# Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 03:58 PM EST

| | | |
|---|---|---|
| PDB ID | : | 2YQQ |
| Title | : | Solution structure of the zf-HIT domain in zinc finger HIT domain-containing protein 3 (TRIP-3) |
| Authors | : | Suzuki, S.; He, F.; Suzuki, S.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI) |
| Deposited on | : | 2007-03-30 |

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 (i)) were used in the production of this report:

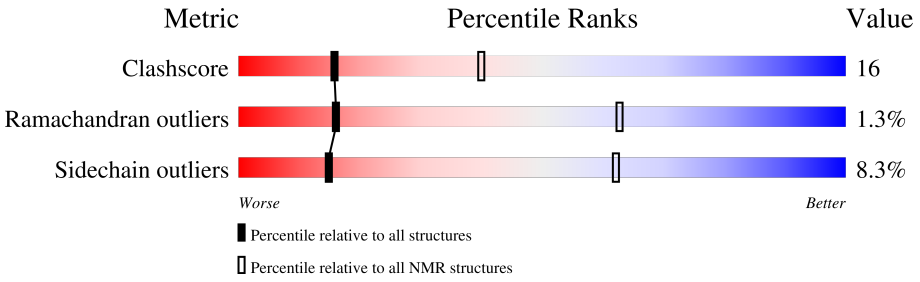
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.27 |
| Ideal geometry (proteins) | : | 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 | 56 | 45% 12% • 39% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:13-A:46 (34) | 0.12 | 12 |

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 4 clusters and 4 single-model clusters were found.

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

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 815 atoms, of which 404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger HIT domain-containing protein 3.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 56 | 813 | 250 | 404 | 74 | 77 | 8 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | expression tag | UNP Q15649 |
| A | 2 | SER | - | expression tag | UNP Q15649 |
| A | 3 | SER | - | expression tag | UNP Q15649 |
| A | 4 | GLY | - | expression tag | UNP Q15649 |
| A | 5 | SER | - | expression tag | UNP Q15649 |
| A | 6 | SER | - | expression tag | UNP Q15649 |
| A | 7 | GLY | - | expression tag | UNP Q15649 |
| A | 51 | SER | - | expression tag | UNP Q15649 |
| A | 52 | GLY | - | expression tag | UNP Q15649 |
| A | 53 | PRO | - | expression tag | UNP Q15649 |
| A | 54 | SER | - | expression tag | UNP Q15649 |
| A | 55 | SER | - | expression tag | UNP Q15649 |
| A | 56 | GLY | - | expression tag | UNP Q15649 |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

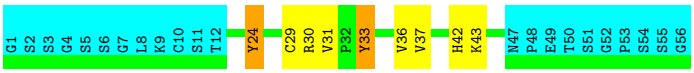
# 4 Residue-property plots (i)

## 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: Zinc finger HIT domain-containing protein 3

Chain A: 45% 12% • 39%



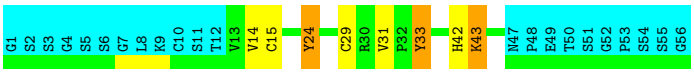

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Zinc finger HIT domain-containing protein 3

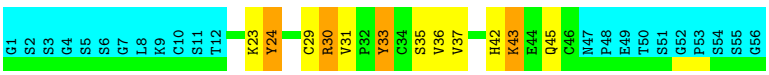
Chain A: 46% 9% 5% 39%




### 4.2.2 Score per residue for model 2

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 39% 14% 7% 39%



### 4.2.3 Score per residue for model 3

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 46% 12% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 K23 Y24 C29 R30 V31 P32 Y33 V36 V37 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 43% 14% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V16 Y24 R25 C29 R30 V31 P32 Y33 C34 S35 Q45 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.5 Score per residue for model 5

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 46% 9% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 Y24 C29 R30 V31 P32 Y33 V37 H42 K43 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.6 Score per residue for model 6

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 46% 11% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 Y24 R25 C29 R30 V31 P32 Y33 C34 S35 V36 V37 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.7 Score per residue for model 7

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 41% 18% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 Y24 C29 R30 V31 P32 Y33 C34 S35 F39 H42 K43 E44 Q45 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.8 Score per residue for model 8

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 43% 12% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 Y24 Y33 V36 V37 C38 F39 H42 K43 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.9 Score per residue for model 9

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 46% 12% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V16 K21 P22 K23 Y24 C29 R30 V31 P32 Y33 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.10 Score per residue for model 10

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 36% 18% 7% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 V16 K23 Y24 C29 R30 V31 P32 Y33 V36 V37 H42 Q45 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.11 Score per residue for model 11

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 46% 9% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 K23 Y24 Y33 H42 K43 E44 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 41% 14% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 Y24 R25 C26 P27 A28 Y33 V36 V37 C38 F39 H42 K43 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.13 Score per residue for model 13

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 41% 14% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 E20 K21 Y24 P32 Y33 V36 V37 C38 F39 H42 K43 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.14 Score per residue for model 14

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 39% 16% 5% 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 Y24 C29 R30 V31 P32 Y33 V36 V37 R40 K41 H42 K43 E44 Q45 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.15 Score per residue for model 15

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 48% 9% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 Y24 P32 Y33 V36 V37 Q45 C46 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.16 Score per residue for model 16

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 48% 9% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 V13 V14 C15 Y24 Y33 V36 F39 K43 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.17 Score per residue for model 17

• Molecule 1: Zinc finger HIT domain-containing protein 3

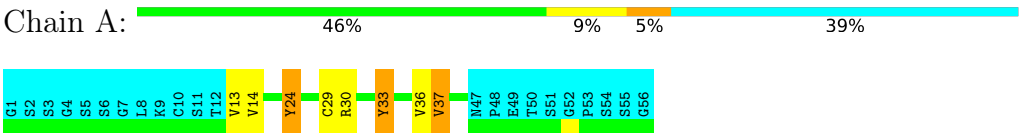
Chain A: 45% 12% • 39%

G1 S2 S3 G4 S5 S6 G7 L8 K9 C10 S11 T12 C18 L19 E20 K21 Y24 Y33 C34 S35 H42 K43 N47 P48 E49 T50 S51 G52 P53 S54 S55 G56

### 4.2.18 Score per residue for model 18

- Molecule 1: Zinc finger HIT domain-containing protein 3

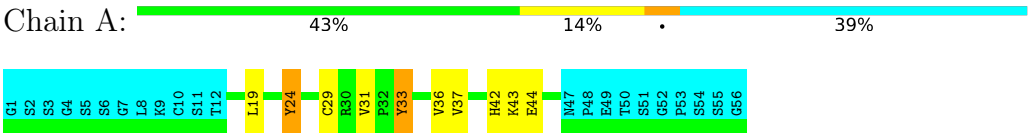
Chain A:




### 4.2.19 Score per residue for model 19

- Molecule 1: Zinc finger HIT domain-containing protein 3

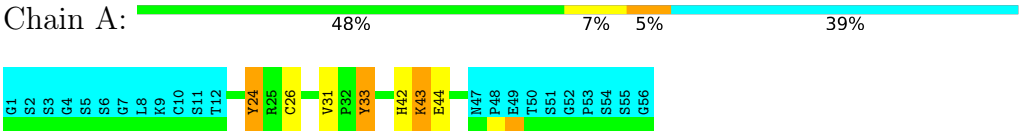
Chain A:




### 4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A:



# 5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

| Software name | Classification | Version |
|---|---|---|
| CYANA | structure solution | 2.0.17 |
| CYANA | refinement | 2.0.17 |

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: ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts (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 | 273 | 280 | 280 | 9±2 |
| All | All | 5500 | 5600 | 5600 | 180 |

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 16.

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:CYS:SG | 1:A:31:VAL:HG13 | 0.74 | 2.22 | 9 | 11 |
| 1:A:33:TYR:CD1 | 1:A:33:TYR:C | 0.65 | 2.69 | 2 | 20 |
| 1:A:33:TYR:O | 1:A:33:TYR:CD1 | 0.62 | 2.53 | 9 | 11 |
| 1:A:23:LYS:CG | 1:A:24:TYR:CE2 | 0.62 | 2.82 | 9 | 1 |
| 1:A:33:TYR:CD1 | 1:A:33:TYR:O | 0.61 | 2.53 | 4 | 9 |
| 1:A:23:LYS:CG | 1:A:24:TYR:CZ | 0.60 | 2.85 | 9 | 1 |
| 1:A:23:LYS:HG2 | 1:A:24:TYR:CE2 | 0.56 | 2.36 | 9 | 1 |
| 1:A:33:TYR:CD1 | 1:A:35:SER:O | 0.56 | 2.58 | 2 | 4 |
| 1:A:23:LYS:HG3 | 1:A:24:TYR:CZ | 0.52 | 2.40 | 9 | 1 |
| 1:A:13:VAL:HG22 | 1:A:32:PRO:HG3 | 0.52 | 1.80 | 13 | 2 |
| 1:A:39:PHE:CE1 | 1:A:43:LYS:HG2 | 0.52 | 2.40 | 16 | 1 |
| 1:A:33:TYR:CG | 1:A:33:TYR:O | 0.51 | 2.62 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:23:LYS:HG2 | 1:A:24:TYR:CZ | 0.51 | 2.41 | 9 | 1 |
| 1:A:29:CYS:C | 1:A:30:ARG:CD | 0.51 | 2.78 | 2 | 3 |
| 1:A:33:TYR:O | 1:A:33:TYR:CG | 0.50 | 2.64 | 9 | 16 |
| 1:A:25:ARG:NE | 1:A:30:ARG:O | 0.50 | 2.45 | 4 | 1 |
| 1:A:36:VAL:HG23 | 1:A:37:VAL:N | 0.49 | 2.22 | 19 | 3 |
| 1:A:16:VAL:HG13 | 1:A:32:PRO:HG2 | 0.49 | 1.83 | 9 | 3 |
| 1:A:23:LYS:HB2 | 1:A:24:TYR:CE1 | 0.49 | 2.43 | 10 | 2 |
| 1:A:42:HIS:CE1 | 1:A:46:CYS:HA | 0.48 | 2.43 | 8 | 2 |
| 1:A:29:CYS:SG | 1:A:31:VAL:CG1 | 0.48 | 3.02 | 5 | 7 |
| 1:A:30:ARG:CD | 1:A:30:ARG:N | 0.48 | 2.77 | 2 | 1 |
| 1:A:19:LEU:HD12 | 1:A:19:LEU:N | 0.47 | 2.24 | 19 | 2 |
| 1:A:39:PHE:O | 1:A:39:PHE:CD1 | 0.47 | 2.67 | 7 | 1 |
| 1:A:36:VAL:O | 1:A:39:PHE:N | 0.47 | 2.47 | 12 | 3 |
| 1:A:42:HIS:O | 1:A:44:GLU:N | 0.47 | 2.48 | 11 | 2 |
| 1:A:36:VAL:CG1 | 1:A:37:VAL:N | 0.47 | 2.78 | 10 | 4 |
| 1:A:39:PHE:CZ | 1:A:43:LYS:HD2 | 0.47 | 2.45 | 13 | 1 |
| 1:A:42:HIS:O | 1:A:43:LYS:C | 0.46 | 2.53 | 11 | 11 |
| 1:A:36:VAL:O | 1:A:37:VAL:C | 0.46 | 2.54 | 12 | 3 |
| 1:A:14:VAL:O | 1:A:15:CYS:C | 0.46 | 2.54 | 11 | 7 |
| 1:A:25:ARG:NH2 | 1:A:30:ARG:O | 0.45 | 2.50 | 6 | 2 |
| 1:A:30:ARG:N | 1:A:30:ARG:HD2 | 0.45 | 2.27 | 2 | 1 |
| 1:A:42:HIS:CD2 | 1:A:43:LYS:N | 0.44 | 2.85 | 11 | 1 |
| 1:A:18:CYS:C | 1:A:19:LEU:HD12 | 0.44 | 2.33 | 17 | 1 |
| 1:A:23:LYS:CB | 1:A:24:TYR:CE1 | 0.44 | 3.01 | 10 | 1 |
| 1:A:24:TYR:HB2 | 1:A:33:TYR:CZ | 0.43 | 2.49 | 8 | 15 |
| 1:A:24:TYR:CD1 | 1:A:24:TYR:N | 0.43 | 2.86 | 6 | 2 |
| 1:A:42:HIS:O | 1:A:45:GLN:N | 0.42 | 2.52 | 10 | 2 |
| 1:A:20:GLU:O | 1:A:21:LYS:C | 0.42 | 2.58 | 17 | 2 |
| 1:A:29:CYS:C | 1:A:30:ARG:HD2 | 0.42 | 2.35 | 18 | 2 |
| 1:A:30:ARG:N | 1:A:30:ARG:CD | 0.42 | 2.83 | 10 | 2 |
| 1:A:23:LYS:HB2 | 1:A:24:TYR:CD1 | 0.42 | 2.50 | 10 | 1 |
| 1:A:29:CYS:C | 1:A:30:ARG:HD3 | 0.41 | 2.36 | 2 | 1 |
| 1:A:26:CYS:HB3 | 1:A:31:VAL:HG22 | 0.41 | 1.92 | 20 | 1 |
| 1:A:36:VAL:HG13 | 1:A:37:VAL:N | 0.41 | 2.31 | 14 | 3 |
| 1:A:39:PHE:CE1 | 1:A:43:LYS:CG | 0.41 | 3.03 | 16 | 1 |
| 1:A:39:PHE:CD1 | 1:A:39:PHE:C | 0.41 | 2.93 | 8 | 1 |
| 1:A:36:VAL:CG2 | 1:A:37:VAL:N | 0.41 | 2.83 | 19 | 1 |
| 1:A:43:LYS:O | 1:A:44:GLU:C | 0.40 | 2.60 | 19 | 1 |
| 1:A:26:CYS:SG | 1:A:28:ALA:HB3 | 0.40 | 2.56 | 12 | 1 |
| 1:A:40:ARG:O | 1:A:44:GLU:CD | 0.40 | 2.60 | 14 | 1 |
| 1:A:13:VAL:HG22 | 1:A:14:VAL:N | 0.40 | 2.32 | 18 | 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 | 34/56 (61%) | 23±2 (67±5%) | 11±2 (32±5%) | 0±0 (1±1%) | 16 63 |
| All | All | 680/1120 (61%) | 456 (67%) | 215 (32%) | 9 (1%) | 16 63 |

All 2 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 | 37 | VAL | 7 |
| 1 | A | 43 | LYS | 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 | 33/50 (66%) | 30±1 (92±3%) | 3±1 (8±3%) | 15 62 |
| All | All | 660/1000 (66%) | 605 (92%) | 55 (8%) | 15 62 |

All 9 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 | 33 | TYR | 20 |
| 1 | A | 24 | TYR | 19 |
| 1 | A | 45 | GLN | 4 |
| 1 | A | 43 | LYS | 3 |
| 1 | A | 30 | ARG | 3 |
| 1 | A | 23 | LYS | 2 |
| 1 | A | 35 | SER | 2 |
| 1 | A | 21 | LYS | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 44 | 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)

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

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

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