wwPDB EM Validation Summary Report

May 19, 2024 – 10:03 am BST

PDB ID	:	8RQ0
EMDB ID	:	EMD-19428
Title	:	Escherichia coli 50S subunit in complex with the antimicrobial peptide Api88 - conformation II
Authors	:	Lauer, S.; Nikolay, R.; Spahn, C.
Deposited on	:	2024-01-17
Resolution	:	2.44 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:

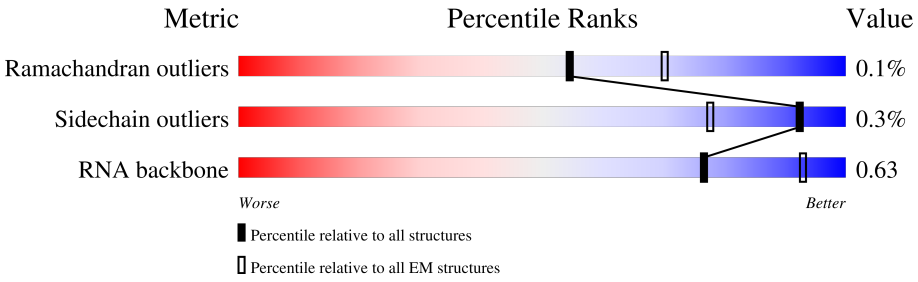
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.44 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	100%
2	1	50	100%
3	2	46	100%
4	3	64	100%
5	4	38	100%
6	6	66	6% 65% 35%
7	A	2903	87% 13%
8	B	120	87% 13%

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Mol	Chain	Length	Quality of chain
9	C	271	100%
10	D	209	100%
11	E	201	100%
12	F	177	5% 100%
13	G	176	99%
14	H	149	63% 100%
15	J	142	100%
16	K	122	100%
17	L	143	100%
18	M	136	100%
19	N	120	100%
20	O	116	100%
21	P	114	100%
22	Q	117	100%
23	R	103	99%
24	S	110	99%
25	T	93	100%
26	U	102	100%
27	V	94	100%
28	W	75	100%
29	X	77	100%
30	Y	63	6% 100%
31	Z	58	100%
32	x	18	50% 67% 6% 28%
32	y	18	6% 83% 17%

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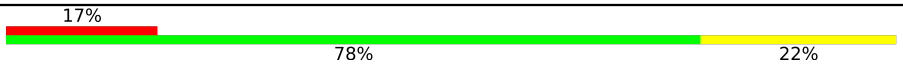
Mol	Chain	Length	Quality of chain
32	z	18	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90661 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
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	43	333	206	59	62	6	0	0

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2900	Total	C	N	O	P	1	0
			62282	27783	11462	20136	2901		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 32 is a protein called Apidaecins type 88.

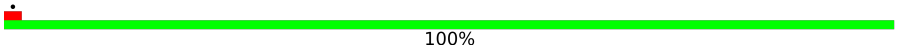
Mol	Chain	Residues	Atoms				AltConf	Trace
32	x	13	Total	C	N	O	0	0
			112	74	24	14		
32	y	15	Total	C	N	O	0	1
			121	80	26	15		
32	z	18	Total	C	N	O	0	1
			148	94	34	20		

3 Residue-property plots (i)

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.

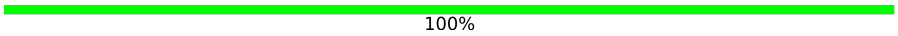
• Molecule 1: Large ribosomal subunit protein bL32

Chain 0:



• Molecule 2: Large ribosomal subunit protein bL33

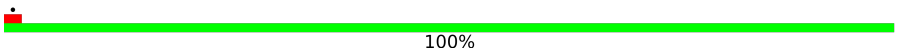
Chain 1:



There are no outlier residues recorded for this chain.

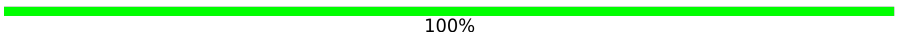
• Molecule 3: Large ribosomal subunit protein bL34

Chain 2:



• Molecule 4: Large ribosomal subunit protein bL35

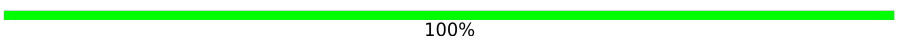
Chain 3:



There are no outlier residues recorded for this chain.

• Molecule 5: Large ribosomal subunit protein bL36A

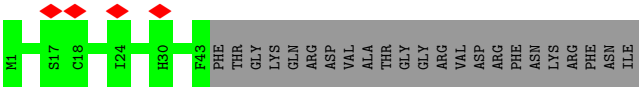
Chain 4:



There are no outlier residues recorded for this chain.

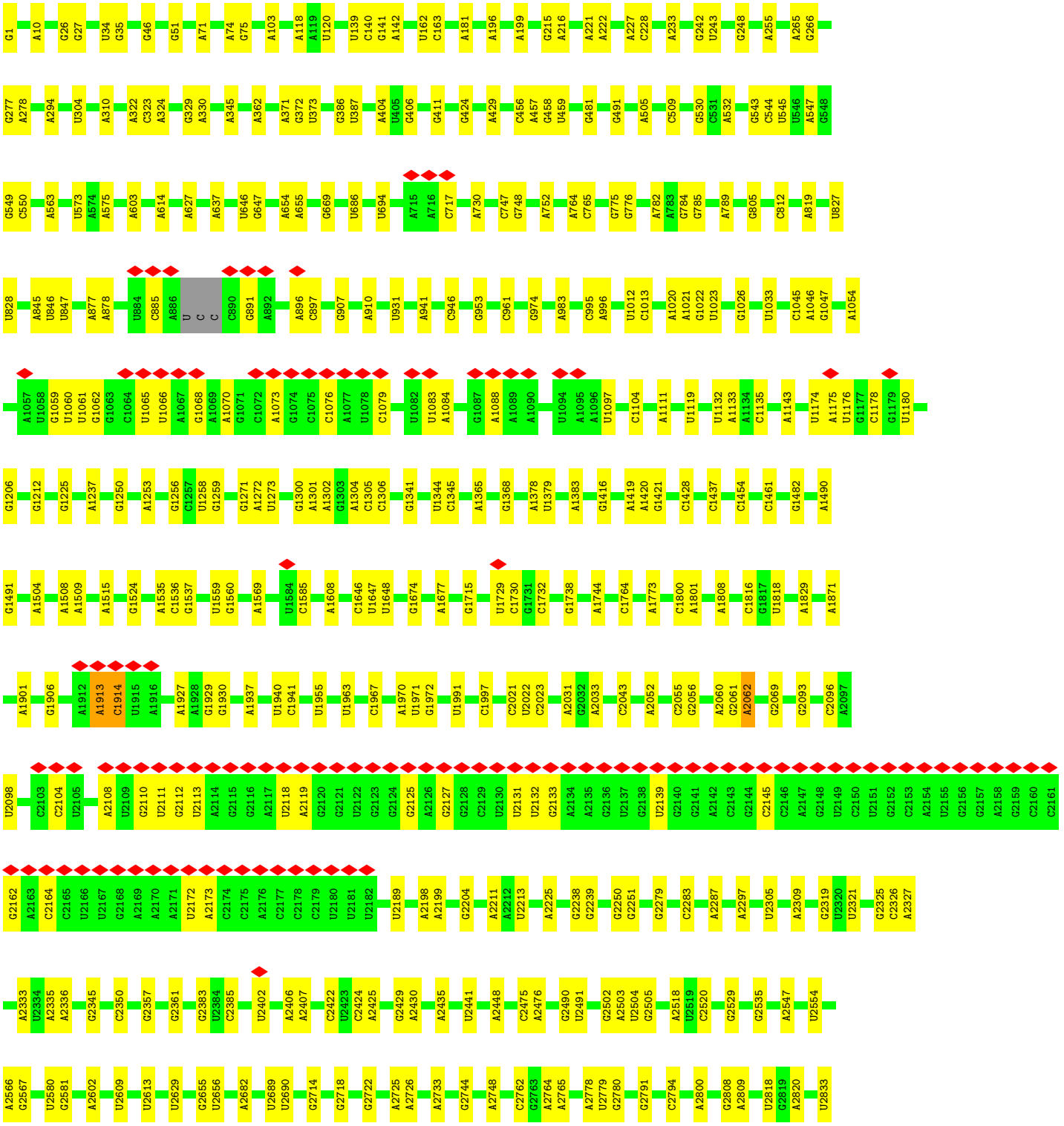
• Molecule 6: Large ribosomal subunit protein bL31

