



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:17 PM UTC

PDB ID : 2LVU / pdb_00002lvu
BMRB ID : 18586
Title : Solution structure of Miz-1 zinc finger 10
Authors : Bedard, M.; Maltais, L.; Beaulieu, M.; Bernard, D.; Lavigne, P.
Deposited on : 2012-07-11

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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
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

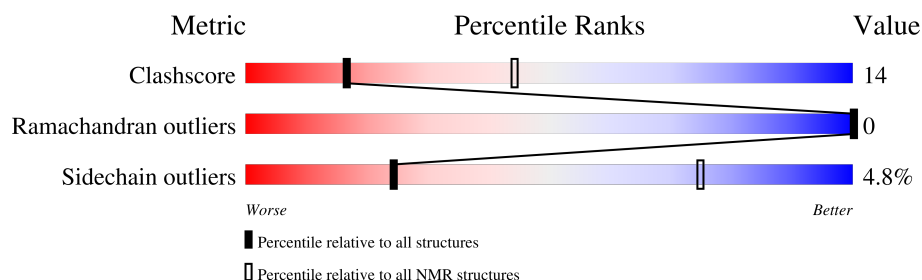
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	83	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:60-A:82 (23)	0.34	17

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. No single-model clusters were found.

Cluster number	Models
1	3, 6, 9, 11, 13, 15, 18
2	5, 8, 10, 12, 14, 17
3	4, 7, 19, 20
4	1, 2, 16

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 429 atoms, of which 210 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger and BTB domain-containing protein 17.

Mol	Chain	Residues	Atoms						Trace
1	A	26	Total	C	H	N	O	S	0
			428	133	210	46	37	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13105

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

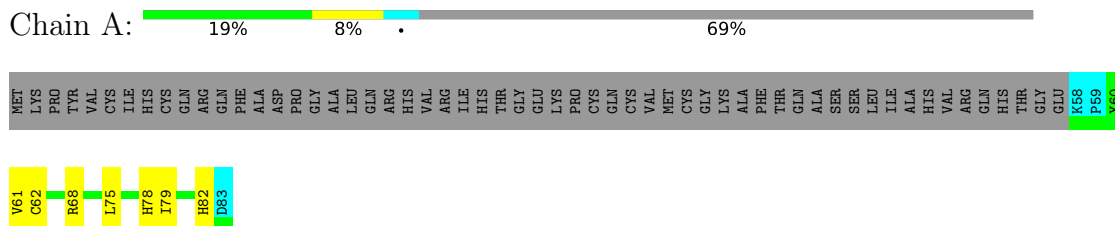
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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.

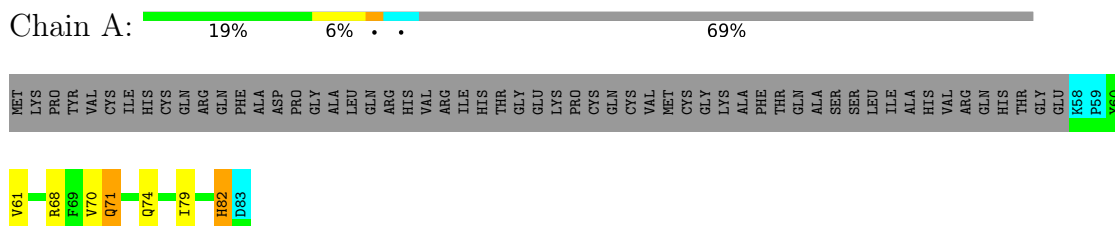
- Molecule 1: Zinc finger and BTB domain-containing protein 17



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

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Zinc finger and BTB domain-containing protein 17



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 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
ARIA	structure calculation	2.2
ARIA	refinement	2.2
CNS	structure calculation	1.21
CNS	refinement	1.21

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	877
Number of shifts mapped to atoms	283
Number of unparsed shifts	0
Number of shifts with mapping errors	594
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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: ZN

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	0.60±0.02	0±0/198 (0.0± 0.0%)	0.90±0.04	0±0/265 (0.0± 0.1%)
All	All	0.60	0/3960 (0.0%)	0.90	2/5300 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	VAL	N-CA-C	-5.37	108.27	113.53	13	2

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	193	186	185	5±2
All	All	3880	3720	3700	106

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 14.

5 of 34 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:TYR:HB3	1:A:75:LEU:HG	0.88	1.42	11	6
1:A:61:VAL:HG22	1:A:68:ARG:HG2	0.76	1.54	12	5
1:A:62:CYS:HA	1:A:79:ILE:HD11	0.73	1.61	9	8
1:A:62:CYS:SG	1:A:79:ILE:HG12	0.64	2.32	19	3
1:A:75:LEU:O	1:A:78:HIS:HB3	0.63	1.93	14	11

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	23/83 (28%)	22±1 (97±3%)	1±1 (3±3%)	0±0 (0±0%)	100	100
All	All	460/1660 (28%)	447 (97%)	13 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	21/72 (29%)	20±1 (95±5%)	1±1 (5±5%)	24	75
All	All	420/1440 (29%)	400 (95%)	20 (5%)	24	75

5 of 8 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	82	HIS	5
1	A	70	VAL	4
1	A	71	GLN	3
1	A	75	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	80	ARG	2

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 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 77% for the well-defined parts and 76% 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

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	877
Number of shifts mapped to atoms	283
Number of unparsed shifts	0
Number of shifts with mapping errors	594
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 594) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	PRO	HA	4.187	0.013	1
1	A	3	PRO	HB2	1.233	0.003	2
1	A	3	PRO	HB3	1.904	0.011	2
1	A	3	PRO	HD2	3.596	0.006	2
1	A	3	PRO	HD3	3.667	0.022	2
1	A	3	PRO	HG2	1.551	0.009	2
1	A	3	PRO	HG3	1.743	0.028	2
1	A	3	PRO	C	176.021	.	1
1	A	3	PRO	CA	63.467	0.033	1
1	A	3	PRO	CB	32.306	0.069	1
1	A	3	PRO	CD	49.929	0.034	1
1	A	3	PRO	CG	26.582	0.016	1
1	A	4	TYR	H	7.733	0.008	1
1	A	4	TYR	HA	4.5	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	TYR	HB2	2.734	0.011	2
1	A	4	TYR	HB3	2.861	0.004	2
1	A	4	TYR	HD1	6.878	0.009	3
1	A	4	TYR	HD2	6.878	0.009	3
1	A	4	TYR	C	174.332	.	1
1	A	4	TYR	CA	57.954	0.034	1
1	A	4	TYR	CB	38.475	0.034	1
1	A	4	TYR	CD1	136.107	0.009	3
1	A	4	TYR	CD2	136.107	0.009	3
1	A	4	TYR	N	118.693	0.043	1
1	A	5	VAL	H	8.42	0.008	1
1	A	5	VAL	HA	4.634	0.009	1
1	A	5	VAL	HB	1.712	0.011	1
1	A	5	VAL	HG11	0.64	0.011	2
1	A	5	VAL	HG12	0.64	0.011	2
1	A	5	VAL	HG13	0.64	0.011	2
1	A	5	VAL	HG21	0.653	0.012	2
1	A	5	VAL	HG22	0.653	0.012	2
1	A	5	VAL	HG23	0.653	0.012	2
1	A	5	VAL	C	174.141	.	1
1	A	5	VAL	CA	60.269	0.012	1
1	A	5	VAL	CB	34.83	0.027	1
1	A	5	VAL	CG1	20.921	.	1
1	A	5	VAL	CG2	20.921	.	1
1	A	5	VAL	N	123.592	0.033	1
1	A	6	CYS	H	9.004	0.005	1
1	A	6	CYS	HA	4.486	0.015	1
1	A	6	CYS	HB2	2.747	0.016	1
1	A	6	CYS	HB3	3.281	0.015	1
1	A	6	CYS	C	177.123	.	1
1	A	6	CYS	CA	59.271	0.045	1
1	A	6	CYS	CB	29.754	0.045	1
1	A	6	CYS	N	128.449	0.031	1
1	A	7	ILE	H	8.658	0.006	1
1	A	7	ILE	HA	3.929	0.015	1
1	A	7	ILE	HB	1.71	0.009	1
1	A	7	ILE	HD11	0.597	0.004	1
1	A	7	ILE	HD12	0.597	0.004	1
1	A	7	ILE	HD13	0.597	0.004	1
1	A	7	ILE	HG12	0.968	0.007	1
1	A	7	ILE	HG13	0.968	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ILE	HG21	0.658	0.007	1
1	A	7	ILE	HG22	0.658	0.007	1
1	A	7	ILE	HG23	0.658	0.007	1
1	A	7	ILE	C	175.653	.	1
1	A	7	ILE	CA	63.258	0.023	1
1	A	7	ILE	CB	37.975	0.06	1
1	A	7	ILE	CD1	13.836	0.09	1
1	A	7	ILE	CG1	26.684	0.059	1
1	A	7	ILE	CG2	17.445	0.056	1
1	A	7	ILE	N	128.379	0.044	1
1	A	8	HIS	H	8.502	0.011	1
1	A	8	HIS	HA	4.238	0.017	1
1	A	8	HIS	HB2	1.802	0.011	1
1	A	8	HIS	HB3	2.231	0.015	1
1	A	8	HIS	C	176.78	.	1
1	A	8	HIS	CA	57.836	0.054	1
1	A	8	HIS	CB	29.345	0.03	1
1	A	8	HIS	N	121.674	0.03	1
1	A	9	CYS	H	7.942	0.007	1
1	A	9	CYS	HA	5.041	0.018	1
1	A	9	CYS	HB2	2.745	0.012	2
1	A	9	CYS	HB3	3.346	0.014	2
1	A	9	CYS	C	174.989	.	1
1	A	9	CYS	CA	58.494	0.016	1
1	A	9	CYS	CB	32.209	0.03	1
1	A	9	CYS	N	115.764	0.035	1
1	A	10	GLN	H	8.191	0.006	1
1	A	10	GLN	HA	3.88	0.015	1
1	A	10	GLN	HB2	2.189	0.003	2
1	A	10	GLN	HB3	2.333	0.003	2
1	A	10	GLN	HE21	6.363	0.004	1
1	A	10	GLN	HE22	7.092	0.003	1
1	A	10	GLN	HG2	2.115	0.013	1
1	A	10	GLN	HG3	2.115	0.013	1
1	A	10	GLN	C	174.724	.	1
1	A	10	GLN	CA	58.438	0.035	1
1	A	10	GLN	CB	25.356	0.013	1
1	A	10	GLN	CG	34.322	0.035	1
1	A	10	GLN	N	116.329	0.021	1
1	A	10	GLN	NE2	111.99	0.022	1
1	A	11	ARG	H	7.844	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ARG	HA	3.935	0.013	1
1	A	11	ARG	HB2	1.219	0.015	2
1	A	11	ARG	HB3	1.383	0.008	2
1	A	11	ARG	HD2	2.789	0.007	2
1	A	11	ARG	HD3	3.001	0.011	2
1	A	11	ARG	HG2	1.724	0.011	1
1	A	11	ARG	HG3	1.724	0.011	1
1	A	11	ARG	C	174.125	.	1
1	A	11	ARG	CA	57.912	0.025	1
1	A	11	ARG	CB	31.307	0.048	1
1	A	11	ARG	CD	43.622	.	1
1	A	11	ARG	CG	28.383	.	1
1	A	11	ARG	N	121.213	0.028	1
1	A	12	GLN	H	7.86	0.007	1
1	A	12	GLN	HA	4.856	0.014	1
1	A	12	GLN	HB2	1.63	0.013	2
1	A	12	GLN	HB3	1.758	0.005	2
1	A	12	GLN	HE21	6.637	0.008	1
1	A	12	GLN	HE22	7.488	0.003	1
1	A	12	GLN	HG2	2.031	0.01	2
1	A	12	GLN	HG3	2.255	0.016	2
1	A	12	GLN	C	175.08	.	1
1	A	12	GLN	CA	54.345	0.059	1
1	A	12	GLN	CB	31.148	0.069	1
1	A	12	GLN	CG	33.754	0.048	1
1	A	12	GLN	N	119.072	0.031	1
1	A	12	GLN	NE2	111.271	0.003	1
1	A	13	PHE	H	8.888	0.011	1
1	A	13	PHE	HA	4.487	0.003	1
1	A	13	PHE	HB2	2.566	0.015	1
1	A	13	PHE	HB3	3.133	0.012	1
1	A	13	PHE	HD1	7.031	0.002	3
1	A	13	PHE	HD2	7.031	0.002	3
1	A	13	PHE	C	174.976	.	1
1	A	13	PHE	CA	57.278	0.019	1
1	A	13	PHE	CB	43.35	0.034	1
1	A	13	PHE	CD1	135.106	0.013	3
1	A	13	PHE	CD2	135.106	0.013	3
1	A	13	PHE	N	119.084	0.026	1
1	A	14	ALA	H	8.962	0.003	1
1	A	14	ALA	HA	4.432	0.014	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	ALA	HB1	1.444	0.01	1
1	A	14	ALA	HB2	1.444	0.01	1
1	A	14	ALA	HB3	1.444	0.01	1
1	A	14	ALA	C	176.59	.	1
1	A	14	ALA	CA	53.149	0.044	1
1	A	14	ALA	CB	19.805	0.029	1
1	A	14	ALA	N	121.775	0.047	1
1	A	15	ASP	H	7.351	0.006	1
1	A	15	ASP	HA	4.737	0.02	1
1	A	15	ASP	HB2	2.565	0.014	2
1	A	15	ASP	HB3	2.69	0.013	2
1	A	15	ASP	CA	51.23	0.058	1
1	A	15	ASP	CB	42.66	0.014	1
1	A	15	ASP	N	114.226	0.019	1
1	A	16	PRO	HA	3.446	0.005	1
1	A	16	PRO	HD2	3.075	0.01	2
1	A	16	PRO	HD3	3.614	0.063	2
1	A	16	PRO	C	178.827	.	1
1	A	16	PRO	CA	64.165	0.026	1
1	A	16	PRO	CB	31.085	0.022	1
1	A	16	PRO	CD	49.894	0.036	1
1	A	16	PRO	CG	26.784	.	1
1	A	17	GLY	H	8.254	0.006	1
1	A	17	GLY	HA2	3.639	0.019	1
1	A	17	GLY	HA3	3.639	0.019	1
1	A	17	GLY	C	175.863	.	1
1	A	17	GLY	CA	46.69	0.027	1
1	A	17	GLY	N	110.007	0.066	1
1	A	18	ALA	H	8.022	0.008	1
1	A	18	ALA	HA	3.841	0.022	1
1	A	18	ALA	HB1	1.497	0.011	1
1	A	18	ALA	HB2	1.497	0.011	1
1	A	18	ALA	HB3	1.497	0.011	1
1	A	18	ALA	C	180.54	.	1
1	A	18	ALA	CA	54.562	0.027	1
1	A	18	ALA	CB	18.794	0.027	1
1	A	18	ALA	N	125.453	0.028	1
1	A	19	LEU	H	6.804	0.006	1
1	A	19	LEU	HA	3.013	0.013	1
1	A	19	LEU	HB2	1.039	0.006	1
1	A	19	LEU	HB3	1.731	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	HD11	0.791	0.011	2
1	A	19	LEU	HD12	0.791	0.011	2
1	A	19	LEU	HD13	0.791	0.011	2
1	A	19	LEU	HD21	0.879	0.023	2
1	A	19	LEU	HD22	0.879	0.023	2
1	A	19	LEU	HD23	0.879	0.023	2
1	A	19	LEU	C	176.841	.	1
1	A	19	LEU	CA	57.723	0.029	1
1	A	19	LEU	CB	40.447	0.06	1
1	A	19	LEU	CD1	23.328	.	1
1	A	19	LEU	CD2	23.328	.	1
1	A	19	LEU	N	118.428	0.012	1
1	A	20	GLN	H	7.931	0.008	1
1	A	20	GLN	HA	3.79	0.014	1
1	A	20	GLN	HB2	2.027	0.014	2
1	A	20	GLN	HB3	2.045	0.013	2
1	A	20	GLN	HG2	2.21	0.002	2
1	A	20	GLN	HG3	2.288	0.004	2
1	A	20	GLN	C	178.29	.	1
1	A	20	GLN	CA	58.675	0.009	1
1	A	20	GLN	CB	27.969	0.006	1
1	A	20	GLN	CG	33.427	0.022	1
1	A	20	GLN	N	118.513	0.023	1
1	A	21	ARG	H	7.727	0.004	1
1	A	21	ARG	HA	3.822	0.011	1
1	A	21	ARG	HB2	1.661	0.006	2
1	A	21	ARG	HB3	1.72	0.004	2
1	A	21	ARG	HD2	3.01	0.003	2
1	A	21	ARG	HD3	3.154	0.004	2
1	A	21	ARG	HG2	1.36	0.008	1
1	A	21	ARG	HG3	1.36	0.008	1
1	A	21	ARG	C	178.324	.	1
1	A	21	ARG	CA	58.956	0.09	1
1	A	21	ARG	CB	30.353	0.003	1
1	A	21	ARG	CD	43.232	0.012	1
1	A	21	ARG	CG	28.086	0.0	1
1	A	21	ARG	N	116.497	0.045	1
1	A	22	HIS	H	7.374	0.008	1
1	A	22	HIS	HA	4.131	0.016	1
1	A	22	HIS	HB2	2.723	0.014	1
1	A	22	HIS	HB3	2.911	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	HIS	HD2	6.848	0.008	1
1	A	22	HIS	C	176.672	.	1
1	A	22	HIS	CA	59.068	0.032	1
1	A	22	HIS	CB	28.49	0.025	1
1	A	22	HIS	CD2	130.313	0.0	1
1	A	22	HIS	N	118.228	0.022	1
1	A	23	VAL	H	8.27	0.007	1
1	A	23	VAL	HA	3.494	0.018	1
1	A	23	VAL	HB	2.243	0.012	1
1	A	23	VAL	HG11	1.232	0.009	1
1	A	23	VAL	HG12	1.232	0.009	1
1	A	23	VAL	HG13	1.232	0.009	1
1	A	23	VAL	HG21	1.232	0.009	1
1	A	23	VAL	HG22	1.232	0.009	1
1	A	23	VAL	HG23	1.232	0.009	1
1	A	23	VAL	C	176.856	.	1
1	A	23	VAL	CA	65.99	0.054	1
1	A	23	VAL	CB	31.834	0.06	1
1	A	23	VAL	CG1	21.94	0.03	1
1	A	23	VAL	CG2	21.94	0.03	1
1	A	23	VAL	N	114.222	0.038	1
1	A	24	ARG	H	6.764	0.01	1
1	A	24	ARG	HA	3.974	0.005	1
1	A	24	ARG	HB2	1.741	0.0	1
1	A	24	ARG	HB3	1.741	0.0	1
1	A	24	ARG	HD2	3.061	0.006	1
1	A	24	ARG	HD3	3.067	0.002	1
1	A	24	ARG	HG2	1.55	0.003	2
1	A	24	ARG	HG3	1.655	0.003	2
1	A	24	ARG	C	178.102	.	1
1	A	24	ARG	CA	57.94	0.0	1
1	A	24	ARG	CB	29.865	0.005	1
1	A	24	ARG	CD	43.555	.	1
1	A	24	ARG	CG	27.154	0.0	1
1	A	24	ARG	N	118.135	0.046	1
1	A	25	ILE	H	7.682	0.009	1
1	A	25	ILE	HA	3.844	0.011	1
1	A	25	ILE	HB	1.589	0.009	1
1	A	25	ILE	HD11	0.544	0.006	1
1	A	25	ILE	HD12	0.544	0.006	1
1	A	25	ILE	HD13	0.544	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	ILE	HG12	0.763	0.018	1
1	A	25	ILE	HG13	0.763	0.018	1
1	A	25	ILE	HG21	0.455	0.005	1
1	A	25	ILE	HG22	0.455	0.005	1
1	A	25	ILE	HG23	0.455	0.005	1
1	A	25	ILE	C	177.015	.	1
1	A	25	ILE	CA	62.939	0.017	1
1	A	25	ILE	CB	37.491	0.025	1
1	A	25	ILE	CD1	14.433	0.014	1
1	A	25	ILE	CG1	26.244	0.058	1
1	A	25	ILE	CG2	16.211	0.044	1
1	A	25	ILE	N	115.964	0.027	1
1	A	26	HIS	H	7.282	0.009	1
1	A	26	HIS	HA	4.551	0.01	1
1	A	26	HIS	HB2	2.524	0.007	2
1	A	26	HIS	HB3	2.624	0.011	2
1	A	26	HIS	HD2	6.57	0.006	1
1	A	26	HIS	HE1	7.93	0.006	1
1	A	26	HIS	C	175.472	.	1
1	A	26	HIS	CA	55.107	0.077	1
1	A	26	HIS	CB	27.955	0.062	1
1	A	26	HIS	CD2	131.261	0.018	1
1	A	26	HIS	CE1	142.684	.	1
1	A	26	HIS	N	117.871	0.051	1
1	A	27	THR	H	7.534	0.014	1
1	A	27	THR	HA	4.125	0.018	1
1	A	27	THR	HB	4.156	0.007	1
1	A	27	THR	HG21	1.069	0.019	1
1	A	27	THR	HG22	1.069	0.019	1
1	A	27	THR	HG23	1.069	0.019	1
1	A	27	THR	C	175.062	.	1
1	A	27	THR	CA	62.725	0.038	1
1	A	27	THR	CB	69.495	0.054	1
1	A	27	THR	N	112.24	0.029	1
1	A	28	GLY	H	8.112	0.011	1
1	A	28	GLY	HA2	3.879	0.007	2
1	A	28	GLY	HA3	3.813	0.003	2
1	A	28	GLY	C	173.918	.	1
1	A	28	GLY	CA	45.243	0.046	1
1	A	28	GLY	N	110.227	0.029	1
1	A	29	GLU	H	7.885	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	GLU	HA	4.048	0.015	1
1	A	29	GLU	HB2	1.842	0.018	2
1	A	29	GLU	HB3	1.893	0.004	2
1	A	29	GLU	HG2	2.169	0.006	2
1	A	29	GLU	HG3	2.115	0.01	2
1	A	29	GLU	C	176.166	.	1
1	A	29	GLU	CA	56.901	0.02	1
1	A	29	GLU	CB	30.255	0.05	1
1	A	29	GLU	CG	36.152	0.019	1
1	A	29	GLU	N	119.771	0.041	1
1	A	30	LYS	H	8.075	0.003	1
1	A	30	LYS	HA	4.455	0.021	1
1	A	30	LYS	CA	53.768	.	1
1	A	30	LYS	CB	33.52	.	1
1	A	30	LYS	N	120.594	0.045	1
1	A	31	PRO	HA	4.401	0.008	1
1	A	31	PRO	HB2	2.123	0.006	2
1	A	31	PRO	HB3	2.081	0.009	2
1	A	31	PRO	HD2	3.568	0.013	2
1	A	31	PRO	HD3	3.62	0.022	2
1	A	31	PRO	HG2	1.839	0.004	2
1	A	31	PRO	HG3	1.901	0.01	2
1	A	31	PRO	C	176.585	.	1
1	A	31	PRO	CA	63.434	0.063	1
1	A	31	PRO	CB	32.293	0.025	1
1	A	31	PRO	CG	26.643	0.002	1
1	A	32	CYS	H	8.356	0.007	1
1	A	32	CYS	HA	4.514	.	1
1	A	32	CYS	C	173.747	.	1
1	A	32	CYS	CA	57.325	0.07	1
1	A	32	CYS	CB	35.049	.	1
1	A	32	CYS	N	117.577	0.046	1
1	A	33	GLN	H	8.372	0.01	1
1	A	33	GLN	HA	5.021	0.011	1
1	A	33	GLN	HB2	1.656	0.008	2
1	A	33	GLN	HB3	1.714	0.006	2
1	A	33	GLN	HG2	1.912	0.016	1
1	A	33	GLN	HG3	1.912	0.016	1
1	A	33	GLN	C	175.002	.	1
1	A	33	GLN	CA	54.101	0.038	1
1	A	33	GLN	CB	32.361	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	GLN	CG	33.837	.	1
1	A	33	GLN	N	120.137	0.023	1
1	A	34	CYS	H	8.993	0.008	1
1	A	34	CYS	HA	4.425	0.007	1
1	A	34	CYS	HB2	2.783	0.014	1
1	A	34	CYS	HB3	3.272	0.013	1
1	A	34	CYS	C	178.038	.	1
1	A	34	CYS	CA	59.22	0.045	1
1	A	34	CYS	CB	29.956	0.033	1
1	A	34	CYS	N	126.003	0.054	1
1	A	35	VAL	H	9.01	0.013	1
1	A	35	VAL	HA	3.971	0.02	1
1	A	35	VAL	HB	2.185	0.025	1
1	A	35	VAL	HG11	0.925	0.014	1
1	A	35	VAL	HG12	0.925	0.014	1
1	A	35	VAL	HG13	0.925	0.014	1
1	A	35	VAL	HG21	0.928	0.012	1
1	A	35	VAL	HG22	0.928	0.012	1
1	A	35	VAL	HG23	0.928	0.012	1
1	A	35	VAL	C	176.03	.	1
1	A	35	VAL	CA	64.03	0.051	1
1	A	35	VAL	CB	31.734	0.068	1
1	A	35	VAL	CG1	20.386	0.007	1
1	A	35	VAL	CG2	20.386	0.007	1
1	A	35	VAL	N	129.398	0.04	1
1	A	36	MET	H	8.726	0.007	1
1	A	36	MET	HA	4.215	0.031	1
1	A	36	MET	HB2	2.17	0.015	1
1	A	36	MET	HB3	2.17	0.015	1
1	A	36	MET	HG2	2.208	0.001	1
1	A	36	MET	HG3	2.208	0.001	1
1	A	36	MET	C	176.951	.	1
1	A	36	MET	CA	57.631	0.057	1
1	A	36	MET	CB	32.113	0.066	1
1	A	36	MET	CG	30.113	.	1
1	A	36	MET	N	120.946	0.056	1
1	A	37	CYS	H	8.038	0.012	1
1	A	37	CYS	HA	5.064	0.008	1
1	A	37	CYS	HB2	2.756	0.011	1
1	A	37	CYS	HB3	3.348	0.013	1
1	A	37	CYS	C	175.989	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	CYS	CA	58.484	0.023	1
1	A	37	CYS	CB	32.235	0.053	1
1	A	37	CYS	N	115.594	0.05	1
1	A	38	GLY	H	8.119	0.007	1
1	A	38	GLY	HA2	3.68	0.017	2
1	A	38	GLY	HA3	4.156	0.016	2
1	A	38	GLY	C	173.535	.	1
1	A	38	GLY	CA	45.994	0.03	1
1	A	38	GLY	N	113.363	0.031	1
1	A	39	LYS	H	7.877	0.005	1
1	A	39	LYS	HA	3.831	0.006	1
1	A	39	LYS	HB2	1.13	0.005	2
1	A	39	LYS	HB3	1.482	0.003	2
1	A	39	LYS	HD2	1.243	0.003	2
1	A	39	LYS	HD3	1.395	0.01	2
1	A	39	LYS	HE2	2.709	0.002	2
1	A	39	LYS	HE3	2.796	0.021	2
1	A	39	LYS	HG2	0.835	0.007	2
1	A	39	LYS	HG3	1.208	0.002	2
1	A	39	LYS	C	173.961	.	1
1	A	39	LYS	CA	58.248	0.036	1
1	A	39	LYS	CB	33.551	0.002	1
1	A	39	LYS	CD	29.114	0.0	1
1	A	39	LYS	CE	42.282	0.0	1
1	A	39	LYS	CG	25.737	.	1
1	A	39	LYS	N	123.49	0.03	1
1	A	40	ALA	H	7.89	0.005	1
1	A	40	ALA	HA	4.868	0.023	1
1	A	40	ALA	HB1	1.116	0.009	1
1	A	40	ALA	HB2	1.116	0.009	1
1	A	40	ALA	HB3	1.116	0.009	1
1	A	40	ALA	C	176.533	.	1
1	A	40	ALA	CA	50.845	0.053	1
1	A	40	ALA	CB	21.18	0.063	1
1	A	40	ALA	N	125.467	0.039	1
1	A	41	PHE	H	8.342	0.006	1
1	A	41	PHE	HA	4.538	0.012	1
1	A	41	PHE	HB2	2.497	0.014	1
1	A	41	PHE	HB3	3.11	0.017	1
1	A	41	PHE	HD1	7.032	0.003	3
1	A	41	PHE	HD2	7.032	0.003	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	PHE	C	174.934	.	1
1	A	41	PHE	CA	57.395	0.015	1
1	A	41	PHE	CB	44.113	0.039	1
1	A	41	PHE	CD1	135.325	0.029	3
1	A	41	PHE	CD2	135.325	0.029	3
1	A	41	PHE	N	117.232	0.03	1
1	A	42	THR	H	8.732	0.005	1
1	A	42	THR	HA	4.42	0.004	1
1	A	42	THR	HB	4.331	0.009	1
1	A	42	THR	HG21	1.079	0.011	1
1	A	42	THR	HG22	1.079	0.011	1
1	A	42	THR	HG23	1.079	0.011	1
1	A	42	THR	C	174.386	.	1
1	A	42	THR	CA	62.005	0.074	1
1	A	42	THR	CB	69.488	0.083	1
1	A	42	THR	CG2	22.213	.	1
1	A	42	THR	N	108.612	0.056	1
1	A	43	GLN	H	7.257	0.006	1
1	A	43	GLN	HA	4.623	0.008	1
1	A	43	GLN	CA	54.332	.	1
1	A	43	GLN	CB	31.631	.	1
1	A	43	GLN	N	118.161	0.025	1
1	A	44	ALA	HA	3.864	0.01	1
1	A	44	ALA	HB1	1.353	0.016	1
1	A	44	ALA	HB2	1.353	0.016	1
1	A	44	ALA	HB3	1.353	0.016	1
1	A	44	ALA	C	179.325	.	1
1	A	44	ALA	CA	55.569	0.055	1
1	A	44	ALA	CB	17.913	0.04	1
1	A	45	SER	H	8.744	0.001	1
1	A	45	SER	HA	2.864	0.01	1
1	A	45	SER	HB2	3.409	0.014	2
1	A	45	SER	HB3	3.217	0.011	2
1	A	45	SER	C	177.517	.	1
1	A	45	SER	CA	61.015	0.053	1
1	A	45	SER	CB	61.493	0.038	1
1	A	45	SER	N	111.824	0.018	1
1	A	46	SER	H	6.932	0.011	1
1	A	46	SER	HA	4.185	0.017	1
1	A	46	SER	HB2	4.231	.	2
1	A	46	SER	HB3	3.974	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	SER	C	175.729	.	1
1	A	46	SER	CA	60.656	0.059	1
1	A	46	SER	CB	62.578	0.085	1
1	A	46	SER	N	118.211	0.025	1
1	A	47	LEU	H	7.132	0.008	1
1	A	47	LEU	HA	2.801	0.01	1
1	A	47	LEU	HB2	0.992	0.013	1
1	A	47	LEU	HB3	1.848	0.012	1
1	A	47	LEU	HD11	0.641	0.014	2
1	A	47	LEU	HD12	0.641	0.014	2
1	A	47	LEU	HD13	0.641	0.014	2
1	A	47	LEU	HD21	0.78	0.007	2
1	A	47	LEU	HD22	0.78	0.007	2
1	A	47	LEU	HD23	0.78	0.007	2
1	A	47	LEU	HG	1.311	0.009	1
1	A	47	LEU	C	177.273	.	1
1	A	47	LEU	CA	57.883	0.074	1
1	A	47	LEU	CB	40.99	0.067	1
1	A	47	LEU	N	124.822	0.038	1
1	A	48	ILE	H	8.152	0.007	1
1	A	48	ILE	HA	3.457	0.012	1
1	A	48	ILE	HB	1.647	0.016	1
1	A	48	ILE	HD11	0.67	0.009	1
1	A	48	ILE	HD12	0.67	0.009	1
1	A	48	ILE	HD13	0.67	0.009	1
1	A	48	ILE	HG12	1.472	0.015	2
1	A	48	ILE	HG13	1.041	0.008	2
1	A	48	ILE	HG21	0.748	0.017	1
1	A	48	ILE	HG22	0.748	0.017	1
1	A	48	ILE	HG23	0.748	0.017	1
1	A	48	ILE	C	178.059	.	1
1	A	48	ILE	CA	64.674	0.051	1
1	A	48	ILE	CB	37.786	0.039	1
1	A	48	ILE	CD1	12.592	0.021	1
1	A	48	ILE	CG1	29.124	0.065	1
1	A	48	ILE	CG2	16.934	0.044	1
1	A	48	ILE	N	118.672	0.05	1
1	A	49	ALA	H	7.237	0.006	1
1	A	49	ALA	HA	3.902	0.01	1
1	A	49	ALA	HB1	1.326	0.013	1
1	A	49	ALA	HB2	1.326	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	ALA	HB3	1.326	0.013	1
1	A	49	ALA	C	179.603	.	1
1	A	49	ALA	CA	54.762	0.041	1
1	A	49	ALA	CB	18.004	0.051	1
1	A	49	ALA	N	120.061	0.041	1
1	A	50	HIS	H	7.429	0.009	1
1	A	50	HIS	HA	4.078	0.017	1
1	A	50	HIS	HB2	2.868	0.01	1
1	A	50	HIS	HB3	3.05	0.015	1
1	A	50	HIS	HD2	6.889	0.005	1
1	A	50	HIS	C	177.439	.	1
1	A	50	HIS	CA	59.262	0.025	1
1	A	50	HIS	CB	28.579	0.049	1
1	A	50	HIS	CD2	130.313	0.0	1
1	A	50	HIS	N	117.236	0.063	1
1	A	51	VAL	H	8.581	0.007	1
1	A	51	VAL	HA	3.484	0.017	1
1	A	51	VAL	HB	2.112	0.014	1
1	A	51	VAL	HG11	0.989	0.019	1
1	A	51	VAL	HG12	0.989	0.019	1
1	A	51	VAL	HG13	0.989	0.019	1
1	A	51	VAL	HG21	1.213	0.015	1
1	A	51	VAL	HG22	1.213	0.015	1
1	A	51	VAL	HG23	1.213	0.015	1
1	A	51	VAL	C	178.46	.	1
1	A	51	VAL	CA	66.744	0.029	1
1	A	51	VAL	CB	31.657	0.046	1
1	A	51	VAL	CG1	22.318	0.082	1
1	A	51	VAL	CG2	22.318	0.082	1
1	A	51	VAL	N	119.094	0.02	1
1	A	52	ARG	H	7.397	0.01	1
1	A	52	ARG	HA	4.086	0.01	1
1	A	52	ARG	C	178.13	.	1
1	A	52	ARG	CA	58.801	.	1
1	A	52	ARG	CB	29.78	0.008	1
1	A	52	ARG	CD	43.414	.	1
1	A	52	ARG	CG	27.738	.	1
1	A	52	ARG	N	118.214	0.022	1
1	A	53	GLN	H	7.525	0.009	1
1	A	53	GLN	HA	3.992	0.013	1
1	A	53	GLN	HB2	1.791	0.012	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	GLN	HB3	1.836	0.01	2
1	A	53	GLN	HG2	2.145	0.006	2
1	A	53	GLN	HG3	2.231	0.011	2
1	A	53	GLN	C	177.537	.	1
1	A	53	GLN	CA	57.204	0.019	1
1	A	53	GLN	CB	27.94	0.015	1
1	A	53	GLN	CG	33.51	0.015	1
1	A	53	GLN	N	116.882	0.018	1
1	A	54	HIS	H	7.325	0.01	1
1	A	54	HIS	HA	4.585	0.004	1
1	A	54	HIS	HB2	3.05	0.014	1
1	A	54	HIS	HB3	3.24	0.012	1
1	A	54	HIS	HD2	6.562	0.008	1
1	A	54	HIS	HE1	7.926	0.007	1
1	A	54	HIS	C	175.986	.	1
1	A	54	HIS	CA	56.657	0.056	1
1	A	54	HIS	CB	28.544	0.017	1
1	A	54	HIS	CD2	130.312	0.0	1
1	A	54	HIS	CE1	142.684	.	1
1	A	54	HIS	N	116.588	0.026	1
1	A	55	THR	H	7.707	0.004	1
1	A	55	THR	HA	4.138	0.006	1
1	A	55	THR	HB	4.17	0.006	1
1	A	55	THR	HG21	1.078	0.016	1
1	A	55	THR	HG22	1.078	0.016	1
1	A	55	THR	HG23	1.078	0.016	1
1	A	55	THR	C	175.14	.	1
1	A	55	THR	CA	62.768	0.041	1
1	A	55	THR	CB	69.576	0.052	1
1	A	55	THR	N	112.615	0.017	1
1	A	56	GLY	H	8.22	0.01	1
1	A	56	GLY	HA2	3.816	0.002	2
1	A	56	GLY	HA3	3.875	0.008	2
1	A	56	GLY	C	173.958	.	1
1	A	56	GLY	CA	45.302	0.018	1
1	A	56	GLY	N	111.071	0.044	1
1	A	57	GLU	H	7.9	0.004	1
1	A	57	GLU	HA	4.141	0.016	1
1	A	57	GLU	HB2	1.814	0.008	2
1	A	57	GLU	HB3	1.905	0.006	2
1	A	57	GLU	HG2	2.091	0.004	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	GLU	HG3	2.133	0.008	2
1	A	57	GLU	C	176.139	.	1
1	A	57	GLU	CA	56.455	0.087	1
1	A	57	GLU	CB	30.322	0.026	1
1	A	57	GLU	CG	36.063	0.005	1
1	A	57	GLU	N	120.313	0.005	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.28 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	75	0.29 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	0.11 ± 0.30	None needed (< 0.5 ppm)
^{15}N	74	-0.58 ± 0.66	None needed (imprecise)

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 77%, i.e. 259 atoms were assigned a chemical shift out of a possible 335. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	108/116 (93%)	44/47 (94%)	43/46 (93%)	21/23 (91%)
Sidechain	137/178 (77%)	93/114 (82%)	43/51 (84%)	1/13 (8%)
Aromatic	14/41 (34%)	7/21 (33%)	7/16 (44%)	0/4 (0%)
Overall	259/335 (77%)	144/182 (79%)	93/113 (82%)	22/40 (55%)

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:

