# Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 11:54 PM EST

| | | |
|---|---|---|
| PDB ID | : | 2DLE |
| Title | : | Solution structure of the fourth fn3 domain of human receptor-type tyrosine-protein phosphatase eta |
| Authors | : | Izumi, K.; Yoshida, M.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI) |
| Deposited on | : | 2006-04-18 |

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

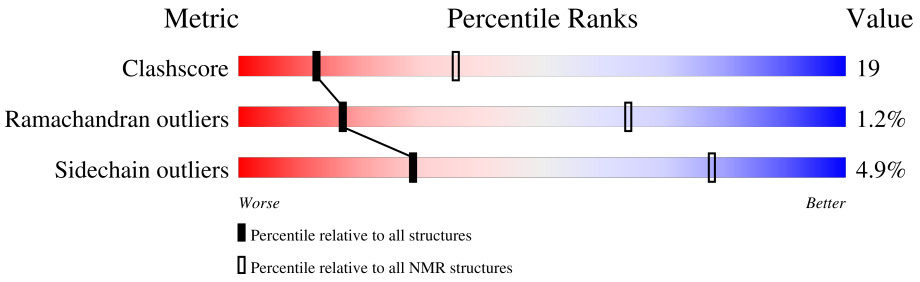
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.27 |
| Ideal geometry (proteins) | : | 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 | 104 | 54% 20% • 25% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 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:9-A:31, A:39-A:47, A:51-A:96 (78) | 0.20 | 16 |

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. No single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1491 atoms, of which 735 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase eta.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 104 | 1491 | 472 | 735 | 125 | 158 | 1 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | cloning artifact | UNP Q12913 |
| A | 2 | SER | - | cloning artifact | UNP Q12913 |
| A | 3 | SER | - | cloning artifact | UNP Q12913 |
| A | 4 | GLY | - | cloning artifact | UNP Q12913 |
| A | 5 | SER | - | cloning artifact | UNP Q12913 |
| A | 6 | SER | - | cloning artifact | UNP Q12913 |
| A | 7 | GLY | - | cloning artifact | UNP Q12913 |
| A | 99 | SER | - | cloning artifact | UNP Q12913 |
| A | 100 | GLY | - | cloning artifact | UNP Q12913 |
| A | 101 | PRO | - | cloning artifact | UNP Q12913 |
| A | 102 | SER | - | cloning artifact | UNP Q12913 |
| A | 103 | SER | - | cloning artifact | UNP Q12913 |
| A | 104 | GLY | - | cloning artifact | UNP Q12913 |

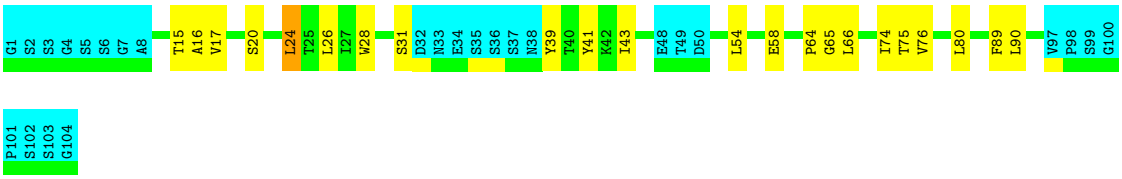
# 4 Residue-property plots (i)

## 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: Receptor-type tyrosine-protein phosphatase eta

Chain A: 54% 20% • 25%



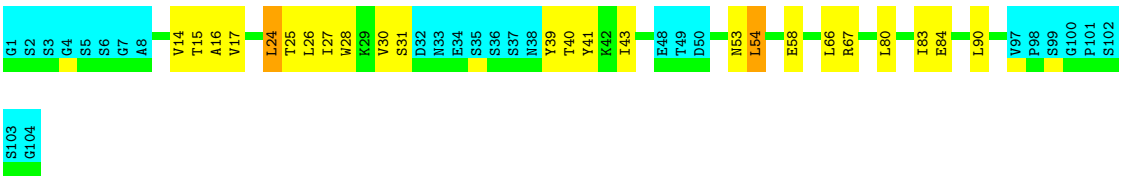

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 52% 21% • 25%




### 4.2.2 Score per residue for model 2

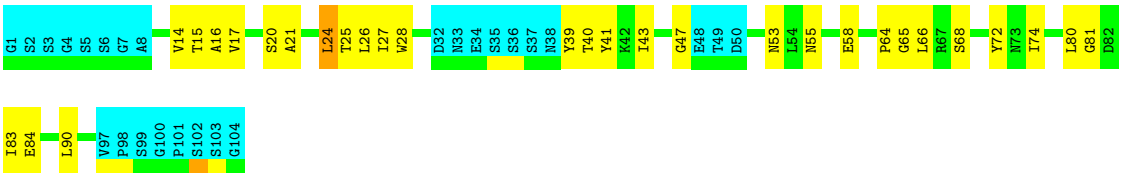
• Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 52% 21% • 25%

### 4.2.3 Score per residue for model 3

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

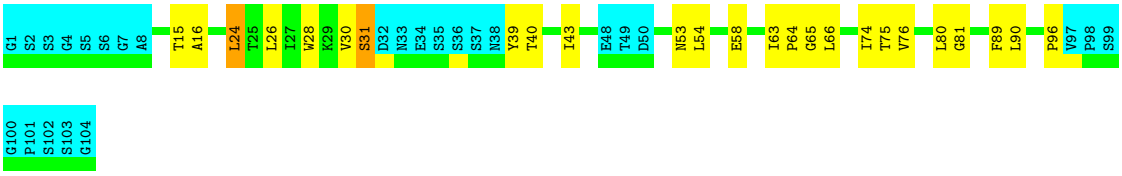
Chain A:




### 4.2.4 Score per residue for model 4

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

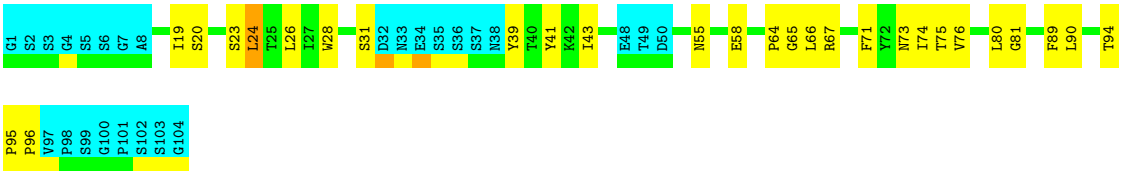
Chain A:




### 4.2.5 Score per residue for model 5

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A:




### 4.2.6 Score per residue for model 6

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 52% 21% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 F12 T15 A16 V17 L24 T25 L26 I27 W28 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 L54 E58 P59 R60 A61 P64 G65 I74 T75 V76 L80 F89 L90 V97 P98 S99 G100 P101 S102 S103 G104

### 4.2.7 Score per residue for model 7

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 44% 26% 5% 25%

G1 S2 S3 G4 S5 S6 G7 A8 I9 V14 T15 A16 V17 S20 S23 L24 T25 L26 I27 W28 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 I43 E48 T49 D50 L54 E58 A61 V62 I63 P64 G65 L66 R67 I74 T75 V76 C77 P78 V79 L80 G81 D82 L90 P96 V97 P98 S99 G100 P101 S102 S103 G104

### 4.2.8 Score per residue for model 8

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 56% 17% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 V14 T15 A16 L24 T25 L26 I27 W28 K29 V30 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 E58 P64 G65 L66 R67 I74 T75 V76 L80 L90 V97 P98 S99 G100 P101 S102 S103 G104

### 4.2.9 Score per residue for model 9

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 45% 29% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 V17 N18 I19 S20 S23 L24 T25 L26 I27 W28 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 A46 G47 E48 T49 D50 L54 E58 I63 P64 G65 L66 R67 S68 N73 I74 T75 V76 L80 G81 G85 F89 L90 T94 V97 P98 S99 G100 P101 S102 S103 G104

### 4.2.10 Score per residue for model 10

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 51% 21% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 V14 T15 A16 V17 S20 S23 L24 T25 L26 I27 W28 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 E48 T49 D50 L54 E58 L66 R67 T75 V76 L80 G81 D82 F89 L90 T94 V97 P98

S99 G100 P101 S102 S103 G104

### 4.2.11 Score per residue for model 11

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 54% 19% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 I9 V17 L24 T25 L26 I27 W28 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 N55 E58 V62 I63 P64 G65 L66 R67 I74 T75 V76 L80 L90 T94 V97 P98 S99

G100 P101 S102 S103 G104

### 4.2.12 Score per residue for model 12

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 51% 20% • 25%

G1 S2 S3 G4 S5 S6 G7 A8 S20 S23 L24 T25 L26 I27 W28 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 L54 E58 P59 I63 P64 G65 L66 F71 Y72 N73 I74 T75 V76 L80 G81 F89 L90 Q91 V97

P98 S99 G100 P101 S102 S103 G104

### 4.2.13 Score per residue for model 13

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 53% 20% • 25%

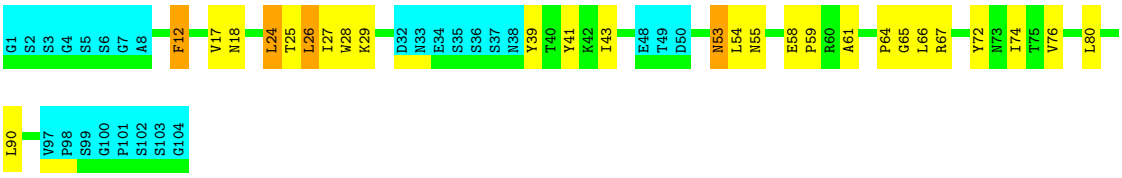
G1 S2 S3 G4 S5 S6 G7 A8 T15 A16 V17 S20 S23 L24 T25 L26 I27 W28 S31 D32 N33 E34 S35 S36 S37 N38 Y39 T40 Y41 K42 I43 E48 T49 D50 E58 P64 G65 L66 I74 T75 V76 G81 P87 L90 V97 P98 S99 G100

P101 S102 S103 G104

### 4.2.14 Score per residue for model 14

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

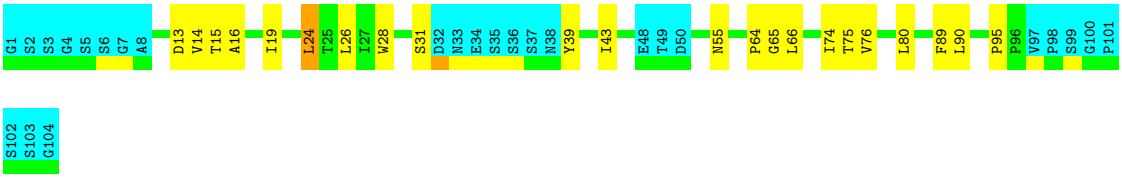
Chain A: 49% 22% • 25%




### 4.2.15 Score per residue for model 15

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

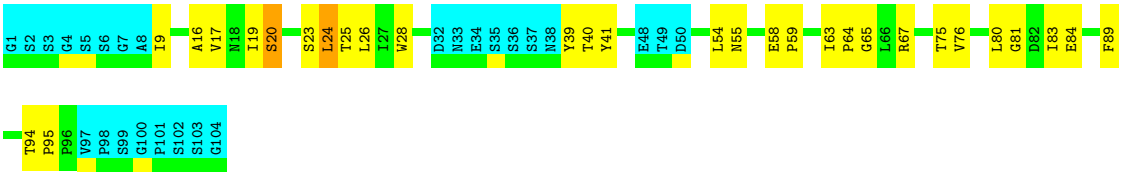
Chain A: 54% 20% • 25%




### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 46% 27% • 25%




### 4.2.17 Score per residue for model 17

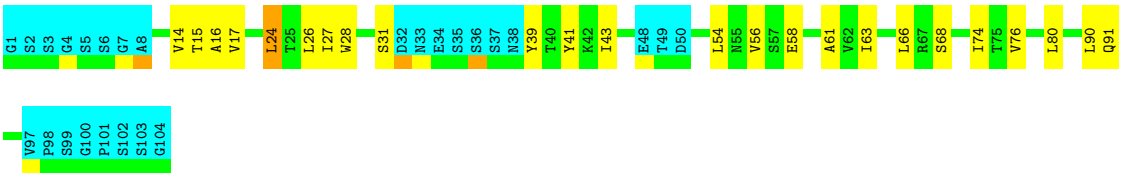
- Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 50% 24% • 25%

### 4.2.18 Score per residue for model 18

• Molecule 1: Receptor-type tyrosine-protein phosphatase eta

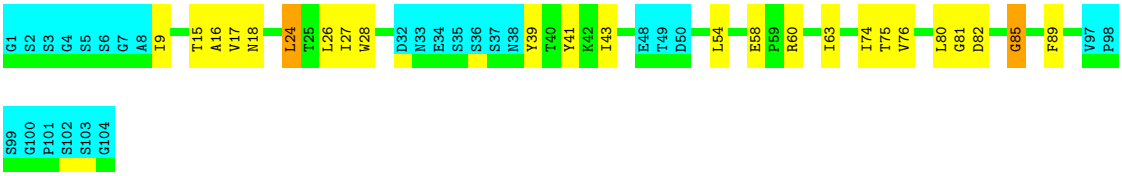
Chain A: 52% 22% • 25%




### 4.2.19 Score per residue for model 19

• Molecule 1: Receptor-type tyrosine-protein phosphatase eta

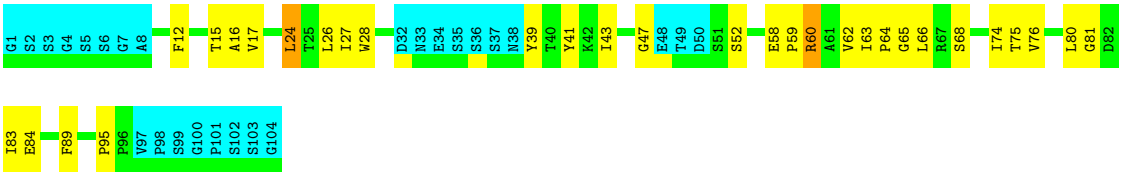
Chain A: 52% 21% • 25%




### 4.2.20 Score per residue for model 20

• Molecule 1: Receptor-type tyrosine-protein phosphatase eta

Chain A: 45% 28% • 25%



# 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: *target function,structures with the lowest energy,structures with the least restraint violations*.

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)

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 | 593 | 603 | 601 | 22±3 |
| All | All | 11860 | 12060 | 12020 | 444 |

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 19.

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:LEU:HD11 | 1:A:90:LEU:HD23 | 1.01 | 1.32 | 17 | 15 |
| 1:A:39:TYR:CD1 | 1:A:80:LEU:HD13 | 0.99 | 1.93 | 11 | 7 |
| 1:A:43:ILE:HG23 | 1:A:74:ILE:HG23 | 0.83 | 1.51 | 5 | 15 |
| 1:A:54:LEU:N | 1:A:54:LEU:HD23 | 0.79 | 1.92 | 10 | 2 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:HD13 | 0.74 | 2.17 | 6 | 12 |
| 1:A:26:LEU:HD23 | 1:A:28:TRP:CZ3 | 0.74 | 2.18 | 16 | 11 |
| 1:A:14:VAL:HG12 | 1:A:90:LEU:HD22 | 0.74 | 1.57 | 3 | 8 |
| 1:A:39:TYR:CD1 | 1:A:80:LEU:HD23 | 0.73 | 2.17 | 9 | 2 |
| 1:A:24:LEU:HD23 | 1:A:66:LEU:CD1 | 0.71 | 2.16 | 7 | 17 |
| 1:A:24:LEU:C | 1:A:24:LEU:HD12 | 0.70 | 2.05 | 12 | 20 |
| 1:A:54:LEU:HD22 | 1:A:63:ILE:CD1 | 0.69 | 2.18 | 12 | 6 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:HD22 | 0.69 | 2.23 | 11 | 4 |
| 1:A:28:TRP:CE2 | 1:A:76:VAL:HG11 | 0.68 | 2.23 | 13 | 18 |
| 1:A:26:LEU:HD11 | 1:A:90:LEU:CD2 | 0.66 | 2.18 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:28:TRP:CE3 | 1:A:76:VAL:HG21 | 0.65 | 2.25 | 15 | 14 |
| 1:A:26:LEU:HD22 | 1:A:74:ILE:HG21 | 0.65 | 1.69 | 6 | 11 |
| 1:A:17:VAL:HG23 | 1:A:25:THR:HB | 0.65 | 1.68 | 7 | 3 |
| 1:A:24:LEU:HD12 | 1:A:24:LEU:O | 0.64 | 1.92 | 2 | 6 |
| 1:A:75:THR:HG23 | 1:A:89:PHE:CE1 | 0.64 | 2.27 | 5 | 5 |
| 1:A:16:ALA:HB1 | 1:A:19:ILE:HD11 | 0.63 | 1.67 | 16 | 1 |
| 1:A:80:LEU:HD23 | 1:A:80:LEU:O | 0.63 | 1.94 | 2 | 2 |
| 1:A:39:TYR:HE1 | 1:A:80:LEU:HD13 | 0.62 | 1.54 | 12 | 3 |
| 1:A:54:LEU:N | 1:A:54:LEU:CD2 | 0.62 | 2.62 | 10 | 2 |
| 1:A:16:ALA:CB | 1:A:19:ILE:HD11 | 0.61 | 2.25 | 16 | 1 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:HD23 | 0.61 | 2.31 | 9 | 2 |
| 1:A:28:TRP:CZ3 | 1:A:76:VAL:HG21 | 0.61 | 2.31 | 18 | 6 |
| 1:A:26:LEU:HD13 | 1:A:74:ILE:HD13 | 0.61 | 1.73 | 4 | 9 |
| 1:A:19:ILE:HG22 | 1:A:95:PRO:HD3 | 0.60 | 1.71 | 16 | 5 |
| 1:A:41:TYR:CD2 | 1:A:58:GLU:O | 0.60 | 2.55 | 12 | 16 |
| 1:A:26:LEU:HD23 | 1:A:74:ILE:HD13 | 0.60 | 1.73 | 7 | 1 |
| 1:A:54:LEU:HD23 | 1:A:61:ALA:HB1 | 0.57 | 1.76 | 7 | 3 |
| 1:A:26:LEU:HD21 | 1:A:90:LEU:HD23 | 0.56 | 1.76 | 14 | 1 |
| 1:A:43:ILE:CG2 | 1:A:74:ILE:HG23 | 0.56 | 2.29 | 2 | 3 |
| 1:A:26:LEU:HD23 | 1:A:28:TRP:HZ3 | 0.56 | 1.60 | 16 | 3 |
| 1:A:21:ALA:HB1 | 1:A:68:SER:OG | 0.56 | 2.01 | 3 | 1 |
| 1:A:83:ILE:HG22 | 1:A:84:GLU:N | 0.55 | 2.16 | 1 | 4 |
| 1:A:24:LEU:HD23 | 1:A:66:LEU:HD11 | 0.55 | 1.78 | 5 | 12 |
| 1:A:28:TRP:CE2 | 1:A:59:PRO:O | 0.54 | 2.60 | 12 | 5 |
| 1:A:25:THR:HG23 | 1:A:62:VAL:HG22 | 0.54 | 1.79 | 11 | 1 |
| 1:A:43:ILE:HG23 | 1:A:74:ILE:CG2 | 0.54 | 2.32 | 8 | 6 |
| 1:A:24:LEU:HD23 | 1:A:66:LEU:HD13 | 0.54 | 1.80 | 7 | 5 |
| 1:A:26:LEU:CD2 | 1:A:74:ILE:HD13 | 0.54 | 2.33 | 7 | 1 |
| 1:A:60:ARG:NH1 | 1:A:62:VAL:CG2 | 0.54 | 2.71 | 20 | 1 |
| 1:A:17:VAL:CG1 | 1:A:27:ILE:HG21 | 0.53 | 2.33 | 19 | 2 |
| 1:A:54:LEU:HD22 | 1:A:63:ILE:HD13 | 0.52 | 1.81 | 12 | 1 |
| 1:A:47:GLY:HA2 | 1:A:72:TYR:CE1 | 0.51 | 2.40 | 3 | 1 |
| 1:A:67:ARG:O | 1:A:94:THR:HG21 | 0.51 | 2.06 | 5 | 5 |
| 1:A:12:PHE:CD1 | 1:A:12:PHE:N | 0.51 | 2.78 | 14 | 3 |
| 1:A:54:LEU:CD2 | 1:A:63:ILE:HD13 | 0.51 | 2.36 | 4 | 1 |
| 1:A:54:LEU:CD2 | 1:A:63:ILE:CD1 | 0.51 | 2.89 | 18 | 2 |
| 1:A:30:VAL:HG21 | 1:A:41:TYR:OH | 0.51 | 2.05 | 1 | 1 |
| 1:A:75:THR:CG2 | 1:A:89:PHE:CE1 | 0.50 | 2.95 | 5 | 5 |
| 1:A:80:LEU:O | 1:A:80:LEU:CD2 | 0.50 | 2.60 | 1 | 3 |
| 1:A:75:THR:OG1 | 1:A:89:PHE:CE2 | 0.50 | 2.65 | 15 | 7 |
| 1:A:75:THR:OG1 | 1:A:89:PHE:CE1 | 0.50 | 2.60 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:82:ASP:N | 1:A:82:ASP:OD1 | 0.50 | 2.45 | 7 | 1 |
| 1:A:75:THR:HG23 | 1:A:87:PRO:HB2 | 0.50 | 1.82 | 13 | 1 |
| 1:A:53:ASN:O | 1:A:54:LEU:HD12 | 0.50 | 2.07 | 4 | 1 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:HG | 0.50 | 2.42 | 1 | 5 |
| 1:A:15:THR:HG22 | 1:A:16:ALA:N | 0.50 | 2.20 | 6 | 11 |
| 1:A:20:SER:CB | 1:A:23:SER:O | 0.49 | 2.60 | 9 | 7 |
| 1:A:17:VAL:HG13 | 1:A:18:ASN:N | 0.49 | 2.22 | 14 | 1 |
| 1:A:53:ASN:HD22 | 1:A:54:LEU:N | 0.49 | 2.05 | 14 | 1 |
| 1:A:26:LEU:CD2 | 1:A:74:ILE:HG21 | 0.49 | 2.36 | 6 | 3 |
| 1:A:80:LEU:C | 1:A:80:LEU:HD13 | 0.49 | 2.27 | 9 | 1 |
| 1:A:20:SER:N | 1:A:23:SER:O | 0.49 | 2.45 | 5 | 2 |
| 1:A:43:ILE:O | 1:A:54:LEU:CD2 | 0.49 | 2.60 | 2 | 1 |
| 1:A:26:LEU:CD1 | 1:A:90:LEU:HD23 | 0.48 | 2.33 | 18 | 2 |
| 1:A:17:VAL:CG1 | 1:A:25:THR:CG2 | 0.48 | 2.92 | 9 | 2 |
| 1:A:43:ILE:HG13 | 1:A:76:VAL:HG22 | 0.48 | 1.86 | 6 | 1 |
| 1:A:17:VAL:CG1 | 1:A:27:ILE:HD13 | 0.47 | 2.38 | 6 | 4 |
| 1:A:15:THR:CG2 | 1:A:16:ALA:N | 0.47 | 2.77 | 1 | 3 |
| 1:A:60:ARG:NH1 | 1:A:62:VAL:HG23 | 0.47 | 2.24 | 20 | 1 |
| 1:A:28:TRP:CD2 | 1:A:59:PRO:O | 0.47 | 2.68 | 12 | 3 |
| 1:A:24:LEU:C | 1:A:24:LEU:CD1 | 0.47 | 2.78 | 12 | 4 |
| 1:A:16:ALA:HB1 | 1:A:19:ILE:CD1 | 0.47 | 2.39 | 16 | 1 |
| 1:A:54:LEU:HD21 | 1:A:63:ILE:HD11 | 0.47 | 1.85 | 18 | 1 |
| 1:A:56:VAL:HG21 | 1:A:61:ALA:HB2 | 0.47 | 1.87 | 18 | 1 |
| 1:A:17:VAL:HG13 | 1:A:27:ILE:HG21 | 0.47 | 1.85 | 19 | 1 |
| 1:A:17:VAL:CG2 | 1:A:27:ILE:HG23 | 0.46 | 2.40 | 13 | 1 |
| 1:A:39:TYR:CD1 | 1:A:80:LEU:HG | 0.46 | 2.46 | 10 | 2 |
| 1:A:43:ILE:HD12 | 1:A:43:ILE:N | 0.46 | 2.25 | 2 | 3 |
| 1:A:75:THR:OG1 | 1:A:89:PHE:CZ | 0.46 | 2.68 | 19 | 3 |
| 1:A:64:PRO:O | 1:A:65:GLY:C | 0.46 | 2.54 | 7 | 16 |
| 1:A:24:LEU:O | 1:A:24:LEU:CD1 | 0.46 | 2.63 | 2 | 2 |
| 1:A:83:ILE:CG2 | 1:A:84:GLU:N | 0.45 | 2.79 | 1 | 1 |
| 1:A:54:LEU:HD23 | 1:A:54:LEU:H | 0.45 | 1.69 | 10 | 1 |
| 1:A:47:GLY:HA2 | 1:A:72:TYR:CD1 | 0.45 | 2.46 | 3 | 1 |
| 1:A:12:PHE:CD1 | 1:A:29:LYS:O | 0.45 | 2.70 | 14 | 2 |
| 1:A:68:SER:CB | 1:A:95:PRO:O | 0.45 | 2.65 | 20 | 1 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:CD1 | 0.45 | 2.97 | 11 | 2 |
| 1:A:71:PHE:CD1 | 1:A:72:TYR:N | 0.45 | 2.85 | 12 | 2 |
| 1:A:63:ILE:HB | 1:A:66:LEU:HD11 | 0.44 | 1.88 | 7 | 2 |
| 1:A:58:GLU:N | 1:A:58:GLU:OE1 | 0.44 | 2.49 | 1 | 2 |
| 1:A:18:ASN:C | 1:A:18:ASN:OD1 | 0.44 | 2.55 | 19 | 1 |
| 1:A:41:TYR:CE2 | 1:A:58:GLU:C | 0.44 | 2.90 | 9 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:46:ALA:HB3 | 1:A:73:ASN:HB2 | 0.44 | 1.88 | 9 | 1 |
| 1:A:54:LEU:HD21 | 1:A:63:ILE:CD1 | 0.44 | 2.42 | 18 | 1 |
| 1:A:17:VAL:HG13 | 1:A:27:ILE:CG2 | 0.44 | 2.42 | 19 | 1 |
| 1:A:74:ILE:CG2 | 1:A:75:THR:N | 0.44 | 2.81 | 13 | 3 |
| 1:A:17:VAL:CG1 | 1:A:18:ASN:N | 0.44 | 2.81 | 14 | 1 |
| 1:A:67:ARG:CB | 1:A:72:TYR:OH | 0.44 | 2.65 | 14 | 1 |
| 1:A:47:GLY:HA3 | 1:A:72:TYR:CE1 | 0.44 | 2.48 | 17 | 1 |
| 1:A:17:VAL:HG12 | 1:A:25:THR:O | 0.44 | 2.12 | 17 | 1 |
| 1:A:43:ILE:HB | 1:A:54:LEU:CD2 | 0.44 | 2.43 | 18 | 1 |
| 1:A:43:ILE:HD13 | 1:A:54:LEU:CD1 | 0.43 | 2.43 | 2 | 1 |
| 1:A:43:ILE:CD1 | 1:A:54:LEU:O | 0.43 | 2.67 | 1 | 1 |
| 1:A:39:TYR:HD1 | 1:A:80:LEU:HD13 | 0.43 | 1.64 | 8 | 1 |
| 1:A:9:ILE:HG21 | 1:A:78:PRO:HB2 | 0.43 | 1.91 | 7 | 1 |
| 1:A:28:TRP:CD2 | 1:A:76:VAL:HG11 | 0.43 | 2.48 | 15 | 1 |
| 1:A:17:VAL:HG13 | 1:A:27:ILE:HD13 | 0.43 | 1.90 | 3 | 2 |
| 1:A:43:ILE:HD12 | 1:A:43:ILE:H | 0.42 | 1.73 | 2 | 1 |
| 1:A:15:THR:O | 1:A:27:ILE:CG1 | 0.42 | 2.68 | 18 | 1 |
| 1:A:39:TYR:CE1 | 1:A:80:LEU:CD2 | 0.42 | 2.99 | 11 | 1 |
| 1:A:39:TYR:CZ | 1:A:80:LEU:HD22 | 0.42 | 2.49 | 11 | 1 |
| 1:A:26:LEU:CD1 | 1:A:27:ILE:N | 0.41 | 2.83 | 14 | 1 |
| 1:A:17:VAL:CG1 | 1:A:25:THR:HB | 0.41 | 2.46 | 9 | 3 |
| 1:A:9:ILE:O | 1:A:85:GLY:CA | 0.41 | 2.69 | 19 | 1 |
| 1:A:80:LEU:O | 1:A:80:LEU:HD22 | 0.41 | 2.15 | 9 | 1 |
| 1:A:53:ASN:C | 1:A:54:LEU:HD23 | 0.41 | 2.35 | 1 | 1 |
| 1:A:71:PHE:CZ | 1:A:73:ASN:OD1 | 0.41 | 2.74 | 5 | 1 |
| 1:A:75:THR:CG2 | 1:A:87:PRO:HB2 | 0.41 | 2.45 | 13 | 1 |
| 1:A:71:PHE:CE1 | 1:A:91:GLN:CG | 0.40 | 3.05 | 12 | 1 |
| 1:A:58:GLU:OE1 | 1:A:58:GLU:N | 0.40 | 2.54 | 11 | 1 |
| 1:A:40:THR:O | 1:A:41:TYR:CD1 | 0.40 | 2.74 | 6 | 1 |
| 1:A:17:VAL:HG13 | 1:A:27:ILE:CD1 | 0.40 | 2.47 | 7 | 1 |
| 1:A:74:ILE:HG22 | 1:A:75:THR:N | 0.40 | 2.31 | 20 | 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 | 78/104 (75%) | 71±1 (91±2%) | 6±1 (7±2%) | 1±1 (1±1%) | 17 | 64 |
| All | All | 1560/2080 (75%) | 1427 (91%) | 115 (7%) | 18 (1%) | 17 | 64 |

All 4 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 | 81 | GLY | 10 |
| 1 | A | 31 | SER | 4 |
| 1 | A | 85 | GLY | 2 |
| 1 | A | 9 | ILE | 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 | 69/89 (78%) | 66±1 (95±2%) | 3±1 (5±2%) | 29 | 78 |
| All | All | 1380/1780 (78%) | 1313 (95%) | 67 (5%) | 29 | 78 |

All 19 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 | 24 | LEU | 20 |
| 1 | A | 40 | THR | 8 |
| 1 | A | 55 | ASN | 7 |
| 1 | A | 20 | SER | 5 |
| 1 | A | 54 | LEU | 3 |
| 1 | A | 17 | VAL | 3 |
| 1 | A | 67 | ARG | 2 |
| 1 | A | 53 | ASN | 2 |
| 1 | A | 12 | PHE | 2 |
| 1 | A | 26 | LEU | 2 |
| 1 | A | 58 | GLU | 2 |
| 1 | A | 82 | ASP | 2 |
| 1 | A | 91 | GLN | 2 |
| 1 | A | 60 | ARG | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 31 | SER | 1 |
| 1 | A | 18 | ASN | 1 |
| 1 | A | 13 | ASP | 1 |
| 1 | A | 57 | SER | 1 |
| 1 | A | 52 | SER | 1 |

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry (i)

There are no ligands in this entry.

### 6.7 Other polymers (i)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided