



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M6N
BMRB ID : 19147
Title : 3D solution structure of EMI1 (Early Mitotic Inhibitor 1)
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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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 : 4.02b-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

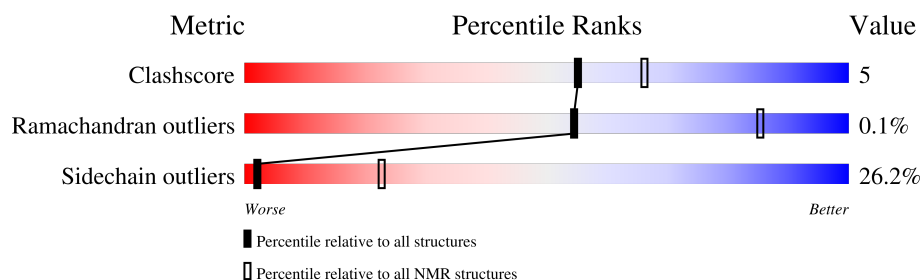
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	86	<div> <div>31%</div> <div>13%</div> <div>9%</div> <div>47%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:15-A:52 (38)	0.31	3

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 and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 712 atoms, of which 349 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-box only protein 5.

Mol	Chain	Residues	Atoms						Trace
1	A	46	Total	C	H	N	O	S	0
			710	220	349	65	67	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9UKT4
A	2	SER	-	expression tag	UNP Q9UKT4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

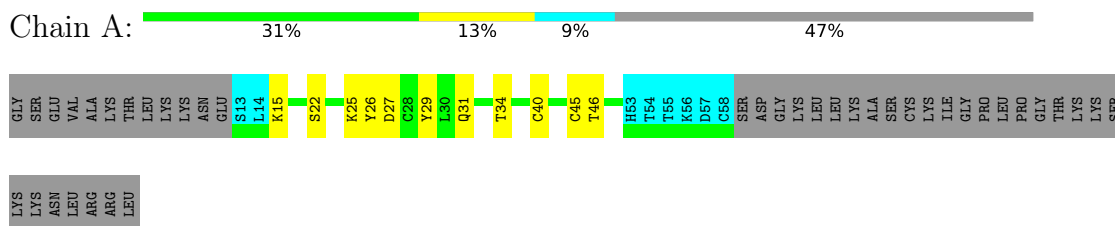
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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.

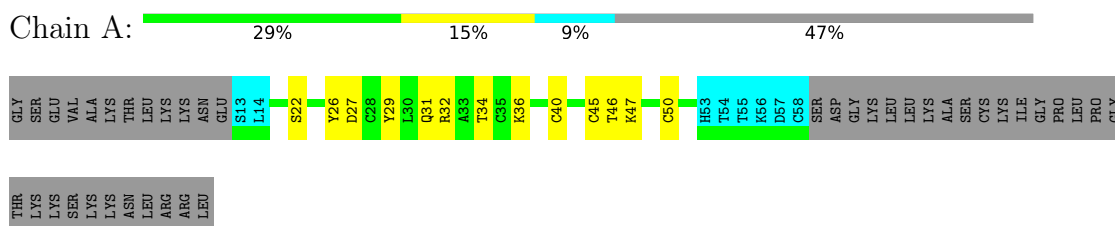
- Molecule 1: F-box only protein 5



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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: F-box only protein 5



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	1043
Number of shifts mapped to atoms	542
Number of unparsed shifts	0
Number of shifts with mapping errors	501
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

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

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	300	290	290	3±2
All	All	6040	5800	5800	63

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 5.

5 of 14 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:CE1	1:A:46:THR:HG21	0.65	2.26	12	15
1:A:31:GLN:O	1:A:46:THR:HG22	0.61	1.95	11	16
1:A:18:ILE:HG22	1:A:49:LEU:HD13	0.58	1.75	1	4
1:A:31:GLN:C	1:A:46:THR:HG22	0.57	2.20	1	15
1:A:18:ILE:CG2	1:A:49:LEU:HD22	0.54	2.32	5	2

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	38/86 (44%)	32±2 (84±5%)	6±2 (16±4%)	0±0 (0±1%)	54	85
All	All	760/1720 (44%)	641 (84%)	118 (16%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	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	33/75 (44%)	24±1 (74±3%)	9±1 (26±3%)	2	23
All	All	660/1500 (44%)	487 (74%)	173 (26%)	2	23

