



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 5OGU
BMRB ID : 34163
Title : Structure of DNA-binding HU protein from micoplasma Spiroplasma mel-
liferum
Authors : Altukhov, D.A.; Talyzina, A.A.; Agapova, Y.K.; Vlaskina, A.V.; Ko-
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Deposited on : 2017-07-13

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

<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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

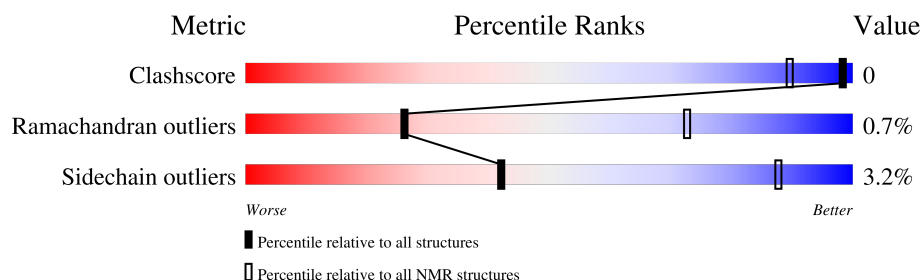
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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	95	
1	B	95	

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 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:-1-A:55, A:77-A:93, B:-1-B:55, B:77-B:93 (148)	0.46	4
2	B:58-B:76 (19)	0.39	6

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2948 atoms, of which 1500 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1474	456	750	130	137	1	
1	B	95	Total	C	H	N	O	S	0
			1474	456	750	130	137	1	

There are 4 discrepancies between the modelled and reference sequences:

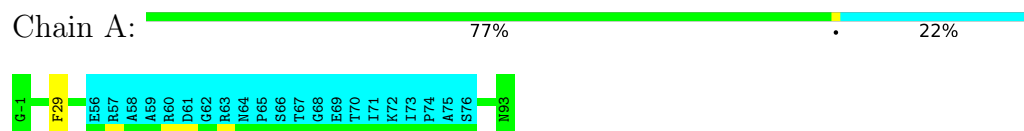
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A037USE5
A	0	HIS	-	expression tag	UNP A0A037USE5
B	-1	GLY	-	expression tag	UNP A0A037USE5
B	0	HIS	-	expression tag	UNP A0A037USE5

4 Residue-property plots

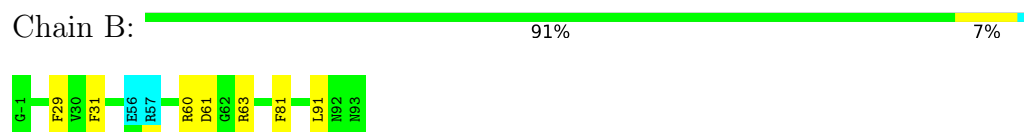
4.1 Average score per residue in the NMR ensemble

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: DNA-binding protein



- Molecule 1: DNA-binding protein

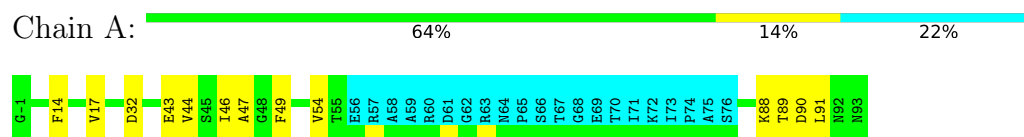


4.2 Scores per residue for each member of the ensemble

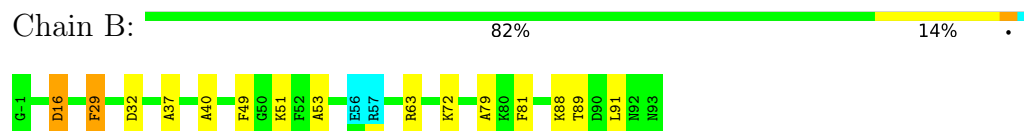
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: DNA-binding protein

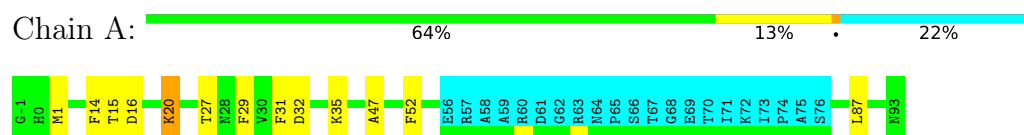


- Molecule 1: DNA-binding protein

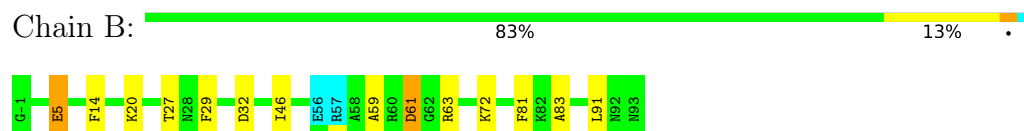


4.2.2 Score per residue for model 2

- Molecule 1: DNA-binding protein

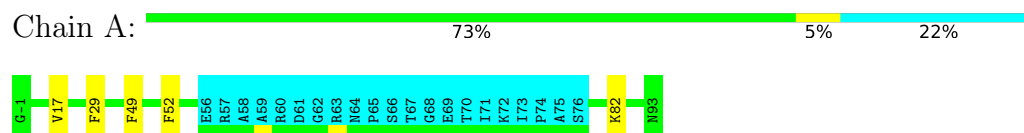


- Molecule 1: DNA-binding protein

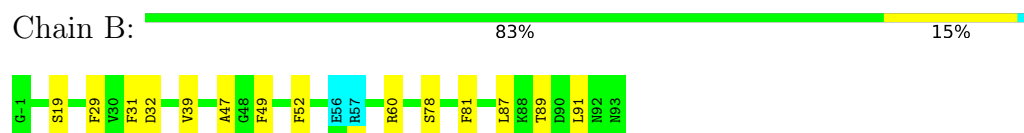


4.2.3 Score per residue for model 3

- Molecule 1: DNA-binding protein

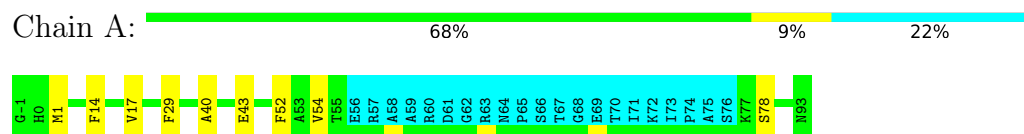


- Molecule 1: DNA-binding protein

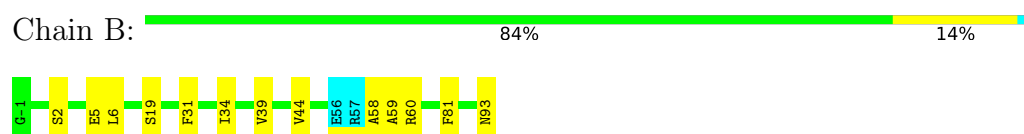


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: DNA-binding protein

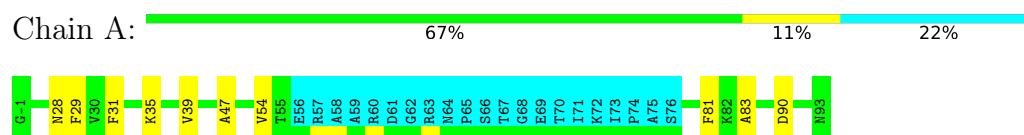


- Molecule 1: DNA-binding protein

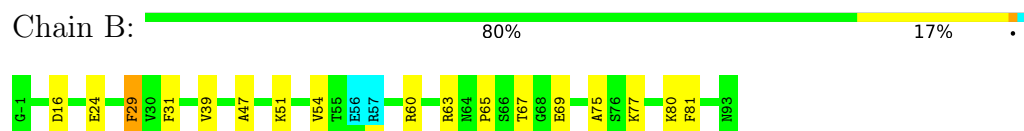


4.2.5 Score per residue for model 5

- Molecule 1: DNA-binding protein

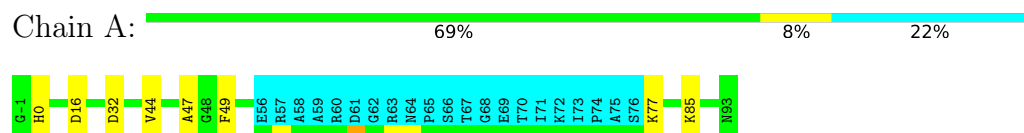


- Molecule 1: DNA-binding protein

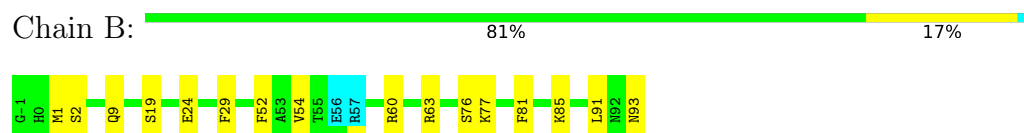


4.2.6 Score per residue for model 6

- Molecule 1: DNA-binding protein

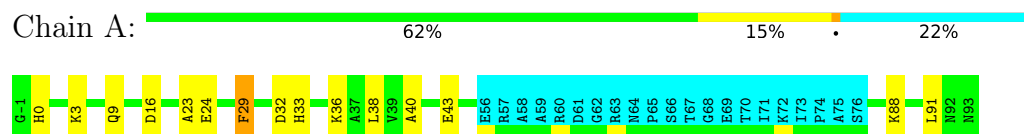


- Molecule 1: DNA-binding protein

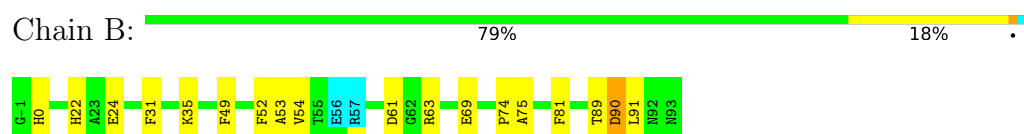


4.2.7 Score per residue for model 7

- Molecule 1: DNA-binding protein

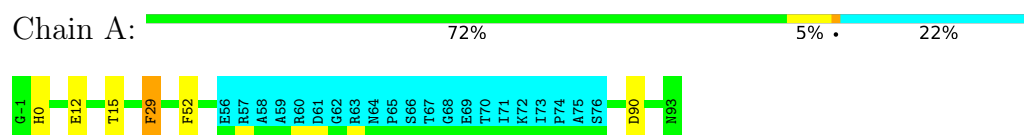


- Molecule 1: DNA-binding protein

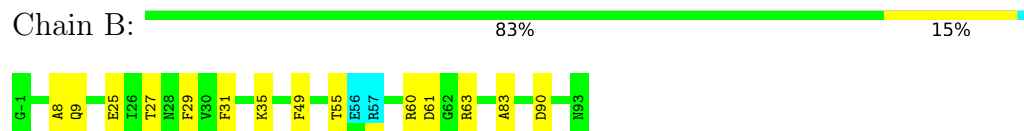


4.2.8 Score per residue for model 8

- Molecule 1: DNA-binding protein

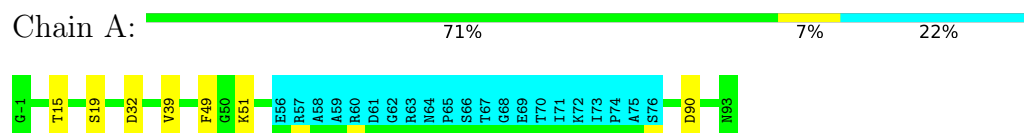


- Molecule 1: DNA-binding protein

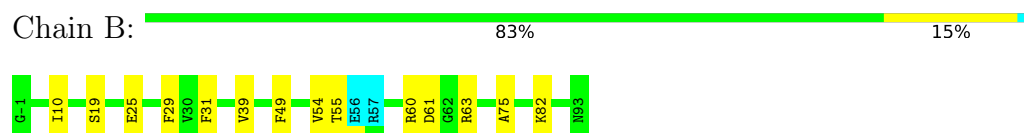


4.2.9 Score per residue for model 9

- Molecule 1: DNA-binding protein

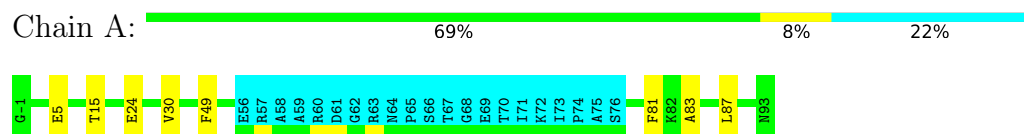


- Molecule 1: DNA-binding protein

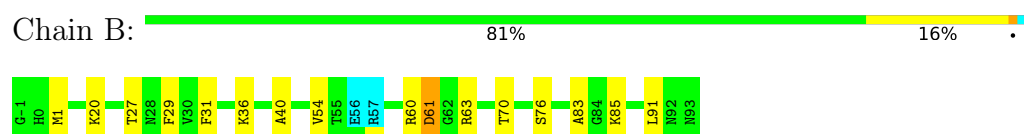


4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein

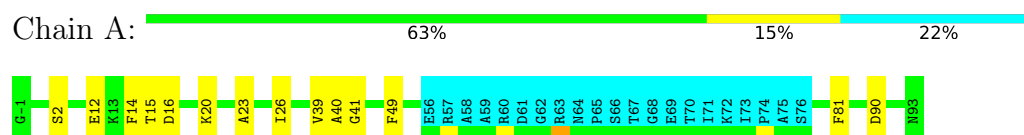


- Molecule 1: DNA-binding protein

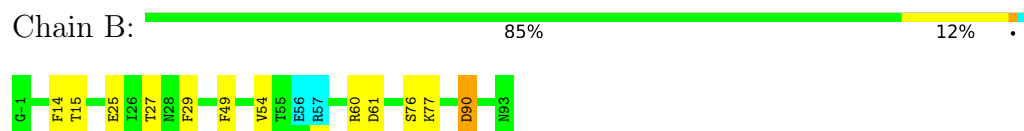


4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein

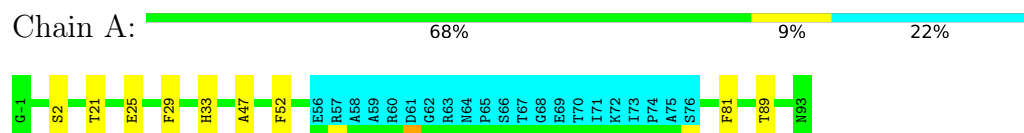


- Molecule 1: DNA-binding protein

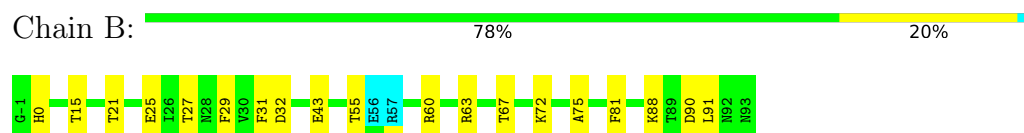


4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding protein

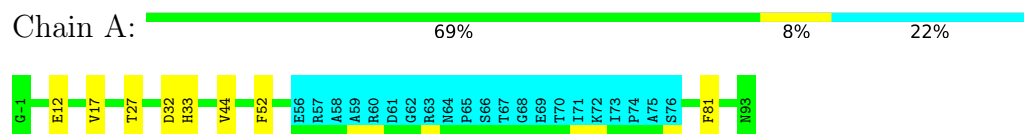


- Molecule 1: DNA-binding protein

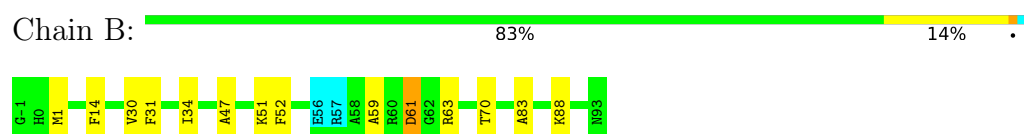


4.2.13 Score per residue for model 13

- Molecule 1: DNA-binding protein

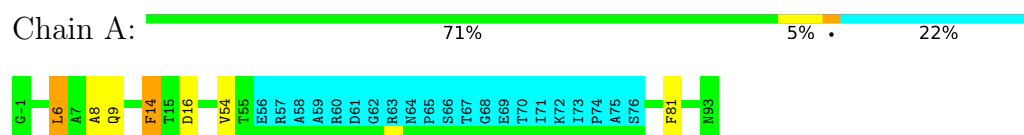


- Molecule 1: DNA-binding protein

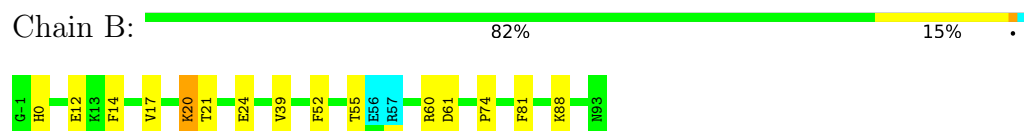


4.2.14 Score per residue for model 14

- Molecule 1: DNA-binding protein

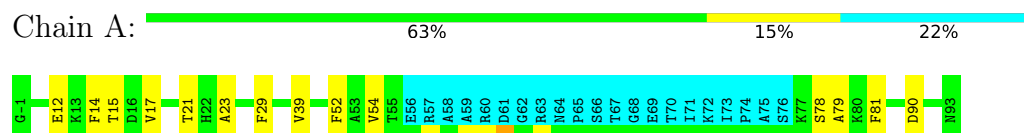


- Molecule 1: DNA-binding protein

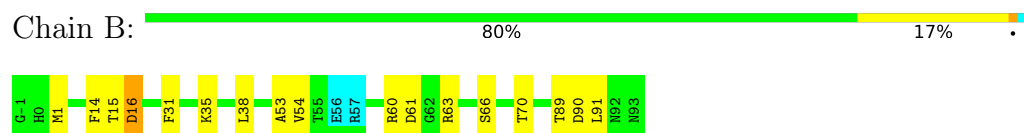


4.2.15 Score per residue for model 15

- Molecule 1: DNA-binding protein



- Molecule 1: DNA-binding protein



5 Refinement protocol and experimental data overview

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

Of the 5000 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
GROMACS	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	320
Number of shifts mapped to atoms	320
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.50±0.01	0±0/577 (0.0± 0.0%)	1.79±0.08	8±3/767 (1.1± 0.3%)
1	B	0.51±0.01	0±0/714 (0.0± 0.0%)	1.86±0.07	14±3/953 (1.4± 0.3%)
All	All	0.51	0/19365 (0.0%)	1.83	328/25800 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.7±1.1
1	A	0.0±0.0	0.6±0.9
All	All	0	20

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	63	ARG	NE-CZ-NH2	15.75	128.17	120.30	6	4
1	B	63	ARG	NE-CZ-NH1	14.54	127.57	120.30	13	5
1	B	31	PHE	CB-CG-CD2	-13.42	111.41	120.80	8	5
1	B	60	ARG	NE-CZ-NH1	12.47	126.54	120.30	11	6
1	B	60	ARG	NE-CZ-NH2	-12.41	114.09	120.30	11	3
1	B	29	PHE	CB-CG-CD2	-11.77	112.56	120.80	10	2
1	A	49	PHE	CB-CG-CD1	-11.47	112.77	120.80	10	3
1	A	49	PHE	CB-CG-CD2	-10.91	113.16	120.80	9	4
1	B	29	PHE	CB-CG-CD1	10.69	128.28	120.80	10	2
1	B	49	PHE	CB-CG-CD1	-10.51	113.44	120.80	11	5
1	B	81	PHE	CB-CG-CD1	-9.85	113.91	120.80	14	6
1	A	21	THR	CA-CB-CG2	9.73	126.02	112.40	12	2
1	B	49	PHE	CB-CG-CD2	-9.56	114.11	120.80	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	PHE	CB-CG-CD1	9.15	127.21	120.80	8	5
1	B	90	ASP	CB-CG-OD1	-8.81	110.37	118.30	15	4
1	B	24	GLU	OE1-CD-OE2	-8.72	112.84	123.30	14	3
1	A	14	PHE	CB-CG-CD2	-8.57	114.80	120.80	1	4
1	A	32	ASP	CB-CG-OD2	8.54	125.99	118.30	9	3
1	B	58	ALA	CB-CA-C	-8.36	97.56	110.10	4	1
1	A	29	PHE	CB-CG-CD1	-8.30	114.99	120.80	8	3
1	A	15	THR	CA-CB-CG2	8.22	123.91	112.40	15	5
1	A	12	GLU	OE1-CD-OE2	-8.06	113.63	123.30	11	2
1	B	14	PHE	CB-CG-CD2	-8.03	115.18	120.80	11	2
1	A	29	PHE	CB-CG-CD2	7.91	126.34	120.80	8	3
1	A	90	ASP	CB-CG-OD2	7.80	125.32	118.30	1	4
1	B	14	PHE	CZ-CE2-CD2	7.80	129.46	120.10	2	1
1	B	16	ASP	CB-CG-OD2	7.75	125.28	118.30	15	2
1	A	47	ALA	C-N-CA	7.71	138.49	122.30	1	1
1	B	14	PHE	CB-CG-CD1	7.43	126.00	120.80	11	2
1	B	60	ARG	CD-NE-CZ	7.37	133.92	123.60	11	2
1	A	16	ASP	CB-CG-OD1	7.36	124.92	118.30	6	2
1	A	78	SER	CB-CA-C	7.35	124.06	110.10	15	2
1	A	30	VAL	CA-CB-CG1	7.30	121.86	110.90	10	1
1	A	6	LEU	CB-CG-CD1	7.25	123.33	111.00	14	1
1	A	17	VAL	CA-CB-CG1	7.24	121.75	110.90	4	4
1	A	40	ALA	N-CA-CB	-7.23	99.98	110.10	7	2
1	A	90	ASP	CB-CG-OD1	-7.20	111.82	118.30	11	2
1	A	43	GLU	OE1-CD-OE2	-7.20	114.66	123.30	1	2
1	A	25	GLU	OE1-CD-OE2	-7.09	114.79	123.30	12	1
1	A	5	GLU	CA-CB-CG	7.08	128.99	113.40	10	1
1	B	90	ASP	CB-CG-OD2	7.03	124.63	118.30	12	2
1	B	81	PHE	CB-CG-CD2	7.02	125.72	120.80	12	2
1	B	32	ASP	CB-CG-OD1	-6.98	112.02	118.30	12	3
1	A	52	PHE	CB-CG-CD2	-6.98	115.91	120.80	8	4
1	B	29	PHE	CD1-CG-CD2	6.90	127.27	118.30	5	1
1	B	83	ALA	CB-CA-C	-6.88	99.78	110.10	13	2
1	B	60	ARG	C-N-CA	6.87	138.86	121.70	14	1
1	B	91	LEU	CB-CG-CD2	6.86	122.66	111.00	7	1
1	A	82	LYS	N-CA-CB	-6.80	98.35	110.60	3	1
1	B	76	SER	CB-CA-C	6.78	122.98	110.10	6	2
1	B	61	ASP	CB-CG-OD1	6.77	124.39	118.30	2	3
1	A	2	SER	N-CA-CB	-6.72	100.42	110.50	12	2
1	B	21	THR	CA-CB-CG2	-6.70	103.03	112.40	12	2
1	B	52	PHE	CB-CG-CD1	-6.67	116.13	120.80	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	19	SER	CB-CA-C	6.67	122.76	110.10	4	2
1	B	31	PHE	CB-CG-CD1	-6.65	116.15	120.80	10	5
1	B	65	PRO	N-CA-CB	6.65	111.28	103.30	5	1
1	B	54	VAL	CA-CB-CG2	6.61	120.82	110.90	9	2
1	A	23	ALA	CB-CA-C	-6.60	100.20	110.10	15	1
1	A	19	SER	CB-CA-C	6.58	122.60	110.10	9	1
1	B	88	LYS	CB-CA-C	6.57	123.54	110.40	13	2
1	A	81	PHE	CB-CG-CD1	-6.55	116.21	120.80	5	2
1	A	44	VAL	CA-CB-CG1	6.53	120.69	110.90	6	1
1	B	12	GLU	O-C-N	-6.49	112.32	122.70	14	1
1	A	8	ALA	N-CA-CB	-6.44	101.08	110.10	14	1
1	B	81	PHE	CZ-CE2-CD2	-6.44	112.38	120.10	6	1
1	B	54	VAL	C-N-CA	6.38	137.66	121.70	10	2
1	B	46	ILE	CA-CB-CG1	6.33	123.04	111.00	2	1
1	A	83	ALA	CB-CA-C	-6.33	100.60	110.10	5	1
1	B	63	ARG	CB-CA-C	6.31	123.02	110.40	9	1
1	B	39	VAL	CG1-CB-CG2	-6.30	100.81	110.90	14	1
1	A	23	ALA	N-CA-CB	6.30	118.92	110.10	7	1
1	A	39	VAL	CA-CB-CG1	6.29	120.33	110.90	5	4
1	B	27	THR	CA-CB-CG2	6.28	121.20	112.40	8	4
1	A	46	ILE	CA-CB-CG1	6.24	122.85	111.00	1	1
1	A	29	PHE	CG-CD2-CE2	-6.21	113.97	120.80	2	1
1	B	75	ALA	N-CA-CB	-6.21	101.41	110.10	12	1
1	B	43	GLU	OE1-CD-OE2	-6.18	115.88	123.30	12	1
1	B	63	ARG	CD-NE-CZ	6.10	132.14	123.60	6	4
1	B	74	PRO	N-CD-CG	6.10	112.35	103.20	14	1
1	A	40	ALA	CB-CA-C	-6.08	100.98	110.10	4	1
1	A	38	LEU	CB-CG-CD2	6.07	121.33	111.00	7	1
1	B	66	SER	N-CA-CB	-6.07	101.39	110.50	15	1
1	B	15	THR	CA-CB-CG2	6.05	120.88	112.40	11	1
1	A	12	GLU	O-C-N	-6.04	113.04	122.70	13	1
1	B	27	THR	CA-CB-OG1	6.03	121.66	109.00	10	1
1	B	5	GLU	OE1-CD-OE2	-6.00	116.09	123.30	2	2
1	B	88	LYS	CA-CB-CG	6.00	126.60	113.40	12	1
1	A	44	VAL	C-N-CA	5.98	136.64	121.70	1	1
1	B	63	ARG	NH1-CZ-NH2	-5.96	112.84	119.40	6	2
1	B	31	PHE	CG-CD2-CE2	-5.96	114.25	120.80	8	1
1	B	55	THR	CA-CB-CG2	5.95	120.72	112.40	12	2
1	B	59	ALA	CB-CA-C	-5.94	101.19	110.10	4	2
1	B	76	SER	N-CA-CB	-5.94	101.60	110.50	10	1
1	B	49	PHE	CD1-CG-CD2	5.93	126.01	118.30	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	70	THR	CA-CB-OG1	5.93	121.45	109.00	13	1
1	B	31	PHE	CZ-CE2-CD2	5.91	127.19	120.10	12	1
1	A	27	THR	CA-CB-CG2	5.90	120.66	112.40	2	2
1	B	54	VAL	CG1-CB-CG2	-5.88	101.50	110.90	7	1
1	B	32	ASP	CB-CG-OD2	5.87	123.59	118.30	2	1
1	A	28	ASN	C-N-CA	5.85	136.33	121.70	5	1
1	B	67	THR	CA-CB-CG2	5.84	120.58	112.40	12	1
1	B	70	THR	CA-CB-CG2	5.82	120.55	112.40	15	1
1	B	53	ALA	CB-CA-C	5.79	118.78	110.10	15	3
1	A	32	ASP	CB-CG-OD1	-5.76	113.12	118.30	1	2
1	B	19	SER	C-N-CA	5.74	136.04	121.70	3	1
1	A	77	LYS	CA-CB-CG	5.71	125.96	113.40	6	1
1	B	75	ALA	CB-CA-C	-5.70	101.56	110.10	9	1
1	A	89	THR	N-CA-C	5.68	126.34	111.00	1	1
1	B	29	PHE	CG-CD2-CE2	-5.67	114.56	120.80	5	3
1	A	31	PHE	CB-CG-CD1	-5.67	116.83	120.80	2	1
1	A	54	VAL	CA-CB-CG1	5.66	119.39	110.90	1	2
1	B	61	ASP	CB-CA-C	5.62	121.64	110.40	7	2
1	B	39	VAL	CA-CB-CG1	5.61	119.32	110.90	4	3
1	A	1	MET	N-CA-CB	-5.58	100.56	110.60	4	1
1	A	81	PHE	CB-CG-CD2	-5.58	116.89	120.80	12	3
1	B	60	ARG	CB-CA-C	5.57	121.54	110.40	5	2
1	B	51	LYS	CB-CA-C	5.57	121.53	110.40	13	2
1	B	30	VAL	CA-CB-CG1	5.56	119.24	110.90	13	1
1	B	54	VAL	CA-CB-CG1	5.53	119.20	110.90	15	2
1	B	0	HIS	N-CA-CB	-5.53	100.64	110.60	12	1
1	B	2	SER	N-CA-CB	-5.52	102.22	110.50	6	2
1	B	15	THR	CA-CB-OG1	5.52	120.59	109.00	12	1
1	B	14	PHE	CG-CD2-CE2	-5.50	114.75	120.80	2	2
1	B	36	LYS	CB-CA-C	5.50	121.40	110.40	10	1
1	B	47	ALA	C-N-CA	5.50	133.84	122.30	3	1
1	A	79	ALA	CB-CA-C	-5.49	101.87	110.10	15	1
1	A	20	LYS	CB-CA-C	5.47	121.34	110.40	2	1
1	A	51	LYS	CB-CA-C	5.45	121.30	110.40	9	1
1	A	87	LEU	O-C-N	-5.45	113.99	122.70	2	1
1	B	29	PHE	CZ-CE2-CD2	5.43	126.62	120.10	2	1
1	B	20	LYS	N-CA-C	5.40	125.59	111.00	14	1
1	B	69	GLU	C-N-CA	5.39	135.19	121.70	5	1
1	A	26	ILE	CA-CB-CG1	5.39	121.25	111.00	11	1
1	B	37	ALA	CB-CA-C	-5.39	102.01	110.10	1	1
1	A	49	PHE	CG-CD1-CE1	-5.39	114.88	120.80	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	HIS	CA-CB-CG	5.38	122.75	113.60	12	1
1	B	31	PHE	CD1-CE1-CZ	-5.37	113.66	120.10	5	1
1	A	43	GLU	N-CA-CB	-5.37	100.94	110.60	1	1
1	B	35	LYS	CA-CB-CG	5.37	125.21	113.40	15	1
1	B	74	PRO	N-CA-CB	5.37	109.74	103.30	7	1
1	B	72	LYS	CB-CA-C	5.36	121.12	110.40	1	2
1	B	83	ALA	O-C-N	-5.36	114.09	123.20	8	1
1	A	44	VAL	O-C-N	-5.34	114.16	122.70	13	1
1	B	0	HIS	C-N-CA	5.33	135.03	121.70	7	1
1	A	83	ALA	N-CA-CB	-5.30	102.68	110.10	10	1
1	B	51	LYS	C-N-CA	5.29	134.93	121.70	1	1
1	B	77	LYS	CB-CA-C	-5.28	99.84	110.40	6	1
1	B	91	LEU	CB-CG-CD1	5.28	119.98	111.00	2	1
1	B	55	THR	CA-CB-OG1	5.28	120.08	109.00	9	1
1	B	59	ALA	N-CA-CB	-5.28	102.71	110.10	13	1
1	A	54	VAL	CG1-CB-CG2	-5.28	102.46	110.90	5	1
1	A	41	GLY	CA-C-O	-5.27	111.12	120.60	11	1
1	B	79	ALA	CB-CA-C	5.26	118.00	110.10	1	1
1	B	66	SER	CB-CA-C	-5.26	100.11	110.10	15	1
1	B	55	THR	C-N-CA	5.26	134.84	121.70	14	1
1	B	6	LEU	CB-CG-CD1	5.25	119.93	111.00	4	1
1	B	70	THR	OG1-CB-CG2	-5.23	97.97	110.00	10	1
1	A	87	LEU	CB-CA-C	5.22	120.12	110.20	10	1
1	B	39	VAL	CA-CB-CG2	5.22	118.73	110.90	9	2
1	B	8	ALA	N-CA-CB	-5.21	102.80	110.10	8	1
1	B	0	HIS	CA-CB-CG	5.20	122.44	113.60	14	1
1	B	61	ASP	CB-CG-OD2	5.19	122.97	118.30	10	1
1	A	88	LYS	CB-CA-C	5.18	120.77	110.40	1	1
1	B	47	ALA	CB-CA-C	5.18	117.87	110.10	5	1
1	B	25	GLU	OE1-CD-OE2	-5.17	117.09	123.30	11	1
1	B	81	PHE	C-N-CA	5.17	134.62	121.70	2	1
1	B	74	PRO	CA-N-CD	-5.16	104.28	111.50	14	1
1	A	29	PHE	CZ-CE2-CD2	5.16	126.29	120.10	12	1
1	B	40	ALA	CB-CA-C	-5.15	102.37	110.10	1	1
1	A	81	PHE	CG-CD2-CE2	-5.14	115.14	120.80	11	1
1	A	24	GLU	OE1-CD-OE2	-5.14	117.13	123.30	10	1
1	A	0	HIS	CA-CB-CG	5.14	122.33	113.60	8	1
1	B	35	LYS	N-CA-CB	-5.14	101.36	110.60	8	1
1	A	17	VAL	O-C-N	5.13	130.90	122.70	4	1
1	B	20	LYS	CA-CB-CG	5.11	124.65	113.40	2	2
1	B	78	SER	CB-CA-C	5.11	119.81	110.10	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	40	ALA	N-CA-CB	-5.11	102.95	110.10	10	1
1	A	43	GLU	C-N-CA	5.11	134.47	121.70	7	1
1	B	1	MET	CB-CA-C	5.10	120.60	110.40	15	2
1	B	82	LYS	N-CA-C	-5.09	97.25	111.00	9	1
1	B	89	THR	N-CA-CB	-5.09	100.63	110.30	15	1
1	B	81	PHE	CG-CD2-CE2	-5.09	115.20	120.80	5	1
1	A	14	PHE	CB-CG-CD1	5.09	124.36	120.80	11	1
1	A	0	HIS	N-CA-CB	-5.08	101.45	110.60	7	1
1	A	54	VAL	CA-CB-CG2	5.07	118.50	110.90	4	1
1	A	88	LYS	C-N-CA	5.06	134.36	121.70	7	1
1	B	16	ASP	CB-CG-OD1	5.06	122.86	118.30	1	1
1	B	1	MET	C-N-CA	5.05	134.32	121.70	10	1
1	B	9	GLN	CB-CG-CD	5.04	124.71	111.60	8	1
1	B	91	LEU	CA-CB-CG	5.03	126.88	115.30	15	1
1	A	21	THR	O-C-N	-5.01	114.68	122.70	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	14	PHE	Sidechain	3
1	B	63	ARG	Sidechain	2
1	A	81	PHE	Sidechain	2
1	B	81	PHE	Sidechain	1
1	B	67	THR	Mainchain	1
1	A	0	HIS	Peptide	1
1	A	33	HIS	Sidechain	1
1	B	22	HIS	Sidechain	1
1	B	69	GLU	Sidechain	1
1	B	75	ALA	Peptide	1
1	B	60	ARG	Sidechain	1
1	B	10	ILE	Mainchain	1
1	A	49	PHE	Sidechain	1
1	A	12	GLU	Sidechain	1
1	B	31	PHE	Sidechain	1
1	B	38	LEU	Mainchain	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	704	731	731	0±0
1	A	569	595	595	0±0
All	All	19095	19890	19890	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ILE:HG23	1:B:44:VAL:HG11	0.56	1.78	4	1
1:B:88:LYS:HG3	1:B:89:THR:H	0.55	1.61	1	1
1:A:33:HIS:CE1	1:B:1:MET:CE	0.47	2.97	13	1
1:A:32:ASP:OD2	1:A:36:LYS:NZ	0.47	2.44	7	1
1:A:31:PHE:CD1	1:A:31:PHE:N	0.43	2.87	5	1
1:A:20:LYS:O	1:A:23:ALA:HB3	0.42	2.14	11	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	72/95 (76%)	66±2 (92±3%)	5±2 (7±3%)	0±1 (1±1%)	29	74
1	B	91/95 (96%)	82±3 (90±3%)	8±2 (9±2%)	1±1 (1±1%)	26	73
All	All	2445/2850 (86%)	2229 (91%)	200 (8%)	16 (1%)	26	73

All 12 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	47	ALA	4
1	B	85	LYS	2
1	A	20	LYS	1
1	B	83	ALA	1
1	A	29	PHE	1
1	B	75	ALA	1
1	A	85	LYS	1
1	B	9	GLN	1
1	B	35	LYS	1
1	B	34	ILE	1
1	B	47	ALA	1
1	B	20	LYS	1

6.3.2 Protein sidechains ⓘ

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	59/75 (79%)	57±1 (97±2%)	2±1 (3±2%)	49	91
1	B	73/75 (97%)	70±1 (96±2%)	3±1 (4±2%)	37	85
All	All	1980/2250 (88%)	1917 (97%)	63 (3%)	42	88

All 33 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	B	29	PHE	7
1	B	61	ASP	6
1	B	91	LEU	5
1	A	16	ASP	3
1	A	29	PHE	3
1	B	25	GLU	3
1	A	91	LEU	2
1	B	16	ASP	2
1	A	35	LYS	2
1	B	89	THR	2
1	B	93	ASN	2
1	B	77	LYS	2
1	A	9	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	B	90	ASP	2
1	A	90	ASP	2
1	A	1	MET	1
1	B	5	GLU	1
1	B	87	LEU	1
1	B	24	GLU	1
1	B	80	LYS	1
1	A	32	ASP	1
1	B	1	MET	1
1	B	19	SER	1
1	A	3	LYS	1
1	A	24	GLU	1
1	A	15	THR	1
1	A	89	THR	1
1	B	72	LYS	1
1	A	6	LEU	1
1	B	17	VAL	1
1	A	17	VAL	1
1	A	54	VAL	1
1	B	15	THR	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 monosaccharides in this entry.

6.6 Ligand geometry ⓘ

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 13% for the well-defined parts and 14% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Spm_BMRB.tab*

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	320
Number of shifts mapped to atoms	320
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	-0.07 ± 0.34	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	41	0.54 ± 0.19	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	78	0.40 ± 0.31	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 13%, i.e. 260 atoms were assigned a chemical shift out of a possible 2014. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	225/831 (27%)	103/332 (31%)	61/334 (18%)	61/165 (37%)
Sidechain	35/1033 (3%)	0/603 (0%)	35/386 (9%)	0/44 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/150 (0%)	0/84 (0%)	0/60 (0%)	0/6 (0%)
Overall	260/2014 (13%)	103/1019 (10%)	96/780 (12%)	61/215 (28%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 14%, i.e. 319 atoms were assigned a chemical shift out of a possible 2298. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	278/942 (30%)	122/376 (32%)	78/380 (21%)	78/186 (42%)
Sidechain	41/1206 (3%)	0/706 (0%)	41/442 (9%)	0/58 (0%)
Aromatic	0/150 (0%)	0/84 (0%)	0/60 (0%)	0/6 (0%)
Overall	319/2298 (14%)	122/1166 (10%)	119/882 (13%)	78/250 (31%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

