



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2022 – 10:36 PM EST

PDB ID : 1ILO  
Title : NMR structure of a thioredoxin, MtH895, from the archeon Methanobacterium thermoautotrophicum strain delta H.  
Authors : Bhattacharyya, S.; Habibi-Nazhad, B.; Slupsky, C.M.; Sykes, B.D.; Wishart, D.S.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2001-05-08

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.26  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

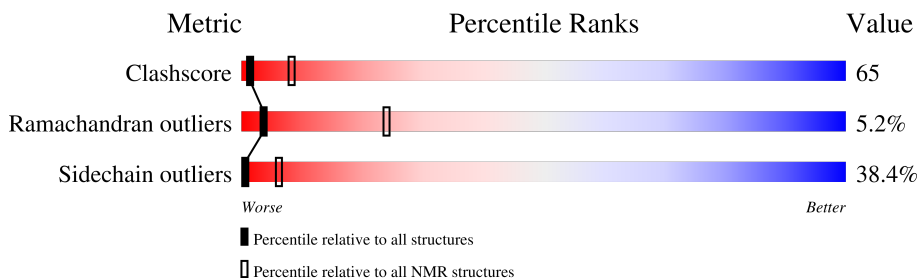
# 1 Overall quality at a glance

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            | 158937                   | 12864                  |
| Ramachandran outliers | 154571                   | 11451                  |
| Sidechain outliers    | 154315                   | 11428                  |

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  $\geq 3$ , 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     | 77     |                  |

## 2 Ensemble composition and analysis

This entry contains 21 models. Model 21 is the overall representative, medoid model (most similar to other models). The authors have identified model 14 as representative, based on the following criterion: *closest to the average*.

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:1-A:73 (73)         | 0.28              | 21           |

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 2 clusters. No single-model clusters were found.

| Cluster number | Models                                                             |
|----------------|--------------------------------------------------------------------|
| 1              | 1, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21 |
| 2              | 2, 10                                                              |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1207 atoms, of which 621 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called conserved hypothetical protein MtH895.

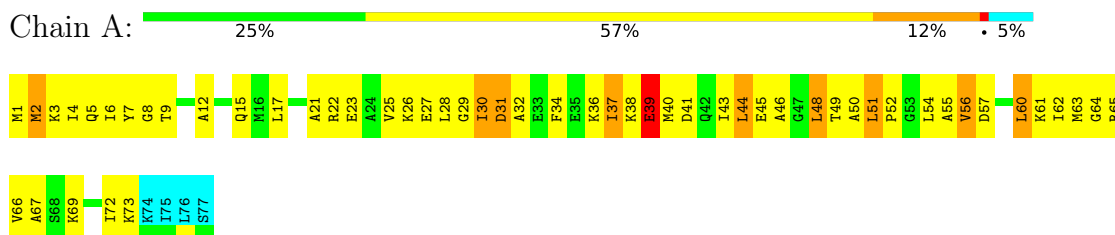
| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
|     |       |          | Total | C   | H   | N  | O   | S |       |
| 1   | A     | 77       | 1207  | 368 | 621 | 97 | 114 | 7 | 0     |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: conserved hypothetical protein MtH895

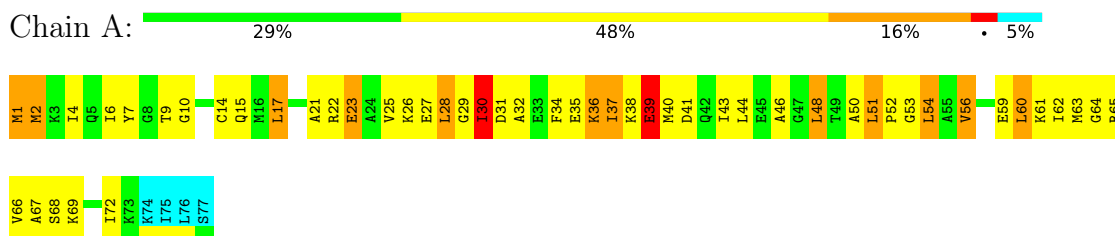


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

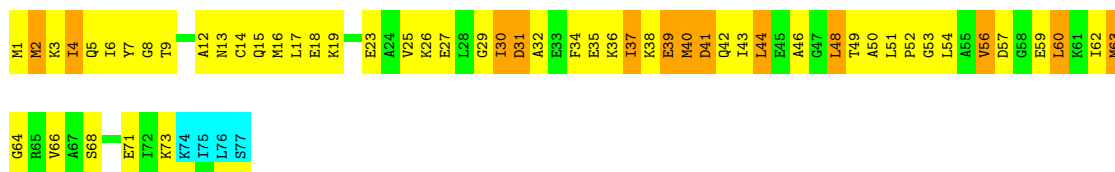
- Molecule 1: conserved hypothetical protein MtH895



#### 4.2.2 Score per residue for model 2

- Molecule 1: conserved hypothetical protein MtH895

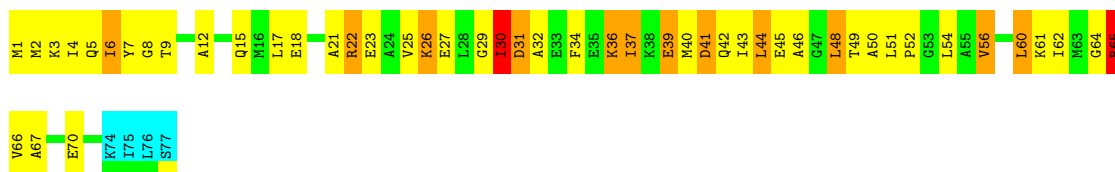




### 4.2.3 Score per residue for model 3

- Molecule 1: conserved hypothetical protein MtH895

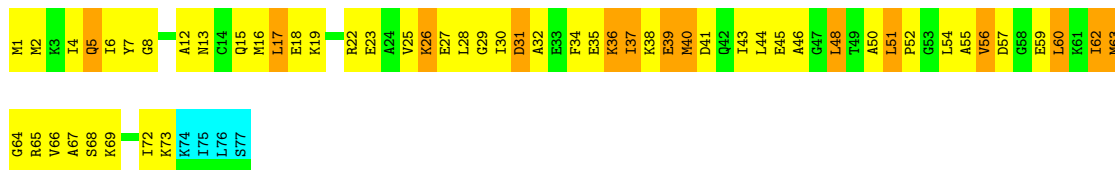
Chain A: 31% 45% 16% 5%



### 4.2.4 Score per residue for model 4

- Molecule 1: conserved hypothetical protein MtH895

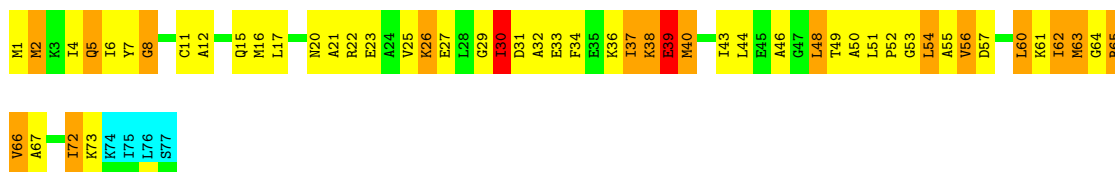
Chain A: 22% 55% 18% 5%



### 4.2.5 Score per residue for model 5

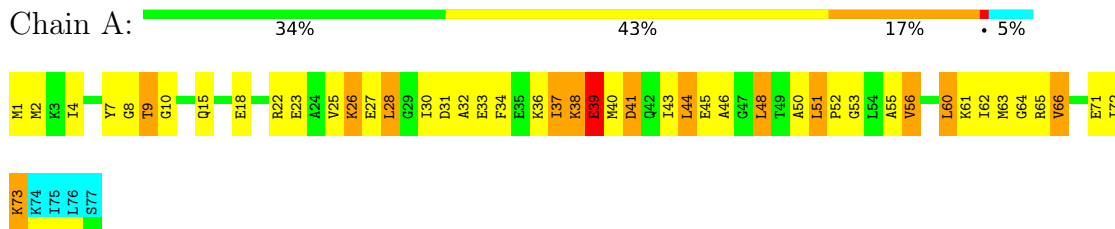
- Molecule 1: conserved hypothetical protein MtH895

Chain A: 26% 45% 21% 5%



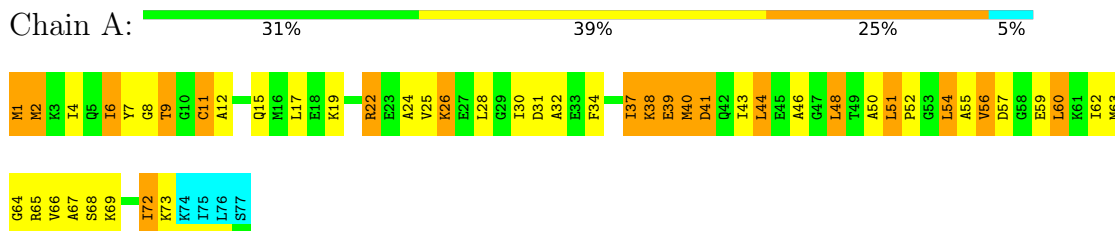
### 4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein MtH895



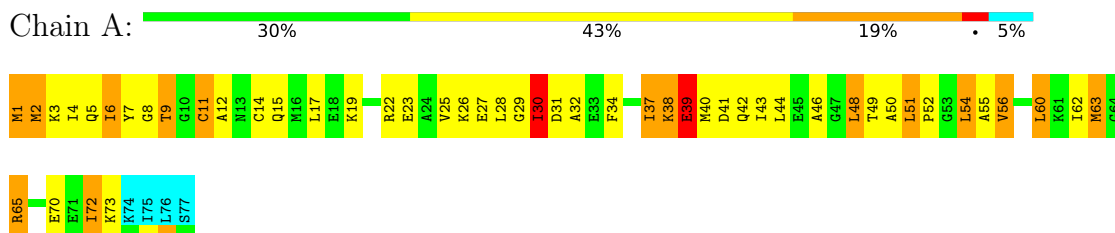
#### 4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein MtH895



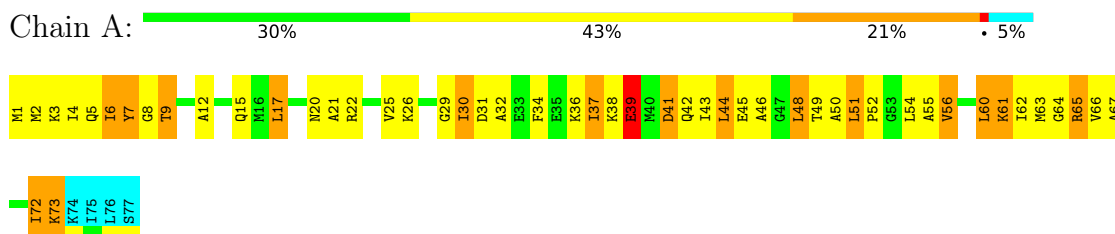
#### 4.2.8 Score per residue for model 8

- Molecule 1: conserved hypothetical protein MtH895



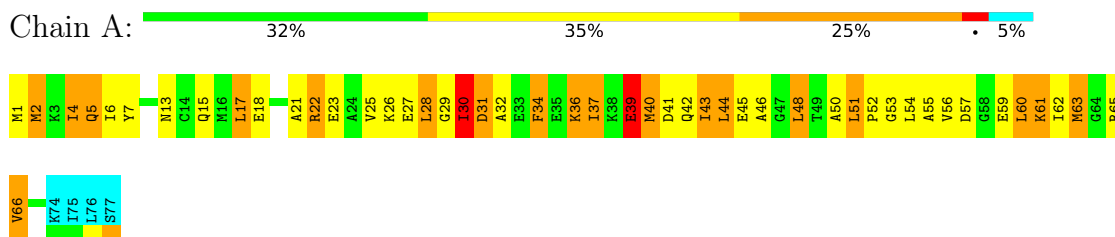
#### 4.2.9 Score per residue for model 9

- Molecule 1: conserved hypothetical protein MtH895



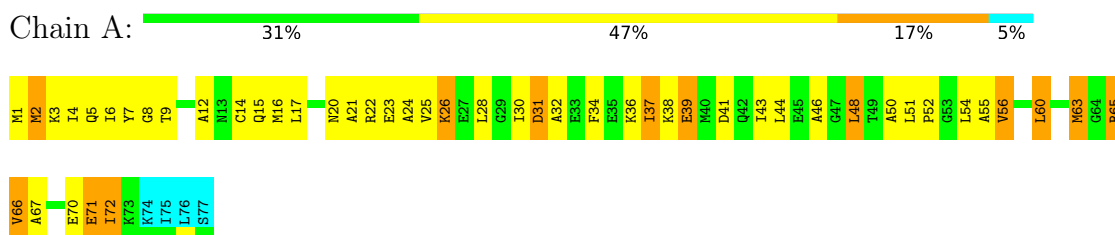
#### 4.2.10 Score per residue for model 10

- Molecule 1: conserved hypothetical protein MtH895



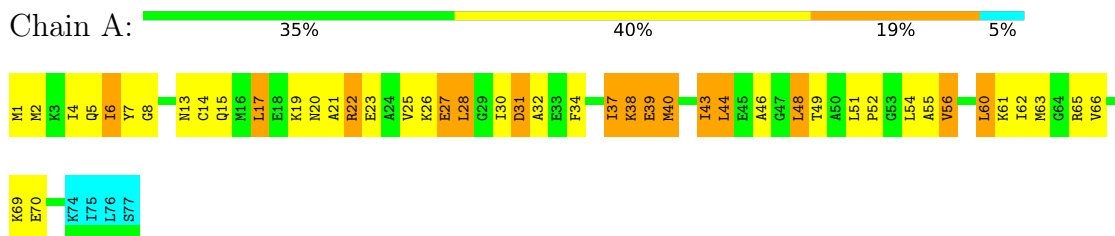
#### 4.2.11 Score per residue for model 11

- Molecule 1: conserved hypothetical protein MtH895



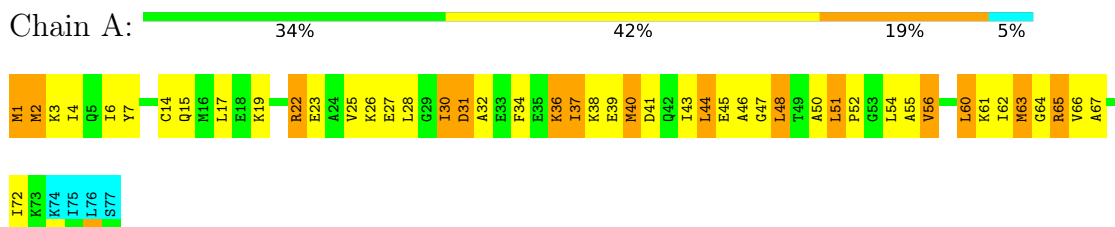
#### 4.2.12 Score per residue for model 12

- Molecule 1: conserved hypothetical protein MtH895



#### 4.2.13 Score per residue for model 13

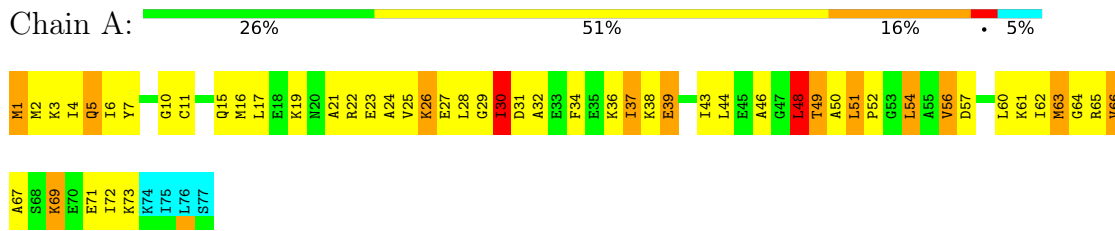
- Molecule 1: conserved hypothetical protein MtH895





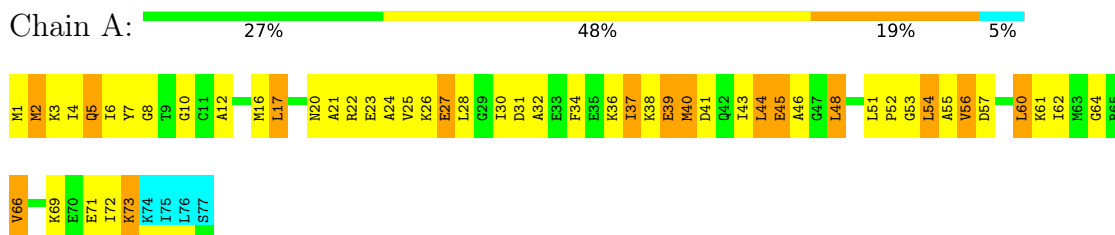
#### 4.2.14 Score per residue for model 14

- Molecule 1: conserved hypothetical protein MtH895



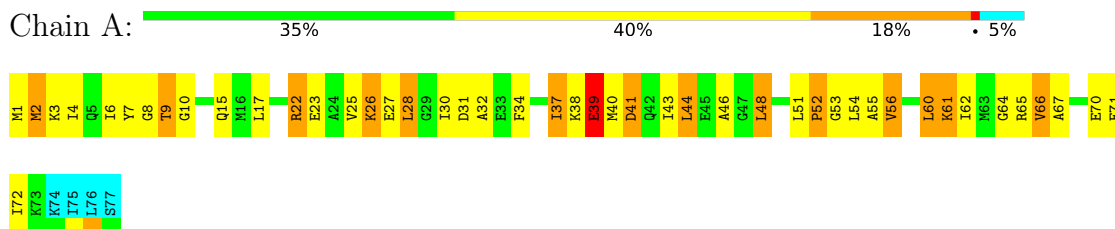
#### 4.2.15 Score per residue for model 15

- Molecule 1: conserved hypothetical protein MtH895



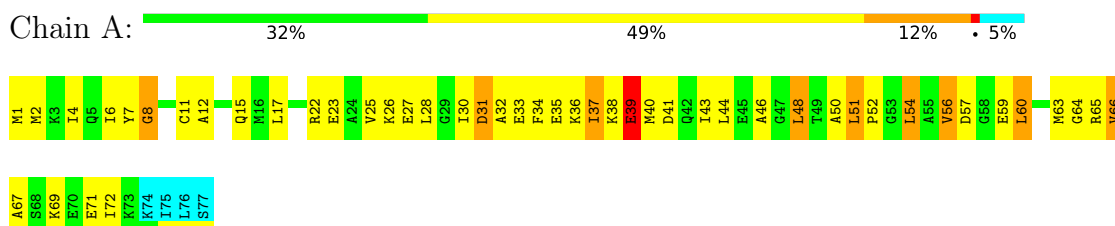
#### 4.2.16 Score per residue for model 16

- Molecule 1: conserved hypothetical protein MtH895



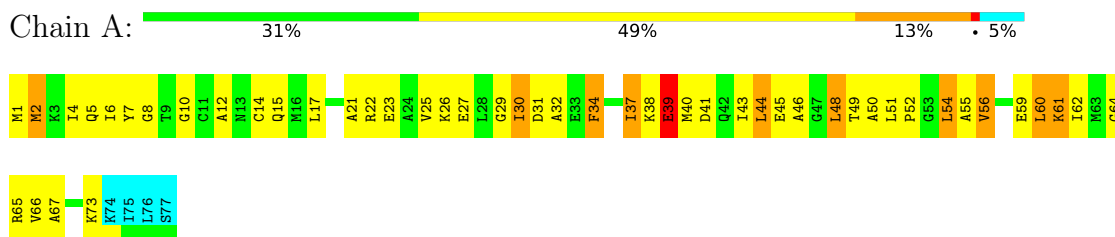
#### 4.2.17 Score per residue for model 17

- Molecule 1: conserved hypothetical protein MtH895



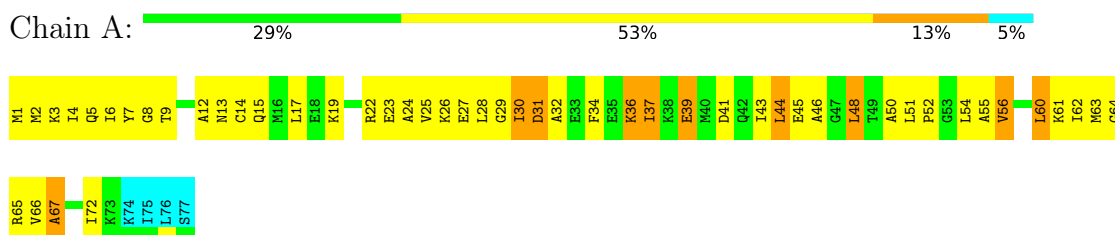
#### 4.2.18 Score per residue for model 18

- Molecule 1: conserved hypothetical protein MtH895



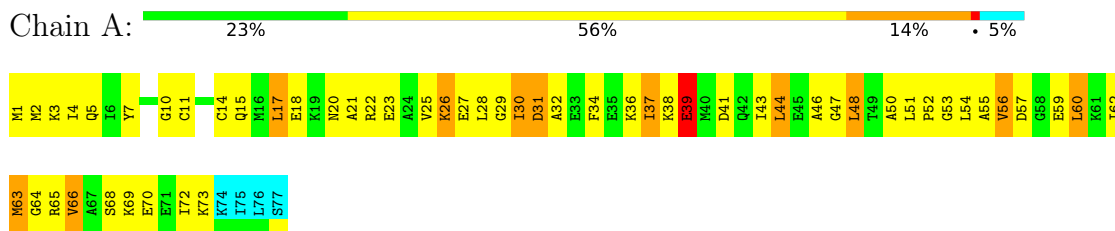
#### 4.2.19 Score per residue for model 19

- Molecule 1: conserved hypothetical protein MtH895



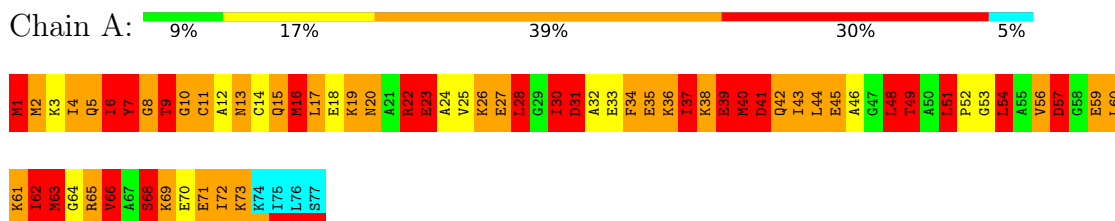
#### 4.2.20 Score per residue for model 20

- Molecule 1: conserved hypothetical protein MtH895



#### 4.2.21 Score per residue for model 21 (medoid)

- Molecule 1: conserved hypothetical protein MtH895



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing molecular dynamics*.

Of the 50 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | structure solution | 3.851   |
| X-PLOR        | refinement         | 3.851   |

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                       | Bond angles |                       |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                  | RMSZ        | #Z>5                  |
| 1   | A     | 1.36±4.35    | 8±37/557 ( 1.5± 6.7%) | 1.22±3.43   | 9±38/742 ( 1.2± 5.1%) |
| All | All   | 4.56         | 177/11697 ( 1.5%)     | 3.64        | 183/15582 ( 1.2%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.1±0.6   | 0.0±0.0   |
| All | All   | 3         | 0         |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|--------|-------------|----------|--------|-------|
|     |       |     |      |        |        |             |          | Worst  | Total |
| 1   | A     | 45  | GLU  | CD-OE1 | -94.08 | 0.22        | 1.25     | 21     | 1     |
| 1   | A     | 39  | GLU  | CD-OE1 | -88.04 | 0.28        | 1.25     | 21     | 1     |
| 1   | A     | 65  | ARG  | CZ-NH1 | -87.68 | 0.19        | 1.33     | 21     | 1     |
| 1   | A     | 22  | ARG  | CZ-NH1 | -86.24 | 0.20        | 1.33     | 21     | 1     |
| 1   | A     | 33  | GLU  | CD-OE1 | -84.25 | 0.33        | 1.25     | 21     | 1     |
| 1   | A     | 71  | GLU  | CD-OE2 | -82.80 | 0.34        | 1.25     | 21     | 1     |
| 1   | A     | 35  | GLU  | CD-OE2 | -82.53 | 0.34        | 1.25     | 21     | 1     |
| 1   | A     | 27  | GLU  | CD-OE2 | -81.12 | 0.36        | 1.25     | 21     | 1     |
| 1   | A     | 59  | GLU  | CD-OE2 | -80.00 | 0.37        | 1.25     | 21     | 1     |
| 1   | A     | 59  | GLU  | CD-OE1 | -79.48 | 0.38        | 1.25     | 21     | 1     |
| 1   | A     | 23  | GLU  | CD-OE1 | -77.03 | 0.41        | 1.25     | 21     | 1     |
| 1   | A     | 70  | GLU  | CD-OE2 | -76.09 | 0.41        | 1.25     | 21     | 1     |
| 1   | A     | 71  | GLU  | CD-OE1 | -75.72 | 0.42        | 1.25     | 21     | 1     |
| 1   | A     | 70  | GLU  | CD-OE1 | -74.22 | 0.44        | 1.25     | 21     | 1     |
| 1   | A     | 18  | GLU  | CD-OE2 | -72.14 | 0.46        | 1.25     | 21     | 1     |
| 1   | A     | 35  | GLU  | CD-OE1 | -70.83 | 0.47        | 1.25     | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
|     |       |     |      |         |        |             |          | Worst  | Total |
| 1   | A     | 27  | GLU  | CD-OE1  | -69.67 | 0.49        | 1.25     | 21     | 1     |
| 1   | A     | 23  | GLU  | CD-OE2  | -69.52 | 0.49        | 1.25     | 21     | 1     |
| 1   | A     | 18  | GLU  | CD-OE1  | -69.07 | 0.49        | 1.25     | 21     | 1     |
| 1   | A     | 33  | GLU  | CD-OE2  | -65.97 | 0.53        | 1.25     | 21     | 1     |
| 1   | A     | 45  | GLU  | CD-OE2  | -63.10 | 0.56        | 1.25     | 21     | 1     |
| 1   | A     | 39  | GLU  | CD-OE2  | -62.05 | 0.57        | 1.25     | 21     | 1     |
| 1   | A     | 7   | TYR  | CE2-CZ  | 58.13  | 2.14        | 1.38     | 9      | 2     |
| 1   | A     | 65  | ARG  | NE-CZ   | -57.56 | 0.58        | 1.33     | 21     | 1     |
| 1   | A     | 68  | SER  | CB-OG   | -57.18 | 0.68        | 1.42     | 21     | 1     |
| 1   | A     | 7   | TYR  | CE1-CZ  | -52.82 | 0.69        | 1.38     | 21     | 1     |
| 1   | A     | 7   | TYR  | CG-CD2  | -50.82 | 0.73        | 1.39     | 21     | 1     |
| 1   | A     | 7   | TYR  | CG-CD1  | -50.05 | 0.74        | 1.39     | 21     | 1     |
| 1   | A     | 7   | TYR  | CD2-CE2 | 49.83  | 2.14        | 1.39     | 9      | 1     |
| 1   | A     | 65  | ARG  | CZ-NH2  | -49.22 | 0.69        | 1.33     | 21     | 1     |
| 1   | A     | 22  | ARG  | CZ-NH2  | -46.06 | 0.73        | 1.33     | 21     | 1     |
| 1   | A     | 45  | GLU  | CG-CD   | -44.93 | 0.84        | 1.51     | 21     | 1     |
| 1   | A     | 34  | PHE  | CG-CD2  | -42.83 | 0.74        | 1.38     | 21     | 1     |
| 1   | A     | 38  | LYS  | CE-NZ   | -42.50 | 0.42        | 1.49     | 21     | 1     |
| 1   | A     | 49  | THR  | CB-OG1  | -41.78 | 0.59        | 1.43     | 21     | 1     |
| 1   | A     | 35  | GLU  | CG-CD   | -41.65 | 0.89        | 1.51     | 21     | 1     |
| 1   | A     | 34  | PHE  | CG-CD1  | -41.60 | 0.76        | 1.38     | 21     | 1     |
| 1   | A     | 65  | ARG  | CD-NE   | -40.48 | 0.77        | 1.46     | 21     | 1     |
| 1   | A     | 42  | GLN  | CD-OE1  | -39.85 | 0.36        | 1.24     | 21     | 1     |
| 1   | A     | 11  | CYS  | CB-SG   | -39.76 | 1.14        | 1.82     | 21     | 1     |
| 1   | A     | 59  | GLU  | CG-CD   | -39.30 | 0.93        | 1.51     | 21     | 1     |
| 1   | A     | 9   | THR  | C-O     | -39.24 | 0.48        | 1.23     | 21     | 1     |
| 1   | A     | 27  | GLU  | CG-CD   | -38.22 | 0.94        | 1.51     | 21     | 1     |
| 1   | A     | 33  | GLU  | CG-CD   | -37.78 | 0.95        | 1.51     | 21     | 1     |
| 1   | A     | 22  | ARG  | NE-CZ   | -37.17 | 0.84        | 1.33     | 21     | 1     |
| 1   | A     | 71  | GLU  | CG-CD   | -36.80 | 0.96        | 1.51     | 21     | 1     |
| 1   | A     | 22  | ARG  | CD-NE   | -36.51 | 0.84        | 1.46     | 21     | 1     |
| 1   | A     | 39  | GLU  | CG-CD   | -36.40 | 0.97        | 1.51     | 21     | 1     |
| 1   | A     | 31  | ASP  | CG-OD1  | -34.39 | 0.46        | 1.25     | 21     | 1     |
| 1   | A     | 34  | PHE  | CE1-CZ  | -33.78 | 0.73        | 1.37     | 21     | 1     |
| 1   | A     | 34  | PHE  | CE2-CZ  | -32.91 | 0.74        | 1.37     | 21     | 1     |
| 1   | A     | 57  | ASP  | CG-OD1  | -32.78 | 0.49        | 1.25     | 21     | 1     |
| 1   | A     | 41  | ASP  | CG-OD2  | -32.50 | 0.50        | 1.25     | 21     | 1     |
| 1   | A     | 2   | MET  | CG-SD   | -32.10 | 0.97        | 1.81     | 21     | 1     |
| 1   | A     | 66  | VAL  | CB-CG2  | -31.86 | 0.85        | 1.52     | 21     | 1     |
| 1   | A     | 61  | LYS  | CE-NZ   | -31.44 | 0.70        | 1.49     | 21     | 1     |
| 1   | A     | 13  | ASN  | CG-OD1  | -30.91 | 0.56        | 1.24     | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|--------|-------------|----------|--------|-------|
|     |       |     |      |        |        |             |          | Worst  | Total |
| 1   | A     | 70  | GLU  | CG-CD  | -30.75 | 1.05        | 1.51     | 21     | 1     |
| 1   | A     | 57  | ASP  | CG-OD2 | -30.37 | 0.55        | 1.25     | 21     | 1     |
| 1   | A     | 31  | ASP  | CG-OD2 | -30.32 | 0.55        | 1.25     | 21     | 1     |
| 1   | A     | 26  | LYS  | CE-NZ  | -30.05 | 0.73        | 1.49     | 21     | 1     |
| 1   | A     | 23  | GLU  | CB-CG  | -29.79 | 0.95        | 1.52     | 21     | 1     |
| 1   | A     | 54  | LEU  | CG-CD2 | -29.69 | 0.42        | 1.51     | 21     | 1     |
| 1   | A     | 9   | THR  | CB-OG1 | -29.66 | 0.83        | 1.43     | 21     | 1     |
| 1   | A     | 38  | LYS  | CD-CE  | -29.60 | 0.77        | 1.51     | 21     | 1     |
| 1   | A     | 66  | VAL  | CB-CG1 | -29.58 | 0.90        | 1.52     | 21     | 1     |
| 1   | A     | 26  | LYS  | CD-CE  | -29.33 | 0.78        | 1.51     | 21     | 1     |
| 1   | A     | 69  | LYS  | CB-CG  | -29.05 | 0.74        | 1.52     | 21     | 1     |
| 1   | A     | 35  | GLU  | CB-CG  | -29.00 | 0.97        | 1.52     | 21     | 1     |
| 1   | A     | 17  | LEU  | CG-CD2 | -28.93 | 0.44        | 1.51     | 21     | 1     |
| 1   | A     | 9   | THR  | C-N    | -28.81 | 0.81        | 1.33     | 21     | 1     |
| 1   | A     | 69  | LYS  | CE-NZ  | -28.11 | 0.78        | 1.49     | 21     | 1     |
| 1   | A     | 70  | GLU  | CB-CG  | -28.05 | 0.98        | 1.52     | 21     | 1     |
| 1   | A     | 40  | MET  | CB-CG  | -28.01 | 0.61        | 1.51     | 21     | 1     |
| 1   | A     | 42  | GLN  | CG-CD  | -27.91 | 0.86        | 1.51     | 21     | 1     |
| 1   | A     | 73  | LYS  | CE-NZ  | -27.84 | 0.79        | 1.49     | 21     | 1     |
| 1   | A     | 5   | GLN  | CD-OE1 | -27.66 | 0.63        | 1.24     | 21     | 1     |
| 1   | A     | 16  | MET  | CG-SD  | -27.52 | 1.09        | 1.81     | 21     | 1     |
| 1   | A     | 23  | GLU  | CG-CD  | -27.41 | 1.10        | 1.51     | 21     | 1     |
| 1   | A     | 36  | LYS  | CD-CE  | -27.11 | 0.83        | 1.51     | 21     | 1     |
| 1   | A     | 42  | GLN  | CD-NE2 | -27.03 | 0.65        | 1.32     | 21     | 1     |
| 1   | A     | 20  | ASN  | CG-OD1 | -26.70 | 0.65        | 1.24     | 21     | 1     |
| 1   | A     | 41  | ASP  | CG-OD1 | -26.55 | 0.64        | 1.25     | 21     | 1     |
| 1   | A     | 19  | LYS  | CD-CE  | -26.46 | 0.85        | 1.51     | 21     | 1     |
| 1   | A     | 69  | LYS  | CD-CE  | -26.35 | 0.85        | 1.51     | 21     | 1     |
| 1   | A     | 73  | LYS  | CD-CE  | -25.88 | 0.86        | 1.51     | 21     | 1     |
| 1   | A     | 18  | GLU  | CG-CD  | -25.76 | 1.13        | 1.51     | 21     | 1     |
| 1   | A     | 30  | ILE  | CB-CG1 | -25.14 | 0.83        | 1.54     | 21     | 1     |
| 1   | A     | 63  | MET  | CG-SD  | -24.98 | 1.16        | 1.81     | 21     | 1     |
| 1   | A     | 49  | THR  | CB-CG2 | -24.83 | 0.70        | 1.52     | 21     | 1     |
| 1   | A     | 13  | ASN  | CG-ND2 | -24.68 | 0.71        | 1.32     | 21     | 1     |
| 1   | A     | 60  | LEU  | CG-CD1 | -24.68 | 0.60        | 1.51     | 21     | 1     |
| 1   | A     | 1   | MET  | CG-SD  | -24.07 | 1.18        | 1.81     | 21     | 1     |
| 1   | A     | 19  | LYS  | CE-NZ  | -23.73 | 0.89        | 1.49     | 21     | 1     |
| 1   | A     | 65  | ARG  | CG-CD  | -23.36 | 0.93        | 1.51     | 21     | 1     |
| 1   | A     | 17  | LEU  | CG-CD1 | -22.72 | 0.67        | 1.51     | 21     | 1     |
| 1   | A     | 28  | LEU  | CG-CD2 | -22.34 | 0.69        | 1.51     | 21     | 1     |
| 1   | A     | 54  | LEU  | CG-CD1 | -22.30 | 0.69        | 1.51     | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
|     |       |     |      |         |        |             |          | Worst  | Total |
| 1   | A     | 61  | LYS  | CD-CE   | -21.78 | 0.96        | 1.51     | 21     | 1     |
| 1   | A     | 1   | MET  | CB-CG   | -21.78 | 0.81        | 1.51     | 21     | 1     |
| 1   | A     | 39  | GLU  | CB-CG   | -21.76 | 1.10        | 1.52     | 21     | 1     |
| 1   | A     | 36  | LYS  | CE-NZ   | -21.65 | 0.94        | 1.49     | 21     | 1     |
| 1   | A     | 30  | ILE  | CB-CG2  | -21.55 | 0.86        | 1.52     | 21     | 1     |
| 1   | A     | 3   | LYS  | CE-NZ   | -21.28 | 0.95        | 1.49     | 21     | 1     |
| 1   | A     | 40  | MET  | CG-SD   | -20.63 | 1.27        | 1.81     | 21     | 1     |
| 1   | A     | 62  | ILE  | CB-CG1  | -19.84 | 0.98        | 1.54     | 21     | 1     |
| 1   | A     | 3   | LYS  | CB-CG   | -19.56 | 0.99        | 1.52     | 21     | 1     |
| 1   | A     | 10  | GLY  | C-O     | -19.09 | 0.93        | 1.23     | 21     | 1     |
| 1   | A     | 5   | GLN  | CG-CD   | -19.05 | 1.07        | 1.51     | 21     | 1     |
| 1   | A     | 63  | MET  | CB-CG   | -18.64 | 0.91        | 1.51     | 21     | 1     |
| 1   | A     | 65  | ARG  | CB-CG   | -18.15 | 1.03        | 1.52     | 21     | 1     |
| 1   | A     | 62  | ILE  | CB-CG2  | -18.09 | 0.96        | 1.52     | 21     | 1     |
| 1   | A     | 3   | LYS  | CD-CE   | -17.80 | 1.06        | 1.51     | 21     | 1     |
| 1   | A     | 59  | GLU  | CB-CG   | -17.76 | 1.18        | 1.52     | 21     | 1     |
| 1   | A     | 72  | ILE  | CB-CG1  | -17.76 | 1.04        | 1.54     | 21     | 1     |
| 1   | A     | 16  | MET  | SD-CE   | -17.72 | 0.78        | 1.77     | 21     | 1     |
| 1   | A     | 1   | MET  | SD-CE   | -17.55 | 0.79        | 1.77     | 21     | 1     |
| 1   | A     | 48  | LEU  | C-O     | -17.52 | 0.90        | 1.23     | 21     | 1     |
| 1   | A     | 40  | MET  | SD-CE   | -17.42 | 0.80        | 1.77     | 21     | 1     |
| 1   | A     | 9   | THR  | CB-CG2  | -17.29 | 0.95        | 1.52     | 21     | 1     |
| 1   | A     | 51  | LEU  | CG-CD1  | -17.11 | 0.88        | 1.51     | 21     | 1     |
| 1   | A     | 60  | LEU  | CG-CD2  | -16.73 | 0.90        | 1.51     | 21     | 1     |
| 1   | A     | 28  | LEU  | CG-CD1  | -16.43 | 0.91        | 1.51     | 21     | 1     |
| 1   | A     | 33  | GLU  | CB-CG   | -16.30 | 1.21        | 1.52     | 21     | 1     |
| 1   | A     | 51  | LEU  | CG-CD2  | -15.94 | 0.92        | 1.51     | 21     | 1     |
| 1   | A     | 6   | ILE  | CB-CG1  | -15.85 | 1.09        | 1.54     | 21     | 1     |
| 1   | A     | 72  | ILE  | CB-CG2  | -15.76 | 1.03        | 1.52     | 21     | 1     |
| 1   | A     | 6   | ILE  | CB-CG2  | -14.79 | 1.07        | 1.52     | 21     | 1     |
| 1   | A     | 38  | LYS  | CG-CD   | -14.63 | 1.02        | 1.52     | 21     | 1     |
| 1   | A     | 62  | ILE  | CG1-CD1 | -14.59 | 0.49        | 1.50     | 21     | 1     |
| 1   | A     | 38  | LYS  | CB-CG   | -14.22 | 1.14        | 1.52     | 21     | 1     |
| 1   | A     | 63  | MET  | SD-CE   | -14.20 | 0.98        | 1.77     | 21     | 1     |
| 1   | A     | 61  | LYS  | CG-CD   | -14.12 | 1.04        | 1.52     | 21     | 1     |
| 1   | A     | 37  | ILE  | CB-CG1  | -13.94 | 1.15        | 1.54     | 21     | 1     |
| 1   | A     | 20  | ASN  | CB-CG   | -13.79 | 1.19        | 1.51     | 21     | 1     |
| 1   | A     | 31  | ASP  | CB-CG   | -13.55 | 1.23        | 1.51     | 21     | 1     |
| 1   | A     | 43  | ILE  | CB-CG1  | -13.41 | 1.16        | 1.54     | 21     | 1     |
| 1   | A     | 61  | LYS  | CB-CG   | -12.92 | 1.17        | 1.52     | 21     | 1     |
| 1   | A     | 37  | ILE  | C-O     | -12.84 | 0.98        | 1.23     | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
|     |       |     |      |         |        |             |          | Worst  | Total |
| 1   | A     | 15  | GLN  | CD-OE1  | -12.68 | 0.96        | 1.24     | 21     | 1     |
| 1   | A     | 2   | MET  | SD-CE   | -12.49 | 1.07        | 1.77     | 21     | 1     |
| 1   | A     | 36  | LYS  | CB-CG   | -12.26 | 1.19        | 1.52     | 21     | 1     |
| 1   | A     | 72  | ILE  | CG1-CD1 | -11.90 | 0.68        | 1.50     | 21     | 1     |
| 1   | A     | 13  | ASN  | CB-CG   | -11.86 | 1.23        | 1.51     | 21     | 1     |
| 1   | A     | 43  | ILE  | CB-CG2  | -11.81 | 1.16        | 1.52     | 21     | 1     |
| 1   | A     | 73  | LYS  | CG-CD   | -11.74 | 1.12        | 1.52     | 21     | 1     |
| 1   | A     | 60  | LEU  | CB-CG   | -11.69 | 1.18        | 1.52     | 21     | 1     |
| 1   | A     | 10  | GLY  | C-N     | -11.20 | 1.08        | 1.34     | 21     | 1     |
| 1   | A     | 3   | LYS  | CG-CD   | -11.12 | 1.14        | 1.52     | 21     | 1     |
| 1   | A     | 57  | ASP  | CB-CG   | -10.82 | 1.29        | 1.51     | 21     | 1     |
| 1   | A     | 19  | LYS  | CG-CD   | -10.75 | 1.15        | 1.52     | 21     | 1     |
| 1   | A     | 71  | GLU  | CB-CG   | -10.59 | 1.32        | 1.52     | 21     | 1     |
| 1   | A     | 15  | GLN  | CG-CD   | -10.53 | 1.26        | 1.51     | 21     | 1     |
| 1   | A     | 28  | LEU  | CB-CG   | -10.51 | 1.22        | 1.52     | 21     | 1     |
| 1   | A     | 69  | LYS  | CG-CD   | -10.25 | 1.17        | 1.52     | 21     | 1     |
| 1   | A     | 54  | LEU  | CB-CG   | -10.21 | 1.23        | 1.52     | 21     | 1     |
| 1   | A     | 48  | LEU  | C-N     | -9.77  | 1.11        | 1.34     | 21     | 1     |
| 1   | A     | 5   | GLN  | CB-CG   | -9.76  | 1.26        | 1.52     | 21     | 1     |
| 1   | A     | 16  | MET  | CB-CG   | -9.08  | 1.22        | 1.51     | 21     | 1     |
| 1   | A     | 37  | ILE  | CB-CG2  | -9.05  | 1.24        | 1.52     | 21     | 1     |
| 1   | A     | 22  | ARG  | CG-CD   | -9.00  | 1.29        | 1.51     | 21     | 1     |
| 1   | A     | 6   | ILE  | CG1-CD1 | -8.98  | 0.88        | 1.50     | 21     | 1     |
| 1   | A     | 37  | ILE  | C-N     | -8.89  | 1.13        | 1.34     | 21     | 1     |
| 1   | A     | 11  | CYS  | C-O     | -8.33  | 1.07        | 1.23     | 21     | 1     |
| 1   | A     | 20  | ASN  | CG-ND2  | -8.24  | 1.12        | 1.32     | 21     | 1     |
| 1   | A     | 26  | LYS  | CG-CD   | -7.43  | 1.27        | 1.52     | 21     | 1     |
| 1   | A     | 8   | GLY  | C-O     | -7.38  | 1.11        | 1.23     | 21     | 1     |
| 1   | A     | 37  | ILE  | CG1-CD1 | -6.71  | 1.04        | 1.50     | 21     | 1     |
| 1   | A     | 5   | GLN  | CD-NE2  | -6.64  | 1.16        | 1.32     | 21     | 1     |
| 1   | A     | 11  | CYS  | C-N     | -6.62  | 1.18        | 1.34     | 21     | 1     |
| 1   | A     | 1   | MET  | CA-CB   | -6.31  | 1.40        | 1.53     | 21     | 1     |
| 1   | A     | 26  | LYS  | CB-CG   | -6.24  | 1.35        | 1.52     | 21     | 1     |
| 1   | A     | 49  | THR  | C-O     | -5.67  | 1.12        | 1.23     | 21     | 1     |
| 1   | A     | 49  | THR  | C-N     | -5.55  | 1.21        | 1.34     | 21     | 1     |
| 1   | A     | 36  | LYS  | CG-CD   | -5.51  | 1.33        | 1.52     | 21     | 1     |
| 1   | A     | 30  | ILE  | CG1-CD1 | -5.20  | 1.14        | 1.50     | 21     | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.



| Mol | Chain | Res | Type | Atoms      | Z       | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|---------|-------------|----------|--------|-------|
|     |       |     |      |            |         |             |          | Worst  | Total |
| 1   | A     | 65  | ARG  | NE-CZ-NH1  | -115.00 | 62.80       | 120.30   | 21     | 1     |
| 1   | A     | 22  | ARG  | NE-CZ-NH2  | 94.72   | 167.66      | 120.30   | 21     | 1     |
| 1   | A     | 65  | ARG  | NE-CZ-NH2  | 91.33   | 165.97      | 120.30   | 21     | 1     |
| 1   | A     | 71  | GLU  | OE1-CD-OE2 | -91.33  | 13.70       | 123.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CD1-CG-CD2 | -85.23  | 24.15       | 117.90   | 21     | 1     |
| 1   | A     | 70  | GLU  | OE1-CD-OE2 | -80.24  | 27.01       | 123.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CB-CG-CD2  | 79.59   | 168.75      | 121.00   | 21     | 1     |
| 1   | A     | 23  | GLU  | OE1-CD-OE2 | -79.48  | 27.92       | 123.30   | 21     | 1     |
| 1   | A     | 59  | GLU  | OE1-CD-OE2 | -77.68  | 30.09       | 123.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CB-CG-CD1  | 76.81   | 167.09      | 121.00   | 21     | 1     |
| 1   | A     | 18  | GLU  | OE1-CD-OE2 | -67.06  | 42.83       | 123.30   | 21     | 1     |
| 1   | A     | 34  | PHE  | CD1-CG-CD2 | -59.66  | 40.74       | 118.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CE1-CZ-CE2 | -59.19  | 25.10       | 119.80   | 21     | 2     |
| 1   | A     | 7   | TYR  | CG-CD1-CE1 | 58.72   | 168.27      | 121.30   | 21     | 1     |
| 1   | A     | 41  | ASP  | CB-CG-OD1  | 58.20   | 170.68      | 118.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CG-CD2-CE2 | 57.73   | 167.49      | 121.30   | 21     | 2     |
| 1   | A     | 7   | TYR  | CZ-CE2-CD2 | -57.64  | 67.92       | 119.80   | 9      | 2     |
| 1   | A     | 34  | PHE  | CB-CG-CD1  | 55.88   | 159.91      | 120.80   | 21     | 1     |
| 1   | A     | 41  | ASP  | CB-CG-OD2  | 55.28   | 168.06      | 118.30   | 21     | 1     |
| 1   | A     | 34  | PHE  | CB-CG-CD2  | 55.04   | 159.33      | 120.80   | 21     | 1     |
| 1   | A     | 39  | GLU  | OE1-CD-OE2 | -54.09  | 58.39       | 123.30   | 21     | 1     |
| 1   | A     | 41  | ASP  | OD1-CG-OD2 | -53.70  | 21.27       | 123.30   | 21     | 1     |
| 1   | A     | 27  | GLU  | OE1-CD-OE2 | -53.23  | 59.42       | 123.30   | 21     | 1     |
| 1   | A     | 7   | TYR  | CD1-CE1-CZ | 52.87   | 167.38      | 119.80   | 21     | 1     |
| 1   | A     | 22  | ARG  | NH1-CZ-NH2 | -52.71  | 61.42       | 119.40   | 21     | 1     |
| 1   | A     | 57  | ASP  | CB-CG-OD2  | 52.01   | 165.11      | 118.30   | 21     | 1     |
| 1   | A     | 33  | GLU  | OE1-CD-OE2 | -51.83  | 61.10       | 123.30   | 21     | 1     |
| 1   | A     | 31  | ASP  | CB-CG-OD2  | 50.84   | 164.06      | 118.30   | 21     | 1     |
| 1   | A     | 57  | ASP  | CB-CG-OD1  | 50.04   | 163.33      | 118.30   | 21     | 1     |
| 1   | A     | 35  | GLU  | OE1-CD-OE2 | -49.65  | 63.72       | 123.30   | 21     | 1     |
| 1   | A     | 63  | MET  | CG-SD-CE   | 48.32   | 177.52      | 100.20   | 21     | 1     |
| 1   | A     | 57  | ASP  | OD1-CG-OD2 | -48.28  | 31.56       | 123.30   | 21     | 1     |
| 1   | A     | 31  | ASP  | CB-CG-OD1  | 46.98   | 160.58      | 118.30   | 21     | 1     |
| 1   | A     | 31  | ASP  | OD1-CG-OD2 | -46.28  | 35.36       | 123.30   | 21     | 1     |
| 1   | A     | 34  | PHE  | CE1-CZ-CE2 | -43.51  | 41.68       | 120.00   | 21     | 1     |
| 1   | A     | 45  | GLU  | OE1-CD-OE2 | -42.73  | 72.03       | 123.30   | 21     | 1     |
| 1   | A     | 9   | THR  | O-C-N      | -42.61  | 50.77       | 123.20   | 21     | 1     |
| 1   | A     | 40  | MET  | CG-SD-CE   | 39.61   | 163.58      | 100.20   | 21     | 1     |
| 1   | A     | 2   | MET  | CG-SD-CE   | 37.95   | 160.93      | 100.20   | 21     | 1     |
| 1   | A     | 34  | PHE  | CG-CD1-CE1 | 35.56   | 159.92      | 120.80   | 21     | 1     |
| 1   | A     | 54  | LEU  | CB-CG-CD1  | 35.11   | 170.69      | 111.00   | 21     | 1     |
| 1   | A     | 34  | PHE  | CG-CD2-CE2 | 35.09   | 159.40      | 120.80   | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
|     |       |     |      |            |        |             |          | Worst  | Total |
| 1   | A     | 17  | LEU  | CB-CG-CD1  | 33.57  | 168.08      | 111.00   | 21     | 1     |
| 1   | A     | 34  | PHE  | CZ-CE2-CD2 | 32.82  | 159.48      | 120.10   | 21     | 1     |
| 1   | A     | 22  | ARG  | CD-NE-CZ   | 32.26  | 168.76      | 123.60   | 21     | 1     |
| 1   | A     | 34  | PHE  | CD1-CE1-CZ | 32.23  | 158.78      | 120.10   | 21     | 1     |
| 1   | A     | 16  | MET  | CG-SD-CE   | 31.38  | 150.40      | 100.20   | 21     | 1     |
| 1   | A     | 54  | LEU  | CB-CG-CD2  | 31.18  | 164.00      | 111.00   | 21     | 1     |
| 1   | A     | 65  | ARG  | CD-NE-CZ   | 30.91  | 166.87      | 123.60   | 21     | 1     |
| 1   | A     | 1   | MET  | CG-SD-CE   | 30.81  | 149.49      | 100.20   | 21     | 1     |
| 1   | A     | 54  | LEU  | CD1-CG-CD2 | -30.65 | 18.55       | 110.50   | 21     | 1     |
| 1   | A     | 40  | MET  | CA-CB-CG   | 30.20  | 164.65      | 113.30   | 21     | 1     |
| 1   | A     | 17  | LEU  | CB-CG-CD2  | 29.70  | 161.49      | 111.00   | 21     | 1     |
| 1   | A     | 71  | GLU  | CG-CD-OE1  | 27.75  | 173.81      | 118.30   | 21     | 1     |
| 1   | A     | 17  | LEU  | CD1-CG-CD2 | -27.68 | 27.47       | 110.50   | 21     | 1     |
| 1   | A     | 71  | GLU  | CG-CD-OE2  | 27.10  | 172.49      | 118.30   | 21     | 1     |
| 1   | A     | 22  | ARG  | CG-CD-NE   | 26.34  | 167.11      | 111.80   | 21     | 1     |
| 1   | A     | 65  | ARG  | CG-CD-NE   | 25.79  | 165.95      | 111.80   | 21     | 1     |
| 1   | A     | 26  | LYS  | CD-CE-NZ   | 24.92  | 169.01      | 111.70   | 21     | 1     |
| 1   | A     | 23  | GLU  | CG-CD-OE2  | 24.54  | 167.37      | 118.30   | 21     | 1     |
| 1   | A     | 70  | GLU  | CG-CD-OE1  | 24.26  | 166.81      | 118.30   | 21     | 1     |
| 1   | A     | 61  | LYS  | CD-CE-NZ   | 23.99  | 166.88      | 111.70   | 21     | 1     |
| 1   | A     | 70  | GLU  | CG-CD-OE2  | 23.94  | 166.17      | 118.30   | 21     | 1     |
| 1   | A     | 59  | GLU  | CG-CD-OE1  | 23.41  | 165.12      | 118.30   | 21     | 1     |
| 1   | A     | 59  | GLU  | CG-CD-OE2  | 23.24  | 164.79      | 118.30   | 21     | 1     |
| 1   | A     | 23  | GLU  | CG-CD-OE1  | 23.21  | 164.71      | 118.30   | 21     | 1     |
| 1   | A     | 69  | LYS  | CD-CE-NZ   | 22.50  | 163.45      | 111.70   | 21     | 1     |
| 1   | A     | 49  | THR  | CA-CB-CG2  | 22.41  | 143.77      | 112.40   | 21     | 1     |
| 1   | A     | 66  | VAL  | CG1-CB-CG2 | -22.23 | 75.34       | 110.90   | 21     | 1     |
| 1   | A     | 9   | THR  | CA-C-N     | 21.83  | 159.86      | 116.20   | 21     | 1     |
| 1   | A     | 45  | GLU  | CG-CD-OE2  | 21.72  | 161.73      | 118.30   | 21     | 1     |
| 1   | A     | 39  | GLU  | CG-CD-OE2  | 21.55  | 161.40      | 118.30   | 21     | 1     |
| 1   | A     | 63  | MET  | CA-CB-CG   | 21.48  | 149.82      | 113.30   | 21     | 1     |
| 1   | A     | 22  | ARG  | NE-CZ-NH1  | 21.23  | 130.92      | 120.30   | 21     | 1     |
| 1   | A     | 5   | GLN  | CB-CG-CD   | 21.20  | 166.71      | 111.60   | 21     | 1     |
| 1   | A     | 69  | LYS  | CB-CG-CD   | 21.17  | 166.64      | 111.60   | 21     | 1     |
| 1   | A     | 38  | LYS  | CD-CE-NZ   | 21.02  | 160.06      | 111.70   | 21     | 1     |
| 1   | A     | 18  | GLU  | CG-CD-OE1  | 20.54  | 159.37      | 118.30   | 21     | 1     |
| 1   | A     | 13  | ASN  | OD1-CG-ND2 | -20.48 | 74.80       | 121.90   | 21     | 1     |
| 1   | A     | 36  | LYS  | CD-CE-NZ   | 20.27  | 158.31      | 111.70   | 21     | 1     |
| 1   | A     | 18  | GLU  | CG-CD-OE2  | 19.75  | 157.79      | 118.30   | 21     | 1     |
| 1   | A     | 49  | THR  | OG1-CB-CG2 | -19.55 | 65.03       | 110.00   | 21     | 1     |
| 1   | A     | 33  | GLU  | CG-CD-OE2  | 19.52  | 157.33      | 118.30   | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
|     |       |     |      |            |        |             |          | Worst  | Total |
| 1   | A     | 19  | LYS  | CD-CE-NZ   | 19.46  | 156.46      | 111.70   | 21     | 1     |
| 1   | A     | 40  | MET  | CB-CG-SD   | 18.99  | 169.37      | 112.40   | 21     | 1     |
| 1   | A     | 69  | LYS  | CG-CD-CE   | 18.68  | 167.94      | 111.90   | 21     | 1     |
| 1   | A     | 9   | THR  | C-N-CA     | 18.42  | 160.98      | 122.30   | 21     | 1     |
| 1   | A     | 27  | GLU  | CG-CD-OE1  | 18.36  | 155.01      | 118.30   | 21     | 1     |
| 1   | A     | 66  | VAL  | CA-CB-CG1  | 17.81  | 137.61      | 110.90   | 21     | 1     |
| 1   | A     | 35  | GLU  | CG-CD-OE1  | 17.76  | 153.82      | 118.30   | 21     | 1     |
| 1   | A     | 42  | GLN  | CB-CG-CD   | 17.73  | 157.69      | 111.60   | 21     | 1     |
| 1   | A     | 7   | TYR  | OH-CZ-CE2  | 17.57  | 167.53      | 120.10   | 21     | 2     |
| 1   | A     | 7   | TYR  | CE1-CZ-OH  | 17.51  | 167.37      | 120.10   | 21     | 1     |
| 1   | A     | 69  | LYS  | CA-CB-CG   | 17.49  | 151.87      | 113.40   | 21     | 1     |
| 1   | A     | 26  | LYS  | CG-CD-CE   | 17.14  | 163.32      | 111.90   | 21     | 1     |
| 1   | A     | 3   | LYS  | CD-CE-NZ   | 16.88  | 150.52      | 111.70   | 21     | 1     |
| 1   | A     | 35  | GLU  | CB-CG-CD   | 16.50  | 158.74      | 114.20   | 21     | 1     |
| 1   | A     | 2   | MET  | CB-CG-SD   | 16.02  | 160.47      | 112.40   | 21     | 1     |
| 1   | A     | 66  | VAL  | CA-CB-CG2  | 15.76  | 134.54      | 110.90   | 21     | 1     |
| 1   | A     | 5   | GLN  | CG-CD-OE1  | -15.73 | 90.13       | 121.60   | 21     | 1     |
| 1   | A     | 6   | ILE  | CB-CG1-CD1 | 15.57  | 157.49      | 113.90   | 21     | 1     |
| 1   | A     | 61  | LYS  | CB-CG-CD   | 15.51  | 151.92      | 111.60   | 21     | 1     |
| 1   | A     | 3   | LYS  | CG-CD-CE   | 15.12  | 157.28      | 111.90   | 21     | 1     |
| 1   | A     | 71  | GLU  | CB-CG-CD   | 15.04  | 154.80      | 114.20   | 21     | 1     |
| 1   | A     | 72  | ILE  | CB-CG1-CD1 | 14.93  | 155.71      | 113.90   | 21     | 1     |
| 1   | A     | 73  | LYS  | CD-CE-NZ   | 14.52  | 145.09      | 111.70   | 21     | 1     |
| 1   | A     | 1   | MET  | CA-CB-CG   | 14.13  | 137.32      | 113.30   | 21     | 1     |
| 1   | A     | 28  | LEU  | CB-CG-CD1  | 14.00  | 134.80      | 111.00   | 21     | 1     |
| 1   | A     | 19  | LYS  | CG-CD-CE   | 13.97  | 153.82      | 111.90   | 21     | 1     |
| 1   | A     | 9   | THR  | CA-C-O     | 13.94  | 149.37      | 120.10   | 21     | 1     |
| 1   | A     | 49  | THR  | CA-CB-OG1  | 13.92  | 138.24      | 109.00   | 21     | 1     |
| 1   | A     | 27  | GLU  | CG-CD-OE2  | 13.63  | 145.57      | 118.30   | 21     | 1     |
| 1   | A     | 30  | ILE  | CG1-CB-CG2 | -13.03 | 82.74       | 111.40   | 21     | 1     |
| 1   | A     | 42  | GLN  | CG-CD-NE2  | 12.71  | 147.21      | 116.70   | 21     | 1     |
| 1   | A     | 60  | LEU  | CB-CG-CD2  | 12.62  | 132.45      | 111.00   | 21     | 1     |
| 1   | A     | 36  | LYS  | CG-CD-CE   | 12.59  | 149.67      | 111.90   | 21     | 1     |
| 1   | A     | 42  | GLN  | OE1-CD-NE2 | -12.48 | 93.19       | 121.90   | 21     | 1     |
| 1   | A     | 59  | GLU  | CB-CG-CD   | 12.43  | 147.75      | 114.20   | 21     | 1     |
| 1   | A     | 35  | GLU  | CG-CD-OE2  | 12.08  | 142.46      | 118.30   | 21     | 1     |
| 1   | A     | 51  | LEU  | CB-CG-CD2  | 11.97  | 131.35      | 111.00   | 21     | 1     |
| 1   | A     | 13  | ASN  | CB-CG-ND2  | 11.94  | 145.36      | 116.70   | 21     | 1     |
| 1   | A     | 61  | LYS  | CG-CD-CE   | 11.77  | 147.21      | 111.90   | 21     | 1     |
| 1   | A     | 9   | THR  | CA-CB-CG2  | 11.72  | 128.81      | 112.40   | 21     | 1     |
| 1   | A     | 33  | GLU  | CG-CD-OE1  | 11.63  | 141.57      | 118.30   | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 65  | ARG  | CB-CG-CD   | 11.46 | 141.40      | 111.60   | 21     | 1     |
| 1   | A     | 73  | LYS  | CG-CD-CE   | 11.40 | 146.11      | 111.90   | 21     | 1     |
| 1   | A     | 39  | GLU  | CG-CD-OE1  | 10.96 | 140.21      | 118.30   | 21     | 1     |
| 1   | A     | 1   | MET  | CB-CG-SD   | 10.91 | 145.13      | 112.40   | 21     | 1     |
| 1   | A     | 28  | LEU  | CB-CG-CD2  | 10.79 | 129.34      | 111.00   | 21     | 1     |
| 1   | A     | 65  | ARG  | NH1-CZ-NH2 | 10.76 | 131.23      | 119.40   | 21     | 1     |
| 1   | A     | 5   | GLN  | CG-CD-NE2  | 10.74 | 142.48      | 116.70   | 21     | 1     |
| 1   | A     | 30  | ILE  | CA-CB-CG2  | 10.62 | 132.14      | 110.90   | 21     | 1     |
| 1   | A     | 45  | GLU  | CB-CG-CD   | 10.39 | 142.26      | 114.20   | 21     | 1     |
| 1   | A     | 16  | MET  | CB-CG-SD   | 10.32 | 143.37      | 112.40   | 21     | 1     |
| 1   | A     | 33  | GLU  | CB-CG-CD   | 10.20 | 141.74      | 114.20   | 21     | 1     |
| 1   | A     | 30  | ILE  | CA-CB-CG1  | 10.13 | 130.24      | 111.00   | 21     | 1     |
| 1   | A     | 20  | ASN  | CB-CG-ND2  | 9.80  | 140.21      | 116.70   | 21     | 1     |
| 1   | A     | 20  | ASN  | CB-CG-OD1  | -9.38 | 102.84      | 121.60   | 21     | 1     |
| 1   | A     | 51  | LEU  | CB-CG-CD1  | 9.21  | 126.65      | 111.00   | 21     | 1     |
| 1   | A     | 38  | LYS  | CG-CD-CE   | 9.20  | 139.51      | 111.90   | 21     | 1     |
| 1   | A     | 13  | ASN  | CB-CG-OD1  | 9.12  | 139.85      | 121.60   | 21     | 1     |
| 1   | A     | 10  | GLY  | O-C-N      | -8.99 | 108.32      | 122.70   | 21     | 1     |
| 1   | A     | 51  | LEU  | CD1-CG-CD2 | -8.91 | 83.78       | 110.50   | 21     | 1     |
| 1   | A     | 68  | SER  | CA-CB-OG   | 8.82  | 135.02      | 111.20   | 21     | 1     |
| 1   | A     | 39  | GLU  | CB-CG-CD   | 8.72  | 137.75      | 114.20   | 21     | 1     |
| 1   | A     | 3   | LYS  | CB-CG-CD   | 8.72  | 134.27      | 111.60   | 21     | 1     |
| 1   | A     | 28  | LEU  | CD1-CG-CD2 | -8.62 | 84.64       | 110.50   | 21     | 1     |
| 1   | A     | 48  | LEU  | O-C-N      | -8.51 | 109.08      | 122.70   | 21     | 1     |
| 1   | A     | 62  | ILE  | CG1-CB-CG2 | -8.46 | 92.80       | 111.40   | 21     | 1     |
| 1   | A     | 9   | THR  | OG1-CB-CG2 | -8.40 | 90.69       | 110.00   | 21     | 1     |
| 1   | A     | 62  | ILE  | CB-CG1-CD1 | 8.14  | 136.70      | 113.90   | 21     | 1     |
| 1   | A     | 37  | ILE  | O-C-N      | -8.11 | 109.72      | 122.70   | 21     | 1     |
| 1   | A     | 23  | GLU  | CA-CB-CG   | 8.10  | 131.21      | 113.40   | 21     | 1     |
| 1   | A     | 72  | ILE  | CG1-CB-CG2 | -8.05 | 93.69       | 111.40   | 21     | 1     |
| 1   | A     | 11  | CYS  | CA-CB-SG   | 7.99  | 128.38      | 114.00   | 21     | 1     |
| 1   | A     | 35  | GLU  | CA-CB-CG   | 7.79  | 130.54      | 113.40   | 21     | 1     |
| 1   | A     | 70  | GLU  | CB-CG-CD   | 7.49  | 134.42      | 114.20   | 21     | 1     |
| 1   | A     | 4   | ILE  | CB-CG1-CD1 | 7.39  | 134.60      | 113.90   | 21     | 1     |
| 1   | A     | 62  | ILE  | CA-CB-CG1  | 7.38  | 125.02      | 111.00   | 21     | 1     |
| 1   | A     | 15  | GLN  | CG-CD-OE1  | -7.11 | 107.38      | 121.60   | 21     | 1     |
| 1   | A     | 23  | GLU  | CB-CG-CD   | 7.05  | 133.23      | 114.20   | 21     | 1     |
| 1   | A     | 73  | LYS  | CB-CG-CD   | 7.04  | 129.90      | 111.60   | 21     | 1     |
| 1   | A     | 3   | LYS  | CA-CB-CG   | 6.93  | 128.65      | 113.40   | 21     | 1     |
| 1   | A     | 65  | ARG  | CA-CB-CG   | 6.92  | 128.62      | 113.40   | 21     | 1     |
| 1   | A     | 72  | ILE  | CA-CB-CG2  | 6.64  | 124.18      | 110.90   | 21     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 6   | ILE  | CG1-CB-CG2 | -6.59 | 96.89       | 111.40   | 21     | 1     |
| 1   | A     | 62  | ILE  | CA-CB-CG2  | 6.44  | 123.78      | 110.90   | 21     | 1     |
| 1   | A     | 72  | ILE  | CA-CB-CG1  | 6.41  | 123.18      | 111.00   | 21     | 1     |
| 1   | A     | 30  | ILE  | CB-CG1-CD1 | 6.40  | 131.83      | 113.90   | 21     | 1     |
| 1   | A     | 60  | LEU  | CA-CB-CG   | 6.13  | 129.41      | 115.30   | 21     | 1     |
| 1   | A     | 60  | LEU  | CD1-CG-CD2 | -6.13 | 92.11       | 110.50   | 21     | 1     |
| 1   | A     | 9   | THR  | CA-CB-OG1  | 5.93  | 121.45      | 109.00   | 21     | 1     |
| 1   | A     | 6   | ILE  | CA-CB-CG1  | 5.88  | 122.16      | 111.00   | 21     | 1     |
| 1   | A     | 70  | GLU  | CA-CB-CG   | 5.84  | 126.25      | 113.40   | 21     | 1     |
| 1   | A     | 27  | GLU  | CB-CG-CD   | 5.74  | 129.70      | 114.20   | 21     | 1     |
| 1   | A     | 37  | ILE  | CA-CB-CG2  | 5.55  | 122.01      | 110.90   | 21     | 1     |
| 1   | A     | 48  | LEU  | CA-C-N     | 5.47  | 129.23      | 117.20   | 21     | 1     |
| 1   | A     | 43  | ILE  | CG1-CB-CG2 | -5.43 | 99.45       | 111.40   | 21     | 1     |
| 1   | A     | 39  | GLU  | CA-CB-CG   | 5.36  | 125.19      | 113.40   | 21     | 1     |

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

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------|----------------|
| 1   | A     | 9   | THR  | CB    | 1              |
| 1   | A     | 30  | ILE  | CB    | 1              |
| 1   | A     | 49  | THR  | CB    | 1              |

There are no planarity outliers.

## 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 554   | 581      | 575      | 73±66   |
| All | All   | 11634 | 12201    | 12195    | 1540    |

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 65.

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

| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:16:MET:CG  | 1:A:16:MET:CE  | 1.59     | 1.81        | 21     | 1     |
| 1:A:30:ILE:CB  | 1:A:30:ILE:CD1 | 1.55     | 1.81        | 21     | 1     |
| 1:A:65:ARG:CD  | 1:A:65:ARG:CB  | 1.54     | 1.85        | 21     | 1     |
| 1:A:65:ARG:CG  | 1:A:65:ARG:NE  | 1.54     | 1.69        | 21     | 1     |
| 1:A:17:LEU:CD2 | 1:A:17:LEU:CB  | 1.49     | 1.90        | 21     | 1     |
| 1:A:54:LEU:CD1 | 1:A:54:LEU:CB  | 1.48     | 1.91        | 21     | 1     |
| 1:A:35:GLU:CD  | 1:A:35:GLU:CB  | 1.47     | 1.82        | 21     | 1     |
| 1:A:19:LYS:CD  | 1:A:19:LYS:NZ  | 1.47     | 1.70        | 21     | 1     |
| 1:A:69:LYS:CB  | 1:A:69:LYS:CD  | 1.47     | 1.90        | 21     | 1     |
| 1:A:73:LYS:CE  | 1:A:73:LYS:CG  | 1.46     | 1.90        | 21     | 1     |
| 1:A:6:ILE:CD1  | 1:A:6:ILE:CB   | 1.45     | 1.94        | 21     | 1     |
| 1:A:1:MET:CE   | 1:A:1:MET:CG   | 1.44     | 1.91        | 21     | 1     |
| 1:A:34:PHE:CZ  | 1:A:34:PHE:CD1 | 1.43     | 2.07        | 21     | 1     |
| 1:A:19:LYS:CE  | 1:A:19:LYS:CG  | 1.42     | 1.95        | 21     | 1     |
| 1:A:31:ASP:OD1 | 1:A:31:ASP:CB  | 1.42     | 1.67        | 21     | 1     |
| 1:A:7:TYR:CZ   | 1:A:7:TYR:CD1  | 1.42     | 2.06        | 21     | 1     |
| 1:A:36:LYS:CD  | 1:A:36:LYS:NZ  | 1.41     | 1.74        | 21     | 1     |
| 1:A:34:PHE:CG  | 1:A:34:PHE:CE2 | 1.40     | 2.08        | 21     | 1     |
| 1:A:7:TYR:CZ   | 1:A:7:TYR:CD2  | 1.39     | 2.07        | 21     | 1     |
| 1:A:7:TYR:CG   | 1:A:7:TYR:CE2  | 1.39     | 2.09        | 21     | 1     |
| 1:A:13:ASN:OD1 | 1:A:13:ASN:CB  | 1.39     | 1.70        | 21     | 1     |
| 1:A:34:PHE:CZ  | 1:A:34:PHE:CD2 | 1.39     | 2.09        | 21     | 1     |
| 1:A:13:ASN:CB  | 1:A:13:ASN:ND2 | 1.39     | 1.86        | 21     | 1     |
| 1:A:2:MET:CG   | 1:A:2:MET:CE   | 1.38     | 2.02        | 21     | 1     |
| 1:A:34:PHE:CG  | 1:A:34:PHE:CE1 | 1.38     | 2.10        | 21     | 1     |
| 1:A:7:TYR:CD2  | 1:A:7:TYR:CE2  | 1.36     | 2.14        | 9      | 1     |
| 1:A:26:LYS:CE  | 1:A:26:LYS:CG  | 1.36     | 2.02        | 21     | 1     |
| 1:A:69:LYS:CE  | 1:A:69:LYS:CG  | 1.36     | 2.01        | 21     | 1     |
| 1:A:7:TYR:CG   | 1:A:7:TYR:CE1  | 1.36     | 2.10        | 21     | 1     |
| 1:A:7:TYR:CE2  | 1:A:7:TYR:CZ   | 1.35     | 2.14        | 9      | 1     |
| 1:A:40:MET:CE  | 1:A:40:MET:CG  | 1.35     | 2.05        | 21     | 1     |
| 1:A:51:LEU:CD1 | 1:A:51:LEU:CB  | 1.33     | 2.05        | 21     | 1     |
| 1:A:1:MET:CG   | 1:A:1:MET:CA   | 1.30     | 2.07        | 21     | 1     |
| 1:A:49:THR:CG2 | 1:A:49:THR:CA  | 1.30     | 2.07        | 21     | 1     |
| 1:A:31:ASP:CB  | 1:A:31:ASP:OD2 | 1.30     | 1.77        | 21     | 1     |
| 1:A:57:ASP:OD1 | 1:A:57:ASP:CB  | 1.30     | 1.77        | 21     | 1     |
| 1:A:16:MET:SD  | 1:A:16:MET:CB  | 1.30     | 2.19        | 21     | 1     |
| 1:A:9:THR:O    | 1:A:10:GLY:CA  | 1.28     | 1.82        | 21     | 1     |
| 1:A:36:LYS:CE  | 1:A:36:LYS:CG  | 1.27     | 2.09        | 21     | 1     |
| 1:A:59:GLU:CD  | 1:A:59:GLU:CB  | 1.27     | 2.02        | 21     | 1     |
| 1:A:1:MET:CG   | 1:A:1:MET:SD   | 1.26     | 1.18        | 21     | 1     |
| 1:A:51:LEU:CB  | 1:A:51:LEU:CD2 | 1.26     | 2.13        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:LEU:CB   | 1:A:17:LEU:CD1  | 1.26     | 2.14        | 21     | 1     |
| 1:A:57:ASP:CB   | 1:A:57:ASP:OD2  | 1.25     | 1.82        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:SD   | 1.25     | 1.16        | 21     | 1     |
| 1:A:34:PHE:CD2  | 1:A:34:PHE:CB   | 1.24     | 2.20        | 21     | 1     |
| 1:A:11:CYS:CB   | 1:A:11:CYS:SG   | 1.23     | 1.14        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:CE   | 1.23     | 2.14        | 21     | 1     |
| 1:A:9:THR:O     | 1:A:9:THR:CA    | 1.22     | 1.88        | 21     | 1     |
| 1:A:30:ILE:CG1  | 1:A:30:ILE:CA   | 1.22     | 2.17        | 21     | 1     |
| 1:A:69:LYS:CG   | 1:A:69:LYS:CA   | 1.19     | 2.19        | 21     | 1     |
| 1:A:7:TYR:CD1   | 1:A:7:TYR:CB    | 1.19     | 2.24        | 21     | 1     |
| 1:A:66:VAL:CG2  | 1:A:66:VAL:CA   | 1.18     | 2.19        | 21     | 1     |
| 1:A:30:ILE:CA   | 1:A:30:ILE:CG2  | 1.18     | 2.20        | 21     | 1     |
| 1:A:34:PHE:CD1  | 1:A:34:PHE:CB   | 1.18     | 2.22        | 21     | 1     |
| 1:A:7:TYR:CD2   | 1:A:7:TYR:CB    | 1.17     | 2.23        | 21     | 1     |
| 1:A:41:ASP:OD2  | 1:A:41:ASP:CB   | 1.17     | 1.93        | 21     | 1     |
| 1:A:6:ILE:CD1   | 1:A:6:ILE:CG2   | 1.15     | 2.25        | 21     | 1     |
| 1:A:16:MET:CG   | 1:A:16:MET:SD   | 1.15     | 1.09        | 21     | 1     |
| 1:A:2:MET:CE    | 1:A:2:MET:SD    | 1.14     | 1.07        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:CB    | 1.13     | 2.34        | 21     | 1     |
| 1:A:49:THR:CA   | 1:A:49:THR:OG1  | 1.13     | 1.95        | 21     | 1     |
| 1:A:11:CYS:SG   | 1:A:11:CYS:CA   | 1.13     | 2.36        | 21     | 1     |
| 1:A:22:ARG:NE   | 1:A:22:ARG:CG   | 1.13     | 2.12        | 21     | 1     |
| 1:A:9:THR:C     | 1:A:10:GLY:CA   | 1.11     | 2.17        | 21     | 1     |
| 1:A:66:VAL:CG2  | 1:A:66:VAL:HB   | 1.11     | 1.68        | 21     | 1     |
| 1:A:51:LEU:CD1  | 1:A:51:LEU:HG   | 1.09     | 1.66        | 21     | 1     |
| 1:A:66:VAL:CA   | 1:A:66:VAL:CG1  | 1.09     | 2.26        | 21     | 1     |
| 1:A:45:GLU:CD   | 1:A:45:GLU:CB   | 1.09     | 2.19        | 21     | 1     |
| 1:A:51:LEU:CD2  | 1:A:51:LEU:HG   | 1.09     | 1.66        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:CA   | 1.08     | 2.31        | 21     | 1     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:CB   | 1.08     | 2.21        | 21     | 1     |
| 1:A:49:THR:OG1  | 1:A:49:THR:HB   | 1.07     | 1.48        | 21     | 1     |
| 1:A:17:LEU:HD21 | 1:A:72:ILE:HD11 | 1.05     | 1.27        | 20     | 3     |
| 1:A:68:SER:OG   | 1:A:68:SER:CA   | 1.05     | 2.04        | 21     | 1     |
| 1:A:68:SER:OG   | 1:A:68:SER:HB2  | 1.05     | 1.30        | 21     | 1     |
| 1:A:66:VAL:HB   | 1:A:66:VAL:CG1  | 1.04     | 1.70        | 21     | 1     |
| 1:A:2:MET:CG    | 1:A:2:MET:SD    | 1.03     | 0.97        | 21     | 1     |
| 1:A:7:TYR:CE1   | 1:A:7:TYR:OH    | 1.03     | 2.06        | 21     | 1     |
| 1:A:68:SER:OG   | 1:A:68:SER:HB3  | 1.03     | 1.30        | 21     | 1     |
| 1:A:7:TYR:CE2   | 1:A:7:TYR:OH    | 1.03     | 2.07        | 21     | 2     |
| 1:A:41:ASP:CB   | 1:A:41:ASP:OD1  | 1.02     | 2.06        | 21     | 1     |
| 1:A:9:THR:CA    | 1:A:10:GLY:N    | 1.02     | 2.22        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:59:GLU:CD   | 1:A:59:GLU:CG   | 1.02     | 0.93        | 21     | 1     |
| 1:A:43:ILE:HG22 | 1:A:48:LEU:HD21 | 1.02     | 1.30        | 6      | 18    |
| 1:A:63:MET:CB   | 1:A:63:MET:HG2  | 1.02     | 1.55        | 21     | 1     |
| 1:A:11:CYS:SG   | 1:A:11:CYS:HB3  | 1.01     | 1.68        | 21     | 1     |
| 1:A:49:THR:CG2  | 1:A:49:THR:HB   | 1.01     | 1.55        | 21     | 1     |
| 1:A:37:ILE:HD13 | 1:A:37:ILE:N    | 1.01     | 1.54        | 21     | 9     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD23 | 1.01     | 1.55        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:HE2   | 1.01     | 1.67        | 21     | 1     |
| 1:A:30:ILE:CG1  | 1:A:30:ILE:HB   | 1.01     | 1.62        | 21     | 1     |
| 1:A:59:GLU:CD   | 1:A:59:GLU:HG3  | 1.00     | 1.45        | 21     | 1     |
| 1:A:49:THR:CG2  | 1:A:49:THR:OG1  | 1.00     | 0.70        | 21     | 1     |
| 1:A:59:GLU:CD   | 1:A:59:GLU:HG2  | 1.00     | 1.45        | 21     | 1     |
| 1:A:63:MET:SD   | 1:A:63:MET:CE   | 1.00     | 0.98        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG11 | 1.00     | 1.53        | 21     | 1     |
| 1:A:11:CYS:SG   | 1:A:11:CYS:HB2  | 0.99     | 1.68        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:HE1   | 0.99     | 1.67        | 21     | 1     |
| 1:A:7:TYR:CD2   | 1:A:7:TYR:CZ    | 0.98     | 2.39        | 9      | 1     |
| 1:A:49:THR:OG1  | 1:A:49:THR:HG23 | 0.98     | 1.24        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG13 | 0.98     | 1.53        | 21     | 1     |
| 1:A:17:LEU:HD11 | 1:A:72:ILE:HD11 | 0.98     | 1.31        | 1      | 5     |
| 1:A:25:VAL:HG21 | 1:A:32:ALA:HB2  | 0.98     | 1.30        | 6      | 16    |
| 1:A:63:MET:SD   | 1:A:63:MET:HG2  | 0.98     | 1.75        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG12 | 0.98     | 1.53        | 21     | 1     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD21 | 0.98     | 1.55        | 21     | 1     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD12 | 0.97     | 1.51        | 21     | 1     |
| 1:A:68:SER:OG   | 1:A:68:SER:CB   | 0.97     | 0.67        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:HE3   | 0.97     | 1.67        | 21     | 1     |
| 1:A:63:MET:CB   | 1:A:63:MET:HG3  | 0.97     | 1.55        | 21     | 1     |
| 1:A:22:ARG:NE   | 1:A:22:ARG:CD   | 0.96     | 0.84        | 21     | 1     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD22 | 0.96     | 1.55        | 21     | 1     |
| 1:A:6:ILE:CG1   | 1:A:6:ILE:HD12  | 0.96     | 1.51        | 21     | 1     |
| 1:A:30:ILE:CG2  | 1:A:30:ILE:HB   | 0.96     | 1.62        | 21     | 1     |
| 1:A:45:GLU:CD   | 1:A:45:GLU:HG3  | 0.96     | 1.40        | 21     | 1     |
| 1:A:6:ILE:CG1   | 1:A:6:ILE:HD13  | 0.96     | 1.51        | 21     | 1     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:CG   | 0.96     | 0.86        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HG21 | 0.95     | 1.49        | 21     | 1     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD13 | 0.95     | 1.51        | 21     | 1     |
| 1:A:63:MET:SD   | 1:A:63:MET:HE2  | 0.95     | 1.59        | 21     | 1     |
| 1:A:6:ILE:CG1   | 1:A:6:ILE:HD11  | 0.95     | 1.51        | 21     | 1     |
| 1:A:63:MET:SD   | 1:A:63:MET:HE1  | 0.95     | 1.59        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HG22 | 0.95     | 1.49        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:35:GLU:CD   | 1:A:35:GLU:HG2  | 0.94     | 1.39        | 21     | 1     |
| 1:A:37:ILE:HD13 | 1:A:37:ILE:H    | 0.94     | 1.03        | 21     | 1     |
| 1:A:22:ARG:NE   | 1:A:22:ARG:HD2  | 0.94     | 1.32        | 21     | 1     |
| 1:A:51:LEU:CG   | 1:A:51:LEU:HD11 | 0.94     | 1.51        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG22 | 0.94     | 1.49        | 21     | 1     |
| 1:A:65:ARG:CD   | 1:A:65:ARG:HG3  | 0.94     | 1.47        | 21     | 1     |
| 1:A:63:MET:SD   | 1:A:63:MET:HE3  | 0.94     | 1.59        | 21     | 1     |
| 1:A:45:GLU:CD   | 1:A:45:GLU:CG   | 0.93     | 0.84        | 21     | 1     |
| 1:A:45:GLU:CD   | 1:A:45:GLU:HG2  | 0.93     | 1.40        | 21     | 1     |
| 1:A:16:MET:SD   | 1:A:16:MET:HG3  | 0.93     | 1.59        | 21     | 1     |
| 1:A:22:ARG:NE   | 1:A:22:ARG:HD3  | 0.93     | 1.32        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG21 | 0.93     | 1.49        | 21     | 1     |
| 1:A:66:VAL:CB   | 1:A:66:VAL:HG23 | 0.93     | 1.49        | 21     | 1     |
| 1:A:16:MET:SD   | 1:A:16:MET:HG2  | 0.93     | 1.59        | 21     | 1     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:HG3  | 0.93     | 1.37        | 21     | 1     |
| 1:A:35:GLU:CD   | 1:A:35:GLU:HG3  | 0.92     | 1.39        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HG23 | 0.92     | 1.49        | 21     | 1     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:HG2  | 0.92     | 1.37        | 21     | 1     |
| 1:A:35:GLU:CD   | 1:A:35:GLU:CG   | 0.92     | 0.89        | 21     | 1     |
| 1:A:51:LEU:CD2  | 1:A:51:LEU:CG   | 0.92     | 0.92        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:CB   | 0.91     | 0.91        | 21     | 1     |
| 1:A:4:ILE:HD13  | 1:A:34:PHE:CZ   | 0.91     | 2.01        | 13     | 13    |
| 1:A:65:ARG:CD   | 1:A:65:ARG:HG2  | 0.91     | 1.47        | 21     | 1     |
| 1:A:63:MET:SD   | 1:A:63:MET:HG3  | 0.91     | 1.75        | 21     | 1     |
| 1:A:65:ARG:CD   | 1:A:65:ARG:CG   | 0.91     | 0.93        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:HB2  | 0.90     | 1.43        | 21     | 1     |
| 1:A:66:VAL:CG1  | 1:A:66:VAL:CB   | 0.90     | 0.90        | 21     | 1     |
| 1:A:6:ILE:CD1   | 1:A:6:ILE:HG21  | 0.89     | 1.98        | 21     | 1     |
| 1:A:49:THR:OG1  | 1:A:49:THR:CB   | 0.89     | 0.59        | 21     | 1     |
| 1:A:7:TYR:CE2   | 1:A:42:GLN:O    | 0.88     | 2.26        | 9      | 1     |
| 1:A:62:ILE:HD13 | 1:A:66:VAL:HG12 | 0.88     | 1.45        | 15     | 1     |
| 1:A:7:TYR:CD2   | 1:A:48:LEU:HD11 | 0.88     | 2.03        | 12     | 5     |
| 1:A:6:ILE:CD1   | 1:A:6:ILE:CG1   | 0.88     | 0.88        | 21     | 1     |
| 1:A:51:LEU:CD1  | 1:A:51:LEU:CG   | 0.88     | 0.88        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HG13 | 0.87     | 1.42        | 21     | 1     |
| 1:A:63:MET:CG   | 1:A:63:MET:HB3  | 0.87     | 1.43        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HG12 | 0.87     | 1.42        | 21     | 1     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HD3  | 0.86     | 1.40        | 21     | 1     |
| 1:A:2:MET:O     | 1:A:32:ALA:HB1  | 0.86     | 1.70        | 18     | 20    |
| 1:A:1:MET:CE    | 1:A:1:MET:SD    | 0.86     | 0.79        | 21     | 1     |
| 1:A:65:ARG:CG   | 1:A:65:ARG:HD2  | 0.86     | 1.39        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:73:LYS:NZ   | 1:A:73:LYS:HE3  | 0.86     | 1.36        | 21     | 1     |
| 1:A:4:ILE:HG13  | 1:A:56:VAL:HG12 | 0.86     | 1.48        | 14     | 14    |
| 1:A:1:MET:CG    | 1:A:1:MET:HB2   | 0.85     | 1.39        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:CG2  | 0.85     | 0.86        | 21     | 1     |
| 1:A:66:VAL:CG2  | 1:A:66:VAL:CB   | 0.85     | 0.85        | 21     | 1     |
| 1:A:4:ILE:HD13  | 1:A:34:PHE:CE2  | 0.85     | 2.06        | 8      | 12    |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:HD21 | 0.85     | 1.45        | 14     | 3     |
| 1:A:1:MET:CG    | 1:A:1:MET:HB3   | 0.85     | 1.39        | 21     | 1     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HD2  | 0.85     | 1.40        | 21     | 1     |
| 1:A:55:ALA:HB2  | 1:A:60:LEU:HD23 | 0.84     | 1.47        | 18     | 2     |
| 1:A:65:ARG:CG   | 1:A:65:ARG:HD3  | 0.84     | 1.39        | 21     | 1     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:CD   | 0.84     | 0.86        | 21     | 1     |
| 1:A:7:TYR:CD1   | 1:A:43:ILE:HA   | 0.84     | 2.07        | 16     | 12    |
| 1:A:19:LYS:CE   | 1:A:19:LYS:HD3  | 0.84     | 1.37        | 21     | 1     |
| 1:A:49:THR:HG23 | 1:A:49:THR:CB   | 0.84     | 1.37        | 21     | 1     |
| 1:A:73:LYS:HE3  | 1:A:73:LYS:CD   | 0.84     | 1.41        | 21     | 1     |
| 1:A:9:THR:C     | 1:A:10:GLY:N    | 0.84     | 0.81        | 21     | 1     |
| 1:A:16:MET:CE   | 1:A:16:MET:SD   | 0.84     | 0.78        | 21     | 1     |
| 1:A:36:LYS:CE   | 1:A:36:LYS:HD2  | 0.84     | 1.37        | 21     | 1     |
| 1:A:40:MET:CE   | 1:A:40:MET:SD   | 0.84     | 0.80        | 21     | 1     |
| 1:A:7:TYR:CD1   | 1:A:37:ILE:HD12 | 0.83     | 2.07        | 12     | 5     |
| 1:A:49:THR:CB   | 1:A:49:THR:HG21 | 0.83     | 1.37        | 21     | 1     |
| 1:A:30:ILE:CB   | 1:A:30:ILE:CG1  | 0.83     | 0.83        | 21     | 1     |
| 1:A:55:ALA:HB2  | 1:A:60:LEU:CD2  | 0.83     | 2.04        | 10     | 3     |
| 1:A:49:THR:CB   | 1:A:49:THR:HG22 | 0.83     | 1.37        | 21     | 1     |
| 1:A:6:ILE:CD1   | 1:A:6:ILE:HG12  | 0.83     | 1.38        | 21     | 1     |
| 1:A:19:LYS:CD   | 1:A:19:LYS:HE2  | 0.82     | 1.36        | 21     | 1     |
| 1:A:6:ILE:CD1   | 1:A:6:ILE:HG13  | 0.82     | 1.38        | 21     | 1     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD12 | 0.82     | 1.35        | 21     | 1     |
| 1:A:7:TYR:CD2   | 1:A:43:ILE:HA   | 0.82     | 2.09        | 7      | 8     |
| 1:A:19:LYS:CE   | 1:A:19:LYS:HD2  | 0.82     | 1.37        | 21     | 1     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD13 | 0.82     | 1.35        | 21     | 1     |
| 1:A:19:LYS:CD   | 1:A:19:LYS:HE3  | 0.82     | 1.36        | 21     | 1     |
| 1:A:36:LYS:CE   | 1:A:36:LYS:HD3  | 0.82     | 1.37        | 21     | 1     |
| 1:A:40:MET:SD   | 1:A:40:MET:HE2  | 0.82     | 1.45        | 21     | 1     |
| 1:A:4:ILE:HD12  | 1:A:34:PHE:CE2  | 0.81     | 2.10        | 2      | 5     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD11 | 0.81     | 1.35        | 21     | 1     |
| 1:A:40:MET:SD   | 1:A:40:MET:HE1  | 0.81     | 1.45        | 21     | 1     |
| 1:A:73:LYS:CD   | 1:A:73:LYS:HE2  | 0.81     | 1.41        | 21     | 1     |
| 1:A:34:PHE:CE2  | 1:A:34:PHE:HZ   | 0.81     | 1.65        | 21     | 1     |
| 1:A:36:LYS:CD   | 1:A:36:LYS:HE2  | 0.81     | 1.35        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:54:LEU:HD11 | 1:A:66:VAL:HG23 | 0.81     | 1.50        | 14     | 1     |
| 1:A:36:LYS:CD   | 1:A:36:LYS:CE   | 0.81     | 0.83        | 21     | 1     |
| 1:A:36:LYS:CD   | 1:A:36:LYS:HE3  | 0.81     | 1.35        | 21     | 1     |
| 1:A:50:ALA:HB3  | 1:A:63:MET:CB   | 0.81     | 2.06        | 5      | 3     |
| 1:A:1:MET:CB    | 1:A:1:MET:HG2   | 0.81     | 1.37        | 21     | 1     |
| 1:A:19:LYS:CD   | 1:A:19:LYS:CE   | 0.81     | 0.85        | 21     | 1     |
| 1:A:50:ALA:HB3  | 1:A:63:MET:HB2  | 0.80     | 1.50        | 8      | 3     |
| 1:A:1:MET:SD    | 1:A:1:MET:HE2   | 0.80     | 1.44        | 21     | 1     |
| 1:A:1:MET:CG    | 1:A:1:MET:CB    | 0.80     | 0.81        | 21     | 1     |
| 1:A:5:GLN:O     | 1:A:54:LEU:HD13 | 0.80     | 1.77        | 12     | 3     |
| 1:A:1:MET:SD    | 1:A:1:MET:HE1   | 0.80     | 1.44        | 21     | 1     |
| 1:A:41:ASP:OD1  | 1:A:41:ASP:CG   | 0.80     | 0.64        | 21     | 1     |
| 1:A:25:VAL:HG11 | 1:A:32:ALA:HB3  | 0.80     | 1.54        | 1      | 16    |
| 1:A:40:MET:SD   | 1:A:40:MET:HE3  | 0.80     | 1.45        | 21     | 1     |
| 1:A:16:MET:SD   | 1:A:16:MET:HE1  | 0.80     | 1.43        | 21     | 1     |
| 1:A:34:PHE:CE1  | 1:A:34:PHE:HZ   | 0.80     | 1.63        | 21     | 1     |
| 1:A:65:ARG:CG   | 1:A:65:ARG:HE   | 0.80     | 1.89        | 21     | 1     |
| 1:A:16:MET:SD   | 1:A:16:MET:HE3  | 0.80     | 1.43        | 21     | 1     |
| 1:A:49:THR:CG2  | 1:A:49:THR:HG1  | 0.80     | 1.54        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:HG2   | 0.80     | 1.44        | 21     | 1     |
| 1:A:1:MET:SD    | 1:A:1:MET:HE3   | 0.80     | 1.44        | 21     | 1     |
| 1:A:1:MET:SD    | 1:A:1:MET:HG3   | 0.79     | 1.66        | 21     | 1     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HD3  | 0.79     | 1.33        | 21     | 1     |
| 1:A:16:MET:CE   | 1:A:16:MET:HG2  | 0.79     | 2.05        | 21     | 1     |
| 1:A:2:MET:SD    | 1:A:2:MET:HG3   | 0.79     | 1.44        | 21     | 1     |
| 1:A:7:TYR:HA    | 1:A:37:ILE:CD1  | 0.79     | 2.07        | 18     | 8     |
| 1:A:1:MET:CB    | 1:A:1:MET:HG3   | 0.79     | 1.37        | 21     | 1     |
| 1:A:73:LYS:NZ   | 1:A:73:LYS:HE2  | 0.78     | 1.36        | 21     | 1     |
| 1:A:17:LEU:HB2  | 1:A:66:VAL:HG13 | 0.78     | 1.53        | 21     | 4     |
| 1:A:4:ILE:HD12  | 1:A:32:ALA:HB1  | 0.78     | 1.55        | 12     | 4     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HD2  | 0.78     | 1.33        | 21     | 1     |
| 1:A:29:GLY:O    | 1:A:30:ILE:HD13 | 0.78     | 1.78        | 19     | 1     |
| 1:A:16:MET:SD   | 1:A:16:MET:HE2  | 0.78     | 1.44        | 21     | 1     |
| 1:A:17:LEU:HD11 | 1:A:72:ILE:CD1  | 0.78     | 2.07        | 1      | 2     |
| 1:A:69:LYS:CD   | 1:A:69:LYS:HE2  | 0.77     | 1.34        | 21     | 1     |
| 1:A:4:ILE:HD12  | 1:A:34:PHE:CZ   | 0.77     | 2.13        | 1      | 5     |
| 1:A:52:PRO:O    | 1:A:62:ILE:HD12 | 0.77     | 1.78        | 15     | 2     |
| 1:A:9:THR:O     | 1:A:10:GLY:N    | 0.77     | 0.63        | 21     | 1     |
| 1:A:55:ALA:HB2  | 1:A:60:LEU:HD12 | 0.77     | 1.56        | 8      | 7     |
| 1:A:7:TYR:CZ    | 1:A:46:ALA:HB2  | 0.77     | 2.14        | 13     | 16    |
| 1:A:69:LYS:CG   | 1:A:69:LYS:HB2  | 0.77     | 1.30        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:2:MET:O     | 1:A:4:ILE:HD12  | 0.76     | 1.80        | 17     | 9     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:HD3  | 0.75     | 1.29        | 21     | 1     |
| 1:A:13:ASN:CG   | 1:A:13:ASN:HD22 | 0.75     | 1.36        | 21     | 1     |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:HD11 | 0.75     | 1.59        | 12     | 2     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:HD2  | 0.74     | 1.29        | 21     | 1     |
| 1:A:49:THR:OG1  | 1:A:49:THR:HG21 | 0.74     | 0.99        | 21     | 1     |
| 1:A:69:LYS:CG   | 1:A:69:LYS:HB3  | 0.74     | 1.30        | 21     | 1     |
| 1:A:6:ILE:N     | 1:A:37:ILE:HD11 | 0.74     | 1.97        | 10     | 5     |
| 1:A:61:LYS:O    | 1:A:62:ILE:HD13 | 0.74     | 1.81        | 9      | 2     |
| 1:A:55:ALA:HB2  | 1:A:60:LEU:HD22 | 0.74     | 1.60        | 7      | 5     |
| 1:A:4:ILE:HG12  | 1:A:56:VAL:HG12 | 0.74     | 1.58        | 16     | 4     |
| 1:A:63:MET:CE   | 1:A:63:MET:HB2  | 0.74     | 2.13        | 21     | 1     |
| 1:A:69:LYS:CD   | 1:A:69:LYS:HE3  | 0.74     | 1.34        | 21     | 1     |
| 1:A:4:ILE:CG1   | 1:A:56:VAL:HG12 | 0.73     | 2.14        | 5      | 18    |
| 1:A:69:LYS:CD   | 1:A:69:LYS:CE   | 0.73     | 0.85        | 21     | 1     |
| 1:A:36:LYS:C    | 1:A:37:ILE:HD13 | 0.73     | 2.04        | 3      | 8     |
| 1:A:13:ASN:CG   | 1:A:13:ASN:HD21 | 0.73     | 1.36        | 21     | 1     |
| 1:A:17:LEU:HD13 | 1:A:17:LEU:O    | 0.72     | 1.84        | 8      | 6     |
| 1:A:69:LYS:CB   | 1:A:69:LYS:HG3  | 0.72     | 1.26        | 21     | 1     |
| 1:A:69:LYS:CB   | 1:A:69:LYS:CG   | 0.72     | 0.74        | 21     | 1     |
| 1:A:48:LEU:HD22 | 1:A:48:LEU:N    | 0.72     | 1.99        | 14     | 7     |
| 1:A:69:LYS:HE2  | 1:A:69:LYS:NZ   | 0.72     | 1.30        | 21     | 1     |
| 1:A:7:TYR:CD1   | 1:A:37:ILE:HG13 | 0.72     | 2.19        | 16     | 10    |
| 1:A:37:ILE:HD13 | 1:A:37:ILE:O    | 0.72     | 1.84        | 8      | 3     |
| 1:A:43:ILE:CG2  | 1:A:48:LEU:HD21 | 0.72     | 2.14        | 2      | 14    |
| 1:A:26:LYS:CD   | 1:A:26:LYS:HE3  | 0.71     | 1.28        | 21     | 1     |
| 1:A:8:GLY:HA3   | 1:A:12:ALA:HB3  | 0.71     | 1.61        | 9      | 13    |
| 1:A:17:LEU:HD11 | 1:A:54:LEU:HG   | 0.71     | 1.62        | 10     | 1     |
| 1:A:22:ARG:HD3  | 1:A:22:ARG:HE   | 0.71     | 1.00        | 21     | 1     |
| 1:A:7:TYR:CE2   | 1:A:37:ILE:HG13 | 0.71     | 2.21        | 17     | 1     |
| 1:A:5:GLN:O     | 1:A:54:LEU:HD22 | 0.70     | 1.86        | 2      | 5     |
| 1:A:69:LYS:CB   | 1:A:69:LYS:HG2  | 0.70     | 1.26        | 21     | 1     |
| 1:A:48:LEU:HD13 | 1:A:60:LEU:HD21 | 0.70     | 1.62        | 4      | 4     |
| 1:A:1:MET:CE    | 1:A:1:MET:HG2   | 0.70     | 2.11        | 21     | 1     |
| 1:A:1:MET:SD    | 1:A:1:MET:HG2   | 0.70     | 1.66        | 21     | 1     |
| 1:A:34:PHE:CD1  | 1:A:34:PHE:CG   | 0.70     | 0.76        | 21     | 1     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:HE21 | 0.70     | 1.31        | 21     | 1     |
| 1:A:5:GLN:C     | 1:A:6:ILE:HD13  | 0.70     | 2.07        | 8      | 1     |
| 1:A:49:THR:CG2  | 1:A:49:THR:CB   | 0.70     | 0.70        | 21     | 1     |
| 1:A:4:ILE:HG23  | 1:A:54:LEU:HD21 | 0.70     | 1.63        | 4      | 3     |
| 1:A:26:LYS:CD   | 1:A:26:LYS:HE2  | 0.69     | 1.27        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:LEU:HD23 | 1:A:67:ALA:O    | 0.69     | 1.88        | 17     | 6     |
| 1:A:7:TYR:CD2   | 1:A:37:ILE:HG13 | 0.69     | 2.22        | 7      | 2     |
| 1:A:69:LYS:HE3  | 1:A:69:LYS:NZ   | 0.69     | 1.30        | 21     | 1     |
| 1:A:6:ILE:HG22  | 1:A:54:LEU:HD12 | 0.69     | 1.63        | 4      | 2     |
| 1:A:62:ILE:CD1  | 1:A:66:VAL:HG12 | 0.69     | 2.18        | 15     | 2     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:HE22 | 0.69     | 1.31        | 21     | 1     |
| 1:A:17:LEU:CD1  | 1:A:67:ALA:HB3  | 0.69     | 2.18        | 7      | 2     |
| 1:A:65:ARG:HG3  | 1:A:65:ARG:HD2  | 0.69     | 1.19        | 21     | 1     |
| 1:A:17:LEU:HD21 | 1:A:72:ILE:CD1  | 0.68     | 2.15        | 20     | 2     |
| 1:A:29:GLY:O    | 1:A:30:ILE:HG23 | 0.68     | 1.88        | 5      | 11    |
| 1:A:48:LEU:HD22 | 1:A:48:LEU:H    | 0.68     | 1.48        | 14     | 1     |
| 1:A:13:ASN:O    | 1:A:66:VAL:HG21 | 0.68     | 1.87        | 10     | 4     |
| 1:A:48:LEU:HD12 | 1:A:60:LEU:HD11 | 0.68     | 1.63        | 7      | 1     |
| 1:A:34:PHE:CG   | 1:A:34:PHE:CD2  | 0.68     | 0.74        | 21     | 1     |
| 1:A:46:ALA:O    | 1:A:60:LEU:HD21 | 0.68     | 1.89        | 16     | 11    |
| 1:A:26:LYS:CE   | 1:A:26:LYS:CD   | 0.68     | 0.77        | 21     | 1     |
| 1:A:55:ALA:CB   | 1:A:60:LEU:HD12 | 0.68     | 2.19        | 8      | 2     |
| 1:A:26:LYS:HD2  | 1:A:26:LYS:HE3  | 0.68     | 1.01        | 21     | 1     |
| 1:A:7:TYR:CE1   | 1:A:37:ILE:HG13 | 0.67     | 2.24        | 1      | 8     |
| 1:A:25:VAL:CG2  | 1:A:32:ALA:HB2  | 0.67     | 2.18        | 3      | 13    |
| 1:A:54:LEU:HD11 | 1:A:56:VAL:HG13 | 0.67     | 1.67        | 15     | 1     |
| 1:A:9:THR:O     | 1:A:9:THR:C     | 0.67     | 0.48        | 21     | 1     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HZ2  | 0.67     | 1.37        | 21     | 1     |
| 1:A:17:LEU:CD1  | 1:A:17:LEU:CG   | 0.67     | 0.67        | 21     | 1     |
| 1:A:22:ARG:CZ   | 1:A:22:ARG:HH21 | 0.67     | 1.38        | 21     | 1     |
| 1:A:11:CYS:CB   | 1:A:11:CYS:HG   | 0.67     | 1.91        | 21     | 1     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HZ3  | 0.67     | 1.37        | 21     | 1     |
| 1:A:22:ARG:CZ   | 1:A:22:ARG:HH22 | 0.67     | 1.38        | 21     | 1     |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:O    | 0.67     | 1.90        | 5      | 10    |
| 1:A:60:LEU:HD13 | 1:A:60:LEU:N    | 0.66     | 2.05        | 8      | 5     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HZ3  | 0.66     | 1.37        | 21     | 1     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD21 | 0.66     | 1.19        | 21     | 1     |
| 1:A:31:ASP:OD2  | 1:A:31:ASP:CG   | 0.66     | 0.55        | 21     | 1     |
| 1:A:25:VAL:HA   | 1:A:28:LEU:HD23 | 0.66     | 1.67        | 16     | 1     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD22 | 0.66     | 1.19        | 21     | 1     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HZ1  | 0.66     | 1.37        | 21     | 1     |
| 1:A:69:LYS:CB   | 1:A:69:LYS:HD2  | 0.66     | 2.12        | 21     | 1     |
| 1:A:57:ASP:OD2  | 1:A:57:ASP:CG   | 0.66     | 0.55        | 21     | 1     |
| 1:A:55:ALA:HB2  | 1:A:60:LEU:CD1  | 0.66     | 2.20        | 15     | 7     |
| 1:A:17:LEU:CG   | 1:A:17:LEU:HD23 | 0.66     | 1.19        | 21     | 1     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HZ1  | 0.66     | 1.37        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:ILE:N    | 1:A:30:ILE:HD13 | 0.65     | 2.05        | 1      | 2     |
| 1:A:50:ALA:HB3  | 1:A:63:MET:HG2  | 0.65     | 1.66        | 10     | 3     |
| 1:A:67:ALA:HB1  | 1:A:71:GLU:HB3  | 0.65     | 1.67        | 11     | 1     |
| 1:A:17:LEU:CD2  | 1:A:72:ILE:HD11 | 0.65     | 2.16        | 20     | 1     |
| 1:A:38:LYS:O    | 1:A:38:LYS:HG3  | 0.65     | 1.92        | 21     | 1     |
| 1:A:25:VAL:HG21 | 1:A:32:ALA:CB   | 0.65     | 2.22        | 10     | 10    |
| 1:A:13:ASN:ND2  | 1:A:13:ASN:CG   | 0.65     | 0.71        | 21     | 1     |
| 1:A:34:PHE:CZ   | 1:A:34:PHE:CE2  | 0.65     | 0.74        | 21     | 1     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HZ2  | 0.65     | 1.37        | 21     | 1     |
| 1:A:43:ILE:HG22 | 1:A:48:LEU:CD2  | 0.65     | 2.22        | 16     | 16    |
| 1:A:26:LYS:HE3  | 1:A:26:LYS:NZ   | 0.65     | 1.25        | 21     | 1     |
| 1:A:34:PHE:CZ   | 1:A:34:PHE:CE1  | 0.65     | 0.73        | 21     | 1     |
| 1:A:4:ILE:CD1   | 1:A:32:ALA:HB1  | 0.65     | 2.22        | 3      | 4     |
| 1:A:54:LEU:HB3  | 1:A:62:ILE:HD11 | 0.64     | 1.69        | 15     | 2     |
| 1:A:61:LYS:O    | 1:A:62:ILE:HD12 | 0.64     | 1.92        | 16     | 2     |
| 1:A:6:ILE:HG23  | 1:A:14:CYS:HB2  | 0.64     | 1.68        | 13     | 2     |
| 1:A:46:ALA:O    | 1:A:60:LEU:HD11 | 0.64     | 1.92        | 18     | 9     |
| 1:A:69:LYS:HA   | 1:A:72:ILE:HD12 | 0.64     | 1.69        | 14     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:HG13 | 0.64     | 1.70        | 21     | 1     |
| 1:A:60:LEU:HD12 | 1:A:63:MET:SD   | 0.64     | 2.32        | 7      | 1     |
| 1:A:4:ILE:HG21  | 1:A:34:PHE:CD2  | 0.64     | 2.27        | 15     | 8     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:NZ   | 0.64     | 0.79        | 21     | 1     |
| 1:A:72:ILE:O    | 1:A:72:ILE:HD13 | 0.64     | 1.93        | 8      | 4     |
| 1:A:7:TYR:HD1   | 1:A:37:ILE:HD12 | 0.64     | 1.52        | 8      | 3     |
| 1:A:17:LEU:CB   | 1:A:66:VAL:HG22 | 0.63     | 2.23        | 17     | 7     |
| 1:A:60:LEU:H    | 1:A:60:LEU:HD22 | 0.63     | 1.51        | 2      | 9     |
| 1:A:28:LEU:O    | 1:A:28:LEU:HD13 | 0.63     | 1.94        | 12     | 3     |
| 1:A:7:TYR:HD2   | 1:A:48:LEU:HD11 | 0.63     | 1.53        | 8      | 3     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:NZ   | 0.63     | 0.78        | 21     | 1     |
| 1:A:54:LEU:CD1  | 1:A:66:VAL:HG23 | 0.63     | 2.22        | 14     | 1     |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:HD23 | 0.63     | 1.68        | 10     | 1     |
| 1:A:17:LEU:CD1  | 1:A:17:LEU:HD23 | 0.63     | 1.18        | 21     | 1     |
| 1:A:65:ARG:CD   | 1:A:65:ARG:HB2  | 0.63     | 2.13        | 21     | 1     |
| 1:A:57:ASP:OD1  | 1:A:57:ASP:CG   | 0.62     | 0.49        | 21     | 1     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:HZ1  | 0.62     | 1.33        | 21     | 1     |
| 1:A:50:ALA:HB3  | 1:A:63:MET:HB3  | 0.62     | 1.68        | 5      | 3     |
| 1:A:5:GLN:CB    | 1:A:37:ILE:HD11 | 0.62     | 2.25        | 4      | 2     |
| 1:A:7:TYR:CE2   | 1:A:42:GLN:C    | 0.62     | 2.73        | 9      | 1     |
| 1:A:41:ASP:OD2  | 1:A:41:ASP:CG   | 0.62     | 0.50        | 21     | 1     |
| 1:A:48:LEU:H    | 1:A:48:LEU:HD22 | 0.62     | 1.53        | 2      | 2     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:HZ3  | 0.62     | 1.33        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:THR:O     | 1:A:9:THR:HB    | 0.61     | 1.95        | 21     | 1     |
| 1:A:7:TYR:CE2   | 1:A:43:ILE:HA   | 0.61     | 2.30        | 12     | 3     |
| 1:A:7:TYR:CE2   | 1:A:37:ILE:HG21 | 0.61     | 2.29        | 9      | 1     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:HZ2  | 0.61     | 1.33        | 21     | 1     |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:HD12 | 0.61     | 1.71        | 2      | 1     |
| 1:A:17:LEU:HD22 | 1:A:20:ASN:OD1  | 0.61     | 1.95        | 15     | 2     |
| 1:A:17:LEU:HD13 | 1:A:67:ALA:C    | 0.61     | 2.15        | 19     | 1     |
| 1:A:7:TYR:CD1   | 1:A:7:TYR:CG    | 0.61     | 0.74        | 21     | 1     |
| 1:A:26:LYS:HE2  | 1:A:26:LYS:NZ   | 0.61     | 1.25        | 21     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:CG1  | 0.61     | 2.26        | 21     | 8     |
| 1:A:17:LEU:HD22 | 1:A:54:LEU:HD13 | 0.61     | 1.70        | 3      | 3     |
| 1:A:62:ILE:HG21 | 1:A:66:VAL:HA   | 0.60     | 1.73        | 14     | 5     |
| 1:A:65:ARG:HD3  | 1:A:65:ARG:HB2  | 0.60     | 1.72        | 21     | 1     |
| 1:A:6:ILE:HD13  | 1:A:6:ILE:N     | 0.60     | 2.12        | 9      | 3     |
| 1:A:65:ARG:CB   | 1:A:65:ARG:HD3  | 0.60     | 1.85        | 21     | 1     |
| 1:A:4:ILE:CG2   | 1:A:54:LEU:HD11 | 0.60     | 2.26        | 2      | 2     |
| 1:A:7:TYR:CE2   | 1:A:48:LEU:HD11 | 0.60     | 2.31        | 12     | 3     |
| 1:A:7:TYR:CD2   | 1:A:37:ILE:CD1  | 0.60     | 2.85        | 18     | 4     |
| 1:A:54:LEU:HD11 | 1:A:66:VAL:CG2  | 0.60     | 2.26        | 14     | 1     |
| 1:A:17:LEU:HD11 | 1:A:17:LEU:HD23 | 0.60     | 0.68        | 21     | 1     |
| 1:A:17:LEU:CB   | 1:A:66:VAL:HG21 | 0.60     | 2.27        | 15     | 1     |
| 1:A:7:TYR:CB    | 1:A:43:ILE:HG23 | 0.60     | 2.27        | 9      | 4     |
| 1:A:42:GLN:CD   | 1:A:42:GLN:NE2  | 0.59     | 0.65        | 21     | 1     |
| 1:A:37:ILE:C    | 1:A:37:ILE:HD13 | 0.59     | 2.18        | 5      | 1     |
| 1:A:7:TYR:CZ    | 1:A:7:TYR:CE2   | 0.59     | 0.71        | 21     | 1     |
| 1:A:7:TYR:OH    | 1:A:46:ALA:HB2  | 0.59     | 1.98        | 13     | 6     |
| 1:A:25:VAL:CG1  | 1:A:32:ALA:HB3  | 0.59     | 2.28        | 1      | 4     |
| 1:A:73:LYS:CE   | 1:A:73:LYS:HG2  | 0.59     | 2.19        | 21     | 1     |
| 1:A:39:GLU:O    | 1:A:43:ILE:HG23 | 0.59     | 1.97        | 10     | 1     |
| 1:A:17:LEU:HD11 | 1:A:62:ILE:HD12 | 0.59     | 1.73        | 12     | 1     |
| 1:A:7:TYR:CD2   | 1:A:7:TYR:CG    | 0.59     | 0.73        | 21     | 1     |
| 1:A:17:LEU:HD12 | 1:A:67:ALA:O    | 0.59     | 1.98        | 3      | 2     |
| 1:A:37:ILE:N    | 1:A:37:ILE:CD1  | 0.58     | 2.39        | 21     | 9     |
| 1:A:26:LYS:CE   | 1:A:26:LYS:NZ   | 0.58     | 0.73        | 21     | 1     |
| 1:A:7:TYR:CZ    | 1:A:7:TYR:CE1   | 0.58     | 0.69        | 21     | 1     |
| 1:A:17:LEU:HD22 | 1:A:17:LEU:O    | 0.58     | 1.99        | 15     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:HB   | 0.58     | 1.75        | 5      | 3     |
| 1:A:12:ALA:HB1  | 1:A:52:PRO:HB3  | 0.57     | 1.76        | 8      | 2     |
| 1:A:7:TYR:HB3   | 1:A:43:ILE:HG23 | 0.57     | 1.76        | 7      | 7     |
| 1:A:22:ARG:CZ   | 1:A:22:ARG:NH2  | 0.57     | 0.73        | 21     | 1     |
| 1:A:54:LEU:CD1  | 1:A:54:LEU:HD23 | 0.57     | 1.11        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:54:LEU:HD21 | 1:A:54:LEU:HD12 | 0.57     | 0.62        | 21     | 1     |
| 1:A:17:LEU:HD23 | 1:A:67:ALA:C    | 0.57     | 2.19        | 9      | 3     |
| 1:A:50:ALA:HB3  | 1:A:63:MET:CG   | 0.57     | 2.29        | 10     | 3     |
| 1:A:31:ASP:OD1  | 1:A:31:ASP:CG   | 0.57     | 0.46        | 21     | 1     |
| 1:A:62:ILE:HD13 | 1:A:66:VAL:CG1  | 0.57     | 2.27        | 15     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:HG23 | 0.56     | 1.77        | 13     | 3     |
| 1:A:61:LYS:C    | 1:A:62:ILE:HD12 | 0.56     | 2.20        | 16     | 1     |
| 1:A:69:LYS:CB   | 1:A:69:LYS:HD3  | 0.56     | 2.16        | 21     | 1     |
| 1:A:34:PHE:CD1  | 1:A:34:PHE:N    | 0.56     | 2.73        | 18     | 6     |
| 1:A:21:ALA:O    | 1:A:25:VAL:HG12 | 0.56     | 2.00        | 14     | 4     |
| 1:A:51:LEU:CB   | 1:A:52:PRO:CD   | 0.56     | 2.83        | 4      | 6     |
| 1:A:17:LEU:HD12 | 1:A:67:ALA:C    | 0.56     | 2.20        | 7      | 1     |
| 1:A:17:LEU:HD23 | 1:A:54:LEU:CD2  | 0.56     | 2.30        | 19     | 1     |
| 1:A:17:LEU:HB3  | 1:A:66:VAL:HG21 | 0.56     | 1.78        | 15     | 2     |
| 1:A:6:ILE:HG23  | 1:A:54:LEU:HD21 | 0.56     | 1.77        | 8      | 1     |
| 1:A:54:LEU:HD12 | 1:A:54:LEU:CD2  | 0.56     | 1.22        | 21     | 1     |
| 1:A:51:LEU:CB   | 1:A:52:PRO:HD3  | 0.56     | 2.30        | 13     | 14    |
| 1:A:46:ALA:C    | 1:A:60:LEU:HD21 | 0.56     | 2.21        | 18     | 2     |
| 1:A:40:MET:HA   | 1:A:43:ILE:HD12 | 0.56     | 1.77        | 2      | 4     |
| 1:A:17:LEU:CD2  | 1:A:54:LEU:HD13 | 0.56     | 2.31        | 3      | 1     |
| 1:A:6:ILE:HG22  | 1:A:14:CYS:HB2  | 0.56     | 1.77        | 8      | 3     |
| 1:A:6:ILE:HD13  | 1:A:6:ILE:HG21  | 0.56     | 1.62        | 21     | 1     |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:CD1  | 0.55     | 2.31        | 2      | 1     |
| 1:A:50:ALA:HB3  | 1:A:64:GLY:N    | 0.55     | 2.16        | 14     | 2     |
| 1:A:1:MET:HB3   | 1:A:1:MET:HG2   | 0.55     | 1.21        | 21     | 1     |
| 1:A:17:LEU:HB2  | 1:A:66:VAL:HG22 | 0.55     | 1.79        | 21     | 5     |
| 1:A:7:TYR:HA    | 1:A:37:ILE:HD12 | 0.55     | 1.79        | 20     | 7     |
| 1:A:54:LEU:HD12 | 1:A:66:VAL:CG2  | 0.55     | 2.32        | 5      | 1     |
| 1:A:24:ALA:O    | 1:A:28:LEU:HD23 | 0.55     | 2.02        | 15     | 4     |
| 1:A:25:VAL:HG13 | 1:A:26:LYS:N    | 0.54     | 2.17        | 6      | 21    |
| 1:A:7:TYR:CD1   | 1:A:37:ILE:CD1  | 0.54     | 2.90        | 6      | 5     |
| 1:A:22:ARG:HA   | 1:A:34:PHE:CZ   | 0.54     | 2.36        | 18     | 2     |
| 1:A:1:MET:H3    | 1:A:31:ASP:C    | 0.54     | 2.06        | 3      | 1     |
| 1:A:68:SER:CB   | 1:A:68:SER:HG   | 0.54     | 1.24        | 21     | 1     |
| 1:A:17:LEU:CB   | 1:A:66:VAL:HG13 | 0.54     | 2.32        | 10     | 1     |
| 1:A:2:MET:HB2   | 1:A:32:ALA:HB2  | 0.54     | 1.78        | 1      | 2     |
| 1:A:54:LEU:HD13 | 1:A:54:LEU:O    | 0.54     | 2.03        | 11     | 2     |
| 1:A:6:ILE:HD11  | 1:A:36:LYS:CG   | 0.54     | 2.32        | 10     | 1     |
| 1:A:47:GLY:HA3  | 1:A:60:LEU:HD21 | 0.54     | 1.79        | 13     | 2     |
| 1:A:2:MET:SD    | 1:A:30:ILE:HD12 | 0.54     | 2.43        | 2      | 1     |
| 1:A:34:PHE:CZ   | 1:A:34:PHE:HE2  | 0.54     | 1.29        | 21     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:53:GLY:O    | 1:A:54:LEU:HD22 | 0.53     | 2.04        | 20     | 1     |
| 1:A:34:PHE:CG   | 1:A:34:PHE:HD2  | 0.53     | 1.29        | 21     | 1     |
| 1:A:54:LEU:O    | 1:A:54:LEU:HD23 | 0.53     | 2.04        | 3      | 1     |
| 1:A:54:LEU:HD13 | 1:A:54:LEU:C    | 0.53     | 2.24        | 11     | 1     |
| 1:A:34:PHE:CG   | 1:A:34:PHE:HD1  | 0.53     | 1.30        | 21     | 1     |
| 1:A:37:ILE:HD13 | 1:A:37:ILE:C    | 0.53     | 2.24        | 8      | 2     |
| 1:A:4:ILE:HG23  | 1:A:54:LEU:CD1  | 0.53     | 2.33        | 19     | 1     |
| 1:A:17:LEU:C    | 1:A:17:LEU:HD13 | 0.53     | 2.23        | 15     | 1     |
| 1:A:34:PHE:CZ   | 1:A:34:PHE:HE1  | 0.53     | 1.28        | 21     | 1     |
| 1:A:54:LEU:CD1  | 1:A:54:LEU:CG   | 0.53     | 0.69        | 21     | 1     |
| 1:A:51:LEU:O    | 1:A:53:GLY:N    | 0.53     | 2.42        | 16     | 3     |
| 1:A:46:ALA:CB   | 1:A:60:LEU:HD21 | 0.52     | 2.28        | 14     | 1     |
| 1:A:54:LEU:CD2  | 1:A:54:LEU:HD11 | 0.52     | 1.06        | 21     | 1     |
| 1:A:54:LEU:HD23 | 1:A:54:LEU:HD11 | 0.52     | 0.85        | 21     | 1     |
| 1:A:54:LEU:HB2  | 1:A:62:ILE:HD11 | 0.52     | 1.82        | 4      | 1     |
| 1:A:51:LEU:HD23 | 1:A:51:LEU:N    | 0.52     | 2.19        | 17     | 1     |
| 1:A:7:TYR:CD1   | 1:A:37:ILE:CG1  | 0.52     | 2.93        | 3      | 9     |
| 1:A:26:LYS:HE2  | 1:A:26:LYS:HZ3  | 0.52     | 1.10        | 21     | 1     |
| 1:A:48:LEU:O    | 1:A:49:THR:HG23 | 0.52     | 2.05        | 2      | 1     |
| 1:A:48:LEU:C    | 1:A:48:LEU:HD23 | 0.52     | 2.24        | 3      | 4     |
| 1:A:6:ILE:HG22  | 1:A:54:LEU:CD1  | 0.52     | 2.34        | 4      | 1     |
| 1:A:17:LEU:HD21 | 1:A:72:ILE:HB   | 0.52     | 1.82        | 5      | 1     |
| 1:A:48:LEU:C    | 1:A:49:THR:HG23 | 0.51     | 2.25        | 2      | 1     |
| 1:A:17:LEU:HD13 | 1:A:21:ALA:HB2  | 0.51     | 1.80        | 5      | 1     |
| 1:A:54:LEU:HD22 | 1:A:62:ILE:HD12 | 0.51     | 1.81        | 7      | 1     |
| 1:A:21:ALA:HB3  | 1:A:34:PHE:HE2  | 0.51     | 1.65        | 18     | 2     |
| 1:A:44:LEU:HD23 | 1:A:45:GLU:H    | 0.51     | 1.65        | 3      | 6     |
| 1:A:17:LEU:HD23 | 1:A:54:LEU:HD22 | 0.51     | 1.83        | 19     | 1     |
| 1:A:54:LEU:C    | 1:A:54:LEU:HD13 | 0.51     | 2.26        | 9      | 3     |
| 1:A:55:ALA:CB   | 1:A:60:LEU:HD22 | 0.51     | 2.34        | 7      | 2     |
| 1:A:17:LEU:HD13 | 1:A:67:ALA:HB3  | 0.51     | 1.81        | 14     | 1     |
| 1:A:52:PRO:HD2  | 1:A:64:GLY:HA2  | 0.51     | 1.83        | 17     | 8     |
| 1:A:50:ALA:CB   | 1:A:64:GLY:N    | 0.51     | 2.74        | 20     | 13    |
| 1:A:72:ILE:HD13 | 1:A:72:ILE:C    | 0.51     | 2.26        | 11     | 3     |
| 1:A:38:LYS:O    | 1:A:39:GLU:HG3  | 0.51     | 2.07        | 21     | 1     |
| 1:A:72:ILE:C    | 1:A:72:ILE:HD13 | 0.50     | 2.26        | 7      | 1     |
| 1:A:25:VAL:CG1  | 1:A:26:LYS:N    | 0.50     | 2.74        | 18     | 21    |
| 1:A:17:LEU:CD2  | 1:A:17:LEU:HD13 | 0.50     | 1.11        | 21     | 1     |
| 1:A:4:ILE:HG23  | 1:A:56:VAL:HG13 | 0.50     | 1.83        | 2      | 4     |
| 1:A:4:ILE:CG2   | 1:A:34:PHE:CD2  | 0.50     | 2.95        | 19     | 10    |
| 1:A:44:LEU:HD23 | 1:A:45:GLU:N    | 0.50     | 2.21        | 3      | 6     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:46:ALA:HB1  | 1:A:60:LEU:CD2  | 0.50     | 2.36        | 18     | 2     |
| 1:A:62:ILE:HD11 | 1:A:67:ALA:HB2  | 0.50     | 1.83        | 18     | 1     |
| 1:A:69:LYS:CE   | 1:A:69:LYS:HG3  | 0.50     | 2.23        | 21     | 1     |
| 1:A:29:GLY:C    | 1:A:30:ILE:HD13 | 0.50     | 2.26        | 1      | 1     |
| 1:A:20:ASN:OD1  | 1:A:21:ALA:N    | 0.50     | 2.45        | 12     | 6     |
| 1:A:46:ALA:CB   | 1:A:60:LEU:HD11 | 0.50     | 2.36        | 12     | 1     |
| 1:A:1:MET:CA    | 1:A:1:MET:HG3   | 0.50     | 2.01        | 21     | 1     |
| 1:A:48:LEU:O    | 1:A:49:THR:CB   | 0.49     | 2.59        | 14     | 2     |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:C    | 0.49     | 2.26        | 5      | 5     |
| 1:A:32:ALA:HB3  | 1:A:34:PHE:HE1  | 0.49     | 1.68        | 10     | 2     |
| 1:A:43:ILE:CG1  | 1:A:44:LEU:N    | 0.49     | 2.76        | 12     | 3     |
| 1:A:7:TYR:CD2   | 1:A:37:ILE:CG1  | 0.49     | 2.95        | 7      | 2     |
| 1:A:7:TYR:CD2   | 1:A:37:ILE:HD12 | 0.49     | 2.43        | 18     | 3     |
| 1:A:17:LEU:CD2  | 1:A:54:LEU:HD22 | 0.49     | 2.38        | 13     | 1     |
| 1:A:23:GLU:O    | 1:A:27:GLU:CB   | 0.49     | 2.60        | 10     | 18    |
| 1:A:30:ILE:CB   | 1:A:30:ILE:HD12 | 0.49     | 2.18        | 21     | 1     |
| 1:A:60:LEU:HD22 | 1:A:60:LEU:N    | 0.49     | 2.21        | 2      | 1     |
| 1:A:1:MET:CG    | 1:A:1:MET:HE3   | 0.49     | 2.19        | 21     | 1     |
| 1:A:17:LEU:HD13 | 1:A:17:LEU:HD22 | 0.49     | 0.59        | 21     | 1     |
| 1:A:7:TYR:HE2   | 1:A:46:ALA:CB   | 0.49     | 2.21        | 8      | 3     |
| 1:A:6:ILE:HD11  | 1:A:34:PHE:HB3  | 0.49     | 1.84        | 11     | 1     |
| 1:A:43:ILE:HG23 | 1:A:48:LEU:HD21 | 0.49     | 1.84        | 5      | 1     |
| 1:A:26:LYS:HE3  | 1:A:26:LYS:HZ1  | 0.49     | 1.10        | 21     | 1     |
| 1:A:48:LEU:HB2  | 1:A:63:MET:HG2  | 0.48     | 1.85        | 19     | 6     |
| 1:A:5:GLN:CA    | 1:A:37:ILE:HD11 | 0.48     | 2.38        | 14     | 1     |
| 1:A:17:LEU:HD13 | 1:A:67:ALA:O    | 0.48     | 2.08        | 13     | 2     |
| 1:A:4:ILE:HG23  | 1:A:54:LEU:HD11 | 0.48     | 1.85        | 1      | 3     |
| 1:A:32:ALA:HB3  | 1:A:34:PHE:CE1  | 0.48     | 2.43        | 14     | 3     |
| 1:A:17:LEU:HD23 | 1:A:18:GLU:N    | 0.48     | 2.22        | 10     | 1     |
| 1:A:48:LEU:N    | 1:A:48:LEU:CD2  | 0.48     | 2.73        | 14     | 1     |
| 1:A:7:TYR:CG    | 1:A:7:TYR:HD1   | 0.48     | 1.24        | 21     | 1     |
| 1:A:7:TYR:CG    | 1:A:7:TYR:HD2   | 0.48     | 1.24        | 21     | 1     |
| 1:A:39:GLU:O    | 1:A:43:ILE:HG13 | 0.48     | 2.08        | 17     | 9     |
| 1:A:1:MET:N     | 1:A:31:ASP:O    | 0.48     | 2.46        | 21     | 6     |
| 1:A:62:ILE:HD13 | 1:A:66:VAL:HA   | 0.48     | 1.86        | 19     | 3     |
| 1:A:5:GLN:HB3   | 1:A:7:TYR:CE1   | 0.48     | 2.44        | 5      | 1     |
| 1:A:25:VAL:HG22 | 1:A:30:ILE:O    | 0.48     | 2.09        | 14     | 2     |
| 1:A:22:ARG:HA   | 1:A:34:PHE:CE1  | 0.48     | 2.44        | 5      | 13    |
| 1:A:17:LEU:HD11 | 1:A:62:ILE:CD1  | 0.48     | 2.37        | 12     | 1     |
| 1:A:6:ILE:HG22  | 1:A:14:CYS:SG   | 0.48     | 2.49        | 18     | 3     |
| 1:A:22:ARG:CG   | 1:A:34:PHE:CD1  | 0.48     | 2.96        | 6      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:THR:CB   | 1:A:49:THR:HG1  | 0.48     | 1.18        | 21     | 1     |
| 1:A:7:TYR:CE2   | 1:A:46:ALA:HB2  | 0.47     | 2.44        | 6      | 3     |
| 1:A:6:ILE:HD11  | 1:A:36:LYS:HG3  | 0.47     | 1.85        | 10     | 1     |
| 1:A:7:TYR:CZ    | 1:A:7:TYR:HE2   | 0.47     | 1.23        | 21     | 1     |
| 1:A:53:GLY:HA2  | 1:A:62:ILE:O    | 0.47     | 2.09        | 10     | 4     |
| 1:A:50:ALA:HB1  | 1:A:64:GLY:N    | 0.47     | 2.25        | 20     | 4     |
| 1:A:46:ALA:HB3  | 1:A:48:LEU:HD13 | 0.47     | 1.86        | 6      | 3     |
| 1:A:54:LEU:HD12 | 1:A:62:ILE:CB   | 0.47     | 2.38        | 14     | 1     |
| 1:A:66:VAL:CG1  | 1:A:66:VAL:C    | 0.47     | 2.82        | 21     | 1     |
| 1:A:54:LEU:HD23 | 1:A:54:LEU:C    | 0.47     | 2.30        | 3      | 1     |
| 1:A:48:LEU:CD1  | 1:A:60:LEU:HD21 | 0.47     | 2.39        | 19     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:CG2  | 0.47     | 2.40        | 13     | 1     |
| 1:A:17:LEU:HD22 | 1:A:66:VAL:HB   | 0.47     | 1.86        | 13     | 1     |
| 1:A:6:ILE:HG22  | 1:A:54:LEU:HD22 | 0.47     | 1.87        | 14     | 1     |
| 1:A:48:LEU:C    | 1:A:48:LEU:CD2  | 0.47     | 2.83        | 3      | 2     |
| 1:A:4:ILE:HG12  | 1:A:56:VAL:CG1  | 0.46     | 2.40        | 15     | 3     |
| 1:A:72:ILE:HD13 | 1:A:72:ILE:O    | 0.46     | 2.10        | 7      | 1     |
| 1:A:17:LEU:HD13 | 1:A:17:LEU:C    | 0.46     | 2.30        | 18     | 2     |
| 1:A:54:LEU:N    | 1:A:62:ILE:O    | 0.46     | 2.48        | 8      | 1     |
| 1:A:7:TYR:CZ    | 1:A:7:TYR:HE1   | 0.46     | 1.22        | 21     | 1     |
| 1:A:17:LEU:HB3  | 1:A:66:VAL:HG22 | 0.46     | 1.87        | 10     | 2     |
| 1:A:48:LEU:CD2  | 1:A:48:LEU:C    | 0.46     | 2.83        | 15     | 8     |
| 1:A:4:ILE:CG2   | 1:A:54:LEU:HD21 | 0.46     | 2.40        | 11     | 1     |
| 1:A:54:LEU:HD12 | 1:A:62:ILE:CG1  | 0.46     | 2.40        | 14     | 1     |
| 1:A:4:ILE:CD1   | 1:A:34:PHE:CE2  | 0.46     | 2.99        | 15     | 1     |
| 1:A:28:LEU:HD21 | 1:A:73:LYS:HG2  | 0.46     | 1.86        | 15     | 1     |
| 1:A:1:MET:CG    | 1:A:1:MET:N     | 0.46     | 2.72        | 21     | 1     |
| 1:A:6:ILE:HD11  | 1:A:36:LYS:HB2  | 0.46     | 1.87        | 5      | 1     |
| 1:A:59:GLU:CG   | 1:A:59:GLU:O    | 0.46     | 2.64        | 1      | 1     |
| 1:A:16:MET:CB   | 1:A:66:VAL:HG11 | 0.46     | 2.40        | 2      | 1     |
| 1:A:38:LYS:O    | 1:A:39:GLU:CB   | 0.46     | 2.63        | 12     | 11    |
| 1:A:17:LEU:HD22 | 1:A:20:ASN:HD21 | 0.46     | 1.69        | 20     | 2     |
| 1:A:40:MET:HA   | 1:A:43:ILE:HG12 | 0.46     | 1.87        | 10     | 2     |
| 1:A:17:LEU:HD13 | 1:A:66:VAL:HG22 | 0.46     | 1.87        | 11     | 1     |
| 1:A:50:ALA:CB   | 1:A:63:MET:HB2  | 0.46     | 2.41        | 20     | 2     |
| 1:A:1:MET:CA    | 1:A:31:ASP:O    | 0.46     | 2.64        | 10     | 19    |
| 1:A:6:ILE:HD13  | 1:A:18:GLU:HG3  | 0.46     | 1.87        | 3      | 1     |
| 1:A:6:ILE:HG23  | 1:A:54:LEU:CD2  | 0.46     | 2.41        | 8      | 1     |
| 1:A:7:TYR:CE1   | 1:A:37:ILE:HD12 | 0.46     | 2.46        | 16     | 2     |
| 1:A:62:ILE:HG21 | 1:A:66:VAL:HG12 | 0.46     | 1.86        | 3      | 1     |
| 1:A:1:MET:CB    | 1:A:31:ASP:O    | 0.45     | 2.64        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:24:ALA:O    | 1:A:28:LEU:HB2  | 0.45     | 2.10        | 21     | 1     |
| 1:A:60:LEU:N    | 1:A:60:LEU:HD13 | 0.45     | 2.26        | 2      | 2     |
| 1:A:72:ILE:HG23 | 1:A:73:LYS:N    | 0.45     | 2.26        | 15     | 4     |
| 1:A:46:ALA:HB3  | 1:A:48:LEU:CD1  | 0.45     | 2.41        | 9      | 1     |
| 1:A:17:LEU:HB2  | 1:A:66:VAL:CG1  | 0.45     | 2.36        | 21     | 1     |
| 1:A:6:ILE:C     | 1:A:37:ILE:HD11 | 0.45     | 2.31        | 15     | 2     |
| 1:A:36:LYS:HD2  | 1:A:36:LYS:HE3  | 0.45     | 1.31        | 21     | 1     |
| 1:A:46:ALA:O    | 1:A:60:LEU:CD2  | 0.45     | 2.64        | 21     | 1     |
| 1:A:7:TYR:HE2   | 1:A:46:ALA:HB2  | 0.45     | 1.72        | 8      | 1     |
| 1:A:6:ILE:HG23  | 1:A:54:LEU:HD11 | 0.45     | 1.88        | 12     | 1     |
| 1:A:40:MET:HA   | 1:A:43:ILE:CD1  | 0.45     | 2.41        | 21     | 1     |
| 1:A:4:ILE:O     | 1:A:34:PHE:HA   | 0.45     | 2.11        | 7      | 1     |
| 1:A:8:GLY:CA    | 1:A:12:ALA:HB3  | 0.45     | 2.42        | 17     | 2     |
| 1:A:48:LEU:CB   | 1:A:63:MET:CG   | 0.45     | 2.94        | 14     | 3     |
| 1:A:73:LYS:CG   | 1:A:73:LYS:HE2  | 0.45     | 2.00        | 21     | 1     |
| 1:A:40:MET:CA   | 1:A:43:ILE:HD12 | 0.44     | 2.42        | 2      | 1     |
| 1:A:7:TYR:CE2   | 1:A:37:ILE:HD12 | 0.44     | 2.46        | 7      | 1     |
| 1:A:54:LEU:HD12 | 1:A:54:LEU:CG   | 0.44     | 1.36        | 21     | 1     |
| 1:A:65:ARG:CD   | 1:A:65:ARG:HB3  | 0.44     | 2.18        | 21     | 1     |
| 1:A:8:GLY:O     | 1:A:10:GLY:N    | 0.44     | 2.50        | 6      | 2     |
| 1:A:43:ILE:O    | 1:A:48:LEU:HD22 | 0.44     | 2.12        | 13     | 1     |
| 1:A:41:ASP:O    | 1:A:44:LEU:HD23 | 0.44     | 2.13        | 13     | 11    |
| 1:A:73:LYS:HE3  | 1:A:73:LYS:HD2  | 0.44     | 1.31        | 21     | 1     |
| 1:A:17:LEU:CD1  | 1:A:72:ILE:HD11 | 0.44     | 2.22        | 1      | 1     |
| 1:A:12:ALA:HB1  | 1:A:52:PRO:CB   | 0.44     | 2.43        | 4      | 2     |
| 1:A:46:ALA:CB   | 1:A:60:LEU:HD12 | 0.44     | 2.43        | 2      | 1     |
| 1:A:6:ILE:HD13  | 1:A:18:GLU:CD   | 0.44     | 2.33        | 4      | 1     |
| 1:A:60:LEU:HD13 | 1:A:60:LEU:H    | 0.44     | 1.70        | 11     | 1     |
| 1:A:7:TYR:CD1   | 1:A:37:ILE:HB   | 0.44     | 2.47        | 4      | 1     |
| 1:A:7:TYR:CD1   | 1:A:7:TYR:N     | 0.44     | 2.84        | 8      | 3     |
| 1:A:6:ILE:N     | 1:A:6:ILE:CD1   | 0.44     | 2.81        | 8      | 2     |
| 1:A:50:ALA:CB   | 1:A:63:MET:CB   | 0.43     | 2.90        | 5      | 1     |
| 1:A:48:LEU:O    | 1:A:48:LEU:CD2  | 0.43     | 2.66        | 9      | 4     |
| 1:A:2:MET:N     | 1:A:32:ALA:HA   | 0.43     | 2.28        | 17     | 5     |
| 1:A:26:LYS:HG2  | 1:A:31:ASP:HA   | 0.43     | 1.89        | 21     | 1     |
| 1:A:6:ILE:CG2   | 1:A:14:CYS:CB   | 0.43     | 2.96        | 1      | 1     |
| 1:A:48:LEU:HB2  | 1:A:63:MET:CG   | 0.43     | 2.43        | 9      | 5     |
| 1:A:17:LEU:CD2  | 1:A:62:ILE:HD11 | 0.43     | 2.43        | 2      | 1     |
| 1:A:6:ILE:HD13  | 1:A:6:ILE:H     | 0.43     | 1.74        | 7      | 1     |
| 1:A:7:TYR:CE1   | 1:A:37:ILE:HG21 | 0.43     | 2.48        | 8      | 1     |
| 1:A:34:PHE:N    | 1:A:34:PHE:HD1  | 0.43     | 2.09        | 18     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:4:ILE:CG1   | 1:A:56:VAL:CG1  | 0.43     | 2.95        | 20     | 4     |
| 1:A:7:TYR:CE1   | 1:A:37:ILE:CG2  | 0.43     | 3.02        | 8      | 2     |
| 1:A:2:MET:CE    | 1:A:30:ILE:HG21 | 0.43     | 2.43        | 13     | 1     |
| 1:A:1:MET:HA    | 1:A:31:ASP:O    | 0.43     | 2.14        | 10     | 4     |
| 1:A:37:ILE:HG12 | 1:A:38:LYS:N    | 0.43     | 2.28        | 20     | 2     |
| 1:A:17:LEU:O    | 1:A:20:ASN:OD1  | 0.43     | 2.37        | 20     | 1     |
| 1:A:13:ASN:OD1  | 1:A:13:ASN:CG   | 0.43     | 0.55        | 21     | 1     |
| 1:A:22:ARG:HG3  | 1:A:34:PHE:CD1  | 0.43     | 2.49        | 9      | 6     |
| 1:A:7:TYR:HA    | 1:A:37:ILE:HD11 | 0.43     | 1.87        | 18     | 1     |
| 1:A:48:LEU:CB   | 1:A:63:MET:HG2  | 0.43     | 2.44        | 7      | 1     |
| 1:A:23:GLU:HG3  | 1:A:24:ALA:N    | 0.43     | 2.28        | 14     | 1     |
| 1:A:17:LEU:CD1  | 1:A:17:LEU:HD22 | 0.43     | 1.03        | 21     | 1     |
| 1:A:2:MET:CE    | 1:A:30:ILE:HD12 | 0.43     | 2.44        | 3      | 1     |
| 1:A:4:ILE:HB    | 1:A:34:PHE:CD2  | 0.43     | 2.49        | 14     | 4     |
| 1:A:54:LEU:HD21 | 1:A:56:VAL:HG13 | 0.43     | 1.89        | 3      | 1     |
| 1:A:7:TYR:HA    | 1:A:37:ILE:CG1  | 0.43     | 2.44        | 7      | 3     |
| 1:A:48:LEU:CD2  | 1:A:48:LEU:O    | 0.42     | 2.67        | 4      | 3     |
| 1:A:14:CYS:HA   | 1:A:66:VAL:HG21 | 0.42     | 1.90        | 20     | 1     |
| 1:A:30:ILE:N    | 1:A:30:ILE:CD1  | 0.42     | 2.76        | 1      | 1     |
| 1:A:17:LEU:CD2  | 1:A:17:LEU:HD11 | 0.42     | 0.96        | 21     | 1     |
| 1:A:2:MET:HE3   | 1:A:30:ILE:HD12 | 0.42     | 1.89        | 3      | 1     |
| 1:A:48:LEU:HD12 | 1:A:53:GLY:HA3  | 0.42     | 1.91        | 6      | 1     |
| 1:A:5:GLN:C     | 1:A:37:ILE:HD11 | 0.42     | 2.34        | 10     | 1     |
| 1:A:17:LEU:HD12 | 1:A:17:LEU:HD21 | 0.42     | 0.43        | 21     | 1     |
| 1:A:17:LEU:CB   | 1:A:66:VAL:CG2  | 0.42     | 2.96        | 17     | 3     |
| 1:A:8:GLY:C     | 1:A:9:THR:HG1   | 0.42     | 2.17        | 16     | 1     |
| 1:A:43:ILE:O    | 1:A:48:LEU:HD21 | 0.42     | 2.13        | 17     | 1     |
| 1:A:8:GLY:HA3   | 1:A:12:ALA:CB   | 0.42     | 2.44        | 21     | 1     |
| 1:A:5:GLN:HB2   | 1:A:37:ILE:HD11 | 0.42     | 1.92        | 14     | 1     |
| 1:A:72:ILE:CG2  | 1:A:73:LYS:N    | 0.42     | 2.83        | 5      | 1     |
| 1:A:7:TYR:HD1   | 1:A:43:ILE:HG22 | 0.42     | 1.75        | 10     | 1     |
| 1:A:17:LEU:HG   | 1:A:67:ALA:HB3  | 0.42     | 1.91        | 1      | 1     |
| 1:A:48:LEU:CB   | 1:A:63:MET:CB   | 0.42     | 2.98        | 2      | 1     |
| 1:A:5:GLN:O     | 1:A:54:LEU:HA   | 0.42     | 2.15        | 15     | 1     |
| 1:A:46:ALA:C    | 1:A:60:LEU:HD11 | 0.42     | 2.35        | 20     | 1     |
| 1:A:17:LEU:CD2  | 1:A:17:LEU:CA   | 0.42     | 2.88        | 21     | 1     |
| 1:A:54:LEU:C    | 1:A:54:LEU:HD12 | 0.42     | 2.35        | 15     | 1     |
| 1:A:48:LEU:N    | 1:A:48:LEU:HD22 | 0.41     | 2.30        | 9      | 2     |
| 1:A:17:LEU:HD21 | 1:A:72:ILE:HG12 | 0.41     | 1.91        | 1      | 1     |
| 1:A:62:ILE:HG21 | 1:A:66:VAL:CA   | 0.41     | 2.45        | 9      | 1     |
| 1:A:43:ILE:O    | 1:A:48:LEU:CD2  | 0.41     | 2.67        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:4:ILE:HG13  | 1:A:56:VAL:CG1  | 0.41     | 2.44        | 19     | 1     |
| 1:A:52:PRO:O    | 1:A:62:ILE:CG2  | 0.41     | 2.68        | 18     | 1     |
| 1:A:25:VAL:HG11 | 1:A:32:ALA:CB   | 0.41     | 2.37        | 1      | 2     |
| 1:A:5:GLN:CB    | 1:A:37:ILE:CD1  | 0.41     | 2.97        | 4      | 2     |
| 1:A:54:LEU:CD1  | 1:A:66:VAL:CG2  | 0.41     | 2.98        | 5      | 1     |
| 1:A:62:ILE:HD13 | 1:A:67:ALA:H    | 0.41     | 1.75        | 13     | 1     |
| 1:A:48:LEU:HD13 | 1:A:60:LEU:CD1  | 0.41     | 2.45        | 12     | 1     |
| 1:A:22:ARG:HG2  | 1:A:34:PHE:CD1  | 0.41     | 2.50        | 19     | 1     |
| 1:A:51:LEU:HD12 | 1:A:52:PRO:HD3  | 0.41     | 1.92        | 7      | 1     |
| 1:A:60:LEU:N    | 1:A:60:LEU:CD1  | 0.41     | 2.77        | 8      | 1     |
| 1:A:5:GLN:O     | 1:A:54:LEU:CD2  | 0.41     | 2.68        | 11     | 1     |
| 1:A:2:MET:CG    | 1:A:25:VAL:CG2  | 0.41     | 2.99        | 19     | 1     |
| 1:A:38:LYS:O    | 1:A:38:LYS:CG   | 0.41     | 2.62        | 21     | 1     |
| 1:A:4:ILE:HG22  | 1:A:54:LEU:HD21 | 0.41     | 1.93        | 2      | 1     |
| 1:A:6:ILE:HG22  | 1:A:54:LEU:HD23 | 0.41     | 1.93        | 10     | 1     |
| 1:A:62:ILE:HD12 | 1:A:62:ILE:N    | 0.41     | 2.31        | 14     | 1     |
| 1:A:48:LEU:O    | 1:A:63:MET:HG3  | 0.41     | 2.16        | 2      | 1     |
| 1:A:17:LEU:O    | 1:A:17:LEU:HD13 | 0.41     | 2.16        | 4      | 1     |
| 1:A:68:SER:HB3  | 1:A:68:SER:HG   | 0.41     | 1.36        | 21     | 1     |
| 1:A:4:ILE:HG21  | 1:A:34:PHE:CE2  | 0.40     | 2.51        | 4      | 1     |
| 1:A:17:LEU:HD21 | 1:A:72:ILE:CG1  | 0.40     | 2.46        | 1      | 1     |
| 1:A:6:ILE:H     | 1:A:37:ILE:HD11 | 0.40     | 1.70        | 2      | 1     |
| 1:A:41:ASP:O    | 1:A:44:LEU:CD2  | 0.40     | 2.70        | 10     | 1     |
| 1:A:17:LEU:CD2  | 1:A:17:LEU:CG   | 0.40     | 0.44        | 21     | 1     |
| 1:A:17:LEU:HD23 | 1:A:62:ILE:HD11 | 0.40     | 1.94        | 2      | 1     |
| 1:A:52:PRO:HG2  | 1:A:65:ARG:N    | 0.40     | 2.31        | 3      | 1     |
| 1:A:7:TYR:O     | 1:A:51:LEU:O    | 0.40     | 2.39        | 11     | 1     |
| 1:A:22:ARG:HG2  | 1:A:34:PHE:CE1  | 0.40     | 2.51        | 11     | 1     |
| 1:A:40:MET:O    | 1:A:43:ILE:HG12 | 0.40     | 2.17        | 13     | 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     | 72/77 (94%) | 58±2 (80±2%) | 11±1 (15±2%) | 4±1 (5±1%) | <b>4</b> <b>24</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| All | All   | 1512/1617 (94%) | 1209 (80%) | 225 (15%) | 78 (5%)  | 4           | 24 |

All 13 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     | 39  | GLU  | 21             |
| 1   | A     | 30  | ILE  | 16             |
| 1   | A     | 65  | ARG  | 15             |
| 1   | A     | 9   | THR  | 8              |
| 1   | A     | 10  | GLY  | 5              |
| 1   | A     | 8   | GLY  | 3              |
| 1   | A     | 66  | VAL  | 3              |
| 1   | A     | 11  | CYS  | 2              |
| 1   | A     | 51  | LEU  | 1              |
| 1   | A     | 48  | LEU  | 1              |
| 1   | A     | 49  | THR  | 1              |
| 1   | A     | 52  | PRO  | 1              |
| 1   | A     | 67  | ALA  | 1              |

### 6.3.2 Protein sidechains [i](#)

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     | 58/62 (94%)     | 36±4 (62±6%) | 22±4 (38±6%) | 0           | 6 |
| All | All   | 1218/1302 (94%) | 750 (62%)    | 468 (38%)    | 0           | 6 |

All 55 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     | 37  | ILE  | 21             |
| 1   | A     | 44  | LEU  | 21             |
| 1   | A     | 48  | LEU  | 21             |
| 1   | A     | 56  | VAL  | 21             |
| 1   | A     | 15  | GLN  | 20             |
| 1   | A     | 60  | LEU  | 19             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 41  | ASP  | 14             |
| 1   | A     | 61  | LYS  | 14             |
| 1   | A     | 36  | LYS  | 12             |
| 1   | A     | 38  | LYS  | 12             |
| 1   | A     | 2   | MET  | 11             |
| 1   | A     | 39  | GLU  | 11             |
| 1   | A     | 3   | LYS  | 11             |
| 1   | A     | 31  | ASP  | 11             |
| 1   | A     | 40  | MET  | 11             |
| 1   | A     | 63  | MET  | 11             |
| 1   | A     | 30  | ILE  | 10             |
| 1   | A     | 51  | LEU  | 10             |
| 1   | A     | 57  | ASP  | 10             |
| 1   | A     | 28  | LEU  | 9              |
| 1   | A     | 54  | LEU  | 9              |
| 1   | A     | 73  | LYS  | 9              |
| 1   | A     | 26  | LYS  | 9              |
| 1   | A     | 65  | ARG  | 9              |
| 1   | A     | 69  | LYS  | 8              |
| 1   | A     | 19  | LYS  | 8              |
| 1   | A     | 5   | GLN  | 8              |
| 1   | A     | 22  | ARG  | 8              |
| 1   | A     | 66  | VAL  | 8              |
| 1   | A     | 9   | THR  | 7              |
| 1   | A     | 17  | LEU  | 7              |
| 1   | A     | 59  | GLU  | 7              |
| 1   | A     | 6   | ILE  | 7              |
| 1   | A     | 49  | THR  | 7              |
| 1   | A     | 1   | MET  | 6              |
| 1   | A     | 68  | SER  | 6              |
| 1   | A     | 70  | GLU  | 6              |
| 1   | A     | 16  | MET  | 6              |
| 1   | A     | 11  | CYS  | 6              |
| 1   | A     | 72  | ILE  | 6              |
| 1   | A     | 71  | GLU  | 5              |
| 1   | A     | 35  | GLU  | 4              |
| 1   | A     | 42  | GLN  | 4              |
| 1   | A     | 45  | GLU  | 4              |
| 1   | A     | 62  | ILE  | 4              |
| 1   | A     | 23  | GLU  | 3              |
| 1   | A     | 18  | GLU  | 3              |
| 1   | A     | 33  | GLU  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 4   | ILE  | 2              |
| 1   | A     | 34  | PHE  | 2              |
| 1   | A     | 43  | ILE  | 2              |
| 1   | A     | 27  | GLU  | 2              |
| 1   | A     | 13  | ASN  | 1              |
| 1   | A     | 7   | TYR  | 1              |
| 1   | A     | 20  | ASN  | 1              |

### 6.3.3 RNA [i](#)

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 monosaccharides 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 21-A  | 5                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 21    | A     | 11:CYS    | C      | 12:ALA    | N      | 1.18         |
| 21    | A     | 37:ILE    | C      | 38:LYS    | N      | 1.13         |
| 21    | A     | 48:LEU    | C      | 49:THR    | N      | 1.11         |
| 21    | A     | 10:GLY    | C      | 11:CYS    | N      | 1.08         |
| 21    | A     | 9:THR     | C      | 10:GLY    | N      | 0.81         |

## 7 Chemical shift validation

No chemical shift data were provided