# Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 01:58 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2MJ3 |
| BMRB ID | : | 19703 |
| Title | : | Backbone 1H, 13C, and 15N Chemical Shift Assignments and structure of Iron-sulfur cluster binding protein from Ehrlichia chaffeensis |
| Authors | : | Barnwal, R.; Varani, G.; Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID) |
| Deposited on | : | 2013-12-23 |

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:

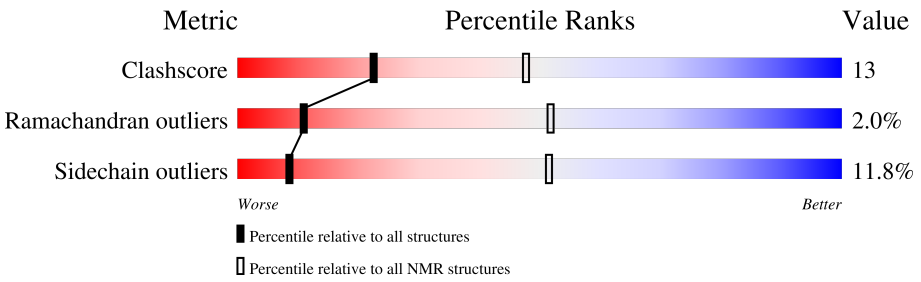
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | 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 78%.

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 | 116 | 55% 18% • 26% |

# 2 Ensemble composition and analysis (i)

This entry contains 9 models. Model 6 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:1-A:29, A:50-A:106 (86) | 0.96 | 6 |

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. No single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 1, 6, 7, 8, 9 |
| 2 | 2, 3, 4, 5 |

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1764 atoms, of which 867 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Iron-sulfur cluster binding protein.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 116 | 1764 | 558 | 867 | 146 | 186 | 7 | 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: Iron-sulfur cluster binding protein

Chain A: 55% 18% • 26%

M1 P2 L3 I4 S8 T15 Y16 E17 A18 Y19 T23 L24 L27 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 I52 D53 P54 I66 T83 S84 I90 I91 L92 T93 K94 E95 L96 V101 T107

R108 N109 I110 S111 F112 V113 K114 N115 S116

## 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: Iron-sulfur cluster binding protein

Chain A: 57% 16% •• 26%

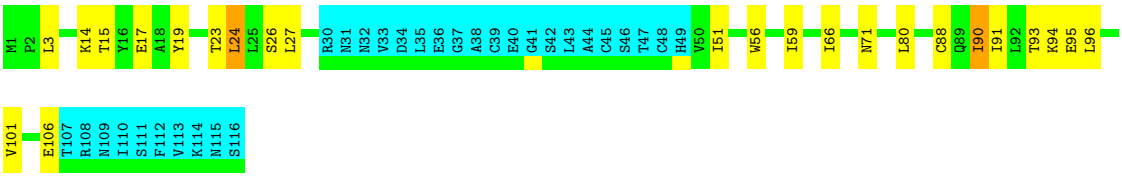
M1 P2 L3 I4 T15 Y16 E17 T23 L27 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 I52 D53 P54 T83 S84 I90 I91 L92 T93 K94 E95 L96 L99 C100 V101 T107 R108 N109 I110 S111 F112

V113 K114 N115 S116

### 4.2.2 Score per residue for model 2

• Molecule 1: Iron-sulfur cluster binding protein

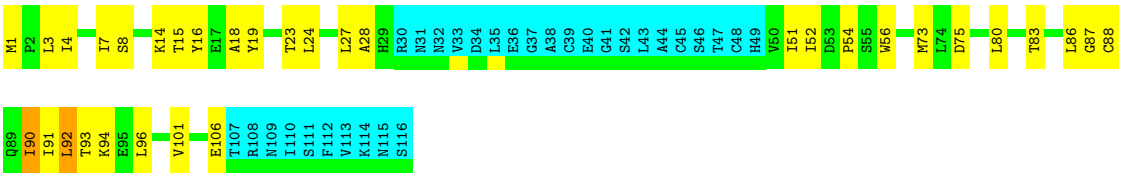
Chain A: 53% 19% • 26%




### 4.2.3 Score per residue for model 3

- Molecule 1: Iron-sulfur cluster binding protein

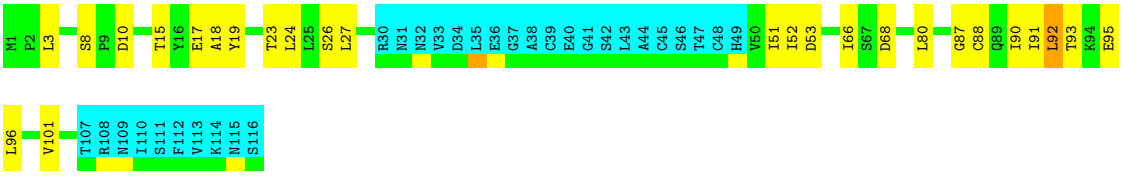
Chain A: 46% 27% • 26%




### 4.2.4 Score per residue for model 4

- Molecule 1: Iron-sulfur cluster binding protein

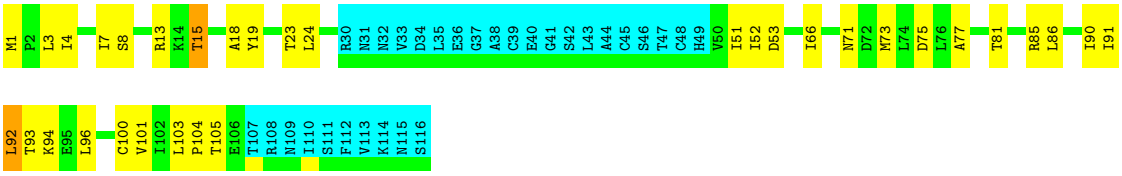
Chain A: 52% 22% • 26%




### 4.2.5 Score per residue for model 5

- Molecule 1: Iron-sulfur cluster binding protein

Chain A: 46% 27% • 26%




### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Iron-sulfur cluster binding protein

Chain A: 52% 22% • 26%

M1 P2 L3 S8 R13 K14 T15 Y16 E17 G21 E22 T23 L24 L27 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 P54 S55 W56 I66 T81 D82 T83 S84 R85 I90 I91 L92 T93 L96

L99 C100 V101 T105 E106 T107 R108 N109 I110 S111 F112 V113 K114 N115 S116

### 4.2.7 Score per residue for model 7

- Molecule 1: Iron-sulfur cluster binding protein

Chain A: 50% 22% •• 26%

M1 P2 L3 I4 T5 F6 I7 S8 R13 K14 T15 Y16 Y19 E22 T23 L24 L25 S26 L27 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 I52 D53 P54 I66 N71 L74 T83 S84 I90 I91

L92 T93 K94 E95 L96 V101 T107 R108 N109 I110 S111 F112 V113 K114 N115 S116

### 4.2.8 Score per residue for model 8

- Molecule 1: Iron-sulfur cluster binding protein

Chain A: 51% 22% •• 26%

M1 P2 L3 I4 T5 F6 I7 S8 T15 Y16 E17 A18 Y19 D20 G21 L24 L25 S26 L27 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 P54 S55 W56 E65 D75 T83 S84 R85 L86 I90 I91

L92 T93 K94 E95 L96 V101 I102 L103 T107 R108 N109 I110 S111 F112 V113 K114 N115 S116

### 4.2.9 Score per residue for model 9

- Molecule 1: Iron-sulfur cluster binding protein

Chain A: 48% 23% •• 26%

M1 P2 L3 F6 I7 S8 T15 Y16 E17 A18 Y19 D20 G21 E22 T23 L24 L27 A28 H29 R30 N31 N32 V33 D34 L35 E36 G37 A38 C39 E40 G41 S42 L43 A44 C45 S46 T47 C48 H49 V50 I51 I52 D53 I66 S67 E70 N71 D72 M73 L74 D75 S84 I90

I91 L92 T93 K94 E95 L96 V101 T107 R108 N109 I110 S111 F112 V113 K114 N115 S116

# 5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 9 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification | Version |
|---|---|---|
| CCPNMR | refinement | |
| CYANA | structure solution | |
| 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 | 1 |
| Total number of shifts | 1054 |
| Number of shifts mapped to atoms | 1054 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 78% |

# 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 | 675 | 656 | 658 | 17±2 |
| All | All | 6075 | 5904 | 5922 | 151 |

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 13.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:51:ILE:HD12 | 1:A:90:ILE:HG22 | 0.95 | 1.38 | 7 | 5 |
| 1:A:18:ALA:HB1 | 1:A:92:LEU:HD13 | 0.92 | 1.39 | 4 | 1 |
| 1:A:96:LEU:HD23 | 1:A:101:VAL:HG11 | 0.85 | 1.49 | 4 | 8 |
| 1:A:23:THR:HG23 | 1:A:91:ILE:HG22 | 0.76 | 1.57 | 1 | 1 |
| 1:A:3:LEU:HD21 | 1:A:15:THR:HG23 | 0.69 | 1.63 | 3 | 8 |
| 1:A:6:PHE:CZ | 1:A:24:LEU:HD11 | 0.68 | 2.24 | 8 | 1 |
| 1:A:18:ALA:HB1 | 1:A:92:LEU:HD12 | 0.64 | 1.70 | 3 | 2 |
| 1:A:17:GLU:O | 1:A:27:LEU:HD11 | 0.62 | 1.95 | 1 | 6 |
| 1:A:73:MET:HB3 | 1:A:86:LEU:HD11 | 0.62 | 1.71 | 3 | 1 |
| 1:A:23:THR:HG23 | 1:A:91:ILE:CG2 | 0.61 | 2.25 | 1 | 1 |
| 1:A:24:LEU:HD11 | 1:A:104:PRO:CG | 0.60 | 2.25 | 5 | 1 |
| 1:A:66:ILE:HD12 | 1:A:71:ASN:CB | 0.60 | 2.27 | 9 | 3 |
| 1:A:77:ALA:HB2 | 1:A:86:LEU:HD13 | 0.60 | 1.74 | 5 | 1 |
| 1:A:3:LEU:HD21 | 1:A:15:THR:HG22 | 0.59 | 1.74 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:51:ILE:CD1 | 1:A:90:ILE:HG22 | 0.59 | 2.27 | 9 | 4 |
| 1:A:51:ILE:O | 1:A:96:LEU:HD21 | 0.59 | 1.97 | 8 | 6 |
| 1:A:84:SER:HB2 | 1:A:90:ILE:HG23 | 0.57 | 1.74 | 9 | 5 |
| 1:A:3:LEU:HD21 | 1:A:15:THR:CG2 | 0.57 | 2.29 | 5 | 8 |
| 1:A:54:PRO:HB3 | 1:A:83:THR:HG22 | 0.57 | 1.76 | 3 | 5 |
| 1:A:73:MET:CB | 1:A:86:LEU:HD11 | 0.56 | 2.29 | 3 | 1 |
| 1:A:18:ALA:HB1 | 1:A:92:LEU:CD1 | 0.56 | 2.23 | 4 | 1 |
| 1:A:16:TYR:CD1 | 1:A:27:LEU:HD21 | 0.55 | 2.37 | 7 | 2 |
| 1:A:23:THR:HB | 1:A:91:ILE:HG22 | 0.55 | 1.78 | 6 | 7 |
| 1:A:96:LEU:HD22 | 1:A:101:VAL:HG21 | 0.55 | 1.76 | 1 | 4 |
| 1:A:96:LEU:HD23 | 1:A:101:VAL:CG1 | 0.55 | 2.28 | 9 | 3 |
| 1:A:73:MET:CG | 1:A:86:LEU:HD21 | 0.55 | 2.32 | 5 | 1 |
| 1:A:7:ILE:HD12 | 1:A:101:VAL:O | 0.54 | 2.02 | 5 | 3 |
| 1:A:56:TRP:CH2 | 1:A:99:LEU:HD12 | 0.54 | 2.38 | 6 | 1 |
| 1:A:51:ILE:HD12 | 1:A:90:ILE:CG2 | 0.54 | 2.25 | 7 | 6 |
| 1:A:96:LEU:CD2 | 1:A:101:VAL:HG11 | 0.53 | 2.33 | 8 | 8 |
| 1:A:3:LEU:HD11 | 1:A:15:THR:CG2 | 0.53 | 2.34 | 8 | 2 |
| 1:A:80:LEU:HD13 | 1:A:88:CYS:H | 0.52 | 1.64 | 3 | 1 |
| 1:A:3:LEU:O | 1:A:4:ILE:HD13 | 0.52 | 2.05 | 1 | 2 |
| 1:A:81:THR:HG21 | 1:A:104:PRO:O | 0.52 | 2.04 | 5 | 1 |
| 1:A:21:GLY:O | 1:A:91:ILE:HD12 | 0.52 | 2.05 | 8 | 3 |
| 1:A:24:LEU:HD11 | 1:A:104:PRO:HG3 | 0.51 | 1.83 | 5 | 1 |
| 1:A:66:ILE:HD12 | 1:A:71:ASN:HB2 | 0.51 | 1.81 | 9 | 1 |
| 1:A:53:ASP:OD1 | 1:A:101:VAL:HG12 | 0.51 | 2.06 | 9 | 1 |
| 1:A:6:PHE:CE2 | 1:A:24:LEU:HD11 | 0.48 | 2.43 | 9 | 1 |
| 1:A:24:LEU:CD1 | 1:A:27:LEU:HD22 | 0.48 | 2.39 | 4 | 1 |
| 1:A:66:ILE:O | 1:A:66:ILE:HD12 | 0.47 | 2.09 | 2 | 3 |
| 1:A:96:LEU:CD2 | 1:A:101:VAL:HG21 | 0.47 | 2.40 | 1 | 2 |
| 1:A:66:ILE:HD12 | 1:A:71:ASN:ND2 | 0.47 | 2.25 | 5 | 1 |
| 1:A:81:THR:OG1 | 1:A:90:ILE:HD13 | 0.46 | 2.11 | 6 | 1 |
| 1:A:56:TRP:HA | 1:A:59:ILE:HD12 | 0.45 | 1.89 | 2 | 1 |
| 1:A:7:ILE:HD11 | 1:A:100:CYS:HB2 | 0.45 | 1.88 | 5 | 1 |
| 1:A:6:PHE:CZ | 1:A:92:LEU:HD21 | 0.44 | 2.48 | 7 | 1 |
| 1:A:3:LEU:HD11 | 1:A:15:THR:HG22 | 0.44 | 1.88 | 8 | 1 |
| 1:A:50:VAL:HG23 | 1:A:85:ARG:CG | 0.44 | 2.42 | 6 | 1 |
| 1:A:51:ILE:HD12 | 1:A:90:ILE:HG23 | 0.43 | 1.90 | 2 | 2 |
| 1:A:4:ILE:HD12 | 1:A:96:LEU:HB2 | 0.43 | 1.89 | 3 | 3 |
| 1:A:80:LEU:HD13 | 1:A:88:CYS:O | 0.43 | 2.12 | 4 | 1 |
| 1:A:3:LEU:HD11 | 1:A:15:THR:HG23 | 0.43 | 1.90 | 1 | 1 |
| 1:A:96:LEU:HA | 1:A:99:LEU:HD12 | 0.43 | 1.90 | 1 | 1 |
| 1:A:52:ILE:HD12 | 1:A:52:ILE:O | 0.42 | 2.13 | 9 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:66:ILE:HD13 | 1:A:71:ASN:HB2 | 0.42 | 1.92 | 2 | 1 |
| 1:A:3:LEU:HD12 | 1:A:4:ILE:H | 0.42 | 1.75 | 7 | 1 |
| 1:A:80:LEU:HD11 | 1:A:88:CYS:SG | 0.41 | 2.55 | 2 | 1 |
| 1:A:80:LEU:HA | 1:A:90:ILE:HD11 | 0.41 | 1.91 | 3 | 1 |
| 1:A:66:ILE:HD12 | 1:A:71:ASN:CG | 0.41 | 2.36 | 9 | 1 |
| 1:A:66:ILE:HG22 | 1:A:70:GLU:CG | 0.41 | 2.45 | 9 | 1 |
| 1:A:24:LEU:HD13 | 1:A:27:LEU:HD22 | 0.41 | 1.93 | 2 | 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 | 85/116 (73%) | 77±2 (90±2%) | 6±2 (8±2%) | 2±1 (2±1%) | 11 | 52 |
| All | All | 765/1044 (73%) | 692 (90%) | 58 (8%) | 15 (2%) | 11 | 52 |

All 3 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 | 90 | ILE | 7 |
| 1 | A | 92 | LEU | 6 |
| 1 | A | 87 | GLY | 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 | 78/104 (75%) | 69±3 (88±4%) | 9±3 (12±4%) | 8 | 51 |
| All | All | 702/936 (75%) | 619 (88%) | 83 (12%) | 8 | 51 |

All 31 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 | 93 | THR | 9 |
| 1 | A | 19 | TYR | 7 |
| 1 | A | 8 | SER | 7 |
| 1 | A | 94 | LYS | 6 |
| 1 | A | 90 | ILE | 4 |
| 1 | A | 95 | GLU | 4 |
| 1 | A | 24 | LEU | 4 |
| 1 | A | 75 | ASP | 4 |
| 1 | A | 1 | MET | 3 |
| 1 | A | 26 | SER | 3 |
| 1 | A | 92 | LEU | 3 |
| 1 | A | 53 | ASP | 3 |
| 1 | A | 13 | ARG | 3 |
| 1 | A | 14 | LYS | 2 |
| 1 | A | 106 | GLU | 2 |
| 1 | A | 56 | TRP | 2 |
| 1 | A | 103 | LEU | 2 |
| 1 | A | 105 | THR | 2 |
| 1 | A | 23 | THR | 1 |
| 1 | A | 52 | ILE | 1 |
| 1 | A | 10 | ASP | 1 |
| 1 | A | 68 | ASP | 1 |
| 1 | A | 15 | THR | 1 |
| 1 | A | 85 | ARG | 1 |
| 1 | A | 22 | GLU | 1 |
| 1 | A | 25 | LEU | 1 |
| 1 | A | 74 | LEU | 1 |
| 1 | A | 65 | GLU | 1 |
| 1 | A | 86 | LEU | 1 |
| 1 | A | 67 | SER | 1 |
| 1 | A | 73 | MET | 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 78% for the well-defined parts and 69% 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 | 1054 |
| Number of shifts mapped to atoms | 1054 |
| 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 |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 99 | -0.06 ± 0.17 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 94 | 0.10 ± 0.23 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 99 | 0.17 ± 0.18 | None needed (< 0.5 ppm) |
| $^{15}N$ | 94 | -0.28 ± 0.28 | 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 78%, i.e. 894 atoms were assigned a chemical shift out of a possible 1149. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 403/427 (94%) | 161/173 (93%) | 164/172 (95%) | 78/82 (95%) |
| Sidechain | 470/649 (72%) | 301/425 (71%) | 168/212 (79%) | 1/12 (8%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 21/73 (29%) | 20/36 (56%) | 0/34 (0%) | 1/3 (33%) |
| Overall | 894/1149 (78%) | 482/634 (76%) | 332/418 (79%) | 80/97 (82%) |

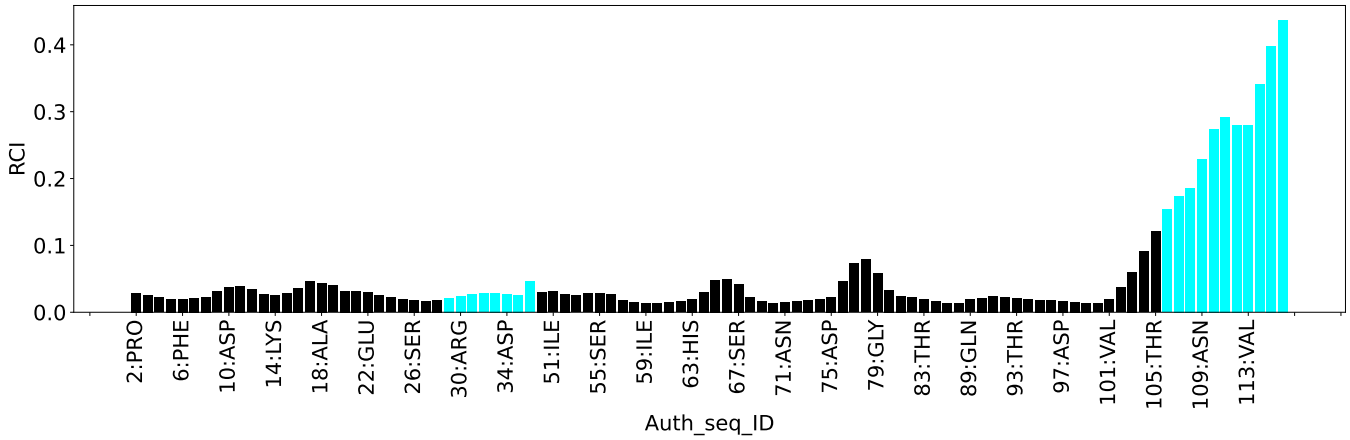
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1054 atoms were assigned a chemical shift out of a possible 1519. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 486/579 (84%) | 194/235 (83%) | 198/232 (85%) | 94/112 (84%) |
| Sidechain | 543/850 (64%) | 345/554 (62%) | 195/273 (71%) | 3/23 (13%) |
| Aromatic | 25/90 (28%) | 24/45 (53%) | 0/41 (0%) | 1/4 (25%) |
| Overall | 1054/1519 (69%) | 563/834 (68%) | 393/546 (72%) | 98/139 (71%) |

### 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: