



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 10:34 AM UTC

PDB ID : 7BL4 / pdb_00007bl4
EMDB ID : EMD-12217
Title : in vitro reconstituted 50S-ObgE-GMPPNP-RsfS particle
Authors : Hilal, T.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2021-01-18
Resolution : 2.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

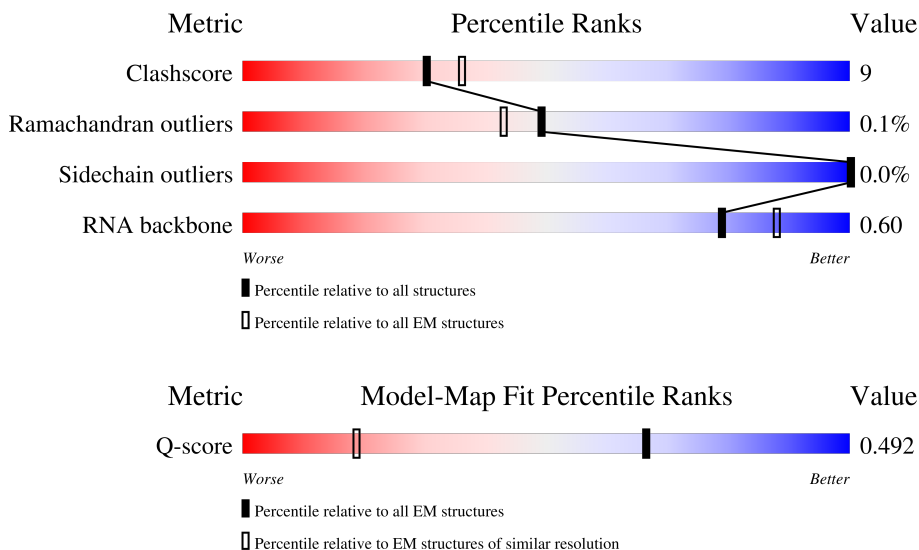
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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.



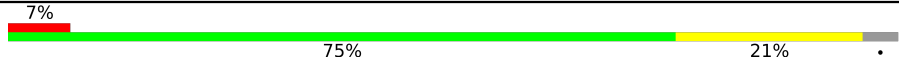

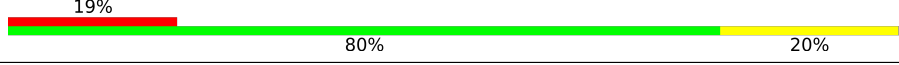

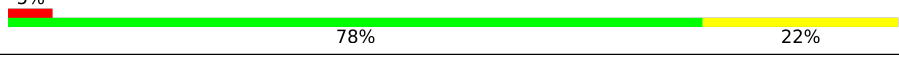
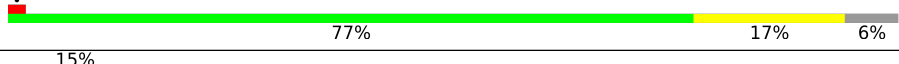
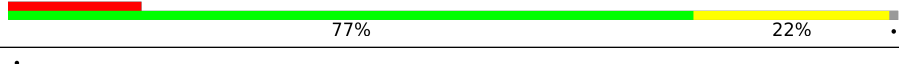

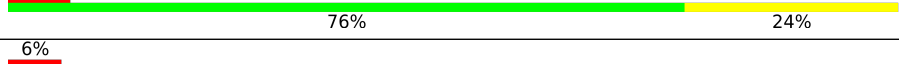


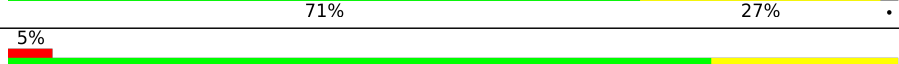
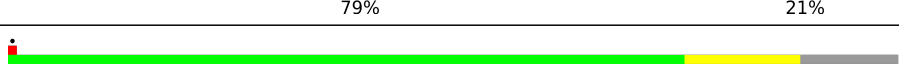
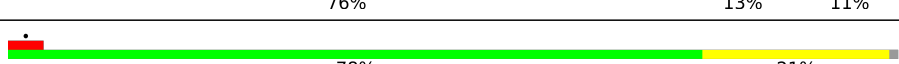

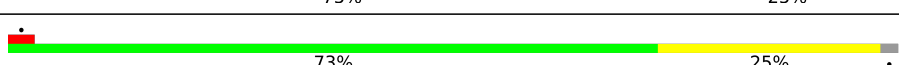
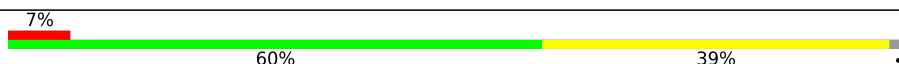
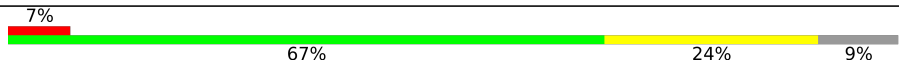
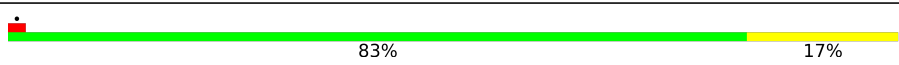


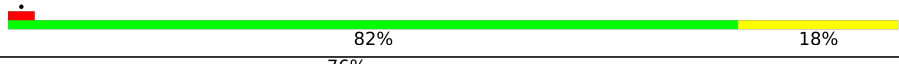
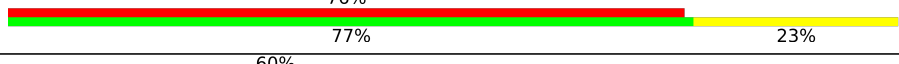


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	g	38	8% (red), 71% (green), 29% (yellow)
2	C	273	73% (green), 26% (yellow), 1% (grey)
3	D	209	6% (red), 78% (green), 22% (yellow)

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Mol	Chain	Length	Quality of chain
4	E	201	
5	F	179	
6	G	177	
7	J	142	
8	L	144	
9	N	127	
10	O	117	
11	Q	118	
12	R	103	
13	S	110	
14	T	100	
15	U	104	
16	V	94	
17	W	85	
18	X	78	
19	Y	63	
20	Z	59	
21	0	57	
22	1	55	
23	2	46	
24	K	123	
25	P	115	
26	M	136	
27	H	149	
28	d	70	

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Mol	Chain	Length	Quality of chain
29	A	2904	<p>5% 56% 40% .</p>
30	B	119	<p>1% 58% 40% .</p>
31	6	105	<p>9% 70% 27% .</p>
32	9	390	<p>12% 65% 22% 13% .</p>
33	3	65	<p>1% 71% 25% . .</p>

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 93560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	g	38	302	185	65	48	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	271	2082	1288	423	364	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	209	1565	979	288	294	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	193	1483	932	266	280	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	177	1410	899	249	256	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	176	1323	832	243	246	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	142	1129	714	212	199	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	144	1053	654	207	190	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	N	120	960	593	196	166	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	O	116	892	552	178	162	0	0

- Molecule 11 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	Q	117	947	604	192	151	0	0

- Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	103	816	516	153	145	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	110	857	532	166	156	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	93	738	466	139	131	2	0	0

- Molecule 15 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	U	102	779	492	146	141		0	0

- Molecule 16 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	94	753	479	137	134	3	0	0

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	76	577	357	117	102	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	77	625	388	129	106	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Y	63	509	313	99	95	2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Z	58	449	281	87	79	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 26 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 27 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 31 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 32 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

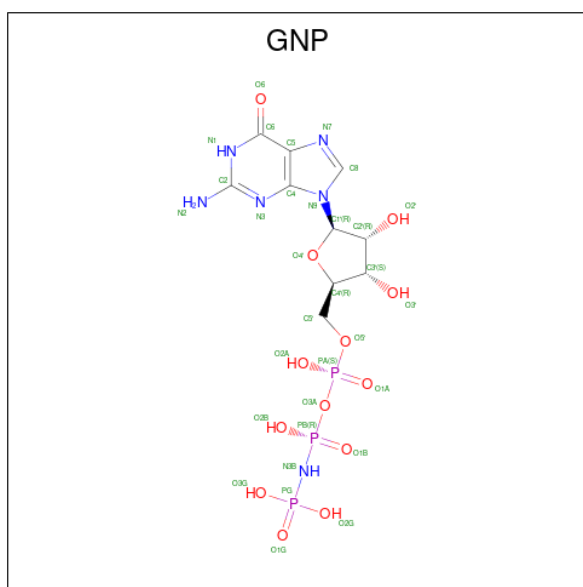
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Zn	0
			1	1	
34	d	1	Total	Zn	0
			1	1	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	A	3	Total Mg 3 3	0
35	6	2	Total Mg 2 2	0
35	9	1	Total Mg 1 1	0

- Molecule 36 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
36	9	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	AltConf
37	C	2	Total O 2 2	0
37	F	1	Total O 1 1	0
37	L	1	Total O 1 1	0
37	N	3	Total O 3 3	0
37	S	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
37	A	18	Total 18	O 18	0
37	B	1	Total 1	O 1	0
37	6	3	Total 3	O 3	0
37	9	5	Total 5	O 5	0

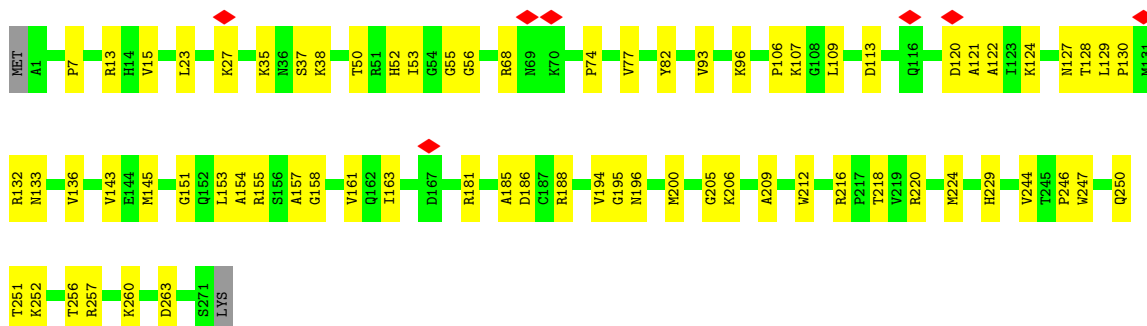
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

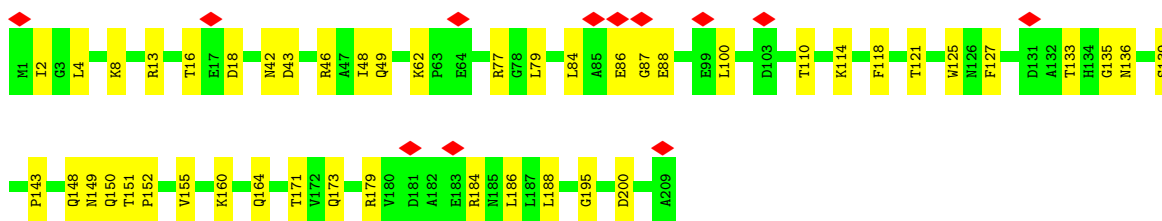
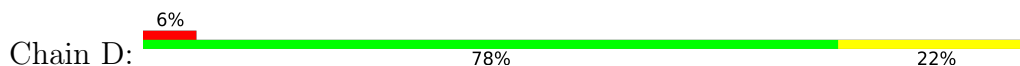
- Molecule 1: 50S ribosomal protein L36



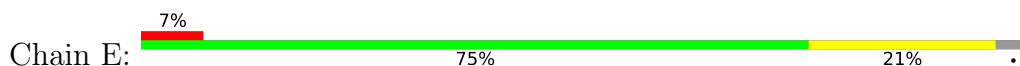
- Molecule 2: 50S ribosomal protein L2

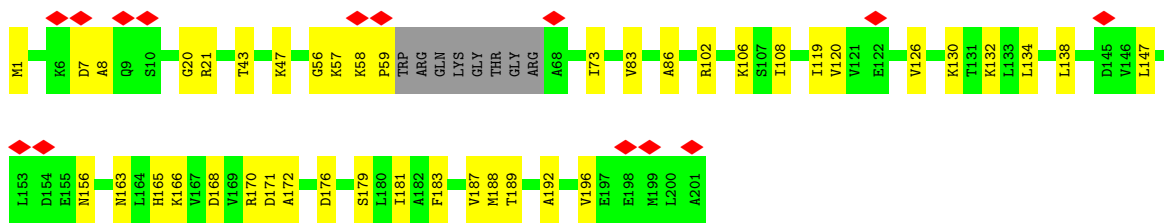


- Molecule 3: 50S ribosomal protein L3

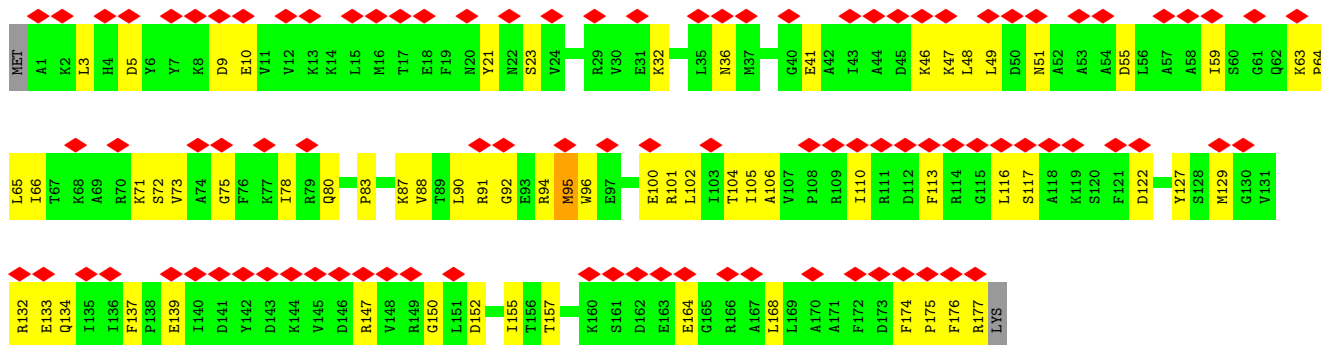


- Molecule 4: 50S ribosomal protein L4

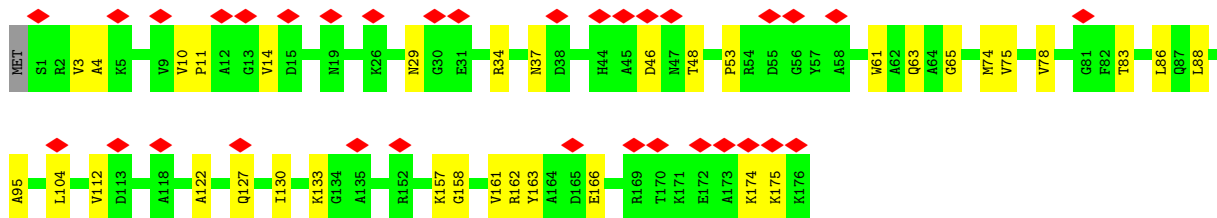
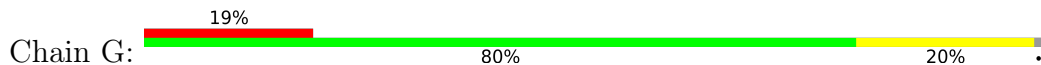




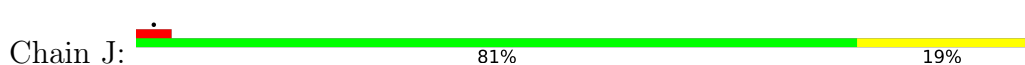
• Molecule 5: 50S ribosomal protein L5



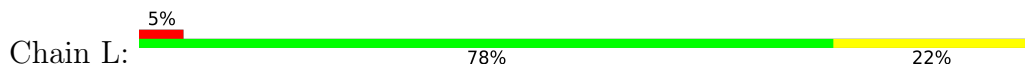
• Molecule 6: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L13



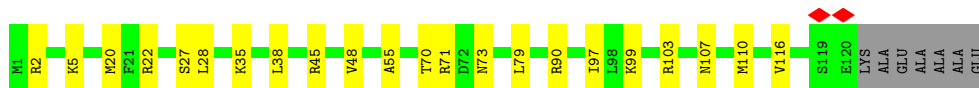
• Molecule 8: 50S ribosomal protein L15





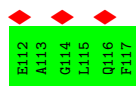
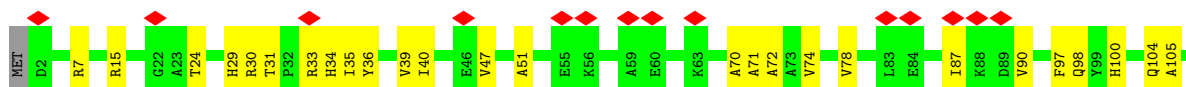
- Molecule 9: 50S ribosomal protein L17

Chain N: 77% 17% 6%



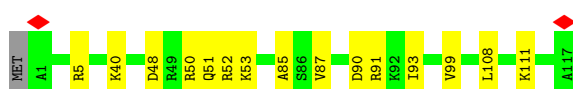
- Molecule 10: 50S ribosomal protein L18

Chain O: 15% 77% 22%



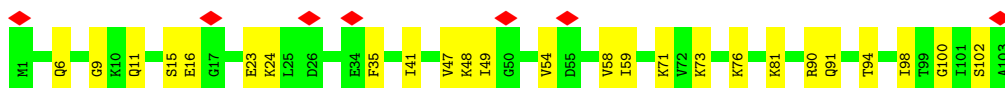
- Molecule 11: 50S ribosomal protein L20

Chain Q: 86% 13%



- Molecule 12: 50S ribosomal protein L21

Chain R: 7% 76% 24%



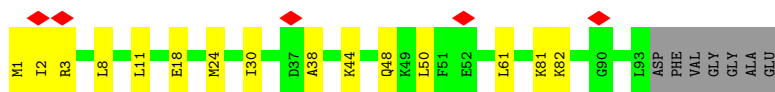
- Molecule 13: 50S ribosomal protein L22

Chain S: 6% 71% 29%



- Molecule 14: 50S ribosomal protein L23

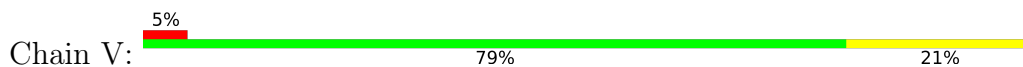
Chain T: 5% 78% 15% 7%



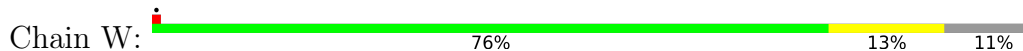
- Molecule 15: 50S ribosomal protein L24



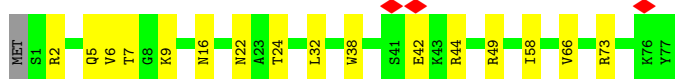
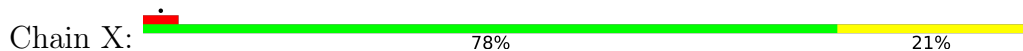
- Molecule 16: 50S ribosomal protein L25



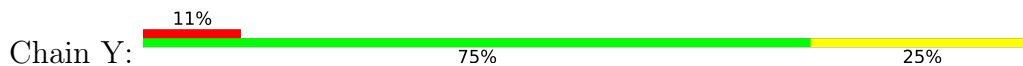
- Molecule 17: 50S ribosomal protein L27



- Molecule 18: 50S ribosomal protein L28



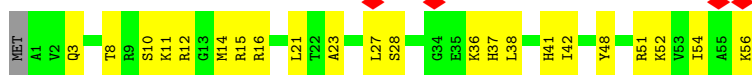
- Molecule 19: 50S ribosomal protein L29



- Molecule 20: 50S ribosomal protein L30



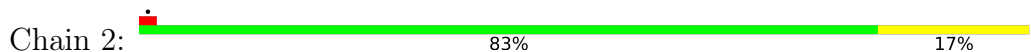
- Molecule 21: 50S ribosomal protein L32



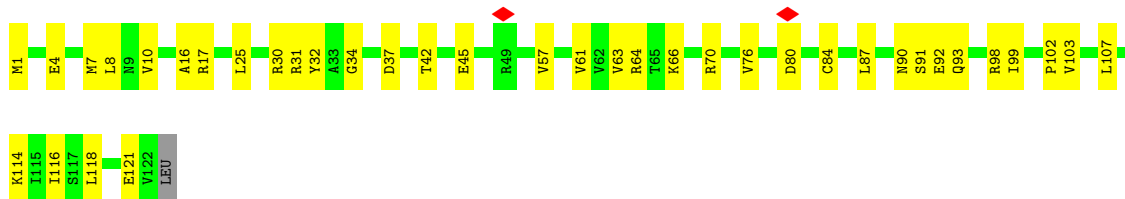
- Molecule 22: 50S ribosomal protein L33



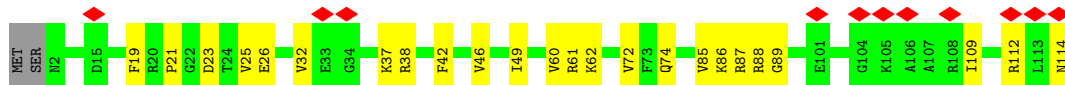
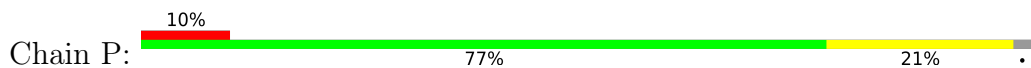
- Molecule 23: 50S ribosomal protein L34



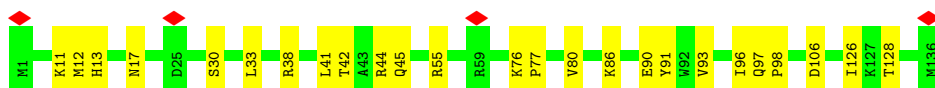
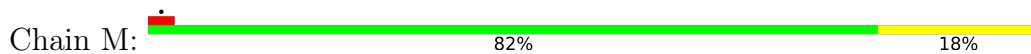
- Molecule 24: 50S ribosomal protein L14



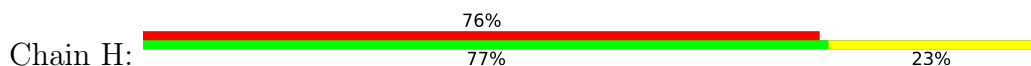
- Molecule 25: 50S ribosomal protein L19

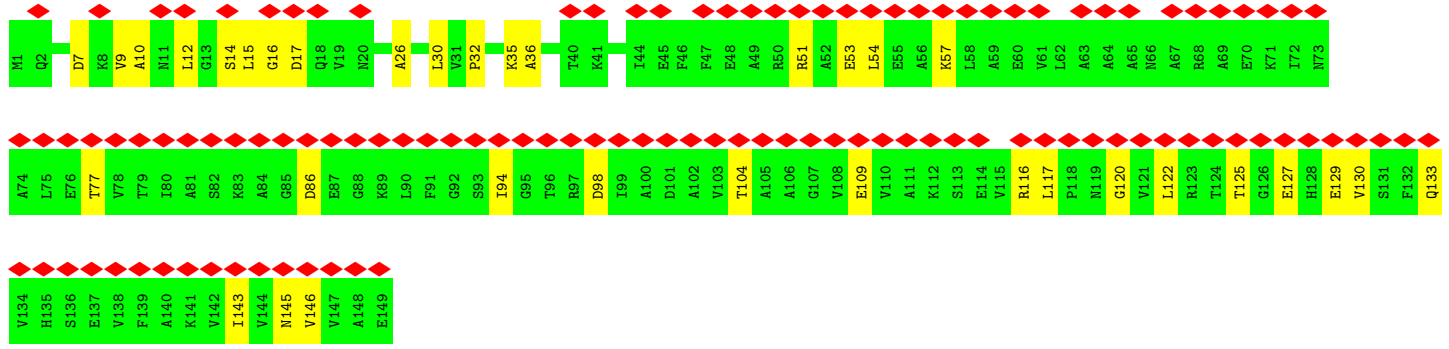


- Molecule 26: 50S ribosomal protein L16



- Molecule 27: 50S ribosomal protein L9

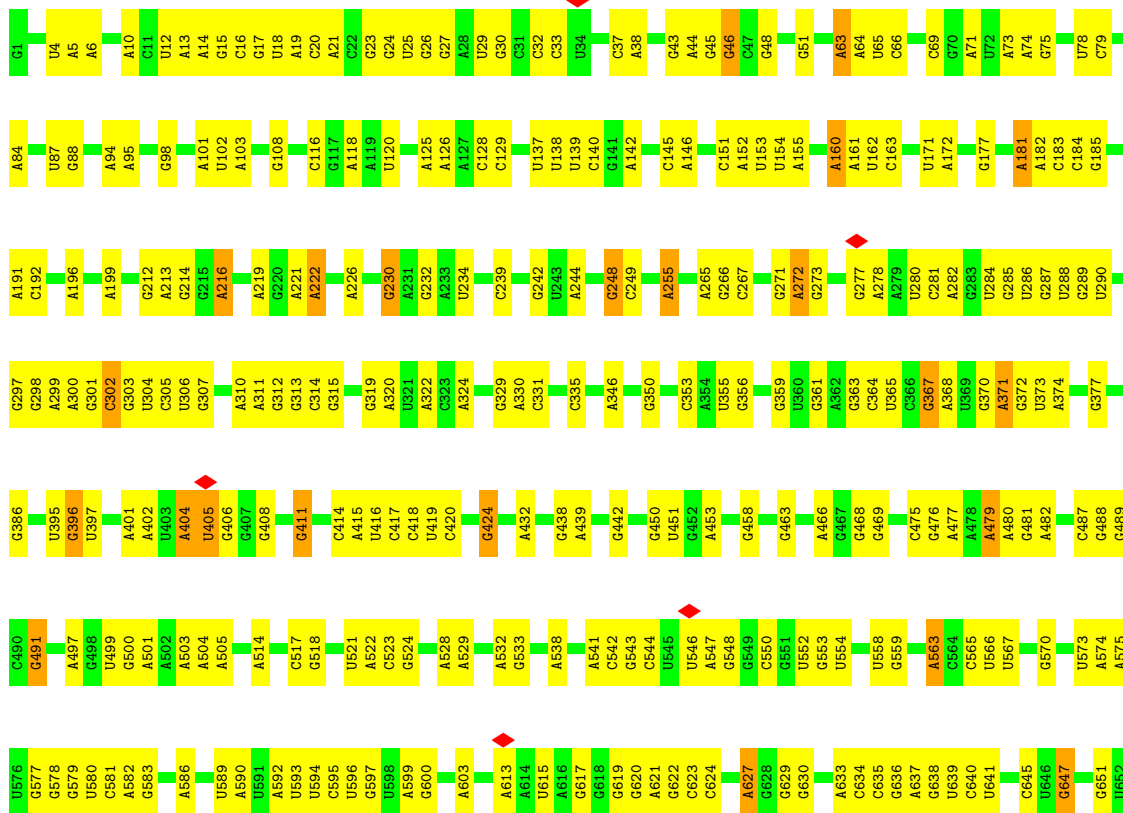


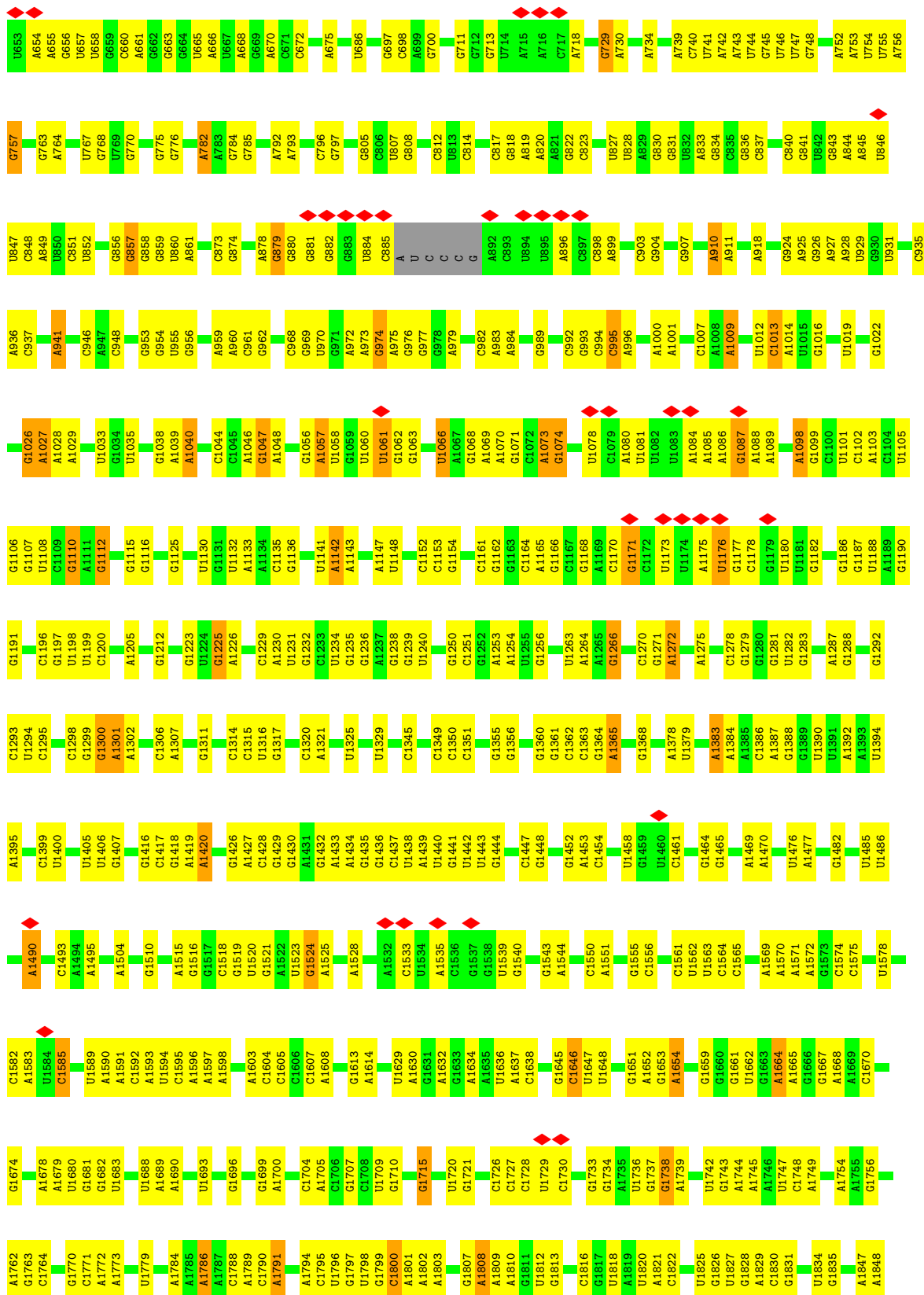


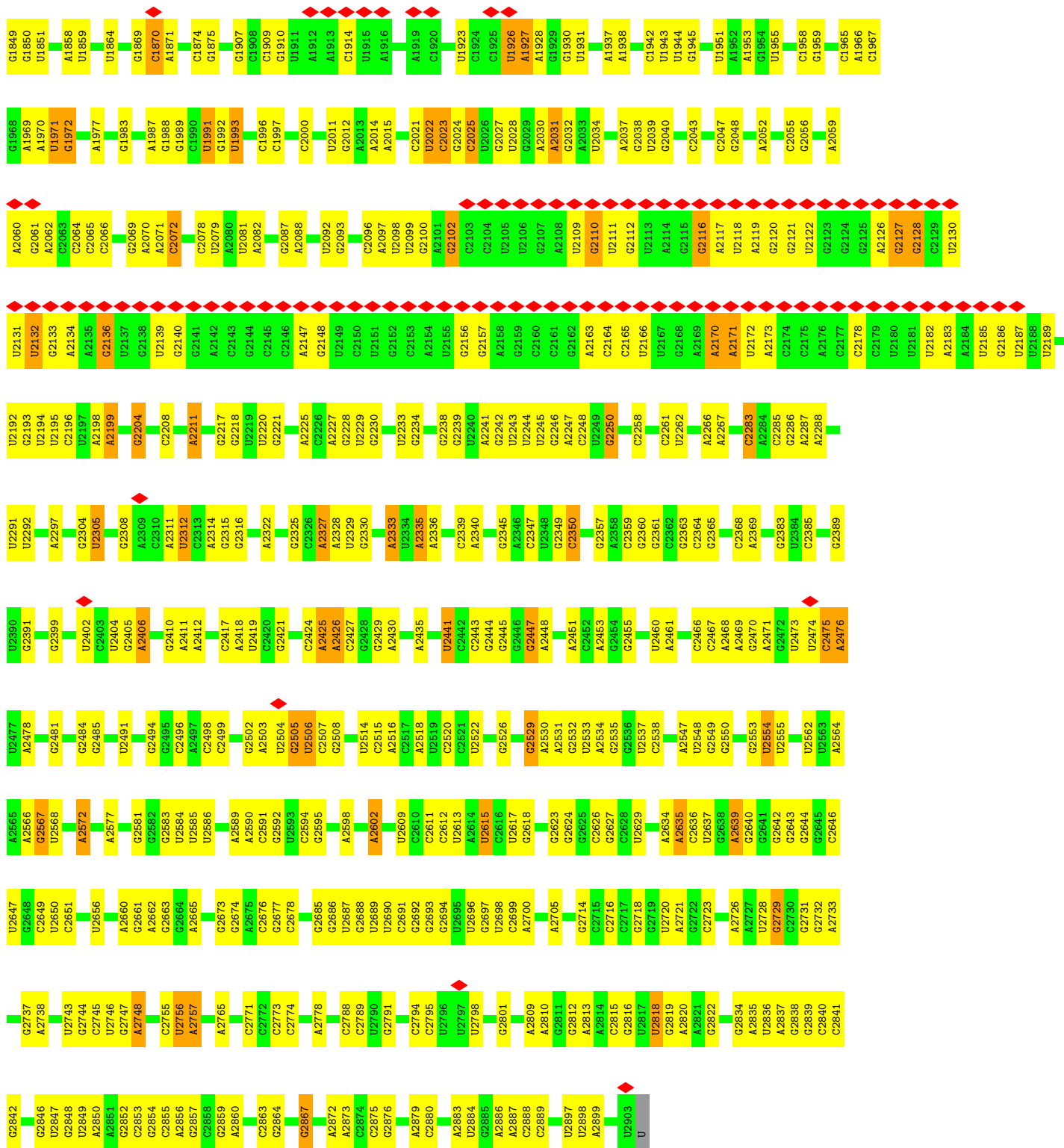
• Molecule 28: 50S ribosomal protein L31



• Molecule 29: 23S ribosomal RNA

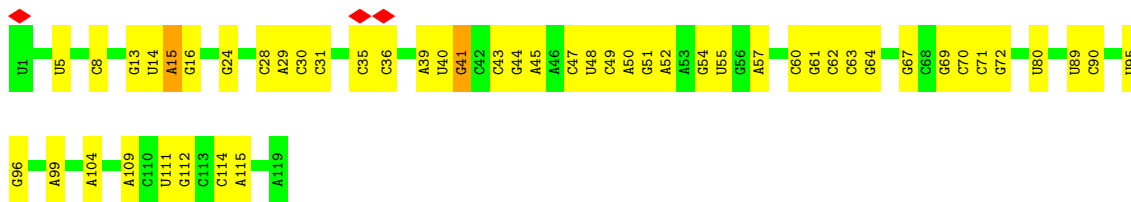




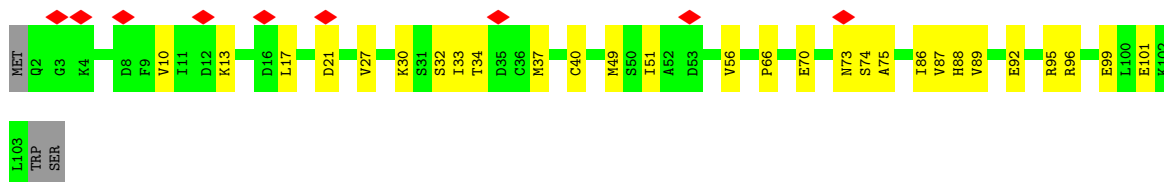


• Molecule 30: 5S ribosomal RNA

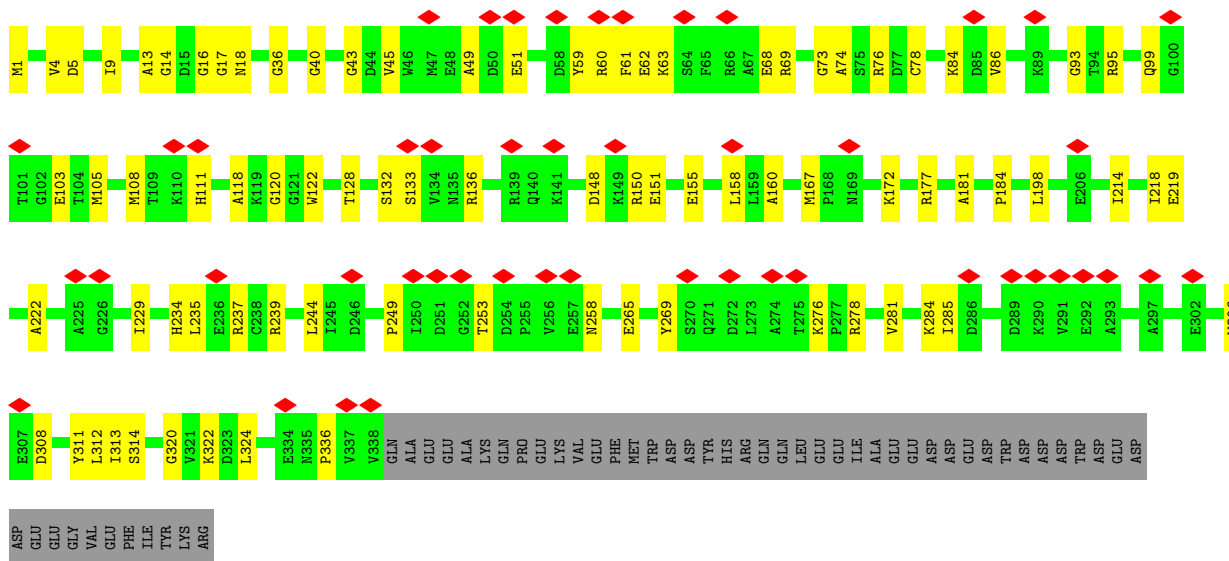




• Molecule 31: Ribosomal silencing factor RsfS



• Molecule 32: GTPase ObgE/CgtA



• Molecule 33: 50S ribosomal protein L35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	190393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	Not provided	
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	22.582	Depositor
Minimum map value	-9.349	Depositor
Average map value	-0.044	Depositor
Map value standard deviation	0.814	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	363.6, 363.6, 363.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.01, 1.01, 1.01	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GNP, MG

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 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	g	0.14	0/303	0.34	0/397
2	C	0.12	0/2121	0.34	0/2852
3	D	0.12	0/1586	0.32	0/2134
4	E	0.11	0/1499	0.34	0/2016
5	F	0.14	0/1434	0.46	3/1926 (0.2%)
6	G	0.11	0/1343	0.32	0/1816
7	J	0.12	0/1152	0.32	0/1551
8	L	0.12	0/1062	0.37	0/1413
9	N	0.12	0/973	0.38	0/1301
10	O	0.12	0/902	0.35	0/1209
11	Q	0.12	0/960	0.36	0/1278
12	R	0.12	0/829	0.37	0/1107
13	S	0.12	0/864	0.33	0/1156
14	T	0.13	0/744	0.37	0/994
15	U	0.15	0/787	0.40	0/1051
16	V	0.11	0/766	0.32	0/1025
17	W	0.11	0/584	0.29	0/772
18	X	0.13	0/635	0.32	0/848
19	Y	0.12	0/510	0.36	0/677
20	Z	0.12	0/453	0.35	0/605
21	0	0.13	0/450	0.36	0/599
22	1	0.12	0/416	0.32	0/554
23	2	0.12	0/380	0.36	0/498
24	K	0.14	0/947	0.34	0/1268
25	P	0.11	0/923	0.32	0/1234
26	M	0.13	0/1093	0.33	0/1460
27	H	0.13	0/1121	0.34	0/1515
28	d	0.08	0/371	0.25	0/496
29	A	0.09	0/69659	0.20	0/108672
30	B	0.07	0/2847	0.15	0/4440
31	6	0.11	0/787	0.29	0/1062
32	9	0.13	0/2626	0.36	0/3542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	3	0.13	0/513	0.46	0/676
All	All	0.10	0/101640	0.25	3/152144 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	175	PRO	CA-C-N	5.85	132.71	121.54
5	F	175	PRO	C-N-CA	5.85	132.71	121.54
5	F	95	MET	CA-CB-CG	5.28	124.65	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	302	0	340	7	0
2	C	2082	0	2157	56	0
3	D	1565	0	1616	35	0
4	E	1483	0	1548	28	0
5	F	1410	0	1447	53	0
6	G	1323	0	1374	22	0
7	J	1129	0	1162	24	0
8	L	1053	0	1129	27	0
9	N	960	0	1000	19	0
10	O	892	0	923	16	0
11	Q	947	0	1022	18	0
12	R	816	0	839	18	0
13	S	857	0	922	23	0
14	T	738	0	807	10	0
15	U	779	0	834	26	0
16	V	753	0	780	12	0
17	W	577	0	594	9	0
18	X	625	0	655	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	509	0	543	12	0
20	Z	449	0	491	11	0
21	0	444	0	461	17	0
22	1	409	0	440	9	0
23	2	377	0	418	6	0
24	K	938	0	1012	30	0
25	P	911	0	957	18	0
26	M	1074	0	1157	18	0
27	H	1110	0	1148	22	0
28	d	364	0	364	7	0
29	A	62195	0	31280	850	0
30	B	2548	0	1292	35	0
31	6	780	0	783	20	0
32	9	2582	0	2606	65	0
33	3	504	0	574	17	0
34	d	1	0	0	0	0
34	g	1	0	0	0	0
35	6	2	0	0	0	0
35	9	1	0	0	0	0
35	A	3	0	0	0	0
36	9	32	0	13	1	0
37	6	3	0	0	0	0
37	9	5	0	0	0	0
37	A	18	0	0	2	0
37	B	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	L	1	0	0	0	0
37	N	3	0	0	0	0
37	S	1	0	0	0	0
All	All	93560	0	62688	1371	0

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 9.

The worst 5 of 1371 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1040:A:N6	29:A:1115:G:H1	1.68	0.89
29:A:285:G:H1	29:A:355:U:H3	1.19	0.89
29:A:1040:A:H61	29:A:1115:G:H1	0.93	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:1171:G:N1	29:A:1178:C:N3	2.27	0.81
4:E:56:GLY:HA2	4:E:73:ILE:HG12	1.65	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	g	36/38 (95%)	36 (100%)	0	0	100	100
2	C	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
3	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
4	E	189/201 (94%)	185 (98%)	4 (2%)	0	100	100
5	F	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
6	G	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
8	L	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
9	N	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
10	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
11	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
12	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
13	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
14	T	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
15	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
16	V	92/94 (98%)	92 (100%)	0	0	100	100
17	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
18	X	75/78 (96%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
20	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
21	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
22	1	48/55 (87%)	48 (100%)	0	0	100	100
23	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
24	K	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
25	P	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
26	M	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
27	H	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
28	d	45/70 (64%)	44 (98%)	1 (2%)	0	100	100
31	6	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
32	9	336/390 (86%)	319 (95%)	17 (5%)	0	100	100
33	3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	3
All	All	3638/3832 (95%)	3452 (95%)	184 (5%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	3	31	ILE
33	3	32	LEU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	g	34/34 (100%)	34 (100%)	0	100	100
2	C	216/218 (99%)	216 (100%)	0	100	100
3	D	164/164 (100%)	164 (100%)	0	100	100
4	E	159/165 (96%)	159 (100%)	0	100	100
5	F	148/150 (99%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	137/138 (99%)	137 (100%)	0	100	100
7	J	116/116 (100%)	116 (100%)	0	100	100
8	L	103/103 (100%)	103 (100%)	0	100	100
9	N	100/103 (97%)	100 (100%)	0	100	100
10	O	86/87 (99%)	86 (100%)	0	100	100
11	Q	89/90 (99%)	89 (100%)	0	100	100
12	R	84/84 (100%)	84 (100%)	0	100	100
13	S	93/93 (100%)	93 (100%)	0	100	100
14	T	80/84 (95%)	80 (100%)	0	100	100
15	U	83/85 (98%)	83 (100%)	0	100	100
16	V	78/78 (100%)	77 (99%)	1 (1%)	61	80
17	W	57/63 (90%)	57 (100%)	0	100	100
18	X	67/68 (98%)	67 (100%)	0	100	100
19	Y	55/55 (100%)	55 (100%)	0	100	100
20	Z	48/49 (98%)	48 (100%)	0	100	100
21	0	47/48 (98%)	47 (100%)	0	100	100
22	1	45/49 (92%)	45 (100%)	0	100	100
23	2	38/38 (100%)	38 (100%)	0	100	100
24	K	103/104 (99%)	103 (100%)	0	100	100
25	P	98/100 (98%)	98 (100%)	0	100	100
26	M	109/109 (100%)	109 (100%)	0	100	100
27	H	114/114 (100%)	114 (100%)	0	100	100
28	d	43/62 (69%)	43 (100%)	0	100	100
31	6	88/91 (97%)	88 (100%)	0	100	100
32	9	273/321 (85%)	273 (100%)	0	100	100
33	3	51/52 (98%)	51 (100%)	0	100	100
All	All	3006/3115 (96%)	3005 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
12	R	11	GLN
19	Y	25	GLN
19	Y	20	ASN
19	Y	27	ASN
5	F	126	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	A	2895/2904 (99%)	377 (13%)	9 (0%)
30	B	118/119 (99%)	11 (9%)	0
All	All	3013/3023 (99%)	388 (12%)	9 (0%)

5 of 388 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	A	10	A
29	A	12	U
29	A	14	A
29	A	27	G
29	A	46	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	A	2505	G
29	A	2756	U
29	A	1057	A
29	A	1378	A
29	A	2127	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	GNP	9	402	35	34,34,34	1.28	5 (14%)	47,54,54	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GNP	9	402	35	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	402	GNP	PB-O3A	4.39	1.64	1.59
36	9	402	GNP	PB-O1B	3.12	1.50	1.46
36	9	402	GNP	PG-N3B	2.90	1.70	1.63
36	9	402	GNP	PG-O1G	2.72	1.50	1.46
36	9	402	GNP	PB-O2B	-2.30	1.50	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

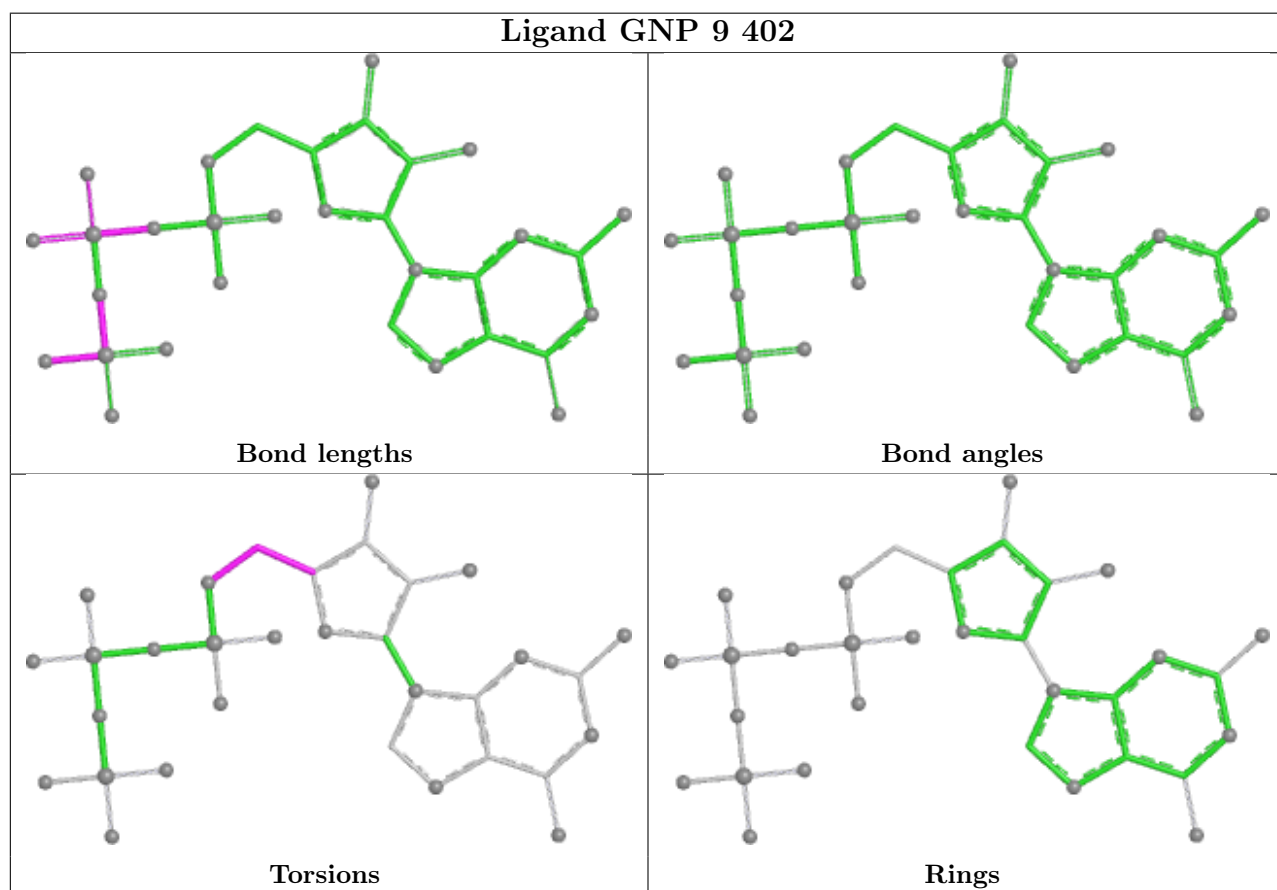
Mol	Chain	Res	Type	Atoms
36	9	402	GNP	O4'-C4'-C5'-O5'
36	9	402	GNP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	9	402	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

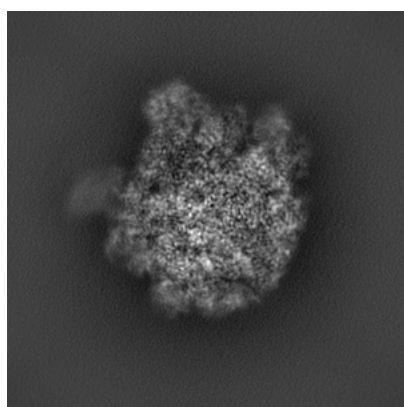
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12217. These allow visual inspection of the internal detail of the map and identification of artifacts.

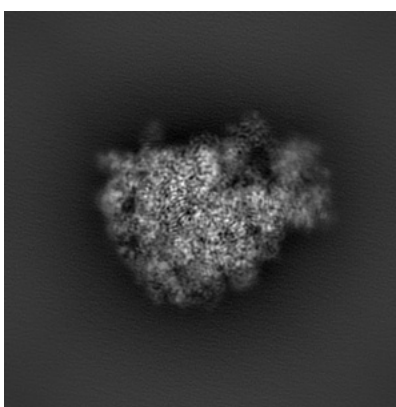
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

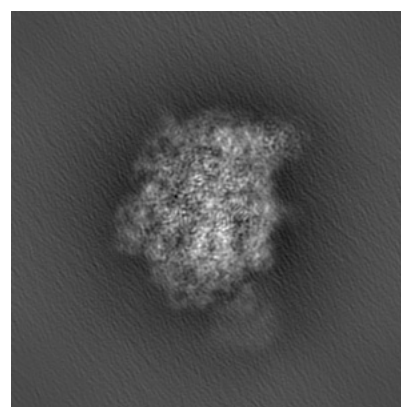
6.1.1 Primary map



X



Y

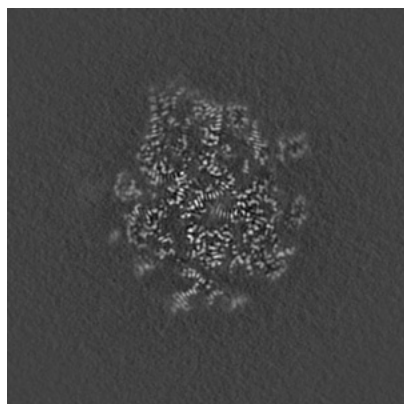


Z

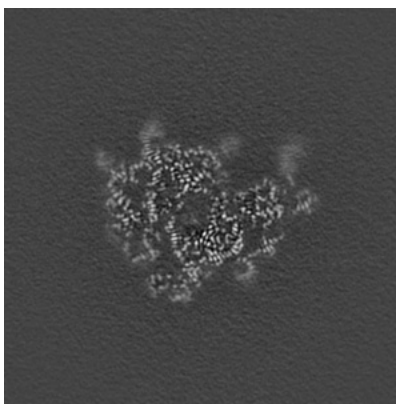
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

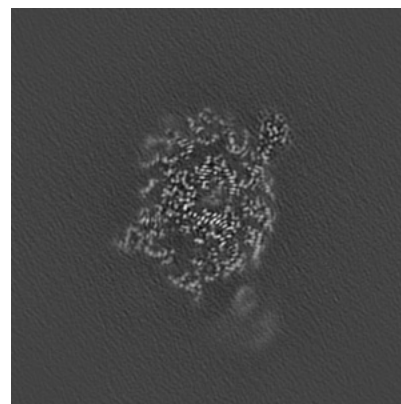
6.2.1 Primary map



X Index: 180



Y Index: 180

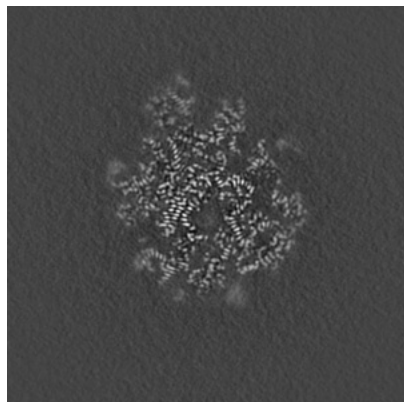


Z Index: 180

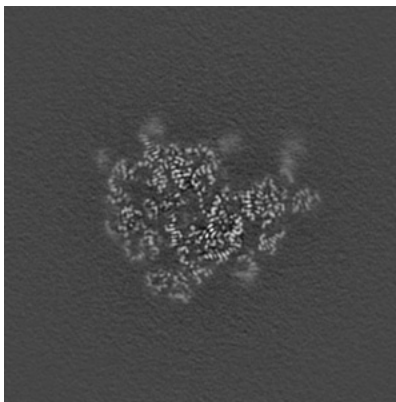
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

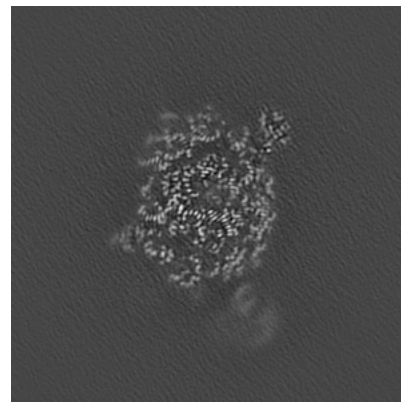
6.3.1 Primary map



X Index: 170



Y Index: 178

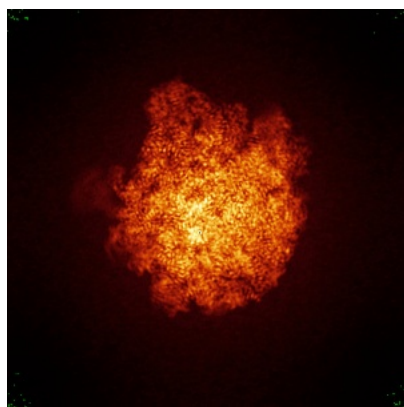


Z Index: 182

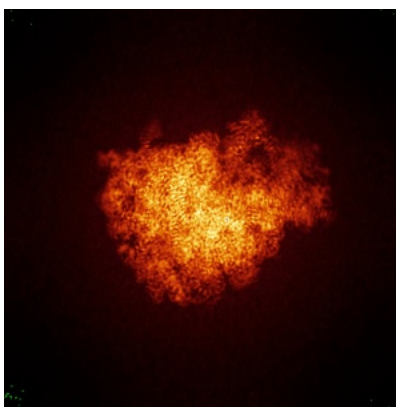
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

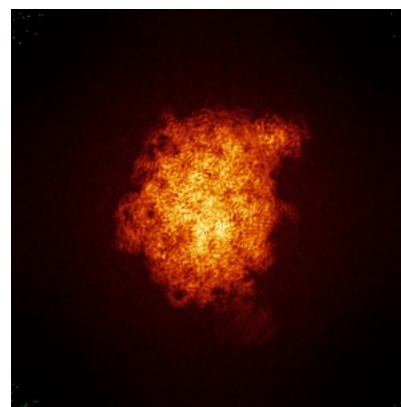
6.4.1 Primary map



X



Y

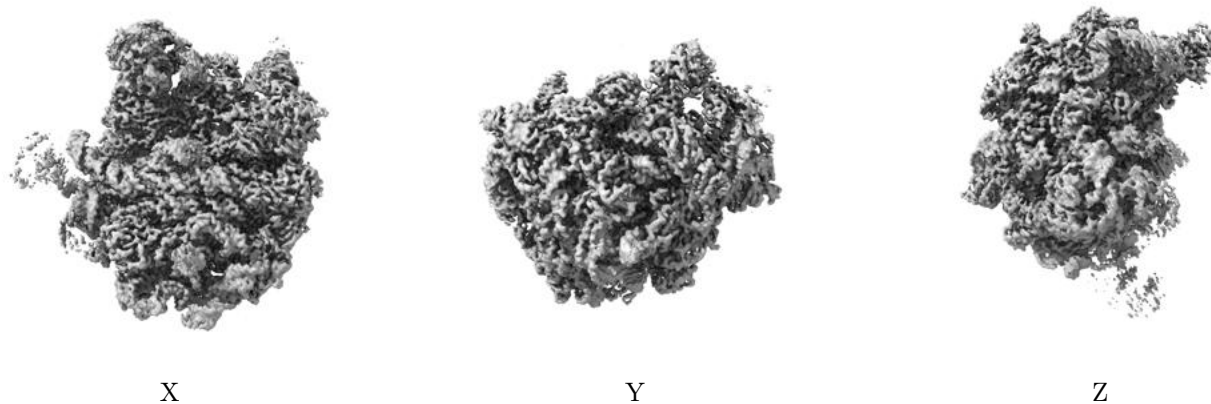


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

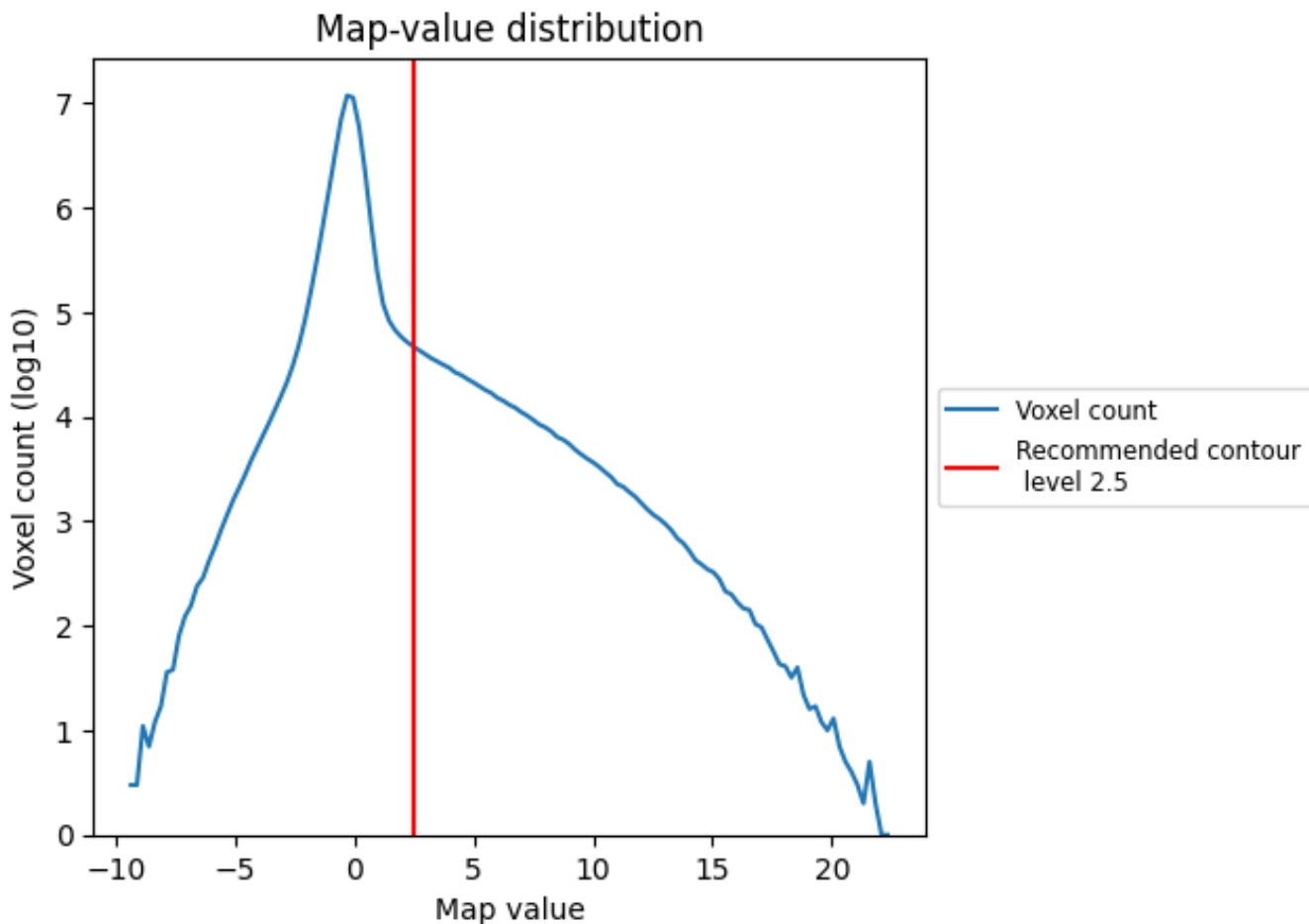
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

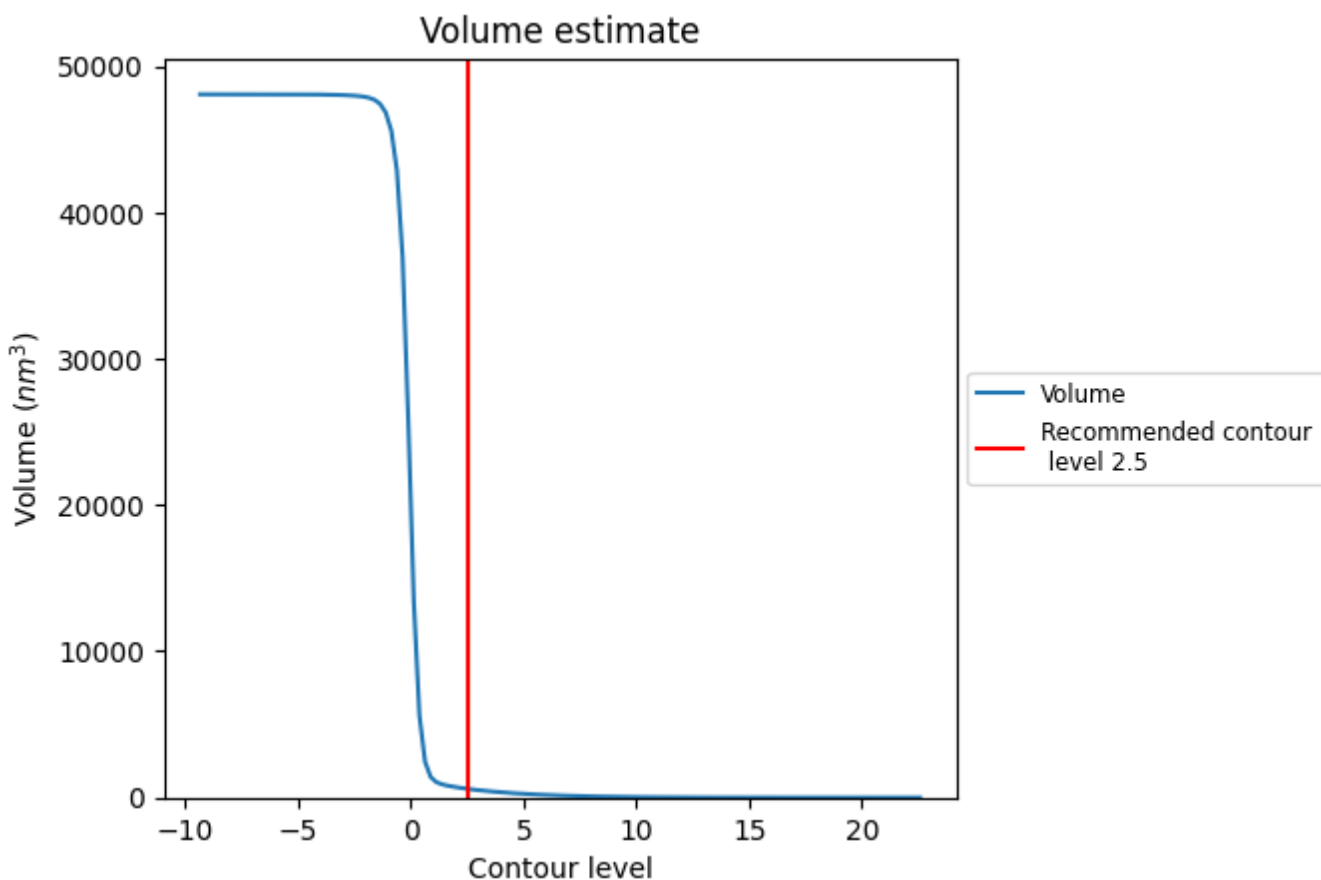
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

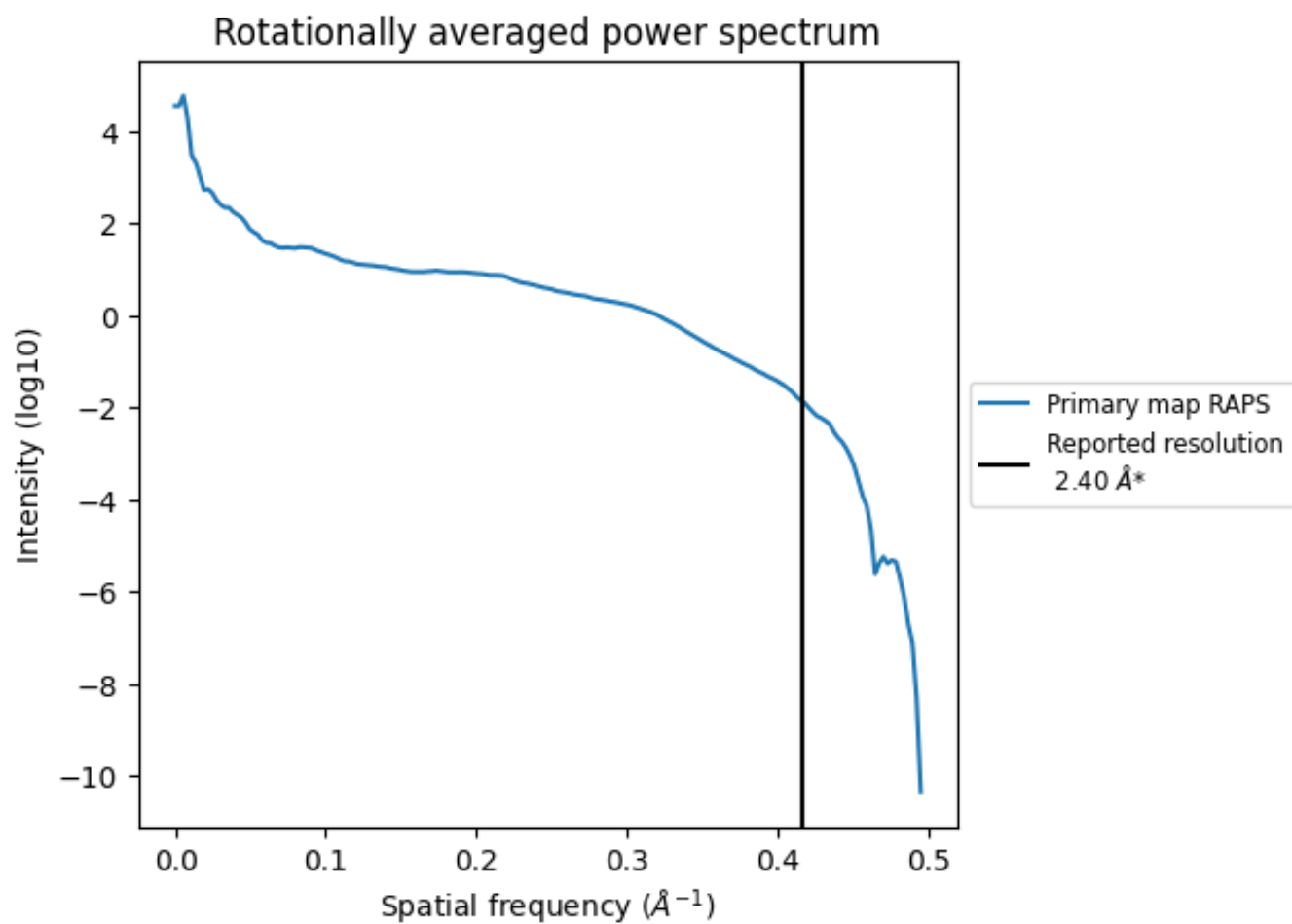
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 597 nm³; this corresponds to an approximate mass of 540 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

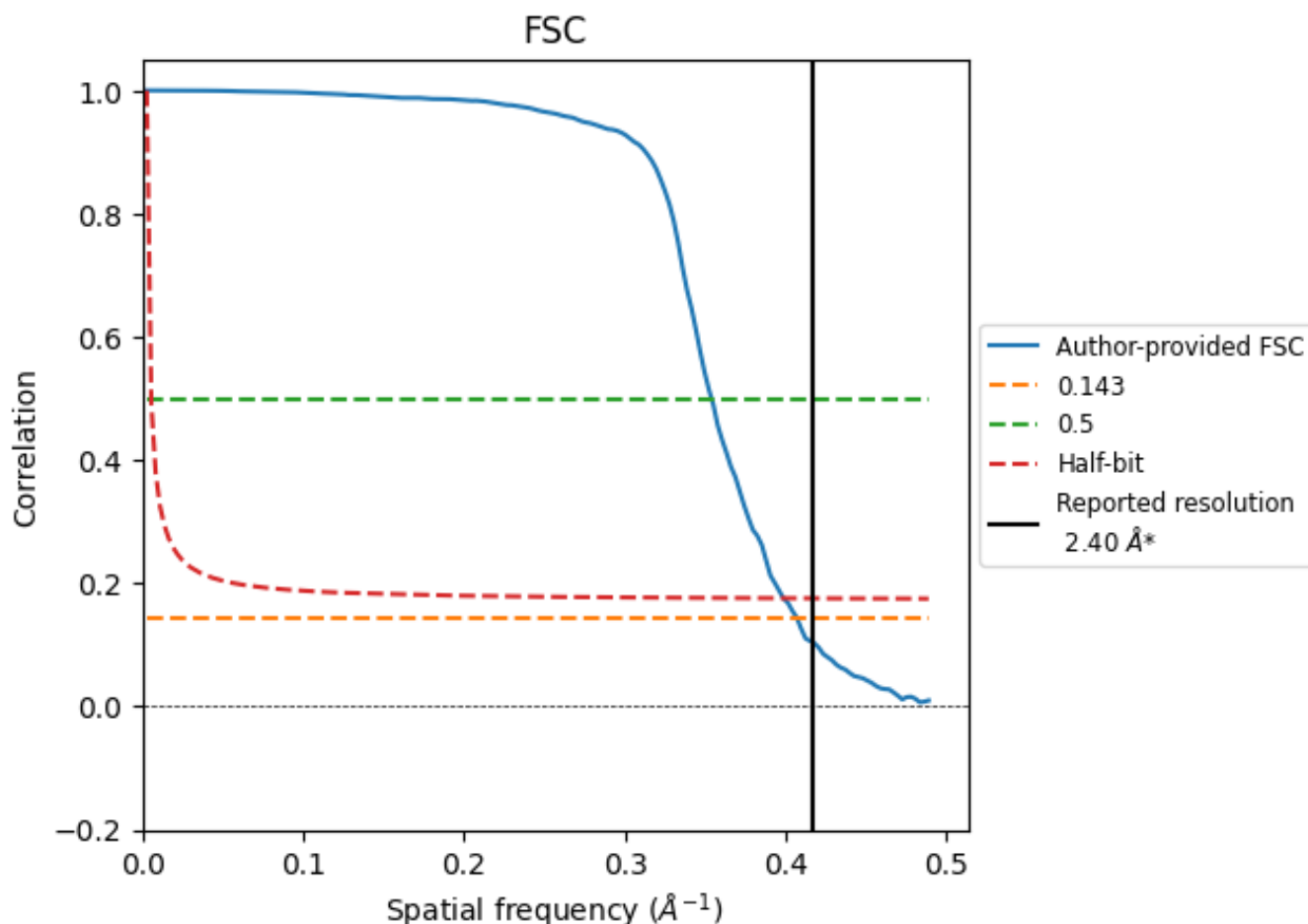


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

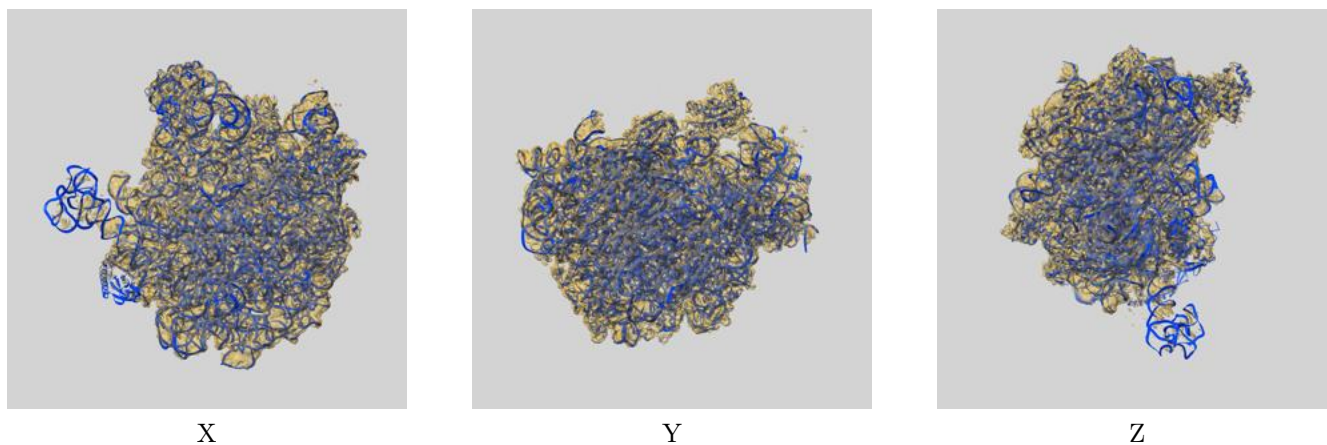
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.46	2.83	2.51
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

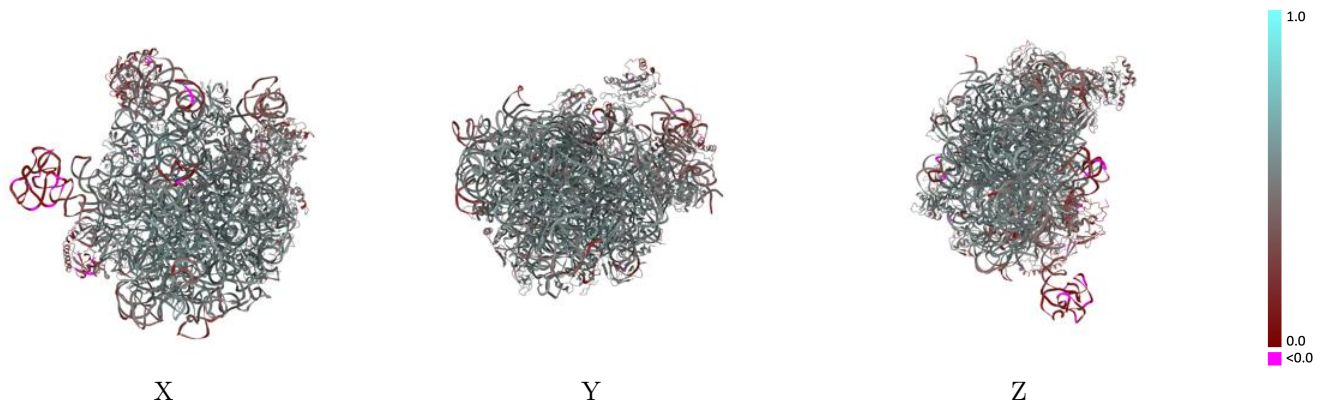
This section contains information regarding the fit between EMDB map EMD-12217 and PDB model 7BL4. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



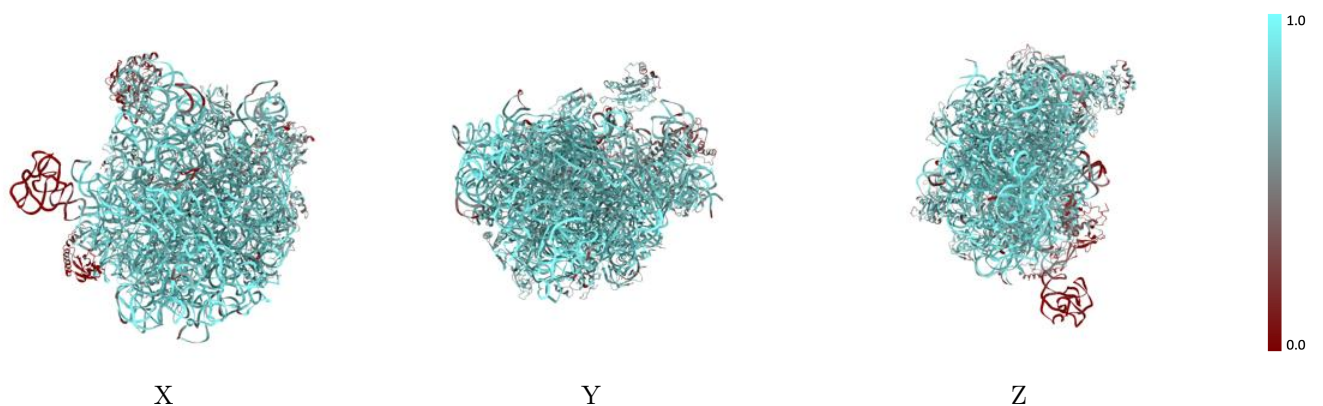
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



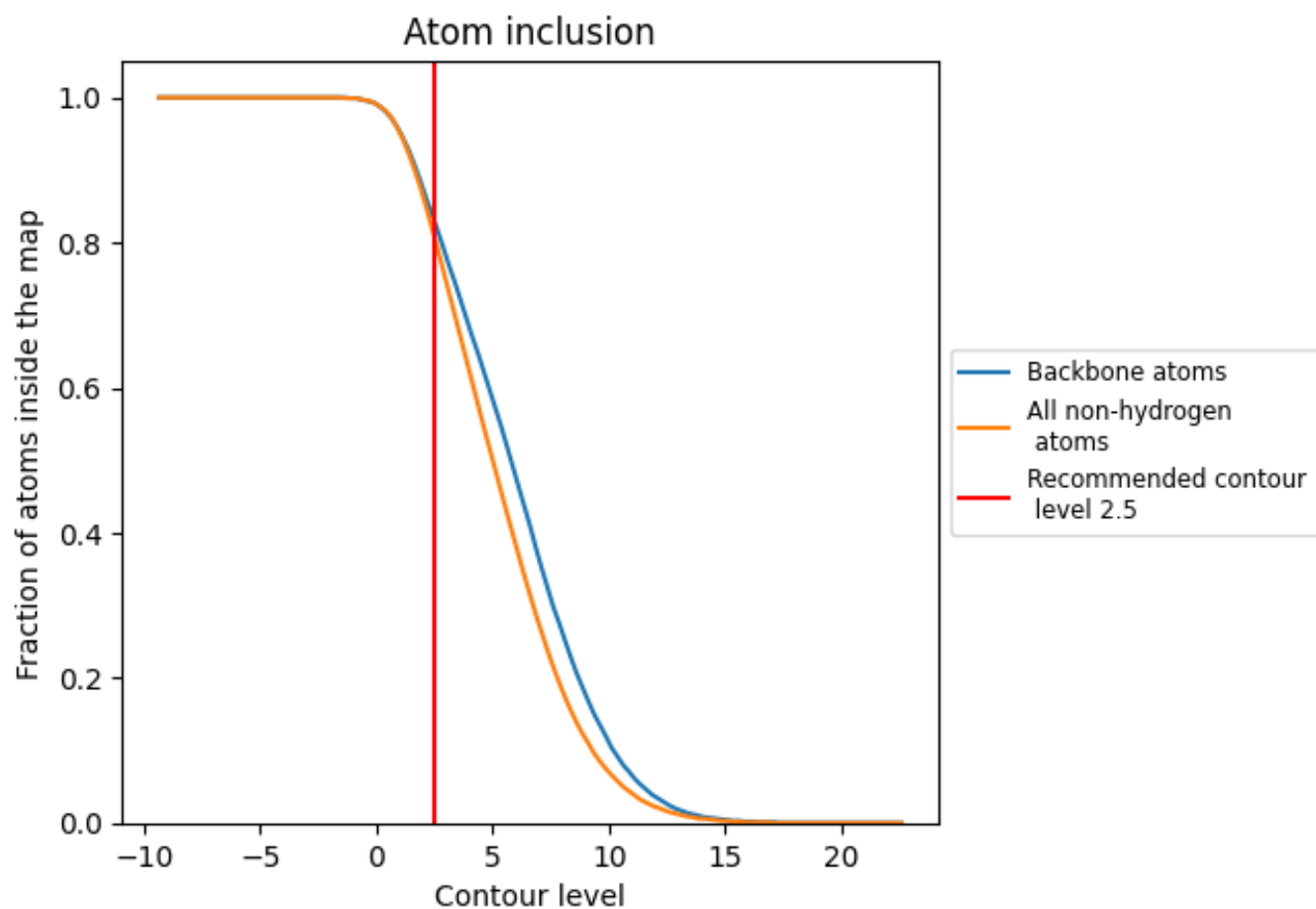
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.4920
0	 0.7340	 0.4890
1	 0.7060	 0.5000
2	 0.8340	 0.5840
3	 0.8110	 0.5410
6	 0.7070	 0.4610
9	 0.6450	 0.4460
A	 0.8680	 0.5010
B	 0.8530	 0.4730
C	 0.7890	 0.5260
D	 0.7160	 0.5110
E	 0.6990	 0.4970
F	 0.3930	 0.3250
G	 0.5710	 0.4280
H	 0.2090	 0.2510
J	 0.7420	 0.5190
K	 0.7770	 0.5130
L	 0.7470	 0.5010
M	 0.7590	 0.5180
N	 0.7650	 0.5210
O	 0.6490	 0.4340
P	 0.7060	 0.4870
Q	 0.8060	 0.5420
R	 0.7370	 0.4910
S	 0.7610	 0.5280
T	 0.7160	 0.5000
U	 0.6320	 0.4350
V	 0.7140	 0.4850
W	 0.7860	 0.5350
X	 0.7740	 0.5210
Y	 0.6780	 0.4250
Z	 0.7390	 0.4940
d	 0.1960	 0.2170
g	 0.6450	 0.5040

