Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 05:19 AM EDT

PDB ID	:	2MFE
BMRB ID	:	19546
Title	:	Csr/Rsm protein-RNA recognition - A molecular affinity ruler: RsmZ(SL2)/ RsmE(dimer) 2:1 complex
Authors	:	Duss, O.; Diarra Dit Konte, N.; Michel, E.; Schubert, M.; Allain, F.H.-T.
Deposited on	:	2013-10-11

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

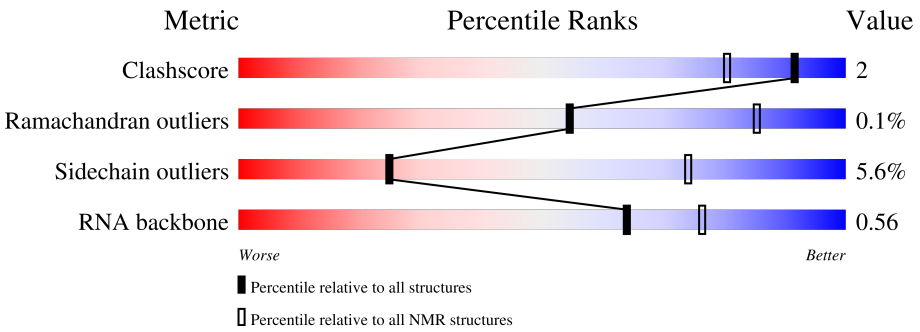
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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
RNA backbone	4643	676

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	70	77% 7% 16%
1	C	70	76% 6% • 16%
2	B	22	82% 9% 9%
2	D	22	82% 9% 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:59, C:1-C:57 (116)	0.50	1

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 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3264 atoms, of which 1426 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Carbon storage regulator homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	59	920	280	472	81	86	1	0
1	C	59	920	280	472	81	86	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	LYS	-	expression tag	UNP Q5MXB2
A	61	ARG	-	expression tag	UNP Q5MXB2
A	62	GLU	-	expression tag	UNP Q5MXB2
A	63	THR	-	expression tag	UNP Q5MXB2
A	64	PRO	-	expression tag	UNP Q5MXB2
A	65	HIS	-	expression tag	UNP Q5MXB2
A	66	HIS	-	expression tag	UNP Q5MXB2
A	67	HIS	-	expression tag	UNP Q5MXB2
A	68	HIS	-	expression tag	UNP Q5MXB2
A	69	HIS	-	expression tag	UNP Q5MXB2
A	70	HIS	-	expression tag	UNP Q5MXB2
C	60	LYS	-	expression tag	UNP Q5MXB2
C	61	ARG	-	expression tag	UNP Q5MXB2
C	62	GLU	-	expression tag	UNP Q5MXB2
C	63	THR	-	expression tag	UNP Q5MXB2
C	64	PRO	-	expression tag	UNP Q5MXB2
C	65	HIS	-	expression tag	UNP Q5MXB2
C	66	HIS	-	expression tag	UNP Q5MXB2
C	67	HIS	-	expression tag	UNP Q5MXB2
C	68	HIS	-	expression tag	UNP Q5MXB2
C	69	HIS	-	expression tag	UNP Q5MXB2
C	70	HIS	-	expression tag	UNP Q5MXB2

- Molecule 2 is a RNA chain called SL2(RsmZ) RNA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	22	712	211	241	89	150	21	0

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Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	D	22	712	211	241	89	150	21	0

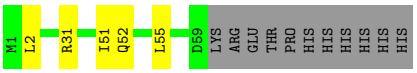
4 Residue-property plots (i)

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.

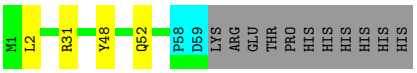
• Molecule 1: Carbon storage regulator homolog

Chain A:



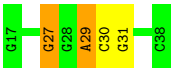
• Molecule 1: Carbon storage regulator homolog

Chain C:



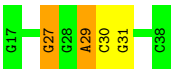
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

Chain D:



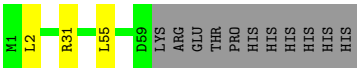
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

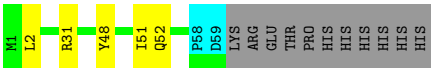
- Molecule 1: Carbon storage regulator homolog

Chain A:



- Molecule 1: Carbon storage regulator homolog

Chain C:

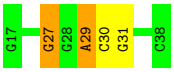


- Molecule 2: SL2(RsmZ) RNA

Chain B:

- Molecule 2: SL2(RsmZ) RNA

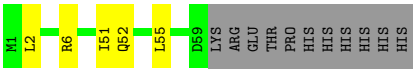
Chain D:



4.2.2 Score per residue for model 2

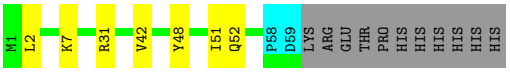
- Molecule 1: Carbon storage regulator homolog

Chain A:



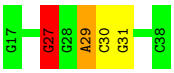
- Molecule 1: Carbon storage regulator homolog

Chain C:



- Molecule 2: SL2(RsmZ) RNA

Chain B:



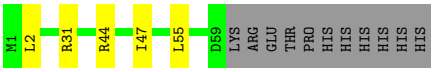
• Molecule 2: SL2(RsmZ) RNA

Chain D:

4.2.3 Score per residue for model 3

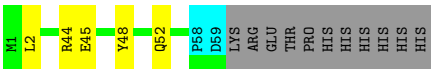
• Molecule 1: Carbon storage regulator homolog

Chain A:



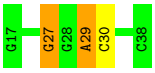
• Molecule 1: Carbon storage regulator homolog

Chain C:



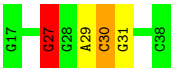
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

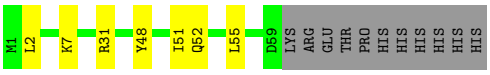
Chain D:



4.2.4 Score per residue for model 4

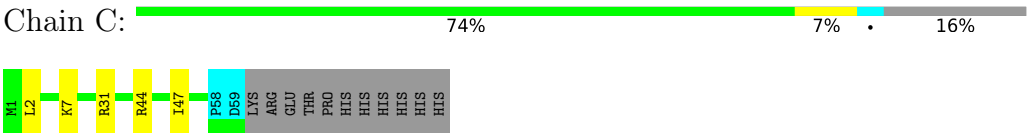
• Molecule 1: Carbon storage regulator homolog

Chain A:



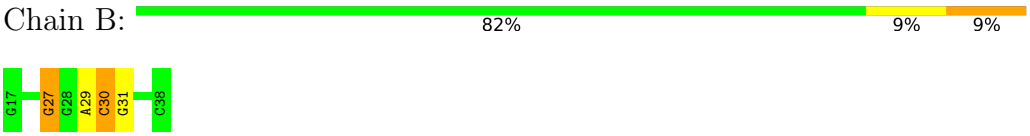
- Molecule 1: Carbon storage regulator homolog

Chain C:



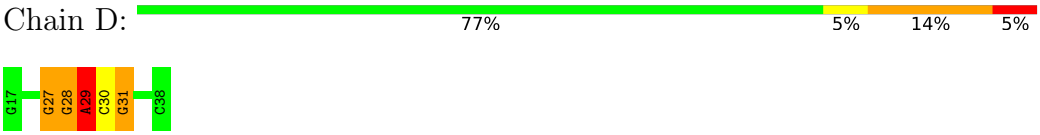
- Molecule 2: SL2(RsmZ) RNA

Chain B:



- Molecule 2: SL2(RsmZ) RNA

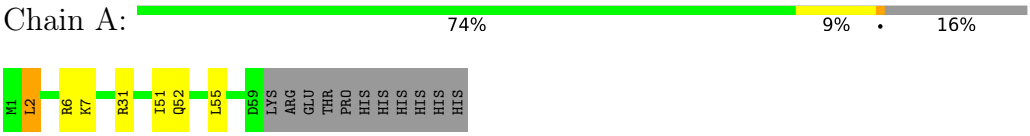
Chain D:



4.2.5 Score per residue for model 5

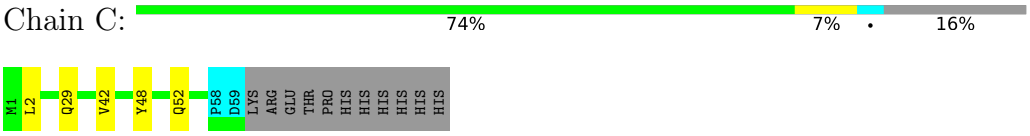
- Molecule 1: Carbon storage regulator homolog

Chain A:



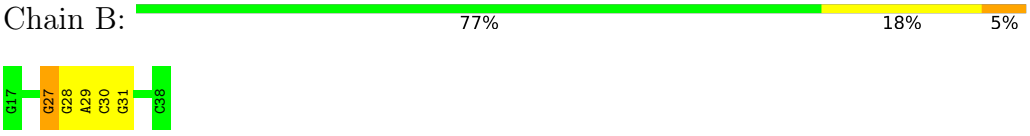
- Molecule 1: Carbon storage regulator homolog

Chain C:



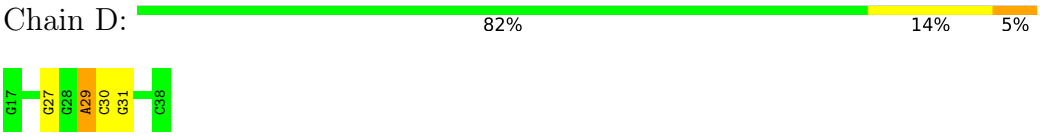
- Molecule 2: SL2(RsmZ) RNA

Chain B:



- Molecule 2: SL2(RsmZ) RNA

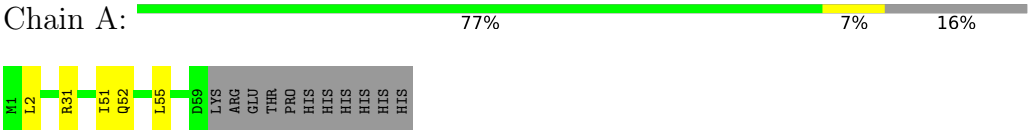
Chain D:



4.2.6 Score per residue for model 6

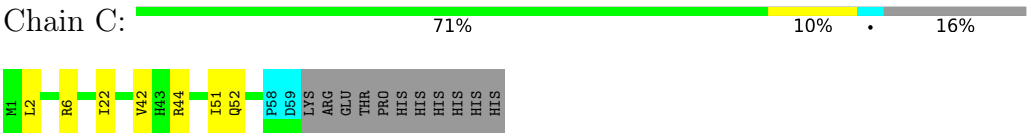
- Molecule 1: Carbon storage regulator homolog

Chain A:



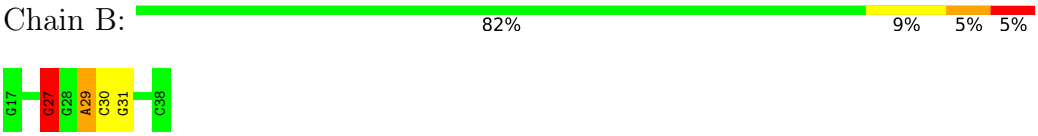
- Molecule 1: Carbon storage regulator homolog

Chain C:



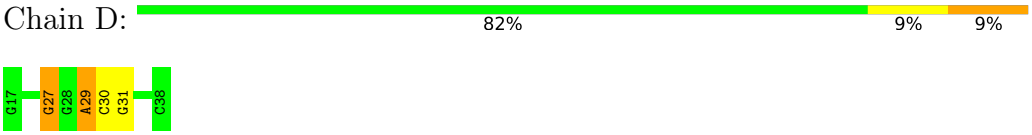
- Molecule 2: SL2(RsmZ) RNA

Chain B:



- Molecule 2: SL2(RsmZ) RNA

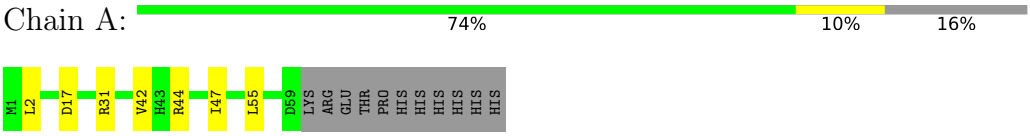
Chain D:



4.2.7 Score per residue for model 7

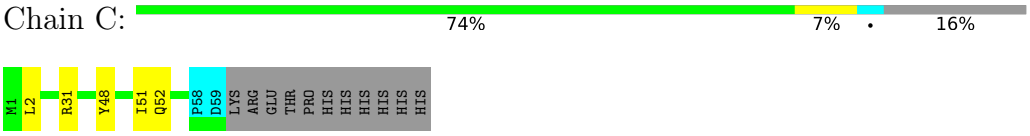
- Molecule 1: Carbon storage regulator homolog

Chain A:



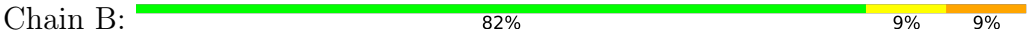
- Molecule 1: Carbon storage regulator homolog

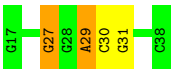
Chain C:



- Molecule 2: SL2(RsmZ) RNA

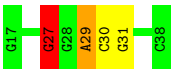
Chain B:





• Molecule 2: SL2(RsmZ) RNA

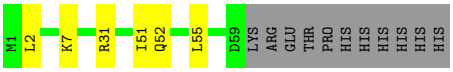
Chain D:



4.2.8 Score per residue for model 8

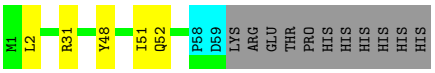
• Molecule 1: Carbon storage regulator homolog

Chain A:



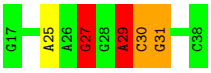
• Molecule 1: Carbon storage regulator homolog

Chain C:



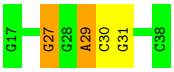
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

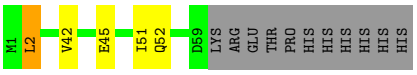
Chain D:



4.2.9 Score per residue for model 9

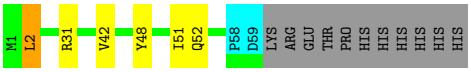
• Molecule 1: Carbon storage regulator homolog

Chain A:



- Molecule 1: Carbon storage regulator homolog

Chain C:



- Molecule 2: SL2(RsmZ) RNA

Chain B:

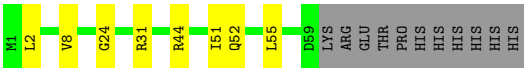
- Molecule 2: SL2(RsmZ) RNA

Chain D:

4.2.10 Score per residue for model 10

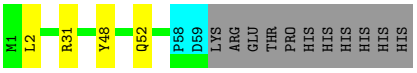
- Molecule 1: Carbon storage regulator homolog

Chain A:



- Molecule 1: Carbon storage regulator homolog

Chain C:

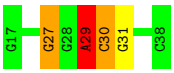


- Molecule 2: SL2(RsmZ) RNA

Chain B:

- Molecule 2: SL2(RsmZ) RNA

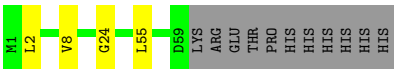
Chain D:



4.2.11 Score per residue for model 11

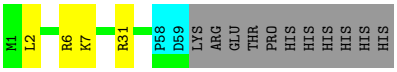
- Molecule 1: Carbon storage regulator homolog

Chain A: 79% 6% 16%



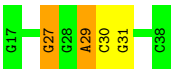
- Molecule 1: Carbon storage regulator homolog

Chain C: 76% 6% • 16%



- Molecule 2: SL2(RsmZ) RNA

Chain B: 82% 9% 9%



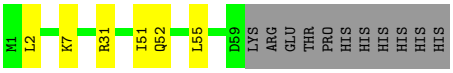
- Molecule 2: SL2(RsmZ) RNA

Chain D: 73% 14% 14%

4.2.12 Score per residue for model 12

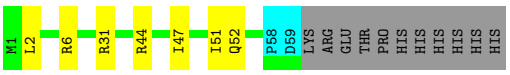
- Molecule 1: Carbon storage regulator homolog

Chain A: 76% 9% 16%



- Molecule 1: Carbon storage regulator homolog

Chain C: 71% 10% • 16%

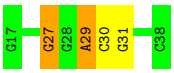


- Molecule 2: SL2(RsmZ) RNA

Chain B: 77% 9% 14%

• Molecule 2: SL2(RsmZ) RNA

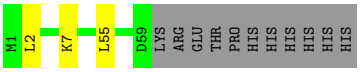
Chain D:



4.2.13 Score per residue for model 13

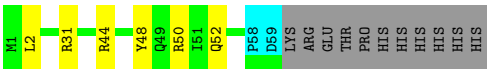
• Molecule 1: Carbon storage regulator homolog

Chain A:



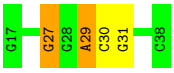
• Molecule 1: Carbon storage regulator homolog

Chain C:



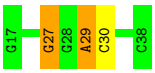
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

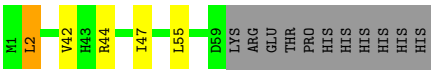
Chain D:



4.2.14 Score per residue for model 14

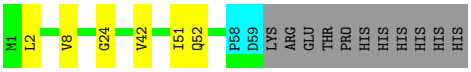
• Molecule 1: Carbon storage regulator homolog

Chain A:



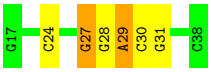
• Molecule 1: Carbon storage regulator homolog

Chain C:



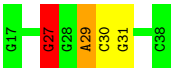
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

Chain D:



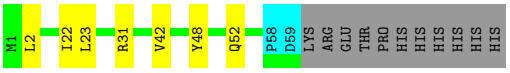
4.2.15 Score per residue for model 15

• Molecule 1: Carbon storage regulator homolog

Chain A:

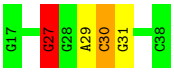
• Molecule 1: Carbon storage regulator homolog

Chain C:



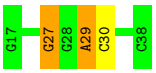
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

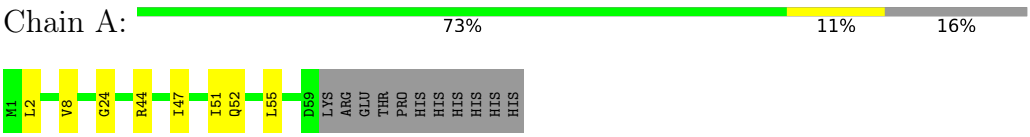
Chain D:



4.2.16 Score per residue for model 16

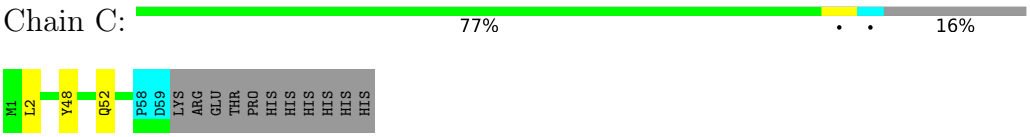
- Molecule 1: Carbon storage regulator homolog

Chain A:



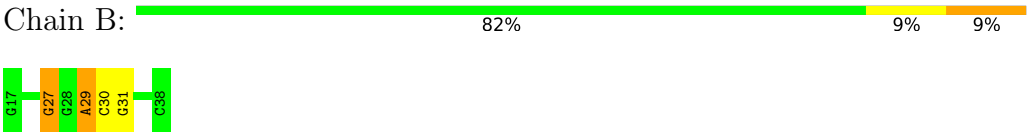
- Molecule 1: Carbon storage regulator homolog

Chain C:



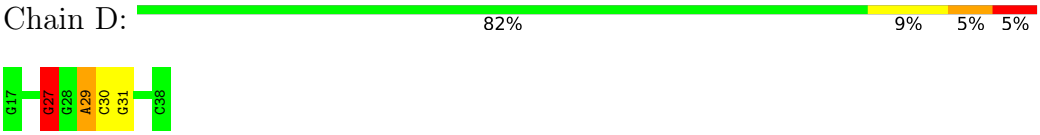
- Molecule 2: SL2(RsmZ) RNA

Chain B:



- Molecule 2: SL2(RsmZ) RNA

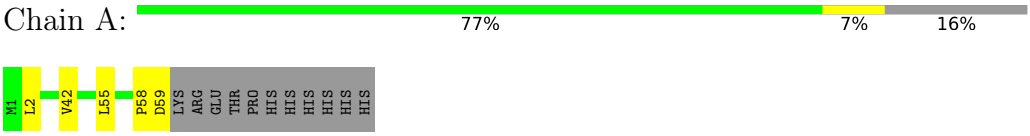
Chain D:



4.2.17 Score per residue for model 17

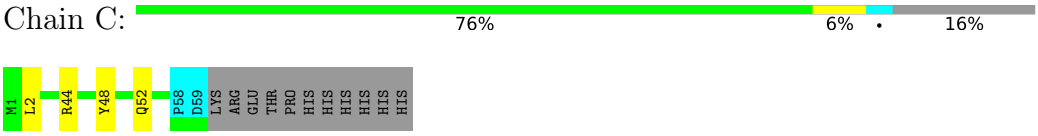
- Molecule 1: Carbon storage regulator homolog

Chain A:



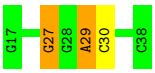
- Molecule 1: Carbon storage regulator homolog

Chain C:



- Molecule 2: SL2(RsmZ) RNA

Chain B:



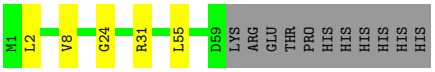
• Molecule 2: SL2(RsmZ) RNA

Chain D:

4.2.18 Score per residue for model 18

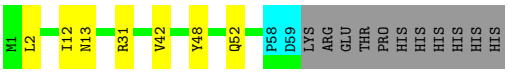
• Molecule 1: Carbon storage regulator homolog

Chain A:



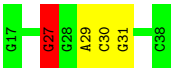
• Molecule 1: Carbon storage regulator homolog

Chain C:



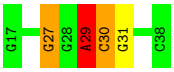
• Molecule 2: SL2(RsmZ) RNA

Chain B:



• Molecule 2: SL2(RsmZ) RNA

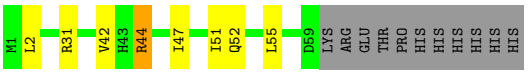
Chain D:



4.2.19 Score per residue for model 19

• Molecule 1: Carbon storage regulator homolog

Chain A:



• Molecule 1: Carbon storage regulator homolog

Chain C: 71% 10% • 16%

M1 L2 R31 V42 H43 R44 Y48 Q49 R50 I51 Q52 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: SL2(RsmZ) RNA

Chain B: 77% 14% 9%

G17 G27 G28 A29 C30 G31 C38

• Molecule 2: SL2(RsmZ) RNA

Chain D: 77% 14% 5% 5%

G17 G27 G28 A29 C30 G31 C38

4.2.20 Score per residue for model 20

• Molecule 1: Carbon storage regulator homolog

Chain A: 76% 9% 16%

M1 L2 R44 R50 I51 Q52 L55 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 71% 10% • 16%

M1 L2 D17 I18 T19 L23 Y48 I51 Q52 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: SL2(RsmZ) RNA

Chain B: 82% 9% 9%

G17 G27 G28 A29 C30 G31 C38

• Molecule 2: SL2(RsmZ) RNA

Chain D: 86% 5% 9%

G17 G27 G28 A29 C30 C38

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 999 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
Amber	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	1048
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	65
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

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	0.40±0.00	0±0/451 (0.0± 0.0%)	0.74±0.02	0±0/610 (0.0± 0.0%)
1	C	0.38±0.01	0±0/436 (0.0± 0.0%)	0.73±0.02	0±0/591 (0.0± 0.0%)
2	B	0.97±0.01	0±0/527 (0.0± 0.0%)	1.46±0.01	0±0/821 (0.0± 0.1%)
2	D	0.96±0.01	0±0/527 (0.0± 0.0%)	1.45±0.02	0±0/821 (0.0± 0.0%)
All	All	0.76	0/38820 (0.0%)	1.20	9/56860 (0.0%)

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
2	B	0.0±0.0	2.0±0.4
2	D	0.0±0.0	1.8±0.6
All	All	0	75

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	D	28	G	O4'-C1'-N9	6.07	113.05	108.20	4	2
2	B	28	G	O4'-C1'-N9	5.74	112.79	108.20	10	3
2	D	30	C	C5'-C4'-C3'	-5.25	107.60	116.00	3	1
2	D	29	A	O4'-C1'-N9	5.20	112.36	108.20	18	1
2	B	30	C	C5'-C4'-C3'	-5.12	107.81	116.00	4	1
2	B	24	C	O4'-C1'-N1	5.03	112.22	108.20	14	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)
2	B	29	A	Sidechain	20
2	D	29	A	Sidechain	18
2	B	27	G	Sidechain	18
2	D	27	G	Sidechain	15
2	D	31	G	Sidechain	2
2	B	31	G	Sidechain	2

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	A	448	472	472	2±1
1	C	433	461	461	2±1
2	B	471	241	241	1±1
2	D	471	241	241	1±1
All	All	36460	28300	28300	97

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:29:A:H2'	2:D:30:C:H5"	0.59	1.74	10	2
2:B:29:A:H2'	2:B:30:C:H5"	0.58	1.75	8	1
1:C:51:ILE:HG22	1:C:52:GLN:HE21	0.48	1.69	14	8
1:A:55:LEU:HD12	1:A:55:LEU:C	0.47	2.30	2	18
1:A:44:ARG:CZ	1:A:47:ILE:HD12	0.46	2.40	19	1
1:A:51:ILE:HG22	1:A:52:GLN:NE2	0.45	2.26	4	9
1:A:51:ILE:HG22	1:A:52:GLN:HE21	0.45	1.71	2	3
2:B:28:G:N1	1:C:42:VAL:HG12	0.44	2.28	5	4
2:D:27:G:N3	2:D:27:G:H2'	0.44	2.28	3	4
1:A:2:LEU:HD12	1:C:42:VAL:HG13	0.43	1.88	9	3
2:B:25:A:C2	2:B:31:G:C6	0.43	3.07	8	1
1:A:8:VAL:CG1	1:A:24:GLY:HA2	0.43	2.44	16	4
1:A:58:PRO:O	1:A:59:ASP:CB	0.43	2.66	17	1
1:C:8:VAL:CG1	1:C:24:GLY:HA2	0.42	2.44	14	1
1:C:48:TYR:CE2	1:C:52:GLN:HG3	0.42	2.49	1	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:27:G:N3	2:D:27:G:C2'	0.42	2.82	4	3
1:A:42:VAL:HG12	2:D:28:G:N1	0.42	2.29	9	1
2:B:27:G:H2'	2:B:27:G:N3	0.42	2.30	8	1
1:C:48:TYR:CE1	1:C:52:GLN:HG3	0.42	2.49	13	2
2:D:29:A:C2	2:D:31:G:H1'	0.42	2.48	4	1
1:A:42:VAL:HG13	1:C:2:LEU:HD12	0.42	1.92	9	1
1:C:12:ILE:HG22	1:C:13:ASN:N	0.42	2.30	18	1
1:A:48:TYR:CZ	1:A:52:GLN:HG3	0.41	2.50	4	1
1:A:42:VAL:O	2:D:27:G:N2	0.41	2.53	17	4
2:B:27:G:N2	1:C:42:VAL:O	0.41	2.54	6	4
1:A:55:LEU:C	1:A:55:LEU:HD12	0.41	2.36	18	1
2:B:30:C:C2	1:C:23:LEU:HD22	0.40	2.51	15	2
2:B:27:G:N3	2:B:27:G:C2'	0.40	2.84	1	1
1:C:51:ILE:HG22	1:C:52:GLN:NE2	0.40	2.31	8	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	57/70 (81%)	50±1 (87±1%)	7±1 (13±1%)	0±0 (0±0%)	54	85
1	C	56/70 (80%)	50±1 (88±2%)	6±1 (11±2%)	0±0 (0±0%)	54	85
All	All	2260/2800 (81%)	1986 (88%)	272 (12%)	2 (0%)	54	85

All 2 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	17	ASP	1
1	C	17	ASP	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	49/60 (82%)	46±1 (95±2%)	3±1 (5±2%)	26	75
1	C	47/60 (78%)	44±1 (94±3%)	3±1 (6±3%)	23	72
All	All	1920/2400 (80%)	1813 (94%)	107 (6%)	25	74

All 19 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	2	LEU	20
1	C	2	LEU	20
1	C	31	ARG	13
1	A	31	ARG	12
1	A	44	ARG	7
1	C	44	ARG	7
1	A	7	LYS	5
1	A	47	ILE	4
1	C	7	LYS	3
1	C	6	ARG	3
1	A	6	ARG	2
1	C	47	ILE	2
1	C	22	ILE	2
1	C	50	ARG	2
1	C	45	GLU	1
1	C	29	GLN	1
1	A	45	GLU	1
1	A	50	ARG	1
1	C	19	THR	1

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	21/22 (95%)	3±1 (15±4%)	1±1 (6±4%)	0.56±0.02
2	D	21/22 (95%)	3±1 (14±4%)	1±1 (7±3%)	0.57±0.02
All	All	840/880 (95%)	119 (14%)	56 (7%)	0.56

The overall RNA backbone suiteness is 0.56.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	27	G	20
2	B	30	C	20
2	D	27	G	20
2	D	30	C	20
2	B	31	G	16
2	D	31	G	14
2	B	28	G	3
2	D	28	G	3
2	B	26	A	1
2	B	29	A	1
2	D	26	A	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	D	29	A	19
2	B	29	A	15
2	B	30	C	9
2	D	30	C	7
2	B	28	G	3
2	D	28	G	2
2	D	27	G	1

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 40% 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 (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	743
Number of shifts mapped to atoms	678
Number of unparsed shifts	0
Number of shifts with mapping errors	65
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 65 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	LYS	CA	56.151	0.050	.
1	A	60	LYS	CB	32.583	0.133	.
1	A	60	LYS	CD	29.001	0.133	.
1	A	60	LYS	CE	41.898	0.000	.
1	A	60	LYS	CG	24.682	0.040	.
1	A	60	LYS	HA	4.255	0.014	.
1	A	60	LYS	HB2	1.811	0.012	.
1	A	60	LYS	HB3	1.675	0.000	.
1	A	60	LYS	HG2	1.376	0.014	.
1	A	60	LYS	HG3	1.344	0.021	.
1	A	60	LYS	H	8.101	0.015	.
1	A	60	LYS	N	122.003	0.046	.
1	A	60	LYS	HD2	1.623	0.014	.
1	A	60	LYS	HD3	1.623	0.014	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	LYS	HE2	2.954	0.006	.
1	A	60	LYS	HE3	2.954	0.006	.
1	A	61	ARG	CA	56.133	0.076	.
1	A	61	ARG	CB	30.784	0.051	.
1	A	61	ARG	CD	43.317	0.084	.
1	A	61	ARG	CG	27.045	0.000	.
1	A	61	ARG	HA	4.25	0.010	.
1	A	61	ARG	HB2	1.788	0.009	.
1	A	61	ARG	HB3	1.723	0.007	.
1	A	61	ARG	H	8.188	0.000	.
1	A	61	ARG	N	121.843	0.000	.
1	A	61	ARG	HD2	3.142	0.010	.
1	A	61	ARG	HD3	3.142	0.010	.
1	A	61	ARG	HG2	1.587	0.004	.
1	A	61	ARG	HG3	1.587	0.004	.
1	A	62	GLU	CA	56.312	0.046	.
1	A	62	GLU	CB	30.428	0.026	.
1	A	62	GLU	CG	36.195	0.020	.
1	A	62	GLU	HA	4.302	0.008	.
1	A	62	GLU	HB2	1.993	0.003	.
1	A	62	GLU	HB3	1.888	0.015	.
1	A	62	GLU	HG2	2.208	0.006	.
1	A	62	GLU	HG3	2.157	0.000	.
1	A	62	GLU	H	8.323	0.000	.
1	A	62	GLU	N	121.766	0.000	.
1	A	63	THR	CA	59.643	0.053	.
1	A	63	THR	CB	69.688	0.054	.
1	A	63	THR	CG2	21.452	0.044	.
1	A	63	THR	HA	4.534	0.006	.
1	A	63	THR	HB	4.082	0.008	.
1	A	63	THR	H	8.154	0.015	.
1	A	63	THR	N	117.672	0.000	.
1	A	63	THR	HG21	1.156	0.010	.
1	A	63	THR	HG22	1.156	0.010	.
1	A	63	THR	HG23	1.156	0.010	.
1	A	64	PRO	CA	63.254	0.039	.
1	A	64	PRO	CB	31.944	0.011	.
1	A	64	PRO	CD	50.959	0.014	.
1	A	64	PRO	CG	27.22	0.000	.
1	A	64	PRO	HA	4.328	0.006	.
1	A	64	PRO	HB2	2.177	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	PRO	HB3	1.685	0.006	.
1	A	64	PRO	HD2	3.612	0.011	.
1	A	64	PRO	HD3	3.755	0.013	.
1	A	64	PRO	HG2	1.903	0.010	.
1	A	64	PRO	HG3	1.903	0.010	.
1	A	65	HIS	CA	57.492	0.046	.
1	A	65	HIS	CB	30.86	0.060	.
1	A	65	HIS	HA	4.361	0.009	.
1	A	65	HIS	HB2	3.115	0.016	.
1	A	65	HIS	HB3	2.965	0.009	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	65	-0.16 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	58	0.26 ± 0.29	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	60	-0.99 ± 0.45	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 28%, i.e. 678 atoms were assigned a chemical shift out of a possible 2447. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	236/586 (40%)	121/241 (50%)	59/232 (25%)	56/113 (50%)
Sidechain	432/989 (44%)	296/648 (46%)	129/301 (43%)	7/40 (18%)
Aromatic	10/32 (31%)	6/16 (38%)	4/14 (29%)	0/2 (0%)
Sugar	0/484 (0%)	0/264 (0%)	0/220 (0%)	0/0 (—%)
Base	0/356 (0%)	0/224 (0%)	0/72 (0%)	0/60 (0%)
Overall	678/2447 (28%)	423/1393 (30%)	192/839 (23%)	63/215 (29%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 678 atoms were assigned a chemical shift out of a possible 2468. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	236/594 (40%)	121/244 (50%)	59/236 (25%)	56/114 (49%)
Sidechain	432/1002 (43%)	296/656 (45%)	129/306 (42%)	7/40 (18%)
Aromatic	10/32 (31%)	6/16 (38%)	4/14 (29%)	0/2 (0%)
Sugar	0/484 (0%)	0/264 (0%)	0/220 (0%)	0/0 (—%)
Base	0/356 (0%)	0/224 (0%)	0/72 (0%)	0/60 (0%)
Overall	678/2468 (27%)	423/1404 (30%)	192/848 (23%)	63/216 (29%)

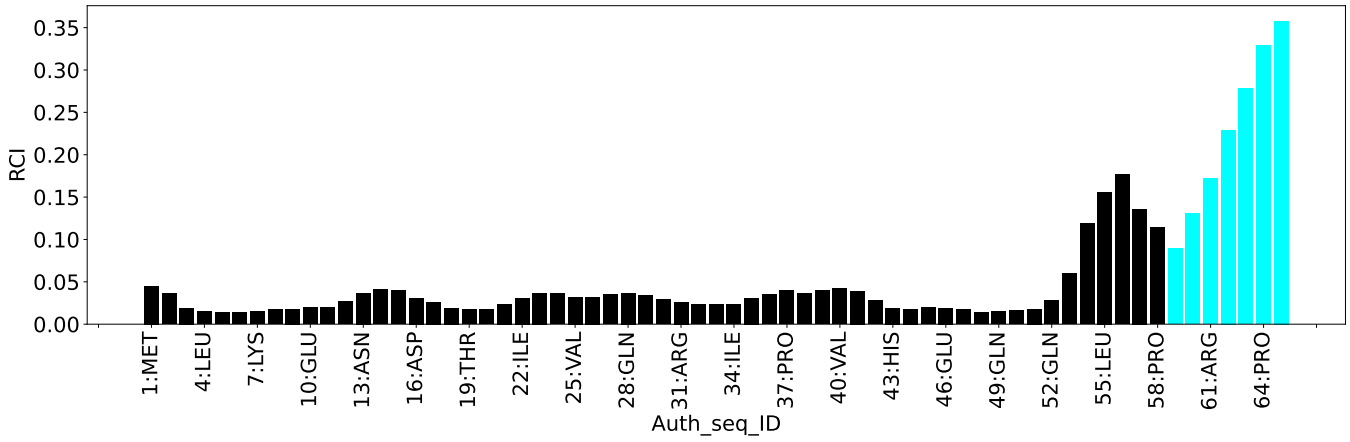
7.1.4 Statistically unusual chemical shifts (i)

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.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:



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	305
Number of shifts mapped to atoms	305
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.2.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 12%, i.e. 299 atoms were assigned a chemical shift out of a possible 2447. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	0/586 (0%)	0/241 (0%)	0/232 (0%)	0/113 (0%)
Sidechain	0/989 (0%)	0/648 (0%)	0/301 (0%)	0/40 (0%)
Aromatic	0/32 (0%)	0/16 (0%)	0/14 (0%)	0/2 (0%)
Sugar	211/484 (44%)	113/264 (43%)	98/220 (45%)	0/0 (—%)
Base	88/356 (25%)	45/224 (20%)	32/72 (44%)	11/60 (18%)
Overall	299/2447 (12%)	158/1393 (11%)	130/839 (15%)	11/215 (5%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 299 atoms were assigned a chemical shift out of a possible 2468. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	0/594 (0%)	0/244 (0%)	0/236 (0%)	0/114 (0%)
Sidechain	0/1002 (0%)	0/656 (0%)	0/306 (0%)	0/40 (0%)
Aromatic	0/32 (0%)	0/16 (0%)	0/14 (0%)	0/2 (0%)
Sugar	211/484 (44%)	113/264 (43%)	98/220 (45%)	0/0 (—%)
Base	88/356 (25%)	45/224 (20%)	32/72 (44%)	11/60 (18%)
Overall	299/2468 (12%)	158/1404 (11%)	130/848 (15%)	11/216 (5%)

7.2.4 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
2	B	26	A	H4'	3.10	3.65 – 5.26	-8.4
2	B	28	G	H5"	2.56	2.98 – 5.38	-6.8

7.2.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins