



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 03:41 AM UTC

PDB ID : 2GA5 / pdb\_00002ga5  
Title : yeast frataxin  
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Deposited on : 2006-03-07

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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

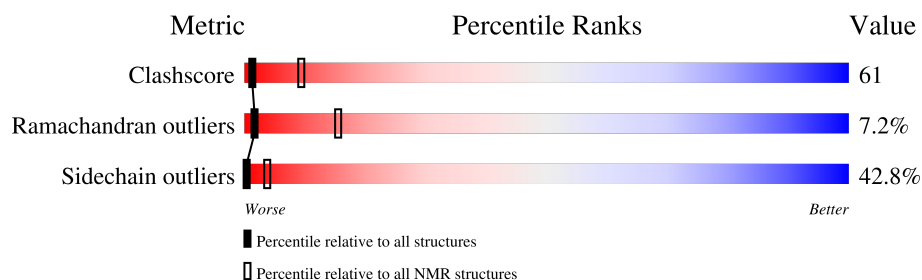
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

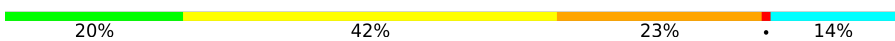
The overall completeness of chemical shifts assignment was not calculated.

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<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

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     | 123    |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:18-A:123 (106)      | 1.02              | 15           |

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1908 atoms, of which 939 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Frataxin homolog, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 123      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1908  | 611 | 939 | 156 | 199 | 3 |       |

There is a discrepancy between the modelled and reference sequences:

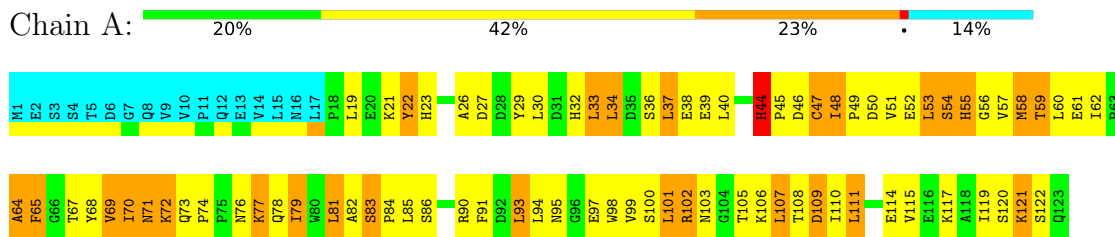
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MET      | -      | cloning artifact | UNP Q07540 |

## 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: Frataxin homolog, mitochondrial

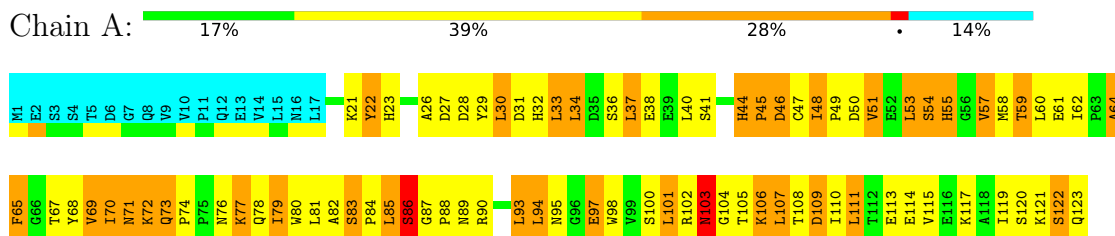


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

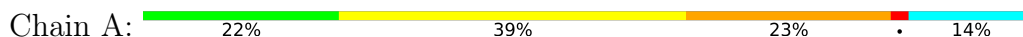
#### 4.2.1 Score per residue for model 1

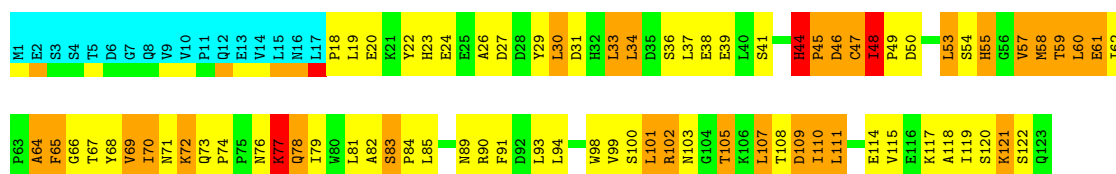
- Molecule 1: Frataxin homolog, mitochondrial



#### 4.2.2 Score per residue for model 2

- Molecule 1: Frataxin homolog, mitochondrial

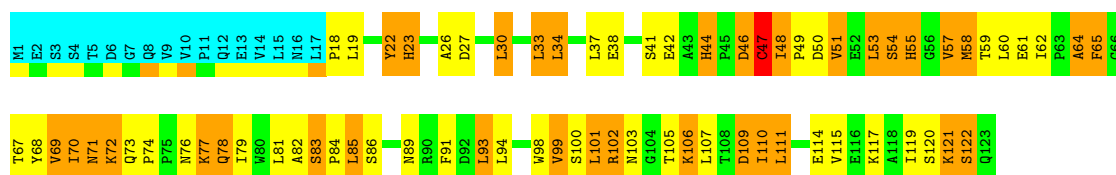




### 4.2.3 Score per residue for model 3

- Molecule 1: Frataxin homolog, mitochondrial

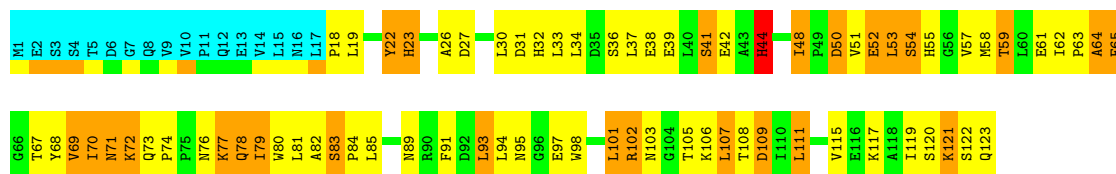
Chain A: 28% 30% 28% 14%



### 4.2.4 Score per residue for model 4

- Molecule 1: Frataxin homolog, mitochondrial

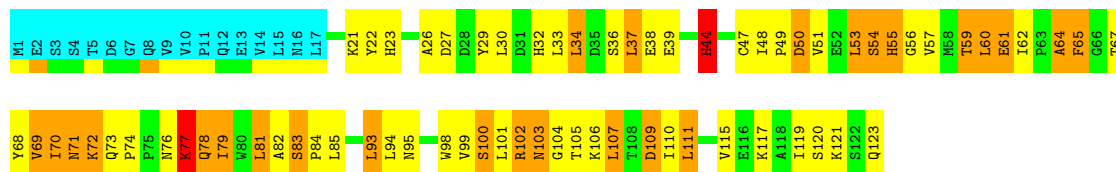
Chain A: 26% 38% 21% 14%



### 4.2.5 Score per residue for model 5

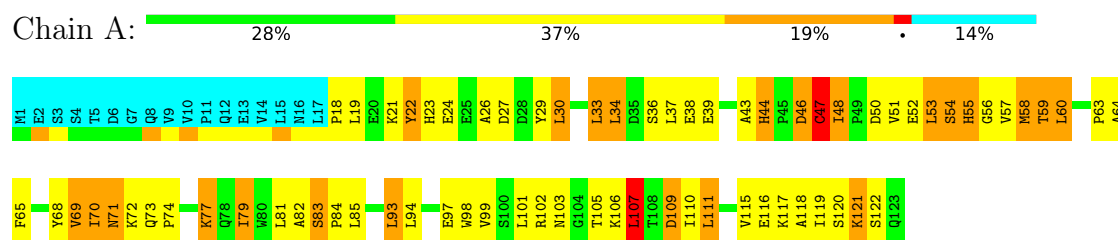
- Molecule 1: Frataxin homolog, mitochondrial

Chain A: 29% 34% 21% 14%



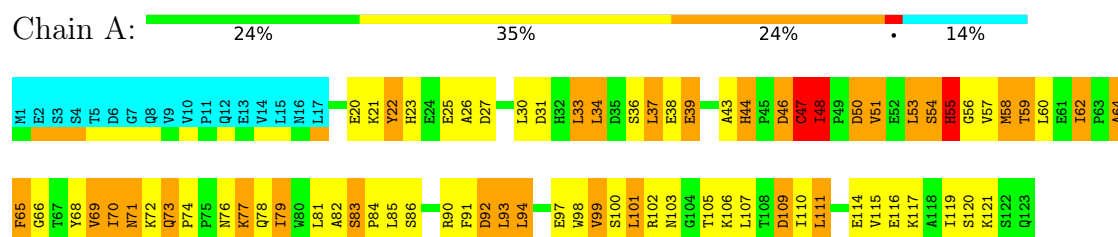
### 4.2.6 Score per residue for model 6

- Molecule 1: Frataxin homolog, mitochondrial



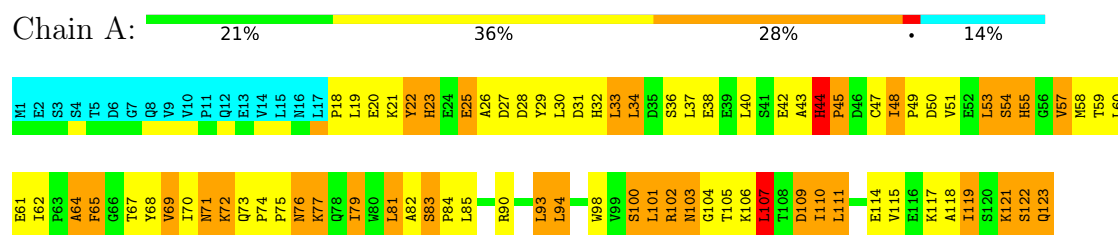
#### 4.2.7 Score per residue for model 7

- Molecule 1: Frataxin homolog, mitochondrial



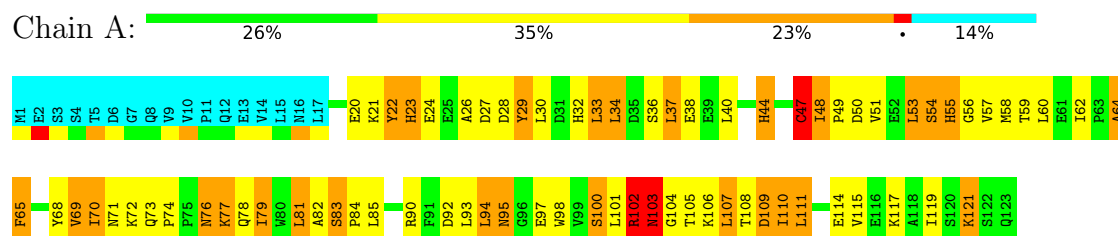
#### 4.2.8 Score per residue for model 8

- Molecule 1: Frataxin homolog, mitochondrial



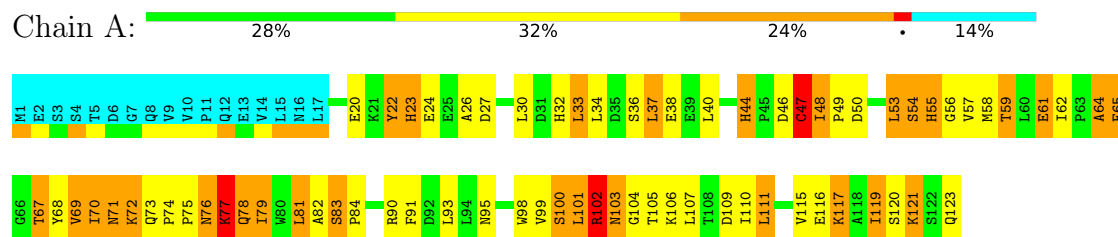
#### 4.2.9 Score per residue for model 9

- Molecule 1: Frataxin homolog, mitochondrial



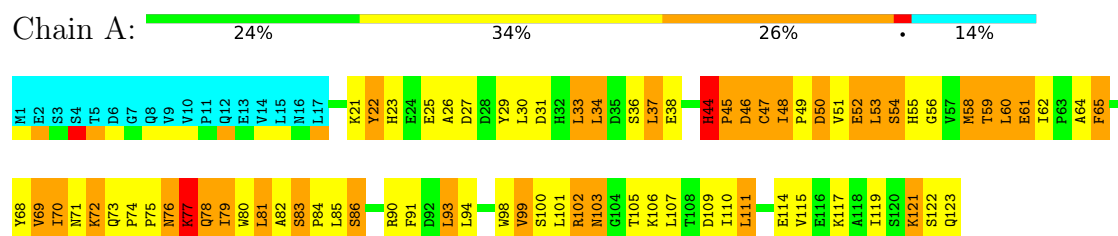
### 4.2.10 Score per residue for model 10

- Molecule 1: Frataxin homolog, mitochondrial



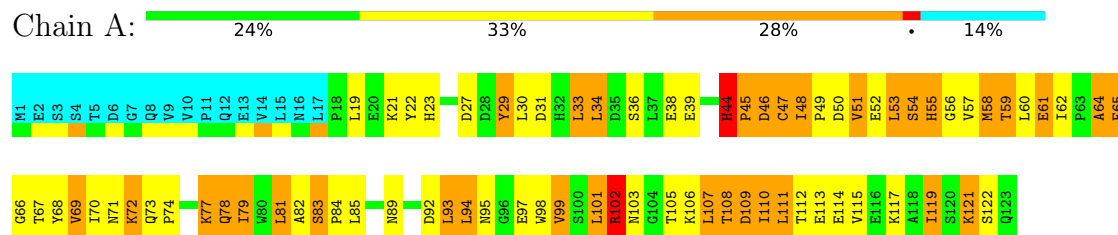
### 4.2.11 Score per residue for model 11

- Molecule 1: Frataxin homolog, mitochondrial



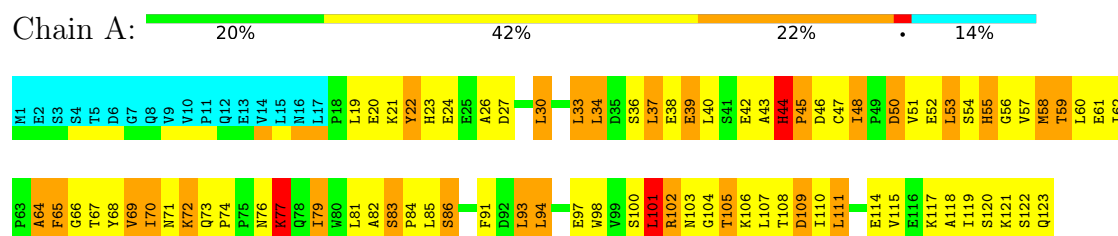
### 4.2.12 Score per residue for model 12

- Molecule 1: Frataxin homolog, mitochondrial



### 4.2.13 Score per residue for model 13

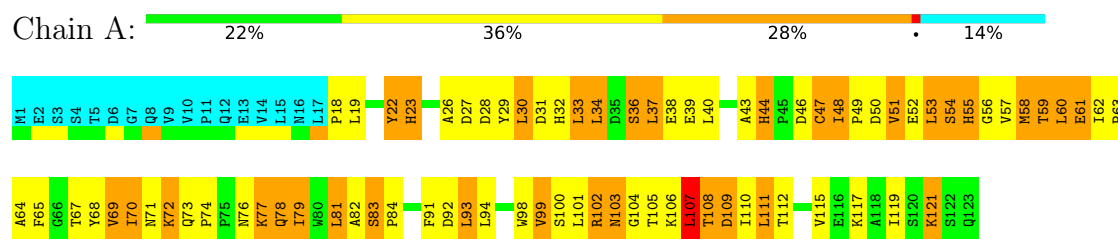
- Molecule 1: Frataxin homolog, mitochondrial





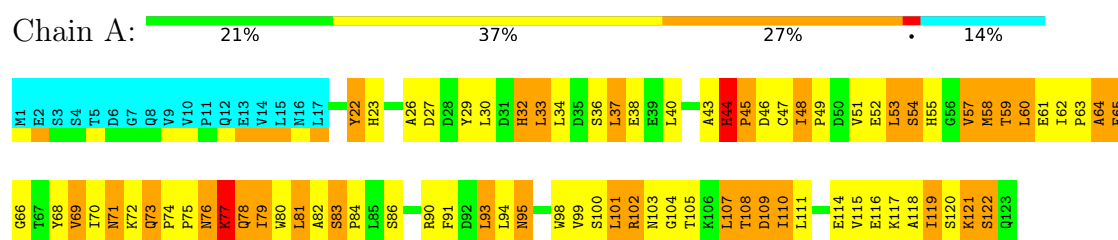
#### 4.2.14 Score per residue for model 14

- Molecule 1: Frataxin homolog, mitochondrial



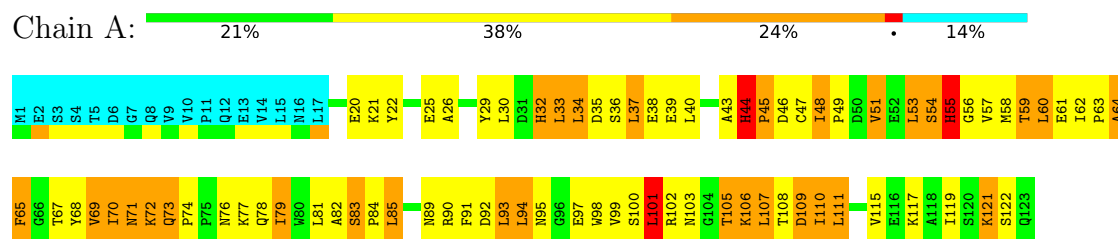
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Frataxin homolog, mitochondrial



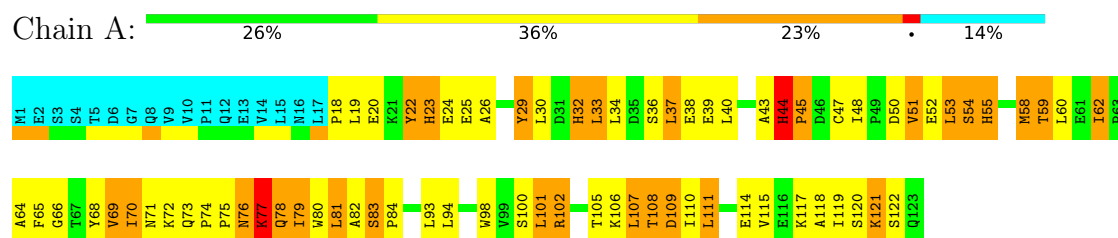
#### 4.2.16 Score per residue for model 16

- Molecule 1: Frataxin homolog, mitochondrial



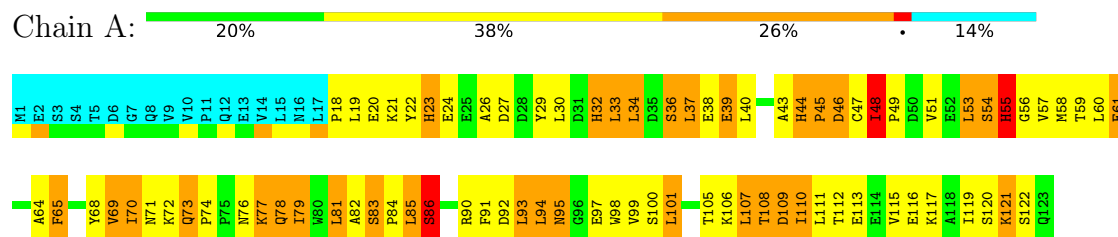
#### 4.2.17 Score per residue for model 17

- Molecule 1: Frataxin homolog, mitochondrial



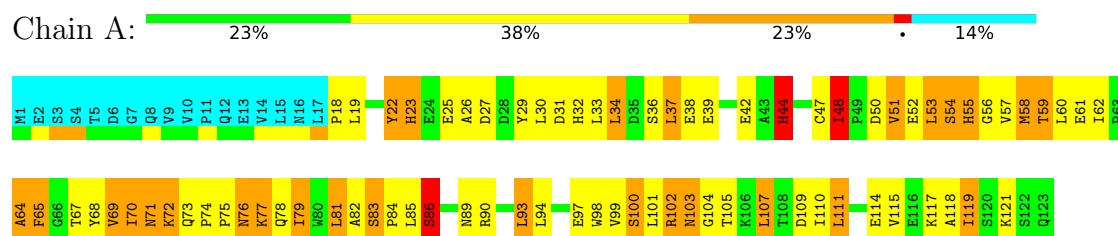
### 4.2.18 Score per residue for model 18

- Molecule 1: Frataxin homolog, mitochondrial



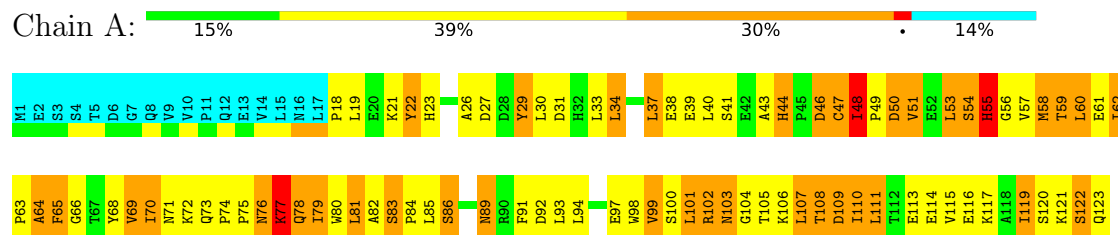
### 4.2.19 Score per residue for model 19

- Molecule 1: Frataxin homolog, mitochondrial



### 4.2.20 Score per residue for model 20

- Molecule 1: Frataxin homolog, mitochondrial



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 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 |
|---------------|--------------------|---------|
| CYANA         | refinement         | 2.1     |
| CYANA         | structure solution | 2.1     |

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 842   | 816      | 816      | 102±12  |
| All | All   | 16840 | 16320    | 16320    | 2033    |

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 61.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:62:ILE:HG21 | 1:A:65:PHE:CE2   | 1.08     | 1.83        | 11     | 17    |
| 1:A:58:MET:HE3  | 1:A:70:ILE:HD13  | 1.04     | 1.30        | 8      | 1     |
| 1:A:81:LEU:HD23 | 1:A:107:LEU:HD11 | 0.99     | 1.35        | 18     | 1     |
| 1:A:68:TYR:CE2  | 1:A:115:VAL:HG12 | 0.98     | 1.94        | 12     | 11    |
| 1:A:62:ILE:HG21 | 1:A:65:PHE:CZ    | 0.97     | 1.94        | 11     | 3     |
| 1:A:65:PHE:CE2  | 1:A:119:ILE:HD11 | 0.96     | 1.96        | 20     | 8     |
| 1:A:68:TYR:CE2  | 1:A:115:VAL:HG22 | 0.91     | 1.99        | 3      | 8     |
| 1:A:115:VAL:O   | 1:A:119:ILE:HD12 | 0.90     | 1.66        | 16     | 7     |
| 1:A:81:LEU:HD11 | 1:A:111:LEU:HD23 | 0.90     | 1.40        | 11     | 7     |
| 1:A:26:ALA:HB1  | 1:A:72:LYS:CG    | 0.90     | 1.96        | 10     | 6     |
| 1:A:81:LEU:HD11 | 1:A:111:LEU:CD2  | 0.90     | 1.96        | 12     | 12    |
| 1:A:79:ILE:HG21 | 1:A:107:LEU:CD2  | 0.87     | 1.99        | 12     | 4     |
| 1:A:79:ILE:HD13 | 1:A:98:TRP:CE3   | 0.87     | 2.05        | 4      | 3     |
| 1:A:53:LEU:HD13 | 1:A:53:LEU:O     | 0.86     | 1.70        | 8      | 20    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:79:ILE:HG21  | 1:A:107:LEU:HD22 | 0.85     | 1.45        | 12     | 8     |
| 1:A:29:TYR:O     | 1:A:33:LEU:HD13  | 0.85     | 1.72        | 5      | 2     |
| 1:A:62:ILE:HG21  | 1:A:65:PHE:CD2   | 0.84     | 2.07        | 4      | 11    |
| 1:A:79:ILE:HD12  | 1:A:98:TRP:CD1   | 0.84     | 2.06        | 6      | 6     |
| 1:A:58:MET:HE2   | 1:A:58:MET:C     | 0.84     | 1.98        | 2      | 5     |
| 1:A:93:LEU:HD22  | 1:A:93:LEU:O     | 0.84     | 1.72        | 1      | 3     |
| 1:A:51:VAL:HG22  | 1:A:60:LEU:HD13  | 0.83     | 1.50        | 9      | 1     |
| 1:A:93:LEU:C     | 1:A:93:LEU:HD22  | 0.83     | 1.98        | 18     | 1     |
| 1:A:81:LEU:HD23  | 1:A:107:LEU:CD1  | 0.83     | 2.03        | 18     | 1     |
| 1:A:111:LEU:O    | 1:A:115:VAL:HG22 | 0.83     | 1.73        | 14     | 11    |
| 1:A:60:LEU:HD23  | 1:A:68:TYR:HB2   | 0.83     | 1.51        | 8      | 10    |
| 1:A:25:GLU:OE1   | 1:A:93:LEU:HD11  | 0.82     | 1.74        | 11     | 1     |
| 1:A:53:LEU:HD22  | 1:A:54:SER:N     | 0.82     | 1.88        | 8      | 17    |
| 1:A:79:ILE:HD12  | 1:A:98:TRP:CD2   | 0.82     | 2.09        | 1      | 4     |
| 1:A:48:ILE:O     | 1:A:48:ILE:HG23  | 0.82     | 1.72        | 14     | 2     |
| 1:A:107:LEU:HD13 | 1:A:108:THR:N    | 0.82     | 1.89        | 16     | 4     |
| 1:A:59:THR:HG23  | 1:A:69:VAL:HG13  | 0.81     | 1.51        | 5      | 10    |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:CD    | 0.81     | 2.05        | 13     | 4     |
| 1:A:111:LEU:O    | 1:A:115:VAL:HG23 | 0.81     | 1.74        | 10     | 9     |
| 1:A:93:LEU:HD13  | 1:A:93:LEU:O     | 0.80     | 1.76        | 18     | 1     |
| 1:A:33:LEU:HD22  | 1:A:70:ILE:HD13  | 0.80     | 1.54        | 2      | 2     |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:HG2   | 0.80     | 1.54        | 10     | 5     |
| 1:A:107:LEU:C    | 1:A:107:LEU:HD12 | 0.79     | 2.03        | 15     | 2     |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:HD2   | 0.79     | 1.55        | 9      | 4     |
| 1:A:79:ILE:CG2   | 1:A:107:LEU:HD13 | 0.78     | 2.08        | 11     | 3     |
| 1:A:48:ILE:HG23  | 1:A:63:PRO:HG3   | 0.78     | 1.52        | 20     | 2     |
| 1:A:53:LEU:HD22  | 1:A:53:LEU:C     | 0.78     | 2.03        | 8      | 11    |
| 1:A:47:CYS:O     | 1:A:48:ILE:HG23  | 0.78     | 1.79        | 7      | 8     |
| 1:A:93:LEU:C     | 1:A:93:LEU:HD12  | 0.77     | 2.05        | 8      | 6     |
| 1:A:61:GLU:HA    | 1:A:67:THR:HG23  | 0.77     | 1.57        | 1      | 11    |
| 1:A:38:GLU:HA    | 1:A:51:VAL:HG11  | 0.76     | 1.55        | 4      | 3     |
| 1:A:70:ILE:HG23  | 1:A:81:LEU:CD2   | 0.76     | 2.10        | 8      | 2     |
| 1:A:79:ILE:HD12  | 1:A:98:TRP:CG    | 0.76     | 2.15        | 10     | 11    |
| 1:A:60:LEU:HD21  | 1:A:62:ILE:HD11  | 0.76     | 1.58        | 11     | 6     |
| 1:A:79:ILE:HG21  | 1:A:107:LEU:HD13 | 0.76     | 1.57        | 11     | 1     |
| 1:A:34:LEU:HD22  | 1:A:53:LEU:HG    | 0.76     | 1.56        | 10     | 11    |
| 1:A:115:VAL:HG12 | 1:A:119:ILE:HD12 | 0.76     | 1.56        | 18     | 6     |
| 1:A:58:MET:CE    | 1:A:70:ILE:HD13  | 0.76     | 2.09        | 8      | 1     |
| 1:A:33:LEU:CD1   | 1:A:70:ILE:HD12  | 0.76     | 2.11        | 7      | 5     |
| 1:A:37:LEU:HG    | 1:A:60:LEU:HD22  | 0.76     | 1.58        | 18     | 8     |
| 1:A:30:LEU:HD11  | 1:A:72:LYS:HB3   | 0.76     | 1.58        | 11     | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:77:LYS:HD3   | 1:A:93:LEU:HD12  | 0.75     | 1.56        | 16     | 1     |
| 1:A:60:LEU:HD23  | 1:A:68:TYR:CB    | 0.75     | 2.11        | 3      | 6     |
| 1:A:79:ILE:HD13  | 1:A:107:LEU:HD22 | 0.75     | 1.59        | 11     | 2     |
| 1:A:33:LEU:HD11  | 1:A:70:ILE:HD12  | 0.75     | 1.57        | 10     | 3     |
| 1:A:53:LEU:HD13  | 1:A:53:LEU:C     | 0.74     | 2.06        | 12     | 19    |
| 1:A:26:ALA:O     | 1:A:30:LEU:HD12  | 0.74     | 1.83        | 20     | 10    |
| 1:A:99:VAL:HG21  | 1:A:103:ASN:HA   | 0.74     | 1.59        | 12     | 3     |
| 1:A:30:LEU:HD11  | 1:A:72:LYS:CB    | 0.74     | 2.13        | 12     | 3     |
| 1:A:33:LEU:HD12  | 1:A:70:ILE:HD12  | 0.73     | 1.60        | 3      | 3     |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:HG3   | 0.73     | 1.60        | 19     | 5     |
| 1:A:69:VAL:HB    | 1:A:82:ALA:HB3   | 0.73     | 1.61        | 19     | 20    |
| 1:A:73:GLN:N     | 1:A:74:PRO:CD    | 0.73     | 2.52        | 17     | 20    |
| 1:A:29:TYR:O     | 1:A:33:LEU:HD23  | 0.73     | 1.84        | 18     | 5     |
| 1:A:37:LEU:CD2   | 1:A:58:MET:HE1   | 0.72     | 2.13        | 8      | 1     |
| 1:A:26:ALA:HB2   | 1:A:98:TRP:CZ2   | 0.72     | 2.19        | 17     | 6     |
| 1:A:111:LEU:O    | 1:A:115:VAL:HG13 | 0.72     | 1.84        | 9      | 8     |
| 1:A:64:ALA:HB3   | 1:A:65:PHE:CE1   | 0.72     | 2.20        | 1      | 15    |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:NZ    | 0.72     | 1.98        | 8      | 1     |
| 1:A:51:VAL:HG22  | 1:A:60:LEU:HD12  | 0.71     | 1.60        | 17     | 4     |
| 1:A:107:LEU:HD23 | 1:A:108:THR:N    | 0.71     | 2.00        | 18     | 2     |
| 1:A:54:SER:O     | 1:A:57:VAL:HG23  | 0.71     | 1.86        | 12     | 1     |
| 1:A:65:PHE:CZ    | 1:A:119:ILE:CG1  | 0.70     | 2.73        | 10     | 11    |
| 1:A:68:TYR:CE1   | 1:A:111:LEU:CD2  | 0.70     | 2.75        | 18     | 8     |
| 1:A:33:LEU:HD12  | 1:A:70:ILE:CD1   | 0.70     | 2.15        | 18     | 2     |
| 1:A:65:PHE:CE2   | 1:A:119:ILE:CD1  | 0.69     | 2.75        | 20     | 6     |
| 1:A:38:GLU:HA    | 1:A:51:VAL:HG21  | 0.69     | 1.64        | 19     | 4     |
| 1:A:93:LEU:HD22  | 1:A:93:LEU:C     | 0.69     | 2.11        | 12     | 2     |
| 1:A:65:PHE:CE2   | 1:A:119:ILE:CG1  | 0.69     | 2.76        | 15     | 11    |
| 1:A:34:LEU:HD22  | 1:A:53:LEU:CG    | 0.68     | 2.18        | 7      | 8     |
| 1:A:79:ILE:CG2   | 1:A:107:LEU:HD22 | 0.68     | 2.19        | 12     | 3     |
| 1:A:58:MET:HE3   | 1:A:70:ILE:CD1   | 0.68     | 2.14        | 8      | 1     |
| 1:A:81:LEU:HD21  | 1:A:111:LEU:CD2  | 0.68     | 2.19        | 12     | 9     |
| 1:A:68:TYR:CD1   | 1:A:111:LEU:CD2  | 0.68     | 2.77        | 15     | 1     |
| 1:A:68:TYR:CE2   | 1:A:115:VAL:CG1  | 0.68     | 2.76        | 17     | 10    |
| 1:A:51:VAL:HG12  | 1:A:60:LEU:HD12  | 0.67     | 1.66        | 15     | 2     |
| 1:A:59:THR:CG2   | 1:A:69:VAL:HG13  | 0.67     | 2.20        | 7      | 3     |
| 1:A:70:ILE:HG23  | 1:A:81:LEU:HD23  | 0.67     | 1.67        | 13     | 8     |
| 1:A:79:ILE:HD13  | 1:A:98:TRP:CZ3   | 0.67     | 2.25        | 4      | 2     |
| 1:A:54:SER:O     | 1:A:55:HIS:C     | 0.66     | 2.39        | 19     | 11    |
| 1:A:68:TYR:CE2   | 1:A:115:VAL:CG2  | 0.66     | 2.78        | 13     | 2     |
| 1:A:29:TYR:O     | 1:A:33:LEU:HD12  | 0.66     | 1.91        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:81:LEU:HD21  | 1:A:111:LEU:HD23 | 0.66     | 1.65        | 19     | 3     |
| 1:A:58:MET:HE2   | 1:A:58:MET:O     | 0.66     | 1.91        | 17     | 2     |
| 1:A:79:ILE:CD1   | 1:A:98:TRP:CD1   | 0.65     | 2.78        | 5      | 6     |
| 1:A:107:LEU:C    | 1:A:107:LEU:HD13 | 0.65     | 2.16        | 1      | 2     |
| 1:A:107:LEU:C    | 1:A:107:LEU:HD23 | 0.65     | 2.16        | 9      | 1     |
| 1:A:51:VAL:HG22  | 1:A:60:LEU:CD1   | 0.65     | 2.22        | 17     | 4     |
| 1:A:65:PHE:CZ    | 1:A:119:ILE:HD11 | 0.65     | 2.26        | 20     | 3     |
| 1:A:99:VAL:HG12  | 1:A:106:LYS:HG3  | 0.65     | 1.69        | 3      | 1     |
| 1:A:77:LYS:HD2   | 1:A:93:LEU:HD11  | 0.65     | 1.67        | 7      | 1     |
| 1:A:37:LEU:HD23  | 1:A:60:LEU:HB2   | 0.65     | 1.68        | 2      | 1     |
| 1:A:115:VAL:CG1  | 1:A:119:ILE:HD12 | 0.64     | 2.21        | 3      | 5     |
| 1:A:37:LEU:HD22  | 1:A:58:MET:HE1   | 0.64     | 1.68        | 8      | 1     |
| 1:A:62:ILE:CG2   | 1:A:65:PHE:CD2   | 0.64     | 2.80        | 4      | 4     |
| 1:A:81:LEU:HG    | 1:A:107:LEU:HD13 | 0.64     | 1.67        | 15     | 2     |
| 1:A:65:PHE:CD1   | 1:A:65:PHE:N     | 0.64     | 2.64        | 15     | 17    |
| 1:A:34:LEU:HA    | 1:A:58:MET:HE2   | 0.64     | 1.69        | 13     | 2     |
| 1:A:72:LYS:CE    | 1:A:98:TRP:CH2   | 0.64     | 2.80        | 17     | 3     |
| 1:A:62:ILE:CG2   | 1:A:65:PHE:CE2   | 0.63     | 2.80        | 15     | 14    |
| 1:A:68:TYR:CE1   | 1:A:111:LEU:HD23 | 0.63     | 2.28        | 18     | 2     |
| 1:A:37:LEU:CD1   | 1:A:60:LEU:HD22  | 0.63     | 2.23        | 5      | 2     |
| 1:A:72:LYS:NZ    | 1:A:98:TRP:CH2   | 0.63     | 2.66        | 6      | 4     |
| 1:A:64:ALA:C     | 1:A:65:PHE:CD1   | 0.63     | 2.77        | 14     | 14    |
| 1:A:70:ILE:HG23  | 1:A:81:LEU:HD22  | 0.63     | 1.71        | 8      | 2     |
| 1:A:69:VAL:O     | 1:A:81:LEU:HD22  | 0.62     | 1.94        | 7      | 9     |
| 1:A:63:PRO:O     | 1:A:64:ALA:HB2   | 0.62     | 1.95        | 4      | 3     |
| 1:A:72:LYS:CE    | 1:A:79:ILE:HD11  | 0.62     | 2.24        | 20     | 1     |
| 1:A:33:LEU:CD1   | 1:A:70:ILE:HG21  | 0.62     | 2.24        | 12     | 3     |
| 1:A:30:LEU:HD11  | 1:A:72:LYS:HG3   | 0.62     | 1.72        | 13     | 1     |
| 1:A:68:TYR:CD1   | 1:A:111:LEU:HD21 | 0.62     | 2.29        | 6      | 11    |
| 1:A:91:PHE:CE1   | 1:A:106:LYS:C    | 0.62     | 2.78        | 16     | 2     |
| 1:A:65:PHE:CZ    | 1:A:119:ILE:CD1  | 0.61     | 2.82        | 1      | 5     |
| 1:A:79:ILE:CD1   | 1:A:79:ILE:N     | 0.61     | 2.64        | 16     | 3     |
| 1:A:63:PRO:O     | 1:A:64:ALA:HB3   | 0.61     | 1.94        | 14     | 2     |
| 1:A:30:LEU:HD21  | 1:A:72:LYS:CB    | 0.61     | 2.25        | 11     | 2     |
| 1:A:115:VAL:HG12 | 1:A:119:ILE:CD1  | 0.61     | 2.25        | 18     | 1     |
| 1:A:51:VAL:HG23  | 1:A:51:VAL:O     | 0.61     | 1.95        | 5      | 1     |
| 1:A:33:LEU:HD22  | 1:A:58:MET:SD    | 0.61     | 2.36        | 6      | 2     |
| 1:A:36:SER:O     | 1:A:40:LEU:HD12  | 0.61     | 1.96        | 18     | 3     |
| 1:A:59:THR:HG23  | 1:A:69:VAL:CG1   | 0.60     | 2.26        | 5      | 3     |
| 1:A:93:LEU:HD12  | 1:A:93:LEU:O     | 0.60     | 1.94        | 10     | 1     |
| 1:A:93:LEU:HD13  | 1:A:93:LEU:H     | 0.60     | 1.54        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:CE    | 0.60     | 2.26        | 8      | 3     |
| 1:A:22:TYR:CD1   | 1:A:23:HIS:N     | 0.60     | 2.70        | 14     | 10    |
| 1:A:60:LEU:HD11  | 1:A:62:ILE:HD11  | 0.60     | 1.71        | 9      | 1     |
| 1:A:26:ALA:HB1   | 1:A:72:LYS:HE3   | 0.60     | 1.72        | 2      | 1     |
| 1:A:107:LEU:CD1  | 1:A:108:THR:N    | 0.60     | 2.65        | 13     | 4     |
| 1:A:48:ILE:O     | 1:A:48:ILE:CG2   | 0.60     | 2.46        | 14     | 1     |
| 1:A:37:LEU:HD22  | 1:A:58:MET:SD    | 0.59     | 2.36        | 2      | 1     |
| 1:A:91:PHE:CE1   | 1:A:107:LEU:HD12 | 0.59     | 2.32        | 10     | 2     |
| 1:A:38:GLU:CD    | 1:A:51:VAL:HG21  | 0.59     | 2.22        | 11     | 4     |
| 1:A:22:TYR:CE2   | 1:A:77:LYS:CD    | 0.59     | 2.85        | 17     | 2     |
| 1:A:79:ILE:CD1   | 1:A:98:TRP:CE3   | 0.59     | 2.83        | 4      | 2     |
| 1:A:85:LEU:CD2   | 1:A:85:LEU:C     | 0.59     | 2.75        | 16     | 1     |
| 1:A:93:LEU:HD13  | 1:A:93:LEU:N     | 0.59     | 2.12        | 19     | 1     |
| 1:A:107:LEU:HD22 | 1:A:107:LEU:C    | 0.59     | 2.23        | 4      | 2     |
| 1:A:33:LEU:CD1   | 1:A:70:ILE:CD1   | 0.59     | 2.80        | 18     | 3     |
| 1:A:93:LEU:CB    | 1:A:98:TRP:CZ3   | 0.59     | 2.86        | 15     | 1     |
| 1:A:72:LYS:C     | 1:A:74:PRO:CD    | 0.58     | 2.76        | 1      | 3     |
| 1:A:43:ALA:O     | 1:A:44:HIS:CB    | 0.58     | 2.51        | 15     | 5     |
| 1:A:33:LEU:HD13  | 1:A:70:ILE:HD13  | 0.58     | 1.74        | 1      | 1     |
| 1:A:22:TYR:C     | 1:A:22:TYR:CD1   | 0.58     | 2.81        | 7      | 10    |
| 1:A:77:LYS:CD    | 1:A:93:LEU:HD11  | 0.58     | 2.28        | 7      | 1     |
| 1:A:30:LEU:HD21  | 1:A:72:LYS:HB2   | 0.58     | 1.73        | 11     | 3     |
| 1:A:93:LEU:C     | 1:A:93:LEU:CD2   | 0.58     | 2.71        | 18     | 3     |
| 1:A:33:LEU:O     | 1:A:37:LEU:HD23  | 0.58     | 1.98        | 7      | 6     |
| 1:A:79:ILE:N     | 1:A:79:ILE:HD12  | 0.57     | 2.14        | 16     | 1     |
| 1:A:37:LEU:HB3   | 1:A:60:LEU:HD13  | 0.57     | 1.75        | 15     | 5     |
| 1:A:28:ASP:O     | 1:A:32:HIS:CD2   | 0.57     | 2.57        | 1      | 2     |
| 1:A:77:LYS:HG2   | 1:A:93:LEU:HD11  | 0.57     | 1.76        | 19     | 1     |
| 1:A:37:LEU:HD12  | 1:A:60:LEU:CD1   | 0.57     | 2.29        | 20     | 1     |
| 1:A:48:ILE:N     | 1:A:49:PRO:CD    | 0.57     | 2.67        | 14     | 8     |
| 1:A:44:HIS:O     | 1:A:44:HIS:CG    | 0.57     | 2.57        | 5      | 19    |
| 1:A:33:LEU:HD11  | 1:A:70:ILE:HG21  | 0.57     | 1.74        | 12     | 2     |
| 1:A:107:LEU:C    | 1:A:107:LEU:CD1  | 0.57     | 2.78        | 8      | 4     |
| 1:A:79:ILE:O     | 1:A:79:ILE:HG22  | 0.57     | 1.98        | 20     | 6     |
| 1:A:77:LYS:HD3   | 1:A:93:LEU:HD23  | 0.57     | 1.77        | 10     | 1     |
| 1:A:26:ALA:HB2   | 1:A:98:TRP:HZ2   | 0.57     | 1.60        | 8      | 6     |
| 1:A:57:VAL:HG13  | 1:A:71:ASN:CB    | 0.57     | 2.30        | 1      | 1     |
| 1:A:72:LYS:HE3   | 1:A:98:TRP:CH2   | 0.57     | 2.35        | 17     | 1     |
| 1:A:85:LEU:HD12  | 1:A:86:SER:N     | 0.57     | 2.15        | 18     | 1     |
| 1:A:37:LEU:HG    | 1:A:60:LEU:HD13  | 0.56     | 1.75        | 1      | 4     |
| 1:A:29:TYR:CE2   | 1:A:98:TRP:CD1   | 0.56     | 2.93        | 12     | 5     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:81:LEU:C    | 1:A:81:LEU:HD13  | 0.56     | 2.26        | 1      | 6     |
| 1:A:44:HIS:ND1  | 1:A:44:HIS:C     | 0.56     | 2.63        | 9      | 15    |
| 1:A:81:LEU:CG   | 1:A:111:LEU:HD23 | 0.56     | 2.31        | 16     | 3     |
| 1:A:60:LEU:CG   | 1:A:62:ILE:HD11  | 0.56     | 2.30        | 3      | 1     |
| 1:A:99:VAL:HG12 | 1:A:106:LYS:CG   | 0.56     | 2.29        | 3      | 1     |
| 1:A:94:LEU:HB2  | 1:A:99:VAL:HG22  | 0.56     | 1.77        | 5      | 3     |
| 1:A:26:ALA:CB   | 1:A:72:LYS:CG    | 0.56     | 2.83        | 11     | 1     |
| 1:A:26:ALA:HB1  | 1:A:72:LYS:HZ2   | 0.56     | 1.57        | 8      | 1     |
| 1:A:30:LEU:HD13 | 1:A:56:GLY:HA2   | 0.56     | 1.76        | 12     | 1     |
| 1:A:93:LEU:H    | 1:A:93:LEU:HD22  | 0.56     | 1.60        | 19     | 1     |
| 1:A:107:LEU:CD2 | 1:A:108:THR:N    | 0.56     | 2.69        | 9      | 2     |
| 1:A:22:TYR:CD2  | 1:A:77:LYS:CG    | 0.56     | 2.88        | 10     | 1     |
| 1:A:65:PHE:CZ   | 1:A:119:ILE:HG12 | 0.56     | 2.36        | 12     | 16    |
| 1:A:105:THR:CG2 | 1:A:110:ILE:HD11 | 0.56     | 2.30        | 13     | 2     |
| 1:A:60:LEU:HG   | 1:A:62:ILE:HD11  | 0.56     | 1.77        | 3      | 1     |
| 1:A:93:LEU:HD12 | 1:A:94:LEU:N     | 0.56     | 2.16        | 3      | 6     |
| 1:A:33:LEU:HD11 | 1:A:70:ILE:CD1   | 0.56     | 2.31        | 13     | 2     |
| 1:A:64:ALA:CB   | 1:A:65:PHE:CE1   | 0.56     | 2.89        | 20     | 14    |
| 1:A:79:ILE:CD1  | 1:A:98:TRP:CZ3   | 0.56     | 2.88        | 4      | 2     |
| 1:A:32:HIS:ND1  | 1:A:32:HIS:C     | 0.56     | 2.64        | 17     | 4     |
| 1:A:58:MET:O    | 1:A:70:ILE:HD12  | 0.55     | 2.01        | 20     | 3     |
| 1:A:81:LEU:CD1  | 1:A:111:LEU:HD23 | 0.55     | 2.31        | 8      | 5     |
| 1:A:22:TYR:CD2  | 1:A:77:LYS:HG3   | 0.55     | 2.36        | 10     | 2     |
| 1:A:72:LYS:CG   | 1:A:79:ILE:CD1   | 0.55     | 2.84        | 2      | 1     |
| 1:A:65:PHE:CE2  | 1:A:119:ILE:HG13 | 0.55     | 2.37        | 4      | 8     |
| 1:A:48:ILE:O    | 1:A:48:ILE:HD12  | 0.55     | 2.01        | 14     | 1     |
| 1:A:48:ILE:HD12 | 1:A:48:ILE:C     | 0.55     | 2.26        | 18     | 1     |
| 1:A:25:GLU:CG   | 1:A:26:ALA:N     | 0.55     | 2.69        | 7      | 4     |
| 1:A:28:ASP:O    | 1:A:32:HIS:CG    | 0.55     | 2.60        | 8      | 3     |
| 1:A:65:PHE:CE1  | 1:A:119:ILE:HG13 | 0.55     | 2.37        | 11     | 1     |
| 1:A:57:VAL:HG22 | 1:A:71:ASN:ND2   | 0.55     | 2.17        | 12     | 1     |
| 1:A:51:VAL:HG12 | 1:A:60:LEU:CD1   | 0.55     | 2.31        | 15     | 1     |
| 1:A:93:LEU:HB2  | 1:A:98:TRP:CZ3   | 0.55     | 2.36        | 15     | 1     |
| 1:A:93:LEU:N    | 1:A:93:LEU:HD22  | 0.55     | 2.17        | 19     | 1     |
| 1:A:59:THR:HA   | 1:A:69:VAL:HG13  | 0.55     | 1.78        | 1      | 1     |
| 1:A:29:TYR:CD2  | 1:A:98:TRP:CD1   | 0.55     | 2.95        | 5      | 5     |
| 1:A:54:SER:O    | 1:A:57:VAL:N     | 0.55     | 2.40        | 9      | 10    |
| 1:A:81:LEU:CD2  | 1:A:107:LEU:HD11 | 0.55     | 2.23        | 18     | 1     |
| 1:A:61:GLU:CA   | 1:A:67:THR:HG23  | 0.55     | 2.32        | 1      | 3     |
| 1:A:94:LEU:HD12 | 1:A:99:VAL:CG2   | 0.55     | 2.32        | 3      | 1     |
| 1:A:25:GLU:OE2  | 1:A:93:LEU:HD21  | 0.55     | 2.01        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:57:VAL:HG13 | 1:A:71:ASN:HB2   | 0.54     | 1.79        | 3      | 3     |
| 1:A:72:LYS:HE2  | 1:A:98:TRP:CH2   | 0.54     | 2.37        | 17     | 3     |
| 1:A:72:LYS:CG   | 1:A:79:ILE:CG1   | 0.54     | 2.86        | 14     | 1     |
| 1:A:34:LEU:HD22 | 1:A:53:LEU:HD23  | 0.54     | 1.77        | 3      | 8     |
| 1:A:76:ASN:CG   | 1:A:77:LYS:N     | 0.54     | 2.66        | 13     | 5     |
| 1:A:93:LEU:C    | 1:A:93:LEU:CD1   | 0.54     | 2.75        | 3      | 6     |
| 1:A:37:LEU:CG   | 1:A:60:LEU:HD13  | 0.54     | 2.33        | 14     | 4     |
| 1:A:53:LEU:C    | 1:A:53:LEU:CD1   | 0.54     | 2.79        | 12     | 9     |
| 1:A:38:GLU:HG3  | 1:A:51:VAL:HG11  | 0.54     | 1.80        | 19     | 1     |
| 1:A:29:TYR:CB   | 1:A:72:LYS:NZ    | 0.54     | 2.70        | 20     | 1     |
| 1:A:25:GLU:OE2  | 1:A:98:TRP:CE2   | 0.54     | 2.60        | 11     | 1     |
| 1:A:51:VAL:HG13 | 1:A:60:LEU:HD13  | 0.54     | 1.77        | 12     | 1     |
| 1:A:121:LYS:C   | 1:A:121:LYS:CD   | 0.54     | 2.81        | 17     | 1     |
| 1:A:60:LEU:CD2  | 1:A:62:ILE:HD11  | 0.54     | 2.30        | 11     | 2     |
| 1:A:30:LEU:HD11 | 1:A:72:LYS:HB2   | 0.54     | 1.78        | 8      | 2     |
| 1:A:73:GLN:N    | 1:A:74:PRO:HD3   | 0.54     | 2.17        | 15     | 19    |
| 1:A:102:ARG:C   | 1:A:103:ASN:CG   | 0.53     | 2.76        | 1      | 2     |
| 1:A:47:CYS:C    | 1:A:48:ILE:CG1   | 0.53     | 2.81        | 19     | 6     |
| 1:A:81:LEU:CD1  | 1:A:111:LEU:CD2  | 0.53     | 2.81        | 12     | 2     |
| 1:A:74:PRO:HB3  | 1:A:80:TRP:CD1   | 0.53     | 2.38        | 11     | 4     |
| 1:A:75:PRO:O    | 1:A:76:ASN:CB    | 0.53     | 2.56        | 17     | 7     |
| 1:A:69:VAL:CB   | 1:A:82:ALA:HB3   | 0.53     | 2.33        | 19     | 20    |
| 1:A:34:LEU:HD13 | 1:A:53:LEU:HG    | 0.53     | 1.79        | 8      | 5     |
| 1:A:79:ILE:HG21 | 1:A:107:LEU:HD23 | 0.53     | 1.81        | 15     | 1     |
| 1:A:58:MET:O    | 1:A:58:MET:HE2   | 0.53     | 2.03        | 3      | 1     |
| 1:A:53:LEU:C    | 1:A:53:LEU:HD22  | 0.53     | 2.27        | 4      | 6     |
| 1:A:51:VAL:HG12 | 1:A:58:MET:CE    | 0.53     | 2.34        | 14     | 1     |
| 1:A:91:PHE:CD2  | 1:A:100:SER:CB   | 0.53     | 2.92        | 18     | 1     |
| 1:A:30:LEU:O    | 1:A:34:LEU:HD23  | 0.53     | 2.04        | 18     | 9     |
| 1:A:77:LYS:CG   | 1:A:93:LEU:HD11  | 0.53     | 2.34        | 19     | 1     |
| 1:A:65:PHE:CZ   | 1:A:119:ILE:HG13 | 0.53     | 2.38        | 11     | 4     |
| 1:A:22:TYR:CD1  | 1:A:77:LYS:HD3   | 0.53     | 2.39        | 18     | 1     |
| 1:A:101:LEU:O   | 1:A:101:LEU:HD13 | 0.52     | 2.05        | 7      | 2     |
| 1:A:37:LEU:HA   | 1:A:40:LEU:HD12  | 0.52     | 1.81        | 9      | 2     |
| 1:A:75:PRO:C    | 1:A:76:ASN:CG    | 0.52     | 2.76        | 17     | 3     |
| 1:A:91:PHE:CE2  | 1:A:100:SER:HB3  | 0.52     | 2.39        | 18     | 1     |
| 1:A:103:ASN:N   | 1:A:103:ASN:ND2  | 0.52     | 2.53        | 1      | 1     |
| 1:A:68:TYR:HE2  | 1:A:115:VAL:HG12 | 0.52     | 1.63        | 2      | 4     |
| 1:A:106:LYS:N   | 1:A:106:LYS:CD   | 0.52     | 2.72        | 16     | 1     |
| 1:A:54:SER:O    | 1:A:56:GLY:N     | 0.52     | 2.43        | 13     | 11    |
| 1:A:72:LYS:CG   | 1:A:72:LYS:O     | 0.52     | 2.58        | 18     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:68:TYR:HE2   | 1:A:115:VAL:HG22 | 0.51     | 1.57        | 13     | 2     |
| 1:A:78:GLN:OE1   | 1:A:78:GLN:C     | 0.51     | 2.53        | 18     | 1     |
| 1:A:79:ILE:CG2   | 1:A:107:LEU:HD23 | 0.51     | 2.35        | 19     | 1     |
| 1:A:48:ILE:HG23  | 1:A:63:PRO:CG    | 0.51     | 2.29        | 20     | 1     |
| 1:A:91:PHE:CE2   | 1:A:107:LEU:HD13 | 0.51     | 2.41        | 7      | 1     |
| 1:A:22:TYR:CD2   | 1:A:77:LYS:HD2   | 0.51     | 2.40        | 17     | 1     |
| 1:A:65:PHE:HE2   | 1:A:119:ILE:HD11 | 0.51     | 1.57        | 20     | 1     |
| 1:A:62:ILE:CG2   | 1:A:65:PHE:CZ    | 0.51     | 2.93        | 1      | 2     |
| 1:A:53:LEU:C     | 1:A:53:LEU:CD2   | 0.51     | 2.83        | 9      | 7     |
| 1:A:93:LEU:O     | 1:A:93:LEU:CD1   | 0.51     | 2.57        | 18     | 3     |
| 1:A:38:GLU:CD    | 1:A:51:VAL:CG2   | 0.51     | 2.83        | 18     | 3     |
| 1:A:34:LEU:HA    | 1:A:58:MET:HE3   | 0.51     | 1.80        | 1      | 1     |
| 1:A:26:ALA:CB    | 1:A:72:LYS:CE    | 0.51     | 2.88        | 2      | 3     |
| 1:A:94:LEU:HD22  | 1:A:99:VAL:HG21  | 0.51     | 1.81        | 7      | 1     |
| 1:A:107:LEU:HD13 | 1:A:107:LEU:C    | 0.51     | 2.30        | 13     | 1     |
| 1:A:91:PHE:CE2   | 1:A:100:SER:HB2  | 0.51     | 2.40        | 15     | 1     |
| 1:A:25:GLU:O     | 1:A:29:TYR:CG    | 0.51     | 2.63        | 19     | 1     |
| 1:A:101:LEU:O    | 1:A:102:ARG:C    | 0.51     | 2.53        | 14     | 17    |
| 1:A:65:PHE:CE2   | 1:A:119:ILE:HG12 | 0.51     | 2.41        | 14     | 9     |
| 1:A:63:PRO:O     | 1:A:64:ALA:CB    | 0.51     | 2.59        | 14     | 4     |
| 1:A:74:PRO:CD    | 1:A:78:GLN:O     | 0.51     | 2.59        | 20     | 4     |
| 1:A:78:GLN:C     | 1:A:78:GLN:CD    | 0.51     | 2.78        | 18     | 1     |
| 1:A:91:PHE:CD2   | 1:A:100:SER:HB2  | 0.51     | 2.41        | 18     | 1     |
| 1:A:30:LEU:O     | 1:A:34:LEU:CD2   | 0.51     | 2.59        | 14     | 9     |
| 1:A:30:LEU:N     | 1:A:30:LEU:HD23  | 0.51     | 2.21        | 13     | 2     |
| 1:A:40:LEU:O     | 1:A:45:PRO:N     | 0.51     | 2.44        | 15     | 5     |
| 1:A:53:LEU:HD22  | 1:A:57:VAL:O     | 0.51     | 2.05        | 12     | 1     |
| 1:A:94:LEU:O     | 1:A:97:GLU:N     | 0.51     | 2.44        | 18     | 3     |
| 1:A:36:SER:C     | 1:A:40:LEU:HD12  | 0.51     | 2.31        | 18     | 1     |
| 1:A:107:LEU:HD23 | 1:A:108:THR:H    | 0.51     | 1.61        | 18     | 1     |
| 1:A:117:LYS:O    | 1:A:121:LYS:CB   | 0.51     | 2.59        | 10     | 14    |
| 1:A:99:VAL:HG23  | 1:A:100:SER:N    | 0.51     | 2.20        | 11     | 2     |
| 1:A:102:ARG:O    | 1:A:102:ARG:CG   | 0.51     | 2.58        | 12     | 1     |
| 1:A:34:LEU:O     | 1:A:38:GLU:CB    | 0.51     | 2.58        | 16     | 1     |
| 1:A:72:LYS:HE2   | 1:A:98:TRP:CZ3   | 0.51     | 2.41        | 17     | 1     |
| 1:A:34:LEU:O     | 1:A:38:GLU:CG    | 0.50     | 2.59        | 9      | 15    |
| 1:A:85:LEU:O     | 1:A:86:SER:CB    | 0.50     | 2.58        | 1      | 3     |
| 1:A:94:LEU:N     | 1:A:97:GLU:O     | 0.50     | 2.44        | 1      | 3     |
| 1:A:77:LYS:O     | 1:A:77:LYS:CD    | 0.50     | 2.59        | 15     | 7     |
| 1:A:64:ALA:HB3   | 1:A:65:PHE:CD1   | 0.50     | 2.41        | 1      | 7     |
| 1:A:70:ILE:HG21  | 1:A:107:LEU:HD21 | 0.50     | 1.83        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:HIS:O    | 1:A:27:ASP:CB   | 0.50     | 2.60        | 20     | 18    |
| 1:A:101:LEU:O   | 1:A:103:ASN:N   | 0.50     | 2.45        | 5      | 13    |
| 1:A:71:ASN:OD1  | 1:A:71:ASN:C    | 0.50     | 2.55        | 20     | 3     |
| 1:A:58:MET:CE   | 1:A:59:THR:O    | 0.50     | 2.60        | 6      | 3     |
| 1:A:34:LEU:HD22 | 1:A:53:LEU:CD2  | 0.50     | 2.35        | 7      | 3     |
| 1:A:50:ASP:N    | 1:A:61:GLU:O    | 0.50     | 2.45        | 4      | 1     |
| 1:A:56:GLY:O    | 1:A:57:VAL:CG2  | 0.50     | 2.59        | 9      | 9     |
| 1:A:77:LYS:O    | 1:A:78:GLN:CD   | 0.50     | 2.55        | 9      | 1     |
| 1:A:79:ILE:CG2  | 1:A:107:LEU:CD1 | 0.50     | 2.86        | 11     | 1     |
| 1:A:36:SER:O    | 1:A:40:LEU:CD1  | 0.50     | 2.60        | 18     | 2     |
| 1:A:48:ILE:CG1  | 1:A:48:ILE:O    | 0.50     | 2.60        | 1      | 4     |
| 1:A:46:ASP:O    | 1:A:47:CYS:CB   | 0.50     | 2.60        | 6      | 4     |
| 1:A:72:LYS:HD3  | 1:A:79:ILE:HD11 | 0.50     | 1.82        | 4      | 1     |
| 1:A:39:GLU:O    | 1:A:43:ALA:CB   | 0.50     | 2.60        | 7      | 7     |
| 1:A:56:GLY:O    | 1:A:71:ASN:ND2  | 0.50     | 2.45        | 11     | 1     |
| 1:A:46:ASP:C    | 1:A:47:CYS:SG   | 0.50     | 2.95        | 20     | 2     |
| 1:A:48:ILE:O    | 1:A:48:ILE:CD1  | 0.50     | 2.60        | 14     | 1     |
| 1:A:58:MET:SD   | 1:A:70:ILE:CD1  | 0.50     | 3.00        | 9      | 2     |
| 1:A:78:GLN:C    | 1:A:79:ILE:HD12 | 0.50     | 2.32        | 4      | 1     |
| 1:A:71:ASN:OD1  | 1:A:72:LYS:N    | 0.50     | 2.45        | 7      | 5     |
| 1:A:77:LYS:CG   | 1:A:77:LYS:O    | 0.50     | 2.58        | 17     | 4     |
| 1:A:77:LYS:O    | 1:A:77:LYS:CE   | 0.50     | 2.60        | 8      | 2     |
| 1:A:81:LEU:HD12 | 1:A:89:ASN:ND2  | 0.50     | 2.21        | 20     | 1     |
| 1:A:77:LYS:O    | 1:A:77:LYS:CG   | 0.50     | 2.59        | 20     | 7     |
| 1:A:117:LYS:O   | 1:A:121:LYS:CG  | 0.50     | 2.60        | 12     | 5     |
| 1:A:33:LEU:CD2  | 1:A:70:ILE:HD13 | 0.50     | 2.33        | 2      | 1     |
| 1:A:78:GLN:CG   | 1:A:91:PHE:O    | 0.50     | 2.60        | 11     | 5     |
| 1:A:54:SER:O    | 1:A:57:VAL:CG2  | 0.50     | 2.59        | 12     | 1     |
| 1:A:26:ALA:O    | 1:A:30:LEU:CD1  | 0.49     | 2.60        | 6      | 4     |
| 1:A:58:MET:N    | 1:A:70:ILE:O    | 0.49     | 2.45        | 11     | 8     |
| 1:A:75:PRO:O    | 1:A:76:ASN:CG   | 0.49     | 2.55        | 10     | 7     |
| 1:A:58:MET:C    | 1:A:58:MET:SD   | 0.49     | 2.95        | 13     | 1     |
| 1:A:115:VAL:O   | 1:A:119:ILE:CD1 | 0.49     | 2.60        | 14     | 2     |
| 1:A:58:MET:HE1  | 1:A:60:LEU:HB2  | 0.49     | 1.83        | 12     | 3     |
| 1:A:58:MET:HE2  | 1:A:59:THR:N    | 0.49     | 2.22        | 2      | 1     |
| 1:A:37:LEU:HD12 | 1:A:60:LEU:HD22 | 0.49     | 1.84        | 5      | 1     |
| 1:A:51:VAL:O    | 1:A:51:VAL:CG2  | 0.49     | 2.60        | 5      | 1     |
| 1:A:37:LEU:CD2  | 1:A:60:LEU:HD22 | 0.49     | 2.37        | 8      | 3     |
| 1:A:76:ASN:O    | 1:A:77:LYS:C    | 0.49     | 2.54        | 15     | 5     |
| 1:A:114:GLU:O   | 1:A:118:ALA:CB  | 0.49     | 2.61        | 13     | 6     |
| 1:A:52:GLU:N    | 1:A:59:THR:O    | 0.49     | 2.46        | 11     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:102:ARG:O   | 1:A:104:GLY:N    | 0.49     | 2.45        | 20     | 6     |
| 1:A:72:LYS:O    | 1:A:72:LYS:CD    | 0.49     | 2.60        | 6      | 1     |
| 1:A:76:ASN:O    | 1:A:78:GLN:CD    | 0.49     | 2.55        | 15     | 2     |
| 1:A:22:TYR:CD1  | 1:A:22:TYR:C     | 0.49     | 2.91        | 13     | 8     |
| 1:A:70:ILE:HG23 | 1:A:107:LEU:HD11 | 0.49     | 1.85        | 6      | 1     |
| 1:A:100:SER:O   | 1:A:101:LEU:CB   | 0.49     | 2.60        | 2      | 8     |
| 1:A:107:LEU:O   | 1:A:109:ASP:N    | 0.49     | 2.45        | 12     | 7     |
| 1:A:71:ASN:C    | 1:A:71:ASN:OD1   | 0.49     | 2.55        | 13     | 4     |
| 1:A:37:LEU:HD12 | 1:A:60:LEU:CD2   | 0.49     | 2.38        | 5      | 1     |
| 1:A:39:GLU:O    | 1:A:43:ALA:HB3   | 0.49     | 2.08        | 18     | 5     |
| 1:A:57:VAL:HG13 | 1:A:71:ASN:ND2   | 0.49     | 2.23        | 15     | 1     |
| 1:A:100:SER:O   | 1:A:101:LEU:C    | 0.49     | 2.56        | 9      | 7     |
| 1:A:38:GLU:OE1  | 1:A:51:VAL:HG21  | 0.49     | 2.06        | 11     | 2     |
| 1:A:81:LEU:HD21 | 1:A:111:LEU:HD21 | 0.49     | 1.85        | 3      | 5     |
| 1:A:70:ILE:CG2  | 1:A:107:LEU:HD21 | 0.49     | 2.38        | 10     | 2     |
| 1:A:74:PRO:CG   | 1:A:78:GLN:O     | 0.49     | 2.61        | 11     | 4     |
| 1:A:47:CYS:O    | 1:A:48:ILE:CG2   | 0.49     | 2.61        | 17     | 2     |
| 1:A:79:ILE:HG21 | 1:A:107:LEU:CD1  | 0.48     | 2.36        | 11     | 1     |
| 1:A:29:TYR:O    | 1:A:33:LEU:CD2   | 0.48     | 2.61        | 17     | 4     |
| 1:A:22:TYR:CE2  | 1:A:77:LYS:CG    | 0.48     | 2.96        | 10     | 1     |
| 1:A:93:LEU:HB2  | 1:A:98:TRP:CE3   | 0.48     | 2.43        | 15     | 2     |
| 1:A:79:ILE:HG22 | 1:A:107:LEU:HD23 | 0.48     | 1.83        | 19     | 1     |
| 1:A:95:ASN:O    | 1:A:95:ASN:ND2   | 0.48     | 2.46        | 5      | 1     |
| 1:A:60:LEU:O    | 1:A:68:TYR:N     | 0.48     | 2.46        | 6      | 4     |
| 1:A:107:LEU:O   | 1:A:110:ILE:N    | 0.48     | 2.47        | 20     | 4     |
| 1:A:72:LYS:C    | 1:A:74:PRO:HD2   | 0.48     | 2.34        | 1      | 2     |
| 1:A:107:LEU:C   | 1:A:109:ASP:N    | 0.48     | 2.71        | 12     | 16    |
| 1:A:102:ARG:O   | 1:A:103:ASN:C    | 0.48     | 2.56        | 9      | 5     |
| 1:A:94:LEU:O    | 1:A:95:ASN:CG    | 0.48     | 2.56        | 5      | 1     |
| 1:A:33:LEU:HD13 | 1:A:70:ILE:HG21  | 0.48     | 1.85        | 8      | 1     |
| 1:A:72:LYS:O    | 1:A:72:LYS:CE    | 0.48     | 2.62        | 13     | 1     |
| 1:A:34:LEU:O    | 1:A:38:GLU:CD    | 0.48     | 2.56        | 4      | 4     |
| 1:A:94:LEU:O    | 1:A:95:ASN:C     | 0.48     | 2.57        | 1      | 4     |
| 1:A:60:LEU:N    | 1:A:68:TYR:O     | 0.48     | 2.47        | 16     | 6     |
| 1:A:116:GLU:O   | 1:A:120:SER:CB   | 0.48     | 2.62        | 6      | 4     |
| 1:A:93:LEU:CB   | 1:A:98:TRP:CE3   | 0.48     | 2.97        | 15     | 1     |
| 1:A:44:HIS:O    | 1:A:44:HIS:ND1   | 0.47     | 2.47        | 14     | 5     |
| 1:A:102:ARG:C   | 1:A:104:GLY:N    | 0.47     | 2.72        | 8      | 7     |
| 1:A:58:MET:SD   | 1:A:70:ILE:HD12  | 0.47     | 2.48        | 9      | 1     |
| 1:A:65:PHE:CE1  | 1:A:119:ILE:HG12 | 0.47     | 2.44        | 5      | 2     |
| 1:A:103:ASN:N   | 1:A:103:ASN:OD1  | 0.47     | 2.47        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:60:LEU:HD12  | 1:A:61:GLU:N     | 0.47     | 2.25        | 18     | 1     |
| 1:A:79:ILE:HD12  | 1:A:98:TRP:CE2   | 0.47     | 2.43        | 1      | 1     |
| 1:A:94:LEU:CB    | 1:A:97:GLU:O     | 0.47     | 2.62        | 12     | 3     |
| 1:A:78:GLN:CB    | 1:A:91:PHE:O     | 0.47     | 2.62        | 2      | 1     |
| 1:A:30:LEU:HD21  | 1:A:79:ILE:CD1   | 0.47     | 2.39        | 9      | 1     |
| 1:A:81:LEU:CD2   | 1:A:107:LEU:CD1  | 0.47     | 2.85        | 18     | 1     |
| 1:A:45:PRO:CB    | 1:A:49:PRO:CG    | 0.47     | 2.92        | 12     | 3     |
| 1:A:93:LEU:HB3   | 1:A:98:TRP:CZ3   | 0.47     | 2.44        | 12     | 4     |
| 1:A:101:LEU:C    | 1:A:103:ASN:N    | 0.47     | 2.71        | 11     | 3     |
| 1:A:50:ASP:N     | 1:A:50:ASP:OD1   | 0.47     | 2.46        | 7      | 1     |
| 1:A:62:ILE:N     | 1:A:66:GLY:O     | 0.47     | 2.47        | 15     | 4     |
| 1:A:92:ASP:OD2   | 1:A:94:LEU:HD13  | 0.47     | 2.09        | 7      | 1     |
| 1:A:111:LEU:HD13 | 1:A:115:VAL:CG1  | 0.47     | 2.40        | 9      | 1     |
| 1:A:26:ALA:CB    | 1:A:72:LYS:HG2   | 0.47     | 2.40        | 11     | 1     |
| 1:A:37:LEU:HD23  | 1:A:58:MET:HE1   | 0.47     | 1.85        | 19     | 2     |
| 1:A:72:LYS:HE2   | 1:A:98:TRP:CZ2   | 0.47     | 2.45        | 15     | 2     |
| 1:A:35:ASP:O     | 1:A:39:GLU:CG    | 0.47     | 2.63        | 16     | 1     |
| 1:A:93:LEU:HG    | 1:A:98:TRP:CZ3   | 0.47     | 2.44        | 16     | 1     |
| 1:A:62:ILE:HG13  | 1:A:65:PHE:CZ    | 0.47     | 2.45        | 17     | 1     |
| 1:A:26:ALA:HB2   | 1:A:72:LYS:HE3   | 0.47     | 1.85        | 1      | 1     |
| 1:A:68:TYR:CE1   | 1:A:84:PRO:HD3   | 0.47     | 2.45        | 18     | 15    |
| 1:A:72:LYS:O     | 1:A:72:LYS:CG    | 0.47     | 2.62        | 1      | 1     |
| 1:A:80:TRP:CE3   | 1:A:88:PRO:HB2   | 0.47     | 2.45        | 1      | 1     |
| 1:A:111:LEU:O    | 1:A:115:VAL:CG2  | 0.47     | 2.60        | 19     | 7     |
| 1:A:25:GLU:CD    | 1:A:98:TRP:CZ2   | 0.47     | 2.93        | 11     | 1     |
| 1:A:101:LEU:O    | 1:A:104:GLY:N    | 0.47     | 2.46        | 14     | 1     |
| 1:A:68:TYR:CD1   | 1:A:111:LEU:HD23 | 0.47     | 2.44        | 15     | 1     |
| 1:A:105:THR:HB   | 1:A:110:ILE:HD13 | 0.47     | 1.86        | 16     | 1     |
| 1:A:56:GLY:C     | 1:A:57:VAL:HG23  | 0.47     | 2.34        | 9      | 9     |
| 1:A:95:ASN:ND2   | 1:A:95:ASN:N     | 0.47     | 2.61        | 15     | 1     |
| 1:A:102:ARG:O    | 1:A:103:ASN:CG   | 0.47     | 2.58        | 13     | 2     |
| 1:A:50:ASP:O     | 1:A:61:GLU:N     | 0.47     | 2.48        | 4      | 6     |
| 1:A:107:LEU:C    | 1:A:107:LEU:CD2  | 0.47     | 2.87        | 9      | 2     |
| 1:A:37:LEU:HD22  | 1:A:58:MET:CE    | 0.47     | 2.38        | 8      | 1     |
| 1:A:72:LYS:C     | 1:A:72:LYS:CD    | 0.47     | 2.88        | 10     | 1     |
| 1:A:71:ASN:N     | 1:A:71:ASN:OD1   | 0.47     | 2.48        | 2      | 1     |
| 1:A:56:GLY:C     | 1:A:57:VAL:CG2   | 0.47     | 2.87        | 19     | 10    |
| 1:A:22:TYR:CE2   | 1:A:72:LYS:HE3   | 0.47     | 2.45        | 6      | 1     |
| 1:A:93:LEU:O     | 1:A:93:LEU:CG    | 0.47     | 2.62        | 10     | 1     |
| 1:A:53:LEU:CD2   | 1:A:57:VAL:O     | 0.47     | 2.63        | 12     | 1     |
| 1:A:32:HIS:CE1   | 1:A:33:LEU:HD22  | 0.47     | 2.45        | 18     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:110:ILE:O   | 1:A:114:GLU:CG   | 0.47     | 2.63        | 20     | 1     |
| 1:A:91:PHE:CZ   | 1:A:107:LEU:HA   | 0.46     | 2.45        | 4      | 2     |
| 1:A:60:LEU:HD11 | 1:A:62:ILE:CD1   | 0.46     | 2.39        | 9      | 1     |
| 1:A:81:LEU:CD2  | 1:A:111:LEU:HD23 | 0.46     | 2.38        | 19     | 2     |
| 1:A:22:TYR:CD2  | 1:A:77:LYS:HD3   | 0.46     | 2.44        | 19     | 1     |
| 1:A:111:LEU:O   | 1:A:115:VAL:CG1  | 0.46     | 2.60        | 9      | 1     |
| 1:A:22:TYR:CE2  | 1:A:77:LYS:HD2   | 0.46     | 2.45        | 17     | 2     |
| 1:A:72:LYS:CD   | 1:A:72:LYS:O     | 0.46     | 2.64        | 18     | 2     |
| 1:A:25:GLU:OE1  | 1:A:93:LEU:CD1   | 0.46     | 2.58        | 11     | 1     |
| 1:A:65:PHE:CE1  | 1:A:119:ILE:CG1  | 0.46     | 2.98        | 11     | 1     |
| 1:A:57:VAL:HG13 | 1:A:71:ASN:HB3   | 0.46     | 1.88        | 1      | 2     |
| 1:A:72:LYS:CD   | 1:A:78:GLN:O     | 0.46     | 2.63        | 3      | 1     |
| 1:A:37:LEU:CG   | 1:A:60:LEU:HD22  | 0.46     | 2.40        | 17     | 2     |
| 1:A:102:ARG:O   | 1:A:103:ASN:CB   | 0.46     | 2.63        | 1      | 1     |
| 1:A:89:ASN:HB3  | 1:A:91:PHE:CE2   | 0.46     | 2.46        | 3      | 1     |
| 1:A:33:LEU:O    | 1:A:37:LEU:CD2   | 0.46     | 2.64        | 7      | 1     |
| 1:A:92:ASP:OD2  | 1:A:94:LEU:CD1   | 0.46     | 2.64        | 7      | 1     |
| 1:A:79:ILE:HD12 | 1:A:98:TRP:CE3   | 0.46     | 2.45        | 1      | 1     |
| 1:A:72:LYS:CE   | 1:A:78:GLN:O     | 0.46     | 2.63        | 5      | 1     |
| 1:A:79:ILE:N    | 1:A:79:ILE:HD13  | 0.46     | 2.26        | 12     | 1     |
| 1:A:84:PRO:O    | 1:A:85:LEU:HD22  | 0.46     | 2.11        | 20     | 1     |
| 1:A:26:ALA:CB   | 1:A:72:LYS:HE2   | 0.46     | 2.41        | 2      | 1     |
| 1:A:27:ASP:C    | 1:A:27:ASP:OD1   | 0.46     | 2.59        | 19     | 2     |
| 1:A:22:TYR:CE2  | 1:A:77:LYS:HD3   | 0.46     | 2.45        | 20     | 2     |
| 1:A:110:ILE:O   | 1:A:114:GLU:CB   | 0.46     | 2.64        | 9      | 4     |
| 1:A:26:ALA:CB   | 1:A:72:LYS:HD3   | 0.46     | 2.41        | 16     | 2     |
| 1:A:68:TYR:OH   | 1:A:114:GLU:CG   | 0.46     | 2.64        | 1      | 5     |
| 1:A:38:GLU:N    | 1:A:51:VAL:HG21  | 0.46     | 2.25        | 3      | 1     |
| 1:A:38:GLU:HG2  | 1:A:51:VAL:HG21  | 0.46     | 1.86        | 4      | 2     |
| 1:A:76:ASN:C    | 1:A:77:LYS:CD    | 0.46     | 2.89        | 9      | 1     |
| 1:A:25:GLU:CD   | 1:A:93:LEU:HD21  | 0.46     | 2.36        | 11     | 1     |
| 1:A:52:GLU:CD   | 1:A:52:GLU:C     | 0.46     | 2.83        | 19     | 1     |
| 1:A:68:TYR:OH   | 1:A:114:GLU:CD   | 0.45     | 2.59        | 3      | 4     |
| 1:A:22:TYR:CE2  | 1:A:72:LYS:NZ    | 0.45     | 2.83        | 3      | 1     |
| 1:A:65:PHE:CE1  | 1:A:118:ALA:O    | 0.45     | 2.69        | 6      | 1     |
| 1:A:40:LEU:O    | 1:A:45:PRO:CA    | 0.45     | 2.64        | 15     | 2     |
| 1:A:58:MET:HE3  | 1:A:58:MET:C     | 0.45     | 2.35        | 15     | 1     |
| 1:A:83:SER:CB   | 1:A:84:PRO:HD2   | 0.45     | 2.41        | 20     | 20    |
| 1:A:61:GLU:CD   | 1:A:62:ILE:N     | 0.45     | 2.74        | 4      | 1     |
| 1:A:72:LYS:CG   | 1:A:79:ILE:HG12  | 0.45     | 2.41        | 14     | 1     |
| 1:A:81:LEU:HD13 | 1:A:81:LEU:O     | 0.45     | 2.11        | 1      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:94:LEU:CB   | 1:A:99:VAL:HG22  | 0.45     | 2.42        | 7      | 1     |
| 1:A:85:LEU:C    | 1:A:85:LEU:HD22  | 0.45     | 2.35        | 16     | 1     |
| 1:A:120:SER:C   | 1:A:122:SER:N    | 0.45     | 2.74        | 3      | 7     |
| 1:A:72:LYS:HE3  | 1:A:98:TRP:CZ3   | 0.45     | 2.46        | 3      | 1     |
| 1:A:111:LEU:C   | 1:A:111:LEU:HD13 | 0.45     | 2.36        | 18     | 2     |
| 1:A:62:ILE:HG13 | 1:A:65:PHE:CE1   | 0.45     | 2.46        | 17     | 1     |
| 1:A:72:LYS:HE3  | 1:A:79:ILE:HD11  | 0.45     | 1.89        | 20     | 1     |
| 1:A:71:ASN:OD1  | 1:A:71:ASN:N     | 0.45     | 2.49        | 4      | 2     |
| 1:A:76:ASN:N    | 1:A:76:ASN:OD1   | 0.45     | 2.48        | 9      | 1     |
| 1:A:45:PRO:HB2  | 1:A:49:PRO:CG    | 0.45     | 2.42        | 12     | 1     |
| 1:A:79:ILE:O    | 1:A:91:PHE:N     | 0.45     | 2.50        | 14     | 1     |
| 1:A:69:VAL:O    | 1:A:82:ALA:N     | 0.45     | 2.50        | 1      | 1     |
| 1:A:83:SER:OG   | 1:A:87:GLY:CA    | 0.45     | 2.64        | 1      | 1     |
| 1:A:47:CYS:C    | 1:A:48:ILE:HG13  | 0.45     | 2.37        | 6      | 1     |
| 1:A:25:GLU:HG3  | 1:A:26:ALA:N     | 0.45     | 2.26        | 7      | 1     |
| 1:A:45:PRO:CB   | 1:A:49:PRO:HG3   | 0.45     | 2.42        | 11     | 4     |
| 1:A:93:LEU:CD1  | 1:A:93:LEU:N     | 0.45     | 2.80        | 1      | 2     |
| 1:A:76:ASN:O    | 1:A:78:GLN:NE2   | 0.45     | 2.50        | 11     | 1     |
| 1:A:72:LYS:O    | 1:A:72:LYS:NZ    | 0.45     | 2.50        | 13     | 2     |
| 1:A:85:LEU:C    | 1:A:86:SER:OG    | 0.45     | 2.60        | 13     | 1     |
| 1:A:91:PHE:CD1  | 1:A:100:SER:N    | 0.45     | 2.84        | 16     | 1     |
| 1:A:91:PHE:CG   | 1:A:100:SER:HB2  | 0.45     | 2.47        | 18     | 2     |
| 1:A:92:ASP:OD1  | 1:A:93:LEU:N     | 0.45     | 2.51        | 16     | 1     |
| 1:A:30:LEU:HD21 | 1:A:72:LYS:HB3   | 0.44     | 1.89        | 16     | 1     |
| 1:A:85:LEU:C    | 1:A:85:LEU:HD12  | 0.44     | 2.37        | 19     | 1     |
| 1:A:89:ASN:N    | 1:A:89:ASN:OD1   | 0.44     | 2.50        | 20     | 1     |
| 1:A:53:LEU:C    | 1:A:53:LEU:HD13  | 0.44     | 2.37        | 1      | 1     |
| 1:A:53:LEU:O    | 1:A:53:LEU:CD1   | 0.44     | 2.59        | 16     | 6     |
| 1:A:44:HIS:ND1  | 1:A:44:HIS:O     | 0.44     | 2.51        | 3      | 2     |
| 1:A:45:PRO:HB2  | 1:A:49:PRO:CD    | 0.44     | 2.43        | 11     | 5     |
| 1:A:70:ILE:HG13 | 1:A:81:LEU:CD2   | 0.44     | 2.43        | 20     | 4     |
| 1:A:101:LEU:O   | 1:A:101:LEU:CD1  | 0.44     | 2.65        | 4      | 2     |
| 1:A:115:VAL:CG1 | 1:A:119:ILE:CD1  | 0.44     | 2.96        | 3      | 2     |
| 1:A:76:ASN:O    | 1:A:77:LYS:CB    | 0.44     | 2.64        | 5      | 1     |
| 1:A:79:ILE:CG2  | 1:A:107:LEU:CD2  | 0.44     | 2.86        | 12     | 2     |
| 1:A:72:LYS:CE   | 1:A:79:ILE:CD1   | 0.44     | 2.94        | 20     | 1     |
| 1:A:70:ILE:HD12 | 1:A:70:ILE:N     | 0.44     | 2.28        | 12     | 3     |
| 1:A:72:LYS:C    | 1:A:74:PRO:HD3   | 0.44     | 2.38        | 1      | 1     |
| 1:A:80:TRP:CE3  | 1:A:88:PRO:CB    | 0.44     | 3.01        | 1      | 1     |
| 1:A:79:ILE:CD1  | 1:A:98:TRP:CG    | 0.44     | 2.96        | 10     | 1     |
| 1:A:50:ASP:CG   | 1:A:52:GLU:OE2   | 0.44     | 2.61        | 17     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:93:LEU:H    | 1:A:93:LEU:CD2   | 0.44     | 2.23        | 19     | 1     |
| 1:A:45:PRO:HB3  | 1:A:49:PRO:CG    | 0.43     | 2.42        | 11     | 2     |
| 1:A:74:PRO:CB   | 1:A:80:TRP:CD1   | 0.43     | 3.01        | 11     | 1     |
| 1:A:107:LEU:O   | 1:A:108:THR:C    | 0.43     | 2.61        | 12     | 6     |
| 1:A:58:MET:HE3  | 1:A:58:MET:O     | 0.43     | 2.13        | 15     | 1     |
| 1:A:26:ALA:CB   | 1:A:72:LYS:CD    | 0.43     | 2.96        | 16     | 1     |
| 1:A:93:LEU:CD1  | 1:A:93:LEU:H     | 0.43     | 2.27        | 1      | 2     |
| 1:A:72:LYS:HD2  | 1:A:79:ILE:CG1   | 0.43     | 2.44        | 5      | 2     |
| 1:A:79:ILE:HG13 | 1:A:98:TRP:CD2   | 0.43     | 2.49        | 10     | 2     |
| 1:A:37:LEU:HD23 | 1:A:60:LEU:HD13  | 0.43     | 1.90        | 14     | 1     |
| 1:A:72:LYS:HE3  | 1:A:79:ILE:CG1   | 0.43     | 2.43        | 20     | 1     |
| 1:A:49:PRO:CB   | 1:A:62:ILE:HD13  | 0.43     | 2.43        | 5      | 1     |
| 1:A:95:ASN:C    | 1:A:97:GLU:N     | 0.43     | 2.76        | 9      | 1     |
| 1:A:72:LYS:C    | 1:A:72:LYS:HD3   | 0.43     | 2.38        | 10     | 2     |
| 1:A:106:LYS:CG  | 1:A:109:ASP:CB   | 0.43     | 2.97        | 16     | 1     |
| 1:A:51:VAL:CG1  | 1:A:58:MET:CE    | 0.43     | 2.96        | 1      | 2     |
| 1:A:48:ILE:CD1  | 1:A:48:ILE:C     | 0.43     | 2.91        | 14     | 1     |
| 1:A:99:VAL:O    | 1:A:99:VAL:HG23  | 0.43     | 2.14        | 18     | 1     |
| 1:A:64:ALA:CB   | 1:A:65:PHE:CD1   | 0.43     | 3.02        | 20     | 6     |
| 1:A:77:LYS:O    | 1:A:78:GLN:NE2   | 0.43     | 2.52        | 11     | 2     |
| 1:A:91:PHE:CD1  | 1:A:100:SER:HB2  | 0.43     | 2.49        | 16     | 2     |
| 1:A:72:LYS:C    | 1:A:72:LYS:HD2   | 0.43     | 2.38        | 17     | 1     |
| 1:A:117:LYS:O   | 1:A:121:LYS:CD   | 0.43     | 2.66        | 1      | 3     |
| 1:A:72:LYS:HD3  | 1:A:98:TRP:CZ2   | 0.43     | 2.48        | 5      | 1     |
| 1:A:37:LEU:HD12 | 1:A:60:LEU:HD13  | 0.43     | 1.89        | 20     | 1     |
| 1:A:68:TYR:CZ   | 1:A:84:PRO:HD3   | 0.43     | 2.49        | 18     | 6     |
| 1:A:34:LEU:CD2  | 1:A:53:LEU:HD23  | 0.43     | 2.44        | 4      | 1     |
| 1:A:70:ILE:CG2  | 1:A:107:LEU:HD11 | 0.43     | 2.44        | 6      | 1     |
| 1:A:70:ILE:CG2  | 1:A:81:LEU:CD2   | 0.43     | 2.92        | 8      | 1     |
| 1:A:78:GLN:C    | 1:A:79:ILE:CD1   | 0.43     | 2.92        | 12     | 1     |
| 1:A:106:LYS:CG  | 1:A:109:ASP:HB2  | 0.43     | 2.43        | 16     | 1     |
| 1:A:72:LYS:HE2  | 1:A:98:TRP:CE2   | 0.43     | 2.48        | 20     | 1     |
| 1:A:77:LYS:O    | 1:A:78:GLN:CG    | 0.43     | 2.67        | 9      | 1     |
| 1:A:28:ASP:O    | 1:A:32:HIS:ND1   | 0.43     | 2.52        | 14     | 1     |
| 1:A:72:LYS:CG   | 1:A:79:ILE:HG13  | 0.43     | 2.42        | 14     | 1     |
| 1:A:34:LEU:CA   | 1:A:58:MET:HE2   | 0.43     | 2.42        | 13     | 1     |
| 1:A:72:LYS:HD3  | 1:A:72:LYS:C     | 0.42     | 2.39        | 6      | 1     |
| 1:A:68:TYR:CE1  | 1:A:111:LEU:HD21 | 0.42     | 2.49        | 11     | 1     |
| 1:A:37:LEU:CD2  | 1:A:58:MET:HE2   | 0.42     | 2.44        | 15     | 1     |
| 1:A:18:PRO:O    | 1:A:19:LEU:C     | 0.42     | 2.62        | 6      | 10    |
| 1:A:71:ASN:CG   | 1:A:72:LYS:N     | 0.42     | 2.76        | 7      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:64:ALA:O     | 1:A:65:PHE:CD1   | 0.42     | 2.72        | 6      | 1     |
| 1:A:69:VAL:C     | 1:A:70:ILE:HG12  | 0.42     | 2.39        | 10     | 1     |
| 1:A:93:LEU:O     | 1:A:93:LEU:CD2   | 0.42     | 2.60        | 12     | 1     |
| 1:A:48:ILE:N     | 1:A:49:PRO:HD3   | 0.42     | 2.29        | 14     | 1     |
| 1:A:72:LYS:HG2   | 1:A:79:ILE:CD1   | 0.42     | 2.43        | 2      | 1     |
| 1:A:72:LYS:HB2   | 1:A:72:LYS:HZ3   | 0.42     | 1.74        | 4      | 1     |
| 1:A:22:TYR:CE2   | 1:A:77:LYS:HG2   | 0.42     | 2.50        | 10     | 1     |
| 1:A:22:TYR:CD1   | 1:A:77:LYS:CD    | 0.42     | 3.02        | 18     | 1     |
| 1:A:68:TYR:CZ    | 1:A:111:LEU:CD2  | 0.42     | 3.02        | 18     | 1     |
| 1:A:99:VAL:HG21  | 1:A:103:ASN:CA   | 0.42     | 2.40        | 12     | 1     |
| 1:A:72:LYS:HG2   | 1:A:79:ILE:CG1   | 0.42     | 2.45        | 14     | 1     |
| 1:A:65:PHE:C     | 1:A:65:PHE:CD1   | 0.42     | 2.97        | 17     | 1     |
| 1:A:120:SER:OG   | 1:A:121:LYS:N    | 0.42     | 2.51        | 5      | 1     |
| 1:A:122:SER:O    | 1:A:123:GLN:C    | 0.42     | 2.63        | 8      | 1     |
| 1:A:112:THR:CG2  | 1:A:113:GLU:N    | 0.42     | 2.83        | 12     | 1     |
| 1:A:93:LEU:H     | 1:A:93:LEU:CD1   | 0.42     | 2.19        | 19     | 1     |
| 1:A:74:PRO:HG2   | 1:A:78:GLN:N     | 0.42     | 2.29        | 20     | 1     |
| 1:A:106:LYS:CE   | 1:A:109:ASP:OD2  | 0.42     | 2.68        | 4      | 1     |
| 1:A:37:LEU:HD23  | 1:A:58:MET:HE2   | 0.42     | 1.91        | 15     | 1     |
| 1:A:97:GLU:OE1   | 1:A:98:TRP:N     | 0.42     | 2.53        | 9      | 1     |
| 1:A:101:LEU:O    | 1:A:101:LEU:HD12 | 0.42     | 2.15        | 11     | 1     |
| 1:A:93:LEU:N     | 1:A:93:LEU:HD13  | 0.42     | 2.30        | 1      | 2     |
| 1:A:91:PHE:CE1   | 1:A:107:LEU:CD1  | 0.42     | 3.03        | 10     | 1     |
| 1:A:62:ILE:O     | 1:A:66:GLY:O     | 0.41     | 2.38        | 20     | 6     |
| 1:A:38:GLU:C     | 1:A:38:GLU:OE1   | 0.41     | 2.62        | 3      | 1     |
| 1:A:71:ASN:OD1   | 1:A:80:TRP:CB    | 0.41     | 2.68        | 4      | 1     |
| 1:A:57:VAL:HG13  | 1:A:71:ASN:HD22  | 0.41     | 1.75        | 15     | 1     |
| 1:A:76:ASN:O     | 1:A:77:LYS:O     | 0.41     | 2.37        | 20     | 3     |
| 1:A:69:VAL:O     | 1:A:81:LEU:HD23  | 0.41     | 2.15        | 9      | 1     |
| 1:A:52:GLU:CD    | 1:A:53:LEU:N     | 0.41     | 2.78        | 19     | 1     |
| 1:A:71:ASN:O     | 1:A:80:TRP:N     | 0.41     | 2.53        | 1      | 1     |
| 1:A:72:LYS:CD    | 1:A:79:ILE:HG13  | 0.41     | 2.45        | 5      | 1     |
| 1:A:62:ILE:CG1   | 1:A:65:PHE:CZ    | 0.41     | 3.03        | 17     | 1     |
| 1:A:76:ASN:O     | 1:A:77:LYS:CE    | 0.41     | 2.68        | 4      | 1     |
| 1:A:101:LEU:O    | 1:A:102:ARG:O    | 0.41     | 2.39        | 12     | 1     |
| 1:A:101:LEU:C    | 1:A:102:ARG:HG2  | 0.41     | 2.41        | 16     | 1     |
| 1:A:106:LYS:CD   | 1:A:106:LYS:N    | 0.41     | 2.84        | 1      | 1     |
| 1:A:107:LEU:HD12 | 1:A:107:LEU:O    | 0.41     | 2.15        | 15     | 2     |
| 1:A:78:GLN:NE2   | 1:A:92:ASP:OD1   | 0.41     | 2.53        | 12     | 1     |
| 1:A:112:THR:HG23 | 1:A:113:GLU:N    | 0.41     | 2.31        | 18     | 1     |
| 1:A:69:VAL:C     | 1:A:70:ILE:HG13  | 0.41     | 2.41        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:72:LYS:HD3   | 1:A:79:ILE:CD1   | 0.41     | 2.46        | 4      | 1     |
| 1:A:56:GLY:HA3   | 1:A:73:GLN:CB    | 0.41     | 2.46        | 10     | 1     |
| 1:A:37:LEU:CD2   | 1:A:60:LEU:HD13  | 0.41     | 2.46        | 14     | 1     |
| 1:A:99:VAL:O     | 1:A:99:VAL:CG2   | 0.41     | 2.67        | 14     | 1     |
| 1:A:26:ALA:HA    | 1:A:72:LYS:CD    | 0.41     | 2.45        | 16     | 1     |
| 1:A:48:ILE:O     | 1:A:48:ILE:CG1   | 0.41     | 2.69        | 18     | 1     |
| 1:A:78:GLN:HG2   | 1:A:79:ILE:N     | 0.41     | 2.30        | 18     | 1     |
| 1:A:71:ASN:ND2   | 1:A:80:TRP:HB2   | 0.41     | 2.30        | 20     | 1     |
| 1:A:29:TYR:CD2   | 1:A:98:TRP:NE1   | 0.41     | 2.89        | 19     | 2     |
| 1:A:68:TYR:CE1   | 1:A:111:LEU:HD22 | 0.41     | 2.51        | 6      | 1     |
| 1:A:34:LEU:HD13  | 1:A:53:LEU:CB    | 0.41     | 2.45        | 9      | 1     |
| 1:A:18:PRO:O     | 1:A:21:LYS:N     | 0.41     | 2.53        | 18     | 1     |
| 1:A:29:TYR:HB3   | 1:A:72:LYS:NZ    | 0.41     | 2.31        | 20     | 1     |
| 1:A:120:SER:O    | 1:A:122:SER:N    | 0.40     | 2.54        | 3      | 3     |
| 1:A:70:ILE:HD13  | 1:A:81:LEU:HD23  | 0.40     | 1.93        | 5      | 1     |
| 1:A:81:LEU:HD12  | 1:A:111:LEU:HD23 | 0.40     | 1.94        | 8      | 1     |
| 1:A:22:TYR:CD2   | 1:A:77:LYS:HG2   | 0.40     | 2.51        | 10     | 1     |
| 1:A:77:LYS:HE2   | 1:A:93:LEU:CD2   | 0.40     | 2.46        | 10     | 1     |
| 1:A:26:ALA:CB    | 1:A:72:LYS:HG3   | 0.40     | 2.41        | 11     | 1     |
| 1:A:36:SER:O     | 1:A:40:LEU:CG    | 0.40     | 2.69        | 18     | 1     |
| 1:A:61:GLU:C     | 1:A:62:ILE:HG12  | 0.40     | 2.41        | 20     | 1     |
| 1:A:81:LEU:HG    | 1:A:107:LEU:CD2  | 0.40     | 2.46        | 13     | 1     |
| 1:A:72:LYS:CG    | 1:A:79:ILE:HD11  | 0.40     | 2.46        | 2      | 1     |
| 1:A:107:LEU:HD13 | 1:A:108:THR:CA   | 0.40     | 2.47        | 16     | 1     |
| 1:A:41:SER:HB3   | 1:A:51:VAL:CG1   | 0.40     | 2.46        | 4      | 1     |
| 1:A:40:LEU:O     | 1:A:44:HIS:C     | 0.40     | 2.64        | 10     | 1     |
| 1:A:115:VAL:C    | 1:A:119:ILE:HD12 | 0.40     | 2.40        | 19     | 1     |
| 1:A:37:LEU:CD1   | 1:A:60:LEU:HD13  | 0.40     | 2.45        | 20     | 1     |
| 1:A:49:PRO:CB    | 1:A:61:GLU:O     | 0.40     | 2.69        | 5      | 1     |
| 1:A:97:GLU:O     | 1:A:99:VAL:HG13  | 0.40     | 2.17        | 7      | 1     |
| 1:A:60:LEU:CD2   | 1:A:68:TYR:HB2   | 0.40     | 2.45        | 9      | 1     |
| 1:A:29:TYR:CZ    | 1:A:107:LEU:HD23 | 0.40     | 2.52        | 14     | 1     |
| 1:A:37:LEU:HD21  | 1:A:60:LEU:HD22  | 0.40     | 1.92        | 14     | 1     |
| 1:A:37:LEU:HD23  | 1:A:58:MET:CE    | 0.40     | 2.47        | 15     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 105/123 (85%)   | 82±2 (78±2%) | 16±2 (15±2%) | 8±2 (7±2%) | 2           | 15 |
| All | All   | 2100/2460 (85%) | 1636 (78%)   | 312 (15%)    | 152 (7%)   | 2           | 15 |

All 18 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     | 55  | HIS  | 20             |
| 1   | A     | 64  | ALA  | 17             |
| 1   | A     | 102 | ARG  | 16             |
| 1   | A     | 44  | HIS  | 12             |
| 1   | A     | 107 | LEU  | 11             |
| 1   | A     | 77  | LYS  | 11             |
| 1   | A     | 45  | PRO  | 10             |
| 1   | A     | 103 | ASN  | 8              |
| 1   | A     | 108 | THR  | 7              |
| 1   | A     | 76  | ASN  | 7              |
| 1   | A     | 46  | ASP  | 6              |
| 1   | A     | 101 | LEU  | 6              |
| 1   | A     | 48  | ILE  | 6              |
| 1   | A     | 86  | SER  | 5              |
| 1   | A     | 47  | CYS  | 5              |
| 1   | A     | 104 | GLY  | 2              |
| 1   | A     | 85  | LEU  | 2              |
| 1   | A     | 95  | ASN  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |   |
|-----|-------|-----------------|--------------|--------------|-------------|---|
| 1   | A     | 96/112 (86%)    | 55±4 (57±4%) | 41±4 (43±4%) | 0           | 4 |
| All | All   | 1920/2240 (86%) | 1098 (57%)   | 822 (43%)    | 0           | 4 |

All 75 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     | 53  | LEU  | 20             |
| 1   | A     | 59  | THR  | 20             |
| 1   | A     | 69  | VAL  | 20             |
| 1   | A     | 83  | SER  | 20             |
| 1   | A     | 105 | THR  | 20             |
| 1   | A     | 109 | ASP  | 20             |
| 1   | A     | 33  | LEU  | 19             |
| 1   | A     | 44  | HIS  | 19             |
| 1   | A     | 54  | SER  | 19             |
| 1   | A     | 48  | ILE  | 18             |
| 1   | A     | 70  | ILE  | 18             |
| 1   | A     | 79  | ILE  | 18             |
| 1   | A     | 93  | LEU  | 18             |
| 1   | A     | 110 | ILE  | 18             |
| 1   | A     | 111 | LEU  | 18             |
| 1   | A     | 37  | LEU  | 17             |
| 1   | A     | 65  | PHE  | 17             |
| 1   | A     | 36  | SER  | 17             |
| 1   | A     | 34  | LEU  | 16             |
| 1   | A     | 77  | LYS  | 16             |
| 1   | A     | 78  | GLN  | 16             |
| 1   | A     | 106 | LYS  | 16             |
| 1   | A     | 22  | TYR  | 15             |
| 1   | A     | 47  | CYS  | 15             |
| 1   | A     | 50  | ASP  | 15             |
| 1   | A     | 94  | LEU  | 15             |
| 1   | A     | 121 | LYS  | 15             |
| 1   | A     | 71  | ASN  | 14             |
| 1   | A     | 58  | MET  | 14             |
| 1   | A     | 72  | LYS  | 13             |
| 1   | A     | 81  | LEU  | 13             |
| 1   | A     | 85  | LEU  | 12             |
| 1   | A     | 21  | LYS  | 11             |
| 1   | A     | 46  | ASP  | 11             |
| 1   | A     | 90  | ARG  | 11             |
| 1   | A     | 122 | SER  | 11             |
| 1   | A     | 99  | VAL  | 11             |
| 1   | A     | 31  | ASP  | 10             |
| 1   | A     | 55  | HIS  | 10             |
| 1   | A     | 101 | LEU  | 10             |
| 1   | A     | 30  | LEU  | 9              |
| 1   | A     | 51  | VAL  | 9              |
| 1   | A     | 20  | GLU  | 9              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 61  | GLU  | 9              |
| 1   | A     | 23  | HIS  | 9              |
| 1   | A     | 86  | SER  | 8              |
| 1   | A     | 123 | GLN  | 8              |
| 1   | A     | 39  | GLU  | 8              |
| 1   | A     | 60  | LEU  | 8              |
| 1   | A     | 32  | HIS  | 8              |
| 1   | A     | 57  | VAL  | 7              |
| 1   | A     | 89  | ASN  | 7              |
| 1   | A     | 97  | GLU  | 7              |
| 1   | A     | 24  | GLU  | 7              |
| 1   | A     | 107 | LEU  | 7              |
| 1   | A     | 119 | ILE  | 7              |
| 1   | A     | 52  | GLU  | 6              |
| 1   | A     | 100 | SER  | 6              |
| 1   | A     | 29  | TYR  | 5              |
| 1   | A     | 41  | SER  | 5              |
| 1   | A     | 73  | GLN  | 5              |
| 1   | A     | 42  | GLU  | 5              |
| 1   | A     | 95  | ASN  | 5              |
| 1   | A     | 92  | ASP  | 5              |
| 1   | A     | 76  | ASN  | 4              |
| 1   | A     | 62  | ILE  | 4              |
| 1   | A     | 102 | ARG  | 4              |
| 1   | A     | 103 | ASN  | 3              |
| 1   | A     | 113 | GLU  | 2              |
| 1   | A     | 67  | THR  | 2              |
| 1   | A     | 117 | LYS  | 2              |
| 1   | A     | 25  | GLU  | 2              |
| 1   | A     | 116 | GLU  | 2              |
| 1   | A     | 120 | SER  | 1              |
| 1   | A     | 112 | THR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided