



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2NDP  
Title : Structure of DNA-binding HU protein from micoplasma Mycoplasma gallisepticum  
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Deposited on : 2016-09-13

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

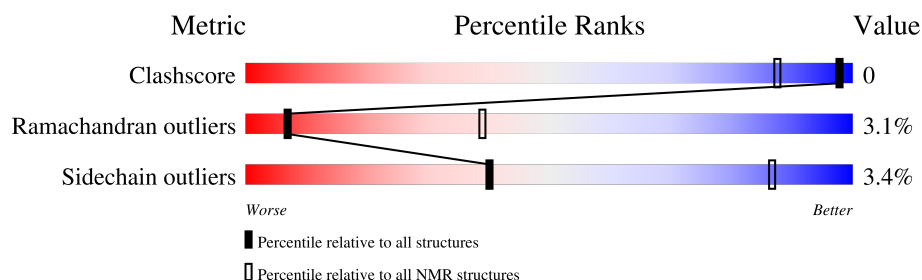
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 22%.

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  $\geq 3$ , 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	99	 68% 9% • 22%
1	B	99	 72% 8% 20%

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:4-A:60, A:80-A:99, B:1-B:61, B:80-B:97 (156)	0.79	9

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 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3252 atoms, of which 1714 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone-like DNA-binding superfamily protein.

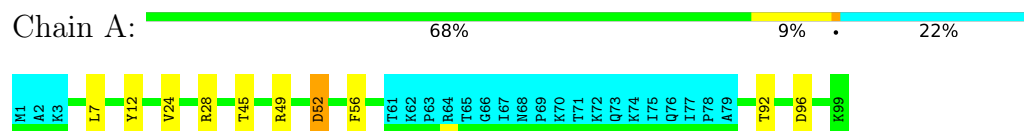
Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1626	492	857	133	142	2	
1	B	99	Total	C	H	N	O	S	0
			1626	492	857	133	142	2	

## 4 Residue-property plots

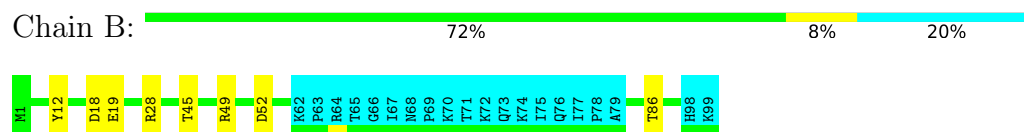
### 4.1 Average score per residue in the NMR ensemble

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: Histone-like DNA-binding superfamily protein



- Molecule 1: Histone-like DNA-binding superfamily protein

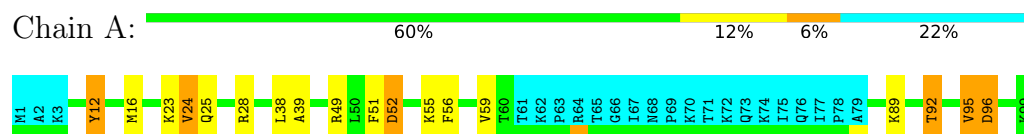


### 4.2 Scores per residue for each member of the ensemble

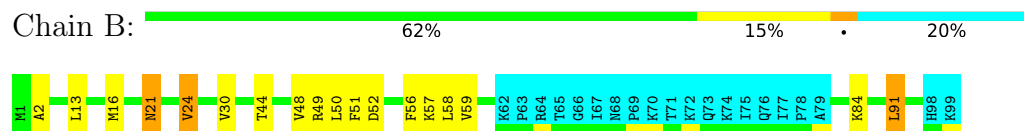
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Histone-like DNA-binding superfamily protein

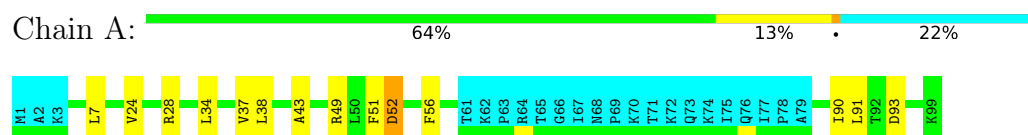


- Molecule 1: Histone-like DNA-binding superfamily protein

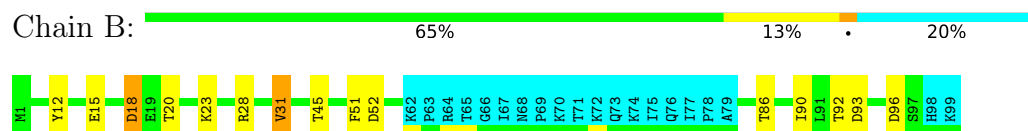


### 4.2.2 Score per residue for model 2

- Molecule 1: Histone-like DNA-binding superfamily protein

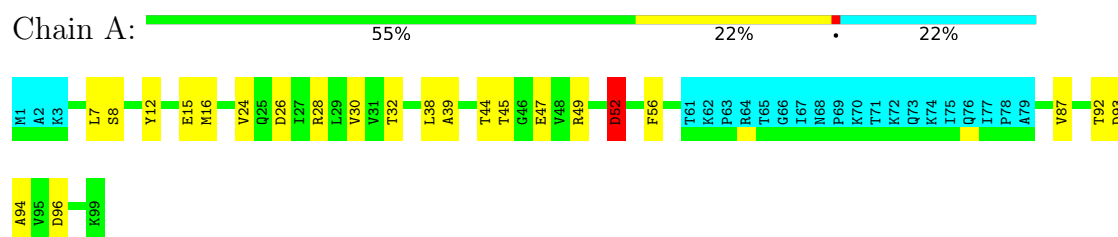


- Molecule 1: Histone-like DNA-binding superfamily protein

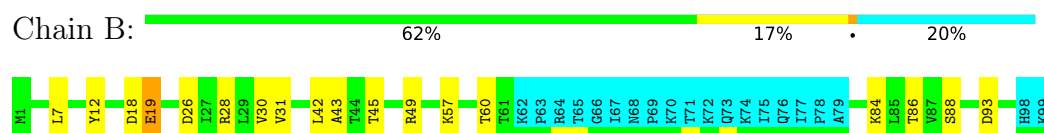


### 4.2.3 Score per residue for model 3

- Molecule 1: Histone-like DNA-binding superfamily protein

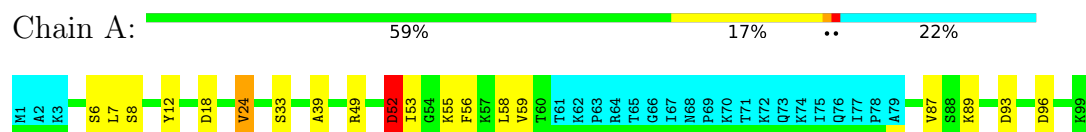


- Molecule 1: Histone-like DNA-binding superfamily protein



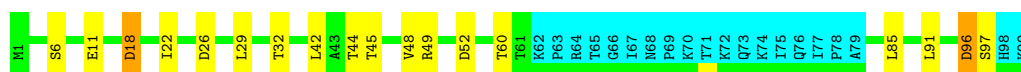
### 4.2.4 Score per residue for model 4

- Molecule 1: Histone-like DNA-binding superfamily protein



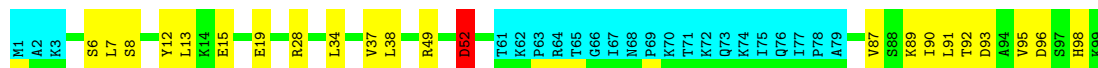
- Molecule 1: Histone-like DNA-binding superfamily protein





#### 4.2.5 Score per residue for model 5

- Molecule 1: Histone-like DNA-binding superfamily protein

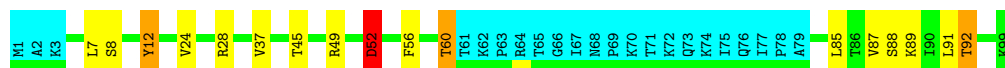


- Molecule 1: Histone-like DNA-binding superfamily protein

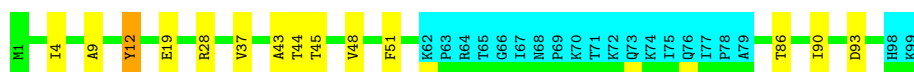


#### 4.2.6 Score per residue for model 6

- Molecule 1: Histone-like DNA-binding superfamily protein

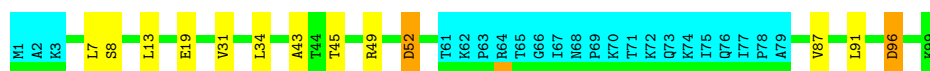


- Molecule 1: Histone-like DNA-binding superfamily protein



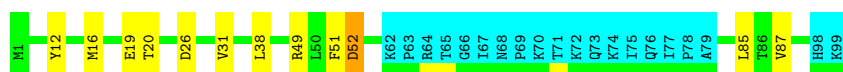
#### 4.2.7 Score per residue for model 7

- Molecule 1: Histone-like DNA-binding superfamily protein



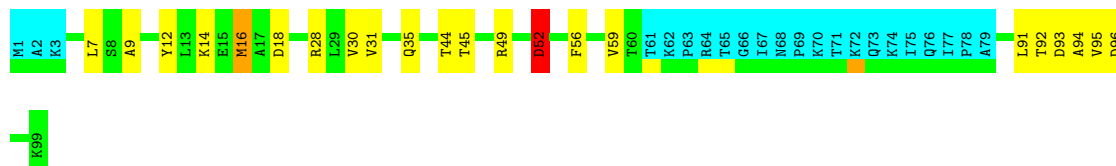
- Molecule 1: Histone-like DNA-binding superfamily protein



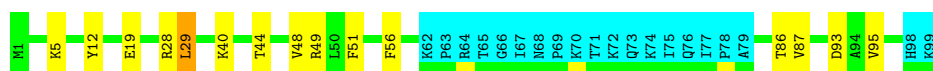


#### 4.2.8 Score per residue for model 8

- Molecule 1: Histone-like DNA-binding superfamily protein

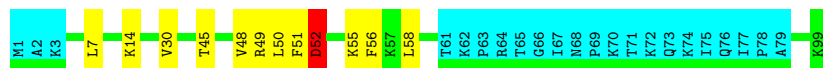


- Molecule 1: Histone-like DNA-binding superfamily protein

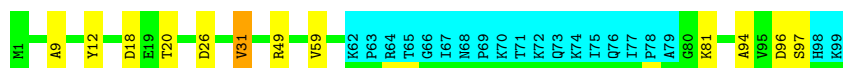


#### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Histone-like DNA-binding superfamily protein

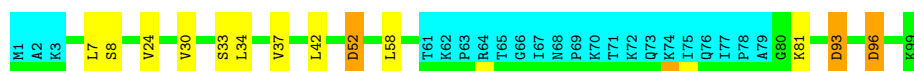


- Molecule 1: Histone-like DNA-binding superfamily protein



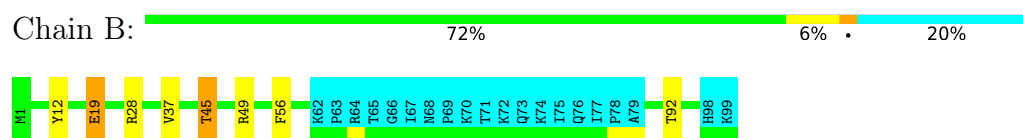
#### 4.2.10 Score per residue for model 10

- Molecule 1: Histone-like DNA-binding superfamily protein



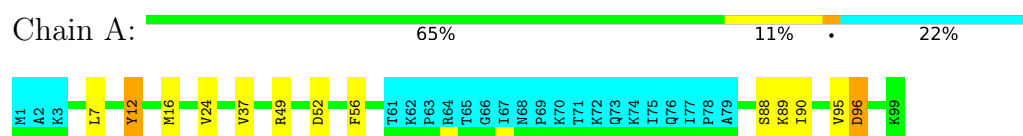


- Molecule 1: Histone-like DNA-binding superfamily protein

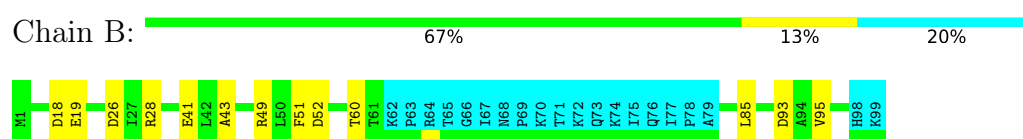


#### 4.2.11 Score per residue for model 11

- Molecule 1: Histone-like DNA-binding superfamily protein

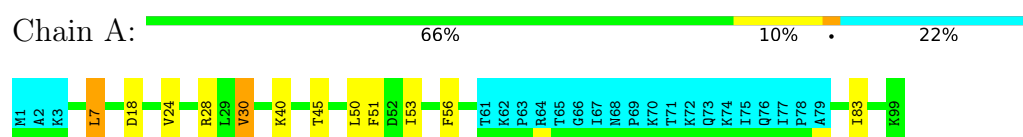


- Molecule 1: Histone-like DNA-binding superfamily protein

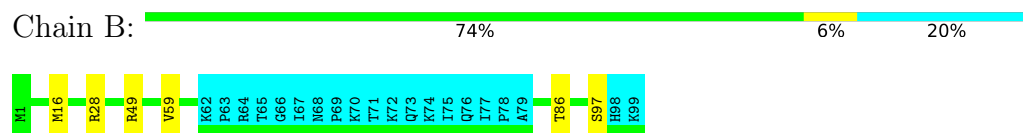


#### 4.2.12 Score per residue for model 12

- Molecule 1: Histone-like DNA-binding superfamily protein

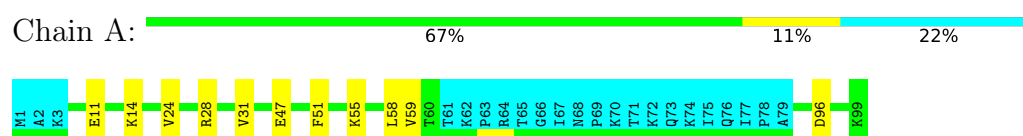


- Molecule 1: Histone-like DNA-binding superfamily protein

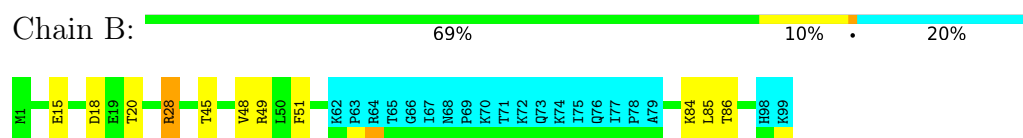


#### 4.2.13 Score per residue for model 13

- Molecule 1: Histone-like DNA-binding superfamily protein

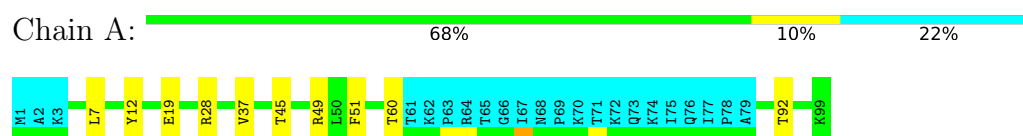


- Molecule 1: Histone-like DNA-binding superfamily protein

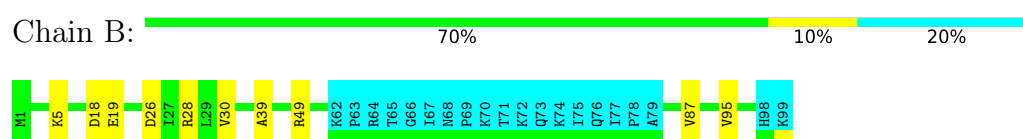


#### 4.2.14 Score per residue for model 14

- Molecule 1: Histone-like DNA-binding superfamily protein

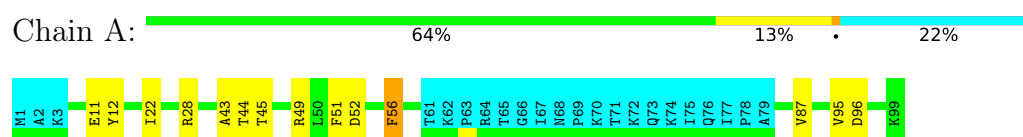


- Molecule 1: Histone-like DNA-binding superfamily protein

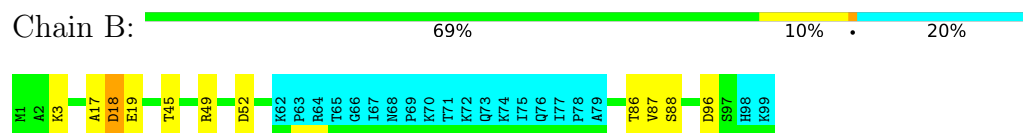


#### 4.2.15 Score per residue for model 15

- Molecule 1: Histone-like DNA-binding superfamily protein



- Molecule 1: Histone-like DNA-binding superfamily 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	2
Total number of shifts	1011
Number of shifts mapped to atoms	1011
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

## 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	0.46±0.01	0±0/602 ( 0.0± 0.0%)	1.89±0.05	12±3/805 ( 1.5± 0.4%)
1	B	0.46±0.01	0±0/611 ( 0.0± 0.0%)	1.90±0.06	12±3/820 ( 1.4± 0.4%)
All	All	0.46	0/18195 ( 0.0%)	1.90	352/24375 ( 1.4%)

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	A	0.0±0.0	1.1±1.0
1	B	0.0±0.0	0.9±1.1
All	All	0	30

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	A	49	ARG	NE-CZ-NH1	16.09	128.35	120.30	1	6
1	A	49	ARG	NE-CZ-NH2	-15.61	112.50	120.30	11	8
1	B	28	ARG	NE-CZ-NH2	-15.24	112.68	120.30	6	7
1	B	49	ARG	NE-CZ-NH2	-14.40	113.10	120.30	7	9
1	A	28	ARG	NE-CZ-NH1	13.09	126.84	120.30	13	5
1	B	56	PHE	CB-CG-CD2	-12.59	111.99	120.80	8	3
1	B	49	ARG	NE-CZ-NH1	12.11	126.35	120.30	12	8
1	A	12	TYR	CB-CG-CD2	-11.40	114.16	121.00	6	2
1	A	28	ARG	NE-CZ-NH2	-11.29	114.66	120.30	13	7
1	B	52	ASP	CB-CG-OD1	10.66	127.89	118.30	2	3
1	B	28	ARG	NE-CZ-NH1	10.19	125.40	120.30	10	7
1	A	12	TYR	CB-CG-CD1	-10.18	114.89	121.00	3	5
1	A	96	ASP	CB-CG-OD1	9.71	127.04	118.30	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	94	ALA	CB-CA-C	9.45	124.28	110.10	3	2
1	B	12	TYR	CB-CG-CD1	9.20	126.52	121.00	5	1
1	B	18	ASP	CB-CG-OD1	8.88	126.29	118.30	13	1
1	B	31	VAL	CA-CB-CG1	8.85	124.18	110.90	3	2
1	B	26	ASP	CB-CG-OD1	8.64	126.07	118.30	7	4
1	B	51	PHE	CB-CG-CD1	-8.23	115.04	120.80	7	3
1	B	26	ASP	CB-CG-OD2	8.23	125.71	118.30	14	3
1	A	9	ALA	CB-CA-C	-8.14	97.89	110.10	8	1
1	B	51	PHE	CB-CG-CD2	8.02	126.41	120.80	6	5
1	A	56	PHE	CB-CG-CD1	-7.82	115.32	120.80	11	6
1	B	93	ASP	CB-CG-OD2	7.80	125.32	118.30	2	4
1	A	93	ASP	CB-CG-OD2	-7.50	111.55	118.30	3	3
1	A	51	PHE	CB-CG-CD2	-7.49	115.56	120.80	2	4
1	B	91	LEU	CB-CG-CD2	7.38	123.56	111.00	1	1
1	A	52	ASP	CB-CG-OD1	7.37	124.93	118.30	4	4
1	B	93	ASP	CB-CG-OD1	-7.36	111.67	118.30	6	3
1	B	87	VAL	CA-CB-CG2	7.34	121.92	110.90	14	2
1	B	56	PHE	CB-CG-CD1	-7.34	115.66	120.80	5	2
1	B	43	ALA	N-CA-CB	-7.25	99.95	110.10	11	1
1	B	59	VAL	CA-CB-CG2	7.19	121.68	110.90	9	1
1	B	48	VAL	CA-CB-CG1	7.18	121.67	110.90	8	2
1	A	56	PHE	CB-CG-CD2	7.12	125.79	120.80	11	3
1	A	52	ASP	CB-CA-C	7.08	124.56	110.40	6	4
1	A	37	VAL	CA-CB-CG1	7.03	121.44	110.90	6	5
1	A	47	GLU	OE1-CD-OE2	-6.98	114.92	123.30	3	2
1	A	52	ASP	CB-CG-OD2	-6.98	112.02	118.30	8	2
1	A	49	ARG	CD-NE-CZ	6.94	133.31	123.60	5	4
1	B	18	ASP	CB-CA-C	6.91	124.21	110.40	14	3
1	A	13	LEU	CB-CG-CD1	6.89	122.72	111.00	5	1
1	A	55	LYS	C-N-CA	6.84	138.79	121.70	1	2
1	A	31	VAL	CA-CB-CG1	6.80	121.09	110.90	7	2
1	B	52	ASP	CB-CG-OD2	-6.74	112.24	118.30	2	1
1	B	20	THR	OG1-CB-CG2	-6.70	94.58	110.00	9	1
1	A	7	LEU	O-C-N	-6.66	112.05	122.70	12	1
1	B	11	GLU	OE1-CD-OE2	-6.58	115.40	123.30	4	1
1	B	87	VAL	CA-CB-CG1	6.57	120.76	110.90	7	1
1	B	96	ASP	CB-CG-OD1	-6.56	112.40	118.30	4	2
1	B	95	VAL	CA-CB-CG2	6.54	120.71	110.90	8	1
1	A	28	ARG	CD-NE-CZ	6.48	132.68	123.60	15	2
1	A	96	ASP	CB-CA-C	6.47	123.34	110.40	1	2
1	A	95	VAL	CA-CB-CG1	6.45	120.57	110.90	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	44	THR	C-N-CA	6.45	137.82	121.70	6	1
1	B	86	THR	CA-CB-CG2	6.39	121.35	112.40	12	2
1	B	48	VAL	CG1-CB-CG2	-6.39	100.67	110.90	6	2
1	B	49	ARG	CD-NE-CZ	6.38	132.54	123.60	11	4
1	B	37	VAL	CG1-CB-CG2	-6.38	100.69	110.90	6	1
1	B	84	LYS	N-CA-CB	-6.38	99.11	110.60	1	1
1	A	19	GLU	N-CA-CB	-6.36	99.15	110.60	7	2
1	B	88	SER	N-CA-CB	-6.35	100.98	110.50	15	1
1	B	18	ASP	CB-CG-OD2	6.31	123.98	118.30	4	1
1	B	92	THR	CA-CB-CG2	6.30	121.22	112.40	2	1
1	B	29	LEU	CB-CG-CD1	6.28	121.68	111.00	8	1
1	A	15	GLU	OE1-CD-OE2	-6.28	115.77	123.30	3	2
1	B	96	ASP	CB-CG-OD2	-6.28	112.65	118.30	9	2
1	B	24	VAL	CA-CB-CG2	6.26	120.30	110.90	1	1
1	B	45	THR	N-CA-CB	6.26	122.20	110.30	10	1
1	A	81	LYS	CB-CA-C	6.24	122.88	110.40	10	1
1	B	12	TYR	CG-CD1-CE1	6.24	126.29	121.30	7	1
1	A	35	GLN	O-C-N	-6.24	112.72	122.70	8	1
1	A	38	LEU	CB-CG-CD2	6.23	121.59	111.00	5	1
1	A	85	LEU	O-C-N	-6.23	112.73	122.70	6	1
1	B	37	VAL	CA-CB-CG2	6.23	120.24	110.90	10	1
1	A	8	SER	CB-CA-C	6.22	121.92	110.10	4	5
1	B	87	VAL	CG1-CB-CG2	6.21	120.83	110.90	8	2
1	B	19	GLU	CB-CA-C	6.19	122.77	110.40	10	1
1	B	15	GLU	N-CA-CB	-6.19	99.47	110.60	13	1
1	A	96	ASP	CB-CG-OD2	6.18	123.86	118.30	10	2
1	B	95	VAL	CA-CB-CG1	6.17	120.16	110.90	14	2
1	B	15	GLU	CB-CA-C	-6.16	98.09	110.40	2	1
1	B	91	LEU	CB-CG-CD1	6.14	121.44	111.00	4	1
1	A	30	VAL	CG1-CB-CG2	-6.13	101.09	110.90	8	2
1	A	39	ALA	N-CA-CB	-6.12	101.54	110.10	1	2
1	B	12	TYR	CB-CG-CD2	-6.10	117.34	121.00	5	3
1	B	59	VAL	CB-CA-C	6.03	122.86	111.40	12	2
1	B	4	ILE	C-N-CA	6.02	136.74	121.70	6	1
1	A	93	ASP	CB-CA-C	6.01	122.43	110.40	10	1
1	B	86	THR	CB-CA-C	6.01	127.82	111.60	5	2
1	B	12	TYR	CG-CD2-CE2	6.01	126.11	121.30	8	1
1	A	30	VAL	CA-CB-CG2	6.01	119.91	110.90	10	1
1	A	91	LEU	CB-CA-C	5.99	121.58	110.20	7	2
1	A	92	THR	CA-CB-CG2	5.99	120.78	112.40	3	2
1	A	87	VAL	CA-CB-CG2	5.99	119.88	110.90	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	SER	CB-CA-C	5.98	121.45	110.10	4	1
1	A	6	SER	N-CA-CB	-5.97	101.54	110.50	5	1
1	B	41	GLU	N-CA-CB	-5.97	99.86	110.60	5	1
1	A	56	PHE	CD1-CE1-CZ	5.96	127.25	120.10	2	1
1	B	43	ALA	N-CA-C	5.82	126.71	111.00	6	1
1	B	16	MET	CG-SD-CE	-5.81	90.91	100.20	12	1
1	A	95	VAL	CB-CA-C	5.80	122.42	111.40	8	1
1	A	12	TYR	CG-CD2-CE2	-5.80	116.66	121.30	11	2
1	B	12	TYR	CZ-CE2-CD2	-5.79	114.59	119.80	8	1
1	B	30	VAL	CA-CB-CG1	5.77	119.55	110.90	14	1
1	A	55	LYS	CB-CA-C	5.74	121.88	110.40	4	1
1	A	43	ALA	CB-CA-C	-5.73	101.50	110.10	2	2
1	B	31	VAL	C-N-CA	5.72	136.01	121.70	9	1
1	A	44	THR	CA-CB-CG2	5.71	120.40	112.40	3	1
1	B	6	SER	CB-CA-C	5.71	120.94	110.10	4	1
1	B	2	ALA	CB-CA-C	5.70	118.64	110.10	1	1
1	A	35	GLN	C-N-CA	5.69	135.92	121.70	8	1
1	B	19	GLU	OE1-CD-OE2	5.68	130.11	123.30	3	1
1	B	85	LEU	CB-CG-CD1	5.67	120.64	111.00	7	1
1	A	87	VAL	CA-CB-CG1	5.67	119.40	110.90	15	1
1	B	44	THR	CA-CB-CG2	5.66	120.32	112.40	4	2
1	A	18	ASP	CB-CG-OD1	5.64	123.37	118.30	12	1
1	A	93	ASP	N-CA-CB	5.64	120.75	110.60	4	1
1	A	58	LEU	CB-CG-CD2	5.64	120.58	111.00	9	2
1	B	16	MET	CA-CB-CG	5.62	122.85	113.30	5	2
1	B	90	ILE	O-C-N	-5.61	113.72	122.70	2	1
1	B	41	GLU	OE1-CD-OE2	-5.61	116.57	123.30	11	1
1	A	39	ALA	CB-CA-C	5.60	118.50	110.10	3	1
1	B	48	VAL	CA-CB-CG2	5.59	119.28	110.90	1	1
1	A	45	THR	CA-CB-CG2	5.57	120.20	112.40	3	1
1	A	24	VAL	CB-CA-C	5.56	121.96	111.40	12	1
1	B	51	PHE	C-N-CA	5.55	135.57	121.70	7	1
1	B	30	VAL	CG1-CB-CG2	-5.55	102.02	110.90	14	1
1	A	51	PHE	CG-CD2-CE2	-5.54	114.71	120.80	13	1
1	A	34	LEU	CB-CG-CD2	5.53	120.40	111.00	10	2
1	B	52	ASP	N-CA-CB	5.52	120.54	110.60	5	2
1	A	12	TYR	CA-CB-CG	5.52	123.90	113.40	15	1
1	B	17	ALA	CB-CA-C	-5.52	101.82	110.10	15	1
1	B	56	PHE	CG-CD1-CE1	-5.51	114.73	120.80	8	1
1	B	20	THR	CA-CB-CG2	5.51	120.11	112.40	7	1
1	B	32	THR	CA-CB-CG2	5.51	120.11	112.40	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	56	PHE	CZ-CE2-CD2	5.51	126.71	120.10	5	1
1	B	9	ALA	N-CA-CB	-5.48	102.43	110.10	6	1
1	A	7	LEU	CB-CG-CD2	5.46	120.28	111.00	11	1
1	B	34	LEU	C-N-CA	5.45	135.34	121.70	5	1
1	B	97	SER	N-CA-CB	-5.45	102.33	110.50	5	1
1	A	26	ASP	CB-CG-OD2	5.44	123.20	118.30	3	1
1	A	83	ILE	CA-CB-CG2	5.42	121.74	110.90	12	1
1	A	33	SER	N-CA-CB	-5.42	102.37	110.50	10	1
1	B	18	ASP	C-N-CA	5.41	135.23	121.70	3	1
1	B	16	MET	CB-CA-C	5.41	121.22	110.40	7	1
1	A	40	LYS	N-CA-CB	-5.41	100.86	110.60	12	1
1	A	60	THR	CA-CB-OG1	5.40	120.35	109.00	6	1
1	B	40	LYS	N-CA-CB	-5.40	100.87	110.60	8	1
1	A	52	ASP	OD1-CG-OD2	-5.40	113.04	123.30	5	1
1	A	43	ALA	N-CA-CB	-5.40	102.55	110.10	15	1
1	A	48	VAL	CB-CA-C	5.39	121.65	111.40	9	1
1	B	26	ASP	CB-CA-C	-5.39	99.62	110.40	14	1
1	A	92	THR	O-C-N	-5.39	114.08	122.70	8	3
1	B	29	LEU	N-CA-CB	-5.38	99.64	110.40	4	1
1	B	39	ALA	CB-CA-C	5.37	118.15	110.10	14	2
1	B	5	LYS	CA-CB-CG	5.35	125.16	113.40	8	1
1	A	49	ARG	N-CA-CB	-5.33	101.00	110.60	14	1
1	B	56	PHE	CD1-CG-CD2	5.33	125.23	118.30	8	1
1	A	51	PHE	N-CA-CB	-5.32	101.03	110.60	12	1
1	A	60	THR	CA-CB-CG2	5.28	119.78	112.40	14	1
1	B	57	LYS	CB-CA-C	5.27	120.94	110.40	3	1
1	A	51	PHE	C-N-CA	5.26	134.86	121.70	1	1
1	A	30	VAL	CA-CB-CG1	5.26	118.79	110.90	12	1
1	A	24	VAL	CA-CB-CG2	5.25	118.77	110.90	4	1
1	A	55	LYS	N-CA-CB	-5.24	101.16	110.60	4	1
1	B	58	LEU	CA-CB-CG	5.24	127.34	115.30	1	1
1	A	50	LEU	CB-CG-CD2	5.24	119.90	111.00	9	1
1	B	20	THR	CA-CB-OG1	5.21	119.95	109.00	13	1
1	B	27	ILE	C-N-CA	5.20	134.70	121.70	5	1
1	A	23	LYS	CB-CA-C	5.20	120.79	110.40	1	1
1	A	89	LYS	C-N-CA	5.17	134.62	121.70	6	1
1	A	44	THR	CA-CB-OG1	5.15	119.81	109.00	8	2
1	A	42	LEU	CA-CB-CG	5.14	127.12	115.30	10	1
1	A	59	VAL	CA-CB-CG1	5.14	118.61	110.90	13	1
1	A	88	SER	N-CA-CB	-5.13	102.80	110.50	11	1
1	B	85	LEU	CB-CA-C	-5.13	100.46	110.20	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	60	THR	OG1-CB-CG2	-5.11	98.24	110.00	11	1
1	B	86	THR	CA-C-O	5.11	130.83	120.10	2	1
1	B	7	LEU	CB-CG-CD1	5.10	119.68	111.00	3	1
1	A	33	SER	C-N-CA	5.10	134.46	121.70	4	1
1	A	51	PHE	CD1-CE1-CZ	-5.10	113.98	120.10	13	1
1	A	18	ASP	CB-CG-OD2	5.10	122.89	118.30	4	1
1	A	93	ASP	C-N-CA	5.09	134.42	121.70	2	1
1	A	22	ILE	CA-CB-CG2	5.09	121.08	110.90	15	1
1	B	51	PHE	CB-CA-C	5.08	120.55	110.40	2	1
1	A	51	PHE	CB-CG-CD1	5.08	124.35	120.80	2	1
1	A	32	THR	N-CA-CB	-5.07	100.66	110.30	3	1
1	B	29	LEU	CB-CG-CD2	-5.07	102.38	111.00	5	1
1	B	12	TYR	CD1-CE1-CZ	-5.07	115.24	119.80	7	1
1	A	95	VAL	C-N-CA	5.06	134.35	121.70	1	1
1	A	51	PHE	O-C-N	-5.05	114.61	122.70	12	1
1	B	17	ALA	C-N-CA	5.05	134.33	121.70	5	1
1	A	56	PHE	CG-CD2-CE2	-5.05	115.25	120.80	1	1
1	A	90	ILE	CA-CB-CG1	5.04	120.58	111.00	5	1
1	A	56	PHE	C-N-CA	5.04	134.31	121.70	8	1
1	A	59	VAL	CA-CB-CG2	5.04	118.46	110.90	1	2
1	B	92	THR	CA-CB-OG1	-5.04	98.42	109.00	10	1
1	B	42	LEU	C-N-CA	5.03	134.28	121.70	3	1
1	B	94	ALA	CB-CA-C	-5.03	102.56	110.10	9	1
1	A	93	ASP	CB-CG-OD1	5.03	122.82	118.30	8	1
1	B	97	SER	CB-CA-C	5.02	119.64	110.10	4	1
1	B	88	SER	C-N-CA	5.00	134.21	121.70	3	1
1	B	26	ASP	OD1-CG-OD2	-5.00	113.80	123.30	7	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	12	TYR	Sidechain	6
1	B	12	TYR	Sidechain	3
1	B	18	ASP	Peptide,Mainchain	2
1	B	60	THR	Peptide	2
1	A	56	PHE	Sidechain	2
1	B	86	THR	Mainchain,Peptide	2
1	A	92	THR	Peptide	1
1	B	20	THR	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	98	HIS	Sidechain	1
1	A	16	MET	Mainchain	1
1	A	31	VAL	Mainchain	1
1	B	44	THR	Peptide	1
1	A	51	PHE	Sidechain	1
1	A	55	LYS	Mainchain	1
1	B	97	SER	Peptide	1
1	A	30	VAL	Mainchain	1
1	B	28	ARG	Sidechain	1
1	B	84	LYS	Peptide	1
1	A	95	VAL	Mainchain	1

## 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	599	658	658	1±1
1	B	608	674	674	1±1
All	All	18105	19980	19980	15

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:A:87:VAL:HG23	1:A:92:THR:HG21	0.72	1.61	6	1
1:A:87:VAL:CG2	1:A:92:THR:HG21	0.56	2.30	6	1
1:A:7:LEU:H	1:A:7:LEU:HD23	0.55	1.62	2	1
1:A:34:LEU:HD21	1:B:31:VAL:HG22	0.54	1.79	2	1
1:A:34:LEU:HD12	1:A:34:LEU:H	0.53	1.64	7	1
1:A:30:VAL:HG11	1:B:30:VAL:HG21	0.51	1.83	3	1
1:B:42:LEU:HD21	1:B:48:VAL:HG23	0.51	1.83	4	1
1:B:9:ALA:HA	1:B:12:TYR:CD2	0.47	2.44	9	1
1:B:90:ILE:HD12	1:B:90:ILE:H	0.47	1.70	6	2
1:A:24:VAL:HG13	1:A:25:GLN:H	0.45	1.72	1	1
1:A:88:SER:O	1:A:92:THR:HG22	0.42	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:ALA:HA	1:B:12:TYR:CE2	0.41	2.50	9	1
1:B:22:ILE:N	1:B:22:ILE:HD12	0.41	2.30	4	1
1:A:50:LEU:HB3	1:A:53:ILE:HD12	0.41	1.93	12	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	76/99 (77%)	64±2 (84±3%)	9±2 (12±3%)	3±1 (4±2%)	6	34
1	B	78/99 (79%)	66±3 (84±4%)	10±3 (13±3%)	2±1 (3±2%)	8	44
All	All	2310/2970 (78%)	1950 (84%)	288 (12%)	72 (3%)	7	39

All 23 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	96	ASP	10
1	A	52	ASP	9
1	A	24	VAL	8
1	B	19	GLU	8
1	B	45	THR	6
1	A	45	THR	6
1	B	52	ASP	4
1	B	18	ASP	4
1	A	89	LYS	3
1	A	95	VAL	1
1	B	21	ASN	1
1	B	24	VAL	1
1	B	43	ALA	1
1	A	8	SER	1
1	B	20	THR	1
1	B	33	SER	1
1	B	44	THR	1
1	A	13	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	38	LEU	1
1	B	31	VAL	1
1	A	16	MET	1
1	A	90	ILE	1
1	B	3	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	68/87 (78%)	65±2 (95±3%)	3±2 (5±3%)	27	77
1	B	69/87 (79%)	68±1 (98±2%)	1±1 (2±2%)	62	94
All	All	2055/2610 (79%)	1985 (97%)	70 (3%)	40	87

All 38 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	52	ASP	11
1	A	7	LEU	10
1	A	16	MET	3
1	A	38	LEU	3
1	A	87	VAL	3
1	A	91	LEU	3
1	A	14	LYS	3
1	A	58	LEU	2
1	B	85	LEU	2
1	A	11	GLU	2
1	A	89	LYS	1
1	B	13	LEU	1
1	B	21	ASN	1
1	B	30	VAL	1
1	B	50	LEU	1
1	B	57	LYS	1
1	B	91	LEU	1
1	A	37	VAL	1
1	A	90	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	23	LYS	1
1	B	84	LYS	1
1	A	53	ILE	1
1	A	59	VAL	1
1	B	96	ASP	1
1	A	19	GLU	1
1	A	45	THR	1
1	A	60	THR	1
1	A	92	THR	1
1	B	31	VAL	1
1	A	18	ASP	1
1	B	29	LEU	1
1	B	86	THR	1
1	B	81	LYS	1
1	A	93	ASP	1
1	A	95	VAL	1
1	B	97	SER	1
1	B	45	THR	1
1	B	5	LYS	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 ⓘ

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 20% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *MGal\_BMRB.tab*

#### 7.1.1 Bookkeeping [i](#)

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	508
Number of shifts mapped to atoms	508
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	94	$0.50 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	66	$1.11 \pm 0.15$	Should be applied
$^{13}\text{C}'$	91	$0.54 \pm 0.15$	Should be applied
$^{15}\text{N}$	92	$-0.34 \pm 0.30$	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 22%, i.e. 431 atoms were assigned a chemical shift out of a possible 1932. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	360/780 (46%)	135/312 (43%)	150/312 (48%)	75/156 (48%)
Sidechain	71/1093 (6%)	4/628 (1%)	65/423 (15%)	2/42 (5%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/59 (0%)	0/32 (0%)	0/26 (0%)	0/1 (0%)
Overall	431/1932 (22%)	139/972 (14%)	215/761 (28%)	77/199 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 506 atoms were assigned a chemical shift out of a possible 2502. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	434/978 (44%)	157/390 (40%)	185/396 (47%)	92/192 (48%)
Sidechain	72/1458 (5%)	4/848 (0%)	66/546 (12%)	2/64 (3%)
Aromatic	0/66 (0%)	0/36 (0%)	0/28 (0%)	0/2 (0%)
Overall	506/2502 (20%)	161/1274 (13%)	251/970 (26%)	94/258 (36%)

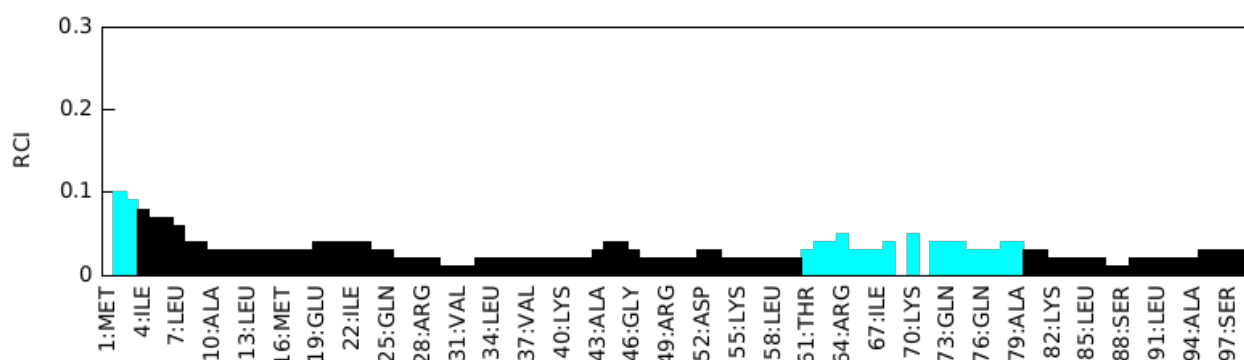
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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:



## 7.2 Chemical shift list 2

File name: working\_cs.cif



Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping [i](#)

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	503
Number of shifts mapped to atoms	503
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

### 7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	92	$0.52 \pm 0.09$	Should be applied
$^{13}\text{C}_\beta$	66	$1.11 \pm 0.11$	Should be applied
$^{13}\text{C}'$	90	$0.53 \pm 0.17$	Should be applied
$^{15}\text{N}$	92	$-0.23 \pm 0.28$	None needed ( $< 0.5$ ppm)

### 7.2.3 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 22%, i.e. 432 atoms were assigned a chemical shift out of a possible 1932. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	361/780 (46%)	135/312 (43%)	150/312 (48%)	76/156 (49%)
Sidechain	71/1093 (6%)	4/628 (1%)	65/423 (15%)	2/42 (5%)
Aromatic	0/59 (0%)	0/32 (0%)	0/26 (0%)	0/1 (0%)
Overall	432/1932 (22%)	139/972 (14%)	215/761 (28%)	78/199 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 501 atoms were assigned a chemical shift out of a possible 2502. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	429/978 (44%)	155/390 (40%)	182/396 (46%)	92/192 (48%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Sidechain	72/1458 (5%)	4/848 (0%)	66/546 (12%)	2/64 (3%)
Aromatic	0/66 (0%)	0/36 (0%)	0/28 (0%)	0/2 (0%)
Overall	501/2502 (20%)	159/1274 (12%)	248/970 (26%)	94/258 (36%)

## 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

## 7.2.5 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:

