



wwPDB EM Validation Summary Report ⓘ

Jan 16, 2025 – 01:23 am GMT

PDB ID : 9H3Z
EMDB ID : EMD-51843
Title : mature 50S subunit
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-10-17
Resolution : 2.98 Å(reported)
Based on initial model : 8RPY

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

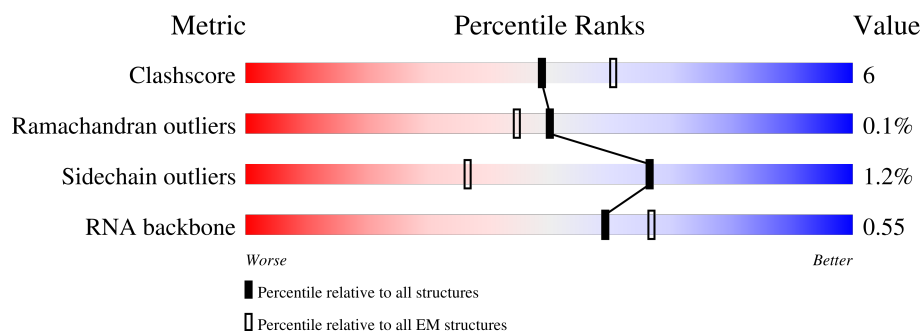
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.





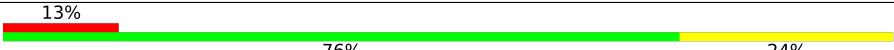
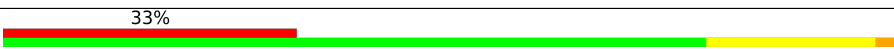

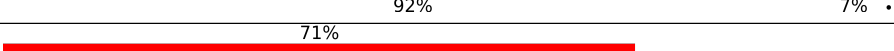
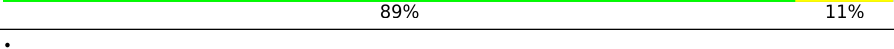
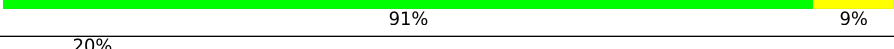
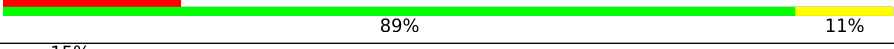



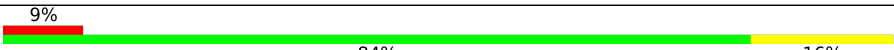


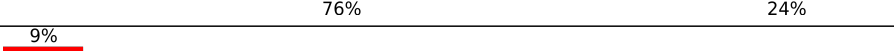
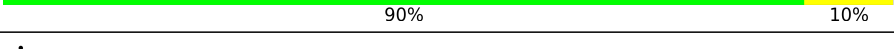




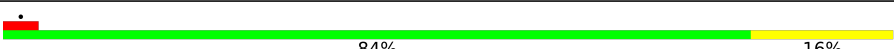

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	56	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	1	50	<div> <div>38%</div> <div>92%</div> <div>8%</div> </div>
3	2	46	<div> <div>.</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
4	3	64	<div> <div>.</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
5	4	38	<div> <div>.</div> <div>84%</div> <div>16%</div> </div>
6	A	2904	<div> <div>5%</div> <div>65%</div> <div>30%</div> <div>5%</div> </div>
7	B	120	<div> <div>.</div> <div>69%</div> <div>25%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	C	271	
9	D	209	
10	E	201	
11	F	177	
12	G	176	
13	H	149	
14	J	142	
15	K	122	
16	L	143	
17	M	136	
18	N	120	
19	O	116	
20	P	114	
21	Q	117	
22	R	103	
23	S	110	
24	T	93	
25	U	102	
26	V	94	
27	W	75	
28	X	77	
29	Y	63	
30	Z	58	

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 89946 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 Large ribosomal subunit protein bL32.

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 23S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2900	Total	C	N	O	P	1	0
			62281	27783	11461	20136	2901		

- Molecule 7 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	S	110	Total	C	N	O	S	1
			868	538	170	157	3	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	75	Total	C	N	O	S	0
			575	356	116	102	1	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL28.

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

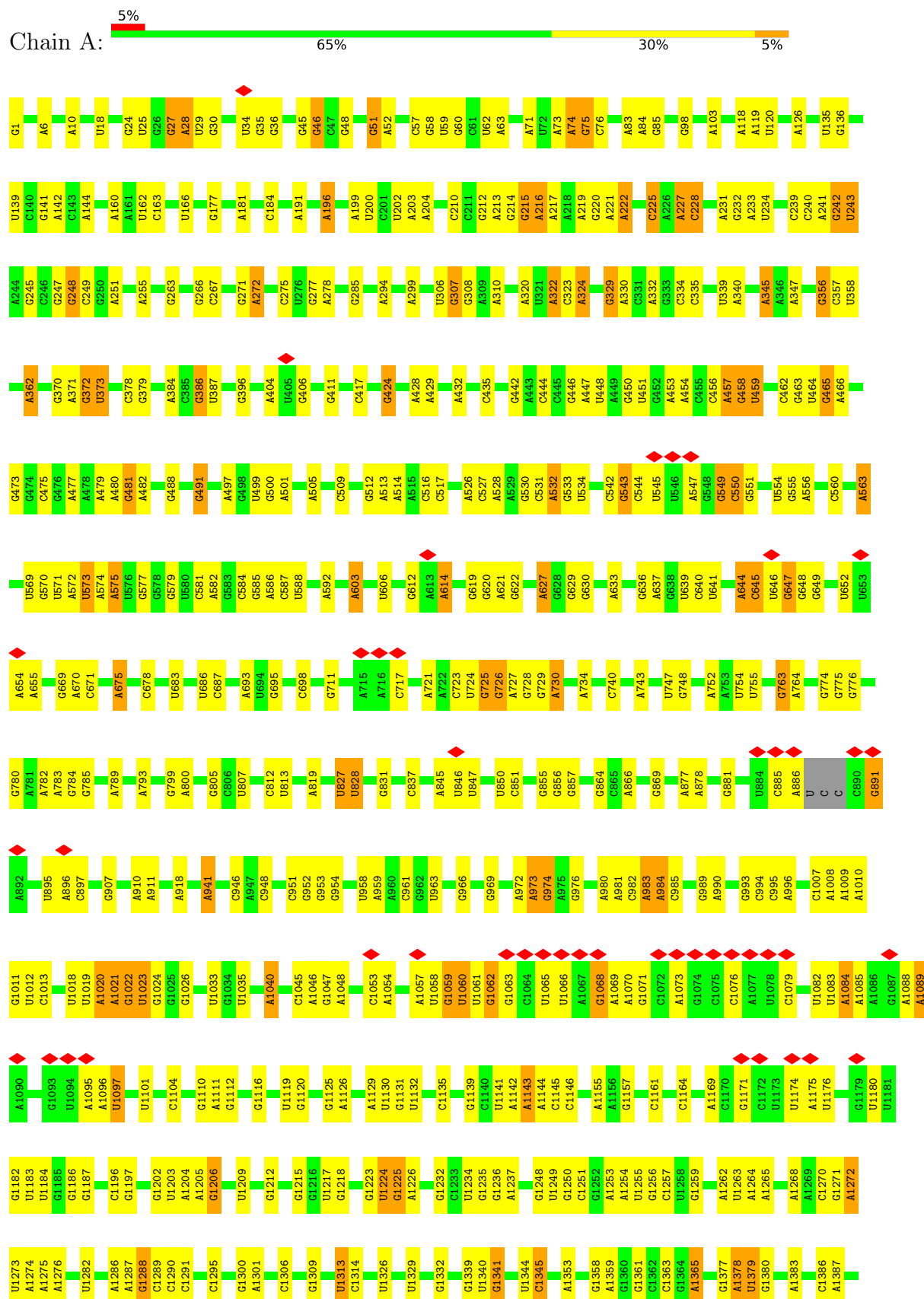
- Molecule 29 is a protein called Large ribosomal subunit protein uL29.

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

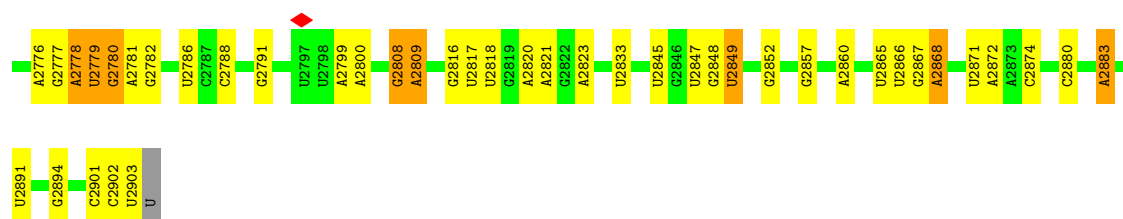
- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

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

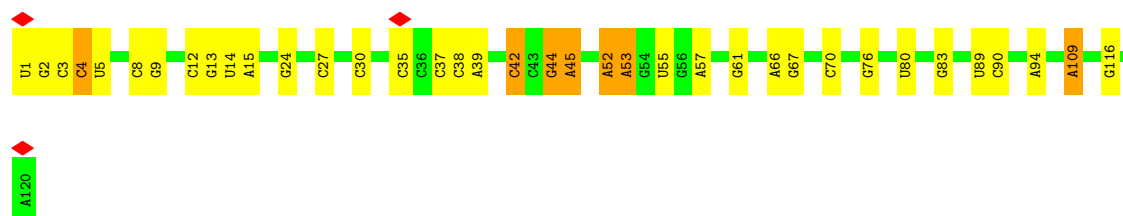
• Molecule 6: 23S ribosomal rRNA



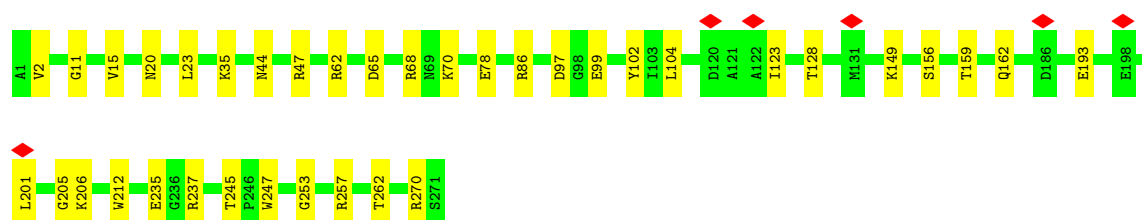
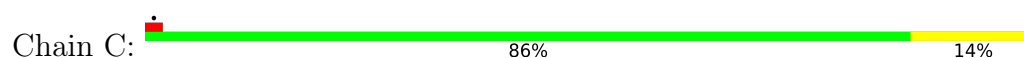




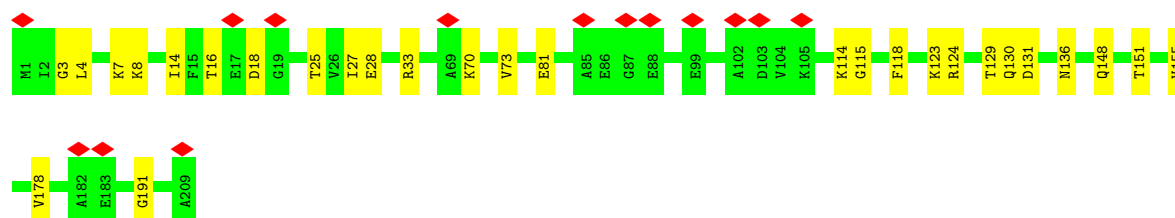
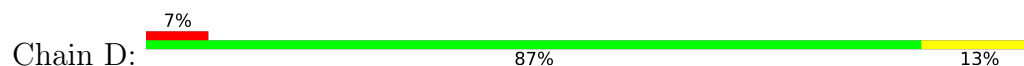
- Molecule 7: 5S ribosomal RNA



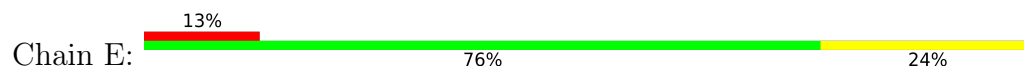
- Molecule 8: Large ribosomal subunit protein uL2



- Molecule 9: 50S ribosomal protein L3

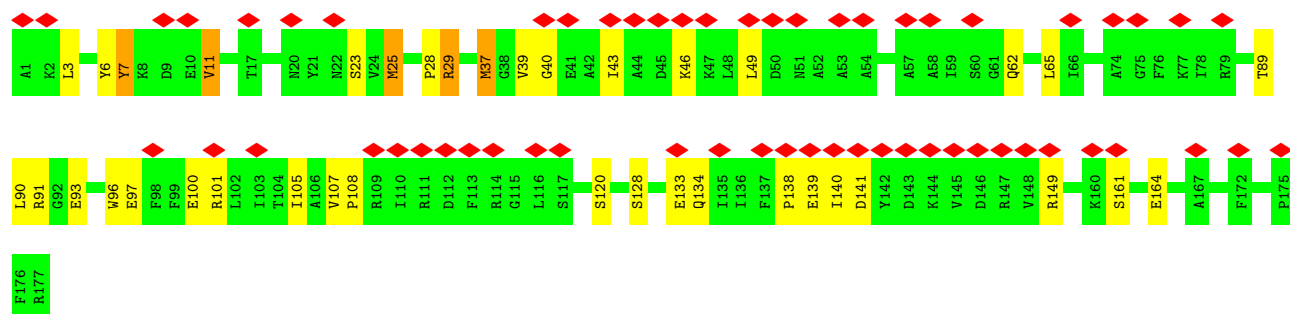
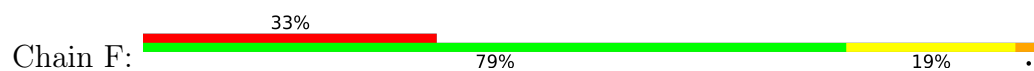


- Molecule 10: Large ribosomal subunit protein uL4

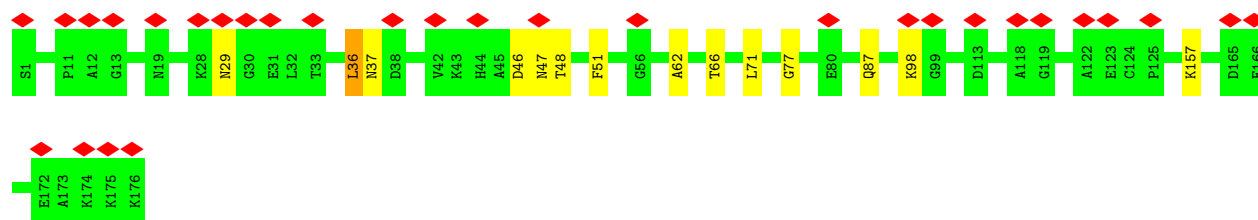
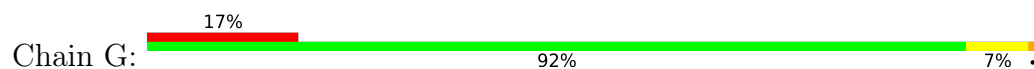




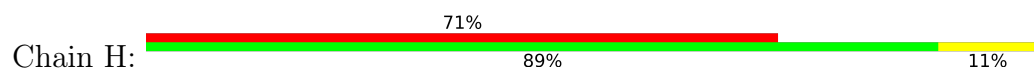
- Molecule 11: Large ribosomal subunit protein uL5



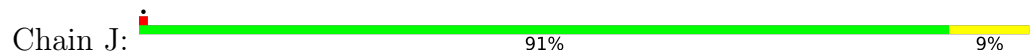
- Molecule 12: Large ribosomal subunit protein uL6



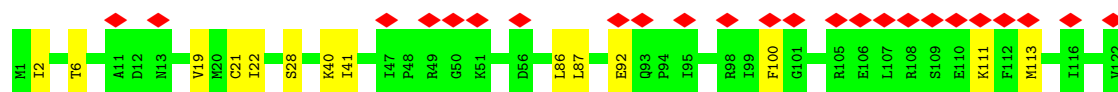
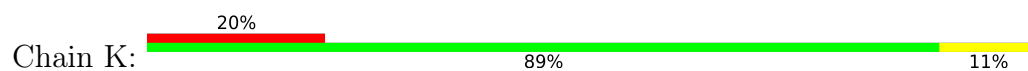
- Molecule 13: Large ribosomal subunit protein bL9



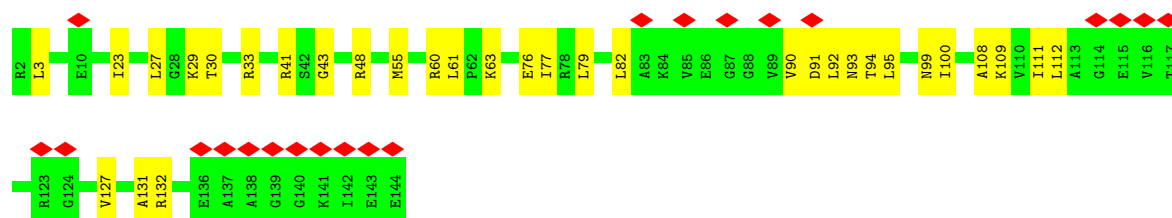
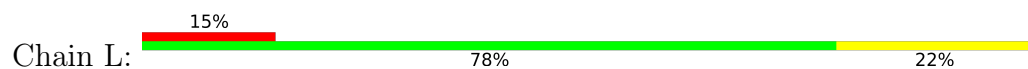
- Molecule 14: Large ribosomal subunit protein uL13



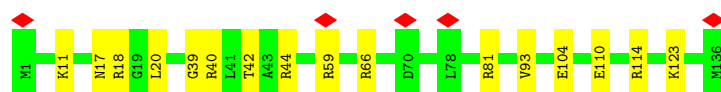
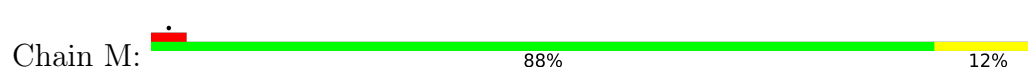
- Molecule 15: Large ribosomal subunit protein uL14



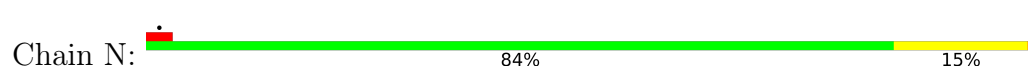
- Molecule 16: Large ribosomal subunit protein uL15



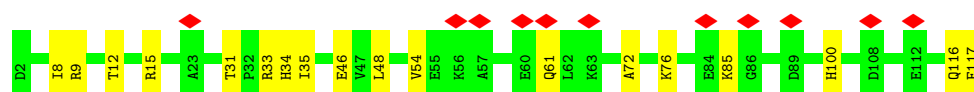
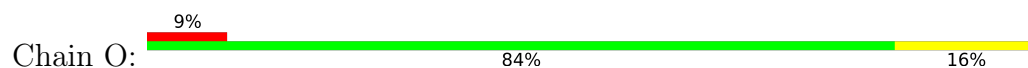
- Molecule 17: 50S ribosomal protein L16



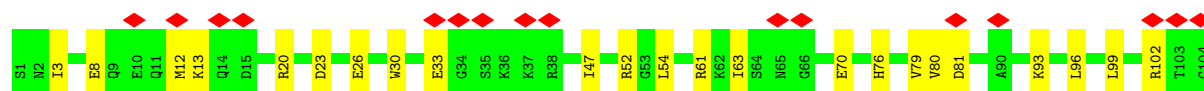
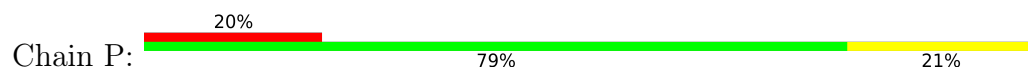
- Molecule 18: Large ribosomal subunit protein bL17

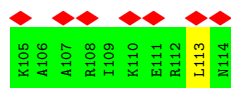


- Molecule 19: Large ribosomal subunit protein uL18

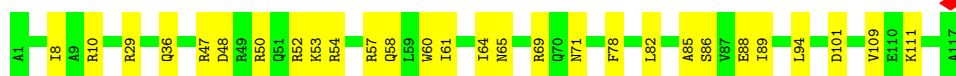
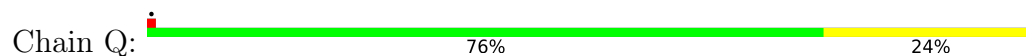


- Molecule 20: Large ribosomal subunit protein bL19

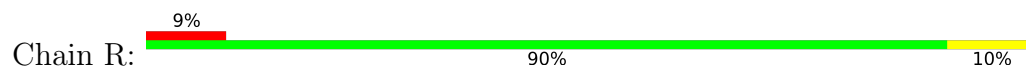




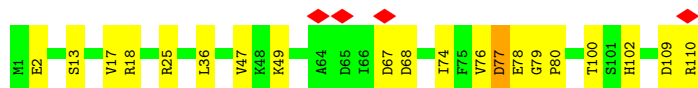
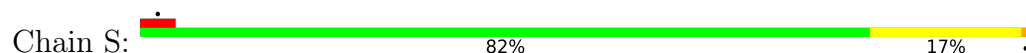
- Molecule 21: Large ribosomal subunit protein bL20



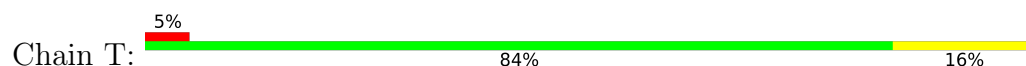
- Molecule 22: Large ribosomal subunit protein bL21



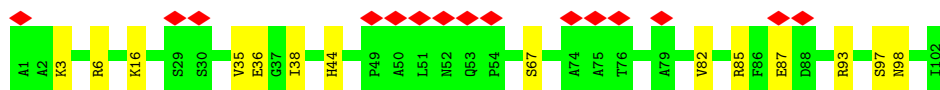
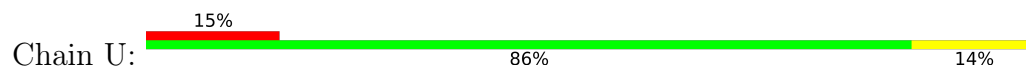
- Molecule 23: Large ribosomal subunit protein uL22



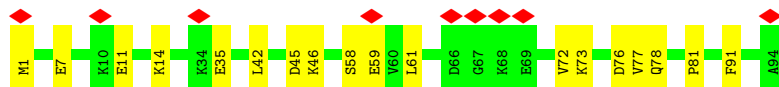
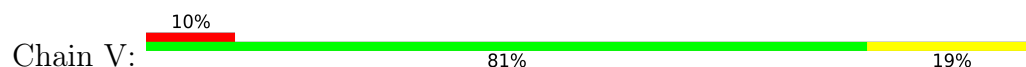
- Molecule 24: Large ribosomal subunit protein uL23




- Molecule 25: Large ribosomal subunit protein uL24



- Molecule 26: Large ribosomal subunit protein bL25




- Molecule 27: Large ribosomal subunit protein bL27

Chain W:  84% 16%




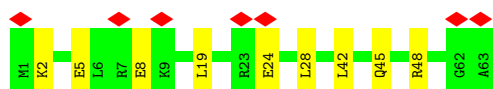
- Molecule 28: Large ribosomal subunit protein bL28

Chain X:  88% 12%




- Molecule 29: Large ribosomal subunit protein uL29

Chain Y:  11% 86% 14%



- Molecule 30: Large ribosomal subunit protein uL30

Chain Z:  81% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.575	Depositor
Minimum map value	-0.980	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.44	Depositor
Map size (\AA)	424.0, 424.0, 424.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4133333, 1.4133333, 1.4133333	Depositor

5 Model quality [i](#)

5.1 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 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	0	0.23	0/450	0.54	0/599
2	1	0.24	0/416	0.48	0/554
3	2	0.25	0/380	0.64	0/498
4	3	0.23	0/513	0.52	0/676
5	4	0.26	0/303	0.56	0/397
6	A	0.15	1/69755 (0.0%)	0.72	8/108820 (0.0%)
7	B	0.24	1/2876 (0.0%)	0.70	0/4483
8	C	0.24	0/2121	0.55	0/2852
9	D	0.24	0/1586	0.50	0/2134
10	E	0.24	0/1571	0.48	0/2113
11	F	0.25	0/1434	0.53	0/1926
12	G	0.24	0/1343	0.48	0/1816
13	H	0.24	0/1122	0.48	0/1515
14	J	0.24	0/1152	0.49	0/1551
15	K	0.24	0/947	0.55	0/1268
16	L	0.25	0/1054	0.57	0/1403
17	M	0.25	0/1093	0.54	0/1460
18	N	0.25	0/973	0.59	0/1301
19	O	0.24	0/902	0.53	0/1209
20	P	0.25	0/929	0.54	0/1242
21	Q	0.24	0/960	0.52	0/1278
22	R	0.25	0/829	0.53	0/1107
23	S	0.23	0/875	0.52	0/1170
24	T	0.23	0/744	0.49	0/994
25	U	0.25	0/787	0.51	0/1051
26	V	0.25	0/766	0.48	0/1025
27	W	0.24	0/582	0.53	0/769
28	X	0.24	0/635	0.57	0/848
29	Y	0.24	0/510	0.49	0/677
30	Z	0.24	0/453	0.54	0/605
All	All	0.18	2/98061 (0.0%)	0.68	8/147341 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	G	OP3-P	-10.57	1.48	1.61
7	B	1	U	OP3-P	-10.54	1.48	1.61

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1913	A	OP1-P-O3'	-10.67	81.72	105.20
6	A	1913	A	OP2-P-O3'	-10.07	83.05	105.20
6	A	1914	C	OP1-P-OP2	7.09	130.23	119.60
6	A	2474	U	C2-N1-C1'	5.73	124.57	117.70
6	A	2321	U	C2-N1-C1'	5.57	124.38	117.70

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	0	444	0	461	7	0
2	1	409	0	440	4	0
3	2	377	0	418	4	0
4	3	504	0	574	12	0
5	4	302	0	343	6	0
6	A	62281	0	31323	517	0
7	B	2572	0	1302	22	0
8	C	2082	0	2157	30	0
9	D	1565	0	1616	20	0
10	E	1552	0	1619	35	0
11	F	1410	0	1447	29	0
12	G	1323	0	1374	10	0
13	H	1111	0	1148	13	0
14	J	1129	0	1162	9	0
15	K	938	0	1012	10	0
16	L	1045	0	1117	28	0
17	M	1074	0	1157	11	0
18	N	960	0	1000	14	0
19	O	892	0	923	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	917	0	965	16	0
21	Q	947	0	1022	24	0
22	R	816	0	839	8	0
23	S	868	0	934	15	0
24	T	738	0	807	11	0
25	U	779	0	834	11	0
26	V	753	0	780	15	0
27	W	575	0	592	10	0
28	X	625	0	655	8	0
29	Y	509	0	543	6	0
30	Z	449	0	491	10	0
All	All	89946	0	59055	786	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 6.

The worst 5 of 786 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)
6:A:727:A:OP2	6:A:1431:A:O2'	1.88	0.91
6:A:177:G:OP2	6:A:177:G:N2	2.05	0.89
16:L:93:ASN:O	16:L:94:THR:OG1	1.91	0.88
6:A:1837:C:O2'	6:A:1927:A:N3	2.05	0.87
6:A:2343:U:HO2'	6:A:2373:G:HO2'	1.13	0.87

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	0	54/56 (96%)	53 (98%)	1 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	60 (97%)	1 (2%)	1 (2%)	8	32
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	C	269/271 (99%)	258 (96%)	11 (4%)	0	100	100
9	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
10	E	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	25	59
11	F	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
12	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
13	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
14	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
15	K	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
16	L	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
17	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
18	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
19	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
20	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
21	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
22	R	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	13	43
23	S	109/110 (99%)	105 (96%)	4 (4%)	0	100	100
24	T	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
25	U	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
26	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
27	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
28	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
29	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
30	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
All	All	3167/3222 (98%)	3050 (96%)	114 (4%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	R	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	E	83	VAL
4	3	31	ILE

5.3.2 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 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	0	47/47 (100%)	45 (96%)	2 (4%)	25	56
2	1	45/45 (100%)	44 (98%)	1 (2%)	47	74
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	70
4	3	51/51 (100%)	49 (96%)	2 (4%)	27	59
5	4	34/34 (100%)	34 (100%)	0	100	100
8	C	216/216 (100%)	215 (100%)	1 (0%)	86	94
9	D	164/164 (100%)	164 (100%)	0	100	100
10	E	165/165 (100%)	162 (98%)	3 (2%)	54	79
11	F	148/148 (100%)	141 (95%)	7 (5%)	22	53
12	G	137/137 (100%)	135 (98%)	2 (2%)	60	82
13	H	114/114 (100%)	114 (100%)	0	100	100
14	J	116/116 (100%)	115 (99%)	1 (1%)	75	88
15	K	103/103 (100%)	102 (99%)	1 (1%)	73	87
16	L	102/102 (100%)	101 (99%)	1 (1%)	73	87
17	M	109/109 (100%)	108 (99%)	1 (1%)	75	88
18	N	100/100 (100%)	98 (98%)	2 (2%)	50	76
19	O	86/86 (100%)	85 (99%)	1 (1%)	67	85
20	P	99/99 (100%)	97 (98%)	2 (2%)	50	76
21	Q	89/89 (100%)	89 (100%)	0	100	100
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	94/93 (101%)	93 (99%)	1 (1%)	70	86
24	T	80/80 (100%)	80 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	U	83/83 (100%)	83 (100%)	0	100	100
26	V	78/78 (100%)	77 (99%)	1 (1%)	65	84
27	W	57/57 (100%)	57 (100%)	0	100	100
28	X	67/67 (100%)	67 (100%)	0	100	100
29	Y	55/55 (100%)	54 (98%)	1 (2%)	54	79
30	Z	48/48 (100%)	47 (98%)	1 (2%)	48	75
All	All	2609/2608 (100%)	2577 (99%)	32 (1%)	66	85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	S	77	ASP
26	V	42	LEU
11	F	11	VAL
11	F	7	TYR
29	Y	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
21	Q	55	GLN
23	S	60	HIS
27	W	72	ASN
26	V	49	ASN
10	E	41	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	A	2897/2904 (99%)	462 (15%)	18 (0%)
7	B	119/120 (99%)	14 (11%)	2 (1%)
All	All	3016/3024 (99%)	476 (15%)	20 (0%)

5 of 476 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	10	A
6	A	27	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	28	A
6	A	34	U
6	A	35	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	2058	A
6	A	2808	G
7	B	66	A
7	B	52	A
6	A	784	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

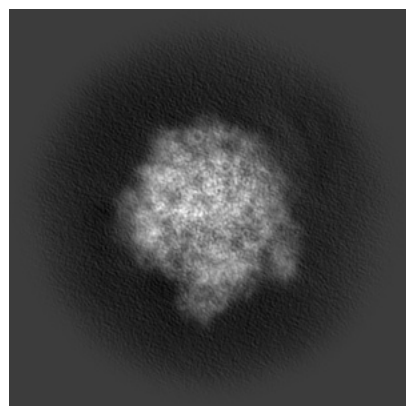
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51843. These allow visual inspection of the internal detail of the map and identification of artifacts.

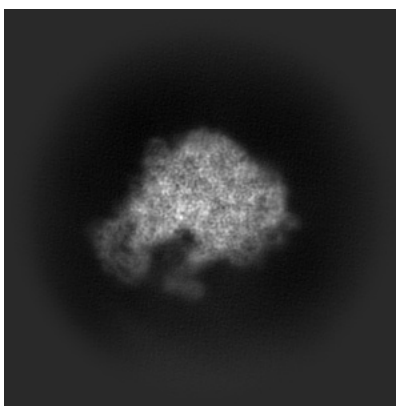
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

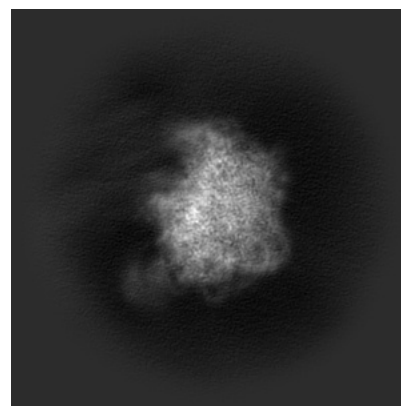
6.1.1 Primary map



X

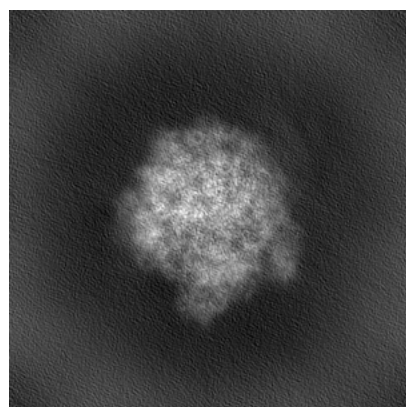


Y

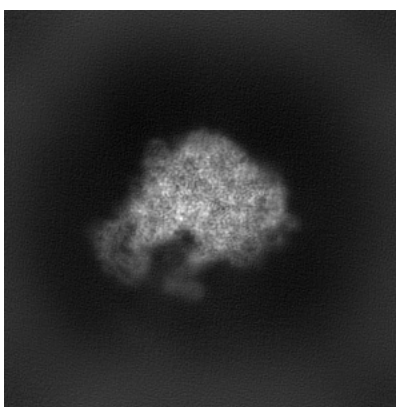


Z

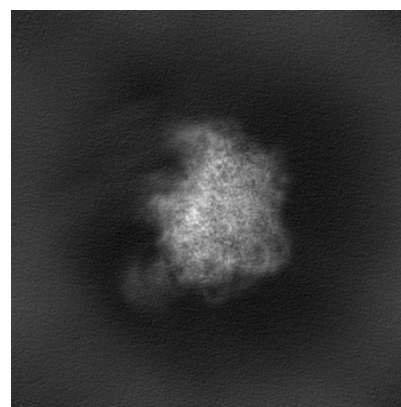
6.1.2 Raw map



X



Y

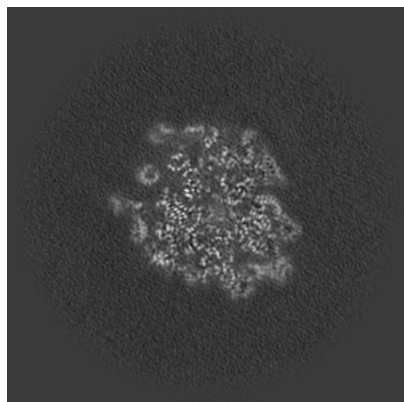


Z

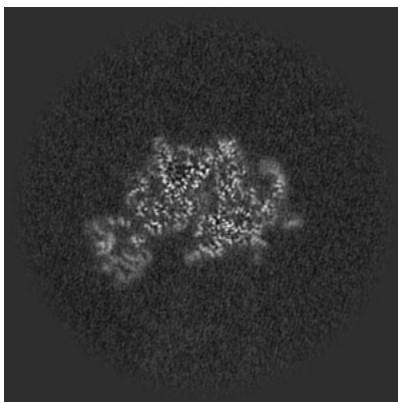
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

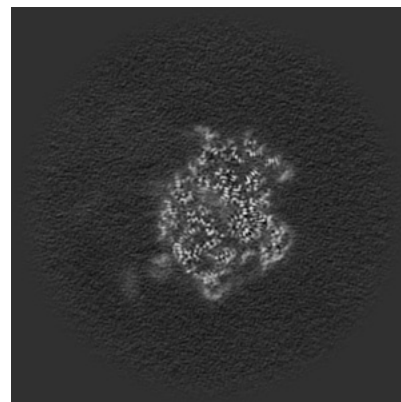
6.2.1 Primary map



X Index: 150

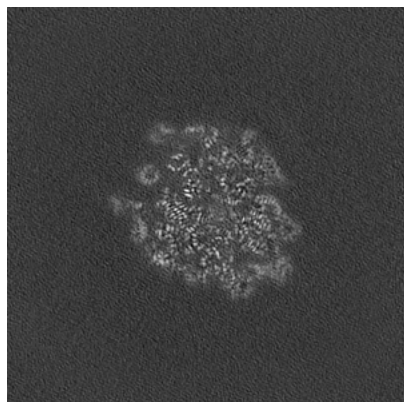


Y Index: 150

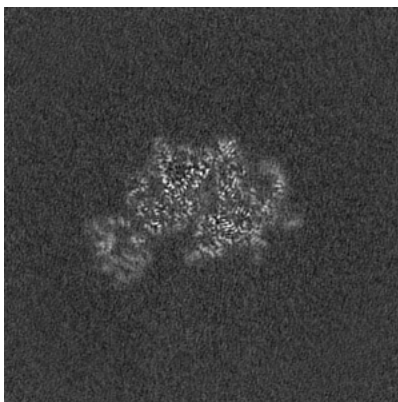


Z Index: 150

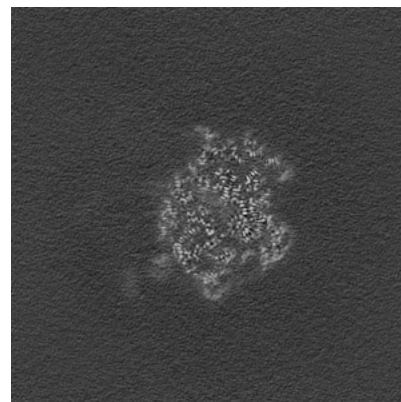
6.2.2 Raw map



X Index: 150



Y Index: 150

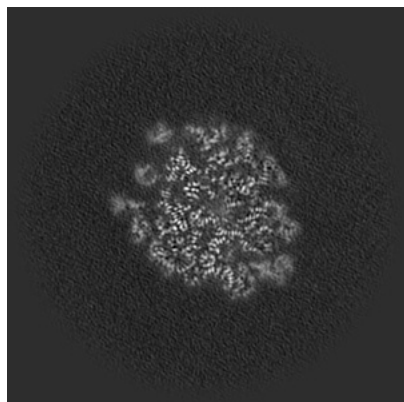


Z Index: 150

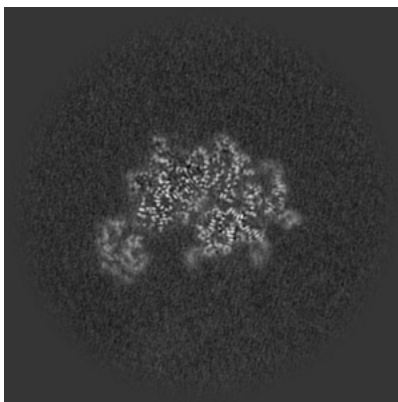
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

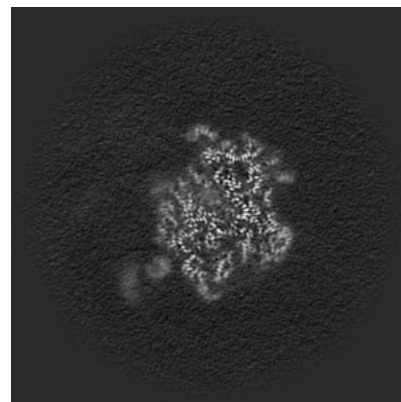
6.3.1 Primary map



X Index: 148

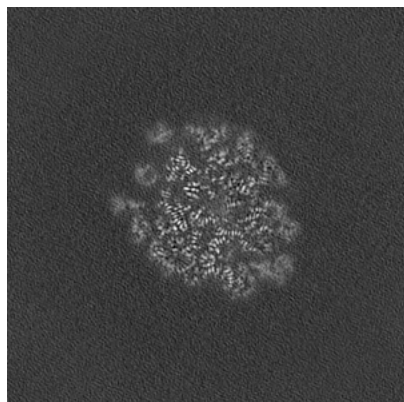


Y Index: 154

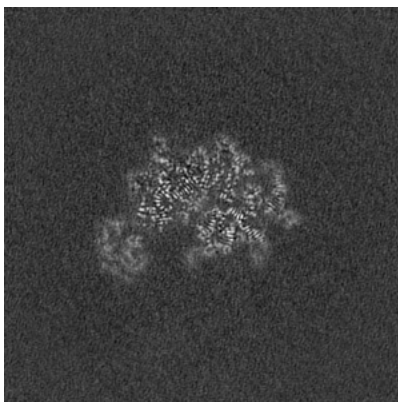


Z Index: 147

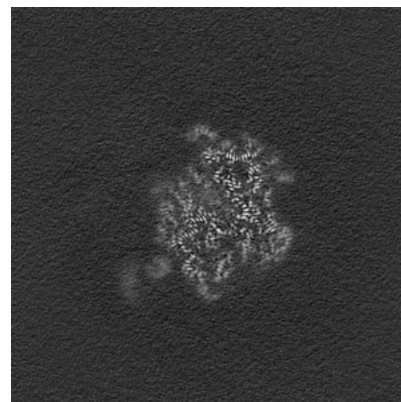
6.3.2 Raw map



X Index: 148



Y Index: 154

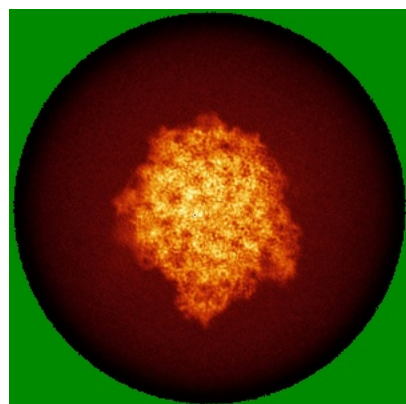


Z Index: 147

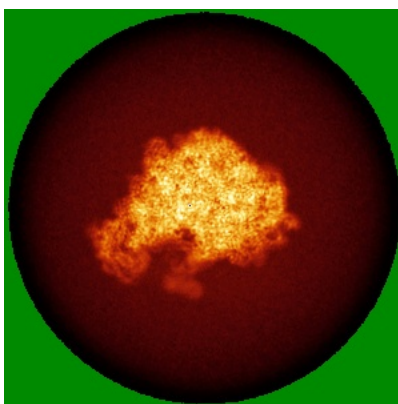
The images above show the largest variance slices of the map in three orthogonal directions.

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

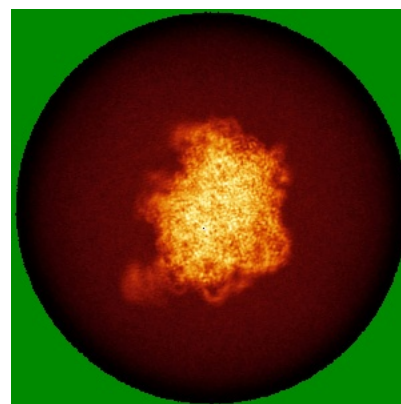
6.4.1 Primary map



X

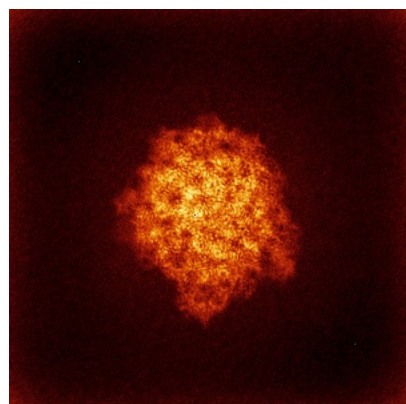


Y

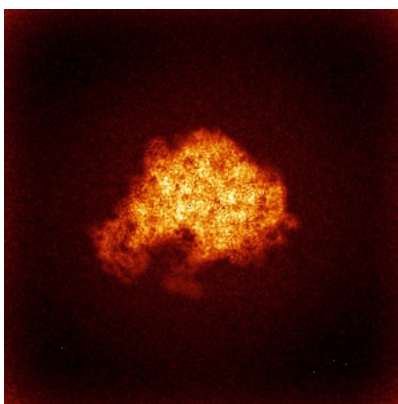


Z

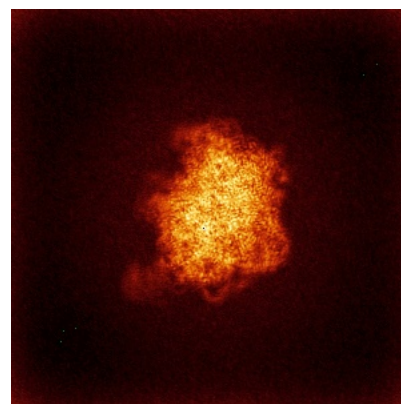
6.4.2 Raw map



X



Y

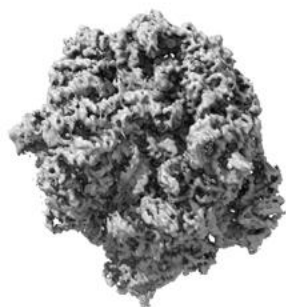


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

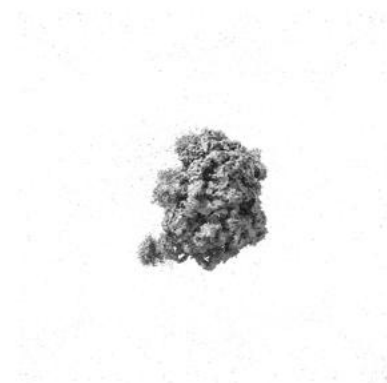
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

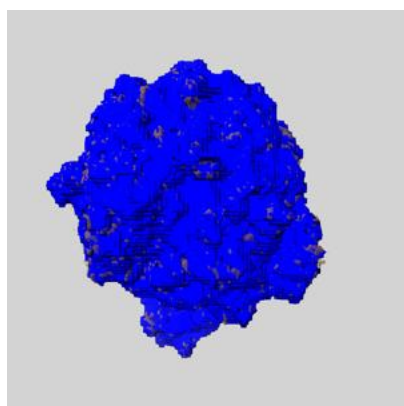
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

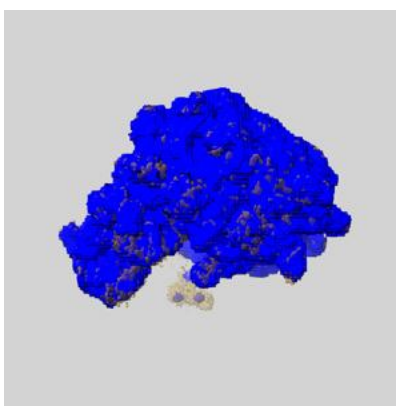
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

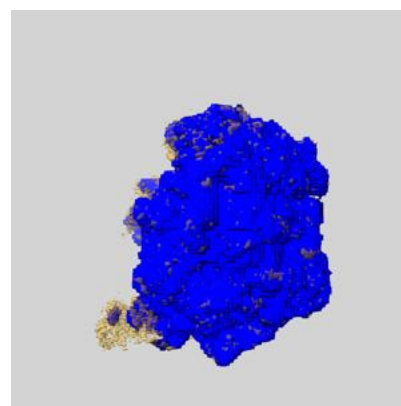
6.6.1 emd_51843_msk_1.map [i](#)



X



Y

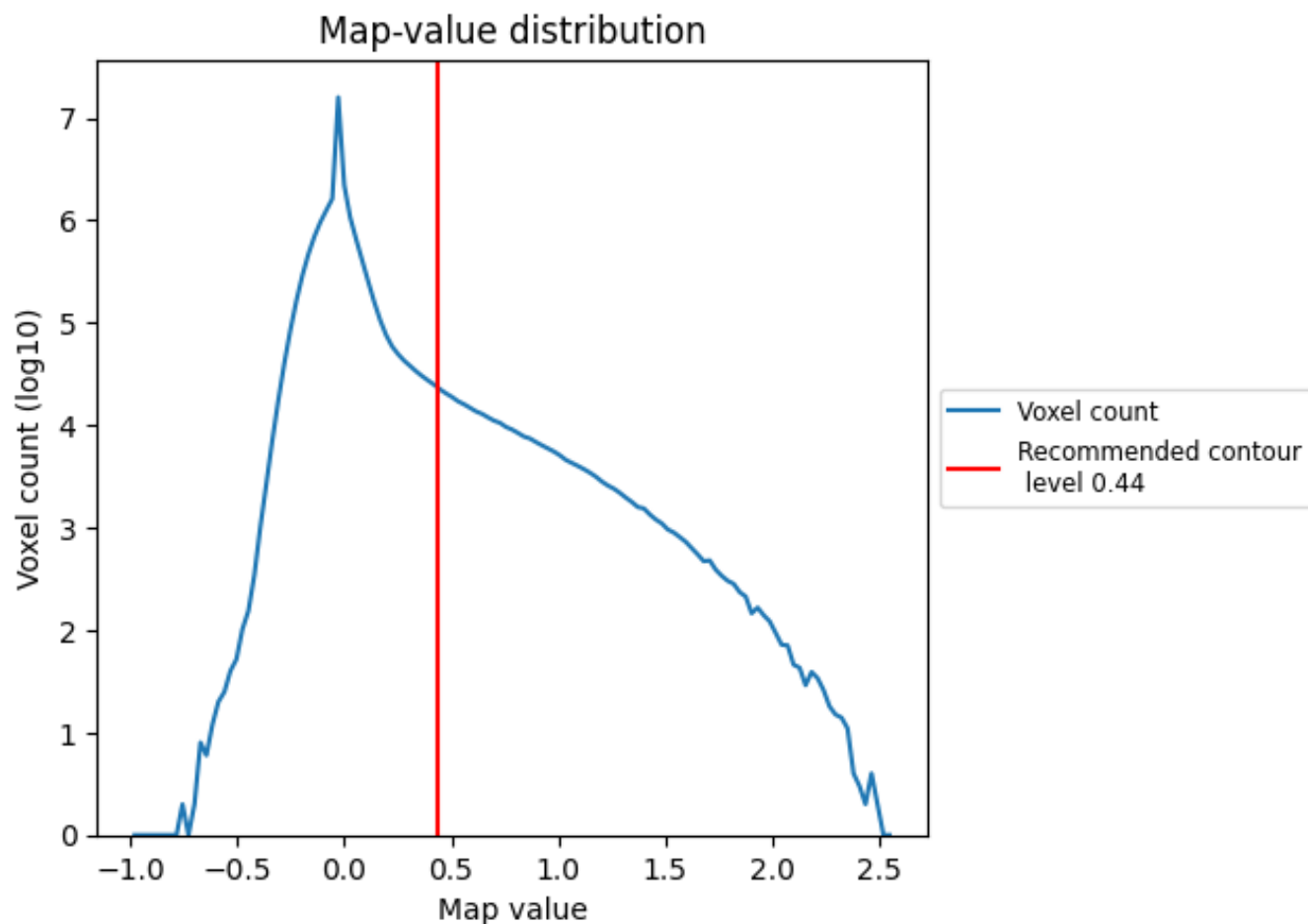


Z

7 Map analysis [i](#)

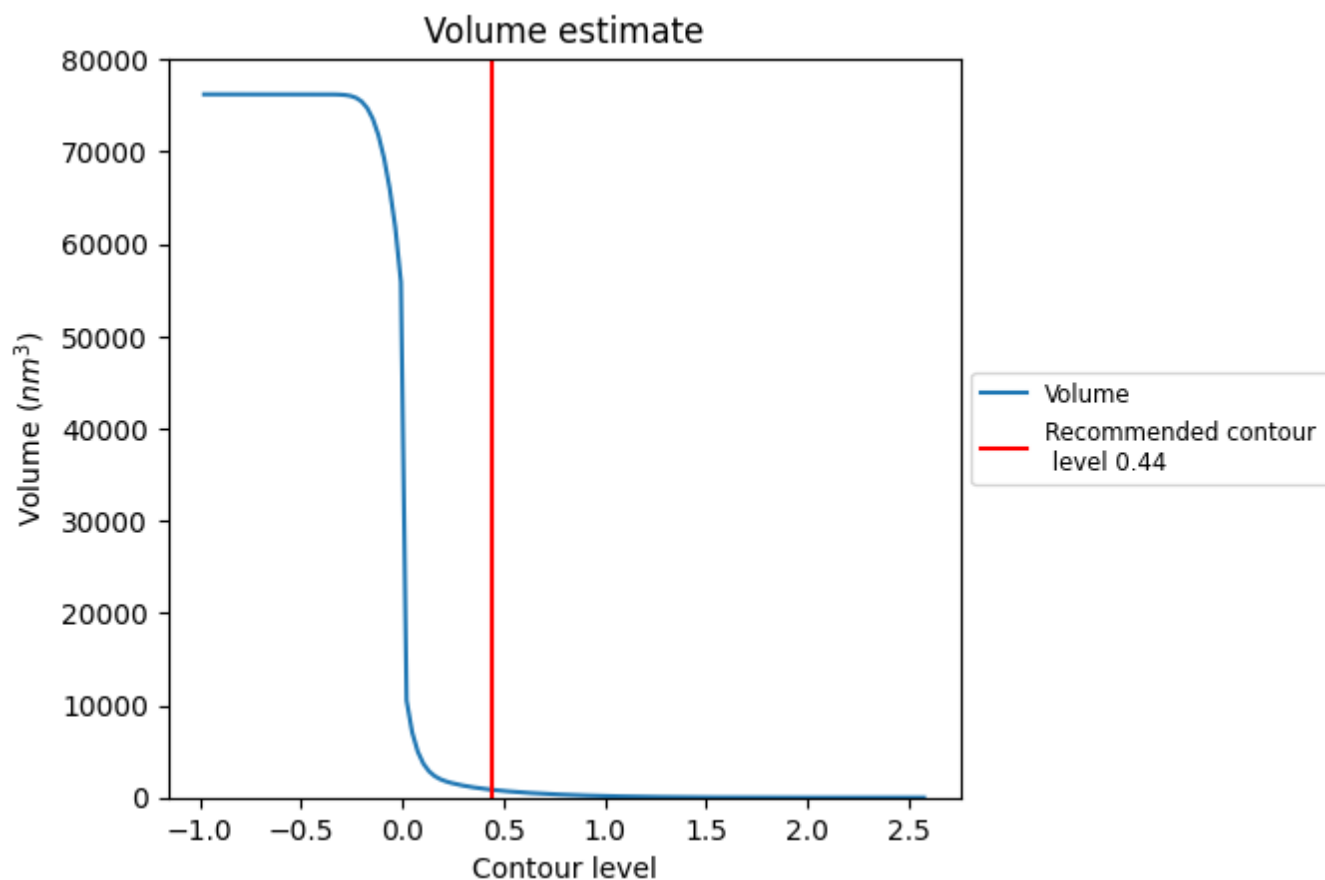
This section contains the results of statistical analysis of the map.

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.

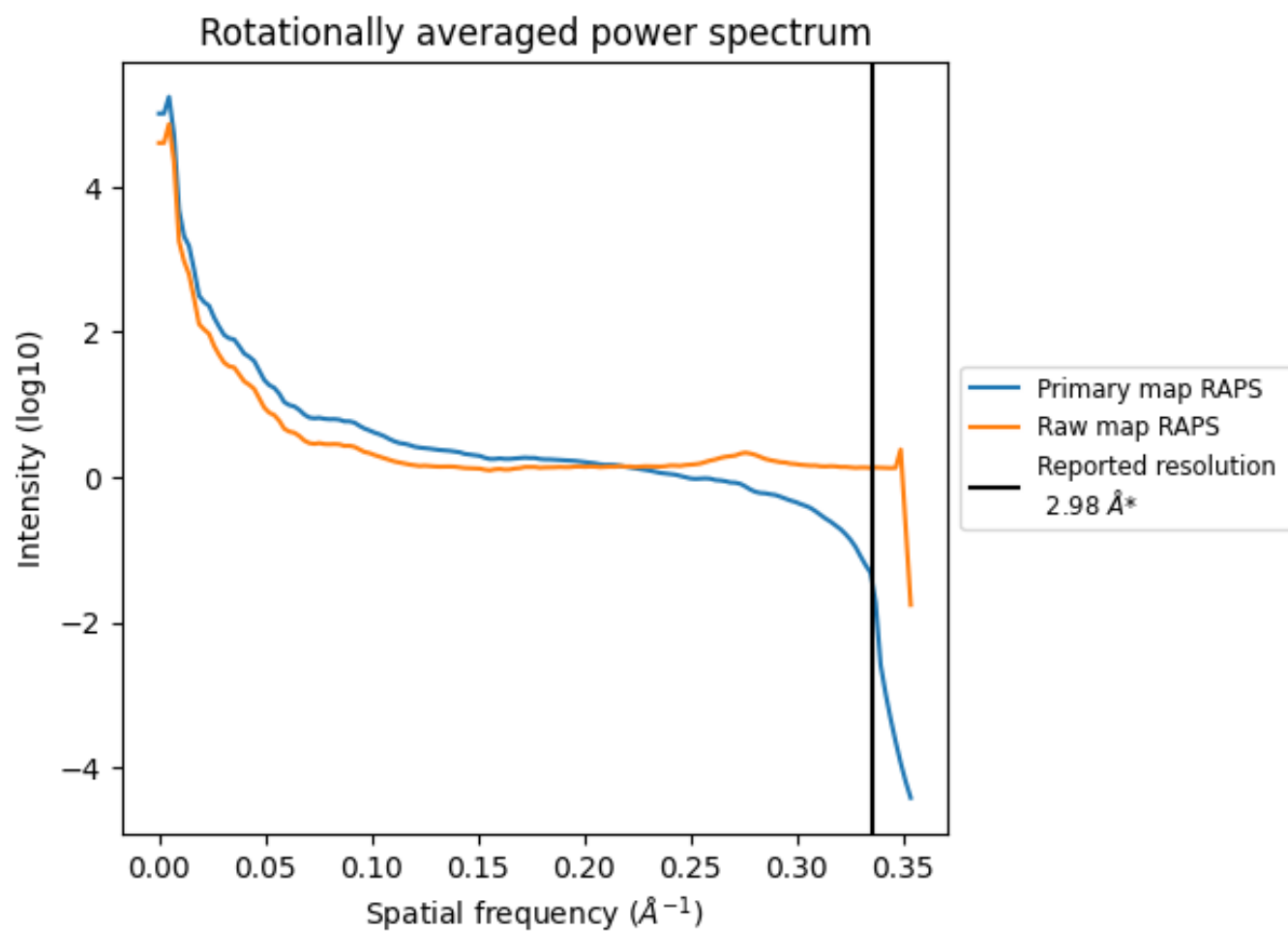
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 849 nm³; this corresponds to an approximate mass of 767 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 ⓘ

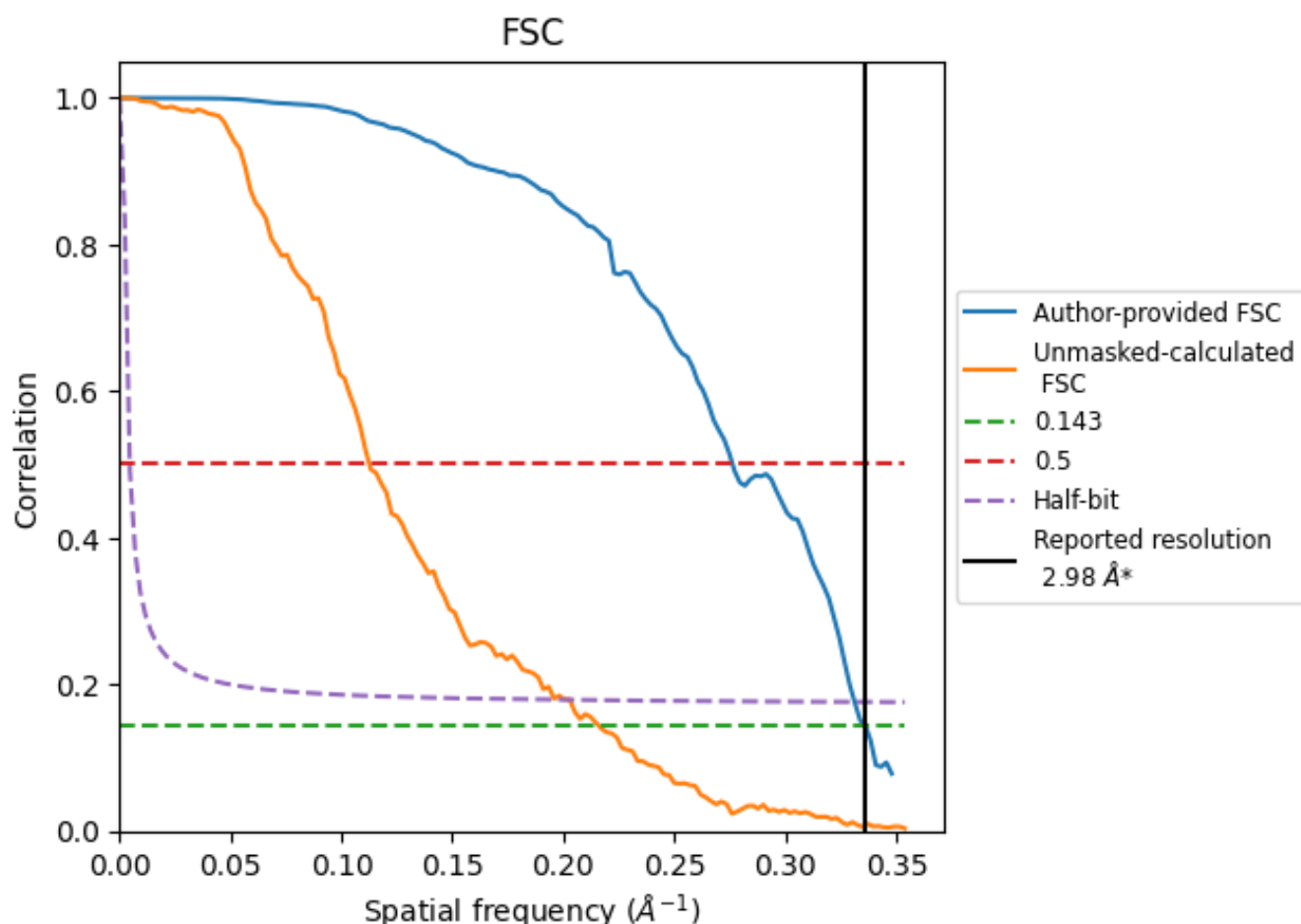


*Reported resolution corresponds to spatial frequency of 0.336 \AA^{-1}

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 0.336 \AA^{-1}

8.2 Resolution estimates [i](#)

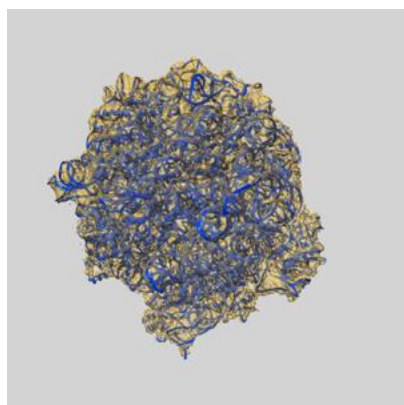
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.62	3.02
Unmasked-calculated*	4.63	8.88	4.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.63 differs from the reported value 2.98 by more than 10 %

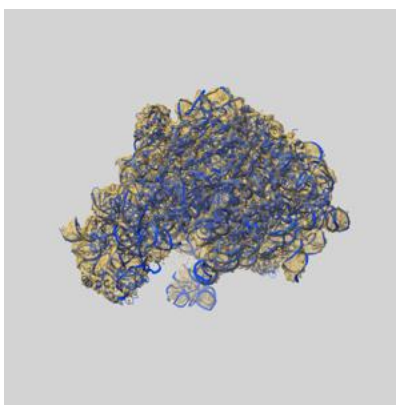
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51843 and PDB model 9H3Z. Per-residue inclusion information can be found in section [3](#) on page [9](#).

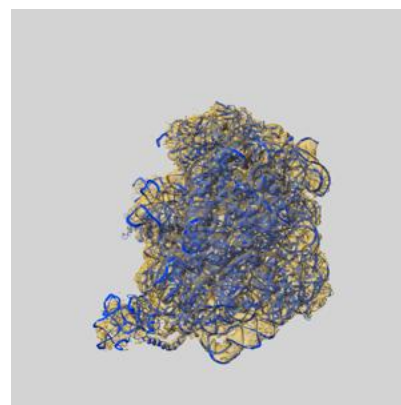
9.1 Map-model overlay [i](#)



X



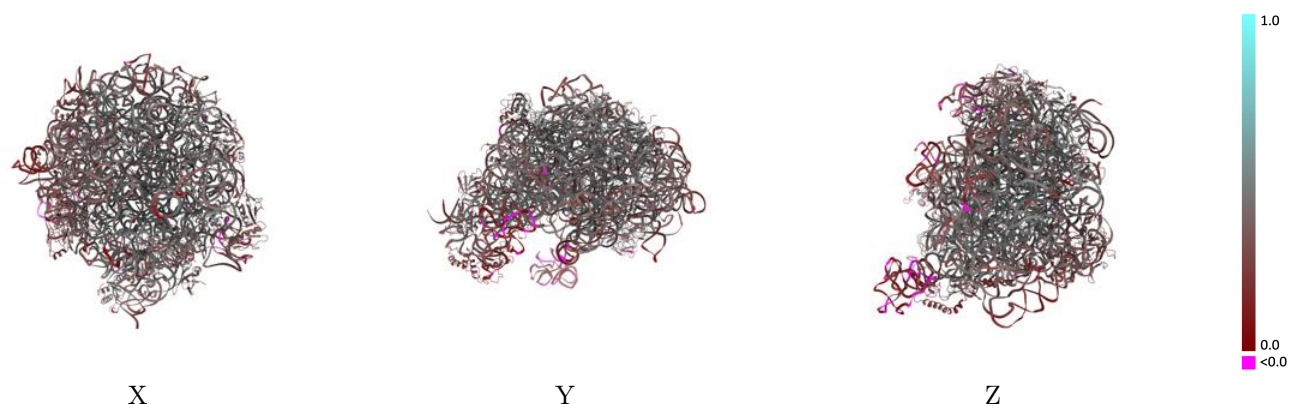
Y



Z

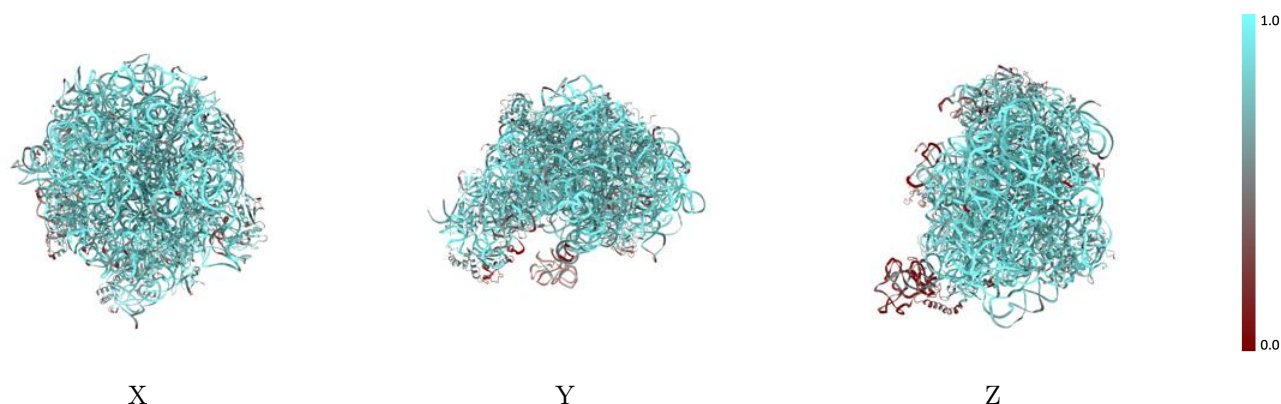
The images above show the 3D surface view of the map at the recommended contour level 0.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



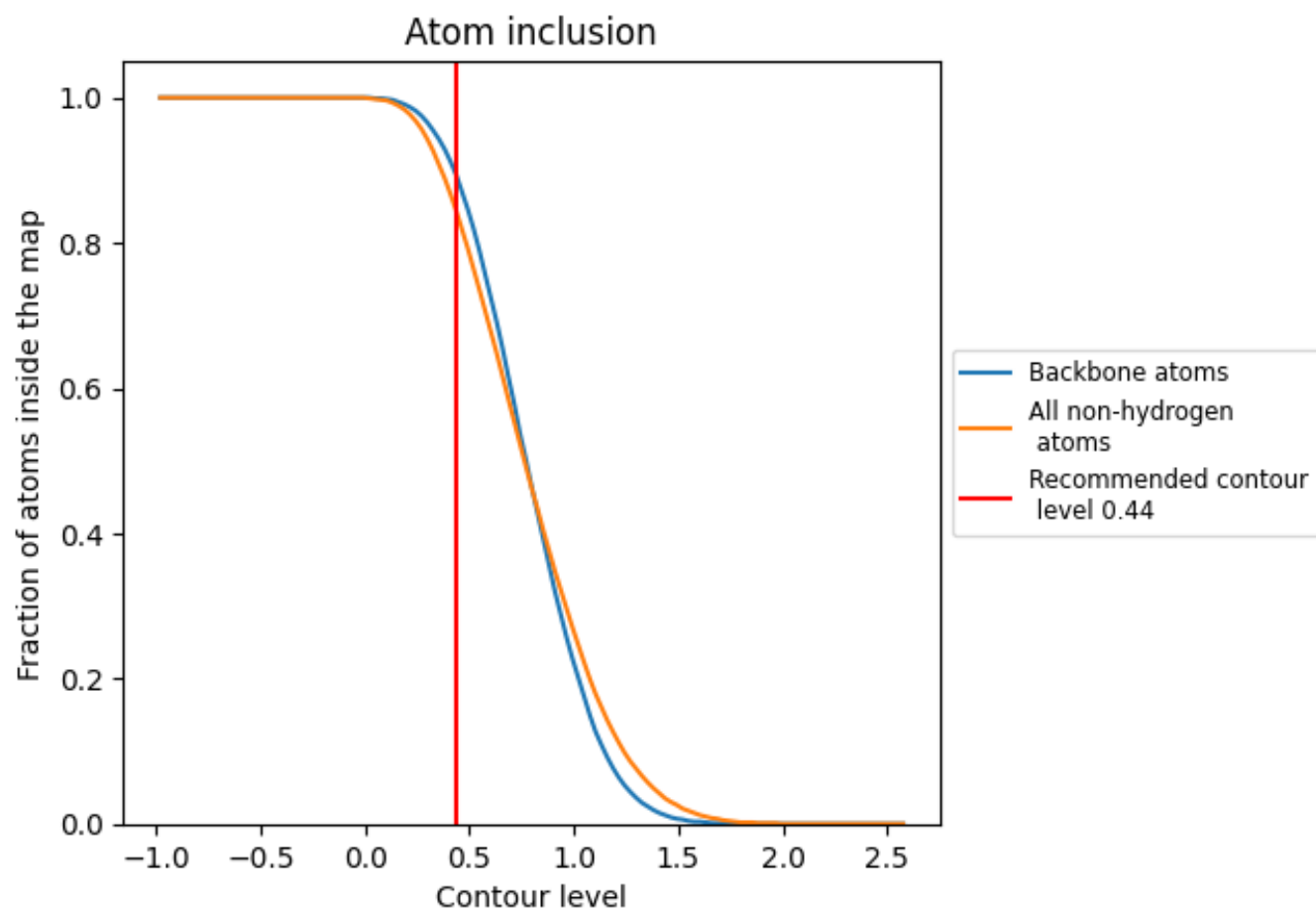
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.44).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.3940
0	 0.7850	 0.4310
1	 0.5090	 0.3950
2	 0.8820	 0.4790
3	 0.8150	 0.4510
4	 0.7600	 0.4280
A	 0.8870	 0.3980
B	 0.9000	 0.3810
C	 0.8250	 0.4440
D	 0.7660	 0.4340
E	 0.6840	 0.3560
F	 0.5050	 0.2500
G	 0.6580	 0.3300
H	 0.2890	 0.2260
J	 0.7980	 0.4420
K	 0.6350	 0.3530
L	 0.7020	 0.3530
M	 0.7900	 0.4430
N	 0.8190	 0.4410
O	 0.7280	 0.3640
P	 0.6350	 0.3660
Q	 0.8510	 0.4400
R	 0.7500	 0.4110
S	 0.7850	 0.4430
T	 0.7820	 0.4120
U	 0.7120	 0.3340
V	 0.7720	 0.3910
W	 0.7780	 0.4410
X	 0.8200	 0.4450
Y	 0.7060	 0.3120
Z	 0.7890	 0.4220

