Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	4D4W
BMRB ID	:	25312
Title	:	Solution structure of human MBD1 CXXC1 domain
Authors	:	Thomson, R.; Smith, B.O.
Deposited on	:	2014-10-31

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:

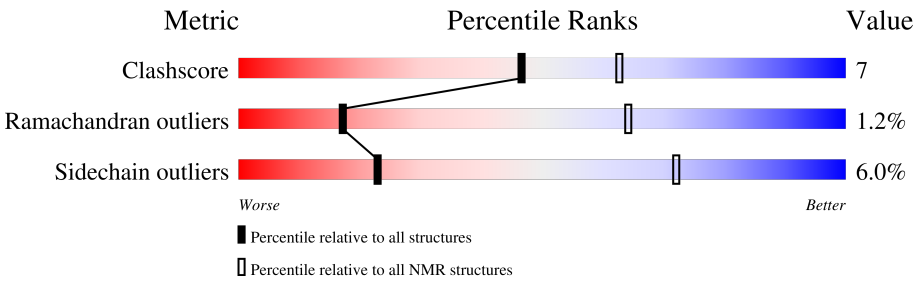
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 57%.

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	61	43% 8% 49%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 2 is the overall representative, medoid model (most similar to other models).

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:15-A:35, A:48-A:57 (31)	0.76	2

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

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

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 7, 8, 9, 10, 11, 12, 15, 16, 18, 24
2	6, 20, 25
3	14, 23
4	17, 21
Single-model clusters	4; 13; 19; 22

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 910 atoms, of which 452 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called METHYL-CPG-BINDING DOMAIN PROTEIN 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	61	910	274	452	89	85	10	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9UIS9
A	2	PRO	-	expression tag	UNP Q9UIS9
A	3	LEU	-	expression tag	UNP Q9UIS9
A	4	GLY	-	expression tag	UNP Q9UIS9
A	5	SER	-	expression tag	UNP Q9UIS9

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: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 43% 8% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 V58 E59 R60 S61

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: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 39% 10% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C30 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 I57 V58 E59 R60 S61

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 8% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R51 R52 V58 E59 R60 S61

4.2.3 Score per residue for model 3

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 38% 11% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 I57 V58 E59 R60 S61

4.2.4 Score per residue for model 4

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 48% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C15 C27 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 V58 E59 R60 S61

4.2.5 Score per residue for model 5

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 39% 11% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 V58 E59 R60 S61

4.2.6 Score per residue for model 6

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 44% 7% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C15 A19 V23 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 V58 E59 R60 S61

4.2.7 Score per residue for model 7

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 43% 7% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 V58 E59 R60 S61

4.2.8 Score per residue for model 8

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 8% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 I57 V58 E59 R60 S61

4.2.9 Score per residue for model 9

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 36% 13% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 D26 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 V58 E59 R60 S61

4.2.10 Score per residue for model 10

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 39% 11% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C27 C30 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 V58 E59 R60 S61

4.2.11 Score per residue for model 11

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 36% 13% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 V58 E59 R60 S61

4.2.12 Score per residue for model 12

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 46% 5% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 V58 E59 R60 S61

4.2.13 Score per residue for model 13

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 8% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 T24 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 R52 I57 V58 E59 R60 S61

4.2.14 Score per residue for model 14

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 43% 8% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 Q22 T32 C33 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 I57 V58 E59 R60 S61

4.2.15 Score per residue for model 15

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 38% 11% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 E50 R51 R52 V58 E59 R60 S61

4.2.16 Score per residue for model 16

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 8% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 G28 A29 C30 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 V58 E59 R60 S61

4.2.17 Score per residue for model 17

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 10% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C27 T32 C33 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 E50 R51 R52 V58 E59 R60 S61

4.2.18 Score per residue for model 18

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 39% 10% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 D26 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 V58 E59 R60 S61

4.2.19 Score per residue for model 19

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 39% 8% • 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 D26 C27 C33 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 V58 E59 R60 S61

4.2.20 Score per residue for model 20

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 38% 13% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 G28 A29 C30 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 K48 C49 R52 V58 E59 R60 S61

4.2.21 Score per residue for model 21

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 38% 13% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 C15 G16 A19 V23 C27 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 R53 C54 I57 V58 E59 R60 S61

4.2.22 Score per residue for model 22

• Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

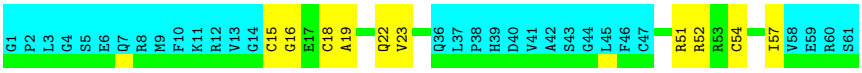
Chain A: 39% 11% 49%

G1 P2 L3 G4 S5 E6 Q7 R8 M9 F10 K11 R12 V13 G14 A19 V23 C30 S31 T32 C33 L34 L35 Q36 L37 P38 H39 D40 V41 A42 S43 G44 L45 F46 C47 R52 I57 V58 E59 R60 S61

4.2.23 Score per residue for model 23

- Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

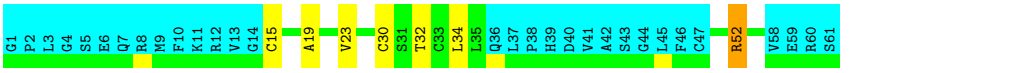
Chain A: 34% 16% 49%



4.2.24 Score per residue for model 24

- Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

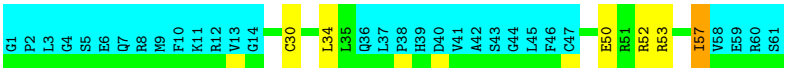
Chain A: 39% 10% • 49%



4.2.25 Score per residue for model 25

- Molecule 1: METHYL-CPG-BINDING DOMAIN PROTEIN 1

Chain A: 41% 8% • 49%



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 25 were deposited, based on the following criterion: *NOE ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
TopSpin	structure solution	1.3
CNS	structure solution	1.2
CcpNmr Analysis	structure solution	2.4
CcpNmr Analysis	structure solution	2.1
CcpNmr Analysis	structure solution	2.2
CcpNmr Analysis	structure solution	1.0
ARIA	structure solution	2.3

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	434
Number of shifts mapped to atoms	428
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	57%

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	227	220	228	3±1
All	All	5675	5500	5700	74

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:HA	1:A:52:ARG:NE	0.59	2.12	2	12
1:A:19:ALA:O	1:A:23:VAL:HG23	0.57	1.99	22	19
1:A:30:CYS:O	1:A:34:LEU:HD13	0.54	2.03	15	17
1:A:15:CYS:SG	1:A:16:GLY:N	0.47	2.86	21	1
1:A:33:CYS:HB3	1:A:49:CYS:HB2	0.45	1.88	14	4
1:A:28:GLY:C	1:A:34:LEU:HD11	0.45	2.32	16	2
1:A:33:CYS:HB3	1:A:49:CYS:HA	0.45	1.89	11	6
1:A:23:VAL:HG11	1:A:52:ARG:NH1	0.44	2.28	22	1
1:A:33:CYS:HB3	1:A:49:CYS:CA	0.43	2.44	1	3
1:A:31:SER:O	1:A:35:LEU:HG	0.42	2.14	11	1
1:A:57:ILE:O	1:A:57:ILE:HG22	0.41	2.15	14	1
1:A:26:ASP:HB2	1:A:49:CYS:CB	0.41	2.45	19	1
1:A:54:CYS:SG	1:A:57:ILE:HA	0.41	2.55	23	2
1:A:18:CYS:O	1:A:22:GLN:HG3	0.41	2.16	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:CYS:HB3	1:A:50:GLU:OE2	0.41	2.16	15	1
1:A:49:CYS:SG	1:A:51:ARG:HB2	0.40	2.55	17	1
1:A:50:GLU:O	1:A:53:ARG:HG2	0.40	2.17	25	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	31/61 (51%)	28±1 (89±4%)	3±1 (10±5%)	0±1 (1±2%)	17	64
All	All	775/1525 (51%)	690 (89%)	76 (10%)	9 (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	57	ILE	6
1	A	24	THR	1
1	A	16	GLY	1
1	A	15	CYS	1

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	26/51 (51%)	24±1 (94±3%)	2±1 (6±3%)	23	72
All	All	650/1275 (51%)	611 (94%)	39 (6%)	23	72

All 7 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	52	ARG	18
1	A	32	THR	8
1	A	27	CYS	5
1	A	26	ASP	3
1	A	51	ARG	2
1	A	15	CYS	2
1	A	33	CYS	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 57% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	434
Number of shifts mapped to atoms	428
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 24 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	GLN	HE21	7.596	0.007	1
1	A	7	GLN	HE22	6.89	0.01	1
1	A	7	GLN	NE2	112.915	0.055	1
1	A	10	PHE	HE2	7.302	.	3
1	A	31	SER	H	9.008	0.006	1
1	A	31	SER	N	114.871	0.087	1
1	A	34	LEU	H	8.031	0.006	1
1	A	34	LEU	HA	4.101	0.012	1
1	A	34	LEU	N	116.799	0.074	1
1	A	35	LEU	H	7.416	0.019	1
1	A	35	LEU	N	119.35	0.055	1
1	A	36	GLN	HE21	6.852	0.01	1
1	A	36	GLN	HE22	7.513	0.016	1
1	A	36	GLN	N	117.603	0.077	1
1	A	36	GLN	NE2	112.793	0.052	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	ALA	H	8.302	0.007	1
1	A	42	ALA	N	124.724	0.1	1
1	A	43	SER	H	7.966	0.014	1
1	A	43	SER	N	113.419	0.081	1
1	A	47	CYS	H	8.121	0.012	1
1	A	47	CYS	HA	4.395	0.01	1
1	A	47	CYS	N	120.279	0.074	1
1	A	57	ILE	H	7.537	0.017	1
1	A	57	ILE	N	121.062	0.156	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	21	CYO	H	8.541	.	1
1	?	21	CYO	N	120.995	.	1
1	?	33	CYO	H	8.935	0.003	1
1	?	33	CYO	N	126.406	0.003	1
1	?	49	CYO	H	8.599	.	1
1	?	49	CYO	N	126.077	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	57	-1.69 ± 0.56	Should be applied

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 57%, i.e. 221 atoms were assigned a chemical shift out of a possible 390. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	95/157 (61%)	64/64 (100%)	0/62 (0%)	31/31 (100%)
Sidechain	126/233 (54%)	123/150 (82%)	0/69 (0%)	3/14 (21%)
Overall	221/390 (57%)	187/214 (87%)	0/131 (0%)	34/45 (76%)

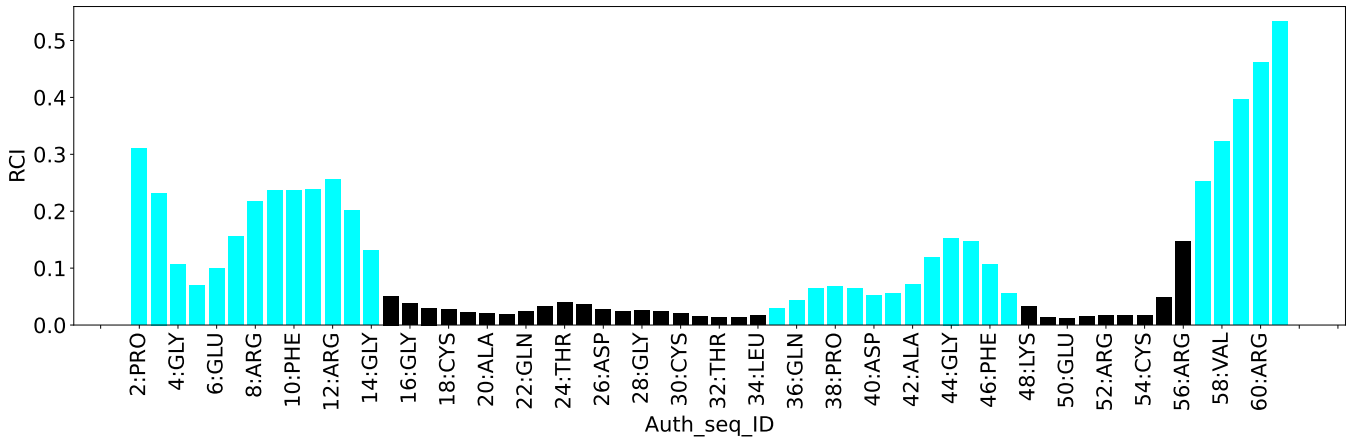
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 404 atoms were assigned a chemical shift out of a possible 795. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	177/307 (58%)	120/126 (95%)	0/122 (0%)	57/59 (97%)
Sidechain	222/460 (48%)	217/297 (73%)	0/137 (0%)	5/26 (19%)
Aromatic	5/28 (18%)	5/14 (36%)	0/12 (0%)	0/2 (0%)
Overall	404/795 (51%)	342/437 (78%)	0/271 (0%)	62/87 (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: