# Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 11:16 AM EST

| | | |
|---|---|---|
| PDB ID | : | 2FUU |
| Title | : | NMR solution structure of the PHD domain from the human BPTF in complex with H3(1-15)K4me3 peptide |
| Authors | : | Ilin, S.; Patel, D.J. |
| Deposited on | : | 2006-01-27 |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

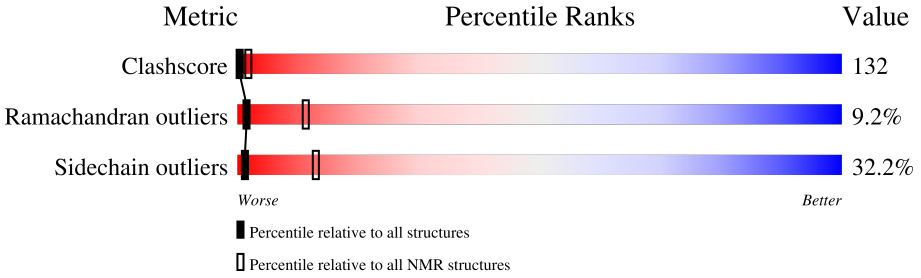
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.27 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.27 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 62 | 13% 40% 21% • 24% |
| 2 | B | 15 | 13% 87% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:10-A:56, B:2-B:3 (49) | 0.21 | 3 |

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

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

The models can be grouped into 2 clusters and 8 single-model clusters were found.

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

# 3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1178 atoms, of which 574 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called bromodomain PHD finger transcription factor.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 62 | 941 | 304 | 451 | 79 | 100 | 7 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | cloning artifact | GB 31322942 |
| A | 2 | PRO | - | cloning artifact | GB 31322942 |
| A | 3 | LEU | - | cloning artifact | GB 31322942 |
| A | 4 | GLY | - | cloning artifact | GB 31322942 |
| A | 5 | SER | - | cloning artifact | GB 31322942 |

- Molecule 2 is a protein called Histone H3.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | |
| 2 | B | 15 | 235 | 66 | 123 | 25 | 21 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 4 | M3L | LYS | modified residue | UNP P61836 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | |
|---|---|---|---|---|
| | | | Total | Zn |
| 3 | A | 2 | 2 | 2 |

# 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: bromodomain PHD finger transcription factor

Chain A: 13% 40% 21% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

• Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

## 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: bromodomain PHD finger transcription factor

Chain A: 16% 37% 21% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

• Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.2 Score per residue for model 2

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 15% 40% 19% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 40% 23% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 P54 Q55 C56 Q57 S58 T59 E60 D61

A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.4 Score per residue for model 4

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 40% 24% 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

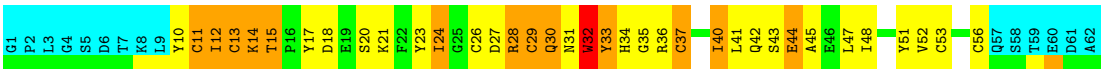
Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.5 Score per residue for model 5

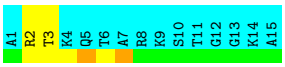
- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 18% 35% 21% • 24%




- Molecule 2: Histone H3

Chain B: 13% 87%



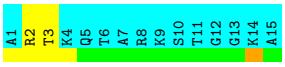

### 4.2.6 Score per residue for model 6

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 10% 37% 24% 5% 24%

- Molecule 2: Histone H3

Chain B: 13% 87%



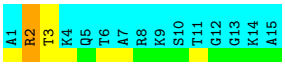

### 4.2.7 Score per residue for model 7

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 18% 31% 26% • 24%

- Molecule 2: Histone H3

Chain B: 7% 7% 87%



### 4.2.8 Score per residue for model 8

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 42% 21% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.9 Score per residue for model 9

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 13% 35% 26% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 F54 Q55 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.10 Score per residue for model 10

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 34% 29% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 V38 G39 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

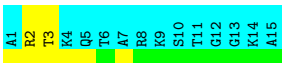
### 4.2.11 Score per residue for model 11

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 16% 35% 23% • 24%

- Molecule 2: Histone H3

Chain B: 13% 87%



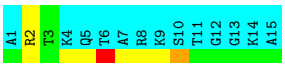

### 4.2.12 Score per residue for model 12

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 45% 19% 24%

- Molecule 2: Histone H3

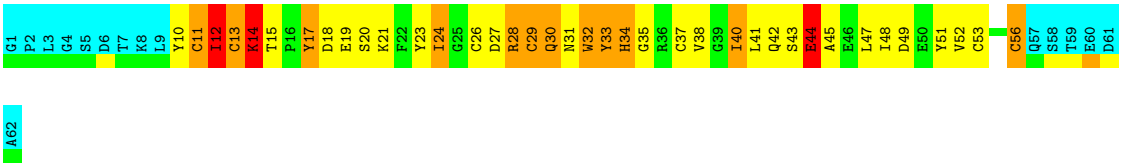
Chain B: 7% 7% 87%




### 4.2.13 Score per residue for model 13

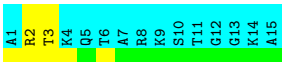
- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 15% 37% 19% 5% 24%




- Molecule 2: Histone H3

Chain B: 13% 87%



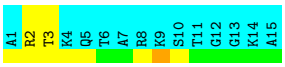
### 4.2.14 Score per residue for model 14

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 10% 45% 21% 24%

- Molecule 2: Histone H3

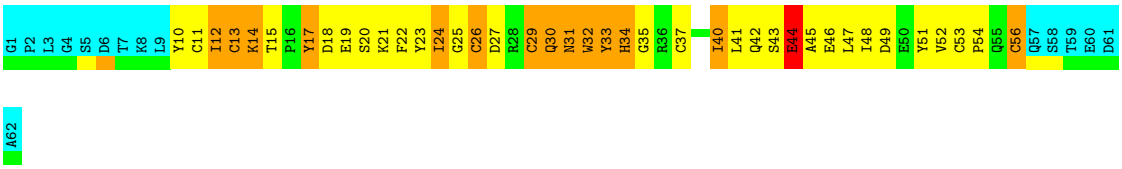
Chain B: 13% 87%




### 4.2.15 Score per residue for model 15

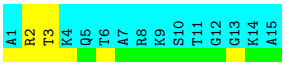
- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 40% 23% • 24%




- Molecule 2: Histone H3

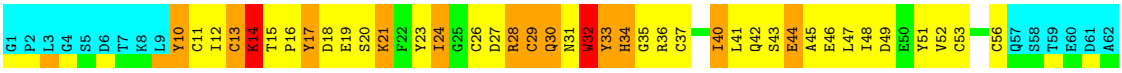
Chain B: 13% 87%




### 4.2.16 Score per residue for model 16

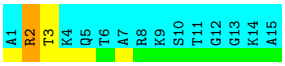
- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 42% 19% • 24%




- Molecule 2: Histone H3

Chain B: 7% 7% 87%



### 4.2.17 Score per residue for model 17

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 15% 34% 24% • 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.18 Score per residue for model 18

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 11% 39% 26% 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 V38 G39 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61

A62

- Molecule 2: Histone H3

Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.19 Score per residue for model 19

- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 16% 35% 24% 24%

G1 P2 L3 G4 S5 D6 T7 K8 L9 Y10 C11 I12 C13 K14 T15 P16 Y17 D18 E19 S20 K21 F22 Y23 I24 G25 C26 D27 R28 C29 Q30 N31 W32 Y33 H34 G35 R36 C37 I40 L41 Q42 S43 E44 A45 E46 L47 I48 D49 E50 Y51 V52 C53 C56 Q57 S58 T59 E60 D61 A62

- Molecule 2: Histone H3

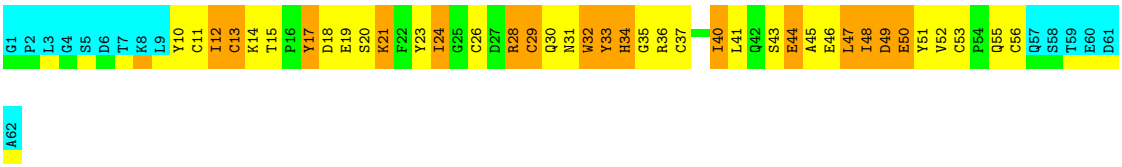
Chain B: 13% 87%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

### 4.2.20 Score per residue for model 20

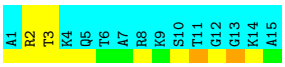
- Molecule 1: bromodomain PHD finger transcription factor

Chain A: 13% 37% 26% 24%




- Molecule 2: Histone H3

Chain B: 13% 87%



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *The structure was solved using a torsion angle simulated annealing protocol.*

Of the 85 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

| Software name | Classification | Version |
|---|---|---|
| X-PLOR | structure solution | 2.13 |
| X-PLOR | refinement | 2.13 |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, ZN

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 | 0.87±0.01 | 0±0/395 ( 0.0± 0.0%) | 1.05±0.01 | 0±0/536 ( 0.1± 0.1%) |
| 2 | B | 0.64±0.02 | 0±0/17 ( 0.0± 0.0%) | 0.79±0.04 | 0±0/21 ( 0.0± 0.0%) |
| All | All | 0.87 | 0/8240 ( 0.0%) | 1.04 | 10/11140 ( 0.1%) |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 32 | TRP | CA-CB-CG | -5.41 | 103.43 | 113.70 | 2 | 10 |

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (i)

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 | 384 | 349 | 352 | 102±11 |
| 2 | B | 18 | 19 | 20 | 5±4 |
| 3 | A | 2 | 0 | 0 | 1±1 |
| All | All | 8080 | 7360 | 7444 | 2049 |

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 132.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:26:CYS:SG | 1:A:53:CYS:CB | 1.48 | 2.02 | 8 | 14 |
| 1:A:29:CYS:CB | 1:A:53:CYS:SG | 1.44 | 2.05 | 6 | 11 |
| 1:A:26:CYS:CB | 1:A:53:CYS:SG | 1.37 | 2.09 | 6 | 14 |
| 1:A:26:CYS:SG | 1:A:29:CYS:CB | 1.35 | 2.11 | 13 | 20 |
| 1:A:26:CYS:CB | 1:A:29:CYS:SG | 1.34 | 2.15 | 16 | 20 |
| 1:A:29:CYS:CB | 1:A:56:CYS:SG | 1.32 | 2.17 | 7 | 20 |
| 1:A:26:CYS:HG | 1:A:53:CYS:CB | 1.24 | 1.44 | 16 | 3 |
| 1:A:29:CYS:CB | 1:A:56:CYS:HG | 1.21 | 1.45 | 7 | 2 |
| 1:A:26:CYS:SG | 1:A:56:CYS:SG | 1.20 | 1.20 | 12 | 20 |
| 1:A:29:CYS:SG | 1:A:53:CYS:CB | 1.16 | 2.34 | 7 | 17 |
| 1:A:53:CYS:SG | 1:A:56:CYS:CB | 1.15 | 2.33 | 14 | 18 |
| 1:A:29:CYS:SG | 1:A:56:CYS:CB | 1.14 | 2.35 | 4 | 20 |
| 1:A:11:CYS:SG | 1:A:13:CYS:CB | 1.08 | 2.41 | 14 | 20 |
| 1:A:53:CYS:CB | 1:A:56:CYS:SG | 1.07 | 2.42 | 14 | 19 |
| 1:A:11:CYS:CB | 1:A:37:CYS:SG | 1.03 | 2.46 | 6 | 20 |
| 1:A:13:CYS:CB | 1:A:37:CYS:SG | 1.00 | 2.49 | 13 | 12 |
| 1:A:47:LEU:HD12 | 1:A:48:ILE:N | 0.99 | 1.70 | 6 | 19 |
| 1:A:11:CYS:SG | 1:A:13:CYS:SG | 0.99 | 1.00 | 1 | 20 |
| 1:A:11:CYS:SG | 1:A:37:CYS:CB | 0.97 | 2.52 | 18 | 15 |
| 1:A:11:CYS:CB | 1:A:13:CYS:SG | 0.97 | 2.52 | 14 | 15 |
| 1:A:34:HIS:CE1 | 1:A:37:CYS:HG | 0.96 | 1.78 | 16 | 9 |
| 1:A:44:GLU:O | 1:A:48:ILE:HB | 0.96 | 1.60 | 1 | 4 |
| 1:A:24:ILE:H | 1:A:24:ILE:HD13 | 0.94 | 1.22 | 7 | 15 |
| 1:A:29:CYS:SG | 1:A:56:CYS:SG | 0.93 | 0.94 | 16 | 20 |
| 1:A:29:CYS:HG | 1:A:53:CYS:CB | 0.91 | 1.77 | 13 | 7 |
| 1:A:29:CYS:CB | 1:A:53:CYS:HG | 0.90 | 1.79 | 20 | 2 |
| 1:A:24:ILE:HD13 | 1:A:24:ILE:N | 0.90 | 1.80 | 7 | 15 |
| 1:A:34:HIS:ND1 | 1:A:37:CYS:SG | 0.90 | 2.45 | 6 | 12 |
| 1:A:26:CYS:SG | 1:A:53:CYS:SG | 0.90 | 0.90 | 7 | 14 |
| 1:A:26:CYS:HB2 | 1:A:53:CYS:N | 0.90 | 1.81 | 6 | 2 |
| 1:A:44:GLU:O | 1:A:48:ILE:HG13 | 0.88 | 1.68 | 12 | 16 |
| 1:A:41:LEU:N | 1:A:44:GLU:OE2 | 0.87 | 2.06 | 17 | 2 |
| 1:A:34:HIS:HD1 | 1:A:37:CYS:CB | 0.87 | 1.82 | 13 | 8 |
| 1:A:24:ILE:N | 1:A:24:ILE:HD13 | 0.85 | 1.85 | 17 | 5 |
| 1:A:11:CYS:HG | 1:A:37:CYS:CB | 0.85 | 1.83 | 7 | 4 |
| 1:A:11:CYS:HG | 1:A:34:HIS:HD1 | 0.84 | 1.10 | 11 | 5 |
| 1:A:13:CYS:SG | 1:A:37:CYS:CB | 0.84 | 2.64 | 11 | 1 |
| 1:A:11:CYS:SG | 1:A:34:HIS:CE1 | 0.84 | 2.70 | 17 | 10 |
| 1:A:21:LYS:HG2 | 1:A:34:HIS:CD2 | 0.84 | 2.06 | 2 | 16 |
| 1:A:24:ILE:HD13 | 1:A:24:ILE:H | 0.84 | 1.30 | 11 | 5 |
| 1:A:45:ALA:O | 2:B:3:THR:HG21 | 0.84 | 1.73 | 6 | 19 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:26:CYS:SG | 1:A:56:CYS:CB | 0.83 | 2.65 | 2 | 3 |
| 1:A:11:CYS:HB3 | 1:A:34:HIS:CE1 | 0.83 | 2.08 | 13 | 9 |
| 1:A:28:ARG:CD | 1:A:28:ARG:N | 0.82 | 2.41 | 13 | 2 |
| 1:A:24:ILE:N | 1:A:24:ILE:CD1 | 0.82 | 2.43 | 7 | 20 |
| 1:A:53:CYS:HG | 1:A:56:CYS:CB | 0.81 | 1.86 | 8 | 2 |
| 1:A:51:TYR:CZ | 1:A:52:VAL:O | 0.81 | 2.33 | 19 | 20 |
| 1:A:24:ILE:CD1 | 1:A:33:TYR:O | 0.80 | 2.30 | 6 | 20 |
| 1:A:34:HIS:HD1 | 1:A:37:CYS:HG | 0.79 | 1.17 | 9 | 3 |
| 1:A:11:CYS:HG | 1:A:34:HIS:CE1 | 0.79 | 1.95 | 2 | 3 |
| 1:A:34:HIS:ND1 | 1:A:37:CYS:CB | 0.79 | 2.45 | 9 | 8 |
| 1:A:44:GLU:CD | 1:A:45:ALA:N | 0.77 | 2.37 | 12 | 1 |
| 1:A:44:GLU:HA | 1:A:47:LEU:HD11 | 0.77 | 1.57 | 10 | 20 |
| 1:A:22:PHE:CZ | 1:A:42:GLN:NE2 | 0.76 | 2.53 | 12 | 3 |
| 1:A:41:LEU:N | 1:A:44:GLU:OE1 | 0.76 | 2.18 | 5 | 1 |
| 1:A:12:ILE:HG23 | 1:A:33:TYR:CD2 | 0.75 | 2.16 | 18 | 4 |
| 1:A:11:CYS:CB | 1:A:34:HIS:CE1 | 0.74 | 2.71 | 2 | 10 |
| 1:A:26:CYS:HG | 1:A:29:CYS:HG | 0.74 | 0.75 | 6 | 1 |
| 1:A:34:HIS:ND1 | 1:A:37:CYS:HB2 | 0.73 | 1.98 | 11 | 6 |
| 1:A:33:TYR:OH | 1:A:53:CYS:HB3 | 0.73 | 1.83 | 7 | 2 |
| 1:A:44:GLU:OE2 | 1:A:47:LEU:HD21 | 0.73 | 1.83 | 6 | 1 |
| 1:A:26:CYS:CB | 1:A:53:CYS:CB | 0.73 | 2.67 | 7 | 14 |
| 1:A:34:HIS:O | 1:A:37:CYS:N | 0.73 | 2.21 | 10 | 18 |
| 1:A:29:CYS:N | 1:A:56:CYS:SG | 0.72 | 2.63 | 7 | 2 |
| 1:A:14:LYS:CG | 1:A:14:LYS:O | 0.72 | 2.36 | 13 | 3 |
| 1:A:29:CYS:CA | 1:A:56:CYS:HG | 0.71 | 1.98 | 7 | 1 |
| 1:A:32:TRP:CH2 | 2:B:2:ARG:NH1 | 0.71 | 2.59 | 10 | 1 |
| 1:A:11:CYS:SG | 1:A:34:HIS:ND1 | 0.71 | 2.63 | 14 | 10 |
| 1:A:13:CYS:HG | 1:A:37:CYS:CB | 0.71 | 1.94 | 6 | 3 |
| 1:A:47:LEU:CD1 | 1:A:48:ILE:HG23 | 0.71 | 2.16 | 6 | 15 |
| 1:A:22:PHE:O | 1:A:34:HIS:HA | 0.71 | 1.86 | 11 | 2 |
| 1:A:31:ASN:ND2 | 1:A:33:TYR:OH | 0.70 | 2.24 | 6 | 5 |
| 1:A:44:GLU:O | 1:A:48:ILE:CG1 | 0.70 | 2.39 | 12 | 16 |
| 1:A:44:GLU:CG | 1:A:45:ALA:N | 0.70 | 2.54 | 12 | 1 |
| 1:A:12:ILE:HG23 | 1:A:33:TYR:CD1 | 0.69 | 2.22 | 14 | 16 |
| 1:A:26:CYS:O | 2:B:2:ARG:NH2 | 0.69 | 2.25 | 13 | 16 |
| 1:A:34:HIS:CE1 | 1:A:37:CYS:SG | 0.69 | 2.85 | 11 | 5 |
| 1:A:21:LYS:CG | 1:A:34:HIS:CD2 | 0.69 | 2.75 | 19 | 14 |
| 1:A:26:CYS:HB3 | 1:A:30:GLN:N | 0.69 | 2.03 | 3 | 15 |
| 1:A:32:TRP:CZ3 | 2:B:2:ARG:NH1 | 0.69 | 2.60 | 10 | 5 |
| 1:A:29:CYS:N | 1:A:56:CYS:HG | 0.68 | 1.86 | 7 | 1 |
| 1:A:13:CYS:HG | 1:A:34:HIS:CE1 | 0.68 | 2.06 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:18:ASP:C | 1:A:20:SER:H | 0.68 | 1.92 | 11 | 19 |
| 1:A:40:ILE:HG23 | 1:A:41:LEU:O | 0.68 | 1.88 | 18 | 8 |
| 1:A:11:CYS:CB | 1:A:37:CYS:HG | 0.68 | 1.94 | 10 | 2 |
| 1:A:34:HIS:HD1 | 1:A:37:CYS:HB2 | 0.68 | 1.47 | 13 | 1 |
| 1:A:41:LEU:HD22 | 1:A:41:LEU:N | 0.68 | 2.04 | 7 | 2 |
| 1:A:42:GLN:HE21 | 1:A:42:GLN:C | 0.68 | 1.91 | 6 | 1 |
| 1:A:21:LYS:NZ | 1:A:34:HIS:CE1 | 0.68 | 2.62 | 8 | 3 |
| 1:A:35:GLY:CA | 1:A:40:ILE:HG22 | 0.67 | 2.20 | 18 | 17 |
| 1:A:26:CYS:SG | 1:A:53:CYS:HB3 | 0.67 | 2.26 | 18 | 9 |
| 1:A:31:ASN:N | 2:B:2:ARG:HH22 | 0.67 | 1.87 | 6 | 2 |
| 1:A:35:GLY:HA3 | 1:A:40:ILE:HG22 | 0.67 | 1.67 | 18 | 1 |
| 1:A:11:CYS:O | 1:A:13:CYS:N | 0.66 | 2.28 | 13 | 16 |
| 1:A:21:LYS:NZ | 1:A:34:HIS:CD2 | 0.66 | 2.62 | 9 | 1 |
| 1:A:36:ARG:N | 1:A:36:ARG:CD | 0.66 | 2.56 | 9 | 2 |
| 1:A:44:GLU:O | 1:A:48:ILE:CB | 0.66 | 2.43 | 1 | 4 |
| 1:A:23:TYR:CD1 | 1:A:23:TYR:N | 0.66 | 2.61 | 7 | 19 |
| 1:A:33:TYR:OH | 1:A:53:CYS:HB2 | 0.66 | 1.91 | 1 | 13 |
| 1:A:26:CYS:HG | 1:A:29:CYS:CB | 0.65 | 1.90 | 6 | 1 |
| 1:A:17:TYR:CE1 | 1:A:23:TYR:CE1 | 0.65 | 2.84 | 7 | 20 |
| 1:A:26:CYS:N | 2:B:2:ARG:NH2 | 0.65 | 2.44 | 6 | 6 |
| 1:A:26:CYS:CB | 1:A:53:CYS:N | 0.65 | 2.59 | 6 | 2 |
| 1:A:26:CYS:N | 2:B:2:ARG:HH21 | 0.65 | 1.89 | 15 | 4 |
| 1:A:33:TYR:OH | 1:A:53:CYS:CB | 0.65 | 2.45 | 1 | 19 |
| 1:A:44:GLU:CA | 1:A:47:LEU:HD11 | 0.65 | 2.21 | 20 | 3 |
| 1:A:28:ARG:N | 1:A:28:ARG:HD2 | 0.64 | 2.07 | 13 | 2 |
| 1:A:21:LYS:HZ3 | 1:A:34:HIS:CD2 | 0.64 | 2.11 | 9 | 1 |
| 1:A:12:ILE:HG22 | 1:A:55:GLN:NE2 | 0.64 | 2.07 | 3 | 2 |
| 1:A:11:CYS:C | 1:A:13:CYS:N | 0.64 | 2.52 | 20 | 20 |
| 1:A:11:CYS:C | 1:A:13:CYS:H | 0.63 | 1.95 | 20 | 20 |
| 1:A:27:ASP:O | 2:B:2:ARG:NH2 | 0.63 | 2.31 | 18 | 11 |
| 1:A:31:ASN:OD1 | 1:A:33:TYR:CZ | 0.63 | 2.51 | 20 | 12 |
| 1:A:21:LYS:HG3 | 1:A:23:TYR:OH | 0.62 | 1.93 | 7 | 1 |
| 1:A:47:LEU:HD12 | 1:A:47:LEU:C | 0.62 | 2.15 | 1 | 16 |
| 1:A:21:LYS:NZ | 1:A:34:HIS:CG | 0.62 | 2.68 | 9 | 1 |
| 1:A:42:GLN:C | 1:A:42:GLN:HE21 | 0.62 | 1.97 | 12 | 1 |
| 1:A:28:ARG:H | 1:A:28:ARG:HD3 | 0.62 | 1.55 | 13 | 2 |
| 1:A:21:LYS:NZ | 1:A:34:HIS:ND1 | 0.62 | 2.47 | 18 | 2 |
| 1:A:51:TYR:C | 1:A:51:TYR:CD1 | 0.62 | 2.73 | 18 | 17 |
| 1:A:24:ILE:CG1 | 1:A:51:TYR:CZ | 0.62 | 2.82 | 18 | 16 |
| 1:A:18:ASP:O | 1:A:20:SER:N | 0.62 | 2.33 | 16 | 17 |
| 1:A:26:CYS:CB | 1:A:29:CYS:CB | 0.62 | 2.77 | 16 | 18 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:31:ASN:N | 1:A:31:ASN:HD22 | 0.62 | 1.93 | 10 | 2 |
| 1:A:31:ASN:HD22 | 1:A:31:ASN:H | 0.61 | 1.37 | 10 | 1 |
| 1:A:26:CYS:O | 2:B:2:ARG:NE | 0.61 | 2.34 | 15 | 1 |
| 1:A:26:CYS:O | 1:A:30:GLN:N | 0.60 | 2.33 | 18 | 14 |
| 1:A:31:ASN:H | 1:A:31:ASN:HD22 | 0.60 | 1.36 | 6 | 2 |
| 1:A:45:ALA:O | 1:A:48:ILE:HD11 | 0.60 | 1.95 | 2 | 11 |
| 1:A:34:HIS:N | 1:A:34:HIS:CD2 | 0.60 | 2.68 | 3 | 2 |
| 1:A:23:TYR:CE2 | 1:A:34:HIS:CD2 | 0.60 | 2.89 | 13 | 2 |
| 1:A:13:CYS:SG | 1:A:34:HIS:CE1 | 0.60 | 2.94 | 6 | 10 |
| 1:A:22:PHE:CE1 | 1:A:42:GLN:NE2 | 0.60 | 2.70 | 6 | 2 |
| 1:A:31:ASN:OD1 | 1:A:33:TYR:OH | 0.60 | 2.17 | 14 | 9 |
| 1:A:15:THR:OG1 | 1:A:34:HIS:CE1 | 0.59 | 2.54 | 13 | 9 |
| 1:A:15:THR:OG1 | 1:A:34:HIS:NE2 | 0.59 | 2.35 | 8 | 7 |
| 1:A:13:CYS:SG | 1:A:34:HIS:ND1 | 0.59 | 2.74 | 19 | 7 |
| 1:A:34:HIS:CD2 | 1:A:34:HIS:N | 0.59 | 2.69 | 20 | 6 |
| 1:A:48:ILE:HD13 | 1:A:49:ASP:H | 0.59 | 1.57 | 1 | 4 |
| 1:A:36:ARG:N | 1:A:36:ARG:HD3 | 0.59 | 2.13 | 10 | 2 |
| 1:A:18:ASP:C | 1:A:20:SER:N | 0.59 | 2.55 | 11 | 19 |
| 1:A:41:LEU:N | 1:A:41:LEU:CD2 | 0.59 | 2.66 | 7 | 2 |
| 1:A:21:LYS:HZ3 | 1:A:34:HIS:CE1 | 0.59 | 2.14 | 8 | 1 |
| 1:A:44:GLU:HG3 | 1:A:45:ALA:H | 0.59 | 1.57 | 12 | 1 |
| 1:A:35:GLY:O | 1:A:39:GLY:N | 0.58 | 2.36 | 18 | 1 |
| 1:A:10:TYR:CD1 | 1:A:32:TRP:CD1 | 0.58 | 2.92 | 11 | 18 |
| 1:A:47:LEU:C | 1:A:47:LEU:CD1 | 0.58 | 2.72 | 10 | 4 |
| 1:A:51:TYR:CG | 1:A:52:VAL:N | 0.58 | 2.72 | 13 | 20 |
| 1:A:26:CYS:HB2 | 1:A:53:CYS:CB | 0.57 | 2.28 | 7 | 1 |
| 1:A:24:ILE:HG12 | 1:A:51:TYR:CZ | 0.57 | 2.34 | 18 | 13 |
| 1:A:52:VAL:HG12 | 1:A:53:CYS:N | 0.57 | 2.13 | 19 | 18 |
| 1:A:34:HIS:O | 1:A:37:CYS:HB2 | 0.57 | 1.98 | 9 | 2 |
| 1:A:43:SER:O | 1:A:45:ALA:N | 0.57 | 2.38 | 20 | 19 |
| 1:A:24:ILE:HD11 | 1:A:33:TYR:O | 0.56 | 2.00 | 19 | 17 |
| 1:A:43:SER:O | 1:A:47:LEU:HG | 0.56 | 2.01 | 6 | 15 |
| 1:A:29:CYS:O | 1:A:30:GLN:NE2 | 0.56 | 2.39 | 16 | 1 |
| 1:A:11:CYS:SG | 1:A:13:CYS:N | 0.56 | 2.76 | 4 | 17 |
| 1:A:34:HIS:O | 1:A:37:CYS:CB | 0.56 | 2.53 | 11 | 3 |
| 1:A:26:CYS:CB | 1:A:56:CYS:HG | 0.56 | 2.07 | 4 | 3 |
| 1:A:14:LYS:O | 1:A:14:LYS:HG3 | 0.56 | 1.99 | 13 | 3 |
| 1:A:30:GLN:CG | 1:A:30:GLN:O | 0.56 | 2.54 | 17 | 10 |
| 1:A:13:CYS:O | 1:A:14:LYS:CG | 0.56 | 2.54 | 7 | 4 |
| 1:A:12:ILE:CG2 | 1:A:55:GLN:NE2 | 0.55 | 2.69 | 3 | 1 |
| 1:A:27:ASP:HB2 | 1:A:52:VAL:HG22 | 0.55 | 1.76 | 14 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:29:CYS:O | 1:A:31:ASN:N | 0.55 | 2.40 | 6 | 5 |
| 1:A:26:CYS:HB2 | 1:A:53:CYS:CA | 0.55 | 2.31 | 6 | 2 |
| 1:A:47:LEU:C | 1:A:47:LEU:HD12 | 0.55 | 2.21 | 10 | 3 |
| 1:A:26:CYS:CB | 1:A:53:CYS:HB3 | 0.55 | 2.32 | 18 | 11 |
| 1:A:31:ASN:OD1 | 1:A:33:TYR:CE1 | 0.55 | 2.59 | 20 | 7 |
| 1:A:44:GLU:O | 1:A:48:ILE:HG12 | 0.55 | 2.02 | 11 | 14 |
| 1:A:13:CYS:O | 1:A:14:LYS:HG2 | 0.55 | 2.02 | 7 | 2 |
| 1:A:26:CYS:N | 2:B:2:ARG:HH22 | 0.54 | 2.00 | 3 | 1 |
| 1:A:26:CYS:SG | 1:A:29:CYS:N | 0.54 | 2.80 | 6 | 4 |
| 1:A:34:HIS:H | 1:A:34:HIS:HD1 | 0.54 | 1.44 | 14 | 1 |
| 1:A:17:TYR:CD1 | 1:A:18:ASP:N | 0.54 | 2.76 | 7 | 8 |
| 1:A:29:CYS:CA | 1:A:56:CYS:SG | 0.54 | 2.92 | 6 | 2 |
| 1:A:30:GLN:C | 2:B:2:ARG:NH2 | 0.54 | 2.60 | 10 | 3 |
| 1:A:41:LEU:N | 1:A:41:LEU:HD12 | 0.54 | 2.17 | 9 | 5 |
| 1:A:29:CYS:O | 1:A:31:ASN:ND2 | 0.54 | 2.40 | 6 | 7 |
| 1:A:11:CYS:HB2 | 1:A:34:HIS:H | 0.54 | 1.63 | 6 | 5 |
| 1:A:28:ARG:CD | 1:A:28:ARG:H | 0.54 | 2.11 | 13 | 3 |
| 1:A:21:LYS:HB3 | 1:A:23:TYR:CZ | 0.54 | 2.37 | 14 | 1 |
| 1:A:27:ASP:OD2 | 1:A:28:ARG:NH1 | 0.54 | 2.41 | 13 | 1 |
| 1:A:13:CYS:O | 1:A:14:LYS:HB2 | 0.54 | 2.03 | 3 | 9 |
| 1:A:51:TYR:CE2 | 1:A:52:VAL:O | 0.53 | 2.61 | 19 | 6 |
| 1:A:25:GLY:C | 2:B:2:ARG:NH2 | 0.53 | 2.61 | 7 | 5 |
| 1:A:44:GLU:OE1 | 1:A:45:ALA:HB2 | 0.53 | 2.03 | 12 | 1 |
| 1:A:15:THR:HG22 | 1:A:34:HIS:NE2 | 0.53 | 2.18 | 5 | 1 |
| 1:A:33:TYR:CD1 | 1:A:33:TYR:N | 0.53 | 2.73 | 18 | 2 |
| 1:A:41:LEU:O | 1:A:44:GLU:CG | 0.53 | 2.56 | 12 | 1 |
| 1:A:35:GLY:O | 1:A:40:ILE:N | 0.53 | 2.34 | 18 | 2 |
| 1:A:11:CYS:CB | 1:A:34:HIS:ND1 | 0.53 | 2.72 | 13 | 2 |
| 1:A:34:HIS:CE1 | 1:A:37:CYS:CA | 0.53 | 2.92 | 9 | 1 |
| 1:A:36:ARG:NH1 | 1:A:36:ARG:CG | 0.53 | 2.72 | 9 | 1 |
| 1:A:26:CYS:N | 1:A:31:ASN:O | 0.53 | 2.33 | 10 | 2 |
| 1:A:44:GLU:CG | 1:A:45:ALA:H | 0.53 | 2.16 | 12 | 1 |
| 1:A:44:GLU:HA | 1:A:47:LEU:HD21 | 0.52 | 1.79 | 17 | 13 |
| 1:A:43:SER:O | 1:A:47:LEU:CD1 | 0.52 | 2.57 | 20 | 1 |
| 1:A:26:CYS:SG | 1:A:53:CYS:N | 0.52 | 2.79 | 7 | 2 |
| 1:A:34:HIS:O | 1:A:38:VAL:HG12 | 0.52 | 2.04 | 10 | 2 |
| 1:A:51:TYR:CD2 | 1:A:51:TYR:C | 0.52 | 2.83 | 5 | 3 |
| 1:A:26:CYS:HB3 | 1:A:53:CYS:SG | 0.52 | 2.33 | 6 | 1 |
| 1:A:26:CYS:CB | 1:A:53:CYS:H | 0.52 | 2.17 | 6 | 2 |
| 1:A:34:HIS:CB | 1:A:37:CYS:HB2 | 0.52 | 2.35 | 19 | 9 |
| 1:A:28:ARG:N | 1:A:28:ARG:CD | 0.52 | 2.72 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:36:ARG:CG | 1:A:36:ARG:HH11 | 0.52 | 2.16 | 9 | 1 |
| 1:A:43:SER:C | 1:A:45:ALA:N | 0.51 | 2.64 | 10 | 19 |
| 1:A:27:ASP:CG | 1:A:51:TYR:O | 0.51 | 2.48 | 8 | 4 |
| 1:A:29:CYS:H | 1:A:56:CYS:HG | 0.51 | 1.46 | 17 | 3 |
| 1:A:44:GLU:HA | 1:A:47:LEU:CD1 | 0.51 | 2.35 | 18 | 16 |
| 1:A:18:ASP:O | 1:A:21:LYS:N | 0.51 | 2.34 | 2 | 10 |
| 1:A:26:CYS:SG | 3:A:201:ZN:ZN | 0.51 | 1.65 | 6 | 12 |
| 1:A:51:TYR:CD1 | 1:A:52:VAL:N | 0.51 | 2.79 | 12 | 16 |
| 1:A:17:TYR:CD1 | 1:A:23:TYR:CE1 | 0.51 | 2.99 | 10 | 5 |
| 1:A:56:CYS:SG | 3:A:201:ZN:ZN | 0.51 | 1.20 | 6 | 1 |
| 1:A:31:ASN:OD1 | 1:A:33:TYR:CE2 | 0.51 | 2.63 | 18 | 2 |
| 1:A:42:GLN:NE2 | 1:A:42:GLN:CA | 0.51 | 2.74 | 6 | 2 |
| 1:A:10:TYR:C | 1:A:32:TRP:O | 0.51 | 2.49 | 14 | 1 |
| 1:A:34:HIS:NE2 | 1:A:36:ARG:CD | 0.51 | 2.74 | 11 | 1 |
| 1:A:26:CYS:HB3 | 1:A:29:CYS:C | 0.51 | 2.26 | 14 | 2 |
| 1:A:10:TYR:HE2 | 1:A:17:TYR:N | 0.51 | 2.04 | 8 | 7 |
| 1:A:26:CYS:O | 2:B:2:ARG:NH1 | 0.50 | 2.41 | 8 | 2 |
| 1:A:26:CYS:C | 2:B:2:ARG:HH21 | 0.50 | 2.09 | 6 | 3 |
| 1:A:51:TYR:OH | 1:A:53:CYS:HA | 0.50 | 2.06 | 10 | 1 |
| 1:A:11:CYS:O | 1:A:14:LYS:N | 0.50 | 2.45 | 2 | 5 |
| 1:A:26:CYS:C | 2:B:2:ARG:HE | 0.50 | 2.09 | 6 | 1 |
| 1:A:27:ASP:HB3 | 1:A:52:VAL:HG22 | 0.50 | 1.84 | 4 | 4 |
| 1:A:26:CYS:HB3 | 1:A:30:GLN:H | 0.50 | 1.64 | 10 | 6 |
| 1:A:47:LEU:HD12 | 1:A:47:LEU:O | 0.50 | 2.06 | 1 | 1 |
| 1:A:48:ILE:CD1 | 1:A:49:ASP:H | 0.50 | 2.20 | 1 | 3 |
| 1:A:34:HIS:NE2 | 1:A:36:ARG:HD2 | 0.50 | 2.21 | 11 | 1 |
| 1:A:43:SER:O | 1:A:46:GLU:N | 0.50 | 2.45 | 1 | 6 |
| 1:A:34:HIS:N | 1:A:37:CYS:HB2 | 0.50 | 2.22 | 19 | 3 |
| 1:A:51:TYR:CE1 | 1:A:52:VAL:C | 0.50 | 2.86 | 18 | 12 |
| 1:A:41:LEU:CD2 | 1:A:41:LEU:H | 0.50 | 2.20 | 7 | 1 |
| 1:A:30:GLN:OE1 | 2:B:2:ARG:NH2 | 0.50 | 2.45 | 20 | 1 |
| 1:A:42:GLN:NE2 | 1:A:42:GLN:O | 0.49 | 2.27 | 6 | 2 |
| 1:A:51:TYR:CD2 | 1:A:52:VAL:N | 0.49 | 2.81 | 5 | 2 |
| 1:A:27:ASP:OD2 | 1:A:51:TYR:O | 0.49 | 2.31 | 19 | 2 |
| 1:A:31:ASN:HD22 | 1:A:31:ASN:N | 0.49 | 2.03 | 7 | 1 |
| 1:A:34:HIS:NE2 | 1:A:36:ARG:NE | 0.49 | 2.59 | 11 | 1 |
| 1:A:13:CYS:O | 1:A:14:LYS:CB | 0.49 | 2.60 | 16 | 10 |
| 1:A:14:LYS:O | 1:A:14:LYS:HG2 | 0.49 | 2.07 | 7 | 2 |
| 1:A:29:CYS:N | 1:A:56:CYS:CB | 0.49 | 2.75 | 7 | 1 |
| 1:A:26:CYS:C | 2:B:2:ARG:HH22 | 0.49 | 2.11 | 13 | 1 |
| 1:A:17:TYR:O | 1:A:18:ASP:OD1 | 0.49 | 2.30 | 17 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:30:GLN:C | 2:B:2:ARG:HH22 | 0.49 | 2.11 | 6 | 2 |
| 1:A:30:GLN:CD | 1:A:30:GLN:O | 0.49 | 2.51 | 16 | 1 |
| 1:A:51:TYR:CE1 | 1:A:52:VAL:O | 0.48 | 2.66 | 14 | 4 |
| 1:A:29:CYS:O | 1:A:30:GLN:CG | 0.48 | 2.61 | 10 | 3 |
| 1:A:17:TYR:HE1 | 1:A:23:TYR:HE1 | 0.48 | 1.51 | 7 | 1 |
| 1:A:45:ALA:O | 2:B:3:THR:CG2 | 0.48 | 2.61 | 13 | 1 |
| 1:A:24:ILE:HG22 | 2:B:3:THR:HG23 | 0.48 | 1.84 | 6 | 3 |
| 1:A:10:TYR:N | 1:A:10:TYR:CD1 | 0.48 | 2.76 | 17 | 2 |
| 1:A:48:ILE:HD12 | 1:A:48:ILE:C | 0.48 | 2.28 | 15 | 10 |
| 1:A:40:ILE:HG13 | 1:A:44:GLU:CD | 0.48 | 2.29 | 18 | 1 |
| 1:A:41:LEU:HB2 | 1:A:44:GLU:OE2 | 0.48 | 2.09 | 6 | 1 |
| 1:A:22:PHE:CD1 | 1:A:22:PHE:N | 0.48 | 2.81 | 8 | 3 |
| 1:A:42:GLN:NE2 | 1:A:42:GLN:C | 0.47 | 2.67 | 6 | 1 |
| 1:A:36:ARG:CD | 1:A:36:ARG:C | 0.47 | 2.82 | 11 | 1 |
| 1:A:24:ILE:HD13 | 1:A:33:TYR:O | 0.47 | 2.08 | 11 | 1 |
| 1:A:51:TYR:CE2 | 1:A:52:VAL:C | 0.47 | 2.88 | 2 | 2 |
| 1:A:40:ILE:CD1 | 1:A:44:GLU:OE1 | 0.47 | 2.62 | 19 | 1 |
| 1:A:21:LYS:HZ2 | 1:A:34:HIS:CG | 0.47 | 2.27 | 18 | 1 |
| 1:A:17:TYR:CE1 | 1:A:23:TYR:HE1 | 0.47 | 2.26 | 7 | 1 |
| 1:A:15:THR:HG1 | 1:A:34:HIS:HE2 | 0.47 | 1.52 | 20 | 1 |
| 1:A:34:HIS:O | 1:A:35:GLY:C | 0.47 | 2.53 | 18 | 15 |
| 1:A:40:ILE:HG23 | 1:A:41:LEU:N | 0.47 | 2.24 | 20 | 18 |
| 1:A:46:GLU:C | 1:A:48:ILE:H | 0.47 | 2.12 | 1 | 4 |
| 1:A:30:GLN:O | 1:A:30:GLN:CG | 0.47 | 2.62 | 19 | 1 |
| 1:A:47:LEU:HD12 | 1:A:48:ILE:HG23 | 0.47 | 1.87 | 11 | 13 |
| 1:A:29:CYS:CB | 1:A:56:CYS:CB | 0.46 | 2.91 | 6 | 1 |
| 1:A:12:ILE:CD1 | 1:A:38:VAL:HG12 | 0.46 | 2.39 | 13 | 1 |
| 1:A:34:HIS:HB2 | 1:A:37:CYS:HB2 | 0.46 | 1.87 | 13 | 1 |
| 1:A:25:GLY:C | 2:B:2:ARG:HH21 | 0.46 | 2.14 | 10 | 1 |
| 1:A:17:TYR:O | 1:A:18:ASP:OD2 | 0.46 | 2.34 | 15 | 8 |
| 1:A:10:TYR:CE2 | 1:A:17:TYR:HB2 | 0.46 | 2.45 | 5 | 2 |
| 1:A:21:LYS:HZ3 | 1:A:34:HIS:CG | 0.46 | 2.27 | 9 | 1 |
| 1:A:22:PHE:CD2 | 1:A:22:PHE:O | 0.46 | 2.68 | 17 | 2 |
| 1:A:28:ARG:HG2 | 1:A:56:CYS:SG | 0.46 | 2.51 | 6 | 1 |
| 1:A:10:TYR:CD1 | 1:A:32:TRP:HD1 | 0.46 | 2.29 | 1 | 6 |
| 1:A:21:LYS:CG | 1:A:34:HIS:CG | 0.46 | 2.99 | 10 | 6 |
| 1:A:27:ASP:C | 2:B:2:ARG:NH2 | 0.46 | 2.69 | 5 | 4 |
| 1:A:48:ILE:HD13 | 1:A:49:ASP:N | 0.46 | 2.26 | 10 | 2 |
| 1:A:52:VAL:CG1 | 1:A:53:CYS:N | 0.46 | 2.79 | 19 | 2 |
| 1:A:49:ASP:OD1 | 1:A:49:ASP:O | 0.46 | 2.34 | 13 | 6 |
| 1:A:34:HIS:CE1 | 1:A:37:CYS:CB | 0.46 | 2.99 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:34:HIS:CG | 1:A:37:CYS:HB2 | 0.46 | 2.46 | 9 | 3 |
| 1:A:48:ILE:CD1 | 1:A:49:ASP:N | 0.46 | 2.79 | 1 | 2 |
| 1:A:22:PHE:CE1 | 1:A:42:GLN:CD | 0.46 | 2.89 | 14 | 1 |
| 1:A:29:CYS:N | 1:A:56:CYS:HB3 | 0.46 | 2.26 | 7 | 1 |
| 1:A:11:CYS:SG | 3:A:202:ZN:ZN | 0.45 | 1.55 | 5 | 5 |
| 1:A:41:LEU:O | 1:A:44:GLU:HG2 | 0.45 | 2.09 | 12 | 1 |
| 1:A:26:CYS:C | 2:B:2:ARG:NH2 | 0.45 | 2.69 | 13 | 1 |
| 1:A:30:GLN:HA | 2:B:2:ARG:CZ | 0.45 | 2.42 | 7 | 1 |
| 1:A:30:GLN:HA | 2:B:2:ARG:NH2 | 0.45 | 2.25 | 7 | 1 |
| 1:A:33:TYR:CZ | 1:A:53:CYS:HB3 | 0.45 | 2.45 | 7 | 1 |
| 1:A:23:TYR:CE2 | 1:A:34:HIS:HD2 | 0.45 | 2.29 | 10 | 2 |
| 1:A:31:ASN:N | 2:B:2:ARG:NH2 | 0.45 | 2.63 | 10 | 2 |
| 1:A:40:ILE:CG2 | 1:A:44:GLU:HG2 | 0.45 | 2.42 | 12 | 1 |
| 1:A:27:ASP:CB | 1:A:52:VAL:HG22 | 0.45 | 2.40 | 14 | 4 |
| 1:A:29:CYS:O | 1:A:30:GLN:CB | 0.45 | 2.63 | 10 | 2 |
| 1:A:28:ARG:C | 1:A:30:GLN:HE21 | 0.45 | 2.14 | 20 | 1 |
| 1:A:45:ALA:O | 1:A:48:ILE:CD1 | 0.45 | 2.65 | 2 | 3 |
| 1:A:34:HIS:CE1 | 1:A:37:CYS:HA | 0.45 | 2.47 | 9 | 1 |
| 1:A:49:ASP:OD2 | 1:A:49:ASP:O | 0.45 | 2.35 | 8 | 2 |
| 1:A:33:TYR:CE2 | 1:A:53:CYS:CB | 0.45 | 3.00 | 13 | 1 |
| 1:A:24:ILE:HG12 | 1:A:51:TYR:CE1 | 0.45 | 2.46 | 17 | 5 |
| 1:A:24:ILE:CG2 | 1:A:44:GLU:OE1 | 0.45 | 2.65 | 12 | 1 |
| 1:A:31:ASN:ND2 | 1:A:31:ASN:N | 0.44 | 2.65 | 7 | 2 |
| 1:A:49:ASP:O | 1:A:49:ASP:OD1 | 0.44 | 2.34 | 15 | 1 |
| 1:A:30:GLN:CA | 2:B:2:ARG:NH2 | 0.44 | 2.80 | 6 | 1 |
| 1:A:47:LEU:CD1 | 1:A:47:LEU:C | 0.44 | 2.85 | 6 | 3 |
| 1:A:35:GLY:HA2 | 1:A:38:VAL:HG13 | 0.44 | 1.89 | 18 | 2 |
| 1:A:27:ASP:OD1 | 1:A:51:TYR:O | 0.44 | 2.35 | 18 | 2 |
| 1:A:27:ASP:N | 2:B:2:ARG:HE | 0.44 | 2.09 | 6 | 1 |
| 1:A:47:LEU:HD12 | 1:A:48:ILE:H | 0.44 | 1.67 | 3 | 1 |
| 1:A:34:HIS:CD2 | 1:A:34:HIS:H | 0.44 | 2.29 | 3 | 1 |
| 1:A:40:ILE:HG12 | 1:A:44:GLU:OE1 | 0.44 | 2.12 | 5 | 1 |
| 1:A:42:GLN:C | 1:A:44:GLU:N | 0.44 | 2.70 | 12 | 1 |
| 1:A:21:LYS:HZ1 | 1:A:34:HIS:CG | 0.43 | 2.30 | 1 | 1 |
| 1:A:44:GLU:O | 1:A:44:GLU:OE1 | 0.43 | 2.36 | 13 | 1 |
| 1:A:43:SER:CB | 1:A:47:LEU:HD23 | 0.43 | 2.43 | 6 | 1 |
| 1:A:53:CYS:HB2 | 1:A:54:PRO:HD2 | 0.43 | 1.89 | 15 | 2 |
| 1:A:35:GLY:C | 1:A:40:ILE:HG22 | 0.43 | 2.33 | 14 | 1 |
| 1:A:15:THR:HG1 | 1:A:34:HIS:CE1 | 0.43 | 2.31 | 20 | 2 |
| 1:A:22:PHE:O | 1:A:22:PHE:CD1 | 0.43 | 2.71 | 7 | 1 |
| 1:A:44:GLU:CD | 1:A:44:GLU:C | 0.43 | 2.76 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:40:ILE:HG12 | 1:A:44:GLU:OE2 | 0.43 | 2.14 | 8 | 1 |
| 1:A:28:ARG:O | 1:A:30:GLN:NE2 | 0.43 | 2.40 | 20 | 1 |
| 1:A:43:SER:C | 1:A:45:ALA:H | 0.43 | 2.17 | 20 | 2 |
| 1:A:21:LYS:HZ2 | 1:A:34:HIS:CE1 | 0.43 | 2.25 | 18 | 1 |
| 1:A:32:TRP:CD2 | 1:A:32:TRP:N | 0.43 | 2.75 | 6 | 3 |
| 1:A:44:GLU:HA | 1:A:47:LEU:CG | 0.43 | 2.44 | 19 | 2 |
| 1:A:12:ILE:CG2 | 1:A:33:TYR:CD1 | 0.43 | 3.01 | 4 | 2 |
| 1:A:29:CYS:CB | 1:A:53:CYS:CB | 0.43 | 2.91 | 6 | 1 |
| 1:A:26:CYS:HB2 | 1:A:31:ASN:HD22 | 0.43 | 1.73 | 11 | 1 |
| 1:A:10:TYR:O | 1:A:11:CYS:C | 0.43 | 2.57 | 13 | 1 |
| 1:A:21:LYS:HB3 | 1:A:23:TYR:CE1 | 0.43 | 2.49 | 14 | 1 |
| 1:A:48:ILE:CG2 | 2:B:3:THR:OG1 | 0.42 | 2.67 | 10 | 1 |
| 1:A:19:GLU:H | 1:A:19:GLU:CD | 0.42 | 2.18 | 20 | 1 |
| 1:A:50:GLU:CD | 1:A:50:GLU:O | 0.42 | 2.58 | 4 | 1 |
| 1:A:14:LYS:O | 1:A:15:THR:HG23 | 0.42 | 2.15 | 6 | 1 |
| 1:A:17:TYR:HE1 | 1:A:23:TYR:CE1 | 0.42 | 2.27 | 7 | 1 |
| 1:A:24:ILE:HG12 | 1:A:51:TYR:CE2 | 0.42 | 2.50 | 7 | 1 |
| 1:A:29:CYS:O | 1:A:30:GLN:HG2 | 0.42 | 2.15 | 10 | 1 |
| 1:A:41:LEU:HB2 | 1:A:44:GLU:HB2 | 0.42 | 1.89 | 17 | 1 |
| 1:A:29:CYS:SG | 3:A:201:ZN:ZN | 0.42 | 1.52 | 11 | 7 |
| 1:A:11:CYS:HA | 1:A:33:TYR:HA | 0.42 | 1.91 | 14 | 4 |
| 1:A:25:GLY:C | 2:B:2:ARG:CZ | 0.42 | 2.88 | 6 | 1 |
| 1:A:48:ILE:CD1 | 2:B:3:THR:OG1 | 0.42 | 2.68 | 3 | 2 |
| 1:A:24:ILE:HB | 1:A:51:TYR:CD1 | 0.42 | 2.49 | 18 | 2 |
| 1:A:29:CYS:O | 1:A:30:GLN:C | 0.42 | 2.58 | 2 | 1 |
| 1:A:52:VAL:HG12 | 1:A:56:CYS:HB2 | 0.42 | 1.92 | 19 | 1 |
| 1:A:55:GLN:O | 1:A:55:GLN:OE1 | 0.41 | 2.37 | 9 | 1 |
| 1:A:10:TYR:CE2 | 1:A:17:TYR:N | 0.41 | 2.89 | 10 | 1 |
| 1:A:21:LYS:CE | 1:A:34:HIS:ND1 | 0.41 | 2.83 | 10 | 1 |
| 1:A:24:ILE:HG21 | 1:A:44:GLU:OE2 | 0.41 | 2.15 | 12 | 1 |
| 1:A:11:CYS:N | 1:A:32:TRP:O | 0.41 | 2.53 | 14 | 1 |
| 1:A:36:ARG:HD2 | 1:A:36:ARG:H | 0.41 | 1.75 | 18 | 1 |
| 1:A:11:CYS:HB2 | 1:A:34:HIS:CD2 | 0.41 | 2.51 | 20 | 1 |
| 1:A:15:THR:CG2 | 1:A:34:HIS:NE2 | 0.41 | 2.83 | 5 | 1 |
| 1:A:24:ILE:HG13 | 1:A:51:TYR:CZ | 0.41 | 2.50 | 5 | 1 |
| 1:A:14:LYS:C | 1:A:15:THR:CG2 | 0.41 | 2.89 | 13 | 1 |
| 1:A:27:ASP:C | 2:B:2:ARG:HH21 | 0.41 | 2.19 | 16 | 1 |
| 1:A:28:ARG:C | 1:A:30:GLN:NE2 | 0.41 | 2.73 | 20 | 1 |
| 1:A:25:GLY:O | 2:B:2:ARG:CG | 0.41 | 2.68 | 6 | 1 |
| 1:A:44:GLU:OE1 | 1:A:45:ALA:CA | 0.41 | 2.69 | 12 | 1 |
| 1:A:21:LYS:O | 1:A:23:TYR:CE1 | 0.41 | 2.74 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:29:CYS:C | 1:A:30:GLN:HG3 | 0.41 | 2.36 | 6 | 1 |
| 1:A:47:LEU:HD11 | 1:A:48:ILE:HG23 | 0.41 | 1.91 | 6 | 1 |
| 1:A:22:PHE:CD1 | 1:A:22:PHE:C | 0.41 | 2.94 | 10 | 2 |
| 1:A:44:GLU:HA | 1:A:47:LEU:CD2 | 0.41 | 2.46 | 19 | 1 |
| 1:A:26:CYS:CB | 1:A:31:ASN:H | 0.41 | 2.29 | 4 | 1 |
| 2:B:2:ARG:CZ | 2:B:2:ARG:CB | 0.40 | 3.00 | 7 | 1 |
| 1:A:31:ASN:N | 1:A:31:ASN:ND2 | 0.40 | 2.64 | 10 | 1 |
| 1:A:11:CYS:CA | 1:A:33:TYR:HA | 0.40 | 2.46 | 13 | 1 |
| 1:A:33:TYR:CE1 | 1:A:53:CYS:CB | 0.40 | 3.04 | 18 | 1 |
| 1:A:26:CYS:HB3 | 1:A:29:CYS:CB | 0.40 | 2.45 | 2 | 1 |
| 1:A:42:GLN:HE21 | 1:A:42:GLN:CA | 0.40 | 2.29 | 6 | 1 |
| 1:A:41:LEU:N | 1:A:41:LEU:CD1 | 0.40 | 2.85 | 9 | 1 |
| 1:A:48:ILE:HG13 | 1:A:48:ILE:H | 0.40 | 1.37 | 12 | 1 |
| 1:A:24:ILE:O | 1:A:32:TRP:HA | 0.40 | 2.17 | 5 | 1 |
| 1:A:26:CYS:SG | 1:A:29:CYS:HB2 | 0.40 | 2.37 | 13 | 1 |
| 1:A:44:GLU:OE2 | 1:A:48:ILE:HG13 | 0.40 | 2.16 | 1 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 47/62 (76%) | 36±1 (76±2%) | 7±1 (14±2%) | 4±1 (9±2%) | 1 | 11 |
| 2 | B | 2/15 (13%) | 1±0 (65±23%) | 1±0 (30±24%) | 0±0 (5±15%) | 4 | 25 |
| All | All | 980/1540 (64%) | 744 (76%) | 146 (15%) | 90 (9%) | 1 | 11 |

All 10 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 | 44 | GLU | 19 |
| 1 | A | 19 | GLU | 17 |
| 1 | A | 12 | ILE | 14 |
| 1 | A | 10 | TYR | 11 |
| 1 | A | 14 | LYS | 9 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 30 | GLN | 7 |
| 1 | A | 50 | GLU | 5 |
| 1 | A | 49 | ASP | 3 |
| 1 | A | 16 | PRO | 3 |
| 2 | B | 2 | ARG | 2 |

### 6.3.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 43/55 (78%) | 28±2 (66±4%) | 14±2 (34±4%) | 1 11 |
| 2 | B | 2/9 (22%) | 2±0 (100±0%) | 0±0 (0±0%) | 100 100 |
| All | All | 900/1280 (70%) | 610 (68%) | 290 (32%) | 1 13 |

All 28 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 | 13 | CYS | 20 |
| 1 | A | 24 | ILE | 20 |
| 1 | A | 29 | CYS | 20 |
| 1 | A | 32 | TRP | 20 |
| 1 | A | 33 | TYR | 20 |
| 1 | A | 40 | ILE | 19 |
| 1 | A | 17 | TYR | 17 |
| 1 | A | 42 | GLN | 17 |
| 1 | A | 34 | HIS | 15 |
| 1 | A | 36 | ARG | 15 |
| 1 | A | 30 | GLN | 13 |
| 1 | A | 28 | ARG | 13 |
| 1 | A | 56 | CYS | 11 |
| 1 | A | 21 | LYS | 10 |
| 1 | A | 15 | THR | 9 |
| 1 | A | 26 | CYS | 9 |
| 1 | A | 11 | CYS | 7 |
| 1 | A | 37 | CYS | 6 |
| 1 | A | 44 | GLU | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 31 | ASN | 6 |
| 1 | A | 48 | ILE | 5 |
| 1 | A | 47 | LEU | 3 |
| 1 | A | 53 | CYS | 2 |
| 1 | A | 38 | VAL | 2 |
| 1 | A | 14 | LYS | 2 |
| 1 | A | 18 | ASP | 1 |
| 1 | A | 12 | ILE | 1 |
| 1 | A | 50 | GLU | 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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | M3L | B | 4 | 2 | 10,11,12 | 0.57±0.03 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | M3L | B | 4 | 2 | 9,14,16 | 0.61±0.05 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | M3L | B | 4 | 2 | - | 0±0,9,10,12 | - |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 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 (i)

No chemical shift data were provided