wwPDB EM Validation Summary Report

Apr 22, 2025 – 08:46 AM EDT

PDB ID	:	8VK7 / pdb_00008vk7
EMDB ID	:	EMD-43305
Title	:	Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-B
Authors	:	Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on	:	2024-01-08
Resolution	:	3.09 Å(reported)
Based on initial models	:	5O61, 6DZI

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 (i) 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 (1)) were used in the production of this report:

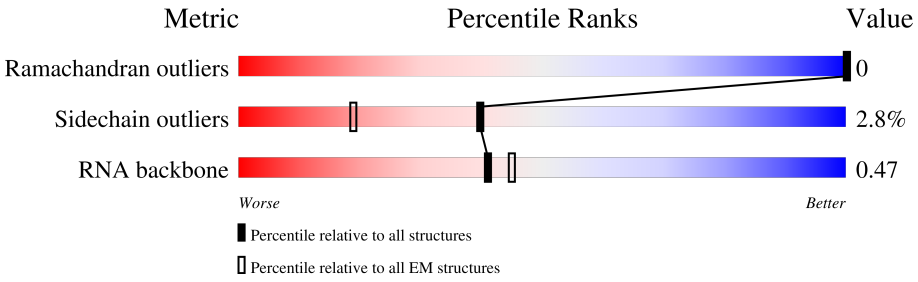
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.09 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	61	5% 97%
2	3	24	92%
3	4	470	21% 97%
4	A	3120	72% 22% 5%
5	B	118	66% 31%
6	C	278	98%
7	D	217	96%
8	E	215	95%

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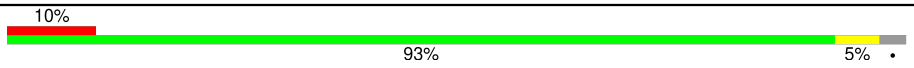
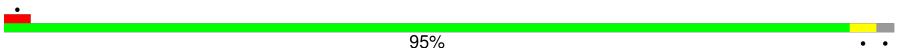
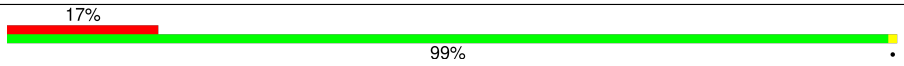
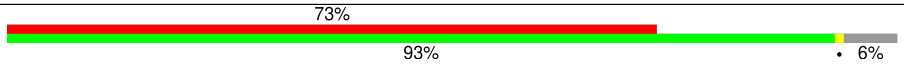
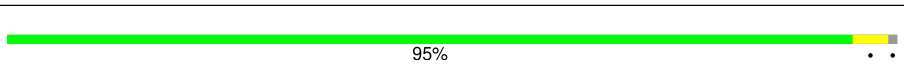
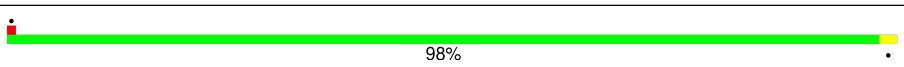
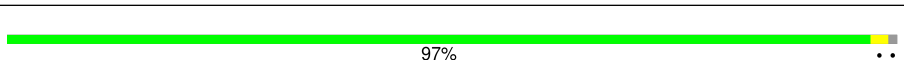
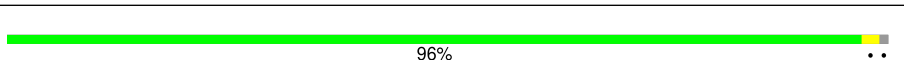
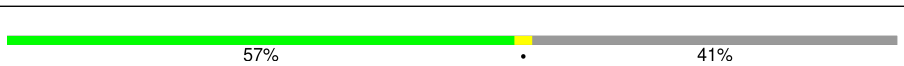
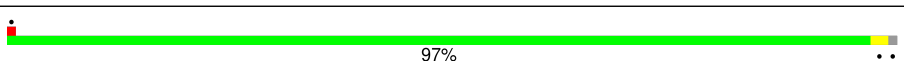
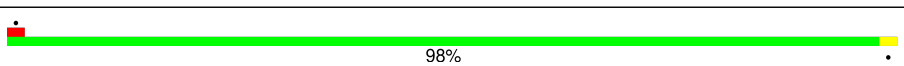
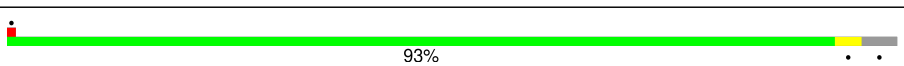
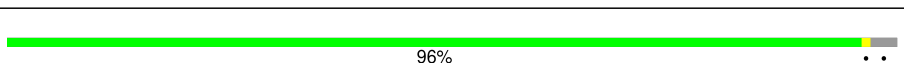
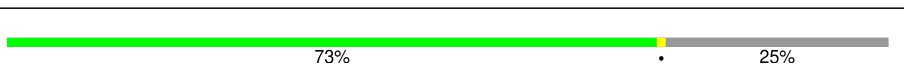
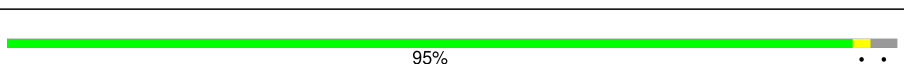
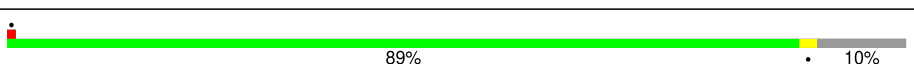
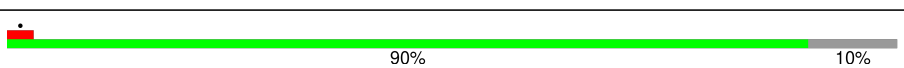
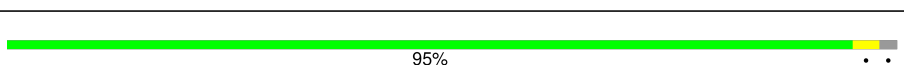
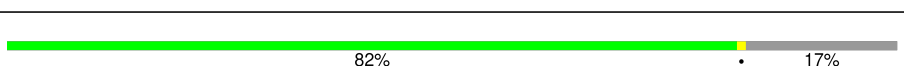
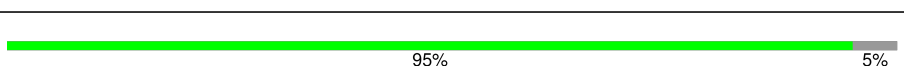
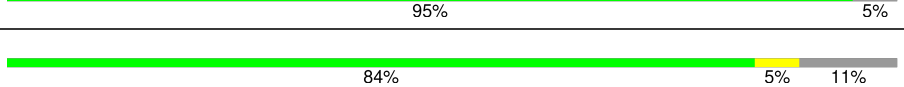
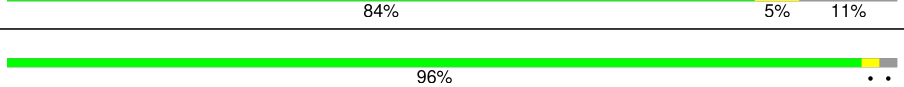
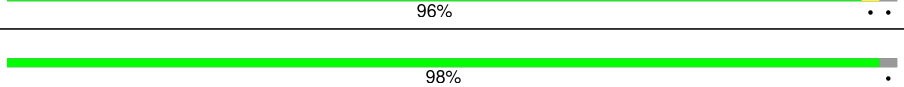
Mol	Chain	Length	Quality of chain
9	F	187	
10	G	179	
11	H	151	
12	I	175	
13	J	142	
14	K	147	
15	L	122	
16	M	147	
17	N	138	
18	O	199	
19	P	127	
20	Q	113	
21	R	129	
22	S	103	
23	T	153	
24	U	100	
25	V	105	
26	W	215	
27	X	88	
28	Y	64	
29	Z	77	
30	b	57	
31	c	55	
32	d	47	
33	e	64	

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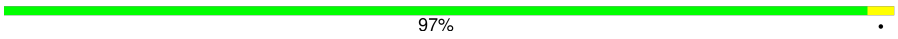
Mol	Chain	Length	Quality of chain
34	f	37	
35	g	75	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 96832 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total 474	C 292	N 95	O 87	0	0

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total 189	C 111	N 50	O 28	0	0

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	468	Total 3539	C 2187	N 651	O 694	S 7	0	0

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2950	Total 63364	C 28241	N 11658	O 20515	P 2950	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	114	Total 2438	C 1088	N 452	O 784	P 114	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	275	Total 2110	C 1298	N 438	O 370	S 4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 14 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 19 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	P	126	Total	C	N	O	0	0
			956	586	199	171		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 21 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 22 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	100	Total 754	C 478	N 137	O 139	0	0

- Molecule 23 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	114	Total 873	C 543	N 171	O 159	0	0

- Molecule 24 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	97	Total 756	C 479	N 138	O 139	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	95	Total 719	C 448	N 135	O 134	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	95	Total 735	C 452	N 149	O 134	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	79	Total 586	C 361	N 123	O 102	0	0

- Molecule 28 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 31 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	e	63	Total	C	N	O	0	0
			502	302	115	85		

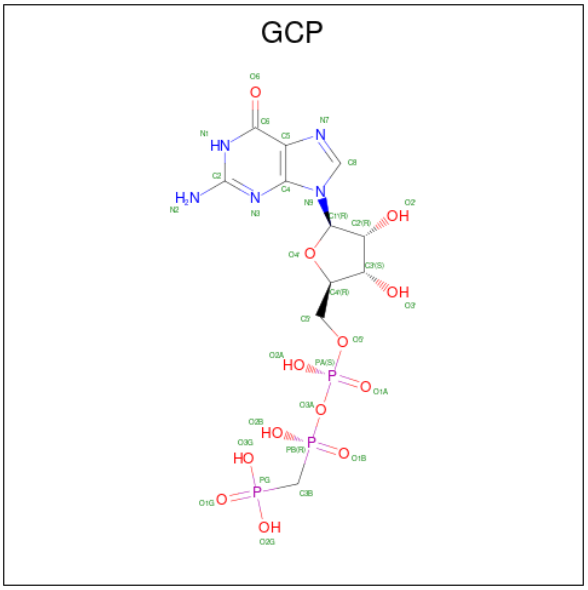
- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 35 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 36 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



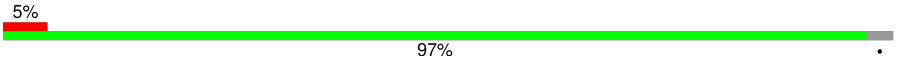
Mol	Chain	Residues	Atoms					AltConf
36	4	1	Total	C	N	O	P	0
			32	11	5	13	3	

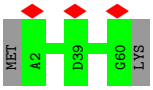
3 Residue-property plots (i)

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: 50S ribosomal protein L30

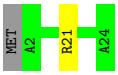
Chain 2:





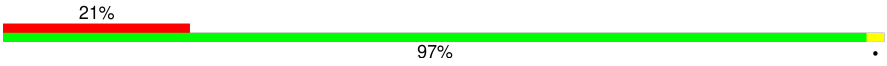
• Molecule 2: 50S Ribosomal Protein L37

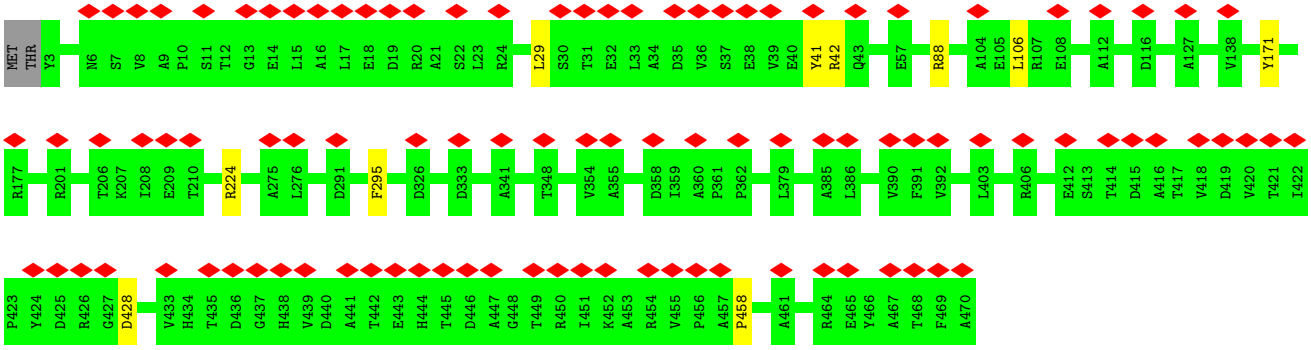
Chain 3:



• Molecule 3: GTPase HflX

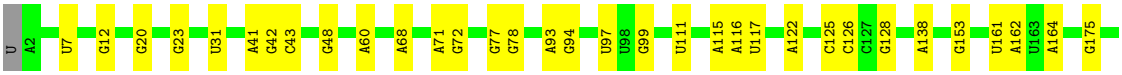
Chain 4:

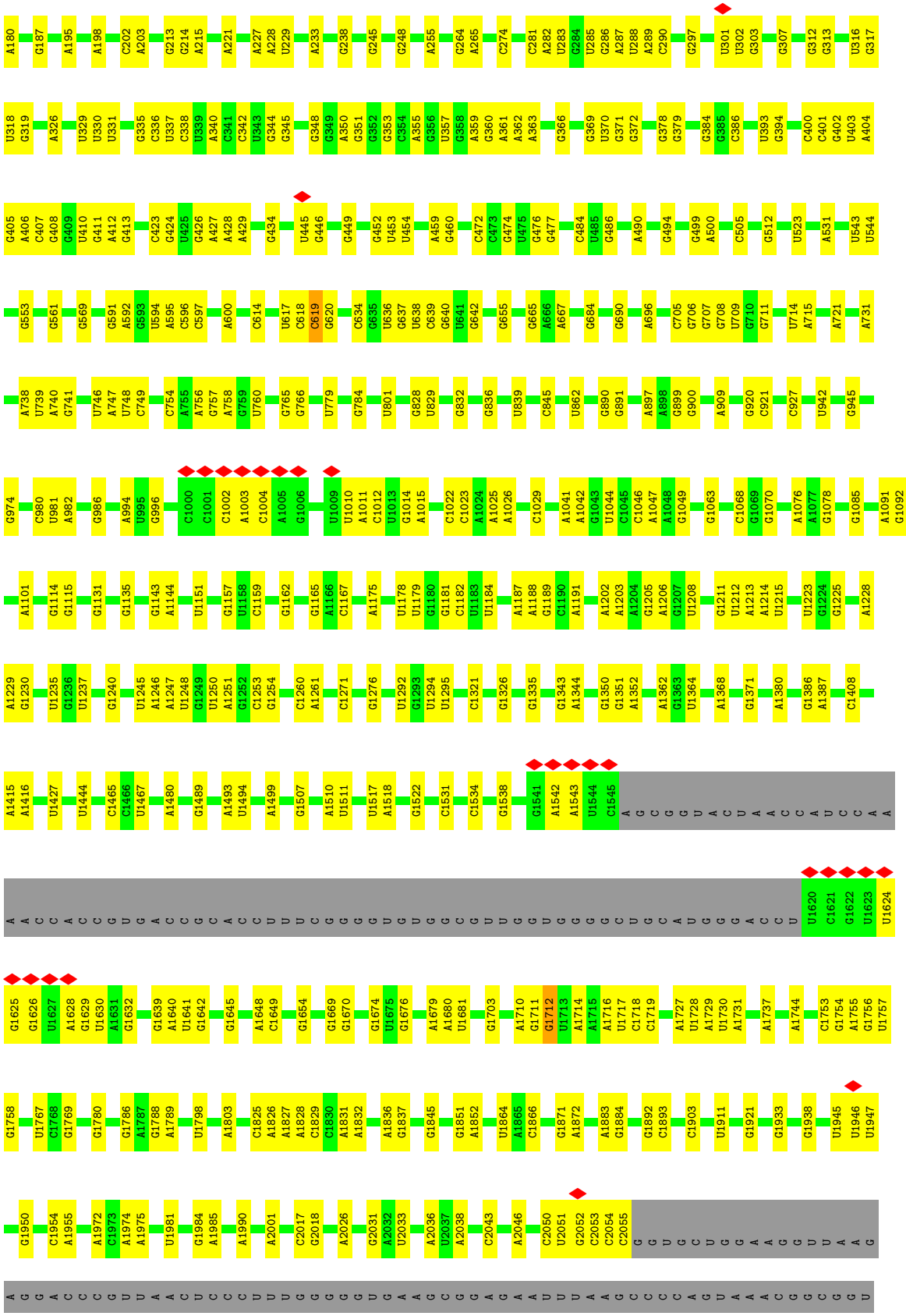


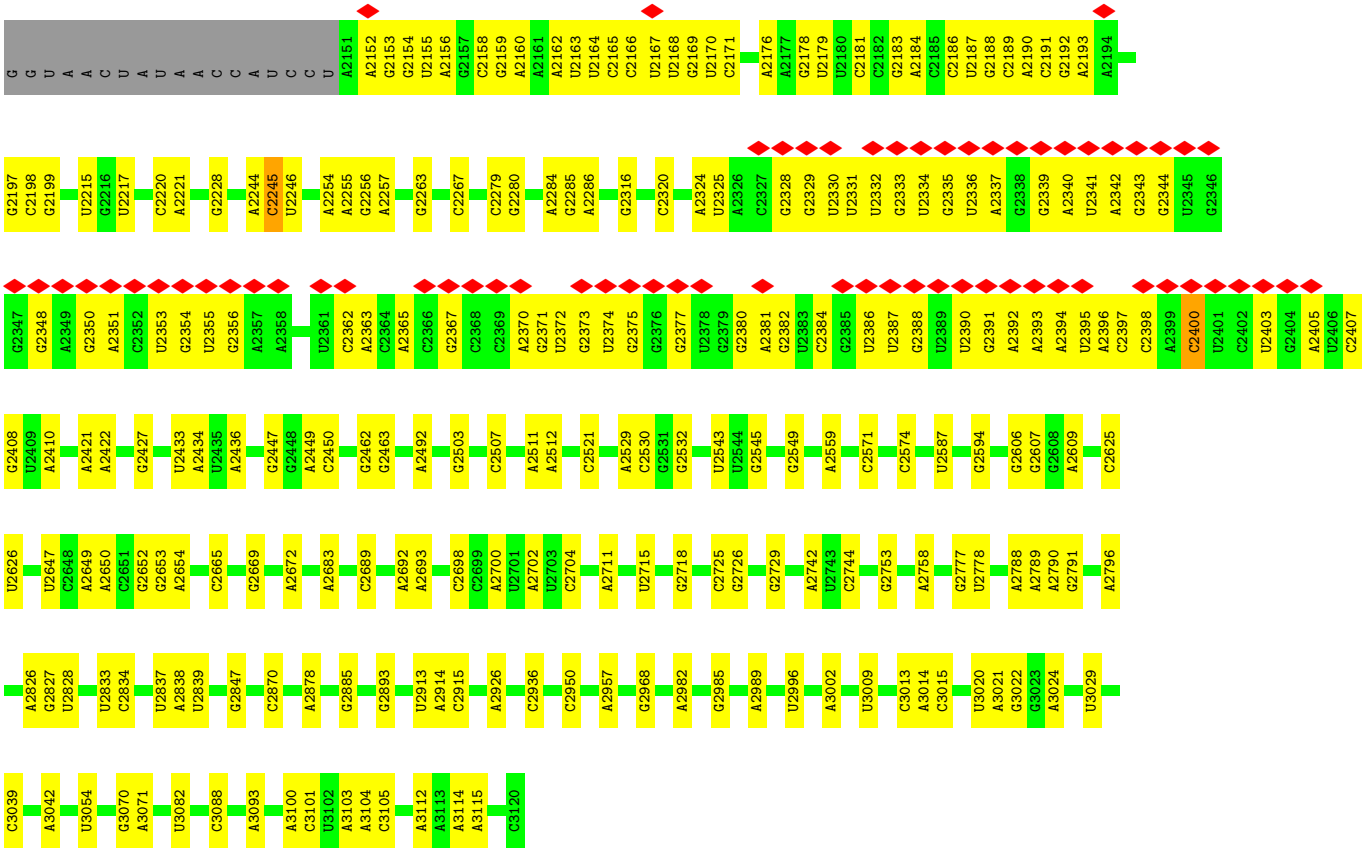


• Molecule 4: 23S ribosomal RNA

Chain A:

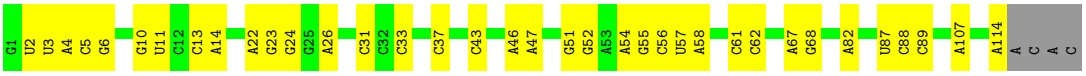






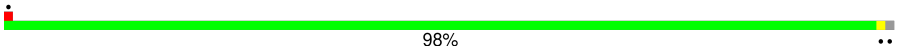
• Molecule 5: 5S ribosomal RNA

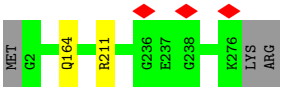
Chain B:



• Molecule 6: 50S ribosomal protein L2

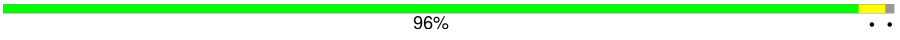
Chain C:

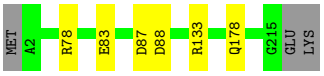




• Molecule 7: 50S ribosomal protein L3

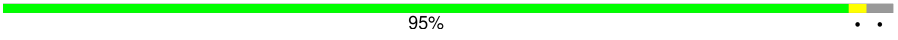
Chain D:





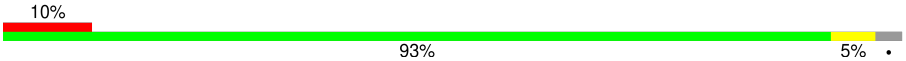
• Molecule 8: 50S Ribosomal Protein L4

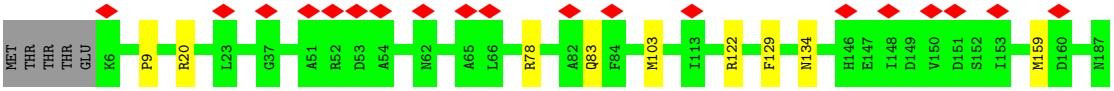
Chain E:



• Molecule 9: 50S Ribosomal Protein L5

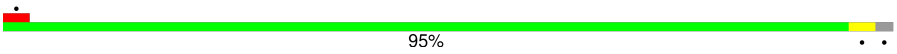
Chain F:

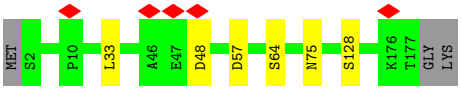




• Molecule 10: 50S ribosomal protein L6

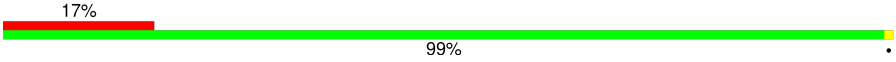
Chain G:

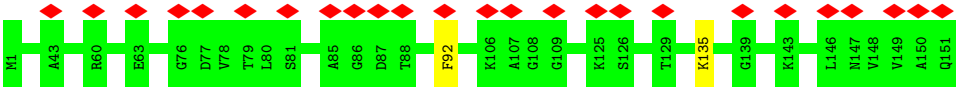




• Molecule 11: 50S ribosomal protein L9

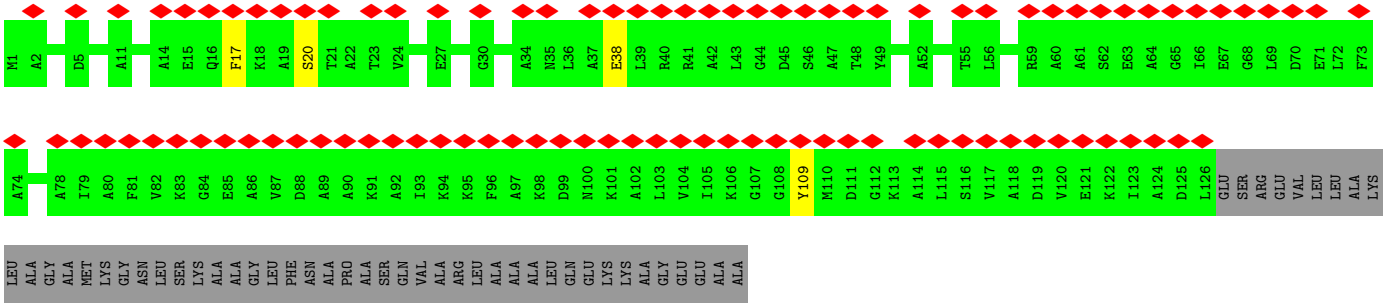
Chain H:





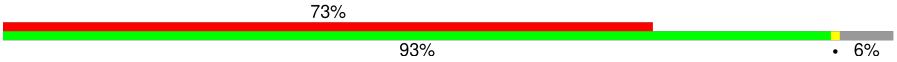
• Molecule 12: 50S ribosomal protein L10

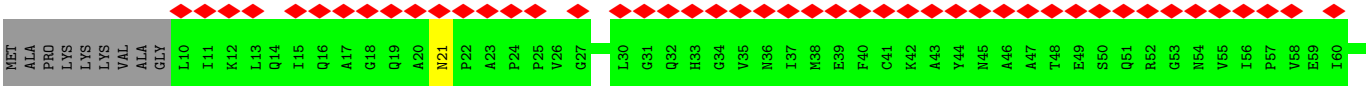
Chain I:

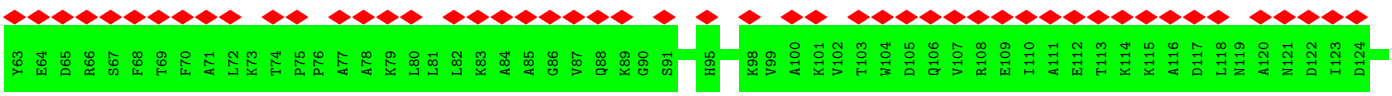


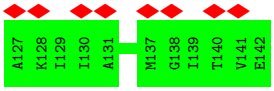
• Molecule 13: 50S ribosomal protein L11

Chain J:



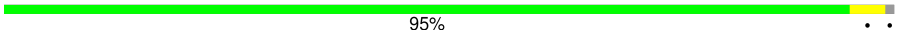


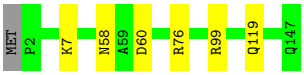




• Molecule 14: 50S Ribosomal Protein L13

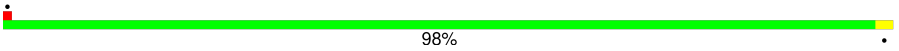
Chain K:

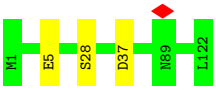




• Molecule 15: 50S ribosomal protein L14

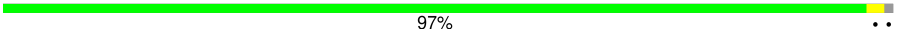
Chain L:

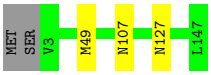




• Molecule 16: 50S ribosomal protein L15

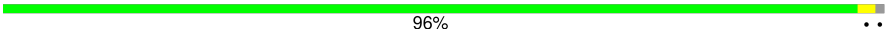
Chain M:





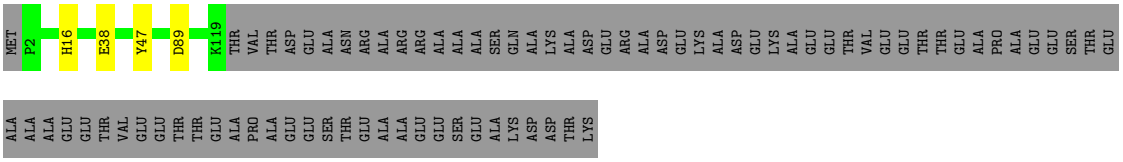
• Molecule 17: Large ribosomal subunit protein uL16

Chain N:



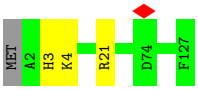
• Molecule 18: 50S ribosomal protein L17

Chain O:



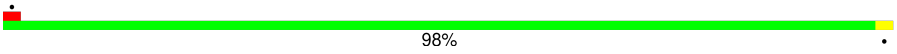
• Molecule 19: 50S Ribosomal Protein L18

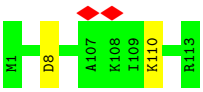
Chain P:



• Molecule 20: 50S ribosomal protein L19

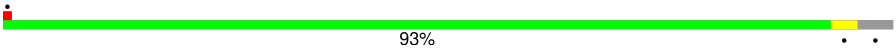
Chain Q:

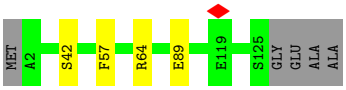




• Molecule 21: 50S Ribosomal Protein L20

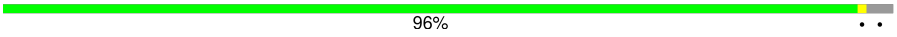
Chain R:





• Molecule 22: 50S Ribosomal Protein L21

Chain S:

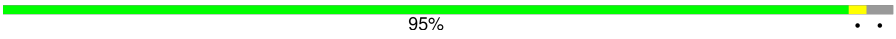


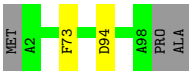
• Molecule 23: 50S Ribosomal Protein L22

Chain T:

• Molecule 24: 50S Ribosomal Protein L23

Chain U:



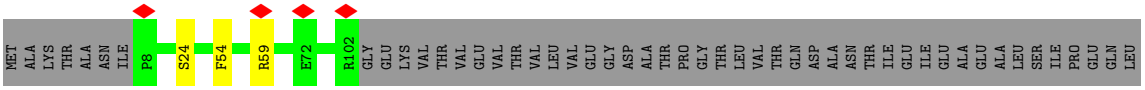


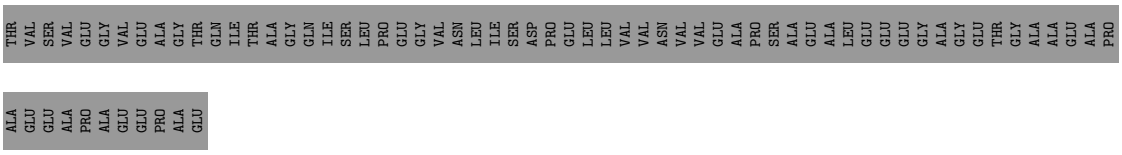
• Molecule 25: 50S ribosomal protein L24

Chain V:

• Molecule 26: 50S ribosomal protein L25

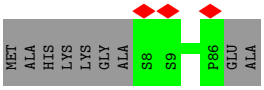
Chain W:





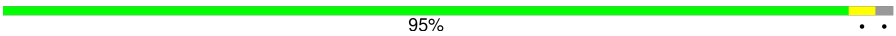
• Molecule 27: 50S ribosomal protein L27

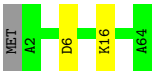
Chain X:



• Molecule 28: 50S Ribosomal Protein L28

Chain Y:



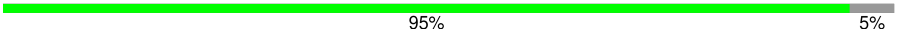


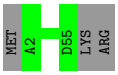
• Molecule 29: 50S ribosomal protein L29

Chain Z:

• Molecule 30: 50S ribosomal protein L32

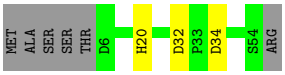
Chain b:





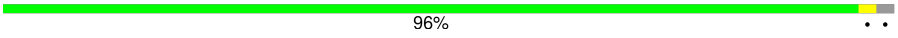
• Molecule 31: 50S Ribosomal Protein L33

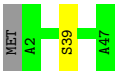
Chain c:



• Molecule 32: 50S ribosomal protein L34

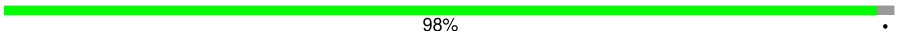
Chain d:





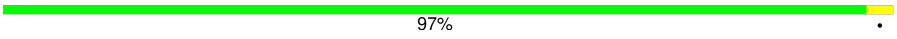
• Molecule 33: 50S ribosomal protein L35

Chain e:



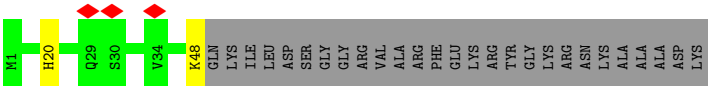
• Molecule 34: 50S ribosomal protein L36

Chain f:



• Molecule 35: 50S Ribosomal Protein L31

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.85	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.755	Depositor
Minimum map value	-0.985	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	430.4, 430.4, 430.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2	0.28	0/477	0.58	0/640
2	3	0.29	0/191	0.65	0/247
3	4	0.49	2/3583 (0.1%)	0.69	3/4857 (0.1%)
4	A	0.73	0/70952	0.82	23/110707 (0.0%)
5	B	0.56	0/2727	0.80	1/4250 (0.0%)
6	C	0.35	0/2153	0.59	0/2895
7	D	0.37	0/1609	0.58	0/2165
8	E	0.34	0/1592	0.52	0/2153
9	F	0.30	0/1467	0.62	2/1973 (0.1%)
10	G	0.31	0/1369	0.56	0/1848
11	H	0.28	0/1027	0.50	0/1398
12	I	0.27	0/925	0.50	0/1246
13	J	0.26	0/1006	0.48	0/1364
14	K	0.35	0/1157	0.51	0/1567
15	L	0.35	0/946	0.58	0/1268
16	M	0.34	0/1091	0.54	0/1457
17	N	0.36	0/1118	0.56	0/1506
18	O	0.36	0/945	0.53	0/1267
19	P	0.30	0/966	0.59	0/1298
20	Q	0.36	0/921	0.57	0/1236
21	R	0.38	0/1000	0.57	0/1341
22	S	0.35	0/764	0.51	0/1030
23	T	0.33	0/887	0.57	0/1204
24	U	0.33	0/766	0.53	0/1030
25	V	0.31	0/725	0.54	0/969
26	W	0.30	0/745	0.59	0/1008
27	X	0.36	0/595	0.61	0/798
28	Y	0.34	0/478	0.60	0/641
29	Z	0.32	0/534	0.59	0/713
30	b	0.34	0/427	0.60	0/572
31	c	0.33	0/413	0.54	0/553
32	d	0.35	0/380	0.71	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.34	0/507	0.63	0/672
34	f	0.33	0/303	0.60	0/401
35	g	0.28	0/372	0.47	0/503
All	All	0.64	2/105118 (0.0%)	0.76	29/157277 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	458	PRO	CG-CD	-21.90	0.78	1.50
3	4	458	PRO	N-CD	9.75	1.61	1.47

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4	458	PRO	N-CD-CG	-20.42	72.57	103.20
3	4	458	PRO	CA-CB-CG	-10.78	83.52	104.00
4	A	1023	C	N3-C2-O2	-9.24	115.43	121.90
3	4	458	PRO	CA-N-CD	-8.96	98.95	111.50
4	A	986	G	C5-C6-O6	7.59	133.16	128.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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	
1	2	57/61 (93%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
3	4	466/470 (99%)	369 (79%)	97 (21%)	0	100	100
6	C	273/278 (98%)	248 (91%)	25 (9%)	0	100	100
7	D	212/217 (98%)	200 (94%)	12 (6%)	0	100	100
8	E	207/215 (96%)	185 (89%)	22 (11%)	0	100	100
9	F	180/187 (96%)	156 (87%)	24 (13%)	0	100	100
10	G	174/179 (97%)	160 (92%)	14 (8%)	0	100	100
11	H	149/151 (99%)	126 (85%)	23 (15%)	0	100	100
12	I	124/175 (71%)	110 (89%)	14 (11%)	0	100	100
13	J	131/142 (92%)	113 (86%)	18 (14%)	0	100	100
14	K	144/147 (98%)	127 (88%)	17 (12%)	0	100	100
15	L	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
16	M	143/147 (97%)	127 (89%)	16 (11%)	0	100	100
17	N	134/138 (97%)	120 (90%)	14 (10%)	0	100	100
18	O	116/199 (58%)	109 (94%)	7 (6%)	0	100	100
19	P	124/127 (98%)	115 (93%)	9 (7%)	0	100	100
20	Q	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
21	R	122/129 (95%)	114 (93%)	8 (7%)	0	100	100
22	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
23	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
24	U	95/100 (95%)	86 (90%)	9 (10%)	0	100	100
25	V	91/105 (87%)	80 (88%)	11 (12%)	0	100	100
26	W	93/215 (43%)	87 (94%)	6 (6%)	0	100	100
27	X	77/88 (88%)	74 (96%)	3 (4%)	0	100	100
28	Y	61/64 (95%)	56 (92%)	5 (8%)	0	100	100
29	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
30	b	52/57 (91%)	46 (88%)	6 (12%)	0	100	100
31	c	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
32	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
33	e	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
34	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	g	46/75 (61%)	33 (72%)	13 (28%)	0	100	100
All	All	3982/4461 (89%)	3559 (89%)	423 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	17 (94%)	1 (6%)	17	46
3	4	370/372 (100%)	361 (98%)	9 (2%)	44	70
6	C	215/218 (99%)	213 (99%)	2 (1%)	75	88
7	D	160/163 (98%)	154 (96%)	6 (4%)	28	59
8	E	169/173 (98%)	165 (98%)	4 (2%)	44	70
9	F	151/156 (97%)	143 (95%)	8 (5%)	19	48
10	G	148/150 (99%)	142 (96%)	6 (4%)	26	57
11	H	90/116 (78%)	88 (98%)	2 (2%)	47	71
12	I	89/120 (74%)	85 (96%)	4 (4%)	23	53
13	J	102/108 (94%)	101 (99%)	1 (1%)	73	86
14	K	119/120 (99%)	113 (95%)	6 (5%)	20	50
15	L	100/100 (100%)	97 (97%)	3 (3%)	36	64
16	M	112/114 (98%)	109 (97%)	3 (3%)	40	67
17	N	114/116 (98%)	111 (97%)	3 (3%)	41	68
18	O	97/158 (61%)	93 (96%)	4 (4%)	26	57
19	P	93/94 (99%)	90 (97%)	3 (3%)	34	63
20	Q	100/100 (100%)	98 (98%)	2 (2%)	50	74
21	R	97/99 (98%)	93 (96%)	4 (4%)	26	57
22	S	81/83 (98%)	80 (99%)	1 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	T	90/117 (77%)	88 (98%)	2 (2%)	47 71
24	U	83/85 (98%)	81 (98%)	2 (2%)	44 70
25	V	79/86 (92%)	77 (98%)	2 (2%)	42 69
26	W	77/168 (46%)	74 (96%)	3 (4%)	27 58
27	X	58/63 (92%)	58 (100%)	0	100 100
28	Y	50/51 (98%)	48 (96%)	2 (4%)	27 58
29	Z	58/66 (88%)	57 (98%)	1 (2%)	56 78
30	b	43/46 (94%)	43 (100%)	0	100 100
31	c	47/52 (90%)	44 (94%)	3 (6%)	14 42
32	d	35/36 (97%)	34 (97%)	1 (3%)	37 65
33	e	53/54 (98%)	53 (100%)	0	100 100
34	f	35/35 (100%)	34 (97%)	1 (3%)	37 65
35	g	43/63 (68%)	41 (95%)	2 (5%)	22 52
All	All	3228/3555 (91%)	3137 (97%)	91 (3%)	40 66

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	N	116	ASP
22	S	78	PHE
18	O	38	GLU
20	Q	8	ASP
24	U	94	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	434	HIS
6	C	135	ASN
7	D	183	HIS
8	E	171	ASN
12	I	54	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	2947/3120 (94%)	675 (22%)	20 (0%)
5	B	113/118 (95%)	32 (28%)	6 (5%)
All	All	3060/3238 (94%)	707 (23%)	26 (0%)

5 of 707 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	7	U
4	A	12	G
4	A	20	G
4	A	23	G
4	A	31	U

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	2155	U
4	A	2362	C
5	B	57	U
4	A	2343	G
4	A	2374	U

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)

1 ligand is 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	$\#\|Z\|>2$
36	GCP	4	501	-	27,34,34	1.33	4 (14%)	35,54,54	1.86	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	GCP	4	501	-	-	1/15/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	501	GCP	C5-C6	3.78	1.47	1.41
36	4	501	GCP	PG-O3G	2.70	1.61	1.55
36	4	501	GCP	PG-O2G	2.61	1.60	1.55
36	4	501	GCP	PB-O3A	2.09	1.60	1.58

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	4	501	GCP	PB-O3A-PA	-4.62	117.30	132.37
36	4	501	GCP	C2-N1-C6	4.39	122.07	115.96
36	4	501	GCP	C5-C6-N1	-4.32	117.65	123.42
36	4	501	GCP	C2-N3-C4	4.05	119.86	115.48
36	4	501	GCP	N3-C2-N1	-2.71	123.77	127.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	4	501	GCP	C5'-O5'-PA-O1A

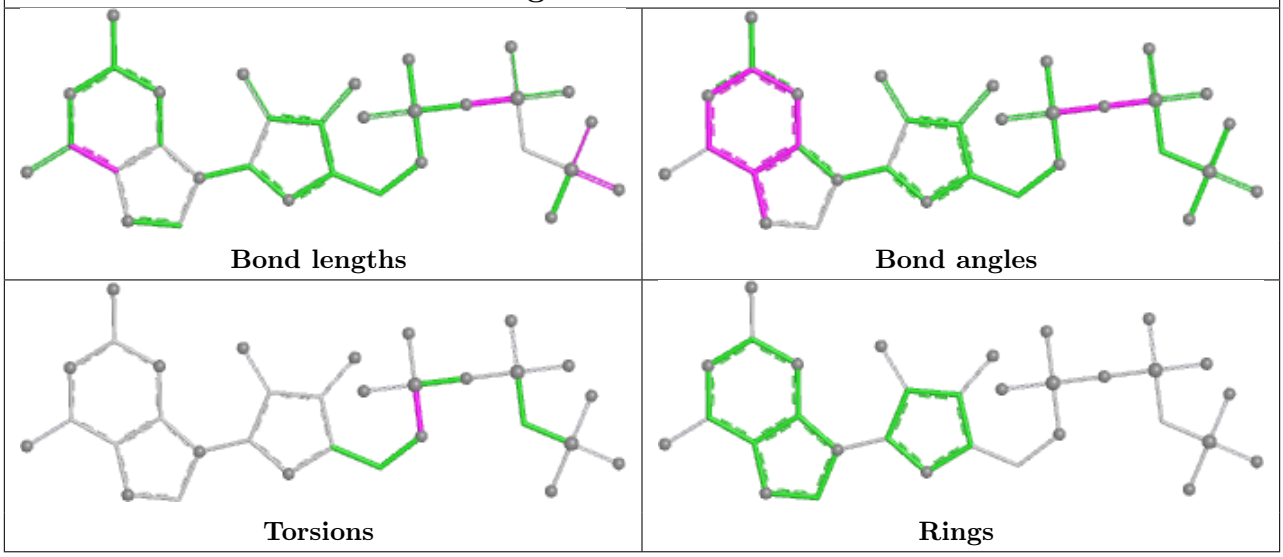
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GCP 4 501



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.

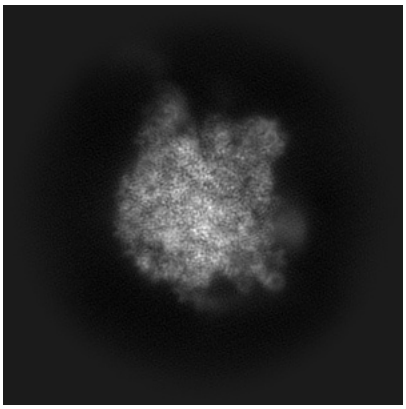
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43305. These allow visual inspection of the internal detail of the map and identification of artifacts.

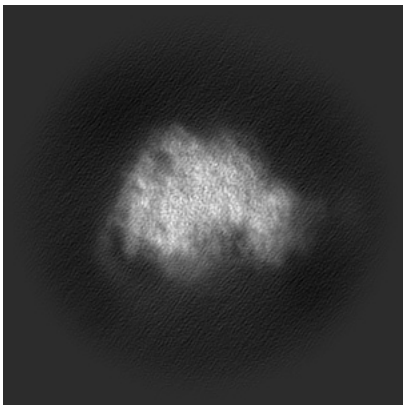
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

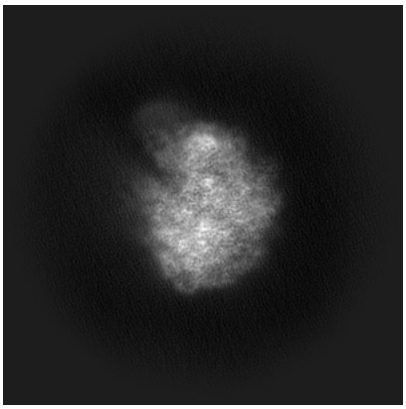
6.1.1 Primary map



X

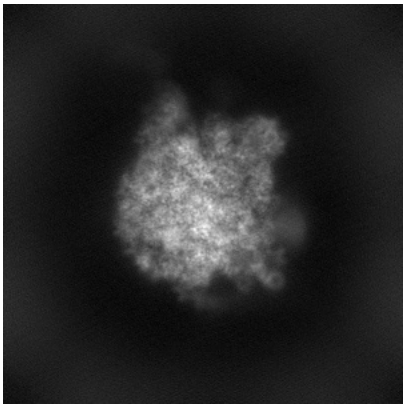


Y

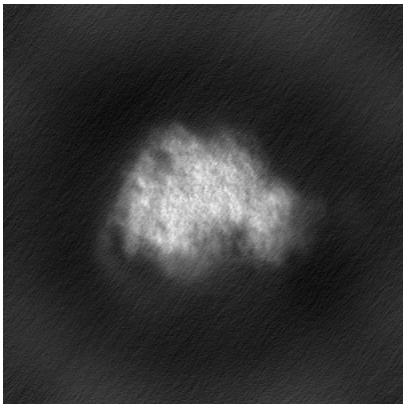


Z

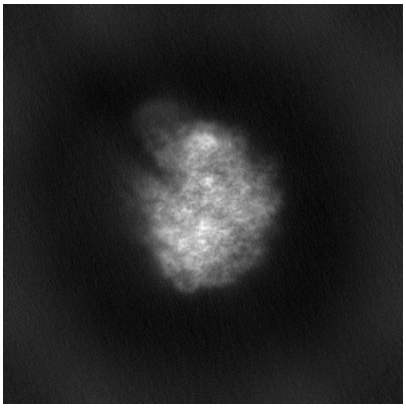
6.1.2 Raw map



X



Y

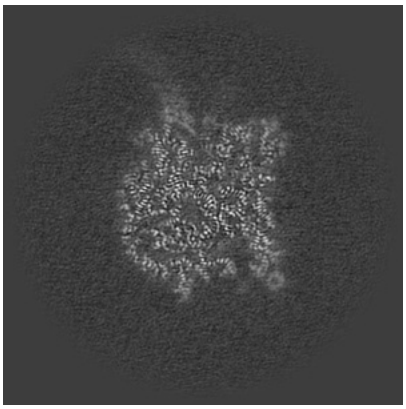


Z

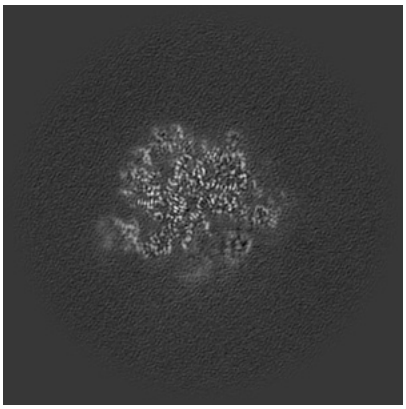
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

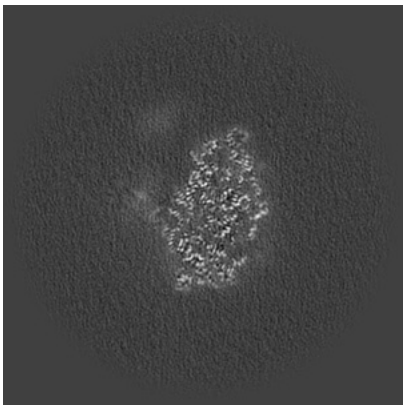
6.2.1 Primary map



X Index: 200

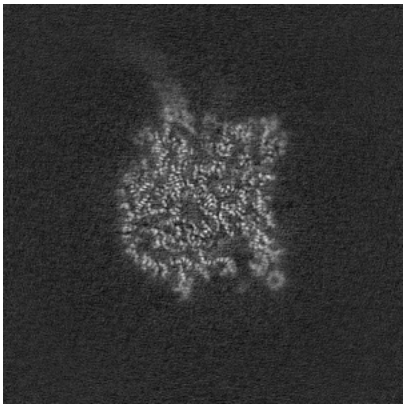


Y Index: 200

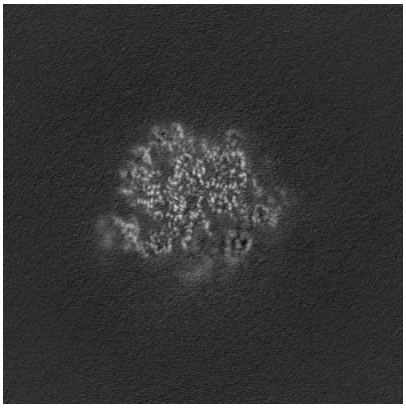


Z Index: 200

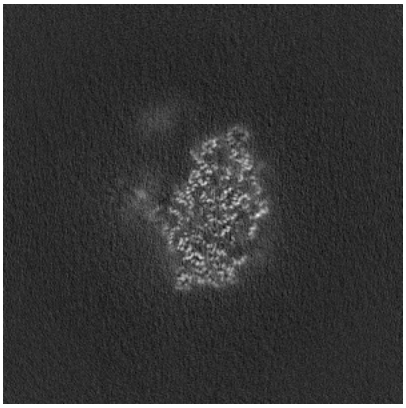
6.2.2 Raw map



X Index: 200



Y Index: 200

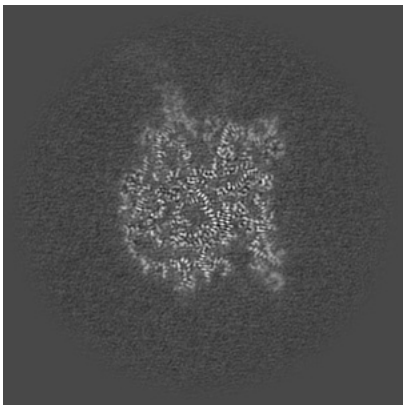


Z Index: 200

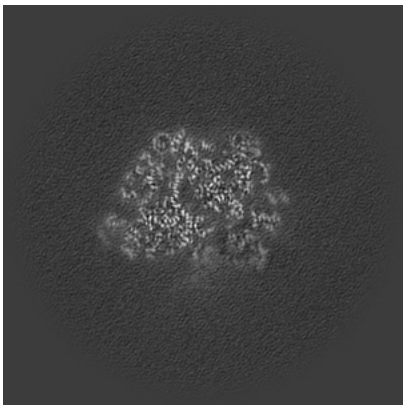
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

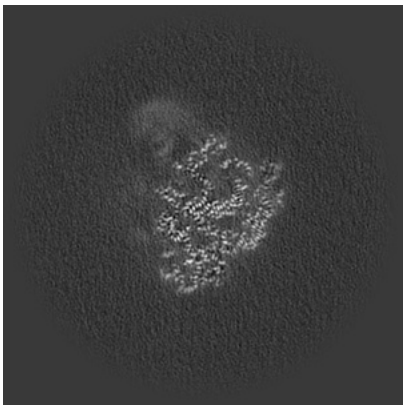
6.3.1 Primary map



X Index: 203

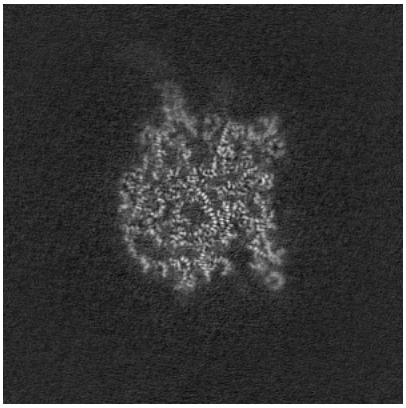


Y Index: 192

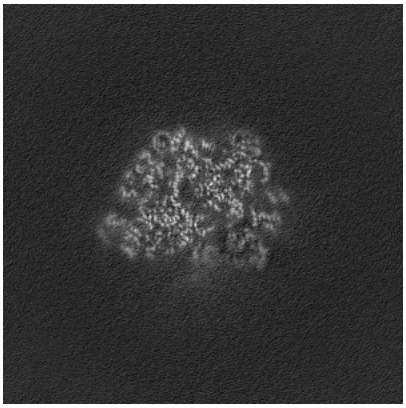


Z Index: 173

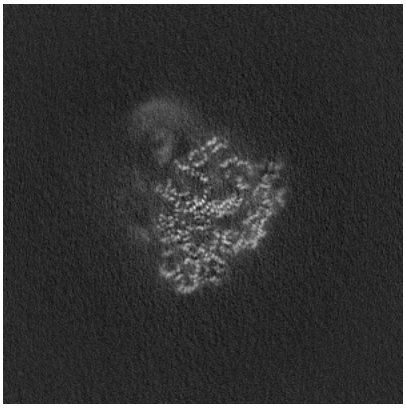
6.3.2 Raw map



X Index: 203



Y Index: 192

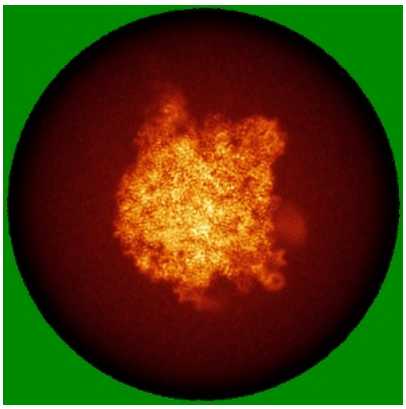


Z Index: 172

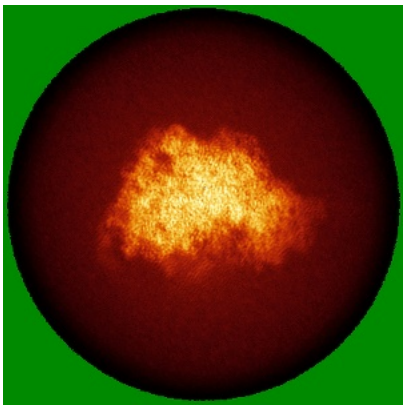
The images above show the largest variance slices of the map in three orthogonal directions.

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

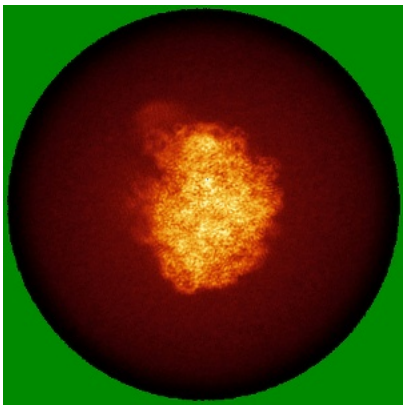
6.4.1 Primary map



X

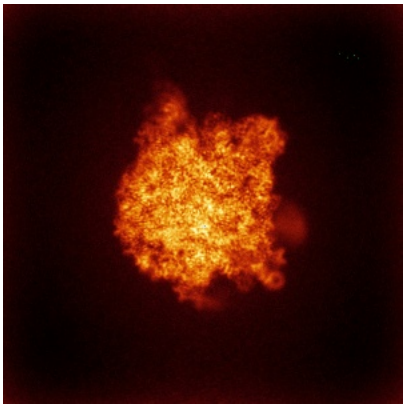


Y

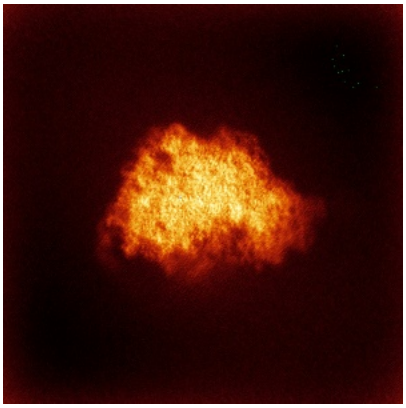


Z

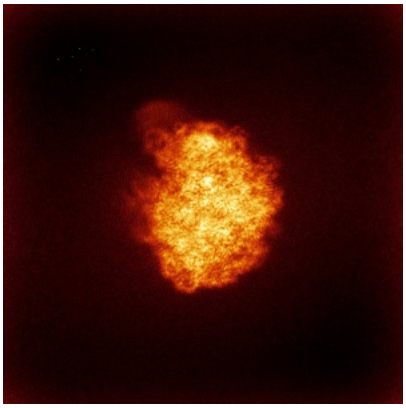
6.4.2 Raw map



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 0.35. 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.

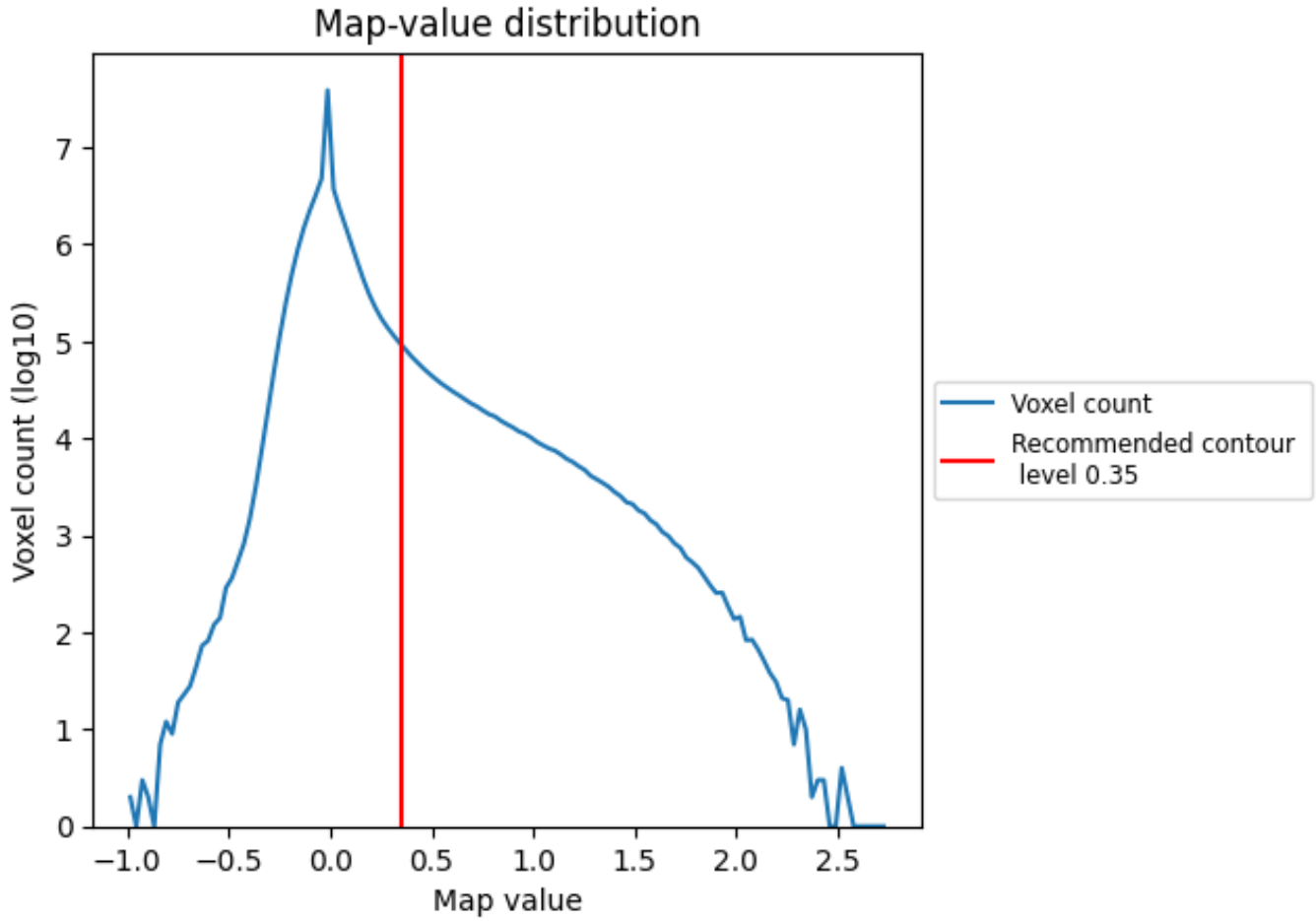
6.6 Mask visualisation (i)

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

7 Map analysis

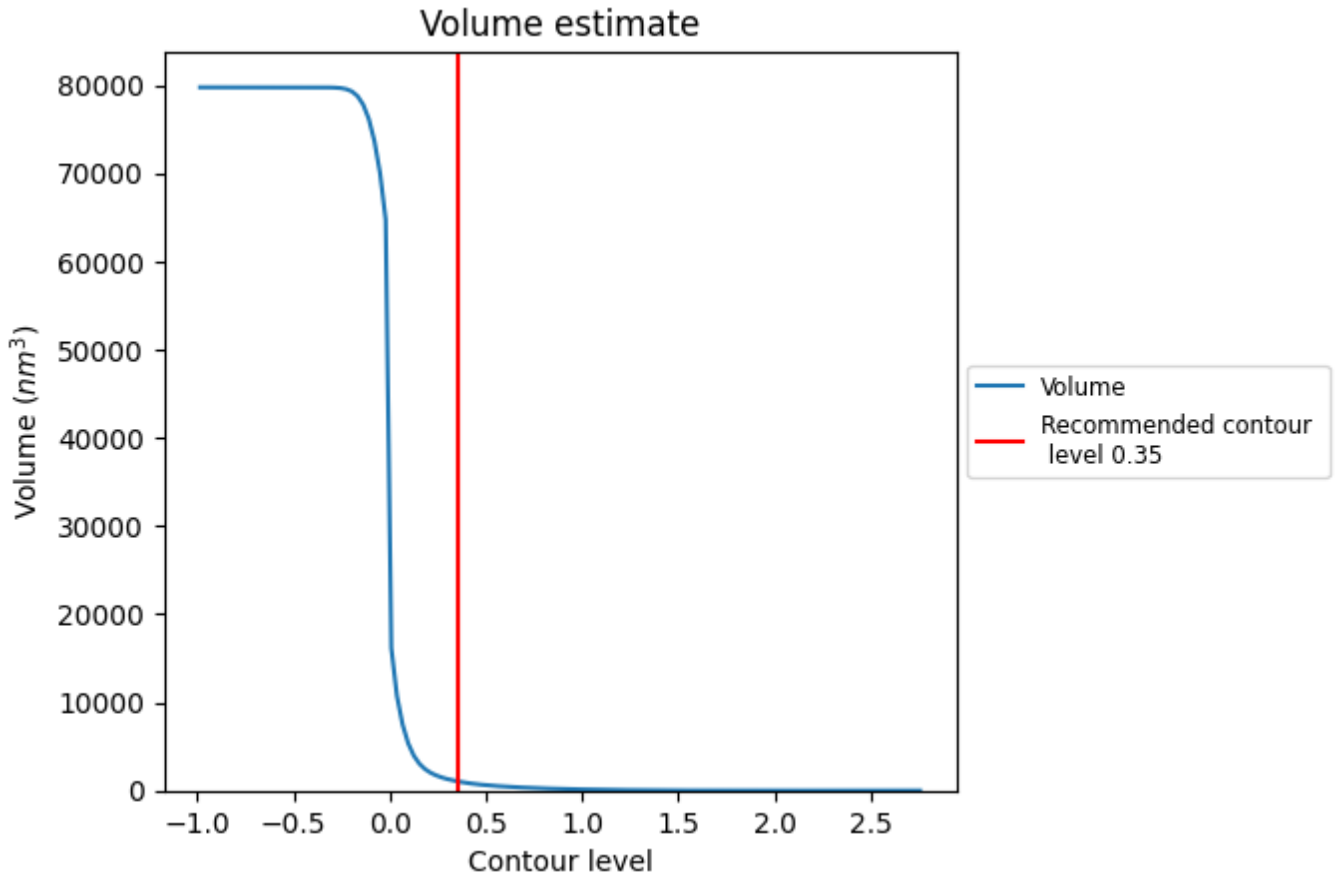
This section contains the results of statistical analysis of the map.

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.

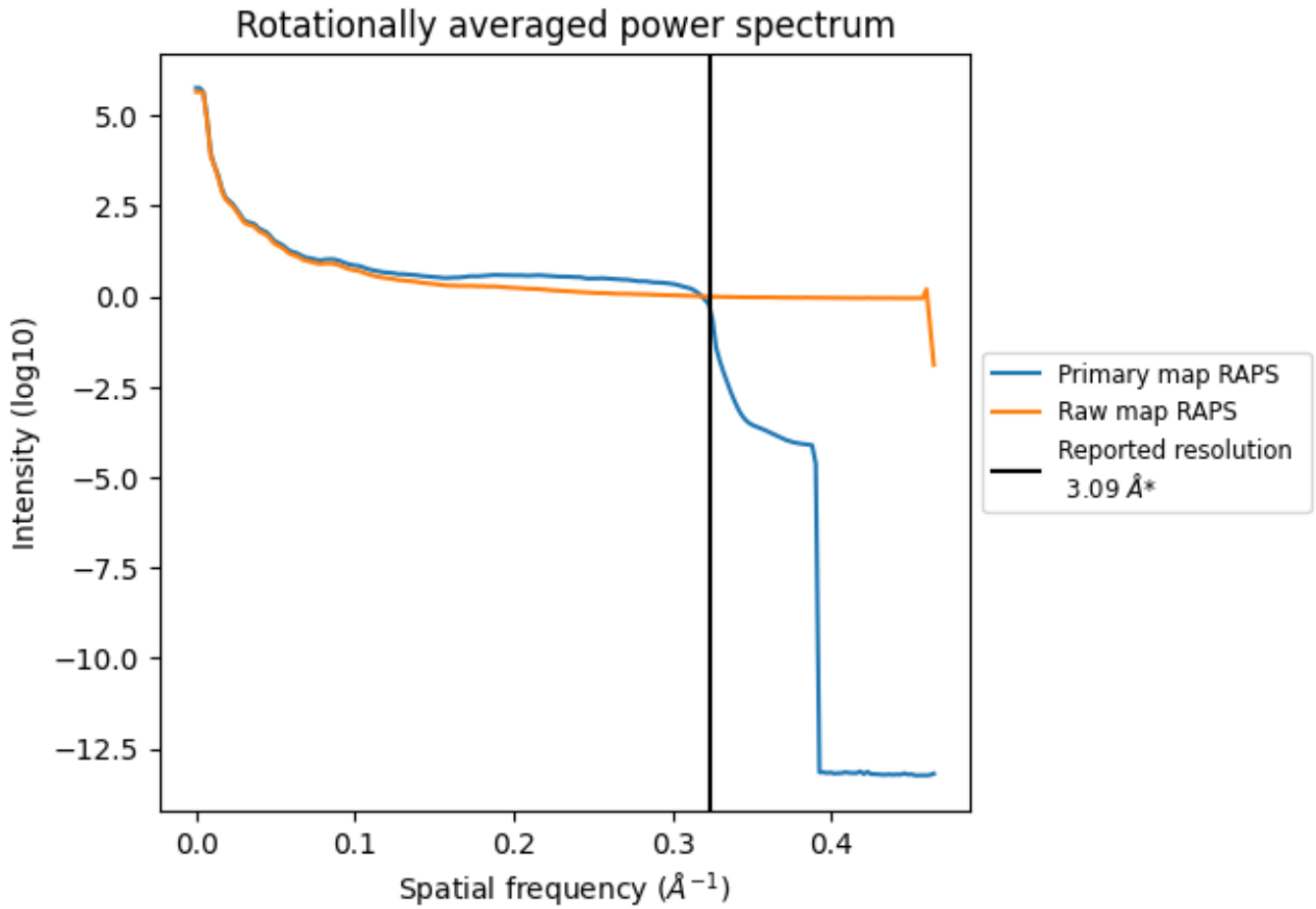
7.2 Volume estimate (i)



The volume at the recommended contour level is 1055 nm^3; this corresponds to an approximate mass of 953 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)

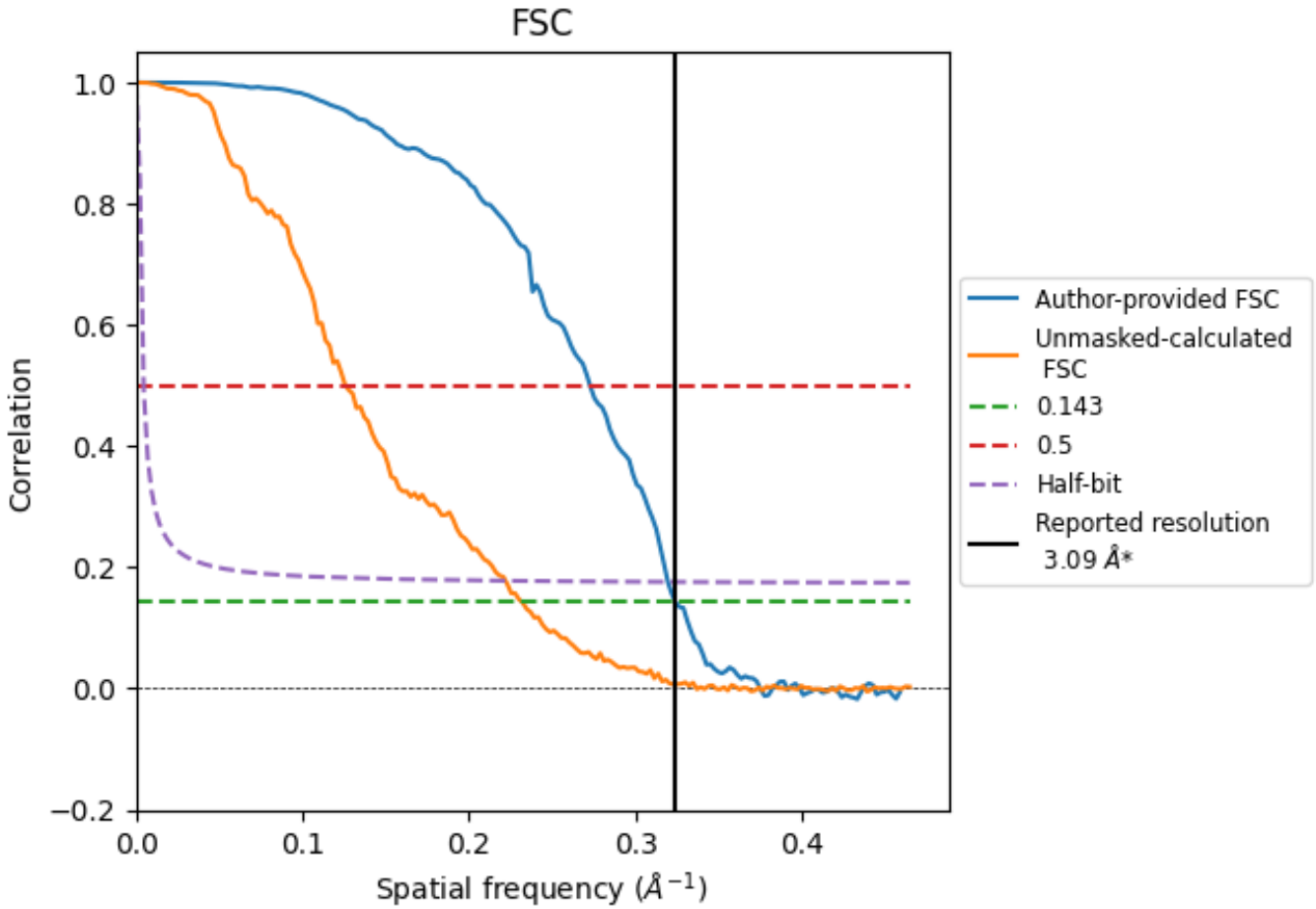


*Reported resolution corresponds to spatial frequency of 0.324 $Å^{-1}$

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 0.324 Å^{-1}

8.2 Resolution estimates (i)

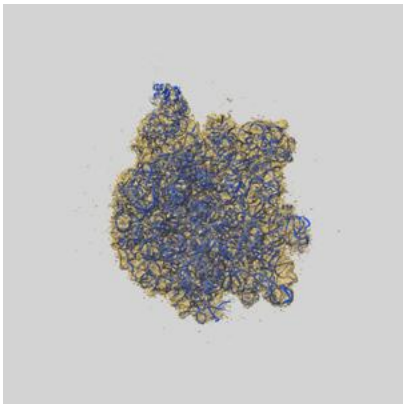
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.67	3.13
Unmasked-calculated*	4.32	7.95	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.09 by more than 10 %

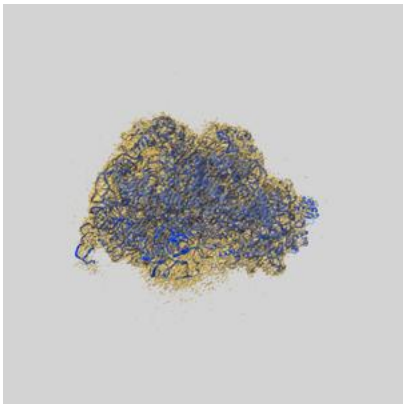
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43305 and PDB model 8VK7. Per-residue inclusion information can be found in section 3 on page 11.

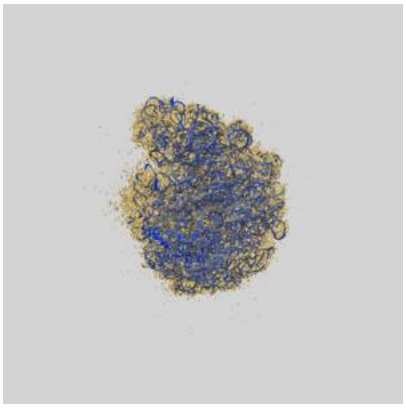
9.1 Map-model overlay



X



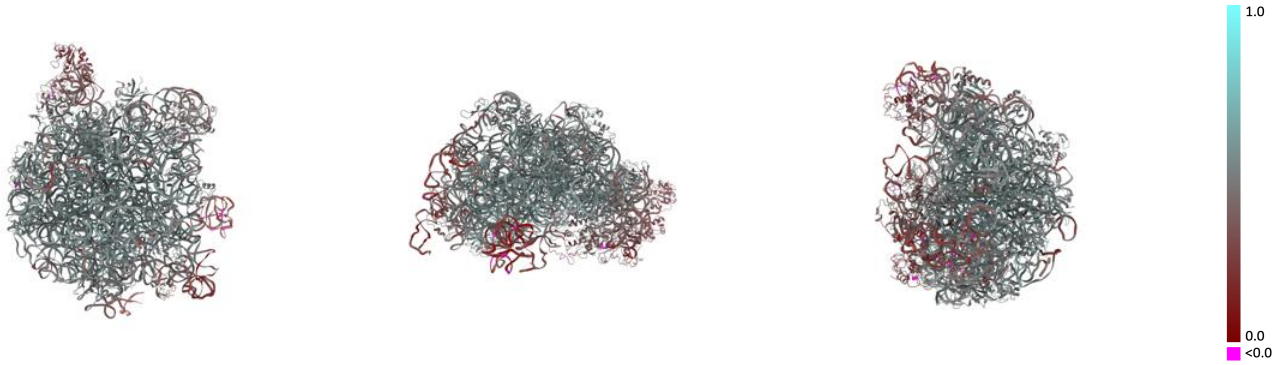
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

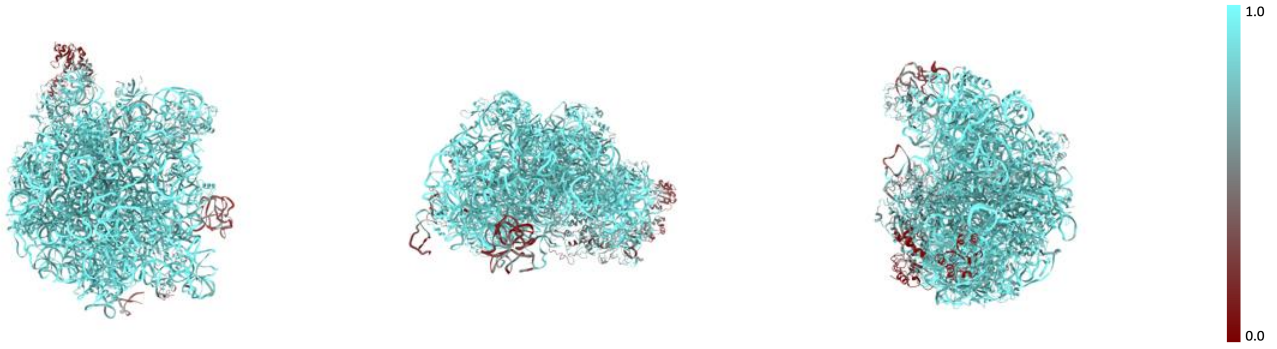
9.2 Q-score mapped to coordinate model (i)



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.

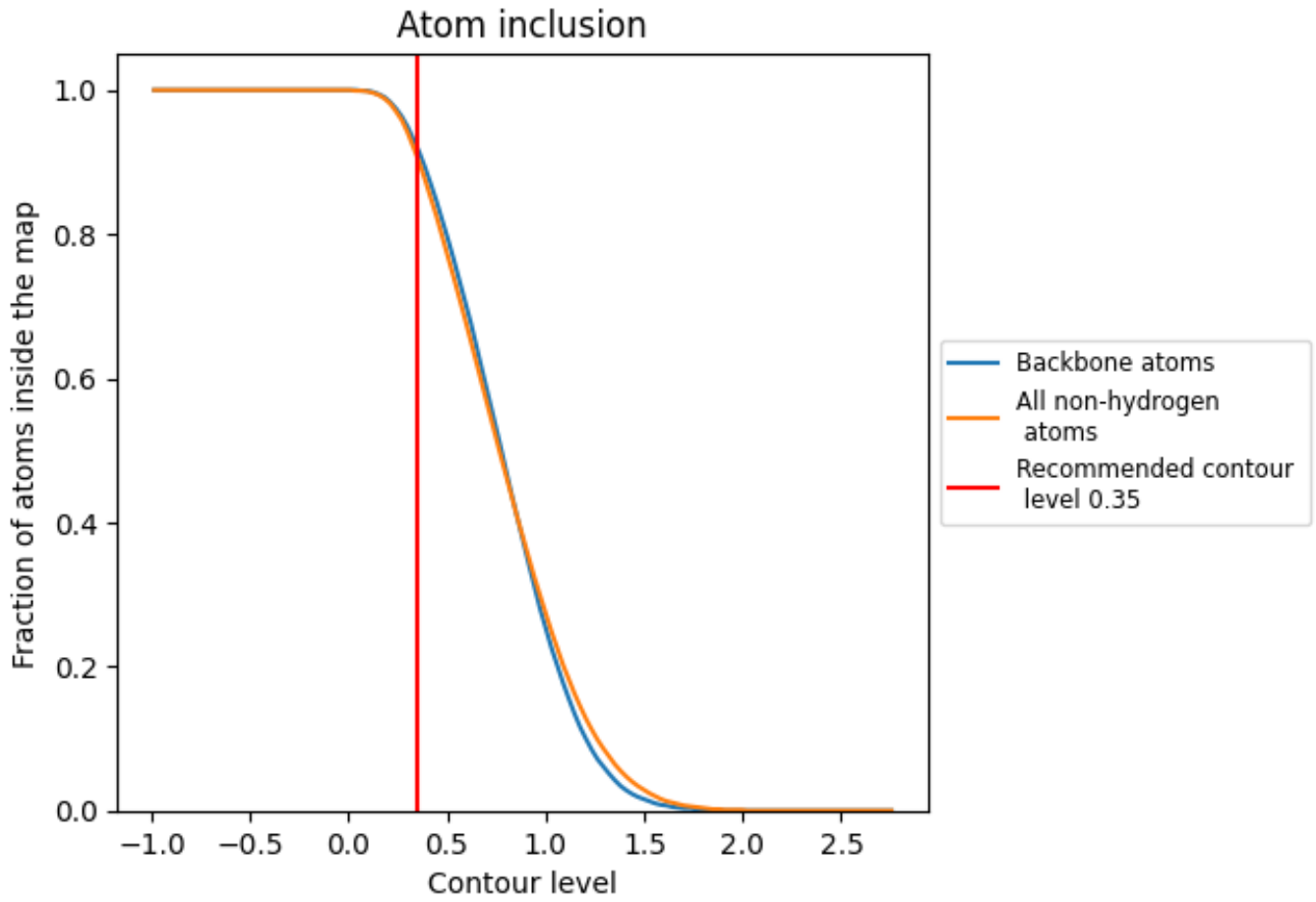
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.4850
2	0.8950	0.5340
3	0.9890	0.5670
4	0.6310	0.3740
A	0.9420	0.4910
B	0.9730	0.4640
C	0.9250	0.5360
D	0.9450	0.5340
E	0.9220	0.5180
F	0.7480	0.3540
G	0.8360	0.4420
H	0.6990	0.4140
I	0.2450	0.2810
J	0.2290	0.2680
K	0.9490	0.5390
L	0.9330	0.5200
M	0.9310	0.5280
N	0.9350	0.5170
O	0.9390	0.5360
P	0.8950	0.4620
Q	0.9100	0.5010
R	0.9440	0.5360
S	0.9100	0.5370
T	0.9530	0.5390
U	0.9410	0.5140
V	0.8980	0.4800
W	0.8110	0.4810
X	0.9440	0.5450
Y	0.9630	0.5500
Z	0.9040	0.4950
b	0.9400	0.5490
c	0.9520	0.5440
d	0.9660	0.5650
e	0.9670	0.5480
f	0.9620	0.5510
g	0.6610	0.3260