wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LHU
BMRB ID	:	17867
Title	:	Structural Insight into the Unique Cardiac Myosin Binding Protein-C Motif: A Partially Folded Domain
Authors	:	Howarth, J.W.; Rosevear, P.R.; Ramisetti, S.; Nolan, K.; Sadayappan, S.
Deposited on	:	2011-08-18

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:

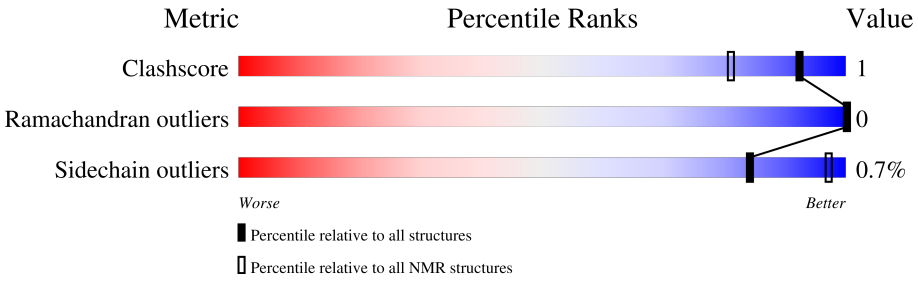
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 38%.

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	124	27% · 72%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:317-A:349 (33)	0.56	15

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 1 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 589 atoms, of which 295 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mybpc3 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	35	589	187	295	54	52	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	MET	-	expression tag	UNP A9JR55
A	235	GLY	-	expression tag	UNP A9JR55
A	236	SER	-	expression tag	UNP A9JR55
A	237	SER	-	expression tag	UNP A9JR55
A	238	HIS	-	expression tag	UNP A9JR55
A	239	HIS	-	expression tag	UNP A9JR55
A	240	HIS	-	expression tag	UNP A9JR55
A	241	HIS	-	expression tag	UNP A9JR55
A	242	HIS	-	expression tag	UNP A9JR55
A	243	HIS	-	expression tag	UNP A9JR55
A	244	SER	-	expression tag	UNP A9JR55
A	245	SER	-	expression tag	UNP A9JR55
A	246	GLY	-	expression tag	UNP A9JR55
A	247	LEU	-	expression tag	UNP A9JR55
A	249	PRO	-	expression tag	UNP A9JR55
A	250	ARG	-	expression tag	UNP A9JR55
A	251	GLY	-	expression tag	UNP A9JR55
A	252	SER	-	expression tag	UNP A9JR55
A	253	HIS	-	expression tag	UNP A9JR55
A	254	MET	-	expression tag	UNP A9JR55

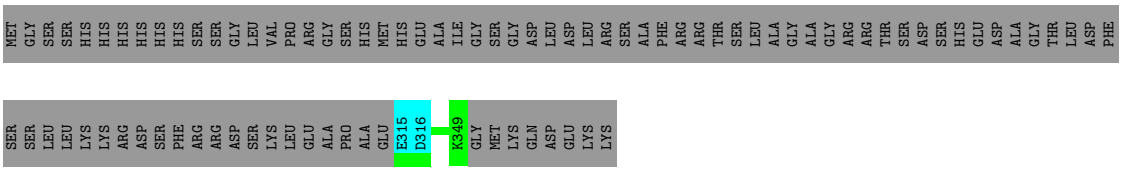
4 Residue-property plots (i)

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: Mybpc3 protein

Chain A: 

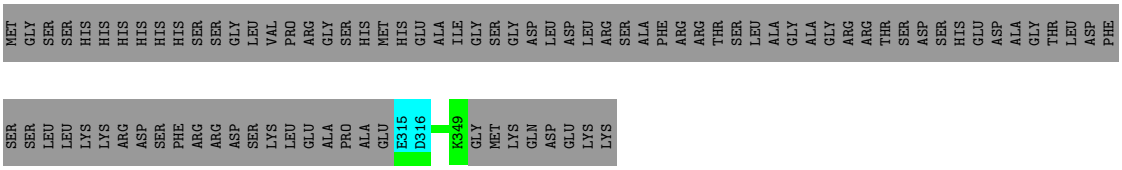


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: Mybpc3 protein

Chain A: 



5 Refinement protocol and experimental data overview

Of the 5000 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
CS-ROSETTA	structure solution	
CS-ROSETTA	refinement	

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	608
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	406
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

6 Model quality

6.1 Standard geometry

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	277	285	286	1±1
All	All	5540	5700	5720	16

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:348:LEU:HD23	1:A:348:LEU:C	0.61	2.16	14	8
1:A:348:LEU:HD23	1:A:348:LEU:O	0.56	2.00	14	4
1:A:348:LEU:C	1:A:348:LEU:CD2	0.49	2.80	17	3
1:A:348:LEU:C	1:A:348:LEU:HD12	0.48	2.28	10	1

6.3 Torsion angles

6.3.1 Protein backbone

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	32/124 (26%)	32±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	640/2480 (26%)	639 (100%)	1 (0%)	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	29/104 (28%)	29±0 (99±1%)	0±0 (1±1%)	84	97
All	All	580/2080 (28%)	576 (99%)	4 (1%)	84	97

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	321	LEU	4

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

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 38% for the well-defined parts and 39% 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	608
Number of shifts mapped to atoms	202
Number of unparsed shifts	0
Number of shifts with mapping errors	406
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 406) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	255	HIS	H	8.33	0.007	1
1	A	255	HIS	HA	4.57	0.016	1
1	A	255	HIS	C	175.2	0.073	1
1	A	255	HIS	CA	56.38	0.167	1
1	A	255	HIS	CB	30.64	0.167	1
1	A	255	HIS	N	120.208	0.039	1
1	A	256	GLU	H	8.303	0.007	1
1	A	256	GLU	HA	4.23	0.016	1
1	A	256	GLU	C	175.9	0.073	1
1	A	256	GLU	CA	56.42	0.167	1
1	A	256	GLU	CB	30.36	0.167	1
1	A	256	GLU	N	121.928	0.039	1
1	A	257	ALA	H	8.4	0.007	1
1	A	257	ALA	HA	4.33	0.016	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	257	ALA	C	177.6	0.073	1
1	A	257	ALA	CA	52.33	0.167	1
1	A	257	ALA	CB	19.07	0.167	1
1	A	257	ALA	N	125.223	0.039	1
1	A	258	ILE	H	8.196	0.007	1
1	A	258	ILE	HA	4.14	0.016	1
1	A	258	ILE	C	176.9	0.073	1
1	A	258	ILE	CA	61.35	0.167	1
1	A	258	ILE	CB	38.6	0.167	1
1	A	258	ILE	N	120.444	0.039	1
1	A	259	GLY	H	8.582	0.007	1
1	A	259	GLY	HA2	3.993	0.016	.
1	A	259	GLY	HA3	3.993	0.016	.
1	A	259	GLY	C	174.2	0.073	1
1	A	259	GLY	CA	45.19	0.167	1
1	A	259	GLY	N	113.111	0.039	1
1	A	260	SER	H	8.339	0.007	1
1	A	260	SER	HA	4.43	0.016	1
1	A	260	SER	C	175.2	0.073	1
1	A	260	SER	CA	58.6	0.167	1
1	A	260	SER	CB	63.79	0.167	1
1	A	260	SER	N	115.659	0.039	1
1	A	261	GLY	H	8.584	0.007	1
1	A	261	GLY	HA2	3.973	0.016	.
1	A	261	GLY	HA3	3.973	0.016	.
1	A	261	GLY	C	174.0	0.073	1
1	A	261	GLY	CA	45.38	0.167	1
1	A	261	GLY	N	110.945	0.039	1
1	A	262	ASP	H	8.226	0.007	1
1	A	262	ASP	HA	4.58	0.016	1
1	A	262	ASP	C	176.5	0.073	1
1	A	262	ASP	CA	54.63	0.167	1
1	A	262	ASP	CB	41.07	0.167	1
1	A	262	ASP	N	120.407	0.039	1
1	A	263	LEU	H	8.205	0.007	1
1	A	263	LEU	HA	4.22	0.016	1
1	A	263	LEU	C	177.2	0.073	1
1	A	263	LEU	CA	55.69	0.167	1
1	A	263	LEU	CB	42.17	0.167	1
1	A	263	LEU	N	121.88	0.039	1
1	A	264	ASP	H	8.327	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	264	ASP	HA	4.58	0.016	1
1	A	264	ASP	C	176.8	0.073	1
1	A	264	ASP	CA	54.3	0.167	1
1	A	264	ASP	CB	40.88	0.167	1
1	A	264	ASP	N	120.806	0.039	1
1	A	265	LEU	H	8.263	0.007	1
1	A	265	LEU	HA	4.22	0.016	1
1	A	265	LEU	C	178.2	0.073	1
1	A	265	LEU	CA	56.02	0.167	1
1	A	265	LEU	CB	41.78	0.167	1
1	A	265	LEU	N	123.224	0.039	1
1	A	266	ARG	H	8.279	0.007	1
1	A	266	ARG	HA	4.23	0.016	1
1	A	266	ARG	C	177.3	0.073	1
1	A	266	ARG	CA	57.15	0.167	1
1	A	266	ARG	CB	30.14	0.167	1
1	A	266	ARG	N	119.27	0.039	1
1	A	267	SER	H	8.097	0.007	1
1	A	267	SER	HA	4.32	0.016	1
1	A	267	SER	C	174.9	0.073	1
1	A	267	SER	CA	59.05	0.167	1
1	A	267	SER	CB	63.41	0.167	1
1	A	267	SER	N	115.229	0.039	1
1	A	268	ALA	H	8.214	0.007	1
1	A	268	ALA	HA	4.19	0.016	1
1	A	268	ALA	C	177.9	0.073	1
1	A	268	ALA	CA	53.3	0.167	1
1	A	268	ALA	CB	18.74	0.167	1
1	A	268	ALA	N	125.076	0.039	1
1	A	269	PHE	H	8.055	0.007	1
1	A	269	PHE	HA	4.52	0.016	1
1	A	269	PHE	C	175.9	0.073	1
1	A	269	PHE	CA	58.11	0.167	1
1	A	269	PHE	CB	39.2	0.167	1
1	A	269	PHE	N	118.0	0.039	1
1	A	270	ARG	H	8.009	0.007	1
1	A	270	ARG	HA	4.27	0.016	1
1	A	270	ARG	C	176.1	0.073	1
1	A	270	ARG	CA	56.25	0.167	1
1	A	270	ARG	CB	30.68	0.167	1
1	A	270	ARG	N	121.802	0.039	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	271	ARG	H	8.324	0.007	1
1	A	271	ARG	HA	4.29	0.016	1
1	A	271	ARG	C	176.7	0.073	1
1	A	271	ARG	CA	56.62	0.167	1
1	A	271	ARG	CB	30.68	0.167	1
1	A	271	ARG	N	121.751	0.039	1
1	A	272	THR	H	8.188	0.007	1
1	A	272	THR	HA	4.33	0.016	1
1	A	272	THR	C	174.6	0.073	1
1	A	272	THR	CA	62.14	0.167	1
1	A	272	THR	CB	69.71	0.167	1
1	A	272	THR	N	114.707	0.039	1
1	A	273	SER	H	8.318	0.007	1
1	A	273	SER	HA	4.43	0.016	1
1	A	273	SER	C	174.6	0.073	1
1	A	273	SER	CA	58.4	0.167	1
1	A	273	SER	CB	63.7	0.167	1
1	A	273	SER	N	117.928	0.039	1
1	A	274	LEU	H	8.305	0.007	1
1	A	274	LEU	HA	4.31	0.016	1
1	A	274	LEU	C	177.3	0.073	1
1	A	274	LEU	CA	55.28	.	1
1	A	274	LEU	CB	42.1	.	1
1	A	274	LEU	N	124.04	0.039	1
1	A	275	ALA	H	8.257	0.007	1
1	A	275	ALA	HA	4.27	0.016	1
1	A	275	ALA	C	178.3	0.073	1
1	A	275	ALA	CA	52.79	0.167	1
1	A	275	ALA	CB	18.97	0.167	1
1	A	275	ALA	N	124.156	0.039	1
1	A	276	GLY	H	8.345	0.007	1
1	A	276	GLY	HA2	3.923	0.016	.
1	A	276	GLY	HA3	3.923	0.016	.
1	A	276	GLY	C	174.1	0.073	1
1	A	276	GLY	CA	45.24	0.167	1
1	A	276	GLY	N	108.114	0.039	1
1	A	277	ALA	H	8.181	0.007	1
1	A	277	ALA	HA	4.31	0.016	1
1	A	277	ALA	C	178.3	0.073	1
1	A	277	ALA	CA	52.7	0.167	1
1	A	277	ALA	CB	19.15	0.167	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	277	ALA	N	123.558	0.039	1
1	A	278	GLY	H	8.461	0.007	1
1	A	278	GLY	HA2	3.922	0.016	.
1	A	278	GLY	HA3	3.922	0.016	.
1	A	278	GLY	C	173.9	0.073	1
1	A	278	GLY	CA	45.2	0.167	1
1	A	278	GLY	N	107.956	0.039	1
1	A	279	ARG	H	8.136	0.007	1
1	A	279	ARG	HA	4.34	0.016	1
1	A	279	ARG	C	176.2	0.073	1
1	A	279	ARG	CA	55.9	0.167	1
1	A	279	ARG	CB	30.86	0.167	1
1	A	279	ARG	N	120.427	0.039	1
1	A	280	ARG	H	8.576	0.007	1
1	A	280	ARG	HA	4.45	0.016	1
1	A	280	ARG	C	176.7	0.073	1
1	A	280	ARG	CA	56.0	0.167	1
1	A	280	ARG	CB	30.89	0.167	1
1	A	280	ARG	N	122.881	0.039	1
1	A	281	THR	H	8.378	0.007	1
1	A	281	THR	HA	4.37	0.016	1
1	A	281	THR	C	174.7	0.073	1
1	A	281	THR	CA	61.86	0.167	1
1	A	281	THR	CB	69.78	0.167	1
1	A	281	THR	N	115.435	0.039	1
1	A	282	SER	H	8.37	0.007	1
1	A	282	SER	HA	4.45	0.016	1
1	A	282	SER	C	174.2	0.073	1
1	A	282	SER	CA	58.36	0.167	1
1	A	282	SER	CB	63.7	0.167	1
1	A	282	SER	N	116.949	0.039	1
1	A	283	ASP	H	8.365	0.007	1
1	A	283	ASP	HA	4.65	0.016	1
1	A	283	ASP	C	176.1	0.073	1
1	A	283	ASP	CA	54.36	0.167	1
1	A	283	ASP	CB	41.18	0.167	1
1	A	283	ASP	N	122.083	0.039	1
1	A	284	SER	H	8.236	0.007	1
1	A	284	SER	HA	4.39	0.016	1
1	A	284	SER	C	174.4	0.073	1
1	A	284	SER	CA	58.44	0.167	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	284	SER	CB	63.68	0.167	1
1	A	284	SER	N	115.614	0.039	1
1	A	285	HIS	H	8.449	0.007	1
1	A	285	HIS	HA	4.6	0.016	1
1	A	285	HIS	C	175.2	0.073	1
1	A	285	HIS	CA	56.36	0.167	1
1	A	285	HIS	CB	30.16	0.167	1
1	A	285	HIS	N	121.148	0.039	1
1	A	286	GLU	H	8.378	0.007	1
1	A	286	GLU	HA	4.23	0.016	1
1	A	286	GLU	C	176.0	0.073	1
1	A	286	GLU	CA	56.66	0.167	1
1	A	286	GLU	CB	30.21	0.167	1
1	A	286	GLU	N	121.889	0.039	1
1	A	287	ASP	H	8.488	0.007	1
1	A	287	ASP	HA	4.59	0.016	1
1	A	287	ASP	C	176.1	0.073	1
1	A	287	ASP	CA	54.29	0.167	1
1	A	287	ASP	CB	41.3	0.167	1
1	A	287	ASP	N	121.574	0.039	1
1	A	288	ALA	H	8.373	0.007	1
1	A	288	ALA	HA	4.26	0.016	1
1	A	288	ALA	C	178.3	0.073	1
1	A	288	ALA	CA	52.99	0.167	1
1	A	288	ALA	CB	19.07	0.167	1
1	A	288	ALA	N	124.918	0.039	1
1	A	289	GLY	H	8.486	0.007	1
1	A	289	GLY	HA2	3.962	0.016	.
1	A	289	GLY	HA3	3.962	0.016	.
1	A	289	GLY	C	174.4	0.073	1
1	A	289	GLY	CA	45.39	0.167	1
1	A	289	GLY	N	107.444	0.039	1
1	A	290	THR	H	7.993	0.007	1
1	A	290	THR	HA	4.29	0.016	1
1	A	290	THR	C	174.5	0.073	1
1	A	290	THR	CA	61.98	0.167	1
1	A	290	THR	CB	69.97	0.167	1
1	A	290	THR	N	113.643	0.039	1
1	A	291	LEU	H	8.236	0.007	1
1	A	291	LEU	HA	4.26	0.016	1
1	A	291	LEU	C	176.4	0.073	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	291	LEU	CA	55.08	0.167	1
1	A	291	LEU	CB	42.34	0.167	1
1	A	291	LEU	N	124.342	0.039	1
1	A	292	ASP	H	8.219	0.007	1
1	A	292	ASP	HA	4.6	0.016	1
1	A	292	ASP	C	176.3	0.073	1
1	A	292	ASP	CA	53.53	0.167	1
1	A	292	ASP	CB	41.02	0.167	1
1	A	292	ASP	N	120.791	0.039	1
1	A	293	PHE	H	8.438	0.007	1
1	A	293	PHE	HA	4.47	0.016	1
1	A	293	PHE	C	176.7	0.073	1
1	A	293	PHE	CA	59.1	0.167	1
1	A	293	PHE	CB	38.93	0.167	1
1	A	293	PHE	N	122.385	0.039	1
1	A	294	SER	H	8.409	0.007	1
1	A	294	SER	HA	4.23	0.016	1
1	A	294	SER	C	175.8	0.073	1
1	A	294	SER	CA	60.25	0.167	1
1	A	294	SER	CB	63.13	0.167	1
1	A	294	SER	N	116.025	0.039	1
1	A	295	SER	H	8.176	0.007	1
1	A	295	SER	HA	4.33	0.016	1
1	A	295	SER	C	175.3	0.073	1
1	A	295	SER	CA	59.72	0.167	1
1	A	295	SER	CB	63.16	0.167	1
1	A	295	SER	N	117.523	0.039	1
1	A	296	LEU	H	7.957	0.007	1
1	A	296	LEU	HA	4.21	0.016	1
1	A	296	LEU	C	177.9	0.073	1
1	A	296	LEU	CA	56.22	0.167	1
1	A	296	LEU	CB	41.91	0.167	1
1	A	296	LEU	N	122.815	0.039	1
1	A	297	LEU	H	7.888	0.007	1
1	A	297	LEU	HA	4.21	0.016	1
1	A	297	LEU	C	177.6	0.073	1
1	A	297	LEU	CA	55.77	0.167	1
1	A	297	LEU	CB	41.87	0.167	1
1	A	297	LEU	N	120.13	0.039	1
1	A	298	LYS	H	7.936	0.007	1
1	A	298	LYS	HA	4.23	0.016	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	298	LYS	C	176.9	0.073	1
1	A	298	LYS	CA	56.71	0.167	1
1	A	298	LYS	CB	32.75	0.167	1
1	A	298	LYS	NZ	120.407	0.039	1
1	A	299	LYS	H	8.162	0.007	1
1	A	299	LYS	HA	4.25	0.016	1
1	A	299	LYS	C	177.0	0.073	1
1	A	299	LYS	CA	56.74	0.167	1
1	A	299	LYS	CB	32.78	0.167	1
1	A	299	LYS	N	121.806	0.039	1
1	A	300	ARG	H	8.351	0.007	1
1	A	300	ARG	HA	4.25	0.016	1
1	A	300	ARG	C	176.4	0.073	1
1	A	300	ARG	CA	56.65	0.167	1
1	A	300	ARG	CB	30.68	0.167	1
1	A	300	ARG	N	122.073	0.039	1
1	A	301	ASP	H	8.386	0.007	1
1	A	301	ASP	HA	4.58	0.016	1
1	A	301	ASP	C	176.5	0.073	1
1	A	301	ASP	CA	54.69	0.167	1
1	A	301	ASP	CB	41.08	0.167	1
1	A	301	ASP	N	121.143	0.039	1
1	A	302	SER	H	8.197	0.007	1
1	A	302	SER	HA	4.32	0.016	1
1	A	302	SER	C	174.3	0.073	1
1	A	302	SER	CA	58.88	0.167	1
1	A	302	SER	CB	63.55	0.167	1
1	A	302	SER	N	115.733	0.039	1
1	A	303	PHE	H	8.143	0.007	1
1	A	303	PHE	HA	4.58	0.016	1
1	A	303	PHE	C	175.6	0.073	1
1	A	303	PHE	CA	57.99	0.167	1
1	A	303	PHE	CB	39.27	0.167	1
1	A	303	PHE	N	121.56	0.039	1
1	A	304	ARG	H	8.127	0.007	1
1	A	304	ARG	HA	4.29	0.016	1
1	A	304	ARG	C	176.0	0.073	1
1	A	304	ARG	CA	56.01	0.167	1
1	A	304	ARG	CB	30.75	0.167	1
1	A	304	ARG	N	122.425	0.039	1
1	A	305	ARG	H	8.417	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	305	ARG	HA	4.25	0.016	1
1	A	305	ARG	C	176.0	0.073	1
1	A	305	ARG	CA	56.29	0.167	1
1	A	305	ARG	CB	30.68	0.167	1
1	A	305	ARG	N	122.681	0.039	1
1	A	306	ASP	H	8.443	0.007	1
1	A	306	ASP	HA	4.6	0.016	1
1	A	306	ASP	C	176.3	0.073	1
1	A	306	ASP	CA	54.25	0.167	1
1	A	306	ASP	CB	41.09	0.167	1
1	A	306	ASP	N	121.143	0.039	1
1	A	307	SER	H	8.23	0.007	1
1	A	307	SER	HA	4.36	0.016	1
1	A	307	SER	C	174.6	0.073	1
1	A	307	SER	CA	58.75	0.167	1
1	A	307	SER	CB	63.64	0.167	1
1	A	307	SER	N	116.593	0.039	1
1	A	308	LYS	H	8.411	0.007	1
1	A	308	LYS	HA	4.29	0.016	1
1	A	308	LYS	C	176.5	0.073	1
1	A	308	LYS	CA	56.55	0.167	1
1	A	308	LYS	CB	32.52	0.167	1
1	A	308	LYS	N	122.558	0.039	1
1	A	309	LEU	H	8.129	0.007	1
1	A	309	LEU	HA	4.3	0.016	1
1	A	309	LEU	C	177.1	0.073	1
1	A	309	LEU	CA	55.05	0.167	1
1	A	309	LEU	CB	42.27	0.167	1
1	A	309	LEU	N	122.172	0.039	1
1	A	310	GLU	H	8.32	0.007	1
1	A	310	GLU	HA	4.27	0.016	1
1	A	310	GLU	C	175.5	0.073	1
1	A	310	GLU	CA	56.1	0.167	1
1	A	310	GLU	CB	30.35	0.167	1
1	A	310	GLU	N	121.45	0.039	1
1	A	311	ALA	H	8.313	0.007	1
1	A	311	ALA	HA	4.56	0.016	1
1	A	311	ALA	C	175.1	0.073	1
1	A	311	ALA	CA	50.39	0.167	1
1	A	311	ALA	CB	18.24	0.167	1
1	A	311	ALA	N	126.059	0.039	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	312	PRO	HA	4.4	0.016	1
1	A	312	PRO	C	176.5	0.073	1
1	A	312	PRO	CA	62.85	0.167	1
1	A	312	PRO	CB	32.0	0.167	1
1	A	313	ALA	H	8.569	0.007	1
1	A	313	ALA	HA	4.32	0.016	1
1	A	313	ALA	C	178.1	0.073	1
1	A	313	ALA	CA	52.31	0.167	1
1	A	313	ALA	CB	19.16	0.167	1
1	A	313	ALA	N	124.622	0.039	1
1	A	314	GLU	H	8.589	0.007	1
1	A	314	GLU	HA	4.13	0.016	1
1	A	314	GLU	C	176.9	0.073	1
1	A	314	GLU	CA	57.51	0.167	1
1	A	314	GLU	CB	30.002	0.167	1
1	A	314	GLU	N	120.659	0.039	1
1	A	350	GLY	H	7.903	0.007	1
1	A	350	GLY	HA2	4.153	0.016	.
1	A	350	GLY	HA3	4.153	0.016	.
1	A	350	GLY	C	174.6	0.073	1
1	A	350	GLY	CA	45.67	0.167	1
1	A	350	GLY	N	106.846	0.039	1
1	A	351	MET	H	7.884	0.007	1
1	A	351	MET	HA	4.38	0.016	1
1	A	351	MET	C	176.5	0.073	1
1	A	351	MET	CA	56.23	0.167	1
1	A	351	MET	CB	33.18	0.167	1
1	A	351	MET	N	119.551	0.039	1
1	A	352	LYS	H	8.239	0.007	1
1	A	352	LYS	HA	4.29	0.016	1
1	A	352	LYS	C	176.7	0.073	1
1	A	352	LYS	CA	56.47	0.167	1
1	A	352	LYS	CB	32.75	0.167	1
1	A	352	LYS	N	121.578	0.039	1
1	A	353	GLN	H	8.432	0.007	1
1	A	353	GLN	HA	4.3	0.016	1
1	A	353	GLN	C	175.8	0.073	1
1	A	353	GLN	CA	56.1	0.167	1
1	A	353	GLN	CB	29.38	0.167	1
1	A	353	GLN	N	121.539	0.039	1
1	A	354	ASP	H	8.418	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	354	ASP	HA	4.58	0.016	1
1	A	354	ASP	C	176.1	0.073	1
1	A	354	ASP	CA	54.47	0.167	1
1	A	354	ASP	CB	41.05	0.167	1
1	A	354	ASP	N	121.262	0.039	1
1	A	355	GLU	H	8.295	0.007	1
1	A	355	GLU	HA	4.25	0.016	1
1	A	355	GLU	C	176.1	0.073	1
1	A	355	GLU	CA	56.53	0.167	1
1	A	355	GLU	CB	30.35	0.167	1
1	A	355	GLU	N	121.272	0.039	1
1	A	356	LYS	H	8.384	0.007	1
1	A	356	LYS	HA	4.31	0.016	1
1	A	356	LYS	C	175.5	0.073	1
1	A	356	LYS	CA	56.24	0.167	1
1	A	356	LYS	CB	32.63	0.167	1
1	A	356	LYS	N	123.191	0.039	1
1	A	357	LYS	H	8.03	0.007	1
1	A	357	LYS	HA	4.16	0.016	1
1	A	357	LYS	C	181.3	0.073	1
1	A	357	LYS	CA	57.49	0.167	1
1	A	357	LYS	CB	33.68	0.167	1
1	A	357	LYS	N	128.55	0.039	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	102	0.11 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	94	0.34 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	102	-0.15 ± 0.26	None needed (< 0.5 ppm)
^{15}N	99	0.28 ± 0.31	None needed (< 0.5 ppm)

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 38%, i.e. 190 atoms were assigned a chemical shift out of a possible 498. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	160/163 (98%)	65/66 (98%)	64/66 (97%)	31/31 (100%)
Sidechain	30/298 (10%)	0/193 (0%)	30/89 (34%)	0/16 (0%)
Aromatic	0/37 (0%)	0/19 (0%)	0/17 (0%)	0/1 (0%)
Overall	190/498 (38%)	65/278 (23%)	94/172 (55%)	31/48 (65%)

7.1.4 Statistically unusual chemical shifts (i)

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	298	LYS	NZ	120.41	19.79 – 46.09	33.3
1	A	331	ARG	CB	41.06	21.74 – 39.52	5.9

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: