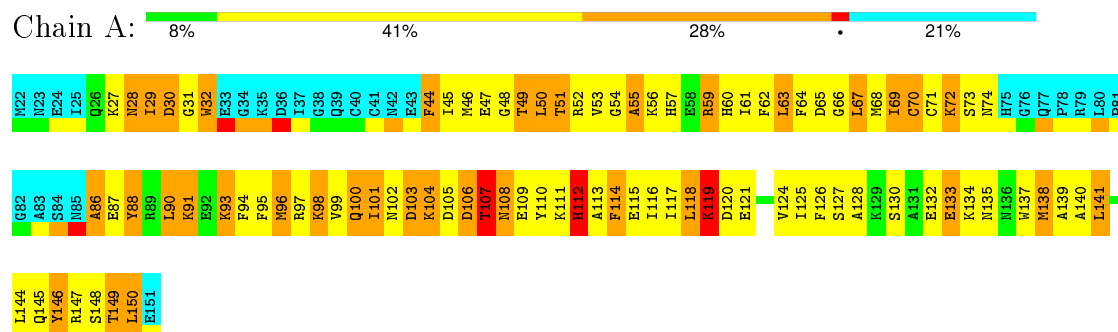
4.2.18 Score per residue for model 18

• Molecule 1: SOS1



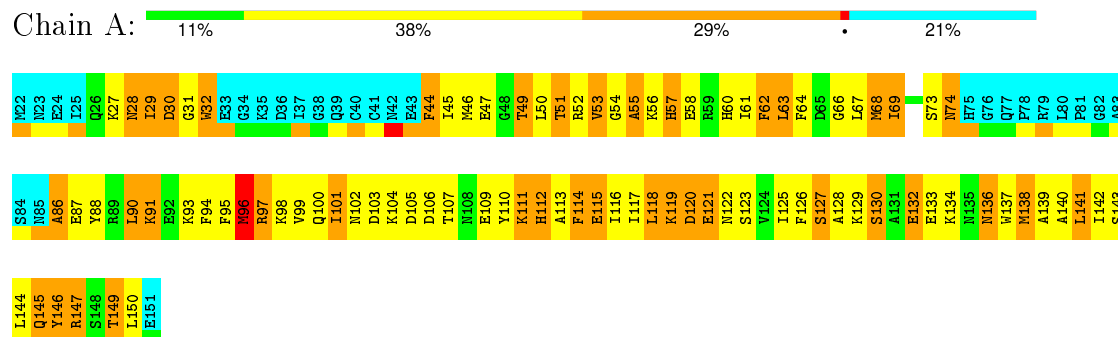
4.2.19 Score per residue for model 19

• Molecule 1: SOS1



4.2.20 Score per residue for model 20

• Molecule 1: SOS1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 750 calculated structures, 20 were deposited, based on the following criterion: *TARGET FUNCTION*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| DYANA | refinement | |
| DYANA | structure solution | |

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 ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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 | 853 | 704 | 848 | 153±11 |
| All | All | 17060 | 14080 | 16960 | 3062 |

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 90.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:63:LEU:HD13 | 1:A:144:LEU:HD11 | 1.15 | 1.15 | 18 | 11 |
| 1:A:95:PHE:CE2 | 1:A:118:LEU:HD22 | 1.14 | 1.77 | 1 | 1 |
| 1:A:128:ALA:HB2 | 1:A:137:TRP:CZ3 | 1.10 | 1.82 | 19 | 20 |
| 1:A:86:ALA:O | 1:A:88:TYR:N | 1.09 | 1.85 | 6 | 5 |
| 1:A:128:ALA:HB2 | 1:A:137:TRP:CE3 | 1.07 | 1.84 | 16 | 20 |
| 1:A:61:ILE:HD11 | 1:A:126:PHE:CZ | 1.04 | 1.87 | 13 | 1 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:HD13 | 1.04 | 1.86 | 9 | 5 |
| 1:A:101:ILE:HD12 | 1:A:116:ILE:HD12 | 1.03 | 1.20 | 19 | 10 |
| 1:A:45:ILE:CD1 | 1:A:144:LEU:HD21 | 1.03 | 1.83 | 9 | 5 |
| 1:A:63:LEU:CD1 | 1:A:144:LEU:HD11 | 1.02 | 1.83 | 20 | 11 |
| 1:A:95:PHE:CE2 | 1:A:118:LEU:HD13 | 1.01 | 1.90 | 6 | 8 |
| 1:A:69:ILE:HD12 | 1:A:90:LEU:HD21 | 1.00 | 1.30 | 7 | 2 |
| 1:A:29:ILE:O | 1:A:86:ALA:HB1 | 0.99 | 1.56 | 11 | 18 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:HD22 | 0.97 | 1.94 | 4 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:90:LEU:O | 1:A:90:LEU:HD13 | 0.96 | 1.60 | 5 | 7 |
| 1:A:90:LEU:HD13 | 1:A:90:LEU:O | 0.96 | 1.61 | 18 | 11 |
| 1:A:64:PHE:O | 1:A:66:GLY:N | 0.93 | 2.00 | 14 | 2 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:CD1 | 0.93 | 1.98 | 7 | 3 |
| 1:A:45:ILE:HD12 | 1:A:144:LEU:HD21 | 0.92 | 1.40 | 20 | 8 |
| 1:A:101:ILE:CD1 | 1:A:116:ILE:HD12 | 0.92 | 1.94 | 20 | 5 |
| 1:A:95:PHE:CE1 | 1:A:118:LEU:HD22 | 0.90 | 2.02 | 8 | 5 |
| 1:A:113:ALA:HB2 | 1:A:127:SER:OG | 0.88 | 1.69 | 7 | 13 |
| 1:A:69:ILE:HD12 | 1:A:70:CYS:N | 0.88 | 1.83 | 6 | 2 |
| 1:A:90:LEU:HD22 | 1:A:91:LYS:N | 0.88 | 1.83 | 2 | 14 |
| 1:A:107:THR:HG22 | 1:A:111:LYS:O | 0.87 | 1.70 | 15 | 8 |
| 1:A:95:PHE:CZ | 1:A:118:LEU:HD22 | 0.87 | 2.05 | 8 | 5 |
| 1:A:96:MET:CB | 1:A:144:LEU:HD13 | 0.87 | 2.00 | 19 | 6 |
| 1:A:63:LEU:HD21 | 1:A:144:LEU:HD11 | 0.86 | 1.46 | 12 | 3 |
| 1:A:63:LEU:HD13 | 1:A:144:LEU:CD1 | 0.86 | 2.00 | 20 | 8 |
| 1:A:46:MET:SD | 1:A:63:LEU:HD23 | 0.85 | 2.10 | 6 | 2 |
| 1:A:146:TYR:O | 1:A:150:LEU:HD23 | 0.85 | 1.71 | 7 | 19 |
| 1:A:53:VAL:HG12 | 1:A:53:VAL:O | 0.85 | 1.72 | 5 | 4 |
| 1:A:45:ILE:HB | 1:A:63:LEU:HD23 | 0.84 | 1.49 | 12 | 1 |
| 1:A:106:ASP:O | 1:A:108:ASN:N | 0.84 | 2.10 | 16 | 11 |
| 1:A:50:LEU:HD13 | 1:A:61:ILE:CG1 | 0.84 | 2.01 | 2 | 19 |
| 1:A:69:ILE:HD13 | 1:A:69:ILE:O | 0.84 | 1.72 | 20 | 2 |
| 1:A:96:MET:HB2 | 1:A:144:LEU:HD13 | 0.84 | 1.47 | 15 | 6 |
| 1:A:63:LEU:HD21 | 1:A:144:LEU:CD1 | 0.83 | 2.03 | 16 | 4 |
| 1:A:50:LEU:HD13 | 1:A:61:ILE:HG13 | 0.83 | 1.50 | 3 | 18 |
| 1:A:53:VAL:O | 1:A:53:VAL:HG12 | 0.83 | 1.74 | 2 | 8 |
| 1:A:63:LEU:HD22 | 1:A:96:MET:SD | 0.81 | 2.16 | 1 | 1 |
| 1:A:50:LEU:HD22 | 1:A:126:PHE:CD2 | 0.81 | 2.10 | 1 | 17 |
| 1:A:133:GLU:O | 1:A:137:TRP:N | 0.81 | 2.14 | 13 | 20 |
| 1:A:46:MET:HG2 | 1:A:63:LEU:HD23 | 0.80 | 1.54 | 1 | 4 |
| 1:A:118:LEU:HD12 | 1:A:119:LYS:O | 0.80 | 1.77 | 1 | 3 |
| 1:A:128:ALA:CB | 1:A:137:TRP:CZ3 | 0.79 | 2.64 | 2 | 19 |
| 1:A:90:LEU:C | 1:A:90:LEU:HD13 | 0.79 | 1.96 | 7 | 6 |
| 1:A:50:LEU:CD2 | 1:A:137:TRP:CE3 | 0.79 | 2.66 | 4 | 19 |
| 1:A:124:VAL:O | 1:A:125:ILE:HD13 | 0.78 | 1.79 | 18 | 3 |
| 1:A:50:LEU:HD23 | 1:A:137:TRP:CE3 | 0.78 | 2.14 | 19 | 19 |
| 1:A:69:ILE:HD12 | 1:A:90:LEU:CD2 | 0.77 | 2.10 | 8 | 2 |
| 1:A:118:LEU:O | 1:A:119:LYS:O | 0.77 | 2.02 | 10 | 12 |
| 1:A:115:GLU:C | 1:A:116:ILE:HD13 | 0.77 | 1.99 | 20 | 8 |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:CE1 | 0.77 | 2.14 | 4 | 1 |
| 1:A:53:VAL:O | 1:A:125:ILE:HG21 | 0.76 | 1.80 | 10 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:ILE:HG13 | 1:A:90:LEU:HD23 | 0.76 | 1.55 | 2 | 5 |
| 1:A:95:PHE:CD2 | 1:A:99:VAL:HG11 | 0.76 | 2.16 | 11 | 1 |
| 1:A:53:VAL:HG12 | 1:A:125:ILE:HG21 | 0.76 | 1.55 | 11 | 4 |
| 1:A:30:ASP:HB3 | 1:A:90:LEU:HD12 | 0.76 | 1.55 | 18 | 1 |
| 1:A:114:PHE:CD1 | 1:A:126:PHE:O | 0.76 | 2.38 | 13 | 2 |
| 1:A:31:GLY:O | 1:A:32:TRP:C | 0.75 | 2.25 | 3 | 20 |
| 1:A:50:LEU:HD12 | 1:A:50:LEU:N | 0.75 | 1.96 | 18 | 4 |
| 1:A:90:LEU:HD13 | 1:A:90:LEU:C | 0.75 | 2.02 | 9 | 8 |
| 1:A:69:ILE:HD13 | 1:A:69:ILE:C | 0.75 | 2.02 | 20 | 4 |
| 1:A:133:GLU:O | 1:A:137:TRP:CG | 0.74 | 2.40 | 17 | 20 |
| 1:A:90:LEU:HD22 | 1:A:90:LEU:C | 0.74 | 2.03 | 15 | 7 |
| 1:A:50:LEU:N | 1:A:50:LEU:HD12 | 0.74 | 1.98 | 13 | 13 |
| 1:A:103:ASP:HA | 1:A:114:PHE:HB2 | 0.74 | 1.59 | 16 | 4 |
| 1:A:96:MET:CG | 1:A:144:LEU:HD13 | 0.73 | 2.13 | 10 | 2 |
| 1:A:116:ILE:CD1 | 1:A:126:PHE:CD2 | 0.73 | 2.71 | 17 | 2 |
| 1:A:113:ALA:HB1 | 1:A:125:ILE:HG22 | 0.73 | 1.60 | 18 | 2 |
| 1:A:95:PHE:CE2 | 1:A:141:LEU:HD11 | 0.73 | 2.19 | 20 | 4 |
| 1:A:128:ALA:HB3 | 1:A:134:LYS:HG2 | 0.73 | 1.61 | 17 | 1 |
| 1:A:96:MET:HA | 1:A:144:LEU:HD13 | 0.72 | 1.61 | 13 | 4 |
| 1:A:29:ILE:HG22 | 1:A:90:LEU:HB3 | 0.72 | 1.61 | 16 | 7 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:HG21 | 0.72 | 2.19 | 6 | 7 |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:C | 0.72 | 2.03 | 3 | 1 |
| 1:A:69:ILE:C | 1:A:69:ILE:HD13 | 0.72 | 2.05 | 18 | 2 |
| 1:A:63:LEU:HD12 | 1:A:64:PHE:N | 0.72 | 1.99 | 17 | 7 |
| 1:A:69:ILE:HD12 | 1:A:69:ILE:C | 0.71 | 2.04 | 13 | 1 |
| 1:A:66:GLY:O | 1:A:67:LEU:HD23 | 0.71 | 1.85 | 13 | 4 |
| 1:A:63:LEU:HD11 | 1:A:144:LEU:CD1 | 0.71 | 2.15 | 4 | 2 |
| 1:A:61:ILE:HD12 | 1:A:70:CYS:CB | 0.71 | 2.15 | 19 | 2 |
| 1:A:119:LYS:O | 1:A:121:GLU:N | 0.71 | 2.23 | 10 | 4 |
| 1:A:96:MET:N | 1:A:144:LEU:HD13 | 0.70 | 2.01 | 8 | 5 |
| 1:A:45:ILE:HD13 | 1:A:144:LEU:HD21 | 0.70 | 1.62 | 9 | 1 |
| 1:A:133:GLU:O | 1:A:137:TRP:CD1 | 0.70 | 2.44 | 4 | 20 |
| 1:A:59:ARG:HB3 | 1:A:71:CYS:O | 0.70 | 1.86 | 8 | 2 |
| 1:A:63:LEU:HA | 1:A:68:MET:HA | 0.70 | 1.63 | 5 | 7 |
| 1:A:111:LYS:O | 1:A:113:ALA:N | 0.70 | 2.23 | 18 | 2 |
| 1:A:69:ILE:HD13 | 1:A:70:CYS:N | 0.70 | 2.00 | 18 | 2 |
| 1:A:53:VAL:CG1 | 1:A:53:VAL:O | 0.70 | 2.40 | 5 | 6 |
| 1:A:68:MET:CB | 1:A:95:PHE:CD2 | 0.70 | 2.74 | 3 | 2 |
| 1:A:49:THR:C | 1:A:50:LEU:HD12 | 0.69 | 2.07 | 18 | 5 |
| 1:A:69:ILE:HG23 | 1:A:90:LEU:CD2 | 0.69 | 2.17 | 7 | 3 |
| 1:A:63:LEU:HD12 | 1:A:68:MET:HB2 | 0.69 | 1.63 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:99:VAL:HG22 | 1:A:145:GLN:HB2 | 0.69 | 1.64 | 2 | 1 |
| 1:A:68:MET:SD | 1:A:95:PHE:CE2 | 0.69 | 2.85 | 11 | 7 |
| 1:A:69:ILE:HD12 | 1:A:90:LEU:HD23 | 0.69 | 1.64 | 8 | 1 |
| 1:A:28:ASN:ND2 | 1:A:88:TYR:CE2 | 0.69 | 2.61 | 19 | 4 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:CD1 | 0.69 | 2.74 | 9 | 2 |
| 1:A:50:LEU:CD2 | 1:A:126:PHE:CD2 | 0.69 | 2.76 | 8 | 7 |
| 1:A:53:VAL:O | 1:A:53:VAL:CG1 | 0.69 | 2.41 | 2 | 6 |
| 1:A:105:ASP:CB | 1:A:113:ALA:O | 0.69 | 2.41 | 20 | 4 |
| 1:A:106:ASP:C | 1:A:107:THR:HG23 | 0.69 | 2.07 | 7 | 4 |
| 1:A:114:PHE:N | 1:A:114:PHE:CD1 | 0.68 | 2.60 | 7 | 6 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CZ3 | 0.68 | 2.23 | 7 | 20 |
| 1:A:54:GLY:O | 1:A:55:ALA:HB3 | 0.68 | 1.87 | 12 | 2 |
| 1:A:95:PHE:CE2 | 1:A:118:LEU:CD1 | 0.68 | 2.75 | 6 | 2 |
| 1:A:68:MET:SD | 1:A:95:PHE:CD2 | 0.68 | 2.87 | 11 | 5 |
| 1:A:45:ILE:CB | 1:A:63:LEU:HD23 | 0.68 | 2.17 | 12 | 1 |
| 1:A:101:ILE:HG12 | 1:A:116:ILE:HG23 | 0.68 | 1.66 | 13 | 3 |
| 1:A:96:MET:HB3 | 1:A:144:LEU:HD12 | 0.68 | 1.62 | 1 | 1 |
| 1:A:53:VAL:CG1 | 1:A:125:ILE:HG21 | 0.68 | 2.18 | 7 | 4 |
| 1:A:116:ILE:N | 1:A:116:ILE:HD13 | 0.68 | 2.04 | 7 | 3 |
| 1:A:94:PHE:CD2 | 1:A:94:PHE:O | 0.68 | 2.47 | 15 | 2 |
| 1:A:101:ILE:HG12 | 1:A:116:ILE:HD12 | 0.68 | 1.64 | 14 | 2 |
| 1:A:99:VAL:HG21 | 1:A:141:LEU:HG | 0.68 | 1.66 | 12 | 3 |
| 1:A:53:VAL:HG21 | 1:A:113:ALA:CB | 0.67 | 2.19 | 12 | 3 |
| 1:A:44:PHE:CD1 | 1:A:62:PHE:CE1 | 0.67 | 2.83 | 18 | 1 |
| 1:A:112:HIS:CD2 | 1:A:112:HIS:O | 0.67 | 2.47 | 10 | 1 |
| 1:A:118:LEU:HD12 | 1:A:120:ASP:HB3 | 0.67 | 1.66 | 8 | 1 |
| 1:A:54:GLY:O | 1:A:55:ALA:HB2 | 0.67 | 1.90 | 15 | 12 |
| 1:A:95:PHE:HD2 | 1:A:118:LEU:HD22 | 0.67 | 1.49 | 16 | 3 |
| 1:A:61:ILE:HD13 | 1:A:70:CYS:HB3 | 0.67 | 1.66 | 3 | 4 |
| 1:A:95:PHE:CZ | 1:A:118:LEU:HD13 | 0.67 | 2.25 | 7 | 3 |
| 1:A:63:LEU:C | 1:A:63:LEU:HD12 | 0.67 | 2.10 | 20 | 6 |
| 1:A:114:PHE:CE1 | 1:A:126:PHE:O | 0.67 | 2.48 | 13 | 2 |
| 1:A:105:ASP:O | 1:A:110:TYR:CG | 0.67 | 2.48 | 9 | 1 |
| 1:A:45:ILE:HD11 | 1:A:65:ASP:HA | 0.67 | 1.66 | 9 | 3 |
| 1:A:69:ILE:CG1 | 1:A:90:LEU:HD23 | 0.66 | 2.21 | 5 | 3 |
| 1:A:61:ILE:HD13 | 1:A:70:CYS:CB | 0.66 | 2.20 | 3 | 3 |
| 1:A:29:ILE:HG22 | 1:A:90:LEU:HB2 | 0.66 | 1.68 | 6 | 4 |
| 1:A:53:VAL:HG21 | 1:A:113:ALA:HB3 | 0.66 | 1.66 | 13 | 1 |
| 1:A:69:ILE:HG23 | 1:A:90:LEU:HD23 | 0.66 | 1.64 | 8 | 1 |
| 1:A:32:TRP:O | 1:A:32:TRP:CD1 | 0.66 | 2.49 | 14 | 6 |
| 1:A:96:MET:HB3 | 1:A:144:LEU:HD13 | 0.66 | 1.68 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:CZ | 0.66 | 2.26 | 16 | 2 |
| 1:A:63:LEU:HD13 | 1:A:96:MET:SD | 0.66 | 2.30 | 1 | 1 |
| 1:A:59:ARG:NE | 1:A:88:TYR:CE2 | 0.66 | 2.64 | 8 | 1 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CE3 | 0.65 | 2.26 | 18 | 20 |
| 1:A:128:ALA:CA | 1:A:137:TRP:CZ3 | 0.65 | 2.80 | 18 | 18 |
| 1:A:106:ASP:O | 1:A:107:THR:C | 0.65 | 2.35 | 8 | 11 |
| 1:A:118:LEU:O | 1:A:118:LEU:HD12 | 0.65 | 1.91 | 10 | 1 |
| 1:A:29:ILE:HG22 | 1:A:90:LEU:CB | 0.65 | 2.21 | 5 | 8 |
| 1:A:94:PHE:O | 1:A:94:PHE:CD2 | 0.65 | 2.49 | 12 | 2 |
| 1:A:28:ASN:ND2 | 1:A:88:TYR:CD2 | 0.65 | 2.65 | 17 | 6 |
| 1:A:50:LEU:HD13 | 1:A:61:ILE:CB | 0.65 | 2.20 | 7 | 19 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CH2 | 0.65 | 2.27 | 7 | 20 |
| 1:A:61:ILE:O | 1:A:62:PHE:CD2 | 0.65 | 2.50 | 14 | 3 |
| 1:A:118:LEU:HD12 | 1:A:122:ASN:HB3 | 0.65 | 1.67 | 4 | 2 |
| 1:A:28:ASN:OD1 | 1:A:88:TYR:CD2 | 0.65 | 2.49 | 18 | 8 |
| 1:A:28:ASN:CG | 1:A:88:TYR:CD2 | 0.65 | 2.70 | 2 | 9 |
| 1:A:55:ALA:O | 1:A:56:LYS:CB | 0.65 | 2.45 | 8 | 11 |
| 1:A:61:ILE:HD12 | 1:A:70:CYS:HB2 | 0.65 | 1.67 | 8 | 2 |
| 1:A:107:THR:CG2 | 1:A:112:HIS:CG | 0.65 | 2.79 | 18 | 1 |
| 1:A:95:PHE:CG | 1:A:99:VAL:HG11 | 0.65 | 2.26 | 2 | 5 |
| 1:A:68:MET:CB | 1:A:95:PHE:CG | 0.65 | 2.80 | 3 | 4 |
| 1:A:45:ILE:HG22 | 1:A:46:MET:HG3 | 0.65 | 1.68 | 20 | 4 |
| 1:A:63:LEU:HD12 | 1:A:63:LEU:C | 0.65 | 2.12 | 2 | 5 |
| 1:A:69:ILE:C | 1:A:69:ILE:HD12 | 0.65 | 2.12 | 6 | 1 |
| 1:A:53:VAL:HG12 | 1:A:125:ILE:CG2 | 0.65 | 2.20 | 11 | 4 |
| 1:A:95:PHE:CE1 | 1:A:120:ASP:CG | 0.65 | 2.69 | 18 | 2 |
| 1:A:60:HIS:ND1 | 1:A:88:TYR:CE2 | 0.65 | 2.65 | 12 | 1 |
| 1:A:107:THR:O | 1:A:109:GLU:N | 0.65 | 2.30 | 6 | 15 |
| 1:A:44:PHE:CG | 1:A:44:PHE:O | 0.65 | 2.48 | 16 | 4 |
| 1:A:67:LEU:HD12 | 1:A:68:MET:N | 0.64 | 2.06 | 9 | 4 |
| 1:A:96:MET:HG2 | 1:A:144:LEU:HD22 | 0.64 | 1.68 | 13 | 1 |
| 1:A:28:ASN:OD1 | 1:A:88:TYR:CE2 | 0.64 | 2.50 | 8 | 2 |
| 1:A:95:PHE:CZ | 1:A:118:LEU:CD2 | 0.64 | 2.80 | 14 | 4 |
| 1:A:31:GLY:H | 1:A:90:LEU:HD12 | 0.64 | 1.53 | 2 | 4 |
| 1:A:44:PHE:CD1 | 1:A:44:PHE:O | 0.64 | 2.50 | 12 | 1 |
| 1:A:99:VAL:HG22 | 1:A:145:GLN:HB3 | 0.64 | 1.70 | 3 | 9 |
| 1:A:64:PHE:CZ | 1:A:69:ILE:HG21 | 0.64 | 2.27 | 1 | 3 |
| 1:A:44:PHE:O | 1:A:44:PHE:CD2 | 0.64 | 2.51 | 1 | 2 |
| 1:A:95:PHE:CG | 1:A:118:LEU:HD13 | 0.64 | 2.27 | 9 | 1 |
| 1:A:53:VAL:HG12 | 1:A:54:GLY:H | 0.64 | 1.53 | 9 | 3 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:CE1 | 0.64 | 2.27 | 18 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:ARG:CG | 1:A:71:CYS:O | 0.63 | 2.47 | 19 | 2 |
| 1:A:47:GLU:CB | 1:A:62:PHE:CE1 | 0.63 | 2.81 | 5 | 5 |
| 1:A:68:MET:HB3 | 1:A:95:PHE:CE1 | 0.63 | 2.28 | 15 | 1 |
| 1:A:53:VAL:HB | 1:A:125:ILE:HG22 | 0.63 | 1.70 | 14 | 5 |
| 1:A:63:LEU:HD22 | 1:A:68:MET:HE3 | 0.63 | 1.68 | 11 | 1 |
| 1:A:68:MET:CE | 1:A:95:PHE:CE2 | 0.63 | 2.82 | 8 | 2 |
| 1:A:133:GLU:HB3 | 1:A:137:TRP:CE2 | 0.63 | 2.28 | 9 | 20 |
| 1:A:50:LEU:HD13 | 1:A:61:ILE:HB | 0.63 | 1.70 | 18 | 12 |
| 1:A:53:VAL:HG21 | 1:A:113:ALA:HB2 | 0.63 | 1.68 | 9 | 2 |
| 1:A:53:VAL:HG13 | 1:A:54:GLY:N | 0.63 | 2.08 | 7 | 5 |
| 1:A:142:ILE:CG2 | 1:A:146:TYR:CE1 | 0.63 | 2.81 | 12 | 4 |
| 1:A:67:LEU:HD12 | 1:A:68:MET:O | 0.63 | 1.94 | 5 | 5 |
| 1:A:53:VAL:HG23 | 1:A:127:SER:OG | 0.63 | 1.93 | 10 | 7 |
| 1:A:116:ILE:HD12 | 1:A:116:ILE:N | 0.63 | 2.08 | 13 | 2 |
| 1:A:73:SER:CB | 1:A:88:TYR:CE2 | 0.63 | 2.82 | 15 | 2 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CD2 | 0.62 | 2.28 | 18 | 20 |
| 1:A:50:LEU:CB | 1:A:126:PHE:CD1 | 0.62 | 2.82 | 14 | 7 |
| 1:A:116:ILE:HD11 | 1:A:126:PHE:CD2 | 0.62 | 2.29 | 17 | 2 |
| 1:A:116:ILE:HD13 | 1:A:126:PHE:CD2 | 0.62 | 2.29 | 18 | 2 |
| 1:A:95:PHE:CD2 | 1:A:99:VAL:HG12 | 0.62 | 2.29 | 15 | 1 |
| 1:A:64:PHE:CZ | 1:A:69:ILE:HD12 | 0.62 | 2.30 | 3 | 2 |
| 1:A:49:THR:O | 1:A:137:TRP:CZ2 | 0.62 | 2.52 | 19 | 9 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:CG2 | 0.62 | 2.82 | 16 | 3 |
| 1:A:93:LYS:HB3 | 1:A:95:PHE:CE2 | 0.62 | 2.30 | 1 | 9 |
| 1:A:96:MET:CA | 1:A:144:LEU:HD13 | 0.62 | 2.25 | 8 | 3 |
| 1:A:44:PHE:C | 1:A:44:PHE:CD1 | 0.62 | 2.71 | 20 | 2 |
| 1:A:44:PHE:CD2 | 1:A:44:PHE:O | 0.61 | 2.54 | 6 | 3 |
| 1:A:68:MET:HB3 | 1:A:93:LYS:O | 0.61 | 1.95 | 12 | 7 |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:CE2 | 0.61 | 2.30 | 16 | 1 |
| 1:A:68:MET:SD | 1:A:95:PHE:CZ | 0.61 | 2.93 | 20 | 6 |
| 1:A:103:ASP:HA | 1:A:114:PHE:CB | 0.61 | 2.26 | 16 | 18 |
| 1:A:49:THR:HG23 | 1:A:60:HIS:HA | 0.61 | 1.71 | 15 | 5 |
| 1:A:45:ILE:CG2 | 1:A:63:LEU:HD23 | 0.61 | 2.25 | 12 | 1 |
| 1:A:44:PHE:CD1 | 1:A:44:PHE:C | 0.61 | 2.73 | 9 | 2 |
| 1:A:88:TYR:N | 1:A:88:TYR:CD1 | 0.61 | 2.65 | 19 | 5 |
| 1:A:114:PHE:CZ | 1:A:126:PHE:CB | 0.61 | 2.84 | 13 | 2 |
| 1:A:44:PHE:O | 1:A:44:PHE:CG | 0.61 | 2.53 | 15 | 5 |
| 1:A:105:ASP:O | 1:A:106:ASP:CB | 0.61 | 2.49 | 9 | 3 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:CB | 0.61 | 2.84 | 12 | 2 |
| 1:A:103:ASP:HA | 1:A:114:PHE:HB3 | 0.61 | 1.72 | 15 | 8 |
| 1:A:101:ILE:HD12 | 1:A:116:ILE:CD1 | 0.61 | 2.26 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:53:VAL:CG1 | 1:A:54:GLY:N | 0.60 | 2.64 | 11 | 5 |
| 1:A:107:THR:O | 1:A:110:TYR:O | 0.60 | 2.20 | 1 | 14 |
| 1:A:53:VAL:CG1 | 1:A:125:ILE:CG2 | 0.60 | 2.80 | 7 | 3 |
| 1:A:29:ILE:HG21 | 1:A:32:TRP:CE3 | 0.60 | 2.32 | 2 | 2 |
| 1:A:118:LEU:O | 1:A:119:LYS:C | 0.60 | 2.39 | 10 | 2 |
| 1:A:50:LEU:CD1 | 1:A:50:LEU:N | 0.60 | 2.65 | 13 | 3 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:CA | 0.60 | 2.26 | 19 | 3 |
| 1:A:95:PHE:CG | 1:A:118:LEU:HB2 | 0.60 | 2.32 | 15 | 3 |
| 1:A:45:ILE:HD11 | 1:A:65:ASP:OD1 | 0.60 | 1.97 | 19 | 1 |
| 1:A:29:ILE:O | 1:A:29:ILE:HD12 | 0.60 | 1.96 | 6 | 1 |
| 1:A:113:ALA:C | 1:A:114:PHE:CG | 0.60 | 2.74 | 15 | 2 |
| 1:A:125:ILE:N | 1:A:125:ILE:HD12 | 0.59 | 2.11 | 7 | 1 |
| 1:A:60:HIS:CB | 1:A:88:TYR:CD2 | 0.59 | 2.85 | 9 | 1 |
| 1:A:45:ILE:HG21 | 1:A:63:LEU:HD12 | 0.59 | 1.74 | 11 | 1 |
| 1:A:64:PHE:CD2 | 1:A:69:ILE:HG21 | 0.59 | 2.33 | 6 | 2 |
| 1:A:68:MET:CG | 1:A:95:PHE:CD2 | 0.59 | 2.85 | 3 | 2 |
| 1:A:113:ALA:HB1 | 1:A:126:PHE:O | 0.59 | 1.96 | 17 | 6 |
| 1:A:108:ASN:O | 1:A:109:GLU:CG | 0.59 | 2.51 | 10 | 1 |
| 1:A:86:ALA:O | 1:A:88:TYR:O | 0.59 | 2.20 | 17 | 15 |
| 1:A:46:MET:SD | 1:A:140:ALA:HB3 | 0.59 | 2.37 | 12 | 2 |
| 1:A:95:PHE:CE1 | 1:A:120:ASP:HB2 | 0.59 | 2.32 | 12 | 6 |
| 1:A:108:ASN:O | 1:A:109:GLU:CB | 0.59 | 2.51 | 13 | 2 |
| 1:A:106:ASP:O | 1:A:107:THR:OG1 | 0.59 | 2.17 | 17 | 3 |
| 1:A:58:GLU:O | 1:A:73:SER:O | 0.59 | 2.21 | 11 | 15 |
| 1:A:45:ILE:HG22 | 1:A:46:MET:CG | 0.59 | 2.28 | 10 | 7 |
| 1:A:56:LYS:O | 1:A:57:HIS:CG | 0.59 | 2.56 | 6 | 4 |
| 1:A:57:HIS:CE1 | 1:A:74:ASN:ND2 | 0.59 | 2.71 | 13 | 2 |
| 1:A:51:THR:HG22 | 1:A:127:SER:HB2 | 0.58 | 1.75 | 17 | 10 |
| 1:A:73:SER:OG | 1:A:88:TYR:CE2 | 0.58 | 2.53 | 1 | 3 |
| 1:A:90:LEU:HD22 | 1:A:90:LEU:O | 0.58 | 1.97 | 1 | 1 |
| 1:A:86:ALA:O | 1:A:87:GLU:C | 0.58 | 2.41 | 10 | 18 |
| 1:A:60:HIS:O | 1:A:61:ILE:HD13 | 0.58 | 1.98 | 19 | 2 |
| 1:A:59:ARG:CB | 1:A:71:CYS:O | 0.58 | 2.51 | 19 | 4 |
| 1:A:133:GLU:O | 1:A:137:TRP:CB | 0.58 | 2.52 | 13 | 19 |
| 1:A:54:GLY:O | 1:A:55:ALA:CB | 0.58 | 2.52 | 12 | 12 |
| 1:A:29:ILE:HG21 | 1:A:32:TRP:HE3 | 0.58 | 1.57 | 2 | 2 |
| 1:A:28:ASN:O | 1:A:29:ILE:O | 0.58 | 2.21 | 17 | 9 |
| 1:A:44:PHE:CE1 | 1:A:64:PHE:CE1 | 0.58 | 2.91 | 5 | 1 |
| 1:A:68:MET:CE | 1:A:141:LEU:HD11 | 0.58 | 2.28 | 10 | 3 |
| 1:A:73:SER:OG | 1:A:88:TYR:CD2 | 0.58 | 2.52 | 1 | 3 |
| 1:A:133:GLU:HB3 | 1:A:137:TRP:NE1 | 0.58 | 2.14 | 8 | 20 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:114:PHE:CE2 | 1:A:126:PHE:HB2 | 0.58 | 2.33 | 13 | 2 |
| 1:A:100:GLN:N | 1:A:117:ILE:O | 0.58 | 2.37 | 14 | 12 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CD1 | 0.58 | 2.34 | 19 | 6 |
| 1:A:99:VAL:HG21 | 1:A:141:LEU:HD23 | 0.58 | 1.76 | 14 | 1 |
| 1:A:95:PHE:CD2 | 1:A:99:VAL:CG1 | 0.58 | 2.86 | 15 | 2 |
| 1:A:73:SER:OG | 1:A:88:TYR:CE1 | 0.58 | 2.53 | 3 | 1 |
| 1:A:28:ASN:OD1 | 1:A:88:TYR:CG | 0.58 | 2.57 | 7 | 5 |
| 1:A:90:LEU:HD13 | 1:A:91:LYS:N | 0.58 | 2.13 | 7 | 2 |
| 1:A:134:LYS:O | 1:A:138:MET:HG2 | 0.57 | 1.98 | 1 | 16 |
| 1:A:114:PHE:CZ | 1:A:126:PHE:HB2 | 0.57 | 2.34 | 13 | 2 |
| 1:A:96:MET:HA | 1:A:99:VAL:CG1 | 0.57 | 2.29 | 1 | 1 |
| 1:A:66:GLY:O | 1:A:67:LEU:CD2 | 0.57 | 2.52 | 7 | 2 |
| 1:A:120:ASP:O | 1:A:121:GLU:CB | 0.57 | 2.52 | 18 | 7 |
| 1:A:113:ALA:CB | 1:A:126:PHE:O | 0.57 | 2.52 | 17 | 5 |
| 1:A:69:ILE:CD1 | 1:A:90:LEU:HD21 | 0.57 | 2.18 | 7 | 1 |
| 1:A:135:ASN:O | 1:A:139:ALA:CB | 0.57 | 2.53 | 7 | 16 |
| 1:A:61:ILE:CG2 | 1:A:68:MET:CE | 0.57 | 2.83 | 11 | 2 |
| 1:A:99:VAL:CG2 | 1:A:141:LEU:HD23 | 0.57 | 2.30 | 14 | 2 |
| 1:A:119:LYS:O | 1:A:120:ASP:C | 0.57 | 2.43 | 10 | 1 |
| 1:A:61:ILE:HD12 | 1:A:70:CYS:SG | 0.57 | 2.39 | 16 | 2 |
| 1:A:50:LEU:N | 1:A:50:LEU:CD1 | 0.57 | 2.67 | 7 | 2 |
| 1:A:69:ILE:CG2 | 1:A:90:LEU:HD23 | 0.57 | 2.30 | 8 | 1 |
| 1:A:29:ILE:HD12 | 1:A:29:ILE:C | 0.57 | 2.20 | 6 | 3 |
| 1:A:56:LYS:O | 1:A:57:HIS:CD2 | 0.57 | 2.58 | 6 | 1 |
| 1:A:53:VAL:CG2 | 1:A:127:SER:OG | 0.57 | 2.52 | 10 | 9 |
| 1:A:27:LYS:HG2 | 1:A:27:LYS:O | 0.57 | 1.98 | 10 | 2 |
| 1:A:116:ILE:HD13 | 1:A:116:ILE:N | 0.57 | 2.14 | 8 | 3 |
| 1:A:88:TYR:CD1 | 1:A:88:TYR:N | 0.56 | 2.71 | 2 | 1 |
| 1:A:44:PHE:CE1 | 1:A:62:PHE:CE1 | 0.56 | 2.93 | 18 | 1 |
| 1:A:66:GLY:O | 1:A:67:LEU:HG | 0.56 | 2.00 | 20 | 3 |
| 1:A:105:ASP:HB2 | 1:A:113:ALA:O | 0.56 | 2.00 | 20 | 2 |
| 1:A:106:ASP:OD2 | 1:A:110:TYR:CZ | 0.56 | 2.58 | 5 | 1 |
| 1:A:90:LEU:C | 1:A:90:LEU:CD1 | 0.56 | 2.72 | 13 | 4 |
| 1:A:63:LEU:HD11 | 1:A:144:LEU:HD11 | 0.56 | 1.77 | 4 | 2 |
| 1:A:73:SER:HA | 1:A:88:TYR:CG | 0.56 | 2.35 | 6 | 1 |
| 1:A:68:MET:HB2 | 1:A:95:PHE:CD2 | 0.56 | 2.35 | 5 | 2 |
| 1:A:128:ALA:HA | 1:A:137:TRP:CH2 | 0.56 | 2.36 | 4 | 20 |
| 1:A:50:LEU:HD23 | 1:A:114:PHE:HZ | 0.56 | 1.59 | 13 | 1 |
| 1:A:68:MET:SD | 1:A:144:LEU:HD12 | 0.56 | 2.40 | 15 | 1 |
| 1:A:107:THR:OG1 | 1:A:108:ASN:N | 0.56 | 2.38 | 13 | 1 |
| 1:A:114:PHE:CD1 | 1:A:116:ILE:HD11 | 0.56 | 2.36 | 2 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:101:ILE:HD12 | 1:A:116:ILE:CG1 | 0.56 | 2.30 | 12 | 2 |
| 1:A:28:ASN:CG | 1:A:88:TYR:CE2 | 0.56 | 2.79 | 2 | 2 |
| 1:A:29:ILE:O | 1:A:86:ALA:CB | 0.56 | 2.54 | 6 | 1 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:HB2 | 0.56 | 2.36 | 15 | 4 |
| 1:A:73:SER:OG | 1:A:88:TYR:CZ | 0.56 | 2.59 | 17 | 3 |
| 1:A:125:ILE:HD12 | 1:A:125:ILE:N | 0.56 | 2.16 | 17 | 1 |
| 1:A:113:ALA:HB2 | 1:A:127:SER:HB2 | 0.56 | 1.77 | 11 | 1 |
| 1:A:116:ILE:HG13 | 1:A:126:PHE:CD2 | 0.55 | 2.36 | 10 | 10 |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:HA | 0.55 | 1.78 | 11 | 2 |
| 1:A:142:ILE:O | 1:A:146:TYR:CD1 | 0.55 | 2.58 | 12 | 5 |
| 1:A:95:PHE:O | 1:A:99:VAL:CG1 | 0.55 | 2.54 | 13 | 9 |
| 1:A:95:PHE:CZ | 1:A:118:LEU:HB3 | 0.55 | 2.36 | 11 | 2 |
| 1:A:46:MET:HB2 | 1:A:63:LEU:HD21 | 0.55 | 1.77 | 15 | 1 |
| 1:A:62:PHE:O | 1:A:69:ILE:HG22 | 0.55 | 2.01 | 1 | 4 |
| 1:A:26:GLN:CD | 1:A:27:LYS:CE | 0.55 | 2.74 | 11 | 2 |
| 1:A:63:LEU:HD21 | 1:A:144:LEU:HD12 | 0.55 | 1.76 | 7 | 1 |
| 1:A:93:LYS:HB3 | 1:A:95:PHE:CE1 | 0.55 | 2.36 | 14 | 8 |
| 1:A:106:ASP:HB2 | 1:A:110:TYR:CD2 | 0.55 | 2.36 | 19 | 3 |
| 1:A:73:SER:HB3 | 1:A:88:TYR:CE2 | 0.55 | 2.37 | 15 | 2 |
| 1:A:46:MET:CE | 1:A:63:LEU:HD23 | 0.55 | 2.32 | 19 | 1 |
| 1:A:106:ASP:CB | 1:A:110:TYR:CG | 0.55 | 2.89 | 19 | 1 |
| 1:A:26:GLN:HG3 | 1:A:27:LYS:CE | 0.55 | 2.32 | 5 | 1 |
| 1:A:68:MET:HB2 | 1:A:95:PHE:CG | 0.55 | 2.36 | 5 | 2 |
| 1:A:102:ASN:O | 1:A:104:LYS:N | 0.55 | 2.40 | 13 | 13 |
| 1:A:142:ILE:O | 1:A:146:TYR:CG | 0.55 | 2.60 | 5 | 5 |
| 1:A:113:ALA:HB2 | 1:A:127:SER:CB | 0.55 | 2.32 | 13 | 1 |
| 1:A:113:ALA:HB2 | 1:A:127:SER:HG | 0.55 | 1.62 | 7 | 2 |
| 1:A:32:TRP:CD1 | 1:A:32:TRP:O | 0.55 | 2.60 | 18 | 1 |
| 1:A:68:MET:HB3 | 1:A:95:PHE:CG | 0.55 | 2.37 | 3 | 5 |
| 1:A:26:GLN:HA | 1:A:29:ILE:CG1 | 0.55 | 2.32 | 9 | 6 |
| 1:A:32:TRP:O | 1:A:32:TRP:CG | 0.55 | 2.60 | 6 | 1 |
| 1:A:111:LYS:CG | 1:A:112:HIS:N | 0.55 | 2.69 | 15 | 4 |
| 1:A:50:LEU:HA | 1:A:137:TRP:CH2 | 0.55 | 2.37 | 16 | 18 |
| 1:A:90:LEU:C | 1:A:90:LEU:HD22 | 0.55 | 2.23 | 4 | 5 |
| 1:A:95:PHE:O | 1:A:99:VAL:HG12 | 0.55 | 2.02 | 18 | 3 |
| 1:A:116:ILE:CD1 | 1:A:126:PHE:CG | 0.55 | 2.89 | 18 | 1 |
| 1:A:70:CYS:O | 1:A:91:LYS:CB | 0.55 | 2.55 | 6 | 5 |
| 1:A:95:PHE:CE2 | 1:A:118:LEU:CD2 | 0.55 | 2.72 | 1 | 1 |
| 1:A:50:LEU:HD23 | 1:A:126:PHE:HB3 | 0.55 | 1.78 | 18 | 1 |
| 1:A:144:LEU:O | 1:A:147:ARG:N | 0.54 | 2.40 | 2 | 15 |
| 1:A:59:ARG:NH2 | 1:A:124:VAL:HG12 | 0.54 | 2.17 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:MET:HG3 | 1:A:95:PHE:CD2 | 0.54 | 2.36 | 3 | 2 |
| 1:A:99:VAL:CG2 | 1:A:141:LEU:O | 0.54 | 2.55 | 8 | 12 |
| 1:A:59:ARG:CA | 1:A:71:CYS:O | 0.54 | 2.55 | 7 | 2 |
| 1:A:73:SER:CB | 1:A:88:TYR:CD2 | 0.54 | 2.89 | 1 | 1 |
| 1:A:119:LYS:C | 1:A:121:GLU:N | 0.54 | 2.60 | 10 | 11 |
| 1:A:29:ILE:CD1 | 1:A:30:ASP:N | 0.54 | 2.70 | 2 | 10 |
| 1:A:72:LYS:O | 1:A:88:TYR:CB | 0.54 | 2.55 | 17 | 4 |
| 1:A:47:GLU:HB2 | 1:A:62:PHE:CZ | 0.54 | 2.38 | 20 | 3 |
| 1:A:116:ILE:N | 1:A:116:ILE:HD12 | 0.54 | 2.17 | 16 | 1 |
| 1:A:47:GLU:HB3 | 1:A:62:PHE:CE1 | 0.54 | 2.37 | 5 | 10 |
| 1:A:142:ILE:O | 1:A:146:TYR:CD2 | 0.54 | 2.60 | 10 | 4 |
| 1:A:105:ASP:O | 1:A:110:TYR:CD2 | 0.54 | 2.61 | 9 | 1 |
| 1:A:93:LYS:HA | 1:A:95:PHE:CZ | 0.54 | 2.37 | 12 | 1 |
| 1:A:72:LYS:O | 1:A:88:TYR:HB2 | 0.54 | 2.03 | 6 | 1 |
| 1:A:95:PHE:O | 1:A:99:VAL:HG13 | 0.54 | 2.03 | 6 | 3 |
| 1:A:59:ARG:NH1 | 1:A:72:LYS:CG | 0.54 | 2.71 | 7 | 1 |
| 1:A:61:ILE:HD13 | 1:A:70:CYS:HB2 | 0.54 | 1.79 | 18 | 1 |
| 1:A:69:ILE:CD1 | 1:A:69:ILE:C | 0.54 | 2.72 | 20 | 5 |
| 1:A:106:ASP:O | 1:A:107:THR:HG23 | 0.54 | 2.02 | 20 | 2 |
| 1:A:95:PHE:HE2 | 1:A:141:LEU:HD11 | 0.54 | 1.61 | 3 | 3 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CE2 | 0.54 | 2.37 | 17 | 20 |
| 1:A:92:GLU:HB3 | 1:A:94:PHE:CZ | 0.54 | 2.38 | 18 | 1 |
| 1:A:29:ILE:HD12 | 1:A:30:ASP:N | 0.54 | 2.18 | 2 | 6 |
| 1:A:47:GLU:HB2 | 1:A:62:PHE:CE1 | 0.54 | 2.38 | 5 | 3 |
| 1:A:95:PHE:CB | 1:A:144:LEU:HD12 | 0.54 | 2.32 | 2 | 1 |
| 1:A:60:HIS:ND1 | 1:A:88:TYR:CZ | 0.54 | 2.76 | 12 | 1 |
| 1:A:107:THR:C | 1:A:109:GLU:N | 0.53 | 2.61 | 16 | 18 |
| 1:A:45:ILE:HD11 | 1:A:65:ASP:CG | 0.53 | 2.22 | 19 | 1 |
| 1:A:45:ILE:HG22 | 1:A:46:MET:N | 0.53 | 2.18 | 10 | 5 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CE2 | 0.53 | 2.38 | 18 | 5 |
| 1:A:50:LEU:HB3 | 1:A:126:PHE:CD1 | 0.53 | 2.37 | 5 | 5 |
| 1:A:116:ILE:CG2 | 1:A:141:LEU:CD2 | 0.53 | 2.86 | 9 | 1 |
| 1:A:55:ALA:O | 1:A:56:LYS:CD | 0.53 | 2.57 | 9 | 1 |
| 1:A:66:GLY:O | 1:A:67:LEU:CG | 0.53 | 2.56 | 20 | 3 |
| 1:A:96:MET:HA | 1:A:144:LEU:HD22 | 0.53 | 1.78 | 8 | 1 |
| 1:A:73:SER:CB | 1:A:88:TYR:CZ | 0.53 | 2.92 | 16 | 4 |
| 1:A:63:LEU:HD11 | 1:A:144:LEU:HD12 | 0.53 | 1.80 | 16 | 3 |
| 1:A:61:ILE:HG23 | 1:A:70:CYS:SG | 0.53 | 2.44 | 12 | 1 |
| 1:A:95:PHE:HA | 1:A:99:VAL:CG1 | 0.53 | 2.34 | 11 | 8 |
| 1:A:93:LYS:CB | 1:A:95:PHE:CE2 | 0.53 | 2.92 | 12 | 3 |
| 1:A:73:SER:HB3 | 1:A:88:TYR:CE1 | 0.53 | 2.39 | 11 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:MET:O | 1:A:93:LYS:O | 0.53 | 2.25 | 12 | 4 |
| 1:A:68:MET:O | 1:A:93:LYS:N | 0.53 | 2.42 | 13 | 9 |
| 1:A:57:HIS:CD2 | 1:A:58:GLU:O | 0.53 | 2.61 | 9 | 1 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CD2 | 0.53 | 2.37 | 1 | 3 |
| 1:A:117:ILE:O | 1:A:117:ILE:HG22 | 0.53 | 2.03 | 17 | 1 |
| 1:A:106:ASP:HB2 | 1:A:110:TYR:CD1 | 0.53 | 2.39 | 16 | 1 |
| 1:A:95:PHE:CD1 | 1:A:99:VAL:HG12 | 0.53 | 2.39 | 1 | 1 |
| 1:A:60:HIS:ND1 | 1:A:62:PHE:CE1 | 0.53 | 2.77 | 8 | 1 |
| 1:A:114:PHE:HZ | 1:A:128:ALA:HB3 | 0.52 | 1.63 | 9 | 4 |
| 1:A:102:ASN:O | 1:A:115:GLU:N | 0.52 | 2.40 | 18 | 2 |
| 1:A:90:LEU:CD1 | 1:A:90:LEU:C | 0.52 | 2.71 | 7 | 5 |
| 1:A:60:HIS:HB2 | 1:A:88:TYR:CD2 | 0.52 | 2.39 | 9 | 2 |
| 1:A:109:GLU:HG2 | 1:A:110:TYR:CE1 | 0.52 | 2.40 | 15 | 3 |
| 1:A:46:MET:HB2 | 1:A:63:LEU:HB3 | 0.52 | 1.80 | 12 | 1 |
| 1:A:90:LEU:CD1 | 1:A:90:LEU:O | 0.52 | 2.53 | 15 | 1 |
| 1:A:50:LEU:HG | 1:A:137:TRP:CZ2 | 0.52 | 2.39 | 2 | 20 |
| 1:A:93:LYS:HB3 | 1:A:95:PHE:CD2 | 0.52 | 2.39 | 16 | 6 |
| 1:A:68:MET:CB | 1:A:93:LYS:O | 0.52 | 2.57 | 1 | 3 |
| 1:A:111:LYS:HG3 | 1:A:112:HIS:CD2 | 0.52 | 2.39 | 10 | 2 |
| 1:A:146:TYR:O | 1:A:150:LEU:CD2 | 0.52 | 2.57 | 20 | 19 |
| 1:A:60:HIS:CB | 1:A:71:CYS:SG | 0.52 | 2.98 | 3 | 3 |
| 1:A:45:ILE:CG2 | 1:A:63:LEU:HD12 | 0.52 | 2.33 | 11 | 2 |
| 1:A:106:ASP:OD2 | 1:A:110:TYR:CE2 | 0.52 | 2.62 | 5 | 2 |
| 1:A:46:MET:CG | 1:A:63:LEU:HD23 | 0.52 | 2.34 | 6 | 2 |
| 1:A:47:GLU:CB | 1:A:62:PHE:CZ | 0.52 | 2.93 | 20 | 2 |
| 1:A:44:PHE:CD1 | 1:A:47:GLU:CG | 0.52 | 2.92 | 12 | 1 |
| 1:A:107:THR:O | 1:A:108:ASN:C | 0.52 | 2.48 | 8 | 13 |
| 1:A:112:HIS:CG | 1:A:112:HIS:O | 0.52 | 2.62 | 6 | 1 |
| 1:A:95:PHE:CD1 | 1:A:119:LYS:CB | 0.52 | 2.93 | 13 | 1 |
| 1:A:64:PHE:N | 1:A:67:LEU:O | 0.52 | 2.41 | 12 | 2 |
| 1:A:96:MET:HG3 | 1:A:144:LEU:HD13 | 0.52 | 1.81 | 18 | 1 |
| 1:A:95:PHE:CE1 | 1:A:120:ASP:CB | 0.52 | 2.91 | 12 | 2 |
| 1:A:46:MET:HG3 | 1:A:63:LEU:HD22 | 0.52 | 1.81 | 12 | 1 |
| 1:A:95:PHE:HB3 | 1:A:144:LEU:HD12 | 0.52 | 1.81 | 2 | 3 |
| 1:A:60:HIS:N | 1:A:71:CYS:O | 0.52 | 2.43 | 2 | 8 |
| 1:A:106:ASP:O | 1:A:107:THR:CG2 | 0.52 | 2.57 | 20 | 2 |
| 1:A:61:ILE:CD1 | 1:A:70:CYS:SG | 0.52 | 2.98 | 5 | 2 |
| 1:A:50:LEU:HB2 | 1:A:126:PHE:CD1 | 0.52 | 2.39 | 14 | 4 |
| 1:A:60:HIS:NE2 | 1:A:62:PHE:CD2 | 0.52 | 2.78 | 4 | 1 |
| 1:A:103:ASP:CG | 1:A:103:ASP:O | 0.52 | 2.48 | 16 | 3 |
| 1:A:26:GLN:HG2 | 1:A:32:TRP:CZ3 | 0.52 | 2.39 | 18 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:113:ALA:O | 1:A:114:PHE:CD2 | 0.52 | 2.63 | 15 | 1 |
| 1:A:69:ILE:C | 1:A:69:ILE:CD1 | 0.52 | 2.78 | 18 | 3 |
| 1:A:44:PHE:CG | 1:A:47:GLU:OE2 | 0.52 | 2.63 | 12 | 1 |
| 1:A:46:MET:SD | 1:A:140:ALA:CB | 0.52 | 2.98 | 13 | 9 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:N | 0.52 | 2.20 | 6 | 3 |
| 1:A:95:PHE:CD1 | 1:A:118:LEU:HB2 | 0.52 | 2.40 | 1 | 2 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:HG23 | 0.52 | 2.39 | 20 | 1 |
| 1:A:95:PHE:CD2 | 1:A:141:LEU:HD11 | 0.52 | 2.40 | 8 | 1 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CZ | 0.51 | 2.39 | 17 | 5 |
| 1:A:67:LEU:CD1 | 1:A:93:LYS:C | 0.51 | 2.78 | 19 | 2 |
| 1:A:142:ILE:HG23 | 1:A:146:TYR:CE1 | 0.51 | 2.40 | 5 | 5 |
| 1:A:63:LEU:HD22 | 1:A:68:MET:CE | 0.51 | 2.35 | 11 | 1 |
| 1:A:109:GLU:C | 1:A:110:TYR:CD1 | 0.51 | 2.84 | 15 | 1 |
| 1:A:73:SER:CB | 1:A:88:TYR:CD1 | 0.51 | 2.92 | 12 | 5 |
| 1:A:95:PHE:CZ | 1:A:120:ASP:OD2 | 0.51 | 2.63 | 18 | 1 |
| 1:A:70:CYS:O | 1:A:91:LYS:N | 0.51 | 2.43 | 4 | 5 |
| 1:A:96:MET:N | 1:A:96:MET:SD | 0.51 | 2.84 | 15 | 2 |
| 1:A:94:PHE:O | 1:A:95:PHE:CD1 | 0.51 | 2.64 | 13 | 2 |
| 1:A:95:PHE:CD1 | 1:A:96:MET:N | 0.51 | 2.78 | 1 | 1 |
| 1:A:101:ILE:HD11 | 1:A:114:PHE:CE2 | 0.51 | 2.40 | 16 | 1 |
| 1:A:49:THR:HB | 1:A:60:HIS:CD2 | 0.51 | 2.40 | 19 | 2 |
| 1:A:29:ILE:C | 1:A:29:ILE:HD12 | 0.51 | 2.26 | 2 | 5 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CE1 | 0.51 | 2.41 | 10 | 2 |
| 1:A:101:ILE:HD12 | 1:A:116:ILE:HG12 | 0.51 | 1.81 | 12 | 1 |
| 1:A:59:ARG:CB | 1:A:72:LYS:HA | 0.51 | 2.36 | 8 | 2 |
| 1:A:68:MET:CB | 1:A:95:PHE:CE1 | 0.51 | 2.94 | 15 | 1 |
| 1:A:99:VAL:HG21 | 1:A:141:LEU:O | 0.51 | 2.05 | 3 | 3 |
| 1:A:73:SER:CB | 1:A:88:TYR:CE1 | 0.51 | 2.94 | 3 | 4 |
| 1:A:107:THR:O | 1:A:110:TYR:N | 0.51 | 2.44 | 5 | 11 |
| 1:A:139:ALA:O | 1:A:143:SER:N | 0.51 | 2.44 | 20 | 10 |
| 1:A:72:LYS:N | 1:A:89:ARG:O | 0.51 | 2.43 | 13 | 4 |
| 1:A:26:GLN:OE1 | 1:A:32:TRP:CD2 | 0.51 | 2.64 | 18 | 1 |
| 1:A:73:SER:HA | 1:A:88:TYR:HB2 | 0.51 | 1.83 | 6 | 1 |
| 1:A:99:VAL:HG21 | 1:A:141:LEU:HD13 | 0.51 | 1.82 | 8 | 2 |
| 1:A:68:MET:SD | 1:A:144:LEU:CD1 | 0.51 | 2.99 | 15 | 1 |
| 1:A:64:PHE:CD2 | 1:A:69:ILE:CG2 | 0.50 | 2.94 | 16 | 3 |
| 1:A:46:MET:SD | 1:A:140:ALA:HB2 | 0.50 | 2.45 | 8 | 3 |
| 1:A:28:ASN:ND2 | 1:A:88:TYR:CZ | 0.50 | 2.79 | 19 | 1 |
| 1:A:45:ILE:HD12 | 1:A:63:LEU:HD11 | 0.50 | 1.82 | 20 | 3 |
| 1:A:101:ILE:HB | 1:A:141:LEU:HD22 | 0.50 | 1.84 | 13 | 2 |
| 1:A:68:MET:HG2 | 1:A:95:PHE:CE1 | 0.50 | 2.41 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:MET:SD | 1:A:93:LYS:CB | 0.50 | 3.00 | 3 | 2 |
| 1:A:50:LEU:CG | 1:A:137:TRP:CE3 | 0.50 | 2.94 | 9 | 19 |
| 1:A:105:ASP:HB2 | 1:A:112:HIS:O | 0.50 | 2.07 | 13 | 1 |
| 1:A:95:PHE:CE1 | 1:A:118:LEU:CB | 0.50 | 2.94 | 17 | 2 |
| 1:A:93:LYS:CG | 1:A:118:LEU:HD13 | 0.50 | 2.36 | 2 | 1 |
| 1:A:29:ILE:CG2 | 1:A:90:LEU:HB3 | 0.50 | 2.36 | 1 | 3 |
| 1:A:106:ASP:HB3 | 1:A:110:TYR:CD1 | 0.50 | 2.41 | 9 | 2 |
| 1:A:65:ASP:O | 1:A:96:MET:HE1 | 0.50 | 2.07 | 18 | 1 |
| 1:A:112:HIS:O | 1:A:114:PHE:CE1 | 0.50 | 2.65 | 18 | 1 |
| 1:A:112:HIS:CD2 | 1:A:128:ALA:O | 0.50 | 2.65 | 5 | 5 |
| 1:A:112:HIS:ND1 | 1:A:112:HIS:O | 0.50 | 2.45 | 20 | 2 |
| 1:A:106:ASP:HB3 | 1:A:110:TYR:CG | 0.50 | 2.42 | 19 | 1 |
| 1:A:26:GLN:NE2 | 1:A:27:LYS:NZ | 0.50 | 2.60 | 11 | 1 |
| 1:A:113:ALA:HA | 1:A:126:PHE:O | 0.50 | 2.06 | 9 | 14 |
| 1:A:128:ALA:HB2 | 1:A:137:TRP:CH2 | 0.50 | 2.39 | 14 | 2 |
| 1:A:32:TRP:CH2 | 1:A:64:PHE:CE2 | 0.50 | 3.00 | 19 | 1 |
| 1:A:113:ALA:CA | 1:A:126:PHE:O | 0.50 | 2.59 | 17 | 5 |
| 1:A:101:ILE:CG1 | 1:A:116:ILE:HD12 | 0.50 | 2.36 | 14 | 1 |
| 1:A:29:ILE:HD12 | 1:A:29:ILE:N | 0.50 | 2.21 | 14 | 1 |
| 1:A:47:GLU:HB3 | 1:A:62:PHE:CZ | 0.50 | 2.41 | 3 | 2 |
| 1:A:44:PHE:CD1 | 1:A:47:GLU:CD | 0.50 | 2.86 | 12 | 1 |
| 1:A:31:GLY:O | 1:A:32:TRP:O | 0.49 | 2.30 | 16 | 2 |
| 1:A:93:LYS:O | 1:A:95:PHE:N | 0.49 | 2.45 | 8 | 5 |
| 1:A:50:LEU:CD2 | 1:A:137:TRP:CD2 | 0.49 | 2.96 | 17 | 16 |
| 1:A:51:THR:CG2 | 1:A:127:SER:HB2 | 0.49 | 2.37 | 7 | 4 |
| 1:A:29:ILE:O | 1:A:88:TYR:O | 0.49 | 2.29 | 12 | 9 |
| 1:A:97:ARG:O | 1:A:98:LYS:CG | 0.49 | 2.60 | 13 | 1 |
| 1:A:95:PHE:CZ | 1:A:120:ASP:HB2 | 0.49 | 2.42 | 12 | 2 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:HG13 | 0.49 | 2.42 | 10 | 2 |
| 1:A:98:LYS:CG | 1:A:145:GLN:OE1 | 0.49 | 2.60 | 10 | 1 |
| 1:A:112:HIS:O | 1:A:127:SER:HA | 0.49 | 2.07 | 9 | 1 |
| 1:A:136:ASN:O | 1:A:140:ALA:CB | 0.49 | 2.61 | 17 | 3 |
| 1:A:62:PHE:HB3 | 1:A:64:PHE:CE1 | 0.49 | 2.42 | 16 | 2 |
| 1:A:96:MET:HG2 | 1:A:97:ARG:N | 0.49 | 2.22 | 15 | 1 |
| 1:A:50:LEU:HD22 | 1:A:126:PHE:CG | 0.49 | 2.42 | 14 | 4 |
| 1:A:44:PHE:CE2 | 1:A:47:GLU:OE2 | 0.49 | 2.66 | 13 | 1 |
| 1:A:95:PHE:CD1 | 1:A:120:ASP:HB2 | 0.49 | 2.42 | 18 | 1 |
| 1:A:50:LEU:CD1 | 1:A:61:ILE:HB | 0.49 | 2.38 | 12 | 17 |
| 1:A:131:ALA:O | 1:A:134:LYS:CG | 0.49 | 2.60 | 13 | 3 |
| 1:A:94:PHE:C | 1:A:95:PHE:CD1 | 0.49 | 2.85 | 12 | 3 |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:CB | 0.49 | 2.37 | 15 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:48:GLY:O | 1:A:61:ILE:O | 0.49 | 2.31 | 11 | 12 |
| 1:A:114:PHE:O | 1:A:125:ILE:HA | 0.49 | 2.06 | 11 | 10 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:HB | 0.49 | 2.42 | 2 | 3 |
| 1:A:60:HIS:HB2 | 1:A:88:TYR:CE2 | 0.49 | 2.42 | 15 | 2 |
| 1:A:57:HIS:CE1 | 1:A:73:SER:O | 0.49 | 2.65 | 9 | 1 |
| 1:A:93:LYS:HG2 | 1:A:118:LEU:HD13 | 0.49 | 1.84 | 2 | 1 |
| 1:A:44:PHE:CD1 | 1:A:47:GLU:OE2 | 0.49 | 2.66 | 12 | 1 |
| 1:A:28:ASN:OD1 | 1:A:88:TYR:CD1 | 0.49 | 2.65 | 15 | 1 |
| 1:A:106:ASP:O | 1:A:109:GLU:N | 0.49 | 2.40 | 4 | 8 |
| 1:A:105:ASP:OD2 | 1:A:107:THR:HG23 | 0.49 | 2.08 | 5 | 2 |
| 1:A:67:LEU:HD21 | 1:A:92:GLU:CD | 0.49 | 2.27 | 6 | 1 |
| 1:A:114:PHE:HD1 | 1:A:116:ILE:HD11 | 0.49 | 1.68 | 2 | 4 |
| 1:A:72:LYS:O | 1:A:89:ARG:N | 0.49 | 2.45 | 9 | 2 |
| 1:A:68:MET:HG2 | 1:A:95:PHE:CE2 | 0.49 | 2.42 | 2 | 1 |
| 1:A:95:PHE:O | 1:A:97:ARG:N | 0.49 | 2.46 | 5 | 8 |
| 1:A:28:ASN:O | 1:A:88:TYR:C | 0.49 | 2.52 | 3 | 5 |
| 1:A:64:PHE:HB2 | 1:A:67:LEU:O | 0.49 | 2.08 | 16 | 11 |
| 1:A:57:HIS:ND1 | 1:A:74:ASN:ND2 | 0.49 | 2.60 | 13 | 2 |
| 1:A:92:GLU:O | 1:A:93:LYS:CE | 0.49 | 2.61 | 1 | 1 |
| 1:A:68:MET:CG | 1:A:95:PHE:CE2 | 0.49 | 2.96 | 5 | 2 |
| 1:A:118:LEU:O | 1:A:118:LEU:CD1 | 0.49 | 2.60 | 10 | 1 |
| 1:A:68:MET:HE1 | 1:A:141:LEU:HD11 | 0.49 | 1.85 | 12 | 2 |
| 1:A:45:ILE:HG21 | 1:A:63:LEU:HD21 | 0.49 | 1.84 | 17 | 2 |
| 1:A:63:LEU:HD23 | 1:A:63:LEU:H | 0.49 | 1.68 | 11 | 2 |
| 1:A:30:ASP:CG | 1:A:31:GLY:N | 0.48 | 2.65 | 1 | 13 |
| 1:A:50:LEU:CD2 | 1:A:126:PHE:CG | 0.48 | 2.95 | 15 | 6 |
| 1:A:105:ASP:CG | 1:A:106:ASP:N | 0.48 | 2.63 | 17 | 2 |
| 1:A:73:SER:HA | 1:A:88:TYR:CD1 | 0.48 | 2.43 | 20 | 3 |
| 1:A:120:ASP:O | 1:A:122:ASN:N | 0.48 | 2.46 | 10 | 1 |
| 1:A:68:MET:HG2 | 1:A:95:PHE:CZ | 0.48 | 2.42 | 15 | 2 |
| 1:A:93:LYS:HB3 | 1:A:95:PHE:CD1 | 0.48 | 2.43 | 11 | 1 |
| 1:A:128:ALA:HA | 1:A:137:TRP:CZ3 | 0.48 | 2.43 | 13 | 3 |
| 1:A:64:PHE:CZ | 1:A:69:ILE:CG2 | 0.48 | 2.96 | 2 | 1 |
| 1:A:70:CYS:SG | 1:A:93:LYS:CD | 0.48 | 3.01 | 16 | 2 |
| 1:A:62:PHE:O | 1:A:69:ILE:CG2 | 0.48 | 2.62 | 18 | 2 |
| 1:A:60:HIS:CE1 | 1:A:88:TYR:CZ | 0.48 | 3.01 | 12 | 1 |
| 1:A:59:ARG:HD2 | 1:A:61:ILE:HD11 | 0.48 | 1.84 | 7 | 1 |
| 1:A:99:VAL:HG23 | 1:A:100:GLN:N | 0.48 | 2.23 | 15 | 1 |
| 1:A:111:LYS:HG3 | 1:A:112:HIS:N | 0.48 | 2.23 | 12 | 7 |
| 1:A:61:ILE:CG2 | 1:A:68:MET:HE1 | 0.48 | 2.38 | 11 | 1 |
| 1:A:51:THR:O | 1:A:127:SER:N | 0.48 | 2.46 | 9 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:MET:O | 1:A:144:LEU:HB3 | 0.48 | 2.08 | 18 | 4 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:HA | 0.48 | 1.86 | 19 | 2 |
| 1:A:28:ASN:O | 1:A:88:TYR:HB2 | 0.48 | 2.08 | 17 | 3 |
| 1:A:112:HIS:O | 1:A:127:SER:OG | 0.48 | 2.31 | 12 | 1 |
| 1:A:59:ARG:CD | 1:A:88:TYR:CE2 | 0.48 | 2.96 | 8 | 1 |
| 1:A:118:LEU:O | 1:A:120:ASP:N | 0.48 | 2.47 | 12 | 3 |
| 1:A:86:ALA:C | 1:A:88:TYR:N | 0.48 | 2.64 | 6 | 4 |
| 1:A:71:CYS:SG | 1:A:71:CYS:O | 0.48 | 2.71 | 4 | 1 |
| 1:A:116:ILE:HD11 | 1:A:126:PHE:CG | 0.48 | 2.44 | 18 | 2 |
| 1:A:109:GLU:CG | 1:A:109:GLU:O | 0.48 | 2.61 | 15 | 2 |
| 1:A:69:ILE:CD1 | 1:A:71:CYS:SG | 0.47 | 3.02 | 1 | 1 |
| 1:A:96:MET:SD | 1:A:97:ARG:N | 0.47 | 2.87 | 10 | 2 |
| 1:A:106:ASP:C | 1:A:107:THR:CG2 | 0.47 | 2.76 | 7 | 3 |
| 1:A:26:GLN:HG2 | 1:A:32:TRP:CE3 | 0.47 | 2.43 | 18 | 1 |
| 1:A:100:GLN:O | 1:A:117:ILE:N | 0.47 | 2.47 | 6 | 9 |
| 1:A:61:ILE:HG23 | 1:A:70:CYS:HB3 | 0.47 | 1.86 | 19 | 1 |
| 1:A:105:ASP:HB3 | 1:A:114:PHE:N | 0.47 | 2.23 | 13 | 1 |
| 1:A:117:ILE:HA | 1:A:122:ASN:O | 0.47 | 2.08 | 18 | 3 |
| 1:A:59:ARG:HD3 | 1:A:88:TYR:CE1 | 0.47 | 2.44 | 8 | 1 |
| 1:A:61:ILE:CD1 | 1:A:70:CYS:HB3 | 0.47 | 2.40 | 6 | 4 |
| 1:A:110:TYR:CD1 | 1:A:110:TYR:N | 0.47 | 2.82 | 15 | 4 |
| 1:A:52:ARG:N | 1:A:57:HIS:O | 0.47 | 2.47 | 17 | 3 |
| 1:A:112:HIS:O | 1:A:112:HIS:ND1 | 0.47 | 2.46 | 2 | 2 |
| 1:A:29:ILE:HD12 | 1:A:86:ALA:CB | 0.47 | 2.40 | 16 | 1 |
| 1:A:47:GLU:OE1 | 1:A:62:PHE:CE1 | 0.47 | 2.67 | 12 | 1 |
| 1:A:101:ILE:HG21 | 1:A:138:MET:HA | 0.47 | 1.86 | 13 | 1 |
| 1:A:55:ALA:O | 1:A:56:LYS:HB3 | 0.47 | 2.08 | 11 | 2 |
| 1:A:95:PHE:CE2 | 1:A:141:LEU:HD21 | 0.47 | 2.43 | 2 | 1 |
| 1:A:111:LYS:HE2 | 1:A:112:HIS:CE1 | 0.47 | 2.43 | 20 | 1 |
| 1:A:132:GLU:O | 1:A:136:ASN:N | 0.47 | 2.39 | 17 | 4 |
| 1:A:68:MET:HB2 | 1:A:95:PHE:HB2 | 0.47 | 1.86 | 3 | 2 |
| 1:A:50:LEU:CG | 1:A:137:TRP:CZ3 | 0.47 | 2.97 | 19 | 17 |
| 1:A:66:GLY:C | 1:A:96:MET:SD | 0.47 | 2.93 | 6 | 2 |
| 1:A:106:ASP:CB | 1:A:110:TYR:CD2 | 0.47 | 2.98 | 19 | 1 |
| 1:A:52:ARG:O | 1:A:52:ARG:CG | 0.47 | 2.63 | 4 | 1 |
| 1:A:47:GLU:HB3 | 1:A:62:PHE:CE2 | 0.47 | 2.44 | 8 | 1 |
| 1:A:58:GLU:C | 1:A:59:ARG:CG | 0.47 | 2.82 | 5 | 1 |
| 1:A:116:ILE:O | 1:A:123:SER:HA | 0.47 | 2.09 | 13 | 4 |
| 1:A:110:TYR:N | 1:A:110:TYR:CD1 | 0.47 | 2.81 | 20 | 5 |
| 1:A:120:ASP:O | 1:A:121:GLU:C | 0.47 | 2.53 | 10 | 1 |
| 1:A:136:ASN:O | 1:A:140:ALA:HB2 | 0.47 | 2.10 | 11 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:27:LYS:HE3 | 1:A:27:LYS:N | 0.47 | 2.25 | 14 | 1 |
| 1:A:57:HIS:NE2 | 1:A:74:ASN:ND2 | 0.47 | 2.63 | 2 | 1 |
| 1:A:90:LEU:HD22 | 1:A:91:LYS:H | 0.47 | 1.70 | 9 | 1 |
| 1:A:95:PHE:CE1 | 1:A:118:LEU:HB2 | 0.47 | 2.45 | 17 | 1 |
| 1:A:51:THR:HG22 | 1:A:127:SER:CB | 0.47 | 2.39 | 17 | 1 |
| 1:A:69:ILE:CD1 | 1:A:91:LYS:O | 0.47 | 2.63 | 14 | 1 |
| 1:A:116:ILE:N | 1:A:116:ILE:CD1 | 0.47 | 2.74 | 20 | 3 |
| 1:A:111:LYS:HE3 | 1:A:112:HIS:CG | 0.47 | 2.45 | 10 | 1 |
| 1:A:44:PHE:CE2 | 1:A:47:GLU:HB3 | 0.47 | 2.45 | 11 | 1 |
| 1:A:111:LYS:CE | 1:A:112:HIS:NE2 | 0.47 | 2.77 | 20 | 1 |
| 1:A:95:PHE:O | 1:A:98:LYS:N | 0.47 | 2.39 | 1 | 3 |
| 1:A:118:LEU:C | 1:A:119:LYS:O | 0.47 | 2.53 | 10 | 1 |
| 1:A:116:ILE:CD1 | 1:A:116:ILE:N | 0.47 | 2.72 | 7 | 2 |
| 1:A:58:GLU:O | 1:A:59:ARG:CG | 0.47 | 2.63 | 12 | 1 |
| 1:A:102:ASN:O | 1:A:115:GLU:O | 0.46 | 2.34 | 14 | 9 |
| 1:A:134:LYS:HG3 | 1:A:135:ASN:N | 0.46 | 2.25 | 1 | 5 |
| 1:A:53:VAL:HB | 1:A:125:ILE:CG2 | 0.46 | 2.40 | 9 | 1 |
| 1:A:67:LEU:HD13 | 1:A:94:PHE:HD1 | 0.46 | 1.59 | 7 | 1 |
| 1:A:56:LYS:O | 1:A:57:HIS:ND1 | 0.46 | 2.49 | 5 | 7 |
| 1:A:45:ILE:HG12 | 1:A:65:ASP:N | 0.46 | 2.25 | 16 | 2 |
| 1:A:95:PHE:HD1 | 1:A:99:VAL:HG12 | 0.46 | 1.68 | 1 | 1 |
| 1:A:73:SER:HB3 | 1:A:88:TYR:CZ | 0.46 | 2.46 | 11 | 2 |
| 1:A:112:HIS:ND1 | 1:A:128:ALA:O | 0.46 | 2.47 | 7 | 1 |
| 1:A:67:LEU:CD1 | 1:A:68:MET:O | 0.46 | 2.62 | 16 | 2 |
| 1:A:95:PHE:CG | 1:A:99:VAL:CG1 | 0.46 | 2.96 | 2 | 3 |
| 1:A:59:ARG:HD3 | 1:A:73:SER:CB | 0.46 | 2.40 | 19 | 1 |
| 1:A:59:ARG:NH2 | 1:A:124:VAL:CG1 | 0.46 | 2.78 | 13 | 2 |
| 1:A:95:PHE:C | 1:A:95:PHE:CD1 | 0.46 | 2.89 | 1 | 1 |
| 1:A:95:PHE:C | 1:A:97:ARG:N | 0.46 | 2.68 | 5 | 9 |
| 1:A:116:ILE:O | 1:A:117:ILE:CG1 | 0.46 | 2.63 | 4 | 4 |
| 1:A:62:PHE:O | 1:A:64:PHE:CE1 | 0.46 | 2.68 | 6 | 2 |
| 1:A:106:ASP:HB2 | 1:A:110:TYR:CE2 | 0.46 | 2.45 | 1 | 3 |
| 1:A:145:GLN:O | 1:A:145:GLN:NE2 | 0.46 | 2.48 | 13 | 1 |
| 1:A:116:ILE:HG13 | 1:A:126:PHE:CG | 0.46 | 2.45 | 1 | 3 |
| 1:A:71:CYS:HA | 1:A:89:ARG:O | 0.46 | 2.10 | 12 | 2 |
| 1:A:142:ILE:HD13 | 1:A:145:GLN:HG2 | 0.46 | 1.88 | 16 | 1 |
| 1:A:95:PHE:CD2 | 1:A:118:LEU:HB3 | 0.46 | 2.46 | 15 | 1 |
| 1:A:130:SER:HB3 | 1:A:133:GLU:CG | 0.46 | 2.40 | 10 | 5 |
| 1:A:142:ILE:HG22 | 1:A:146:TYR:CE2 | 0.46 | 2.44 | 15 | 3 |
| 1:A:111:LYS:CE | 1:A:112:HIS:CD2 | 0.46 | 2.99 | 17 | 1 |
| 1:A:31:GLY:N | 1:A:90:LEU:HD12 | 0.46 | 2.24 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:51:THR:CG2 | 1:A:127:SER:HB3 | 0.46 | 2.40 | 11 | 1 |
| 1:A:68:MET:CG | 1:A:95:PHE:CZ | 0.46 | 2.98 | 15 | 1 |
| 1:A:61:ILE:HG23 | 1:A:68:MET:CE | 0.46 | 2.41 | 1 | 1 |
| 1:A:130:SER:HB2 | 1:A:133:GLU:CG | 0.46 | 2.40 | 14 | 6 |
| 1:A:100:GLN:O | 1:A:117:ILE:O | 0.46 | 2.34 | 19 | 3 |
| 1:A:68:MET:HG3 | 1:A:95:PHE:CE2 | 0.46 | 2.46 | 5 | 1 |
| 1:A:32:TRP:CG | 1:A:32:TRP:O | 0.46 | 2.68 | 14 | 2 |
| 1:A:114:PHE:CZ | 1:A:128:ALA:HB3 | 0.46 | 2.46 | 9 | 1 |
| 1:A:118:LEU:C | 1:A:120:ASP:N | 0.46 | 2.68 | 12 | 6 |
| 1:A:45:ILE:HG22 | 1:A:46:MET:HG2 | 0.46 | 1.88 | 10 | 1 |
| 1:A:72:LYS:O | 1:A:88:TYR:CG | 0.46 | 2.69 | 17 | 1 |
| 1:A:128:ALA:CB | 1:A:137:TRP:CH2 | 0.46 | 2.99 | 2 | 4 |
| 1:A:98:LYS:O | 1:A:99:VAL:CG1 | 0.46 | 2.64 | 8 | 3 |
| 1:A:30:ASP:OD2 | 1:A:89:ARG:CZ | 0.46 | 2.63 | 10 | 1 |
| 1:A:93:LYS:C | 1:A:95:PHE:CD2 | 0.46 | 2.89 | 7 | 1 |
| 1:A:50:LEU:HD22 | 1:A:126:PHE:CE2 | 0.45 | 2.46 | 1 | 4 |
| 1:A:26:GLN:O | 1:A:29:ILE:HD11 | 0.45 | 2.11 | 10 | 1 |
| 1:A:132:GLU:O | 1:A:135:ASN:N | 0.45 | 2.48 | 17 | 1 |
| 1:A:92:GLU:O | 1:A:92:GLU:CG | 0.45 | 2.63 | 16 | 1 |
| 1:A:118:LEU:O | 1:A:121:GLU:N | 0.45 | 2.47 | 20 | 1 |
| 1:A:105:ASP:HB3 | 1:A:113:ALA:O | 0.45 | 2.09 | 15 | 2 |
| 1:A:59:ARG:HD3 | 1:A:88:TYR:CZ | 0.45 | 2.46 | 8 | 1 |
| 1:A:59:ARG:CD | 1:A:73:SER:CB | 0.45 | 2.95 | 8 | 2 |
| 1:A:92:GLU:HG2 | 1:A:94:PHE:CZ | 0.45 | 2.46 | 13 | 1 |
| 1:A:112:HIS:O | 1:A:112:HIS:CG | 0.45 | 2.69 | 8 | 2 |
| 1:A:130:SER:O | 1:A:131:ALA:C | 0.45 | 2.55 | 17 | 1 |
| 1:A:29:ILE:CD1 | 1:A:29:ILE:C | 0.45 | 2.84 | 6 | 1 |
| 1:A:68:MET:CG | 1:A:96:MET:HG2 | 0.45 | 2.41 | 1 | 1 |
| 1:A:117:ILE:HG22 | 1:A:117:ILE:O | 0.45 | 2.11 | 11 | 1 |
| 1:A:68:MET:CG | 1:A:95:PHE:CE1 | 0.45 | 2.99 | 15 | 1 |
| 1:A:57:HIS:CD2 | 1:A:74:ASN:HB2 | 0.45 | 2.47 | 5 | 1 |
| 1:A:50:LEU:CD1 | 1:A:61:ILE:CG1 | 0.45 | 2.91 | 12 | 2 |
| 1:A:130:SER:O | 1:A:133:GLU:N | 0.45 | 2.50 | 8 | 5 |
| 1:A:135:ASN:O | 1:A:138:MET:HE2 | 0.45 | 2.12 | 16 | 1 |
| 1:A:59:ARG:HD3 | 1:A:88:TYR:CD1 | 0.45 | 2.46 | 8 | 1 |
| 1:A:59:ARG:CD | 1:A:73:SER:HB3 | 0.45 | 2.42 | 19 | 2 |
| 1:A:29:ILE:C | 1:A:86:ALA:HB1 | 0.45 | 2.29 | 19 | 1 |
| 1:A:68:MET:CB | 1:A:95:PHE:HB2 | 0.45 | 2.42 | 17 | 4 |
| 1:A:32:TRP:CZ3 | 1:A:64:PHE:CE2 | 0.45 | 3.05 | 7 | 1 |
| 1:A:116:ILE:O | 1:A:124:VAL:N | 0.45 | 2.50 | 12 | 1 |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:O | 0.45 | 2.12 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:62:PHE:O | 1:A:69:ILE:O | 0.45 | 2.35 | 19 | 2 |
| 1:A:128:ALA:CA | 1:A:137:TRP:CH2 | 0.45 | 3.00 | 2 | 5 |
| 1:A:28:ASN:O | 1:A:28:ASN:OD1 | 0.45 | 2.35 | 6 | 1 |
| 1:A:55:ALA:O | 1:A:56:LYS:C | 0.45 | 2.55 | 18 | 2 |
| 1:A:106:ASP:C | 1:A:110:TYR:HB2 | 0.45 | 2.31 | 15 | 1 |
| 1:A:105:ASP:CG | 1:A:113:ALA:O | 0.45 | 2.55 | 3 | 8 |
| 1:A:53:VAL:O | 1:A:125:ILE:CG2 | 0.45 | 2.63 | 8 | 4 |
| 1:A:57:HIS:NE2 | 1:A:58:GLU:O | 0.45 | 2.50 | 9 | 1 |
| 1:A:95:PHE:CZ | 1:A:120:ASP:CG | 0.45 | 2.90 | 12 | 1 |
| 1:A:45:ILE:CD1 | 1:A:65:ASP:HA | 0.45 | 2.42 | 7 | 1 |
| 1:A:114:PHE:CE2 | 1:A:134:LYS:HG3 | 0.45 | 2.46 | 15 | 1 |
| 1:A:68:MET:O | 1:A:93:LYS:CA | 0.45 | 2.65 | 13 | 2 |
| 1:A:30:ASP:CB | 1:A:89:ARG:CG | 0.45 | 2.94 | 14 | 1 |
| 1:A:133:GLU:OE1 | 1:A:137:TRP:NE1 | 0.45 | 2.50 | 1 | 1 |
| 1:A:63:LEU:CD2 | 1:A:96:MET:SD | 0.45 | 2.99 | 1 | 1 |
| 1:A:51:THR:HB | 1:A:127:SER:CB | 0.45 | 2.42 | 11 | 1 |
| 1:A:28:ASN:ND2 | 1:A:87:GLU:OE1 | 0.44 | 2.51 | 6 | 1 |
| 1:A:101:ILE:HG22 | 1:A:142:ILE:HG12 | 0.44 | 1.89 | 14 | 1 |
| 1:A:90:LEU:C | 1:A:90:LEU:CD2 | 0.44 | 2.76 | 15 | 1 |
| 1:A:48:GLY:O | 1:A:61:ILE:N | 0.44 | 2.51 | 9 | 3 |
| 1:A:114:PHE:CZ | 1:A:126:PHE:HB3 | 0.44 | 2.46 | 13 | 1 |
| 1:A:120:ASP:OD1 | 1:A:120:ASP:N | 0.44 | 2.50 | 20 | 1 |
| 1:A:99:VAL:N | 1:A:145:GLN:OE1 | 0.44 | 2.50 | 13 | 2 |
| 1:A:28:ASN:CA | 1:A:86:ALA:HA | 0.44 | 2.43 | 20 | 4 |
| 1:A:52:ARG:HA | 1:A:125:ILE:O | 0.44 | 2.12 | 15 | 4 |
| 1:A:112:HIS:CG | 1:A:128:ALA:O | 0.44 | 2.71 | 1 | 1 |
| 1:A:63:LEU:HD12 | 1:A:68:MET:CB | 0.44 | 2.38 | 12 | 1 |
| 1:A:100:GLN:CB | 1:A:117:ILE:O | 0.44 | 2.65 | 1 | 1 |
| 1:A:111:LYS:HE3 | 1:A:112:HIS:CE1 | 0.44 | 2.48 | 9 | 1 |
| 1:A:113:ALA:C | 1:A:114:PHE:CD1 | 0.44 | 2.90 | 14 | 2 |
| 1:A:47:GLU:O | 1:A:47:GLU:CG | 0.44 | 2.65 | 2 | 1 |
| 1:A:123:SER:C | 1:A:124:VAL:CG2 | 0.44 | 2.85 | 18 | 1 |
| 1:A:61:ILE:CG2 | 1:A:68:MET:HE2 | 0.44 | 2.42 | 11 | 1 |
| 1:A:95:PHE:CB | 1:A:99:VAL:HG11 | 0.44 | 2.42 | 17 | 4 |
| 1:A:28:ASN:N | 1:A:86:ALA:HA | 0.44 | 2.28 | 20 | 3 |
| 1:A:125:ILE:CD1 | 1:A:125:ILE:N | 0.44 | 2.78 | 7 | 1 |
| 1:A:96:MET:SD | 1:A:96:MET:C | 0.44 | 2.96 | 7 | 1 |
| 1:A:46:MET:HE2 | 1:A:63:LEU:HD23 | 0.44 | 1.90 | 19 | 1 |
| 1:A:49:THR:HG23 | 1:A:60:HIS:CG | 0.44 | 2.48 | 7 | 3 |
| 1:A:72:LYS:O | 1:A:88:TYR:HA | 0.44 | 2.13 | 12 | 2 |
| 1:A:112:HIS:O | 1:A:113:ALA:O | 0.44 | 2.36 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:119:LYS:C | 1:A:121:GLU:H | 0.44 | 2.16 | 20 | 1 |
| 1:A:63:LEU:CD1 | 1:A:63:LEU:C | 0.44 | 2.81 | 20 | 1 |
| 1:A:49:THR:HB | 1:A:60:HIS:CG | 0.44 | 2.47 | 11 | 3 |
| 1:A:96:MET:HG3 | 1:A:97:ARG:N | 0.44 | 2.26 | 6 | 1 |
| 1:A:100:GLN:CA | 1:A:117:ILE:O | 0.44 | 2.66 | 7 | 2 |
| 1:A:99:VAL:HB | 1:A:141:LEU:HD23 | 0.44 | 1.90 | 1 | 1 |
| 1:A:53:VAL:HG12 | 1:A:54:GLY:N | 0.44 | 2.24 | 9 | 1 |
| 1:A:55:ALA:C | 1:A:56:LYS:CG | 0.44 | 2.86 | 9 | 1 |
| 1:A:64:PHE:O | 1:A:67:LEU:N | 0.44 | 2.50 | 2 | 1 |
| 1:A:68:MET:O | 1:A:93:LYS:HB2 | 0.43 | 2.14 | 9 | 5 |
| 1:A:69:ILE:HD11 | 1:A:90:LEU:HA | 0.43 | 1.90 | 1 | 1 |
| 1:A:72:LYS:O | 1:A:88:TYR:CA | 0.43 | 2.67 | 9 | 3 |
| 1:A:107:THR:HG23 | 1:A:112:HIS:CD2 | 0.43 | 2.49 | 18 | 1 |
| 1:A:29:ILE:CB | 1:A:90:LEU:HB2 | 0.43 | 2.43 | 7 | 1 |
| 1:A:28:ASN:O | 1:A:88:TYR:O | 0.43 | 2.35 | 17 | 3 |
| 1:A:93:LYS:HG2 | 1:A:118:LEU:CD1 | 0.43 | 2.44 | 2 | 1 |
| 1:A:57:HIS:CD2 | 1:A:72:LYS:HD2 | 0.43 | 2.49 | 19 | 1 |
| 1:A:118:LEU:HD12 | 1:A:122:ASN:HB2 | 0.43 | 1.90 | 7 | 1 |
| 1:A:28:ASN:ND2 | 1:A:88:TYR:CG | 0.43 | 2.86 | 15 | 1 |
| 1:A:73:SER:HB2 | 1:A:88:TYR:CG | 0.43 | 2.49 | 5 | 3 |
| 1:A:101:ILE:HD13 | 1:A:138:MET:HA | 0.43 | 1.89 | 17 | 4 |
| 1:A:105:ASP:HA | 1:A:112:HIS:O | 0.43 | 2.13 | 13 | 1 |
| 1:A:98:LYS:C | 1:A:99:VAL:CG1 | 0.43 | 2.87 | 13 | 4 |
| 1:A:106:ASP:HB2 | 1:A:110:TYR:CE1 | 0.43 | 2.48 | 16 | 1 |
| 1:A:95:PHE:CA | 1:A:99:VAL:CG1 | 0.43 | 2.96 | 11 | 2 |
| 1:A:59:ARG:NH2 | 1:A:124:VAL:HG11 | 0.43 | 2.29 | 12 | 1 |
| 1:A:139:ALA:O | 1:A:143:SER:CB | 0.43 | 2.67 | 20 | 1 |
| 1:A:70:CYS:SG | 1:A:93:LYS:CE | 0.43 | 3.07 | 7 | 1 |
| 1:A:95:PHE:CE1 | 1:A:118:LEU:HB3 | 0.43 | 2.49 | 3 | 2 |
| 1:A:57:HIS:CG | 1:A:72:LYS:HD2 | 0.43 | 2.49 | 19 | 1 |
| 1:A:98:LYS:C | 1:A:99:VAL:HG13 | 0.43 | 2.33 | 8 | 3 |
| 1:A:101:ILE:O | 1:A:101:ILE:HG23 | 0.43 | 2.12 | 14 | 1 |
| 1:A:27:LYS:O | 1:A:28:ASN:ND2 | 0.43 | 2.52 | 18 | 1 |
| 1:A:96:MET:O | 1:A:96:MET:SD | 0.43 | 2.76 | 12 | 1 |
| 1:A:99:VAL:O | 1:A:145:GLN:CG | 0.43 | 2.66 | 12 | 1 |
| 1:A:59:ARG:NE | 1:A:59:ARG:HA | 0.43 | 2.27 | 8 | 2 |
| 1:A:65:ASP:O | 1:A:96:MET:SD | 0.43 | 2.76 | 13 | 1 |
| 1:A:30:ASP:OD2 | 1:A:89:ARG:NH1 | 0.43 | 2.52 | 14 | 1 |
| 1:A:135:ASN:O | 1:A:139:ALA:HB2 | 0.43 | 2.12 | 7 | 2 |
| 1:A:45:ILE:CG1 | 1:A:65:ASP:HA | 0.43 | 2.44 | 11 | 1 |
| 1:A:44:PHE:CZ | 1:A:47:GLU:HB3 | 0.43 | 2.49 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:144:LEU:C | 1:A:146:TYR:N | 0.43 | 2.71 | 10 | 12 |
| 1:A:95:PHE:O | 1:A:98:LYS:O | 0.43 | 2.37 | 9 | 3 |
| 1:A:59:ARG:HA | 1:A:71:CYS:O | 0.43 | 2.14 | 13 | 1 |
| 1:A:113:ALA:CB | 1:A:127:SER:OG | 0.43 | 2.57 | 4 | 2 |
| 1:A:124:VAL:C | 1:A:125:ILE:HD12 | 0.43 | 2.34 | 8 | 2 |
| 1:A:26:GLN:HG3 | 1:A:27:LYS:N | 0.43 | 2.29 | 16 | 1 |
| 1:A:61:ILE:CD1 | 1:A:70:CYS:HB2 | 0.43 | 2.44 | 4 | 2 |
| 1:A:51:THR:CB | 1:A:127:SER:HB2 | 0.43 | 2.43 | 10 | 2 |
| 1:A:44:PHE:CZ | 1:A:62:PHE:CE1 | 0.43 | 3.07 | 10 | 1 |
| 1:A:45:ILE:HG13 | 1:A:65:ASP:N | 0.43 | 2.29 | 9 | 1 |
| 1:A:142:ILE:HG22 | 1:A:146:TYR:CD2 | 0.43 | 2.49 | 15 | 1 |
| 1:A:114:PHE:CD1 | 1:A:114:PHE:N | 0.42 | 2.84 | 12 | 2 |
| 1:A:49:THR:HG23 | 1:A:60:HIS:CD2 | 0.42 | 2.49 | 5 | 1 |
| 1:A:29:ILE:HA | 1:A:90:LEU:HB3 | 0.42 | 1.91 | 6 | 1 |
| 1:A:64:PHE:C | 1:A:66:GLY:N | 0.42 | 2.72 | 2 | 4 |
| 1:A:63:LEU:H | 1:A:63:LEU:HD23 | 0.42 | 1.74 | 15 | 2 |
| 1:A:128:ALA:HB3 | 1:A:134:LYS:CG | 0.42 | 2.41 | 17 | 1 |
| 1:A:47:GLU:OE1 | 1:A:47:GLU:N | 0.42 | 2.51 | 17 | 1 |
| 1:A:101:ILE:CG2 | 1:A:142:ILE:HG12 | 0.42 | 2.44 | 4 | 4 |
| 1:A:142:ILE:CG2 | 1:A:146:TYR:CE2 | 0.42 | 3.02 | 10 | 1 |
| 1:A:64:PHE:O | 1:A:96:MET:SD | 0.42 | 2.77 | 9 | 1 |
| 1:A:120:ASP:C | 1:A:122:ASN:N | 0.42 | 2.72 | 10 | 1 |
| 1:A:59:ARG:CD | 1:A:88:TYR:CD2 | 0.42 | 3.02 | 8 | 1 |
| 1:A:95:PHE:CG | 1:A:118:LEU:HB3 | 0.42 | 2.49 | 4 | 1 |
| 1:A:101:ILE:HG13 | 1:A:102:ASN:N | 0.42 | 2.29 | 9 | 1 |
| 1:A:51:THR:HG22 | 1:A:127:SER:HB3 | 0.42 | 1.90 | 11 | 1 |
| 1:A:61:ILE:HG21 | 1:A:68:MET:HE1 | 0.42 | 1.90 | 11 | 1 |
| 1:A:64:PHE:O | 1:A:67:LEU:O | 0.42 | 2.37 | 12 | 1 |
| 1:A:96:MET:CG | 1:A:96:MET:O | 0.42 | 2.66 | 7 | 1 |
| 1:A:128:ALA:CB | 1:A:137:TRP:CE3 | 0.42 | 2.86 | 13 | 1 |
| 1:A:95:PHE:O | 1:A:98:LYS:C | 0.42 | 2.58 | 18 | 1 |
| 1:A:66:GLY:O | 1:A:96:MET:CE | 0.42 | 2.68 | 19 | 1 |
| 1:A:116:ILE:HD11 | 1:A:126:PHE:HB2 | 0.42 | 1.91 | 12 | 2 |
| 1:A:52:ARG:CG | 1:A:57:HIS:HB2 | 0.42 | 2.44 | 4 | 1 |
| 1:A:68:MET:HE3 | 1:A:141:LEU:HD11 | 0.42 | 1.91 | 10 | 1 |
| 1:A:90:LEU:CD2 | 1:A:90:LEU:C | 0.42 | 2.88 | 17 | 1 |
| 1:A:65:ASP:O | 1:A:66:GLY:C | 0.42 | 2.58 | 14 | 1 |
| 1:A:114:PHE:CZ | 1:A:134:LYS:HB2 | 0.42 | 2.49 | 18 | 1 |
| 1:A:106:ASP:CB | 1:A:110:TYR:CD1 | 0.42 | 3.03 | 16 | 1 |
| 1:A:59:ARG:HB2 | 1:A:71:CYS:O | 0.42 | 2.15 | 11 | 1 |
| 1:A:60:HIS:HB2 | 1:A:71:CYS:SG | 0.42 | 2.55 | 11 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:MET:CE | 1:A:69:ILE:C | 0.42 | 2.88 | 20 | 1 |
| 1:A:89:ARG:CG | 1:A:90:LEU:N | 0.42 | 2.82 | 7 | 1 |
| 1:A:94:PHE:CG | 1:A:94:PHE:O | 0.42 | 2.71 | 15 | 1 |
| 1:A:119:LYS:O | 1:A:120:ASP:CB | 0.42 | 2.67 | 9 | 1 |
| 1:A:53:VAL:HG13 | 1:A:54:GLY:H | 0.42 | 1.73 | 7 | 2 |
| 1:A:56:LYS:O | 1:A:74:ASN:ND2 | 0.42 | 2.53 | 8 | 1 |
| 1:A:44:PHE:CZ | 1:A:47:GLU:OE1 | 0.42 | 2.73 | 3 | 1 |
| 1:A:73:SER:HA | 1:A:88:TYR:CB | 0.42 | 2.44 | 6 | 1 |
| 1:A:63:LEU:CB | 1:A:68:MET:HA | 0.42 | 2.45 | 14 | 1 |
| 1:A:58:GLU:O | 1:A:59:ARG:HG2 | 0.42 | 2.15 | 12 | 1 |
| 1:A:142:ILE:HG22 | 1:A:146:TYR:CE1 | 0.42 | 2.50 | 20 | 1 |
| 1:A:67:LEU:HD22 | 1:A:94:PHE:HB3 | 0.42 | 1.92 | 15 | 1 |
| 1:A:67:LEU:CD1 | 1:A:94:PHE:N | 0.42 | 2.83 | 19 | 1 |
| 1:A:63:LEU:C | 1:A:63:LEU:CD1 | 0.42 | 2.82 | 2 | 1 |
| 1:A:61:ILE:HD11 | 1:A:70:CYS:SG | 0.42 | 2.55 | 2 | 1 |
| 1:A:51:THR:O | 1:A:125:ILE:O | 0.42 | 2.37 | 18 | 1 |
| 1:A:44:PHE:CE2 | 1:A:62:PHE:CD1 | 0.41 | 3.08 | 5 | 1 |
| 1:A:55:ALA:O | 1:A:56:LYS:HB2 | 0.41 | 2.15 | 9 | 2 |
| 1:A:145:GLN:OE1 | 1:A:145:GLN:O | 0.41 | 2.38 | 20 | 1 |
| 1:A:59:ARG:HG3 | 1:A:71:CYS:O | 0.41 | 2.14 | 8 | 1 |
| 1:A:68:MET:HB2 | 1:A:95:PHE:CB | 0.41 | 2.46 | 3 | 1 |
| 1:A:26:GLN:CD | 1:A:26:GLN:O | 0.41 | 2.59 | 5 | 1 |
| 1:A:46:MET:HG2 | 1:A:63:LEU:CD2 | 0.41 | 2.45 | 5 | 1 |
| 1:A:103:ASP:CB | 1:A:114:PHE:HB3 | 0.41 | 2.44 | 14 | 1 |
| 1:A:45:ILE:CG2 | 1:A:63:LEU:CD2 | 0.41 | 2.97 | 12 | 1 |
| 1:A:98:LYS:HG3 | 1:A:119:LYS:CB | 0.41 | 2.45 | 8 | 1 |
| 1:A:144:LEU:O | 1:A:146:TYR:N | 0.41 | 2.54 | 2 | 1 |
| 1:A:44:PHE:O | 1:A:45:ILE:C | 0.41 | 2.59 | 2 | 1 |
| 1:A:26:GLN:O | 1:A:29:ILE:HG13 | 0.41 | 2.15 | 3 | 1 |
| 1:A:68:MET:O | 1:A:93:LYS:CB | 0.41 | 2.69 | 13 | 1 |
| 1:A:63:LEU:HD22 | 1:A:96:MET:CE | 0.41 | 2.45 | 1 | 1 |
| 1:A:64:PHE:C | 1:A:66:GLY:H | 0.41 | 2.18 | 1 | 1 |
| 1:A:99:VAL:HG21 | 1:A:141:LEU:CB | 0.41 | 2.46 | 1 | 1 |
| 1:A:59:ARG:CG | 1:A:72:LYS:HA | 0.41 | 2.45 | 2 | 1 |
| 1:A:29:ILE:CB | 1:A:90:LEU:HB3 | 0.41 | 2.45 | 20 | 1 |
| 1:A:130:SER:CB | 1:A:133:GLU:HG3 | 0.41 | 2.46 | 13 | 1 |
| 1:A:107:THR:C | 1:A:109:GLU:H | 0.41 | 2.18 | 10 | 1 |
| 1:A:47:GLU:HB2 | 1:A:62:PHE:CE2 | 0.41 | 2.49 | 20 | 1 |
| 1:A:67:LEU:CD1 | 1:A:67:LEU:C | 0.41 | 2.78 | 3 | 1 |
| 1:A:46:MET:SD | 1:A:140:ALA:HB1 | 0.41 | 2.55 | 6 | 1 |
| 1:A:103:ASP:O | 1:A:103:ASP:CG | 0.41 | 2.59 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:60:HIS:O | 1:A:71:CYS:SG | 0.41 | 2.79 | 13 | 1 |
| 1:A:105:ASP:O | 1:A:106:ASP:CG | 0.41 | 2.58 | 10 | 1 |
| 1:A:134:LYS:O | 1:A:138:MET:CG | 0.41 | 2.68 | 9 | 1 |
| 1:A:52:ARG:HB2 | 1:A:52:ARG:CZ | 0.41 | 2.45 | 9 | 1 |
| 1:A:72:LYS:O | 1:A:88:TYR:HB3 | 0.41 | 2.15 | 17 | 1 |
| 1:A:49:THR:CG2 | 1:A:60:HIS:HA | 0.41 | 2.46 | 20 | 1 |
| 1:A:51:THR:OG1 | 1:A:58:GLU:CG | 0.41 | 2.69 | 8 | 1 |
| 1:A:46:MET:HG2 | 1:A:63:LEU:HB3 | 0.41 | 1.93 | 6 | 1 |
| 1:A:132:GLU:CG | 1:A:133:GLU:N | 0.41 | 2.82 | 17 | 1 |
| 1:A:45:ILE:C | 1:A:46:MET:HG2 | 0.41 | 2.36 | 14 | 1 |
| 1:A:95:PHE:CZ | 1:A:118:LEU:CB | 0.41 | 3.03 | 11 | 1 |
| 1:A:120:ASP:O | 1:A:121:GLU:HB2 | 0.41 | 2.15 | 8 | 1 |
| 1:A:68:MET:HB2 | 1:A:93:LYS:O | 0.41 | 2.15 | 6 | 1 |
| 1:A:64:PHE:N | 1:A:64:PHE:CD1 | 0.41 | 2.87 | 6 | 2 |
| 1:A:62:PHE:O | 1:A:69:ILE:HG23 | 0.41 | 2.16 | 4 | 1 |
| 1:A:63:LEU:HB3 | 1:A:68:MET:CG | 0.41 | 2.46 | 14 | 1 |
| 1:A:30:ASP:CB | 1:A:89:ARG:HG3 | 0.41 | 2.46 | 14 | 1 |
| 1:A:55:ALA:O | 1:A:56:LYS:CG | 0.41 | 2.69 | 14 | 1 |
| 1:A:68:MET:SD | 1:A:68:MET:C | 0.41 | 2.99 | 18 | 1 |
| 1:A:101:ILE:CD1 | 1:A:116:ILE:CD1 | 0.41 | 2.85 | 20 | 1 |
| 1:A:57:HIS:CD2 | 1:A:74:ASN:HA | 0.41 | 2.51 | 20 | 1 |
| 1:A:96:MET:C | 1:A:98:LYS:N | 0.41 | 2.74 | 19 | 1 |
| 1:A:64:PHE:CE2 | 1:A:69:ILE:HG12 | 0.41 | 2.51 | 13 | 1 |
| 1:A:130:SER:CB | 1:A:133:GLU:HG2 | 0.41 | 2.46 | 4 | 1 |
| 1:A:44:PHE:CD1 | 1:A:47:GLU:HG3 | 0.41 | 2.51 | 12 | 1 |
| 1:A:72:LYS:CB | 1:A:89:ARG:HG3 | 0.40 | 2.46 | 3 | 1 |
| 1:A:45:ILE:CG2 | 1:A:46:MET:CG | 0.40 | 2.99 | 14 | 1 |
| 1:A:64:PHE:CD1 | 1:A:64:PHE:N | 0.40 | 2.87 | 3 | 1 |
| 1:A:98:LYS:C | 1:A:145:GLN:OE1 | 0.40 | 2.60 | 10 | 1 |
| 1:A:118:LEU:CD1 | 1:A:119:LYS:O | 0.40 | 2.66 | 9 | 1 |
| 1:A:135:ASN:O | 1:A:138:MET:HG3 | 0.40 | 2.15 | 9 | 1 |
| 1:A:101:ILE:HG22 | 1:A:142:ILE:CG1 | 0.40 | 2.47 | 14 | 1 |
| 1:A:124:VAL:O | 1:A:125:ILE:CD1 | 0.40 | 2.60 | 18 | 1 |
| 1:A:92:GLU:OE2 | 1:A:94:PHE:CE2 | 0.40 | 2.74 | 5 | 1 |
| 1:A:61:ILE:HD12 | 1:A:68:MET:CE | 0.40 | 2.46 | 2 | 1 |
| 1:A:58:GLU:O | 1:A:73:SER:N | 0.40 | 2.45 | 12 | 1 |
| 1:A:95:PHE:CE1 | 1:A:118:LEU:HD13 | 0.40 | 2.51 | 7 | 1 |
| 1:A:59:ARG:CD | 1:A:61:ILE:HD11 | 0.40 | 2.46 | 7 | 1 |
| 1:A:45:ILE:HB | 1:A:63:LEU:CD1 | 0.40 | 2.47 | 19 | 1 |
| 1:A:46:MET:HG2 | 1:A:63:LEU:CG | 0.40 | 2.46 | 6 | 1 |
| 1:A:68:MET:HG3 | 1:A:95:PHE:CE1 | 0.40 | 2.52 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:46:MET:O | 1:A:46:MET:CG | 0.40 | 2.70 | 17 | 1 |
| 1:A:58:GLU:O | 1:A:59:ARG:HG3 | 0.40 | 2.16 | 2 | 1 |
| 1:A:30:ASP:OD2 | 1:A:31:GLY:N | 0.40 | 2.55 | 18 | 1 |
| 1:A:132:GLU:O | 1:A:136:ASN:HB2 | 0.40 | 2.16 | 12 | 1 |
| 1:A:95:PHE:HD2 | 1:A:99:VAL:HG12 | 0.40 | 1.75 | 15 | 1 |
| 1:A:50:LEU:CD1 | 1:A:61:ILE:HG13 | 0.40 | 2.35 | 3 | 1 |
| 1:A:118:LEU:HD12 | 1:A:118:LEU:C | 0.40 | 2.37 | 9 | 1 |
| 1:A:46:MET:HE2 | 1:A:46:MET:O | 0.40 | 2.17 | 2 | 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 | 103/130 (79%) | 65±3 (63±3%) | 26±2 (25±2%) | 13±1 (12±1%) | 1 | 7 |
| All | All | 2060/2600 (79%) | 1292 (63%) | 515 (25%) | 253 (12%) | 1 | 7 |

All 29 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 | 149 | THR | 20 |
| 1 | A | 112 | HIS | 20 |
| 1 | A | 29 | ILE | 17 |
| 1 | A | 32 | TRP | 17 |
| 1 | A | 55 | ALA | 15 |
| 1 | A | 108 | ASN | 15 |
| 1 | A | 107 | THR | 13 |
| 1 | A | 119 | LYS | 13 |
| 1 | A | 56 | LYS | 12 |
| 1 | A | 103 | ASP | 12 |
| 1 | A | 86 | ALA | 12 |
| 1 | A | 44 | PHE | 11 |
| 1 | A | 28 | ASN | 10 |
| 1 | A | 121 | GLU | 9 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 30 | ASP | 8 |
| 1 | A | 94 | PHE | 8 |
| 1 | A | 96 | MET | 8 |
| 1 | A | 111 | LYS | 7 |
| 1 | A | 106 | ASP | 6 |
| 1 | A | 87 | GLU | 5 |
| 1 | A | 109 | GLU | 4 |
| 1 | A | 88 | TYR | 2 |
| 1 | A | 117 | ILE | 2 |
| 1 | A | 45 | ILE | 2 |
| 1 | A | 120 | ASP | 1 |
| 1 | A | 65 | ASP | 1 |
| 1 | A | 113 | ALA | 1 |
| 1 | A | 105 | ASP | 1 |
| 1 | A | 98 | LYS | 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 | 92/114 (81%) | 52±4 (57±4%) | 40±4 (43±4%) | 0 3 |
| All | All | 1840/2280 (81%) | 1047 (57%) | 793 (43%) | 0 3 |

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 | 146 | TYR | 20 |
| 1 | A | 149 | THR | 20 |
| 1 | A | 132 | GLU | 20 |
| 1 | A | 49 | THR | 20 |
| 1 | A | 101 | ILE | 20 |
| 1 | A | 90 | LEU | 20 |
| 1 | A | 51 | THR | 20 |
| 1 | A | 141 | LEU | 19 |
| 1 | A | 148 | SER | 19 |
| 1 | A | 138 | MET | 19 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 27 | LYS | 18 |
| 1 | A | 114 | PHE | 18 |
| 1 | A | 30 | ASP | 17 |
| 1 | A | 63 | LEU | 17 |
| 1 | A | 111 | LYS | 17 |
| 1 | A | 124 | VAL | 15 |
| 1 | A | 91 | LYS | 15 |
| 1 | A | 67 | LEU | 15 |
| 1 | A | 119 | LYS | 15 |
| 1 | A | 118 | LEU | 14 |
| 1 | A | 115 | GLU | 14 |
| 1 | A | 96 | MET | 14 |
| 1 | A | 62 | PHE | 13 |
| 1 | A | 150 | LEU | 13 |
| 1 | A | 104 | LYS | 13 |
| 1 | A | 123 | SER | 12 |
| 1 | A | 68 | MET | 12 |
| 1 | A | 112 | HIS | 12 |
| 1 | A | 134 | LYS | 12 |
| 1 | A | 127 | SER | 12 |
| 1 | A | 92 | GLU | 12 |
| 1 | A | 46 | MET | 12 |
| 1 | A | 130 | SER | 12 |
| 1 | A | 145 | GLN | 11 |
| 1 | A | 60 | HIS | 11 |
| 1 | A | 136 | ASN | 11 |
| 1 | A | 107 | THR | 10 |
| 1 | A | 52 | ARG | 10 |
| 1 | A | 56 | LYS | 10 |
| 1 | A | 72 | LYS | 10 |
| 1 | A | 97 | ARG | 10 |
| 1 | A | 93 | LYS | 10 |
| 1 | A | 69 | ILE | 10 |
| 1 | A | 47 | GLU | 10 |
| 1 | A | 100 | GLN | 9 |
| 1 | A | 106 | ASP | 9 |
| 1 | A | 59 | ARG | 9 |
| 1 | A | 98 | LYS | 9 |
| 1 | A | 147 | ARG | 9 |
| 1 | A | 89 | ARG | 8 |
| 1 | A | 121 | GLU | 8 |
| 1 | A | 26 | GLN | 8 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 44 | PHE | 7 |
| 1 | A | 122 | ASN | 7 |
| 1 | A | 129 | LYS | 7 |
| 1 | A | 143 | SER | 6 |
| 1 | A | 102 | ASN | 5 |
| 1 | A | 120 | ASP | 5 |
| 1 | A | 105 | ASP | 5 |
| 1 | A | 50 | LEU | 4 |
| 1 | A | 45 | ILE | 4 |
| 1 | A | 57 | HIS | 3 |
| 1 | A | 116 | ILE | 3 |
| 1 | A | 71 | CYS | 3 |
| 1 | A | 28 | ASN | 3 |
| 1 | A | 135 | ASN | 3 |
| 1 | A | 65 | ASP | 3 |
| 1 | A | 53 | VAL | 3 |
| 1 | A | 88 | TYR | 2 |
| 1 | A | 108 | ASN | 2 |
| 1 | A | 70 | CYS | 2 |
| 1 | A | 74 | ASN | 2 |
| 1 | A | 73 | SER | 2 |
| 1 | A | 109 | GLU | 1 |
| 1 | A | 133 | GLU | 1 |
| 1 | A | 125 | ILE | 1 |
| 1 | A | 29 | ILE | 1 |
| 1 | A | 110 | TYR | 1 |
| 1 | A | 103 | ASP | 1 |
| 1 | A | 95 | PHE | 1 |
| 1 | A | 99 | VAL | 1 |
| 1 | A | 58 | GLU | 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