5 of 15 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	27	ASP	20
1	A	29	TYR	20
1	A	34	THR	20
1	A	40	CYS	19
1	A	45	CYS	19

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](#)

Of 2 ligands modelled in this entry, 2 are 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 90% for the well-defined parts and 90% 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	1043
Number of shifts mapped to atoms	542
Number of unparsed shifts	0
Number of shifts with mapping errors	501
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 501) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	LEU	H	7.862	0.020	.
1	A	86	LEU	N	129.646	0.300	.
1	A	5	ALA	H	8.274	0.020	.
1	A	5	ALA	N	127.448	0.300	.
1	A	8	LEU	H	8.153	0.020	.
1	A	8	LEU	N	124.868	0.300	.
1	A	77	LYS	H	8.347	0.020	.
1	A	77	LYS	N	123.805	0.300	.
1	A	69	LYS	H	8.302	0.020	.
1	A	69	LYS	N	123.832	0.300	.
1	A	73	LEU	H	8.324	0.020	.
1	A	73	LEU	N	123.76	0.300	.
1	A	85	ARG	H	8.25	0.020	.
1	A	85	ARG	N	123.315	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	GLU	H	8.675	0.020	.
1	A	3	GLU	N	123.284	0.300	.
1	A	78	LYS	H	8.309	0.020	.
1	A	78	LYS	N	122.668	0.300	.
1	A	65	LYS	H	8.27	0.020	.
1	A	65	LYS	N	122.764	0.300	.
1	A	83	LEU	H	8.115	0.020	.
1	A	83	LEU	N	122.869	0.300	.
1	A	70	ILE	H	8.08	0.020	.
1	A	70	ILE	N	122.258	0.300	.
1	A	64	LEU	H	7.988	0.020	.
1	A	64	LEU	N	122.593	0.300	.
1	A	9	LYS	H	8.099	0.020	.
1	A	9	LYS	N	121.871	0.300	.
1	A	10	LYS	H	8.079	0.020	.
1	A	10	LYS	N	122.056	0.300	.
1	A	60	ASP	H	8.086	0.020	.
1	A	60	ASP	N	122.154	0.300	.
1	A	4	VAL	H	8.1	0.020	.
1	A	4	VAL	N	121.453	0.300	.
1	A	12	GLU	H	8.298	0.020	.
1	A	12	GLU	N	121.687	0.300	.
1	A	84	ARG	H	8.18	0.020	.
1	A	84	ARG	N	121.586	0.300	.
1	A	63	LEU	H	8.012	0.020	.
1	A	63	LEU	N	121.439	0.300	.
1	A	68	CYS	H	8.195	0.020	.
1	A	68	CYS	N	121.407	0.300	.
1	A	6	LYS	H	8.212	0.020	.
1	A	6	LYS	N	120.601	0.300	.
1	A	62	LYS	H	8.014	0.020	.
1	A	62	LYS	N	120.306	0.300	.
1	A	82	ASN	H	8.372	0.020	.
1	A	82	ASN	N	119.696	0.300	.
1	A	11	ASN	H	8.455	0.020	.
1	A	11	ASN	N	119.458	0.300	.
1	A	79	SER	H	8.268	0.020	.
1	A	79	SER	N	117.303	0.300	.
1	A	59	SER	H	8.293	0.020	.
1	A	59	SER	N	115.879	0.300	.
1	A	7	THR	H	8.0	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	THR	N	115.127	0.300	.
1	A	67	SER	H	8.201	0.020	.
1	A	67	SER	N	114.679	0.300	.
1	A	71	GLY	H	8.214	0.020	.
1	A	71	GLY	N	113.226	0.300	.
1	A	76	THR	H	7.908	0.020	.
1	A	76	THR	N	113.511	0.300	.
1	A	61	GLY	H	8.323	0.020	.
1	A	61	GLY	N	109.614	0.300	.
1	A	75	GLY	H	8.431	0.020	.
1	A	75	GLY	N	109.007	0.300	.
1	A	80	LYS	H	8.324	0.020	.
1	A	80	LYS	N	123.959	0.300	.
1	A	86	LEU	CA	56.494	0.300	.
1	A	86	LEU	CB	42.902	0.300	.
1	A	5	ALA	CA	52.245	0.300	.
1	A	5	ALA	CB	18.705	0.300	.
1	A	8	LEU	CA	54.689	0.300	.
1	A	8	LEU	CB	41.856	0.300	.
1	A	77	LYS	CA	56.052	0.300	.
1	A	77	LYS	CB	32.529	0.300	.
1	A	69	LYS	CA	56.059	0.300	.
1	A	69	LYS	CB	32.494	0.300	.
1	A	73	LEU	CA	52.74	0.300	.
1	A	85	ARG	CA	55.611	0.300	.
1	A	3	GLU	CA	56.16	0.300	.
1	A	3	GLU	CB	29.45	0.300	.
1	A	85	ARG	CB	30.364	0.300	.
1	A	78	LYS	CA	56.195	0.300	.
1	A	78	LYS	CB	32.826	0.300	.
1	A	65	LYS	CA	55.965	0.300	.
1	A	65	LYS	CB	32.443	0.300	.
1	A	83	LEU	CA	54.888	0.300	.
1	A	83	LEU	CB	42.242	0.300	.
1	A	70	ILE	CA	60.619	0.300	.
1	A	70	ILE	CB	38.407	0.300	.
1	A	64	LEU	CA	54.84	0.300	.
1	A	64	LEU	CB	41.681	0.300	.
1	A	60	ASP	CA	54.262	0.300	.
1	A	60	ASP	CB	40.84	0.300	.
1	A	9	LYS	CA	55.405	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	LYS	CB	32.467	0.300	.
1	A	10	LYS	CA	56.518	0.300	.
1	A	10	LYS	CB	32.825	0.300	.
1	A	4	VAL	CA	62.034	0.300	.
1	A	4	VAL	CB	32.213	0.300	.
1	A	12	GLU	CA	56.171	0.300	.
1	A	12	GLU	CB	30.369	0.300	.
1	A	84	ARG	CA	55.545	0.300	.
1	A	84	ARG	CB	30.218	0.300	.
1	A	63	LEU	CA	55.168	0.300	.
1	A	63	LEU	CB	41.675	0.300	.
1	A	68	CYS	CA	58.153	0.300	.
1	A	6	LYS	CA	56.123	0.300	.
1	A	6	LYS	CB	32.499	0.300	.
1	A	68	CYS	CB	27.648	0.300	.
1	A	62	LYS	CA	56.56	0.300	.
1	A	62	LYS	CB	32.351	0.300	.
1	A	82	ASN	CA	53.008	0.300	.
1	A	82	ASN	CB	38.42	0.300	.
1	A	11	ASN	CA	52.699	0.300	.
1	A	11	ASN	CB	38.192	0.300	.
1	A	79	SER	CA	57.852	0.300	.
1	A	79	SER	CB	63.473	0.300	.
1	A	59	SER	CA	58.168	0.300	.
1	A	59	SER	CB	63.177	0.300	.
1	A	7	THR	CA	61.555	0.300	.
1	A	7	THR	CB	69.505	0.300	.
1	A	67	SER	CA	58.266	0.300	.
1	A	67	SER	CB	63.615	0.300	.
1	A	71	GLY	CA	43.952	0.300	.
1	A	76	THR	CA	61.478	0.300	.
1	A	76	THR	CB	69.369	0.300	.
1	A	75	GLY	CA	44.951	0.300	.
1	A	61	GLY	CA	45.597	0.300	.
1	A	80	LYS	CA	56.564	0.300	.
1	A	80	LYS	CB	32.496	0.300	.
1	A	66	ALA	H	8.184	0.020	.
1	A	66	ALA	N	124.736	0.300	.
1	A	66	ALA	CB	18.837	0.300	.
1	A	66	ALA	CA	52.199	0.300	.
1	A	81	LYS	H	8.217	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	LYS	N	121.975	0.300	.
1	A	81	LYS	CB	32.643	0.300	.
1	A	81	LYS	CA	56.036	0.300	.
1	A	4	VAL	HA	3.963	0.020	.
1	A	4	VAL	HB	1.971	0.020	.
1	A	4	VAL	HG11	0.862	0.020	.
1	A	4	VAL	HG12	0.862	0.020	.
1	A	4	VAL	HG13	0.862	0.020	.
1	A	4	VAL	CG1	20.212	0.300	.
1	A	3	GLU	HA	4.246	0.020	.
1	A	3	GLU	HB2	1.958	0.020	.
1	A	5	ALA	HA	4.202	0.020	.
1	A	5	ALA	HB1	1.299	0.020	.
1	A	5	ALA	HB2	1.299	0.020	.
1	A	5	ALA	HB3	1.299	0.020	.
1	A	6	LYS	HA	4.23	0.020	.
1	A	6	LYS	HB3	1.673	0.020	.
1	A	6	LYS	CD	29.064	0.300	.
1	A	6	LYS	CG	24.37	0.300	.
1	A	6	LYS	CE	41.747	0.300	.
1	A	6	LYS	HB2	1.746	0.020	.
1	A	6	LYS	HG2	1.358	0.020	.
1	A	6	LYS	HG3	1.358	0.020	.
1	A	6	LYS	HD2	1.714	0.020	.
1	A	6	LYS	HD3	1.714	0.020	.
1	A	6	LYS	HE2	2.903	0.020	.
1	A	6	LYS	HE3	2.903	0.020	.
1	A	7	THR	HA	4.232	0.020	.
1	A	7	THR	HB	4.129	0.020	.
1	A	7	THR	HG21	1.111	0.020	.
1	A	7	THR	HG22	1.111	0.020	.
1	A	7	THR	HG23	1.111	0.020	.
1	A	7	THR	CG2	21.212	0.300	.
1	A	8	LEU	HA	4.271	0.020	.
1	A	8	LEU	HB2	1.553	0.020	.
1	A	8	LEU	HD11	0.83	0.020	.
1	A	8	LEU	HD12	0.83	0.020	.
1	A	8	LEU	HD13	0.83	0.020	.
1	A	8	LEU	CG	26.469	0.300	.
1	A	8	LEU	CD1	24.484	0.300	.
1	A	8	LEU	CD2	23.098	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	LEU	HB3	1.499	0.020	.
1	A	8	LEU	HD21	0.78	0.020	.
1	A	8	LEU	HD22	0.78	0.020	.
1	A	8	LEU	HD23	0.78	0.020	.
1	A	9	LYS	HA	4.213	0.020	.
1	A	9	LYS	HE2	2.921	0.020	.
1	A	9	LYS	HE3	2.921	0.020	.
1	A	9	LYS	HB2	1.627	0.020	.
1	A	9	LYS	HB3	1.627	0.020	.
1	A	9	LYS	HD2	1.727	0.020	.
1	A	9	LYS	HD3	1.727	0.020	.
1	A	9	LYS	HG2	1.318	0.020	.
1	A	9	LYS	HG3	1.318	0.020	.
1	A	11	ASN	HA	4.597	0.020	.
1	A	11	ASN	HB3	2.66	0.020	.
1	A	11	ASN	HB2	2.75	0.020	.
1	A	12	GLU	HA	4.373	0.020	.
1	A	12	GLU	HB3	1.898	0.020	.
1	A	12	GLU	HG2	2.181	0.020	.
1	A	12	GLU	HG3	2.181	0.020	.
1	A	12	GLU	CG	36.011	0.300	.
1	A	68	CYS	HA	4.432	0.020	.
1	A	68	CYS	HB2	2.856	0.020	.
1	A	68	CYS	HB3	2.856	0.020	.
1	A	60	ASP	HA	4.433	0.020	.
1	A	60	ASP	HB2	2.6	0.020	.
1	A	60	ASP	HB3	2.6	0.020	.
1	A	59	SER	HA	4.25	0.020	.
1	A	59	SER	HB2	3.759	0.020	.
1	A	59	SER	HB3	3.759	0.020	.
1	A	61	GLY	HA2	3.805	0.020	.
1	A	61	GLY	HA3	3.805	0.020	.
1	A	62	LYS	HA	4.156	0.020	.
1	A	62	LYS	HB2	1.744	0.020	.
1	A	62	LYS	HB3	1.744	0.020	.
1	A	62	LYS	HD2	1.59	0.020	.
1	A	62	LYS	HD3	1.59	0.020	.
1	A	62	LYS	HG2	1.346	0.020	.
1	A	62	LYS	HG3	1.346	0.020	.
1	A	62	LYS	HE2	2.9	0.020	.
1	A	62	LYS	HE3	2.9	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	LYS	CD	28.42	0.300	.
1	A	62	LYS	CG	24.157	0.300	.
1	A	62	LYS	CE	41.487	0.300	.
1	A	63	LEU	HA	4.212	0.020	.
1	A	63	LEU	HB2	1.496	0.020	.
1	A	63	LEU	HB3	1.496	0.020	.
1	A	63	LEU	HD11	0.826	0.020	.
1	A	63	LEU	HD12	0.826	0.020	.
1	A	63	LEU	HD13	0.826	0.020	.
1	A	63	LEU	HD21	0.826	0.020	.
1	A	63	LEU	HD22	0.826	0.020	.
1	A	63	LEU	HD23	0.826	0.020	.
1	A	63	LEU	CD1	24.2	0.300	.
1	A	64	LEU	HA	4.243	0.020	.
1	A	64	LEU	HB2	1.572	0.020	.
1	A	64	LEU	HB3	1.572	0.020	.
1	A	65	LYS	HA	4.226	0.020	.
1	A	66	ALA	HA	4.222	0.020	.
1	A	66	ALA	HB1	1.328	0.020	.
1	A	66	ALA	HB2	1.328	0.020	.
1	A	66	ALA	HB3	1.328	0.020	.
1	A	70	ILE	HA	4.122	0.020	.
1	A	70	ILE	HB	1.778	0.020	.
1	A	70	ILE	CG1	26.513	0.300	.
1	A	70	ILE	CG2	17.046	0.300	.
1	A	70	ILE	CD1	12.431	0.300	.
1	A	70	ILE	HG12	1.397	0.020	.
1	A	70	ILE	HG13	1.094	0.020	.
1	A	70	ILE	HG21	0.839	0.020	.
1	A	70	ILE	HG22	0.839	0.020	.
1	A	70	ILE	HG23	0.839	0.020	.
1	A	71	GLY	HA3	3.926	0.020	.
1	A	72	PRO	HA	4.334	0.020	.
1	A	72	PRO	CA	62.334	0.300	.
1	A	74	PRO	HA	4.329	0.020	.
1	A	74	PRO	CA	63.078	0.300	.
1	A	72	PRO	CB	31.687	0.300	.
1	A	72	PRO	CG	26.597	0.300	.
1	A	72	PRO	HB3	1.794	0.020	.
1	A	72	PRO	CD	49.324	0.300	.
1	A	72	PRO	HG2	1.896	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	PRO	HG3	1.896	0.020	.
1	A	72	PRO	HD2	3.527	0.020	.
1	A	72	PRO	HD3	3.527	0.020	.
1	A	74	PRO	CD	50.145	0.300	.
1	A	74	PRO	CB	31.672	0.300	.
1	A	74	PRO	CG	26.979	0.300	.
1	A	74	PRO	HB3	1.845	0.020	.
1	A	74	PRO	HB2	2.231	0.020	.
1	A	74	PRO	HG2	1.961	0.020	.
1	A	74	PRO	HG3	1.961	0.020	.
1	A	74	PRO	HD2	3.772	0.020	.
1	A	74	PRO	HD3	3.576	0.020	.
1	A	75	GLY	HA2	3.908	0.020	.
1	A	75	GLY	HA3	3.908	0.020	.
1	A	77	LYS	HA	4.209	0.020	.
1	A	82	ASN	HA	4.609	0.020	.
1	A	82	ASN	HB2	2.69	0.020	.
1	A	82	ASN	HB3	2.69	0.020	.
1	A	83	LEU	HA	4.224	0.020	.
1	A	83	LEU	HB2	1.49	0.020	.
1	A	83	LEU	HB3	1.49	0.020	.
1	A	83	LEU	HD11	0.839	0.020	.
1	A	83	LEU	HD12	0.839	0.020	.
1	A	83	LEU	HD13	0.839	0.020	.
1	A	83	LEU	HD21	0.839	0.020	.
1	A	83	LEU	HD22	0.839	0.020	.
1	A	83	LEU	HD23	0.839	0.020	.
1	A	84	ARG	HA	4.23	0.020	.
1	A	84	ARG	HB3	1.463	0.020	.
1	A	84	ARG	CD	41.134	0.300	.
1	A	84	ARG	CG	24.604	0.300	.
1	A	84	ARG	HG2	1.597	0.020	.
1	A	84	ARG	HG3	1.597	0.020	.
1	A	84	ARG	HD2	3.146	0.020	.
1	A	84	ARG	HD3	3.146	0.020	.
1	A	85	ARG	HA	4.217	0.020	.
1	A	85	ARG	HB2	1.741	0.020	.
1	A	85	ARG	CG	26.962	0.300	.
1	A	85	ARG	CD	42.872	0.300	.
1	A	85	ARG	HG2	1.533	0.020	.
1	A	85	ARG	HG3	1.533	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	ARG	HD2	3.108	0.020	.
1	A	85	ARG	HD3	3.108	0.020	.
1	A	86	LEU	HA	4.094	0.020	.
1	A	86	LEU	HB2	1.485	0.020	.
1	A	86	LEU	HB3	1.485	0.020	.
1	A	86	LEU	CD1	24.735	0.300	.
1	A	76	THR	HB	4.089	0.020	.
1	A	76	THR	HA	4.197	0.020	.
1	A	76	THR	CG2	21.295	0.300	.
1	A	76	THR	HG21	1.118	0.020	.
1	A	76	THR	HG22	1.118	0.020	.
1	A	76	THR	HG23	1.118	0.020	.
1	A	73	LEU	HB2	1.524	0.020	.
1	A	73	LEU	CB	41.166	0.300	.
1	A	73	LEU	HB3	1.476	0.020	.
1	A	73	LEU	HA	4.495	0.020	.
1	A	73	LEU	CG	26.406	0.300	.
1	A	73	LEU	CD1	24.801	0.300	.
1	A	73	LEU	CD2	22.586	0.300	.
1	A	73	LEU	HD11	0.872	0.020	.
1	A	73	LEU	HD12	0.872	0.020	.
1	A	73	LEU	HD13	0.872	0.020	.
1	A	73	LEU	HD21	0.834	0.020	.
1	A	73	LEU	HD22	0.834	0.020	.
1	A	73	LEU	HD23	0.834	0.020	.
1	A	73	LEU	HG	1.567	0.020	.
1	A	79	SER	HA	4.347	0.020	.
1	A	79	SER	HB2	3.731	0.020	.
1	A	79	SER	HB3	3.731	0.020	.
1	A	3	GLU	HB3	1.854	0.020	.
1	A	82	ASN	HD21	7.579	0.020	.
1	A	82	ASN	ND2	113.098	0.300	.
1	A	82	ASN	HD22	6.879	0.020	.
1	A	4	VAL	HG21	0.855	0.020	.
1	A	4	VAL	HG22	0.855	0.020	.
1	A	4	VAL	HG23	0.855	0.020	.
1	A	4	VAL	CG2	20.678	0.300	.
1	A	77	LYS	HE2	2.92	0.020	.
1	A	77	LYS	HE3	2.92	0.020	.
1	A	77	LYS	HB2	1.643	0.020	.
1	A	77	LYS	HB3	1.643	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	LYS	HD2	1.709	0.020	.
1	A	77	LYS	HD3	1.709	0.020	.
1	A	77	LYS	HG2	1.36	0.020	.
1	A	77	LYS	HG3	1.36	0.020	.
1	A	78	LYS	HE2	2.88	0.020	.
1	A	78	LYS	HE3	2.88	0.020	.
1	A	78	LYS	HD2	1.714	0.020	.
1	A	78	LYS	HD3	1.714	0.020	.
1	A	78	LYS	HG2	1.401	0.020	.
1	A	78	LYS	HG3	1.401	0.020	.
1	A	78	LYS	HB2	1.638	0.020	.
1	A	78	LYS	HB3	1.638	0.020	.
1	A	80	LYS	HA	4.23	0.020	.
1	A	80	LYS	HE2	2.914	0.020	.
1	A	80	LYS	HE3	2.914	0.020	.
1	A	80	LYS	HD2	1.777	0.020	.
1	A	80	LYS	HD3	1.777	0.020	.
1	A	80	LYS	HB2	1.641	0.020	.
1	A	80	LYS	HB3	1.641	0.020	.
1	A	80	LYS	HG2	1.367	0.020	.
1	A	80	LYS	HG3	1.367	0.020	.
1	A	78	LYS	HA	4.241	0.020	.
1	A	2	SER	HB2	3.788	0.020	.
1	A	2	SER	HB3	3.788	0.020	.
1	A	2	SER	CB	63.354	0.300	.
1	A	2	SER	HA	4.341	0.020	.
1	A	2	SER	CA	58.096	0.300	.
1	A	3	GLU	CG	36.237	0.300	.
1	A	3	GLU	HG2	2.11	0.020	.
1	A	3	GLU	HG3	2.11	0.020	.
1	A	8	LEU	HG	1.504	0.020	.
1	A	9	LYS	CG	24.277	0.300	.
1	A	9	LYS	CD	28.642	0.300	.
1	A	9	LYS	CE	41.652	0.300	.
1	A	10	LYS	HA	4.216	0.020	.
1	A	10	LYS	HB2	1.602	0.020	.
1	A	10	LYS	HB3	1.602	0.020	.
1	A	10	LYS	HG2	1.323	0.020	.
1	A	10	LYS	HG3	1.323	0.020	.
1	A	10	LYS	HD2	1.713	0.020	.
1	A	10	LYS	HD3	1.713	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	LYS	HE2	2.915	0.020	.
1	A	10	LYS	HE3	2.915	0.020	.
1	A	10	LYS	CG	24.229	0.300	.
1	A	10	LYS	CD	28.595	0.300	.
1	A	10	LYS	CE	41.666	0.300	.
1	A	11	ASN	HD21	7.553	0.020	.
1	A	11	ASN	ND2	112.766	0.300	.
1	A	11	ASN	HD22	6.86	0.020	.
1	A	63	LEU	HG	1.527	0.020	.
1	A	63	LEU	CG	26.473	0.300	.
1	A	64	LEU	HG	1.5	0.020	.
1	A	64	LEU	CG	26.411	0.300	.
1	A	64	LEU	CD1	24.753	0.300	.
1	A	65	LYS	HE2	2.913	0.020	.
1	A	65	LYS	HE3	2.913	0.020	.
1	A	65	LYS	HD2	1.721	0.020	.
1	A	65	LYS	HD3	1.721	0.020	.
1	A	65	LYS	HB2	1.635	0.020	.
1	A	65	LYS	HB3	1.635	0.020	.
1	A	65	LYS	HG2	1.376	0.020	.
1	A	65	LYS	HG3	1.376	0.020	.
1	A	65	LYS	CG	24.302	0.300	.
1	A	65	LYS	CD	28.583	0.300	.
1	A	65	LYS	CE	41.606	0.300	.
1	A	67	SER	HB2	3.754	0.020	.
1	A	67	SER	HB3	3.754	0.020	.
1	A	67	SER	HA	4.377	0.020	.
1	A	69	LYS	HA	4.268	0.020	.
1	A	69	LYS	HE2	2.921	0.020	.
1	A	69	LYS	HE3	2.921	0.020	.
1	A	69	LYS	HB2	1.621	0.020	.
1	A	69	LYS	HB3	1.621	0.020	.
1	A	69	LYS	HD2	1.726	0.020	.
1	A	69	LYS	HD3	1.726	0.020	.
1	A	69	LYS	HG2	1.325	0.020	.
1	A	69	LYS	HG3	1.325	0.020	.
1	A	69	LYS	CG	24.242	0.300	.
1	A	69	LYS	CD	28.583	0.300	.
1	A	69	LYS	CE	41.666	0.300	.
1	A	77	LYS	CG	24.242	0.300	.
1	A	77	LYS	CD	28.643	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	77	LYS	CE	41.666	0.300	.
1	A	78	LYS	CG	24.193	0.300	.
1	A	78	LYS	CD	28.342	0.300	.
1	A	78	LYS	CE	41.666	0.300	.
1	A	80	LYS	CG	24.302	0.300	.
1	A	80	LYS	CD	30.175	0.300	.
1	A	80	LYS	CE	41.606	0.300	.
1	A	81	LYS	HA	4.148	0.020	.
1	A	81	LYS	HE2	2.915	0.020	.
1	A	81	LYS	HE3	2.915	0.020	.
1	A	81	LYS	HB2	1.638	0.020	.
1	A	81	LYS	HB3	1.638	0.020	.
1	A	81	LYS	HD2	1.715	0.020	.
1	A	81	LYS	HD3	1.715	0.020	.
1	A	81	LYS	HG2	1.304	0.020	.
1	A	81	LYS	HG3	1.304	0.020	.
1	A	81	LYS	CG	24.182	0.300	.
1	A	81	LYS	CD	28.707	0.300	.
1	A	81	LYS	CE	41.854	0.300	.
1	A	83	LEU	HG	1.492	0.020	.
1	A	83	LEU	CG	26.917	0.300	.
1	A	83	LEU	CD1	22.756	0.300	.
1	A	86	LEU	HD11	0.861	0.020	.
1	A	86	LEU	HD12	0.861	0.020	.
1	A	86	LEU	HD13	0.861	0.020	.
1	A	86	LEU	HD21	0.861	0.020	.
1	A	86	LEU	HD22	0.861	0.020	.
1	A	86	LEU	HD23	0.861	0.020	.
1	A	86	LEU	HG	1.378	0.020	.
1	A	86	LEU	CG	26.78	0.300	.
1	A	3	GLU	C	176.655	0.300	.
1	A	4	VAL	C	176.11	0.300	.
1	A	5	ALA	C	177.887	0.300	.
1	A	6	LYS	C	175.28	0.300	.
1	A	7	THR	C	174.332	0.300	.
1	A	8	LEU	C	174.474	0.300	.
1	A	9	LYS	C	176.252	0.300	.
1	A	10	LYS	C	176.394	0.300	.
1	A	11	ASN	C	175.209	0.300	.
1	A	12	GLU	C	176.252	0.300	.
1	A	59	SER	C	174.356	0.300	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	ASP	C	177.176	0.300	.
1	A	61	GLY	C	174.83	0.300	.
1	A	62	LYS	C	177.01	0.300	.
1	A	63	LEU	C	177.461	0.300	.
1	A	64	LEU	C	177.176	0.300	.
1	A	65	LYS	C	176.489	0.300	.
1	A	66	ALA	C	177.959	0.300	.
1	A	67	SER	C	177.129	0.300	.
1	A	68	CYS	C	174.427	0.300	.
1	A	69	LYS	C	176.821	0.300	.
1	A	70	ILE	C	176.299	0.300	.
1	A	75	GLY	C	174.545	0.300	.
1	A	76	THR	C	174.759	0.300	.
1	A	77	LYS	C	176.679	0.300	.
1	A	78	LYS	C	176.536	0.300	.
1	A	79	SER	C	177.034	0.300	.
1	A	80	LYS	C	176.607	0.300	.
1	A	81	LYS	C	176.276	0.300	.
1	A	82	ASN	C	174.996	0.300	.
1	A	83	LEU	C	177.153	0.300	.
1	A	84	ARG	C	175.802	0.300	.
1	A	85	ARG	C	175.091	0.300	.
1	A	72	PRO	HB2	2.154	0.020	.
1	A	12	GLU	HB2	1.98	0.020	.
1	A	85	ARG	HB3	1.678	0.020	.
1	A	84	ARG	HB2	1.652	0.020	.
1	A	70	ILE	HD11	0.766	0.020	.
1	A	70	ILE	HD12	0.766	0.020	.
1	A	70	ILE	HD13	0.766	0.020	.
1	A	71	GLY	HA2	4.077	0.020	.
1	A	64	LEU	HD11	0.815	0.020	.
1	A	64	LEU	HD12	0.815	0.020	.
1	A	64	LEU	HD13	0.815	0.020	.
1	A	64	LEU	HD21	0.815	0.020	.
1	A	64	LEU	HD22	0.815	0.020	.
1	A	64	LEU	HD23	0.815	0.020	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	85	0.43 ± 0.44	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	80	0.63 ± 0.22	Should be applied
$^{13}\text{C}'$	77	0.32 ± 0.28	None needed (< 0.5 ppm)
^{15}N	81	-1.76 ± 0.56	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 444 atoms were assigned a chemical shift out of a possible 495. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	188/190 (99%)	77/77 (100%)	74/76 (97%)	37/37 (100%)
Sidechain	224/259 (86%)	152/165 (92%)	68/78 (87%)	4/16 (25%)
Aromatic	32/46 (70%)	21/21 (100%)	11/25 (44%)	0/0 (—%)
Overall	444/495 (90%)	250/263 (95%)	153/179 (85%)	41/53 (77%)

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	32	ARG	NE	116.02	76.53 – 92.65	19.5
1	A	32	ARG	HD3	1.09	1.81 – 4.39	-7.8

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:

