WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 03:37 AM EDT

PDB ID	:	2MF0
BMRB ID	:	19534
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

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

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

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 5%.

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.
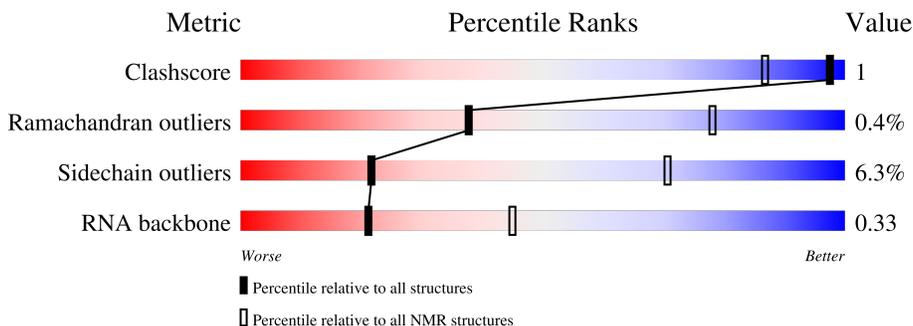
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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	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)	0.43	4
2	E:2-E:48, F:1-F:48 (95)	0.24	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

Continued on next page...

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).

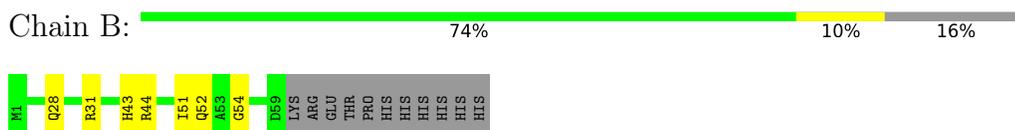| Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	G	72	2332	693	783	295	490	71	0

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Carbon storage regulator homolog
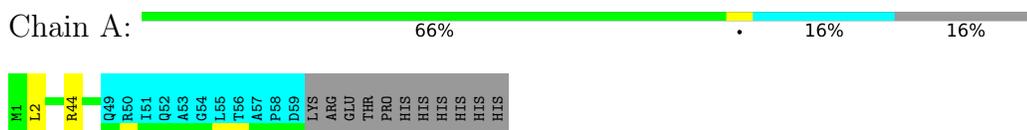
Chain A:

- Molecule 1: Carbon storage regulator homolog

Chain B:

- Molecule 1: Carbon storage regulator homolog

Chain C:

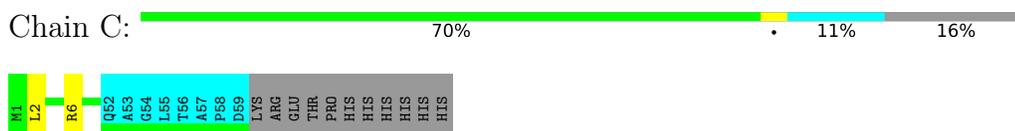- Molecule 1: Carbon storage regulator homolog

Chain D:

- Molecule 1: Carbon storage regulator homolog

Chain E:

- Molecule 1: Carbon storage regulator homolog

Chain F: 66% • 16% 16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 36% 49% 15%

U1 G2 U3 C4 G5 A6 C7 G8 G9 A10 U11 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65 A66 C67

G68 A72

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: 63% 6% 16% 16%

M1 L2 K7 I22 L23 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 71% 13% 16%

M1 R31 H43 R44 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 69% • 11% 16%

M1 L2 Q28 Q29 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 66% 7% 11% 16%

M1 L2 I3 R6 I22 V42 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E:

• Molecule 1: Carbon storage regulator homolog

Chain F:

• Molecule 2: RNA_(72-MER)

Chain G:
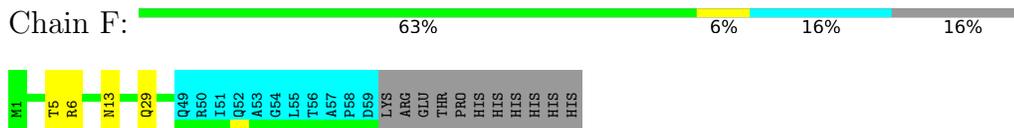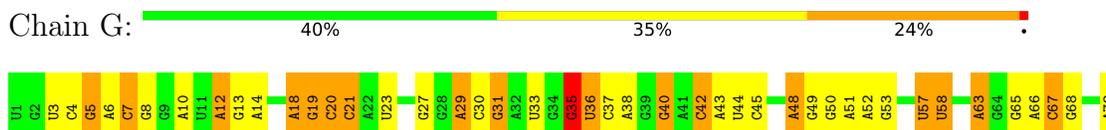
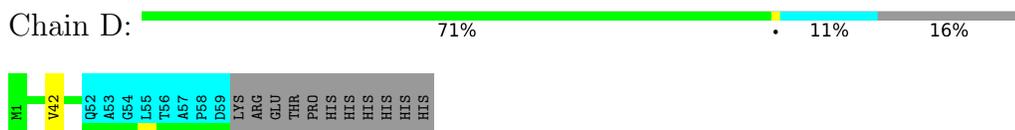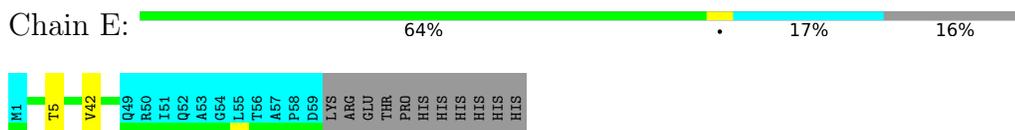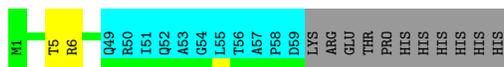### 4.2.2 Score per residue for model 2

• Molecule 1: Carbon storage regulator homolog
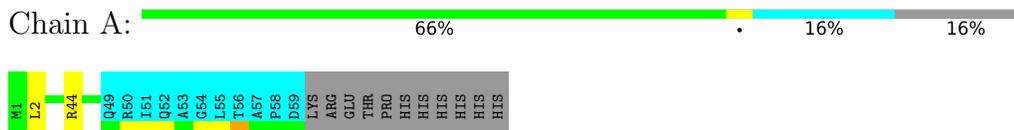
Chain A:

• Molecule 1: Carbon storage regulator homolog

Chain B:

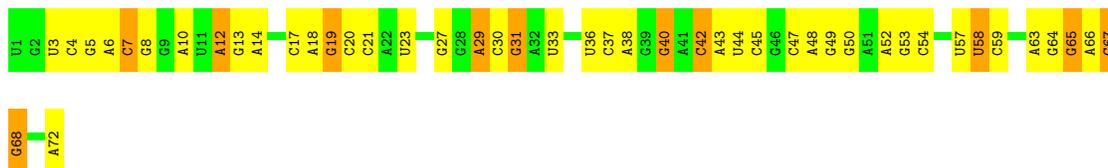• Molecule 1: Carbon storage regulator homolog

Chain C:

• Molecule 1: Carbon storage regulator homolog

Chain D:

• Molecule 1: Carbon storage regulator homolog

Chain E:

• Molecule 1: Carbon storage regulator homolog
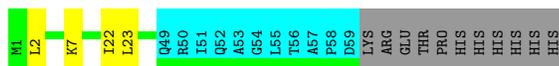
Chain F:

• Molecule 2: RNA_(72-MER)

Chain G:
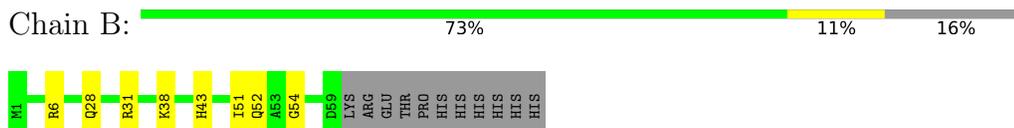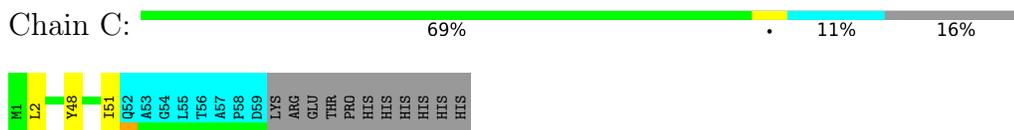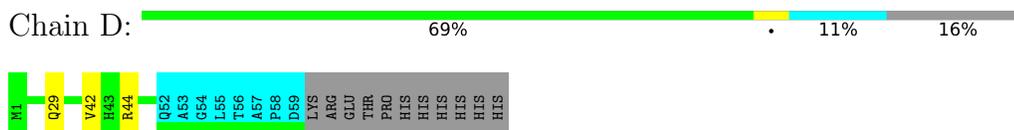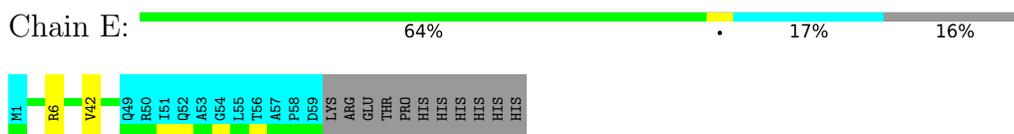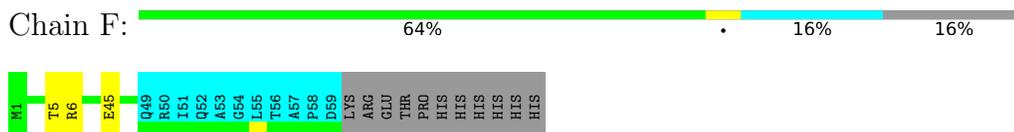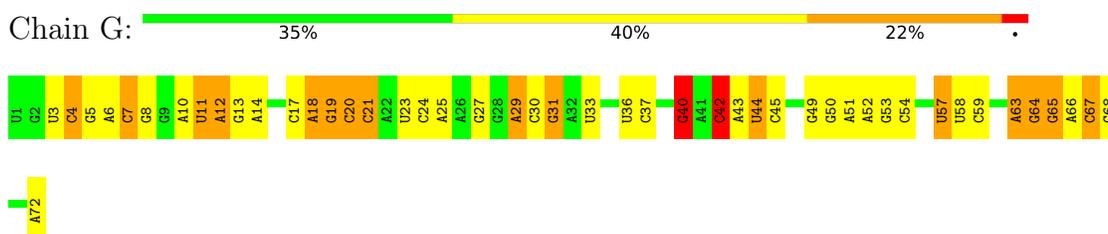
4.2.3   Score per residue for model 3

• Molecule 1: Carbon storage regulator homolog
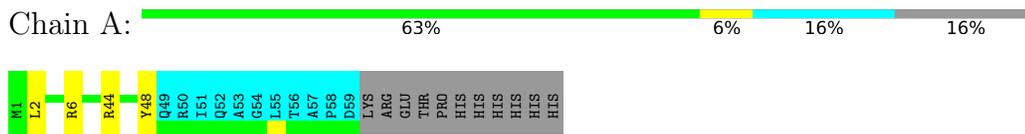
Chain A:

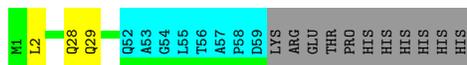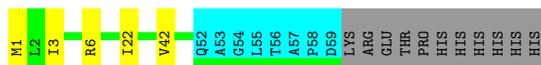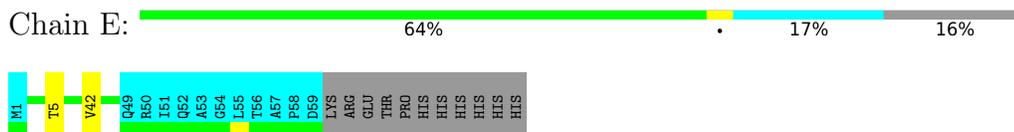

• Molecule 1: Carbon storage regulator homolog

Chain B:

• Molecule 1: Carbon storage regulator homolog

Chain C:

• Molecule 1: Carbon storage regulator homolog

Chain D:

M1 Q29 V42 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 63% • 17% 16%

M1 T5 R6 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 66% • 16% 16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 39% 35% 21% 6%

U1 G2 U3 C4 G5 A6 C7 G8 G9 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 A43 U44 C45 A48 G49 G50 A51 A52 G53 U57 U58 C59 A63 G64 G65 A66 C67 G68 A69 U70

G71 A72
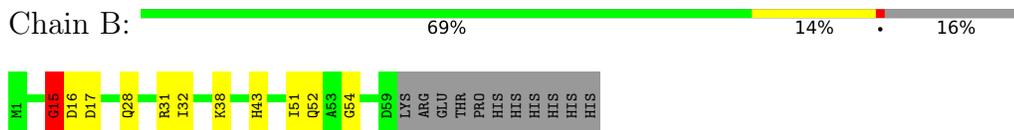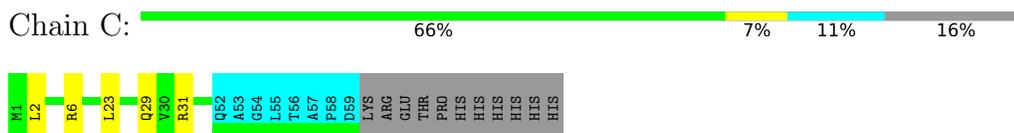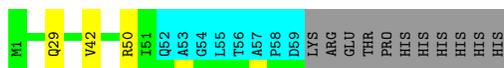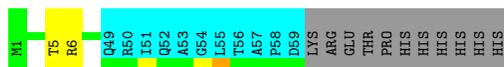
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Carbon storage regulator homolog

Chain A: 66% • 16% 16%

M1 L2 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 74% 10% 16%

M1 I22 V25 R31 H43 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 70% • 11% 16%

M1 L2 R44 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D:

66%   7%   11%   16%

M1 L4 T5 V8 V25 V42 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain E:

63%   .   17%   16%

M1 L2 T5 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain F:

66%   .   16%   16%

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

- Molecule 2: RNA_(72-MER)

Chain G:

42%   40%   14%   .

U1 G2 U3 C4 G5 A6 C7 G8 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 C24 A25 A26 G27 G28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U58 C59 A63 G64 G65 A66 C67 G68

A72

4.2.5 Score per residue for model 5

- Molecule 1: Carbon storage regulator homolog

Chain A:

66%   .   16%   16%

M1 L2 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain B:

77%   7%   16%

M1 R31 D39 H43 R44 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain C:

70%   .   11%   16%

M1 L2 R6 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain D:

71% · 11% 16%

M1 V42 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain E:

64% · 17% 16%

M1 T5 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain F:

63% 6% 16% 16%

M1 T5 R6 Q29 E45 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 2: RNA_(72-MER)

Chain G:

40% 36% 19% ·

U1 G2 U3 C4 G5 A6 C7 G8 G9 A12 G13 C17 A18 G19 C20 C21 A22 U23 C24 A25 A26 C27 G28 A29 C30 G31 A32 U33 U36 C37 G40 A41 C42 A43 U44 C45 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65 A66 C67 G68

A72

4.2.6 Score per residue for model 6

- Molecule 1: Carbon storage regulator homolog

Chain A:

63% · · 16% 16%

M1 L2 L23 H43 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain B:

73% 11% 16%

M1 Q28 R31 K38 H43 R44 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain C: 69% 11% 16%

M1 L2 Q28 Q29 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 67% 6% 11% 16%

M1 L2 I3 L4 V42 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 63% 17% 16%

M1 T5 R6 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 64% 16% 16%

M1 T5 R6 E45 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 2: RNA_(72-MER)

Chain G: 33% 51% 14%

U1 G2 U3 C4 G5 A6 C7 G8 G9 A10 U11 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 G55 A56 U57 U58 C59 C62 G65 A66

C67 G68 A72

4.2.7 Score per residue for model 7

• Molecule 1: Carbon storage regulator homolog

Chain A: 63% 6% 16% 16%

M1 L2 R6 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 71% 13% 16%

M1 Q28 I32 K38 H43 R44 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 71%   •   11%   16%

M1 L2 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 69%   •   11%   16%

M1 L4 T5 R6 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 66%   •   17%   16%

M1 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 67%   •   16%   16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 40%   38%   17%   6%

U1 G2 U3 C4 G5 A6 C7 G8 G9 A10 U11 A12 G13 A14 G19 C20 C21 A22 U23 G27 C28 A29 C30 G31 A32 U33 A38 G39 G40 A41 C42 A43 U44 C45 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65 A66 C67 G68 A72

4.2.8   Score per residue for model 8

• Molecule 1: Carbon storage regulator homolog

Chain A: 64%   •   16%   16%

M1 L2 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS
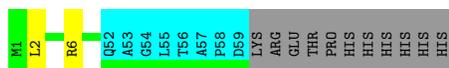
• Molecule 1: Carbon storage regulator homolog

Chain B: 71%   11%   •   16%

- Molecule 1: Carbon storage regulator homolog

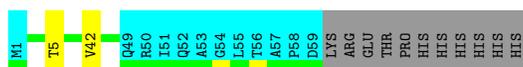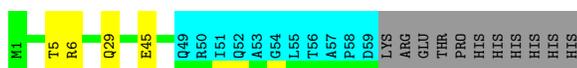Chain C:

- 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:

4.2.9 Score per residue for model 9

- Molecule 1: Carbon storage regulator homolog
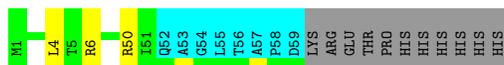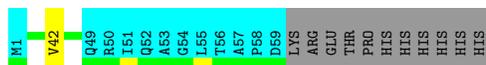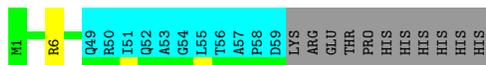
Chain A:

- Molecule 1: Carbon storage regulator homolog

Chain B:

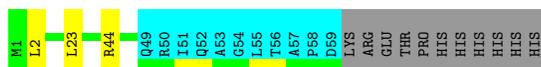• Molecule 1: Carbon storage regulator homolog

Chain C:
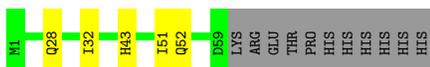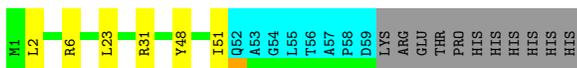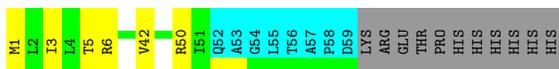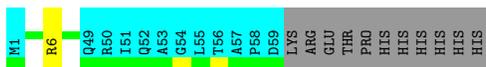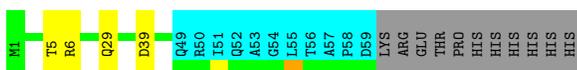

• Molecule 1: Carbon storage regulator homolog
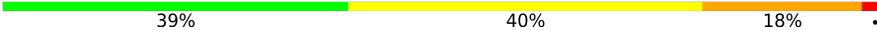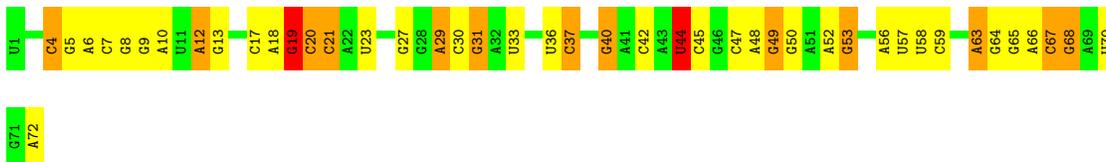
Chain D:

• Molecule 1: Carbon storage regulator homolog

Chain E:

• Molecule 1: Carbon storage regulator homolog

Chain F:

• Molecule 2: RNA_(72-MER)

Chain G:

4.2.10　Score per residue for model 10

• Molecule 1: Carbon storage regulator homolog

Chain A:

M1 L2 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 69% 16% 16%

M1 Q28 R31 I32 V42 H43 R44 R50 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 64% 9% 11% 16%

M1 L2 R6 L23 Q29 V30 R31 R44 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 64% 9% 11% 16%

M1 T5 R6 V42 H43 R44 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 60% 7% 17% 16%

M1 L2 T5 R6 V42 E45 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 67% . 16% 16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 32% 42% 24% .

U1 G2 U3 C4 G5 A6 C7 G8 G9 A10 U11 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 C24 A25 A26 G27 C28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65

A66 C67 G68 A69 U70 G71 A72

4.2.11 Score per residue for model 11

• Molecule 1: Carbon storage regulator homolog

Chain A:

63% 6% 16% 16%

M1 L2 R6 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain B:

74% 10% 16%

M1 V25 Q28 R31 H43 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain C:

69% 11% 16%

M1 L2 R6 I22 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain D:

64% 9% 11% 16%

M1 L4 T5 V8 V25 V42 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain E:

63% 17% 16%

M1 T5 R6 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 1: Carbon storage regulator homolog

Chain F:

64% 16% 16%

M1 T5 R6 Q29 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

- Molecule 2: RNA_(72-MER)

Chain G:

43% 39% 15%

U1 G2 U3 C4 G5 A6 C7 G8 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 U36 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U58 C59 A63 G64 G65 A66 C67 G68 A69 U70 G71 A72

4.2.12 Score per residue for model 12

- Molecule 1: Carbon storage regulator homolog

Chain A: 64% · 16% 16%

M1 L2 R44 Y48 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 74% 10% 16%

M1 V25 Q28 R31 H43 I51 Q52 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 70% · 11% 16%

M1 L2 R6 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 69% · 11% 16%

M1 T5 V42 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 66% · 17% 16%

M1 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 67% · 16% 16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 36% 44% 18% ·

U1 G2 U3 C4 G5 A6 C7 G8 G9 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 C24 A25 A26 G27 Q28 A29 C30 G31 A32 U33 U36 C37 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 C62 A63 G64 G65 A66

C67 G68 A69 U70 G71 A72

4.2.13   Score per residue for model 13

• 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
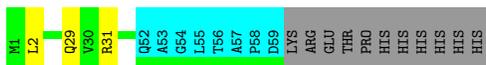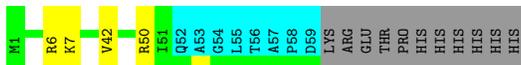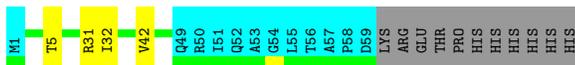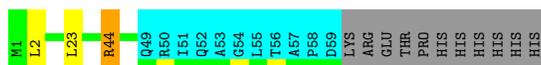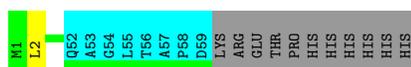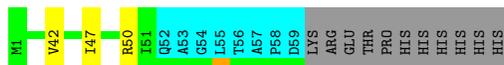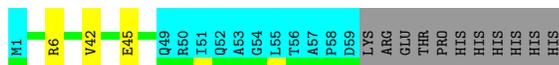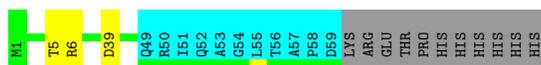
Chain F:

• Molecule 2: RNA_(72-MER)

Chain G:

C67 G68 A69 U70 G71 A72

4.2.14 Score per residue for model 14

• Molecule 1: Carbon storage regulator homolog
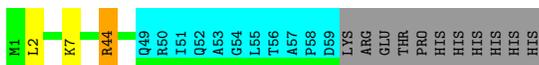
Chain A:

64%   16%   16%

M1 L2 K7 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B:

74%   10%   16%

M1 Q28 I32 H43 E46 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C:

69%   11%   16%

M1 L2 Q29 V30 R31 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D:

67%   6% 11%   16%

M1 R6 K7 V42 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E:

61%   6% 17%   16%

M1 T5 R31 I32 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F:

66%   16%   16%

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

• Molecule 2: RNA_(72-MER)

Chain G:

38%   46%   12%

U1 G2 U3 C4 C7 G8 G9 A10 U11 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 U36 C37 A38 G39 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 G55 A56 U57 U58 C59 A63 G64 G65 A66 C67

G68 A72
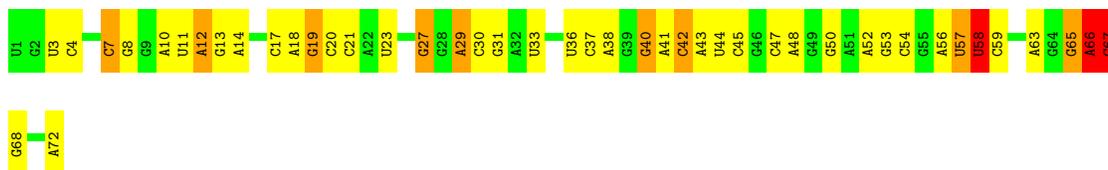
4.2.15 Score per residue for model 15

• Molecule 1: Carbon storage regulator homolog

Chain A: 64%   • •   16%   16%

M1 L2 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 79%   6%   16%

M1 R31 H43 I51 Q52 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 71%   •   11%   16%

M1 L2 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 69%   •   11%   16%

M1 V42 I47 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 63%   •   17%   16%

M1 R6 V42 E45 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 64%   •   16%   16%

M1 T5 R6 D39 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: RNA_(72-MER)

Chain G:

4.2.16 Score per residue for model 16

• Molecule 1: Carbon storage regulator homolog
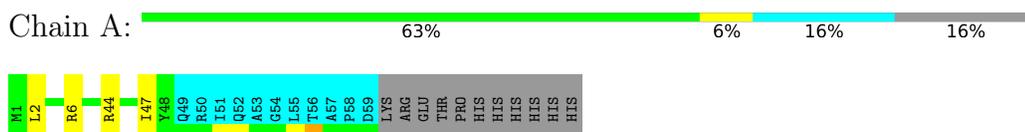
Chain A:

• Molecule 1: Carbon storage regulator homolog

Chain B:

• Molecule 1: Carbon storage regulator homolog

Chain C:

• Molecule 1: Carbon storage regulator homolog

Chain D:

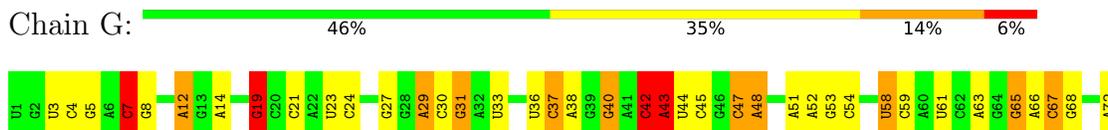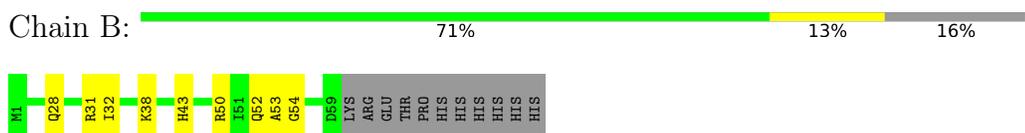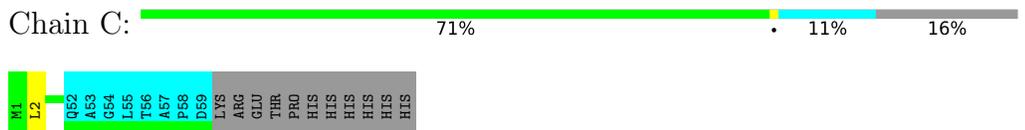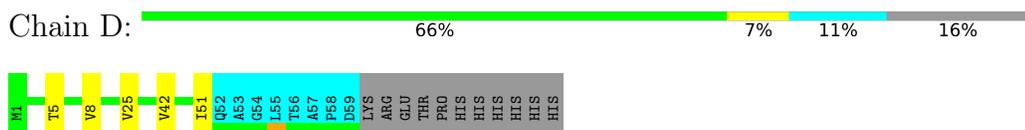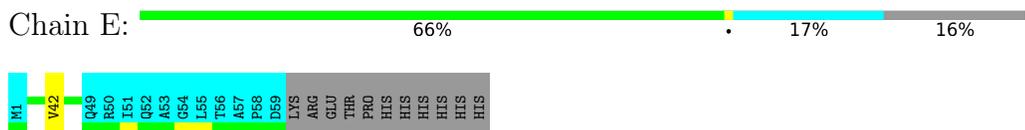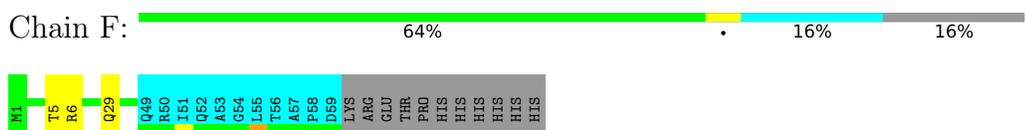• Molecule 1: Carbon storage regulator homolog

Chain E:

• Molecule 1: Carbon storage regulator homolog
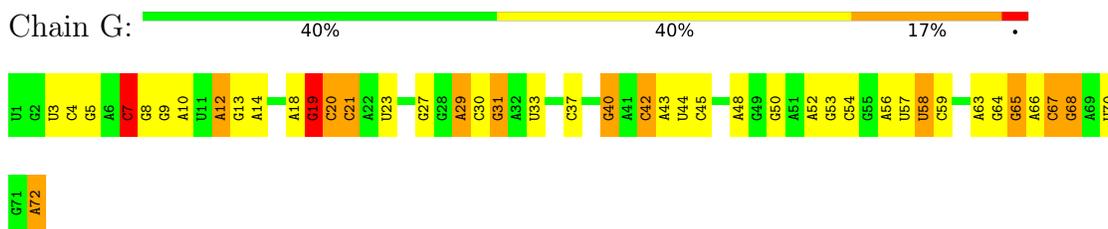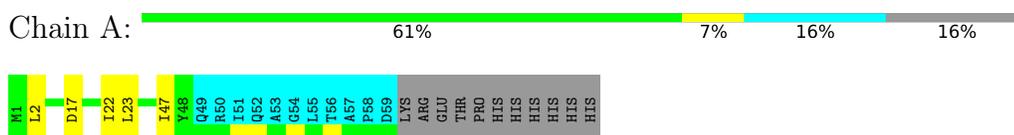
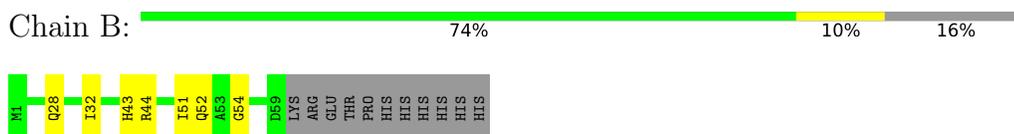Chain F:

● Molecule 2: RNA_(72-MER)

Chain G:

4.2.17 Score per residue for model 17

● Molecule 1: Carbon storage regulator homolog

Chain A:

● Molecule 1: Carbon storage regulator homolog

Chain B:

● Molecule 1: Carbon storage regulator homolog

Chain C:

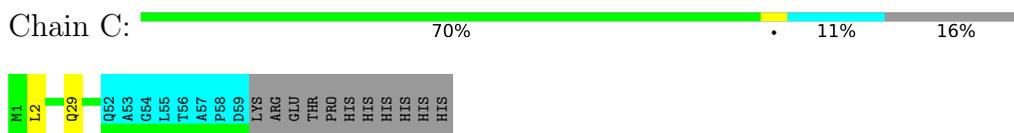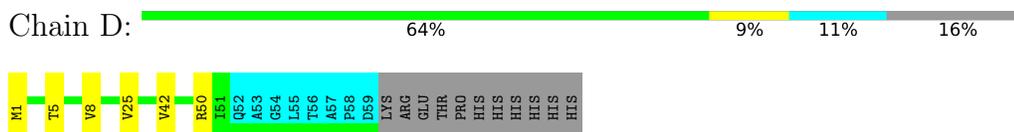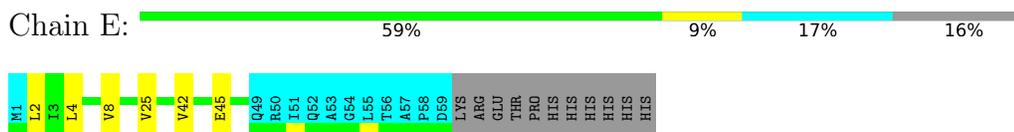

● Molecule 1: Carbon storage regulator homolog

Chain D:

● Molecule 1: Carbon storage regulator homolog

Chain E:

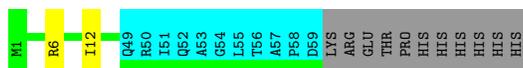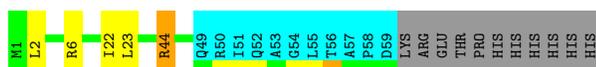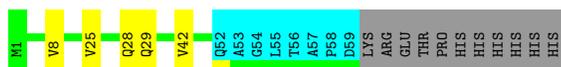● Molecule 1: Carbon storage regulator homolog

Chain F:

M1 R6 I12 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: RNA_(72-MER)

Chain G: 51%   31%   14%   •

U1 G2 U3 C4 C7 G8 A12 G13 A14 A18 G19 C20 C21 A22 U23 G27 C28 A29 C30 G31 A32 U33 A38 G39 G40 A41 C42 A43 U44 C45 G49 G50 A51 A52 G53 C54 U58 C59 C62 A63 G64 G65 A66 C67 G68 A72

4.2.18   Score per residue for model 18

• Molecule 1: Carbon storage regulator homolog

Chain A: 61%   6%   •   16%   16%

M1 L2 R6 I22 L23 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B: 77%   7%   16%

M1 R6 H43 E46 I51 Q52 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C: 70%   •   11%   16%

M1 L2 R6 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D: 66%   7%   11%   16%

M1 V8 V25 Q28 Q29 V42 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E: 61%   6%   17%   16%

M1 T5 R6 I32 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 66%   ••   16%   16%

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

• Molecule 2: RNA_(72-MER)

Chain G:

U1 G2 U3 C4 G5 A6 C7 G8 U11 A12 G13 A14 A18 G19 C20 G21 A22 U23 C24 G27 C28 A29 C30 C31 A32 U33 C37 A38 G39 G40 A41 C42 A43 U44 C47 A48 Q49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65 A66 C67 G68 A69 U70

G71 A72

4.2.19　Score per residue for model 19

• Molecule 1: Carbon storage regulator homolog
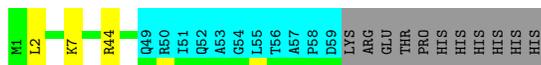
Chain A:

M1 L2 K7 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain B:

M1 R6 Q28 R31 K38 H43 R44 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C:

M1 L2 R6 Q29 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D:

M1 L2 I3 L4 T5 R6 I22 V42 H43 R44 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E:

M1 V42 E45 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F:

66%   ·   16%   16%

M1 T5 Q29 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 2: RNA_(72-MER)

Chain G:

39%   44%   11%   6%

U1 G2 U3 C4 G7 G8 G9 A10 U11 A12 G13 A14 A18 G19 C20 C21 A22 U23 G27 G28 A29 C30 G31 A32 U33 C37 A38 G39 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 C54 U57 U58 C59 A63 G64 G65 A66 C67 G68 A69 U70

G71 A72
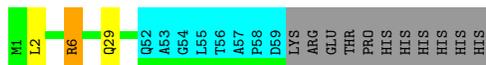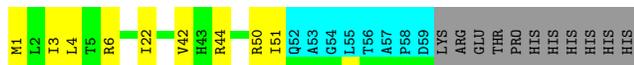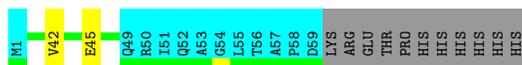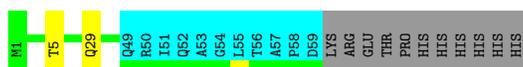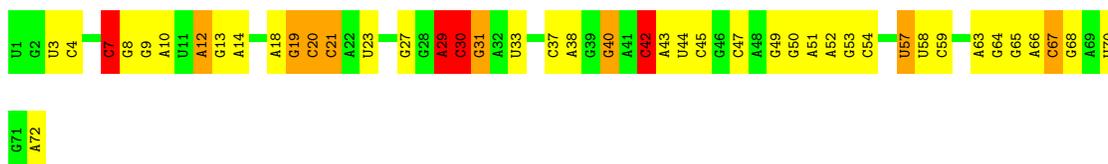
4.2.20   Score per residue for model 20

• Molecule 1: Carbon storage regulator homolog

Chain A:

64%   ·   16%   16%

M1 L2 R6 R44 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS
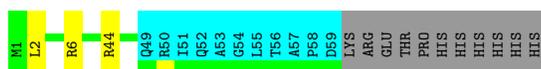
• Molecule 1: Carbon storage regulator homolog

Chain B:

70%   13%   ·   16%

M1 G15 D16 D17 Q28 I32 H43 R44 I51 Q52 A53 G54 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain C:

70%   ··   11%   16%

M1 L2 R44 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain D:

64%   9%   11%   16%

M1 L4 T5 R6 V42 H43 R44 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain E:

64%   ·   17%   16%

M1 T5 V42 Q49 R50 I51 Q52 A53 G54 L55 T56 A57 P58 D59 LYS ARG GLU THR PRO HIS HIS HIS HIS HIS HIS

• Molecule 1: Carbon storage regulator homolog

Chain F: 66% .. 16% 16%

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

• Molecule 2: RNA_(72-MER)

Chain G: 39% 39% 15% 7%

U1 G2 U3 C4 G5 A6 C7 G8 U11 A12 G13 A14 C17 A18 G19 C20 C21 A22 U23 C24 G27 G28 A29 C30 G31 A32 U33 U36 C37 G40 A41 C42 A43 U44 C45 G46 C47 A48 G49 G50 A51 A52 G53 U57 U58 C59 A63 G64 G65 A66 C67 G68

A72

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)	working_cs.cif
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)	5%

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	0.38±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	0±0/610 (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(^{o})	Ideal(^{o})	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	Models 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(^{o})	Ideal(^{o})	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	12	A	Sidechain	20
2	G	29	A	Sidechain	20
2	G	31	G	Sidechain	20
2	G	66	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	4	C	Sidechain	10
2	G	64	G	Sidechain	10
2	G	68	G	Sidechain	10
2	G	36	U	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	51	A	Sidechain	7
2	G	9	G	Sidechain	7
2	G	5	G	Sidechain	6
2	G	25	A	Sidechain	6
1	C	6	ARG	Sidechain	5
2	G	53	G	Sidechain	5
2	G	58	U	Sidechain	5
2	G	56	A	Sidechain	5
2	G	37	C	Sidechain	4
2	G	67	C	Sidechain	4
1	A	44	ARG	Sidechain	4
2	G	6	A	Sidechain	4
2	G	18	A	Sidechain	3
1	C	31	ARG	Sidechain	3
2	G	17	C	Sidechain	3
2	G	8	G	Sidechain	3
2	G	27	G	Sidechain	3
2	G	43	A	Sidechain	3
2	G	62	C	Sidechain	3
2	G	20	C	Sidechain	3
1	A	48	TYR	Sidechain	2
1	B	15	GLY	Mainchain	2
1	E	6	ARG	Sidechain	2
2	G	57	U	Sidechain	2
1	C	44	ARG	Sidechain	2
2	G	35	G	Sidechain	1
2	G	24	C	Sidechain	1
2	G	40	G	Sidechain	1
2	G	54	C	Sidechain	1
1	C	15	GLY	Mainchain	1
2	G	15	C	Sidechain	1
2	G	44	U	Sidechain	1
2	G	39	G	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	G	72	A	Sidechain	1
2	G	38	A	Sidechain	1
2	G	61	U	Sidechain	1
1	E	31	ARG	Sidechain	1
2	G	41	A	Sidechain	1
2	G	45	C	Sidechain	1

6.2   Too-close contacts   ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	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:HD12	1:D:51:ILE:N	0.57	2.15	10	5
1:D:51:ILE:HD12	1:D:51:ILE:H	0.56	1.61	8	3
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
1:C:6:ARG:HE	1:C:22:ILE:CG2	0.46	2.24	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:B:56:THR:HG22	1:B:57:ALA:H	0.46	1.70	1	1
2:G:27:G:H2'	2:G:27:G:N3	0.45	2.27	5	1
1:C:23:LEU:HD13	2:G:67:C:H1'	0.45	1.88	3	2
1:C:48:TYR:HA	1:C:51:ILE:HD13	0.45	1.88	2	2
1:C:44:ARG:HH21	1:D:4:LEU:HD22	0.45	1.72	20	1
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:N	1:D:51:ILE:CD1	0.44	2.81	20	3
2:G:12:A:C8	2:G:12:A:H5"	0.43	2.49	20	2
1:D:8:VAL:HG11	1:D:25:VAL:CG1	0.43	2.41	17	2
1:D:51:ILE:H	1:D:51:ILE:CD1	0.43	2.25	8	1
1:C:23:LEU:HD12	1:C:31:ARG:HG2	0.42	1.91	10	2
1:F:6:ARG:HD2	1:F:12:ILE:HD11	0.42	1.90	17	1
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
2:G:12:A:H5"	2:G:12:A:C8	0.40	2.51	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%)	54	85
1	B	57/70 (81%)	52±1 (90±2%)	4±1 (8±2%)	1±1 (2±1%)	12	54
1	C	50/70 (71%)	50±1 (100±1%)	0±0 (0±1%)	0±0 (0±1%)	50	82
1	D	50/70 (71%)	49±1 (97±2%)	1±1 (3±2%)	0±0 (0±0%)	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5960/8400 (71%)	5645 (95%)	291 (5%)	24 (0%)	38	78

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	C	15	GLY	1
1	C	16	ASP	1
1	B	58	PRO	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%)	17	65
1	B	49/60 (82%)	45±1 (92±3%)	4±1 (8±3%)	15	62
1	C	44/60 (73%)	42±1 (96±2%)	2±1 (4±2%)	33	81
1	D	44/60 (73%)	41±1 (94±2%)	3±1 (6±2%)	22	71
1	E	40/60 (67%)	38±1 (94±3%)	2±1 (6±3%)	22	71
1	F	41/60 (68%)	39±1 (95±3%)	2±1 (5±3%)	28	77
All	All	5180/7200 (72%)	4855 (94%)	325 (6%)	21	70

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
1	C	2	LEU	20
1	D	42	VAL	19
1	E	42	VAL	19

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Mol	Chain	Res	Type	Models (Total)
1	F	5	THR	16
1	A	44	ARG	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	D	6	ARG	8
1	A	6	ARG	8
1	C	29	GLN	7
1	F	29	GLN	6
1	E	6	ARG	6
1	C	6	ARG	6
1	B	38	LYS	5
1	D	4	LEU	5
1	D	50	ARG	5
1	E	45	GLU	5
1	A	22	ILE	4
1	B	25	VAL	4
1	A	7	LYS	3
1	B	52	GLN	3
1	B	6	ARG	3
1	D	29	GLN	3
1	F	45	GLU	3
1	E	2	LEU	3
1	C	28	GLN	2
1	D	22	ILE	2
1	C	44	ARG	2
1	B	39	ASP	2
1	F	39	ASP	2
1	B	46	GLU	2
1	E	32	ILE	2
1	A	47	ILE	2
1	F	13	ASN	1
1	B	22	ILE	1
1	B	44	ARG	1
1	C	22	ILE	1
1	F	10	GLU	1
1	F	38	LYS	1
1	B	42	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	D	1	MET	1
1	E	29	GLN	1
1	E	4	LEU	1
1	D	28	GLN	1

6.3.3   RNA (i)

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	8	G	20
2	G	12	A	20
2	G	19	G	20
2	G	27	G	20
2	G	30	C	20
2	G	40	G	20
2	G	42	C	20
2	G	52	A	20
2	G	53	G	20
2	G	65	G	20
2	G	67	C	20
2	G	68	G	20
2	G	50	G	19
2	G	7	C	18
2	G	13	G	18
2	G	44	U	18
2	G	43	A	17
2	G	59	C	17
2	G	31	G	16
2	G	57	U	14
2	G	58	U	13
2	G	5	G	12
2	G	38	A	11
2	G	49	G	11
2	G	6	A	9
2	G	48	A	8

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Mol	Chain	Res	Type	Models (Total)
2	G	63	A	8
2	G	72	A	8
2	G	18	A	7
2	G	64	G	7
2	G	20	C	5
2	G	11	U	5
2	G	29	A	5
2	G	37	C	4
2	G	17	C	3
2	G	35	G	1
2	G	36	U	1
2	G	51	A	1
2	G	9	G	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	12	A	7
2	G	63	A	7
2	G	19	G	5
2	G	38	A	4
2	G	30	C	4
2	G	18	A	3
2	G	42	C	3
2	G	57	U	2
2	G	4	C	2
2	G	35	G	1
2	G	17	C	1
2	G	52	A	1
2	G	58	U	1
2	G	37	C	1
2	G	47	C	1
2	G	21	C	1
2	G	43	A	1
2	G	7	C	1

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 5% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping ⓘ

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

Total number of shifts	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)	0

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 5%, i.e. 274 atoms were assigned a chemical shift out of a possible 5624. 0 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/1537 (0%)	0/632 (0%)	0/608 (0%)	0/297 (0%)
Sidechain	0/2623 (0%)	0/1718 (0%)	0/802 (0%)	0/103 (0%)
Aromatic	0/96 (0%)	0/48 (0%)	0/42 (0%)	0/6 (0%)
Sugar	84/792 (11%)	42/432 (10%)	42/360 (12%)	0/0 (—%)
Base	190/576 (33%)	95/360 (26%)	75/122 (61%)	20/94 (21%)
Overall	274/5624 (5%)	137/3190 (4%)	117/1934 (6%)	20/500 (4%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 4%, i.e. 274 atoms were assigned a chemical shift out of a possible 6252. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/1782 (0%)	0/732 (0%)	0/708 (0%)	0/342 (0%)
Sidechain	0/3006 (0%)	0/1968 (0%)	0/918 (0%)	0/120 (0%)
Aromatic	0/96 (0%)	0/48 (0%)	0/42 (0%)	0/6 (0%)
Sugar	84/792 (11%)	42/432 (10%)	42/360 (12%)	0/0 (—%)
Base	190/576 (33%)	95/360 (26%)	75/122 (61%)	20/94 (21%)
Overall	274/6252 (4%)	137/3540 (4%)	117/2150 (5%)	20/562 (4%)

7.1.4   Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5   Random Coil Index (RCI) plots ⓘ

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

7.2   Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1   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	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 ⓘ

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

7.2.3   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 0%, i.e. 12 atoms were assigned a chemical shift out of a possible 5624. 0 out of 49 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/1537 (0%)	0/632 (0%)	0/608 (0%)	0/297 (0%)
Sidechain	0/2623 (0%)	0/1718 (0%)	0/802 (0%)	0/103 (0%)
Aromatic	0/96 (0%)	0/48 (0%)	0/42 (0%)	0/6 (0%)
Sugar	4/792 (1%)	2/432 (0%)	2/360 (1%)	0/0 (—%)
Base	8/576 (1%)	4/360 (1%)	3/122 (2%)	1/94 (1%)
Overall	12/5624 (0%)	6/3190 (0%)	5/1934 (0%)	1/500 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 12 atoms were assigned a chemical shift out of a possible 6252. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/1782 (0%)	0/732 (0%)	0/708 (0%)	0/342 (0%)
Sidechain	0/3006 (0%)	0/1968 (0%)	0/918 (0%)	0/120 (0%)
Aromatic	0/96 (0%)	0/48 (0%)	0/42 (0%)	0/6 (0%)
Sugar	4/792 (1%)	2/432 (0%)	2/360 (1%)	0/0 (—%)
Base	8/576 (1%)	4/360 (1%)	3/122 (2%)	1/94 (1%)
Overall	12/6252 (0%)	6/3540 (0%)	5/2150 (0%)	1/562 (0%)

7.2.4   Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.2.5   Random Coil Index (RCI) plots ⓘ

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