



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2K7B / pdb_00002k7b
BMRB ID : 15197
Title : NMR structure of Mg²⁺-bound CaBP1 N-domain
Authors : Ames, J.
Deposited on : 2008-08-08

This is a wwPDB NMR Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

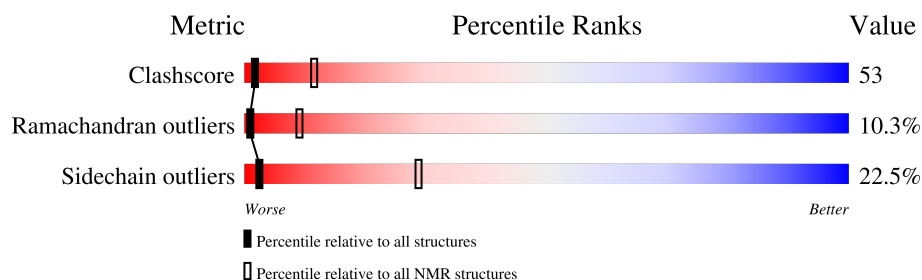
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	76	17% 62% 14% • 5%

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 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:20-A:91 (72)	1.27	13

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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1214 atoms, of which 592 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1213	384	592	105	124	8	

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

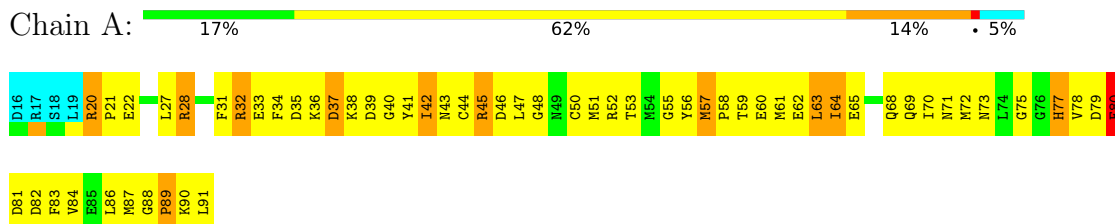
Mol	Chain	Residues	Atoms	
2	A	1	Total	Mg
			1	1

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.

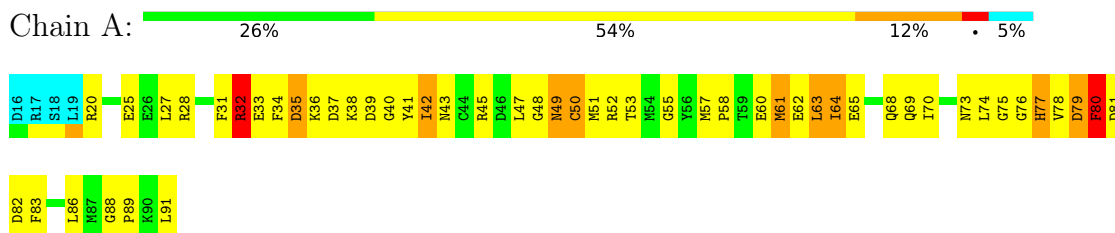
- Molecule 1: Calcium-binding protein 1



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Calcium-binding protein 1



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 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
X-PLOR	refinement	3.1

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	924
Number of shifts mapped to atoms	747
Number of unparsed shifts	0
Number of shifts with mapping errors	177
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.42±0.01	2±0/597 (0.3± 0.0%)	1.43±0.02	2±0/798 (0.3± 0.1%)
All	All	1.42	30/8955 (0.3%)	1.43	33/11970 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.5±0.6
All	All	0	67

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	77	HIS	CG-ND1	-12.05	1.25	1.38	14	15
1	A	77	HIS	ND1-CE1	-5.52	1.27	1.32	3	15

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	77	HIS	CE1-NE2-CD2	-7.55	101.45	109.00	14	15
1	A	80	PHE	CA-CB-CG	-6.67	107.13	113.80	11	15
1	A	56	TYR	CB-CA-C	-6.44	109.16	116.63	3	1
1	A	34	PHE	CA-CB-CG	-5.29	108.51	113.80	2	2

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	ARG	Sidechain	15
1	A	52	ARG	Sidechain	14
1	A	28	ARG	Sidechain	13
1	A	45	ARG	Sidechain	13
1	A	20	ARG	Sidechain	12

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	588	559	559	61±8
All	All	8835	8385	8385	910

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 53.

5 of 338 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:H	1:A:63:LEU:HD13	1.01	1.15	5	1
1:A:59:THR:HG22	1:A:60:GLU:H	0.88	1.28	8	3
1:A:59:THR:HG22	1:A:60:GLU:N	0.86	1.85	4	2
1:A:63:LEU:HD23	1:A:64:ILE:H	0.83	1.33	8	1
1:A:91:LEU:N	1:A:91:LEU:HD22	0.82	1.89	9	2

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	71/76 (93%)	51±2 (72±3%)	13±2 (18±3%)	7±2 (10±2%)	1	9
All	All	1065/1140 (93%)	762 (72%)	193 (18%)	110 (10%)	1	9

5 of 22 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	80	PHE	15
1	A	75	GLY	12
1	A	89	PRO	9
1	A	61	MET	8
1	A	58	PRO	8

6.3.2 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	65/69 (94%)	50±2 (78±3%)	15±2 (22±3%)	2	29
All	All	975/1035 (94%)	756 (78%)	219 (22%)	2	29

5 of 51 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	64	ILE	15
1	A	78	VAL	15
1	A	53	THR	13
1	A	42	ILE	10
1	A	20	ARG	9

6.3.3 RNA ⓘ

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 71% 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

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	924
Number of shifts mapped to atoms	747
Number of unparsed shifts	0
Number of shifts with mapping errors	177
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 177) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	LEU	H	8.31	0.04	1
1	A	12	LEU	HA	4.35	0.04	1
1	A	12	LEU	HB2	1.63	0.04	2
1	A	12	LEU	HD11	0.84	0.04	2
1	A	12	LEU	HD12	0.84	0.04	2
1	A	12	LEU	HD13	0.84	0.04	2
1	A	12	LEU	HD21	0.89	0.04	2
1	A	12	LEU	HD22	0.89	0.04	2
1	A	12	LEU	HD23	0.89	0.04	2
1	A	12	LEU	CA	55.83	0.2	1
1	A	12	LEU	CB	42.37	0.2	1
1	A	12	LEU	CG	26.71	0.2	1
1	A	12	LEU	CD1	23.54	0.2	1
1	A	12	LEU	CD2	25.32	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	LEU	N	122.66	0.2	1
1	A	13	SER	H	8.26	0.04	1
1	A	13	SER	HA	4.43	0.04	1
1	A	13	SER	HB2	3.87	0.04	2
1	A	13	SER	C	174.72	0.2	1
1	A	13	SER	CA	58.67	0.2	1
1	A	13	SER	CB	64.03	0.2	1
1	A	13	SER	N	115.72	0.2	1
1	A	14	ARG	H	8.22	0.04	1
1	A	14	ARG	HA	4.06	0.04	1
1	A	14	ARG	HB2	2.02	0.04	2
1	A	14	ARG	CA	56.4	0.2	1
1	A	14	ARG	CB	32.64	0.2	1
1	A	14	ARG	N	122.72	0.2	1
1	A	15	LYS	HA	4.29	0.04	1
1	A	15	LYS	HB2	1.76	0.04	2
1	A	15	LYS	HG2	1.42	0.04	2
1	A	15	LYS	HD2	1.68	0.04	2
1	A	15	LYS	HE2	3.01	0.04	2
1	A	15	LYS	C	176.14	0.2	1
1	A	15	LYS	CA	56.43	0.2	1
1	A	15	LYS	CB	32.91	0.2	1
1	A	15	LYS	CG	24.8	0.2	1
1	A	15	LYS	CD	29.02	0.2	1
1	A	15	LYS	CE	42.25	0.2	1
1	A	16	ASP	H	8.28	0.04	1
1	A	92	LEU	HG	1.6	0.04	1
1	A	92	LEU	C	177.44	0.2	1
1	A	93	ALA	H	7.44	0.04	1
1	A	93	ALA	HA	4.26	0.04	1
1	A	93	ALA	HB1	1.49	0.04	1
1	A	93	ALA	HB2	1.49	0.04	1
1	A	93	ALA	HB3	1.49	0.04	1
1	A	93	ALA	C	177.96	0.2	1
1	A	93	ALA	CA	53.17	0.2	1
1	A	93	ALA	CB	19.13	0.2	1
1	A	93	ALA	N	121.93	0.2	1
1	A	94	GLU	H	8.12	0.04	1
1	A	94	GLU	HA	4.4	0.04	1
1	A	94	GLU	HB2	2.37	0.04	2
1	A	94	GLU	HG2	2.36	0.04	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	GLU	C	176.9	0.2	1
1	A	94	GLU	CA	56.88	0.2	1
1	A	94	GLU	CB	30.45	0.2	1
1	A	94	GLU	CG	36.45	0.2	1
1	A	94	GLU	N	118.94	0.2	1
1	A	95	THR	H	8.02	0.04	1
1	A	95	THR	HA	4.4	0.04	1
1	A	95	THR	HB	4.33	0.04	1
1	A	95	THR	HG21	1.24	0.04	1
1	A	95	THR	HG22	1.24	0.04	1
1	A	95	THR	HG23	1.24	0.04	1
1	A	95	THR	C	174.65	0.2	1
1	A	95	THR	CA	62.08	0.2	1
1	A	95	THR	CB	69.99	0.2	1
1	A	95	THR	CG2	21.86	0.2	1
1	A	95	THR	N	113.59	0.2	1
1	A	97	ASP	H	8.29	0.04	1
1	A	97	ASP	HA	4.61	0.04	1
1	A	97	ASP	HB2	2.6	0.04	2
1	A	97	ASP	HB3	2.75	0.04	2
1	A	97	ASP	C	176.06	0.2	1
1	A	97	ASP	CA	54.86	0.2	1
1	A	97	ASP	CB	41.13	0.2	1
1	A	97	ASP	N	118.64	0.2	1
1	A	98	MET	H	8.11	0.04	1
1	A	98	MET	HA	4.49	0.04	1
1	A	98	MET	HB2	2.07	0.04	2
1	A	98	MET	HG2	2.61	0.04	2
1	A	98	MET	C	176.22	0.2	1
1	A	98	MET	CA	55.87	0.2	1
1	A	98	MET	CB	33.36	0.2	1
1	A	98	MET	CG	32.07	0.2	1
1	A	98	MET	N	119.8	0.2	1
1	A	99	ILE	H	8.21	0.04	1
1	A	99	ILE	HA	4.06	0.04	1
1	A	99	ILE	HB	1.82	0.04	1
1	A	99	ILE	HG12	1.56	0.04	1
1	A	99	ILE	HG13	1.17	0.04	1
1	A	99	ILE	HG21	0.96	0.04	1
1	A	99	ILE	HG22	0.96	0.04	1
1	A	99	ILE	HG23	0.96	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	ILE	HD11	0.84	0.04	1
1	A	99	ILE	HD12	0.84	0.04	1
1	A	99	ILE	HD13	0.84	0.04	1
1	A	99	ILE	C	176.02	0.2	1
1	A	99	ILE	CA	62.14	0.2	1
1	A	99	ILE	CB	38.57	0.2	1
1	A	99	ILE	CG1	27.77	0.2	1
1	A	99	ILE	CG2	17.98	0.2	1
1	A	99	ILE	CD1	13.45	0.2	1
1	A	99	ILE	N	122.28	0.2	1
1	A	100	GLY	H	8.61	0.04	1
1	A	100	GLY	HA2	4.0	0.04	2
1	A	100	GLY	HA3	4.27	0.04	2
1	A	100	GLY	C	174.55	0.2	1
1	A	100	GLY	CA	45.31	0.2	1
1	A	100	GLY	N	113.55	0.2	1
1	A	101	VAL	H	8.27	0.04	1
1	A	101	VAL	HA	3.86	0.04	1
1	A	101	VAL	HB	2.19	0.04	1
1	A	101	VAL	HG11	1.12	0.04	2
1	A	101	VAL	HG12	1.12	0.04	2
1	A	101	VAL	HG13	1.12	0.04	2
1	A	101	VAL	HG21	1.07	0.04	2
1	A	101	VAL	HG22	1.07	0.04	2
1	A	101	VAL	HG23	1.07	0.04	2
1	A	101	VAL	C	177.42	0.2	1
1	A	101	VAL	CA	66.17	0.2	1
1	A	101	VAL	CB	31.8	0.2	1
1	A	101	VAL	CG1	22.35	0.2	1
1	A	101	VAL	CG2	21.36	0.2	1
1	A	101	VAL	N	119.81	0.2	1
1	A	102	LYS	H	8.49	0.04	1
1	A	102	LYS	HB3	1.96	0.04	2
1	A	102	LYS	N	121.87	0.2	1
1	A	103	GLU	HB3	2.37	0.04	2
1	A	103	GLU	HG3	2.84	0.04	2
1	A	104	LEU	HB3	1.58	0.04	2
1	A	105	ARG	HG2	1.39	0.04	2
1	A	105	ARG	HD2	2.93	0.04	2
1	A	105	ARG	HD3	2.84	0.04	2
1	A	105	ARG	C	178.68	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	ARG	CG	27.23	0.2	1
1	A	105	ARG	CD	42.99	0.2	1
1	A	108	PHE	H	8.61	0.04	1
1	A	108	PHE	HA	3.54	0.04	1
1	A	108	PHE	HB2	3.19	0.04	2
1	A	108	PHE	HB3	3.04	0.04	2
1	A	108	PHE	HD1	7.09	0.04	3
1	A	108	PHE	HE1	7.42	0.04	3
1	A	108	PHE	C	177.02	0.2	1
1	A	108	PHE	CA	62.12	0.2	1
1	A	108	PHE	CB	40.21	0.2	1
1	A	108	PHE	N	118.51	0.2	1
1	A	114	ASN	H	7.81	0.04	1
1	A	114	ASN	HA	4.78	0.04	1
1	A	114	ASN	HB2	3.27	0.04	2
1	A	114	ASN	HB3	2.86	0.04	2
1	A	114	ASN	C	176.25	0.2	1
1	A	114	ASN	CA	51.54	0.2	1
1	A	114	ASN	CB	36.77	0.2	1
1	A	114	ASN	N	115.05	0.2	1
1	A	125	ARG	HG3	1.63	0.04	2
1	A	130	LYS	HD3	1.52	0.04	2
1	A	134	HIS	HA	4.61	0.04	1
1	A	134	HIS	HB2	3.16	0.04	2
1	A	134	HIS	HD2	7.008	0.04	1
1	A	134	HIS	C	175.7	0.2	1
1	A	134	HIS	CA	56.86	0.2	1
1	A	134	HIS	CB	30.29	0.2	1
1	A	135	GLN	H	8.09	0.04	1
1	A	135	GLN	HA	4.36	0.04	1
1	A	135	GLN	HB2	2.11	0.04	2
1	A	135	GLN	HB3	1.97	0.04	2
1	A	135	GLN	HG2	2.18	0.04	2
1	A	135	GLN	C	175.71	0.2	1
1	A	135	GLN	CA	56.48	0.2	1
1	A	135	GLN	CB	29.63	0.2	1
1	A	135	GLN	CG	33.7	0.2	1
1	A	135	GLN	N	119.42	0.2	1
1	A	138	HIS	HB3	3.34	0.04	2
1	A	164	MET	HB3	2.18	0.04	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	-0.42 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	0.11 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	84	-0.33 ± 0.13	None needed (< 0.5 ppm)
^{15}N	84	0.47 ± 0.37	None needed (< 0.5 ppm)

7.1.3 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 72%, i.e. 716 atoms were assigned a chemical shift out of a possible 996. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	340/360 (94%)	140/147 (95%)	134/144 (93%)	66/69 (96%)
Sidechain	359/571 (63%)	228/365 (62%)	131/182 (72%)	0/24 (0%)
Aromatic	17/65 (26%)	15/32 (47%)	2/32 (6%)	0/1 (0%)
Overall	716/996 (72%)	383/544 (70%)	267/358 (75%)	66/94 (70%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