Chain 6:



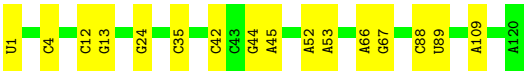
• Molecule 7: 23S ribosomal RNA

Chain A:



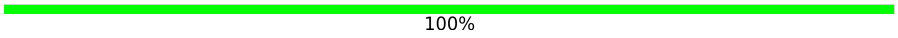
• Molecule 8: 5S ribosomal RNA

Chain B:



• Molecule 9: Large ribosomal subunit protein uL2

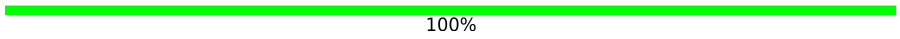
Chain C:



There are no outlier residues recorded for this chain.

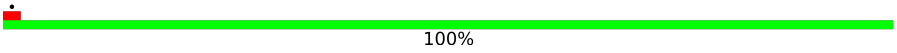
• Molecule 10: Large ribosomal subunit protein uL3

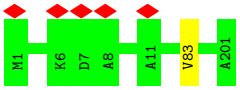
Chain D:



• Molecule 11: Large ribosomal subunit protein uL4

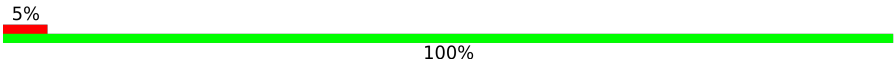
Chain E:

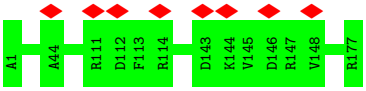




• Molecule 12: Large ribosomal subunit protein uL5

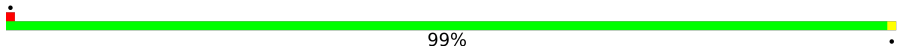
Chain F:

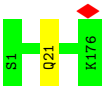




• Molecule 13: Large ribosomal subunit protein uL6

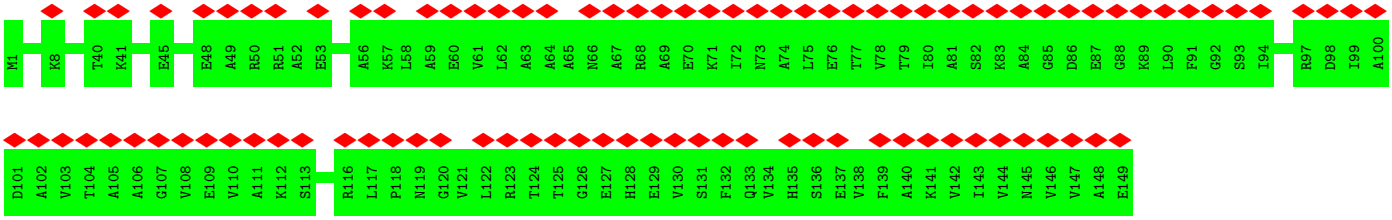
Chain G:





• Molecule 14: Large ribosomal subunit protein bL9

Chain H:



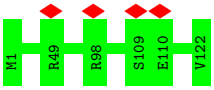
• Molecule 15: Large ribosomal subunit protein uL13

Chain J: 100%

There are no outlier residues recorded for this chain.

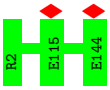
• Molecule 16: Large ribosomal subunit protein uL14

Chain K: 100%



• Molecule 17: Large ribosomal subunit protein uL15

Chain L: 100%



• Molecule 18: Large ribosomal subunit protein uL16

Chain M: 100%

There are no outlier residues recorded for this chain.

• Molecule 19: Large ribosomal subunit protein bL17

Chain N: 100%

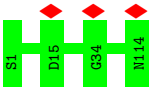
• Molecule 20: Large ribosomal subunit protein uL18

Chain O: 100%

There are no outlier residues recorded for this chain.

• Molecule 21: Large ribosomal subunit protein bL19

Chain P: 100%

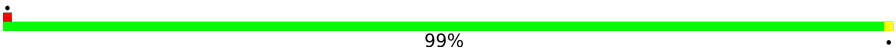


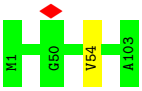
• Molecule 22: Large ribosomal subunit protein bL20

Chain Q: 

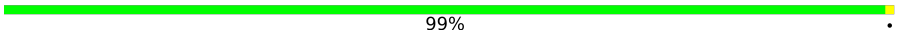
There are no outlier residues recorded for this chain.

• Molecule 23: Large ribosomal subunit protein bL21

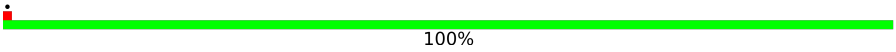
Chain R: 



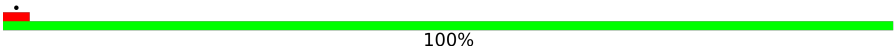
• Molecule 24: Large ribosomal subunit protein uL22

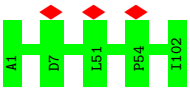
Chain S: 

• Molecule 25: Large ribosomal subunit protein uL23

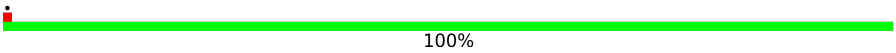
Chain T: 

• Molecule 26: Large ribosomal subunit protein uL24

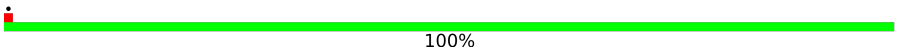
Chain U: 



• Molecule 27: Large ribosomal subunit protein bL25

Chain V: 

• Molecule 28: Large ribosomal subunit protein bL27

Chain W: 

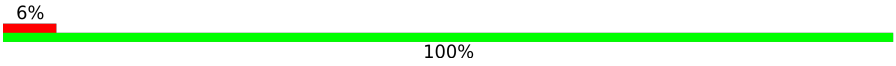
• Molecule 29: Large ribosomal subunit protein bL28

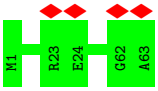
Chain X:

There are no outlier residues recorded for this chain.

• Molecule 30: Large ribosomal subunit protein uL29

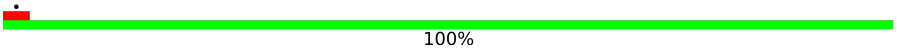
Chain Y:





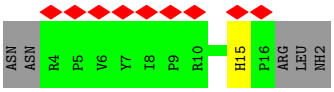
• Molecule 31: Large ribosomal subunit protein uL30

Chain Z:



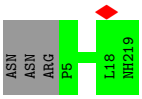
• Molecule 32: Apidaecins type 88

Chain x:



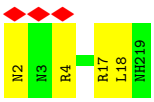
• Molecule 32: Apidaecins type 88

Chain y:



• Molecule 32: Apidaecins type 88

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	260475	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 ($e^-/Å^2$)	26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.762	Depositor
Minimum map value	-0.250	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	359.28, 359.28, 359.28	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.998, 0.998, 0.998	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.25	0/450	0.55	0/599
2	1	0.25	0/416	0.50	0/554
3	2	0.25	0/380	0.64	0/498
4	3	0.25	0/513	0.58	0/676
5	4	0.26	0/303	0.56	0/397
6	6	0.25	0/339	0.47	0/454
7	A	0.30	1/69756 (0.0%)	0.67	11/108822 (0.0%)
8	B	0.30	1/2876 (0.0%)	0.66	0/4483
9	C	0.26	0/2121	0.57	0/2852
10	D	0.27	0/1586	0.52	0/2134
11	E	0.25	0/1571	0.50	0/2113
12	F	0.25	0/1434	0.53	0/1926
13	G	0.24	0/1343	0.49	0/1816
14	H	0.25	0/1122	0.49	0/1515
15	J	0.26	0/1152	0.49	0/1551
16	K	0.26	0/947	0.59	0/1268
17	L	0.26	0/1054	0.59	0/1403
18	M	0.26	0/1093	0.55	0/1460
19	N	0.26	0/973	0.61	0/1301
20	O	0.25	0/902	0.54	0/1209
21	P	0.27	0/929	0.55	0/1242
22	Q	0.27	0/960	0.51	0/1278
23	R	0.26	0/829	0.54	0/1107
24	S	0.25	0/875	0.53	0/1170
25	T	0.25	0/744	0.51	0/994
26	U	0.28	0/787	0.53	0/1051
27	V	0.26	0/766	0.50	0/1025
28	W	0.26	0/582	0.56	0/769
29	X	0.25	0/635	0.57	0/848
30	Y	0.24	0/510	0.52	0/677
31	Z	0.25	0/453	0.53	0/605
32	x	0.33	0/119	0.62	0/165

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	y	0.28	0/127	0.58	0/175
32	z	0.54	0/154	0.60	0/212
All	All	0.29	2/98801 (0.0%)	0.64	11/148349 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	G	OP3-P	-10.62	1.48	1.61
8	B	1	U	OP3-P	-10.59	1.48	1.61

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1913	A	OP1-P-O3'	-11.07	80.84	105.20
7	A	1259	G	P-O3'-C3'	-9.21	108.64	119.70
7	A	1913	A	OP2-P-O3'	-9.17	85.03	105.20
7	A	1305	C	P-O3'-C3'	-9.04	108.85	119.70
7	A	1258	U	P-O3'-C3'	-7.86	110.27	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	52 (96%)	2 (4%)	0	100	100
2	1	48/50 (96%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
5	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
6	6	41/66 (62%)	38 (93%)	3 (7%)	0	100	100
9	C	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
10	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
11	E	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	29	34
12	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
13	G	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
14	H	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
15	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
16	K	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
17	L	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
18	M	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
19	N	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
20	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
21	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
22	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
23	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	16
24	S	109/110 (99%)	105 (96%)	4 (4%)	0	100	100
25	T	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
26	U	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
27	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
28	W	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
29	X	75/77 (97%)	75 (100%)	0	0	100	100
30	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
31	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
32	x	11/18 (61%)	10 (91%)	1 (9%)	0	100	100
32	y	13/18 (72%)	10 (77%)	3 (23%)	0	100	100
32	z	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
All	All	3248/3342 (97%)	3115 (96%)	131 (4%)	2 (0%)	54	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	R	54	VAL
11	E	83	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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
5	4	34/34 (100%)	34 (100%)	0	100	100
6	6	40/59 (68%)	40 (100%)	0	100	100
9	C	216/216 (100%)	216 (100%)	0	100	100
10	D	164/164 (100%)	164 (100%)	0	100	100
11	E	165/165 (100%)	165 (100%)	0	100	100
12	F	148/148 (100%)	148 (100%)	0	100	100
13	G	137/137 (100%)	136 (99%)	1 (1%)	84	90
14	H	114/114 (100%)	114 (100%)	0	100	100
15	J	116/116 (100%)	116 (100%)	0	100	100
16	K	103/103 (100%)	103 (100%)	0	100	100
17	L	102/102 (100%)	102 (100%)	0	100	100
18	M	109/109 (100%)	109 (100%)	0	100	100
19	N	100/100 (100%)	100 (100%)	0	100	100
20	O	86/86 (100%)	86 (100%)	0	100	100
21	P	99/99 (100%)	99 (100%)	0	100	100
22	Q	89/89 (100%)	89 (100%)	0	100	100
23	R	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	S	94/93 (101%)	93 (99%)	1 (1%)	73 83
25	T	80/80 (100%)	80 (100%)	0	100 100
26	U	83/83 (100%)	83 (100%)	0	100 100
27	V	78/78 (100%)	78 (100%)	0	100 100
28	W	57/57 (100%)	57 (100%)	0	100 100
29	X	67/67 (100%)	67 (100%)	0	100 100
30	Y	55/55 (100%)	55 (100%)	0	100 100
31	Z	48/48 (100%)	48 (100%)	0	100 100
32	x	13/17 (76%)	12 (92%)	1 (8%)	13 15
32	y	14/17 (82%)	14 (100%)	0	100 100
32	z	17/17 (100%)	13 (76%)	4 (24%)	1 0
All	All	2693/2718 (99%)	2686 (100%)	7 (0%)	92 95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	z	2	ASN
32	z	4	ARG
32	z	18	LEU
32	z	17	ARG
32	x	15	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
32	z	2	ASN
32	z	15	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	2897/2903 (99%)	371 (12%)	16 (0%)
8	B	119/120 (99%)	13 (10%)	2 (1%)
All	All	3016/3023 (99%)	384 (12%)	18 (0%)

5 of 384 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	10	A
7	A	26	G
7	A	27	G
7	A	34	U
7	A	35	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	2725	A
8	B	66	A
8	B	52	A
7	A	1378	A
7	A	2655	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 monosaccharides 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.

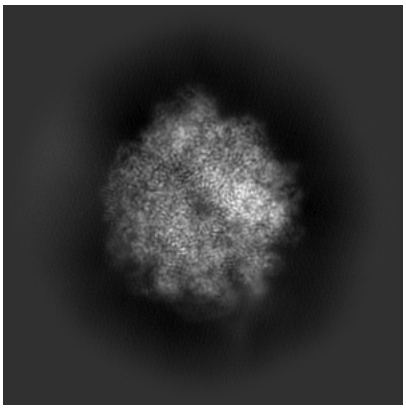
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19428. These allow visual inspection of the internal detail of the map and identification of artifacts.

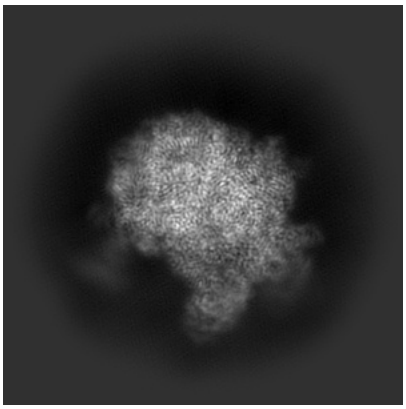
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

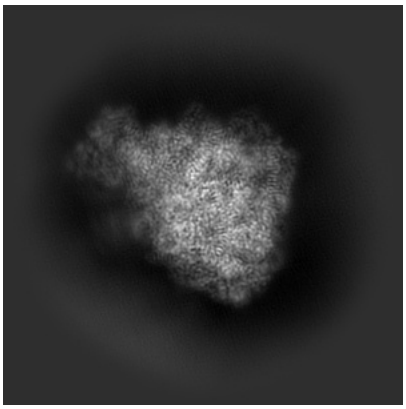
6.1.1 Primary map



X

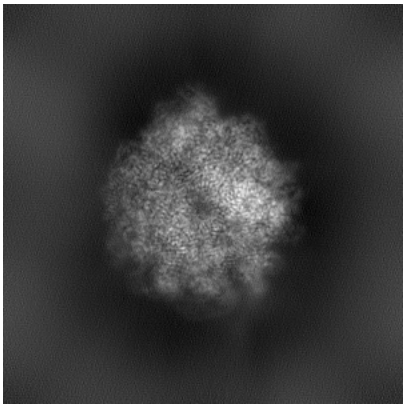


Y

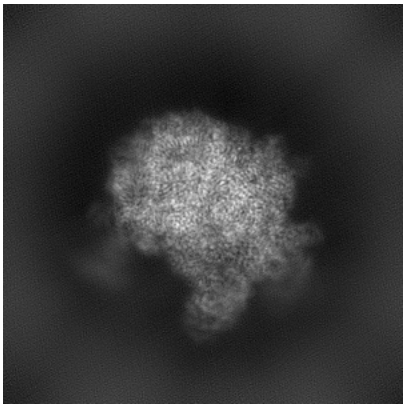


Z

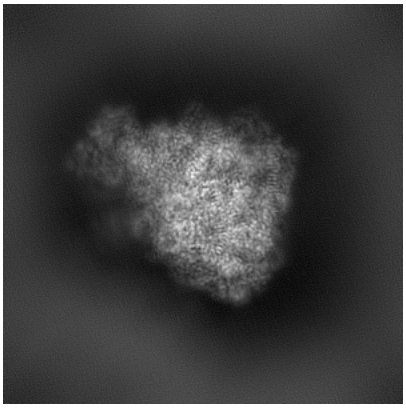
6.1.2 Raw map



X



Y

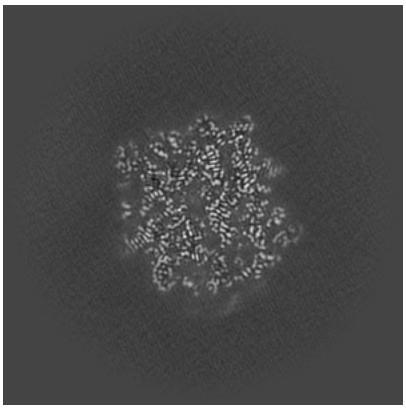


Z

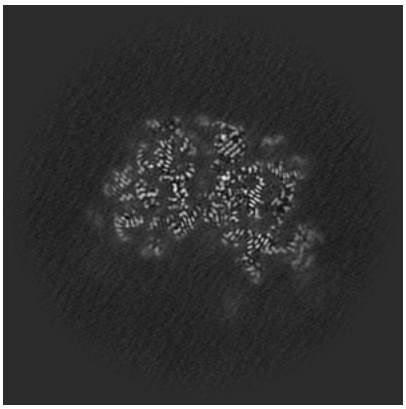
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

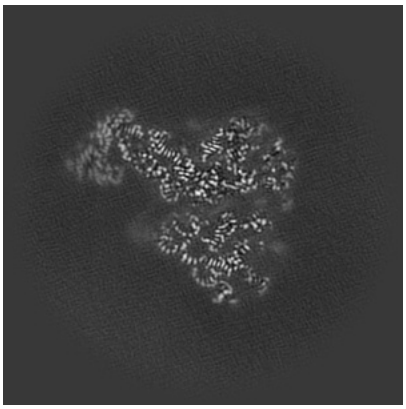
6.2.1 Primary map



X Index: 180

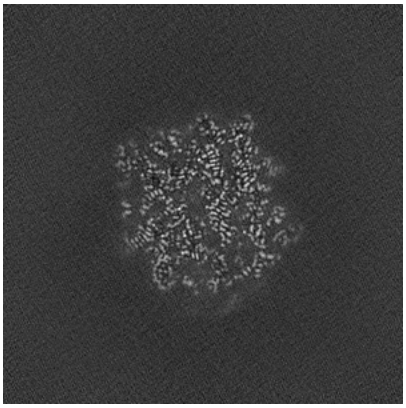


Y Index: 180

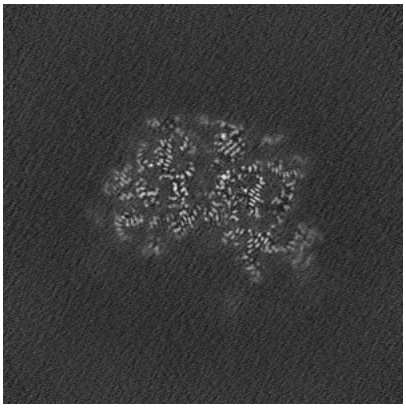


Z Index: 180

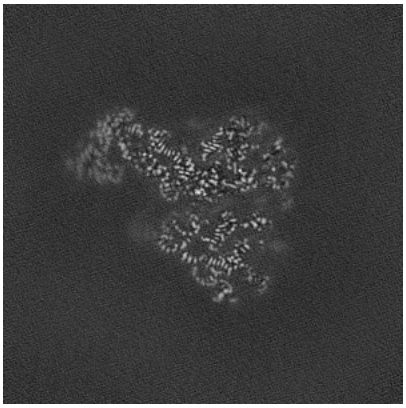
6.2.2 Raw map



X Index: 180



Y Index: 180

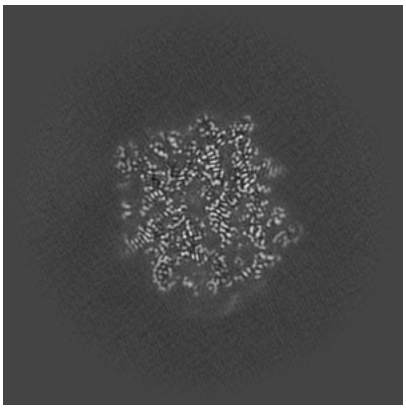


Z Index: 180

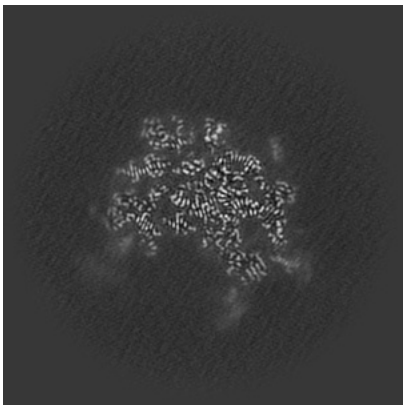
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

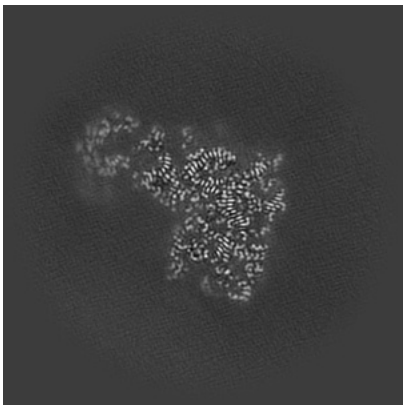
6.3.1 Primary map



X Index: 180

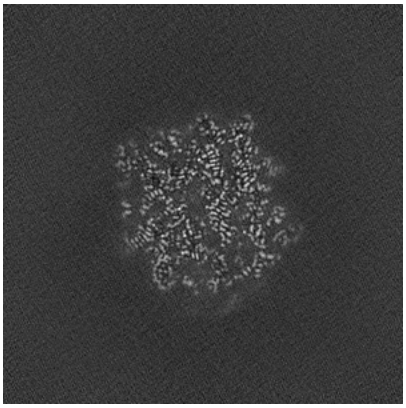


Y Index: 192

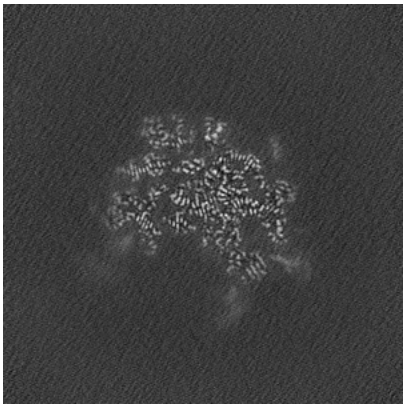


Z Index: 198

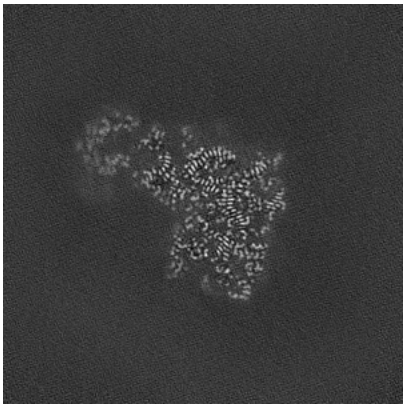
6.3.2 Raw map



X Index: 180



Y Index: 192

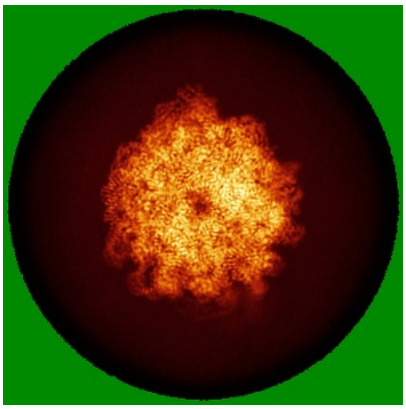


Z Index: 198

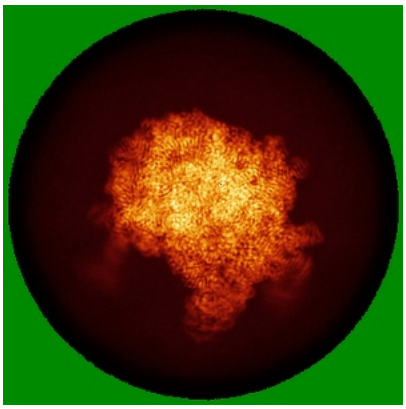
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

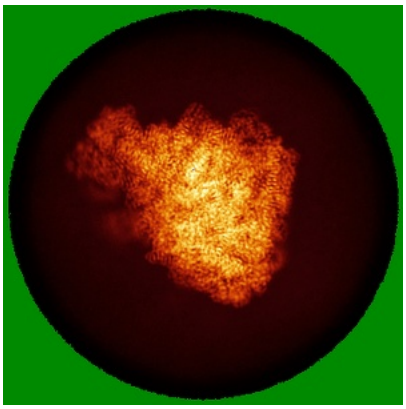
6.4.1 Primary map



X

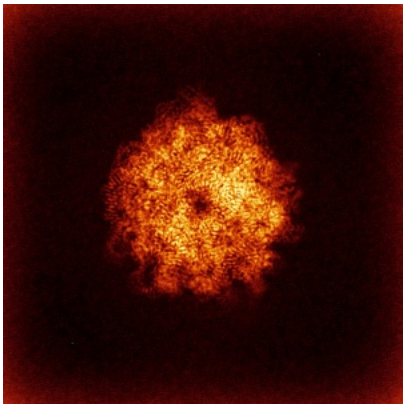


Y

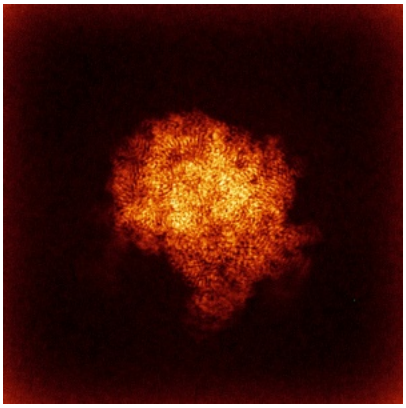


Z

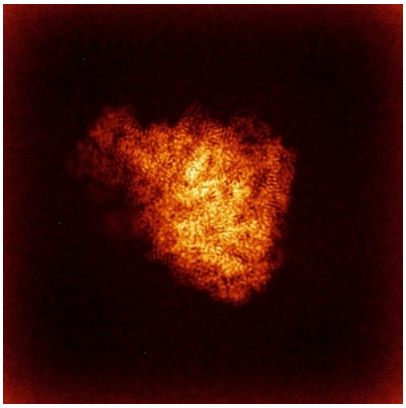
6.4.2 Raw map



X



Y

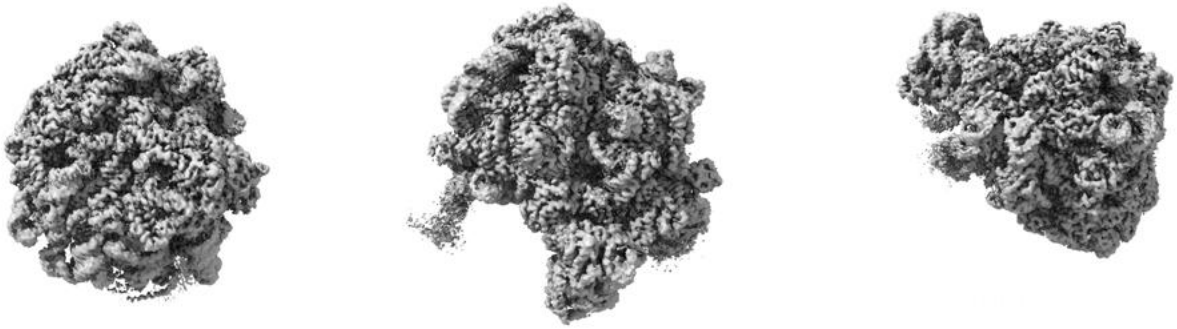


Z

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 0.06. 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.

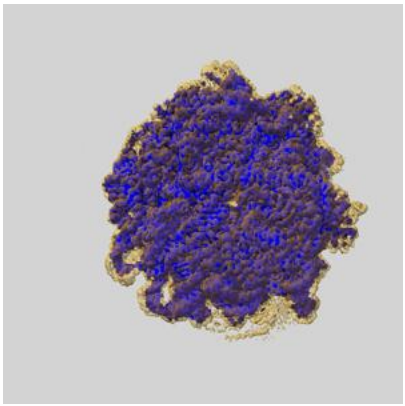
6.6 Mask visualisation (i)

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

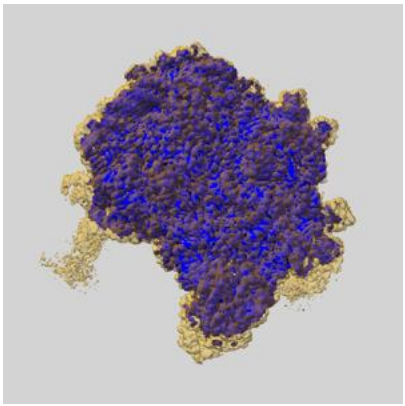
A mask typically either:

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

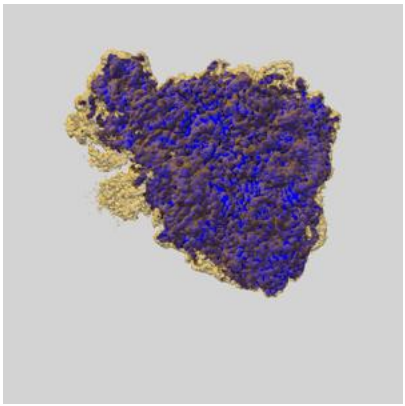
6.6.1 emd_19428_msk_1.map (i)



X



Y

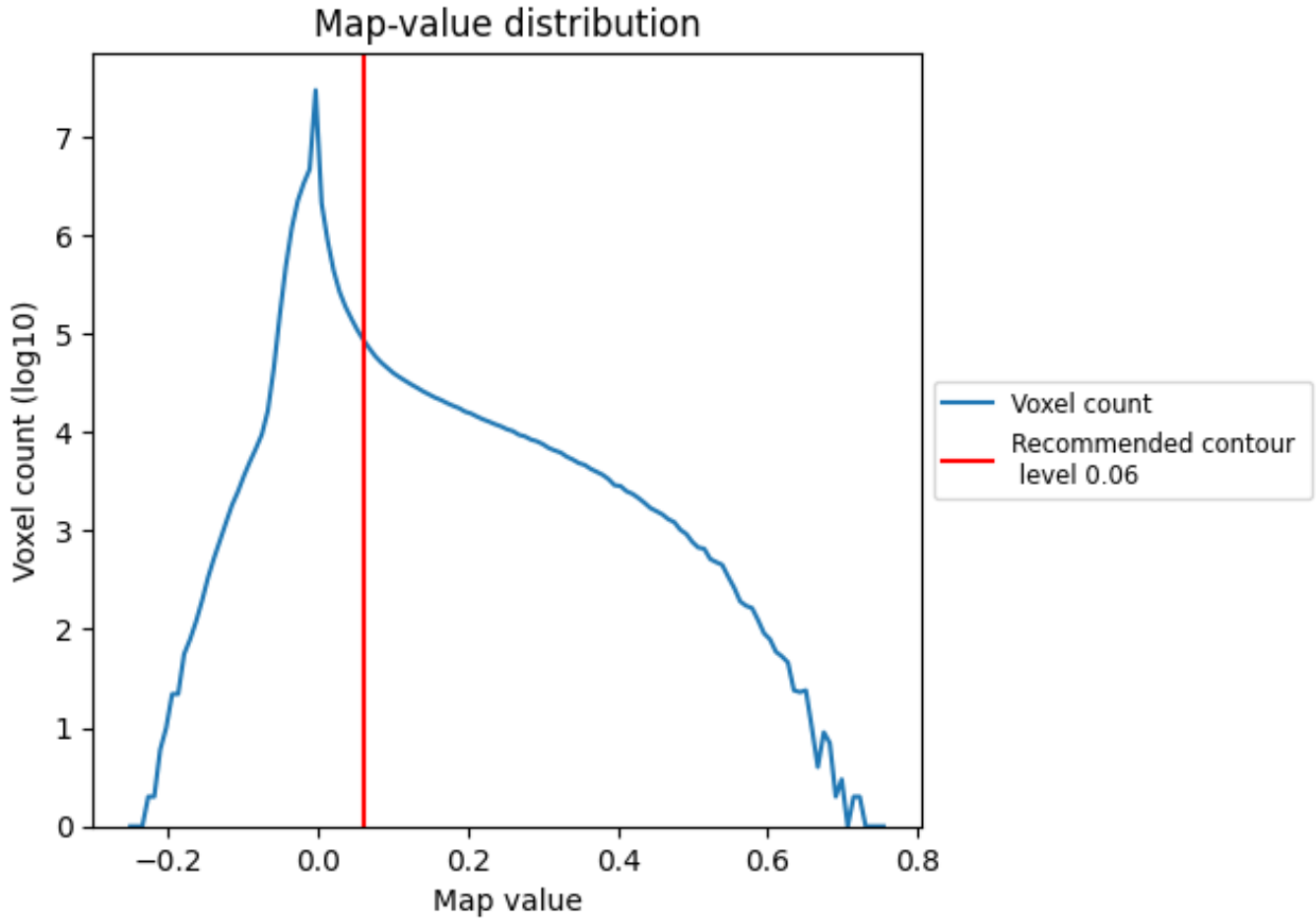


Z

7 Map analysis

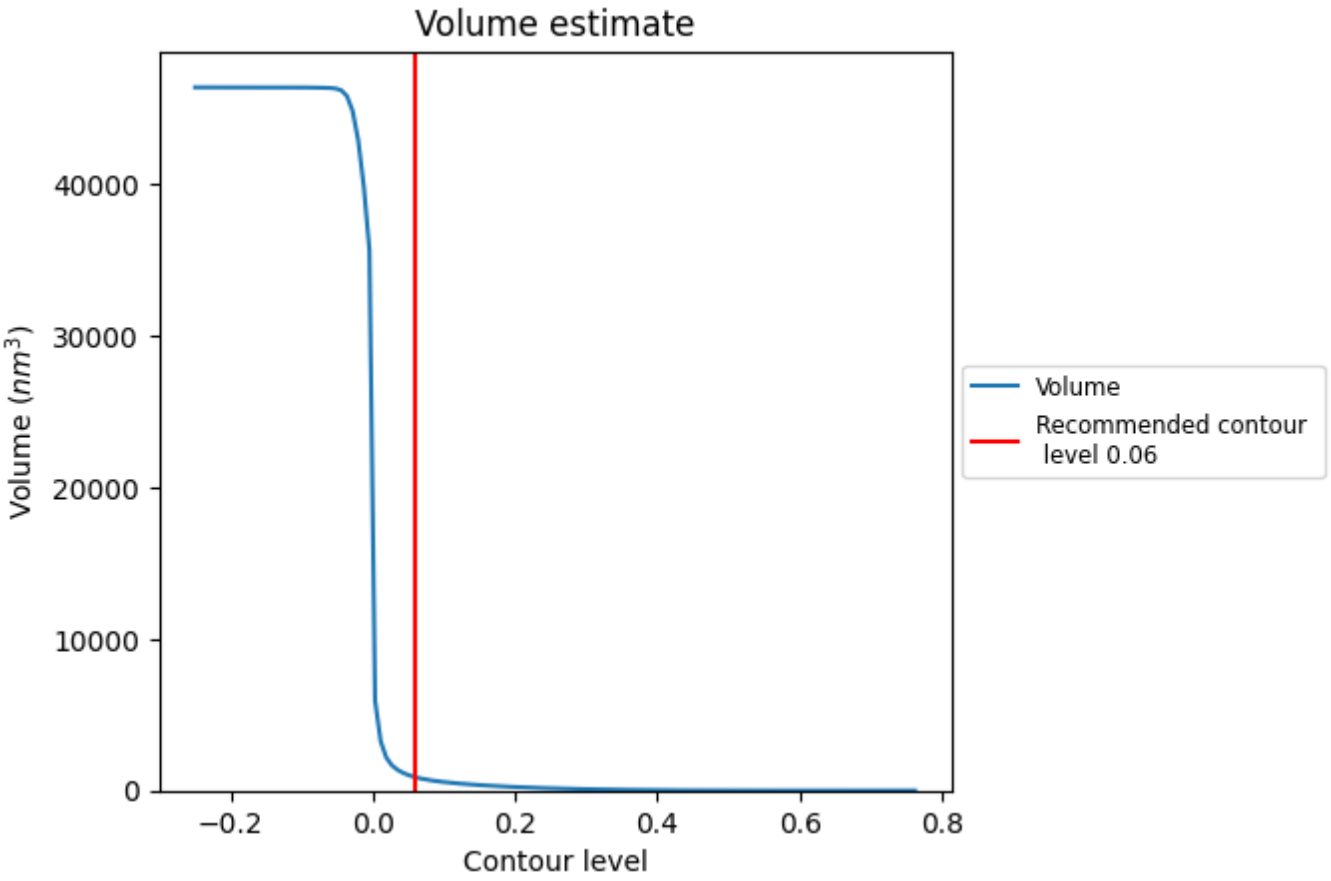
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

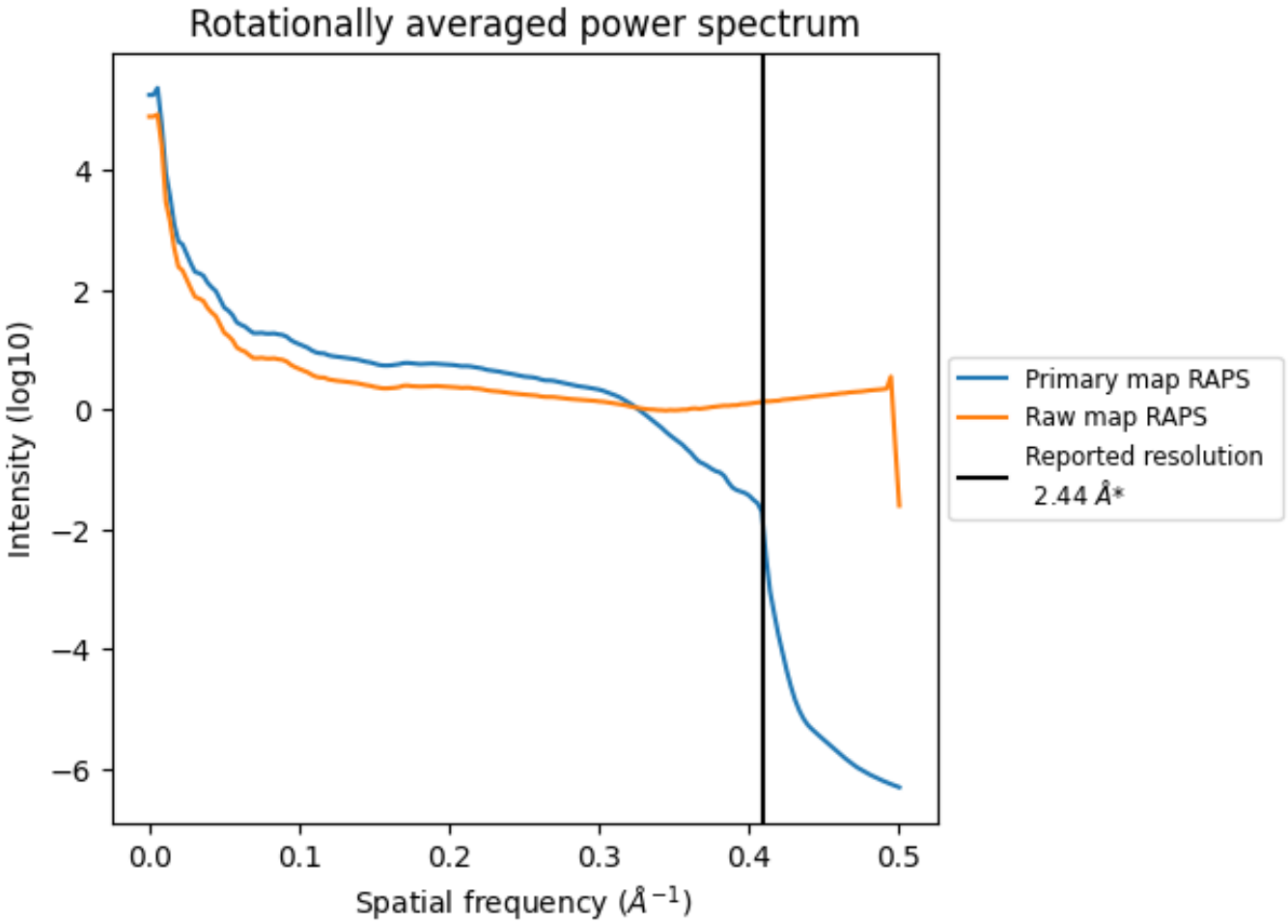
7.2 Volume estimate (i)



The volume at the recommended contour level is 878 nm^3; this corresponds to an approximate mass of 793 kDa.

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

7.3 Rotationally averaged power spectrum (i)

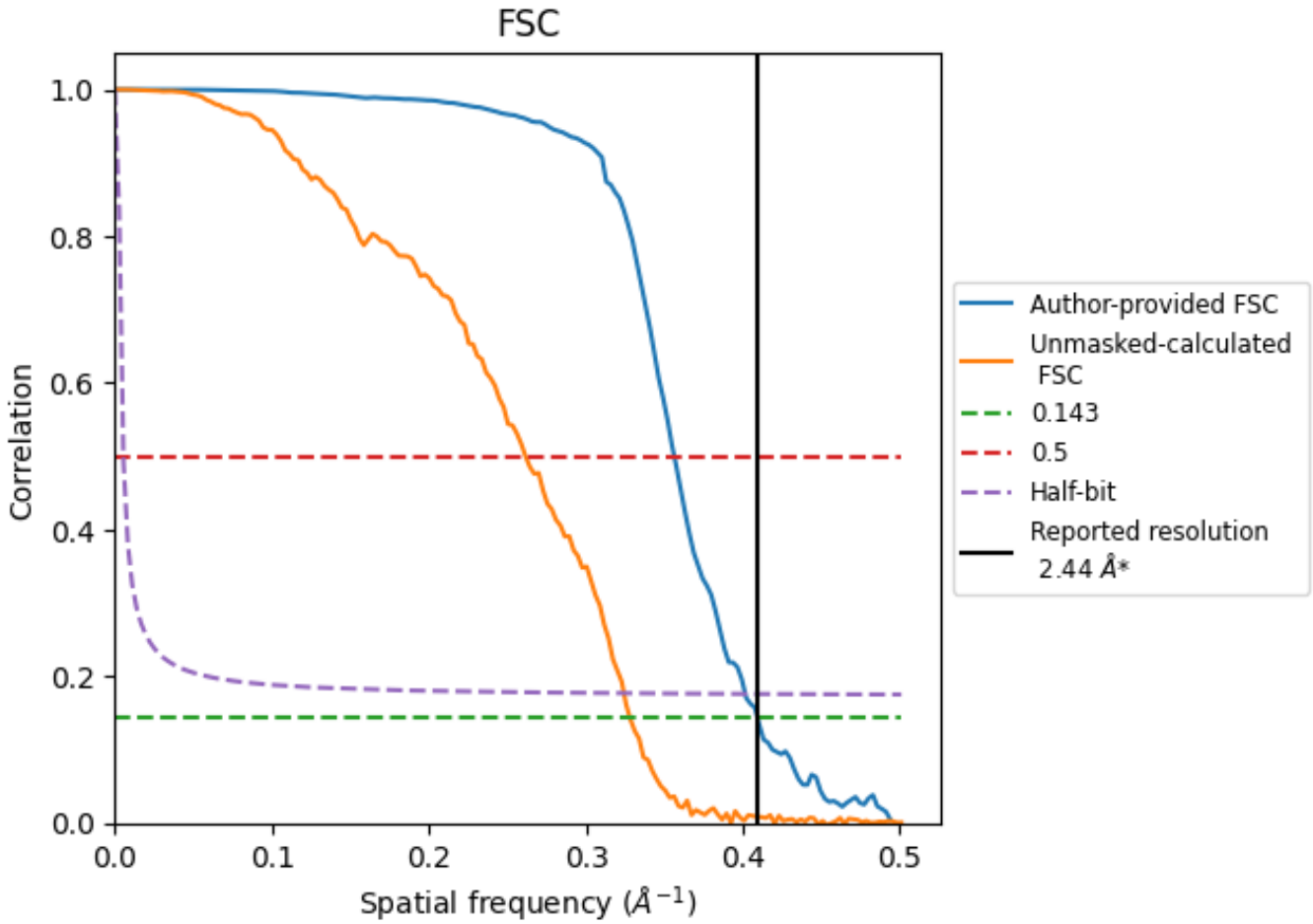


*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8.2 Resolution estimates (i)

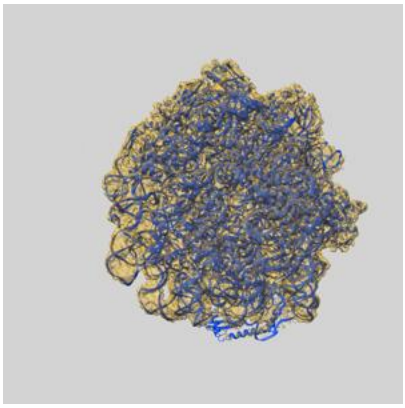
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.81	2.49
Unmasked-calculated*	3.05	3.82	3.08

*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 3.05 differs from the reported value 2.44 by more than 10 %

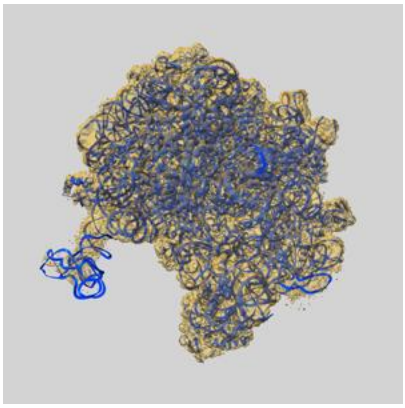
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19428 and PDB model 8RQ0. Per-residue inclusion information can be found in section 3 on page 10.

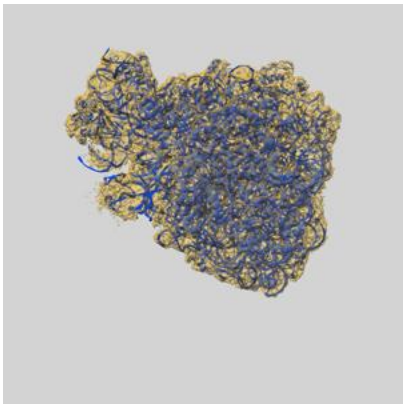
9.1 Map-model overlay



X



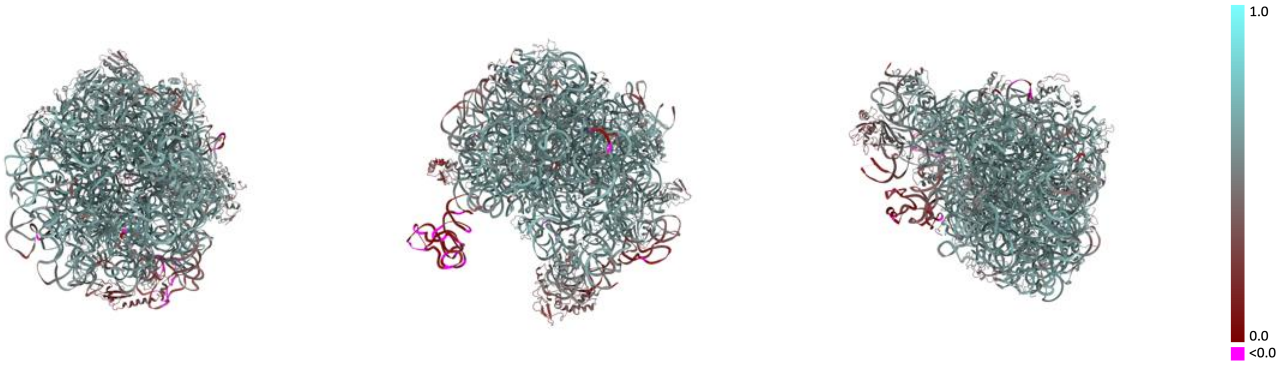
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

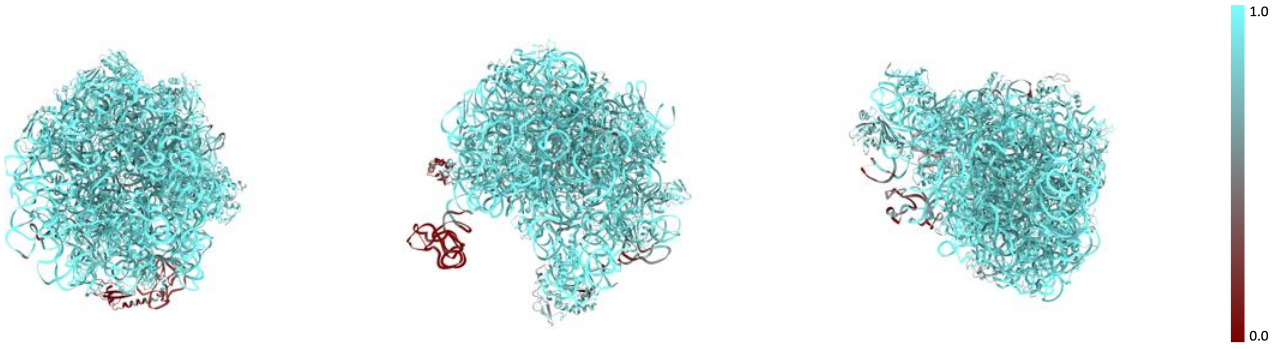
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

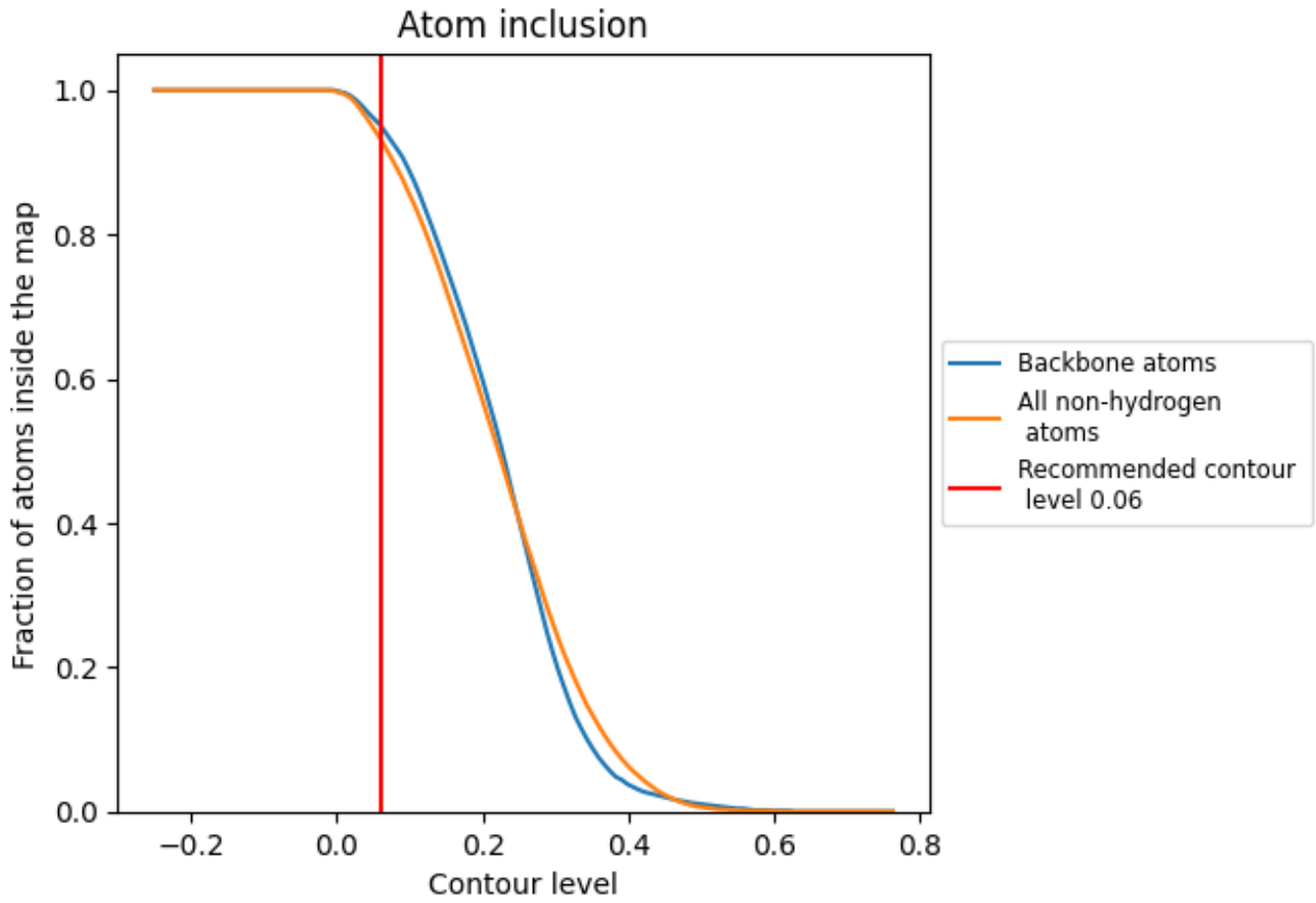
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.5570
0	0.9490	0.5850
1	0.9180	0.5610
2	0.9720	0.6030
3	0.9760	0.6080
4	0.9450	0.5610
6	0.6730	0.3040
A	0.9470	0.5690
B	0.9800	0.5320
C	0.9680	0.5940
D	0.9470	0.5810
E	0.9010	0.5390
F	0.7880	0.3760
G	0.8740	0.4960
H	0.3490	0.2870
J	0.9480	0.5840
K	0.8640	0.5300
L	0.9320	0.5470
M	0.9470	0.5780
N	0.9650	0.5920
O	0.9330	0.5100
P	0.8850	0.5530
Q	0.9800	0.6080
R	0.9150	0.5490
S	0.9440	0.5720
T	0.9290	0.5460
U	0.9170	0.5140
V	0.9210	0.5420
W	0.9410	0.5980
X	0.9700	0.5790
Y	0.8810	0.4910
Z	0.9220	0.5610
x	0.3520	0.3190
y	0.6670	0.3740
z	0.6910	0.3700