



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 7M2M / pdb_00007m2m
BMRB ID : 30888
Title : NMR Structure of GCAP5
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Deposited on : 2021-03-17

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

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

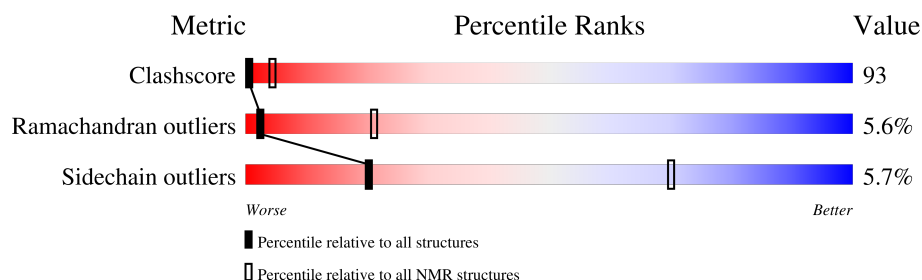
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

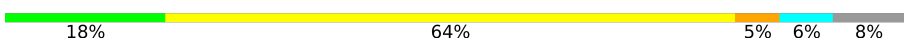
The overall completeness of chemical shifts assignment is 57%.

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	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	198	

2 Ensemble composition and analysis

This entry contains 9 models. Model 1 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:2-A:100, A:104-A:122, A:128-A:143, A:147-A:183 (171)	1.80	1

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 and 5 single-model clusters were found.

Cluster number	Models
1	2, 9
2	1, 6
Single-model clusters	3; 4; 5; 7; 8

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2873 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Guanylate cyclase activator 1A.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			2872	929	1420	223	288	12	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MYR	-	insertion	UNP Q5MAC8

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

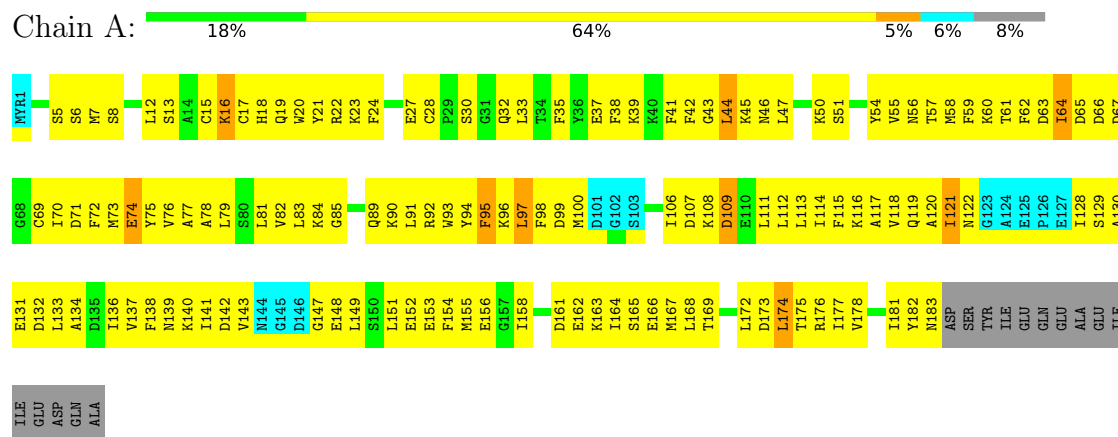
Mol	Chain	Residues	Atoms	
2	A	1	Total	Mg
			1	1

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.

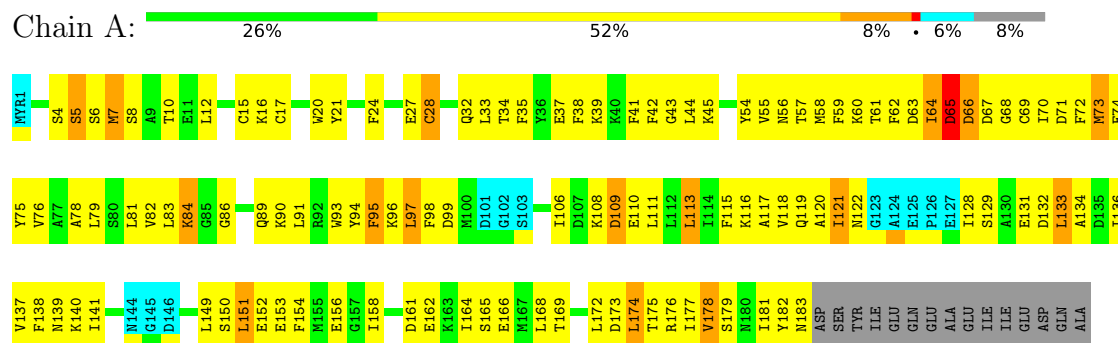
- Molecule 1: Guanylate cyclase activator 1A



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Guanylate cyclase activator 1A



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 50 calculated structures, 9 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure calculation	

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	1551
Number of shifts mapped to atoms	1384
Number of unparsed shifts	0
Number of shifts with mapping errors	167
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	57%

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, MYR

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	0.54±0.00	0±0/1389 (0.0± 0.0%)	1.02±0.01	1±1/1866 (0.1± 0.0%)
All	All	0.54	0/12501 (0.0%)	1.02	9/16794 (0.1%)

There are no bond-length outliers.

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	95	PHE	CA-CB-CG	-6.00	107.80	113.80	7	7
1	A	154	PHE	CA-CB-CG	-5.84	107.95	113.80	4	1
1	A	35	PHE	CA-CB-CG	-5.16	108.64	113.80	4	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	1365	1341	1340	252±28
All	All	12294	12069	12060	2268

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 93.

5 of 1697 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD11	1:A:164:ILE:HG22	1.12	1.14	3	1
1:A:121:ILE:HD13	1:A:122:ASN:N	1.09	1.61	7	5
1:A:133:LEU:HD22	1:A:167:MET:SD	1.09	1.87	7	1
1:A:115:PHE:CD1	1:A:130:ALA:HB3	1.08	1.84	6	1
1:A:118:VAL:O	1:A:121:ILE:HD12	1.06	1.48	7	5

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	169/198 (85%)	148±3 (88±2%)	11±3 (7±2%)	9±2 (6±1%)	2	21
All	All	1521/1782 (85%)	1335 (88%)	101 (7%)	85 (6%)	2	21

5 of 39 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	16	LYS	7
1	A	64	ILE	6
1	A	109	ASP	6
1	A	148	GLU	5
1	A	5	SER	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	152/172 (88%)	143±1 (94±1%)	9±1 (6±1%)	20	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1368/1548 (88%)	1290 (94%)	78 (6%)	20 70

5 of 42 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	121	ILE	8
1	A	174	LEU	7
1	A	44	LEU	6
1	A	97	LEU	5
1	A	74	GLU	3

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 57% for the well-defined parts and 57% 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	1551
Number of shifts mapped to atoms	1384
Number of unparsed shifts	0
Number of shifts with mapping errors	167
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 167) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	184	ASP	HA	4.559	0	1
1	A	184	ASP	HB2	2.675	0	1
1	A	184	ASP	HB3	2.675	0	1
1	A	184	ASP	C	176.37	0	1
1	A	184	ASP	CA	53.513	0.13	1
1	A	184	ASP	CB	39.884	0.03	1
1	A	185	SER	H	8.131	0.01	1
1	A	185	SER	HA	4.412	0.01	1
1	A	185	SER	HB2	3.822	0.01	1
1	A	185	SER	HB3	3.822	0.01	1
1	A	185	SER	C	174.185	0	1
1	A	185	SER	CA	57.564	0.03	1
1	A	185	SER	CB	62.77	0.06	1
1	A	185	SER	N	115.477	0.04	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	186	TYR	H	8.077	0.01	1
1	A	186	TYR	HA	4.516	0.05	1
1	A	186	TYR	HB2	3.006	0.01	1
1	A	186	TYR	HB3	3.006	0.01	1
1	A	186	TYR	C	175.449	0	1
1	A	186	TYR	CA	57.189	0.12	1
1	A	186	TYR	CB	37.449	0.04	1
1	A	186	TYR	N	122.551	0.04	1
1	A	187	ILE	H	7.788	0	1
1	A	187	ILE	HA	4.077	0.01	1
1	A	187	ILE	HB	1.771	0.03	1
1	A	187	ILE	HD11	0.846	0.01	1
1	A	187	ILE	HD12	0.846	0.01	1
1	A	187	ILE	HD13	0.846	0.01	1
1	A	187	ILE	HG12	1.42	0.01	2
1	A	187	ILE	HG13	1.094	0.07	2
1	A	187	ILE	HG21	0.858	0.01	1
1	A	187	ILE	HG22	0.858	0.01	1
1	A	187	ILE	HG23	0.858	0.01	1
1	A	187	ILE	C	175.727	0	1
1	A	187	ILE	CA	59.657	0.06	1
1	A	187	ILE	CB	37.813	0.12	1
1	A	187	ILE	CD1	11.67	0.07	1
1	A	187	ILE	CG1	26.056	0.04	1
1	A	187	ILE	CG2	16.21	0.03	1
1	A	187	ILE	N	123.641	0.04	1
1	A	188	GLU	H	8.318	0.01	1
1	A	188	GLU	HA	4.166	0.05	1
1	A	188	GLU	HB2	1.977	0.01	1
1	A	188	GLU	HB3	1.977	0.01	1
1	A	188	GLU	HG2	2.278	0.01	1
1	A	188	GLU	HG3	2.278	0.01	1
1	A	188	GLU	C	176.389	0	1
1	A	188	GLU	CA	55.599	0.04	1
1	A	188	GLU	CB	28.989	0.02	1
1	A	188	GLU	CG	35.103	0	1
1	A	188	GLU	N	125.353	0.04	1
1	A	189	GLN	H	8.311	0.01	1
1	A	189	GLN	HA	4.305	0.06	1
1	A	189	GLN	HB2	2.07	0	2
1	A	189	GLN	HB3	2.004	0.01	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	GLN	HG2	2.363	0.02	1
1	A	189	GLN	HG3	2.363	0.02	1
1	A	189	GLN	C	175.997	0	1
1	A	189	GLN	CA	54.753	0.07	1
1	A	189	GLN	CB	28.581	0.05	1
1	A	189	GLN	CG	32.608	0	1
1	A	189	GLN	N	122.091	0.05	1
1	A	190	GLU	H	8.457	0.02	1
1	A	190	GLU	HA	4.262	0.02	1
1	A	190	GLU	HB2	2.05	0.01	2
1	A	190	GLU	HB3	1.957	0	2
1	A	190	GLU	HG2	2.276	0	1
1	A	190	GLU	HG3	2.276	0	1
1	A	190	GLU	C	176.203	0	1
1	A	190	GLU	CA	55.537	0.03	1
1	A	190	GLU	CB	29.053	0.07	1
1	A	190	GLU	CG	35.102	0	1
1	A	190	GLU	N	122.845	0.04	1
1	A	191	ALA	H	8.255	0	1
1	A	191	ALA	HA	4.311	0.02	1
1	A	191	ALA	HB1	1.399	0.01	1
1	A	191	ALA	HB2	1.399	0.01	1
1	A	191	ALA	HB3	1.399	0.01	1
1	A	191	ALA	C	177.565	0	1
1	A	191	ALA	CA	51.35	0.14	1
1	A	191	ALA	CB	18.275	0.02	1
1	A	191	ALA	N	125.271	0.04	1
1	A	192	GLU	H	8.304	0.01	1
1	A	192	GLU	HA	4.276	0.01	1
1	A	192	GLU	HB2	1.962	0.01	1
1	A	192	GLU	HB3	1.962	0.01	1
1	A	192	GLU	HG2	2.25	0.01	1
1	A	192	GLU	HG3	2.25	0.01	1
1	A	192	GLU	C	176.284	0	1
1	A	192	GLU	CA	55.355	0.05	1
1	A	192	GLU	CB	29.231	0.01	1
1	A	192	GLU	CG	35.072	0	1
1	A	192	GLU	N	120.834	0.05	1
1	A	193	ILE	H	8.201	0	1
1	A	193	ILE	HA	4.191	0.03	1
1	A	193	ILE	HB	1.857	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	193	ILE	HD11	0.869	0	1
1	A	193	ILE	HD12	0.869	0	1
1	A	193	ILE	HD13	0.869	0	1
1	A	193	ILE	HG12	1.182	0.01	2
1	A	193	ILE	HG13	1.489	0.02	2
1	A	193	ILE	HG21	0.883	0	1
1	A	193	ILE	HG22	0.883	0	1
1	A	193	ILE	HG23	0.883	0	1
1	A	193	ILE	C	176.074	0	1
1	A	193	ILE	CA	59.815	0.03	1
1	A	193	ILE	CB	37.374	0.05	1
1	A	193	ILE	CD1	11.512	0.02	1
1	A	193	ILE	CG1	26.07	0	1
1	A	193	ILE	CG2	16.32	0.02	1
1	A	193	ILE	N	123.217	0.04	1
1	A	194	ILE	H	8.272	0.01	1
1	A	194	ILE	HA	4.19	0.01	1
1	A	194	ILE	HB	1.863	0.01	1
1	A	194	ILE	HD11	0.887	0.01	1
1	A	194	ILE	HD12	0.887	0.01	1
1	A	194	ILE	HD13	0.887	0.01	1
1	A	194	ILE	HG12	1.485	0.01	2
1	A	194	ILE	HG13	1.196	0.01	2
1	A	194	ILE	HG21	0.898	0.02	1
1	A	194	ILE	HG22	0.898	0.02	1
1	A	194	ILE	HG23	0.898	0.02	1
1	A	194	ILE	C	176.222	0	1
1	A	194	ILE	CA	59.67	0.04	1
1	A	194	ILE	CB	37.433	0.05	1
1	A	194	ILE	CD1	11.456	0	1
1	A	194	ILE	CG1	26.057	0.04	1
1	A	194	ILE	CG2	16.366	0.02	1
1	A	194	ILE	N	126.578	0.04	1
1	A	195	GLU	H	8.491	0.01	1
1	A	195	GLU	HA	4.305	0.01	1
1	A	195	GLU	HB2	2.019	0.02	2
1	A	195	GLU	HB3	1.958	0.01	2
1	A	195	GLU	HG2	2.281	0.02	1
1	A	195	GLU	HG3	2.281	0.02	1
1	A	195	GLU	C	176.114	0	1
1	A	195	GLU	CA	55.465	0.06	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	195	GLU	CB	29.279	0.1	1
1	A	195	GLU	CG	35.107	0.05	1
1	A	195	GLU	N	126.137	0.04	1
1	A	196	ASP	H	8.358	0	1
1	A	196	ASP	HA	4.582	0.01	1
1	A	196	ASP	HB2	2.663	0.01	1
1	A	196	ASP	HB3	2.663	0.01	1
1	A	196	ASP	C	176.106	0	1
1	A	196	ASP	CA	53.314	0.14	1
1	A	196	ASP	CB	39.988	0.02	1
1	A	196	ASP	N	122.064	0.04	1
1	A	197	GLN	H	8.269	0.01	1
1	A	197	GLN	HA	4.346	0.01	1
1	A	197	GLN	HB2	2.164	0.01	2
1	A	197	GLN	HB3	1.984	0.01	2
1	A	197	GLN	HG2	2.382	0.01	1
1	A	197	GLN	HG3	2.382	0.01	1
1	A	197	GLN	C	174.824	0	1
1	A	197	GLN	CA	54.553	0.03	1
1	A	197	GLN	CB	28.477	0.03	1
1	A	197	GLN	CG	32.64	0.02	1
1	A	197	GLN	N	121.194	0.04	1
1	A	198	ALA	H	7.994	0.01	1
1	A	198	ALA	HA	4.125	0.04	1
1	A	198	ALA	HB1	1.365	0.01	1
1	A	198	ALA	HB2	1.365	0.01	1
1	A	198	ALA	HB3	1.365	0.01	1
1	A	198	ALA	CA	52.815	0.02	1
1	A	198	ALA	CB	18.922	0.05	1
1	A	198	ALA	N	131.589	0.03	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	0.55 ± 0.10	Should be checked
$^{13}\text{C}_\beta$	164	1.40 ± 0.10	Should be checked
$^{13}\text{C}'$	156	-0.48 ± 0.08	None needed (< 0.5 ppm)
^{15}N	158	0.72 ± 0.25	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. 1329 atoms were assigned a chemical shift out of a possible 2326. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	696/862 (81%)	272/350 (78%)	287/342 (84%)	137/170 (81%)
Sidechain	629/1249 (50%)	417/812 (51%)	212/401 (53%)	0/36 (0%)
Aromatic	4/215 (2%)	2/105 (2%)	0/107 (0%)	2/3 (67%)
Overall	1329/2326 (57%)	691/1267 (55%)	499/850 (59%)	139/209 (67%)

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:

