



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:06 pm GMT

PDB ID : 1FHT
Title : RNA-BINDING DOMAIN OF THE U1A SPLICEOSOMAL PROTEIN
U1A117, NMR, 43 STRUCTURES
Authors : Allain, F.H.-T.; Gubser, C.C.; Howe, P.W.A.; Nagai, K.; Neuhaus, D.; Varani, G.
Deposited on : 1996-02-21

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 | : | trunk28760 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

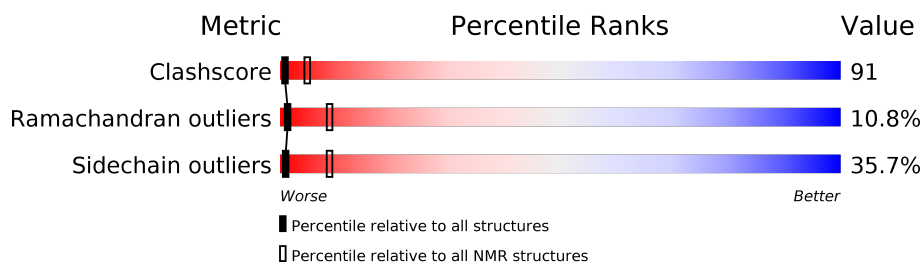
1 Overall quality at a glance

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 | 116 | |

2 Ensemble composition and analysis

This entry contains 43 models. Model 12 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:6-A:94 (89) | 0.43 | 12 |
| 2 | A:105-A:113 (9) | 1.23 | 19 |

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 9 clusters and 3 single-model clusters were found.

| Cluster number | Models |
|-----------------------|--|
| 1 | 8, 9, 13, 15, 25, 27, 32, 34, 35, 36, 37, 38 |
| 2 | 4, 21, 23, 29, 41 |
| 3 | 17, 22, 33, 39, 40 |
| 4 | 5, 6, 14, 20, 26 |
| 5 | 2, 11, 28, 31 |
| 6 | 1, 19, 30 |
| 7 | 12, 24 |
| 8 | 3, 43 |
| 9 | 7, 42 |
| Single-model clusters | 10; 16; 18 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 953 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A.

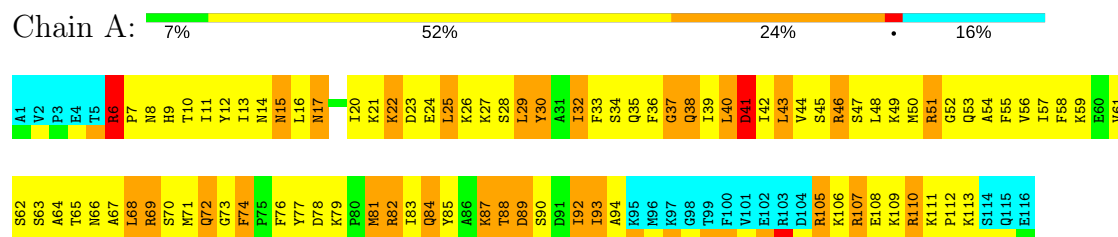
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|-------|
| 1 | A | 116 | Total | C | N | O | S | 0 |
| | | | 953 | 606 | 171 | 172 | 4 | |

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: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

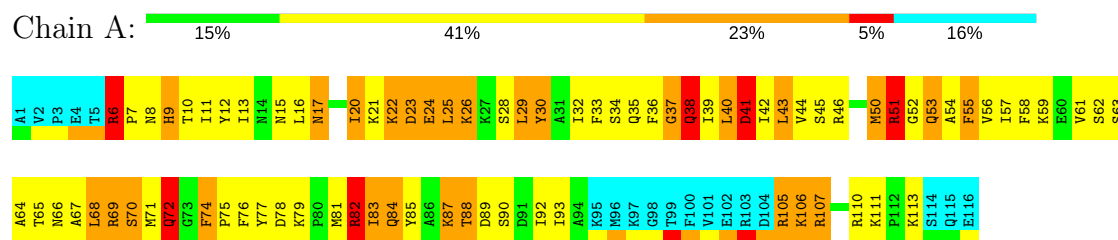


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

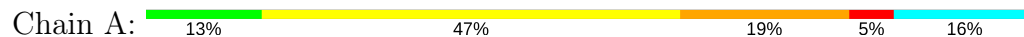
4.2.1 Score per residue for model 1

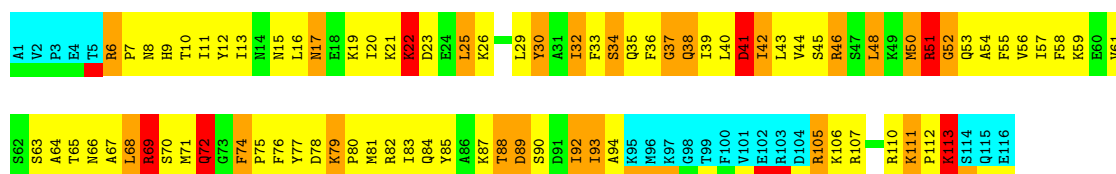
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



4.2.2 Score per residue for model 2

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

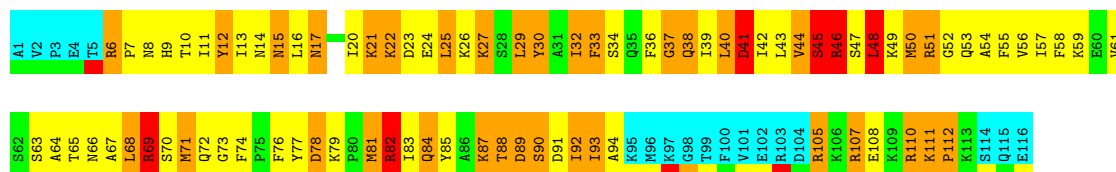




4.2.3 Score per residue for model 3

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

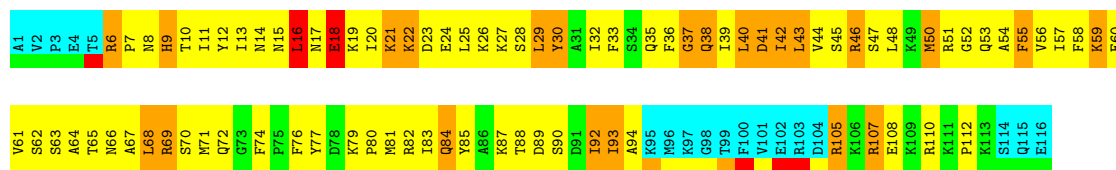
Chain A: 11% 39% 29% 5% 16%



4.2.4 Score per residue for model 4

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

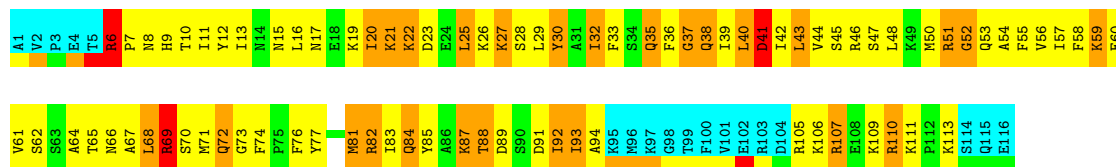
Chain A: 10% 53% 20% 16%



4.2.5 Score per residue for model 5

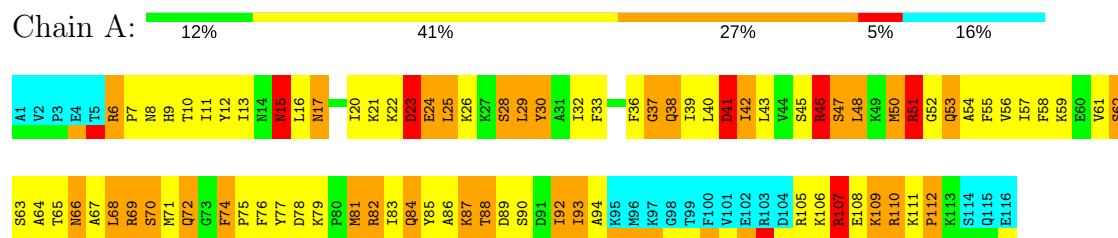
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 13% 47% 22% 16%



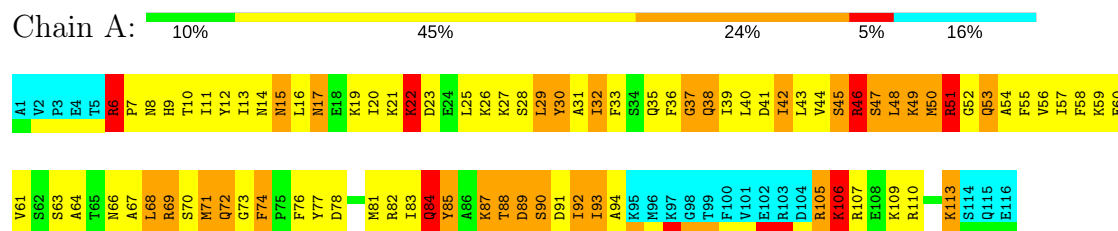
4.2.6 Score per residue for model 6

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



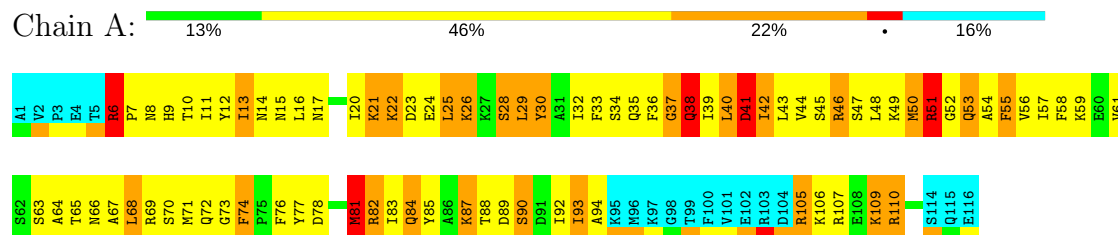
4.2.7 Score per residue for model 7

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



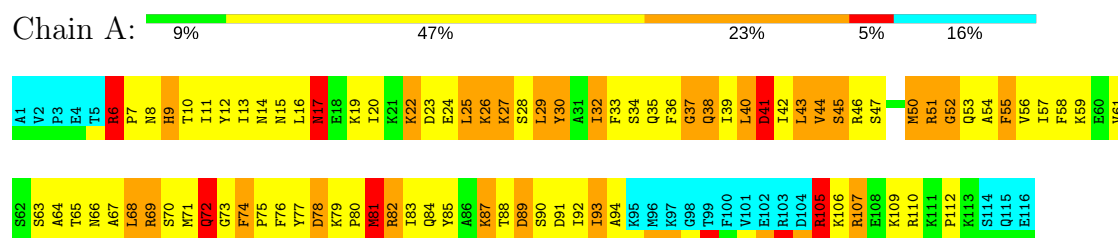
4.2.8 Score per residue for model 8

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



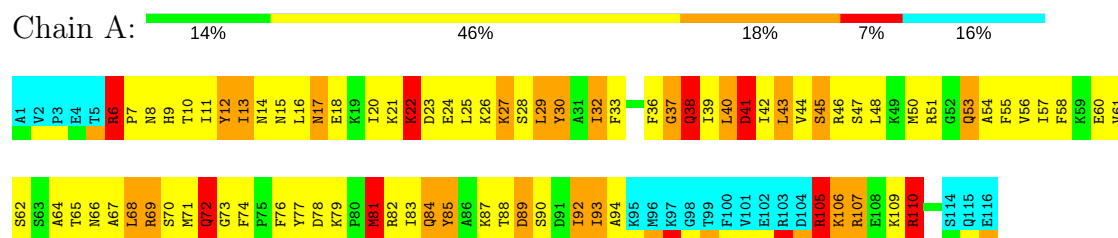
4.2.9 Score per residue for model 9

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



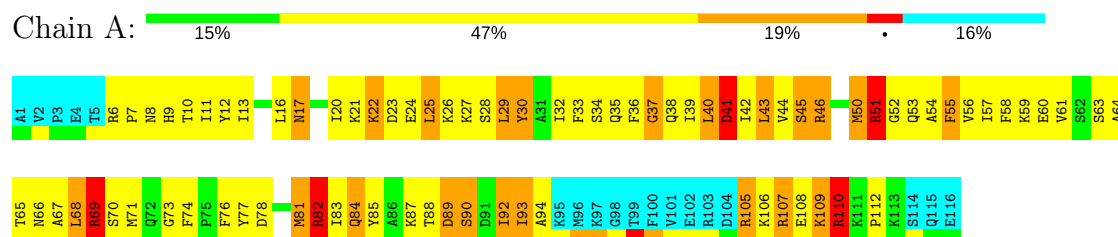
4.2.10 Score per residue for model 10

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



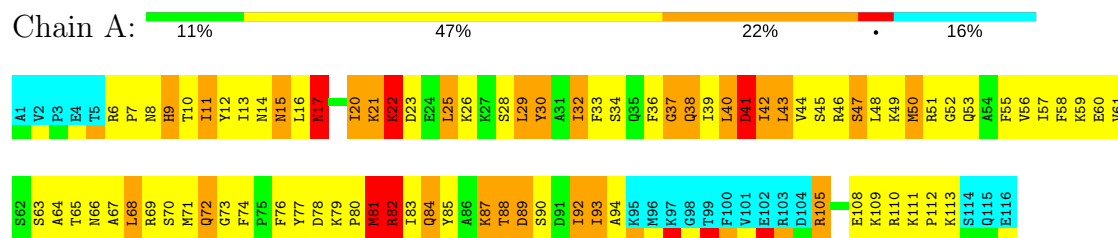
4.2.11 Score per residue for model 11

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



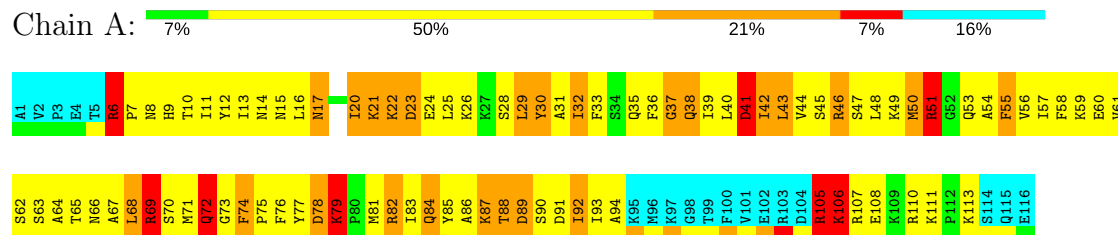
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



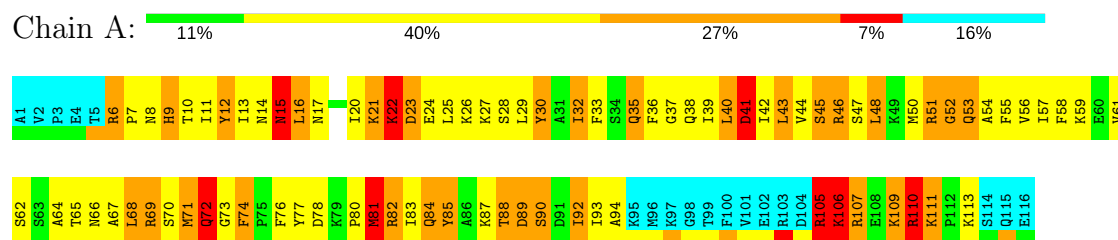
4.2.13 Score per residue for model 13

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



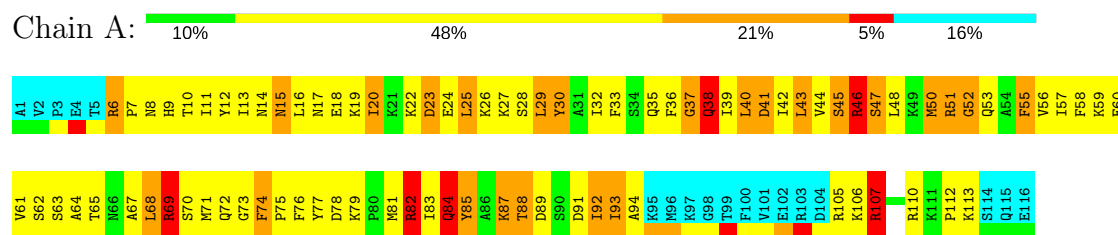
4.2.14 Score per residue for model 14

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



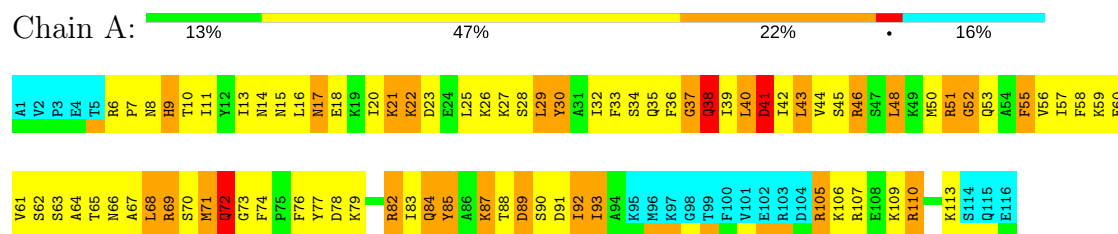
4.2.15 Score per residue for model 15

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



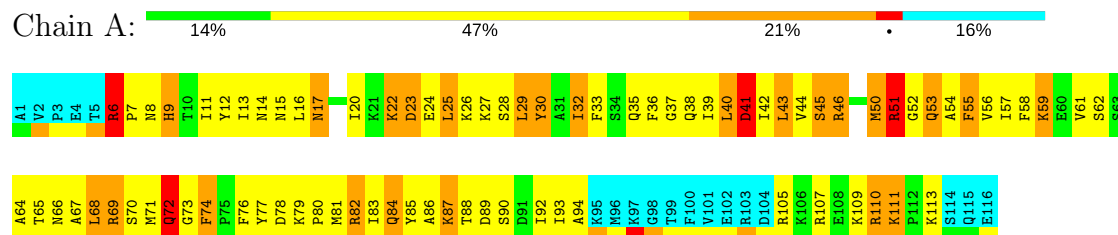
4.2.16 Score per residue for model 16

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



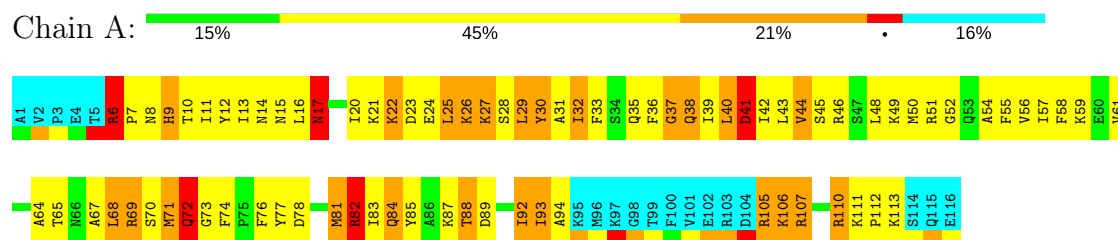
4.2.17 Score per residue for model 17

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



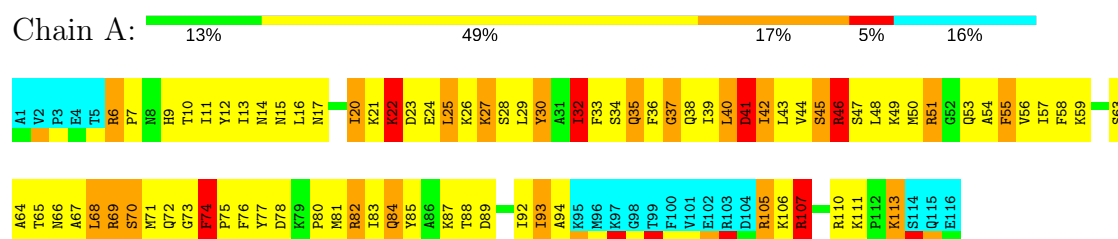
4.2.18 Score per residue for model 18

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



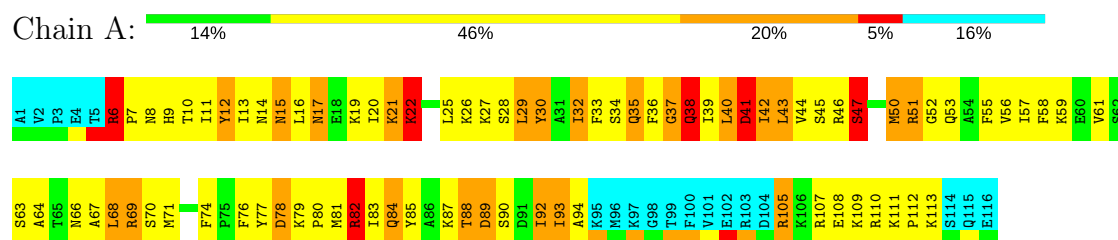
4.2.19 Score per residue for model 19

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



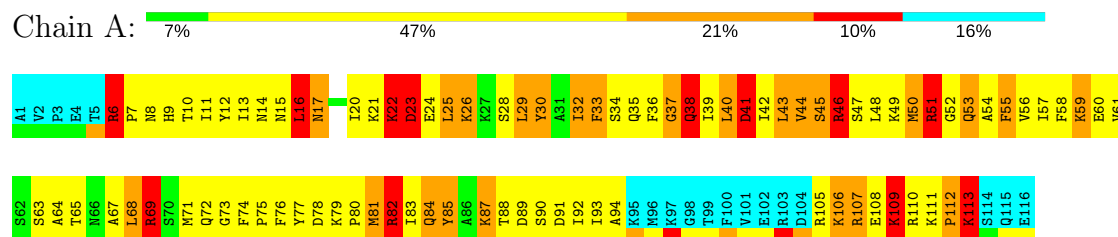
4.2.20 Score per residue for model 20

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



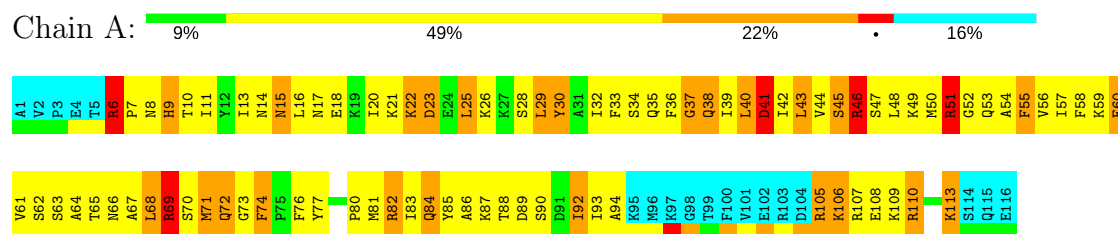
4.2.21 Score per residue for model 21

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



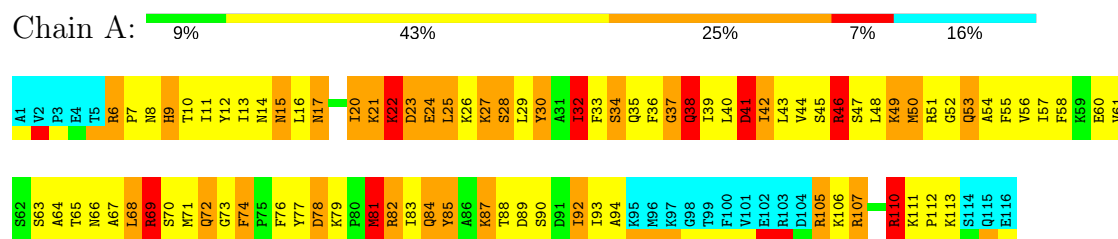
4.2.22 Score per residue for model 22

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



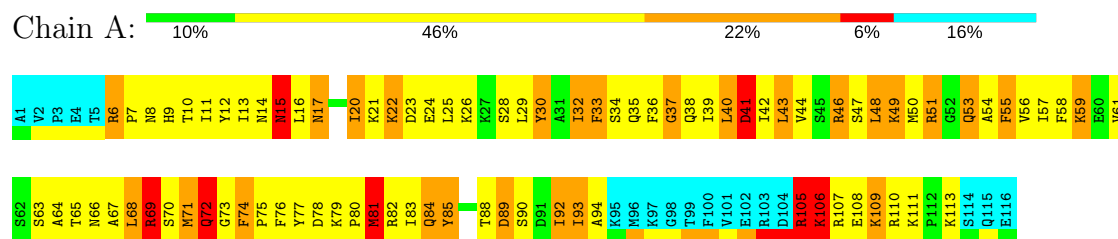
4.2.23 Score per residue for model 23

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



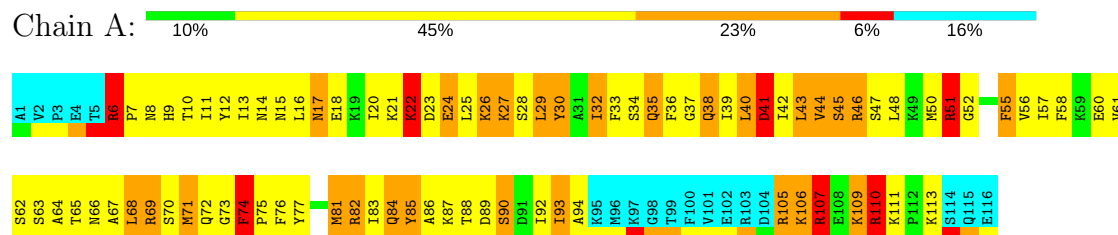
4.2.24 Score per residue for model 24

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



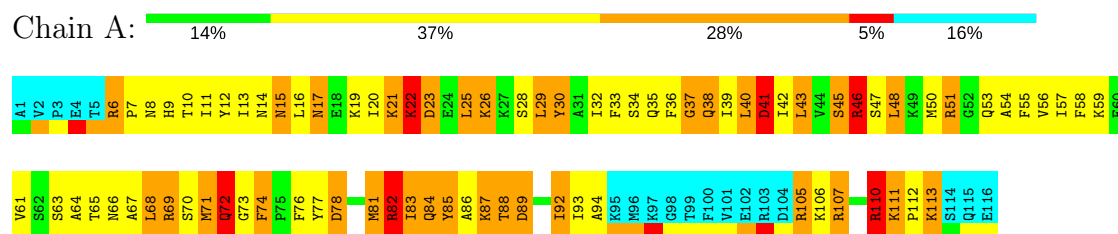
4.2.25 Score per residue for model 25

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



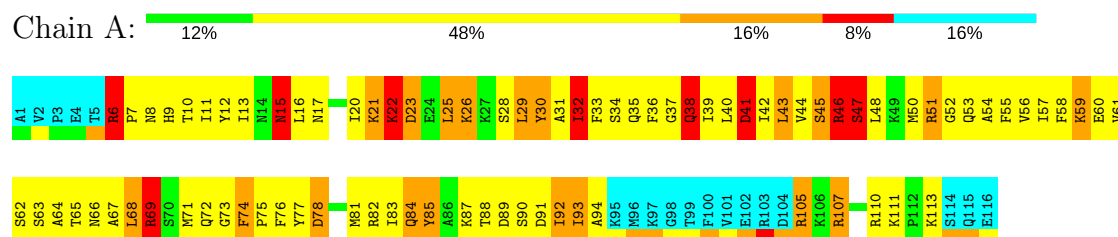
4.2.26 Score per residue for model 26

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



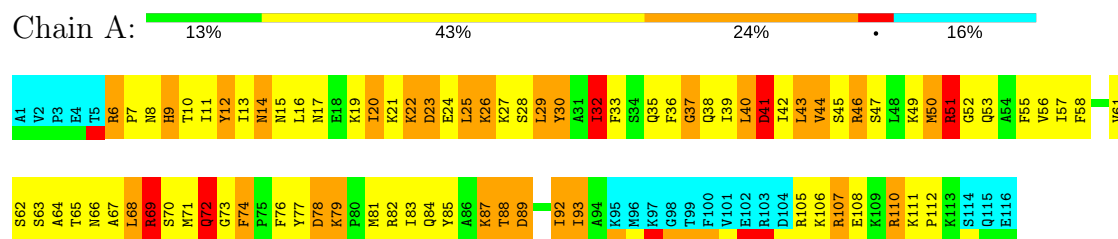
4.2.27 Score per residue for model 27

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



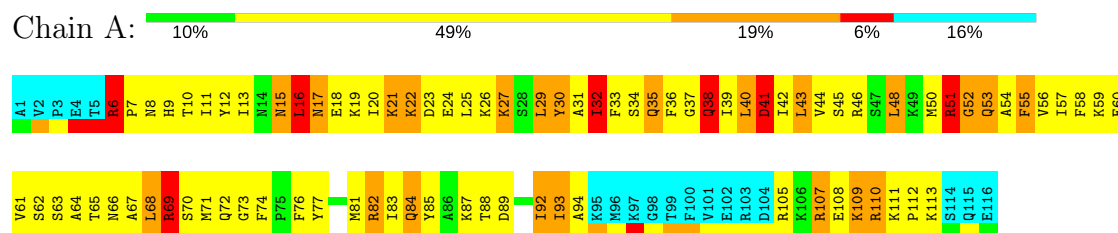
4.2.28 Score per residue for model 28

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



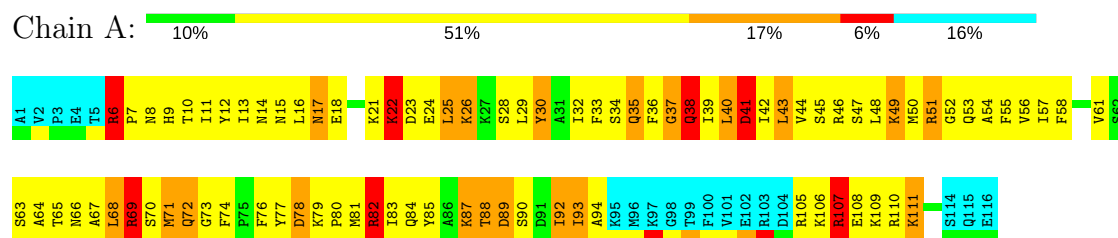
4.2.29 Score per residue for model 29

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



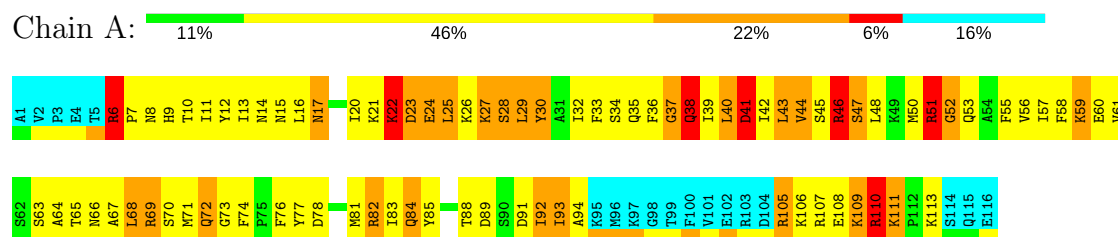
4.2.30 Score per residue for model 30

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



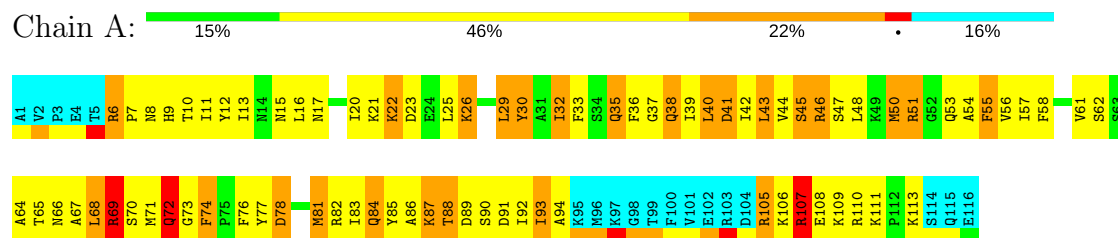
4.2.31 Score per residue for model 31

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



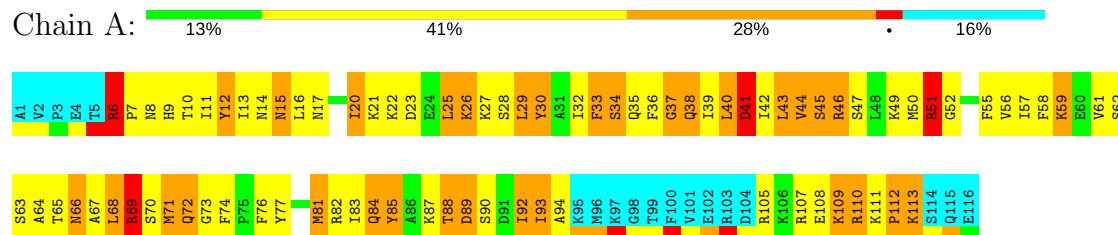
4.2.32 Score per residue for model 32

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



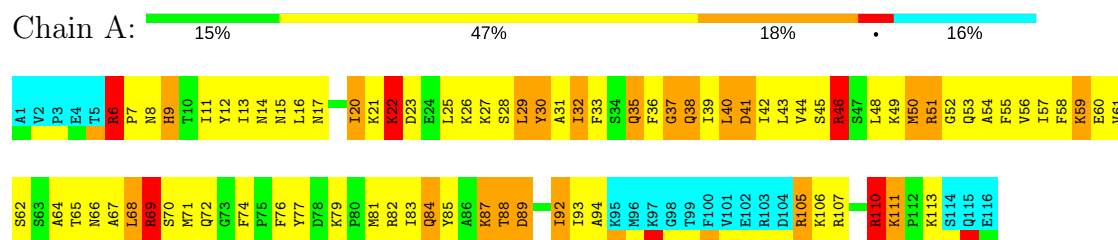
4.2.33 Score per residue for model 33

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



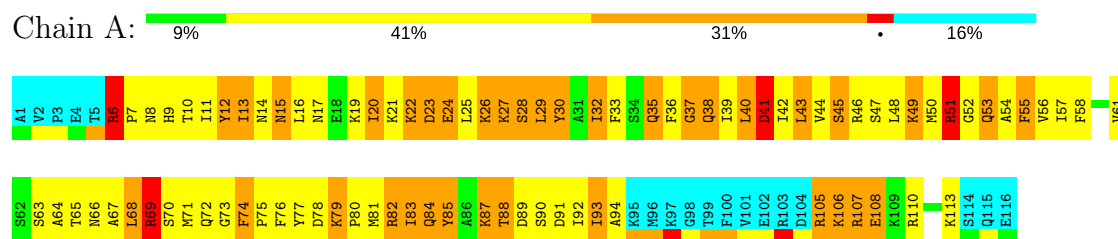
4.2.34 Score per residue for model 34

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



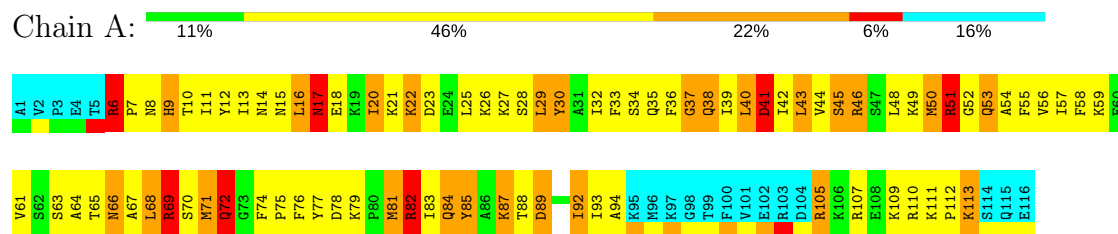
4.2.35 Score per residue for model 35

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



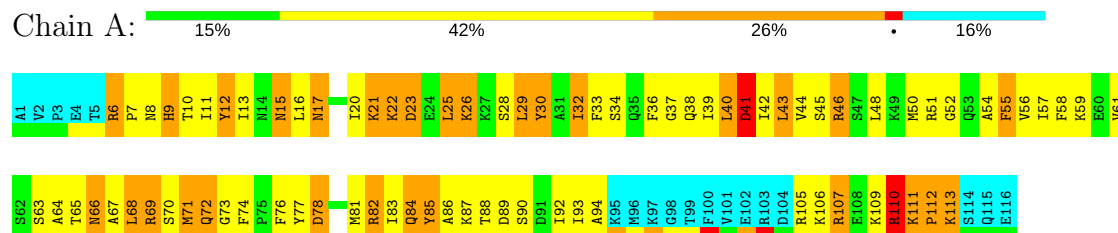
4.2.36 Score per residue for model 36

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



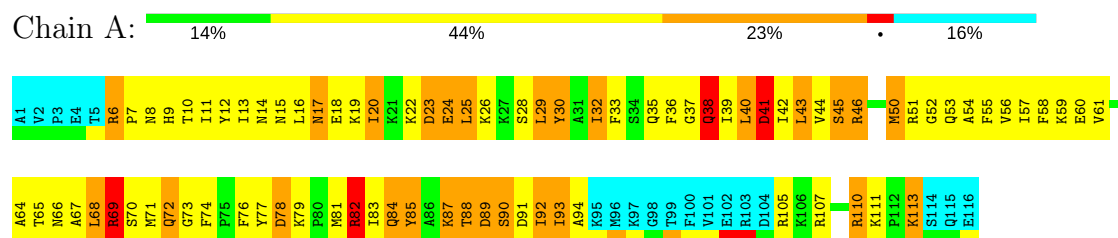
4.2.37 Score per residue for model 37

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



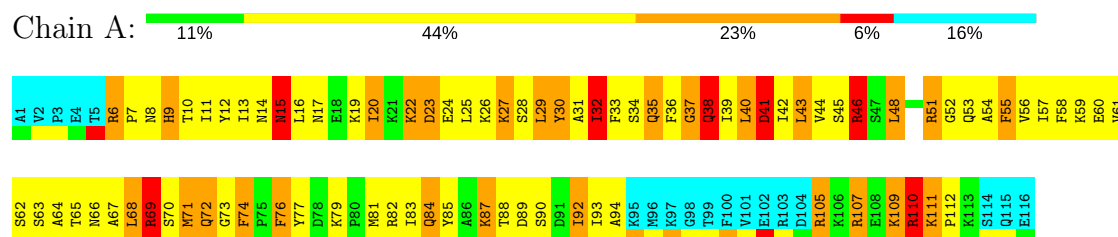
4.2.38 Score per residue for model 38

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



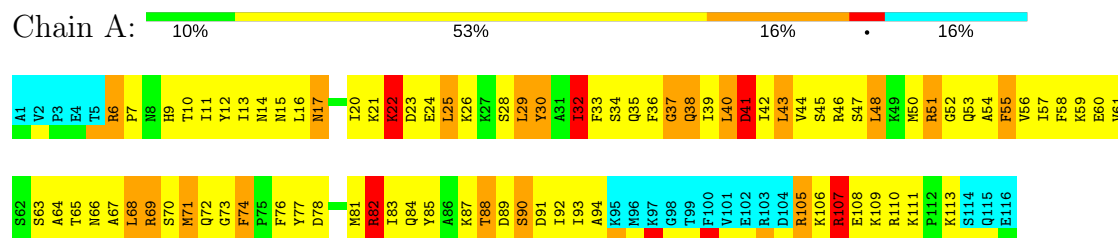
4.2.39 Score per residue for model 39

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



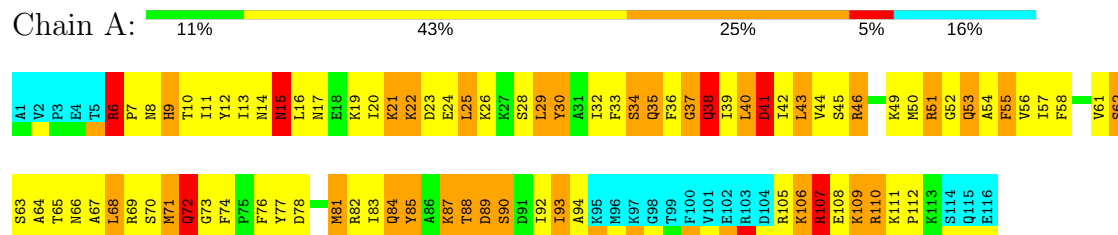
4.2.40 Score per residue for model 40

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



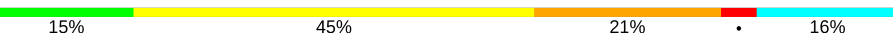
4.2.41 Score per residue for model 41

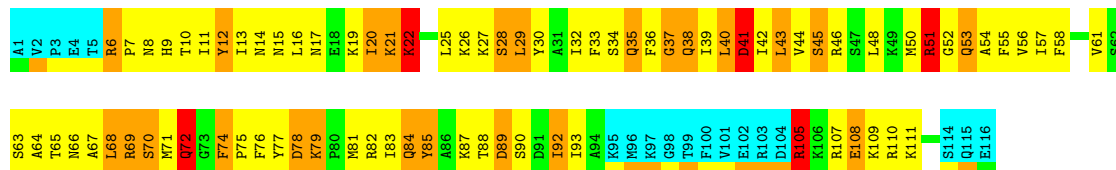
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



4.2.42 Score per residue for model 42

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

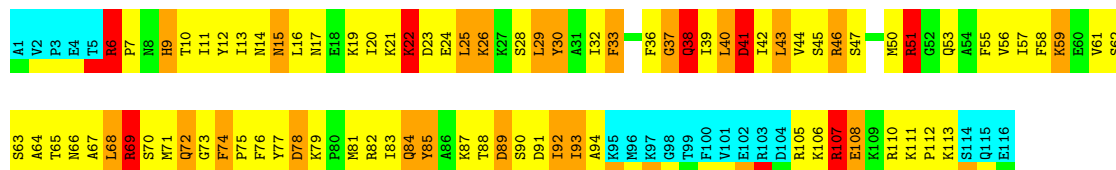
Chain A: 



4.2.43 Score per residue for model 43

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 43 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 | 3.1 |

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.

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 7.7±0.6 |
| All | All | 0 | 331 |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 110 | ARG | Sidechain | 43 |
| 1 | A | 6 | ARG | Sidechain | 43 |
| 1 | A | 82 | ARG | Sidechain | 42 |
| 1 | A | 51 | ARG | Sidechain | 41 |
| 1 | A | 105 | ARG | Sidechain | 41 |
| 1 | A | 107 | ARG | Sidechain | 41 |
| 1 | A | 46 | ARG | Sidechain | 41 |
| 1 | A | 69 | ARG | Sidechain | 39 |

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 | 810 | 0 | 853 | 151±13 |
| All | All | 34830 | 0 | 36679 | 6493 |

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 91.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HD13 | 1.07 | 1.10 | 14 | 3 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:HD11 | 1.04 | 1.27 | 25 | 25 |
| 1:A:29:LEU:HD13 | 1:A:42:ILE:HG21 | 1.00 | 1.31 | 23 | 11 |
| 1:A:13:ILE:CG2 | 1:A:16:LEU:HD21 | 1.00 | 1.86 | 24 | 28 |
| 1:A:30:TYR:CD2 | 1:A:42:ILE:HD11 | 1.00 | 1.91 | 19 | 9 |
| 1:A:57:ILE:HD11 | 1:A:93:ILE:HD11 | 0.99 | 1.32 | 31 | 37 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:HD13 | 0.98 | 1.93 | 41 | 33 |
| 1:A:40:LEU:HD21 | 1:A:59:LYS:N | 0.98 | 1.73 | 4 | 7 |
| 1:A:44:VAL:HG12 | 1:A:54:ALA:HB2 | 0.97 | 1.36 | 29 | 23 |
| 1:A:68:LEU:HD13 | 1:A:69:ARG:N | 0.96 | 1.76 | 33 | 41 |
| 1:A:39:ILE:O | 1:A:40:LEU:HD13 | 0.96 | 1.60 | 40 | 4 |
| 1:A:10:THR:OG1 | 1:A:57:ILE:HD13 | 0.95 | 1.61 | 11 | 20 |
| 1:A:39:ILE:C | 1:A:40:LEU:HD13 | 0.94 | 1.82 | 43 | 10 |
| 1:A:8:ASN:O | 1:A:61:VAL:HG13 | 0.94 | 1.62 | 31 | 8 |
| 1:A:33:PHE:CB | 1:A:39:ILE:HD11 | 0.94 | 1.92 | 35 | 21 |
| 1:A:16:LEU:HD23 | 1:A:52:GLY:O | 0.93 | 1.62 | 30 | 13 |
| 1:A:71:MET:CB | 1:A:83:ILE:HD11 | 0.93 | 1.93 | 18 | 7 |
| 1:A:40:LEU:HD11 | 1:A:59:LYS:CA | 0.93 | 1.94 | 1 | 8 |
| 1:A:55:PHE:CE1 | 1:A:92:ILE:HG21 | 0.93 | 1.98 | 21 | 12 |
| 1:A:55:PHE:CE2 | 1:A:92:ILE:HD13 | 0.92 | 1.98 | 4 | 15 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:CD1 | 0.92 | 1.93 | 14 | 2 |
| 1:A:17:ASN:OD1 | 1:A:20:ILE:HD11 | 0.92 | 1.65 | 43 | 1 |
| 1:A:16:LEU:HD12 | 1:A:77:TYR:CD2 | 0.91 | 2.01 | 15 | 10 |
| 1:A:68:LEU:HG | 1:A:85:TYR:CE1 | 0.91 | 2.01 | 8 | 26 |
| 1:A:68:LEU:HD13 | 1:A:68:LEU:C | 0.90 | 1.87 | 3 | 23 |
| 1:A:44:VAL:HG12 | 1:A:54:ALA:CB | 0.90 | 1.97 | 35 | 19 |
| 1:A:42:ILE:O | 1:A:43:LEU:HD23 | 0.90 | 1.67 | 13 | 5 |
| 1:A:55:PHE:CE1 | 1:A:92:ILE:HD13 | 0.90 | 2.02 | 33 | 16 |
| 1:A:68:LEU:C | 1:A:68:LEU:HD13 | 0.89 | 1.88 | 12 | 20 |
| 1:A:40:LEU:HD11 | 1:A:59:LYS:N | 0.89 | 1.82 | 38 | 7 |
| 1:A:15:ASN:C | 1:A:16:LEU:HD22 | 0.89 | 1.88 | 38 | 23 |
| 1:A:13:ILE:HD13 | 1:A:29:LEU:HD22 | 0.88 | 1.45 | 33 | 5 |
| 1:A:11:ILE:HD11 | 1:A:56:VAL:HG21 | 0.88 | 1.44 | 5 | 33 |
| 1:A:16:LEU:HG | 1:A:25:LEU:HD11 | 0.87 | 1.44 | 16 | 17 |
| 1:A:7:PRO:HB2 | 1:A:61:VAL:HG12 | 0.87 | 1.46 | 21 | 33 |
| 1:A:26:LYS:HA | 1:A:29:LEU:HD12 | 0.87 | 1.47 | 6 | 41 |
| 1:A:43:LEU:HD21 | 1:A:57:ILE:HG12 | 0.86 | 1.43 | 23 | 1 |
| 1:A:42:ILE:C | 1:A:43:LEU:HD22 | 0.86 | 1.90 | 23 | 2 |
| 1:A:13:ILE:HG22 | 1:A:16:LEU:HD21 | 0.85 | 1.47 | 31 | 17 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:LEU:HB3 | 1:A:25:LEU:HD11 | 0.85 | 1.45 | 12 | 9 |
| 1:A:55:PHE:CE2 | 1:A:92:ILE:HG21 | 0.85 | 2.06 | 32 | 7 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD21 | 0.85 | 1.48 | 10 | 4 |
| 1:A:40:LEU:N | 1:A:40:LEU:HD13 | 0.85 | 1.85 | 17 | 2 |
| 1:A:43:LEU:HD11 | 1:A:57:ILE:CG1 | 0.85 | 2.00 | 39 | 11 |
| 1:A:29:LEU:N | 1:A:29:LEU:HD13 | 0.84 | 1.87 | 20 | 2 |
| 1:A:89:ASP:OD2 | 1:A:92:ILE:HD12 | 0.84 | 1.70 | 33 | 3 |
| 1:A:43:LEU:HD11 | 1:A:93:ILE:HD12 | 0.84 | 1.49 | 15 | 1 |
| 1:A:29:LEU:HB2 | 1:A:42:ILE:HG21 | 0.84 | 1.48 | 20 | 6 |
| 1:A:43:LEU:HD11 | 1:A:93:ILE:CG1 | 0.84 | 2.01 | 42 | 4 |
| 1:A:40:LEU:HD22 | 1:A:40:LEU:N | 0.84 | 1.88 | 33 | 3 |
| 1:A:13:ILE:HG21 | 1:A:16:LEU:HD21 | 0.83 | 1.48 | 7 | 7 |
| 1:A:10:THR:HG23 | 1:A:56:VAL:O | 0.83 | 1.73 | 37 | 16 |
| 1:A:16:LEU:N | 1:A:16:LEU:HD22 | 0.83 | 1.89 | 29 | 15 |
| 1:A:39:ILE:O | 1:A:40:LEU:HD22 | 0.83 | 1.74 | 31 | 9 |
| 1:A:30:TYR:CZ | 1:A:39:ILE:HG22 | 0.82 | 2.09 | 29 | 27 |
| 1:A:43:LEU:CD2 | 1:A:93:ILE:HG23 | 0.82 | 2.04 | 11 | 2 |
| 1:A:16:LEU:CG | 1:A:25:LEU:HD21 | 0.82 | 2.04 | 2 | 3 |
| 1:A:32:ILE:HD12 | 1:A:33:PHE:CD1 | 0.82 | 2.09 | 13 | 5 |
| 1:A:29:LEU:HB2 | 1:A:42:ILE:HD13 | 0.82 | 1.49 | 42 | 11 |
| 1:A:40:LEU:HD13 | 1:A:40:LEU:N | 0.82 | 1.89 | 4 | 4 |
| 1:A:10:THR:HG21 | 1:A:89:ASP:CB | 0.82 | 2.05 | 35 | 2 |
| 1:A:71:MET:HB3 | 1:A:83:ILE:HD11 | 0.82 | 1.48 | 30 | 6 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:CG1 | 0.82 | 2.03 | 12 | 6 |
| 1:A:16:LEU:CB | 1:A:25:LEU:HD21 | 0.81 | 2.05 | 24 | 4 |
| 1:A:29:LEU:CD1 | 1:A:42:ILE:HG21 | 0.81 | 2.05 | 23 | 10 |
| 1:A:16:LEU:CD1 | 1:A:25:LEU:HD21 | 0.81 | 2.06 | 41 | 1 |
| 1:A:43:LEU:HD11 | 1:A:57:ILE:HD11 | 0.81 | 1.48 | 19 | 4 |
| 1:A:33:PHE:HB2 | 1:A:39:ILE:HD11 | 0.81 | 1.51 | 6 | 39 |
| 1:A:40:LEU:HD11 | 1:A:59:LYS:HA | 0.81 | 1.49 | 15 | 8 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:HG21 | 0.81 | 2.10 | 21 | 8 |
| 1:A:16:LEU:HG | 1:A:25:LEU:HD21 | 0.81 | 1.53 | 12 | 8 |
| 1:A:40:LEU:N | 1:A:40:LEU:HD22 | 0.81 | 1.90 | 40 | 5 |
| 1:A:16:LEU:HD12 | 1:A:25:LEU:HD21 | 0.81 | 1.51 | 41 | 1 |
| 1:A:39:ILE:HD11 | 1:A:58:PHE:CE2 | 0.80 | 2.11 | 10 | 17 |
| 1:A:40:LEU:HD21 | 1:A:58:PHE:C | 0.80 | 1.96 | 4 | 5 |
| 1:A:71:MET:HB2 | 1:A:83:ILE:HD11 | 0.80 | 1.52 | 28 | 25 |
| 1:A:68:LEU:HG | 1:A:85:TYR:CE2 | 0.80 | 2.10 | 2 | 17 |
| 1:A:57:ILE:HD11 | 1:A:93:ILE:HD13 | 0.80 | 1.54 | 11 | 3 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HD12 | 0.80 | 1.54 | 12 | 1 |
| 1:A:9:HIS:N | 1:A:61:VAL:HG13 | 0.79 | 1.92 | 41 | 32 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:31:ALA:O | 1:A:32:ILE:HG23 | 0.79 | 1.75 | 39 | 5 |
| 1:A:32:ILE:HD13 | 1:A:76:PHE:CE1 | 0.79 | 2.12 | 24 | 3 |
| 1:A:16:LEU:CG | 1:A:25:LEU:HD11 | 0.79 | 2.07 | 37 | 11 |
| 1:A:16:LEU:HB2 | 1:A:25:LEU:HD21 | 0.79 | 1.52 | 24 | 2 |
| 1:A:17:ASN:O | 1:A:20:ILE:HD12 | 0.78 | 1.77 | 10 | 23 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:CD1 | 0.78 | 2.08 | 28 | 24 |
| 1:A:40:LEU:HD22 | 1:A:57:ILE:O | 0.78 | 1.78 | 4 | 5 |
| 1:A:43:LEU:HD21 | 1:A:93:ILE:HG12 | 0.78 | 1.54 | 24 | 4 |
| 1:A:43:LEU:HD11 | 1:A:93:ILE:CD1 | 0.78 | 2.09 | 15 | 2 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD12 | 0.78 | 1.55 | 43 | 5 |
| 1:A:40:LEU:HD22 | 1:A:40:LEU:H | 0.77 | 1.37 | 43 | 2 |
| 1:A:16:LEU:HB3 | 1:A:25:LEU:HD21 | 0.77 | 1.55 | 30 | 8 |
| 1:A:16:LEU:HD12 | 1:A:25:LEU:HD11 | 0.77 | 1.56 | 9 | 8 |
| 1:A:68:LEU:HD12 | 1:A:85:TYR:OH | 0.77 | 1.80 | 31 | 40 |
| 1:A:29:LEU:CB | 1:A:42:ILE:HG21 | 0.77 | 2.09 | 19 | 5 |
| 1:A:40:LEU:N | 1:A:40:LEU:HD12 | 0.77 | 1.95 | 25 | 2 |
| 1:A:10:THR:HG21 | 1:A:89:ASP:HB3 | 0.76 | 1.57 | 1 | 2 |
| 1:A:33:PHE:HB3 | 1:A:39:ILE:HD11 | 0.76 | 1.56 | 27 | 14 |
| 1:A:86:ALA:HB1 | 1:A:89:ASP:OD2 | 0.76 | 1.80 | 32 | 5 |
| 1:A:48:LEU:N | 1:A:48:LEU:HD22 | 0.76 | 1.95 | 18 | 1 |
| 1:A:16:LEU:HD22 | 1:A:16:LEU:N | 0.76 | 1.95 | 16 | 20 |
| 1:A:32:ILE:HD12 | 1:A:33:PHE:N | 0.76 | 1.95 | 16 | 3 |
| 1:A:43:LEU:N | 1:A:43:LEU:HD22 | 0.76 | 1.96 | 23 | 1 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:HG13 | 0.76 | 1.57 | 9 | 5 |
| 1:A:44:VAL:HG22 | 1:A:45:SER:N | 0.76 | 1.96 | 21 | 2 |
| 1:A:10:THR:HG23 | 1:A:57:ILE:HD13 | 0.75 | 1.58 | 12 | 9 |
| 1:A:42:ILE:HD13 | 1:A:42:ILE:N | 0.75 | 1.95 | 4 | 4 |
| 1:A:89:ASP:HB3 | 1:A:92:ILE:HD12 | 0.75 | 1.56 | 8 | 2 |
| 1:A:11:ILE:HD12 | 1:A:83:ILE:CG2 | 0.75 | 2.10 | 43 | 8 |
| 1:A:9:HIS:H | 1:A:61:VAL:HG13 | 0.75 | 1.42 | 37 | 31 |
| 1:A:43:LEU:HD11 | 1:A:93:ILE:HG13 | 0.75 | 1.59 | 42 | 6 |
| 1:A:42:ILE:N | 1:A:42:ILE:HD13 | 0.75 | 1.96 | 12 | 6 |
| 1:A:16:LEU:CD1 | 1:A:25:LEU:HD11 | 0.75 | 2.11 | 32 | 6 |
| 1:A:48:LEU:O | 1:A:48:LEU:HD13 | 0.74 | 1.82 | 34 | 1 |
| 1:A:44:VAL:HG13 | 1:A:53:GLN:O | 0.74 | 1.82 | 15 | 3 |
| 1:A:57:ILE:HD11 | 1:A:93:ILE:CD1 | 0.74 | 2.13 | 25 | 20 |
| 1:A:30:TYR:CD2 | 1:A:42:ILE:HD12 | 0.74 | 2.18 | 28 | 4 |
| 1:A:89:ASP:O | 1:A:92:ILE:HG22 | 0.74 | 1.83 | 24 | 26 |
| 1:A:48:LEU:HD12 | 1:A:48:LEU:O | 0.74 | 1.83 | 3 | 1 |
| 1:A:16:LEU:HD11 | 1:A:76:PHE:CE2 | 0.74 | 2.17 | 22 | 7 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:HG12 | 0.74 | 1.60 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:ILE:HD11 | 1:A:56:VAL:CG2 | 0.73 | 2.12 | 5 | 16 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD13 | 0.73 | 1.56 | 42 | 5 |
| 1:A:79:LYS:N | 1:A:80:PRO:CD | 0.73 | 2.50 | 35 | 1 |
| 1:A:39:ILE:HD12 | 1:A:56:VAL:CG1 | 0.73 | 2.14 | 9 | 32 |
| 1:A:16:LEU:CB | 1:A:25:LEU:HD11 | 0.73 | 2.13 | 12 | 7 |
| 1:A:9:HIS:N | 1:A:61:VAL:HG23 | 0.73 | 1.98 | 6 | 1 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:CD1 | 0.73 | 2.13 | 43 | 5 |
| 1:A:39:ILE:CG2 | 1:A:42:ILE:HD11 | 0.73 | 2.10 | 28 | 5 |
| 1:A:67:ALA:O | 1:A:83:ILE:HD13 | 0.73 | 1.82 | 16 | 23 |
| 1:A:29:LEU:HD23 | 1:A:76:PHE:CZ | 0.73 | 2.19 | 43 | 4 |
| 1:A:36:PHE:CD2 | 1:A:67:ALA:HA | 0.73 | 2.19 | 8 | 42 |
| 1:A:68:LEU:HD22 | 1:A:83:ILE:HB | 0.72 | 1.60 | 43 | 22 |
| 1:A:33:PHE:CD1 | 1:A:67:ALA:HB1 | 0.72 | 2.19 | 20 | 27 |
| 1:A:68:LEU:HA | 1:A:83:ILE:HG21 | 0.72 | 1.61 | 15 | 24 |
| 1:A:76:PHE:CE2 | 1:A:77:TYR:CE2 | 0.71 | 2.78 | 35 | 7 |
| 1:A:40:LEU:N | 1:A:40:LEU:HD23 | 0.71 | 2.00 | 21 | 1 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:HD12 | 0.71 | 1.60 | 10 | 1 |
| 1:A:9:HIS:NE2 | 1:A:57:ILE:HG23 | 0.71 | 2.00 | 14 | 15 |
| 1:A:7:PRO:HB2 | 1:A:61:VAL:HG22 | 0.71 | 1.59 | 6 | 1 |
| 1:A:11:ILE:HD12 | 1:A:83:ILE:HG21 | 0.71 | 1.63 | 40 | 8 |
| 1:A:8:ASN:C | 1:A:61:VAL:HG13 | 0.71 | 2.06 | 29 | 3 |
| 1:A:43:LEU:HD11 | 1:A:57:ILE:HG12 | 0.71 | 1.62 | 9 | 2 |
| 1:A:40:LEU:HD13 | 1:A:59:LYS:HD2 | 0.71 | 1.63 | 21 | 1 |
| 1:A:17:ASN:CB | 1:A:20:ILE:HD11 | 0.70 | 2.16 | 17 | 7 |
| 1:A:43:LEU:HD21 | 1:A:93:ILE:HG13 | 0.70 | 1.62 | 10 | 3 |
| 1:A:50:MET:O | 1:A:52:GLY:N | 0.70 | 2.25 | 7 | 3 |
| 1:A:43:LEU:HD21 | 1:A:93:ILE:CG1 | 0.70 | 2.16 | 10 | 2 |
| 1:A:12:TYR:CE2 | 1:A:55:PHE:CE2 | 0.70 | 2.79 | 14 | 16 |
| 1:A:76:PHE:CZ | 1:A:77:TYR:CE1 | 0.70 | 2.79 | 26 | 14 |
| 1:A:40:LEU:HD23 | 1:A:59:LYS:HB2 | 0.70 | 1.61 | 31 | 4 |
| 1:A:20:ILE:CG2 | 1:A:25:LEU:HD13 | 0.70 | 2.05 | 14 | 2 |
| 1:A:48:LEU:HD13 | 1:A:48:LEU:C | 0.70 | 2.07 | 34 | 3 |
| 1:A:16:LEU:HD12 | 1:A:76:PHE:CD2 | 0.70 | 2.21 | 21 | 2 |
| 1:A:76:PHE:CE1 | 1:A:77:TYR:CE1 | 0.70 | 2.79 | 29 | 16 |
| 1:A:43:LEU:HD21 | 1:A:57:ILE:HD11 | 0.69 | 1.62 | 20 | 1 |
| 1:A:16:LEU:HD23 | 1:A:52:GLY:C | 0.69 | 2.07 | 31 | 6 |
| 1:A:76:PHE:CE2 | 1:A:77:TYR:CE1 | 0.69 | 2.79 | 24 | 9 |
| 1:A:65:THR:HG22 | 1:A:69:ARG:HD3 | 0.69 | 1.62 | 3 | 4 |
| 1:A:12:TYR:CE2 | 1:A:55:PHE:CZ | 0.69 | 2.80 | 31 | 6 |
| 1:A:68:LEU:HA | 1:A:83:ILE:HD13 | 0.69 | 1.63 | 18 | 7 |
| 1:A:9:HIS:H | 1:A:61:VAL:HG23 | 0.69 | 1.47 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:43:LEU:HD11 | 1:A:57:ILE:HG13 | 0.69 | 1.64 | 39 | 3 |
| 1:A:55:PHE:CE1 | 1:A:92:ILE:HG23 | 0.69 | 2.23 | 29 | 4 |
| 1:A:39:ILE:CD1 | 1:A:56:VAL:CG1 | 0.69 | 2.71 | 20 | 35 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:C | 0.69 | 2.08 | 13 | 4 |
| 1:A:11:ILE:HG22 | 1:A:64:ALA:HB1 | 0.69 | 1.65 | 34 | 30 |
| 1:A:16:LEU:HD11 | 1:A:76:PHE:CD2 | 0.69 | 2.22 | 10 | 7 |
| 1:A:76:PHE:CZ | 1:A:77:TYR:CZ | 0.69 | 2.80 | 35 | 3 |
| 1:A:13:ILE:HG23 | 1:A:81:MET:HG2 | 0.68 | 1.63 | 41 | 1 |
| 1:A:39:ILE:HD12 | 1:A:56:VAL:HG13 | 0.68 | 1.65 | 30 | 22 |
| 1:A:79:LYS:N | 1:A:80:PRO:HD3 | 0.68 | 2.03 | 35 | 1 |
| 1:A:68:LEU:HG | 1:A:85:TYR:CZ | 0.68 | 2.24 | 26 | 43 |
| 1:A:48:LEU:O | 1:A:48:LEU:HD23 | 0.68 | 1.88 | 25 | 5 |
| 1:A:76:PHE:CD1 | 1:A:77:TYR:CD1 | 0.68 | 2.81 | 29 | 3 |
| 1:A:89:ASP:OD1 | 1:A:92:ILE:HD12 | 0.68 | 1.88 | 40 | 3 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:CD1 | 0.68 | 2.19 | 39 | 5 |
| 1:A:76:PHE:CD2 | 1:A:77:TYR:CD1 | 0.68 | 2.82 | 41 | 8 |
| 1:A:68:LEU:C | 1:A:68:LEU:CD1 | 0.68 | 2.62 | 11 | 22 |
| 1:A:33:PHE:CE2 | 1:A:56:VAL:HG21 | 0.68 | 2.24 | 17 | 29 |
| 1:A:29:LEU:HA | 1:A:32:ILE:HD11 | 0.68 | 1.64 | 24 | 16 |
| 1:A:76:PHE:CE2 | 1:A:77:TYR:CZ | 0.68 | 2.81 | 35 | 5 |
| 1:A:20:ILE:HD11 | 1:A:77:TYR:CD2 | 0.68 | 2.24 | 20 | 5 |
| 1:A:89:ASP:CB | 1:A:92:ILE:HD12 | 0.67 | 2.18 | 8 | 5 |
| 1:A:50:MET:CA | 1:A:50:MET:CE | 0.67 | 2.73 | 21 | 2 |
| 1:A:25:LEU:HD12 | 1:A:77:TYR:CE2 | 0.67 | 2.24 | 14 | 6 |
| 1:A:38:GLN:HG2 | 1:A:40:LEU:HD23 | 0.67 | 1.66 | 18 | 1 |
| 1:A:40:LEU:HD11 | 1:A:59:LYS:H | 0.67 | 1.48 | 17 | 2 |
| 1:A:48:LEU:HD23 | 1:A:49:LYS:N | 0.67 | 2.05 | 23 | 1 |
| 1:A:25:LEU:HD23 | 1:A:29:LEU:HD11 | 0.67 | 1.65 | 15 | 1 |
| 1:A:16:LEU:HD13 | 1:A:76:PHE:CD2 | 0.67 | 2.24 | 36 | 1 |
| 1:A:25:LEU:HD13 | 1:A:77:TYR:CE2 | 0.66 | 2.24 | 39 | 1 |
| 1:A:12:TYR:CD2 | 1:A:55:PHE:CE2 | 0.66 | 2.84 | 6 | 4 |
| 1:A:56:VAL:HG11 | 1:A:58:PHE:CZ | 0.66 | 2.26 | 30 | 38 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:CD1 | 0.66 | 2.78 | 15 | 30 |
| 1:A:25:LEU:HD12 | 1:A:77:TYR:CZ | 0.66 | 2.25 | 32 | 3 |
| 1:A:29:LEU:HD13 | 1:A:42:ILE:CG2 | 0.66 | 2.14 | 23 | 8 |
| 1:A:30:TYR:CE1 | 1:A:39:ILE:HG22 | 0.66 | 2.25 | 38 | 3 |
| 1:A:68:LEU:CD1 | 1:A:68:LEU:C | 0.66 | 2.64 | 8 | 21 |
| 1:A:43:LEU:HD12 | 1:A:55:PHE:HB2 | 0.66 | 1.66 | 12 | 5 |
| 1:A:56:VAL:CG1 | 1:A:58:PHE:CE1 | 0.66 | 2.79 | 25 | 34 |
| 1:A:88:THR:HG22 | 1:A:88:THR:O | 0.66 | 1.88 | 31 | 7 |
| 1:A:30:TYR:CD2 | 1:A:42:ILE:CD1 | 0.66 | 2.77 | 19 | 17 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:39:ILE:HD11 | 1:A:58:PHE:CZ | 0.66 | 2.25 | 21 | 14 |
| 1:A:32:ILE:HD13 | 1:A:76:PHE:HE1 | 0.66 | 1.51 | 24 | 1 |
| 1:A:50:MET:HE1 | 1:A:50:MET:O | 0.66 | 1.90 | 20 | 4 |
| 1:A:55:PHE:CE1 | 1:A:92:ILE:CG2 | 0.66 | 2.79 | 22 | 12 |
| 1:A:43:LEU:HD11 | 1:A:93:ILE:HG12 | 0.66 | 1.68 | 42 | 3 |
| 1:A:28:SER:O | 1:A:32:ILE:HD11 | 0.65 | 1.90 | 40 | 5 |
| 1:A:29:LEU:CD1 | 1:A:29:LEU:N | 0.65 | 2.60 | 20 | 1 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:CG2 | 0.65 | 2.79 | 4 | 2 |
| 1:A:72:GLN:HA | 1:A:83:ILE:HD12 | 0.65 | 1.67 | 1 | 1 |
| 1:A:16:LEU:CD1 | 1:A:76:PHE:CD1 | 0.65 | 2.79 | 25 | 3 |
| 1:A:39:ILE:CD1 | 1:A:58:PHE:CE2 | 0.65 | 2.79 | 17 | 20 |
| 1:A:40:LEU:CD1 | 1:A:40:LEU:N | 0.65 | 2.60 | 17 | 3 |
| 1:A:25:LEU:HD11 | 1:A:52:GLY:HA2 | 0.65 | 1.68 | 23 | 1 |
| 1:A:29:LEU:HD11 | 1:A:44:VAL:HG11 | 0.65 | 1.68 | 7 | 1 |
| 1:A:33:PHE:CB | 1:A:39:ILE:CD1 | 0.65 | 2.75 | 28 | 14 |
| 1:A:87:LYS:O | 1:A:88:THR:CB | 0.64 | 2.44 | 6 | 33 |
| 1:A:13:ILE:HD11 | 1:A:33:PHE:CZ | 0.64 | 2.27 | 14 | 4 |
| 1:A:43:LEU:HD21 | 1:A:57:ILE:CG1 | 0.64 | 2.22 | 23 | 1 |
| 1:A:58:PHE:CD2 | 1:A:63:SER:CB | 0.64 | 2.80 | 16 | 10 |
| 1:A:10:THR:HG21 | 1:A:55:PHE:HB3 | 0.64 | 1.70 | 31 | 5 |
| 1:A:56:VAL:CG1 | 1:A:58:PHE:CE2 | 0.64 | 2.81 | 20 | 7 |
| 1:A:43:LEU:O | 1:A:43:LEU:HD12 | 0.64 | 1.93 | 43 | 1 |
| 1:A:50:MET:HA | 1:A:50:MET:HE3 | 0.64 | 1.69 | 4 | 3 |
| 1:A:40:LEU:H | 1:A:40:LEU:HD22 | 0.64 | 1.53 | 8 | 3 |
| 1:A:16:LEU:CD1 | 1:A:76:PHE:CD2 | 0.64 | 2.80 | 36 | 9 |
| 1:A:36:PHE:CE1 | 1:A:70:SER:CB | 0.64 | 2.81 | 39 | 12 |
| 1:A:76:PHE:CD2 | 1:A:81:MET:CE | 0.64 | 2.80 | 29 | 4 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:CE2 | 0.64 | 2.28 | 22 | 4 |
| 1:A:32:ILE:CD1 | 1:A:33:PHE:CE1 | 0.63 | 2.80 | 43 | 4 |
| 1:A:68:LEU:CD1 | 1:A:85:TYR:CZ | 0.63 | 2.81 | 17 | 37 |
| 1:A:25:LEU:CD1 | 1:A:77:TYR:CE2 | 0.63 | 2.80 | 32 | 6 |
| 1:A:43:LEU:HD21 | 1:A:93:ILE:HG23 | 0.63 | 1.70 | 11 | 2 |
| 1:A:43:LEU:CD1 | 1:A:57:ILE:HD11 | 0.63 | 2.24 | 19 | 5 |
| 1:A:32:ILE:HG23 | 1:A:33:PHE:CD1 | 0.63 | 2.28 | 19 | 9 |
| 1:A:38:GLN:HG2 | 1:A:40:LEU:HD12 | 0.63 | 1.69 | 17 | 1 |
| 1:A:29:LEU:CD2 | 1:A:76:PHE:CZ | 0.63 | 2.81 | 43 | 4 |
| 1:A:32:ILE:CG2 | 1:A:33:PHE:CE1 | 0.63 | 2.81 | 2 | 8 |
| 1:A:58:PHE:CD1 | 1:A:63:SER:CB | 0.63 | 2.82 | 11 | 4 |
| 1:A:32:ILE:CD1 | 1:A:33:PHE:CD1 | 0.63 | 2.81 | 16 | 4 |
| 1:A:56:VAL:CG1 | 1:A:58:PHE:CZ | 0.63 | 2.81 | 13 | 4 |
| 1:A:44:VAL:HG13 | 1:A:54:ALA:HB2 | 0.63 | 1.69 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:9:HIS:O | 1:A:9:HIS:CD2 | 0.62 | 2.52 | 26 | 19 |
| 1:A:50:MET:HE3 | 1:A:53:GLN:HB2 | 0.62 | 1.70 | 30 | 6 |
| 1:A:7:PRO:HA | 1:A:85:TYR:CD1 | 0.62 | 2.29 | 31 | 16 |
| 1:A:43:LEU:N | 1:A:43:LEU:CD2 | 0.62 | 2.63 | 8 | 2 |
| 1:A:16:LEU:HD12 | 1:A:76:PHE:CE1 | 0.62 | 2.29 | 25 | 3 |
| 1:A:32:ILE:HD12 | 1:A:76:PHE:CE1 | 0.62 | 2.29 | 37 | 2 |
| 1:A:45:SER:HA | 1:A:50:MET:HB2 | 0.62 | 1.71 | 3 | 3 |
| 1:A:13:ILE:HD13 | 1:A:29:LEU:CD2 | 0.62 | 2.23 | 14 | 1 |
| 1:A:88:THR:O | 1:A:88:THR:HG22 | 0.62 | 1.94 | 11 | 2 |
| 1:A:11:ILE:CG2 | 1:A:64:ALA:HB1 | 0.62 | 2.24 | 34 | 28 |
| 1:A:16:LEU:HD12 | 1:A:76:PHE:CE2 | 0.62 | 2.30 | 30 | 7 |
| 1:A:68:LEU:CD1 | 1:A:69:ARG:N | 0.62 | 2.63 | 36 | 30 |
| 1:A:39:ILE:C | 1:A:40:LEU:HD23 | 0.62 | 2.14 | 36 | 7 |
| 1:A:30:TYR:CE2 | 1:A:39:ILE:HG22 | 0.62 | 2.29 | 6 | 8 |
| 1:A:43:LEU:O | 1:A:54:ALA:HB1 | 0.62 | 1.93 | 26 | 6 |
| 1:A:32:ILE:O | 1:A:36:PHE:CD1 | 0.62 | 2.53 | 21 | 18 |
| 1:A:32:ILE:CG2 | 1:A:33:PHE:CD1 | 0.62 | 2.83 | 33 | 8 |
| 1:A:111:LYS:N | 1:A:112:PRO:CD | 0.62 | 2.63 | 6 | 5 |
| 1:A:9:HIS:CD2 | 1:A:9:HIS:O | 0.62 | 2.53 | 40 | 18 |
| 1:A:89:ASP:CG | 1:A:92:ILE:HD12 | 0.62 | 2.15 | 21 | 3 |
| 1:A:16:LEU:CD1 | 1:A:76:PHE:CE2 | 0.62 | 2.82 | 36 | 7 |
| 1:A:30:TYR:HA | 1:A:42:ILE:HD11 | 0.61 | 1.72 | 31 | 6 |
| 1:A:32:ILE:HG22 | 1:A:33:PHE:CD1 | 0.61 | 2.30 | 37 | 3 |
| 1:A:6:ARG:O | 1:A:85:TYR:CG | 0.61 | 2.53 | 5 | 27 |
| 1:A:55:PHE:HE1 | 1:A:92:ILE:HG21 | 0.61 | 1.55 | 40 | 1 |
| 1:A:39:ILE:CG2 | 1:A:42:ILE:CG1 | 0.61 | 2.79 | 43 | 25 |
| 1:A:15:ASN:O | 1:A:16:LEU:O | 0.61 | 2.18 | 21 | 3 |
| 1:A:44:VAL:CG1 | 1:A:54:ALA:HB2 | 0.61 | 2.23 | 27 | 4 |
| 1:A:50:MET:HE2 | 1:A:50:MET:CA | 0.61 | 2.26 | 21 | 1 |
| 1:A:40:LEU:HD21 | 1:A:59:LYS:CA | 0.61 | 2.26 | 19 | 1 |
| 1:A:32:ILE:CD1 | 1:A:33:PHE:CZ | 0.61 | 2.83 | 6 | 3 |
| 1:A:16:LEU:CD1 | 1:A:77:TYR:CD2 | 0.61 | 2.84 | 23 | 1 |
| 1:A:50:MET:HA | 1:A:50:MET:CE | 0.61 | 2.26 | 21 | 4 |
| 1:A:68:LEU:O | 1:A:68:LEU:HD22 | 0.61 | 1.96 | 33 | 8 |
| 1:A:56:VAL:HG11 | 1:A:58:PHE:CE2 | 0.60 | 2.31 | 20 | 5 |
| 1:A:9:HIS:O | 1:A:9:HIS:CG | 0.60 | 2.55 | 4 | 10 |
| 1:A:9:HIS:CB | 1:A:61:VAL:HG22 | 0.60 | 2.26 | 9 | 8 |
| 1:A:21:LYS:O | 1:A:23:ASP:N | 0.60 | 2.35 | 14 | 1 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:CG1 | 0.60 | 2.80 | 8 | 8 |
| 1:A:25:LEU:HD22 | 1:A:77:TYR:CE2 | 0.60 | 2.32 | 1 | 2 |
| 1:A:40:LEU:N | 1:A:40:LEU:CD1 | 0.60 | 2.63 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:PHE:HB2 | 1:A:39:ILE:CD1 | 0.60 | 2.27 | 13 | 35 |
| 1:A:33:PHE:HB2 | 1:A:39:ILE:CG1 | 0.60 | 2.27 | 27 | 28 |
| 1:A:39:ILE:CG2 | 1:A:42:ILE:CD1 | 0.60 | 2.80 | 4 | 10 |
| 1:A:20:ILE:CD1 | 1:A:77:TYR:CD2 | 0.60 | 2.85 | 35 | 6 |
| 1:A:33:PHE:HD2 | 1:A:42:ILE:HD11 | 0.60 | 1.57 | 10 | 2 |
| 1:A:16:LEU:N | 1:A:16:LEU:CD2 | 0.60 | 2.65 | 39 | 23 |
| 1:A:29:LEU:HD23 | 1:A:76:PHE:CE1 | 0.59 | 2.32 | 43 | 2 |
| 1:A:16:LEU:CD2 | 1:A:16:LEU:N | 0.59 | 2.65 | 37 | 13 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:CG1 | 0.59 | 2.27 | 38 | 16 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:HD12 | 0.59 | 2.26 | 3 | 3 |
| 1:A:33:PHE:HA | 1:A:36:PHE:CD2 | 0.59 | 2.33 | 12 | 20 |
| 1:A:13:ILE:HG22 | 1:A:16:LEU:CD2 | 0.59 | 2.27 | 1 | 6 |
| 1:A:16:LEU:H | 1:A:16:LEU:HD22 | 0.59 | 1.57 | 14 | 1 |
| 1:A:48:LEU:HD13 | 1:A:48:LEU:O | 0.59 | 1.96 | 29 | 2 |
| 1:A:9:HIS:CG | 1:A:9:HIS:O | 0.59 | 2.55 | 37 | 10 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HB2 | 0.59 | 1.73 | 29 | 3 |
| 1:A:13:ILE:HG23 | 1:A:16:LEU:HD21 | 0.59 | 1.73 | 26 | 5 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:CD1 | 0.59 | 2.80 | 18 | 8 |
| 1:A:67:ALA:O | 1:A:83:ILE:HD12 | 0.59 | 1.98 | 41 | 8 |
| 1:A:40:LEU:CD1 | 1:A:59:LYS:N | 0.59 | 2.65 | 27 | 1 |
| 1:A:10:THR:HG21 | 1:A:55:PHE:HB2 | 0.59 | 1.74 | 19 | 1 |
| 1:A:9:HIS:HB2 | 1:A:61:VAL:HG22 | 0.59 | 1.73 | 37 | 11 |
| 1:A:44:VAL:HG23 | 1:A:53:GLN:O | 0.59 | 1.97 | 21 | 1 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HD22 | 0.59 | 1.73 | 10 | 1 |
| 1:A:55:PHE:CE1 | 1:A:89:ASP:OD2 | 0.59 | 2.56 | 10 | 1 |
| 1:A:12:TYR:CB | 1:A:84:GLN:O | 0.59 | 2.51 | 8 | 22 |
| 1:A:58:PHE:CD1 | 1:A:63:SER:HB2 | 0.59 | 2.33 | 11 | 4 |
| 1:A:12:TYR:CD1 | 1:A:13:ILE:N | 0.59 | 2.71 | 5 | 18 |
| 1:A:41:ASP:O | 1:A:43:LEU:HD23 | 0.59 | 1.98 | 25 | 2 |
| 1:A:64:ALA:O | 1:A:68:LEU:HB3 | 0.59 | 1.97 | 29 | 43 |
| 1:A:9:HIS:CE1 | 1:A:57:ILE:HG23 | 0.59 | 2.33 | 42 | 4 |
| 1:A:55:PHE:CD1 | 1:A:55:PHE:N | 0.59 | 2.70 | 24 | 7 |
| 1:A:12:TYR:CE1 | 1:A:53:GLN:OE1 | 0.59 | 2.56 | 10 | 3 |
| 1:A:78:ASP:O | 1:A:79:LYS:CB | 0.59 | 2.51 | 35 | 4 |
| 1:A:22:LYS:O | 1:A:23:ASP:CB | 0.59 | 2.51 | 4 | 28 |
| 1:A:44:VAL:HB | 1:A:54:ALA:HB2 | 0.59 | 1.74 | 9 | 1 |
| 1:A:40:LEU:CD2 | 1:A:40:LEU:N | 0.58 | 2.62 | 33 | 4 |
| 1:A:25:LEU:HD21 | 1:A:52:GLY:O | 0.58 | 1.98 | 36 | 1 |
| 1:A:68:LEU:HD12 | 1:A:85:TYR:CZ | 0.58 | 2.32 | 17 | 27 |
| 1:A:45:SER:O | 1:A:50:MET:HE3 | 0.58 | 1.98 | 42 | 5 |
| 1:A:29:LEU:CD1 | 1:A:76:PHE:CZ | 0.58 | 2.85 | 20 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:PHE:CD1 | 1:A:89:ASP:OD1 | 0.58 | 2.56 | 35 | 2 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:CG2 | 0.58 | 2.80 | 28 | 2 |
| 1:A:43:LEU:HD22 | 1:A:93:ILE:HG13 | 0.58 | 1.76 | 4 | 5 |
| 1:A:30:TYR:CE1 | 1:A:39:ILE:O | 0.58 | 2.56 | 13 | 2 |
| 1:A:22:LYS:HE3 | 1:A:44:VAL:HG23 | 0.58 | 1.75 | 27 | 1 |
| 1:A:48:LEU:N | 1:A:48:LEU:CD2 | 0.58 | 2.66 | 18 | 1 |
| 1:A:9:HIS:CD2 | 1:A:58:PHE:O | 0.58 | 2.56 | 21 | 17 |
| 1:A:42:ILE:C | 1:A:43:LEU:HD23 | 0.58 | 2.18 | 15 | 2 |
| 1:A:32:ILE:HG22 | 1:A:33:PHE:CG | 0.58 | 2.34 | 2 | 2 |
| 1:A:71:MET:SD | 1:A:74:PHE:CD2 | 0.58 | 2.97 | 42 | 3 |
| 1:A:17:ASN:HB3 | 1:A:20:ILE:HD11 | 0.58 | 1.76 | 17 | 5 |
| 1:A:32:ILE:HD12 | 1:A:33:PHE:CE1 | 0.58 | 2.34 | 43 | 2 |
| 1:A:50:MET:CE | 1:A:53:GLN:HB2 | 0.58 | 2.28 | 3 | 13 |
| 1:A:32:ILE:HD12 | 1:A:33:PHE:CG | 0.58 | 2.33 | 18 | 3 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HG | 0.58 | 1.74 | 21 | 1 |
| 1:A:50:MET:HE2 | 1:A:50:MET:HA | 0.58 | 1.73 | 21 | 1 |
| 1:A:32:ILE:HG22 | 1:A:33:PHE:N | 0.58 | 2.13 | 23 | 3 |
| 1:A:38:GLN:CG | 1:A:40:LEU:HD11 | 0.58 | 2.29 | 40 | 1 |
| 1:A:33:PHE:CD1 | 1:A:67:ALA:CB | 0.58 | 2.87 | 20 | 5 |
| 1:A:55:PHE:HE2 | 1:A:92:ILE:HD13 | 0.58 | 1.54 | 28 | 3 |
| 1:A:77:TYR:O | 1:A:78:ASP:CB | 0.58 | 2.50 | 35 | 21 |
| 1:A:12:TYR:CD1 | 1:A:84:GLN:NE2 | 0.58 | 2.72 | 15 | 2 |
| 1:A:89:ASP:O | 1:A:93:ILE:HD12 | 0.58 | 1.98 | 1 | 3 |
| 1:A:74:PHE:CE1 | 1:A:75:PRO:O | 0.58 | 2.57 | 36 | 1 |
| 1:A:55:PHE:CD2 | 1:A:89:ASP:OD2 | 0.57 | 2.57 | 21 | 6 |
| 1:A:36:PHE:CE1 | 1:A:70:SER:HB3 | 0.57 | 2.34 | 32 | 4 |
| 1:A:12:TYR:CZ | 1:A:53:GLN:OE1 | 0.57 | 2.57 | 42 | 4 |
| 1:A:47:SER:O | 1:A:50:MET:CE | 0.57 | 2.52 | 21 | 1 |
| 1:A:36:PHE:CZ | 1:A:71:MET:SD | 0.57 | 2.97 | 16 | 4 |
| 1:A:55:PHE:CG | 1:A:89:ASP:CG | 0.57 | 2.78 | 1 | 2 |
| 1:A:36:PHE:CE2 | 1:A:71:MET:CG | 0.57 | 2.87 | 26 | 4 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:O | 0.57 | 1.98 | 7 | 3 |
| 1:A:40:LEU:HD21 | 1:A:59:LYS:H | 0.57 | 1.58 | 36 | 1 |
| 1:A:58:PHE:CD2 | 1:A:63:SER:HB2 | 0.57 | 2.35 | 43 | 7 |
| 1:A:14:ASN:O | 1:A:15:ASN:CB | 0.57 | 2.53 | 33 | 19 |
| 1:A:17:ASN:HB2 | 1:A:20:ILE:HD11 | 0.57 | 1.75 | 15 | 3 |
| 1:A:32:ILE:CG2 | 1:A:33:PHE:N | 0.57 | 2.67 | 33 | 12 |
| 1:A:32:ILE:CD1 | 1:A:76:PHE:CE1 | 0.57 | 2.87 | 41 | 3 |
| 1:A:68:LEU:CG | 1:A:85:TYR:CE1 | 0.57 | 2.88 | 42 | 26 |
| 1:A:76:PHE:CD2 | 1:A:81:MET:SD | 0.57 | 2.98 | 22 | 6 |
| 1:A:30:TYR:CG | 1:A:42:ILE:HD11 | 0.57 | 2.34 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:SER:CB | 1:A:76:PHE:CZ | 0.57 | 2.88 | 43 | 4 |
| 1:A:11:ILE:CD1 | 1:A:56:VAL:CG2 | 0.57 | 2.83 | 5 | 8 |
| 1:A:76:PHE:CG | 1:A:81:MET:SD | 0.57 | 2.97 | 41 | 1 |
| 1:A:25:LEU:O | 1:A:29:LEU:HD22 | 0.57 | 2.00 | 20 | 1 |
| 1:A:68:LEU:O | 1:A:68:LEU:HD13 | 0.57 | 2.00 | 8 | 6 |
| 1:A:44:VAL:HG22 | 1:A:54:ALA:HB2 | 0.57 | 1.77 | 19 | 3 |
| 1:A:33:PHE:CE1 | 1:A:67:ALA:HB1 | 0.57 | 2.33 | 7 | 4 |
| 1:A:7:PRO:HA | 1:A:85:TYR:CD2 | 0.57 | 2.35 | 11 | 26 |
| 1:A:92:ILE:HG22 | 1:A:93:ILE:HD12 | 0.57 | 1.77 | 23 | 2 |
| 1:A:44:VAL:HG23 | 1:A:44:VAL:O | 0.57 | 1.99 | 29 | 2 |
| 1:A:67:ALA:O | 1:A:83:ILE:CD1 | 0.56 | 2.52 | 7 | 17 |
| 1:A:42:ILE:CD1 | 1:A:42:ILE:N | 0.56 | 2.65 | 12 | 4 |
| 1:A:40:LEU:N | 1:A:40:LEU:CD2 | 0.56 | 2.65 | 40 | 1 |
| 1:A:71:MET:CE | 1:A:81:MET:CE | 0.56 | 2.83 | 19 | 3 |
| 1:A:58:PHE:CD2 | 1:A:63:SER:HB3 | 0.56 | 2.36 | 16 | 13 |
| 1:A:58:PHE:CD1 | 1:A:63:SER:HB3 | 0.56 | 2.35 | 2 | 4 |
| 1:A:76:PHE:CD2 | 1:A:81:MET:HE2 | 0.56 | 2.35 | 31 | 3 |
| 1:A:40:LEU:HD13 | 1:A:59:LYS:HB2 | 0.56 | 1.77 | 7 | 1 |
| 1:A:66:ASN:O | 1:A:70:SER:CB | 0.56 | 2.53 | 19 | 20 |
| 1:A:44:VAL:O | 1:A:44:VAL:HG23 | 0.56 | 2.00 | 38 | 3 |
| 1:A:57:ILE:HD11 | 1:A:93:ILE:CG1 | 0.56 | 2.29 | 23 | 3 |
| 1:A:16:LEU:CD1 | 1:A:76:PHE:CE1 | 0.56 | 2.88 | 25 | 3 |
| 1:A:16:LEU:HD12 | 1:A:77:TYR:CE2 | 0.56 | 2.34 | 23 | 2 |
| 1:A:29:LEU:HB3 | 1:A:33:PHE:CE2 | 0.56 | 2.35 | 33 | 18 |
| 1:A:16:LEU:O | 1:A:17:ASN:C | 0.56 | 2.44 | 35 | 14 |
| 1:A:16:LEU:HD12 | 1:A:77:TYR:HD2 | 0.56 | 1.60 | 8 | 1 |
| 1:A:12:TYR:CZ | 1:A:53:GLN:CD | 0.56 | 2.79 | 28 | 4 |
| 1:A:25:LEU:HB3 | 1:A:44:VAL:HG21 | 0.56 | 1.78 | 7 | 1 |
| 1:A:32:ILE:HD11 | 1:A:33:PHE:CZ | 0.56 | 2.36 | 8 | 4 |
| 1:A:20:ILE:HD12 | 1:A:77:TYR:CD2 | 0.56 | 2.35 | 29 | 4 |
| 1:A:84:GLN:O | 1:A:85:TYR:C | 0.56 | 2.44 | 35 | 43 |
| 1:A:9:HIS:NE2 | 1:A:57:ILE:CG2 | 0.56 | 2.68 | 23 | 11 |
| 1:A:44:VAL:CG2 | 1:A:45:SER:N | 0.56 | 2.69 | 20 | 3 |
| 1:A:22:LYS:HB2 | 1:A:44:VAL:HG21 | 0.56 | 1.76 | 33 | 1 |
| 1:A:50:MET:CE | 1:A:50:MET:O | 0.56 | 2.54 | 22 | 6 |
| 1:A:28:SER:O | 1:A:32:ILE:CG1 | 0.56 | 2.54 | 39 | 7 |
| 1:A:8:ASN:O | 1:A:9:HIS:CB | 0.56 | 2.53 | 33 | 20 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:HA | 0.56 | 1.78 | 5 | 1 |
| 1:A:50:MET:CE | 1:A:53:GLN:CB | 0.56 | 2.84 | 30 | 4 |
| 1:A:6:ARG:O | 1:A:85:TYR:CD2 | 0.56 | 2.59 | 31 | 4 |
| 1:A:9:HIS:NE2 | 1:A:57:ILE:HG22 | 0.55 | 2.16 | 3 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:LEU:CG | 1:A:85:TYR:CE2 | 0.55 | 2.89 | 26 | 17 |
| 1:A:16:LEU:O | 1:A:20:ILE:CD1 | 0.55 | 2.55 | 6 | 12 |
| 1:A:90:SER:HA | 1:A:93:ILE:HD13 | 0.55 | 1.78 | 25 | 3 |
| 1:A:16:LEU:HD13 | 1:A:16:LEU:N | 0.55 | 2.16 | 21 | 3 |
| 1:A:28:SER:HB2 | 1:A:76:PHE:CE2 | 0.55 | 2.37 | 42 | 1 |
| 1:A:56:VAL:HG11 | 1:A:58:PHE:CE1 | 0.55 | 2.37 | 40 | 25 |
| 1:A:40:LEU:HD21 | 1:A:59:LYS:HB2 | 0.55 | 1.77 | 20 | 5 |
| 1:A:10:THR:CG2 | 1:A:57:ILE:HD13 | 0.55 | 2.31 | 32 | 6 |
| 1:A:55:PHE:N | 1:A:55:PHE:CD1 | 0.55 | 2.75 | 8 | 13 |
| 1:A:17:ASN:N | 1:A:17:ASN:OD1 | 0.55 | 2.40 | 43 | 1 |
| 1:A:36:PHE:CE2 | 1:A:71:MET:HG2 | 0.55 | 2.37 | 11 | 6 |
| 1:A:112:PRO:O | 1:A:113:LYS:CG | 0.55 | 2.54 | 26 | 1 |
| 1:A:36:PHE:CZ | 1:A:70:SER:CB | 0.55 | 2.89 | 6 | 5 |
| 1:A:36:PHE:CE1 | 1:A:70:SER:OG | 0.55 | 2.57 | 6 | 1 |
| 1:A:17:ASN:CB | 1:A:20:ILE:CD1 | 0.55 | 2.84 | 17 | 2 |
| 1:A:13:ILE:CG2 | 1:A:16:LEU:CD2 | 0.55 | 2.84 | 25 | 7 |
| 1:A:28:SER:HB2 | 1:A:76:PHE:CZ | 0.55 | 2.37 | 42 | 3 |
| 1:A:89:ASP:OD2 | 1:A:93:ILE:CD1 | 0.55 | 2.55 | 41 | 1 |
| 1:A:68:LEU:CD1 | 1:A:69:ARG:CG | 0.55 | 2.84 | 10 | 7 |
| 1:A:26:LYS:CG | 1:A:44:VAL:HG13 | 0.55 | 2.31 | 37 | 1 |
| 1:A:49:LYS:O | 1:A:50:MET:C | 0.55 | 2.45 | 3 | 3 |
| 1:A:55:PHE:CD1 | 1:A:89:ASP:CG | 0.55 | 2.81 | 1 | 2 |
| 1:A:43:LEU:CD2 | 1:A:57:ILE:CG1 | 0.55 | 2.84 | 20 | 1 |
| 1:A:9:HIS:NE2 | 1:A:58:PHE:O | 0.54 | 2.40 | 13 | 14 |
| 1:A:44:VAL:HG12 | 1:A:45:SER:N | 0.54 | 2.16 | 19 | 2 |
| 1:A:40:LEU:HD11 | 1:A:59:LYS:CB | 0.54 | 2.31 | 24 | 2 |
| 1:A:36:PHE:CE2 | 1:A:70:SER:HB3 | 0.54 | 2.37 | 18 | 3 |
| 1:A:82:ARG:O | 1:A:82:ARG:CG | 0.54 | 2.55 | 31 | 2 |
| 1:A:32:ILE:CD1 | 1:A:76:PHE:CD1 | 0.54 | 2.90 | 41 | 1 |
| 1:A:28:SER:CB | 1:A:77:TYR:OH | 0.54 | 2.55 | 10 | 18 |
| 1:A:51:ARG:O | 1:A:53:GLN:N | 0.54 | 2.39 | 11 | 5 |
| 1:A:13:ILE:HG23 | 1:A:16:LEU:CD2 | 0.54 | 2.32 | 35 | 2 |
| 1:A:55:PHE:CD2 | 1:A:89:ASP:HB2 | 0.54 | 2.38 | 41 | 1 |
| 1:A:50:MET:CG | 1:A:50:MET:O | 0.54 | 2.55 | 14 | 2 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:CD2 | 0.54 | 2.33 | 22 | 4 |
| 1:A:46:ARG:CD | 1:A:46:ARG:N | 0.54 | 2.70 | 39 | 1 |
| 1:A:16:LEU:O | 1:A:20:ILE:HD11 | 0.54 | 2.01 | 12 | 2 |
| 1:A:39:ILE:CD1 | 1:A:56:VAL:HG13 | 0.54 | 2.32 | 20 | 4 |
| 1:A:33:PHE:CD2 | 1:A:42:ILE:HD11 | 0.54 | 2.38 | 10 | 2 |
| 1:A:46:ARG:N | 1:A:50:MET:SD | 0.54 | 2.80 | 22 | 1 |
| 1:A:15:ASN:O | 1:A:16:LEU:HD22 | 0.54 | 2.03 | 38 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:48:LEU:C | 1:A:48:LEU:HD23 | 0.54 | 2.22 | 19 | 3 |
| 1:A:29:LEU:N | 1:A:29:LEU:CD1 | 0.54 | 2.60 | 42 | 1 |
| 1:A:38:GLN:HG2 | 1:A:40:LEU:HD11 | 0.54 | 1.77 | 40 | 1 |
| 1:A:10:THR:OG1 | 1:A:57:ILE:CD1 | 0.54 | 2.55 | 27 | 8 |
| 1:A:33:PHE:HB3 | 1:A:39:ILE:CD1 | 0.54 | 2.33 | 25 | 3 |
| 1:A:22:LYS:HE3 | 1:A:44:VAL:HG11 | 0.54 | 1.79 | 28 | 2 |
| 1:A:45:SER:O | 1:A:50:MET:CE | 0.54 | 2.56 | 42 | 5 |
| 1:A:71:MET:O | 1:A:73:GLY:N | 0.54 | 2.40 | 28 | 21 |
| 1:A:17:ASN:O | 1:A:19:LYS:N | 0.54 | 2.40 | 4 | 1 |
| 1:A:74:PHE:HB3 | 1:A:81:MET:HE3 | 0.54 | 1.80 | 21 | 1 |
| 1:A:68:LEU:CD2 | 1:A:83:ILE:O | 0.54 | 2.55 | 1 | 4 |
| 1:A:40:LEU:O | 1:A:41:ASP:CB | 0.54 | 2.56 | 9 | 32 |
| 1:A:37:GLY:O | 1:A:38:GLN:CB | 0.54 | 2.56 | 21 | 17 |
| 1:A:33:PHE:HA | 1:A:36:PHE:CD1 | 0.54 | 2.38 | 20 | 11 |
| 1:A:8:ASN:O | 1:A:9:HIS:HB3 | 0.54 | 2.03 | 6 | 30 |
| 1:A:7:PRO:HA | 1:A:85:TYR:CE1 | 0.54 | 2.38 | 31 | 11 |
| 1:A:50:MET:HE1 | 1:A:51:ARG:O | 0.54 | 2.02 | 8 | 3 |
| 1:A:68:LEU:O | 1:A:72:GLN:CB | 0.54 | 2.56 | 34 | 1 |
| 1:A:35:GLN:OE1 | 1:A:36:PHE:CE1 | 0.54 | 2.61 | 14 | 1 |
| 1:A:78:ASP:O | 1:A:79:LYS:CG | 0.54 | 2.56 | 28 | 2 |
| 1:A:45:SER:O | 1:A:46:ARG:CD | 0.54 | 2.56 | 7 | 1 |
| 1:A:92:ILE:CG2 | 1:A:93:ILE:N | 0.54 | 2.71 | 42 | 7 |
| 1:A:65:THR:O | 1:A:69:ARG:CG | 0.54 | 2.56 | 19 | 23 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:HD12 | 0.54 | 2.37 | 31 | 6 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD11 | 0.54 | 1.79 | 20 | 1 |
| 1:A:41:ASP:O | 1:A:57:ILE:CG1 | 0.54 | 2.56 | 34 | 8 |
| 1:A:36:PHE:CZ | 1:A:70:SER:HB3 | 0.54 | 2.38 | 6 | 4 |
| 1:A:50:MET:HE3 | 1:A:53:GLN:CB | 0.54 | 2.33 | 30 | 2 |
| 1:A:40:LEU:CB | 1:A:57:ILE:O | 0.53 | 2.56 | 16 | 2 |
| 1:A:45:SER:CB | 1:A:50:MET:SD | 0.53 | 2.97 | 15 | 6 |
| 1:A:24:GLU:O | 1:A:27:LYS:CG | 0.53 | 2.56 | 9 | 7 |
| 1:A:33:PHE:CE2 | 1:A:56:VAL:CG2 | 0.53 | 2.91 | 17 | 5 |
| 1:A:108:GLU:O | 1:A:109:LYS:CG | 0.53 | 2.56 | 6 | 2 |
| 1:A:26:LYS:CG | 1:A:44:VAL:HG23 | 0.53 | 2.33 | 12 | 2 |
| 1:A:50:MET:O | 1:A:50:MET:CE | 0.53 | 2.56 | 31 | 9 |
| 1:A:12:TYR:CE2 | 1:A:89:ASP:OD2 | 0.53 | 2.61 | 21 | 1 |
| 1:A:50:MET:CA | 1:A:50:MET:HE3 | 0.53 | 2.32 | 23 | 1 |
| 1:A:74:PHE:CD2 | 1:A:75:PRO:HD2 | 0.53 | 2.39 | 43 | 9 |
| 1:A:74:PHE:CG | 1:A:75:PRO:HD2 | 0.53 | 2.38 | 19 | 10 |
| 1:A:33:PHE:CE1 | 1:A:71:MET:SD | 0.53 | 3.02 | 32 | 3 |
| 1:A:28:SER:HG | 1:A:76:PHE:HE1 | 0.53 | 1.46 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:43:LEU:HD21 | 1:A:93:ILE:CG2 | 0.53 | 2.33 | 11 | 2 |
| 1:A:36:PHE:CZ | 1:A:71:MET:HG2 | 0.53 | 2.38 | 26 | 3 |
| 1:A:17:ASN:O | 1:A:20:ILE:CD1 | 0.53 | 2.57 | 23 | 14 |
| 1:A:111:LYS:N | 1:A:112:PRO:HD2 | 0.53 | 2.19 | 6 | 5 |
| 1:A:43:LEU:O | 1:A:54:ALA:CB | 0.53 | 2.57 | 26 | 3 |
| 1:A:12:TYR:CZ | 1:A:55:PHE:CZ | 0.53 | 2.95 | 33 | 1 |
| 1:A:20:ILE:CG2 | 1:A:25:LEU:HD12 | 0.53 | 2.32 | 12 | 1 |
| 1:A:29:LEU:H | 1:A:29:LEU:HD22 | 0.53 | 1.63 | 42 | 1 |
| 1:A:17:ASN:CB | 1:A:77:TYR:O | 0.53 | 2.56 | 35 | 1 |
| 1:A:44:VAL:O | 1:A:45:SER:C | 0.53 | 2.47 | 3 | 1 |
| 1:A:30:TYR:CD2 | 1:A:42:ILE:HG13 | 0.53 | 2.38 | 34 | 14 |
| 1:A:50:MET:CE | 1:A:53:GLN:O | 0.53 | 2.56 | 3 | 6 |
| 1:A:81:MET:O | 1:A:83:ILE:N | 0.53 | 2.42 | 18 | 5 |
| 1:A:46:ARG:O | 1:A:47:SER:CB | 0.53 | 2.56 | 15 | 4 |
| 1:A:76:PHE:CE1 | 1:A:77:TYR:CD1 | 0.53 | 2.97 | 29 | 2 |
| 1:A:43:LEU:CD2 | 1:A:57:ILE:HD11 | 0.53 | 2.31 | 20 | 1 |
| 1:A:66:ASN:O | 1:A:70:SER:N | 0.53 | 2.42 | 9 | 8 |
| 1:A:20:ILE:HD11 | 1:A:77:TYR:HD2 | 0.53 | 1.64 | 10 | 5 |
| 1:A:12:TYR:O | 1:A:84:GLN:NE2 | 0.53 | 2.42 | 10 | 5 |
| 1:A:43:LEU:HD21 | 1:A:57:ILE:CD1 | 0.53 | 2.34 | 20 | 1 |
| 1:A:44:VAL:CG1 | 1:A:53:GLN:O | 0.53 | 2.56 | 43 | 2 |
| 1:A:22:LYS:O | 1:A:24:GLU:N | 0.53 | 2.42 | 14 | 5 |
| 1:A:39:ILE:CG2 | 1:A:42:ILE:HG13 | 0.53 | 2.34 | 27 | 13 |
| 1:A:71:MET:HB3 | 1:A:74:PHE:CG | 0.53 | 2.39 | 23 | 5 |
| 1:A:31:ALA:O | 1:A:32:ILE:CG2 | 0.53 | 2.57 | 34 | 6 |
| 1:A:55:PHE:CD2 | 1:A:89:ASP:CB | 0.53 | 2.92 | 41 | 1 |
| 1:A:44:VAL:HG12 | 1:A:54:ALA:HB1 | 0.53 | 1.76 | 7 | 2 |
| 1:A:28:SER:O | 1:A:32:ILE:CD1 | 0.53 | 2.57 | 40 | 2 |
| 1:A:82:ARG:O | 1:A:84:GLN:NE2 | 0.53 | 2.42 | 17 | 8 |
| 1:A:15:ASN:O | 1:A:15:ASN:ND2 | 0.53 | 2.41 | 35 | 1 |
| 1:A:14:ASN:OD1 | 1:A:53:GLN:CG | 0.52 | 2.57 | 36 | 5 |
| 1:A:43:LEU:CD1 | 1:A:57:ILE:CG1 | 0.52 | 2.88 | 4 | 2 |
| 1:A:65:THR:O | 1:A:69:ARG:CD | 0.52 | 2.57 | 36 | 3 |
| 1:A:42:ILE:O | 1:A:43:LEU:CD2 | 0.52 | 2.57 | 18 | 3 |
| 1:A:45:SER:OG | 1:A:50:MET:CB | 0.52 | 2.57 | 42 | 1 |
| 1:A:50:MET:HE3 | 1:A:50:MET:CA | 0.52 | 2.33 | 36 | 1 |
| 1:A:40:LEU:CD2 | 1:A:57:ILE:O | 0.52 | 2.56 | 17 | 3 |
| 1:A:21:LYS:O | 1:A:22:LYS:O | 0.52 | 2.27 | 1 | 30 |
| 1:A:28:SER:OG | 1:A:76:PHE:CZ | 0.52 | 2.60 | 20 | 3 |
| 1:A:22:LYS:CE | 1:A:44:VAL:CG2 | 0.52 | 2.87 | 22 | 2 |
| 1:A:6:ARG:O | 1:A:85:TYR:CB | 0.52 | 2.57 | 9 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:36:PHE:CE1 | 1:A:70:SER:HB2 | 0.52 | 2.39 | 35 | 2 |
| 1:A:18:GLU:O | 1:A:19:LYS:CG | 0.52 | 2.57 | 4 | 2 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:HG12 | 0.52 | 2.34 | 8 | 4 |
| 1:A:55:PHE:CE2 | 1:A:89:ASP:OD2 | 0.52 | 2.62 | 21 | 2 |
| 1:A:71:MET:O | 1:A:81:MET:CG | 0.52 | 2.58 | 5 | 3 |
| 1:A:16:LEU:HD13 | 1:A:16:LEU:H | 0.52 | 1.62 | 21 | 1 |
| 1:A:20:ILE:HB | 1:A:25:LEU:HD11 | 0.52 | 1.81 | 35 | 1 |
| 1:A:28:SER:HB3 | 1:A:76:PHE:CZ | 0.52 | 2.39 | 43 | 10 |
| 1:A:36:PHE:CD2 | 1:A:67:ALA:CA | 0.52 | 2.91 | 4 | 13 |
| 1:A:16:LEU:HD12 | 1:A:77:TYR:CG | 0.52 | 2.40 | 42 | 5 |
| 1:A:44:VAL:HG22 | 1:A:54:ALA:CB | 0.52 | 2.34 | 17 | 2 |
| 1:A:17:ASN:HB3 | 1:A:20:ILE:CD1 | 0.52 | 2.35 | 17 | 2 |
| 1:A:113:LYS:N | 1:A:113:LYS:CD | 0.52 | 2.71 | 31 | 1 |
| 1:A:112:PRO:O | 1:A:113:LYS:CB | 0.52 | 2.57 | 36 | 1 |
| 1:A:43:LEU:HD11 | 1:A:57:ILE:CD1 | 0.52 | 2.34 | 39 | 5 |
| 1:A:55:PHE:CE2 | 1:A:89:ASP:CG | 0.52 | 2.83 | 36 | 2 |
| 1:A:39:ILE:HD13 | 1:A:39:ILE:N | 0.52 | 2.17 | 13 | 3 |
| 1:A:26:LYS:CG | 1:A:44:VAL:CG2 | 0.52 | 2.87 | 12 | 1 |
| 1:A:71:MET:CG | 1:A:83:ILE:HD11 | 0.52 | 2.34 | 27 | 1 |
| 1:A:89:ASP:OD1 | 1:A:89:ASP:N | 0.52 | 2.43 | 13 | 2 |
| 1:A:10:THR:HA | 1:A:56:VAL:O | 0.52 | 2.04 | 25 | 34 |
| 1:A:52:GLY:O | 1:A:53:GLN:CG | 0.52 | 2.57 | 14 | 1 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:CD2 | 0.52 | 2.35 | 10 | 1 |
| 1:A:12:TYR:OH | 1:A:53:GLN:NE2 | 0.52 | 2.43 | 28 | 9 |
| 1:A:68:LEU:CG | 1:A:85:TYR:CZ | 0.52 | 2.93 | 17 | 36 |
| 1:A:68:LEU:CD1 | 1:A:69:ARG:HG2 | 0.52 | 2.35 | 10 | 6 |
| 1:A:57:ILE:CD1 | 1:A:93:ILE:HD11 | 0.52 | 2.33 | 32 | 6 |
| 1:A:36:PHE:CE2 | 1:A:71:MET:SD | 0.52 | 3.03 | 31 | 1 |
| 1:A:68:LEU:HD22 | 1:A:68:LEU:O | 0.52 | 2.04 | 17 | 4 |
| 1:A:39:ILE:HG23 | 1:A:42:ILE:CG1 | 0.52 | 2.35 | 41 | 5 |
| 1:A:13:ILE:HD12 | 1:A:54:ALA:O | 0.52 | 2.05 | 23 | 1 |
| 1:A:69:ARG:O | 1:A:72:GLN:CB | 0.52 | 2.57 | 26 | 2 |
| 1:A:68:LEU:HA | 1:A:83:ILE:HD12 | 0.52 | 1.81 | 31 | 4 |
| 1:A:32:ILE:HG21 | 1:A:71:MET:HE2 | 0.52 | 1.81 | 29 | 2 |
| 1:A:44:VAL:HG12 | 1:A:50:MET:HE1 | 0.52 | 1.82 | 25 | 1 |
| 1:A:14:ASN:O | 1:A:16:LEU:CD2 | 0.52 | 2.58 | 13 | 1 |
| 1:A:68:LEU:O | 1:A:72:GLN:NE2 | 0.52 | 2.42 | 16 | 10 |
| 1:A:43:LEU:O | 1:A:55:PHE:CD1 | 0.52 | 2.62 | 22 | 1 |
| 1:A:32:ILE:O | 1:A:35:GLN:CG | 0.52 | 2.58 | 32 | 3 |
| 1:A:72:GLN:HE21 | 1:A:83:ILE:HD12 | 0.52 | 1.64 | 5 | 2 |
| 1:A:71:MET:SD | 1:A:74:PHE:CB | 0.52 | 2.98 | 1 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:63:SER:O | 1:A:66:ASN:ND2 | 0.52 | 2.42 | 36 | 1 |
| 1:A:43:LEU:O | 1:A:44:VAL:CG1 | 0.52 | 2.58 | 3 | 1 |
| 1:A:14:ASN:OD1 | 1:A:14:ASN:N | 0.52 | 2.43 | 19 | 1 |
| 1:A:68:LEU:HD13 | 1:A:68:LEU:O | 0.51 | 2.05 | 11 | 4 |
| 1:A:71:MET:O | 1:A:72:GLN:C | 0.51 | 2.48 | 1 | 12 |
| 1:A:48:LEU:O | 1:A:51:ARG:CG | 0.51 | 2.59 | 35 | 2 |
| 1:A:26:LYS:HG2 | 1:A:44:VAL:CG2 | 0.51 | 2.35 | 12 | 1 |
| 1:A:16:LEU:O | 1:A:20:ILE:CG1 | 0.51 | 2.58 | 36 | 2 |
| 1:A:106:LYS:O | 1:A:106:LYS:CG | 0.51 | 2.57 | 1 | 2 |
| 1:A:42:ILE:CG1 | 1:A:56:VAL:HG13 | 0.51 | 2.35 | 24 | 2 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:HG13 | 0.51 | 2.35 | 2 | 13 |
| 1:A:80:PRO:O | 1:A:82:ARG:N | 0.51 | 2.43 | 14 | 3 |
| 1:A:7:PRO:HA | 1:A:85:TYR:CE2 | 0.51 | 2.41 | 11 | 16 |
| 1:A:106:LYS:O | 1:A:107:ARG:C | 0.51 | 2.49 | 41 | 2 |
| 1:A:70:SER:O | 1:A:74:PHE:CD1 | 0.51 | 2.64 | 41 | 4 |
| 1:A:13:ILE:CG2 | 1:A:14:ASN:N | 0.51 | 2.73 | 13 | 6 |
| 1:A:36:PHE:CD2 | 1:A:66:ASN:OD1 | 0.51 | 2.63 | 36 | 1 |
| 1:A:17:ASN:ND2 | 1:A:77:TYR:O | 0.51 | 2.43 | 39 | 4 |
| 1:A:42:ILE:N | 1:A:42:ILE:CD1 | 0.51 | 2.65 | 20 | 4 |
| 1:A:50:MET:HE1 | 1:A:53:GLN:C | 0.51 | 2.26 | 3 | 2 |
| 1:A:40:LEU:CD1 | 1:A:59:LYS:HA | 0.51 | 2.35 | 5 | 2 |
| 1:A:71:MET:CG | 1:A:81:MET:CE | 0.51 | 2.88 | 18 | 1 |
| 1:A:71:MET:HG2 | 1:A:74:PHE:CG | 0.51 | 2.40 | 42 | 2 |
| 1:A:77:TYR:N | 1:A:77:TYR:CD1 | 0.51 | 2.77 | 23 | 13 |
| 1:A:22:LYS:HE2 | 1:A:44:VAL:CG2 | 0.51 | 2.36 | 22 | 1 |
| 1:A:20:ILE:HD13 | 1:A:77:TYR:CE2 | 0.51 | 2.41 | 7 | 4 |
| 1:A:37:GLY:O | 1:A:38:GLN:CG | 0.51 | 2.59 | 15 | 6 |
| 1:A:14:ASN:ND2 | 1:A:53:GLN:CG | 0.51 | 2.73 | 35 | 1 |
| 1:A:87:LYS:O | 1:A:88:THR:HB | 0.51 | 2.05 | 13 | 35 |
| 1:A:36:PHE:CE2 | 1:A:70:SER:CB | 0.51 | 2.94 | 18 | 3 |
| 1:A:50:MET:O | 1:A:50:MET:HE2 | 0.51 | 2.06 | 32 | 7 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:HG22 | 0.51 | 2.40 | 1 | 2 |
| 1:A:33:PHE:CB | 1:A:58:PHE:CZ | 0.51 | 2.94 | 31 | 1 |
| 1:A:39:ILE:HG23 | 1:A:42:ILE:HG13 | 0.51 | 1.82 | 24 | 1 |
| 1:A:58:PHE:CG | 1:A:63:SER:HB2 | 0.51 | 2.40 | 42 | 6 |
| 1:A:16:LEU:O | 1:A:17:ASN:O | 0.51 | 2.28 | 20 | 15 |
| 1:A:21:LYS:O | 1:A:21:LYS:CG | 0.51 | 2.58 | 41 | 2 |
| 1:A:71:MET:HB3 | 1:A:81:MET:HE2 | 0.51 | 1.82 | 5 | 1 |
| 1:A:91:ASP:O | 1:A:94:ALA:HB3 | 0.51 | 2.06 | 43 | 1 |
| 1:A:36:PHE:CE2 | 1:A:70:SER:HB2 | 0.51 | 2.41 | 26 | 4 |
| 1:A:68:LEU:CD1 | 1:A:69:ARG:HG3 | 0.51 | 2.35 | 37 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:LEU:HD13 | 1:A:69:ARG:CA | 0.51 | 2.36 | 33 | 7 |
| 1:A:25:LEU:HD23 | 1:A:76:PHE:CE2 | 0.51 | 2.40 | 21 | 1 |
| 1:A:55:PHE:CD1 | 1:A:89:ASP:OD2 | 0.51 | 2.63 | 1 | 1 |
| 1:A:68:LEU:CD1 | 1:A:85:TYR:CE2 | 0.51 | 2.94 | 17 | 17 |
| 1:A:43:LEU:CD1 | 1:A:55:PHE:CD1 | 0.51 | 2.94 | 14 | 2 |
| 1:A:89:ASP:HA | 1:A:92:ILE:HD12 | 0.51 | 1.81 | 1 | 3 |
| 1:A:33:PHE:CB | 1:A:58:PHE:CE1 | 0.51 | 2.94 | 31 | 1 |
| 1:A:77:TYR:C | 1:A:80:PRO:HD3 | 0.51 | 2.26 | 35 | 1 |
| 1:A:30:TYR:CE2 | 1:A:42:ILE:HG13 | 0.51 | 2.41 | 28 | 18 |
| 1:A:30:TYR:CZ | 1:A:39:ILE:CG2 | 0.51 | 2.91 | 29 | 4 |
| 1:A:32:ILE:HD12 | 1:A:33:PHE:CZ | 0.51 | 2.41 | 6 | 1 |
| 1:A:71:MET:HE2 | 1:A:74:PHE:CD2 | 0.51 | 2.40 | 32 | 2 |
| 1:A:39:ILE:O | 1:A:40:LEU:HD23 | 0.51 | 2.06 | 5 | 1 |
| 1:A:71:MET:SD | 1:A:71:MET:N | 0.51 | 2.83 | 15 | 1 |
| 1:A:71:MET:HG2 | 1:A:74:PHE:CD2 | 0.51 | 2.40 | 36 | 2 |
| 1:A:48:LEU:C | 1:A:48:LEU:CD1 | 0.51 | 2.80 | 35 | 2 |
| 1:A:105:ARG:O | 1:A:105:ARG:CG | 0.51 | 2.58 | 42 | 1 |
| 1:A:8:ASN:CG | 1:A:8:ASN:O | 0.50 | 2.50 | 16 | 4 |
| 1:A:33:PHE:O | 1:A:36:PHE:N | 0.50 | 2.44 | 36 | 9 |
| 1:A:105:ARG:O | 1:A:107:ARG:N | 0.50 | 2.44 | 9 | 1 |
| 1:A:8:ASN:ND2 | 1:A:88:THR:OG1 | 0.50 | 2.44 | 39 | 2 |
| 1:A:42:ILE:C | 1:A:43:LEU:CD2 | 0.50 | 2.79 | 8 | 1 |
| 1:A:45:SER:N | 1:A:50:MET:HE1 | 0.50 | 2.20 | 32 | 1 |
| 1:A:36:PHE:CE2 | 1:A:71:MET:HG3 | 0.50 | 2.41 | 2 | 4 |
| 1:A:39:ILE:CD1 | 1:A:56:VAL:HG11 | 0.50 | 2.36 | 22 | 7 |
| 1:A:28:SER:HB3 | 1:A:76:PHE:CE1 | 0.50 | 2.41 | 36 | 3 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:HD12 | 0.50 | 1.83 | 39 | 3 |
| 1:A:9:HIS:CE1 | 1:A:57:ILE:CG2 | 0.50 | 2.95 | 40 | 2 |
| 1:A:109:LYS:O | 1:A:109:LYS:CG | 0.50 | 2.58 | 11 | 3 |
| 1:A:40:LEU:CD2 | 1:A:59:LYS:N | 0.50 | 2.72 | 21 | 3 |
| 1:A:29:LEU:HB3 | 1:A:42:ILE:HG21 | 0.50 | 1.80 | 19 | 1 |
| 1:A:76:PHE:CB | 1:A:81:MET:SD | 0.50 | 2.99 | 37 | 2 |
| 1:A:30:TYR:CE2 | 1:A:39:ILE:CG2 | 0.50 | 2.95 | 11 | 5 |
| 1:A:10:THR:OG1 | 1:A:57:ILE:HD12 | 0.50 | 2.06 | 27 | 3 |
| 1:A:14:ASN:OD1 | 1:A:15:ASN:N | 0.50 | 2.44 | 25 | 2 |
| 1:A:89:ASP:O | 1:A:92:ILE:CG2 | 0.50 | 2.57 | 24 | 6 |
| 1:A:71:MET:O | 1:A:74:PHE:N | 0.50 | 2.45 | 36 | 8 |
| 1:A:43:LEU:N | 1:A:43:LEU:HD23 | 0.50 | 2.22 | 26 | 3 |
| 1:A:74:PHE:CB | 1:A:81:MET:SD | 0.50 | 2.99 | 6 | 3 |
| 1:A:52:GLY:O | 1:A:53:GLN:O | 0.50 | 2.30 | 7 | 6 |
| 1:A:33:PHE:HB3 | 1:A:67:ALA:HB2 | 0.50 | 1.83 | 12 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:15:ASN:H | 1:A:16:LEU:HD22 | 0.50 | 1.67 | 27 | 3 |
| 1:A:40:LEU:HD23 | 1:A:40:LEU:N | 0.50 | 2.22 | 36 | 1 |
| 1:A:39:ILE:N | 1:A:39:ILE:HD13 | 0.50 | 2.21 | 28 | 1 |
| 1:A:71:MET:O | 1:A:81:MET:HB3 | 0.50 | 2.07 | 35 | 1 |
| 1:A:71:MET:HE3 | 1:A:74:PHE:CD2 | 0.50 | 2.41 | 24 | 1 |
| 1:A:22:LYS:CE | 1:A:44:VAL:CG1 | 0.50 | 2.89 | 19 | 1 |
| 1:A:50:MET:HE2 | 1:A:50:MET:O | 0.50 | 2.07 | 22 | 2 |
| 1:A:48:LEU:C | 1:A:48:LEU:CD2 | 0.50 | 2.80 | 26 | 3 |
| 1:A:58:PHE:CD1 | 1:A:58:PHE:N | 0.50 | 2.79 | 13 | 1 |
| 1:A:71:MET:HB3 | 1:A:81:MET:HE3 | 0.50 | 1.84 | 15 | 1 |
| 1:A:33:PHE:CZ | 1:A:67:ALA:HB1 | 0.50 | 2.42 | 42 | 1 |
| 1:A:16:LEU:CB | 1:A:25:LEU:CD2 | 0.50 | 2.87 | 24 | 1 |
| 1:A:41:ASP:CB | 1:A:57:ILE:HB | 0.50 | 2.37 | 25 | 17 |
| 1:A:36:PHE:HB3 | 1:A:66:ASN:CB | 0.50 | 2.36 | 4 | 19 |
| 1:A:26:LYS:HG2 | 1:A:44:VAL:HG23 | 0.50 | 1.84 | 12 | 2 |
| 1:A:16:LEU:CD2 | 1:A:52:GLY:O | 0.50 | 2.53 | 7 | 2 |
| 1:A:10:THR:CG2 | 1:A:55:PHE:HB2 | 0.50 | 2.36 | 19 | 1 |
| 1:A:37:GLY:HA3 | 1:A:63:SER:CB | 0.49 | 2.37 | 31 | 28 |
| 1:A:39:ILE:O | 1:A:40:LEU:CD2 | 0.49 | 2.57 | 31 | 3 |
| 1:A:68:LEU:CD1 | 1:A:85:TYR:CE1 | 0.49 | 2.95 | 28 | 23 |
| 1:A:44:VAL:HG22 | 1:A:45:SER:H | 0.49 | 1.65 | 21 | 1 |
| 1:A:111:LYS:CB | 1:A:112:PRO:HD3 | 0.49 | 2.37 | 2 | 4 |
| 1:A:40:LEU:C | 1:A:40:LEU:CD2 | 0.49 | 2.80 | 38 | 1 |
| 1:A:74:PHE:CB | 1:A:75:PRO:HD2 | 0.49 | 2.37 | 19 | 3 |
| 1:A:12:TYR:CZ | 1:A:55:PHE:CE2 | 0.49 | 2.99 | 33 | 1 |
| 1:A:22:LYS:CE | 1:A:22:LYS:CA | 0.49 | 2.90 | 26 | 1 |
| 1:A:77:TYR:CD1 | 1:A:77:TYR:N | 0.49 | 2.81 | 13 | 15 |
| 1:A:13:ILE:CD1 | 1:A:33:PHE:CZ | 0.49 | 2.95 | 10 | 1 |
| 1:A:55:PHE:HE2 | 1:A:92:ILE:HG21 | 0.49 | 1.60 | 32 | 1 |
| 1:A:13:ILE:O | 1:A:53:GLN:CB | 0.49 | 2.60 | 7 | 1 |
| 1:A:17:ASN:OD1 | 1:A:77:TYR:CB | 0.49 | 2.60 | 43 | 1 |
| 1:A:50:MET:O | 1:A:51:ARG:O | 0.49 | 2.30 | 8 | 6 |
| 1:A:66:ASN:O | 1:A:70:SER:HB3 | 0.49 | 2.07 | 7 | 4 |
| 1:A:12:TYR:CE1 | 1:A:53:GLN:HG2 | 0.49 | 2.42 | 30 | 1 |
| 1:A:22:LYS:CE | 1:A:44:VAL:O | 0.49 | 2.60 | 11 | 1 |
| 1:A:17:ASN:O | 1:A:18:GLU:C | 0.49 | 2.51 | 4 | 1 |
| 1:A:82:ARG:CG | 1:A:82:ARG:O | 0.49 | 2.61 | 30 | 2 |
| 1:A:55:PHE:CE2 | 1:A:92:ILE:CG2 | 0.49 | 2.91 | 32 | 3 |
| 1:A:26:LYS:HA | 1:A:29:LEU:CD2 | 0.49 | 2.37 | 42 | 2 |
| 1:A:45:SER:O | 1:A:46:ARG:HD2 | 0.49 | 2.08 | 7 | 1 |
| 1:A:65:THR:HA | 1:A:85:TYR:OH | 0.49 | 2.08 | 33 | 37 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:SER:N | 1:A:39:ILE:HG12 | 0.49 | 2.23 | 2 | 4 |
| 1:A:108:GLU:O | 1:A:108:GLU:CG | 0.49 | 2.61 | 29 | 4 |
| 1:A:76:PHE:HB2 | 1:A:81:MET:CG | 0.49 | 2.37 | 42 | 3 |
| 1:A:46:ARG:O | 1:A:50:MET:CB | 0.49 | 2.60 | 15 | 1 |
| 1:A:76:PHE:CZ | 1:A:77:TYR:OH | 0.49 | 2.65 | 35 | 1 |
| 1:A:40:LEU:HD22 | 1:A:59:LYS:HA | 0.49 | 1.85 | 7 | 1 |
| 1:A:51:ARG:O | 1:A:52:GLY:C | 0.49 | 2.50 | 3 | 14 |
| 1:A:15:ASN:O | 1:A:79:LYS:CB | 0.49 | 2.60 | 39 | 1 |
| 1:A:32:ILE:HG13 | 1:A:33:PHE:N | 0.49 | 2.23 | 42 | 6 |
| 1:A:10:THR:HG23 | 1:A:56:VAL:C | 0.49 | 2.28 | 42 | 6 |
| 1:A:22:LYS:CE | 1:A:44:VAL:HG21 | 0.49 | 2.38 | 20 | 1 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:HB | 0.49 | 2.37 | 28 | 1 |
| 1:A:17:ASN:HB2 | 1:A:77:TYR:O | 0.49 | 2.08 | 35 | 1 |
| 1:A:45:SER:OG | 1:A:55:PHE:CE1 | 0.49 | 2.66 | 43 | 1 |
| 1:A:55:PHE:CZ | 1:A:92:ILE:HG23 | 0.49 | 2.42 | 4 | 1 |
| 1:A:89:ASP:OD2 | 1:A:92:ILE:CD1 | 0.49 | 2.60 | 8 | 1 |
| 1:A:16:LEU:HG | 1:A:25:LEU:CD2 | 0.49 | 2.38 | 2 | 2 |
| 1:A:11:ILE:CG1 | 1:A:11:ILE:O | 0.49 | 2.61 | 31 | 1 |
| 1:A:72:GLN:NE2 | 1:A:83:ILE:O | 0.49 | 2.45 | 41 | 1 |
| 1:A:42:ILE:CG2 | 1:A:56:VAL:HG22 | 0.49 | 2.37 | 20 | 1 |
| 1:A:48:LEU:CD2 | 1:A:48:LEU:C | 0.49 | 2.81 | 39 | 5 |
| 1:A:106:LYS:O | 1:A:107:ARG:CB | 0.49 | 2.61 | 25 | 1 |
| 1:A:26:LYS:CG | 1:A:27:LYS:N | 0.49 | 2.75 | 7 | 3 |
| 1:A:18:GLU:OE2 | 1:A:51:ARG:CB | 0.49 | 2.60 | 36 | 1 |
| 1:A:50:MET:O | 1:A:51:ARG:C | 0.49 | 2.50 | 25 | 12 |
| 1:A:20:ILE:HD12 | 1:A:77:TYR:HD2 | 0.49 | 1.67 | 14 | 3 |
| 1:A:43:LEU:HG | 1:A:93:ILE:CG1 | 0.49 | 2.37 | 8 | 1 |
| 1:A:11:ILE:HG12 | 1:A:56:VAL:HB | 0.49 | 1.85 | 28 | 6 |
| 1:A:40:LEU:CD2 | 1:A:58:PHE:C | 0.48 | 2.81 | 19 | 3 |
| 1:A:43:LEU:HD12 | 1:A:93:ILE:CG1 | 0.48 | 2.38 | 8 | 1 |
| 1:A:84:GLN:O | 1:A:85:TYR:O | 0.48 | 2.31 | 38 | 10 |
| 1:A:10:THR:HG23 | 1:A:57:ILE:CD1 | 0.48 | 2.35 | 12 | 1 |
| 1:A:58:PHE:CE2 | 1:A:64:ALA:HA | 0.48 | 2.42 | 11 | 3 |
| 1:A:28:SER:CB | 1:A:77:TYR:HH | 0.48 | 2.20 | 20 | 1 |
| 1:A:46:ARG:HD3 | 1:A:46:ARG:N | 0.48 | 2.23 | 39 | 2 |
| 1:A:30:TYR:CZ | 1:A:39:ILE:O | 0.48 | 2.66 | 13 | 2 |
| 1:A:51:ARG:HD3 | 1:A:51:ARG:O | 0.48 | 2.07 | 21 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:HB3 | 0.48 | 2.07 | 16 | 1 |
| 1:A:112:PRO:O | 1:A:113:LYS:O | 0.48 | 2.31 | 26 | 5 |
| 1:A:25:LEU:O | 1:A:25:LEU:HD23 | 0.48 | 2.08 | 5 | 1 |
| 1:A:79:LYS:CG | 1:A:80:PRO:HD2 | 0.48 | 2.39 | 24 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:15:ASN:C | 1:A:16:LEU:CD2 | 0.48 | 2.81 | 36 | 1 |
| 1:A:81:MET:CE | 1:A:81:MET:HA | 0.48 | 2.39 | 35 | 1 |
| 1:A:83:ILE:HG22 | 1:A:84:GLN:H | 0.48 | 1.68 | 15 | 4 |
| 1:A:12:TYR:HB2 | 1:A:84:GLN:O | 0.48 | 2.08 | 9 | 7 |
| 1:A:30:TYR:HA | 1:A:42:ILE:CD1 | 0.48 | 2.39 | 33 | 4 |
| 1:A:70:SER:O | 1:A:74:PHE:CE1 | 0.48 | 2.66 | 41 | 3 |
| 1:A:29:LEU:O | 1:A:32:ILE:CG1 | 0.48 | 2.62 | 24 | 5 |
| 1:A:65:THR:O | 1:A:69:ARG:HG2 | 0.48 | 2.09 | 9 | 20 |
| 1:A:74:PHE:CB | 1:A:75:PRO:CD | 0.48 | 2.91 | 19 | 3 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:CG | 0.48 | 2.38 | 21 | 1 |
| 1:A:46:ARG:O | 1:A:50:MET:HB3 | 0.48 | 2.08 | 15 | 1 |
| 1:A:69:ARG:O | 1:A:70:SER:C | 0.48 | 2.52 | 1 | 2 |
| 1:A:107:ARG:O | 1:A:108:GLU:C | 0.48 | 2.52 | 35 | 2 |
| 1:A:50:MET:O | 1:A:50:MET:SD | 0.48 | 2.72 | 25 | 3 |
| 1:A:43:LEU:HD22 | 1:A:43:LEU:N | 0.48 | 2.20 | 8 | 1 |
| 1:A:71:MET:HA | 1:A:74:PHE:CG | 0.48 | 2.43 | 29 | 3 |
| 1:A:46:ARG:O | 1:A:51:ARG:NH2 | 0.48 | 2.46 | 6 | 1 |
| 1:A:48:LEU:HD22 | 1:A:51:ARG:HD2 | 0.48 | 1.84 | 24 | 1 |
| 1:A:71:MET:O | 1:A:81:MET:HB2 | 0.48 | 2.09 | 39 | 1 |
| 1:A:32:ILE:HD13 | 1:A:71:MET:HE1 | 0.48 | 1.85 | 36 | 1 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:HD11 | 0.48 | 2.39 | 1 | 3 |
| 1:A:48:LEU:C | 1:A:48:LEU:HD13 | 0.48 | 2.26 | 29 | 1 |
| 1:A:12:TYR:O | 1:A:84:GLN:OE1 | 0.48 | 2.32 | 11 | 1 |
| 1:A:29:LEU:CB | 1:A:42:ILE:HD13 | 0.48 | 2.39 | 14 | 2 |
| 1:A:20:ILE:CG2 | 1:A:24:GLU:HB2 | 0.48 | 2.38 | 10 | 1 |
| 1:A:16:LEU:HD12 | 1:A:25:LEU:CD1 | 0.48 | 2.39 | 36 | 1 |
| 1:A:83:ILE:C | 1:A:84:GLN:CG | 0.48 | 2.83 | 18 | 8 |
| 1:A:76:PHE:O | 1:A:77:TYR:HB2 | 0.48 | 2.09 | 19 | 21 |
| 1:A:43:LEU:CD2 | 1:A:93:ILE:HG13 | 0.48 | 2.38 | 10 | 6 |
| 1:A:39:ILE:C | 1:A:40:LEU:HD22 | 0.48 | 2.29 | 40 | 3 |
| 1:A:105:ARG:CG | 1:A:106:LYS:N | 0.48 | 2.75 | 18 | 1 |
| 1:A:88:THR:CG2 | 1:A:88:THR:O | 0.48 | 2.61 | 31 | 1 |
| 1:A:76:PHE:O | 1:A:79:LYS:O | 0.48 | 2.32 | 3 | 2 |
| 1:A:73:GLY:O | 1:A:74:PHE:O | 0.47 | 2.32 | 25 | 14 |
| 1:A:58:PHE:CZ | 1:A:67:ALA:CB | 0.47 | 2.97 | 36 | 5 |
| 1:A:13:ILE:HD11 | 1:A:33:PHE:HZ | 0.47 | 1.69 | 28 | 2 |
| 1:A:45:SER:O | 1:A:46:ARG:HB2 | 0.47 | 2.09 | 7 | 2 |
| 1:A:15:ASN:O | 1:A:16:LEU:HD13 | 0.47 | 2.08 | 24 | 1 |
| 1:A:22:LYS:O | 1:A:23:ASP:C | 0.47 | 2.52 | 14 | 8 |
| 1:A:30:TYR:CD2 | 1:A:39:ILE:HG21 | 0.47 | 2.44 | 11 | 4 |
| 1:A:33:PHE:O | 1:A:35:GLN:N | 0.47 | 2.47 | 40 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:61:VAL:CG1 | 1:A:62:SER:N | 0.47 | 2.77 | 6 | 1 |
| 1:A:109:LYS:C | 1:A:110:ARG:CG | 0.47 | 2.82 | 25 | 1 |
| 1:A:76:PHE:CG | 1:A:81:MET:HE2 | 0.47 | 2.44 | 10 | 1 |
| 1:A:66:ASN:CG | 1:A:67:ALA:N | 0.47 | 2.68 | 36 | 1 |
| 1:A:17:ASN:ND2 | 1:A:78:ASP:OD2 | 0.47 | 2.47 | 16 | 1 |
| 1:A:66:ASN:O | 1:A:70:SER:HB2 | 0.47 | 2.09 | 37 | 23 |
| 1:A:73:GLY:O | 1:A:74:PHE:C | 0.47 | 2.53 | 5 | 19 |
| 1:A:58:PHE:CE1 | 1:A:64:ALA:HA | 0.47 | 2.44 | 41 | 1 |
| 1:A:58:PHE:CB | 1:A:63:SER:HB2 | 0.47 | 2.39 | 13 | 3 |
| 1:A:25:LEU:HD23 | 1:A:44:VAL:HG11 | 0.47 | 1.86 | 4 | 1 |
| 1:A:43:LEU:HD13 | 1:A:93:ILE:HD11 | 0.47 | 1.86 | 12 | 2 |
| 1:A:108:GLU:O | 1:A:110:ARG:N | 0.47 | 2.47 | 33 | 1 |
| 1:A:27:LYS:C | 1:A:27:LYS:CD | 0.47 | 2.83 | 18 | 1 |
| 1:A:45:SER:CB | 1:A:50:MET:HG2 | 0.47 | 2.40 | 43 | 8 |
| 1:A:32:ILE:CD1 | 1:A:33:PHE:N | 0.47 | 2.73 | 16 | 1 |
| 1:A:26:LYS:HG3 | 1:A:27:LYS:N | 0.47 | 2.24 | 20 | 4 |
| 1:A:28:SER:O | 1:A:32:ILE:HG12 | 0.47 | 2.09 | 36 | 8 |
| 1:A:16:LEU:HB3 | 1:A:25:LEU:CD1 | 0.47 | 2.40 | 37 | 2 |
| 1:A:83:ILE:HG22 | 1:A:84:GLN:N | 0.47 | 2.24 | 33 | 4 |
| 1:A:72:GLN:HA | 1:A:72:GLN:NE2 | 0.47 | 2.24 | 6 | 3 |
| 1:A:22:LYS:HD2 | 1:A:44:VAL:CG1 | 0.47 | 2.39 | 12 | 1 |
| 1:A:16:LEU:HD12 | 1:A:76:PHE:CD1 | 0.47 | 2.43 | 18 | 1 |
| 1:A:16:LEU:HA | 1:A:80:PRO:CB | 0.47 | 2.40 | 35 | 1 |
| 1:A:49:LYS:C | 1:A:51:ARG:N | 0.47 | 2.66 | 7 | 1 |
| 1:A:11:ILE:HA | 1:A:85:TYR:HA | 0.47 | 1.86 | 13 | 20 |
| 1:A:45:SER:O | 1:A:46:ARG:CB | 0.47 | 2.62 | 7 | 2 |
| 1:A:112:PRO:O | 1:A:113:LYS:HG3 | 0.47 | 2.09 | 26 | 1 |
| 1:A:45:SER:O | 1:A:46:ARG:CG | 0.47 | 2.62 | 3 | 1 |
| 1:A:15:ASN:ND2 | 1:A:79:LYS:NZ | 0.47 | 2.63 | 38 | 1 |
| 1:A:29:LEU:CD1 | 1:A:44:VAL:HG11 | 0.47 | 2.39 | 7 | 1 |
| 1:A:29:LEU:HA | 1:A:32:ILE:CG1 | 0.47 | 2.40 | 36 | 4 |
| 1:A:28:SER:HB2 | 1:A:77:TYR:OH | 0.47 | 2.10 | 35 | 8 |
| 1:A:22:LYS:N | 1:A:22:LYS:HD2 | 0.47 | 2.24 | 32 | 3 |
| 1:A:12:TYR:HB3 | 1:A:84:GLN:O | 0.47 | 2.09 | 28 | 12 |
| 1:A:46:ARG:O | 1:A:47:SER:O | 0.47 | 2.33 | 6 | 2 |
| 1:A:10:THR:CG2 | 1:A:55:PHE:HB3 | 0.47 | 2.39 | 6 | 5 |
| 1:A:87:LYS:O | 1:A:88:THR:OG1 | 0.47 | 2.33 | 6 | 2 |
| 1:A:28:SER:OG | 1:A:76:PHE:CE1 | 0.47 | 2.62 | 21 | 1 |
| 1:A:45:SER:HA | 1:A:50:MET:CB | 0.47 | 2.39 | 3 | 2 |
| 1:A:15:ASN:OD1 | 1:A:80:PRO:O | 0.47 | 2.33 | 14 | 2 |
| 1:A:33:PHE:HB3 | 1:A:58:PHE:CZ | 0.47 | 2.44 | 14 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:PHE:HB2 | 1:A:89:ASP:OD2 | 0.47 | 2.10 | 41 | 1 |
| 1:A:43:LEU:C | 1:A:44:VAL:HG13 | 0.47 | 2.29 | 3 | 1 |
| 1:A:45:SER:O | 1:A:46:ARG:HG2 | 0.47 | 2.08 | 3 | 1 |
| 1:A:82:ARG:HG3 | 1:A:82:ARG:O | 0.47 | 2.10 | 19 | 2 |
| 1:A:9:HIS:CA | 1:A:61:VAL:HG22 | 0.47 | 2.40 | 9 | 1 |
| 1:A:16:LEU:O | 1:A:20:ILE:HD12 | 0.47 | 2.09 | 31 | 4 |
| 1:A:50:MET:SD | 1:A:53:GLN:CB | 0.47 | 3.03 | 12 | 3 |
| 1:A:89:ASP:O | 1:A:92:ILE:N | 0.47 | 2.48 | 41 | 3 |
| 1:A:44:VAL:HG13 | 1:A:45:SER:H | 0.47 | 1.69 | 21 | 1 |
| 1:A:87:LYS:O | 1:A:87:LYS:CG | 0.47 | 2.60 | 21 | 1 |
| 1:A:50:MET:CE | 1:A:53:GLN:N | 0.47 | 2.78 | 14 | 1 |
| 1:A:57:ILE:HD11 | 1:A:93:ILE:HG12 | 0.47 | 1.87 | 14 | 1 |
| 1:A:65:THR:HG22 | 1:A:69:ARG:CD | 0.47 | 2.39 | 27 | 4 |
| 1:A:6:ARG:CG | 1:A:7:PRO:HD2 | 0.47 | 2.40 | 30 | 1 |
| 1:A:36:PHE:CZ | 1:A:71:MET:HG3 | 0.47 | 2.45 | 42 | 2 |
| 1:A:29:LEU:HD22 | 1:A:29:LEU:H | 0.47 | 1.69 | 20 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:SD | 0.47 | 2.73 | 43 | 3 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:N | 0.47 | 2.22 | 16 | 1 |
| 1:A:21:LYS:O | 1:A:22:LYS:C | 0.47 | 2.54 | 4 | 16 |
| 1:A:81:MET:HA | 1:A:81:MET:CE | 0.47 | 2.40 | 26 | 3 |
| 1:A:45:SER:O | 1:A:50:MET:O | 0.47 | 2.33 | 13 | 6 |
| 1:A:39:ILE:CG2 | 1:A:42:ILE:HG12 | 0.47 | 2.39 | 18 | 1 |
| 1:A:8:ASN:CA | 1:A:61:VAL:HG13 | 0.47 | 2.40 | 29 | 1 |
| 1:A:43:LEU:HD12 | 1:A:55:PHE:HD2 | 0.47 | 1.70 | 42 | 1 |
| 1:A:56:VAL:HG12 | 1:A:58:PHE:CE1 | 0.47 | 2.44 | 41 | 2 |
| 1:A:71:MET:HB3 | 1:A:81:MET:HE1 | 0.47 | 1.86 | 3 | 1 |
| 1:A:44:VAL:O | 1:A:45:SER:O | 0.47 | 2.33 | 7 | 1 |
| 1:A:49:LYS:O | 1:A:51:ARG:N | 0.47 | 2.48 | 7 | 1 |
| 1:A:22:LYS:CE | 1:A:44:VAL:HG12 | 0.47 | 2.40 | 19 | 1 |
| 1:A:71:MET:CB | 1:A:74:PHE:HB2 | 0.47 | 2.40 | 19 | 1 |
| 1:A:22:LYS:HE3 | 1:A:44:VAL:HG21 | 0.47 | 1.87 | 37 | 2 |
| 1:A:110:ARG:O | 1:A:110:ARG:CG | 0.47 | 2.63 | 26 | 1 |
| 1:A:82:ARG:O | 1:A:82:ARG:HG3 | 0.47 | 2.11 | 31 | 2 |
| 1:A:28:SER:HB3 | 1:A:77:TYR:OH | 0.46 | 2.11 | 8 | 5 |
| 1:A:24:GLU:O | 1:A:27:LYS:HG2 | 0.46 | 2.10 | 4 | 4 |
| 1:A:20:ILE:CG2 | 1:A:25:LEU:HB2 | 0.46 | 2.40 | 36 | 3 |
| 1:A:72:GLN:NE2 | 1:A:72:GLN:HA | 0.46 | 2.25 | 8 | 2 |
| 1:A:68:LEU:O | 1:A:72:GLN:HB3 | 0.46 | 2.11 | 34 | 1 |
| 1:A:16:LEU:HD13 | 1:A:76:PHE:CD1 | 0.46 | 2.45 | 25 | 1 |
| 1:A:89:ASP:O | 1:A:89:ASP:OD1 | 0.46 | 2.34 | 1 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:CB | 0.46 | 2.63 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:PHE:O | 1:A:34:SER:C | 0.46 | 2.53 | 20 | 16 |
| 1:A:22:LYS:HD2 | 1:A:22:LYS:N | 0.46 | 2.25 | 4 | 6 |
| 1:A:25:LEU:O | 1:A:29:LEU:CD1 | 0.46 | 2.62 | 21 | 3 |
| 1:A:61:VAL:HG13 | 1:A:62:SER:N | 0.46 | 2.26 | 6 | 1 |
| 1:A:41:ASP:HB3 | 1:A:57:ILE:CG1 | 0.46 | 2.40 | 36 | 3 |
| 1:A:43:LEU:HD22 | 1:A:93:ILE:HG23 | 0.46 | 1.87 | 42 | 2 |
| 1:A:22:LYS:HE3 | 1:A:44:VAL:CG1 | 0.46 | 2.41 | 28 | 2 |
| 1:A:66:ASN:O | 1:A:70:SER:OG | 0.46 | 2.33 | 23 | 8 |
| 1:A:45:SER:N | 1:A:50:MET:HG2 | 0.46 | 2.25 | 16 | 2 |
| 1:A:105:ARG:O | 1:A:106:LYS:O | 0.46 | 2.33 | 14 | 5 |
| 1:A:55:PHE:CE2 | 1:A:92:ILE:CD1 | 0.46 | 2.94 | 39 | 2 |
| 1:A:71:MET:CB | 1:A:81:MET:SD | 0.46 | 3.03 | 10 | 3 |
| 1:A:40:LEU:HD13 | 1:A:59:LYS:N | 0.46 | 2.24 | 27 | 1 |
| 1:A:16:LEU:HD11 | 1:A:81:MET:SD | 0.46 | 2.50 | 7 | 2 |
| 1:A:33:PHE:HB3 | 1:A:58:PHE:CE1 | 0.46 | 2.45 | 31 | 1 |
| 1:A:26:LYS:HG2 | 1:A:44:VAL:HG13 | 0.46 | 1.86 | 36 | 1 |
| 1:A:71:MET:CE | 1:A:81:MET:SD | 0.46 | 3.03 | 19 | 1 |
| 1:A:29:LEU:HA | 1:A:32:ILE:CD1 | 0.46 | 2.41 | 4 | 12 |
| 1:A:11:ILE:CD1 | 1:A:56:VAL:HG21 | 0.46 | 2.36 | 9 | 3 |
| 1:A:38:GLN:C | 1:A:39:ILE:HD13 | 0.46 | 2.31 | 17 | 2 |
| 1:A:90:SER:HA | 1:A:93:ILE:HD12 | 0.46 | 1.88 | 42 | 1 |
| 1:A:26:LYS:O | 1:A:28:SER:N | 0.46 | 2.49 | 23 | 2 |
| 1:A:20:ILE:HG12 | 1:A:77:TYR:CD2 | 0.46 | 2.45 | 35 | 1 |
| 1:A:50:MET:SD | 1:A:50:MET:C | 0.46 | 2.94 | 31 | 4 |
| 1:A:29:LEU:O | 1:A:32:ILE:HG12 | 0.46 | 2.11 | 8 | 4 |
| 1:A:41:ASP:O | 1:A:57:ILE:HG12 | 0.46 | 2.11 | 14 | 15 |
| 1:A:16:LEU:O | 1:A:20:ILE:HG13 | 0.46 | 2.11 | 36 | 2 |
| 1:A:78:ASP:OD1 | 1:A:78:ASP:O | 0.46 | 2.32 | 19 | 2 |
| 1:A:43:LEU:CD1 | 1:A:92:ILE:CG2 | 0.46 | 2.93 | 5 | 1 |
| 1:A:14:ASN:N | 1:A:14:ASN:OD1 | 0.46 | 2.46 | 16 | 1 |
| 1:A:38:GLN:O | 1:A:40:LEU:CD1 | 0.46 | 2.64 | 27 | 2 |
| 1:A:33:PHE:CE1 | 1:A:67:ALA:HA | 0.46 | 2.45 | 42 | 1 |
| 1:A:30:TYR:OH | 1:A:40:LEU:O | 0.46 | 2.34 | 20 | 1 |
| 1:A:32:ILE:CD1 | 1:A:33:PHE:CG | 0.46 | 2.98 | 18 | 2 |
| 1:A:45:SER:HB3 | 1:A:50:MET:CB | 0.46 | 2.41 | 20 | 3 |
| 1:A:8:ASN:OD1 | 1:A:8:ASN:O | 0.46 | 2.34 | 12 | 1 |
| 1:A:48:LEU:O | 1:A:51:ARG:HG2 | 0.46 | 2.11 | 35 | 2 |
| 1:A:33:PHE:CE1 | 1:A:67:ALA:CA | 0.46 | 2.99 | 42 | 1 |
| 1:A:43:LEU:HD23 | 1:A:55:PHE:C | 0.46 | 2.31 | 23 | 1 |
| 1:A:76:PHE:HB2 | 1:A:81:MET:CE | 0.46 | 2.41 | 12 | 3 |
| 1:A:43:LEU:HD22 | 1:A:93:ILE:HA | 0.46 | 1.87 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:71:MET:CB | 1:A:81:MET:HG3 | 0.46 | 2.41 | 12 | 3 |
| 1:A:22:LYS:HE3 | 1:A:46:ARG:CD | 0.46 | 2.41 | 34 | 1 |
| 1:A:37:GLY:O | 1:A:38:GLN:HB2 | 0.46 | 2.11 | 36 | 8 |
| 1:A:110:ARG:CG | 1:A:110:ARG:O | 0.46 | 2.63 | 5 | 1 |
| 1:A:50:MET:HG3 | 1:A:50:MET:O | 0.46 | 2.10 | 14 | 1 |
| 1:A:32:ILE:O | 1:A:36:PHE:CE1 | 0.46 | 2.69 | 30 | 4 |
| 1:A:27:LYS:HG3 | 1:A:28:SER:N | 0.46 | 2.25 | 42 | 2 |
| 1:A:12:TYR:CE2 | 1:A:55:PHE:CE1 | 0.46 | 3.03 | 10 | 3 |
| 1:A:90:SER:O | 1:A:93:ILE:HB | 0.46 | 2.11 | 21 | 17 |
| 1:A:68:LEU:HA | 1:A:83:ILE:CB | 0.46 | 2.41 | 22 | 2 |
| 1:A:15:ASN:ND2 | 1:A:80:PRO:O | 0.46 | 2.48 | 20 | 2 |
| 1:A:76:PHE:CG | 1:A:81:MET:CE | 0.46 | 2.98 | 41 | 2 |
| 1:A:44:VAL:CG1 | 1:A:45:SER:N | 0.46 | 2.79 | 19 | 2 |
| 1:A:49:LYS:O | 1:A:53:GLN:OE1 | 0.46 | 2.34 | 24 | 3 |
| 1:A:51:ARG:CD | 1:A:51:ARG:O | 0.46 | 2.64 | 21 | 1 |
| 1:A:22:LYS:HE3 | 1:A:22:LYS:N | 0.46 | 2.24 | 26 | 1 |
| 1:A:40:LEU:HD12 | 1:A:40:LEU:N | 0.46 | 2.25 | 27 | 1 |
| 1:A:46:ARG:N | 1:A:50:MET:HG3 | 0.46 | 2.26 | 3 | 1 |
| 1:A:58:PHE:HB3 | 1:A:63:SER:HB2 | 0.46 | 1.88 | 13 | 13 |
| 1:A:11:ILE:O | 1:A:55:PHE:HA | 0.46 | 2.11 | 8 | 6 |
| 1:A:50:MET:CE | 1:A:50:MET:CA | 0.46 | 2.94 | 4 | 2 |
| 1:A:109:LYS:O | 1:A:110:ARG:C | 0.46 | 2.55 | 25 | 4 |
| 1:A:33:PHE:CD1 | 1:A:33:PHE:N | 0.46 | 2.84 | 21 | 1 |
| 1:A:71:MET:HE3 | 1:A:74:PHE:CB | 0.46 | 2.40 | 21 | 1 |
| 1:A:69:ARG:O | 1:A:72:GLN:HB3 | 0.46 | 2.11 | 26 | 1 |
| 1:A:71:MET:O | 1:A:71:MET:HG3 | 0.46 | 2.11 | 41 | 2 |
| 1:A:72:GLN:NE2 | 1:A:83:ILE:N | 0.46 | 2.64 | 18 | 1 |
| 1:A:44:VAL:O | 1:A:50:MET:SD | 0.46 | 2.73 | 3 | 1 |
| 1:A:71:MET:CG | 1:A:71:MET:O | 0.46 | 2.64 | 7 | 1 |
| 1:A:71:MET:HB3 | 1:A:74:PHE:HB2 | 0.45 | 1.89 | 9 | 4 |
| 1:A:40:LEU:CD2 | 1:A:59:LYS:HB2 | 0.45 | 2.41 | 20 | 9 |
| 1:A:16:LEU:CB | 1:A:25:LEU:CD1 | 0.45 | 2.90 | 37 | 1 |
| 1:A:71:MET:HG2 | 1:A:81:MET:CE | 0.45 | 2.41 | 22 | 1 |
| 1:A:8:ASN:O | 1:A:8:ASN:CG | 0.45 | 2.55 | 10 | 4 |
| 1:A:23:ASP:OD1 | 1:A:24:GLU:N | 0.45 | 2.49 | 9 | 1 |
| 1:A:90:SER:HA | 1:A:93:ILE:CD1 | 0.45 | 2.41 | 8 | 1 |
| 1:A:43:LEU:HD12 | 1:A:55:PHE:CD1 | 0.45 | 2.46 | 15 | 1 |
| 1:A:25:LEU:HD13 | 1:A:25:LEU:O | 0.45 | 2.10 | 30 | 2 |
| 1:A:38:GLN:O | 1:A:40:LEU:CD2 | 0.45 | 2.64 | 36 | 1 |
| 1:A:45:SER:O | 1:A:46:ARG:HD3 | 0.45 | 2.11 | 3 | 1 |
| 1:A:38:GLN:OE1 | 1:A:59:LYS:CB | 0.45 | 2.64 | 20 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:46:ARG:N | 1:A:46:ARG:HD2 | 0.45 | 2.26 | 16 | 1 |
| 1:A:59:LYS:O | 1:A:60:GLU:OE1 | 0.45 | 2.33 | 22 | 1 |
| 1:A:68:LEU:HA | 1:A:83:ILE:CG2 | 0.45 | 2.38 | 15 | 11 |
| 1:A:68:LEU:HA | 1:A:83:ILE:CD1 | 0.45 | 2.42 | 19 | 5 |
| 1:A:76:PHE:CD2 | 1:A:81:MET:HE1 | 0.45 | 2.46 | 15 | 1 |
| 1:A:110:ARG:CZ | 1:A:110:ARG:CB | 0.45 | 2.94 | 10 | 1 |
| 1:A:50:MET:HE3 | 1:A:50:MET:HA | 0.45 | 1.88 | 36 | 1 |
| 1:A:74:PHE:O | 1:A:81:MET:HG3 | 0.45 | 2.12 | 35 | 1 |
| 1:A:107:ARG:O | 1:A:108:GLU:O | 0.45 | 2.33 | 43 | 1 |
| 1:A:42:ILE:HG12 | 1:A:56:VAL:HG13 | 0.45 | 1.87 | 16 | 1 |
| 1:A:88:THR:O | 1:A:88:THR:CG2 | 0.45 | 2.64 | 29 | 2 |
| 1:A:57:ILE:CD1 | 1:A:93:ILE:HG12 | 0.45 | 2.42 | 23 | 2 |
| 1:A:71:MET:CG | 1:A:81:MET:HE1 | 0.45 | 2.41 | 18 | 1 |
| 1:A:105:ARG:O | 1:A:105:ARG:HG3 | 0.45 | 2.12 | 42 | 1 |
| 1:A:11:ILE:HB | 1:A:83:ILE:CG2 | 0.45 | 2.41 | 41 | 1 |
| 1:A:43:LEU:O | 1:A:43:LEU:HG | 0.45 | 2.11 | 20 | 1 |
| 1:A:30:TYR:O | 1:A:34:SER:CB | 0.45 | 2.65 | 24 | 1 |
| 1:A:17:ASN:OD1 | 1:A:77:TYR:HB3 | 0.45 | 2.11 | 43 | 1 |
| 1:A:7:PRO:HB2 | 1:A:61:VAL:CG1 | 0.45 | 2.41 | 17 | 8 |
| 1:A:83:ILE:C | 1:A:84:GLN:HG3 | 0.45 | 2.32 | 25 | 17 |
| 1:A:14:ASN:O | 1:A:15:ASN:HB2 | 0.45 | 2.11 | 40 | 9 |
| 1:A:71:MET:HB3 | 1:A:81:MET:SD | 0.45 | 2.51 | 31 | 4 |
| 1:A:48:LEU:CD1 | 1:A:48:LEU:C | 0.45 | 2.80 | 34 | 1 |
| 1:A:75:PRO:O | 1:A:81:MET:CE | 0.45 | 2.64 | 21 | 1 |
| 1:A:26:LYS:O | 1:A:27:LYS:C | 0.45 | 2.55 | 23 | 3 |
| 1:A:16:LEU:HD11 | 1:A:76:PHE:HE2 | 0.45 | 1.72 | 11 | 1 |
| 1:A:16:LEU:HA | 1:A:80:PRO:HB2 | 0.45 | 1.89 | 35 | 1 |
| 1:A:28:SER:OG | 1:A:77:TYR:OH | 0.45 | 2.34 | 26 | 4 |
| 1:A:20:ILE:HB | 1:A:25:LEU:CD2 | 0.45 | 2.40 | 22 | 1 |
| 1:A:22:LYS:HD3 | 1:A:46:ARG:CD | 0.45 | 2.42 | 4 | 1 |
| 1:A:42:ILE:O | 1:A:43:LEU:HD22 | 0.45 | 2.11 | 8 | 1 |
| 1:A:50:MET:SD | 1:A:53:GLN:HB2 | 0.45 | 2.51 | 12 | 6 |
| 1:A:22:LYS:HE2 | 1:A:44:VAL:O | 0.45 | 2.12 | 11 | 1 |
| 1:A:45:SER:HB2 | 1:A:50:MET:CB | 0.45 | 2.42 | 10 | 3 |
| 1:A:50:MET:HE1 | 1:A:53:GLN:O | 0.45 | 2.11 | 16 | 4 |
| 1:A:43:LEU:CD1 | 1:A:57:ILE:CD1 | 0.45 | 2.94 | 4 | 1 |
| 1:A:43:LEU:HD23 | 1:A:43:LEU:N | 0.45 | 2.27 | 29 | 1 |
| 1:A:50:MET:HE1 | 1:A:53:GLN:CB | 0.45 | 2.41 | 3 | 1 |
| 1:A:30:TYR:CD2 | 1:A:42:ILE:HG12 | 0.45 | 2.47 | 20 | 1 |
| 1:A:15:ASN:OD1 | 1:A:80:PRO:HA | 0.45 | 2.11 | 35 | 1 |
| 1:A:107:ARG:CD | 1:A:107:ARG:C | 0.45 | 2.85 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:14:ASN:OD1 | 1:A:53:GLN:HG3 | 0.45 | 2.12 | 43 | 3 |
| 1:A:22:LYS:O | 1:A:23:ASP:HB2 | 0.45 | 2.12 | 1 | 3 |
| 1:A:89:ASP:HB3 | 1:A:92:ILE:CG2 | 0.45 | 2.42 | 26 | 9 |
| 1:A:33:PHE:CD2 | 1:A:56:VAL:HG11 | 0.45 | 2.47 | 31 | 1 |
| 1:A:32:ILE:HD11 | 1:A:76:PHE:CE1 | 0.45 | 2.47 | 10 | 1 |
| 1:A:71:MET:CA | 1:A:74:PHE:HB2 | 0.45 | 2.41 | 19 | 1 |
| 1:A:106:LYS:CG | 1:A:106:LYS:O | 0.45 | 2.64 | 43 | 1 |
| 1:A:16:LEU:HB2 | 1:A:52:GLY:CA | 0.45 | 2.41 | 21 | 3 |
| 1:A:22:LYS:O | 1:A:23:ASP:HB3 | 0.45 | 2.12 | 19 | 8 |
| 1:A:41:ASP:O | 1:A:43:LEU:CD2 | 0.45 | 2.64 | 25 | 2 |
| 1:A:24:GLU:O | 1:A:25:LEU:C | 0.45 | 2.55 | 38 | 8 |
| 1:A:48:LEU:CD2 | 1:A:48:LEU:O | 0.45 | 2.65 | 6 | 1 |
| 1:A:22:LYS:N | 1:A:22:LYS:HE2 | 0.45 | 2.27 | 12 | 1 |
| 1:A:84:GLN:O | 1:A:86:ALA:N | 0.45 | 2.50 | 26 | 1 |
| 1:A:39:ILE:HG23 | 1:A:42:ILE:HG12 | 0.45 | 1.88 | 18 | 1 |
| 1:A:50:MET:C | 1:A:50:MET:SD | 0.45 | 2.96 | 42 | 4 |
| 1:A:25:LEU:HD21 | 1:A:52:GLY:HA2 | 0.45 | 1.88 | 42 | 1 |
| 1:A:13:ILE:N | 1:A:54:ALA:O | 0.45 | 2.50 | 23 | 1 |
| 1:A:30:TYR:CE1 | 1:A:39:ILE:CG2 | 0.45 | 2.98 | 38 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:HE1 | 0.45 | 2.12 | 37 | 1 |
| 1:A:71:MET:O | 1:A:81:MET:CB | 0.45 | 2.65 | 39 | 1 |
| 1:A:50:MET:O | 1:A:50:MET:HE3 | 0.45 | 2.11 | 17 | 1 |
| 1:A:24:GLU:HA | 1:A:27:LYS:CG | 0.45 | 2.42 | 18 | 2 |
| 1:A:32:ILE:HG12 | 1:A:71:MET:CE | 0.45 | 2.42 | 38 | 1 |
| 1:A:106:LYS:O | 1:A:107:ARG:CG | 0.45 | 2.65 | 35 | 1 |
| 1:A:50:MET:CE | 1:A:50:MET:HA | 0.45 | 2.38 | 4 | 1 |
| 1:A:47:SER:OG | 1:A:48:LEU:N | 0.45 | 2.50 | 40 | 1 |
| 1:A:71:MET:SD | 1:A:74:PHE:HB2 | 0.45 | 2.51 | 27 | 1 |
| 1:A:32:ILE:HD13 | 1:A:76:PHE:CD1 | 0.45 | 2.47 | 41 | 1 |
| 1:A:44:VAL:O | 1:A:44:VAL:CG2 | 0.45 | 2.65 | 36 | 1 |
| 1:A:43:LEU:HD23 | 1:A:43:LEU:H | 0.45 | 1.71 | 20 | 1 |
| 1:A:65:THR:O | 1:A:69:ARG:HG3 | 0.44 | 2.12 | 19 | 2 |
| 1:A:24:GLU:O | 1:A:27:LYS:HG3 | 0.44 | 2.13 | 25 | 8 |
| 1:A:32:ILE:HD12 | 1:A:71:MET:SD | 0.44 | 2.51 | 4 | 1 |
| 1:A:25:LEU:O | 1:A:29:LEU:HG | 0.44 | 2.12 | 21 | 12 |
| 1:A:52:GLY:O | 1:A:53:GLN:C | 0.44 | 2.54 | 6 | 9 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:HG13 | 0.44 | 1.87 | 38 | 3 |
| 1:A:9:HIS:CA | 1:A:61:VAL:HG13 | 0.44 | 2.42 | 41 | 1 |
| 1:A:76:PHE:CD1 | 1:A:81:MET:CE | 0.44 | 3.01 | 41 | 1 |
| 1:A:26:LYS:HG3 | 1:A:44:VAL:HG13 | 0.44 | 1.90 | 10 | 1 |
| 1:A:29:LEU:O | 1:A:32:ILE:HG13 | 0.44 | 2.12 | 3 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:44:VAL:C | 1:A:50:MET:SD | 0.44 | 2.95 | 3 | 1 |
| 1:A:40:LEU:HD22 | 1:A:40:LEU:C | 0.44 | 2.32 | 38 | 1 |
| 1:A:10:THR:HG21 | 1:A:89:ASP:HB2 | 0.44 | 1.82 | 35 | 1 |
| 1:A:13:ILE:O | 1:A:53:GLN:HA | 0.44 | 2.12 | 5 | 13 |
| 1:A:71:MET:HA | 1:A:74:PHE:CB | 0.44 | 2.42 | 15 | 1 |
| 1:A:16:LEU:HB3 | 1:A:25:LEU:CD2 | 0.44 | 2.42 | 31 | 2 |
| 1:A:89:ASP:O | 1:A:90:SER:C | 0.44 | 2.55 | 42 | 3 |
| 1:A:38:GLN:OE1 | 1:A:40:LEU:HD12 | 0.44 | 2.11 | 38 | 1 |
| 1:A:43:LEU:CD1 | 1:A:93:ILE:HG23 | 0.44 | 2.43 | 38 | 1 |
| 1:A:52:GLY:O | 1:A:53:GLN:HG3 | 0.44 | 2.13 | 14 | 3 |
| 1:A:43:LEU:CD1 | 1:A:55:PHE:HB2 | 0.44 | 2.42 | 2 | 2 |
| 1:A:14:ASN:O | 1:A:15:ASN:HB3 | 0.44 | 2.12 | 10 | 2 |
| 1:A:25:LEU:HD22 | 1:A:77:TYR:HE2 | 0.44 | 1.71 | 27 | 1 |
| 1:A:71:MET:CE | 1:A:81:MET:HE3 | 0.44 | 2.42 | 1 | 1 |
| 1:A:22:LYS:HD3 | 1:A:46:ARG:NH1 | 0.44 | 2.28 | 3 | 1 |
| 1:A:10:THR:CG2 | 1:A:55:PHE:CB | 0.44 | 2.95 | 19 | 1 |
| 1:A:71:MET:HB3 | 1:A:74:PHE:CB | 0.44 | 2.42 | 43 | 3 |
| 1:A:14:ASN:ND2 | 1:A:84:GLN:NE2 | 0.44 | 2.64 | 16 | 2 |
| 1:A:77:TYR:O | 1:A:78:ASP:HB2 | 0.44 | 2.11 | 30 | 6 |
| 1:A:36:PHE:CZ | 1:A:71:MET:CG | 0.44 | 3.01 | 37 | 2 |
| 1:A:7:PRO:O | 1:A:61:VAL:CG1 | 0.44 | 2.65 | 8 | 1 |
| 1:A:17:ASN:ND2 | 1:A:77:TYR:HB3 | 0.44 | 2.27 | 8 | 1 |
| 1:A:69:ARG:NH1 | 1:A:69:ARG:HG2 | 0.44 | 2.26 | 34 | 1 |
| 1:A:71:MET:O | 1:A:81:MET:HG2 | 0.44 | 2.13 | 12 | 1 |
| 1:A:39:ILE:C | 1:A:40:LEU:HD12 | 0.44 | 2.33 | 25 | 1 |
| 1:A:39:ILE:HG22 | 1:A:42:ILE:CD1 | 0.44 | 2.42 | 13 | 1 |
| 1:A:71:MET:HA | 1:A:74:PHE:CD1 | 0.44 | 2.48 | 24 | 2 |
| 1:A:84:GLN:N | 1:A:84:GLN:CD | 0.44 | 2.71 | 11 | 1 |
| 1:A:45:SER:O | 1:A:46:ARG:C | 0.44 | 2.54 | 22 | 4 |
| 1:A:33:PHE:HB3 | 1:A:58:PHE:CE2 | 0.44 | 2.47 | 14 | 6 |
| 1:A:43:LEU:HD22 | 1:A:93:ILE:HG12 | 0.44 | 1.89 | 1 | 1 |
| 1:A:37:GLY:O | 1:A:63:SER:OG | 0.44 | 2.33 | 31 | 1 |
| 1:A:49:LYS:O | 1:A:53:GLN:NE2 | 0.44 | 2.51 | 35 | 1 |
| 1:A:71:MET:HG3 | 1:A:71:MET:O | 0.44 | 2.13 | 7 | 1 |
| 1:A:110:ARG:O | 1:A:111:LYS:C | 0.44 | 2.56 | 14 | 7 |
| 1:A:12:TYR:HB3 | 1:A:84:GLN:NE2 | 0.44 | 2.28 | 15 | 1 |
| 1:A:107:ARG:O | 1:A:107:ARG:CG | 0.44 | 2.65 | 30 | 1 |
| 1:A:10:THR:HG21 | 1:A:89:ASP:OD1 | 0.44 | 2.13 | 41 | 1 |
| 1:A:87:LYS:CD | 1:A:87:LYS:N | 0.44 | 2.80 | 35 | 1 |
| 1:A:87:LYS:N | 1:A:87:LYS:HD2 | 0.44 | 2.27 | 35 | 1 |
| 1:A:26:LYS:HA | 1:A:29:LEU:CD1 | 0.44 | 2.41 | 34 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:40:LEU:HB2 | 1:A:57:ILE:O | 0.44 | 2.12 | 22 | 1 |
| 1:A:74:PHE:O | 1:A:80:PRO:HA | 0.44 | 2.13 | 21 | 2 |
| 1:A:32:ILE:HG23 | 1:A:33:PHE:CE1 | 0.44 | 2.46 | 30 | 2 |
| 1:A:44:VAL:HG12 | 1:A:45:SER:H | 0.44 | 1.72 | 31 | 1 |
| 1:A:55:PHE:CB | 1:A:89:ASP:OD2 | 0.44 | 2.66 | 41 | 1 |
| 1:A:74:PHE:CD1 | 1:A:74:PHE:C | 0.44 | 2.91 | 36 | 1 |
| 1:A:76:PHE:HB2 | 1:A:81:MET:HG2 | 0.44 | 1.90 | 24 | 1 |
| 1:A:79:LYS:HG3 | 1:A:80:PRO:HD2 | 0.44 | 1.89 | 24 | 1 |
| 1:A:15:ASN:CG | 1:A:80:PRO:O | 0.44 | 2.56 | 4 | 1 |
| 1:A:25:LEU:O | 1:A:28:SER:OG | 0.44 | 2.32 | 26 | 2 |
| 1:A:70:SER:O | 1:A:72:GLN:N | 0.44 | 2.50 | 18 | 1 |
| 1:A:39:ILE:HD13 | 1:A:58:PHE:CE1 | 0.44 | 2.47 | 42 | 1 |
| 1:A:69:ARG:O | 1:A:69:ARG:CD | 0.44 | 2.66 | 13 | 1 |
| 1:A:14:ASN:ND2 | 1:A:53:GLN:CD | 0.44 | 2.72 | 35 | 1 |
| 1:A:13:ILE:C | 1:A:14:ASN:OD1 | 0.44 | 2.56 | 35 | 1 |
| 1:A:38:GLN:O | 1:A:39:ILE:C | 0.44 | 2.56 | 34 | 5 |
| 1:A:71:MET:HG3 | 1:A:74:PHE:HB2 | 0.44 | 1.89 | 22 | 1 |
| 1:A:11:ILE:HG12 | 1:A:56:VAL:CG2 | 0.44 | 2.43 | 9 | 2 |
| 1:A:74:PHE:HB2 | 1:A:81:MET:SD | 0.44 | 2.53 | 9 | 1 |
| 1:A:14:ASN:HA | 1:A:53:GLN:CG | 0.44 | 2.43 | 36 | 4 |
| 1:A:68:LEU:HD23 | 1:A:83:ILE:HG22 | 0.44 | 1.89 | 21 | 1 |
| 1:A:32:ILE:CG2 | 1:A:33:PHE:CZ | 0.44 | 3.01 | 30 | 2 |
| 1:A:23:ASP:O | 1:A:27:LYS:HG2 | 0.44 | 2.12 | 29 | 1 |
| 1:A:109:LYS:O | 1:A:109:LYS:HG3 | 0.44 | 2.13 | 41 | 1 |
| 1:A:24:GLU:O | 1:A:26:LYS:N | 0.44 | 2.51 | 24 | 1 |
| 1:A:47:SER:O | 1:A:49:LYS:N | 0.44 | 2.50 | 7 | 1 |
| 1:A:36:PHE:HB3 | 1:A:66:ASN:HB2 | 0.43 | 1.90 | 39 | 4 |
| 1:A:89:ASP:CB | 1:A:92:ILE:HB | 0.43 | 2.43 | 4 | 3 |
| 1:A:68:LEU:CD1 | 1:A:85:TYR:OH | 0.43 | 2.64 | 28 | 8 |
| 1:A:30:TYR:N | 1:A:42:ILE:HD12 | 0.43 | 2.28 | 33 | 1 |
| 1:A:47:SER:O | 1:A:48:LEU:HB2 | 0.43 | 2.13 | 14 | 1 |
| 1:A:46:ARG:O | 1:A:50:MET:O | 0.43 | 2.36 | 15 | 1 |
| 1:A:71:MET:HB3 | 1:A:83:ILE:CD1 | 0.43 | 2.42 | 41 | 2 |
| 1:A:76:PHE:CE2 | 1:A:77:TYR:CD1 | 0.43 | 3.05 | 24 | 2 |
| 1:A:37:GLY:O | 1:A:38:GLN:CD | 0.43 | 2.56 | 43 | 1 |
| 1:A:22:LYS:HE2 | 1:A:22:LYS:N | 0.43 | 2.29 | 34 | 1 |
| 1:A:25:LEU:CD2 | 1:A:77:TYR:CE2 | 0.43 | 3.00 | 1 | 1 |
| 1:A:58:PHE:CZ | 1:A:67:ALA:HB2 | 0.43 | 2.49 | 42 | 1 |
| 1:A:68:LEU:HD12 | 1:A:69:ARG:CG | 0.43 | 2.43 | 42 | 1 |
| 1:A:20:ILE:HB | 1:A:25:LEU:CD1 | 0.43 | 2.43 | 3 | 2 |
| 1:A:50:MET:HA | 1:A:53:GLN:NE2 | 0.43 | 2.28 | 43 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:44:VAL:HG23 | 1:A:45:SER:N | 0.43 | 2.28 | 16 | 3 |
| 1:A:45:SER:HB3 | 1:A:50:MET:SD | 0.43 | 2.52 | 11 | 4 |
| 1:A:108:GLU:O | 1:A:109:LYS:C | 0.43 | 2.56 | 21 | 3 |
| 1:A:17:ASN:O | 1:A:20:ILE:HG12 | 0.43 | 2.13 | 12 | 3 |
| 1:A:71:MET:CE | 1:A:74:PHE:CD2 | 0.43 | 3.01 | 25 | 3 |
| 1:A:25:LEU:O | 1:A:29:LEU:CD2 | 0.43 | 2.66 | 20 | 1 |
| 1:A:29:LEU:HD21 | 1:A:76:PHE:CE2 | 0.43 | 2.48 | 35 | 1 |
| 1:A:76:PHE:HB2 | 1:A:81:MET:SD | 0.43 | 2.53 | 37 | 4 |
| 1:A:43:LEU:HB2 | 1:A:55:PHE:O | 0.43 | 2.13 | 8 | 1 |
| 1:A:45:SER:CB | 1:A:50:MET:HB3 | 0.43 | 2.43 | 17 | 1 |
| 1:A:22:LYS:C | 1:A:24:GLU:N | 0.43 | 2.72 | 21 | 2 |
| 1:A:73:GLY:HA2 | 1:A:80:PRO:CB | 0.43 | 2.44 | 30 | 1 |
| 1:A:68:LEU:HG | 1:A:85:TYR:CD1 | 0.43 | 2.46 | 7 | 3 |
| 1:A:36:PHE:HB3 | 1:A:66:ASN:OD1 | 0.43 | 2.13 | 36 | 1 |
| 1:A:55:PHE:CE1 | 1:A:89:ASP:OD1 | 0.43 | 2.71 | 32 | 1 |
| 1:A:17:ASN:ND2 | 1:A:19:LYS:HB2 | 0.43 | 2.28 | 35 | 1 |
| 1:A:77:TYR:O | 1:A:80:PRO:HD3 | 0.43 | 2.13 | 35 | 1 |
| 1:A:22:LYS:CG | 1:A:45:SER:HB3 | 0.43 | 2.43 | 7 | 1 |
| 1:A:18:GLU:CG | 1:A:51:ARG:HG2 | 0.43 | 2.43 | 22 | 1 |
| 1:A:14:ASN:CB | 1:A:53:GLN:HG2 | 0.43 | 2.43 | 15 | 4 |
| 1:A:30:TYR:OH | 1:A:40:LEU:C | 0.43 | 2.57 | 4 | 3 |
| 1:A:89:ASP:O | 1:A:93:ILE:CD1 | 0.43 | 2.66 | 29 | 1 |
| 1:A:12:TYR:CZ | 1:A:55:PHE:CE1 | 0.43 | 3.06 | 42 | 3 |
| 1:A:43:LEU:CD2 | 1:A:57:ILE:CD1 | 0.43 | 2.97 | 20 | 1 |
| 1:A:32:ILE:CD1 | 1:A:76:PHE:CE2 | 0.43 | 3.02 | 39 | 1 |
| 1:A:15:ASN:O | 1:A:16:LEU:C | 0.43 | 2.56 | 21 | 4 |
| 1:A:38:GLN:O | 1:A:40:LEU:HD23 | 0.43 | 2.14 | 6 | 2 |
| 1:A:32:ILE:HG21 | 1:A:71:MET:CE | 0.43 | 2.43 | 29 | 2 |
| 1:A:70:SER:O | 1:A:71:MET:C | 0.43 | 2.56 | 18 | 1 |
| 1:A:29:LEU:O | 1:A:30:TYR:C | 0.43 | 2.56 | 23 | 1 |
| 1:A:42:ILE:O | 1:A:43:LEU:HD13 | 0.43 | 2.14 | 23 | 1 |
| 1:A:48:LEU:C | 1:A:50:MET:N | 0.43 | 2.72 | 3 | 2 |
| 1:A:10:THR:CG2 | 1:A:56:VAL:O | 0.43 | 2.60 | 37 | 1 |
| 1:A:109:LYS:O | 1:A:110:ARG:HG3 | 0.43 | 2.14 | 25 | 1 |
| 1:A:57:ILE:CD1 | 1:A:93:ILE:CG1 | 0.43 | 2.96 | 23 | 1 |
| 1:A:14:ASN:HA | 1:A:53:GLN:HG2 | 0.43 | 1.89 | 7 | 1 |
| 1:A:15:ASN:O | 1:A:15:ASN:OD1 | 0.43 | 2.36 | 16 | 1 |
| 1:A:68:LEU:HD12 | 1:A:69:ARG:HG3 | 0.43 | 1.90 | 16 | 4 |
| 1:A:25:LEU:HA | 1:A:77:TYR:OH | 0.43 | 2.13 | 4 | 1 |
| 1:A:43:LEU:CG | 1:A:93:ILE:CG1 | 0.43 | 2.97 | 8 | 1 |
| 1:A:108:GLU:O | 1:A:109:LYS:O | 0.43 | 2.36 | 21 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:71:MET:HG3 | 1:A:81:MET:HE3 | 0.43 | 1.91 | 18 | 1 |
| 1:A:55:PHE:CZ | 1:A:89:ASP:OD2 | 0.43 | 2.71 | 10 | 1 |
| 1:A:10:THR:CG2 | 1:A:89:ASP:CB | 0.43 | 2.88 | 35 | 1 |
| 1:A:40:LEU:CG | 1:A:59:LYS:HB2 | 0.43 | 2.44 | 39 | 1 |
| 1:A:76:PHE:CE1 | 1:A:77:TYR:CE2 | 0.43 | 3.07 | 28 | 2 |
| 1:A:16:LEU:CD2 | 1:A:25:LEU:HD21 | 0.43 | 2.44 | 14 | 1 |
| 1:A:55:PHE:CE1 | 1:A:92:ILE:CD1 | 0.43 | 3.02 | 26 | 3 |
| 1:A:30:TYR:CA | 1:A:42:ILE:HD11 | 0.43 | 2.43 | 1 | 2 |
| 1:A:14:ASN:ND2 | 1:A:53:GLN:HG2 | 0.43 | 2.29 | 35 | 1 |
| 1:A:65:THR:HG23 | 1:A:69:ARG:HD2 | 0.43 | 1.91 | 43 | 2 |
| 1:A:15:ASN:OD1 | 1:A:79:LYS:HB3 | 0.43 | 2.14 | 16 | 1 |
| 1:A:36:PHE:CE2 | 1:A:67:ALA:HA | 0.43 | 2.48 | 4 | 4 |
| 1:A:22:LYS:HD2 | 1:A:46:ARG:CD | 0.43 | 2.44 | 8 | 1 |
| 1:A:81:MET:O | 1:A:83:ILE:HG13 | 0.43 | 2.13 | 3 | 4 |
| 1:A:111:LYS:HB2 | 1:A:112:PRO:HD3 | 0.43 | 1.90 | 36 | 3 |
| 1:A:70:SER:C | 1:A:72:GLN:N | 0.43 | 2.72 | 18 | 1 |
| 1:A:89:ASP:CG | 1:A:89:ASP:O | 0.43 | 2.57 | 1 | 1 |
| 1:A:19:LYS:O | 1:A:20:ILE:C | 0.43 | 2.57 | 42 | 1 |
| 1:A:78:ASP:O | 1:A:79:LYS:HB2 | 0.43 | 2.13 | 13 | 2 |
| 1:A:39:ILE:HG23 | 1:A:42:ILE:CD1 | 0.43 | 2.43 | 20 | 2 |
| 1:A:30:TYR:CD1 | 1:A:39:ILE:HB | 0.42 | 2.49 | 6 | 1 |
| 1:A:37:GLY:O | 1:A:38:GLN:O | 0.42 | 2.37 | 31 | 1 |
| 1:A:43:LEU:HB2 | 1:A:55:PHE:CD2 | 0.42 | 2.49 | 19 | 1 |
| 1:A:40:LEU:O | 1:A:41:ASP:HB2 | 0.42 | 2.14 | 42 | 8 |
| 1:A:13:ILE:O | 1:A:53:GLN:HG2 | 0.42 | 2.14 | 32 | 2 |
| 1:A:45:SER:O | 1:A:46:ARG:O | 0.42 | 2.37 | 26 | 1 |
| 1:A:85:TYR:O | 1:A:86:ALA:C | 0.42 | 2.57 | 26 | 2 |
| 1:A:26:LYS:C | 1:A:28:SER:N | 0.42 | 2.70 | 42 | 1 |
| 1:A:71:MET:HE3 | 1:A:81:MET:CE | 0.42 | 2.45 | 36 | 1 |
| 1:A:84:GLN:O | 1:A:84:GLN:HG2 | 0.42 | 2.14 | 28 | 1 |
| 1:A:65:THR:CG2 | 1:A:69:ARG:HD2 | 0.42 | 2.44 | 43 | 1 |
| 1:A:71:MET:HA | 1:A:74:PHE:HB2 | 0.42 | 1.91 | 27 | 3 |
| 1:A:71:MET:HE3 | 1:A:81:MET:SD | 0.42 | 2.53 | 19 | 3 |
| 1:A:89:ASP:OD1 | 1:A:92:ILE:CD1 | 0.42 | 2.66 | 40 | 2 |
| 1:A:77:TYR:O | 1:A:78:ASP:HB3 | 0.42 | 2.13 | 35 | 4 |
| 1:A:30:TYR:OH | 1:A:40:LEU:HA | 0.42 | 2.14 | 29 | 6 |
| 1:A:25:LEU:HD22 | 1:A:52:GLY:HA2 | 0.42 | 1.90 | 34 | 1 |
| 1:A:76:PHE:CD1 | 1:A:81:MET:HE2 | 0.42 | 2.49 | 8 | 1 |
| 1:A:71:MET:HE3 | 1:A:81:MET:HE3 | 0.42 | 1.91 | 1 | 1 |
| 1:A:87:LYS:N | 1:A:87:LYS:CD | 0.42 | 2.81 | 1 | 1 |
| 1:A:30:TYR:CA | 1:A:42:ILE:CD1 | 0.42 | 2.97 | 31 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:ILE:O | 1:A:14:ASN:OD1 | 0.42 | 2.37 | 35 | 1 |
| 1:A:40:LEU:HG | 1:A:59:LYS:CG | 0.42 | 2.45 | 43 | 1 |
| 1:A:50:MET:HA | 1:A:53:GLN:OE1 | 0.42 | 2.14 | 22 | 1 |
| 1:A:71:MET:HB2 | 1:A:83:ILE:CD1 | 0.42 | 2.42 | 21 | 2 |
| 1:A:45:SER:OG | 1:A:50:MET:CE | 0.42 | 2.68 | 27 | 1 |
| 1:A:113:LYS:N | 1:A:113:LYS:HD3 | 0.42 | 2.29 | 31 | 1 |
| 1:A:44:VAL:CG2 | 1:A:44:VAL:O | 0.42 | 2.67 | 29 | 1 |
| 1:A:38:GLN:HG2 | 1:A:63:SER:OG | 0.42 | 2.14 | 42 | 1 |
| 1:A:33:PHE:HB2 | 1:A:39:ILE:HG13 | 0.42 | 1.90 | 28 | 1 |
| 1:A:25:LEU:CD1 | 1:A:77:TYR:CZ | 0.42 | 3.01 | 32 | 1 |
| 1:A:25:LEU:HD12 | 1:A:77:TYR:OH | 0.42 | 2.15 | 32 | 1 |
| 1:A:68:LEU:HG | 1:A:85:TYR:CD2 | 0.42 | 2.48 | 19 | 2 |
| 1:A:7:PRO:HB3 | 1:A:65:THR:OG1 | 0.42 | 2.13 | 2 | 5 |
| 1:A:106:LYS:O | 1:A:107:ARG:CD | 0.42 | 2.68 | 25 | 1 |
| 1:A:28:SER:O | 1:A:32:ILE:HG13 | 0.42 | 2.14 | 25 | 1 |
| 1:A:111:LYS:CB | 1:A:112:PRO:CD | 0.42 | 2.98 | 36 | 4 |
| 1:A:69:ARG:CD | 1:A:69:ARG:O | 0.42 | 2.68 | 2 | 1 |
| 1:A:11:ILE:O | 1:A:11:ILE:CG1 | 0.42 | 2.67 | 41 | 2 |
| 1:A:48:LEU:O | 1:A:51:ARG:HG3 | 0.42 | 2.14 | 13 | 1 |
| 1:A:28:SER:HB2 | 1:A:76:PHE:CE1 | 0.42 | 2.50 | 13 | 1 |
| 1:A:51:ARG:O | 1:A:53:GLN:HG3 | 0.42 | 2.14 | 3 | 1 |
| 1:A:79:LYS:HG3 | 1:A:80:PRO:CD | 0.42 | 2.44 | 24 | 1 |
| 1:A:55:PHE:CD1 | 1:A:92:ILE:HG21 | 0.42 | 2.48 | 37 | 1 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:HG23 | 0.42 | 2.45 | 9 | 1 |
| 1:A:91:ASP:CG | 1:A:92:ILE:N | 0.42 | 2.73 | 40 | 1 |
| 1:A:33:PHE:C | 1:A:39:ILE:HD11 | 0.42 | 2.34 | 17 | 2 |
| 1:A:22:LYS:N | 1:A:22:LYS:CE | 0.42 | 2.83 | 12 | 1 |
| 1:A:106:LYS:O | 1:A:107:ARG:HB2 | 0.42 | 2.15 | 25 | 2 |
| 1:A:22:LYS:HE2 | 1:A:45:SER:O | 0.42 | 2.15 | 25 | 1 |
| 1:A:82:ARG:HG2 | 1:A:82:ARG:NH1 | 0.42 | 2.29 | 21 | 1 |
| 1:A:16:LEU:HD23 | 1:A:53:GLN:N | 0.42 | 2.30 | 14 | 1 |
| 1:A:68:LEU:CD2 | 1:A:83:ILE:C | 0.42 | 2.88 | 2 | 1 |
| 1:A:43:LEU:CD2 | 1:A:93:ILE:HG12 | 0.42 | 2.38 | 24 | 1 |
| 1:A:31:ALA:C | 1:A:32:ILE:CG1 | 0.42 | 2.88 | 39 | 1 |
| 1:A:43:LEU:O | 1:A:54:ALA:HA | 0.42 | 2.14 | 34 | 4 |
| 1:A:50:MET:HE2 | 1:A:50:MET:HB3 | 0.42 | 1.67 | 41 | 1 |
| 1:A:44:VAL:O | 1:A:45:SER:HB2 | 0.42 | 2.15 | 13 | 1 |
| 1:A:110:ARG:NH1 | 1:A:110:ARG:HG2 | 0.42 | 2.30 | 23 | 1 |
| 1:A:40:LEU:HG | 1:A:59:LYS:CD | 0.42 | 2.45 | 11 | 1 |
| 1:A:20:ILE:CB | 1:A:25:LEU:HD13 | 0.42 | 2.45 | 20 | 1 |
| 1:A:12:TYR:O | 1:A:84:GLN:HG2 | 0.42 | 2.14 | 28 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:16:LEU:HG | 1:A:52:GLY:O | 0.42 | 2.15 | 35 | 1 |
| 1:A:25:LEU:CD2 | 1:A:52:GLY:HA2 | 0.42 | 2.44 | 42 | 2 |
| 1:A:86:ALA:CB | 1:A:89:ASP:OD2 | 0.42 | 2.64 | 17 | 1 |
| 1:A:14:ASN:CG | 1:A:14:ASN:O | 0.42 | 2.57 | 15 | 1 |
| 1:A:41:ASP:O | 1:A:57:ILE:HB | 0.42 | 2.14 | 18 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:HE2 | 0.42 | 2.14 | 18 | 1 |
| 1:A:40:LEU:O | 1:A:41:ASP:OD1 | 0.42 | 2.38 | 11 | 1 |
| 1:A:11:ILE:HG13 | 1:A:56:VAL:CG2 | 0.42 | 2.43 | 28 | 1 |
| 1:A:29:LEU:O | 1:A:33:PHE:CD2 | 0.42 | 2.73 | 38 | 1 |
| 1:A:45:SER:H | 1:A:50:MET:HE1 | 0.42 | 1.73 | 38 | 1 |
| 1:A:47:SER:O | 1:A:51:ARG:HG3 | 0.42 | 2.15 | 9 | 1 |
| 1:A:43:LEU:O | 1:A:54:ALA:CA | 0.42 | 2.68 | 34 | 1 |
| 1:A:41:ASP:HB3 | 1:A:57:ILE:HB | 0.42 | 1.92 | 25 | 2 |
| 1:A:108:GLU:O | 1:A:109:LYS:HG3 | 0.42 | 2.15 | 21 | 1 |
| 1:A:91:ASP:N | 1:A:91:ASP:OD1 | 0.42 | 2.51 | 31 | 1 |
| 1:A:76:PHE:CB | 1:A:81:MET:CG | 0.42 | 2.98 | 42 | 1 |
| 1:A:62:SER:O | 1:A:66:ASN:ND2 | 0.42 | 2.53 | 41 | 1 |
| 1:A:14:ASN:O | 1:A:16:LEU:HD22 | 0.42 | 2.14 | 13 | 1 |
| 1:A:13:ILE:HG22 | 1:A:14:ASN:N | 0.42 | 2.30 | 7 | 1 |
| 1:A:20:ILE:HB | 1:A:25:LEU:HD23 | 0.41 | 1.91 | 22 | 1 |
| 1:A:46:ARG:O | 1:A:47:SER:C | 0.41 | 2.59 | 6 | 1 |
| 1:A:112:PRO:O | 1:A:113:LYS:HG2 | 0.41 | 2.15 | 2 | 1 |
| 1:A:48:LEU:HD13 | 1:A:51:ARG:HD3 | 0.41 | 1.92 | 27 | 1 |
| 1:A:78:ASP:O | 1:A:79:LYS:HG3 | 0.41 | 2.15 | 42 | 1 |
| 1:A:92:ILE:O | 1:A:93:ILE:C | 0.41 | 2.57 | 43 | 2 |
| 1:A:32:ILE:HG23 | 1:A:71:MET:SD | 0.41 | 2.55 | 33 | 1 |
| 1:A:12:TYR:CE1 | 1:A:53:GLN:CD | 0.41 | 2.94 | 14 | 1 |
| 1:A:36:PHE:N | 1:A:36:PHE:CD1 | 0.41 | 2.85 | 15 | 2 |
| 1:A:112:PRO:O | 1:A:113:LYS:HB2 | 0.41 | 2.14 | 36 | 1 |
| 1:A:81:MET:O | 1:A:82:ARG:C | 0.41 | 2.57 | 3 | 1 |
| 1:A:16:LEU:HD12 | 1:A:76:PHE:HE2 | 0.41 | 1.73 | 38 | 1 |
| 1:A:55:PHE:CD2 | 1:A:89:ASP:CG | 0.41 | 2.93 | 37 | 1 |
| 1:A:16:LEU:HB2 | 1:A:52:GLY:HA3 | 0.41 | 1.92 | 33 | 1 |
| 1:A:47:SER:C | 1:A:49:LYS:N | 0.41 | 2.74 | 21 | 1 |
| 1:A:58:PHE:CD1 | 1:A:64:ALA:HA | 0.41 | 2.50 | 32 | 1 |
| 1:A:89:ASP:O | 1:A:93:ILE:N | 0.41 | 2.54 | 35 | 1 |
| 1:A:72:GLN:NE2 | 1:A:83:ILE:HB | 0.41 | 2.30 | 17 | 1 |
| 1:A:67:ALA:O | 1:A:71:MET:HG3 | 0.41 | 2.16 | 33 | 1 |
| 1:A:109:LYS:C | 1:A:110:ARG:HG2 | 0.41 | 2.35 | 25 | 1 |
| 1:A:32:ILE:HG21 | 1:A:33:PHE:CZ | 0.41 | 2.50 | 2 | 1 |
| 1:A:30:TYR:O | 1:A:34:SER:HB3 | 0.41 | 2.15 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:48:LEU:HD13 | 1:A:49:LYS:N | 0.41 | 2.30 | 35 | 1 |
| 1:A:23:ASP:HA | 1:A:26:LYS:CE | 0.41 | 2.45 | 24 | 1 |
| 1:A:105:ARG:O | 1:A:106:LYS:CB | 0.41 | 2.66 | 7 | 1 |
| 1:A:28:SER:HG | 1:A:76:PHE:HE2 | 0.41 | 1.51 | 34 | 1 |
| 1:A:32:ILE:HG22 | 1:A:33:PHE:CE1 | 0.41 | 2.48 | 2 | 1 |
| 1:A:69:ARG:O | 1:A:72:GLN:HB2 | 0.41 | 2.16 | 42 | 2 |
| 1:A:22:LYS:HG3 | 1:A:44:VAL:HG21 | 0.41 | 1.92 | 31 | 1 |
| 1:A:34:SER:HB3 | 1:A:35:GLN:NE2 | 0.41 | 2.31 | 29 | 1 |
| 1:A:14:ASN:CG | 1:A:53:GLN:HG2 | 0.41 | 2.36 | 35 | 1 |
| 1:A:43:LEU:HD11 | 1:A:55:PHE:HB2 | 0.41 | 1.92 | 43 | 1 |
| 1:A:68:LEU:HA | 1:A:83:ILE:HB | 0.41 | 1.91 | 22 | 1 |
| 1:A:6:ARG:HB2 | 1:A:6:ARG:NH2 | 0.41 | 2.30 | 9 | 1 |
| 1:A:106:LYS:O | 1:A:107:ARG:HG3 | 0.41 | 2.15 | 41 | 1 |
| 1:A:105:ARG:O | 1:A:106:LYS:HB2 | 0.41 | 2.16 | 10 | 1 |
| 1:A:89:ASP:OD1 | 1:A:92:ILE:HB | 0.41 | 2.15 | 10 | 1 |
| 1:A:43:LEU:C | 1:A:44:VAL:CG1 | 0.41 | 2.89 | 3 | 1 |
| 1:A:30:TYR:OH | 1:A:41:ASP:N | 0.41 | 2.54 | 38 | 1 |
| 1:A:55:PHE:CG | 1:A:89:ASP:OD1 | 0.41 | 2.74 | 35 | 1 |
| 1:A:77:TYR:N | 1:A:80:PRO:HD2 | 0.41 | 2.30 | 35 | 1 |
| 1:A:47:SER:HB3 | 1:A:50:MET:CB | 0.41 | 2.46 | 19 | 1 |
| 1:A:45:SER:HB3 | 1:A:50:MET:HG2 | 0.41 | 1.92 | 19 | 1 |
| 1:A:29:LEU:HB3 | 1:A:33:PHE:CZ | 0.41 | 2.50 | 38 | 2 |
| 1:A:6:ARG:O | 1:A:85:TYR:CD1 | 0.41 | 2.73 | 27 | 1 |
| 1:A:25:LEU:HG | 1:A:25:LEU:O | 0.41 | 2.16 | 37 | 1 |
| 1:A:29:LEU:CD2 | 1:A:76:PHE:CE2 | 0.41 | 3.04 | 8 | 1 |
| 1:A:45:SER:OG | 1:A:46:ARG:N | 0.41 | 2.53 | 21 | 1 |
| 1:A:55:PHE:CG | 1:A:89:ASP:OD2 | 0.41 | 2.74 | 41 | 1 |
| 1:A:40:LEU:CD1 | 1:A:59:LYS:HB2 | 0.41 | 2.46 | 7 | 1 |
| 1:A:46:ARG:N | 1:A:46:ARG:CD | 0.41 | 2.84 | 19 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:CG | 0.41 | 2.68 | 16 | 1 |
| 1:A:21:LYS:CB | 1:A:21:LYS:NZ | 0.41 | 2.84 | 37 | 1 |
| 1:A:44:VAL:HB | 1:A:54:ALA:CB | 0.41 | 2.43 | 9 | 1 |
| 1:A:32:ILE:O | 1:A:35:GLN:HG3 | 0.41 | 2.15 | 39 | 3 |
| 1:A:18:GLU:C | 1:A:19:LYS:HG3 | 0.41 | 2.36 | 4 | 1 |
| 1:A:83:ILE:O | 1:A:84:GLN:HG3 | 0.41 | 2.16 | 8 | 1 |
| 1:A:68:LEU:O | 1:A:72:GLN:HB2 | 0.41 | 2.16 | 34 | 1 |
| 1:A:45:SER:HB2 | 1:A:50:MET:SD | 0.41 | 2.56 | 36 | 3 |
| 1:A:53:GLN:O | 1:A:54:ALA:HB2 | 0.41 | 2.16 | 21 | 1 |
| 1:A:65:THR:O | 1:A:69:ARG:HB2 | 0.41 | 2.16 | 15 | 2 |
| 1:A:12:TYR:N | 1:A:84:GLN:O | 0.41 | 2.54 | 26 | 1 |
| 1:A:48:LEU:HG | 1:A:48:LEU:O | 0.41 | 2.16 | 31 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:77:TYR:HD1 | 1:A:77:TYR:N | 0.41 | 2.13 | 42 | 1 |
| 1:A:33:PHE:CE1 | 1:A:67:ALA:CB | 0.41 | 3.04 | 42 | 1 |
| 1:A:22:LYS:HE3 | 1:A:44:VAL:CG2 | 0.41 | 2.46 | 41 | 1 |
| 1:A:32:ILE:HD11 | 1:A:33:PHE:CE2 | 0.41 | 2.50 | 36 | 1 |
| 1:A:40:LEU:O | 1:A:41:ASP:OD2 | 0.41 | 2.38 | 20 | 1 |
| 1:A:32:ILE:HG23 | 1:A:33:PHE:N | 0.41 | 2.30 | 32 | 1 |
| 1:A:77:TYR:N | 1:A:77:TYR:HD1 | 0.41 | 2.13 | 38 | 1 |
| 1:A:15:ASN:O | 1:A:15:ASN:CG | 0.41 | 2.58 | 35 | 1 |
| 1:A:30:TYR:O | 1:A:34:SER:HB2 | 0.41 | 2.16 | 24 | 1 |
| 1:A:33:PHE:C | 1:A:35:GLN:N | 0.41 | 2.74 | 42 | 2 |
| 1:A:89:ASP:O | 1:A:92:ILE:HB | 0.41 | 2.16 | 8 | 1 |
| 1:A:26:LYS:HG3 | 1:A:44:VAL:HG11 | 0.41 | 1.92 | 21 | 1 |
| 1:A:111:LYS:CD | 1:A:111:LYS:N | 0.41 | 2.80 | 30 | 1 |
| 1:A:30:TYR:CG | 1:A:39:ILE:HG21 | 0.41 | 2.51 | 7 | 1 |
| 1:A:39:ILE:O | 1:A:40:LEU:HD12 | 0.41 | 2.16 | 7 | 1 |
| 1:A:90:SER:O | 1:A:91:ASP:C | 0.40 | 2.59 | 43 | 1 |
| 1:A:14:ASN:OD1 | 1:A:53:GLN:CD | 0.40 | 2.59 | 22 | 1 |
| 1:A:15:ASN:OD1 | 1:A:15:ASN:N | 0.40 | 2.50 | 9 | 1 |
| 1:A:32:ILE:HD11 | 1:A:76:PHE:CE2 | 0.40 | 2.51 | 39 | 1 |
| 1:A:50:MET:HE2 | 1:A:53:GLN:O | 0.40 | 2.16 | 17 | 2 |
| 1:A:16:LEU:CD1 | 1:A:77:TYR:CG | 0.40 | 3.05 | 34 | 1 |
| 1:A:33:PHE:CB | 1:A:58:PHE:CE2 | 0.40 | 3.03 | 33 | 1 |
| 1:A:47:SER:HB2 | 1:A:50:MET:HB2 | 0.40 | 1.92 | 12 | 1 |
| 1:A:109:LYS:O | 1:A:110:ARG:CG | 0.40 | 2.69 | 25 | 1 |
| 1:A:22:LYS:O | 1:A:24:GLU:OE1 | 0.40 | 2.38 | 30 | 1 |
| 1:A:45:SER:O | 1:A:50:MET:HG2 | 0.40 | 2.16 | 31 | 1 |
| 1:A:46:ARG:O | 1:A:47:SER:HB2 | 0.40 | 2.16 | 31 | 1 |
| 1:A:16:LEU:H | 1:A:16:LEU:CD2 | 0.40 | 2.29 | 41 | 1 |
| 1:A:37:GLY:HA3 | 1:A:63:SER:OG | 0.40 | 2.16 | 19 | 1 |
| 1:A:86:ALA:HB1 | 1:A:89:ASP:CG | 0.40 | 2.36 | 22 | 1 |
| 1:A:26:LYS:O | 1:A:30:TYR:HB2 | 0.40 | 2.16 | 8 | 1 |
| 1:A:44:VAL:O | 1:A:50:MET:HG2 | 0.40 | 2.15 | 21 | 1 |
| 1:A:71:MET:O | 1:A:74:PHE:HB2 | 0.40 | 2.16 | 14 | 1 |
| 1:A:31:ALA:C | 1:A:32:ILE:HG12 | 0.40 | 2.37 | 29 | 1 |
| 1:A:35:GLN:O | 1:A:36:PHE:C | 0.40 | 2.57 | 20 | 1 |
| 1:A:68:LEU:CD2 | 1:A:83:ILE:HB | 0.40 | 2.45 | 35 | 1 |
| 1:A:107:ARG:O | 1:A:107:ARG:HD3 | 0.40 | 2.16 | 19 | 1 |
| 1:A:74:PHE:CG | 1:A:75:PRO:CD | 0.40 | 3.04 | 19 | 1 |
| 1:A:69:ARG:HD3 | 1:A:69:ARG:O | 0.40 | 2.17 | 22 | 1 |
| 1:A:25:LEU:HD12 | 1:A:29:LEU:HD11 | 0.40 | 1.94 | 8 | 1 |
| 1:A:86:ALA:C | 1:A:88:THR:N | 0.40 | 2.75 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:107:ARG:CG | 1:A:107:ARG:O | 0.40 | 2.70 | 41 | 1 |
| 1:A:43:LEU:CD2 | 1:A:57:ILE:HG12 | 0.40 | 2.46 | 20 | 1 |
| 1:A:28:SER:O | 1:A:32:ILE:HG23 | 0.40 | 2.16 | 4 | 1 |
| 1:A:31:ALA:C | 1:A:32:ILE:HG23 | 0.40 | 2.37 | 34 | 1 |
| 1:A:38:GLN:HE21 | 1:A:40:LEU:HD11 | 0.40 | 1.75 | 33 | 1 |
| 1:A:50:MET:HB3 | 1:A:50:MET:HE2 | 0.40 | 1.68 | 18 | 1 |
| 1:A:39:ILE:C | 1:A:40:LEU:HG | 0.40 | 2.37 | 10 | 1 |
| 1:A:40:LEU:HG | 1:A:57:ILE:O | 0.40 | 2.17 | 20 | 1 |
| 1:A:14:ASN:CG | 1:A:53:GLN:CG | 0.40 | 2.90 | 35 | 1 |
| 1:A:113:LYS:O | 1:A:113:LYS:HG2 | 0.40 | 2.16 | 7 | 1 |
| 1:A:48:LEU:C | 1:A:50:MET:H | 0.40 | 2.20 | 7 | 1 |
| 1:A:13:ILE:O | 1:A:53:GLN:HB3 | 0.40 | 2.16 | 7 | 1 |
| 1:A:51:ARG:C | 1:A:53:GLN:N | 0.40 | 2.74 | 6 | 1 |
| 1:A:13:ILE:HG21 | 1:A:16:LEU:HG | 0.40 | 1.94 | 25 | 1 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD23 | 0.40 | 1.92 | 26 | 1 |
| 1:A:50:MET:CE | 1:A:53:GLN:HB3 | 0.40 | 2.46 | 30 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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 | 98/116 (84%) | 68±4 (69±4%) | 20±3 (20±3%) | 11±2 (11±2%) | 1 | 9 |
| All | All | 4214/4988 (84%) | 2905 (69%) | 855 (20%) | 454 (11%) | 1 | 9 |

All 39 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 | 41 | ASP | 42 |
| 1 | A | 37 | GLY | 42 |
| 1 | A | 38 | GLN | 40 |
| 1 | A | 22 | LYS | 36 |
| 1 | A | 72 | GLN | 32 |
| 1 | A | 88 | THR | 21 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 85 | TYR | 19 |
| 1 | A | 112 | PRO | 18 |
| 1 | A | 17 | ASN | 18 |
| 1 | A | 32 | ILE | 18 |
| 1 | A | 15 | ASN | 16 |
| 1 | A | 6 | ARG | 14 |
| 1 | A | 106 | LYS | 12 |
| 1 | A | 51 | ARG | 11 |
| 1 | A | 53 | GLN | 11 |
| 1 | A | 81 | MET | 9 |
| 1 | A | 52 | GLY | 9 |
| 1 | A | 113 | LYS | 8 |
| 1 | A | 109 | LYS | 7 |
| 1 | A | 105 | ARG | 6 |
| 1 | A | 47 | SER | 6 |
| 1 | A | 82 | ARG | 6 |
| 1 | A | 46 | ARG | 5 |
| 1 | A | 74 | PHE | 5 |
| 1 | A | 45 | SER | 4 |
| 1 | A | 79 | LYS | 4 |
| 1 | A | 44 | VAL | 4 |
| 1 | A | 48 | LEU | 4 |
| 1 | A | 23 | ASP | 4 |
| 1 | A | 110 | ARG | 3 |
| 1 | A | 34 | SER | 3 |
| 1 | A | 16 | LEU | 3 |
| 1 | A | 78 | ASP | 3 |
| 1 | A | 107 | ARG | 3 |
| 1 | A | 84 | GLN | 2 |
| 1 | A | 70 | SER | 2 |
| 1 | A | 108 | GLU | 2 |
| 1 | A | 18 | GLU | 1 |
| 1 | A | 20 | ILE | 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 | 89/105 (85%) | 57±4 (64±4%) | 32±4 (36±4%) | 1 | 9 |
| All | All | 3827/4515 (85%) | 2459 (64%) | 1368 (36%) | 1 | 9 |

All 73 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 | 68 | LEU | 43 |
| 1 | A | 30 | TYR | 43 |
| 1 | A | 41 | ASP | 40 |
| 1 | A | 84 | GLN | 38 |
| 1 | A | 40 | LEU | 37 |
| 1 | A | 29 | LEU | 36 |
| 1 | A | 43 | LEU | 34 |
| 1 | A | 35 | GLN | 34 |
| 1 | A | 92 | ILE | 31 |
| 1 | A | 111 | LYS | 30 |
| 1 | A | 93 | ILE | 29 |
| 1 | A | 72 | GLN | 29 |
| 1 | A | 87 | LYS | 28 |
| 1 | A | 25 | LEU | 28 |
| 1 | A | 45 | SER | 26 |
| 1 | A | 46 | ARG | 26 |
| 1 | A | 6 | ARG | 26 |
| 1 | A | 38 | GLN | 25 |
| 1 | A | 107 | ARG | 25 |
| 1 | A | 113 | LYS | 24 |
| 1 | A | 89 | ASP | 24 |
| 1 | A | 69 | ARG | 24 |
| 1 | A | 81 | MET | 24 |
| 1 | A | 109 | LYS | 23 |
| 1 | A | 74 | PHE | 23 |
| 1 | A | 90 | SER | 23 |
| 1 | A | 51 | ARG | 22 |
| 1 | A | 82 | ARG | 22 |
| 1 | A | 22 | LYS | 21 |
| 1 | A | 50 | MET | 21 |
| 1 | A | 106 | LYS | 21 |
| 1 | A | 55 | PHE | 21 |
| 1 | A | 62 | SER | 21 |
| 1 | A | 105 | ARG | 20 |
| 1 | A | 60 | GLU | 20 |
| 1 | A | 23 | ASP | 20 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 21 | LYS | 19 |
| 1 | A | 47 | SER | 19 |
| 1 | A | 48 | LEU | 18 |
| 1 | A | 78 | ASP | 17 |
| 1 | A | 9 | HIS | 17 |
| 1 | A | 110 | ARG | 16 |
| 1 | A | 79 | LYS | 16 |
| 1 | A | 71 | MET | 16 |
| 1 | A | 27 | LYS | 16 |
| 1 | A | 32 | ILE | 16 |
| 1 | A | 49 | LYS | 15 |
| 1 | A | 59 | LYS | 15 |
| 1 | A | 26 | LYS | 15 |
| 1 | A | 20 | ILE | 15 |
| 1 | A | 24 | GLU | 13 |
| 1 | A | 17 | ASN | 13 |
| 1 | A | 19 | LYS | 12 |
| 1 | A | 15 | ASN | 11 |
| 1 | A | 91 | ASP | 11 |
| 1 | A | 42 | ILE | 10 |
| 1 | A | 108 | GLU | 10 |
| 1 | A | 28 | SER | 10 |
| 1 | A | 12 | TYR | 9 |
| 1 | A | 34 | SER | 9 |
| 1 | A | 18 | GLU | 7 |
| 1 | A | 70 | SER | 6 |
| 1 | A | 44 | VAL | 5 |
| 1 | A | 33 | PHE | 5 |
| 1 | A | 16 | LEU | 5 |
| 1 | A | 66 | ASN | 4 |
| 1 | A | 53 | GLN | 4 |
| 1 | A | 83 | ILE | 3 |
| 1 | A | 13 | ILE | 3 |
| 1 | A | 14 | ASN | 3 |
| 1 | A | 76 | PHE | 1 |
| 1 | A | 11 | 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 [i](#)

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