



## wwPDB EM Validation Summary Report ⓘ

Jan 22, 2025 – 12:36 am GMT

PDB ID : 9H3X  
EMDB ID : EMD-51841  
Title : 50S subunit precursor C-CP\_H68\_L35  
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.  
Deposited on : 2024-10-17  
Resolution : 4.12 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](mailto: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>.

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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

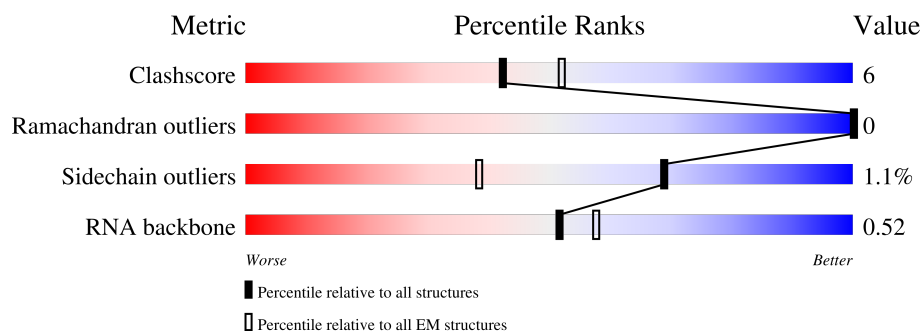
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.12 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  $\geq 3$ , 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>48%</div> <div>77%</div> <div>23%</div> </div>
2	1	50	<div> <div>74%</div> <div>80%</div> <div>20%</div> </div>
3	2	46	<div> <div>7%</div> <div>87%</div> <div>13%</div> </div>
4	3	64	<div> <div>41%</div> <div>84%</div> <div>16%</div> </div>
5	A	2903	<div> <div>7%</div> <div>56%</div> <div>29%</div> <div>5%</div> <div>9%</div> </div>
6	B	120	<div> <div>72%</div> <div>24%</div> <div>..</div> </div>
7	C	271	<div> <div>9%</div> <div>74%</div> <div>15%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
8	D	209	
9	E	201	
10	F	177	
11	H	149	
12	J	142	
13	K	122	
14	L	143	
15	N	120	
16	O	116	
17	P	114	
18	Q	117	
19	R	103	
20	S	110	
21	T	93	
22	U	102	
23	V	94	
24	W	76	
25	X	77	
26	Y	63	
27	Z	58	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 80353 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
			410	263	75	72		

- 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2637	Total	C	N	O	P	0	0
			56640	25266	10450	18287	2637		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	241	Total	C	N	O	S	0	0
			1859	1149	379	325	6		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	186	Total	C	N	O	S	0	0
			1393	880	250	259	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	190	Total	C	N	O	S	0	0
			1462	918	262	277	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 15 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 17 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 23 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 25 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	61	Total	C	N	O	S	0	0
			499	308	97	92	2		

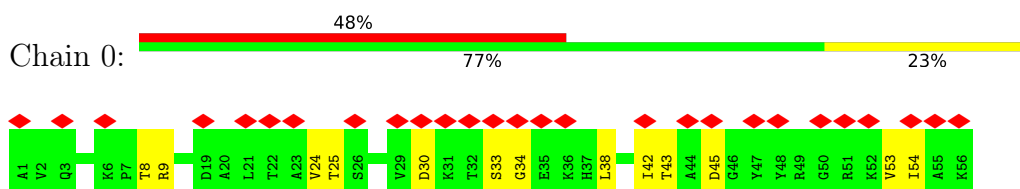
- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

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

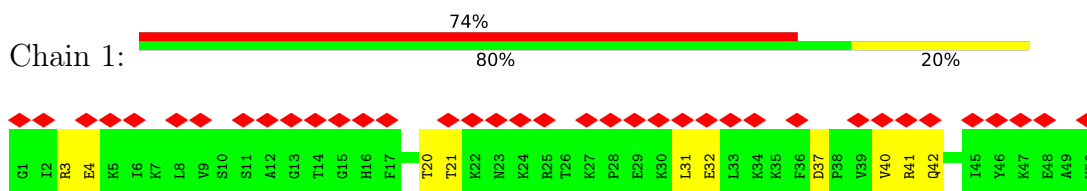
### 3 Residue-property plots

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.

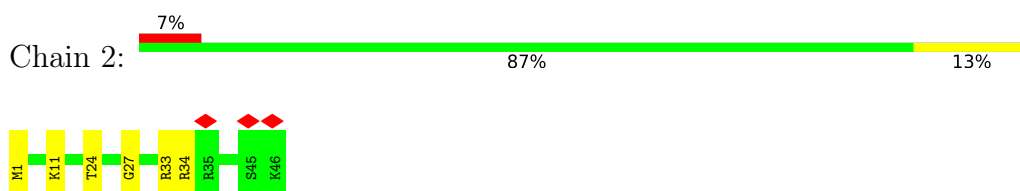
- Molecule 1: Large ribosomal subunit protein bL32



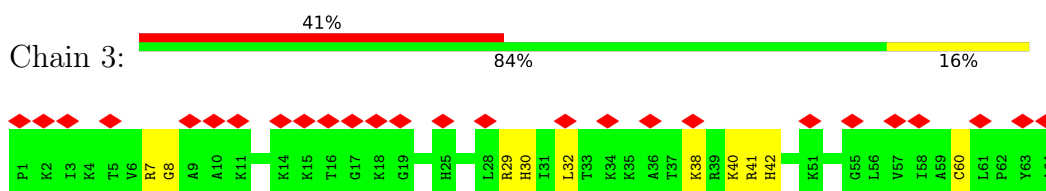
- Molecule 2: Large ribosomal subunit protein bL33



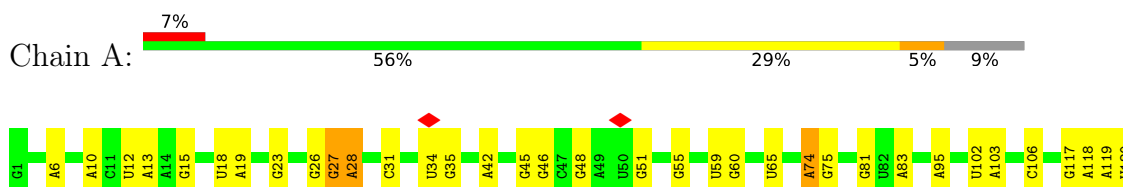
- Molecule 3: Large ribosomal subunit protein bL34



- Molecule 4: Large ribosomal subunit protein bL35



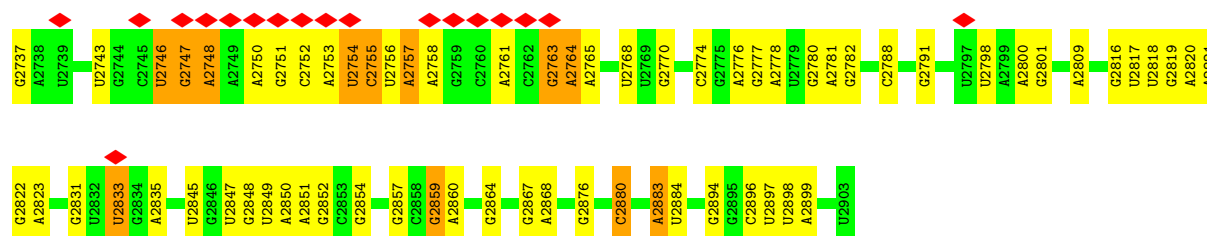
- Molecule 5: 23S ribosomal RNA



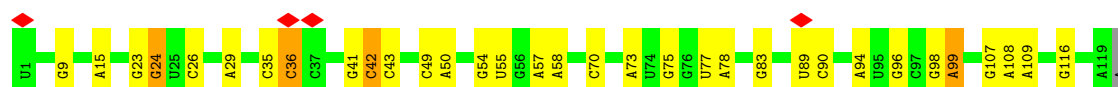




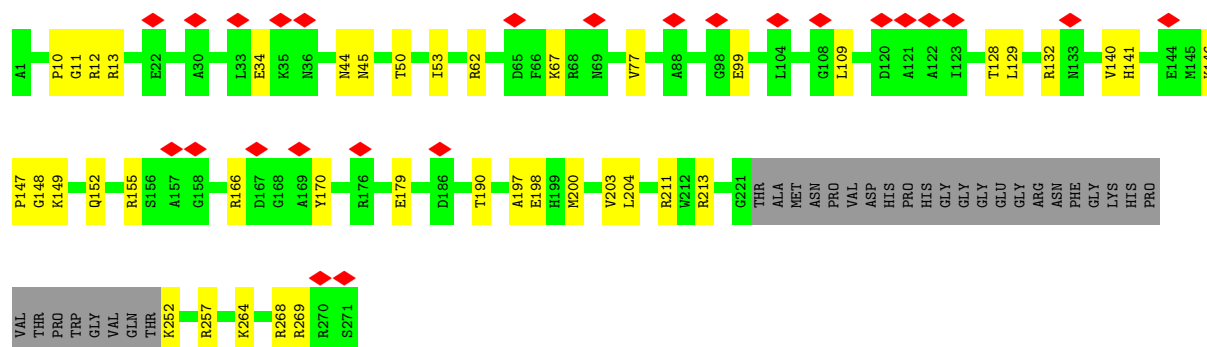
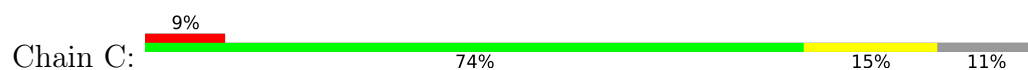




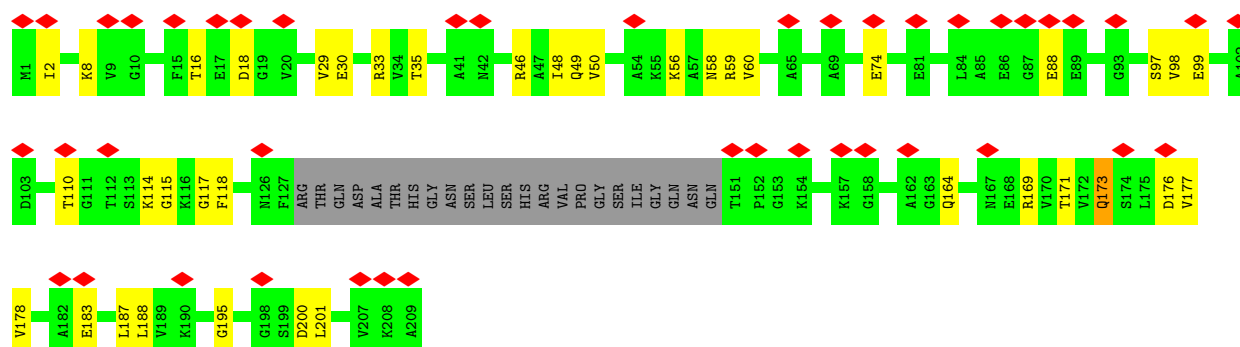
• Molecule 6: 5S ribosomal RNA



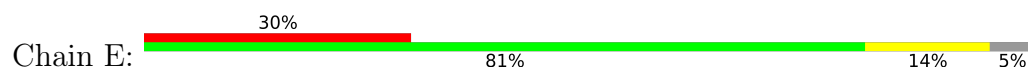
• Molecule 7: Large ribosomal subunit protein uL2



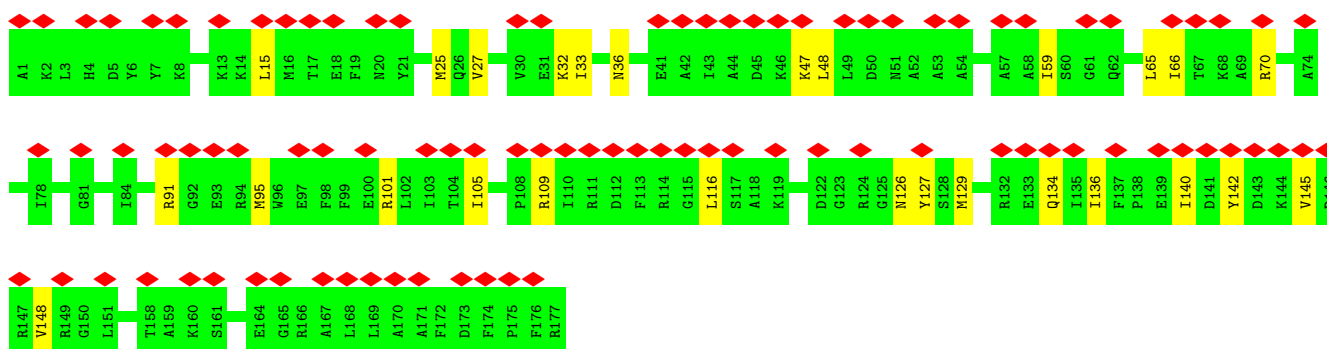
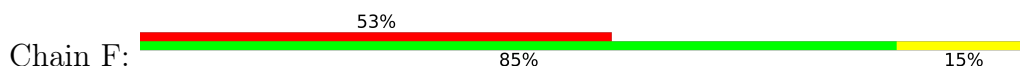
• Molecule 8: 50S ribosomal protein L3



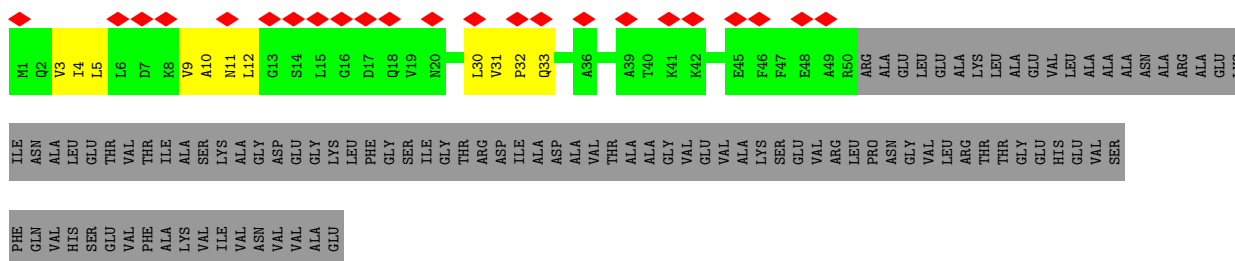
• Molecule 9: Large ribosomal subunit protein uL4



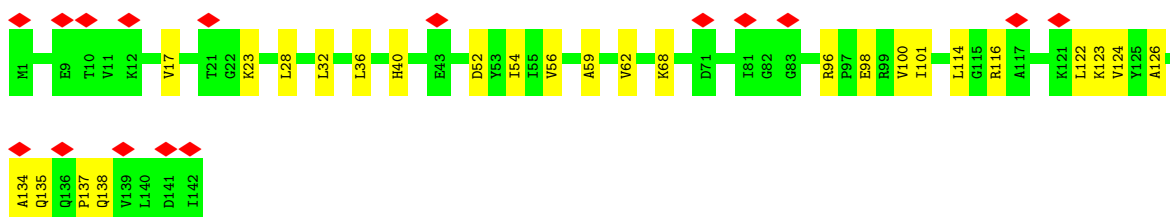
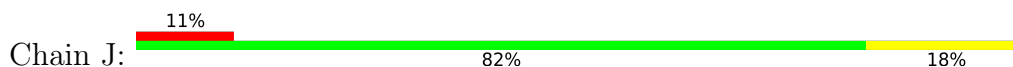
- Molecule 10: Large ribosomal subunit protein uL5



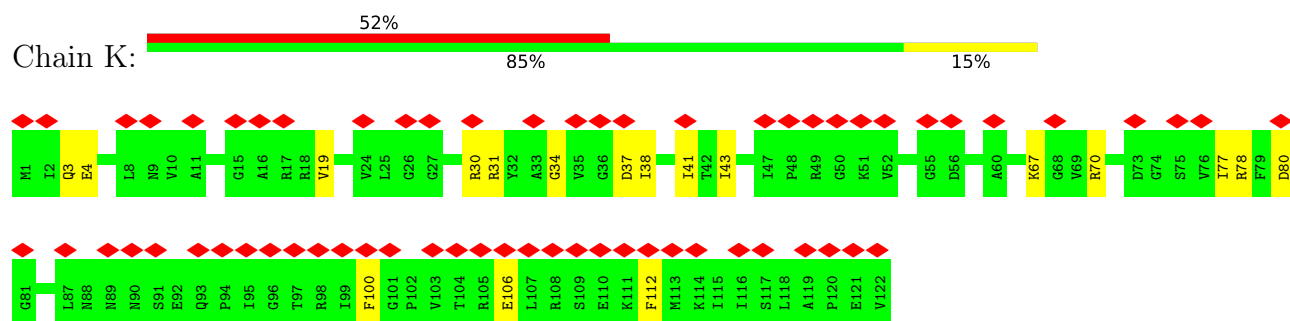
- Molecule 11: Large ribosomal subunit protein bL9



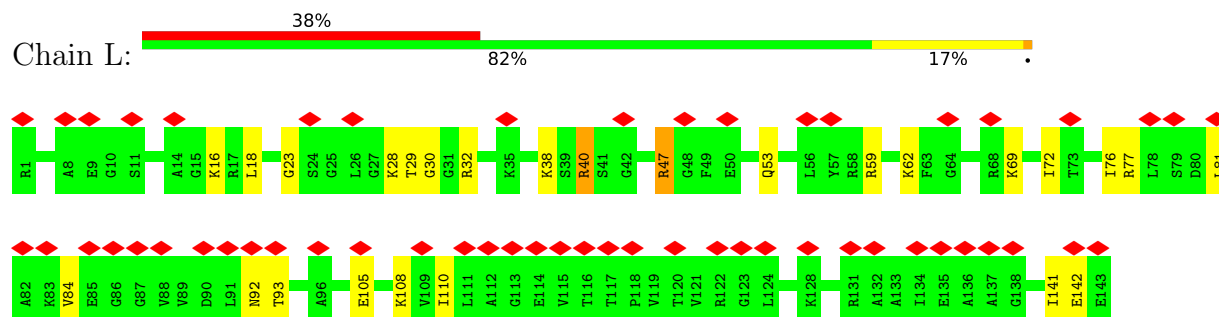
- Molecule 12: Large ribosomal subunit protein uL13



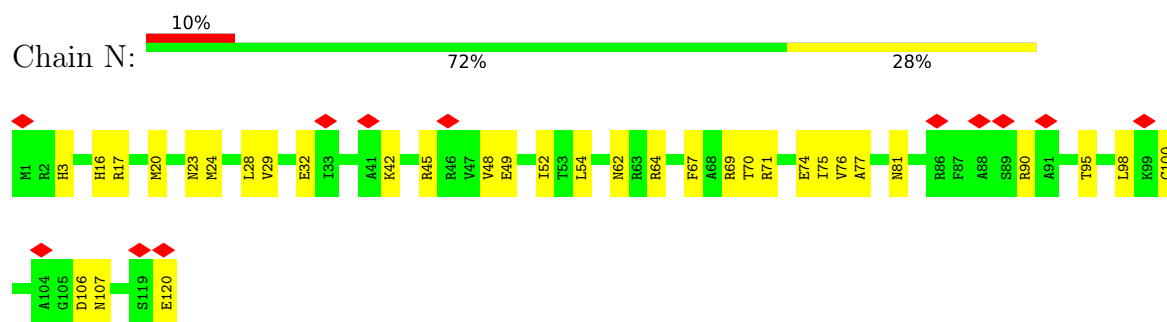
- Molecule 13: Large ribosomal subunit protein uL14



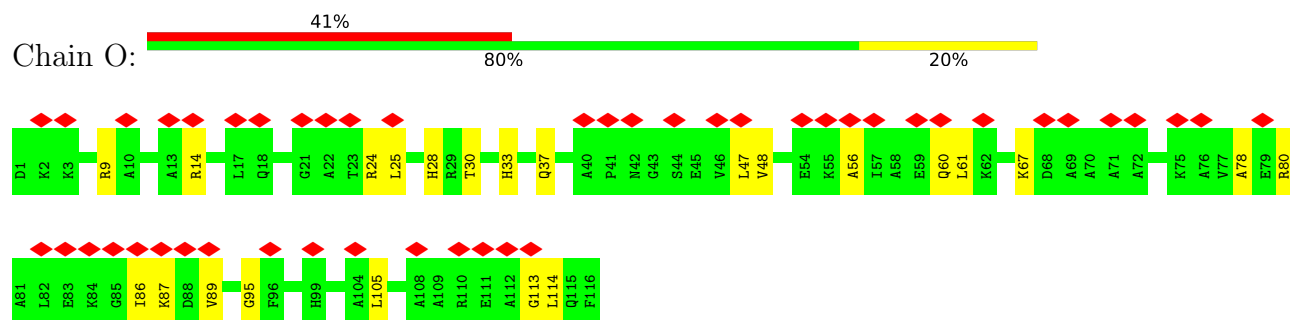
- Molecule 14: Large ribosomal subunit protein uL15



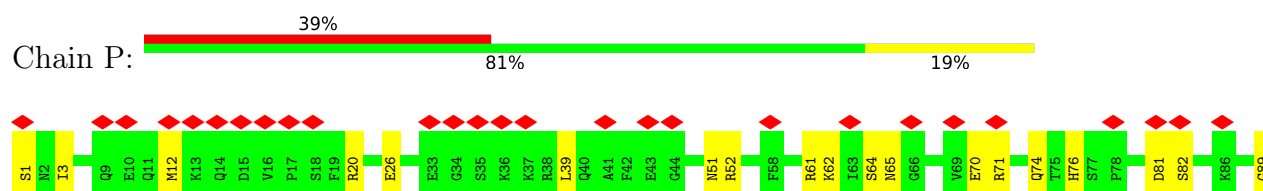
- Molecule 15: Large ribosomal subunit protein bL17

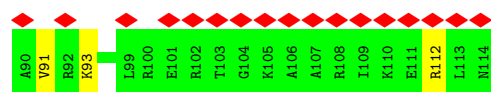


- Molecule 16: Large ribosomal subunit protein uL18

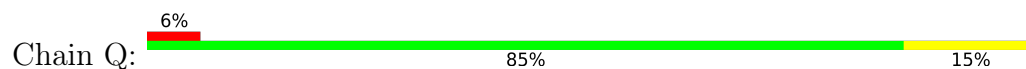


- Molecule 17: Large ribosomal subunit protein bL19

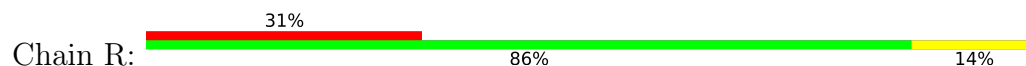




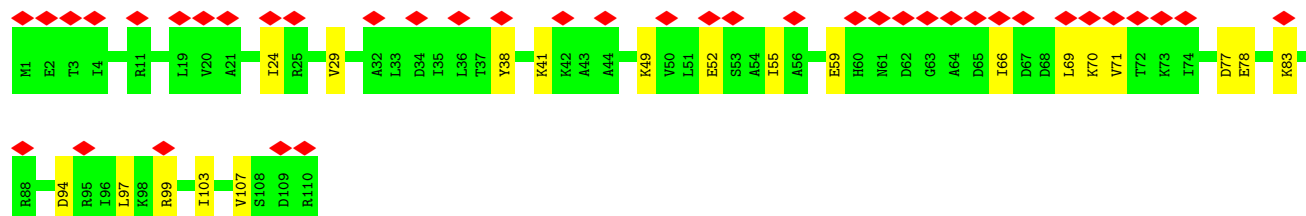
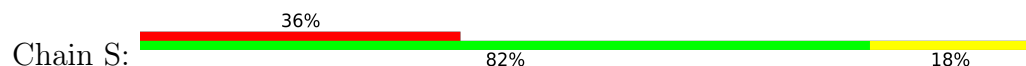
- Molecule 18: Large ribosomal subunit protein bL20



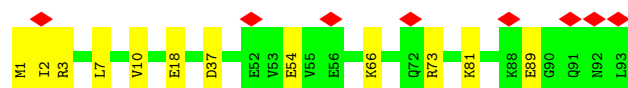
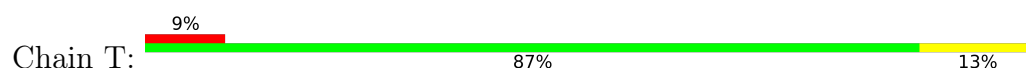
- Molecule 19: Large ribosomal subunit protein bL21



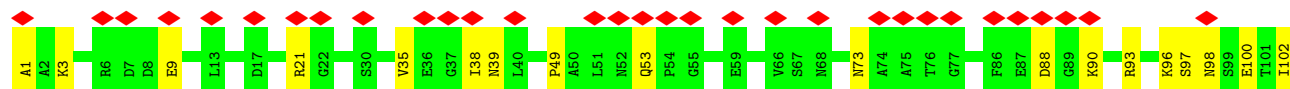
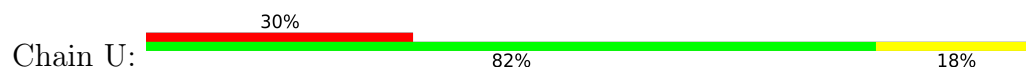
- Molecule 20: Large ribosomal subunit protein uL22



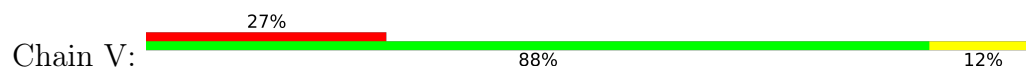
- Molecule 21: Large ribosomal subunit protein uL23

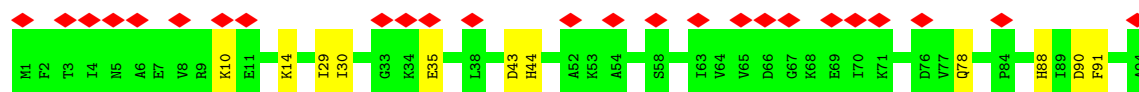


- Molecule 22: Large ribosomal subunit protein uL24

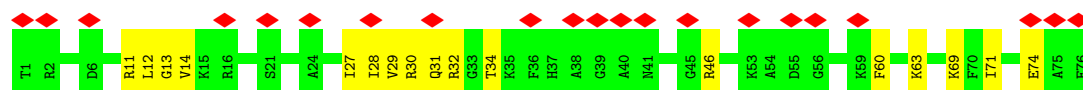
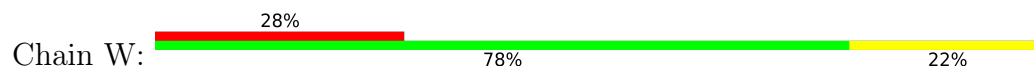


- Molecule 23: Large ribosomal subunit protein bL25





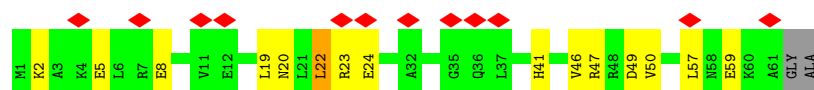
- Molecule 24: Large ribosomal subunit protein bL27



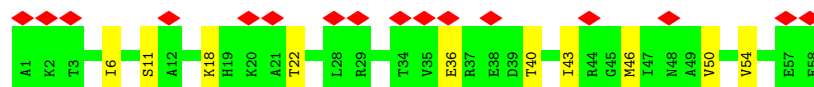
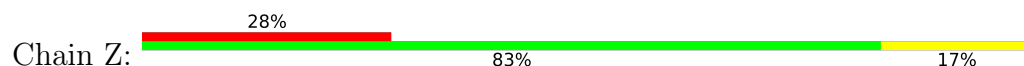
- Molecule 25: Large ribosomal subunit protein bL28



- Molecule 26: Large ribosomal subunit protein uL29



- Molecule 27: Large ribosomal subunit protein uL30



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9591	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	1.526	Depositor
Minimum map value	-0.490	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.437	Depositor
Map size (Å)	424.0, 424.0, 424.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4133333, 1.4133333, 1.4133333	Depositor



## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the 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	0.22	0/450	0.54	0/599
2	1	0.27	0/417	0.49	0/554
3	2	0.25	0/380	0.63	0/498
4	3	0.23	0/513	0.51	0/676
5	A	0.54	12/63442 (0.0%)	0.80	39/98971 (0.0%)
6	B	0.14	0/2847	0.71	0/4440
7	C	0.24	0/1887	0.55	0/2528
8	D	0.25	0/1410	0.51	0/1894
9	E	0.24	0/1477	0.48	0/1986
10	F	0.24	0/1435	0.50	0/1926
11	H	0.26	0/389	0.53	0/523
12	J	0.24	0/1152	0.49	0/1551
13	K	0.24	0/948	0.55	0/1268
14	L	0.25	0/1054	0.58	0/1403
15	N	0.24	0/974	0.58	0/1301
16	O	0.24	0/902	0.54	0/1209
17	P	0.24	0/929	0.53	0/1242
18	Q	0.24	0/960	0.52	0/1278
19	R	0.25	0/829	0.53	0/1107
20	S	0.23	0/864	0.51	0/1156
21	T	0.24	0/745	0.51	0/994
22	U	0.25	0/788	0.51	0/1051
23	V	0.24	0/766	0.47	0/1025
24	W	0.25	0/582	0.55	0/769
25	X	0.24	0/635	0.56	0/848
26	Y	0.25	0/500	0.53	0/665
27	Z	0.24	0/453	0.55	0/605
All	All	0.48	12/87728 (0.0%)	0.74	39/132067 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2721	A	C6-N1	66.27	1.81	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2721	A	N3-C4	60.72	1.71	1.34
5	A	2721	A	N1-C2	42.73	1.72	1.34
5	A	2721	A	C2-N3	39.52	1.69	1.33
5	A	2721	A	C5-C4	37.55	1.65	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2722	G	C8-N9-C4	-73.58	76.97	106.40
5	A	2722	G	N7-C8-N9	38.84	132.52	113.10
5	A	2722	G	N9-C4-C5	37.11	120.25	105.40
5	A	2721	A	N1-C2-N3	-29.63	114.49	129.30
5	A	2722	G	N3-C4-C5	-26.37	115.41	128.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	12	0
2	1	410	0	443	9	0
3	2	377	0	418	6	0
4	3	504	0	574	11	0
5	A	56640	0	28485	534	0
6	B	2546	0	1292	21	0
7	C	1859	0	1952	32	0
8	D	1393	0	1454	27	0
9	E	1462	0	1523	21	0
10	F	1411	0	1447	22	0
11	H	384	0	405	10	0
12	J	1129	0	1162	21	0
13	K	939	0	1012	15	0
14	L	1045	0	1120	22	0
15	N	961	0	1000	24	0
16	O	892	0	926	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	917	0	965	17	0
18	Q	947	0	1022	12	0
19	R	816	0	839	9	0
20	S	857	0	922	20	0
21	T	739	0	807	10	0
22	U	780	0	834	12	0
23	V	753	0	780	6	0
24	W	575	0	592	18	0
25	X	625	0	655	18	0
26	Y	499	0	535	11	0
27	Z	449	0	491	10	0
All	All	80353	0	52116	821	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 821 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)
5:A:2721:A:C2	5:A:2722:G:H1'	1.25	1.64
5:A:2721:A:C2	5:A:2721:A:N3	1.69	1.60
5:A:2721:A:N3	5:A:2721:A:C4	1.71	1.58
5:A:2721:A:C2	5:A:2721:A:N1	1.72	1.55
5:A:2721:A:N1	5:A:2721:A:C6	1.81	1.48

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%)	51 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	48/50 (96%)	48 (100%)	0	0	100	100
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
4	3	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
7	C	237/271 (88%)	224 (94%)	13 (6%)	0	100	100
8	D	182/209 (87%)	176 (97%)	6 (3%)	0	100	100
9	E	186/201 (92%)	184 (99%)	2 (1%)	0	100	100
10	F	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
11	H	48/149 (32%)	42 (88%)	6 (12%)	0	100	100
12	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
13	K	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
14	L	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
15	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
16	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
17	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
18	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
20	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
21	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
22	U	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
23	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
24	W	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
25	X	75/77 (97%)	75 (100%)	0	0	100	100
26	Y	59/63 (94%)	54 (92%)	5 (8%)	0	100	100
27	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
All	All	2652/2873 (92%)	2526 (95%)	126 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	47 (100%)	0	100	100
2	1	45/45 (100%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/51 (100%)	51 (100%)	0	100	100
7	C	193/216 (89%)	193 (100%)	0	100	100
8	D	145/164 (88%)	142 (98%)	3 (2%)	48	66
9	E	157/165 (95%)	154 (98%)	3 (2%)	52	69
10	F	148/148 (100%)	147 (99%)	1 (1%)	81	86
11	H	40/114 (35%)	40 (100%)	0	100	100
12	J	116/116 (100%)	116 (100%)	0	100	100
13	K	103/103 (100%)	102 (99%)	1 (1%)	73	81
14	L	102/102 (100%)	100 (98%)	2 (2%)	50	68
15	N	100/100 (100%)	98 (98%)	2 (2%)	50	68
16	O	86/86 (100%)	84 (98%)	2 (2%)	45	64
17	P	99/99 (100%)	99 (100%)	0	100	100
18	Q	89/89 (100%)	88 (99%)	1 (1%)	70	80
19	R	84/84 (100%)	81 (96%)	3 (4%)	30	53
20	S	93/93 (100%)	93 (100%)	0	100	100
21	T	80/80 (100%)	80 (100%)	0	100	100
22	U	83/83 (100%)	83 (100%)	0	100	100
23	V	78/78 (100%)	76 (97%)	2 (3%)	41	61
24	W	56/58 (97%)	55 (98%)	1 (2%)	54	71
25	X	67/67 (100%)	67 (100%)	0	100	100
26	Y	55/55 (100%)	52 (94%)	3 (6%)	18	42
27	Z	48/48 (100%)	48 (100%)	0	100	100
All	All	2203/2329 (95%)	2179 (99%)	24 (1%)	69	80

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Q	35	PHE
19	R	46	GLU

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Mol	Chain	Res	Type
19	R	40	MET
23	V	10	LYS
10	F	25	MET

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

Mol	Chain	Res	Type
14	L	34	HIS
15	N	23	ASN
23	V	44	HIS
15	N	81	ASN
10	F	126	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2632/2903 (90%)	468 (17%)	20 (0%)
6	B	118/120 (98%)	12 (10%)	0
All	All	2750/3023 (90%)	480 (17%)	20 (0%)

5 of 480 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	A
5	A	12	U
5	A	26	G
5	A	27	G
5	A	28	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	2140	G
5	A	2746	U
5	A	2763	G
5	A	2754	U
5	A	1126	A

## 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.

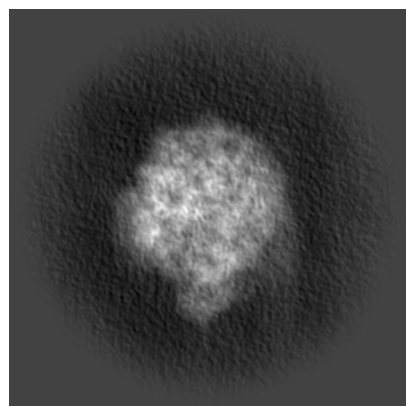
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51841. These allow visual inspection of the internal detail of the map and identification of artifacts.

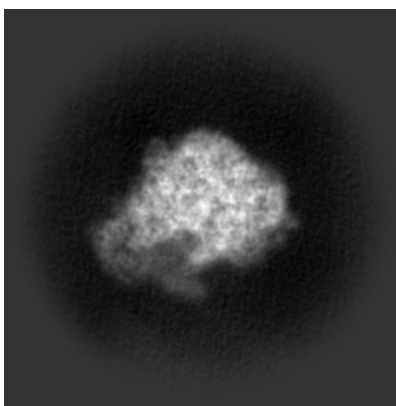
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

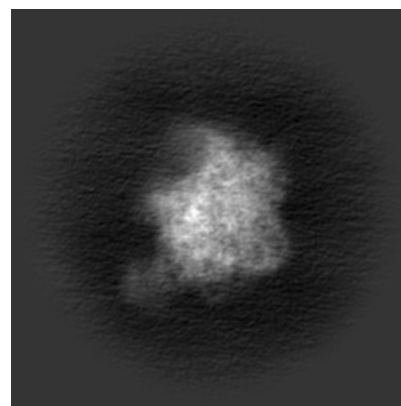
#### 6.1.1 Primary map



X

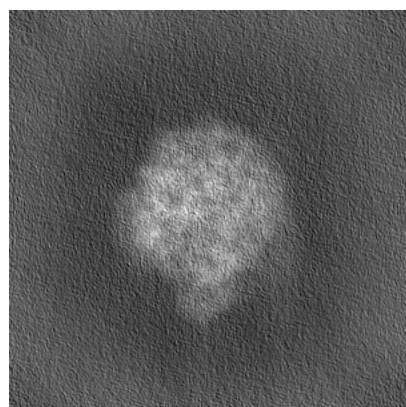


Y

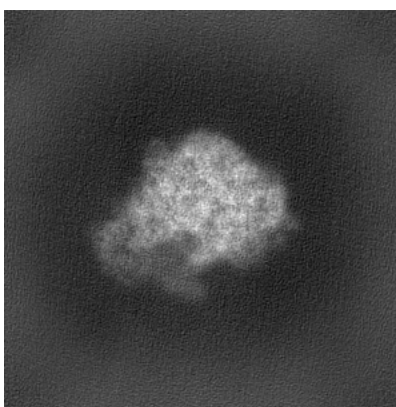


Z

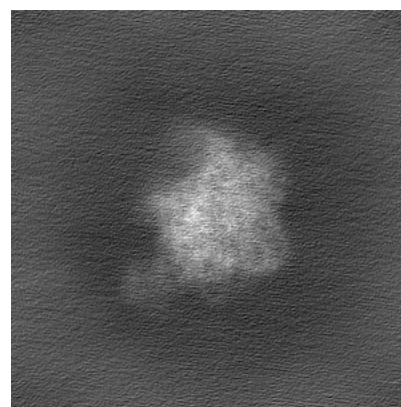
#### 6.1.2 Raw map



X



Y



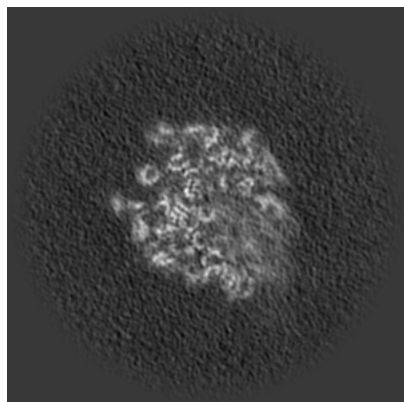
Z

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

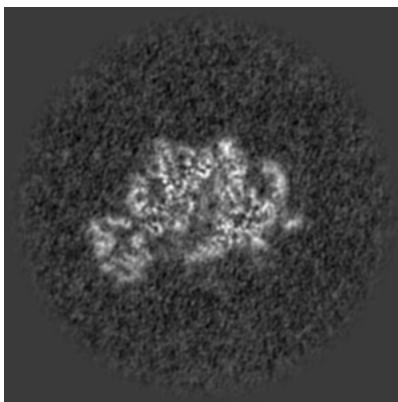


## 6.2 Central slices [i](#)

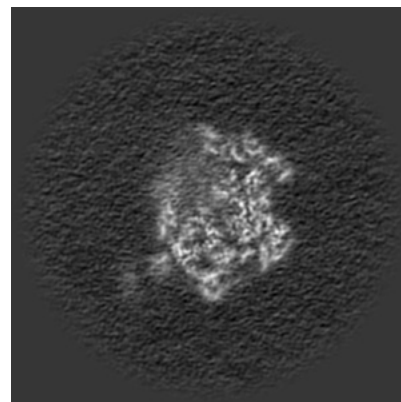
### 6.2.1 Primary map



X Index: 150

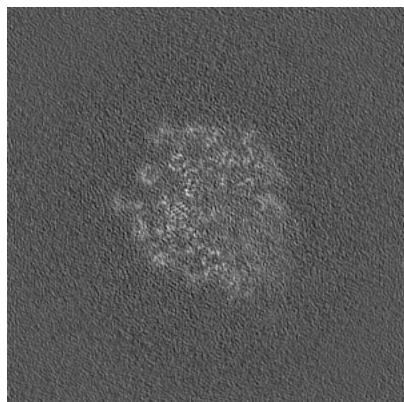


Y Index: 150

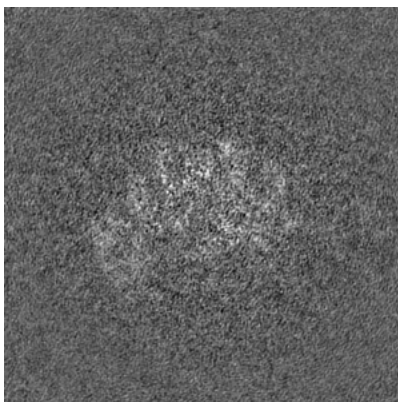


Z Index: 150

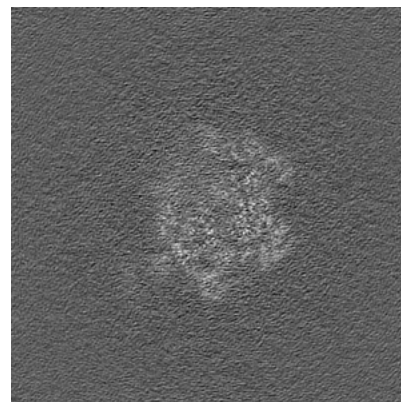
### 6.2.2 Raw map



X Index: 150



Y Index: 150

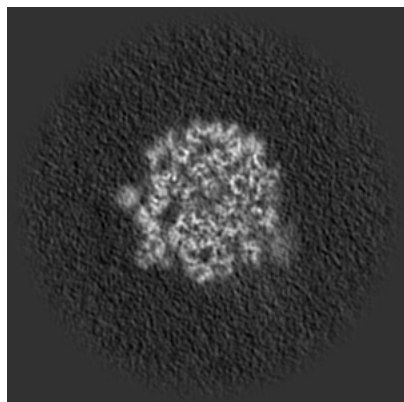


Z Index: 150

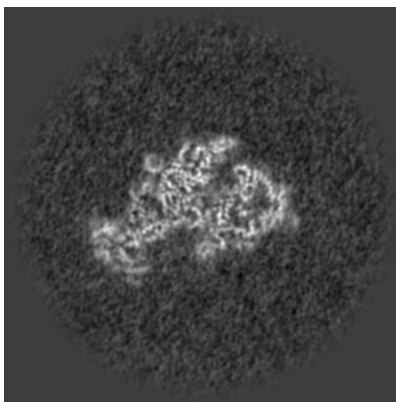
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

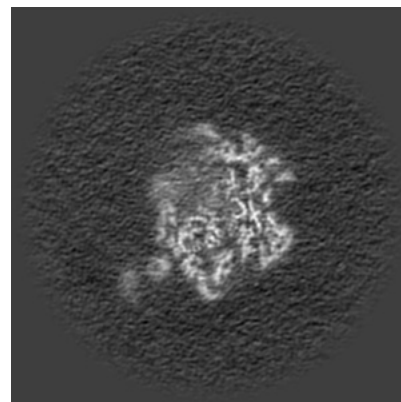
### 6.3.1 Primary map



X Index: 162

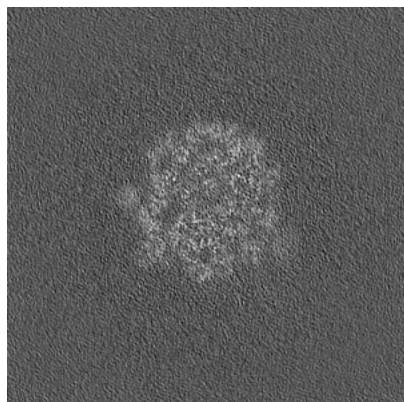


Y Index: 142

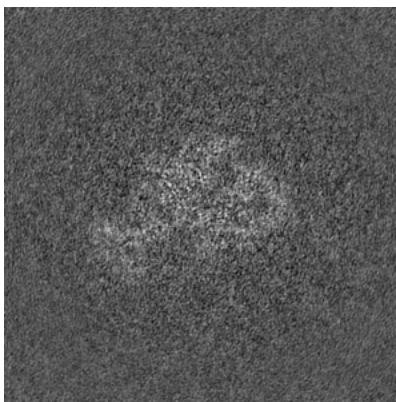


Z Index: 148

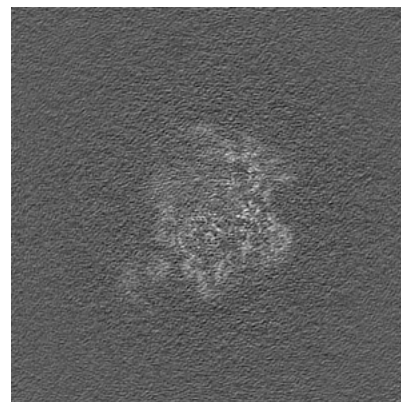
### 6.3.2 Raw map



X Index: 162



Y Index: 142

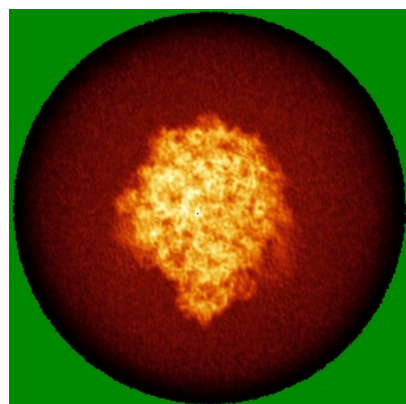


Z Index: 147

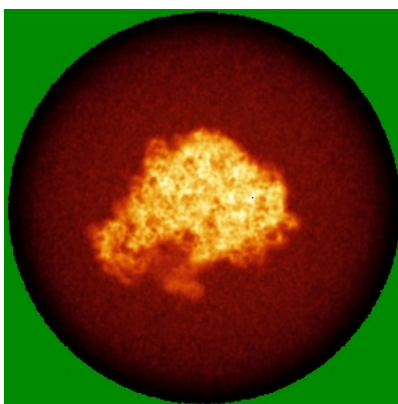
The images above show the largest variance slices of the map in three orthogonal directions.

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

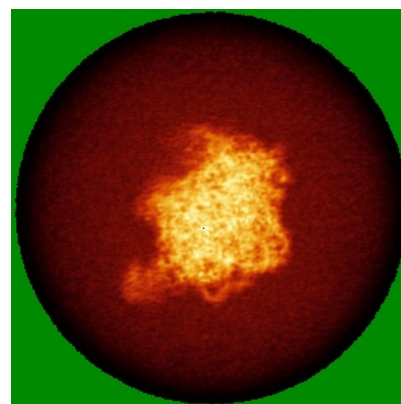
### 6.4.1 Primary map



X

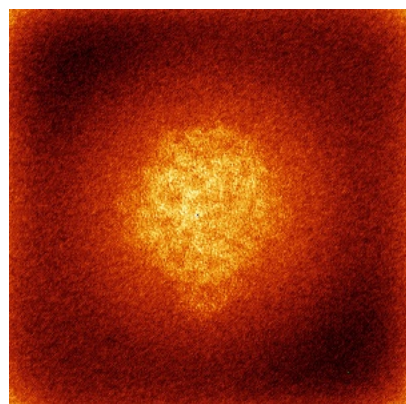


Y

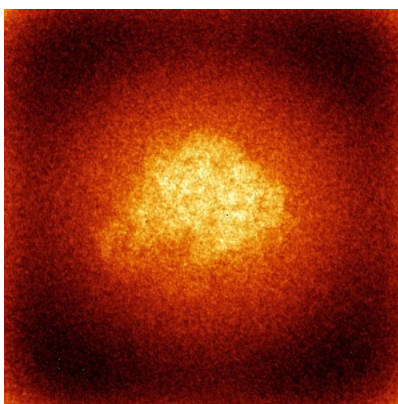


Z

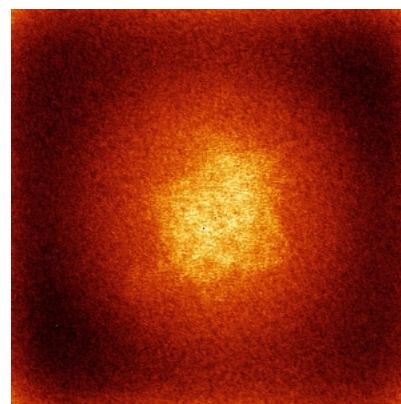
### 6.4.2 Raw map



X



Y



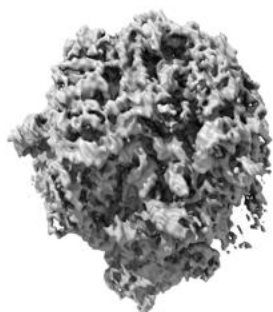
Z

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



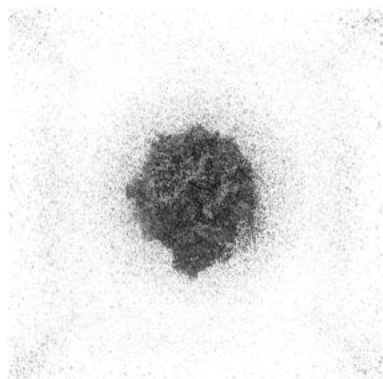
Y



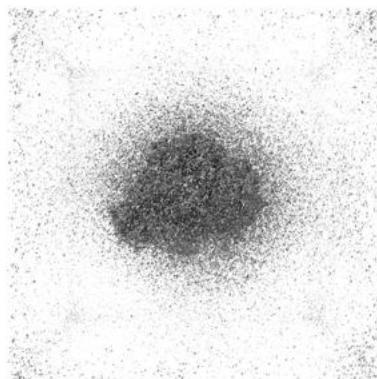
Z

The images above show the 3D surface view of the map at the recommended contour level 0.437. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

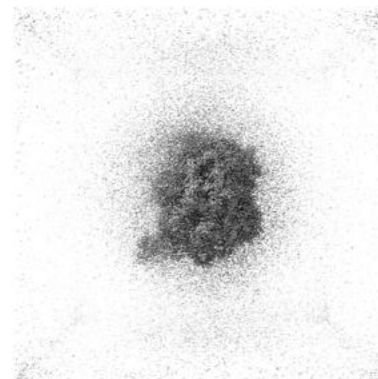
### 6.5.2 Raw map



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.

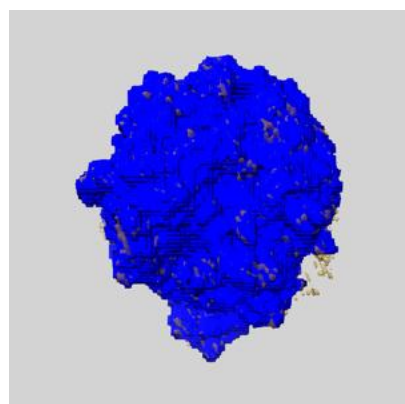
## 6.6 Mask visualisation [i](#)

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

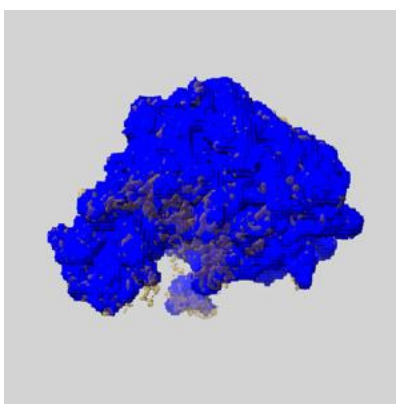
A mask typically either:

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

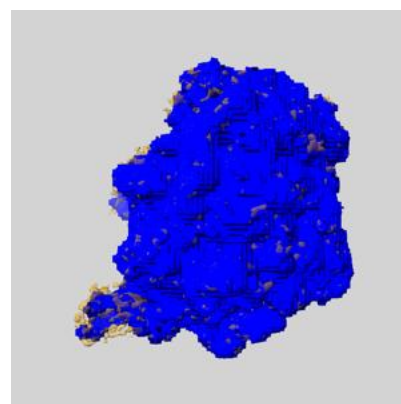
### 6.6.1 emd\_51841\_msk\_1.map [i](#)



X



Y

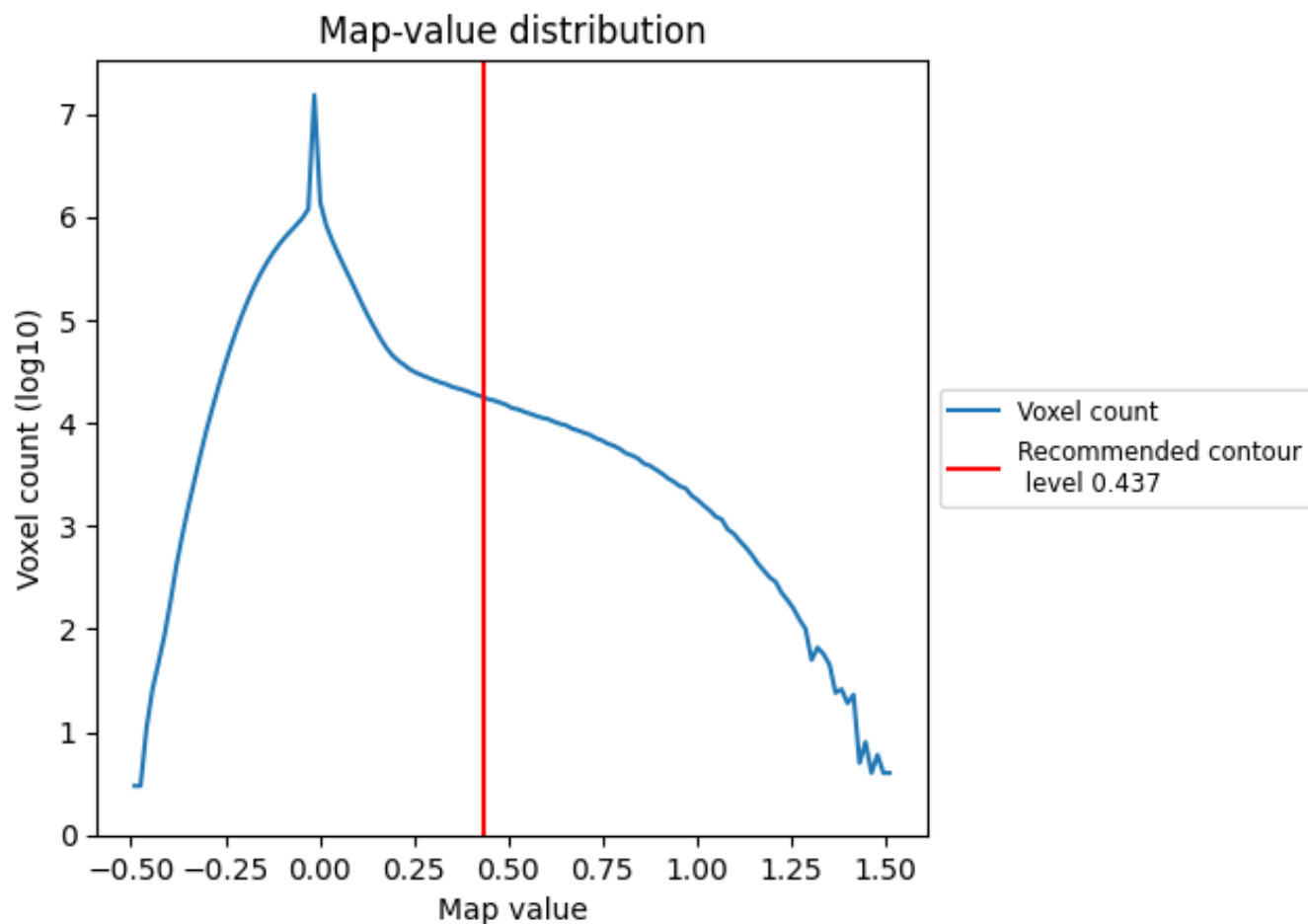


Z

## 7 Map analysis [i](#)

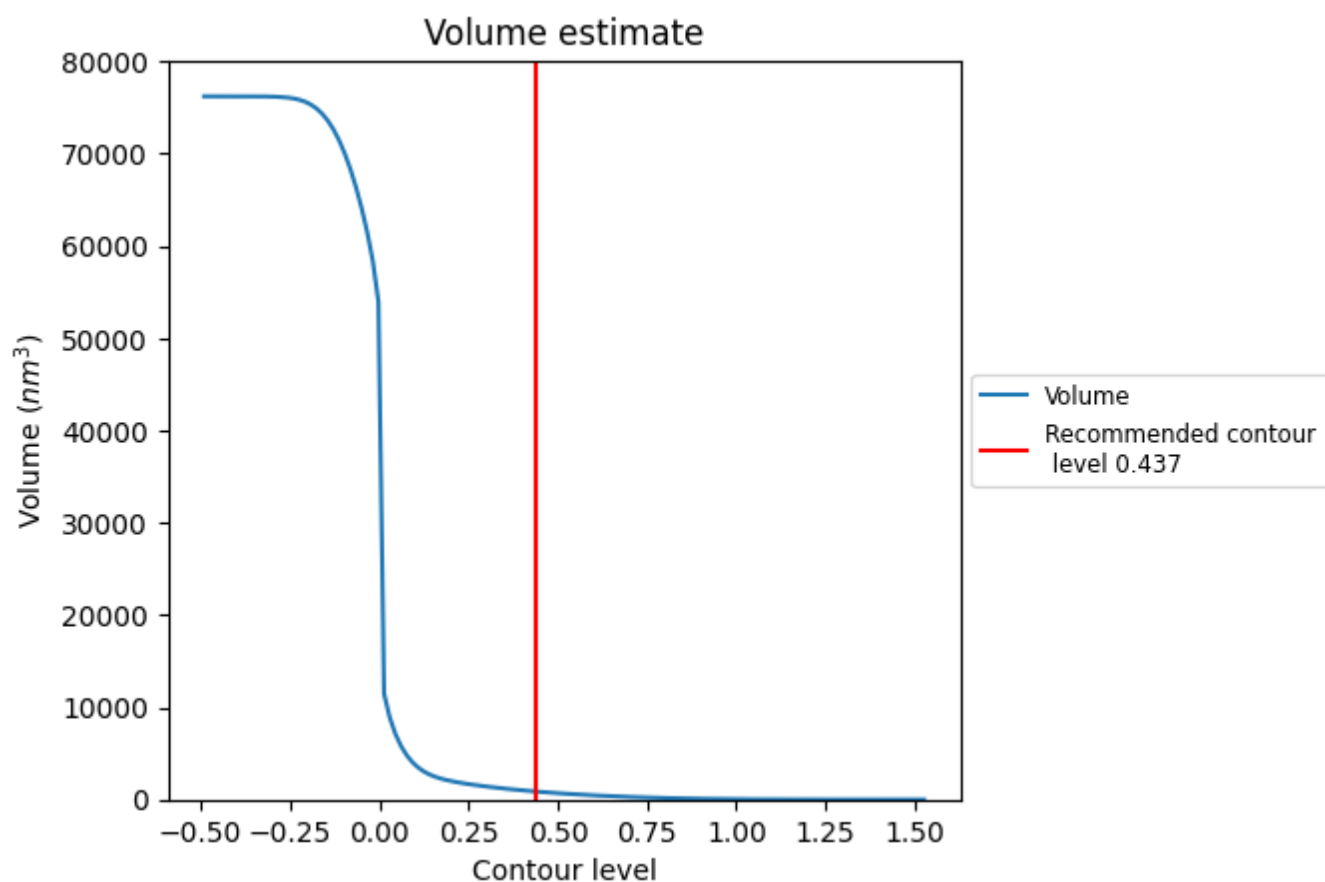
This section contains the results of statistical analysis of the map.

### 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.

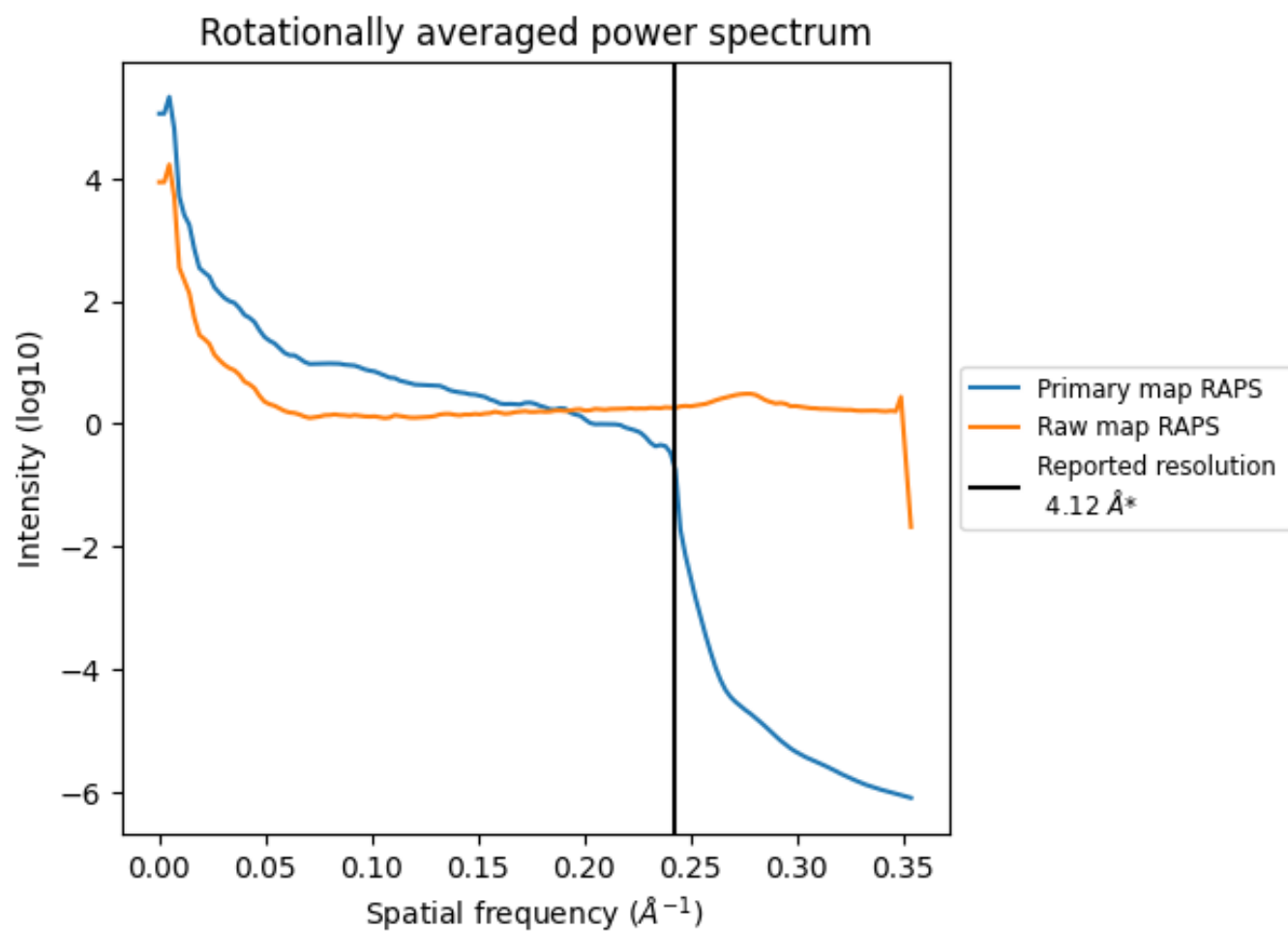
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 875 nm<sup>3</sup>; this corresponds to an approximate mass of 790 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 ⓘ



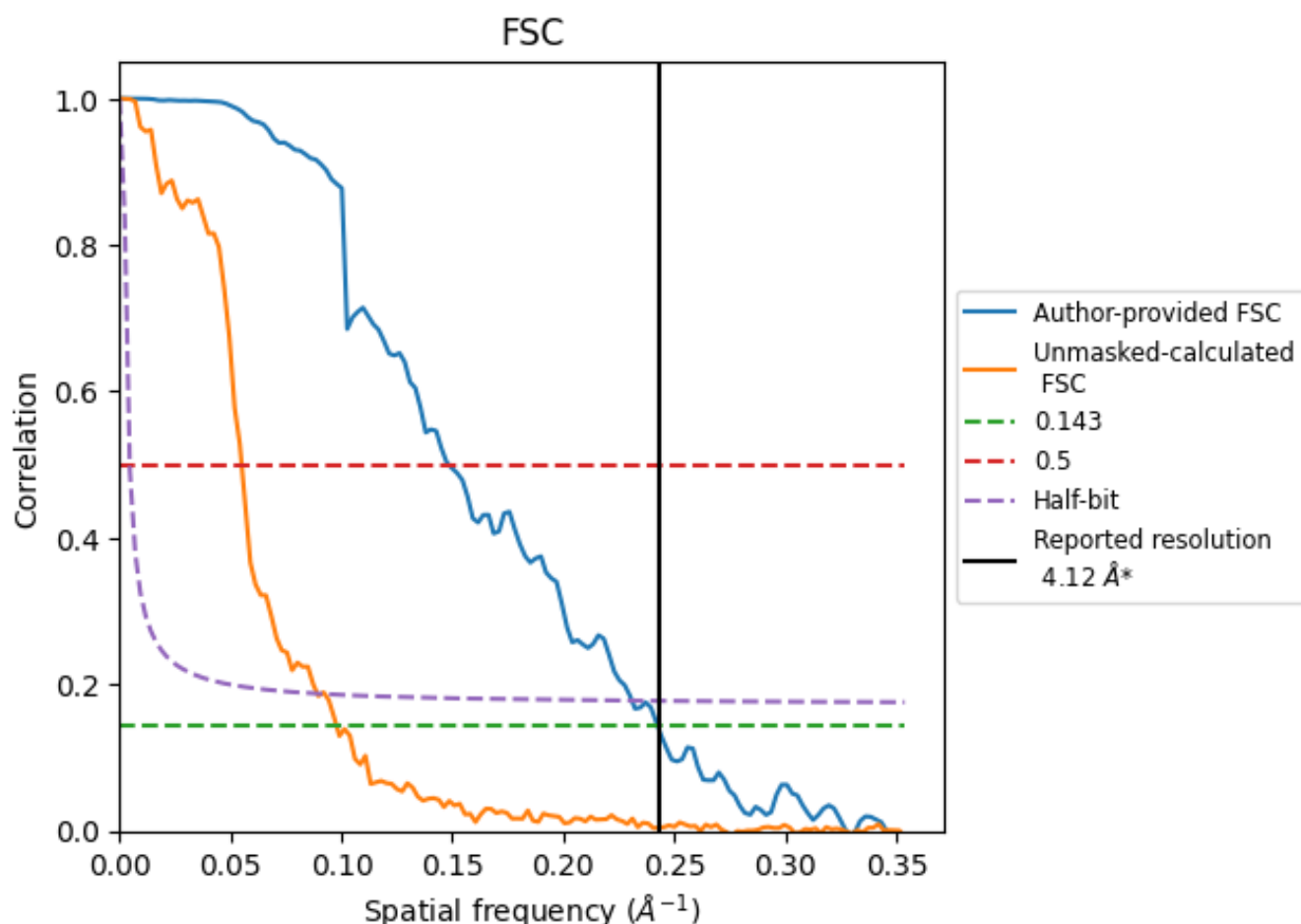
\*Reported resolution corresponds to spatial frequency of 0.243  $\text{\AA}^{-1}$



## 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 0.243 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

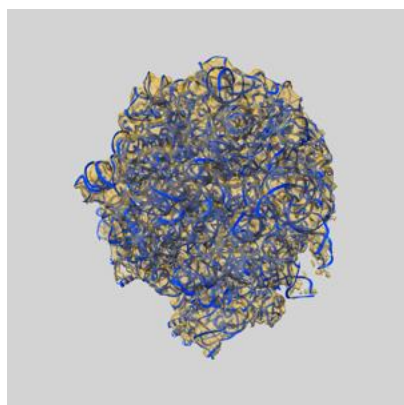
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.12	-	-
Author-provided FSC curve	4.12	6.74	4.33
Unmasked-calculated*	10.22	18.15	11.22

\*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 10.22 differs from the reported value 4.12 by more than 10 %

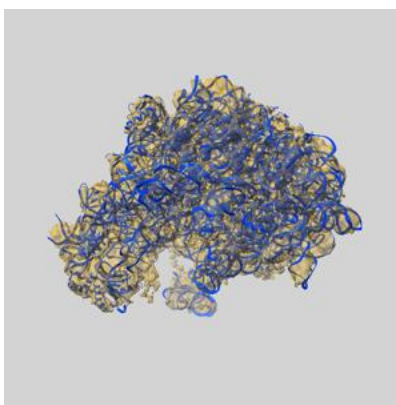
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51841 and PDB model 9H3X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

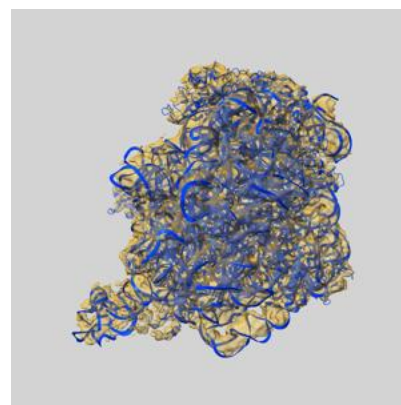
### 9.1 Map-model overlay [i](#)



X



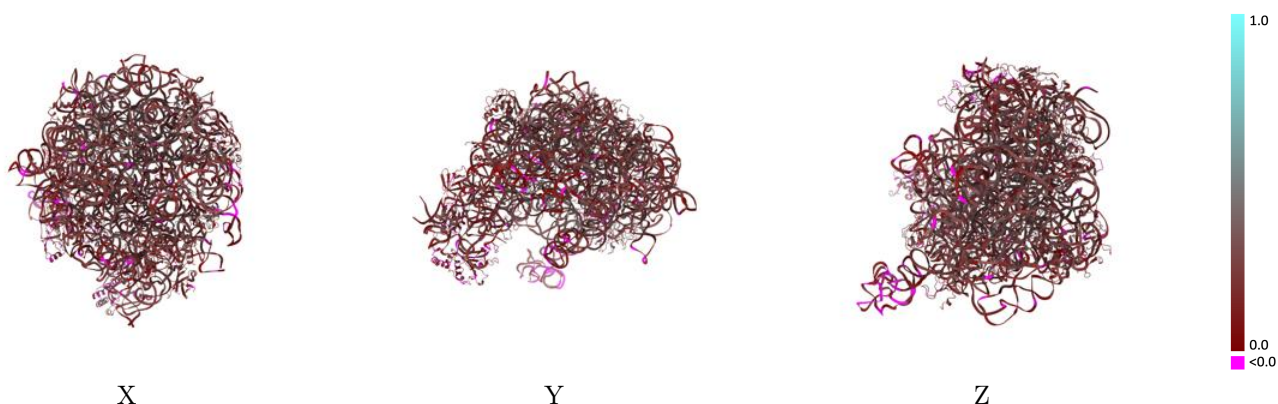
Y



Z

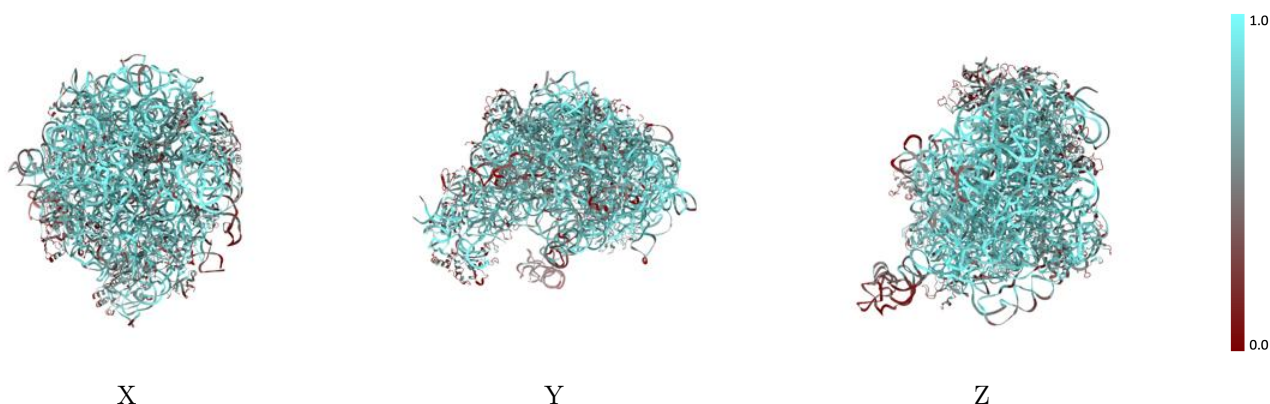
The images above show the 3D surface view of the map at the recommended contour level 0.437 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



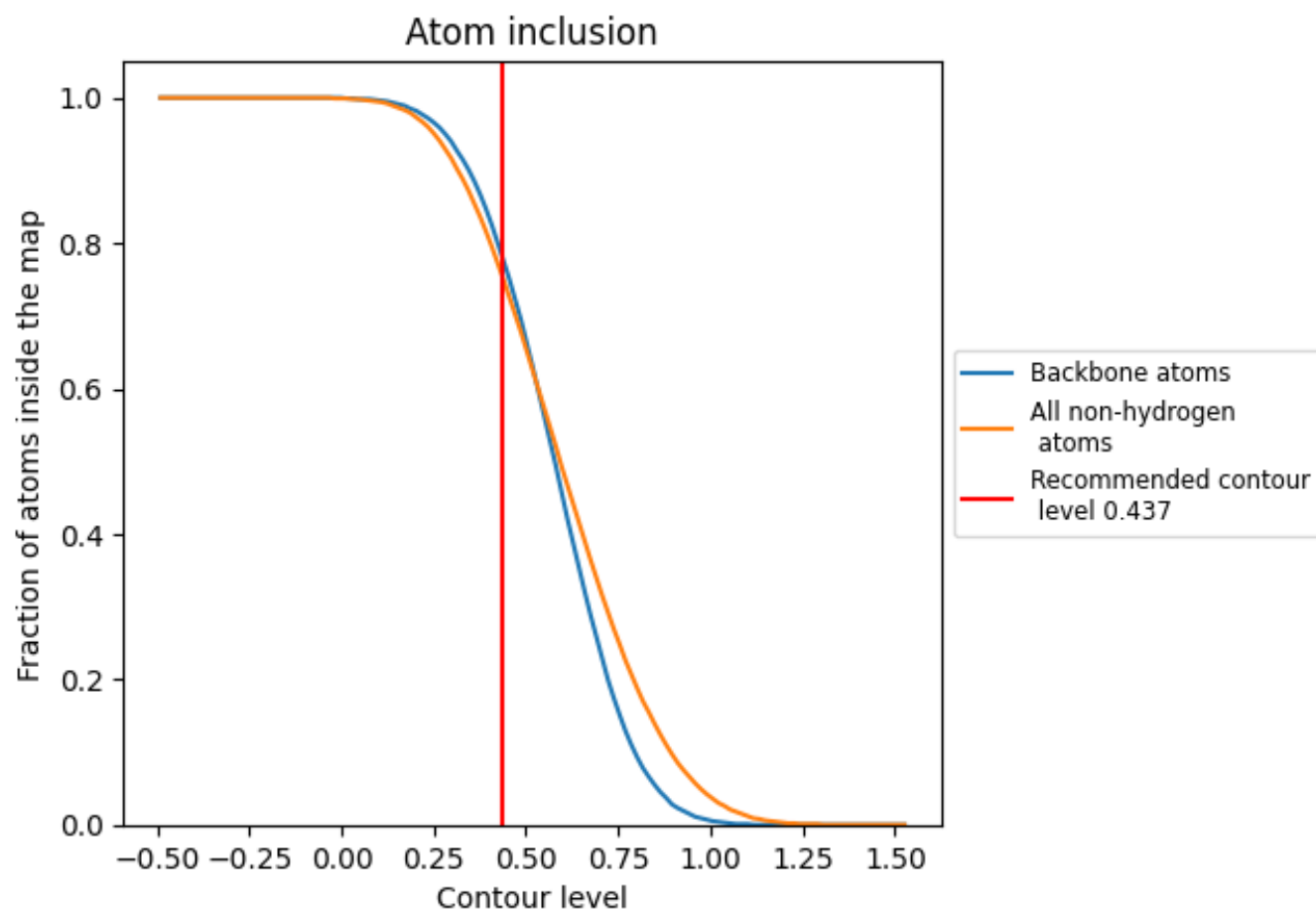
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.437).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 75% 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 (0.437) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.2300
0	 0.4110	 0.2120
1	 0.2460	 0.1570
2	 0.7270	 0.2750
3	 0.5110	 0.1980
A	 0.8190	 0.2370
B	 0.8270	 0.1900
C	 0.6930	 0.2580
D	 0.5750	 0.2460
E	 0.5390	 0.2020
F	 0.4000	 0.1300
H	 0.4510	 0.1840
J	 0.6820	 0.2690
K	 0.3960	 0.1990
L	 0.5070	 0.1870
N	 0.7040	 0.2690
O	 0.5140	 0.1400
P	 0.5070	 0.1960
Q	 0.7140	 0.2680
R	 0.5340	 0.2200
S	 0.4870	 0.2580
T	 0.6850	 0.2630
U	 0.5650	 0.2070
V	 0.5580	 0.2140
W	 0.5580	 0.1780
X	 0.6740	 0.2650
Y	 0.5870	 0.1930
Z	 0.5900	 0.2140

