Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 01:06 AM BST

PDB ID	:	2LC5
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 Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

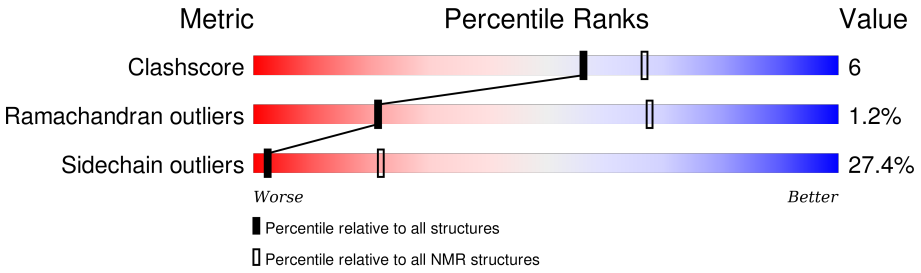
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	85	61% 24% • 14%

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)	0.51	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

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
1	A	85	Total	C	H	N	O	S	0
			1348	426	663	109	147	3	

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

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

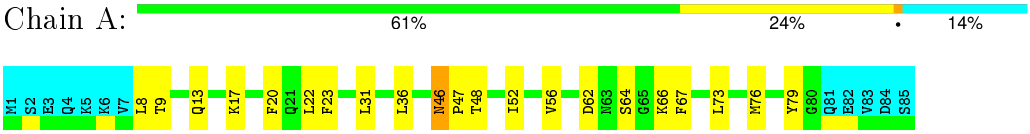
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

Chain A:



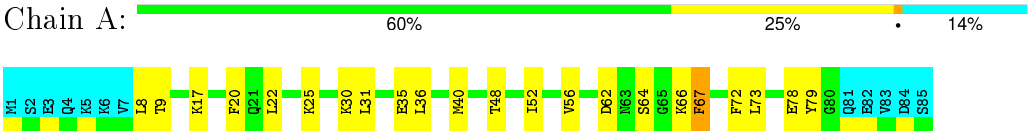
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin, putative

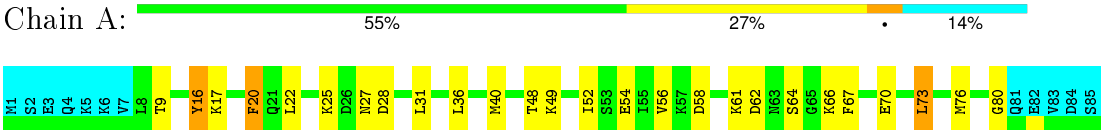
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin, putative

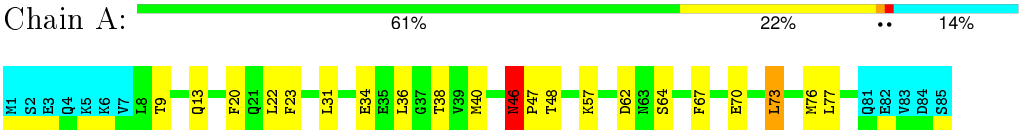
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Calmodulin, putative

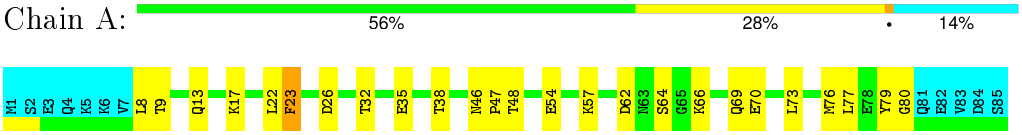
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Calmodulin, putative

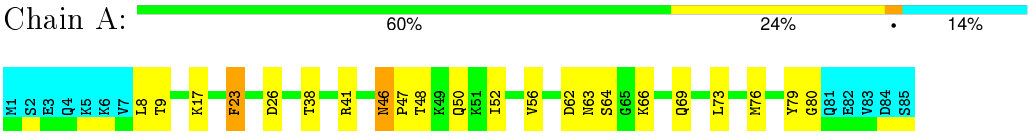
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Calmodulin, putative

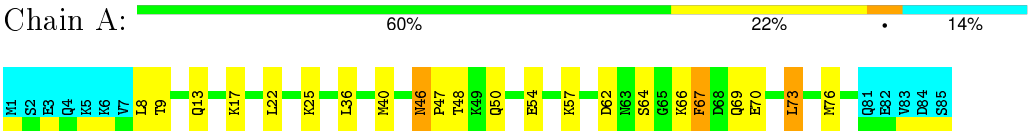
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Calmodulin, putative

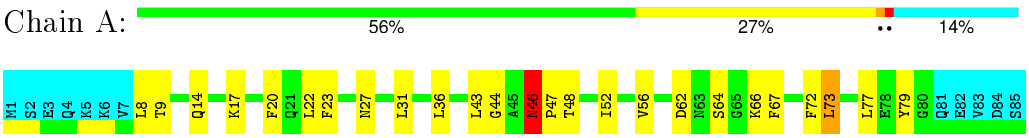
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Calmodulin, putative

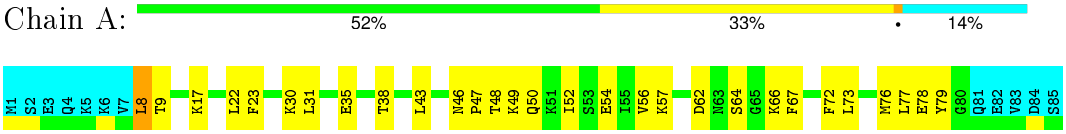
Chain A:



4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Calmodulin, putative

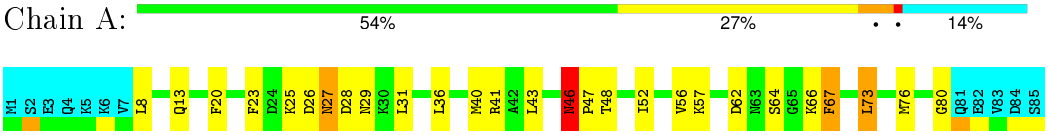
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Calmodulin, putative

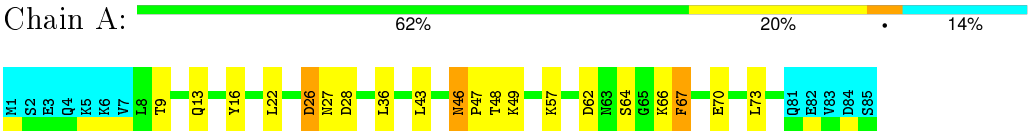
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Calmodulin, putative

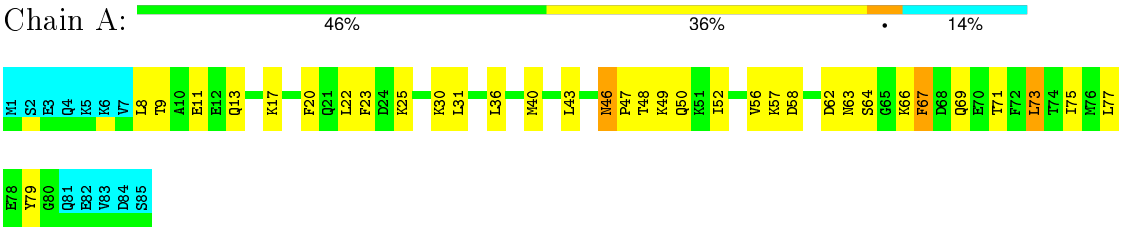
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Calmodulin, putative

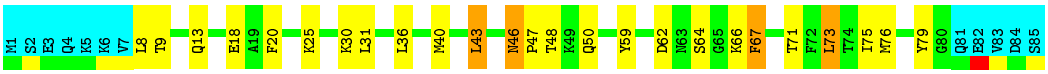
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Calmodulin, putative

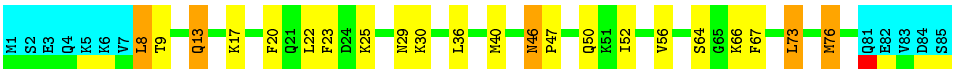
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin, putative

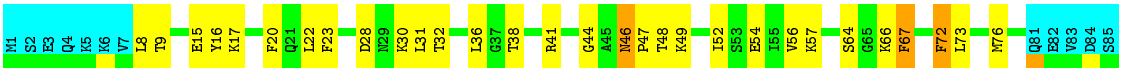
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin, putative

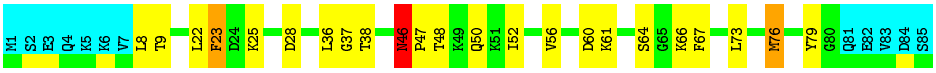
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin, putative

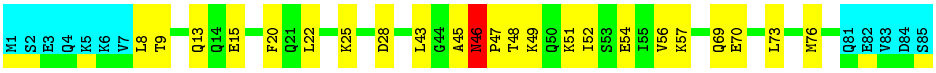
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin, putative

Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin, putative

Chain A:

4.2.18 Score per residue for model 18

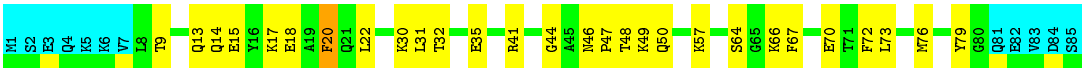
- Molecule 1: Calmodulin, putative

Chain A:

4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin, putative

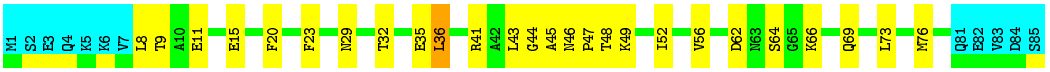
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin, putative

Chain A:



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)	2lc5_cs.str
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)	77%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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.

All 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
1:A:23:PHE:CZ	1:A:38:THR:HG21	0.61	2.30	4	6
1:A:32:THR:HG22	1:A:35:GLU:OE2	0.60	1.95	4	1
1:A:13:GLN:CD	1:A:73:LEU:HD21	0.60	2.16	9	3
1:A:8:LEU:HD21	1:A:76:MET:O	0.59	1.97	13	1
1:A:16:TYR:CE2	1:A:73:LEU:HD12	0.59	2.32	2	1
1:A:20:PHE:HB2	1:A:31:LEU:HD21	0.58	1.76	19	2
1:A:20:PHE:CD2	1:A:31:LEU:HD22	0.58	2.33	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD12	1:A:35:GLU:HB3	0.58	1.75	1	2
1:A:36:LEU:HD22	1:A:67:PHE:CE1	0.57	2.34	2	7
1:A:30:LYS:O	1:A:31:LEU:HD12	0.57	2.00	11	2
1:A:30:LYS:C	1:A:31:LEU:HD22	0.56	2.20	8	2
1:A:17:LYS:HD3	1:A:73:LEU:HD11	0.56	1.78	11	3
1:A:32:THR:HG22	1:A:66:LYS:CE	0.55	2.31	14	1
1:A:20:PHE:O	1:A:31:LEU:HD11	0.54	2.02	3	2
1:A:36:LEU:CD2	1:A:56:VAL:HG21	0.54	2.33	15	2
1:A:36:LEU:HD23	1:A:56:VAL:HG11	0.53	1.81	17	1
1:A:36:LEU:HD13	1:A:67:PHE:CD2	0.52	2.39	7	4
1:A:71:THR:HG22	1:A:75:ILE:HD11	0.49	1.84	11	2
1:A:43:LEU:HD13	1:A:43:LEU:O	0.49	2.08	12	1
1:A:36:LEU:O	1:A:36:LEU:HD13	0.49	2.07	20	1
1:A:36:LEU:HD22	1:A:67:PHE:CZ	0.49	2.43	7	2
1:A:31:LEU:HD12	1:A:35:GLU:CB	0.49	2.37	1	2
1:A:71:THR:HG22	1:A:75:ILE:CD1	0.49	2.38	11	2
1:A:36:LEU:HD22	1:A:67:PHE:CD1	0.48	2.43	12	2
1:A:32:THR:HG23	1:A:35:GLU:OE1	0.47	2.09	19	1
1:A:46:ASN:CB	1:A:47:PRO:CD	0.47	2.93	17	18
1:A:32:THR:HG23	1:A:35:GLU:OE2	0.47	2.10	20	1
1:A:36:LEU:HD21	1:A:56:VAL:HG21	0.47	1.86	15	1
1:A:52:ILE:O	1:A:56:VAL:HG13	0.46	2.10	17	1
1:A:41:ARG:O	1:A:45:ALA:HB2	0.46	2.11	20	1
1:A:36:LEU:HD23	1:A:56:VAL:HG21	0.45	1.88	18	1
1:A:32:THR:HG22	1:A:66:LYS:HE2	0.45	1.89	14	1
1:A:16:TYR:CZ	1:A:73:LEU:HD12	0.45	2.47	2	1
1:A:13:GLN:CG	1:A:73:LEU:HD11	0.45	2.41	13	1
1:A:8:LEU:HD23	1:A:8:LEU:O	0.45	2.12	6	1
1:A:23:PHE:CE2	1:A:38:THR:HG21	0.44	2.47	5	1
1:A:13:GLN:HG3	1:A:73:LEU:HD21	0.44	1.88	3	1
1:A:30:LYS:O	1:A:31:LEU:HD13	0.44	2.13	14	2
1:A:46:ASN:N	1:A:47:PRO:HD2	0.43	2.28	18	18
1:A:31:LEU:HD12	1:A:35:GLU:CD	0.43	2.33	8	2
1:A:69:GLN:O	1:A:73:LEU:HD12	0.43	2.13	6	3
1:A:8:LEU:HD11	1:A:77:LEU:CD2	0.43	2.43	4	1
1:A:36:LEU:HD13	1:A:67:PHE:CE2	0.43	2.49	2	1
1:A:13:GLN:HG3	1:A:73:LEU:HD11	0.42	1.91	13	1
1:A:20:PHE:HD2	1:A:31:LEU:HD13	0.42	1.73	3	1
1:A:20:PHE:HB2	1:A:31:LEU:HD13	0.42	1.90	9	2
1:A:8:LEU:HD13	1:A:76:MET:CE	0.42	2.44	15	1
1:A:77:LEU:HD13	1:A:77:LEU:C	0.42	2.35	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:THR:HG22	1:A:66:LYS:NZ	0.42	2.29	14	1
1:A:52:ILE:O	1:A:56:VAL:HG22	0.42	2.15	17	1
1:A:8:LEU:HD13	1:A:80:GLY:O	0.41	2.14	9	1
1:A:8:LEU:HD11	1:A:76:MET:CE	0.41	2.46	6	1
1:A:20:PHE:CG	1:A:31:LEU:HD13	0.41	2.50	2	1
1:A:36:LEU:CD2	1:A:56:VAL:HG11	0.41	2.45	17	1
1:A:16:TYR:HH	1:A:72:PHE:HD2	0.41	1.56	14	1
1:A:37:GLY:HA2	1:A:52:ILE:HD12	0.41	1.93	15	1
1:A:20:PHE:HB3	1:A:31:LEU:HD13	0.41	1.93	7	1
1:A:36:LEU:HD13	1:A:67:PHE:CZ	0.40	2.50	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/85 (86%)	66±1 (90±2%)	6±1 (8±2%)	1±1 (1±1%)	21	68
All	All	1460/1700 (86%)	1321 (90%)	121 (8%)	18 (1%)	21	68

All 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	45	ALA	1
1	A	27	ASN	1
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	64/76 (84%)	46±2 (73±3%)	18±2 (27±3%)	2 22
All	All	1280/1520 (84%)	929 (73%)	351 (27%)	2 22

All 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	73	LEU	19
1	A	64	SER	19
1	A	9	THR	19
1	A	48	THR	18
1	A	66	LYS	17
1	A	22	LEU	16
1	A	76	MET	15
1	A	46	ASN	13
1	A	62	ASP	13
1	A	67	PHE	13
1	A	8	LEU	11
1	A	79	TYR	11
1	A	25	LYS	10
1	A	57	LYS	10
1	A	40	MET	9
1	A	23	PHE	9
1	A	50	GLN	9
1	A	49	LYS	9
1	A	70	GLU	8
1	A	17	LYS	8
1	A	20	PHE	8
1	A	13	GLN	8
1	A	54	GLU	7
1	A	28	ASP	6
1	A	43	LEU	6
1	A	72	PHE	5
1	A	26	ASP	4
1	A	15	GLU	4
1	A	41	ARG	4
1	A	27	ASN	4
1	A	69	GLN	4
1	A	29	ASN	4
1	A	77	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	78	GLU	3
1	A	30	LYS	3
1	A	59	TYR	2
1	A	16	TYR	2
1	A	63	ASN	2
1	A	14	GLN	2
1	A	18	GLU	2
1	A	51	LYS	2
1	A	61	LYS	2
1	A	11	GLU	2
1	A	58	ASP	2
1	A	60	ASP	1
1	A	35	GLU	1
1	A	36	LEU	1
1	A	34	GLU	1

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 carbohydrates 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 77% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: 2lc5_cs.str

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.

- Residue not found in structure. All 495 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	111	HIS	H	7.76	0.02	1
A	95	ILE	HG21	0.24	0.02	1
A	139	ILE	HG13	1.16	0.02	1
A	119	LYS	N	119.57	0.3	1
A	114	THR	HB	3.85	0.02	1
A	136	GLU	CA	57.24	0.3	1
A	136	GLU	HB2	2.16	0.02	1
A	87	GLU	H	8.21	0.02	1
A	107	SER	C	173.87	0.3	1
A	95	ILE	CG1	24.28	0.3	1
A	146	LYS	C	174.59	0.3	1
A	128	LEU	CA	58.57	0.3	1
A	97	ASP	HA	4.07	0.02	1
A	144	PHE	C	175.59	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	91	LYS	HA	4.75	0.02	1
A	121	THR	HG22	1.28	0.02	1
A	116	LEU	HB3	0.83	0.02	1
A	132	ILE	HG12	1.61	0.02	1
A	90	LYS	N	125.39	0.3	1
A	139	ILE	CB	39.38	0.3	1
A	137	GLY	CA	46.17	0.3	1
A	138	LEU	N	120.51	0.3	1
A	135	GLU	CA	57.44	0.3	1
A	110	LYS	H	7.75	0.02	1
A	120	LEU	H	7.79	0.02	1
A	127	ASP	C	176.18	0.3	1
A	87	GLU	C	173.77	0.3	1
A	134	VAL	C	174.08	0.3	1
A	97	ASP	CA	58.57	0.3	1
A	116	LEU	HD23	-0.6	0.02	1
A	105	SER	HB2	3.85	0.02	1
A	151	LYS	CA	58.33	0.3	1
A	119	LYS	HA	4.21	0.02	1
A	96	PHE	HA	3.19	0.02	1
A	108	GLU	N	122.69	0.3	1
A	151	LYS	HG2	1.37	0.02	1
A	127	ASP	CA	58.88	0.3	1
A	124	GLU	CA	59.82	0.3	1
A	132	ILE	HG21	0.92	0.02	1
A	120	LEU	CB	45.37	0.3	1
A	113	LEU	CG	25.52	0.3	1
A	97	ASP	C	175.2	0.3	1
A	142	ASP	C	176.46	0.3	1
A	98	LYS	H	8.15	0.02	1
A	135	GLU	N	118.41	0.3	1
A	88	ASP	C	175.59	0.3	1
A	115	THR	H	8.25	0.02	1
A	91	LYS	C	172.83	0.3	1
A	111	HIS	HA	3.85	0.02	1
A	110	LYS	N	118.5	0.3	1
A	86	THR	HG23	1.17	0.02	1
A	132	ILE	C	173.11	0.3	1
A	93	PHE	N	117.94	0.3	1
A	124	GLU	N	118.94	0.3	1
A	105	SER	CB	65.55	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	143	ASP	C	176.3	0.3	1
A	122	GLU	HB2	2.26	0.02	1
A	115	THR	CG2	22.14	0.3	1
A	118	GLU	N	120.51	0.3	1
A	151	LYS	HB3	1.7	0.02	1
A	130	LYS	CE	40.73	0.3	1
A	111	HIS	N	119.28	0.3	1
A	120	LEU	CG	28.12	0.3	1
A	86	THR	CA	65.57	0.3	1
A	134	VAL	HA	4.09	0.02	1
A	110	LYS	CA	59.7	0.3	1
A	148	ILE	CA	62.42	0.3	1
A	117	GLY	C	171.87	0.3	1
A	144	PHE	HB3	2.21	0.02	1
A	116	LEU	CB	42.62	0.3	1
A	97	ASP	H	7.54	0.02	1
A	145	VAL	HG12	0.84	0.02	1
A	91	LYS	H	8.3	0.02	1
A	128	LEU	CB	41.58	0.3	1
A	86	THR	C	172.75	0.3	1
A	121	THR	HG21	1.28	0.02	1
A	129	LEU	CA	56.19	0.3	1
A	146	LYS	HA	4.22	0.02	1
A	139	ILE	H	7.92	0.02	1
A	117	GLY	CA	46.79	0.3	1
A	120	LEU	HD23	0.75	0.02	1
A	118	GLU	CA	56.94	0.3	1
A	139	ILE	HG21	0.84	0.02	1
A	112	VAL	H	8.02	0.02	1
A	109	LEU	H	7.78	0.02	1
A	125	VAL	HA	3.46	0.02	1
A	86	THR	N	116.27	0.3	1
A	113	LEU	HA	4.61	0.02	1
A	116	LEU	H	7.57	0.02	1
A	109	LEU	CG	26.82	0.3	1
A	137	GLY	HA2	3.99	0.02	1
A	129	LEU	C	173.58	0.3	1
A	128	LEU	H	8.34	0.02	1
A	105	SER	HG	5.65	0.02	1
A	120	LEU	HB3	1.5	0.02	1
A	101	ASN	HA	4.65	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	124	GLU	CB	31.2	0.3	1
A	131	GLU	CA	62.22	0.3	1
A	149	THR	C	174.52	0.3	1
A	139	ILE	HG12	1.39	0.02	1
A	111	HIS	CB	30.62	0.3	1
A	117	GLY	N	107.6	0.3	1
A	126	ASP	HB3	2.65	0.02	1
A	122	GLU	CA	61.1	0.3	1
A	117	GLY	HA3	3.88	0.02	1
A	134	VAL	CA	62.7	0.3	1
A	150	SER	N	117.37	0.3	1
A	145	VAL	HG21	0.8	0.02	1
A	140	ASN	H	8.26	0.02	1
A	86	THR	H	8.34	0.02	1
A	107	SER	HA	4.12	0.02	1
A	116	LEU	HD13	0.39	0.02	1
A	100	LYS	C	175.09	0.3	1
A	132	ILE	CG2	18.79	0.3	1
A	120	LEU	HD11	0.78	0.02	1
A	105	SER	CA	58.43	0.3	1
A	149	THR	CG2	22.53	0.3	1
A	112	VAL	N	121.09	0.3	1
A	100	LYS	N	118.61	0.3	1
A	107	SER	N	111.89	0.3	1
A	110	LYS	CG	26.17	0.3	1
A	134	VAL	N	120.16	0.3	1
A	140	ASN	CB	39.28	0.3	1
A	86	THR	CB	69.87	0.3	1
A	147	LEU	N	121.9	0.3	1
A	129	LEU	HA	3.85	0.02	1
A	148	ILE	CB	37.06	0.3	1
A	92	ALA	CA	54.28	0.3	1
A	146	LYS	H	8.58	0.02	1
A	116	LEU	CA	56.06	0.3	1
A	119	LYS	CB	32.9	0.3	1
A	134	VAL	CG1	26.26	0.3	1
A	145	VAL	HG11	0.84	0.02	1
A	113	LEU	HB2	2.64	0.02	1
A	110	LYS	HA	4.47	0.02	1
A	109	LEU	HD23	0.75	0.02	1
A	125	VAL	HG12	0.85	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	145	VAL	CG2	21.7	0.3	1
A	107	SER	CA	61.95	0.3	1
A	86	THR	HA	4.24	0.02	1
A	90	LYS	CB	33.63	0.3	1
A	150	SER	C	170.61	0.3	1
A	144	PHE	CA	57.38	0.3	1
A	91	LYS	HB2	2.1	0.02	1
A	138	LEU	CB	41.73	0.3	1
A	89	ILE	C	172.26	0.3	1
A	130	LYS	CA	61.77	0.3	1
A	146	LYS	CB	31.5	0.3	1
A	132	ILE	HD12	0.88	0.02	1
A	126	ASP	CA	58.69	0.3	1
A	132	ILE	HA	4.17	0.02	1
A	150	SER	CB	64.73	0.3	1
A	121	THR	CG2	22.55	0.3	1
A	119	LYS	CG	25.44	0.3	1
A	136	GLU	HA	4.12	0.02	1
A	108	GLU	HA	4.07	0.02	1
A	145	VAL	HB	1.96	0.02	1
A	143	ASP	HA	3.85	0.02	1
A	124	GLU	HB2	2.28	0.02	1
A	106	ALA	HA	4.17	0.02	1
A	124	GLU	CG	38.43	0.3	1
A	90	LYS	H	8.25	0.02	1
A	150	SER	HB3	3.88	0.02	1
A	120	LEU	N	122.71	0.3	1
A	132	ILE	HG13	1.32	0.02	1
A	135	GLU	CB	30.52	0.3	1
A	142	ASP	HA	4.3	0.02	1
A	142	ASP	CA	58.63	0.3	1
A	150	SER	HA	4.39	0.02	1
A	139	ILE	CG1	21.78	0.3	1
A	120	LEU	CD1	25.06	0.3	1
A	134	VAL	CB	32.68	0.3	1
A	123	GLN	CA	59.5	0.3	1
A	147	LEU	CB	41.87	0.3	1
A	135	GLU	C	175.26	0.3	1
A	99	GLU	CA	60.94	0.3	1
A	115	THR	C	172.02	0.3	1
A	144	PHE	N	119.84	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	151	LYS	CB	34.2	0.3	1
A	113	LEU	C	174.53	0.3	1
A	125	VAL	H	8.14	0.02	1
A	145	VAL	HA	4.16	0.02	1
A	120	LEU	HD12	0.78	0.02	1
A	86	THR	CG2	22.37	0.3	1
A	114	THR	C	172.25	0.3	1
A	98	LYS	N	117.31	0.3	1
A	129	LEU	HB2	2.59	0.02	1
A	101	ASN	N	119.79	0.3	1
A	97	ASP	CB	42.19	0.3	1
A	135	GLU	H	7.48	0.02	1
A	151	LYS	C	178.48	0.3	1
A	143	ASP	CA	58.27	0.3	1
A	99	GLU	C	176.36	0.3	1
A	125	VAL	HG11	0.85	0.02	1
A	151	LYS	HB2	1.73	0.02	1
A	109	LEU	HD13	0.75	0.02	1
A	87	GLU	HB3	1.93	0.02	1
A	127	ASP	HB3	0.78	0.02	1
A	146	LYS	N	125.08	0.3	1
A	108	GLU	C	175.59	0.3	1
A	109	LEU	N	115.15	0.3	1
A	90	LYS	C	173.46	0.3	1
A	119	LYS	HG3	1.28	0.02	1
A	106	ALA	C	176.59	0.3	1
A	126	ASP	H	8.13	0.02	1
A	91	LYS	CA	54.51	0.3	1
A	121	THR	H	9.02	0.02	1
A	114	THR	N	116.96	0.3	1
A	118	GLU	H	8.01	0.02	1
A	148	ILE	HB	2.21	0.02	1
A	128	LEU	N	117.88	0.3	1
A	129	LEU	CG	25.68	0.3	1
A	122	GLU	HB3	2.26	0.02	1
A	116	LEU	HA	4.82	0.02	1
A	90	LYS	CA	56.92	0.3	1
A	137	GLY	N	106.3	0.3	1
A	138	LEU	CA	54.94	0.3	1
A	118	GLU	C	173.33	0.3	1
A	109	LEU	HA	3.95	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	132	ILE	HD11	0.88	0.02	1
A	126	ASP	CB	41.2	0.3	1
A	97	ASP	N	119.48	0.3	1
A	124	GLU	HA	4.01	0.02	1
A	127	ASP	HA	4.12	0.02	1
A	115	THR	CA	63.26	0.3	1
A	139	ILE	HD11	0.8	0.02	1
A	95	ILE	HG23	0.24	0.02	1
A	144	PHE	CB	36.87	0.3	1
A	144	PHE	HB2	2.65	0.02	1
A	151	LYS	N	127.6	0.3	1
A	108	GLU	CG	36.69	0.3	1
A	105	SER	HA	4.18	0.02	1
A	110	LYS	C	176.07	0.3	1
A	148	ILE	C	173.16	0.3	1
A	96	PHE	C	175.42	0.3	1
A	108	GLU	H	7.62	0.02	1
A	120	LEU	HD22	0.75	0.02	1
A	93	PHE	C	175.09	0.3	1
A	106	ALA	H	8.81	0.02	1
A	131	GLU	H	9.01	0.02	1
A	100	LYS	H	7.99	0.02	1
A	139	ILE	HG22	0.84	0.02	1
A	121	THR	C	171.85	0.3	1
A	89	ILE	CB	39.63	0.3	1
A	107	SER	H	8.26	0.02	1
A	123	GLN	CB	29.17	0.3	1
A	89	ILE	HA	4.06	0.02	1
A	120	LEU	HA	4.72	0.02	1
A	144	PHE	H	8.08	0.02	1
A	97	ASP	HB2	2.86	0.02	1
A	116	LEU	HD21	-0.6	0.02	1
A	99	GLU	CB	27.19	0.3	1
A	106	ALA	HB1	1.33	0.02	1
A	107	SER	HB3	3.82	0.02	1
A	98	LYS	C	177.38	0.3	1
A	93	PHE	CA	59.04	0.3	1
A	114	THR	CB	64.7	0.3	1
A	101	ASN	C	175.67	0.3	1
A	124	GLU	C	177.27	0.3	1
A	149	THR	HG23	1.17	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	139	ILE	CD1	13.91	0.3	1
A	117	GLY	H	7.97	0.02	1
A	149	THR	CB	71.9	0.3	1
A	131	GLU	CB	32.52	0.3	1
A	132	ILE	HG23	0.92	0.02	1
A	112	VAL	C	176.4	0.3	1
A	89	ILE	CD1	13.85	0.3	1
A	122	GLU	CB	30.03	0.3	1
A	87	GLU	CB	30.63	0.3	1
A	95	ILE	HB	0.84	0.02	1
A	91	LYS	HG2	1.33	0.02	1
A	117	GLY	HA2	3.97	0.02	1
A	129	LEU	HG	1.98	0.02	1
A	149	THR	HG21	1.17	0.02	1
A	112	VAL	CA	67.21	0.3	1
A	123	GLN	HB2	2.35	0.02	1
A	121	THR	HA	4.62	0.02	1
A	86	THR	HG21	1.17	0.02	1
A	145	VAL	HG22	0.8	0.02	1
A	143	ASP	HB2	2.51	0.02	1
A	149	THR	H	7.99	0.02	1
A	116	LEU	HD12	0.39	0.02	1
A	132	ILE	CG1	28.61	0.3	1
A	139	ILE	HA	4.07	0.02	1
A	145	VAL	C	173.02	0.3	1
A	125	VAL	CG1	25.12	0.3	1
A	122	GLU	HA	3.77	0.02	1
A	87	GLU	HA	4.67	0.02	1
A	115	THR	CB	70.4	0.3	1
A	89	ILE	H	8.07	0.02	1
A	139	ILE	HD12	0.8	0.02	1
A	145	VAL	CA	63.08	0.3	1
A	139	ILE	CA	62.07	0.3	1
A	134	VAL	CG2	26.26	0.3	1
A	119	LYS	C	172.97	0.3	1
A	149	THR	N	120.53	0.3	1
A	131	GLU	N	125.87	0.3	1
A	116	LEU	C	174.33	0.3	1
A	92	ALA	HB3	1.28	0.02	1
A	122	GLU	N	120.56	0.3	1
A	101	ASN	H	8.08	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	91	LYS	HB3	2.1	0.02	1
A	133	GLY	CA	46.64	0.3	1
A	89	ILE	HB	2.37	0.02	1
A	132	ILE	HB	1.94	0.02	1
A	133	GLY	HA3	3.82	0.02	1
A	125	VAL	CA	68.21	0.3	1
A	150	SER	CA	59.95	0.3	1
A	123	GLN	C	174.98	0.3	1
A	106	ALA	HB2	1.33	0.02	1
A	139	ILE	N	120.94	0.3	1
A	121	THR	N	113.69	0.3	1
A	124	GLU	HB3	2.25	0.02	1
A	108	GLU	HB2	2.25	0.02	1
A	147	LEU	C	172.66	0.3	1
A	136	GLU	CG	36.98	0.3	1
A	149	THR	CA	63.17	0.3	1
A	98	LYS	CB	32.66	0.3	1
A	133	GLY	C	171.05	0.3	1
A	101	ASN	CB	41.31	0.3	1
A	150	SER	HB2	3.92	0.02	1
A	122	GLU	C	175.59	0.3	1
A	128	LEU	C	176.84	0.3	1
A	95	ILE	HA	3.25	0.02	1
A	95	ILE	CA	67.56	0.3	1
A	119	LYS	HB2	1.66	0.02	1
A	142	ASP	CB	41.01	0.3	1
A	139	ILE	CG2	18.23	0.3	1
A	133	GLY	N	109.87	0.3	1
A	147	LEU	CA	55.27	0.3	1
A	137	GLY	H	8.17	0.02	1
A	95	ILE	C	176.13	0.3	1
A	125	VAL	N	120.31	0.3	1
A	112	VAL	CB	32.52	0.3	1
A	109	LEU	CB	39.6	0.3	1
A	121	THR	HB	4.34	0.02	1
A	116	LEU	HD11	0.39	0.02	1
A	120	LEU	HD13	0.78	0.02	1
A	113	LEU	CA	55.02	0.3	1
A	125	VAL	CG2	22.61	0.3	1
A	124	GLU	H	7.62	0.02	1
A	109	LEU	HD12	0.75	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	87	GLU	HB2	2.21	0.02	1
A	138	LEU	C	170.6	0.3	1
A	127	ASP	HB2	1.93	0.02	1
A	126	ASP	N	120.34	0.3	1
A	133	GLY	H	7.87	0.02	1
A	119	LYS	HG2	1.28	0.02	1
A	145	VAL	CB	33.8	0.3	1
A	116	LEU	CG	27.16	0.3	1
A	91	LYS	CB	35.7	0.3	1
A	108	GLU	CA	58.94	0.3	1
A	127	ASP	N	122.89	0.3	1
A	148	ILE	CG1	30.94	0.3	1
A	106	ALA	CA	56.32	0.3	1
A	121	THR	CA	61.58	0.3	1
A	148	ILE	HA	4.48	0.02	1
A	109	LEU	HD21	0.75	0.02	1
A	132	ILE	H	8.58	0.02	1
A	136	GLU	H	7.92	0.02	1
A	140	ASN	C	172.58	0.3	1
A	130	LYS	C	172.86	0.3	1
A	143	ASP	H	8.23	0.02	1
A	123	GLN	N	117.61	0.3	1
A	145	VAL	H	8.06	0.02	1
A	93	PHE	H	7.97	0.02	1
A	100	LYS	HA	3.85	0.02	1
A	137	GLY	C	173.67	0.3	1
A	136	GLU	CB	30.02	0.3	1
A	136	GLU	HB3	2.16	0.02	1
A	98	LYS	CA	61.07	0.3	1
A	149	THR	HA	4.29	0.02	1
A	106	ALA	N	125.36	0.3	1
A	101	ASN	CA	57.44	0.3	1
A	121	THR	HG23	1.28	0.02	1
A	120	LEU	HD21	0.75	0.02	1
A	87	GLU	N	121.89	0.3	1
A	139	ILE	HG23	0.84	0.02	1
A	111	HIS	CA	59.32	0.3	1
A	132	ILE	N	118.45	0.3	1
A	123	GLN	HA	3.96	0.02	1
A	109	LEU	CA	62.84	0.3	1
A	116	LEU	HD22	-0.6	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	132	ILE	CD1	15.18	0.3	1
A	107	SER	HB2	3.82	0.02	1
A	92	ALA	CB	19.46	0.3	1
A	91	LYS	N	121.65	0.3	1
A	136	GLU	C	171.14	0.3	1
A	86	THR	HG22	1.17	0.02	1
A	114	THR	CA	59.07	0.3	1
A	150	SER	H	7.56	0.02	1
A	145	VAL	HG23	0.8	0.02	1
A	88	ASP	CA	55.56	0.3	1
A	127	ASP	CB	43.05	0.3	1
A	132	ILE	HG22	0.92	0.02	1
A	95	ILE	HG22	0.24	0.02	1
A	129	LEU	N	115.39	0.3	1
A	116	LEU	HB2	1.66	0.02	1
A	87	GLU	CA	59.73	0.3	1
A	109	LEU	HD11	0.75	0.02	1
A	120	LEU	C	174.69	0.3	1
A	126	ASP	HA	4.34	0.02	1
A	132	ILE	CA	63.23	0.3	1
A	119	LYS	H	8.04	0.02	1
A	123	GLN	HB3	2.32	0.02	1
A	115	THR	N	115.99	0.3	1
A	119	LYS	CA	56.46	0.3	1
A	127	ASP	H	7.88	0.02	1
A	89	ILE	CG2	18.21	0.3	1
A	139	ILE	C	180.56	0.3	1
A	95	ILE	CD1	15.7	0.3	1
A	138	LEU	H	7.83	0.02	1
A	129	LEU	H	7.76	0.02	1
A	134	VAL	HB	2.64	0.02	1
A	109	LEU	HB2	1.9	0.02	1
A	139	ILE	HD13	0.8	0.02	1
A	99	GLU	HA	3.79	0.02	1
A	151	LYS	HA	4.13	0.02	1
A	145	VAL	HG13	0.84	0.02	1
A	96	PHE	CA	60.32	0.3	1
A	110	LYS	HB2	1.92	0.02	1
A	121	THR	CB	71.94	0.3	1
A	100	LYS	CA	59.56	0.3	1
A	92	ALA	HB2	1.28	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	LEU	CB	40.86	0.3	1
A	134	VAL	H	7.89	0.02	1
A	147	LEU	H	8.25	0.02	1
A	118	GLU	CB	30.64	0.3	1
A	144	PHE	HA	4.23	0.02	1
A	89	ILE	CA	62.33	0.3	1
A	151	LYS	H	7.5	0.02	1
A	133	GLY	HA2	4.09	0.02	1
A	125	VAL	CB	32.04	0.3	1
A	137	GLY	HA3	3.69	0.02	1
A	139	ILE	HB	1.82	0.02	1
A	92	ALA	N	120.98	0.3	1
A	106	ALA	HB3	1.33	0.02	1
A	131	GLU	C	173.23	0.3	1
A	116	LEU	N	120.79	0.3	1
A	107	SER	CB	63.23	0.3	1
A	109	LEU	CD1	23.85	0.3	1
A	108	GLU	HB3	2.22	0.02	1
A	114	THR	HA	4.47	0.02	1
A	96	PHE	N	120.44	0.3	1
A	88	ASP	CB	41.85	0.3	1
A	120	LEU	HB2	1.53	0.02	1
A	111	HIS	C	175.32	0.3	1
A	142	ASP	HB2	2.64	0.02	1
A	126	ASP	HB2	2.65	0.02	1
A	95	ILE	CB	37.06	0.3	1
A	119	LYS	HB3	1.66	0.02	1
A	143	ASP	CB	41.13	0.3	1
A	130	LYS	N	121.46	0.3	1
A	123	GLN	CG	34.63	0.3	1
A	118	GLU	HA	3.84	0.02	1
A	105	SER	C	172.85	0.3	1
A	99	GLU	CG	39.79	0.3	1
A	145	VAL	N	120.73	0.3	1
A	89	ILE	CG1	27.77	0.3	1
A	131	GLU	CG	37.28	0.3	1
A	120	LEU	CA	54.94	0.3	1
A	113	LEU	CB	41.86	0.3	1
A	92	ALA	H	7.85	0.02	1
A	122	GLU	CG	37.29	0.3	1
A	132	ILE	CB	40.21	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	ALA	C	175.18	0.3	1
A	140	ASN	CA	56.94	0.3	1
A	122	GLU	H	8.83	0.02	1
A	89	ILE	N	121.46	0.3	1
A	130	LYS	H	7.94	0.02	1
A	95	ILE	CG2	22.55	0.3	1
A	108	GLU	CB	30.41	0.3	1
A	96	PHE	CB	42.62	0.3	1
A	92	ALA	HA	4.18	0.02	1
A	136	GLU	N	121.56	0.3	1
A	106	ALA	CB	22.51	0.3	1
A	100	LYS	CB	33.07	0.3	1
A	109	LEU	HD22	0.75	0.02	1
A	125	VAL	HG13	0.85	0.02	1
A	92	ALA	HB1	1.28	0.02	1
A	145	VAL	CG1	21.99	0.3	1
A	126	ASP	C	176.52	0.3	1
A	143	ASP	N	119.5	0.3	1
A	123	GLN	H	8.22	0.02	1
A	86	THR	HB	3.96	0.02	1
A	149	THR	HG22	1.17	0.02	1
A	130	LYS	CB	32.52	0.3	1
A	140	ASN	N	125.93	0.3	1
A	146	LYS	CA	57.19	0.3	1
A	132	ILE	HD13	0.88	0.02	1
A	125	VAL	C	174.21	0.3	1
A	114	THR	H	8.28	0.02	1
A	110	LYS	CB	33.23	0.3	1
A	109	LEU	C	177.07	0.3	1
A	96	PHE	H	7.74	0.02	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	-1.10 ± 0.19	Should be applied
$^{13}C_{\beta}$	136	-0.54 ± 0.06	Should be applied
$^{13}C'$	144	2.52 ± 0.09	Should be applied
^{15}N	135	0.48 ± 0.28	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 77%, i.e. 695 atoms were assigned a chemical shift out of a possible 902. 8 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	363/363 (100%)	145/145 (100%)	146/146 (100%)	72/72 (100%)
Sidechain	332/479 (69%)	186/278 (67%)	146/181 (81%)	0/20 (0%)
Aromatic	0/60 (0%)	0/32 (0%)	0/28 (0%)	0/0 (—%)
Overall	695/902 (77%)	331/455 (73%)	292/355 (82%)	72/92 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 796 atoms were assigned a chemical shift out of a possible 1052. 10 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	411/423 (97%)	164/169 (97%)	166/170 (98%)	81/84 (96%)
Sidechain	385/569 (68%)	215/331 (65%)	170/214 (79%)	0/24 (0%)
Aromatic	0/60 (0%)	0/32 (0%)	0/28 (0%)	0/0 (—%)
Overall	796/1052 (76%)	379/532 (71%)	336/412 (82%)	81/108 (75%)

7.1.4 Statistically unusual chemical shifts

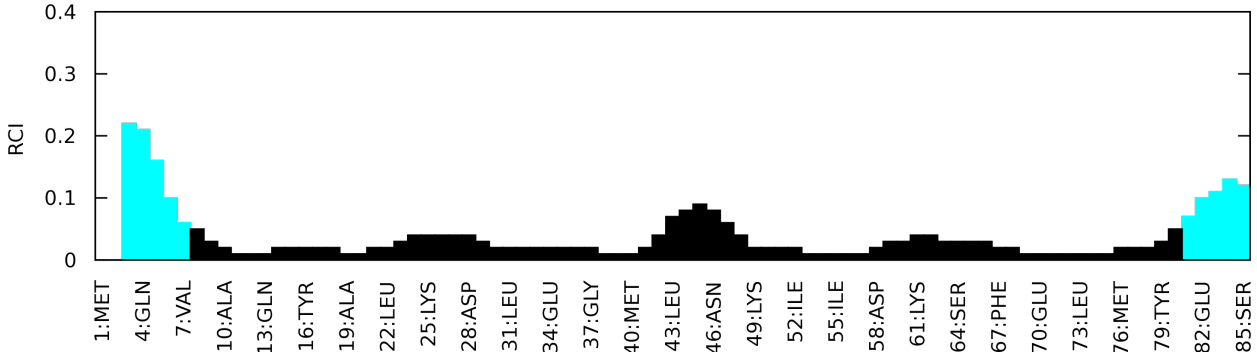
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	127	ASP	HB3	0.78	4.07 – 1.27	-6.7

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.

Random coil index (RCI) for chain A:


RCI
0.4
0.3
0.2
0.1
0
1:MET
4:GLN
7:VAL
10:ALA
13:GLN
16:TYR
19:ALA
22:LEU
25:LYS
28:ASP
31:LEU
34:GLU
37:GLY
40:MET
43:LEU
46:ASN
49:LYS
52:ILE
55:ILE
58:ASP
61:LYS
64:SER
67:PHE
70:GLU
73:LEU
76:MET
79:TYR
82:GLU
85:SER