



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:21 AM BST

PDB ID : 2MF0
Title : Structural basis of the non-coding RNA RsmZ acting as protein sponge: Conformer L of RsmZ(1-72)/RsmE(dimer) 1to3 complex
Authors : Duss, O.; Michel, E.; Yulikov, M.; Schubert, M.; Jeschke, G.; Allain, F.H.-T.
Deposited on : 2013-10-02

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

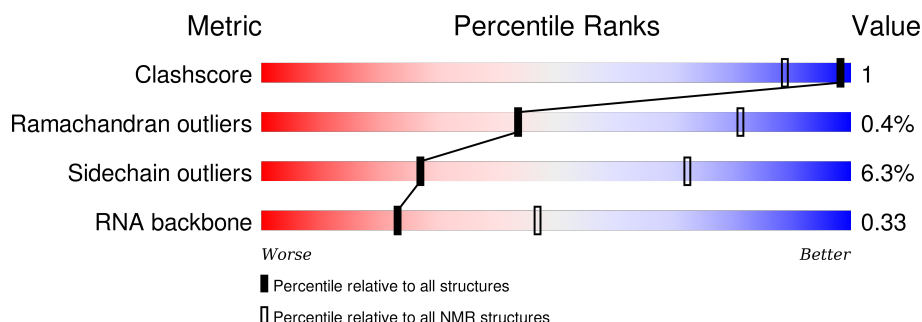
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958
RNA backbone	3027	600

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	70	 66% 16% 16%
1	B	70	 74% 10% 16%
1	C	70	 70% 11% 16%
1	D	70	 71% 11% 16%
1	E	70	 64% 17% 16%
1	F	70	 66% 16% 16%
2	G	72	 36% 49% 15%

2 Ensemble composition and analysis

This entry contains 20 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:48, B:1-B:59, C:1-C:51, D:1-D:51 (209)	0.25	4
2	E:2-E:48, F:1-F:48 (95)	0.14	20

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7852 atoms, of which 3615 are hydrogens and 0 are deuteriums.

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

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

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
A	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
A	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
A	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
A	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
A	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
A	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
A	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0
A	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
A	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0
A	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0
B	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
B	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
B	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
B	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
B	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
B	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
B	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
B	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0
B	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
B	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
C	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
C	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
C	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
C	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
C	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0
C	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
D	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
D	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
D	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
D	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
D	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0
D	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
E	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
E	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
E	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
E	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
E	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0
E	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0
F	60	LYS	-	EXPRESSION TAG	UNP Q4KEY0
F	61	ARG	-	EXPRESSION TAG	UNP Q4KEY0
F	62	GLU	-	EXPRESSION TAG	UNP Q4KEY0
F	63	THR	-	EXPRESSION TAG	UNP Q4KEY0
F	64	PRO	-	EXPRESSION TAG	UNP Q4KEY0
F	65	HIS	-	EXPRESSION TAG	UNP Q4KEY0
F	66	HIS	-	EXPRESSION TAG	UNP Q4KEY0
F	67	HIS	-	EXPRESSION TAG	UNP Q4KEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	68	HIS	-	EXPRESSION TAG	UNP Q4KEY0
F	69	HIS	-	EXPRESSION TAG	UNP Q4KEY0
F	70	HIS	-	EXPRESSION TAG	UNP Q4KEY0

- Molecule 2 is a RNA chain called RNA_(72-MER).

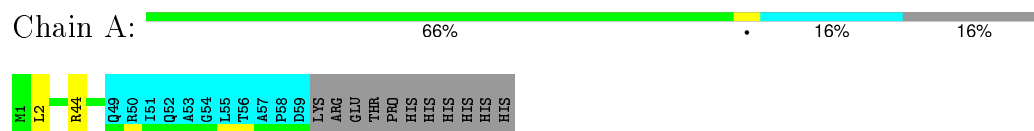
Mol	Chain	Residues	Atoms						Trace
2	G	72	Total	C	H	N	O	P	0
			2332	693	783	295	490	71	

4 Residue-property plots [i](#)

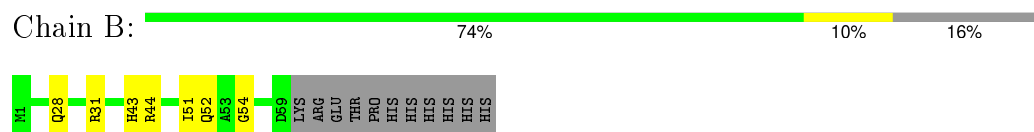
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

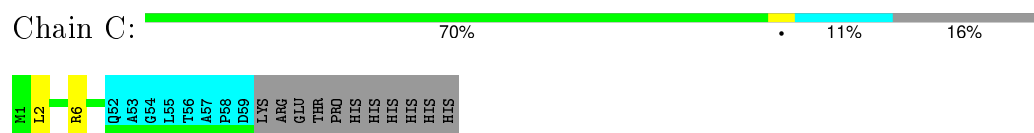
- Molecule 1: Carbon storage regulator homolog



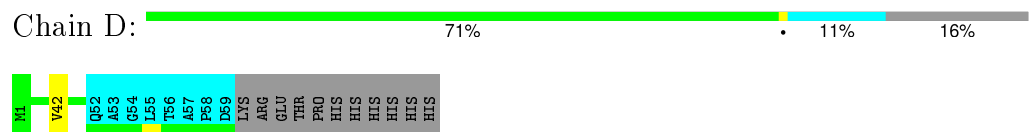
- Molecule 1: Carbon storage regulator homolog



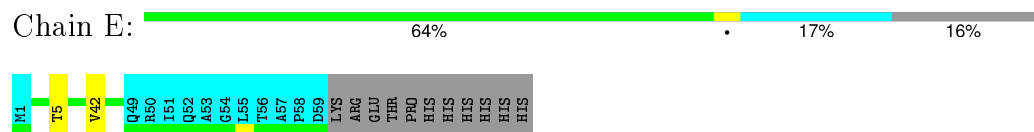
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

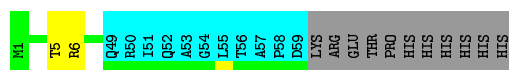


- Molecule 1: Carbon storage regulator homolog



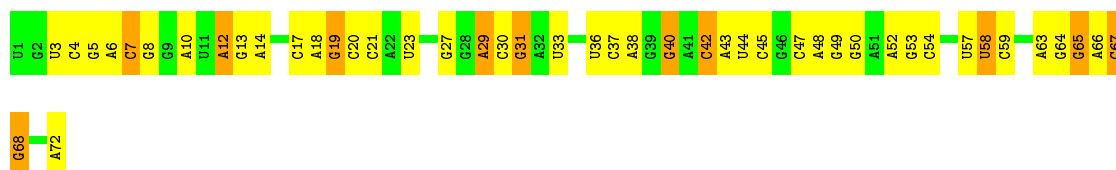
- Molecule 1: Carbon storage regulator homolog

Chain F: 



- Molecule 2: RNA_ (72-MER)

Chain G: 



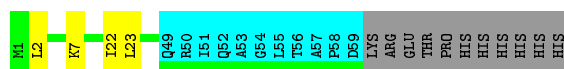
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Carbon storage regulator homolog

Chain A: 



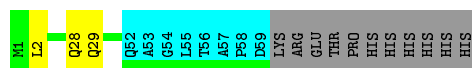
- Molecule 1: Carbon storage regulator homolog

Chain B: 



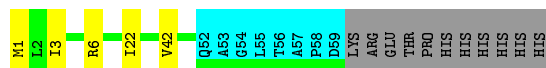
- Molecule 1: Carbon storage regulator homolog

Chain C: 

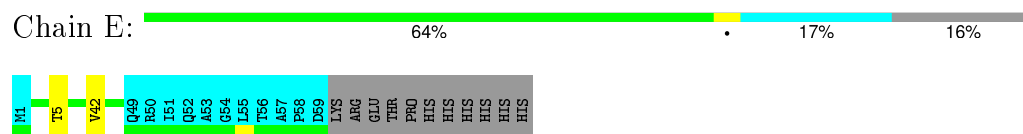


- Molecule 1: Carbon storage regulator homolog

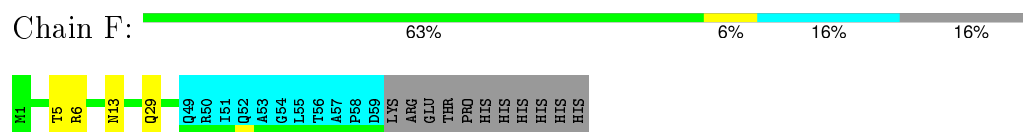
Chain D: 



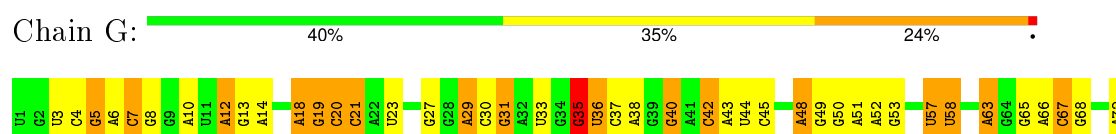
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

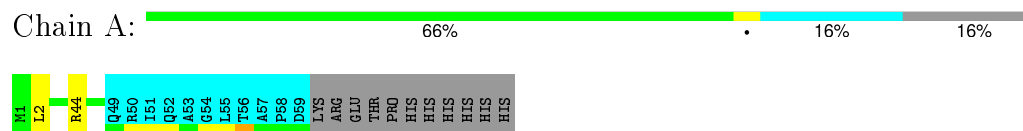


- Molecule 2: RNA_(72-MER)

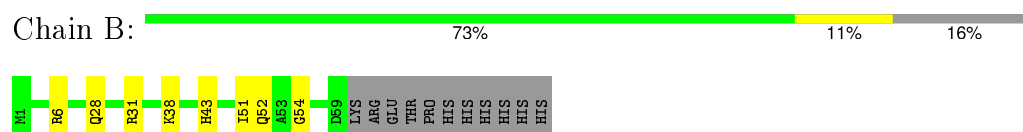


4.2.2 Score per residue for model 2

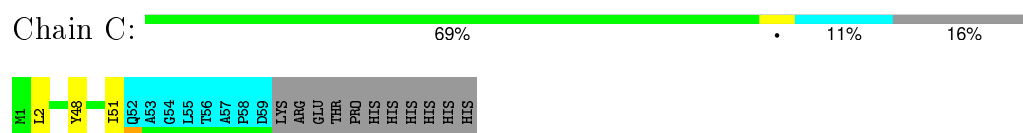
- Molecule 1: Carbon storage regulator homolog



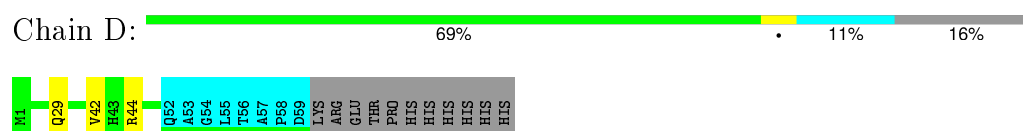
- Molecule 1: Carbon storage regulator homolog



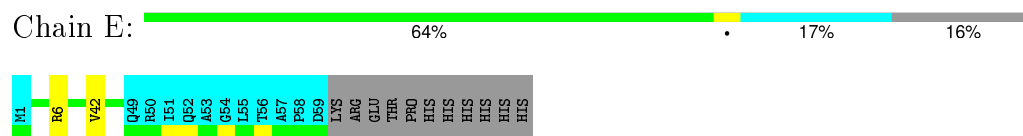
- Molecule 1: Carbon storage regulator homolog



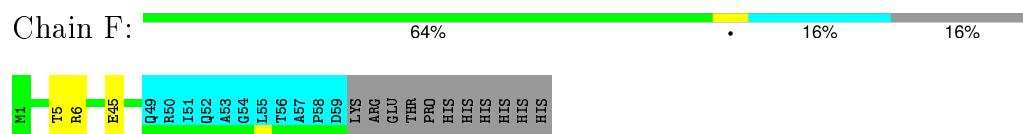
- Molecule 1: Carbon storage regulator homolog



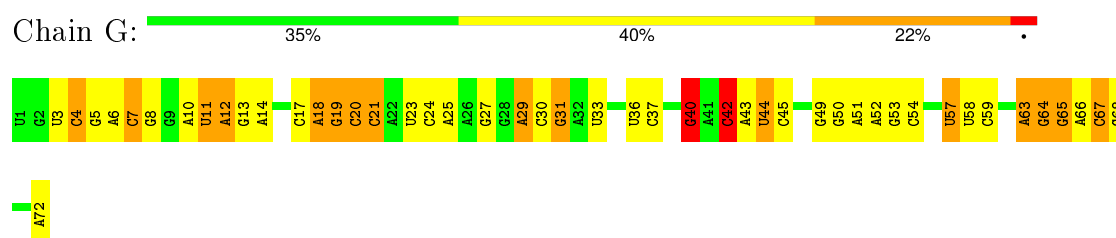
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

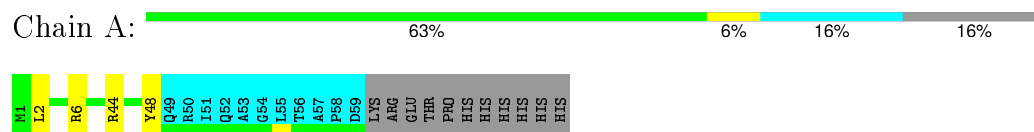


- Molecule 2: RNA_(72-MER)

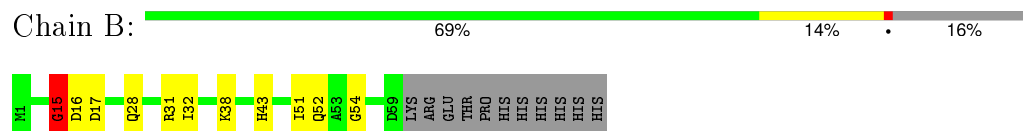


4.2.3 Score per residue for model 3

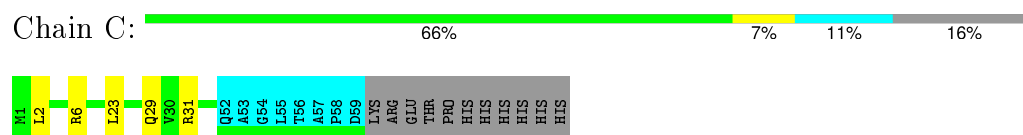
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

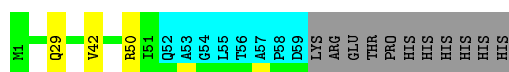


- Molecule 1: Carbon storage regulator homolog

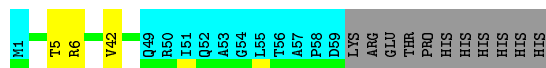


- Molecule 1: Carbon storage regulator homolog

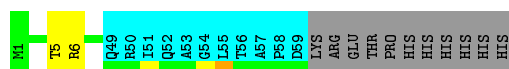




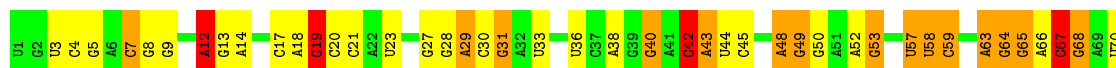
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

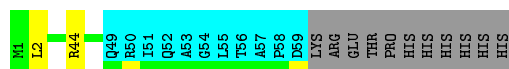


- Molecule 2: RNA_ (72-MER)



4.2.4 Score per residue for model 4 (medoid)

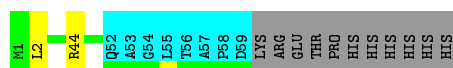
- Molecule 1: Carbon storage regulator homolog



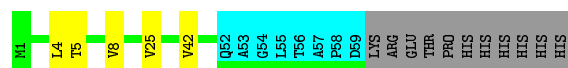
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog



- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | L2 | T5 | V42 | Q49 | R50 | T51 | Q52 | A53 | G54 | L55 | T56 | A57 | P58 | D59 | LVS | ARG | GLU | THR | PRO | HIS | HIS | HIS | HIS | HIS | HIS |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

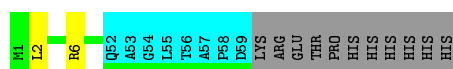
- | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|--|----|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | | T5 | R6 | | Q49 | R50 | I51 | Q52 | A53 | G54 | L55 | T56 | A57 | P58 | D59 | LYS | ARG | GLU | THR | PRO | HIS | HIS | HIS | HIS | HIS | HIS |
|----|--|----|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

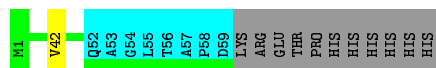
M1	L2	R44	Q49	R50	I51	O52	A53	G54	L55	T56	A57	F58	D59	LYS	ARG	GLU	THR	PRO	HIS	HIS	HIS	HIS	HIS	HIS	HIS
----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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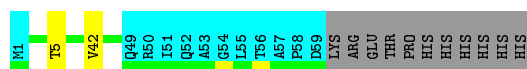
- Chain C:  70% • 11% 16%



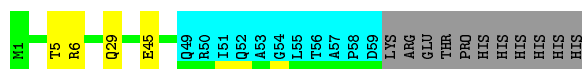
- Molecule 1: Carbon storage regulator homolog



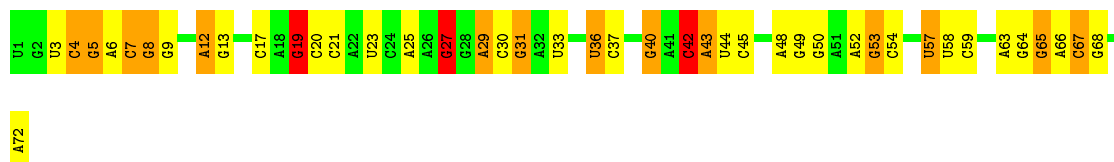
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

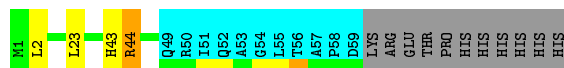


- Molecule 2: RNA_(72-MER)

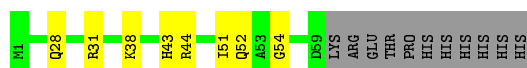


4.2.6 Score per residue for model 6

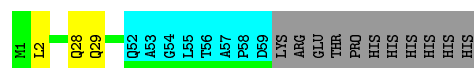
- Molecule 1: Carbon storage regulator homolog



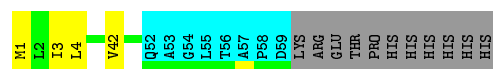
- Molecule 1: Carbon storage regulator homolog



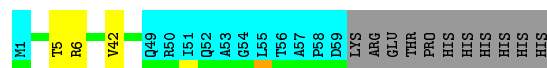
- Molecule 1: Carbon storage regulator homolog



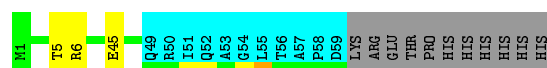
- Molecule 1: Carbon storage regulator homolog



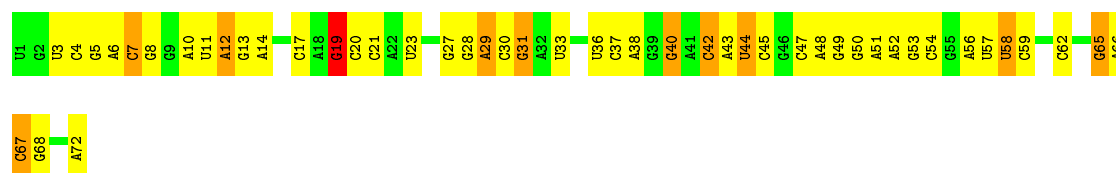
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

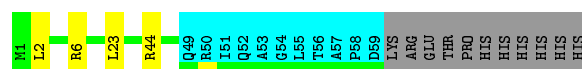


- Molecule 2: RNA_(72-MER)



4.2.7 Score per residue for model 7

- Molecule 1: Carbon storage regulator homolog

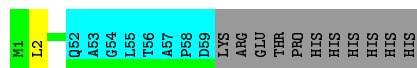


- Molecule 1: Carbon storage regulator homolog

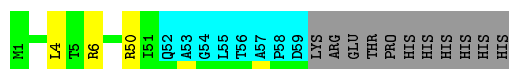




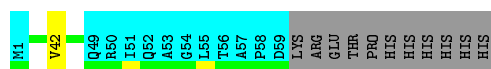
- Molecule 1: Carbon storage regulator homolog



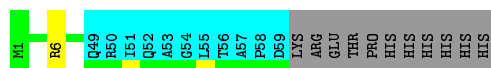
- Molecule 1: Carbon storage regulator homolog



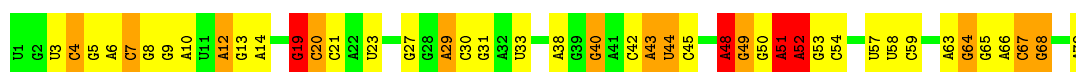
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

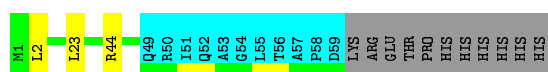


- Molecule 2: RNA_ (72-MER)



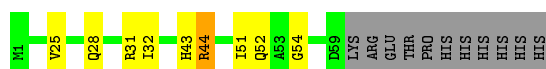
4.2.8 Score per residue for model 8

- Molecule 1: Carbon storage regulator homolog

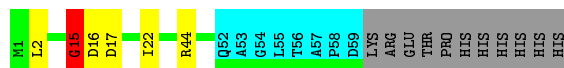


- Molecule 1: Carbon storage regulator homolog

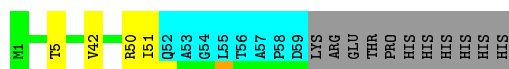




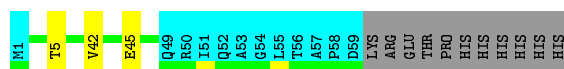
- Molecule 1: Carbon storage regulator homolog



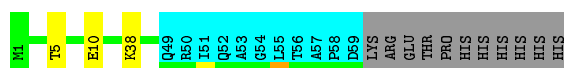
- Molecule 1: Carbon storage regulator homolog



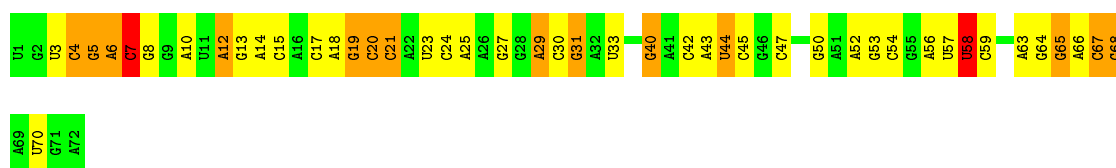
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

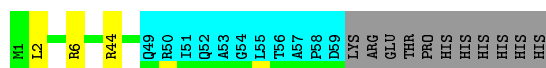


- Molecule 2: RNA_{72-MER}

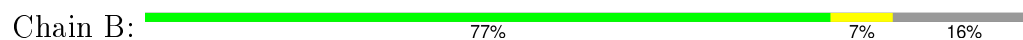


4.2.9 Score per residue for model 9

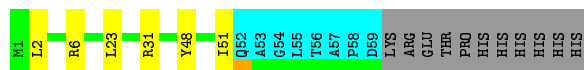
- Molecule 1: Carbon storage regulator homolog



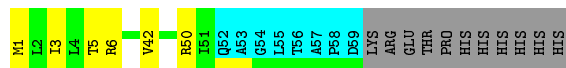
- Molecule 1: Carbon storage regulator homolog



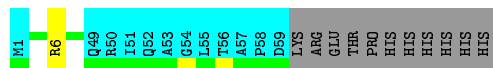
- Molecule 1: Carbon storage regulator homolog



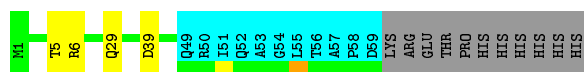
- Molecule 1: Carbon storage regulator homolog



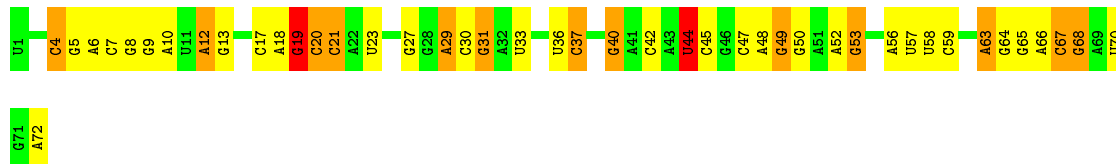
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog



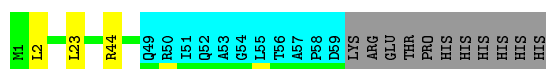
- Molecule 2: RNA_(72-MER)



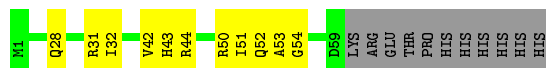
4.2.10 Score per residue for model 10

- Molecule 1: Carbon storage regulator homolog

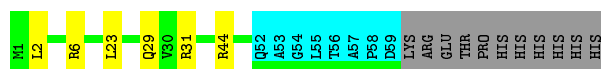




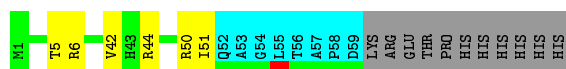
- Molecule 1: Carbon storage regulator homolog



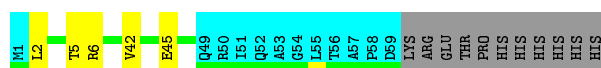
- Molecule 1: Carbon storage regulator homolog



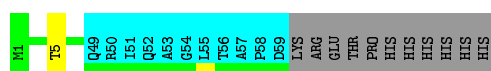
- Molecule 1: Carbon storage regulator homolog



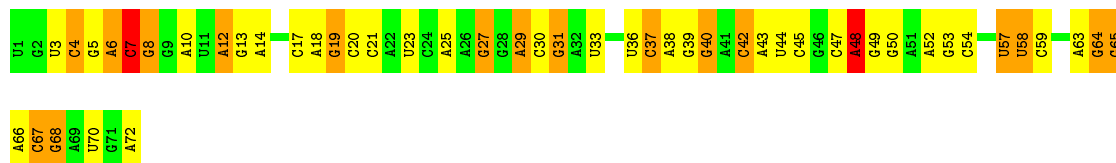
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog



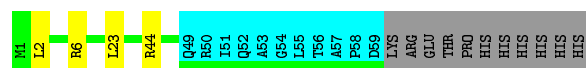
- Molecule 2: RNA₇₂ (72-MER)



4.2.11 Score per residue for model 11

- Molecule 1: Carbon storage regulator homolog

Chain A: 



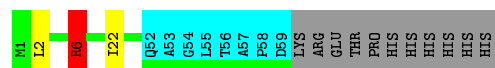
- Molecule 1: Carbon storage regulator homolog

Chain B: 



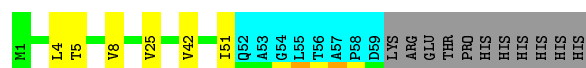
- Molecule 1: Carbon storage regulator homolog

Chain C: 



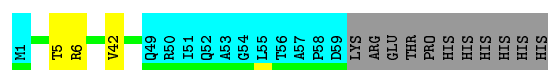
- Molecule 1: Carbon storage regulator homolog

Chain D: 



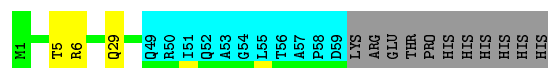
- Molecule 1: Carbon storage regulator homolog

Chain E: 



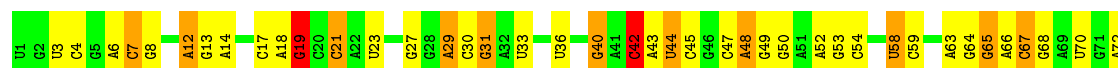
- Molecule 1: Carbon storage regulator homolog

Chain F: 



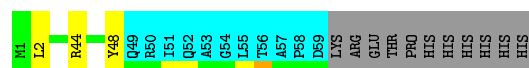
- Molecule 2: RNA_(72-MER)

Chain G: 

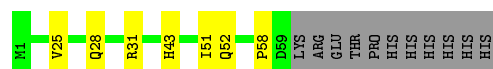


4.2.12 Score per residue for model 12

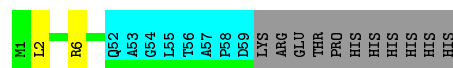
- Molecule 1: Carbon storage regulator homolog



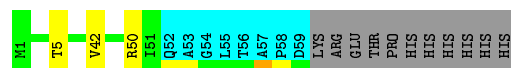
- Chain B:  74% 10% 16%



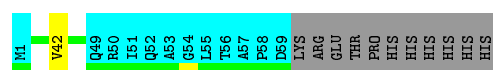
- Chain C:  70% 11% 16%



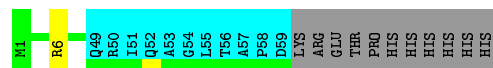
- Chain D:  69% 11% 16%



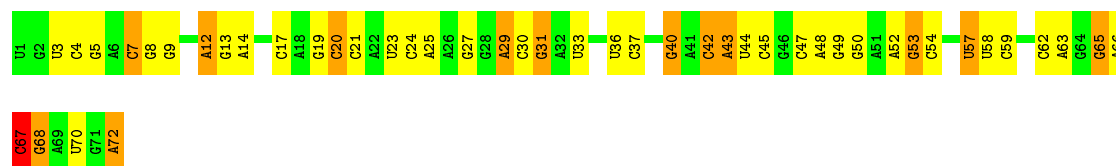
- Chain E:  66% 17% 16%



- Chain F:  67% 16% 16%

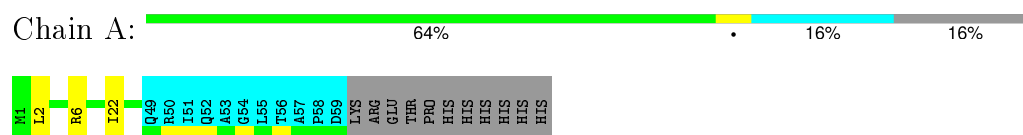


- Chain G: 36% 44% 18%

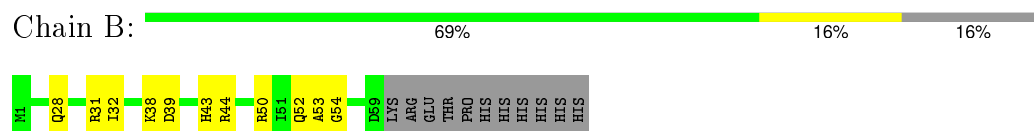


4.2.13 Score per residue for model 13

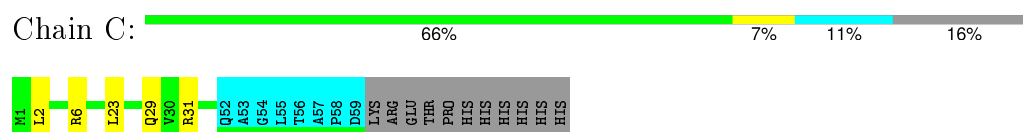
- Molecule 1: Carbon storage regulator homolog



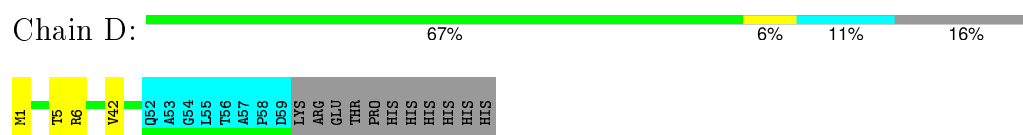
- Molecule 1: Carbon storage regulator homolog



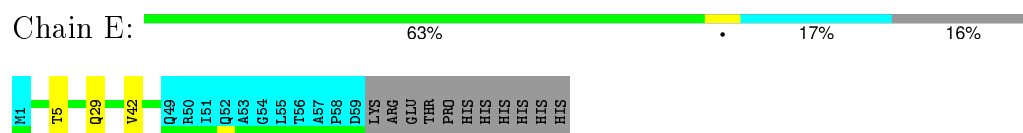
- Molecule 1: Carbon storage regulator homolog



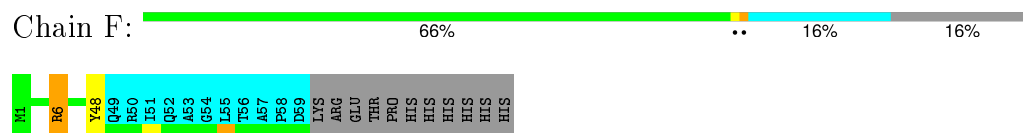
- Molecule 1: Carbon storage regulator homolog



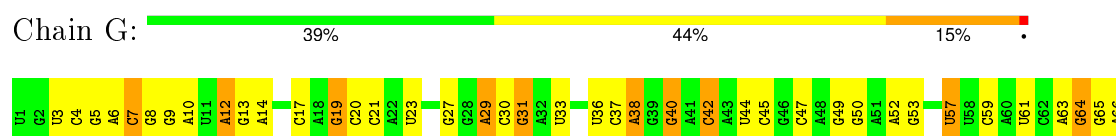
- Molecule 1: Carbon storage regulator homolog

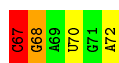


- Molecule 1: Carbon storage regulator homolog



- Molecule 2: RNA_ (72-MER)

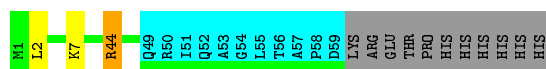




4.2.14 Score per residue for model 14

- Molecule 1: Carbon storage regulator homolog

Chain A: 64% 16% 16%



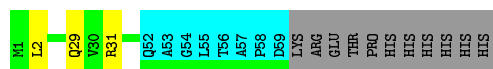
- Molecule 1: Carbon storage regulator homolog

Chain B: 74% 10% 16%



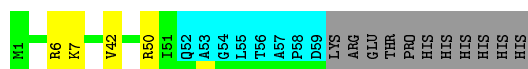
- Molecule 1: Carbon storage regulator homolog

Chain C: 69% 11% 16%



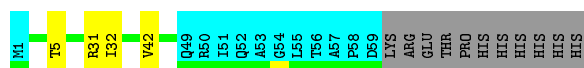
- Molecule 1: Carbon storage regulator homolog

Chain D: 67% 6% 11% 16%



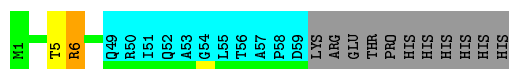
- Molecule 1: Carbon storage regulator homolog

Chain E: 61% 6% 17% 16%



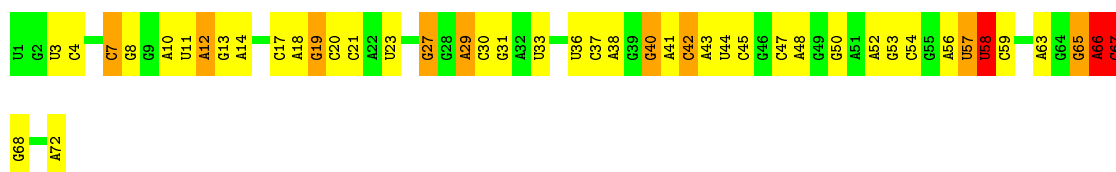
- Molecule 1: Carbon storage regulator homolog

Chain F: 66% 16% 16%



- Molecule 2: RNA_ (72-MER)

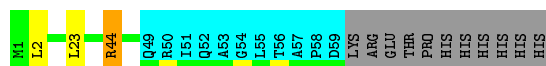
Chain G: 38% 46% 13% 3%



4.2.15 Score per residue for model 15

- Molecule 1: Carbon storage regulator homolog

Chain A: 64% 16% 16%



- Molecule 1: Carbon storage regulator homolog

Chain B: 79% 6% 16%



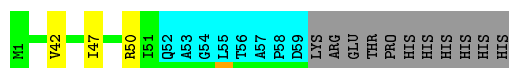
- Molecule 1: Carbon storage regulator homolog

Chain C: 71% 11% 16%



- Molecule 1: Carbon storage regulator homolog

Chain D: 69% 11% 16%



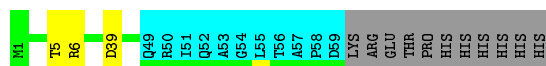
- Molecule 1: Carbon storage regulator homolog

Chain E: 63% 17% 16%

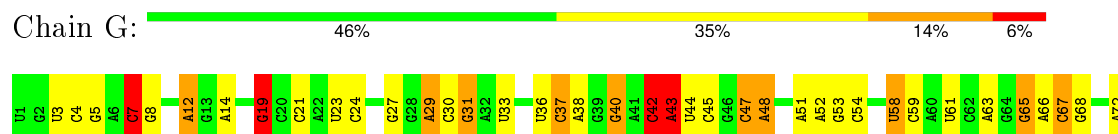


- Molecule 1: Carbon storage regulator homolog

Chain F: 64% 16% 16%

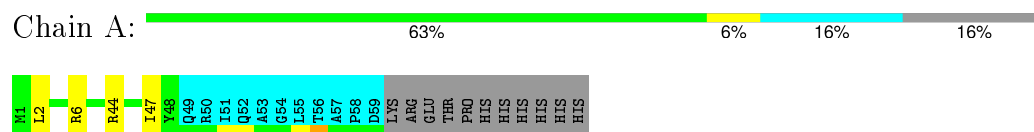


- Molecule 2: RNA_(72-MER)

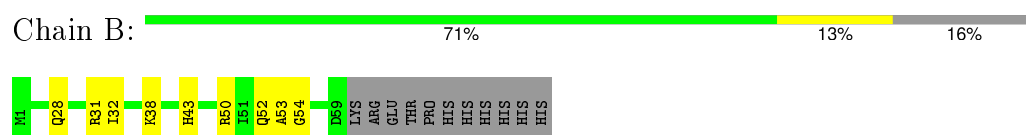


4.2.16 Score per residue for model 16

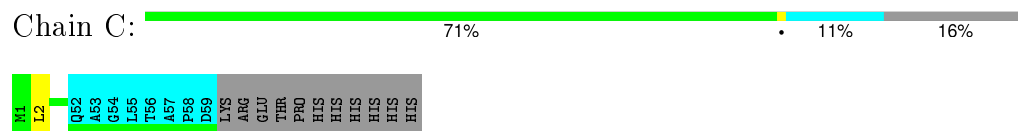
- Molecule 1: Carbon storage regulator homolog



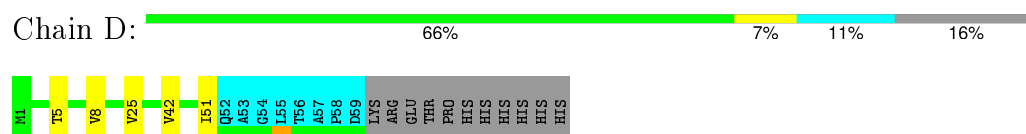
- Molecule 1: Carbon storage regulator homolog



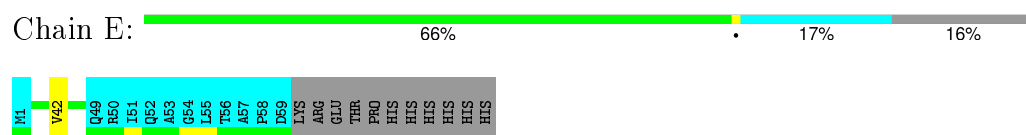
- Molecule 1: Carbon storage regulator homolog



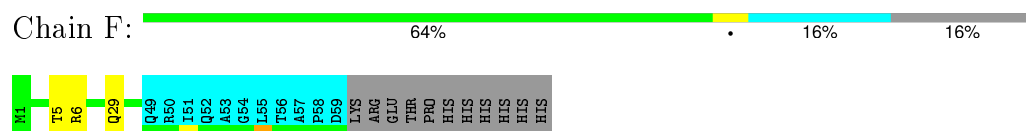
- Molecule 1: Carbon storage regulator homolog



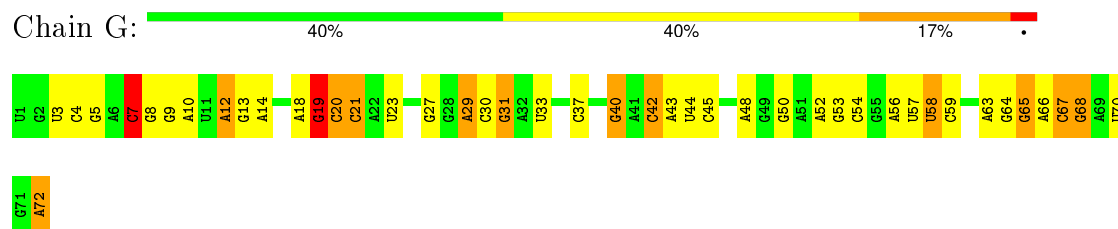
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

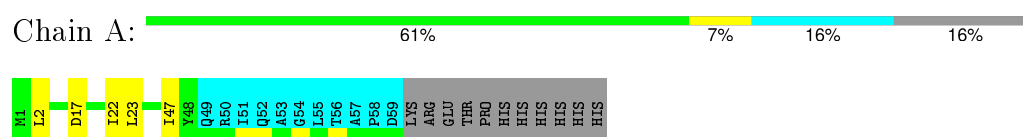


- Molecule 2: RNA_(72-MER)

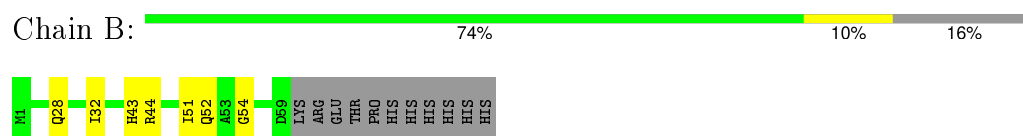


4.2.17 Score per residue for model 17

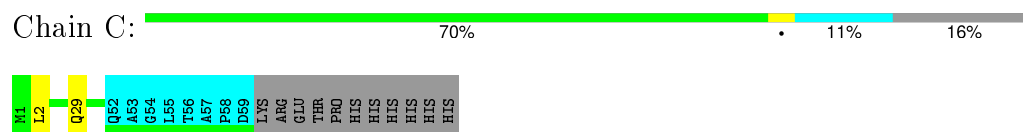
- Molecule 1: Carbon storage regulator homolog



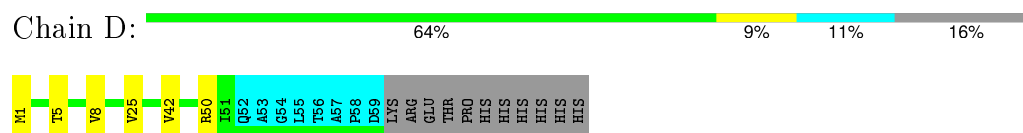
- Molecule 1: Carbon storage regulator homolog



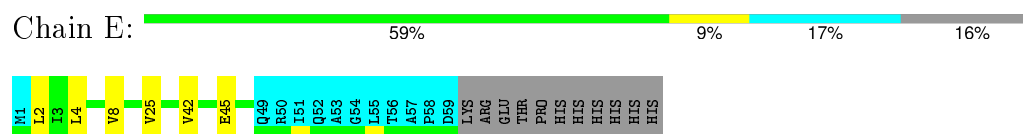
- Molecule 1: Carbon storage regulator homolog



- Molecule 1: Carbon storage regulator homolog

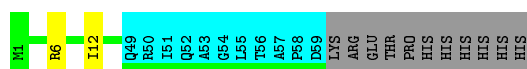


- Molecule 1: Carbon storage regulator homolog



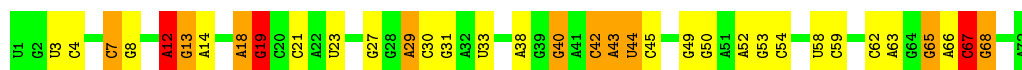
- Molecule 1: Carbon storage regulator homolog





- Molecule 2: RNA_ (72-MER)

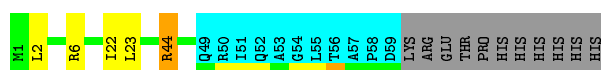
Chain G: 51% 31% 14% •



4.2.18 Score per residue for model 18

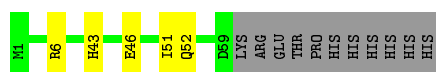
- Molecule 1: Carbon storage regulator homolog

Chain A: 61% 6% • 16% 16%



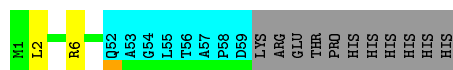
- Molecule 1: Carbon storage regulator homolog

Chain B: 77% 7% 16%



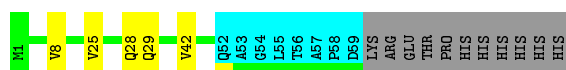
- Molecule 1: Carbon storage regulator homolog

Chain C: 70% • 11% 16%



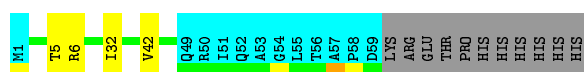
- Molecule 1: Carbon storage regulator homolog

Chain D: 66% 7% 11% 16%



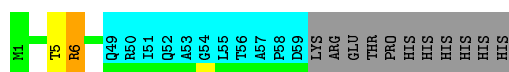
- Molecule 1: Carbon storage regulator homolog

Chain E: 61% 6% 17% 16%



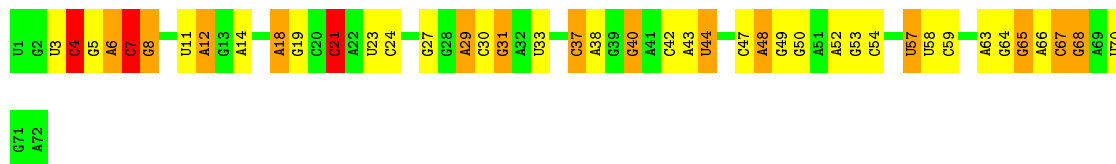
- Molecule 1: Carbon storage regulator homolog

Chain F: 66% •• 16% 16%



- Molecule 2: RNA_(72-MER)

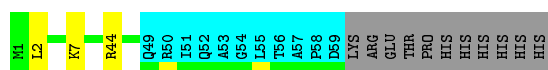
Chain G: 42% 35% 19% .



4.2.19 Score per residue for model 19

- Molecule 1: Carbon storage regulator homolog

Chain A: 64% 16% 16% .



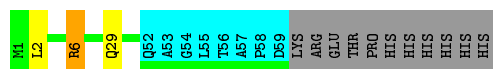
- Molecule 1: Carbon storage regulator homolog

Chain B: 71% 13% 16% .



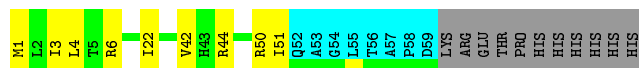
- Molecule 1: Carbon storage regulator homolog

Chain C: 69% 11% 16% .



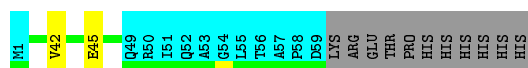
- Molecule 1: Carbon storage regulator homolog

Chain D: 60% 13% 11% 16%



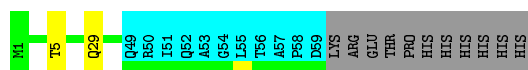
- Molecule 1: Carbon storage regulator homolog

Chain E: 64% 17% 16% .



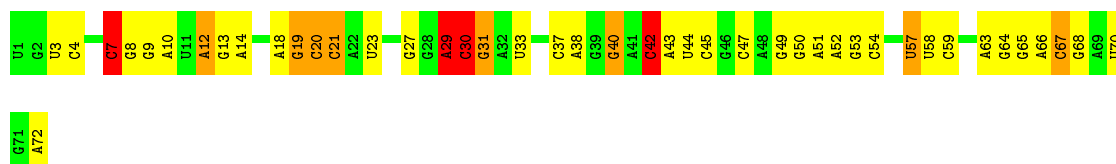
- Molecule 1: Carbon storage regulator homolog

Chain F:  66% 16% 16%



- Molecule 2: RNA_(72-MER)

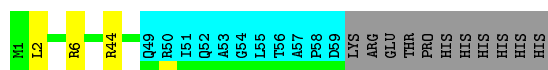
Chain G:  39% 44% 11% 6%



4.2.20 Score per residue for model 20

- Molecule 1: Carbon storage regulator homolog

Chain A:  64% 16% 16%



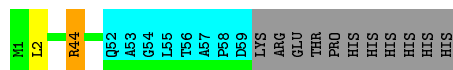
- Molecule 1: Carbon storage regulator homolog

Chain B:  70% 13% 16%



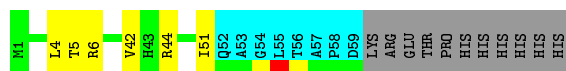
- Molecule 1: Carbon storage regulator homolog

Chain C:  70% 11% 16%



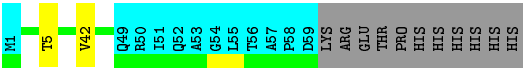
- Molecule 1: Carbon storage regulator homolog

Chain D:  64% 9% 11% 16%

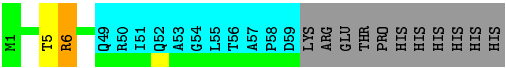


- Molecule 1: Carbon storage regulator homolog

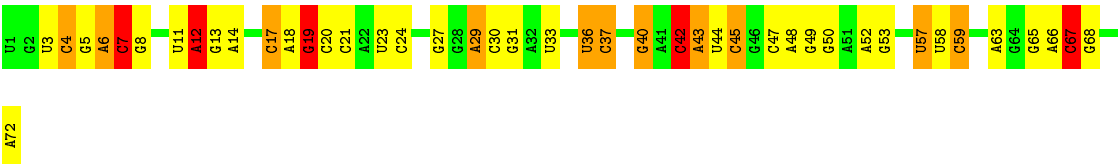
Chain E:  64% 17% 16%



- Molecule 1: Carbon storage regulator homolog



- Molecule 2: RNA_(72-MER)



5 Refinement protocol and experimental data overview

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

Of the 2500 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)	2mf0_cs.str
Number of chemical shift lists	2
Total number of shifts	292
Number of shifts mapped to atoms	292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	0.38±0.00	0±0/370 (0.0±0.0%)	0.80±0.02	0±0/501 (0.0±0.0%)
1	B	0.38±0.00	0±0/451 (0.0±0.0%)	0.87±0.02	1±1/610 (0.1±0.1%)
1	C	0.38±0.00	0±0/398 (0.0±0.0%)	0.80±0.02	0±0/538 (0.0±0.0%)
1	D	0.38±0.00	0±0/398 (0.0±0.0%)	0.84±0.02	0±0/538 (0.0±0.1%)
1	E	0.38±0.00	0±0/362 (0.0±0.0%)	0.80±0.02	0±0/491 (0.0±0.0%)
1	F	0.38±0.00	0±0/370 (0.0±0.0%)	0.78±0.03	0±0/501 (0.0±0.0%)
2	G	1.01±0.00	0±0/1737 (0.0±0.0%)	1.67±0.02	22±3/2709 (0.8±0.1%)
All	All	0.72	0/81720 (0.0%)	1.28	450/117760 (0.4%)

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	C	0.0±0.0	0.6±0.6
1	A	0.0±0.0	0.3±0.5
1	F	0.0±0.0	0.5±0.5
1	E	0.0±0.0	0.1±0.4
1	B	0.0±0.0	0.1±0.3
2	G	0.0±0.0	16.2±2.7
All	All	0	356

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
2	G	17	C	O4'-C1'-N1	10.15	116.32	108.20	12	8
2	G	58	U	O4'-C1'-N1	9.68	115.94	108.20	16	13
2	G	7	C	N3-C2-O2	-9.54	115.22	121.90	8	6
2	G	7	C	N1-C2-O2	9.49	124.59	118.90	16	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	G	37	C	O4'-C1'-N1	9.37	115.70	108.20	13	10
2	G	19	G	O4'-C1'-N9	8.29	114.84	108.20	9	13
2	G	7	C	C2-N1-C1'	8.27	127.89	118.80	8	3
2	G	18	A	O4'-C1'-N9	8.03	114.62	108.20	16	6
2	G	40	G	O4'-C1'-N9	7.97	114.58	108.20	6	20
2	G	42	C	O4'-C1'-N1	7.78	114.42	108.20	19	15
2	G	57	U	O4'-C1'-N1	7.62	114.30	108.20	8	11
2	G	21	C	O4'-C1'-N1	7.43	114.14	108.20	18	20
2	G	72	A	O4'-C1'-N9	7.37	114.09	108.20	20	10
2	G	19	G	C1'-O4'-C4'	-6.72	104.52	109.90	2	6
2	G	7	C	O4'-C1'-N1	6.70	113.56	108.20	15	6
2	G	67	C	C5'-C4'-C3'	-6.66	105.35	116.00	10	12
2	G	21	C	C1'-O4'-C4'	-6.65	104.58	109.90	18	1
2	G	21	C	C4'-C3'-C2'	-6.54	96.06	102.60	18	1
2	G	20	C	O4'-C1'-N1	6.48	113.39	108.20	16	16
2	G	44	U	O4'-C1'-N1	6.46	113.37	108.20	7	10
2	G	37	C	N1-C2-O2	6.31	122.69	118.90	13	10
2	G	7	C	C6-N1-C1'	-6.26	113.28	120.80	8	3
2	G	17	C	N1-C2-O2	6.20	122.62	118.90	12	7
2	G	27	G	C5'-C4'-C3'	-6.14	106.17	116.00	5	1
1	D	44	ARG	NE-CZ-NH1	6.10	123.35	120.30	2	4
2	G	66	A	C3'-C2'-C1'	6.09	106.37	101.50	14	1
2	G	21	C	C5'-C4'-O4'	6.09	116.40	109.10	18	1
1	B	44	ARG	NE-CZ-NH1	6.06	123.33	120.30	10	10
2	G	42	C	C3'-C2'-C1'	6.03	106.33	101.50	15	2
2	G	4	C	N1-C2-O2	6.00	122.50	118.90	16	12
2	G	43	A	O4'-C1'-N9	5.99	112.99	108.20	2	7
2	G	48	A	P-O3'-C3'	5.98	126.88	119.70	18	1
2	G	4	C	O4'-C1'-N1	5.97	112.98	108.20	18	6
2	G	30	C	P-O3'-C3'	5.96	126.85	119.70	19	1
2	G	7	C	C3'-C2'-C1'	-5.95	96.74	101.50	8	1
2	G	35	G	O4'-C1'-N9	5.95	112.96	108.20	1	1
2	G	3	U	O4'-C1'-N1	5.89	112.91	108.20	10	19
2	G	52	A	P-O3'-C3'	5.89	126.76	119.70	7	1
2	G	4	C	N3-C2-O2	-5.86	117.80	121.90	16	17
2	G	30	C	O4'-C1'-N1	5.84	112.87	108.20	19	1
2	G	67	C	C3'-C2'-C1'	-5.82	96.85	101.50	13	6
2	G	23	U	O4'-C1'-N1	5.73	112.79	108.20	10	20
2	G	47	C	O4'-C1'-N1	5.69	112.75	108.20	10	11
2	G	37	C	N3-C2-O2	-5.69	117.92	121.90	13	4
2	G	59	C	O4'-C1'-N1	5.61	112.69	108.20	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	G	45	C	O4'-C1'-N1	5.59	112.67	108.20	15	19
2	G	40	G	C3'-C2'-C1'	-5.56	97.05	101.50	6	1
2	G	17	C	N3-C2-O2	-5.53	118.03	121.90	12	3
2	G	48	A	C3'-C2'-C1'	5.51	105.91	101.50	1	5
2	G	33	U	O4'-C1'-N1	5.48	112.58	108.20	3	20
2	G	7	C	C6-N1-C2	-5.48	118.11	120.30	10	1
2	G	36	U	O4'-C1'-N1	5.46	112.57	108.20	1	6
2	G	7	C	P-O3'-C3'	5.43	126.21	119.70	20	1
2	G	4	C	P-O3'-C3'	5.42	126.20	119.70	18	2
2	G	67	C	P-O3'-C3'	5.37	126.15	119.70	18	3
2	G	54	C	O4'-C1'-N1	5.37	112.50	108.20	8	14
2	G	70	U	O4'-C1'-N1	5.37	112.50	108.20	11	10
2	G	6	A	C5'-C4'-C3'	-5.33	107.47	116.00	18	2
2	G	52	A	O4'-C4'-C3'	5.29	110.33	106.10	7	1
2	G	24	C	O4'-C1'-N1	5.20	112.36	108.20	18	5
2	G	47	C	N1-C2-O2	5.17	122.00	118.90	11	2
2	G	51	A	C3'-C2'-C1'	5.14	105.61	101.50	7	1
1	A	44	ARG	NE-CZ-NH1	5.14	122.87	120.30	16	1
2	G	11	U	O4'-C1'-N1	5.12	112.30	108.20	2	1
2	G	47	C	N3-C2-O2	-5.12	118.32	121.90	11	2
2	G	13	G	C5'-C4'-C3'	-5.11	107.83	116.00	17	1
2	G	5	G	N3-C4-C5	-5.09	126.06	128.60	3	1
2	G	6	A	C5'-C4'-O4'	5.06	115.17	109.10	8	1
2	G	47	C	P-O3'-C3'	5.04	125.74	119.70	15	1
2	G	61	U	O4'-C1'-N1	5.02	112.22	108.20	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)
2	G	31	G	Sidechain	20
2	G	66	A	Sidechain	20
2	G	12	A	Sidechain	20
2	G	29	A	Sidechain	20
2	G	14	A	Sidechain	18
2	G	7	C	Sidechain	17
2	G	63	A	Sidechain	14
2	G	65	G	Sidechain	13
2	G	10	A	Sidechain	11
2	G	19	G	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
2	G	64	G	Sidechain	10
2	G	68	G	Sidechain	10
2	G	36	U	Sidechain	10
2	G	4	C	Sidechain	10
1	F	6	ARG	Sidechain	9
2	G	42	C	Sidechain	9
2	G	21	C	Sidechain	8
2	G	49	G	Sidechain	8
2	G	48	A	Sidechain	8
2	G	9	G	Sidechain	7
2	G	51	A	Sidechain	7
2	G	25	A	Sidechain	6
2	G	5	G	Sidechain	6
2	G	56	A	Sidechain	5
2	G	53	G	Sidechain	5
2	G	58	U	Sidechain	5
1	C	6	ARG	Sidechain	5
2	G	6	A	Sidechain	4
2	G	37	C	Sidechain	4
1	A	44	ARG	Sidechain	4
2	G	67	C	Sidechain	4
2	G	18	A	Sidechain	3
2	G	20	C	Sidechain	3
1	C	31	ARG	Sidechain	3
2	G	27	G	Sidechain	3
2	G	8	G	Sidechain	3
2	G	17	C	Sidechain	3
2	G	62	C	Sidechain	3
2	G	43	A	Sidechain	3
2	G	57	U	Sidechain	2
1	E	6	ARG	Sidechain	2
1	A	48	TYR	Sidechain	2
1	B	15	GLY	Mainchain	2
1	C	44	ARG	Sidechain	2
2	G	38	A	Sidechain	1
2	G	61	U	Sidechain	1
2	G	35	G	Sidechain	1
2	G	44	U	Sidechain	1
2	G	54	C	Sidechain	1
1	E	31	ARG	Sidechain	1
2	G	24	C	Sidechain	1
2	G	15	C	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	G	72	A	Sidechain	1
2	G	39	G	Sidechain	1
2	G	40	G	Sidechain	1
2	G	41	A	Sidechain	1
1	C	15	GLY	Mainchain	1
2	G	45	C	Sidechain	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	448	472	472	1±1
1	D	395	422	422	1±1
1	A	367	390	390	0±0
1	C	395	422	422	0±1
1	F	367	390	390	0±0
1	E	359	379	379	0±0
2	G	1549	783	783	1±1
All	All	77600	65160	65160	74

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:47:ILE:HD12	2:G:7:C:C2	0.65	2.27	15	1
1:D:8:VAL:HG11	1:D:25:VAL:HG12	0.63	1.68	11	5
1:D:51:ILE:HD11	2:G:7:C:C2	0.62	2.29	11	2
2:G:29:A:H2'	2:G:30:C:H5''	0.59	1.75	19	1
1:D:51:ILE:N	1:D:51:ILE:HD12	0.57	2.15	10	3
1:D:51:ILE:H	1:D:51:ILE:HD12	0.56	1.61	8	3
1:D:51:ILE:HD12	1:D:51:ILE:N	0.53	2.18	11	2
2:G:66:A:C2'	2:G:67:C:H5''	0.49	2.37	14	1
1:E:8:VAL:CG1	1:E:25:VAL:HG12	0.47	2.39	17	1
1:B:50:ARG:O	1:B:53:ALA:HB3	0.46	2.11	1	4
1:E:8:VAL:HG11	1:E:25:VAL:HG12	0.46	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:6:ARG:HE	1:C:22:ILE:CG2	0.46	2.24	11	1
1:B:56:THR:HG22	1:B:57:ALA:H	0.46	1.70	1	1
2:G:27:G:N3	2:G:27:G:H2'	0.45	2.27	5	1
1:C:23:LEU:HD13	2:G:67:C:H1'	0.45	1.88	3	2
1:C:44:ARG:HH21	1:D:4:LEU:HD22	0.45	1.72	20	1
1:C:48:TYR:HA	1:C:51:ILE:HD13	0.45	1.88	2	2
1:C:15:GLY:O	1:C:17:ASP:N	0.44	2.51	8	1
1:B:15:GLY:O	1:B:17:ASP:N	0.44	2.50	20	2
1:D:1:MET:HG2	1:D:3:ILE:HD11	0.44	1.90	6	4
1:B:51:ILE:HG22	1:B:52:GLN:NE2	0.44	2.28	9	16
1:B:1:MET:CE	2:G:52:A:C8	0.44	3.00	7	1
1:D:51:ILE:CD1	1:D:51:ILE:N	0.44	2.81	20	2
2:G:12:A:H5''	2:G:12:A:C8	0.43	2.49	20	1
1:D:8:VAL:HG11	1:D:25:VAL:CG1	0.43	2.41	17	2
1:D:51:ILE:N	1:D:51:ILE:CD1	0.43	2.82	10	1
1:D:51:ILE:CD1	1:D:51:ILE:H	0.43	2.25	8	1
2:G:12:A:C8	2:G:12:A:H5''	0.42	2.50	3	2
1:F:6:ARG:HD2	1:F:12:ILE:HD11	0.42	1.90	17	1
1:C:23:LEU:HD12	1:C:31:ARG:HG2	0.42	1.91	10	2
2:G:63:A:H2'	2:G:64:G:C8	0.42	2.49	2	1
1:B:38:LYS:HE3	2:G:28:G:H1'	0.42	1.92	3	2
2:G:66:A:H2'	2:G:67:C:H5''	0.41	1.92	14	1
1:C:29:GLN:HG3	1:D:7:LYS:CG	0.41	2.46	14	1
1:D:1:MET:CE	2:G:67:C:C6	0.40	3.04	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	47/70 (67%)	43±1 (92±1%)	4±1 (8±1%)	0±0 (0±0%)	59	88
1	B	57/70 (81%)	52±1 (90±2%)	4±1 (8±2%)	1±1 (2±1%)	15	58
1	C	50/70 (71%)	50±1 (100±1%)	0±0 (0±1%)	0±0 (0±1%)	56	85
1	D	50/70 (71%)	49±1 (97±2%)	1±1 (3±2%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	47/70 (67%)	45±1 (96±2%)	2±1 (4±2%)	0±0 (0±0%)	100	100
1	F	47/70 (67%)	44±1 (94±2%)	3±1 (6±2%)	0±0 (0±0%)	100	100
All	All	5960/8400 (71%)	5645 (95%)	291 (5%)	24 (0%)	43	81

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	54	GLY	16
1	B	15	GLY	2
1	B	16	ASP	2
1	B	58	PRO	1
1	C	15	GLY	1
1	C	16	ASP	1
1	A	17	ASP	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	41/60 (68%)	38±1 (92±2%)	3±1 (8±2%)	21	66
1	B	49/60 (82%)	45±1 (92±3%)	4±1 (8±3%)	19	64
1	C	44/60 (73%)	42±1 (96±2%)	2±1 (4±2%)	40	83
1	D	44/60 (73%)	41±1 (94±2%)	3±1 (6±2%)	28	73
1	E	40/60 (67%)	38±1 (94±3%)	2±1 (6±3%)	28	73
1	F	41/60 (68%)	39±1 (95±3%)	2±1 (5±3%)	35	79
All	All	5180/7200 (72%)	4855 (94%)	325 (6%)	27	72

All 51 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	B	43	HIS	20

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Mol	Chain	Res	Type	Models (Total)
1	C	2	LEU	20
1	E	42	VAL	19
1	D	42	VAL	19
1	A	44	ARG	16
1	F	5	THR	16
1	B	28	GLN	15
1	B	31	ARG	14
1	E	5	THR	12
1	F	6	ARG	11
1	B	32	ILE	10
1	D	5	THR	10
1	A	23	LEU	9
1	A	6	ARG	8
1	D	6	ARG	8
1	C	29	GLN	7
1	C	6	ARG	6
1	E	6	ARG	6
1	F	29	GLN	6
1	E	45	GLU	5
1	D	4	LEU	5
1	B	38	LYS	5
1	D	50	ARG	5
1	B	25	VAL	4
1	A	22	ILE	4
1	A	7	LYS	3
1	F	45	GLU	3
1	B	6	ARG	3
1	B	52	GLN	3
1	D	29	GLN	3
1	E	2	LEU	3
1	C	44	ARG	2
1	F	39	ASP	2
1	E	32	ILE	2
1	B	39	ASP	2
1	C	28	GLN	2
1	A	47	ILE	2
1	B	46	GLU	2
1	D	22	ILE	2
1	E	29	GLN	1
1	D	28	GLN	1
1	D	1	MET	1
1	E	4	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	F	10	GLU	1
1	B	44	ARG	1
1	F	38	LYS	1
1	B	22	ILE	1
1	C	22	ILE	1
1	B	42	VAL	1
1	F	13	ASN	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	G	71/72 (99%)	25±3 (35±4%)	5±2 (7±2%)	0.33±0.02
All	All	1420/1440 (99%)	497 (35%)	101 (7%)	0.33

The overall RNA backbone suiteness is 0.33.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	G	19	G	20
2	G	52	A	20
2	G	30	C	20
2	G	40	G	20
2	G	8	G	20
2	G	65	G	20
2	G	42	C	20
2	G	68	G	20
2	G	27	G	20
2	G	67	C	20
2	G	53	G	20
2	G	12	A	20
2	G	50	G	19
2	G	13	G	18
2	G	44	U	18
2	G	7	C	18
2	G	59	C	17
2	G	43	A	17
2	G	31	G	16
2	G	57	U	14
2	G	58	U	13
2	G	5	G	12
2	G	49	G	11

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Mol	Chain	Res	Type	Models (Total)
2	G	38	A	11
2	G	6	A	9
2	G	72	A	8
2	G	48	A	8
2	G	63	A	8
2	G	18	A	7
2	G	64	G	7
2	G	20	C	5
2	G	29	A	5
2	G	11	U	5
2	G	37	C	4
2	G	17	C	3
2	G	51	A	1
2	G	9	G	1
2	G	35	G	1
2	G	36	U	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	G	29	A	20
2	G	67	C	15
2	G	5	G	12
2	G	48	A	8
2	G	63	A	7
2	G	12	A	7
2	G	19	G	5
2	G	30	C	4
2	G	38	A	4
2	G	18	A	3
2	G	42	C	3
2	G	4	C	2
2	G	57	U	2
2	G	52	A	1
2	G	58	U	1
2	G	21	C	1
2	G	47	C	1
2	G	37	C	1
2	G	35	G	1
2	G	17	C	1
2	G	43	A	1
2	G	7	C	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: 2mf0_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	280
Number of shifts mapped to atoms	280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

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

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 6%, i.e. 284 atoms were assigned a chemical shift out of a possible 5089. 0 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1506 (0%)	0/601 (0%)	0/608 (0%)	0/297 (0%)
Sidechain	0/2123 (0%)	0/1218 (0%)	0/802 (0%)	0/103 (0%)
Aromatic	0/90 (0%)	0/48 (0%)	0/36 (0%)	0/6 (0%)
Overall	284/5089 (6%)	144/2659 (5%)	117/1928 (6%)	23/502 (5%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 284 atoms were assigned a chemical shift out of a possible 5648. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1746 (0%)	0/696 (0%)	0/708 (0%)	0/342 (0%)
Sidechain	0/2442 (0%)	0/1404 (0%)	0/918 (0%)	0/120 (0%)
Aromatic	0/90 (0%)	0/48 (0%)	0/36 (0%)	0/6 (0%)
Overall	284/5648 (5%)	144/2940 (5%)	117/2144 (5%)	23/564 (4%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	G	41	A	H8	9.24	9.22 – 6.72	5.1

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (`assigned_chem_shift_list_1`). RCI is only applicable to proteins.

7.2 Chemical shift list 2

File name: 2mf0_cs.str

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	12
Number of shifts mapped to atoms	12
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](#)

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 0%, i.e. 24 atoms were assigned a chemical shift out of a possible 5089. 0 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/1506 (0%)	0/601 (0%)	0/608 (0%)	0/297 (0%)
Sidechain	0/2123 (0%)	0/1218 (0%)	0/802 (0%)	0/103 (0%)
Aromatic	0/90 (0%)	0/48 (0%)	0/36 (0%)	0/6 (0%)
Overall	24/5089 (0%)	14/2659 (1%)	6/1928 (0%)	4/502 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 24 atoms were assigned a chemical shift out of a possible 5648. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/1746 (0%)	0/696 (0%)	0/708 (0%)	0/342 (0%)
Sidechain	0/2442 (0%)	0/1404 (0%)	0/918 (0%)	0/120 (0%)
Aromatic	0/90 (0%)	0/48 (0%)	0/36 (0%)	0/6 (0%)
Overall	24/5648 (0%)	14/2940 (0%)	6/2144 (0%)	4/564 (1%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.