



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 1MR6 / pdb\_00001mr6  
Title : Solution Structure of gamma-Bungarotoxin:Implication for the role of the Residues Adjacent to RGD in Integrin Binding  
Authors : Chuang, W.-J.; Shiu, J.-H.; Chen, C.-Y.; Chen, Y.-C.; Chang, L.-S.  
Deposited on : 2002-09-18

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                                                             |

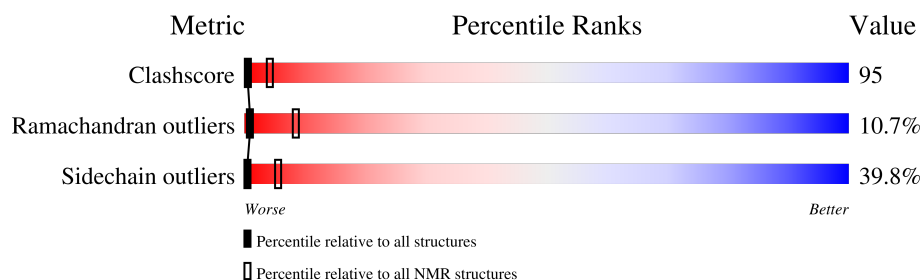
# 1 Overall quality at a glance

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     | 68     |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 6 as representative, based on the following criterion: *fewest violations*.

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:30, A:39-A:48, A:56-A:68 (53) | 1.11              | 9            |

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 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1014 atoms, of which 496 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called neurotoxin.

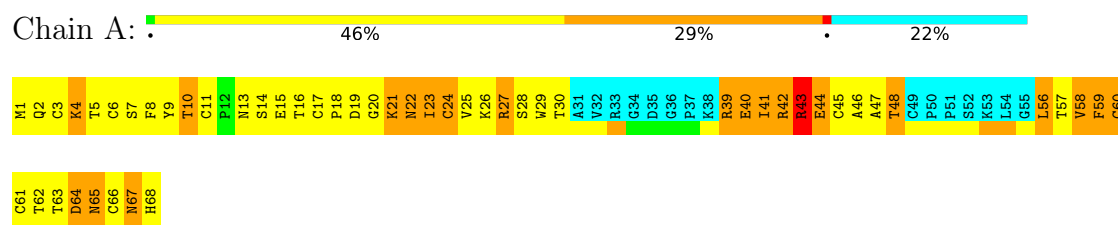
| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 1   | A     | 68       | Total | C   | H   | N  | O  | S  | 0     |
|     |       |          | 1014  | 312 | 496 | 96 | 99 | 11 |       |

## 4 Residue-property plots [i](#)

### 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: neurotoxin

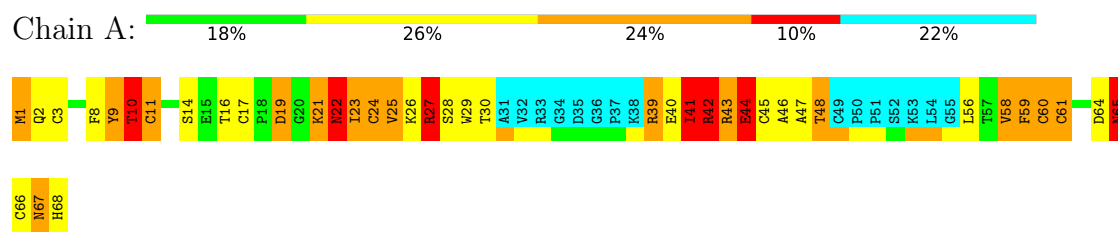


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

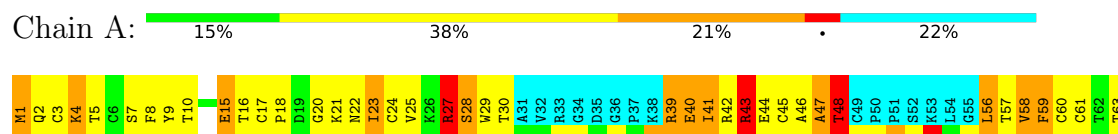
#### 4.2.1 Score per residue for model 1

- Molecule 1: neurotoxin



#### 4.2.2 Score per residue for model 2

- Molecule 1: neurotoxin





### 4.2.3 Score per residue for model 3

- Molecule 1: neurotoxin

Chain A: 16% 24% 34% • 22%



### 4.2.4 Score per residue for model 4

- Molecule 1: neurotoxin

Chain A: 10% 34% 26% 7% 22%



### 4.2.5 Score per residue for model 5

- Molecule 1: neurotoxin

Chain A: 6% 31% 35% 6% 22%

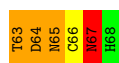


### 4.2.6 Score per residue for model 6

- Molecule 1: neurotoxin

Chain A: 16% 25% 32% • 22%





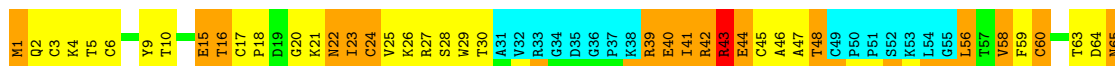
#### 4.2.7 Score per residue for model 7

- Molecule 1: neurotoxin



#### 4.2.8 Score per residue for model 8

- Molecule 1: neurotoxin



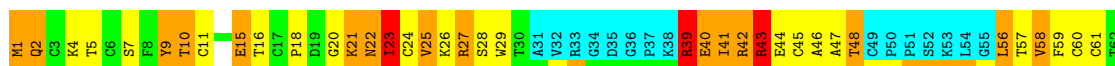
#### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: neurotoxin



#### 4.2.10 Score per residue for model 10

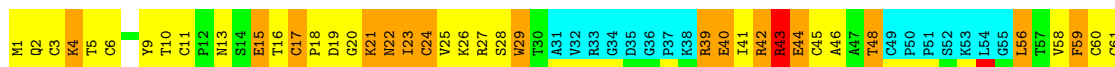
- Molecule 1: neurotoxin





#### 4.2.11 Score per residue for model 11

- Molecule 1: neurotoxin



#### 4.2.12 Score per residue for model 12

- Molecule 1: neurotoxin



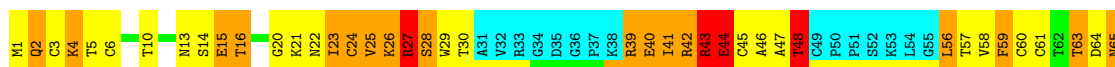
#### 4.2.13 Score per residue for model 13

- Molecule 1: neurotoxin



#### 4.2.14 Score per residue for model 14

- Molecule 1: neurotoxin



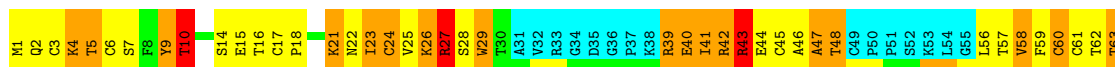




#### 4.2.15 Score per residue for model 15

- Molecule 1: neurotoxin

Chain A: 10% 32% 29% 6% 22%



#### 4.2.16 Score per residue for model 16

- Molecule 1: neurotoxin

Chain A: . 35% 34% . 22%



#### 4.2.17 Score per residue for model 17

- Molecule 1: neurotoxin

Chain A: 15% 37% 26% 22%



#### 4.2.18 Score per residue for model 18

- Molecule 1: neurotoxin

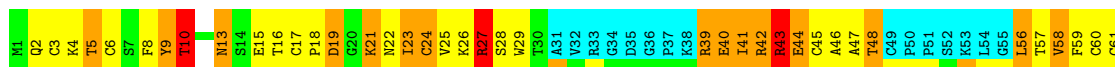
Chain A: 7% 37% 28% 6% 22%





#### 4.2.19 Score per residue for model 19

- Molecule 1: neurotoxin



#### 4.2.20 Score per residue for model 20

- Molecule 1: neurotoxin



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR        | refinement     | 3.85    |

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

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     | 1.41±0.01    | 0±0/423 ( 0.0± 0.0%) | 1.32±0.02   | 1±1/570 ( 0.1± 0.1%) |
| All | All   | 1.41         | 0/8460 ( 0.0%)       | 1.32        | 16/11400 ( 0.1%)     |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 3.7±0.5   |
| All | All   | 0         | 74        |

There are no bond-length outliers.

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     | 59  | PHE  | CA-CB-CG | -6.40 | 107.40      | 113.80   | 12     | 13    |
| 1   | A     | 47  | ALA  | N-CA-C   | -5.63 | 105.53      | 112.90   | 15     | 1     |
| 1   | A     | 68  | HIS  | CA-CB-CG | -5.21 | 108.59      | 113.80   | 7      | 1     |
| 1   | A     | 8   | PHE  | CA-CB-CG | -5.01 | 108.79      | 113.80   | 5      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 39  | ARG  | Sidechain | 20             |
| 1   | A     | 42  | ARG  | Sidechain | 19             |
| 1   | A     | 27  | ARG  | Sidechain | 18             |
| 1   | A     | 43  | ARG  | Sidechain | 17             |

## 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     | 416   | 389      | 389      | 77±9    |
| All | All   | 8320  | 7780     | 7780     | 1535    |

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 95.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:HD12 | 1.03     | 1.24        | 16     | 6     |
| 1:A:25:VAL:HG11 | 1:A:46:ALA:HB3  | 1.01     | 1.29        | 17     | 7     |
| 1:A:5:THR:HG23  | 1:A:24:CYS:SG   | 0.95     | 2.01        | 19     | 3     |
| 1:A:23:ILE:HD12 | 1:A:47:ALA:O    | 0.95     | 1.60        | 5      | 12    |
| 1:A:29:TRP:CB   | 1:A:56:LEU:HD12 | 0.94     | 1.92        | 16     | 1     |
| 1:A:25:VAL:HG22 | 1:A:44:GLU:O    | 0.93     | 1.62        | 7      | 13    |
| 1:A:29:TRP:CE3  | 1:A:56:LEU:HD11 | 0.93     | 1.98        | 15     | 6     |
| 1:A:28:SER:O    | 1:A:56:LEU:HD13 | 0.92     | 1.64        | 16     | 1     |
| 1:A:29:TRP:CE3  | 1:A:56:LEU:HD21 | 0.86     | 2.05        | 1      | 1     |
| 1:A:27:ARG:HB3  | 1:A:56:LEU:HD23 | 0.86     | 1.44        | 1      | 3     |
| 1:A:23:ILE:HD11 | 1:A:62:THR:HG22 | 0.86     | 1.43        | 15     | 4     |
| 1:A:1:MET:HE2   | 1:A:17:CYS:O    | 0.85     | 1.69        | 1      | 1     |
| 1:A:23:ILE:CG2  | 1:A:25:VAL:HG13 | 0.85     | 2.01        | 20     | 2     |
| 1:A:25:VAL:HG12 | 1:A:48:THR:O    | 0.85     | 1.71        | 14     | 3     |
| 1:A:27:ARG:HB3  | 1:A:56:LEU:HD21 | 0.84     | 1.50        | 13     | 4     |
| 1:A:27:ARG:CG   | 1:A:56:LEU:HD21 | 0.83     | 2.04        | 17     | 1     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:HD11 | 0.82     | 1.48        | 1      | 9     |
| 1:A:28:SER:CB   | 1:A:41:ILE:HG22 | 0.82     | 2.05        | 20     | 11    |
| 1:A:28:SER:HB3  | 1:A:41:ILE:HG22 | 0.82     | 1.51        | 18     | 4     |
| 1:A:41:ILE:HD13 | 1:A:41:ILE:O    | 0.80     | 1.76        | 6      | 1     |
| 1:A:25:VAL:CG1  | 1:A:46:ALA:HB3  | 0.80     | 2.06        | 17     | 4     |
| 1:A:27:ARG:CB   | 1:A:56:LEU:HD23 | 0.80     | 2.05        | 6      | 3     |
| 1:A:7:SER:HB3   | 1:A:41:ILE:HD13 | 0.79     | 1.53        | 16     | 1     |
| 1:A:5:THR:O     | 1:A:5:THR:HG23  | 0.77     | 1.79        | 6      | 1     |
| 1:A:28:SER:HB2  | 1:A:41:ILE:HG22 | 0.77     | 1.57        | 20     | 8     |
| 1:A:27:ARG:CB   | 1:A:56:LEU:HD21 | 0.76     | 2.11        | 9      | 4     |
| 1:A:3:CYS:SG    | 1:A:5:THR:HG23  | 0.76     | 2.20        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:41:ILE:HD12 | 1:A:41:ILE:C    | 0.75     | 2.07        | 4      | 3     |
| 1:A:5:THR:HG21  | 1:A:44:GLU:C    | 0.72     | 2.09        | 6      | 2     |
| 1:A:27:ARG:HB2  | 1:A:56:LEU:HD21 | 0.72     | 1.60        | 9      | 1     |
| 1:A:25:VAL:O    | 1:A:25:VAL:HG23 | 0.72     | 1.85        | 4      | 10    |
| 1:A:2:GLN:HB3   | 1:A:16:THR:HG23 | 0.71     | 1.59        | 14     | 2     |
| 1:A:27:ARG:HG2  | 1:A:56:LEU:HD23 | 0.71     | 1.61        | 3      | 1     |
| 1:A:5:THR:HG22  | 1:A:44:GLU:CA   | 0.70     | 2.16        | 14     | 5     |
| 1:A:23:ILE:HG23 | 1:A:24:CYS:N    | 0.70     | 2.01        | 10     | 19    |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:CD1  | 0.69     | 2.16        | 10     | 15    |
| 1:A:23:ILE:CG1  | 1:A:62:THR:HG22 | 0.69     | 2.18        | 18     | 4     |
| 1:A:41:ILE:HD13 | 1:A:41:ILE:C    | 0.68     | 2.12        | 6      | 1     |
| 1:A:23:ILE:CG2  | 1:A:24:CYS:N    | 0.68     | 2.57        | 6      | 20    |
| 1:A:2:GLN:CG    | 1:A:16:THR:HG23 | 0.68     | 2.19        | 6      | 4     |
| 1:A:41:ILE:HD12 | 1:A:41:ILE:O    | 0.68     | 1.87        | 4      | 1     |
| 1:A:23:ILE:CD1  | 1:A:62:THR:HG22 | 0.67     | 2.18        | 15     | 4     |
| 1:A:29:TRP:CE3  | 1:A:40:GLU:O    | 0.67     | 2.48        | 10     | 18    |
| 1:A:64:ASP:O    | 1:A:65:ASN:C    | 0.66     | 2.39        | 12     | 20    |
| 1:A:23:ILE:HG22 | 1:A:25:VAL:HG13 | 0.66     | 1.66        | 11     | 2     |
| 1:A:29:TRP:CA   | 1:A:56:LEU:HD11 | 0.66     | 2.20        | 10     | 1     |
| 1:A:25:VAL:HG11 | 1:A:46:ALA:CB   | 0.66     | 2.15        | 17     | 1     |
| 1:A:2:GLN:HG3   | 1:A:16:THR:HG23 | 0.66     | 1.67        | 9      | 3     |
| 1:A:66:CYS:O    | 1:A:67:ASN:C    | 0.65     | 2.39        | 7      | 4     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:HD21 | 0.65     | 1.67        | 8      | 5     |
| 1:A:2:GLN:HG2   | 1:A:16:THR:HG23 | 0.65     | 1.67        | 15     | 6     |
| 1:A:29:TRP:HA   | 1:A:56:LEU:CD1  | 0.65     | 2.21        | 16     | 1     |
| 1:A:29:TRP:CB   | 1:A:56:LEU:HD11 | 0.64     | 2.22        | 10     | 3     |
| 1:A:56:LEU:N    | 1:A:56:LEU:HD12 | 0.64     | 2.08        | 10     | 1     |
| 1:A:27:ARG:HB2  | 1:A:56:LEU:HD23 | 0.64     | 1.69        | 6      | 1     |
| 1:A:29:TRP:CZ2  | 1:A:40:GLU:HG3  | 0.63     | 2.28        | 10     | 3     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:HD13 | 0.63     | 1.70        | 12     | 3     |
| 1:A:8:PHE:CD1   | 1:A:43:ARG:NH2  | 0.63     | 2.66        | 7      | 1     |
| 1:A:27:ARG:CD   | 1:A:56:LEU:HD21 | 0.63     | 2.24        | 15     | 1     |
| 1:A:68:HIS:N    | 1:A:68:HIS:CD2  | 0.63     | 2.67        | 15     | 3     |
| 1:A:59:PHE:CD1  | 1:A:59:PHE:C    | 0.62     | 2.77        | 7      | 14    |
| 1:A:8:PHE:CG    | 1:A:43:ARG:NH1  | 0.62     | 2.67        | 7      | 1     |
| 1:A:8:PHE:CD1   | 1:A:9:TYR:N     | 0.62     | 2.67        | 7      | 1     |
| 1:A:29:TRP:CE3  | 1:A:56:LEU:CD1  | 0.62     | 2.82        | 17     | 4     |
| 1:A:59:PHE:CE1  | 1:A:67:ASN:ND2  | 0.62     | 2.67        | 9      | 2     |
| 1:A:28:SER:O    | 1:A:56:LEU:CD1  | 0.62     | 2.44        | 16     | 2     |
| 1:A:59:PHE:CZ   | 1:A:67:ASN:ND2  | 0.62     | 2.67        | 16     | 3     |
| 1:A:7:SER:CB    | 1:A:41:ILE:HD13 | 0.62     | 2.23        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:29:TRP:CE3  | 1:A:29:TRP:N    | 0.61     | 2.68        | 15     | 14    |
| 1:A:9:TYR:CD1   | 1:A:9:TYR:N     | 0.61     | 2.67        | 1      | 3     |
| 1:A:1:MET:HE1   | 1:A:19:ASP:O    | 0.61     | 1.95        | 1      | 1     |
| 1:A:29:TRP:CB   | 1:A:56:LEU:HD21 | 0.61     | 2.25        | 8      | 3     |
| 1:A:29:TRP:CA   | 1:A:56:LEU:HD12 | 0.61     | 2.25        | 16     | 1     |
| 1:A:67:ASN:O    | 1:A:68:HIS:CD2  | 0.61     | 2.54        | 7      | 1     |
| 1:A:39:ARG:O    | 1:A:41:ILE:HG23 | 0.60     | 1.96        | 15     | 5     |
| 1:A:41:ILE:O    | 1:A:41:ILE:CD1  | 0.60     | 2.49        | 4      | 1     |
| 1:A:28:SER:O    | 1:A:56:LEU:HD22 | 0.60     | 1.96        | 8      | 3     |
| 1:A:3:CYS:O     | 1:A:5:THR:HG23  | 0.60     | 1.96        | 18     | 3     |
| 1:A:29:TRP:HA   | 1:A:56:LEU:HD11 | 0.60     | 1.72        | 10     | 1     |
| 1:A:1:MET:O     | 1:A:16:THR:HG22 | 0.60     | 1.96        | 3      | 2     |
| 1:A:27:ARG:CG   | 1:A:56:LEU:HD23 | 0.60     | 2.26        | 3      | 1     |
| 1:A:29:TRP:CZ3  | 1:A:40:GLU:O    | 0.60     | 2.55        | 9      | 16    |
| 1:A:23:ILE:CG2  | 1:A:25:VAL:CG1  | 0.60     | 2.77        | 20     | 3     |
| 1:A:25:VAL:O    | 1:A:25:VAL:CG2  | 0.60     | 2.49        | 4      | 6     |
| 1:A:59:PHE:CE1  | 1:A:67:ASN:CG   | 0.60     | 2.80        | 5      | 2     |
| 1:A:3:CYS:HB3   | 1:A:24:CYS:HA   | 0.59     | 1.73        | 5      | 12    |
| 1:A:14:SER:CB   | 1:A:65:ASN:CB   | 0.59     | 2.80        | 5      | 2     |
| 1:A:9:TYR:C     | 1:A:10:THR:HG22 | 0.59     | 2.22        | 1      | 7     |
| 1:A:59:PHE:CZ   | 1:A:67:ASN:CG   | 0.59     | 2.81        | 16     | 1     |
| 1:A:5:THR:HG21  | 1:A:45:CYS:N    | 0.59     | 2.12        | 6      | 2     |
| 1:A:27:ARG:HG2  | 1:A:56:LEU:HD21 | 0.59     | 1.71        | 17     | 1     |
| 1:A:25:VAL:HG22 | 1:A:44:GLU:C    | 0.59     | 2.23        | 1      | 6     |
| 1:A:8:PHE:CD1   | 1:A:43:ARG:CZ   | 0.59     | 2.86        | 7      | 1     |
| 1:A:21:LYS:O    | 1:A:22:ASN:ND2  | 0.59     | 2.36        | 11     | 20    |
| 1:A:29:TRP:CD2  | 1:A:40:GLU:O    | 0.58     | 2.56        | 6      | 10    |
| 1:A:41:ILE:HD12 | 1:A:43:ARG:NH1  | 0.58     | 2.13        | 5      | 1     |
| 1:A:59:PHE:CD2  | 1:A:67:ASN:OD1  | 0.58     | 2.56        | 4      | 1     |
| 1:A:29:TRP:CD2  | 1:A:56:LEU:HD11 | 0.58     | 2.34        | 3      | 2     |
| 1:A:63:THR:O    | 1:A:64:ASP:CB   | 0.58     | 2.51        | 5      | 2     |
| 1:A:29:TRP:CE2  | 1:A:40:GLU:O    | 0.58     | 2.57        | 8      | 6     |
| 1:A:2:GLN:O     | 1:A:65:ASN:N    | 0.58     | 2.37        | 10     | 3     |
| 1:A:1:MET:HE2   | 1:A:22:ASN:CG   | 0.58     | 2.23        | 14     | 1     |
| 1:A:63:THR:HG22 | 1:A:66:CYS:SG   | 0.58     | 2.38        | 5      | 1     |
| 1:A:26:LYS:CE   | 1:A:43:ARG:NH1  | 0.58     | 2.67        | 18     | 1     |
| 1:A:29:TRP:CZ2  | 1:A:40:GLU:CG   | 0.58     | 2.87        | 10     | 1     |
| 1:A:5:THR:OG1   | 1:A:44:GLU:N    | 0.58     | 2.37        | 6      | 1     |
| 1:A:9:TYR:CE2   | 1:A:10:THR:CG2  | 0.58     | 2.87        | 7      | 1     |
| 1:A:29:TRP:CE2  | 1:A:40:GLU:CG   | 0.58     | 2.87        | 10     | 2     |
| 1:A:41:ILE:CD1  | 1:A:41:ILE:C    | 0.57     | 2.77        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:8:PHE:CB    | 1:A:43:ARG:NH1  | 0.57     | 2.66        | 7      | 1     |
| 1:A:29:TRP:CH2  | 1:A:40:GLU:O    | 0.57     | 2.58        | 8      | 5     |
| 1:A:8:PHE:CD1   | 1:A:68:HIS:O    | 0.57     | 2.57        | 16     | 1     |
| 1:A:59:PHE:CD1  | 1:A:67:ASN:OD1  | 0.57     | 2.57        | 11     | 3     |
| 1:A:29:TRP:O    | 1:A:39:ARG:HA   | 0.57     | 1.98        | 15     | 16    |
| 1:A:3:CYS:SG    | 1:A:24:CYS:N    | 0.57     | 2.78        | 7      | 11    |
| 1:A:4:LYS:O     | 1:A:5:THR:HG23  | 0.57     | 1.99        | 11     | 6     |
| 1:A:5:THR:O     | 1:A:5:THR:CG2   | 0.57     | 2.52        | 6      | 1     |
| 1:A:29:TRP:CZ2  | 1:A:40:GLU:O    | 0.57     | 2.58        | 8      | 4     |
| 1:A:5:THR:HA    | 1:A:68:HIS:HE2  | 0.57     | 1.59        | 15     | 1     |
| 1:A:29:TRP:HE3  | 1:A:56:LEU:HD11 | 0.57     | 1.55        | 9      | 1     |
| 1:A:48:THR:O    | 1:A:60:CYS:HB3  | 0.56     | 2.00        | 8      | 7     |
| 1:A:4:LYS:O     | 1:A:68:HIS:NE2  | 0.56     | 2.38        | 15     | 1     |
| 1:A:27:ARG:O    | 1:A:41:ILE:HA   | 0.56     | 2.00        | 4      | 9     |
| 1:A:21:LYS:HD2  | 1:A:21:LYS:C    | 0.56     | 2.25        | 10     | 1     |
| 1:A:29:TRP:CA   | 1:A:56:LEU:CD1  | 0.56     | 2.84        | 16     | 1     |
| 1:A:24:CYS:O    | 1:A:60:CYS:HA   | 0.56     | 2.00        | 4      | 16    |
| 1:A:59:PHE:CE2  | 1:A:67:ASN:ND2  | 0.56     | 2.73        | 3      | 1     |
| 1:A:23:ILE:HB   | 1:A:46:ALA:O    | 0.56     | 2.01        | 11     | 20    |
| 1:A:2:GLN:CB    | 1:A:16:THR:HG23 | 0.56     | 2.30        | 14     | 3     |
| 1:A:59:PHE:CZ   | 1:A:67:ASN:OD1  | 0.56     | 2.59        | 1      | 1     |
| 1:A:9:TYR:CD1   | 1:A:9:TYR:O     | 0.56     | 2.59        | 5      | 3     |
| 1:A:23:ILE:HD12 | 1:A:48:THR:O    | 0.56     | 2.00        | 3      | 2     |
| 1:A:29:TRP:N    | 1:A:29:TRP:CE3  | 0.56     | 2.74        | 16     | 3     |
| 1:A:24:CYS:C    | 1:A:25:VAL:CG1  | 0.55     | 2.78        | 1      | 10    |
| 1:A:64:ASP:O    | 1:A:66:CYS:N    | 0.55     | 2.39        | 9      | 5     |
| 1:A:1:MET:C     | 1:A:2:GLN:CG    | 0.55     | 2.79        | 10     | 6     |
| 1:A:59:PHE:CZ   | 1:A:61:CYS:SG   | 0.55     | 3.00        | 3      | 1     |
| 1:A:29:TRP:CZ3  | 1:A:41:ILE:HA   | 0.55     | 2.37        | 17     | 7     |
| 1:A:41:ILE:C    | 1:A:41:ILE:CD1  | 0.55     | 2.79        | 4      | 1     |
| 1:A:23:ILE:HG22 | 1:A:25:VAL:CG1  | 0.54     | 2.31        | 10     | 4     |
| 1:A:66:CYS:SG   | 1:A:67:ASN:N    | 0.54     | 2.80        | 16     | 3     |
| 1:A:8:PHE:CE2   | 1:A:9:TYR:CE1   | 0.54     | 2.94        | 19     | 1     |
| 1:A:42:ARG:CG   | 1:A:43:ARG:N    | 0.54     | 2.71        | 6      | 10    |
| 1:A:25:VAL:CG2  | 1:A:44:GLU:C    | 0.54     | 2.80        | 12     | 1     |
| 1:A:1:MET:SD    | 1:A:2:GLN:N     | 0.54     | 2.80        | 15     | 1     |
| 1:A:1:MET:HE2   | 1:A:22:ASN:OD1  | 0.54     | 2.02        | 14     | 2     |
| 1:A:29:TRP:CZ2  | 1:A:40:GLU:HB2  | 0.54     | 2.38        | 11     | 9     |
| 1:A:4:LYS:CD    | 1:A:4:LYS:C     | 0.54     | 2.81        | 2      | 1     |
| 1:A:23:ILE:HG23 | 1:A:24:CYS:O    | 0.54     | 2.03        | 5      | 8     |
| 1:A:23:ILE:O    | 1:A:45:CYS:SG   | 0.54     | 2.65        | 3      | 10    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:27:ARG:O    | 1:A:41:ILE:HB   | 0.54     | 2.02        | 6      | 3     |
| 1:A:24:CYS:HB3  | 1:A:67:ASN:ND2  | 0.54     | 2.17        | 4      | 4     |
| 1:A:8:PHE:CD1   | 1:A:8:PHE:O     | 0.54     | 2.61        | 5      | 1     |
| 1:A:2:GLN:CD    | 1:A:64:ASP:CB   | 0.54     | 2.81        | 17     | 2     |
| 1:A:48:THR:O    | 1:A:60:CYS:CB   | 0.54     | 2.56        | 12     | 2     |
| 1:A:21:LYS:HD2  | 1:A:21:LYS:N    | 0.54     | 2.17        | 10     | 1     |
| 1:A:66:CYS:O    | 1:A:67:ASN:ND2  | 0.53     | 2.41        | 4      | 1     |
| 1:A:1:MET:CE    | 1:A:18:PRO:O    | 0.53     | 2.57        | 17     | 1     |
| 1:A:43:ARG:O    | 1:A:44:GLU:CG   | 0.53     | 2.56        | 2      | 2     |
| 1:A:40:GLU:N    | 1:A:40:GLU:OE1  | 0.53     | 2.41        | 13     | 3     |
| 1:A:26:LYS:CD   | 1:A:67:ASN:OD1  | 0.53     | 2.56        | 15     | 2     |
| 1:A:23:ILE:CD1  | 1:A:47:ALA:O    | 0.53     | 2.56        | 2      | 8     |
| 1:A:23:ILE:CB   | 1:A:46:ALA:O    | 0.53     | 2.56        | 11     | 2     |
| 1:A:25:VAL:CG1  | 1:A:48:THR:O    | 0.53     | 2.56        | 16     | 2     |
| 1:A:66:CYS:O    | 1:A:68:HIS:N    | 0.53     | 2.41        | 3      | 4     |
| 1:A:63:THR:CG2  | 1:A:66:CYS:SG   | 0.53     | 2.97        | 8      | 1     |
| 1:A:24:CYS:O    | 1:A:25:VAL:HG12 | 0.53     | 2.04        | 4      | 4     |
| 1:A:40:GLU:OE1  | 1:A:40:GLU:CA   | 0.53     | 2.56        | 17     | 3     |
| 1:A:8:PHE:HA    | 1:A:11:CYS:HB2  | 0.53     | 1.79        | 7      | 1     |
| 1:A:27:ARG:HG2  | 1:A:58:VAL:HG13 | 0.53     | 1.80        | 4      | 1     |
| 1:A:2:GLN:CG    | 1:A:16:THR:OG1  | 0.53     | 2.57        | 16     | 2     |
| 1:A:2:GLN:HA    | 1:A:16:THR:HA   | 0.53     | 1.79        | 5      | 13    |
| 1:A:43:ARG:O    | 1:A:44:GLU:CB   | 0.53     | 2.57        | 14     | 3     |
| 1:A:59:PHE:CE2  | 1:A:67:ASN:OD1  | 0.53     | 2.62        | 4      | 2     |
| 1:A:40:GLU:CD   | 1:A:40:GLU:N    | 0.53     | 2.67        | 6      | 4     |
| 1:A:4:LYS:O     | 1:A:5:THR:CG2   | 0.53     | 2.56        | 2      | 4     |
| 1:A:24:CYS:O    | 1:A:60:CYS:CB   | 0.53     | 2.57        | 4      | 2     |
| 1:A:29:TRP:O    | 1:A:39:ARG:CG   | 0.53     | 2.57        | 20     | 3     |
| 1:A:17:CYS:CB   | 1:A:18:PRO:HD2  | 0.53     | 2.33        | 11     | 1     |
| 1:A:5:THR:HG22  | 1:A:43:ARG:HB3  | 0.53     | 1.80        | 19     | 2     |
| 1:A:6:CYS:O     | 1:A:43:ARG:CG   | 0.53     | 2.57        | 9      | 3     |
| 1:A:29:TRP:CE2  | 1:A:40:GLU:HB2  | 0.53     | 2.38        | 4      | 6     |
| 1:A:63:THR:HG23 | 1:A:64:ASP:CG   | 0.53     | 2.29        | 5      | 1     |
| 1:A:27:ARG:CB   | 1:A:57:THR:O    | 0.53     | 2.56        | 20     | 1     |
| 1:A:41:ILE:C    | 1:A:41:ILE:HD12 | 0.52     | 2.29        | 1      | 1     |
| 1:A:9:TYR:CD2   | 1:A:10:THR:HG22 | 0.52     | 2.39        | 7      | 1     |
| 1:A:27:ARG:HD2  | 1:A:56:LEU:HD21 | 0.52     | 1.79        | 15     | 1     |
| 1:A:4:LYS:NZ    | 1:A:6:CYS:SG    | 0.52     | 2.83        | 7      | 1     |
| 1:A:23:ILE:N    | 1:A:46:ALA:O    | 0.52     | 2.42        | 10     | 4     |
| 1:A:5:THR:CG2   | 1:A:44:GLU:C    | 0.52     | 2.82        | 9      | 4     |
| 1:A:8:PHE:CD1   | 1:A:8:PHE:C     | 0.52     | 2.86        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:2:GLN:HA    | 1:A:16:THR:CA   | 0.52     | 2.34        | 12     | 1     |
| 1:A:1:MET:O     | 1:A:16:THR:HG23 | 0.52     | 2.03        | 1      | 2     |
| 1:A:26:LYS:CE   | 1:A:59:PHE:HB3  | 0.52     | 2.35        | 7      | 1     |
| 1:A:26:LYS:HD3  | 1:A:59:PHE:CD1  | 0.52     | 2.40        | 7      | 1     |
| 1:A:24:CYS:O    | 1:A:25:VAL:CG1  | 0.52     | 2.58        | 4      | 4     |
| 1:A:23:ILE:CD1  | 1:A:48:THR:O    | 0.52     | 2.56        | 3      | 3     |
| 1:A:27:ARG:O    | 1:A:40:GLU:O    | 0.52     | 2.28        | 4      | 1     |
| 1:A:16:THR:CG2  | 1:A:17:CYS:N    | 0.52     | 2.73        | 16     | 3     |
| 1:A:4:LYS:O     | 1:A:67:ASN:CB   | 0.52     | 2.58        | 4      | 1     |
| 1:A:59:PHE:CD1  | 1:A:59:PHE:O    | 0.52     | 2.63        | 10     | 4     |
| 1:A:48:THR:O    | 1:A:60:CYS:SG   | 0.51     | 2.68        | 9      | 6     |
| 1:A:14:SER:HB3  | 1:A:65:ASN:CB   | 0.51     | 2.35        | 5      | 2     |
| 1:A:67:ASN:HB3  | 1:A:68:HIS:CD2  | 0.51     | 2.40        | 15     | 1     |
| 1:A:21:LYS:HD3  | 1:A:45:CYS:C    | 0.51     | 2.29        | 3      | 3     |
| 1:A:28:SER:HA   | 1:A:40:GLU:O    | 0.51     | 2.05        | 1      | 2     |
| 1:A:21:LYS:O    | 1:A:22:ASN:CG   | 0.51     | 2.53        | 10     | 9     |
| 1:A:23:ILE:HG13 | 1:A:62:THR:CG2  | 0.51     | 2.35        | 11     | 1     |
| 1:A:8:PHE:HB3   | 1:A:43:ARG:NH1  | 0.51     | 2.21        | 7      | 1     |
| 1:A:3:CYS:O     | 1:A:15:GLU:O    | 0.51     | 2.28        | 4      | 3     |
| 1:A:7:SER:HB3   | 1:A:9:TYR:CE1   | 0.51     | 2.40        | 7      | 1     |
| 1:A:40:GLU:N    | 1:A:40:GLU:OE2  | 0.51     | 2.43        | 14     | 2     |
| 1:A:66:CYS:O    | 1:A:67:ASN:CB   | 0.51     | 2.56        | 6      | 1     |
| 1:A:28:SER:O    | 1:A:56:LEU:CD2  | 0.51     | 2.58        | 19     | 2     |
| 1:A:5:THR:HG22  | 1:A:44:GLU:C    | 0.51     | 2.31        | 17     | 3     |
| 1:A:4:LYS:HB3   | 1:A:68:HIS:CD2  | 0.51     | 2.40        | 15     | 1     |
| 1:A:29:TRP:CZ3  | 1:A:56:LEU:HD21 | 0.51     | 2.39        | 1      | 1     |
| 1:A:4:LYS:CD    | 1:A:6:CYS:SG    | 0.51     | 2.99        | 7      | 1     |
| 1:A:21:LYS:HG2  | 1:A:45:CYS:C    | 0.51     | 2.31        | 17     | 6     |
| 1:A:41:ILE:O    | 1:A:42:ARG:C    | 0.51     | 2.53        | 1      | 2     |
| 1:A:5:THR:CG2   | 1:A:44:GLU:CA   | 0.51     | 2.89        | 8      | 5     |
| 1:A:5:THR:HG21  | 1:A:44:GLU:HA   | 0.51     | 1.83        | 10     | 2     |
| 1:A:1:MET:HE3   | 1:A:22:ASN:HA   | 0.51     | 1.83        | 11     | 1     |
| 1:A:4:LYS:CD    | 1:A:68:HIS:CB   | 0.51     | 2.89        | 16     | 1     |
| 1:A:26:LYS:HG2  | 1:A:27:ARG:N    | 0.51     | 2.21        | 1      | 1     |
| 1:A:8:PHE:O     | 1:A:43:ARG:CZ   | 0.51     | 2.59        | 17     | 2     |
| 1:A:3:CYS:SG    | 1:A:23:ILE:C    | 0.51     | 2.94        | 13     | 12    |
| 1:A:25:VAL:CG2  | 1:A:44:GLU:O    | 0.51     | 2.57        | 12     | 2     |
| 1:A:5:THR:CG2   | 1:A:44:GLU:HA   | 0.50     | 2.37        | 2      | 9     |
| 1:A:23:ILE:HD13 | 1:A:60:CYS:HB3  | 0.50     | 1.83        | 2      | 1     |
| 1:A:3:CYS:O     | 1:A:4:LYS:C     | 0.50     | 2.53        | 12     | 5     |
| 1:A:23:ILE:HG12 | 1:A:62:THR:HG22 | 0.50     | 1.82        | 19     | 2     |

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| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:29:TRP:NE1  | 1:A:40:GLU:HB3 | 0.50     | 2.21        | 15     | 2     |
| 1:A:4:LYS:CB    | 1:A:67:ASN:O   | 0.50     | 2.58        | 13     | 1     |
| 1:A:26:LYS:HA   | 1:A:42:ARG:O   | 0.50     | 2.07        | 8      | 9     |
| 1:A:26:LYS:C    | 1:A:27:ARG:CG  | 0.50     | 2.85        | 4      | 1     |
| 1:A:59:PHE:O    | 1:A:59:PHE:CD2 | 0.50     | 2.65        | 19     | 1     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:CB  | 0.50     | 2.37        | 7      | 5     |
| 1:A:21:LYS:CB   | 1:A:45:CYS:HB3 | 0.50     | 2.36        | 8      | 2     |
| 1:A:18:PRO:HG2  | 1:A:21:LYS:HZ1 | 0.50     | 1.66        | 10     | 1     |
| 1:A:23:ILE:HD12 | 1:A:48:THR:HA  | 0.50     | 1.83        | 18     | 2     |
| 1:A:25:VAL:CG2  | 1:A:27:ARG:NH1 | 0.50     | 2.75        | 3      | 1     |
| 1:A:25:VAL:HG11 | 1:A:48:THR:O   | 0.50     | 2.07        | 16     | 2     |
| 1:A:8:PHE:CD1   | 1:A:8:PHE:N    | 0.50     | 2.78        | 20     | 1     |
| 1:A:57:THR:HG22 | 1:A:57:THR:O   | 0.50     | 2.07        | 18     | 2     |
| 1:A:27:ARG:O    | 1:A:41:ILE:CB  | 0.50     | 2.59        | 6      | 1     |
| 1:A:67:ASN:N    | 1:A:67:ASN:OD1 | 0.50     | 2.44        | 8      | 2     |
| 1:A:29:TRP:CE2  | 1:A:40:GLU:HB3 | 0.50     | 2.41        | 9      | 2     |
| 1:A:21:LYS:HD2  | 1:A:45:CYS:CB  | 0.50     | 2.37        | 11     | 2     |
| 1:A:21:LYS:CD   | 1:A:45:CYS:C   | 0.50     | 2.85        | 11     | 2     |
| 1:A:66:CYS:O    | 1:A:66:CYS:SG  | 0.50     | 2.70        | 4      | 3     |
| 1:A:56:LEU:HD12 | 1:A:57:THR:N   | 0.50     | 2.22        | 10     | 1     |
| 1:A:23:ILE:CG2  | 1:A:24:CYS:O   | 0.50     | 2.59        | 19     | 2     |
| 1:A:63:THR:O    | 1:A:64:ASP:O   | 0.50     | 2.30        | 9      | 7     |
| 1:A:64:ASP:O    | 1:A:65:ASN:O   | 0.50     | 2.30        | 16     | 2     |
| 1:A:27:ARG:CD   | 1:A:27:ARG:N   | 0.50     | 2.74        | 11     | 1     |
| 1:A:26:LYS:HD3  | 1:A:59:PHE:CD2 | 0.49     | 2.42        | 15     | 4     |
| 1:A:61:CYS:HB2  | 1:A:67:ASN:ND2 | 0.49     | 2.22        | 15     | 1     |
| 1:A:4:LYS:N     | 1:A:4:LYS:CE   | 0.49     | 2.75        | 12     | 1     |
| 1:A:11:CYS:O    | 1:A:68:HIS:C   | 0.49     | 2.56        | 7      | 1     |
| 1:A:63:THR:OG1  | 1:A:64:ASP:N   | 0.49     | 2.43        | 7      | 1     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:CD2 | 0.49     | 2.38        | 8      | 2     |
| 1:A:56:LEU:HD12 | 1:A:57:THR:H   | 0.49     | 1.66        | 10     | 1     |
| 1:A:5:THR:HG22  | 1:A:44:GLU:HA  | 0.49     | 1.83        | 14     | 2     |
| 1:A:4:LYS:O     | 1:A:4:LYS:CD   | 0.49     | 2.59        | 2      | 1     |
| 1:A:63:THR:O    | 1:A:64:ASP:C   | 0.49     | 2.56        | 6      | 7     |
| 1:A:1:MET:N     | 1:A:18:PRO:O   | 0.49     | 2.45        | 15     | 1     |
| 1:A:29:TRP:NE1  | 1:A:40:GLU:HG3 | 0.49     | 2.22        | 2      | 6     |
| 1:A:11:CYS:O    | 1:A:68:HIS:ND1 | 0.49     | 2.45        | 5      | 1     |
| 1:A:3:CYS:CB    | 1:A:24:CYS:HA  | 0.49     | 2.38        | 2      | 5     |
| 1:A:5:THR:C     | 1:A:6:CYS:SG   | 0.49     | 2.95        | 16     | 1     |
| 1:A:1:MET:SD    | 1:A:1:MET:N    | 0.49     | 2.85        | 3      | 8     |
| 1:A:1:MET:HE3   | 1:A:17:CYS:O   | 0.49     | 2.08        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:ILE:HD11 | 1:A:62:THR:CG2  | 0.49     | 2.37        | 18     | 3     |
| 1:A:8:PHE:N     | 1:A:68:HIS:OXT  | 0.49     | 2.46        | 5      | 1     |
| 1:A:8:PHE:HB3   | 1:A:43:ARG:CZ   | 0.49     | 2.38        | 7      | 1     |
| 1:A:6:CYS:O     | 1:A:67:ASN:O    | 0.49     | 2.31        | 16     | 1     |
| 1:A:6:CYS:O     | 1:A:43:ARG:NE   | 0.49     | 2.45        | 18     | 1     |
| 1:A:2:GLN:O     | 1:A:64:ASP:C    | 0.49     | 2.55        | 4      | 4     |
| 1:A:4:LYS:N     | 1:A:24:CYS:SG   | 0.49     | 2.86        | 6      | 3     |
| 1:A:29:TRP:O    | 1:A:39:ARG:CA   | 0.49     | 2.60        | 7      | 2     |
| 1:A:29:TRP:O    | 1:A:40:GLU:N    | 0.49     | 2.46        | 10     | 2     |
| 1:A:42:ARG:HG3  | 1:A:43:ARG:N    | 0.49     | 2.22        | 15     | 4     |
| 1:A:5:THR:HG1   | 1:A:15:GLU:CD   | 0.49     | 2.16        | 9      | 1     |
| 1:A:4:LYS:CE    | 1:A:65:ASN:O    | 0.49     | 2.61        | 15     | 1     |
| 1:A:42:ARG:HG2  | 1:A:43:ARG:N    | 0.48     | 2.22        | 13     | 6     |
| 1:A:18:PRO:O    | 1:A:19:ASP:C    | 0.48     | 2.56        | 16     | 3     |
| 1:A:21:LYS:CE   | 1:A:45:CYS:HB2  | 0.48     | 2.38        | 11     | 1     |
| 1:A:65:ASN:O    | 1:A:66:CYS:C    | 0.48     | 2.56        | 11     | 1     |
| 1:A:21:LYS:HB3  | 1:A:45:CYS:SG   | 0.48     | 2.48        | 16     | 3     |
| 1:A:17:CYS:CB   | 1:A:18:PRO:CD   | 0.48     | 2.92        | 11     | 1     |
| 1:A:48:THR:C    | 1:A:60:CYS:SG   | 0.48     | 2.96        | 14     | 1     |
| 1:A:1:MET:C     | 1:A:2:GLN:CD    | 0.48     | 2.81        | 16     | 1     |
| 1:A:41:ILE:O    | 1:A:42:ARG:O    | 0.48     | 2.31        | 4      | 2     |
| 1:A:65:ASN:ND2  | 1:A:65:ASN:N    | 0.48     | 2.61        | 18     | 1     |
| 1:A:66:CYS:C    | 1:A:67:ASN:OD1  | 0.48     | 2.56        | 7      | 1     |
| 1:A:66:CYS:O    | 1:A:67:ASN:OD1  | 0.48     | 2.31        | 18     | 1     |
| 1:A:17:CYS:HB3  | 1:A:21:LYS:CB   | 0.48     | 2.37        | 19     | 1     |
| 1:A:8:PHE:C     | 1:A:10:THR:H    | 0.48     | 2.15        | 7      | 1     |
| 1:A:5:THR:OG1   | 1:A:15:GLU:CD   | 0.48     | 2.56        | 9      | 2     |
| 1:A:1:MET:CE    | 1:A:22:ASN:OD1  | 0.48     | 2.61        | 14     | 1     |
| 1:A:60:CYS:C    | 1:A:61:CYS:SG   | 0.48     | 2.97        | 2      | 1     |
| 1:A:21:LYS:HB3  | 1:A:45:CYS:HB3  | 0.48     | 1.85        | 8      | 1     |
| 1:A:4:LYS:CE    | 1:A:13:ASN:O    | 0.48     | 2.62        | 19     | 2     |
| 1:A:7:SER:O     | 1:A:8:PHE:CB    | 0.48     | 2.61        | 16     | 1     |
| 1:A:24:CYS:C    | 1:A:25:VAL:HG13 | 0.48     | 2.33        | 6      | 5     |
| 1:A:59:PHE:CD1  | 1:A:67:ASN:CG   | 0.48     | 2.92        | 5      | 1     |
| 1:A:63:THR:C    | 1:A:64:ASP:CG   | 0.48     | 2.82        | 5      | 2     |
| 1:A:1:MET:C     | 1:A:2:GLN:HG3   | 0.48     | 2.33        | 8      | 6     |
| 1:A:3:CYS:HB3   | 1:A:24:CYS:CA   | 0.48     | 2.39        | 5      | 9     |
| 1:A:11:CYS:O    | 1:A:68:HIS:OXT  | 0.48     | 2.32        | 7      | 1     |
| 1:A:43:ARG:NH1  | 1:A:43:ARG:HG2  | 0.48     | 2.24        | 10     | 1     |
| 1:A:2:GLN:O     | 1:A:3:CYS:SG    | 0.48     | 2.72        | 11     | 6     |
| 1:A:4:LYS:C     | 1:A:24:CYS:SG   | 0.48     | 2.96        | 19     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:26:LYS:CB   | 1:A:42:ARG:O    | 0.48     | 2.62        | 15     | 1     |
| 1:A:66:CYS:O    | 1:A:67:ASN:CG   | 0.48     | 2.56        | 19     | 1     |
| 1:A:28:SER:HB2  | 1:A:41:ILE:CG2  | 0.48     | 2.35        | 20     | 1     |
| 1:A:4:LYS:C     | 1:A:5:THR:HG23  | 0.47     | 2.33        | 2      | 3     |
| 1:A:24:CYS:O    | 1:A:59:PHE:O    | 0.47     | 2.32        | 20     | 2     |
| 1:A:4:LYS:O     | 1:A:67:ASN:HB2  | 0.47     | 2.09        | 4      | 1     |
| 1:A:26:LYS:HD3  | 1:A:67:ASN:OD1  | 0.47     | 2.09        | 15     | 2     |
| 1:A:2:GLN:HA    | 1:A:16:THR:CB   | 0.47     | 2.39        | 12     | 1     |
| 1:A:26:LYS:CG   | 1:A:43:ARG:HG3  | 0.47     | 2.38        | 17     | 1     |
| 1:A:11:CYS:SG   | 1:A:68:HIS:C    | 0.47     | 2.97        | 1      | 1     |
| 1:A:24:CYS:SG   | 1:A:61:CYS:SG   | 0.47     | 3.12        | 12     | 1     |
| 1:A:2:GLN:NE2   | 1:A:64:ASP:HB3  | 0.47     | 2.25        | 14     | 2     |
| 1:A:66:CYS:SG   | 1:A:66:CYS:O    | 0.47     | 2.72        | 15     | 1     |
| 1:A:7:SER:O     | 1:A:11:CYS:HB2  | 0.47     | 2.09        | 5      | 2     |
| 1:A:18:PRO:O    | 1:A:19:ASP:CG   | 0.47     | 2.57        | 5      | 1     |
| 1:A:9:TYR:O     | 1:A:9:TYR:CG    | 0.47     | 2.66        | 11     | 3     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:HB3  | 0.47     | 1.86        | 18     | 1     |
| 1:A:24:CYS:O    | 1:A:60:CYS:CA   | 0.47     | 2.62        | 4      | 2     |
| 1:A:4:LYS:HD3   | 1:A:6:CYS:SG    | 0.47     | 2.50        | 7      | 1     |
| 1:A:15:GLU:HG2  | 1:A:16:THR:N    | 0.47     | 2.24        | 8      | 1     |
| 1:A:5:THR:C     | 1:A:15:GLU:OE1  | 0.47     | 2.57        | 19     | 1     |
| 1:A:64:ASP:O    | 1:A:64:ASP:OD1  | 0.47     | 2.33        | 8      | 5     |
| 1:A:5:THR:OG1   | 1:A:43:ARG:HB2  | 0.47     | 2.10        | 6      | 1     |
| 1:A:11:CYS:O    | 1:A:68:HIS:O    | 0.47     | 2.33        | 16     | 1     |
| 1:A:61:CYS:SG   | 1:A:66:CYS:O    | 0.47     | 2.73        | 19     | 1     |
| 1:A:23:ILE:HG21 | 1:A:48:THR:O    | 0.47     | 2.10        | 8      | 5     |
| 1:A:4:LYS:O     | 1:A:24:CYS:SG   | 0.47     | 2.73        | 16     | 4     |
| 1:A:12:PRO:O    | 1:A:13:ASN:O    | 0.47     | 2.33        | 9      | 1     |
| 1:A:29:TRP:CD1  | 1:A:40:GLU:HB3  | 0.47     | 2.44        | 15     | 1     |
| 1:A:1:MET:SD    | 1:A:22:ASN:O    | 0.47     | 2.73        | 12     | 6     |
| 1:A:9:TYR:CE2   | 1:A:10:THR:HG22 | 0.47     | 2.44        | 7      | 1     |
| 1:A:28:SER:HA   | 1:A:41:ILE:HG22 | 0.47     | 1.85        | 17     | 3     |
| 1:A:64:ASP:C    | 1:A:66:CYS:N    | 0.47     | 2.72        | 11     | 1     |
| 1:A:43:ARG:N    | 1:A:43:ARG:HD3  | 0.47     | 2.25        | 17     | 2     |
| 1:A:26:LYS:CB   | 1:A:59:PHE:HB3  | 0.47     | 2.39        | 18     | 1     |
| 1:A:3:CYS:SG    | 1:A:17:CYS:SG   | 0.47     | 3.13        | 15     | 4     |
| 1:A:6:CYS:O     | 1:A:43:ARG:HD2  | 0.47     | 2.10        | 4      | 1     |
| 1:A:64:ASP:C    | 1:A:65:ASN:CG   | 0.47     | 2.83        | 17     | 4     |
| 1:A:5:THR:HA    | 1:A:43:ARG:CG   | 0.47     | 2.39        | 11     | 1     |
| 1:A:16:THR:HG22 | 1:A:17:CYS:N    | 0.47     | 2.23        | 20     | 4     |
| 1:A:1:MET:CB    | 1:A:22:ASN:HA   | 0.47     | 2.40        | 3      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:27:ARG:HG2  | 1:A:56:LEU:CD2  | 0.47     | 2.37        | 3      | 1     |
| 1:A:24:CYS:SG   | 1:A:61:CYS:O    | 0.47     | 2.73        | 18     | 3     |
| 1:A:39:ARG:O    | 1:A:41:ILE:N    | 0.47     | 2.48        | 10     | 2     |
| 1:A:14:SER:HB2  | 1:A:65:ASN:CG   | 0.47     | 2.34        | 16     | 2     |
| 1:A:39:ARG:C    | 1:A:40:GLU:OE1  | 0.47     | 2.58        | 13     | 1     |
| 1:A:23:ILE:CD1  | 1:A:48:THR:HA   | 0.47     | 2.40        | 18     | 2     |
| 1:A:41:ILE:O    | 1:A:41:ILE:HD13 | 0.46     | 2.10        | 1      | 1     |
| 1:A:16:THR:O    | 1:A:17:CYS:C    | 0.46     | 2.58        | 19     | 5     |
| 1:A:7:SER:HB2   | 1:A:9:TYR:CD2   | 0.46     | 2.45        | 5      | 1     |
| 1:A:42:ARG:O    | 1:A:43:ARG:HD2  | 0.46     | 2.10        | 7      | 1     |
| 1:A:1:MET:O     | 1:A:17:CYS:N    | 0.46     | 2.47        | 12     | 3     |
| 1:A:26:LYS:CG   | 1:A:42:ARG:O    | 0.46     | 2.63        | 8      | 1     |
| 1:A:2:GLN:HA    | 1:A:16:THR:OG1  | 0.46     | 2.10        | 12     | 1     |
| 1:A:11:CYS:SG   | 1:A:68:HIS:OXT  | 0.46     | 2.73        | 12     | 1     |
| 1:A:2:GLN:CD    | 1:A:64:ASP:HB3  | 0.46     | 2.35        | 17     | 1     |
| 1:A:11:CYS:SG   | 1:A:43:ARG:NH2  | 0.46     | 2.88        | 17     | 1     |
| 1:A:21:LYS:CG   | 1:A:45:CYS:HB3  | 0.46     | 2.40        | 18     | 1     |
| 1:A:1:MET:O     | 1:A:16:THR:CG2  | 0.46     | 2.64        | 17     | 2     |
| 1:A:42:ARG:C    | 1:A:43:ARG:CD   | 0.46     | 2.89        | 13     | 3     |
| 1:A:26:LYS:NZ   | 1:A:28:SER:HB3  | 0.46     | 2.26        | 8      | 1     |
| 1:A:27:ARG:HB3  | 1:A:56:LEU:CD2  | 0.46     | 2.40        | 11     | 1     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:CB   | 0.46     | 2.40        | 12     | 1     |
| 1:A:1:MET:SD    | 1:A:17:CYS:SG   | 0.46     | 3.13        | 15     | 1     |
| 1:A:2:GLN:C     | 1:A:3:CYS:SG    | 0.46     | 2.98        | 2      | 3     |
| 1:A:1:MET:SD    | 1:A:21:LYS:O    | 0.46     | 2.73        | 16     | 1     |
| 1:A:24:CYS:HB2  | 1:A:67:ASN:ND2  | 0.46     | 2.26        | 1      | 1     |
| 1:A:26:LYS:CG   | 1:A:59:PHE:HB3  | 0.46     | 2.41        | 13     | 4     |
| 1:A:10:THR:O    | 1:A:10:THR:OG1  | 0.46     | 2.31        | 1      | 2     |
| 1:A:26:LYS:O    | 1:A:58:VAL:HA   | 0.46     | 2.10        | 4      | 3     |
| 1:A:8:PHE:O     | 1:A:43:ARG:NH2  | 0.46     | 2.49        | 2      | 1     |
| 1:A:24:CYS:SG   | 1:A:63:THR:O    | 0.46     | 2.74        | 2      | 1     |
| 1:A:23:ILE:HG13 | 1:A:62:THR:HG22 | 0.46     | 1.87        | 4      | 2     |
| 1:A:67:ASN:O    | 1:A:68:HIS:O    | 0.46     | 2.34        | 8      | 1     |
| 1:A:2:GLN:HG2   | 1:A:16:THR:CG2  | 0.46     | 2.39        | 13     | 1     |
| 1:A:63:THR:CB   | 1:A:66:CYS:HB2  | 0.46     | 2.40        | 17     | 1     |
| 1:A:27:ARG:HA   | 1:A:57:THR:O    | 0.46     | 2.11        | 2      | 10    |
| 1:A:5:THR:O     | 1:A:6:CYS:O     | 0.46     | 2.34        | 6      | 1     |
| 1:A:8:PHE:C     | 1:A:10:THR:N    | 0.46     | 2.71        | 7      | 1     |
| 1:A:4:LYS:C     | 1:A:5:THR:CG2   | 0.46     | 2.88        | 10     | 1     |
| 1:A:9:TYR:O     | 1:A:68:HIS:O    | 0.46     | 2.34        | 11     | 1     |
| 1:A:10:THR:O    | 1:A:12:PRO:HD3  | 0.46     | 2.11        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:THR:OG1   | 1:A:15:GLU:OE1  | 0.46     | 2.34        | 9      | 1     |
| 1:A:21:LYS:HG2  | 1:A:22:ASN:N    | 0.46     | 2.26        | 10     | 1     |
| 1:A:29:TRP:NE1  | 1:A:40:GLU:HG2  | 0.46     | 2.26        | 10     | 1     |
| 1:A:7:SER:C     | 1:A:43:ARG:NH1  | 0.46     | 2.74        | 12     | 1     |
| 1:A:29:TRP:N    | 1:A:29:TRP:CD2  | 0.46     | 2.84        | 15     | 2     |
| 1:A:14:SER:CB   | 1:A:65:ASN:CG   | 0.46     | 2.89        | 16     | 2     |
| 1:A:62:THR:C    | 1:A:63:THR:CG2  | 0.46     | 2.89        | 7      | 1     |
| 1:A:56:LEU:CD1  | 1:A:57:THR:N    | 0.46     | 2.79        | 10     | 1     |
| 1:A:1:MET:HE3   | 1:A:22:ASN:CA   | 0.46     | 2.40        | 11     | 1     |
| 1:A:23:ILE:HD13 | 1:A:60:CYS:HB2  | 0.46     | 1.87        | 11     | 1     |
| 1:A:43:ARG:N    | 1:A:43:ARG:CD   | 0.46     | 2.79        | 16     | 2     |
| 1:A:4:LYS:HG3   | 1:A:68:HIS:CD2  | 0.46     | 2.44        | 16     | 1     |
| 1:A:42:ARG:O    | 1:A:43:ARG:HG3  | 0.46     | 2.11        | 16     | 1     |
| 1:A:30:THR:O    | 1:A:30:THR:HG23 | 0.46     | 2.09        | 12     | 4     |
| 1:A:24:CYS:CB   | 1:A:67:ASN:ND2  | 0.46     | 2.79        | 4      | 1     |
| 1:A:18:PRO:O    | 1:A:19:ASP:O    | 0.46     | 2.33        | 5      | 2     |
| 1:A:4:LYS:HD3   | 1:A:68:HIS:O    | 0.46     | 2.11        | 7      | 2     |
| 1:A:9:TYR:CE2   | 1:A:10:THR:HG21 | 0.46     | 2.46        | 7      | 1     |
| 1:A:21:LYS:CB   | 1:A:45:CYS:CB   | 0.46     | 2.94        | 8      | 1     |
| 1:A:41:ILE:HD11 | 1:A:43:ARG:NH1  | 0.46     | 2.26        | 12     | 1     |
| 1:A:17:CYS:HB3  | 1:A:18:PRO:HD2  | 0.45     | 1.88        | 2      | 11    |
| 1:A:21:LYS:HG2  | 1:A:45:CYS:CB   | 0.45     | 2.41        | 13     | 2     |
| 1:A:24:CYS:SG   | 1:A:61:CYS:CB   | 0.45     | 3.04        | 7      | 2     |
| 1:A:26:LYS:NZ   | 1:A:67:ASN:HB3  | 0.45     | 2.25        | 16     | 1     |
| 1:A:64:ASP:C    | 1:A:65:ASN:ND2  | 0.45     | 2.74        | 17     | 1     |
| 1:A:41:ILE:CD1  | 1:A:41:ILE:O    | 0.45     | 2.65        | 1      | 1     |
| 1:A:28:SER:O    | 1:A:57:THR:HB   | 0.45     | 2.11        | 2      | 1     |
| 1:A:4:LYS:HB3   | 1:A:67:ASN:O    | 0.45     | 2.12        | 16     | 3     |
| 1:A:29:TRP:O    | 1:A:39:ARG:HG3  | 0.45     | 2.11        | 8      | 2     |
| 1:A:24:CYS:SG   | 1:A:66:CYS:SG   | 0.45     | 3.15        | 11     | 1     |
| 1:A:1:MET:HG3   | 1:A:17:CYS:HB2  | 0.45     | 1.87        | 15     | 1     |
| 1:A:1:MET:O     | 1:A:2:GLN:HG3   | 0.45     | 2.11        | 2      | 4     |
| 1:A:26:LYS:CG   | 1:A:27:ARG:N    | 0.45     | 2.78        | 5      | 1     |
| 1:A:28:SER:CA   | 1:A:41:ILE:HB   | 0.45     | 2.42        | 6      | 1     |
| 1:A:39:ARG:O    | 1:A:39:ARG:CG   | 0.45     | 2.65        | 7      | 1     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:C    | 0.45     | 2.36        | 10     | 1     |
| 1:A:5:THR:HA    | 1:A:68:HIS:NE2  | 0.45     | 2.26        | 15     | 1     |
| 1:A:21:LYS:C    | 1:A:22:ASN:ND2  | 0.45     | 2.74        | 15     | 1     |
| 1:A:4:LYS:CG    | 1:A:68:HIS:HB3  | 0.45     | 2.41        | 16     | 1     |
| 1:A:4:LYS:N     | 1:A:65:ASN:HA   | 0.45     | 2.25        | 15     | 2     |
| 1:A:3:CYS:O     | 1:A:4:LYS:O     | 0.45     | 2.34        | 12     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:ILE:HG22 | 1:A:24:CYS:O    | 0.45     | 2.11        | 19     | 1     |
| 1:A:4:LYS:HD2   | 1:A:4:LYS:N     | 0.45     | 2.27        | 2      | 1     |
| 1:A:5:THR:OG1   | 1:A:43:ARG:C    | 0.45     | 2.60        | 6      | 1     |
| 1:A:56:LEU:HG   | 1:A:57:THR:N    | 0.45     | 2.26        | 7      | 1     |
| 1:A:2:GLN:C     | 1:A:15:GLU:O    | 0.45     | 2.60        | 10     | 1     |
| 1:A:1:MET:HG2   | 1:A:22:ASN:CA   | 0.45     | 2.42        | 15     | 1     |
| 1:A:8:PHE:CG    | 1:A:43:ARG:CZ   | 0.45     | 3.00        | 7      | 1     |
| 1:A:28:SER:O    | 1:A:28:SER:OG   | 0.45     | 2.35        | 13     | 1     |
| 1:A:24:CYS:HB2  | 1:A:67:ASN:CG   | 0.45     | 2.37        | 18     | 2     |
| 1:A:63:THR:C    | 1:A:64:ASP:O    | 0.45     | 2.58        | 9      | 6     |
| 1:A:26:LYS:CE   | 1:A:67:ASN:HB3  | 0.45     | 2.42        | 12     | 2     |
| 1:A:4:LYS:HD2   | 1:A:11:CYS:CB   | 0.45     | 2.41        | 18     | 1     |
| 1:A:59:PHE:O    | 1:A:59:PHE:CD1  | 0.45     | 2.70        | 20     | 1     |
| 1:A:4:LYS:O     | 1:A:4:LYS:HD2   | 0.45     | 2.12        | 2      | 1     |
| 1:A:27:ARG:HG3  | 1:A:29:TRP:CZ3  | 0.45     | 2.47        | 2      | 1     |
| 1:A:5:THR:HB    | 1:A:24:CYS:SG   | 0.45     | 2.52        | 6      | 1     |
| 1:A:17:CYS:SG   | 1:A:18:PRO:HD2  | 0.45     | 2.52        | 11     | 1     |
| 1:A:29:TRP:CA   | 1:A:56:LEU:HD21 | 0.44     | 2.42        | 8      | 1     |
| 1:A:29:TRP:HB3  | 1:A:56:LEU:CG   | 0.44     | 2.42        | 10     | 1     |
| 1:A:4:LYS:NZ    | 1:A:24:CYS:HB3  | 0.44     | 2.27        | 12     | 1     |
| 1:A:28:SER:CA   | 1:A:41:ILE:HG22 | 0.44     | 2.42        | 20     | 1     |
| 1:A:9:TYR:C     | 1:A:10:THR:CG2  | 0.44     | 2.91        | 1      | 2     |
| 1:A:56:LEU:HD22 | 1:A:57:THR:N    | 0.44     | 2.27        | 2      | 2     |
| 1:A:63:THR:O    | 1:A:64:ASP:OD2  | 0.44     | 2.35        | 5      | 1     |
| 1:A:21:LYS:HD2  | 1:A:46:ALA:HA   | 0.44     | 1.90        | 20     | 3     |
| 1:A:2:GLN:HA    | 1:A:15:GLU:O    | 0.44     | 2.12        | 10     | 1     |
| 1:A:2:GLN:CB    | 1:A:64:ASP:HA   | 0.44     | 2.42        | 11     | 1     |
| 1:A:15:GLU:OE1  | 1:A:16:THR:O    | 0.44     | 2.34        | 17     | 1     |
| 1:A:15:GLU:O    | 1:A:16:THR:O    | 0.44     | 2.35        | 5      | 1     |
| 1:A:7:SER:CB    | 1:A:9:TYR:CE1   | 0.44     | 3.00        | 7      | 1     |
| 1:A:4:LYS:HE3   | 1:A:65:ASN:O    | 0.44     | 2.12        | 15     | 1     |
| 1:A:42:ARG:C    | 1:A:43:ARG:HD3  | 0.44     | 2.38        | 7      | 1     |
| 1:A:21:LYS:C    | 1:A:21:LYS:CD   | 0.44     | 2.88        | 10     | 1     |
| 1:A:5:THR:O     | 1:A:43:ARG:HG2  | 0.44     | 2.13        | 16     | 1     |
| 1:A:61:CYS:SG   | 1:A:67:ASN:OD1  | 0.44     | 2.75        | 1      | 1     |
| 1:A:26:LYS:O    | 1:A:27:ARG:HG2  | 0.44     | 2.13        | 4      | 1     |
| 1:A:56:LEU:HD13 | 1:A:57:THR:H    | 0.44     | 1.72        | 14     | 2     |
| 1:A:9:TYR:HA    | 1:A:41:ILE:HD11 | 0.44     | 1.89        | 3      | 2     |
| 1:A:21:LYS:CG   | 1:A:22:ASN:N    | 0.44     | 2.81        | 10     | 1     |
| 1:A:10:THR:OG1  | 1:A:11:CYS:N    | 0.44     | 2.50        | 13     | 1     |
| 1:A:1:MET:HG3   | 1:A:17:CYS:CB   | 0.44     | 2.43        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:22:ASN:O    | 1:A:23:ILE:CG1  | 0.44     | 2.66        | 15     | 1     |
| 1:A:27:ARG:HB3  | 1:A:57:THR:O    | 0.44     | 2.13        | 20     | 1     |
| 1:A:23:ILE:CG2  | 1:A:25:VAL:HG12 | 0.44     | 2.42        | 10     | 2     |
| 1:A:28:SER:HB3  | 1:A:41:ILE:CG2  | 0.44     | 2.43        | 6      | 1     |
| 1:A:4:LYS:CG    | 1:A:14:SER:HA   | 0.44     | 2.43        | 7      | 1     |
| 1:A:9:TYR:HA    | 1:A:43:ARG:NH1  | 0.44     | 2.27        | 8      | 1     |
| 1:A:21:LYS:CD   | 1:A:45:CYS:HB3  | 0.44     | 2.42        | 18     | 1     |
| 1:A:67:ASN:OD1  | 1:A:67:ASN:N    | 0.44     | 2.51        | 7      | 1     |
| 1:A:18:PRO:HG2  | 1:A:21:LYS:NZ   | 0.44     | 2.28        | 10     | 1     |
| 1:A:24:CYS:SG   | 1:A:61:CYS:HB2  | 0.44     | 2.52        | 13     | 1     |
| 1:A:4:LYS:HA    | 1:A:15:GLU:CB   | 0.44     | 2.43        | 17     | 1     |
| 1:A:17:CYS:HB3  | 1:A:21:LYS:HB2  | 0.44     | 1.89        | 19     | 1     |
| 1:A:63:THR:O    | 1:A:64:ASP:CG   | 0.43     | 2.61        | 5      | 1     |
| 1:A:6:CYS:O     | 1:A:43:ARG:HG2  | 0.43     | 2.12        | 8      | 3     |
| 1:A:27:ARG:HB3  | 1:A:56:LEU:HD11 | 0.43     | 1.89        | 7      | 1     |
| 1:A:2:GLN:CA    | 1:A:15:GLU:O    | 0.43     | 2.66        | 10     | 1     |
| 1:A:63:THR:HG23 | 1:A:64:ASP:N    | 0.43     | 2.28        | 20     | 1     |
| 1:A:1:MET:O     | 1:A:17:CYS:HB2  | 0.43     | 2.14        | 5      | 2     |
| 1:A:24:CYS:SG   | 1:A:67:ASN:HB2  | 0.43     | 2.53        | 6      | 1     |
| 1:A:28:SER:O    | 1:A:56:LEU:HD11 | 0.43     | 2.11        | 10     | 1     |
| 1:A:61:CYS:SG   | 1:A:62:THR:N    | 0.43     | 2.91        | 15     | 1     |
| 1:A:26:LYS:C    | 1:A:27:ARG:HD3  | 0.43     | 2.38        | 3      | 1     |
| 1:A:22:ASN:O    | 1:A:23:ILE:HG13 | 0.43     | 2.12        | 15     | 1     |
| 1:A:2:GLN:O     | 1:A:64:ASP:HA   | 0.43     | 2.14        | 3      | 3     |
| 1:A:21:LYS:HD3  | 1:A:46:ALA:N    | 0.43     | 2.29        | 3      | 1     |
| 1:A:66:CYS:O    | 1:A:67:ASN:HB2  | 0.43     | 2.14        | 6      | 1     |
| 1:A:6:CYS:SG    | 1:A:43:ARG:NH2  | 0.43     | 2.91        | 6      | 1     |
| 1:A:4:LYS:CD    | 1:A:68:HIS:O    | 0.43     | 2.67        | 7      | 1     |
| 1:A:58:VAL:HG12 | 1:A:59:PHE:H    | 0.43     | 1.73        | 10     | 1     |
| 1:A:42:ARG:HD3  | 1:A:43:ARG:N    | 0.43     | 2.28        | 12     | 1     |
| 1:A:28:SER:CB   | 1:A:41:ILE:CG2  | 0.43     | 2.88        | 20     | 1     |
| 1:A:4:LYS:HG2   | 1:A:65:ASN:CB   | 0.43     | 2.43        | 3      | 1     |
| 1:A:14:SER:HB2  | 1:A:65:ASN:ND2  | 0.43     | 2.27        | 13     | 2     |
| 1:A:5:THR:C     | 1:A:43:ARG:HG3  | 0.43     | 2.39        | 6      | 1     |
| 1:A:6:CYS:SG    | 1:A:15:GLU:OE1  | 0.43     | 2.76        | 14     | 1     |
| 1:A:39:ARG:HG2  | 1:A:39:ARG:O    | 0.43     | 2.14        | 14     | 1     |
| 1:A:61:CYS:CB   | 1:A:66:CYS:O    | 0.43     | 2.66        | 15     | 1     |
| 1:A:43:ARG:O    | 1:A:44:GLU:HG2  | 0.43     | 2.13        | 4      | 1     |
| 1:A:25:VAL:HA   | 1:A:59:PHE:O    | 0.43     | 2.13        | 9      | 3     |
| 1:A:21:LYS:HE2  | 1:A:45:CYS:O    | 0.43     | 2.14        | 11     | 1     |
| 1:A:28:SER:CB   | 1:A:41:ILE:HB   | 0.43     | 2.44        | 6      | 1     |

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| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:47:ALA:C    | 1:A:48:THR:OG1 | 0.43     | 2.62        | 10     | 1     |
| 1:A:4:LYS:CB    | 1:A:68:HIS:HB3 | 0.43     | 2.43        | 16     | 1     |
| 1:A:11:CYS:O    | 1:A:68:HIS:HB2 | 0.43     | 2.14        | 16     | 1     |
| 1:A:26:LYS:C    | 1:A:27:ARG:HG3 | 0.43     | 2.39        | 4      | 1     |
| 1:A:4:LYS:HD3   | 1:A:68:HIS:CA  | 0.43     | 2.44        | 14     | 1     |
| 1:A:23:ILE:HG23 | 1:A:24:CYS:H   | 0.42     | 1.71        | 4      | 1     |
| 1:A:26:LYS:CA   | 1:A:42:ARG:O   | 0.42     | 2.67        | 15     | 1     |
| 1:A:43:ARG:O    | 1:A:44:GLU:OE2 | 0.42     | 2.37        | 16     | 1     |
| 1:A:4:LYS:HD3   | 1:A:13:ASN:O   | 0.42     | 2.14        | 18     | 1     |
| 1:A:23:ILE:HG12 | 1:A:61:CYS:O   | 0.42     | 2.13        | 18     | 7     |
| 1:A:1:MET:CG    | 1:A:22:ASN:HA  | 0.42     | 2.45        | 4      | 1     |
| 1:A:59:PHE:CE1  | 1:A:61:CYS:SG  | 0.42     | 3.12        | 20     | 1     |
| 1:A:7:SER:C     | 1:A:11:CYS:HB2 | 0.42     | 2.39        | 7      | 1     |
| 1:A:8:PHE:CG    | 1:A:68:HIS:O   | 0.42     | 2.72        | 16     | 1     |
| 1:A:26:LYS:HE3  | 1:A:43:ARG:NH1 | 0.42     | 2.29        | 3      | 1     |
| 1:A:8:PHE:CB    | 1:A:68:HIS:HB2 | 0.42     | 2.43        | 7      | 1     |
| 1:A:29:TRP:CE2  | 1:A:40:GLU:HG2 | 0.42     | 2.49        | 10     | 1     |
| 1:A:29:TRP:N    | 1:A:39:ARG:HG2 | 0.42     | 2.28        | 16     | 1     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:HB2 | 0.42     | 1.92        | 2      | 2     |
| 1:A:42:ARG:C    | 1:A:43:ARG:HG3 | 0.42     | 2.40        | 4      | 1     |
| 1:A:23:ILE:O    | 1:A:45:CYS:HA  | 0.42     | 2.14        | 19     | 2     |
| 1:A:14:SER:CB   | 1:A:65:ASN:HB3 | 0.42     | 2.44        | 5      | 1     |
| 1:A:63:THR:CG2  | 1:A:64:ASP:N   | 0.42     | 2.83        | 5      | 1     |
| 1:A:28:SER:OG   | 1:A:57:THR:HB  | 0.42     | 2.15        | 12     | 2     |
| 1:A:43:ARG:CZ   | 1:A:67:ASN:O   | 0.42     | 2.68        | 14     | 1     |
| 1:A:9:TYR:C     | 1:A:43:ARG:NH2 | 0.42     | 2.77        | 2      | 1     |
| 1:A:26:LYS:O    | 1:A:27:ARG:CG  | 0.42     | 2.68        | 4      | 1     |
| 1:A:4:LYS:HG2   | 1:A:15:GLU:N   | 0.42     | 2.30        | 5      | 1     |
| 1:A:1:MET:HG2   | 1:A:22:ASN:C   | 0.42     | 2.40        | 15     | 1     |
| 1:A:23:ILE:HB   | 1:A:47:ALA:O   | 0.42     | 2.14        | 2      | 3     |
| 1:A:25:VAL:CG2  | 1:A:25:VAL:O   | 0.42     | 2.68        | 2      | 1     |
| 1:A:29:TRP:CD2  | 1:A:29:TRP:N   | 0.42     | 2.87        | 9      | 2     |
| 1:A:2:GLN:HG3   | 1:A:16:THR:OG1 | 0.42     | 2.15        | 16     | 1     |
| 1:A:27:ARG:O    | 1:A:41:ILE:CA  | 0.42     | 2.68        | 4      | 1     |
| 1:A:15:GLU:OE1  | 1:A:15:GLU:C   | 0.42     | 2.63        | 7      | 1     |
| 1:A:21:LYS:HD2  | 1:A:45:CYS:HB3 | 0.42     | 1.91        | 11     | 2     |
| 1:A:62:THR:C    | 1:A:63:THR:OG1 | 0.42     | 2.61        | 15     | 1     |
| 1:A:3:CYS:HB2   | 1:A:45:CYS:SG  | 0.42     | 2.54        | 18     | 1     |
| 1:A:23:ILE:HG22 | 1:A:46:ALA:O   | 0.42     | 2.14        | 20     | 1     |
| 1:A:21:LYS:HB2  | 1:A:46:ALA:HA  | 0.41     | 1.91        | 10     | 1     |
| 1:A:27:ARG:NH2  | 1:A:42:ARG:HD3 | 0.41     | 2.30        | 14     | 1     |

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| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:21:LYS:HD3  | 1:A:45:CYS:O   | 0.41     | 2.15        | 1      | 1     |
| 1:A:4:LYS:HG3   | 1:A:68:HIS:OXT | 0.41     | 2.14        | 7      | 1     |
| 1:A:43:ARG:O    | 1:A:44:GLU:CD  | 0.41     | 2.63        | 16     | 1     |
| 1:A:6:CYS:HB2   | 1:A:43:ARG:NH2 | 0.41     | 2.30        | 18     | 1     |
| 1:A:4:LYS:O     | 1:A:67:ASN:HB3 | 0.41     | 2.15        | 6      | 1     |
| 1:A:4:LYS:HE3   | 1:A:15:GLU:HB2 | 0.41     | 1.92        | 7      | 1     |
| 1:A:8:PHE:CA    | 1:A:11:CYS:HB2 | 0.41     | 2.44        | 7      | 1     |
| 1:A:40:GLU:N    | 1:A:40:GLU:CD  | 0.41     | 2.77        | 7      | 1     |
| 1:A:4:LYS:HE2   | 1:A:14:SER:C   | 0.41     | 2.41        | 16     | 1     |
| 1:A:7:SER:CB    | 1:A:41:ILE:CD1 | 0.41     | 2.97        | 16     | 1     |
| 1:A:62:THR:O    | 1:A:62:THR:OG1 | 0.41     | 2.32        | 17     | 1     |
| 1:A:64:ASP:O    | 1:A:65:ASN:CG  | 0.41     | 2.63        | 17     | 1     |
| 1:A:63:THR:HG22 | 1:A:66:CYS:HB2 | 0.41     | 1.92        | 20     | 1     |
| 1:A:4:LYS:HD2   | 1:A:68:HIS:OXT | 0.41     | 2.14        | 7      | 1     |
| 1:A:4:LYS:CE    | 1:A:15:GLU:HB2 | 0.41     | 2.45        | 7      | 1     |
| 1:A:4:LYS:HD3   | 1:A:11:CYS:O   | 0.41     | 2.16        | 11     | 1     |
| 1:A:4:LYS:CD    | 1:A:68:HIS:HB3 | 0.41     | 2.45        | 16     | 1     |
| 1:A:1:MET:HE3   | 1:A:18:PRO:O   | 0.41     | 2.16        | 17     | 1     |
| 1:A:11:CYS:SG   | 1:A:68:HIS:O   | 0.41     | 2.79        | 1      | 1     |
| 1:A:66:CYS:O    | 1:A:68:HIS:CD2 | 0.41     | 2.74        | 1      | 1     |
| 1:A:21:LYS:N    | 1:A:21:LYS:CD  | 0.41     | 2.83        | 10     | 1     |
| 1:A:26:LYS:HG3  | 1:A:59:PHE:HB3 | 0.41     | 1.93        | 14     | 1     |
| 1:A:4:LYS:O     | 1:A:26:LYS:NZ  | 0.41     | 2.53        | 16     | 1     |
| 1:A:4:LYS:HE2   | 1:A:15:GLU:N   | 0.41     | 2.30        | 16     | 1     |
| 1:A:21:LYS:HE3  | 1:A:45:CYS:O   | 0.41     | 2.15        | 6      | 1     |
| 1:A:25:VAL:O    | 1:A:43:ARG:HA  | 0.41     | 2.15        | 16     | 2     |
| 1:A:43:ARG:O    | 1:A:44:GLU:HB2 | 0.41     | 2.16        | 15     | 1     |
| 1:A:9:TYR:O     | 1:A:10:THR:HB  | 0.41     | 2.16        | 16     | 1     |
| 1:A:21:LYS:HD3  | 1:A:21:LYS:HA  | 0.41     | 1.68        | 2      | 2     |
| 1:A:43:ARG:CD   | 1:A:43:ARG:N   | 0.41     | 2.83        | 9      | 1     |
| 1:A:4:LYS:N     | 1:A:4:LYS:CD   | 0.41     | 2.84        | 12     | 1     |
| 1:A:63:THR:OG1  | 1:A:66:CYS:HB2 | 0.41     | 2.15        | 17     | 1     |
| 1:A:23:ILE:CG2  | 1:A:46:ALA:O   | 0.41     | 2.68        | 20     | 1     |
| 1:A:19:ASP:OD1  | 1:A:21:LYS:N   | 0.41     | 2.54        | 5      | 1     |
| 1:A:27:ARG:CB   | 1:A:29:TRP:CZ3 | 0.41     | 3.03        | 12     | 1     |
| 1:A:1:MET:HG3   | 1:A:21:LYS:C   | 0.41     | 2.41        | 16     | 1     |
| 1:A:24:CYS:HB2  | 1:A:67:ASN:OD1 | 0.41     | 2.16        | 18     | 1     |
| 1:A:59:PHE:O    | 1:A:67:ASN:ND2 | 0.41     | 2.54        | 1      | 1     |
| 1:A:4:LYS:C     | 1:A:4:LYS:HD3  | 0.41     | 2.41        | 2      | 1     |
| 1:A:28:SER:CB   | 1:A:57:THR:HB  | 0.41     | 2.45        | 2      | 1     |
| 1:A:59:PHE:CE2  | 1:A:66:CYS:SG  | 0.41     | 3.14        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:18:PRO:O    | 1:A:19:ASP:OD1  | 0.41     | 2.39        | 5      | 1     |
| 1:A:63:THR:O    | 1:A:64:ASP:HB3  | 0.41     | 2.14        | 5      | 1     |
| 1:A:21:LYS:CE   | 1:A:45:CYS:O    | 0.41     | 2.69        | 6      | 1     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:O    | 0.41     | 2.16        | 8      | 1     |
| 1:A:29:TRP:HA   | 1:A:56:LEU:HD21 | 0.41     | 1.93        | 8      | 2     |
| 1:A:1:MET:SD    | 1:A:22:ASN:HA   | 0.41     | 2.55        | 11     | 1     |
| 1:A:27:ARG:N    | 1:A:27:ARG:HD3  | 0.41     | 2.31        | 11     | 1     |
| 1:A:21:LYS:CE   | 1:A:21:LYS:HA   | 0.41     | 2.46        | 12     | 1     |
| 1:A:23:ILE:HG22 | 1:A:24:CYS:N    | 0.41     | 2.30        | 15     | 1     |
| 1:A:26:LYS:HE3  | 1:A:68:HIS:CE1  | 0.41     | 2.51        | 15     | 1     |
| 1:A:27:ARG:CG   | 1:A:56:LEU:CD2  | 0.41     | 2.90        | 17     | 1     |
| 1:A:43:ARG:C    | 1:A:44:GLU:CG   | 0.41     | 2.94        | 4      | 1     |
| 1:A:14:SER:HB3  | 1:A:65:ASN:HB2  | 0.41     | 1.92        | 16     | 1     |
| 1:A:2:GLN:HG2   | 1:A:16:THR:CB   | 0.40     | 2.46        | 2      | 2     |
| 1:A:28:SER:HG   | 1:A:57:THR:HB   | 0.40     | 1.75        | 5      | 1     |
| 1:A:11:CYS:O    | 1:A:68:HIS:HB3  | 0.40     | 2.16        | 7      | 1     |
| 1:A:29:TRP:O    | 1:A:39:ARG:HB2  | 0.40     | 2.15        | 7      | 1     |
| 1:A:42:ARG:C    | 1:A:43:ARG:HD2  | 0.40     | 2.41        | 13     | 1     |
| 1:A:5:THR:HA    | 1:A:43:ARG:CB   | 0.40     | 2.45        | 17     | 1     |
| 1:A:4:LYS:HE2   | 1:A:13:ASN:O    | 0.40     | 2.15        | 19     | 1     |
| 1:A:6:CYS:C     | 1:A:7:SER:OG    | 0.40     | 2.63        | 5      | 1     |
| 1:A:8:PHE:CE2   | 1:A:68:HIS:CE1  | 0.40     | 3.09        | 5      | 1     |
| 1:A:6:CYS:SG    | 1:A:43:ARG:CZ   | 0.40     | 3.09        | 6      | 1     |
| 1:A:56:LEU:HD12 | 1:A:56:LEU:HA   | 0.40     | 1.71        | 11     | 1     |
| 1:A:68:HIS:N    | 1:A:68:HIS:HD2  | 0.40     | 2.12        | 15     | 1     |
| 1:A:42:ARG:C    | 1:A:43:ARG:CG   | 0.40     | 2.94        | 16     | 1     |
| 1:A:9:TYR:O     | 1:A:43:ARG:NH1  | 0.40     | 2.54        | 8      | 1     |
| 1:A:26:LYS:HB2  | 1:A:42:ARG:O    | 0.40     | 2.16        | 11     | 1     |
| 1:A:3:CYS:HB2   | 1:A:17:CYS:SG   | 0.40     | 2.56        | 12     | 1     |
| 1:A:56:LEU:HD23 | 1:A:56:LEU:HA   | 0.40     | 1.78        | 2      | 1     |
| 1:A:14:SER:HB3  | 1:A:65:ASN:CG   | 0.40     | 2.42        | 6      | 1     |
| 1:A:24:CYS:O    | 1:A:25:VAL:HG13 | 0.40     | 2.17        | 6      | 1     |
| 1:A:4:LYS:HD2   | 1:A:67:ASN:C    | 0.40     | 2.41        | 12     | 1     |
| 1:A:25:VAL:C    | 1:A:26:LYS:HG3  | 0.40     | 2.41        | 12     | 1     |
| 1:A:41:ILE:HD11 | 1:A:43:ARG:HH11 | 0.40     | 1.76        | 12     | 1     |
| 1:A:56:LEU:N    | 1:A:56:LEU:HD23 | 0.40     | 2.31        | 12     | 1     |
| 1:A:68:HIS:O    | 1:A:68:HIS:CG   | 0.40     | 2.72        | 14     | 1     |
| 1:A:43:ARG:NH1  | 1:A:43:ARG:CG   | 0.40     | 2.81        | 18     | 1     |
| 1:A:21:LYS:HG3  | 1:A:45:CYS:SG   | 0.40     | 2.57        | 19     | 1     |
| 1:A:25:VAL:HG21 | 1:A:46:ALA:HB3  | 0.40     | 1.93        | 20     | 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     | 51/68 (75%)     | 33±3 (64±6%) | 13±3 (25±5%) | 5±2 (11±3%) | <b>1</b>    | <b>8</b> |
| All | All   | 1020/1360 (75%) | 657 (64%)    | 254 (25%)    | 109 (11%)   | <b>1</b>    | <b>8</b> |

All 23 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     | 65  | ASN  | 16             |
| 1   | A     | 20  | GLY  | 12             |
| 1   | A     | 22  | ASN  | 11             |
| 1   | A     | 64  | ASP  | 9              |
| 1   | A     | 10  | THR  | 8              |
| 1   | A     | 67  | ASN  | 7              |
| 1   | A     | 13  | ASN  | 6              |
| 1   | A     | 6   | CYS  | 5              |
| 1   | A     | 44  | GLU  | 4              |
| 1   | A     | 19  | ASP  | 4              |
| 1   | A     | 15  | GLU  | 3              |
| 1   | A     | 48  | THR  | 3              |
| 1   | A     | 4   | LYS  | 3              |
| 1   | A     | 66  | CYS  | 3              |
| 1   | A     | 40  | GLU  | 3              |
| 1   | A     | 41  | ILE  | 2              |
| 1   | A     | 42  | ARG  | 2              |
| 1   | A     | 47  | ALA  | 2              |
| 1   | A     | 7   | SER  | 2              |
| 1   | A     | 25  | VAL  | 1              |
| 1   | A     | 16  | THR  | 1              |
| 1   | A     | 8   | PHE  | 1              |
| 1   | A     | 23  | ILE  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |
|-----|-------|-----------------|--------------|--------------|-------------|
| 1   | A     | 50/61 (82%)     | 30±3 (60±7%) | 20±3 (40±7%) | 0 5         |
| All | All   | 1000/1220 (82%) | 602 (60%)    | 398 (40%)    | 0 5         |

All 47 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     | 23  | ILE  | 20             |
| 1   | A     | 48  | THR  | 20             |
| 1   | A     | 24  | CYS  | 18             |
| 1   | A     | 10  | THR  | 16             |
| 1   | A     | 21  | LYS  | 16             |
| 1   | A     | 58  | VAL  | 16             |
| 1   | A     | 43  | ARG  | 15             |
| 1   | A     | 14  | SER  | 14             |
| 1   | A     | 4   | LYS  | 14             |
| 1   | A     | 40  | GLU  | 14             |
| 1   | A     | 60  | CYS  | 13             |
| 1   | A     | 15  | GLU  | 13             |
| 1   | A     | 44  | GLU  | 12             |
| 1   | A     | 27  | ARG  | 11             |
| 1   | A     | 41  | ILE  | 11             |
| 1   | A     | 67  | ASN  | 11             |
| 1   | A     | 56  | LEU  | 11             |
| 1   | A     | 63  | THR  | 11             |
| 1   | A     | 26  | LYS  | 10             |
| 1   | A     | 1   | MET  | 9              |
| 1   | A     | 9   | TYR  | 9              |
| 1   | A     | 39  | ARG  | 9              |
| 1   | A     | 65  | ASN  | 9              |
| 1   | A     | 7   | SER  | 8              |
| 1   | A     | 25  | VAL  | 7              |
| 1   | A     | 2   | GLN  | 7              |
| 1   | A     | 30  | THR  | 7              |
| 1   | A     | 11  | CYS  | 6              |
| 1   | A     | 61  | CYS  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 28  | SER  | 6              |
| 1   | A     | 16  | THR  | 6              |
| 1   | A     | 8   | PHE  | 5              |
| 1   | A     | 5   | THR  | 5              |
| 1   | A     | 29  | TRP  | 5              |
| 1   | A     | 3   | CYS  | 4              |
| 1   | A     | 57  | THR  | 4              |
| 1   | A     | 19  | ASP  | 3              |
| 1   | A     | 42  | ARG  | 3              |
| 1   | A     | 62  | THR  | 2              |
| 1   | A     | 6   | CYS  | 2              |
| 1   | A     | 64  | ASP  | 2              |
| 1   | A     | 68  | HIS  | 2              |
| 1   | A     | 17  | CYS  | 2              |
| 1   | A     | 22  | ASN  | 1              |
| 1   | A     | 13  | ASN  | 1              |
| 1   | A     | 66  | CYS  | 1              |
| 1   | A     | 45  | CYS  | 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 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 ⓘ

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided