# Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 11:28 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 2MHO |
| BMRB ID | : | 19643 |
| Title | : | Solution State Structure PSD-95 PDZ1 with 5HT2C Receptor peptide |
| Authors | : | Dorr, L.A.; Phelan, M.M.; Lian, L. |
| Deposited on | : | 2013-11-29 |

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

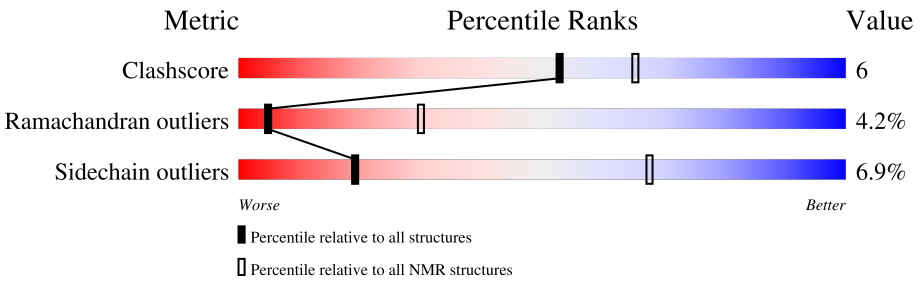
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 is 80%.

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 | 99 | 23% 44% 8% 24% |
| 2 | B | 9 | 11% 11% 78% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 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:6-A:12, A:20-A:29, A:37-A:94, B:8-B:9 (77) | 0.34 | 9 |

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1630 atoms, of which 817 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Disks large homolog 4.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 99 | 1488 | 463 | 743 | 132 | 147 | 3 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | expression tag | UNP P31016 |
| A | 2 | ALA | - | expression tag | UNP P31016 |
| A | 3 | MET | - | expression tag | UNP P31016 |

- Molecule 2 is a protein called peptide from 5-hydroxytryptamine receptor 2C.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | |
| 2 | B | 9 | 142 | 41 | 74 | 12 | 15 | 0 |

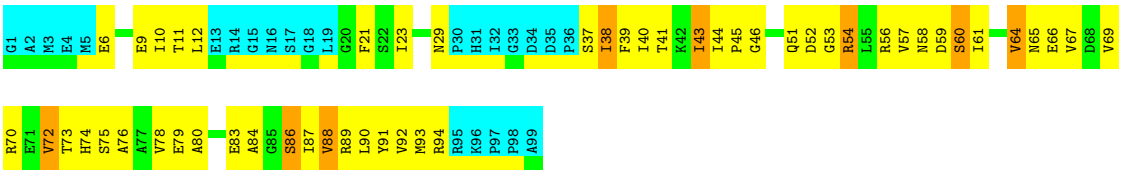
# 4 Residue-property plots (i)

## 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: Disks large homolog 4

Chain A: 23% 44% 8% 24%




• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

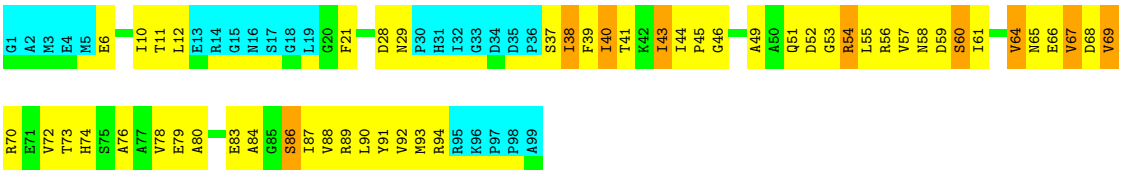
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Disks large homolog 4

Chain A: 22% 44% 9% 24%




• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

V1 V2 S3 E4 R5 I6 S7 S8 V9

### 4.2.2 Score per residue for model 2

- Molecule 1: Disks large homolog 4

Chain A: 20% 48% 7% 24%

G1 A2 M3 E4 M5 E6 E9 I10 T11 L12 E13 R14 G15 N16 S17 G18 L19 G20 F21 S22 I23 T27 D28 N29 P30 H31 I32 G33 D34 D35 P36 S37 I38 F39 I40 T41 K42 I43 I44 P45 G46 Q51 D52 G53 R54 L55 R56 V57 N58 D59 S60 I61 L62 F63 V64 N65 E66

V67 D68 V69 R70 E71 V72 T73 H74 S75 A76 A77 V78 E79 A80 E83 A84 G85 S86 I87 V88 R89 L90 Y91 V92 M93 R94 R95 K96 P97 P98 A99

- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

V1 V2 S3 E4 R5 I6 S7 S8 V9

### 4.2.3 Score per residue for model 3

- Molecule 1: Disks large homolog 4

Chain A: 20% 48% 7% 24%

G1 A2 M3 E4 M5 E6 Y7 E8 E9 I10 T11 L12 E13 R14 G15 N16 S17 G18 L19 G20 F21 S22 I23 N29 P30 H31 I32 G33 D34 D35 P36 S37 I38 F39 I40 T41 K42 I43 I44 P45 G46 Q51 D52 G53 R54 L55 R56 V57 N58 D59 S60 I61 V64 N65 E66 V67 D68

V69 R70 E71 V72 T73 H74 S75 A76 A77 V78 E79 A80 E83 A84 G85 S86 I87 V88 R89 L90 Y91 V92 M93 R94 R95 K96 P97 P98 A99

- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

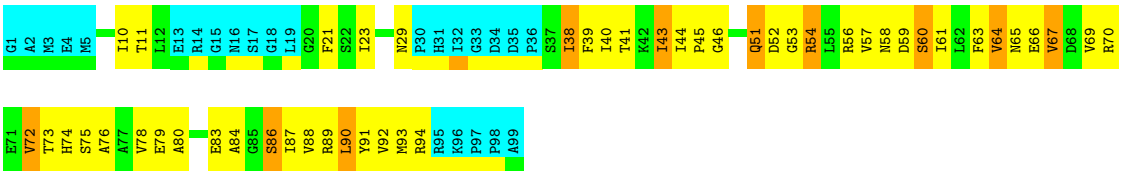
Chain B: 11% 11% 78%

V1 V2 S3 E4 R5 I6 S7 S8 V9

### 4.2.4 Score per residue for model 4

- Molecule 1: Disks large homolog 4

Chain A: 26% 39% 10% 24%



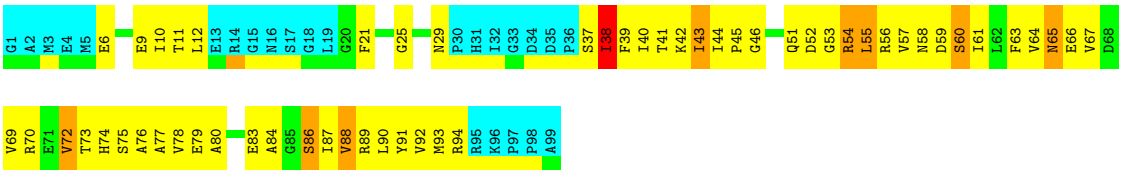

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

### 4.2.5 Score per residue for model 5

• Molecule 1: Disks large homolog 4

Chain A: 19% 47% 8% • 24%



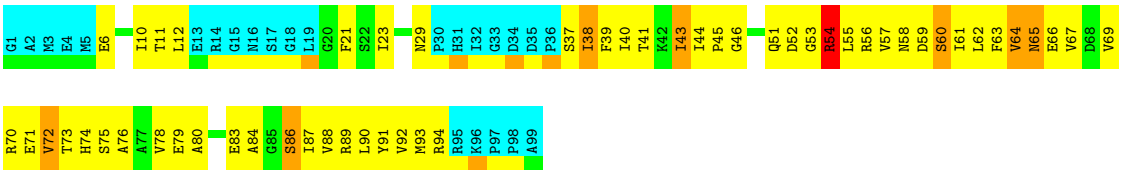

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

### 4.2.6 Score per residue for model 6

• Molecule 1: Disks large homolog 4

Chain A: 20% 47% 7% • 24%



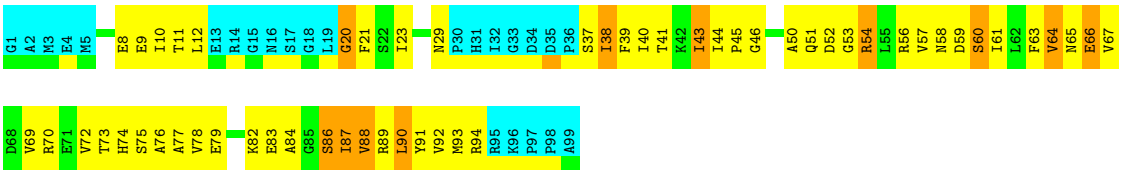

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

### 4.2.7 Score per residue for model 7

- Molecule 1: Disks large homolog 4

Chain A: 19% 45% 11% 24%




- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

### 4.2.8 Score per residue for model 8

- Molecule 1: Disks large homolog 4

Chain A: 18% 46% 8% • 24%

- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

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

- Molecule 1: Disks large homolog 4

Chain A: 18% 48% 9% 24%

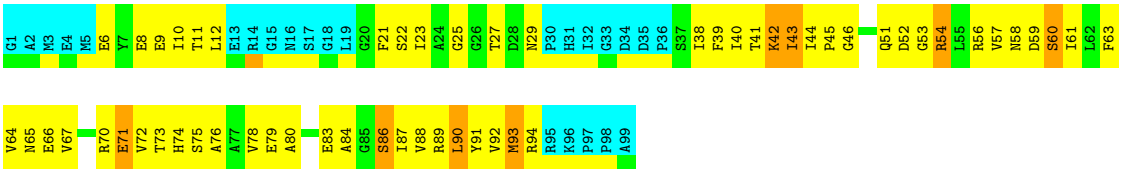
• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

### 4.2.10 Score per residue for model 10

• Molecule 1: Disks large homolog 4

Chain A: 18% 49% 8% 24%



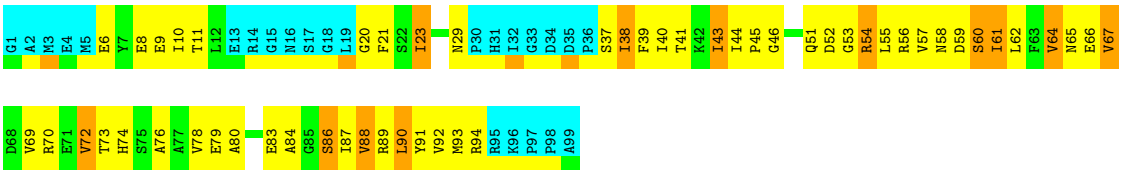

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

### 4.2.11 Score per residue for model 11

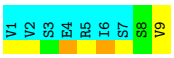
• Molecule 1: Disks large homolog 4

Chain A: 21% 42% 12% 24%




• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%




### 4.2.12 Score per residue for model 12

• Molecule 1: Disks large homolog 4

Chain A: 22% 46% 6% • 24%

G1 A2 M3 E4 M5 E6 Y7 I10 T11 L12 E13 R14 G15 N16 S17 G18 L19 G20 F21 S22 I23 T27 D28 N29 P30 H31 I32 G33 D34 D35 P36 S37 I38 F39 I40 T41 K42 I43 I44 P45 G46 Q51 D52 G53 R54 L55 R56 V57 N58 D59 S60 I61 V64 N65 E66 V67

D68 V69 R70 E71 V72 T73 H74 S75 A76 A77 V78 E79 A80 L81 K82 E83 A84 G85 S86 I87 V88 R89 L90 Y91 V92 M93 R94 R95 K96 P97 P98 A99

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

V1 V2 S3 E4 R5 I6 S7 S8 V9

### 4.2.13 Score per residue for model 13

• Molecule 1: Disks large homolog 4

Chain A: 14% 56% 5% • 24%

G1 A2 M3 E4 M5 E6 Y7 E8 E9 I10 T11 L12 E13 R14 G15 N16 S17 G18 L19 G20 F21 S22 I23 T27 D28 N29 P30 H31 I32 G33 D34 D35 P36 S37 I38 F39 I40 T41 K42 I43 I44 P45 G46 A49 A50 Q51 D52 G53 R54 L55 R56 V57 N58 D59 S60 I61 L62 F63

V64 N65 E66 V67 D68 V69 R70 E71 V72 T73 H74 S75 A76 A77 V78 E79 A80 L81 K82 E83 A84 G85 S86 I87 V88 R89 L90 Y91 V92 M93 R94 R95 K96 P97 P98 A99

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

V1 V2 S3 E4 R5 I6 S7 S8 V9

### 4.2.14 Score per residue for model 14

• Molecule 1: Disks large homolog 4

Chain A: 20% 48% 7% 24%

G1 A2 M3 E4 M5 E6 Y7 E8 E9 I10 T11 L12 E13 R14 G15 N16 S17 G18 L19 G20 F21 S22 I23 N29 P30 H31 I32 G33 D34 D35 P36 S37 I38 F39 I40 T41 K42 I43 I44 P45 G46 Q51 D52 G53 R54 L55 R56 V57 N58 D59 S60 I61 L62 F63 V64 N65 E66 V67

D68 V69 R70 E71 V72 T73 H74 S75 A76 A77 V78 E79 A80 E83 A84 G85 S86 I87 V88 R89 L90 Y91 V92 M93 R94 R95 K96 P97 P98 A99

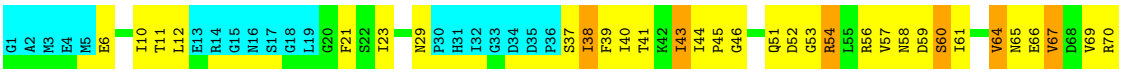
• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

### 4.2.15 Score per residue for model 15

- Molecule 1: Disks large homolog 4

Chain A:



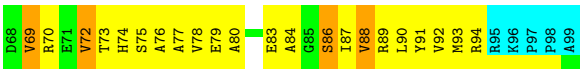
- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B:

### 4.2.16 Score per residue for model 16

- Molecule 1: Disks large homolog 4

Chain A:



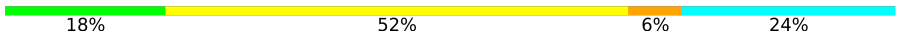

- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

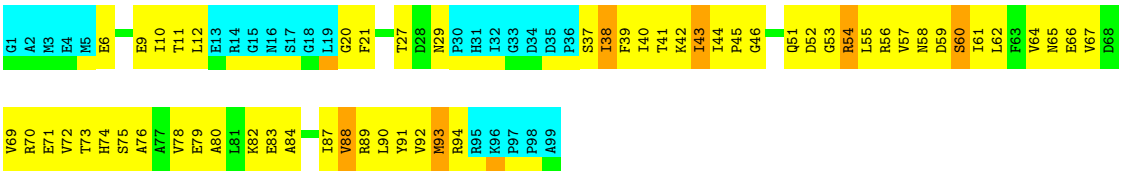
Chain B:

### 4.2.17 Score per residue for model 17

- Molecule 1: Disks large homolog 4

Chain A:





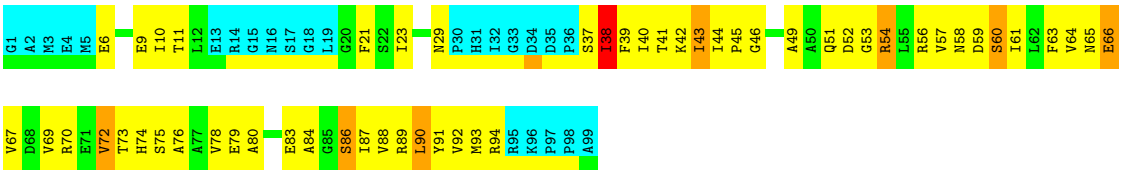

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

### 4.2.18 Score per residue for model 18

• Molecule 1: Disks large homolog 4

Chain A: 21% 46% 7% • 24%



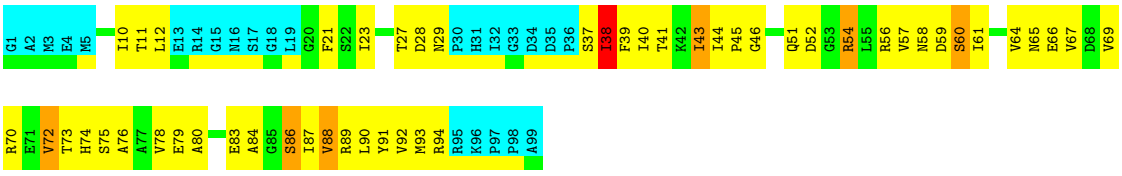

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 22% 78%

### 4.2.19 Score per residue for model 19

• Molecule 1: Disks large homolog 4

Chain A: 24% 44% 6% • 24%



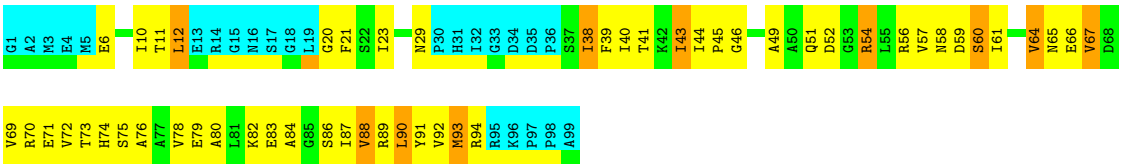

• Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

### 4.2.20 Score per residue for model 20

- Molecule 1: Disks large homolog 4

Chain A: 22% 43% 10% 24%




- Molecule 2: peptide from 5-hydroxytryptamine receptor 2C

Chain B: 11% 11% 78%

# 5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

| **Software name** | **Classification** | **Version** |
|---|---|---|
| CNS | refinement | 1.2 |
| CNS | structure solution | 1.2 |
| CYANA | structure solution | 2.1 |
| CYANA | refinement | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | working_cs.cif |
|---|---|
| Number of chemical shift lists | 2 |
| Total number of shifts | 1051 |
| Number of shifts mapped to atoms | 1051 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 80% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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 | 3.54±0.02 | 80±3/576 ( 14.0± 0.5%) | 1.78±0.03 | 10±1/781 ( 1.3± 0.2%) |
| 2 | B | 3.95±0.12 | 2±1/13 ( 12.3± 5.1%) | 1.54±0.06 | 0±0/15 ( 0.0± 0.0%) |
| All | All | 3.55 | 1641/11780 ( 13.9%) | 1.78 | 203/15920 ( 1.3%) |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 29 | ASN | C-N | 11.30 | 1.55 | 1.34 | 2 | 20 |
| 1 | A | 44 | ILE | C-N | 10.68 | 1.54 | 1.34 | 13 | 20 |
| 1 | A | 72 | VAL | CA-CB | 10.59 | 1.76 | 1.54 | 5 | 20 |
| 2 | B | 9 | VAL | CA-CB | 9.79 | 1.75 | 1.54 | 19 | 20 |
| 1 | A | 38 | ILE | CA-CB | 9.45 | 1.76 | 1.54 | 12 | 20 |
| 1 | A | 43 | ILE | CA-CB | 9.14 | 1.75 | 1.54 | 15 | 20 |
| 1 | A | 57 | VAL | N-CA | 8.73 | 1.63 | 1.46 | 8 | 19 |
| 1 | A | 44 | ILE | CA-CB | 8.71 | 1.74 | 1.54 | 16 | 20 |
| 1 | A | 64 | VAL | CA-CB | 8.62 | 1.72 | 1.54 | 17 | 9 |
| 1 | A | 87 | ILE | CA-CB | 8.58 | 1.74 | 1.54 | 7 | 20 |
| 1 | A | 65 | ASN | N-CA | 8.57 | 1.63 | 1.46 | 17 | 19 |
| 1 | A | 54 | ARG | N-CA | 8.43 | 1.63 | 1.46 | 4 | 20 |
| 1 | A | 67 | VAL | CA-CB | 8.16 | 1.71 | 1.54 | 13 | 20 |
| 1 | A | 88 | VAL | CA-CB | 8.12 | 1.71 | 1.54 | 3 | 12 |
| 1 | A | 61 | ILE | CA-CB | 8.01 | 1.73 | 1.54 | 8 | 20 |
| 1 | A | 78 | VAL | CA-CB | 7.99 | 1.71 | 1.54 | 6 | 20 |
| 1 | A | 52 | ASP | C-N | 7.89 | 1.47 | 1.33 | 20 | 20 |
| 1 | A | 10 | ILE | CA-CB | 7.85 | 1.73 | 1.54 | 11 | 20 |
| 1 | A | 70 | ARG | NE-CZ | 7.71 | 1.43 | 1.33 | 1 | 20 |
| 1 | A | 56 | ARG | NE-CZ | 7.68 | 1.43 | 1.33 | 4 | 20 |
| 1 | A | 89 | ARG | NE-CZ | 7.68 | 1.43 | 1.33 | 5 | 20 |
| 1 | A | 94 | ARG | NE-CZ | 7.63 | 1.43 | 1.33 | 1 | 20 |
| 1 | A | 54 | ARG | NE-CZ | 7.59 | 1.43 | 1.33 | 4 | 20 |
| 1 | A | 58 | ASN | C-N | 7.57 | 1.51 | 1.34 | 15 | 20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 79 | GLU | N-CA | 7.42 | 1.61 | 1.46 | 3 | 20 |
| 1 | A | 78 | VAL | N-CA | 7.33 | 1.60 | 1.46 | 13 | 20 |
| 1 | A | 74 | HIS | N-CA | 7.31 | 1.60 | 1.46 | 16 | 20 |
| 1 | A | 84 | ALA | N-CA | 7.30 | 1.60 | 1.46 | 5 | 15 |
| 1 | A | 92 | VAL | CA-CB | 7.30 | 1.70 | 1.54 | 16 | 20 |
| 1 | A | 66 | GLU | CA-CB | 7.28 | 1.70 | 1.53 | 4 | 17 |
| 1 | A | 40 | ILE | CA-CB | 7.25 | 1.71 | 1.54 | 11 | 20 |
| 1 | A | 86 | SER | CA-CB | 7.19 | 1.63 | 1.52 | 19 | 18 |
| 2 | B | 8 | SER | CA-CB | 7.00 | 1.63 | 1.52 | 1 | 6 |
| 1 | A | 65 | ASN | CA-CB | 6.99 | 1.71 | 1.53 | 12 | 20 |
| 1 | A | 60 | SER | N-CA | 6.98 | 1.60 | 1.46 | 1 | 20 |
| 1 | A | 83 | GLU | N-CA | 6.90 | 1.60 | 1.46 | 10 | 19 |
| 1 | A | 70 | ARG | N-CA | 6.89 | 1.60 | 1.46 | 8 | 18 |
| 1 | A | 21 | PHE | CA-CB | 6.88 | 1.69 | 1.53 | 1 | 20 |
| 1 | A | 70 | ARG | C-N | 6.78 | 1.49 | 1.34 | 10 | 9 |
| 1 | A | 46 | GLY | C-N | 6.74 | 1.45 | 1.33 | 13 | 20 |
| 1 | A | 64 | VAL | N-CA | 6.69 | 1.59 | 1.46 | 19 | 9 |
| 1 | A | 39 | PHE | CA-CB | 6.67 | 1.68 | 1.53 | 11 | 20 |
| 1 | A | 90 | LEU | CA-CB | 6.64 | 1.69 | 1.53 | 12 | 20 |
| 1 | A | 59 | ASP | C-N | 6.61 | 1.49 | 1.34 | 5 | 20 |
| 1 | A | 66 | GLU | N-CA | 6.61 | 1.59 | 1.46 | 4 | 13 |
| 1 | A | 41 | THR | CA-CB | 6.51 | 1.70 | 1.53 | 4 | 6 |
| 1 | A | 93 | MET | CA-CB | 6.43 | 1.68 | 1.53 | 14 | 20 |
| 1 | A | 21 | PHE | CB-CG | 6.40 | 1.62 | 1.51 | 16 | 20 |
| 1 | A | 41 | THR | C-N | 6.32 | 1.48 | 1.34 | 9 | 20 |
| 1 | A | 89 | ARG | CA-CB | 6.31 | 1.67 | 1.53 | 2 | 19 |
| 1 | A | 75 | SER | C-N | 6.31 | 1.48 | 1.34 | 8 | 16 |
| 1 | A | 29 | ASN | CA-C | 6.30 | 1.69 | 1.52 | 19 | 5 |
| 1 | A | 60 | SER | CA-CB | 6.20 | 1.62 | 1.52 | 7 | 6 |
| 1 | A | 94 | ARG | CA-CB | 6.18 | 1.67 | 1.53 | 1 | 9 |
| 1 | A | 66 | GLU | C-N | 6.13 | 1.48 | 1.34 | 15 | 17 |
| 1 | A | 23 | ILE | N-CA | 6.12 | 1.58 | 1.46 | 4 | 17 |
| 1 | A | 53 | GLY | N-CA | 6.11 | 1.55 | 1.46 | 9 | 17 |
| 1 | A | 45 | PRO | N-CA | 6.06 | 1.57 | 1.47 | 13 | 20 |
| 1 | A | 12 | LEU | CA-CB | 6.05 | 1.67 | 1.53 | 15 | 17 |
| 1 | A | 44 | ILE | CA-C | 6.05 | 1.68 | 1.52 | 5 | 20 |
| 1 | A | 56 | ARG | CA-CB | 6.00 | 1.67 | 1.53 | 15 | 1 |
| 1 | A | 9 | GLU | CB-CG | 5.97 | 1.63 | 1.52 | 8 | 10 |
| 1 | A | 42 | LYS | CA-CB | 5.97 | 1.67 | 1.53 | 17 | 6 |
| 1 | A | 45 | PRO | CA-C | 5.96 | 1.64 | 1.52 | 16 | 20 |
| 1 | A | 38 | ILE | CB-CG1 | 5.96 | 1.70 | 1.54 | 7 | 19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 93 | MET | N-CA | 5.94 | 1.58 | 1.46 | 5 | 16 |
| 1 | A | 80 | ALA | C-N | 5.88 | 1.47 | 1.34 | 16 | 18 |
| 1 | A | 86 | SER | N-CA | 5.88 | 1.58 | 1.46 | 10 | 9 |
| 1 | A | 23 | ILE | CB-CG1 | 5.87 | 1.70 | 1.54 | 11 | 1 |
| 1 | A | 73 | THR | N-CA | 5.83 | 1.58 | 1.46 | 4 | 18 |
| 1 | A | 69 | VAL | CA-CB | 5.82 | 1.67 | 1.54 | 16 | 17 |
| 1 | A | 39 | PHE | CB-CG | 5.81 | 1.61 | 1.51 | 17 | 9 |
| 1 | A | 45 | PRO | C-N | 5.81 | 1.43 | 1.33 | 16 | 20 |
| 1 | A | 71 | GLU | CA-CB | 5.80 | 1.66 | 1.53 | 13 | 6 |
| 1 | A | 76 | ALA | C-N | 5.79 | 1.47 | 1.34 | 13 | 20 |
| 1 | A | 37 | SER | CA-CB | 5.79 | 1.61 | 1.52 | 6 | 10 |
| 1 | A | 6 | GLU | CA-CB | 5.78 | 1.66 | 1.53 | 1 | 17 |
| 1 | A | 8 | GLU | CA-CB | 5.77 | 1.66 | 1.53 | 3 | 6 |
| 1 | A | 84 | ALA | C-N | 5.75 | 1.43 | 1.33 | 14 | 20 |
| 1 | A | 92 | VAL | N-CA | 5.74 | 1.57 | 1.46 | 5 | 17 |
| 1 | A | 91 | TYR | CB-CG | 5.74 | 1.60 | 1.51 | 14 | 20 |
| 1 | A | 74 | HIS | CB-CG | 5.73 | 1.60 | 1.50 | 6 | 13 |
| 1 | A | 58 | ASN | CA-C | 5.72 | 1.67 | 1.52 | 2 | 17 |
| 1 | A | 66 | GLU | CA-C | 5.71 | 1.67 | 1.52 | 15 | 3 |
| 1 | A | 70 | ARG | CA-C | 5.71 | 1.67 | 1.52 | 13 | 2 |
| 1 | A | 72 | VAL | N-CA | 5.68 | 1.57 | 1.46 | 8 | 5 |
| 1 | A | 39 | PHE | C-N | 5.66 | 1.47 | 1.34 | 12 | 10 |
| 1 | A | 54 | ARG | CA-CB | 5.64 | 1.66 | 1.53 | 12 | 5 |
| 1 | A | 82 | LYS | C-N | 5.62 | 1.47 | 1.34 | 12 | 5 |
| 1 | A | 75 | SER | N-CA | 5.60 | 1.57 | 1.46 | 4 | 5 |
| 1 | A | 45 | PRO | N-CD | 5.59 | 1.55 | 1.47 | 16 | 20 |
| 1 | A | 83 | GLU | C-N | 5.55 | 1.46 | 1.34 | 15 | 4 |
| 1 | A | 65 | ASN | CA-C | 5.48 | 1.67 | 1.52 | 11 | 4 |
| 1 | A | 9 | GLU | CA-CB | 5.43 | 1.65 | 1.53 | 8 | 2 |
| 1 | A | 8 | GLU | CB-CG | 5.42 | 1.62 | 1.52 | 3 | 6 |
| 1 | A | 51 | GLN | C-N | 5.42 | 1.46 | 1.34 | 18 | 20 |
| 2 | B | 8 | SER | C-N | 5.42 | 1.46 | 1.34 | 19 | 4 |
| 1 | A | 27 | THR | N-CA | 5.41 | 1.57 | 1.46 | 13 | 8 |
| 1 | A | 37 | SER | N-CA | 5.39 | 1.57 | 1.46 | 13 | 3 |
| 1 | A | 20 | GLY | N-CA | 5.38 | 1.54 | 1.46 | 3 | 1 |
| 1 | A | 71 | GLU | CB-CG | 5.36 | 1.62 | 1.52 | 10 | 1 |
| 1 | A | 62 | LEU | CA-CB | 5.36 | 1.66 | 1.53 | 2 | 6 |
| 1 | A | 59 | ASP | N-CA | 5.35 | 1.57 | 1.46 | 7 | 10 |
| 1 | A | 21 | PHE | N-CA | 5.33 | 1.57 | 1.46 | 16 | 1 |
| 1 | A | 65 | ASN | C-N | 5.32 | 1.46 | 1.34 | 15 | 3 |
| 1 | A | 39 | PHE | C-O | 5.32 | 1.33 | 1.23 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 49 | ALA | N-CA | 5.31 | 1.56 | 1.46 | 18 | 3 |
| 1 | A | 83 | GLU | CB-CG | 5.31 | 1.62 | 1.52 | 13 | 4 |
| 1 | A | 54 | ARG | C-N | 5.30 | 1.46 | 1.34 | 20 | 3 |
| 1 | A | 61 | ILE | N-CA | 5.30 | 1.56 | 1.46 | 4 | 11 |
| 1 | A | 20 | GLY | C-N | 5.30 | 1.46 | 1.34 | 11 | 2 |
| 1 | A | 70 | ARG | CD-NE | 5.28 | 1.55 | 1.46 | 3 | 6 |
| 1 | A | 69 | VAL | N-CA | 5.27 | 1.56 | 1.46 | 20 | 6 |
| 1 | A | 38 | ILE | CA-C | 5.27 | 1.66 | 1.52 | 12 | 1 |
| 1 | A | 54 | ARG | CD-NE | 5.27 | 1.55 | 1.46 | 17 | 5 |
| 1 | A | 11 | THR | CA-CB | 5.27 | 1.67 | 1.53 | 15 | 10 |
| 1 | A | 89 | ARG | N-CA | 5.26 | 1.56 | 1.46 | 11 | 5 |
| 1 | A | 57 | VAL | CA-CB | 5.26 | 1.65 | 1.54 | 4 | 6 |
| 1 | A | 10 | ILE | N-CA | 5.26 | 1.56 | 1.46 | 6 | 6 |
| 1 | A | 77 | ALA | C-N | 5.23 | 1.46 | 1.34 | 2 | 8 |
| 1 | A | 74 | HIS | C-N | 5.23 | 1.46 | 1.34 | 10 | 7 |
| 1 | A | 7 | TYR | CB-CG | 5.22 | 1.59 | 1.51 | 13 | 4 |
| 1 | A | 89 | ARG | CD-NE | 5.22 | 1.55 | 1.46 | 13 | 1 |
| 1 | A | 92 | VAL | CA-C | 5.22 | 1.66 | 1.52 | 5 | 9 |
| 1 | A | 25 | GLY | C-N | 5.21 | 1.42 | 1.33 | 5 | 2 |
| 1 | A | 28 | ASP | C-N | 5.21 | 1.46 | 1.34 | 19 | 2 |
| 1 | A | 63 | PHE | CA-CB | 5.21 | 1.65 | 1.53 | 6 | 7 |
| 1 | A | 37 | SER | C-N | 5.20 | 1.46 | 1.34 | 3 | 6 |
| 1 | A | 41 | THR | N-CA | 5.19 | 1.56 | 1.46 | 18 | 2 |
| 1 | A | 94 | ARG | CD-NE | 5.18 | 1.55 | 1.46 | 5 | 4 |
| 1 | A | 21 | PHE | C-N | 5.18 | 1.46 | 1.34 | 5 | 3 |
| 1 | A | 74 | HIS | CA-C | 5.17 | 1.66 | 1.52 | 1 | 3 |
| 1 | A | 23 | ILE | C-N | 5.17 | 1.46 | 1.34 | 9 | 2 |
| 1 | A | 55 | LEU | CA-CB | 5.16 | 1.65 | 1.53 | 5 | 1 |
| 1 | A | 74 | HIS | CA-CB | 5.13 | 1.65 | 1.53 | 7 | 3 |
| 2 | B | 8 | SER | N-CA | 5.12 | 1.56 | 1.46 | 13 | 2 |
| 1 | A | 57 | VAL | CA-C | 5.12 | 1.66 | 1.52 | 7 | 3 |
| 1 | A | 68 | ASP | CA-CB | 5.11 | 1.65 | 1.53 | 8 | 2 |
| 1 | A | 49 | ALA | C-N | 5.09 | 1.45 | 1.34 | 20 | 2 |
| 1 | A | 62 | LEU | C-N | 5.09 | 1.45 | 1.34 | 11 | 1 |
| 1 | A | 47 | GLY | N-CA | 5.07 | 1.53 | 1.46 | 16 | 1 |
| 1 | A | 50 | ALA | C-N | 5.06 | 1.45 | 1.34 | 7 | 2 |
| 1 | A | 39 | PHE | N-CA | 5.06 | 1.56 | 1.46 | 12 | 1 |
| 1 | A | 78 | VAL | CA-C | 5.04 | 1.66 | 1.52 | 15 | 1 |
| 1 | A | 91 | TYR | C-O | 5.02 | 1.32 | 1.23 | 1 | 1 |
| 1 | A | 53 | GLY | C-N | 5.01 | 1.45 | 1.34 | 4 | 1 |
| 1 | A | 73 | THR | C-N | 5.00 | 1.45 | 1.34 | 4 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 88 | VAL | CA-CB-CG2 | 11.05 | 127.48 | 110.90 | 19 | 8 |
| 1 | A | 88 | VAL | CA-CB-CG1 | 10.72 | 126.99 | 110.90 | 16 | 3 |
| 1 | A | 64 | VAL | CA-CB-CG1 | 9.69 | 125.43 | 110.90 | 8 | 6 |
| 1 | A | 69 | VAL | CA-CB-CG1 | 8.49 | 123.64 | 110.90 | 9 | 6 |
| 1 | A | 94 | ARG | NE-CZ-NH1 | 8.22 | 124.41 | 120.30 | 7 | 20 |
| 1 | A | 70 | ARG | NE-CZ-NH1 | 8.16 | 124.38 | 120.30 | 17 | 20 |
| 1 | A | 54 | ARG | NE-CZ-NH1 | 8.12 | 124.36 | 120.30 | 17 | 20 |
| 1 | A | 89 | ARG | NE-CZ-NH1 | 8.10 | 124.35 | 120.30 | 6 | 20 |
| 1 | A | 56 | ARG | NE-CZ-NH1 | 8.08 | 124.34 | 120.30 | 19 | 20 |
| 1 | A | 67 | VAL | CA-CB-CG1 | 7.95 | 122.83 | 110.90 | 4 | 3 |
| 1 | A | 57 | VAL | CA-CB-CG1 | 7.77 | 122.56 | 110.90 | 14 | 14 |
| 1 | A | 72 | VAL | CA-CB-CG2 | 7.38 | 121.97 | 110.90 | 16 | 11 |
| 1 | A | 67 | VAL | CA-CB-CG2 | 6.86 | 121.19 | 110.90 | 13 | 13 |
| 1 | A | 64 | VAL | CA-CB-CG2 | 5.76 | 119.54 | 110.90 | 1 | 8 |
| 1 | A | 23 | ILE | CA-CB-CG1 | 5.75 | 121.92 | 111.00 | 11 | 1 |
| 1 | A | 83 | GLU | N-CA-CB | -5.71 | 100.33 | 110.60 | 15 | 1 |
| 1 | A | 39 | PHE | CB-CG-CD1 | 5.59 | 124.72 | 120.80 | 1 | 2 |
| 1 | A | 90 | LEU | CB-CG-CD1 | 5.47 | 120.30 | 111.00 | 10 | 9 |
| 1 | A | 39 | PHE | CA-CB-CG | 5.41 | 126.89 | 113.90 | 1 | 4 |
| 1 | A | 93 | MET | CA-CB-CG | 5.28 | 122.28 | 113.30 | 14 | 2 |
| 1 | A | 69 | VAL | CA-CB-CG2 | 5.28 | 118.82 | 110.90 | 11 | 3 |
| 1 | A | 65 | ASN | C-N-CA | 5.25 | 134.83 | 121.70 | 5 | 2 |
| 1 | A | 38 | ILE | CA-CB-CG1 | 5.21 | 120.89 | 111.00 | 12 | 3 |
| 1 | A | 74 | HIS | CA-CB-CG | 5.19 | 122.42 | 113.60 | 4 | 1 |
| 1 | A | 83 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 | 15 | 1 |
| 1 | A | 69 | VAL | CB-CA-C | 5.06 | 121.02 | 111.40 | 12 | 1 |
| 1 | A | 42 | LYS | CA-CB-CG | 5.06 | 124.53 | 113.40 | 17 | 1 |

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 | 569 | 573 | 572 | 6±3 |
| 2 | B | 14 | 14 | 14 | 1±1 |
| All | All | 11660 | 11740 | 11720 | 132 |

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 6.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:43:ILE:CA | 1:A:43:ILE:CB | 1.65 | 1.75 | 18 | 19 |
| 1:A:87:ILE:CA | 1:A:87:ILE:CB | 1.62 | 1.74 | 12 | 2 |
| 1:A:38:ILE:CB | 1:A:38:ILE:CA | 1.62 | 1.74 | 5 | 7 |
| 1:A:72:VAL:CA | 1:A:72:VAL:CB | 1.59 | 1.76 | 3 | 10 |
| 1:A:44:ILE:CA | 1:A:44:ILE:CB | 1.57 | 1.74 | 13 | 2 |
| 2:B:9:VAL:CA | 2:B:9:VAL:CB | 1.56 | 1.74 | 7 | 3 |
| 1:A:72:VAL:CA | 1:A:72:VAL:HB | 0.75 | 2.06 | 16 | 10 |
| 1:A:38:ILE:CA | 1:A:38:ILE:HB | 0.74 | 2.07 | 13 | 7 |
| 1:A:43:ILE:CA | 1:A:43:ILE:HB | 0.71 | 2.11 | 11 | 19 |
| 1:A:64:VAL:O | 1:A:67:VAL:HB | 0.63 | 1.93 | 4 | 1 |
| 2:B:9:VAL:CA | 2:B:9:VAL:CG1 | 0.61 | 2.74 | 7 | 3 |
| 1:A:44:ILE:CA | 1:A:44:ILE:HB | 0.60 | 2.10 | 16 | 2 |
| 1:A:87:ILE:CA | 1:A:87:ILE:HB | 0.59 | 2.13 | 7 | 2 |
| 1:A:38:ILE:CA | 1:A:38:ILE:CG2 | 0.56 | 2.77 | 12 | 7 |
| 1:A:72:VAL:CA | 1:A:72:VAL:CG1 | 0.55 | 2.78 | 4 | 10 |
| 2:B:9:VAL:CA | 2:B:9:VAL:CG2 | 0.55 | 2.79 | 19 | 3 |
| 2:B:9:VAL:CA | 2:B:9:VAL:HB | 0.53 | 2.15 | 20 | 2 |
| 1:A:44:ILE:CB | 1:A:44:ILE:N | 0.53 | 2.68 | 16 | 1 |
| 1:A:72:VAL:CB | 1:A:72:VAL:C | 0.47 | 2.77 | 6 | 8 |
| 1:A:44:ILE:CA | 1:A:44:ILE:CG1 | 0.45 | 2.83 | 13 | 1 |
| 1:A:44:ILE:CA | 1:A:44:ILE:CG2 | 0.44 | 2.83 | 16 | 2 |
| 1:A:64:VAL:O | 1:A:67:VAL:HG22 | 0.44 | 2.13 | 15 | 3 |
| 1:A:87:ILE:CA | 1:A:87:ILE:CG1 | 0.42 | 2.87 | 12 | 1 |
| 1:A:64:VAL:O | 1:A:67:VAL:HG12 | 0.42 | 2.15 | 8 | 1 |
| 1:A:87:ILE:CA | 1:A:87:ILE:CG2 | 0.41 | 2.86 | 7 | 1 |
| 1:A:22:SER:HB2 | 1:A:42:LYS:HB3 | 0.41 | 1.92 | 10 | 1 |
| 1:A:43:ILE:CA | 1:A:43:ILE:CG1 | 0.41 | 2.87 | 17 | 3 |
| 1:A:61:ILE:HG21 | 1:A:64:VAL:HG23 | 0.40 | 1.94 | 11 | 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 | 75/99 (76%) | 66±1 (88±2%) | 6±1 (8±2%) | 3±1 (4±1%) | 5 29 |
| 2 | B | 1/9 (11%) | 1±0 (80±40%) | 0±0 (20±40%) | 0±0 (0±0%) | 100 100 |
| All | All | 1520/2160 (70%) | 1333 (88%) | 123 (8%) | 64 (4%) | 5 30 |

All 6 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 | 60 | SER | 20 |
| 1 | A | 54 | ARG | 18 |
| 1 | A | 86 | SER | 15 |
| 1 | A | 20 | GLY | 5 |
| 1 | A | 65 | ASN | 3 |
| 1 | A | 66 | GLU | 3 |

### 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 | 60/78 (77%) | 56±1 (93±2%) | 4±1 (7±2%) | 18 66 |
| 2 | B | 2/9 (22%) | 2±0 (100±0%) | 0±0 (0±0%) | 100 100 |
| All | All | 1240/1740 (71%) | 1154 (93%) | 86 (7%) | 19 68 |

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 | 38 | ILE | 18 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 88 | VAL | 11 |
| 1 | A | 11 | THR | 10 |
| 1 | A | 55 | LEU | 9 |
| 1 | A | 90 | LEU | 9 |
| 1 | A | 64 | VAL | 7 |
| 1 | A | 69 | VAL | 6 |
| 1 | A | 93 | MET | 4 |
| 1 | A | 67 | VAL | 2 |
| 1 | A | 40 | ILE | 1 |
| 1 | A | 89 | ARG | 1 |
| 1 | A | 51 | GLN | 1 |
| 1 | A | 54 | ARG | 1 |
| 1 | A | 9 | GLU | 1 |
| 1 | A | 8 | GLU | 1 |
| 1 | A | 71 | GLU | 1 |
| 1 | A | 23 | ILE | 1 |
| 1 | A | 81 | LEU | 1 |
| 1 | A | 12 | LEU | 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)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 74% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

### 7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 992 |
| Number of shifts mapped to atoms | 992 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 95 | 0.14 ± 0.18 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 84 | -0.05 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 0 | — | None (insufficient data) |
| $^{15}N$ | 90 | 0.07 ± 0.45 | None needed (< 0.5 ppm) |

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 807 atoms were assigned a chemical shift out of a possible 1028. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 301/390 (77%) | 154/160 (96%) | 74/154 (48%) | 73/76 (96%) |
| Sidechain | 464/582 (80%) | 319/382 (84%) | 145/179 (81%) | 0/21 (0%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 42/56 (75%) | 21/27 (78%) | 21/27 (78%) | 0/2 (0%) |
| Overall | 807/1028 (79%) | 494/569 (87%) | 240/360 (67%) | 73/99 (74%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 992 atoms were assigned a chemical shift out of a possible 1425. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 381/541 (70%) | 196/222 (88%) | 95/216 (44%) | 90/103 (87%) |
| Sidechain | 565/820 (69%) | 387/536 (72%) | 178/252 (71%) | 0/32 (0%) |
| Aromatic | 46/64 (72%) | 23/31 (74%) | 23/29 (79%) | 0/4 (0%) |
| Overall | 992/1425 (70%) | 606/789 (77%) | 296/497 (60%) | 90/139 (65%) |

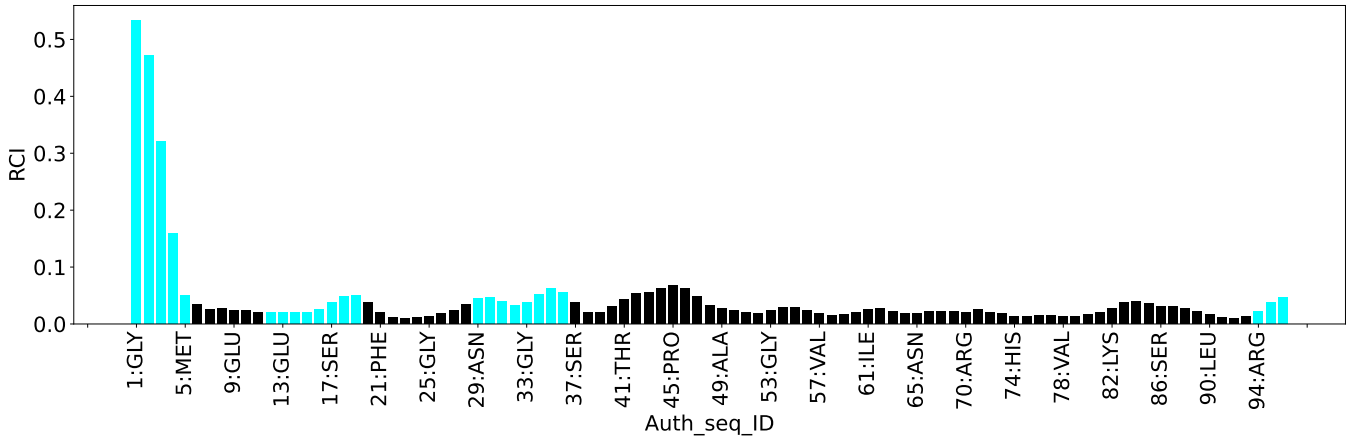
### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

### 7.2.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 59 |
| Number of shifts mapped to atoms | 59 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

### 7.2.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 13 atoms were assigned a chemical shift out of a possible 1028. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | **Total** | $^{1}$**H** | $^{13}$**C** | $^{15}$**N** |
|---|---|---|---|---|
| Backbone | 4/390 (1%) | 4/160 (2%) | 0/154 (0%) | 0/76 (0%) |
| Sidechain | 9/582 (2%) | 9/382 (2%) | 0/179 (0%) | 0/21 (0%) |
| Aromatic | 0/56 (0%) | 0/27 (0%) | 0/27 (0%) | 0/2 (0%) |
| Overall | 13/1028 (1%) | 13/569 (2%) | 0/360 (0%) | 0/99 (0%) |

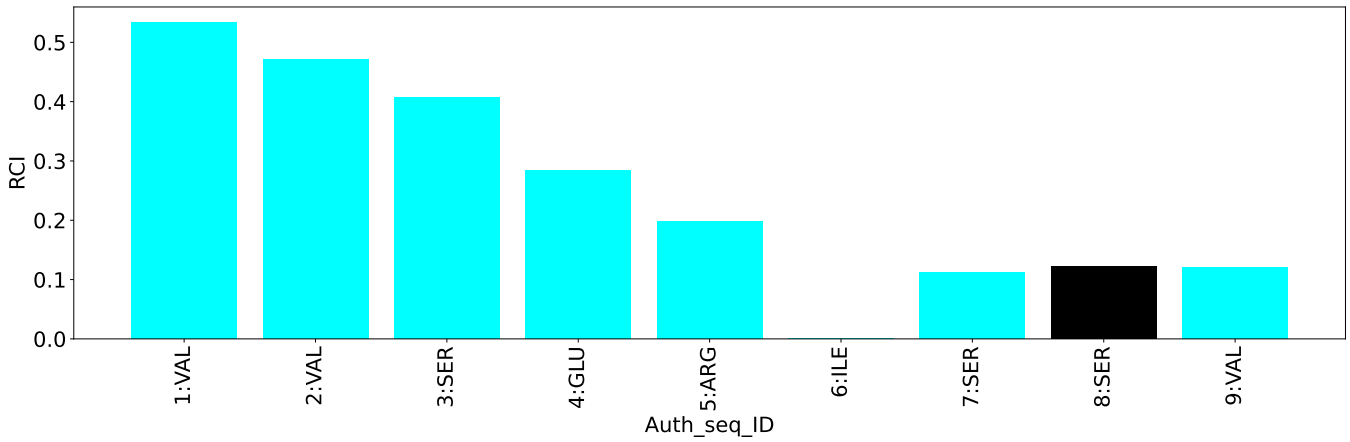
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 59 atoms were assigned a chemical shift out of a possible 1425. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | **Total** | $^{1}$**H** | $^{13}$**C** | $^{15}$**N** |
|---|---|---|---|---|
| Backbone | 14/541 (3%) | 14/222 (6%) | 0/216 (0%) | 0/103 (0%) |
| Sidechain | 45/820 (5%) | 45/536 (8%) | 0/252 (0%) | 0/32 (0%) |
| Aromatic | 0/64 (0%) | 0/31 (0%) | 0/29 (0%) | 0/4 (0%) |
| Overall | 59/1425 (4%) | 59/789 (7%) | 0/497 (0%) | 0/139 (0%) |

### 7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B: