



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 01:17 AM UTC

PDB ID : 6HMA / pdb_00006hma
EMDB ID : EMD-0243
Title : Improved model derived from cryo-EM map of Staphylococcus aureus large ribosomal subunit
Authors : Eyal, Z.; Camicata, G.; Matzov, D.; Fox, T.; de Val, N.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2018-09-12
Resolution : 2.65 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:

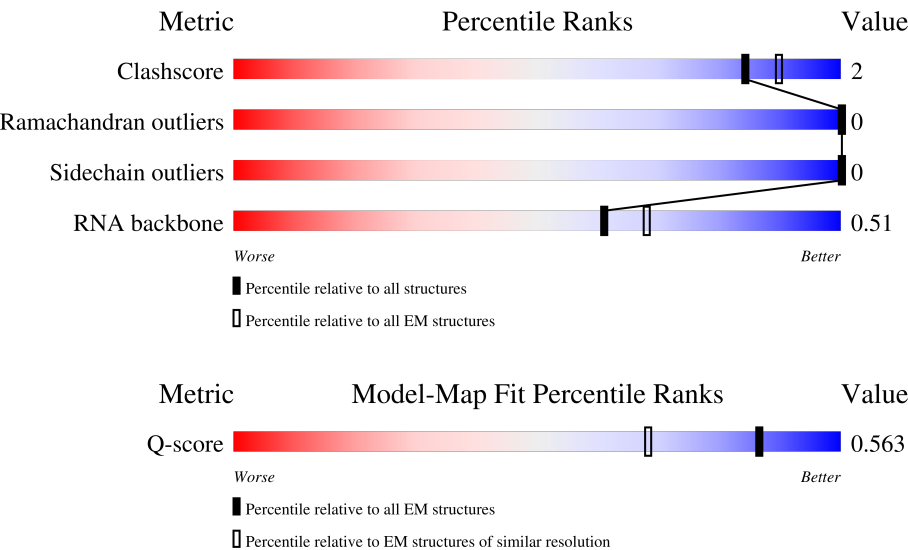
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.65 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	9050 (2.15 - 3.15)

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	A	2923	
2	B	115	
3	C	274	

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Mol	Chain	Length	Quality of chain
4	D	215	
5	E	206	
6	F	158	
7	G	175	
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	119	
14	N	116	
15	O	116	
16	P	102	
17	Q	112	
18	R	89	
19	S	103	
20	T	94	
21	U	79	
22	V	49	
23	W	67	
24	X	58	
25	Z	48	
26	1	47	
27	2	43	
28	3	64	

Continued on next page...

Mol	Chain	Length	Quality of chain
29	4	37	32% 84% 16%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 86401 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2834	Total	C	N	O	P	0	0
			60769	27128	11118	19689	2834		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2448	1094	436	803	115		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O		0	0
			778	462	158	158			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1263	790	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	119	Total	C	N	O	0	0
			882	549	174	159		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	114	Total	C	N	O	0	0
			889	563	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			854	534	164	153	3		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	79	Total	C	N	O	0	0
			597	369	117	111		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	49	Total	C	N	O	0	0
			379	234	82	63		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

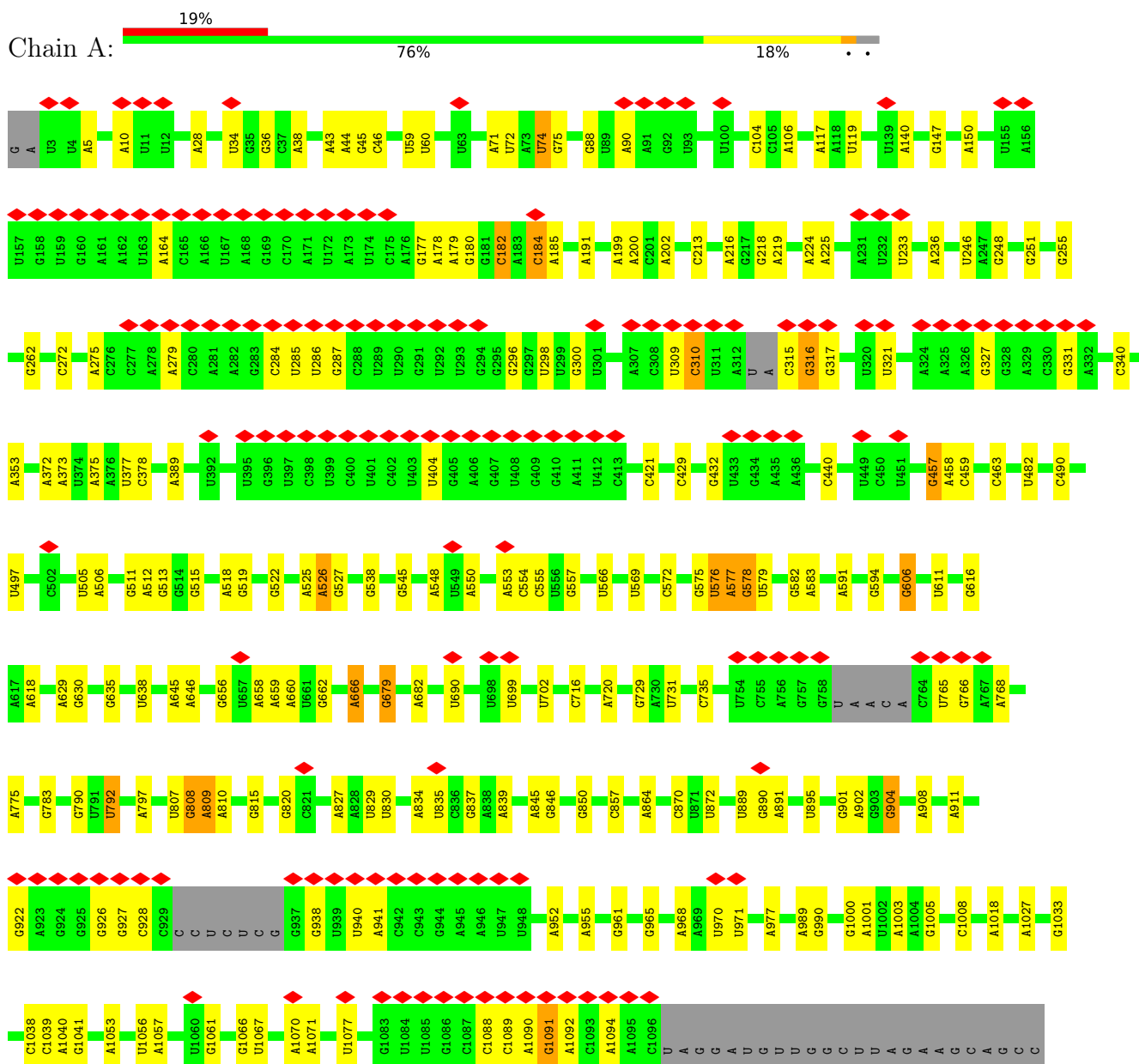
- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

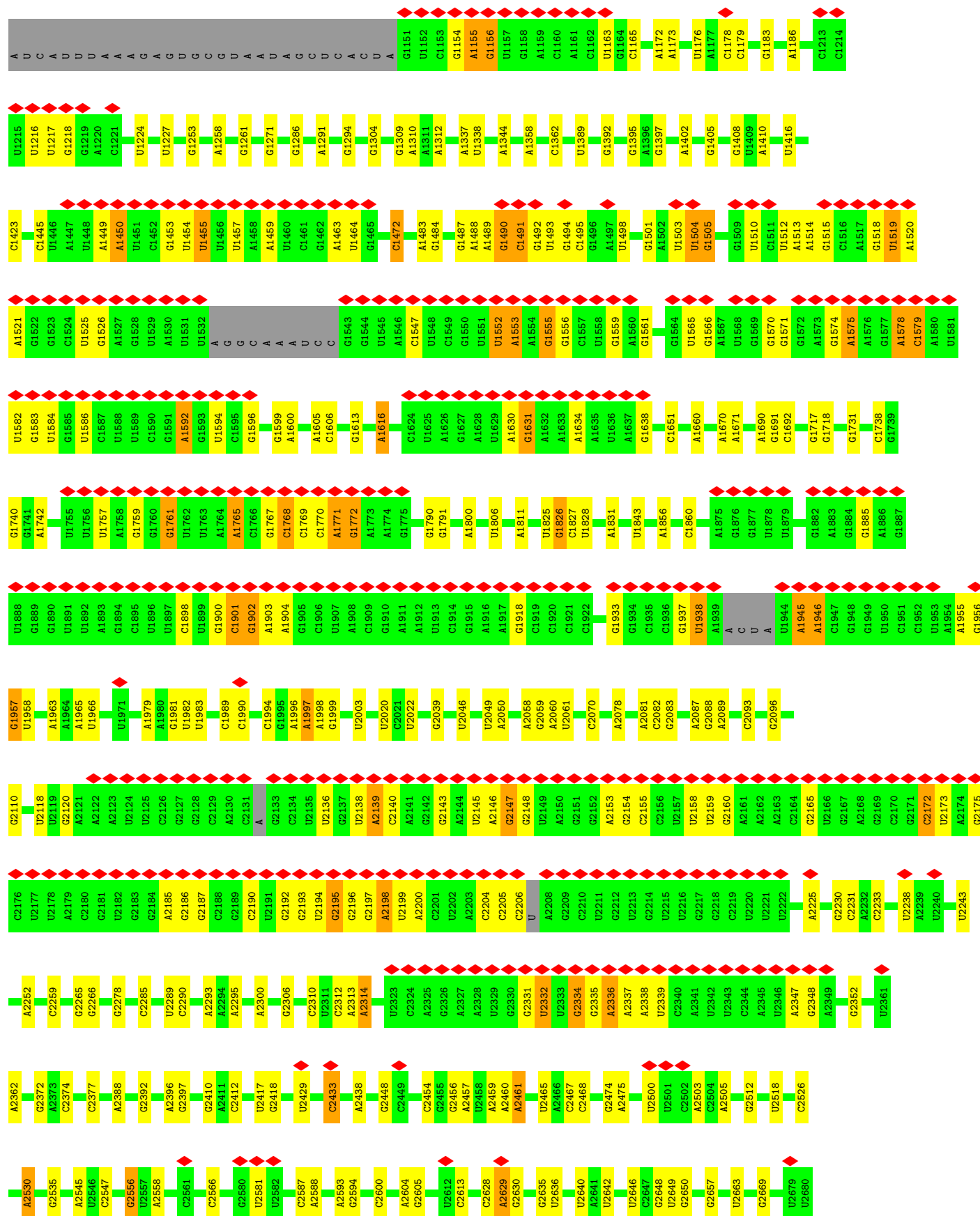
Mol	Chain	Residues	Atoms		AltConf
30	A	229	Total	Mg	0
			229	229	
30	B	2	Total	Mg	0
			2	2	
30	C	2	Total	Mg	0
			2	2	
30	J	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	U	1	Total	Mg	0
			1	1	
30	Z	1	Total	Mg	0
			1	1	

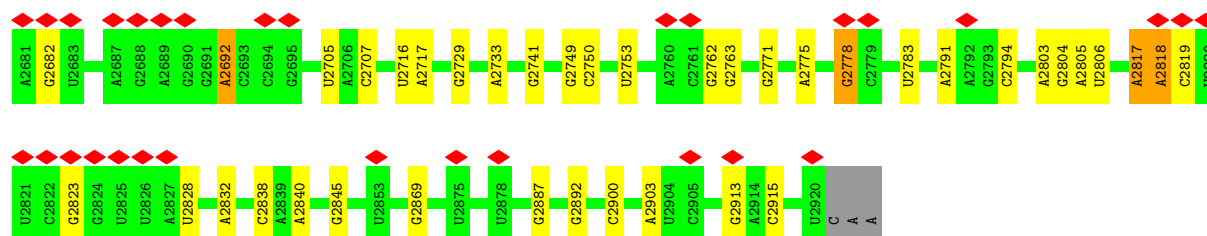
3 Residue-property plots

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.

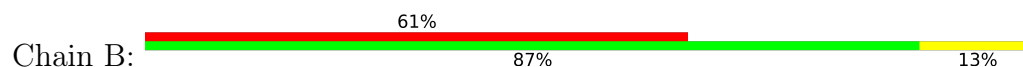
• Molecule 1: 23S ribosomal RNA



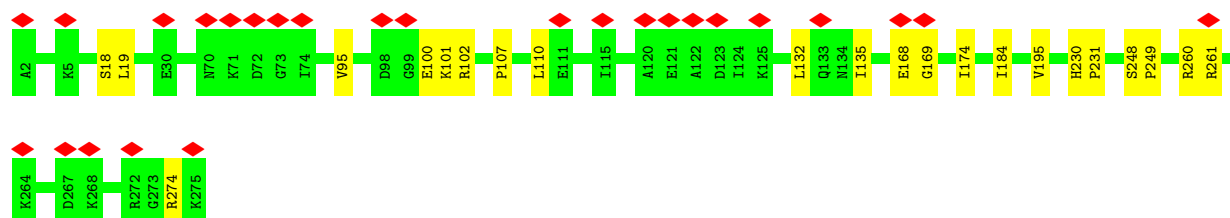




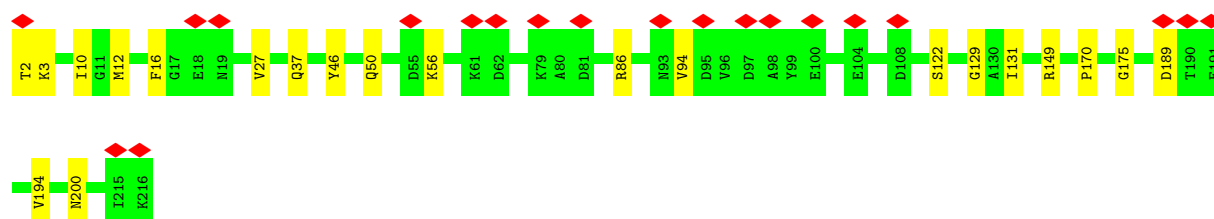
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

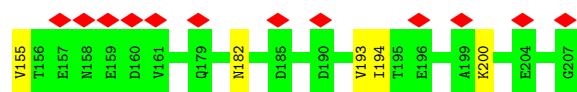


• Molecule 4: 50S ribosomal protein L3



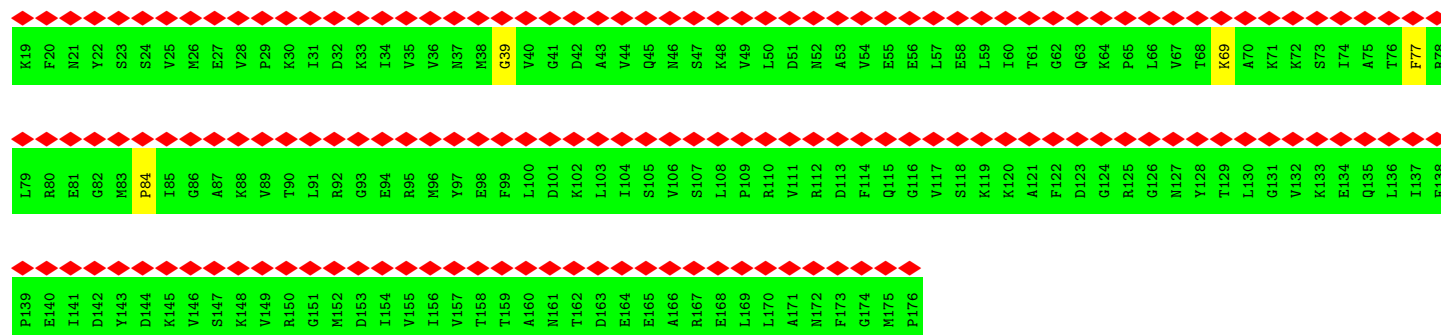
• Molecule 5: 50S ribosomal protein L4





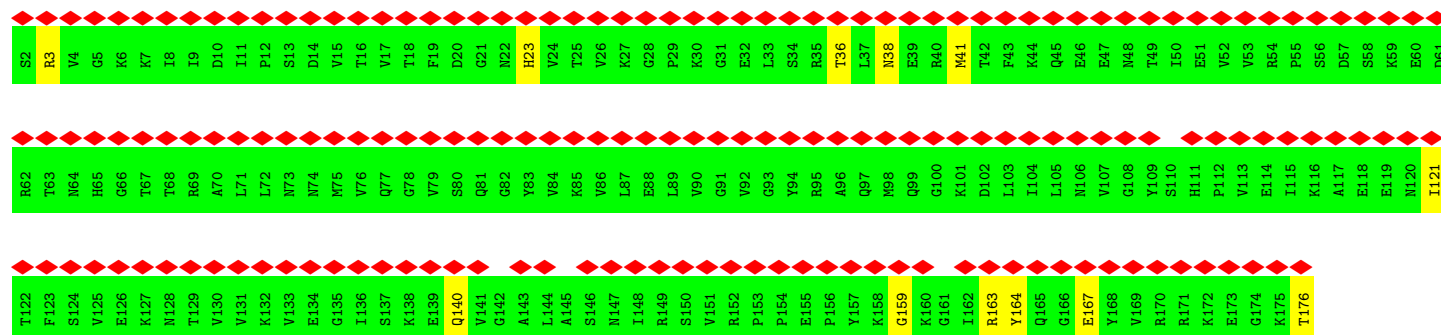
• Molecule 6: 50S ribosomal protein L5

Chain F: 100%
97%



• Molecule 7: 50S ribosomal protein L6

Chain G: 98%
93% 7%



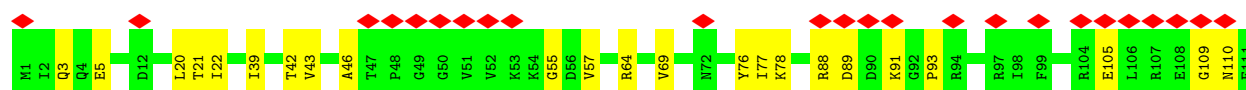
• Molecule 8: 50S ribosomal protein L13

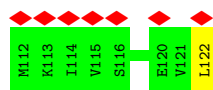
Chain H: 5%
92% 8%



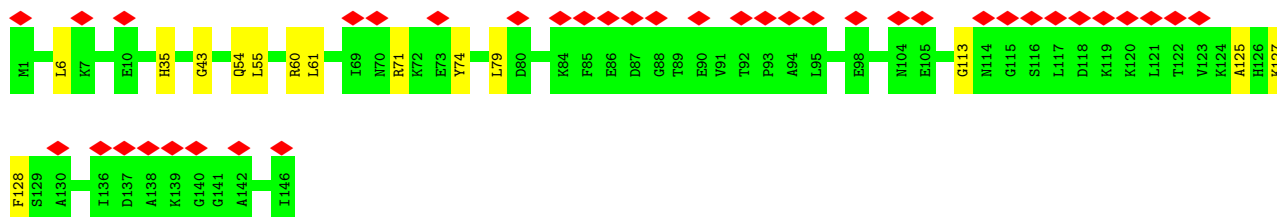
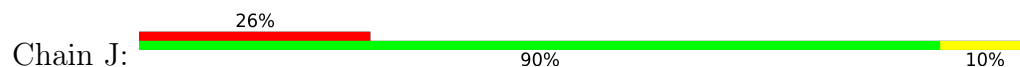
• Molecule 9: 50S ribosomal protein L14

Chain I: 25%
80% 20%

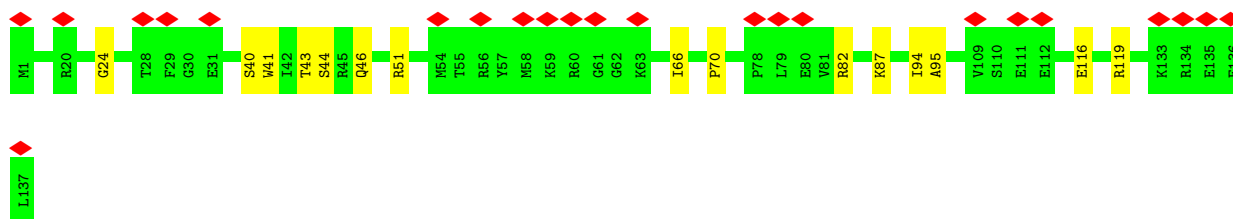
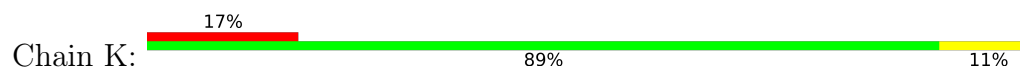




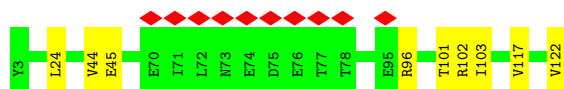
- Molecule 10: 50S ribosomal protein L15



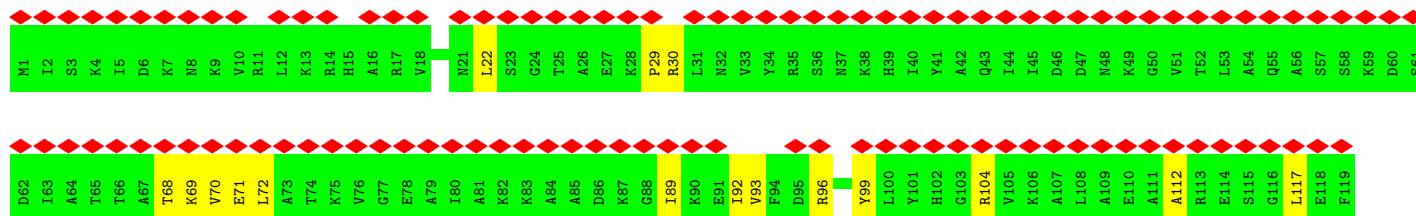
- Molecule 11: 50S ribosomal protein L16



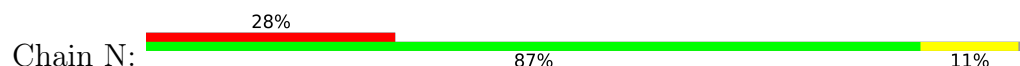
- Molecule 12: 50S ribosomal protein L17

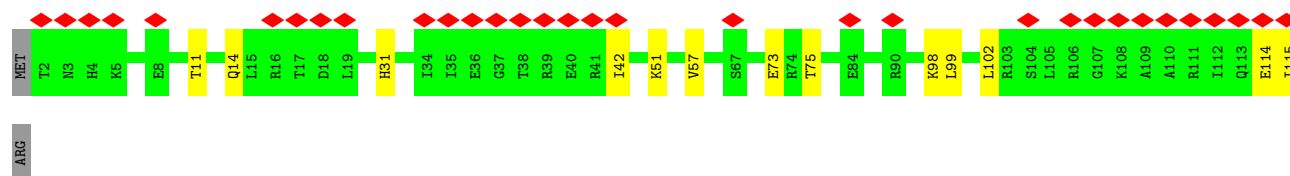


- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

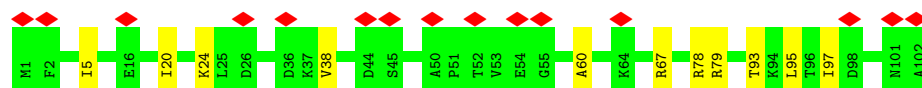
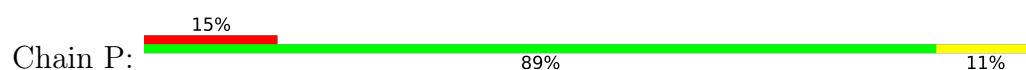




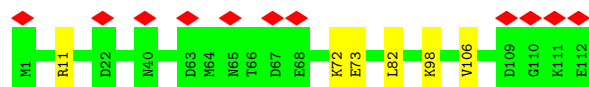
- Molecule 15: 50S ribosomal protein L20



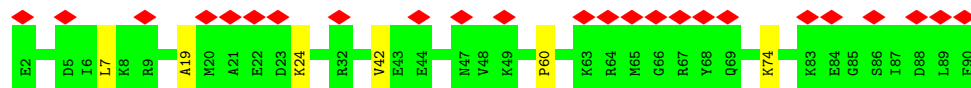
- Molecule 16: 50S ribosomal protein L21



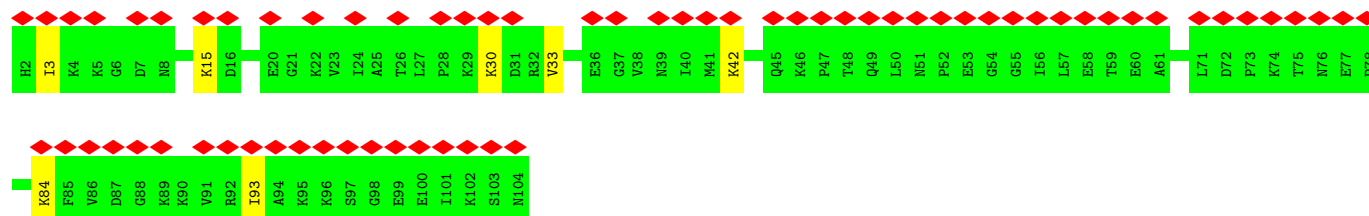
- Molecule 17: 50S ribosomal protein L22



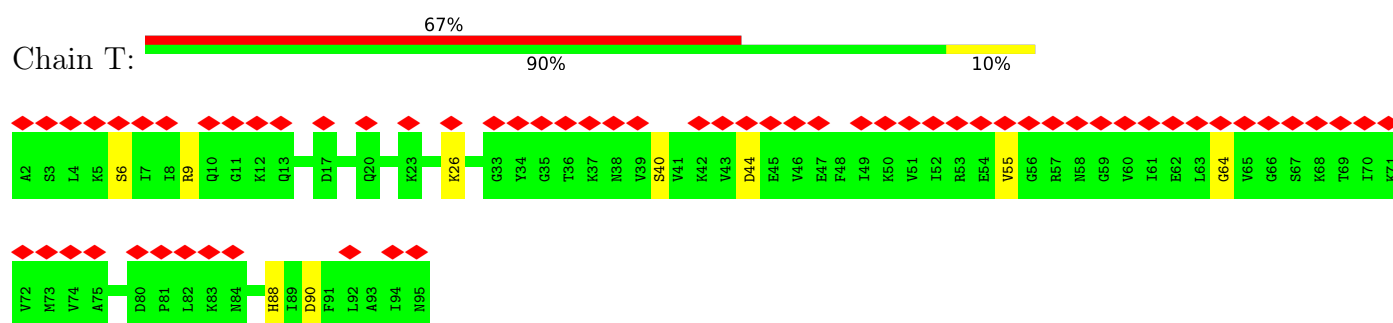
- Molecule 18: 50S ribosomal protein L23



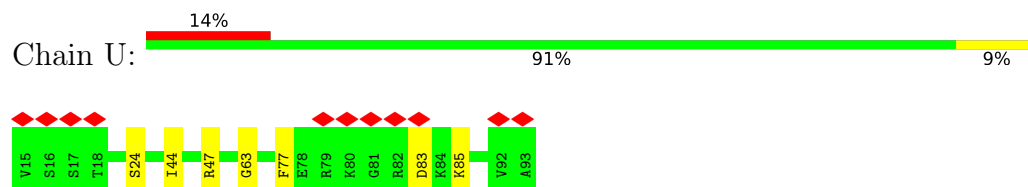
- Molecule 19: 50S ribosomal protein L24



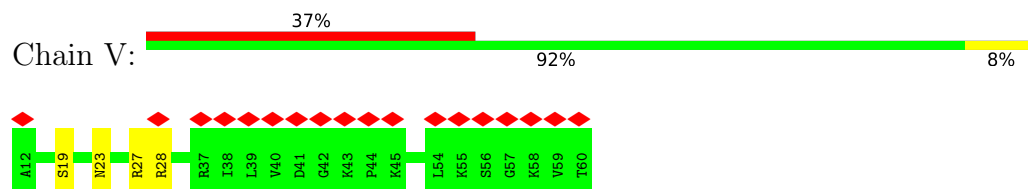
- Molecule 20: 50S ribosomal protein L25



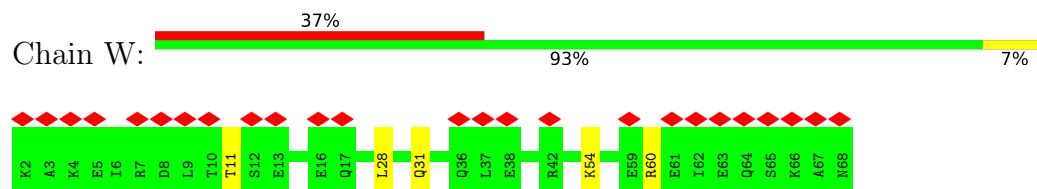
- Molecule 21: 50S ribosomal protein L27



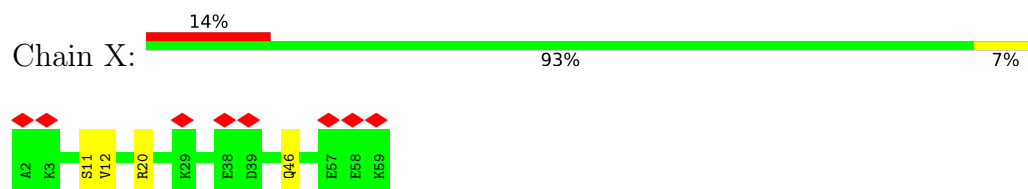
- Molecule 22: 50S ribosomal protein L28



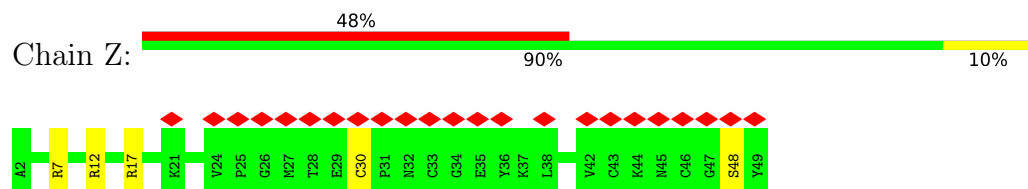
- Molecule 23: 50S ribosomal protein L29



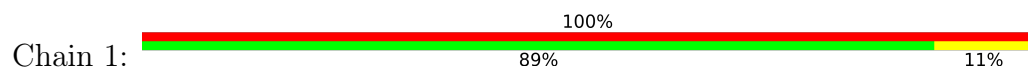
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L33





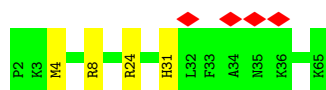
- Molecule 27: 50S ribosomal protein L34

Chain 2: 98%



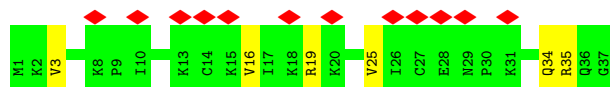
- Molecule 28: 50S ribosomal protein L35

Chain 3: 6% 94% 6%



- Molecule 29: 50S ribosomal protein L36

Chain 4: 32% 84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211046	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.691	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	281.42398, 281.42398, 281.42398	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8579999, 0.8579999, 0.8579999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, 5MU, 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	A	0.54	4/67975 (0.0%)	0.45	19/105995 (0.0%)
2	B	0.45	0/2736	0.38	1/4261 (0.0%)
3	C	0.66	0/2129	0.69	0/2858
4	D	0.66	0/1651	0.74	0/2215
5	E	0.62	0/1595	0.66	0/2154
6	F	0.21	0/777	0.52	0/1079
7	G	0.34	0/1281	0.56	0/1736
8	H	0.67	0/1165	0.72	0/1570
9	I	0.63	0/925	0.81	3/1242 (0.2%)
10	J	0.66	0/1100	0.72	1/1467 (0.1%)
11	K	0.60	0/1095	0.62	0/1472
12	L	0.64	0/936	0.75	0/1253
13	M	0.41	0/891	0.69	1/1194 (0.1%)
14	N	0.60	0/901	0.64	0/1209
15	O	0.72	0/954	0.69	0/1264
16	P	0.65	0/800	0.71	0/1070
17	Q	0.67	0/862	0.74	0/1161
18	R	0.60	0/723	0.70	0/966
19	S	0.47	0/779	0.70	2/1043 (0.2%)
20	T	0.46	0/730	0.69	1/981 (0.1%)
21	U	0.67	0/603	0.68	0/802
22	V	0.55	0/384	0.66	0/515
23	W	0.55	0/542	0.73	0/722
24	X	0.65	0/451	0.66	0/606
25	Z	0.60	0/366	0.73	0/489
26	1	0.25	0/395	0.57	0/530
27	2	0.77	0/371	0.81	0/484
28	3	0.64	0/526	0.73	0/690
29	4	0.52	0/298	0.68	0/392
All	All	0.56	4/93941 (0.0%)	0.51	28/141420 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	5MU	O3'-P	-28.00	1.19	1.61
1	A	790	G	O3'-P	-17.81	1.34	1.61
1	A	1224	U	O3'-P	-8.91	1.47	1.61
1	A	1966	5MU	O3'-P	-8.51	1.48	1.61

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2397	G	OP1-P-OP2	-13.01	80.58	119.60
1	A	2762	G	O3'-P-O5'	-11.89	86.17	104.00
1	A	2397	G	O5'-P-OP1	-11.31	74.06	108.00
1	A	790	G	O3'-P-O5'	11.04	120.57	104.00
1	A	2396	A	OP2-P-O3'	-10.65	76.06	108.00

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	A	60769	0	30549	150	0
2	B	2448	0	1239	1	0
3	C	2094	0	2205	15	0
4	D	1627	0	1667	14	0
5	E	1572	0	1619	22	0
6	F	778	0	348	4	0
7	G	1263	0	1225	9	0
8	H	1143	0	1134	7	0
9	I	918	0	981	19	0
10	J	1086	0	1125	14	0
11	K	1071	0	1123	10	0
12	L	932	0	983	5	0
13	M	882	0	900	9	0
14	N	889	0	937	8	0
15	O	942	0	1014	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	790	0	830	6	0
17	Q	854	0	914	6	0
18	R	715	0	748	3	0
19	S	770	0	809	4	0
20	T	722	0	766	4	0
21	U	597	0	604	6	0
22	V	379	0	400	3	0
23	W	541	0	563	3	0
24	X	449	0	491	3	0
25	Z	360	0	358	4	0
26	1	390	0	394	3	0
27	2	367	0	415	1	0
28	3	521	0	586	4	0
29	4	295	0	340	5	0
30	A	229	0	0	0	0
30	B	2	0	0	0	0
30	C	2	0	0	0	0
30	J	1	0	0	0	0
30	K	1	0	0	0	0
30	U	1	0	0	0	0
30	Z	1	0	0	0	0
All	All	86401	0	55267	285	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 2.

The worst 5 of 285 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)
1:A:2338:A:C2	6:F:77:PHE:CB	2.50	0.95
5:E:34:PHE:CE1	10:J:6:LEU:HD13	2.08	0.88
1:A:2669:G:OP2	8:H:86:LYS:NZ	2.09	0.86
4:D:131:ILE:HD11	4:D:149:ARG:CZ	2.07	0.84
1:A:1825:U:OP2	3:C:274:ARG:NH2	2.14	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	
3	C	272/274 (99%)	259 (95%)	13 (5%)	0	100	100
4	D	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	156/158 (99%)	140 (90%)	16 (10%)	0	100	100
7	G	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
8	H	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
9	I	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
11	K	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
12	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
13	M	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
14	N	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
17	Q	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	S	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
20	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
21	U	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
22	V	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
23	W	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
26	1	45/47 (96%)	45 (100%)	0	0	100	100
27	2	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
29	4	35/37 (95%)	35 (100%)	0	0	100	100
All	All	2985/3041 (98%)	2766 (93%)	219 (7%)	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	
3	C	221/221 (100%)	221 (100%)	0	100	100
4	D	173/173 (100%)	173 (100%)	0	100	100
5	E	168/168 (100%)	168 (100%)	0	100	100
7	G	124/153 (81%)	124 (100%)	0	100	100
8	H	122/123 (99%)	122 (100%)	0	100	100
9	I	100/100 (100%)	100 (100%)	0	100	100
10	J	109/112 (97%)	109 (100%)	0	100	100
11	K	108/114 (95%)	108 (100%)	0	100	100
12	L	96/101 (95%)	96 (100%)	0	100	100
13	M	83/95 (87%)	83 (100%)	0	100	100
14	N	93/102 (91%)	93 (100%)	0	100	100
15	O	96/96 (100%)	96 (100%)	0	100	100
16	P	84/86 (98%)	84 (100%)	0	100	100
17	Q	89/91 (98%)	89 (100%)	0	100	100
18	R	78/80 (98%)	78 (100%)	0	100	100
19	S	81/88 (92%)	81 (100%)	0	100	100
20	T	78/82 (95%)	78 (100%)	0	100	100
21	U	59/62 (95%)	59 (100%)	0	100	100
22	V	39/41 (95%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	58/60 (97%)	58 (100%)	0	100	100
24	X	52/52 (100%)	52 (100%)	0	100	100
25	Z	35/44 (80%)	35 (100%)	0	100	100
26	1	44/45 (98%)	44 (100%)	0	100	100
27	2	39/39 (100%)	39 (100%)	0	100	100
28	3	55/55 (100%)	55 (100%)	0	100	100
29	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2319/2418 (96%)	2319 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	71	HIS
16	P	81	ASN
13	M	39	HIS
22	V	16	ASN
14	N	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2823/2923 (96%)	450 (15%)	6 (0%)
2	B	114/115 (99%)	12 (10%)	0
All	All	2937/3038 (96%)	462 (15%)	6 (0%)

5 of 462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	10	A
1	A	28	A
1	A	34	U
1	A	36	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1670	A
1	A	1957	G
1	A	2749	G
1	A	577	A
1	A	576	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	5MU	A	792	1	19,22,23	4.56	7 (36%)	27,32,35	3.84	10 (37%)
1	5MU	A	1966	1	19,22,23	4.65	7 (36%)	27,32,35	3.81	10 (37%)
1	2MA	A	2530	30,1	22,25,26	1.40	5 (22%)	32,37,40	2.43	11 (34%)

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
1	5MU	A	792	1	-	2/7/25/26	0/2/2/2
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2
1	2MA	A	2530	30,1	-	2/7/25/26	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1966	5MU	C2-N1	10.23	1.54	1.38
1	A	792	5MU	C2-N1	10.12	1.54	1.38
1	A	1966	5MU	C6-N1	9.79	1.54	1.38
1	A	792	5MU	C6-N1	9.45	1.54	1.38
1	A	1966	5MU	C4-C5	9.34	1.60	1.44

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	5MU	C5-C4-N3	12.75	126.40	115.32
1	A	1966	5MU	C5-C4-N3	12.22	125.94	115.32
1	A	1966	5MU	C5-C6-N1	-10.45	111.96	123.31
1	A	792	5MU	C5-C6-N1	-9.87	112.59	123.31
1	A	2530	2MA	C5-C4-N3	-7.82	118.94	127.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	792	5MU	O4'-C4'-C5'-O5'
1	A	2530	2MA	O4'-C4'-C5'-O5'
1	A	792	5MU	C3'-C4'-C5'-O5'
1	A	2530	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 237 ligands modelled in this entry, 237 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1299:U	O3'	1300:G	P	3.08
1	A	1232:G	O3'	1233:A	P	3.01
1	A	1294:G	O3'	1295:C	P	2.95
1	A	790:G	O3'	791:U	P	1.34
1	A	792:5MU	O3'	793:G	P	1.19

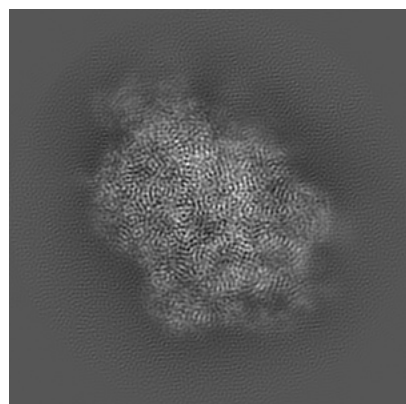
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0243. These allow visual inspection of the internal detail of the map and identification of artifacts.

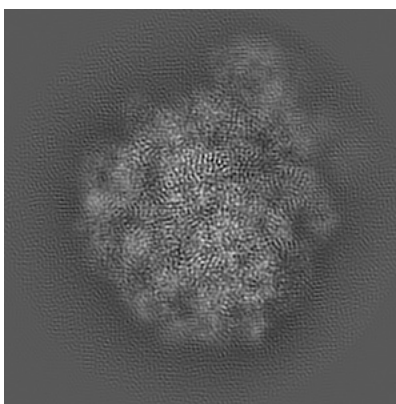
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

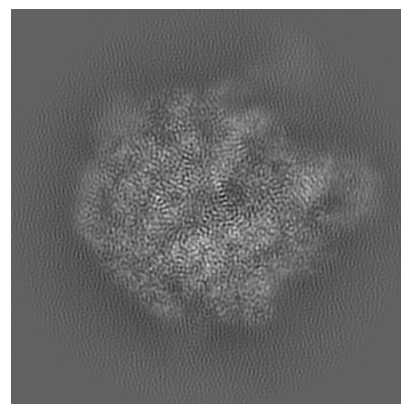
6.1.1 Primary map



X

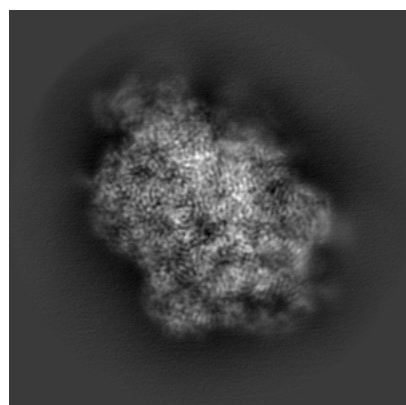


Y

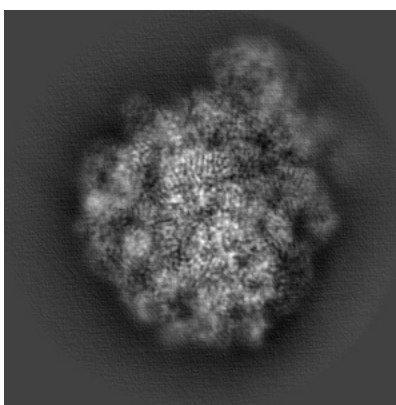


Z

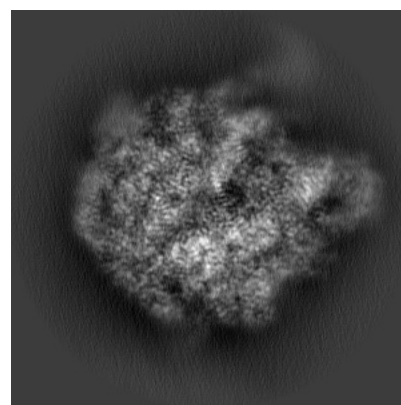
6.1.2 Raw map



X



Y

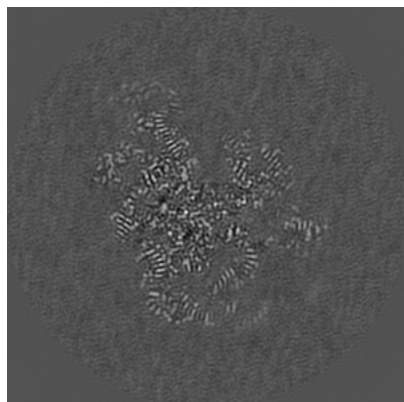


Z

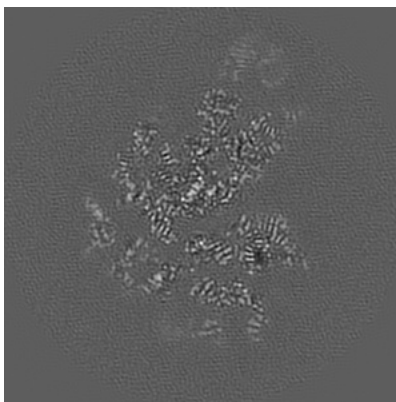
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

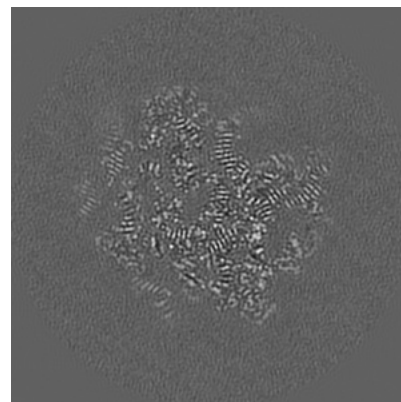
6.2.1 Primary map



X Index: 164

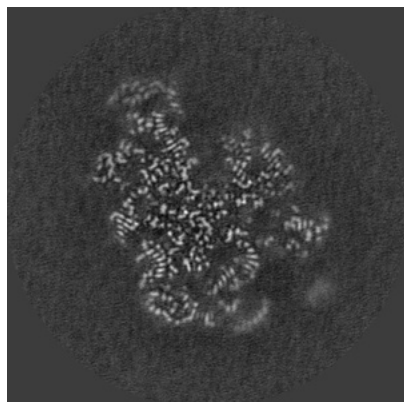


Y Index: 164

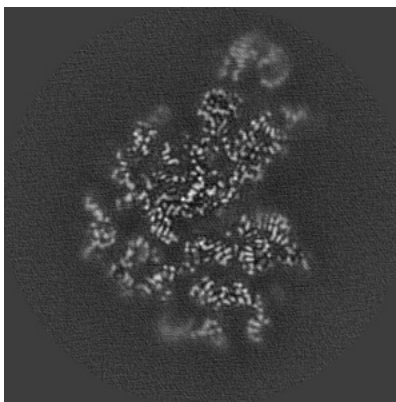


Z Index: 164

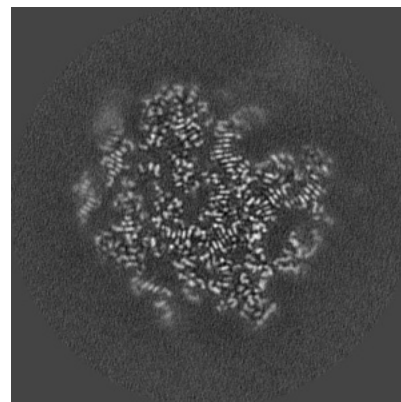
6.2.2 Raw map



X Index: 164



Y Index: 164

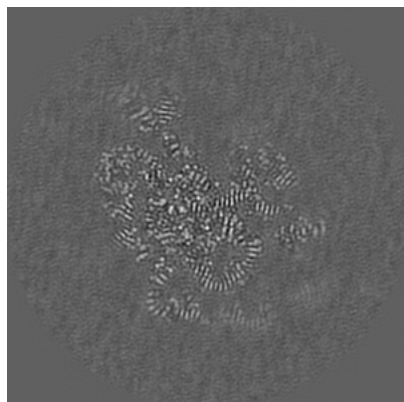


Z Index: 164

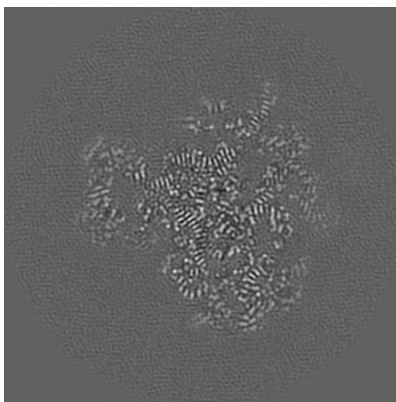
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

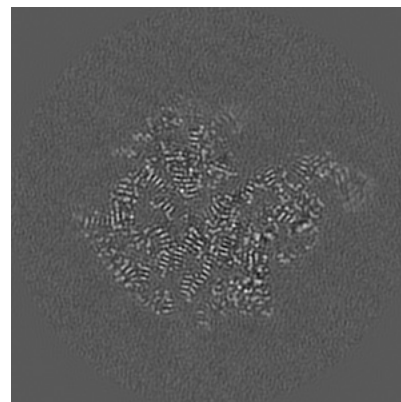
6.3.1 Primary map



X Index: 170

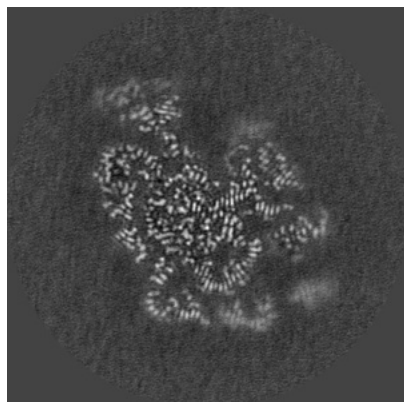


Y Index: 138

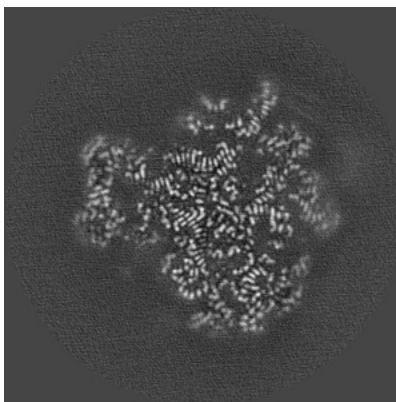


Z Index: 181

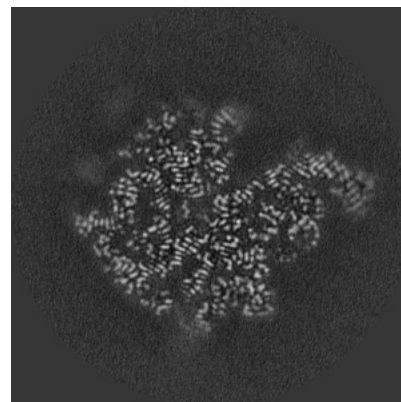
6.3.2 Raw map



X Index: 170



Y Index: 138

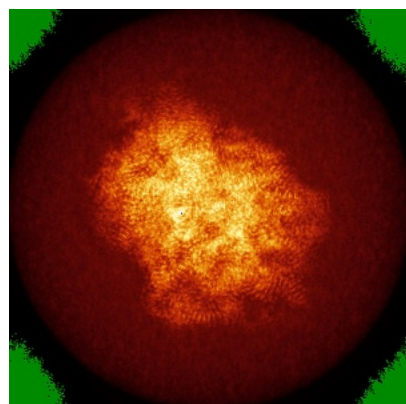


Z Index: 183

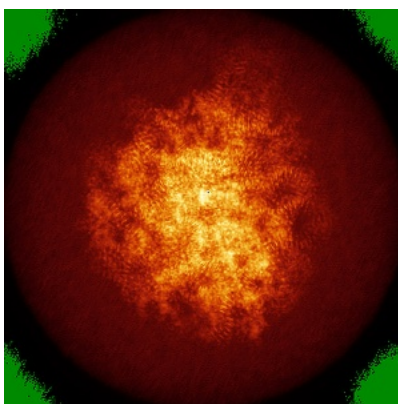
The images above show the largest variance slices of the map in three orthogonal directions.

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

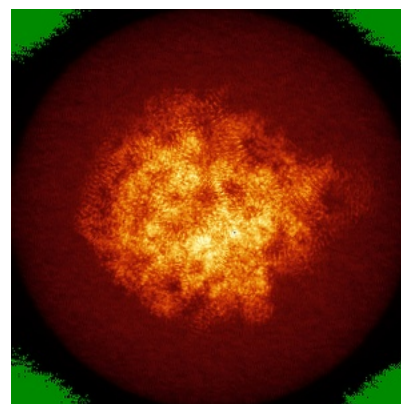
6.4.1 Primary map



X

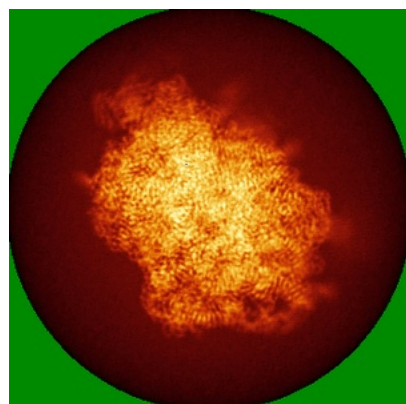


Y

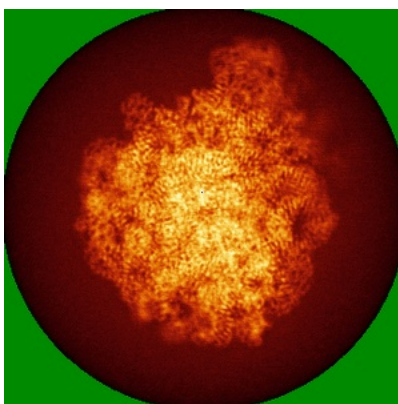


Z

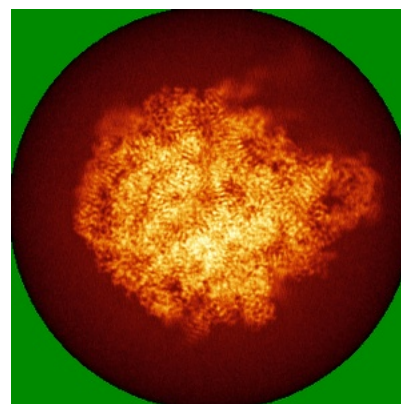
6.4.2 Raw map



X



Y

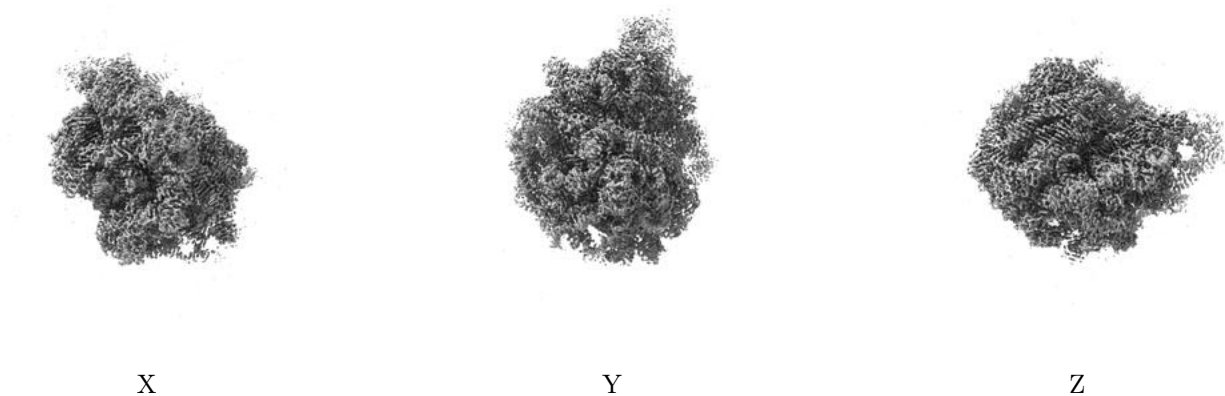


Z

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.

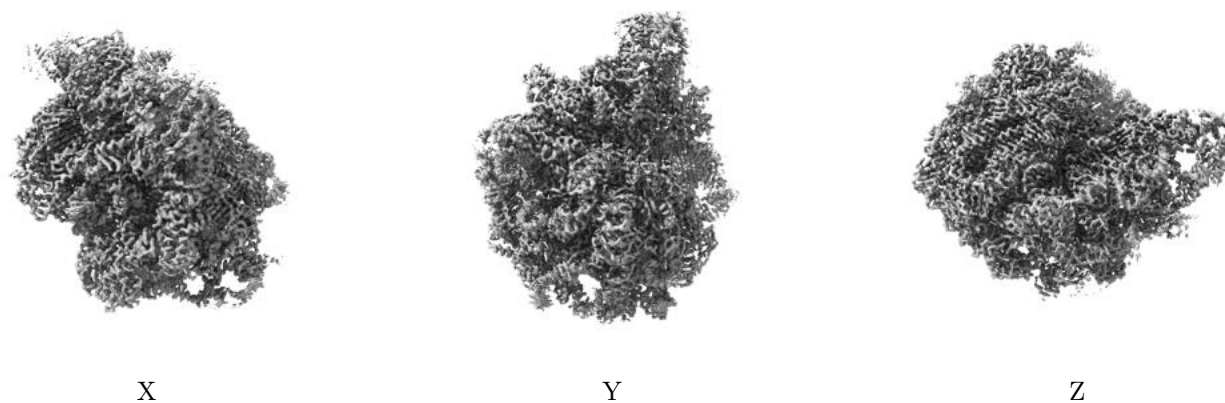
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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.

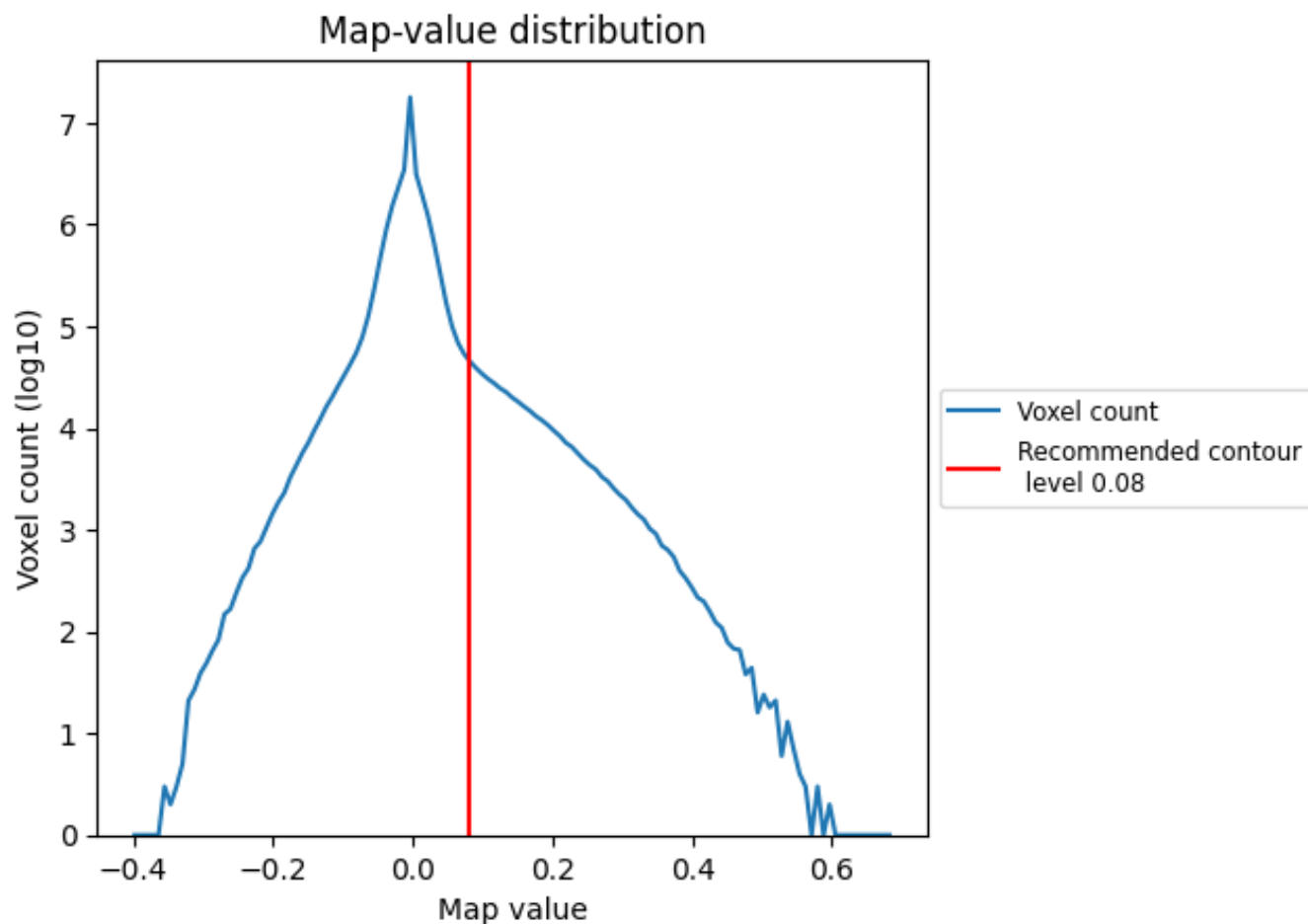
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

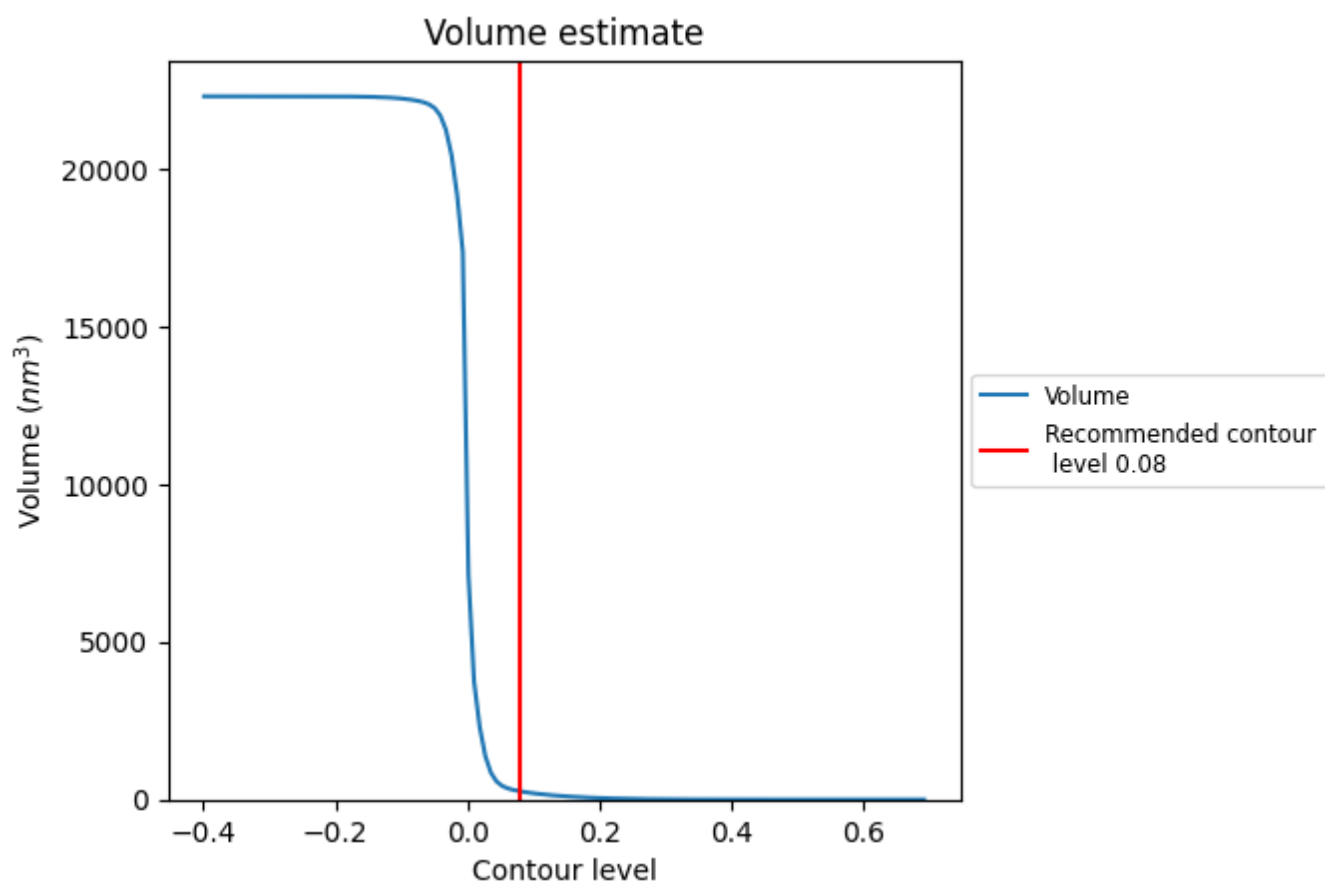
This section contains the results of statistical analysis of the map.

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.

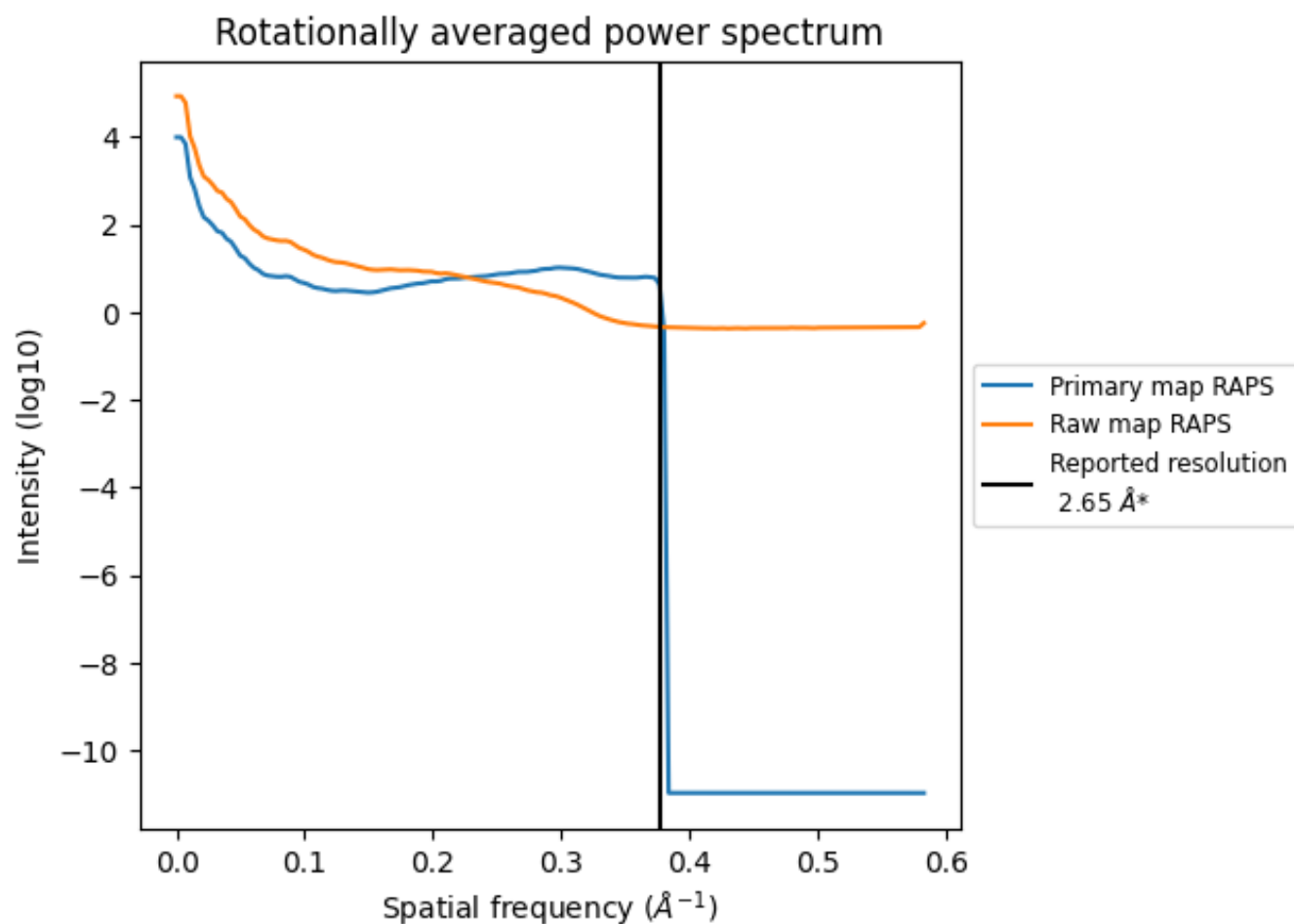
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 236 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 ⓘ

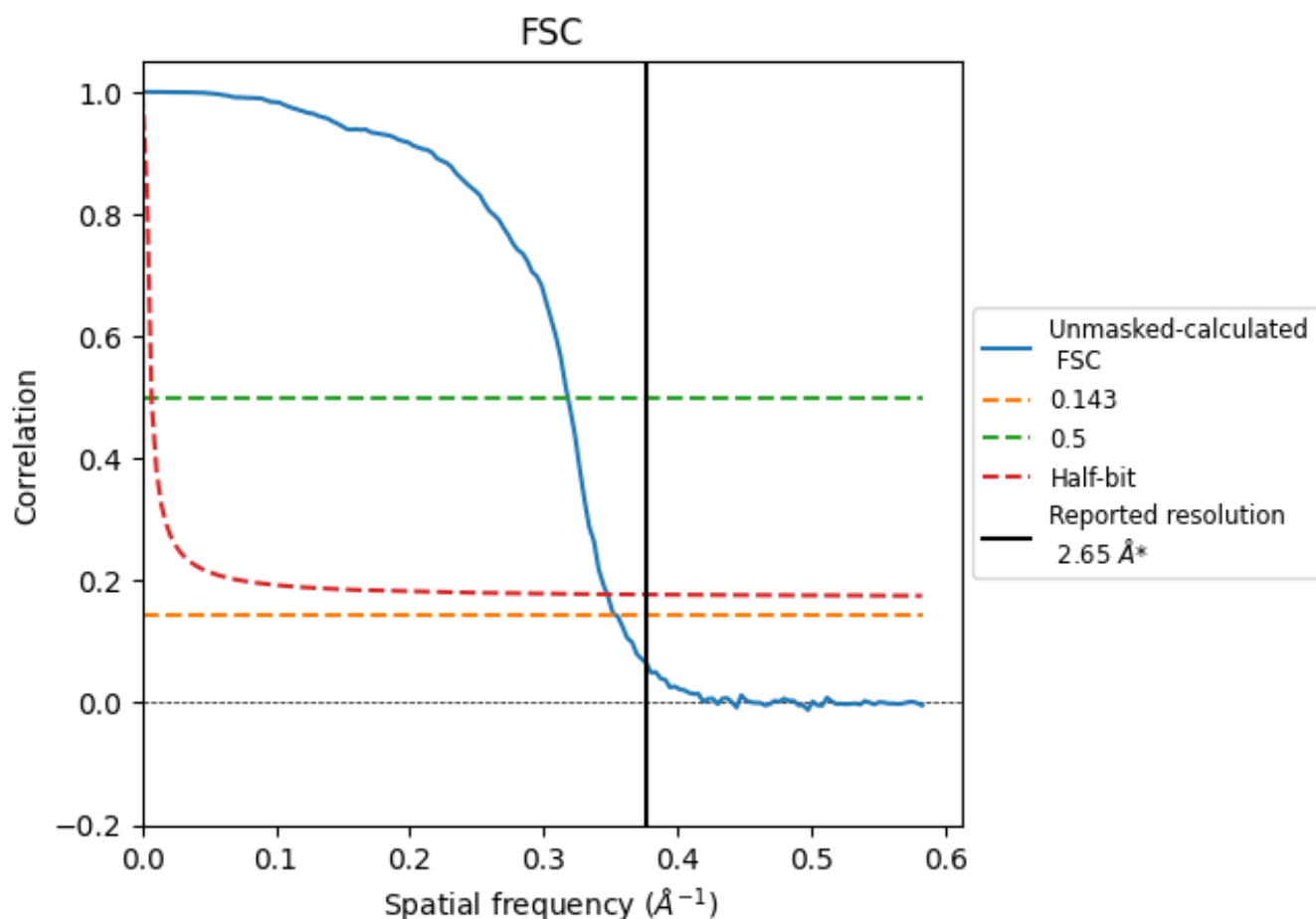


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

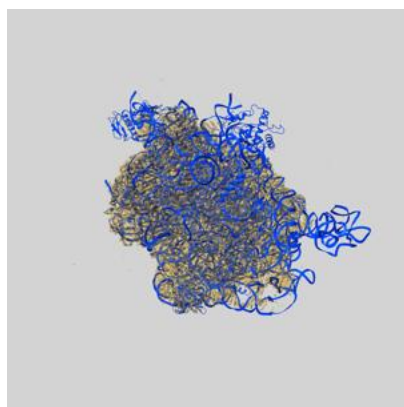
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.14	2.88

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

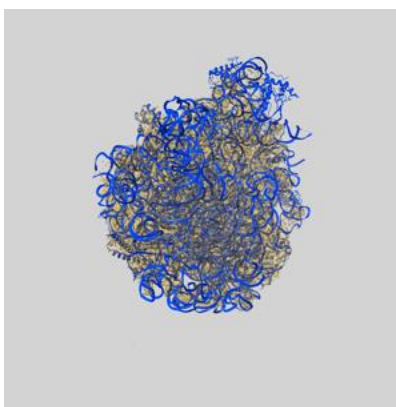
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-0243 and PDB model 6HMA. Per-residue inclusion information can be found in section 3 on page 10.

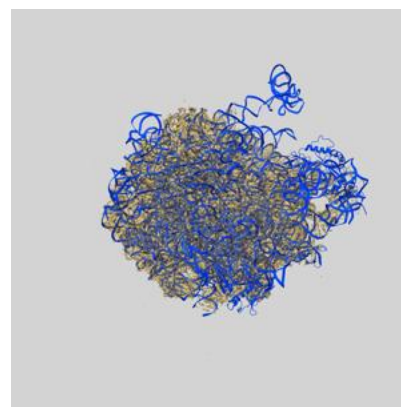
9.1 Map-model overlay ⓘ



X



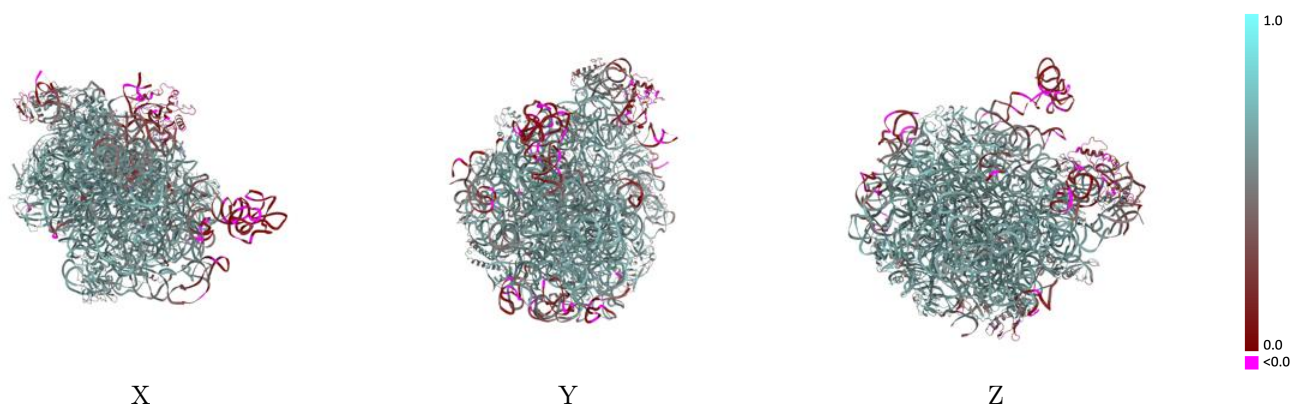
Y



Z

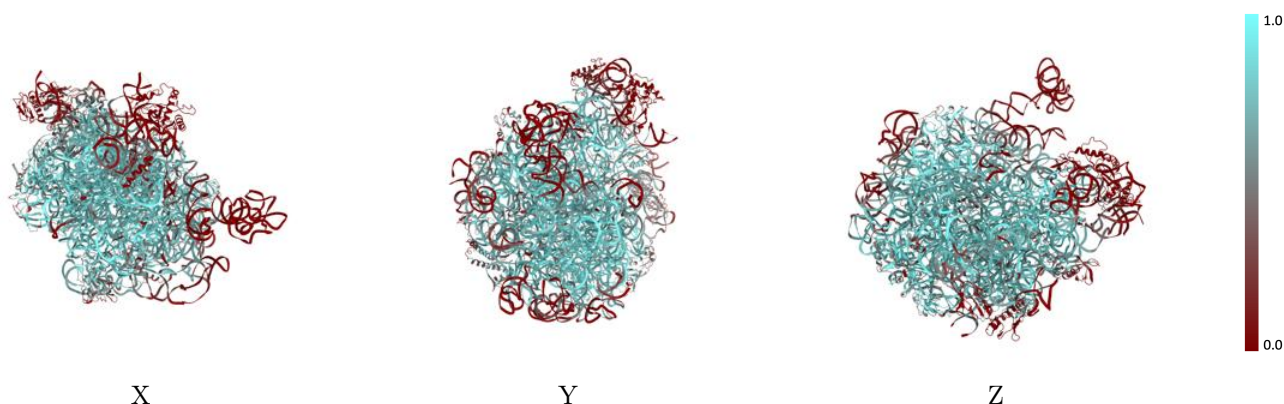
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



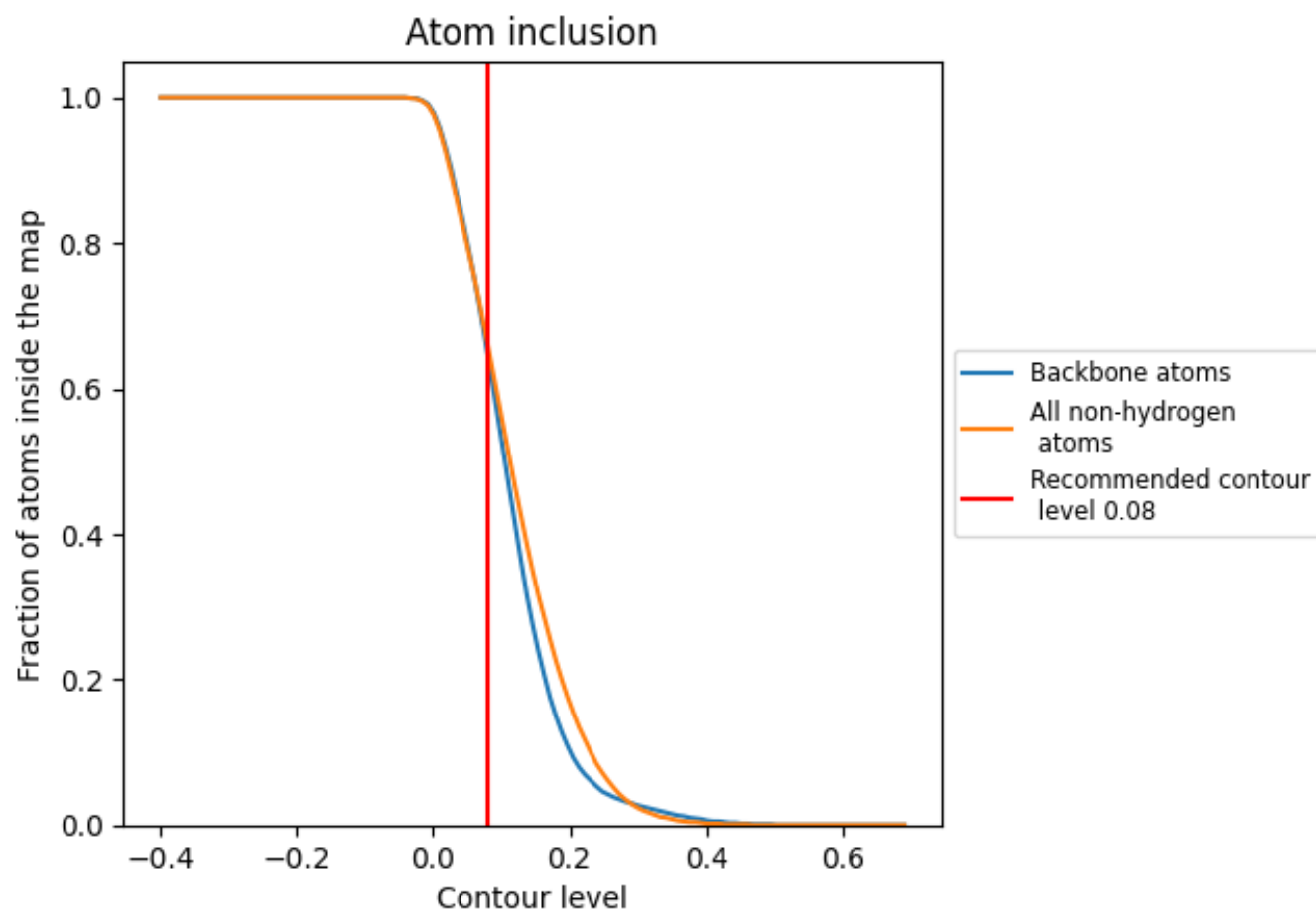
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 66% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.5630
1	 0.0350	 0.4330
2	 0.9020	 0.6430
3	 0.7690	 0.6250
4	 0.4810	 0.5720
A	 0.7050	 0.5680
B	 0.3530	 0.4900
C	 0.7490	 0.6210
D	 0.7640	 0.6120
E	 0.6640	 0.5980
F	 0.0000	 0.1450
G	 0.0700	 0.3980
H	 0.7820	 0.6160
I	 0.6280	 0.5790
J	 0.6320	 0.5870
K	 0.7060	 0.6070
L	 0.7620	 0.6140
M	 0.1570	 0.4320
N	 0.5980	 0.5720
O	 0.8410	 0.6470
P	 0.7060	 0.5890
Q	 0.7680	 0.6190
R	 0.6050	 0.5630
S	 0.3000	 0.4710
T	 0.3030	 0.5070
U	 0.7480	 0.5990
V	 0.5290	 0.5280
W	 0.4820	 0.5290
X	 0.7390	 0.5970
Z	 0.5490	 0.5390

