# Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 10:26 pm BST

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|---|---|---|
| PDB ID | : | 6I2O |
| Title | : | Solution NMR structure of PilE1 from Streptococcus sanguinis |
| Authors | : | Berry, J.L.; Xu, Y. |
| Deposited on | : | 2018-11-01 |

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

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

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

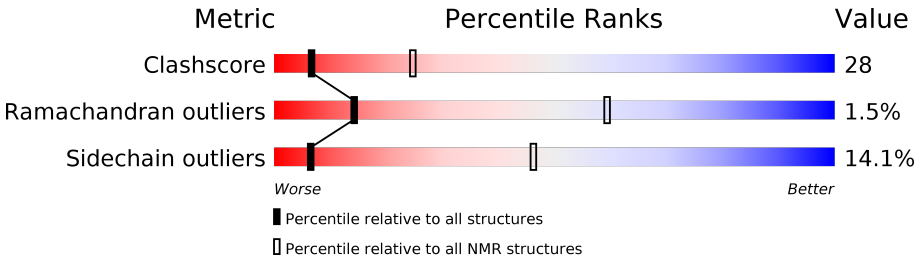
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 89%.

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 | 113 | 43% 38% 6% 12% |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:7-A:96, A:103-A:111 (99) | 0.31 | 7 |

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, 2, 3, 4, 6, 7, 8, 10 |
| 2 | 5, 9 |

# 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1667 atoms, of which 818 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Type IV pilin PilE1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 113 | 1667 | 512 | 818 | 155 | 181 | 1 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 6 | HIS | PHE | conflict | UNP A0A0B7GU52 |

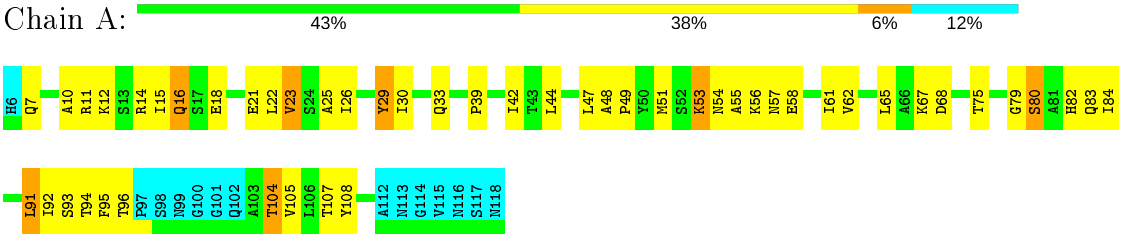
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Type IV pilin PilE1

Chain A:



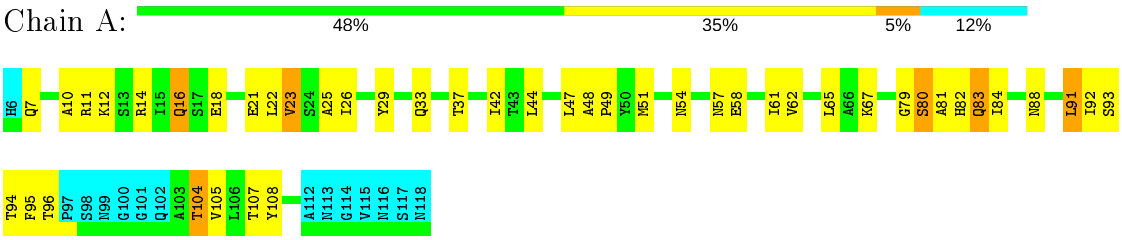

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

- Molecule 1: Type IV pilin PilE1

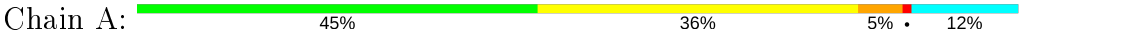
Chain A:

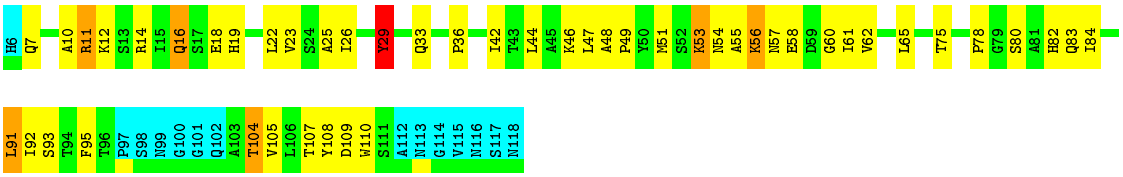



### 4.2.2 Score per residue for model 2

- Molecule 1: Type IV pilin PilE1

Chain A:

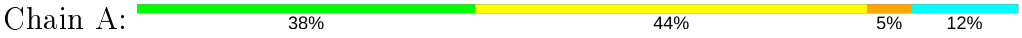


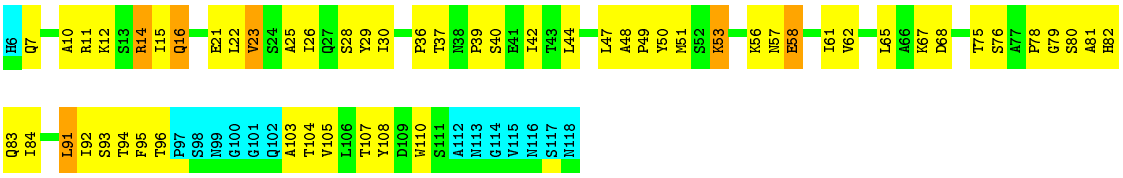



### 4.2.3 Score per residue for model 3

- Molecule 1: Type IV pilin PilE1

Chain A:

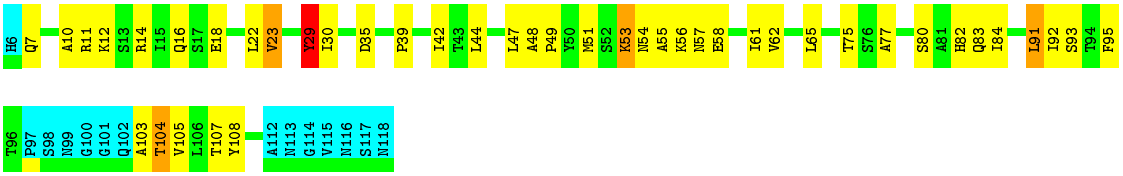



### 4.2.4 Score per residue for model 4

- Molecule 1: Type IV pilin PilE1

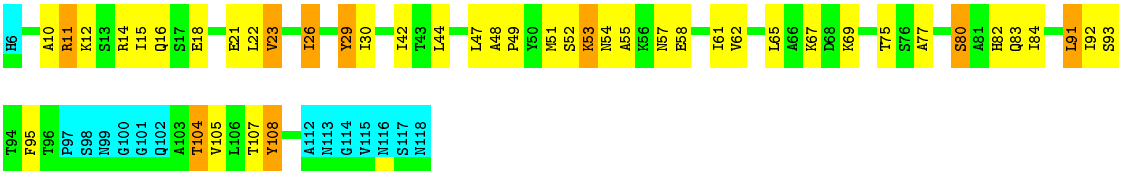
Chain A:


### 4.2.5 Score per residue for model 5

- Molecule 1: Type IV pilin PilE1

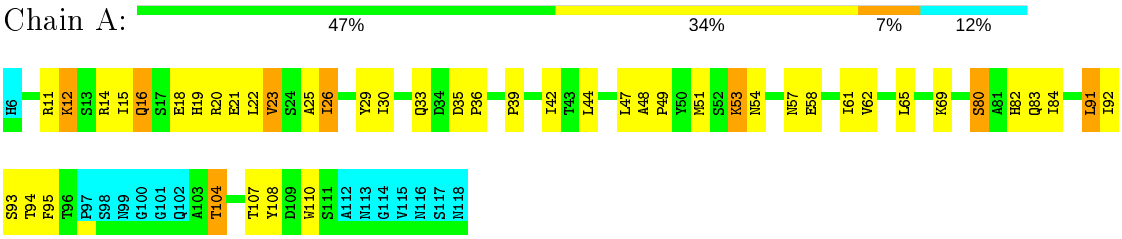
Chain A:


### 4.2.6 Score per residue for model 6

- Molecule 1: Type IV pilin PilE1

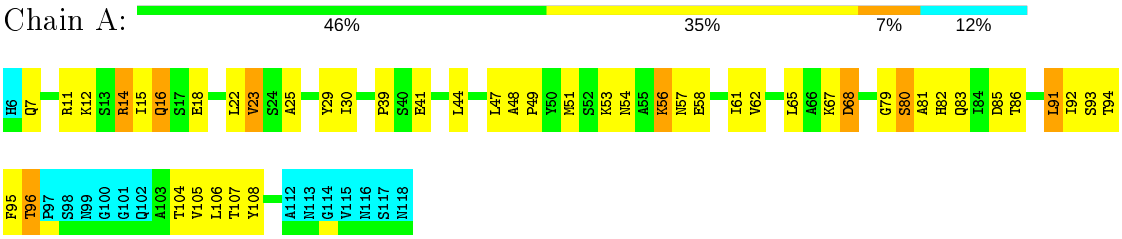
Chain A:




### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Type IV pilin PilE1

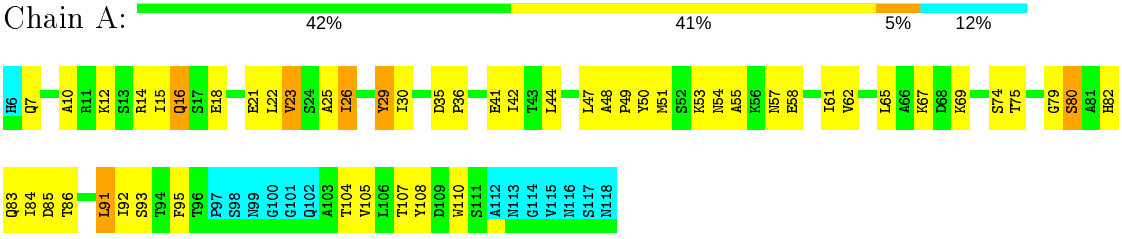
Chain A:




### 4.2.8 Score per residue for model 8

- Molecule 1: Type IV pilin PilE1

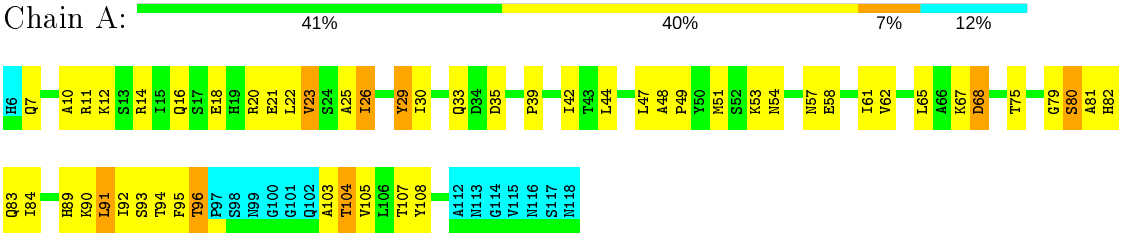
Chain A:




### 4.2.9 Score per residue for model 9

- Molecule 1: Type IV pilin PilE1

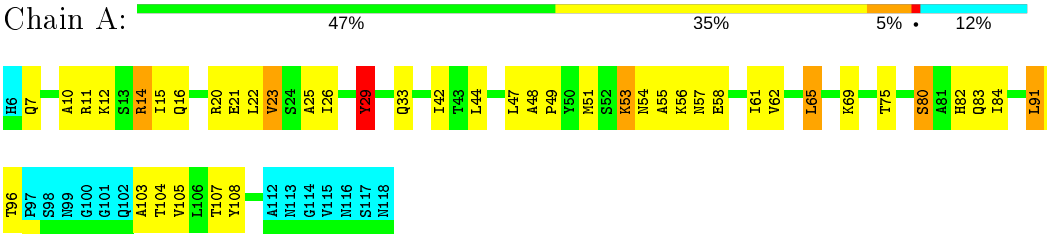
Chain A:



### 4.2.10 Score per residue for model 10

- Molecule 1: Type IV pilin PilE1

Chain A:



# 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

Of the 100 calculated structures, 10 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 | |
| ARIA | structure calculation | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

| Chemical shift file(s) | input_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1272 |
| Number of shifts mapped to atoms | 1272 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 89% |

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

## 5.1 Too-close contacts

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 | 754 | 736 | 733 | 41±3 |
| All | All | 7540 | 7360 | 7330 | 414 |

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 28.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:44:LEU:HD13 | 1:A:65:LEU:HD13 | 1.01 | 1.32 | 10 | 7 |
| 1:A:11:ARG:HB2 | 1:A:104:THR:HG21 | 0.94 | 1.39 | 2 | 7 |
| 1:A:44:LEU:HD11 | 1:A:82:HIS:HB2 | 0.85 | 1.48 | 2 | 10 |
| 1:A:12:LYS:O | 1:A:16:GLN:HB2 | 0.80 | 1.75 | 9 | 10 |
| 1:A:25:ALA:HB2 | 1:A:51:MET:SD | 0.71 | 2.24 | 7 | 8 |
| 1:A:83:GLN:O | 1:A:92:ILE:HB | 0.71 | 1.86 | 2 | 10 |
| 1:A:93:SER:O | 1:A:105:VAL:HA | 0.67 | 1.90 | 3 | 9 |
| 1:A:44:LEU:HD13 | 1:A:65:LEU:CD1 | 0.66 | 2.21 | 1 | 10 |
| 1:A:11:ARG:CB | 1:A:104:THR:HG21 | 0.64 | 2.22 | 10 | 5 |
| 1:A:53:LYS:O | 1:A:53:LYS:HD3 | 0.62 | 1.93 | 2 | 1 |
| 1:A:53:LYS:HD3 | 1:A:53:LYS:O | 0.62 | 1.94 | 4 | 1 |
| 1:A:61:ILE:HG23 | 1:A:62:VAL:HG23 | 0.62 | 1.69 | 1 | 9 |
| 1:A:91:LEU:O | 1:A:107:THR:HA | 0.62 | 1.93 | 4 | 10 |
| 1:A:75:THR:HG21 | 1:A:80:SER:O | 0.61 | 1.95 | 9 | 4 |
| 1:A:41:GLU:HA | 1:A:86:THR:HG21 | 0.61 | 1.73 | 8 | 2 |
| 1:A:47:LEU:O | 1:A:51:MET:HG2 | 0.59 | 1.96 | 8 | 10 |
| 1:A:44:LEU:HD13 | 1:A:65:LEU:HD12 | 0.58 | 1.72 | 7 | 5 |
| 1:A:22:LEU:HD21 | 1:A:65:LEU:HD21 | 0.57 | 1.75 | 10 | 1 |
| 1:A:53:LYS:HD3 | 1:A:54:ASN:N | 0.57 | 2.14 | 6 | 1 |
| 1:A:44:LEU:HD12 | 1:A:80:SER:HB3 | 0.56 | 1.77 | 10 | 5 |
| 1:A:44:LEU:HD21 | 1:A:82:HIS:HB3 | 0.56 | 1.78 | 10 | 2 |
| 1:A:11:ARG:HD2 | 1:A:12:LYS:N | 0.56 | 2.15 | 5 | 4 |
| 1:A:91:LEU:HB3 | 1:A:108:TYR:HB3 | 0.56 | 1.77 | 7 | 3 |
| 1:A:23:VAL:HB | 1:A:108:TYR:CD1 | 0.56 | 2.36 | 2 | 9 |
| 1:A:61:ILE:HD11 | 1:A:65:LEU:HD11 | 0.55 | 1.78 | 8 | 9 |
| 1:A:61:ILE:O | 1:A:65:LEU:HG | 0.55 | 2.00 | 5 | 2 |
| 1:A:57:ASN:O | 1:A:61:ILE:HG22 | 0.55 | 2.02 | 8 | 10 |
| 1:A:44:LEU:HD21 | 1:A:82:HIS:CB | 0.55 | 2.32 | 9 | 7 |
| 1:A:22:LEU:CD1 | 1:A:44:LEU:HD22 | 0.54 | 2.33 | 4 | 10 |
| 1:A:22:LEU:HD11 | 1:A:65:LEU:HD11 | 0.53 | 1.80 | 1 | 4 |
| 1:A:11:ARG:HA | 1:A:14:ARG:CG | 0.53 | 2.34 | 10 | 3 |
| 1:A:81:ALA:HA | 1:A:94:THR:O | 0.53 | 2.04 | 9 | 4 |
| 1:A:11:ARG:HD3 | 1:A:104:THR:CG2 | 0.53 | 2.34 | 5 | 3 |
| 1:A:51:MET:HB2 | 1:A:55:ALA:HB3 | 0.53 | 1.80 | 8 | 4 |
| 1:A:48:ALA:HB3 | 1:A:49:PRO:HD3 | 0.53 | 1.81 | 8 | 10 |
| 1:A:7:GLN:HA | 1:A:10:ALA:HB3 | 0.53 | 1.80 | 1 | 7 |
| 1:A:53:LYS:O | 1:A:55:ALA:N | 0.52 | 2.42 | 4 | 2 |
| 1:A:11:ARG:HD3 | 1:A:104:THR:OG1 | 0.52 | 2.05 | 2 | 2 |
| 1:A:48:ALA:HB2 | 1:A:61:ILE:HG21 | 0.52 | 1.82 | 2 | 6 |
| 1:A:42:ILE:HG22 | 1:A:84:ILE:HD13 | 0.51 | 1.83 | 1 | 9 |
| 1:A:68:ASP:OD1 | 1:A:96:THR:HB | 0.51 | 2.05 | 9 | 1 |
| 1:A:18:GLU:HB3 | 1:A:65:LEU:CD2 | 0.51 | 2.35 | 9 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:44:LEU:HD12 | 1:A:80:SER:CB | 0.51 | 2.36 | 8 | 5 |
| 1:A:25:ALA:CB | 1:A:51:MET:SD | 0.50 | 2.98 | 6 | 6 |
| 1:A:11:ARG:HB3 | 1:A:104:THR:HG21 | 0.50 | 1.83 | 7 | 3 |
| 1:A:41:GLU:HA | 1:A:86:THR:CG2 | 0.50 | 2.36 | 8 | 1 |
| 1:A:15:ILE:HG21 | 1:A:93:SER:CB | 0.50 | 2.37 | 7 | 3 |
| 1:A:18:GLU:HB3 | 1:A:65:LEU:HD22 | 0.50 | 1.82 | 5 | 4 |
| 1:A:22:LEU:HD21 | 1:A:65:LEU:HD22 | 0.50 | 1.83 | 5 | 3 |
| 1:A:75:THR:O | 1:A:83:GLN:HB2 | 0.50 | 2.06 | 8 | 3 |
| 1:A:53:LYS:HB2 | 1:A:53:LYS:NZ | 0.49 | 2.23 | 6 | 1 |
| 1:A:22:LEU:HD13 | 1:A:51:MET:SD | 0.49 | 2.46 | 4 | 3 |
| 1:A:7:GLN:HG2 | 1:A:95:PHE:CZ | 0.49 | 2.42 | 2 | 2 |
| 1:A:26:ILE:HG23 | 1:A:30:ILE:CD1 | 0.49 | 2.37 | 5 | 4 |
| 1:A:21:GLU:CB | 1:A:53:LYS:HZ3 | 0.49 | 2.21 | 10 | 1 |
| 1:A:76:SER:HB3 | 1:A:83:GLN:NE2 | 0.49 | 2.22 | 3 | 1 |
| 1:A:21:GLU:HB3 | 1:A:51:MET:HE3 | 0.48 | 1.86 | 5 | 2 |
| 1:A:55:ALA:HA | 1:A:60:GLY:O | 0.48 | 2.06 | 2 | 1 |
| 1:A:44:LEU:HB2 | 1:A:62:VAL:HG22 | 0.48 | 1.86 | 5 | 4 |
| 1:A:95:PHE:HB3 | 1:A:104:THR:HB | 0.48 | 1.85 | 1 | 10 |
| 1:A:23:VAL:HA | 1:A:91:LEU:HD23 | 0.48 | 1.84 | 5 | 6 |
| 1:A:11:ARG:HD3 | 1:A:104:THR:HG23 | 0.48 | 1.86 | 9 | 1 |
| 1:A:61:ILE:HG23 | 1:A:62:VAL:H | 0.47 | 1.69 | 10 | 5 |
| 1:A:53:LYS:HD3 | 1:A:54:ASN:H | 0.47 | 1.69 | 6 | 1 |
| 1:A:67:LYS:HD2 | 1:A:79:GLY:O | 0.47 | 2.09 | 8 | 3 |
| 1:A:61:ILE:HG23 | 1:A:62:VAL:N | 0.47 | 2.25 | 3 | 10 |
| 1:A:30:ILE:HG23 | 1:A:39:PRO:HG3 | 0.47 | 1.87 | 7 | 3 |
| 1:A:55:ALA:HB1 | 1:A:61:ILE:HB | 0.46 | 1.88 | 4 | 1 |
| 1:A:29:TYR:C | 1:A:29:TYR:CD2 | 0.46 | 2.89 | 2 | 3 |
| 1:A:7:GLN:O | 1:A:11:ARG:HG3 | 0.46 | 2.11 | 3 | 2 |
| 1:A:21:GLU:OE1 | 1:A:53:LYS:HB2 | 0.46 | 2.10 | 9 | 1 |
| 1:A:67:LYS:HE2 | 1:A:79:GLY:O | 0.46 | 2.11 | 1 | 1 |
| 1:A:7:GLN:HG2 | 1:A:11:ARG:HG3 | 0.45 | 1.87 | 7 | 1 |
| 1:A:44:LEU:HD21 | 1:A:82:HIS:HB2 | 0.45 | 1.87 | 8 | 4 |
| 1:A:10:ALA:O | 1:A:14:ARG:HG2 | 0.45 | 2.10 | 8 | 2 |
| 1:A:36:PRO:O | 1:A:110:TRP:HZ2 | 0.45 | 1.95 | 8 | 4 |
| 1:A:21:GLU:OE1 | 1:A:53:LYS:HB3 | 0.45 | 2.12 | 3 | 1 |
| 1:A:82:HIS:HA | 1:A:93:SER:HA | 0.45 | 1.89 | 10 | 5 |
| 1:A:61:ILE:CD1 | 1:A:65:LEU:HD11 | 0.44 | 2.42 | 5 | 1 |
| 1:A:18:GLU:O | 1:A:22:LEU:HD22 | 0.44 | 2.13 | 9 | 2 |
| 1:A:19:HIS:O | 1:A:23:VAL:HG13 | 0.44 | 2.12 | 2 | 2 |
| 1:A:21:GLU:CG | 1:A:53:LYS:HG2 | 0.44 | 2.42 | 6 | 1 |
| 1:A:18:GLU:HA | 1:A:21:GLU:CG | 0.44 | 2.43 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:83:GLN:HG2 | 1:A:94:THR:OG1 | 0.44 | 2.13 | 6 | 1 |
| 1:A:44:LEU:CB | 1:A:62:VAL:HG22 | 0.44 | 2.43 | 7 | 1 |
| 1:A:62:VAL:HG13 | 1:A:80:SER:HB2 | 0.43 | 1.90 | 2 | 2 |
| 1:A:26:ILE:HD11 | 1:A:84:ILE:HG12 | 0.43 | 1.90 | 9 | 2 |
| 1:A:26:ILE:HD12 | 1:A:91:LEU:CD2 | 0.43 | 2.44 | 9 | 1 |
| 1:A:91:LEU:C | 1:A:91:LEU:HD12 | 0.43 | 2.34 | 10 | 1 |
| 1:A:51:MET:CB | 1:A:55:ALA:HB3 | 0.43 | 2.43 | 4 | 1 |
| 1:A:29:TYR:HA | 1:A:50:TYR:CE1 | 0.43 | 2.49 | 8 | 1 |
| 1:A:92:ILE:HG23 | 1:A:105:VAL:HG13 | 0.43 | 1.90 | 1 | 1 |
| 1:A:7:GLN:HG2 | 1:A:95:PHE:CE2 | 0.43 | 2.49 | 4 | 1 |
| 1:A:44:LEU:HG | 1:A:77:ALA:HB2 | 0.43 | 1.91 | 4 | 2 |
| 1:A:26:ILE:HG23 | 1:A:30:ILE:HD12 | 0.42 | 1.89 | 5 | 3 |
| 1:A:84:ILE:HG23 | 1:A:90:LYS:O | 0.42 | 2.14 | 9 | 1 |
| 1:A:67:LYS:HE2 | 1:A:79:GLY:C | 0.42 | 2.35 | 3 | 1 |
| 1:A:58:GLU:HA | 1:A:61:ILE:CG2 | 0.42 | 2.43 | 3 | 1 |
| 1:A:28:SER:HB3 | 1:A:50:TYR:HB3 | 0.42 | 1.91 | 3 | 1 |
| 1:A:83:GLN:HE21 | 1:A:83:GLN:HA | 0.42 | 1.74 | 1 | 1 |
| 1:A:14:ARG:HG3 | 1:A:15:ILE:N | 0.42 | 2.30 | 8 | 2 |
| 1:A:30:ILE:HG12 | 1:A:39:PRO:HG3 | 0.42 | 1.90 | 4 | 3 |
| 1:A:67:LYS:HA | 1:A:80:SER:HA | 0.42 | 1.92 | 8 | 2 |
| 1:A:75:THR:HA | 1:A:83:GLN:HB2 | 0.42 | 1.92 | 10 | 1 |
| 1:A:68:ASP:HB2 | 1:A:96:THR:H | 0.42 | 1.74 | 9 | 2 |
| 1:A:29:TYR:CE1 | 1:A:42:ILE:HG12 | 0.41 | 2.49 | 5 | 1 |
| 1:A:91:LEU:HD12 | 1:A:91:LEU:C | 0.41 | 2.36 | 6 | 1 |
| 1:A:11:ARG:HD2 | 1:A:104:THR:OG1 | 0.41 | 2.16 | 6 | 1 |
| 1:A:91:LEU:C | 1:A:91:LEU:CD1 | 0.41 | 2.88 | 9 | 1 |
| 1:A:46:LYS:O | 1:A:49:PRO:HD2 | 0.41 | 2.15 | 2 | 1 |
| 1:A:23:VAL:HG12 | 1:A:91:LEU:HG | 0.41 | 1.93 | 2 | 2 |
| 1:A:15:ILE:HD11 | 1:A:95:PHE:HB2 | 0.41 | 1.92 | 3 | 1 |
| 1:A:91:LEU:CD1 | 1:A:91:LEU:C | 0.41 | 2.89 | 3 | 1 |
| 1:A:49:PRO:HG2 | 1:A:50:TYR:CD2 | 0.41 | 2.49 | 8 | 1 |
| 1:A:85:ASP:HB2 | 1:A:92:ILE:HD13 | 0.41 | 1.91 | 8 | 2 |
| 1:A:29:TYR:HE2 | 1:A:33:GLN:NE2 | 0.41 | 2.14 | 10 | 1 |
| 1:A:95:PHE:O | 1:A:103:ALA:HA | 0.41 | 2.16 | 3 | 4 |
| 1:A:51:MET:HG3 | 1:A:61:ILE:CD1 | 0.41 | 2.45 | 3 | 1 |
| 1:A:33:GLN:HG3 | 1:A:39:PRO:HB3 | 0.41 | 1.92 | 9 | 1 |
| 1:A:18:GLU:OE2 | 1:A:65:LEU:HD23 | 0.40 | 2.16 | 8 | 1 |
| 1:A:11:ARG:CG | 1:A:12:LYS:N | 0.40 | 2.84 | 6 | 1 |
| 1:A:12:LYS:HA | 1:A:106:LEU:HD21 | 0.40 | 1.93 | 7 | 1 |
| 1:A:58:GLU:HA | 1:A:61:ILE:HG22 | 0.40 | 1.92 | 3 | 1 |

## 5.2 Torsion angles

### 5.2.1 Protein backbone

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 | 99/113 (88%) | 89±2 (90±2%) | 9±2 (9±2%) | 2±1 (2±1%) | 14 59 |
| All | All | 990/1130 (88%) | 889 (90%) | 86 (9%) | 15 (2%) | 14 59 |

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 | 54 | ASN | 7 |
| 1 | A | 56 | LYS | 5 |
| 1 | A | 78 | PRO | 2 |
| 1 | A | 74 | SER | 1 |

### 5.2.2 Protein sidechains

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 | 85/95 (89%) | 73±2 (86±2%) | 12±2 (14±2%) | 6 46 |
| All | All | 850/950 (89%) | 730 (86%) | 120 (14%) | 6 46 |

All 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 58 | GLU | 10 |
| 1 | A | 91 | LEU | 10 |
| 1 | A | 29 | TYR | 10 |
| 1 | A | 23 | VAL | 9 |
| 1 | A | 14 | ARG | 8 |
| 1 | A | 53 | LYS | 8 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 26 | ILE | 8 |
| 1 | A | 80 | SER | 8 |
| 1 | A | 104 | THR | 6 |
| 1 | A | 16 | GLN | 6 |
| 1 | A | 96 | THR | 5 |
| 1 | A | 69 | LYS | 4 |
| 1 | A | 35 | ASP | 4 |
| 1 | A | 33 | GLN | 3 |
| 1 | A | 68 | ASP | 3 |
| 1 | A | 20 | ARG | 3 |
| 1 | A | 11 | ARG | 2 |
| 1 | A | 37 | THR | 2 |
| 1 | A | 56 | LYS | 2 |
| 1 | A | 83 | GLN | 1 |
| 1 | A | 88 | ASN | 1 |
| 1 | A | 12 | LYS | 1 |
| 1 | A | 65 | LEU | 1 |
| 1 | A | 40 | SER | 1 |
| 1 | A | 89 | HIS | 1 |
| 1 | A | 52 | SER | 1 |
| 1 | A | 108 | TYR | 1 |
| 1 | A | 54 | ASN | 1 |

### 5.2.3 RNA

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains

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

## 5.4 Carbohydrates

There are no carbohydrates in this entry.

## 5.5 Ligand geometry

There are no ligands in this entry.

## 5.6 Other polymers

There are no such molecules in this entry.

## 5.7 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

## 6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *2241_shifts_4*

### 6.1.1 Bookkeeping

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 | 1272 |
| Number of shifts mapped to atoms | 1272 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 2 |

### 6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 113 | -0.51 ± 0.25 | Should be applied |
| $^{13}C_{\beta}$ | 106 | 0.22 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 111 | -0.09 ± 0.27 | None needed (< 0.5 ppm) |
| $^{15}N$ | 106 | -0.33 ± 0.30 | None needed (< 0.5 ppm) |

### 6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1033 atoms were assigned a chemical shift out of a possible 1157. 1 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 483/487 (99%) | 193/194 (99%) | 196/198 (99%) | 94/95 (99%) |
| Sidechain | 490/601 (82%) | 304/352 (86%) | 186/221 (84%) | 0/28 (0%) |

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| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 60/69 (87%) | 33/35 (94%) | 26/27 (96%) | 1/7 (14%) |
| Overall | 1033/1157 (89%) | 530/581 (91%) | 408/446 (91%) | 95/130 (73%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1147 atoms were assigned a chemical shift out of a possible 1297. 1 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 549/555 (99%) | 219/221 (99%) | 224/226 (99%) | 106/108 (98%) |
| Sidechain | 534/665 (80%) | 332/390 (85%) | 202/242 (83%) | 0/33 (0%) |
| Aromatic | 64/77 (83%) | 37/39 (95%) | 26/29 (90%) | 1/9 (11%) |
| Overall | 1147/1297 (88%) | 588/650 (90%) | 452/497 (91%) | 107/150 (71%) |

### 6.1.4 Statistically unusual chemical shifts (i)

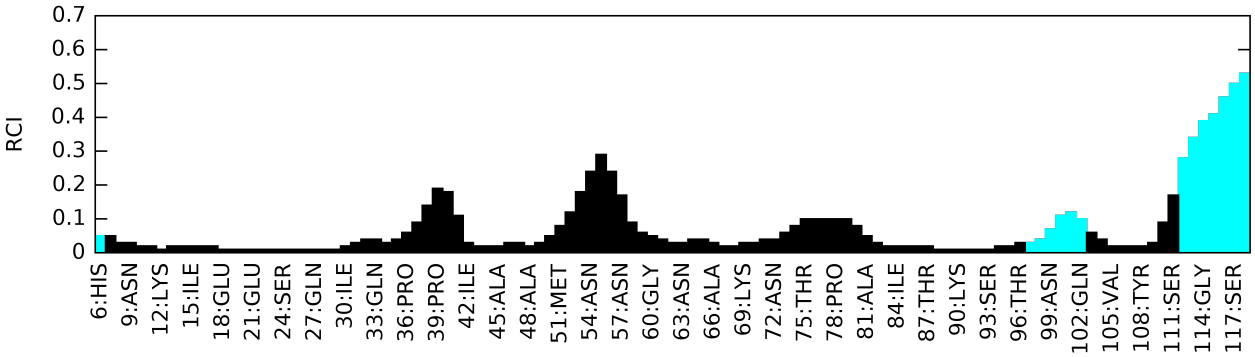
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 110 | TRP | CZ2 | 102.99 | 121.76 – 106.66 | -7.4 |
| 1 | A | 12 | LYS | HB3 | -0.15 | 3.10 – 0.40 | -7.0 |

### 6.1.5 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.

Random coil index (RCI) for chain A:


RCI
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
6:HIS
9:ASN
12:LYS
15:ILE
18:GLU
21:GLU
24:SER
27:GLN
30:ILE
33:GLN
36:PRO
39:PRO
42:ILE
45:ALA
48:ALA
51:MET
54:ASN
57:ASN
60:GLY
63:ASN
66:ALA
69:LYS
72:ASN
75:THR
78:PRO
81:ALA
84:ILE
87:THR
90:LYS
93:SER
96:THR
99:ASN
102:GLN
105:VAL
108:TYR
111:SER
114:GLY
117:SER