wwPDB NMR Structure Validation Summary Report

Apr 21, 2024 – 02:04 PM EDT

PDB ID	:	2LC5
BMRB ID	:	15663
Title	:	Calmodulin-like Protein from Entamoeba histolytica: Solution Structure and Calcium-Binding Properties of a Partially Folded Protein
Authors	:	Rout, A.K.; Padhan, N.; Barnwal, R.P.; Bhattacharya, A.; Chary, K.V.
Deposited on	:	2011-04-23

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 (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:

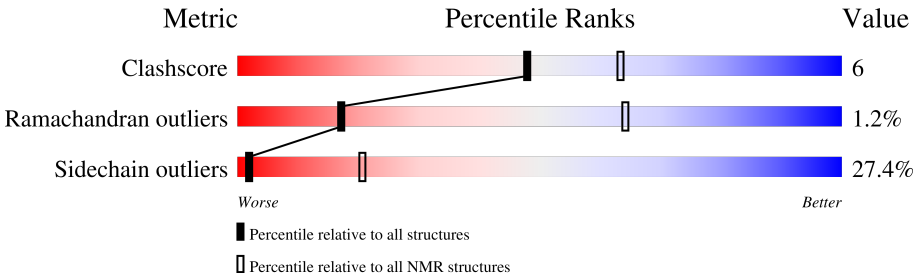
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 79%.

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	151	34% 13% • 8% 44%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:8-A:80 (73)	0.88	8

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 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1350 atoms, of which 663 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin, putative.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1348	426	663	109	147	3	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

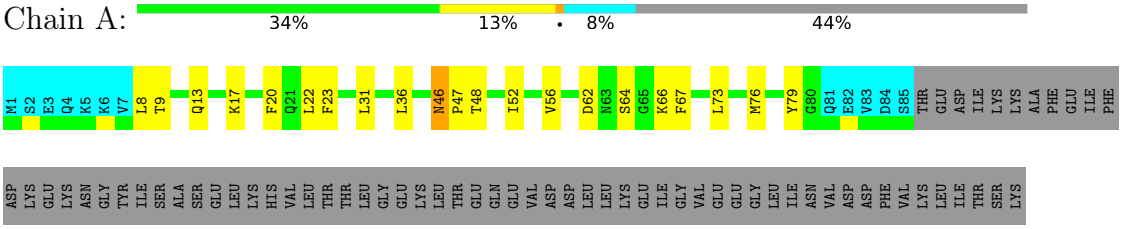
Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

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.

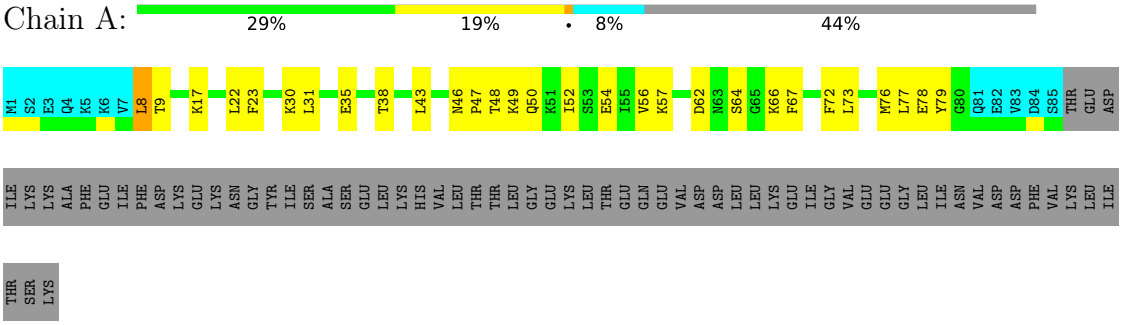
- Molecule 1: Calmodulin, putative



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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Calmodulin, putative



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, DISTANCE GEOMETRY, SIMULATED ANNEALING.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LOWEST ENER.*

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

Software name	Classification	Version
TALOS	structure solution	
CYANA 3.0	refinement	Beta

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	1386
Number of shifts mapped to atoms	891
Number of unparsed shifts	0
Number of shifts with mapping errors	495
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

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

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

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	589	568	568	7±2
All	All	11820	11360	11360	147

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 6.

5 of 63 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD13	1:A:67:PHE:CG	0.65	2.27	12	4
1:A:20:PHE:CD2	1:A:31:LEU:HD13	0.65	2.27	2	2
1:A:8:LEU:HD11	1:A:77:LEU:HD23	0.63	1.70	8	2
1:A:8:LEU:HD13	1:A:80:GLY:C	0.62	2.14	9	1
1:A:52:ILE:O	1:A:56:VAL:HG23	0.61	1.95	2	12

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	73/151 (48%)	66±1 (90±2%)	6±1 (8±2%)	1±1 (1±1%)	17 64
All	All	1460/3020 (48%)	1321 (90%)	121 (8%)	18 (1%)	17 64

5 of 7 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	46	ASN	6
1	A	44	GLY	4
1	A	80	GLY	3
1	A	26	ASP	2
1	A	8	LEU	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	64/136 (47%)	46±2 (73±3%)	18±2 (27±3%)	2 21
All	All	1280/2720 (47%)	929 (73%)	351 (27%)	2 21

5 of 48 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	9	THR	19
1	A	64	SER	19
1	A	73	LEU	19
1	A	48	THR	18
1	A	66	LYS	17

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 monosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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 79% for the well-defined parts and 78% 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	1386
Number of shifts mapped to atoms	891
Number of unparsed shifts	0
Number of shifts with mapping errors	495
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 495) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	THR	H	8.34	0.02	.
1	A	86	THR	HA	4.24	0.02	.
1	A	86	THR	HB	3.96	0.02	.
1	A	86	THR	HG21	1.17	0.02	.
1	A	86	THR	HG22	1.17	0.02	.
1	A	86	THR	HG23	1.17	0.02	.
1	A	86	THR	C	172.75	0.30	.
1	A	86	THR	CA	65.57	0.30	.
1	A	86	THR	CB	69.87	0.30	.
1	A	86	THR	CG2	22.37	0.30	.
1	A	86	THR	N	116.27	0.30	.
1	A	87	GLU	H	8.21	0.02	.
1	A	87	GLU	HA	4.67	0.02	.
1	A	87	GLU	HB2	2.21	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	87	GLU	HB3	1.93	0.02	.
1	A	87	GLU	C	173.77	0.30	.
1	A	87	GLU	CA	59.73	0.30	.
1	A	87	GLU	CB	30.63	0.30	.
1	A	87	GLU	N	121.89	0.30	.
1	A	88	ASP	C	175.59	0.30	.
1	A	88	ASP	CA	55.56	0.30	.
1	A	88	ASP	CB	41.85	0.30	.
1	A	89	ILE	H	8.07	0.02	.
1	A	89	ILE	HA	4.06	0.02	.
1	A	89	ILE	HB	2.37	0.02	.
1	A	89	ILE	C	172.26	0.30	.
1	A	89	ILE	CA	62.33	0.30	.
1	A	89	ILE	CB	39.63	0.30	.
1	A	89	ILE	CD1	13.85	0.30	.
1	A	89	ILE	CG1	27.77	0.30	.
1	A	89	ILE	CG2	18.21	0.30	.
1	A	89	ILE	N	121.46	0.30	.
1	A	90	LYS	H	8.25	0.02	.
1	A	90	LYS	C	173.46	0.30	.
1	A	90	LYS	CA	56.92	0.30	.
1	A	90	LYS	CB	33.63	0.30	.
1	A	90	LYS	N	125.39	0.30	.
1	A	91	LYS	H	8.3	0.02	.
1	A	91	LYS	HA	4.75	0.02	.
1	A	91	LYS	HB2	2.1	0.02	.
1	A	91	LYS	HB3	2.1	0.02	.
1	A	91	LYS	HG2	1.33	0.02	.
1	A	91	LYS	C	172.83	0.30	.
1	A	91	LYS	CA	54.51	0.30	.
1	A	91	LYS	CB	35.7	0.30	.
1	A	91	LYS	N	121.65	0.30	.
1	A	92	ALA	H	7.85	0.02	.
1	A	92	ALA	HA	4.18	0.02	.
1	A	92	ALA	HB1	1.28	0.02	.
1	A	92	ALA	HB2	1.28	0.02	.
1	A	92	ALA	HB3	1.28	0.02	.
1	A	92	ALA	C	175.18	0.30	.
1	A	92	ALA	CA	54.28	0.30	.
1	A	92	ALA	CB	19.46	0.30	.
1	A	92	ALA	N	120.98	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	PHE	H	7.97	0.02	.
1	A	93	PHE	C	175.09	0.30	.
1	A	93	PHE	CA	59.04	0.30	.
1	A	93	PHE	N	117.94	0.30	.
1	A	95	ILE	HA	3.25	0.02	.
1	A	95	ILE	HB	0.84	0.02	.
1	A	95	ILE	HG21	0.24	0.02	.
1	A	95	ILE	HG22	0.24	0.02	.
1	A	95	ILE	HG23	0.24	0.02	.
1	A	95	ILE	C	176.13	0.30	.
1	A	95	ILE	CA	67.56	0.30	.
1	A	95	ILE	CB	37.06	0.30	.
1	A	95	ILE	CD1	15.7	0.30	.
1	A	95	ILE	CG1	24.28	0.30	.
1	A	95	ILE	CG2	22.55	0.30	.
1	A	96	PHE	H	7.74	0.02	.
1	A	96	PHE	HA	3.19	0.02	.
1	A	96	PHE	C	175.42	0.30	.
1	A	96	PHE	CA	60.32	0.30	.
1	A	96	PHE	CB	42.62	0.30	.
1	A	96	PHE	N	120.44	0.30	.
1	A	97	ASP	H	7.54	0.02	.
1	A	97	ASP	HA	4.07	0.02	.
1	A	97	ASP	HB2	2.86	0.02	.
1	A	97	ASP	C	175.2	0.30	.
1	A	97	ASP	CA	58.57	0.30	.
1	A	97	ASP	CB	42.19	0.30	.
1	A	97	ASP	N	119.48	0.30	.
1	A	98	LYS	H	8.15	0.02	.
1	A	98	LYS	C	177.38	0.30	.
1	A	98	LYS	CA	61.07	0.30	.
1	A	98	LYS	CB	32.66	0.30	.
1	A	98	LYS	N	117.31	0.30	.
1	A	99	GLU	HA	3.79	0.02	.
1	A	99	GLU	C	176.36	0.30	.
1	A	99	GLU	CA	60.94	0.30	.
1	A	99	GLU	CB	27.19	0.30	.
1	A	99	GLU	CG	39.79	0.30	.
1	A	100	LYS	H	7.99	0.02	.
1	A	100	LYS	HA	3.85	0.02	.
1	A	100	LYS	C	175.09	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	LYS	CA	59.56	0.30	.
1	A	100	LYS	CB	33.07	0.30	.
1	A	100	LYS	N	118.61	0.30	.
1	A	101	ASN	H	8.08	0.02	.
1	A	101	ASN	HA	4.65	0.02	.
1	A	101	ASN	C	175.67	0.30	.
1	A	101	ASN	CA	57.44	0.30	.
1	A	101	ASN	CB	41.31	0.30	.
1	A	101	ASN	N	119.79	0.30	.
1	A	105	SER	HA	4.18	0.02	.
1	A	105	SER	HB2	3.85	0.02	.
1	A	105	SER	HG	5.65	0.02	.
1	A	105	SER	C	172.85	0.30	.
1	A	105	SER	CA	58.43	0.30	.
1	A	105	SER	CB	65.55	0.30	.
1	A	106	ALA	H	8.81	0.02	.
1	A	106	ALA	HA	4.17	0.02	.
1	A	106	ALA	HB1	1.33	0.02	.
1	A	106	ALA	HB2	1.33	0.02	.
1	A	106	ALA	HB3	1.33	0.02	.
1	A	106	ALA	C	176.59	0.30	.
1	A	106	ALA	CA	56.32	0.30	.
1	A	106	ALA	CB	22.51	0.30	.
1	A	106	ALA	N	125.36	0.30	.
1	A	107	SER	H	8.26	0.02	.
1	A	107	SER	HA	4.12	0.02	.
1	A	107	SER	HB2	3.82	0.02	.
1	A	107	SER	HB3	3.82	0.02	.
1	A	107	SER	C	173.87	0.30	.
1	A	107	SER	CA	61.95	0.30	.
1	A	107	SER	CB	63.23	0.30	.
1	A	107	SER	N	111.89	0.30	.
1	A	108	GLU	H	7.62	0.02	.
1	A	108	GLU	HA	4.07	0.02	.
1	A	108	GLU	HB2	2.25	0.02	.
1	A	108	GLU	HB3	2.22	0.02	.
1	A	108	GLU	C	175.59	0.30	.
1	A	108	GLU	CA	58.94	0.30	.
1	A	108	GLU	CB	30.41	0.30	.
1	A	108	GLU	CG	36.69	0.30	.
1	A	108	GLU	N	122.69	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	LEU	H	7.78	0.02	.
1	A	109	LEU	HA	3.95	0.02	.
1	A	109	LEU	HB2	1.9	0.02	.
1	A	109	LEU	HD11	0.75	0.02	.
1	A	109	LEU	HD12	0.75	0.02	.
1	A	109	LEU	HD13	0.75	0.02	.
1	A	109	LEU	HD21	0.75	0.02	.
1	A	109	LEU	HD22	0.75	0.02	.
1	A	109	LEU	HD23	0.75	0.02	.
1	A	109	LEU	C	177.07	0.30	.
1	A	109	LEU	CA	62.84	0.30	.
1	A	109	LEU	CB	39.6	0.30	.
1	A	109	LEU	CD1	23.85	0.30	.
1	A	109	LEU	CG	26.82	0.30	.
1	A	109	LEU	N	115.15	0.30	.
1	A	110	LYS	H	7.75	0.02	.
1	A	110	LYS	HA	4.47	0.02	.
1	A	110	LYS	HB2	1.92	0.02	.
1	A	110	LYS	C	176.07	0.30	.
1	A	110	LYS	CA	59.7	0.30	.
1	A	110	LYS	CB	33.23	0.30	.
1	A	110	LYS	CG	26.17	0.30	.
1	A	110	LYS	N	118.5	0.30	.
1	A	111	HIS	H	7.76	0.02	.
1	A	111	HIS	HA	3.85	0.02	.
1	A	111	HIS	C	175.32	0.30	.
1	A	111	HIS	CA	59.32	0.30	.
1	A	111	HIS	CB	30.62	0.30	.
1	A	111	HIS	N	119.28	0.30	.
1	A	112	VAL	H	8.02	0.02	.
1	A	112	VAL	C	176.4	0.30	.
1	A	112	VAL	CA	67.21	0.30	.
1	A	112	VAL	CB	32.52	0.30	.
1	A	112	VAL	N	121.09	0.30	.
1	A	113	LEU	HA	4.61	0.02	.
1	A	113	LEU	HB2	2.64	0.02	.
1	A	113	LEU	C	174.53	0.30	.
1	A	113	LEU	CA	55.02	0.30	.
1	A	113	LEU	CB	41.86	0.30	.
1	A	113	LEU	CG	25.52	0.30	.
1	A	114	THR	H	8.28	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	114	THR	HA	4.47	0.02	.
1	A	114	THR	HB	3.85	0.02	.
1	A	114	THR	C	172.25	0.30	.
1	A	114	THR	CA	59.07	0.30	.
1	A	114	THR	CB	64.7	0.30	.
1	A	114	THR	N	116.96	0.30	.
1	A	115	THR	H	8.25	0.02	.
1	A	115	THR	C	172.02	0.30	.
1	A	115	THR	CA	63.26	0.30	.
1	A	115	THR	CB	70.4	0.30	.
1	A	115	THR	CG2	22.14	0.30	.
1	A	115	THR	N	115.99	0.30	.
1	A	116	LEU	H	7.57	0.02	.
1	A	116	LEU	HA	4.82	0.02	.
1	A	116	LEU	HB2	1.66	0.02	.
1	A	116	LEU	HB3	0.83	0.02	.
1	A	116	LEU	HD11	0.39	0.02	.
1	A	116	LEU	HD12	0.39	0.02	.
1	A	116	LEU	HD13	0.39	0.02	.
1	A	116	LEU	HD21	-0.6	0.02	.
1	A	116	LEU	HD22	-0.6	0.02	.
1	A	116	LEU	HD23	-0.6	0.02	.
1	A	116	LEU	C	174.33	0.30	.
1	A	116	LEU	CA	56.06	0.30	.
1	A	116	LEU	CB	42.62	0.30	.
1	A	116	LEU	CG	27.16	0.30	.
1	A	116	LEU	N	120.79	0.30	.
1	A	117	GLY	H	7.97	0.02	.
1	A	117	GLY	HA2	3.97	0.02	.
1	A	117	GLY	HA3	3.88	0.02	.
1	A	117	GLY	C	171.87	0.30	.
1	A	117	GLY	CA	46.79	0.30	.
1	A	117	GLY	N	107.6	0.30	.
1	A	118	GLU	H	8.01	0.02	.
1	A	118	GLU	HA	3.84	0.02	.
1	A	118	GLU	C	173.33	0.30	.
1	A	118	GLU	CA	56.94	0.30	.
1	A	118	GLU	CB	30.64	0.30	.
1	A	118	GLU	N	120.51	0.30	.
1	A	119	LYS	H	8.04	0.02	.
1	A	119	LYS	HA	4.21	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	119	LYS	HB2	1.66	0.02	.
1	A	119	LYS	HB3	1.66	0.02	.
1	A	119	LYS	HG2	1.28	0.02	.
1	A	119	LYS	HG3	1.28	0.02	.
1	A	119	LYS	C	172.97	0.30	.
1	A	119	LYS	CA	56.46	0.30	.
1	A	119	LYS	CB	32.9	0.30	.
1	A	119	LYS	CG	25.44	0.30	.
1	A	119	LYS	N	119.57	0.30	.
1	A	120	LEU	H	7.79	0.02	.
1	A	120	LEU	HA	4.72	0.02	.
1	A	120	LEU	HB2	1.53	0.02	.
1	A	120	LEU	HB3	1.5	0.02	.
1	A	120	LEU	HD11	0.78	0.02	.
1	A	120	LEU	HD12	0.78	0.02	.
1	A	120	LEU	HD13	0.78	0.02	.
1	A	120	LEU	HD21	0.75	0.02	.
1	A	120	LEU	HD22	0.75	0.02	.
1	A	120	LEU	HD23	0.75	0.02	.
1	A	120	LEU	C	174.69	0.30	.
1	A	120	LEU	CA	54.94	0.30	.
1	A	120	LEU	CB	45.37	0.30	.
1	A	120	LEU	CD1	25.06	0.30	.
1	A	120	LEU	CG	28.12	0.30	.
1	A	120	LEU	N	122.71	0.30	.
1	A	121	THR	H	9.02	0.02	.
1	A	121	THR	HA	4.62	0.02	.
1	A	121	THR	HB	4.34	0.02	.
1	A	121	THR	HG21	1.28	0.02	.
1	A	121	THR	HG22	1.28	0.02	.
1	A	121	THR	HG23	1.28	0.02	.
1	A	121	THR	C	171.85	0.30	.
1	A	121	THR	CA	61.58	0.30	.
1	A	121	THR	CB	71.94	0.30	.
1	A	121	THR	CG2	22.55	0.30	.
1	A	121	THR	N	113.69	0.30	.
1	A	122	GLU	H	8.83	0.02	.
1	A	122	GLU	HA	3.77	0.02	.
1	A	122	GLU	HB2	2.26	0.02	.
1	A	122	GLU	HB3	2.26	0.02	.
1	A	122	GLU	C	175.59	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	GLU	CA	61.1	0.30	.
1	A	122	GLU	CB	30.03	0.30	.
1	A	122	GLU	CG	37.29	0.30	.
1	A	122	GLU	N	120.56	0.30	.
1	A	123	GLN	H	8.22	0.02	.
1	A	123	GLN	HA	3.96	0.02	.
1	A	123	GLN	HB2	2.35	0.02	.
1	A	123	GLN	HB3	2.32	0.02	.
1	A	123	GLN	C	174.98	0.30	.
1	A	123	GLN	CA	59.5	0.30	.
1	A	123	GLN	CB	29.17	0.30	.
1	A	123	GLN	CG	34.63	0.30	.
1	A	123	GLN	N	117.61	0.30	.
1	A	124	GLU	H	7.62	0.02	.
1	A	124	GLU	HA	4.01	0.02	.
1	A	124	GLU	HB2	2.28	0.02	.
1	A	124	GLU	HB3	2.25	0.02	.
1	A	124	GLU	C	177.27	0.30	.
1	A	124	GLU	CA	59.82	0.30	.
1	A	124	GLU	CB	31.2	0.30	.
1	A	124	GLU	CG	38.43	0.30	.
1	A	124	GLU	N	118.94	0.30	.
1	A	125	VAL	H	8.14	0.02	.
1	A	125	VAL	HA	3.46	0.02	.
1	A	125	VAL	HG11	0.85	0.02	.
1	A	125	VAL	HG12	0.85	0.02	.
1	A	125	VAL	HG13	0.85	0.02	.
1	A	125	VAL	C	174.21	0.30	.
1	A	125	VAL	CA	68.21	0.30	.
1	A	125	VAL	CB	32.04	0.30	.
1	A	125	VAL	CG1	25.12	0.30	.
1	A	125	VAL	CG2	22.61	0.30	.
1	A	125	VAL	N	120.31	0.30	.
1	A	126	ASP	H	8.13	0.02	.
1	A	126	ASP	HA	4.34	0.02	.
1	A	126	ASP	HB2	2.65	0.02	.
1	A	126	ASP	HB3	2.65	0.02	.
1	A	126	ASP	C	176.52	0.30	.
1	A	126	ASP	CA	58.69	0.30	.
1	A	126	ASP	CB	41.2	0.30	.
1	A	126	ASP	N	120.34	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	ASP	H	7.88	0.02	.
1	A	127	ASP	HA	4.12	0.02	.
1	A	127	ASP	HB2	1.93	0.02	.
1	A	127	ASP	HB3	0.78	0.02	.
1	A	127	ASP	C	176.18	0.30	.
1	A	127	ASP	CA	58.88	0.30	.
1	A	127	ASP	CB	43.05	0.30	.
1	A	127	ASP	N	122.89	0.30	.
1	A	128	LEU	H	8.34	0.02	.
1	A	128	LEU	C	176.84	0.30	.
1	A	128	LEU	CA	58.57	0.30	.
1	A	128	LEU	CB	41.58	0.30	.
1	A	128	LEU	N	117.88	0.30	.
1	A	129	LEU	H	7.76	0.02	.
1	A	129	LEU	HA	3.85	0.02	.
1	A	129	LEU	HB2	2.59	0.02	.
1	A	129	LEU	HG	1.98	0.02	.
1	A	129	LEU	C	173.58	0.30	.
1	A	129	LEU	CA	56.19	0.30	.
1	A	129	LEU	CB	40.86	0.30	.
1	A	129	LEU	CG	25.68	0.30	.
1	A	129	LEU	N	115.39	0.30	.
1	A	130	LYS	H	7.94	0.02	.
1	A	130	LYS	C	172.86	0.30	.
1	A	130	LYS	CA	61.77	0.30	.
1	A	130	LYS	CB	32.52	0.30	.
1	A	130	LYS	CE	40.73	0.30	.
1	A	130	LYS	N	121.46	0.30	.
1	A	131	GLU	H	9.01	0.02	.
1	A	131	GLU	C	173.23	0.30	.
1	A	131	GLU	CA	62.22	0.30	.
1	A	131	GLU	CB	32.52	0.30	.
1	A	131	GLU	CG	37.28	0.30	.
1	A	131	GLU	N	125.87	0.30	.
1	A	132	ILE	H	8.58	0.02	.
1	A	132	ILE	HA	4.17	0.02	.
1	A	132	ILE	HB	1.94	0.02	.
1	A	132	ILE	HD11	0.88	0.02	.
1	A	132	ILE	HD12	0.88	0.02	.
1	A	132	ILE	HD13	0.88	0.02	.
1	A	132	ILE	HG12	1.61	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	132	ILE	HG13	1.32	0.02	.
1	A	132	ILE	HG21	0.92	0.02	.
1	A	132	ILE	HG22	0.92	0.02	.
1	A	132	ILE	HG23	0.92	0.02	.
1	A	132	ILE	C	173.11	0.30	.
1	A	132	ILE	CA	63.23	0.30	.
1	A	132	ILE	CB	40.21	0.30	.
1	A	132	ILE	CD1	15.18	0.30	.
1	A	132	ILE	CG1	28.61	0.30	.
1	A	132	ILE	CG2	18.79	0.30	.
1	A	132	ILE	N	118.45	0.30	.
1	A	133	GLY	H	7.87	0.02	.
1	A	133	GLY	HA2	4.09	0.02	.
1	A	133	GLY	HA3	3.82	0.02	.
1	A	133	GLY	C	171.05	0.30	.
1	A	133	GLY	CA	46.64	0.30	.
1	A	133	GLY	N	109.87	0.30	.
1	A	134	VAL	H	7.89	0.02	.
1	A	134	VAL	HA	4.09	0.02	.
1	A	134	VAL	HB	2.64	0.02	.
1	A	134	VAL	C	174.08	0.30	.
1	A	134	VAL	CA	62.7	0.30	.
1	A	134	VAL	CB	32.68	0.30	.
1	A	134	VAL	CG1	26.26	0.30	.
1	A	134	VAL	CG2	26.26	0.30	.
1	A	134	VAL	N	120.16	0.30	.
1	A	135	GLU	H	7.48	0.02	.
1	A	135	GLU	C	175.26	0.30	.
1	A	135	GLU	CA	57.44	0.30	.
1	A	135	GLU	CB	30.52	0.30	.
1	A	135	GLU	N	118.41	0.30	.
1	A	136	GLU	H	7.92	0.02	.
1	A	136	GLU	HA	4.12	0.02	.
1	A	136	GLU	HB2	2.16	0.02	.
1	A	136	GLU	HB3	2.16	0.02	.
1	A	136	GLU	C	171.14	0.30	.
1	A	136	GLU	CA	57.24	0.30	.
1	A	136	GLU	CB	30.02	0.30	.
1	A	136	GLU	CG	36.98	0.30	.
1	A	136	GLU	N	121.56	0.30	.
1	A	137	GLY	H	8.17	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	GLY	HA2	3.99	0.02	.
1	A	137	GLY	HA3	3.69	0.02	.
1	A	137	GLY	C	173.67	0.30	.
1	A	137	GLY	CA	46.17	0.30	.
1	A	137	GLY	N	106.3	0.30	.
1	A	138	LEU	H	7.83	0.02	.
1	A	138	LEU	C	170.6	0.30	.
1	A	138	LEU	CA	54.94	0.30	.
1	A	138	LEU	CB	41.73	0.30	.
1	A	138	LEU	N	120.51	0.30	.
1	A	139	ILE	H	7.92	0.02	.
1	A	139	ILE	HA	4.07	0.02	.
1	A	139	ILE	HB	1.82	0.02	.
1	A	139	ILE	HD11	0.8	0.02	.
1	A	139	ILE	HD12	0.8	0.02	.
1	A	139	ILE	HD13	0.8	0.02	.
1	A	139	ILE	HG12	1.39	0.02	.
1	A	139	ILE	HG13	1.16	0.02	.
1	A	139	ILE	HG21	0.84	0.02	.
1	A	139	ILE	HG22	0.84	0.02	.
1	A	139	ILE	HG23	0.84	0.02	.
1	A	139	ILE	C	180.56	0.30	.
1	A	139	ILE	CA	62.07	0.30	.
1	A	139	ILE	CB	39.38	0.30	.
1	A	139	ILE	CD1	13.91	0.30	.
1	A	139	ILE	CG1	21.78	0.30	.
1	A	139	ILE	CG2	18.23	0.30	.
1	A	139	ILE	N	120.94	0.30	.
1	A	140	ASN	H	8.26	0.02	.
1	A	140	ASN	C	172.58	0.30	.
1	A	140	ASN	CA	56.94	0.30	.
1	A	140	ASN	CB	39.28	0.30	.
1	A	140	ASN	N	125.93	0.30	.
1	A	142	ASP	HA	4.3	0.02	.
1	A	142	ASP	HB2	2.64	0.02	.
1	A	142	ASP	C	176.46	0.30	.
1	A	142	ASP	CA	58.63	0.30	.
1	A	142	ASP	CB	41.01	0.30	.
1	A	143	ASP	H	8.23	0.02	.
1	A	143	ASP	HA	3.85	0.02	.
1	A	143	ASP	HB2	2.51	0.02	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	143	ASP	C	176.3	0.30	.
1	A	143	ASP	CA	58.27	0.30	.
1	A	143	ASP	CB	41.13	0.30	.
1	A	143	ASP	N	119.5	0.30	.
1	A	144	PHE	H	8.08	0.02	.
1	A	144	PHE	HA	4.23	0.02	.
1	A	144	PHE	HB2	2.65	0.02	.
1	A	144	PHE	HB3	2.21	0.02	.
1	A	144	PHE	C	175.59	0.30	.
1	A	144	PHE	CA	57.38	0.30	.
1	A	144	PHE	CB	36.87	0.30	.
1	A	144	PHE	N	119.84	0.30	.
1	A	145	VAL	H	8.06	0.02	.
1	A	145	VAL	HA	4.16	0.02	.
1	A	145	VAL	HB	1.96	0.02	.
1	A	145	VAL	HG11	0.84	0.02	.
1	A	145	VAL	HG12	0.84	0.02	.
1	A	145	VAL	HG13	0.84	0.02	.
1	A	145	VAL	HG21	0.8	0.02	.
1	A	145	VAL	HG22	0.8	0.02	.
1	A	145	VAL	HG23	0.8	0.02	.
1	A	145	VAL	C	173.02	0.30	.
1	A	145	VAL	CA	63.08	0.30	.
1	A	145	VAL	CB	33.8	0.30	.
1	A	145	VAL	CG1	21.99	0.30	.
1	A	145	VAL	CG2	21.7	0.30	.
1	A	145	VAL	N	120.73	0.30	.
1	A	146	LYS	H	8.58	0.02	.
1	A	146	LYS	HA	4.22	0.02	.
1	A	146	LYS	C	174.59	0.30	.
1	A	146	LYS	CA	57.19	0.30	.
1	A	146	LYS	CB	31.5	0.30	.
1	A	146	LYS	N	125.08	0.30	.
1	A	147	LEU	H	8.25	0.02	.
1	A	147	LEU	C	172.66	0.30	.
1	A	147	LEU	CA	55.27	0.30	.
1	A	147	LEU	CB	41.87	0.30	.
1	A	147	LEU	N	121.9	0.30	.
1	A	148	ILE	HA	4.48	0.02	.
1	A	148	ILE	HB	2.21	0.02	.
1	A	148	ILE	C	173.16	0.30	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	148	ILE	CA	62.42	0.30	.
1	A	148	ILE	CB	37.06	0.30	.
1	A	148	ILE	CG1	30.94	0.30	.
1	A	149	THR	H	7.99	0.02	.
1	A	149	THR	HA	4.29	0.02	.
1	A	149	THR	HG21	1.17	0.02	.
1	A	149	THR	HG22	1.17	0.02	.
1	A	149	THR	HG23	1.17	0.02	.
1	A	149	THR	C	174.52	0.30	.
1	A	149	THR	CA	63.17	0.30	.
1	A	149	THR	CB	71.9	0.30	.
1	A	149	THR	CG2	22.53	0.30	.
1	A	149	THR	N	120.53	0.30	.
1	A	150	SER	H	7.56	0.02	.
1	A	150	SER	HA	4.39	0.02	.
1	A	150	SER	HB2	3.92	0.02	.
1	A	150	SER	HB3	3.88	0.02	.
1	A	150	SER	C	170.61	0.30	.
1	A	150	SER	CA	59.95	0.30	.
1	A	150	SER	CB	64.73	0.30	.
1	A	150	SER	N	117.37	0.30	.
1	A	151	LYS	H	7.5	0.02	.
1	A	151	LYS	HA	4.13	0.02	.
1	A	151	LYS	HB2	1.73	0.02	.
1	A	151	LYS	HB3	1.7	0.02	.
1	A	151	LYS	HG2	1.37	0.02	.
1	A	151	LYS	C	178.48	0.30	.
1	A	151	LYS	CA	58.33	0.30	.
1	A	151	LYS	CB	34.2	0.30	.
1	A	151	LYS	N	127.6	0.30	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	-1.09 ± 0.14	Should be checked
$^{13}C_{\beta}$	136	-0.54 ± 0.15	Should be checked
$^{13}C'$	144	2.52 ± 0.08	Should be applied
^{15}N	135	0.47 ± 0.49	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 79%, i.e. 780 atoms were assigned a chemical shift out of a possible 987. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	367/367 (100%)	149/149 (100%)	146/146 (100%)	72/72 (100%)
Sidechain	413/553 (75%)	261/352 (74%)	152/181 (84%)	0/20 (0%)
Aromatic	0/67 (0%)	0/32 (0%)	0/35 (0%)	0/0 (—%)
Overall	780/987 (79%)	410/533 (77%)	298/362 (82%)	72/92 (78%)

7.1.4 Statistically unusual chemical shifts

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.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	127	ASP	HB3	0.78	1.32 – 4.00	-7.0

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: