wwPDB EM Validation Summary Report

Apr 20, 2024 – 05:23 pm BST

PDB ID	:	7QIY
EMDB ID	:	EMD-14003
Title	:	Specific features and methylation sites of a plant ribosome. 40S head ribosomal subunit.
Authors	:	Cottilli, P.; Itoh, Y.; Amunts, A.
Deposited on	:	2021-12-16
Resolution	:	2.58 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:

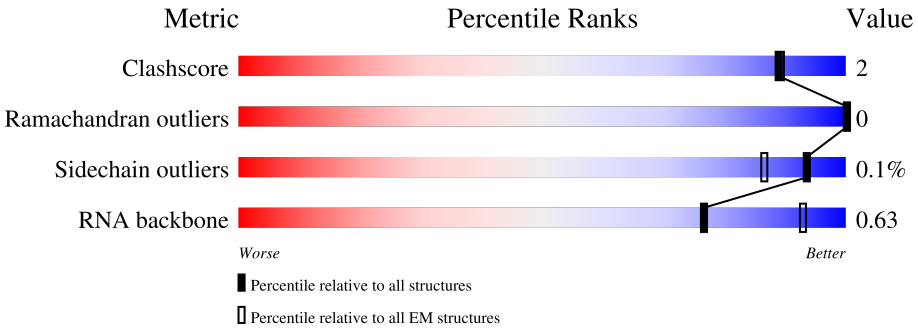
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	2	1806	21% 5% 74%
2	D	239	84% 5% 11%
3	E	211	81% 7% 12%
4	F	180	49% 49%
5	G	151	79% 5% 17%
6	H	147	93% 5%
7	I	144	52% 5% 43%

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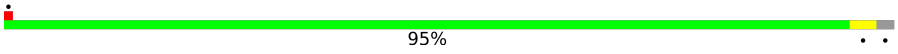
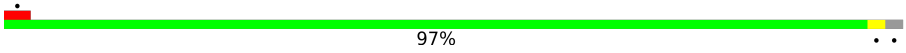
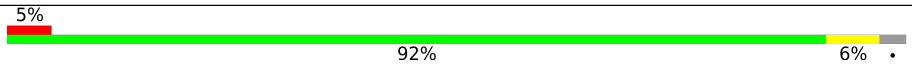
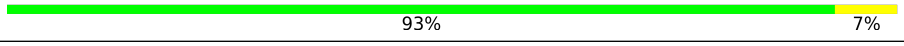
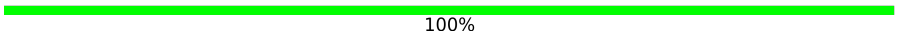
Mol	Chain	Length	Quality of chain
8	J	152	
9	K	143	
10	L	123	
11	M	65	
12	N	56	
13	O	326	
14	P	108	
15	Q	14	
16	R	3	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 44140 atoms, of which 19577 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA head.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	2	474	15216	4518	5115	1765	3344	474	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	?	-	U	deletion	GB 2090998067
2	1194	I2T	U	modified residue	GB 2090998067
2	1282A	4AC	C	modified residue	GB 2090998067
2	?	-	C	deletion	GB 2090998067

- Molecule 2 is a protein called KH type-2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	213	3429	1060	1751	307	302	9	0	0

- Molecule 3 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	185	2965	912	1499	277	269	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	37	GLY	ASP	conflict	UNP A0A3Q7IVL4
E	43	MET	ILE	conflict	UNP A0A3Q7IVL4
E	60	MET	THR	conflict	UNP A0A3Q7IVL4
E	117	GLN	LEU	conflict	UNP A0A3Q7IVL4

- Molecule 4 is a protein called S10_plectin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	92	Total	C	H	N	O	S	0	0
			1572	514	790	128	136	4		

- Molecule 5 is a protein called 40S head ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	126	Total	C	H	N	O	S	0	0
			2096	650	1078	190	173	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	75	GLN	PRO	conflict	UNP A0A3Q7F5X2

- Molecule 6 is a protein called 40S head ribosomal protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	140	Total	C	H	N	O	S	0	0
			2339	722	1204	220	189	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	62	HIS	GLN	conflict	UNP A0A3Q7GDB0
H	105	GLN	THR	conflict	UNP A0A3Q7GDB0

- Molecule 7 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	82	Total	C	H	N	O	S	0	0
			1420	426	738	135	118	3		

- Molecule 8 is a protein called 40S head ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	142	Total	C	H	N	O	S	0	0
			2343	720	1189	227	202	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	67	LEU	VAL	conflict	UNP A0A3Q7FJL7

- Molecule 9 is a protein called 40S head ribosomal protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	140	Total	C	H	N	O	S	0	0
			2208	692	1104	215	194	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	6	SER	ASN	conflict	UNP A0A3Q7FTS1
K	14	ASP	GLU	conflict	UNP A0A3Q7FTS1

- Molecule 10 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	104	Total	C	H	N	O	S	0	0
			1701	515	880	152	150	4		

- Molecule 11 is a protein called 40S head ribosomal protein eS28.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	64	Total	C	H	N	O	S	0	0
			1070	319	551	105	93	2		

- Molecule 12 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	50	Total	C	H	N	O	S	0	0
			805	253	400	82	64	6		

- Molecule 13 is a protein called Mitogen-activated protein kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	317	Total	C	H	N	O	S	0	0
			4898	1554	2434	427	472	11		

- Molecule 14 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	75	Total	C	H	N	O	S	0	0
			1228	373	636	108	108	3		

- Molecule 15 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	14	Total	C	H	N	O	P	0	0
			451	134	152	55	96	14		

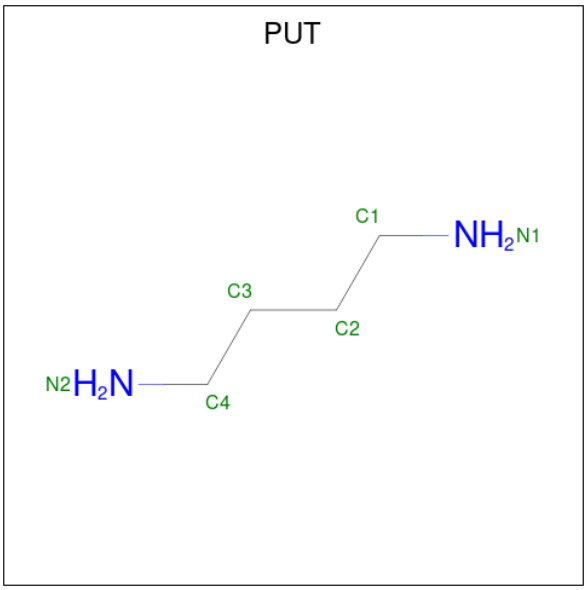
- Molecule 16 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	3	Total	C	H	N	O	P	0	0
			95	28	33	10	21	3		

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
17	2	7	Total	K	0
			7	7	
17	J	1	Total	K	0
			1	1	
17	K	1	Total	K	0
			1	1	
17	N	1	Total	K	0
			1	1	

- Molecule 18 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).

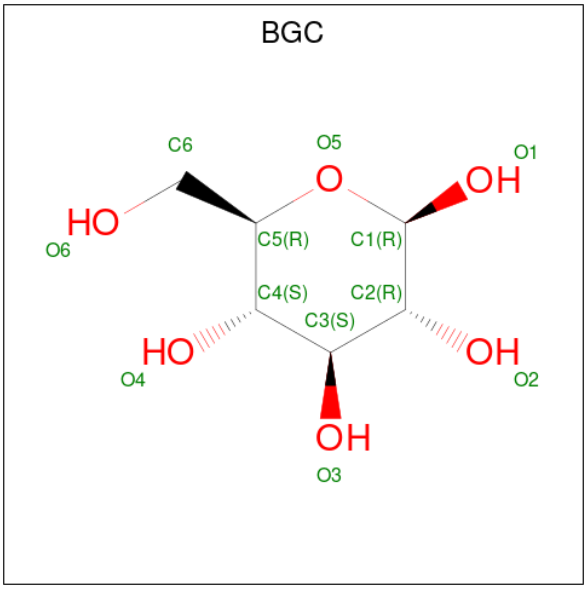


Mol	Chain	Residues	Atoms				AltConf
18	2	1	Total	C	H	N	0
			18	4	12	2	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
19	2	27	Total Mg 27 27	0
19	J	1	Total Mg 1 1	0

- Molecule 20 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	AltConf
20	D	1	Total C H O 22 6 11 5	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	N	1	Total Zn 1 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	2	166	Total O 166 166	0
22	E	10	Total O 10 10	0
22	G	1	Total O 1 1	0

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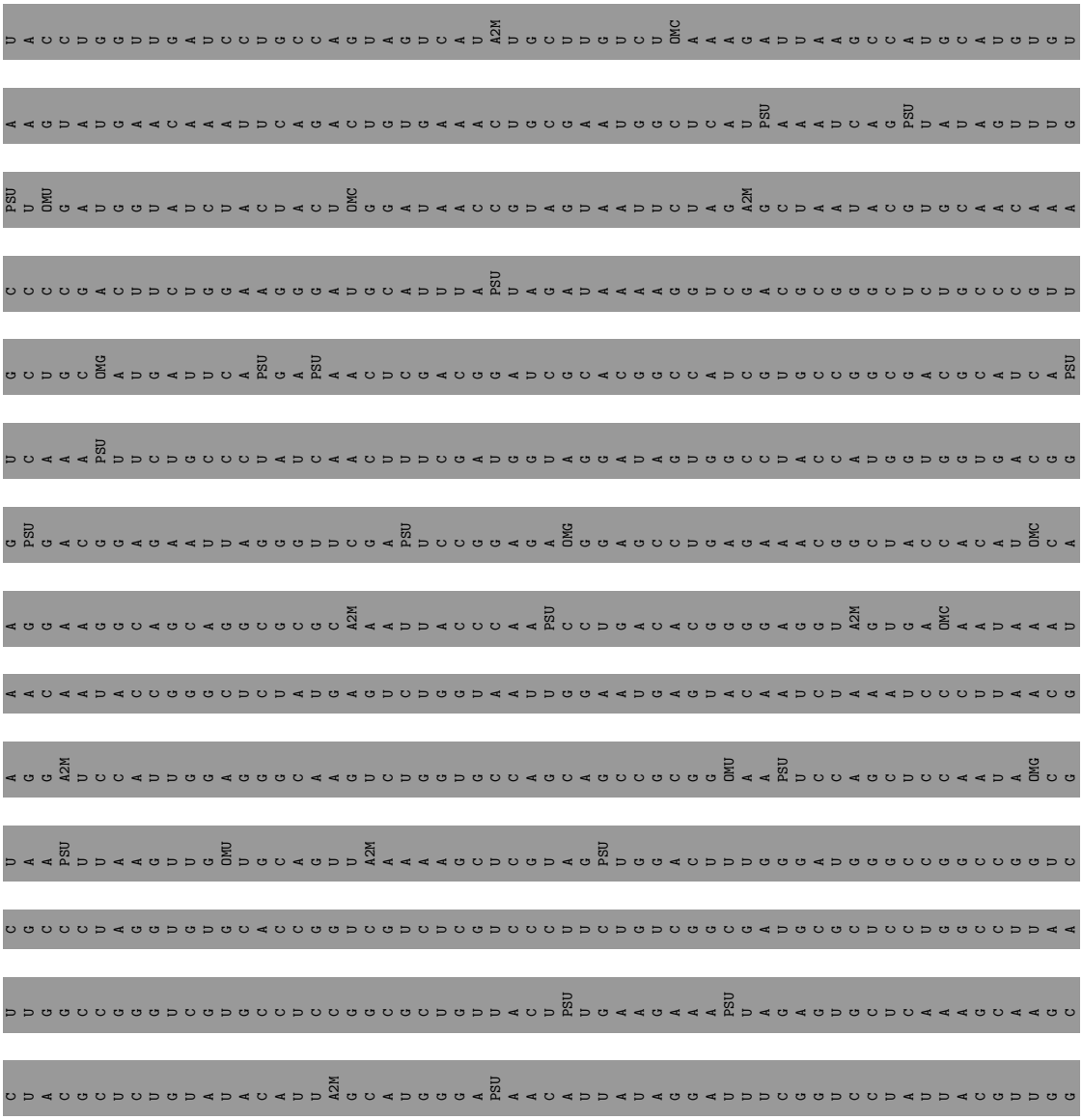
Mol	Chain	Residues	Atoms	AltConf
22	H	4	Total O 4 4	0
22	J	6	Total O 6 6	0
22	K	24	Total O 24 24	0
22	L	7	Total O 7 7	0
22	M	1	Total O 1 1	0
22	N	2	Total O 2 2	0
22	P	4	Total O 4 4	0

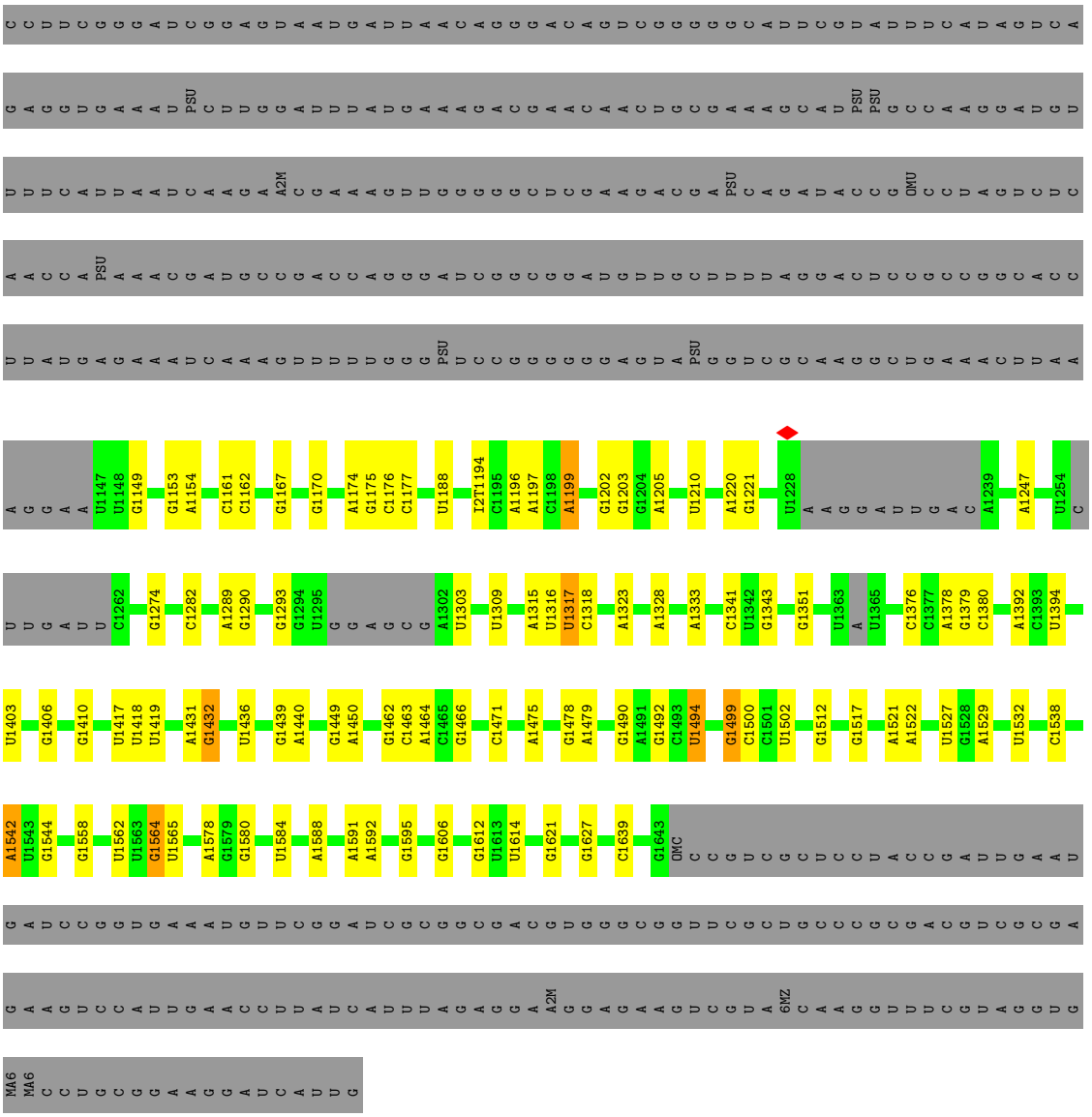
3 Residue-property plots (i)

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: 18S rRNA head

Chain 2: 21% 5% 74%



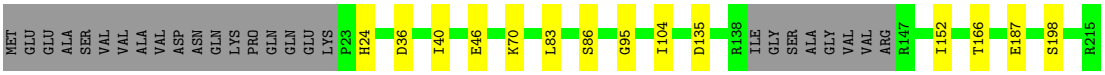


• Molecule 2: KH type-2 domain-containing protein

Chain D:

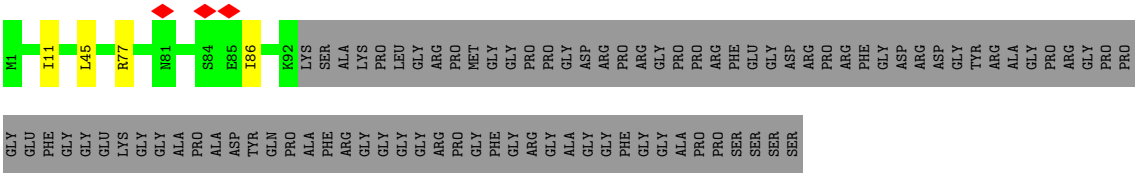
• Molecule 3: Ribosomal_S7 domain-containing protein

Chain E:



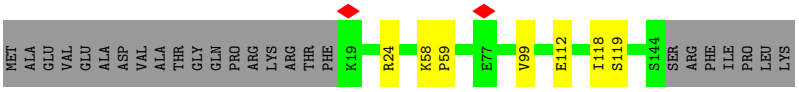
• Molecule 4: S10_plectin domain-containing protein

Chain F:



• Molecule 5: 40S head ribosomal protein uS19

Chain G:

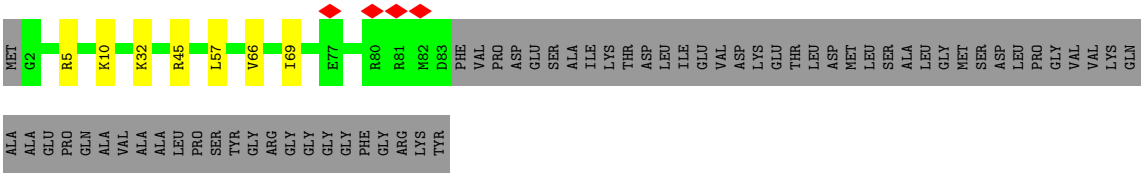


• Molecule 6: 40S head ribosomal protein uS9

Chain H:

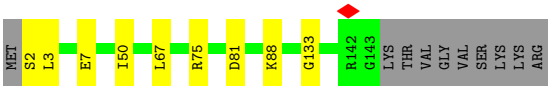
• Molecule 7: 40S ribosomal protein S17

Chain I:



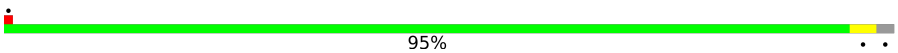
• Molecule 8: 40S head ribosomal protein uS13

Chain J:



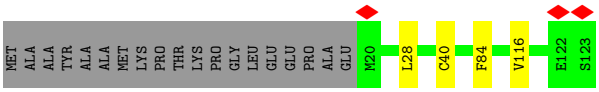
• Molecule 9: 40S head ribosomal protein eS19

Chain K:



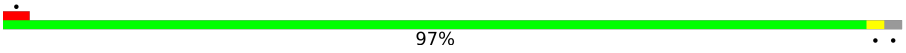
• Molecule 10: Ribosomal_S10 domain-containing protein

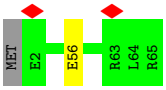
Chain L:



• Molecule 11: 40S head ribosomal protein eS28

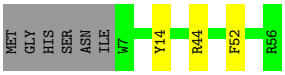
Chain M:





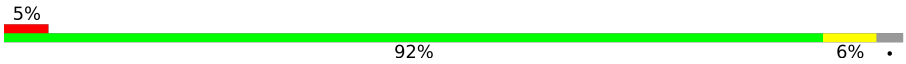
• Molecule 12: 40S ribosomal protein S29

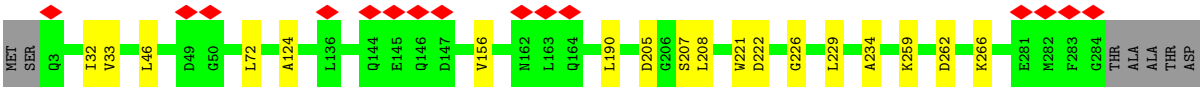
Chain N:

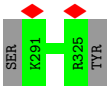


• Molecule 13: Mitogen-activated protein kinase

Chain O:

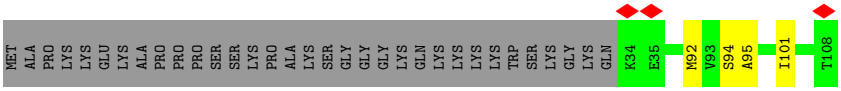






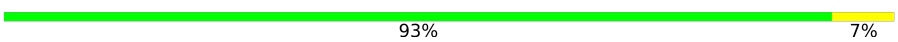
• Molecule 14: 40S ribosomal protein S25

Chain P:



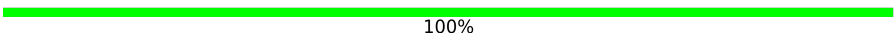
• Molecule 15: tRNA

Chain Q:



• Molecule 16: mRNA

Chain R:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335806	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 ($e^-/Å^2$)	30.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.152	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0197	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, I2T, 4AC, A2M, PUT, OMU, ZN, BGC, OMG, OMC, PSU, 7MG, K

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	0.42	0/10642	0.72	0/16571
2	D	0.26	0/1702	0.51	0/2285
3	E	0.25	0/1488	0.51	0/2005
4	F	0.26	0/804	0.44	0/1087
5	G	0.28	0/1039	0.52	0/1391
6	H	0.26	0/1154	0.56	0/1540
7	I	0.25	0/689	0.53	0/913
8	J	0.25	0/1171	0.53	0/1565
9	K	0.27	0/1128	0.52	0/1515
10	L	0.25	0/831	0.51	0/1118
11	M	0.26	0/522	0.59	0/694
12	N	0.27	0/416	0.54	0/555
13	O	0.24	0/2516	0.49	0/3414
14	P	0.25	0/598	0.52	0/800
15	Q	0.25	0/334	0.65	0/518
16	R	0.21	0/68	0.62	0/103
All	All	0.33	0/25102	0.62	0/36074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	10101	5115	5109	29	0
2	D	1678	1751	1748	8	0
3	E	1466	1499	1497	8	0
4	F	782	790	789	2	0
5	G	1018	1078	1077	4	0
6	H	1135	1204	1202	2	0
7	I	682	738	737	5	0
8	J	1154	1189	1188	6	0
9	K	1104	1104	1116	3	0
10	L	821	880	879	3	0
11	M	519	551	550	1	0
12	N	405	400	398	3	0
13	O	2464	2434	2435	10	0
14	P	592	636	635	2	0
15	Q	299	152	152	1	0
16	R	62	33	33	0	0
17	2	7	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	N	1	0	0	0	0
18	2	6	12	12	0	0
19	2	27	0	0	0	0
19	J	1	0	0	0	0
20	D	11	11	10	1	0
21	N	1	0	0	0	0
22	2	166	0	0	5	0
22	E	10	0	0	0	0
22	G	1	0	0	0	0
22	H	4	0	0	0	0
22	J	6	0	0	0	0
22	K	24	0	0	2	0
22	L	7	0	0	0	0
22	M	1	0	0	0	0
22	N	2	0	0	0	0
22	P	4	0	0	0	0
All	All	24563	19577	19567	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1196:A:OP1	22:2:2001:HOH:O	2.04	0.74
1:2:1558:G:O2'	12:N:14:TYR:OH	2.05	0.73
1:2:1532:U:O4	22:2:2002:HOH:O	2.06	0.72
1:2:1584:U:OP1	22:2:2003:HOH:O	2.12	0.67
11:M:56:GLU:N	11:M:56:GLU:OE1	2.29	0.65

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	211/239 (88%)	207 (98%)	4 (2%)	0	100	100
3	E	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
4	F	90/180 (50%)	88 (98%)	2 (2%)	0	100	100
5	G	124/151 (82%)	123 (99%)	1 (1%)	0	100	100
6	H	138/147 (94%)	135 (98%)	3 (2%)	0	100	100
7	I	80/144 (56%)	79 (99%)	1 (1%)	0	100	100
8	J	140/152 (92%)	137 (98%)	3 (2%)	0	100	100
9	K	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
10	L	102/123 (83%)	101 (99%)	1 (1%)	0	100	100
11	M	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
12	N	48/56 (86%)	48 (100%)	0	0	100	100
13	O	313/326 (96%)	309 (99%)	4 (1%)	0	100	100
14	P	73/108 (68%)	73 (100%)	0	0	100	100
All	All	1700/2045 (83%)	1674 (98%)	26 (2%)	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
2	D	180/204 (88%)	180 (100%)	0	100 100
3	E	157/178 (88%)	157 (100%)	0	100 100
4	F	86/141 (61%)	86 (100%)	0	100 100
5	G	111/132 (84%)	111 (100%)	0	100 100
6	H	118/122 (97%)	117 (99%)	1 (1%)	81 92
7	I	76/123 (62%)	76 (100%)	0	100 100
8	J	122/131 (93%)	122 (100%)	0	100 100
9	K	113/116 (97%)	113 (100%)	0	100 100
10	L	96/109 (88%)	96 (100%)	0	100 100
11	M	57/58 (98%)	57 (100%)	0	100 100
12	N	42/47 (89%)	42 (100%)	0	100 100
13	O	275/282 (98%)	275 (100%)	0	100 100
14	P	65/91 (71%)	65 (100%)	0	100 100
All	All	1498/1734 (86%)	1497 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	30	ARG

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

Mol	Chain	Res	Type
2	D	177	HIS
2	D	214	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	467/1806 (25%)	62 (13%)	1 (0%)
15	Q	13/14 (92%)	0	0
16	R	2/3 (66%)	0	0
All	All	482/1823 (26%)	62 (12%)	1 (0%)

5 of 62 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	1149	G
1	2	1153	G
1	2	1154	A
1	2	1161	C
1	2	1162	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1462	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2	1633	1	18,21,22	0.51	0	22,30,33	0.55	0
1	PSU	2	1190	1	18,21,22	0.48	0	22,30,33	0.56	0
1	PSU	2	1210	1	18,21,22	0.49	0	22,30,33	0.42	0
1	PSU	2	1534	1	18,21,22	0.50	0	22,30,33	0.55	0
1	OMU	2	1265	1	19,22,23	0.28	0	26,31,34	0.49	0
1	PSU	2	1484	1	18,21,22	0.52	0	22,30,33	0.56	0
1	PSU	2	1178	1	18,21,22	0.49	0	22,30,33	0.61	0
1	PSU	2	1217	1	18,21,22	0.52	0	22,30,33	0.55	0
1	PSU	2	1292	1	18,21,22	0.48	0	22,30,33	0.57	0
1	A2M	2	1328	1	18,25,26	0.68	0	18,36,39	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	I2T	2	1194	1	24,29,30	0.61	0	29,42,45	0.66	0
1	PSU	2	1566	1	18,21,22	0.48	0	22,30,33	0.54	0
1	PSU	2	1312	1	18,21,22	0.49	0	22,30,33	0.57	0
1	4AC	2	1282(A)	1	21,24,25	0.33	0	29,34,37	0.43	0
1	OMU	2	1446	1	19,22,23	0.28	0	26,31,34	0.46	0
1	A2M	2	1578	1	18,25,26	0.65	0	18,36,39	0.75	1 (5%)
1	PSU	2	1307	1	18,21,22	0.50	0	22,30,33	0.37	0
1	OMG	2	1274	17,1	18,26,27	0.99	3 (16%)	19,38,41	0.64	0
1	OMC	2	1218	1	19,22,23	0.30	0	26,31,34	0.39	0
1	OMU	2	1382	1,19	19,22,23	0.33	0	26,31,34	0.46	0
1	7MG	2	1580	1,15	22,26,27	1.16	1 (4%)	29,39,42	0.81	1 (3%)
1	PSU	2	1537	1	18,21,22	0.51	0	22,30,33	0.56	0
1	PSU	2	1303	1	18,21,22	0.50	0	22,30,33	0.57	0
1	OMU	2	1272	1,19	19,22,23	0.26	0	26,31,34	0.47	0
1	PSU	2	1184	1	18,21,22	0.50	0	22,30,33	0.57	0
1	OMG	2	1432	1,19	18,26,27	0.99	3 (16%)	19,38,41	0.59	0
1	OMU	2	1263	1	19,22,23	0.28	0	26,31,34	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	1633	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1190	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1210	1	-	1/7/25/26	0/2/2/2
1	PSU	2	1534	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1265	1	-	0/9/27/28	0/2/2/2
1	PSU	2	1484	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1178	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1217	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1292	1	-	0/7/25/26	0/2/2/2
1	A2M	2	1328	1	-	0/5/27/28	0/3/3/3
1	I2T	2	1194	1	-	6/16/34/35	0/2/2/2
1	PSU	2	1566	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1312	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1282(A)	1	-	0/11/29/30	0/2/2/2
1	OMU	2	1446	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1578	1	-	2/5/27/28	0/3/3/3
1	PSU	2	1307	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	1274	17,1	-	0/5/27/28	0/3/3/3
1	OMC	2	1218	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1382	1,19	-	0/9/27/28	0/2/2/2
1	7MG	2	1580	1,15	-	0/7/37/38	0/3/3/3
1	PSU	2	1537	1	-	0/7/25/26	0/2/2/2
1	PSU	2	1303	1	-	2/7/25/26	0/2/2/2
1	OMU	2	1272	1,19	-	1/9/27/28	0/2/2/2
1	PSU	2	1184	1	-	0/7/25/26	0/2/2/2
1	OMG	2	1432	1,19	-	1/5/27/28	0/3/3/3
1	OMU	2	1263	1	-	0/9/27/28	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1580	7MG	C5-N7	4.81	1.41	1.35
1	2	1274	OMG	C5-C6	-2.47	1.42	1.47
1	2	1432	OMG	C5-C6	-2.39	1.42	1.47
1	2	1432	OMG	C8-N7	-2.21	1.31	1.35
1	2	1274	OMG	C8-N7	-2.08	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1328	A2M	C5-C6-N6	2.39	123.98	120.35
1	2	1578	A2M	C5-C6-N6	2.30	123.85	120.35
1	2	1580	7MG	C5-C4-N9	2.27	109.29	106.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1303	PSU	O4'-C4'-C5'-O5'
1	2	1194	I2T	C32-C31-N3-C4
1	2	1194	I2T	N3-C31-C32-C33
1	2	1303	PSU	C3'-C4'-C5'-O5'
1	2	1194	I2T	C32-C31-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1194	I2T	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 39 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
20	BGC	D	301	2	11,11,12	0.20	0	15,15,17	0.37	0
18	PUT	2	1908	-	5,5,5	0.15	0	4,4,4	0.17	0

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
20	BGC	D	301	2	-	1/2/19/22	0/1/1/1
18	PUT	2	1908	-	-	2/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	D	301	BGC	O5-C5-C6-O6
18	2	1908	PUT	C2-C3-C4-N2
18	2	1908	PUT	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	301	BGC	1	0

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.

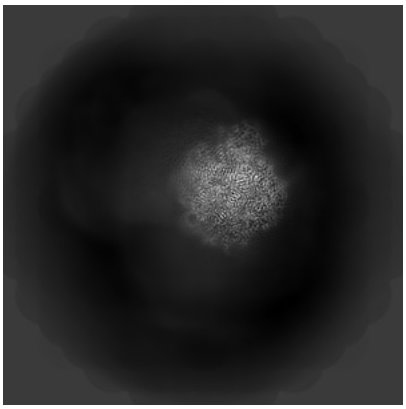
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14003. These allow visual inspection of the internal detail of the map and identification of artifacts.

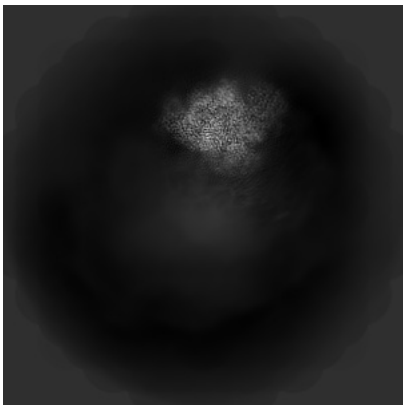
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

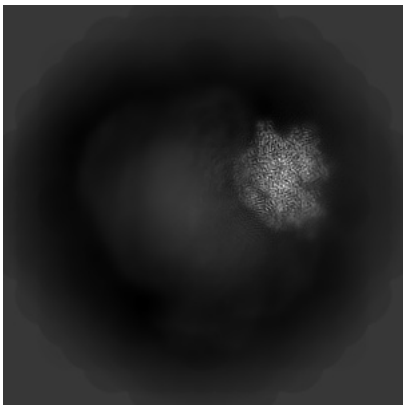
6.1.1 Primary map



X

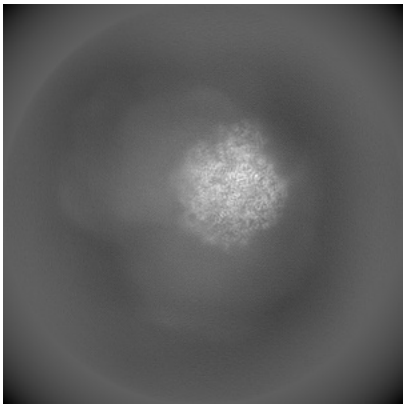


Y

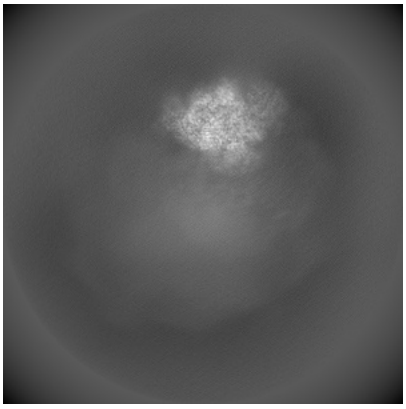


Z

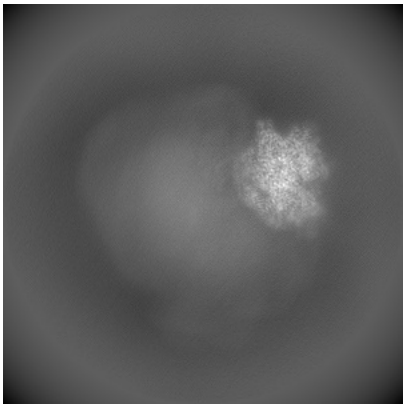
6.1.2 Raw map



X



Y

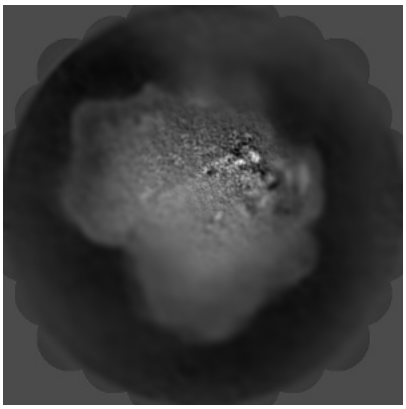


Z

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

6.2 Central slices (i)

6.2.1 Primary map

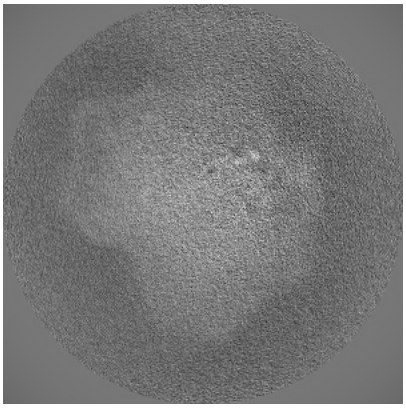


X Index: 270

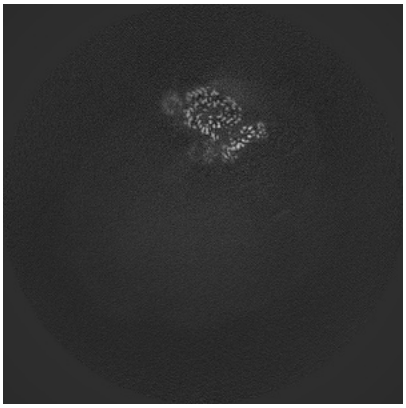
Y Index: 270

Z Index: 270

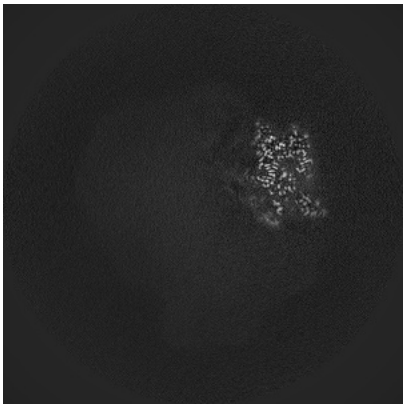
6.2.2 Raw map



X Index: 270



Y Index: 270



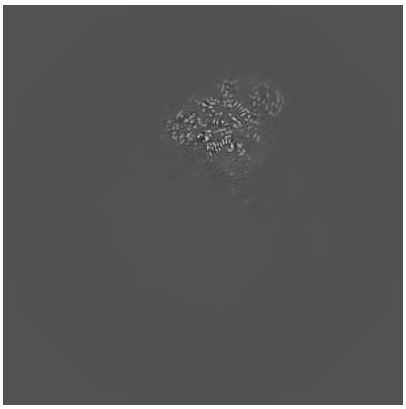
Z Index: 270

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

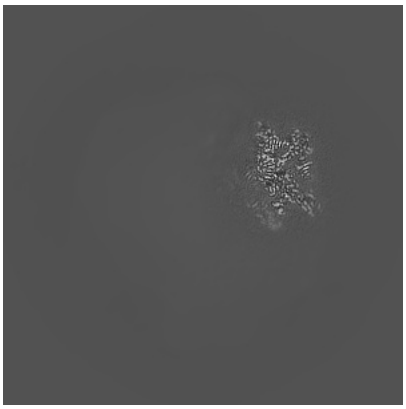
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 373

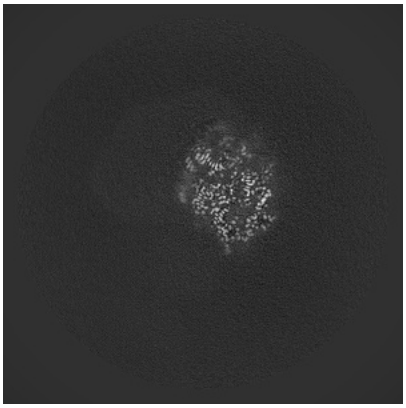


Y Index: 316

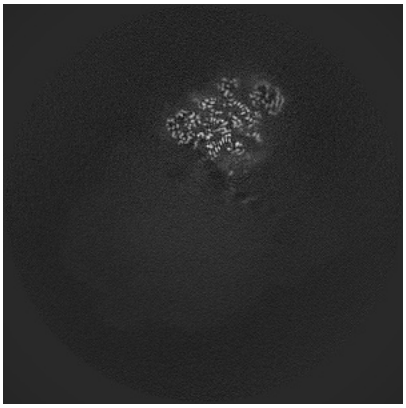


Z Index: 275

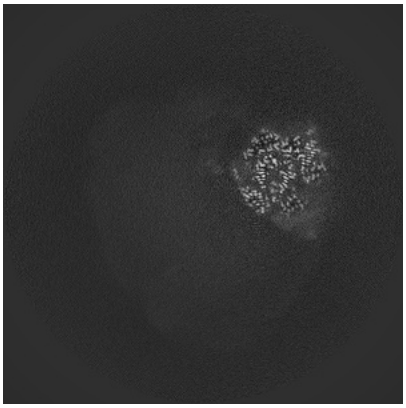
6.3.2 Raw map



X Index: 373



Y Index: 315

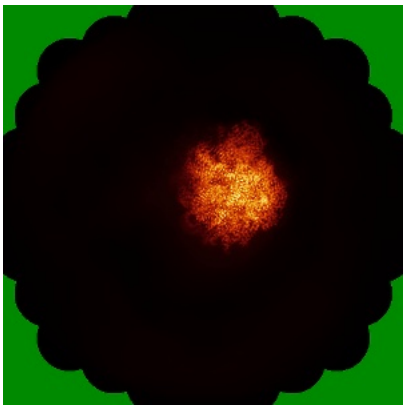


Z Index: 308

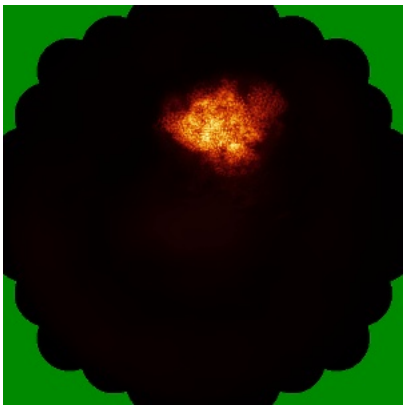
The images above show the largest variance slices of the map in three orthogonal directions.

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

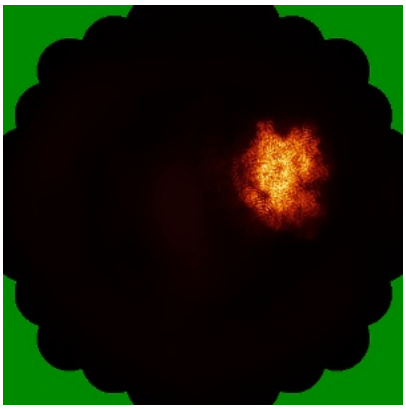
6.4.1 Primary map



X

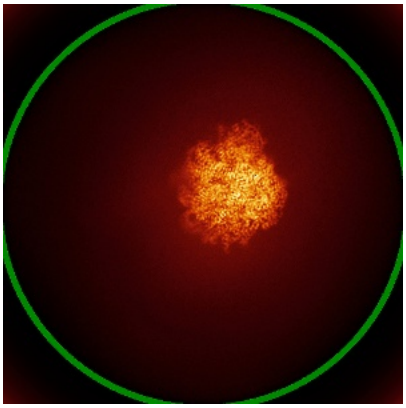


Y

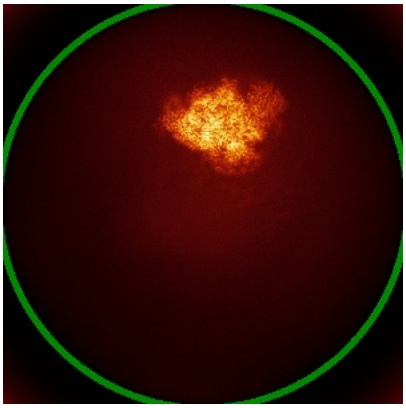


Z

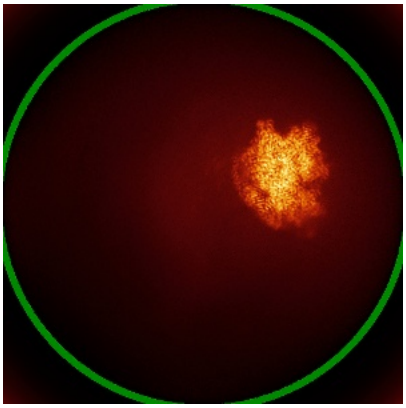
6.4.2 Raw map



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 0.0197. 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.

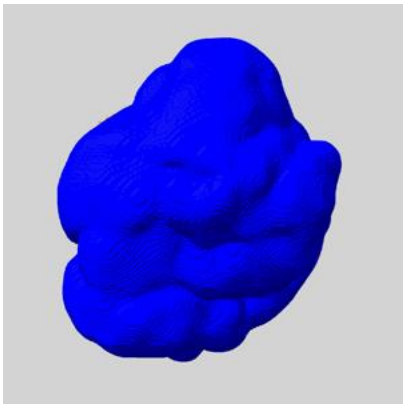
6.6 Mask visualisation (i)

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

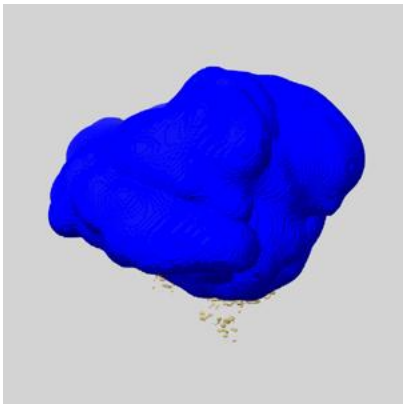
A mask typically either:

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

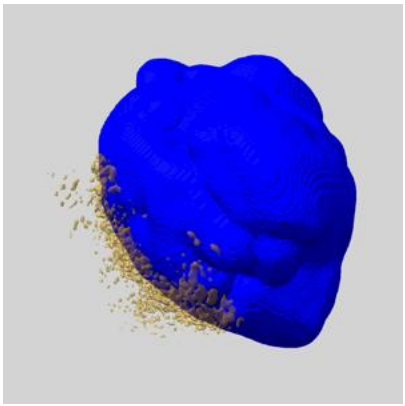
6.6.1 emd_14003_msk_1.map (i)



X



Y

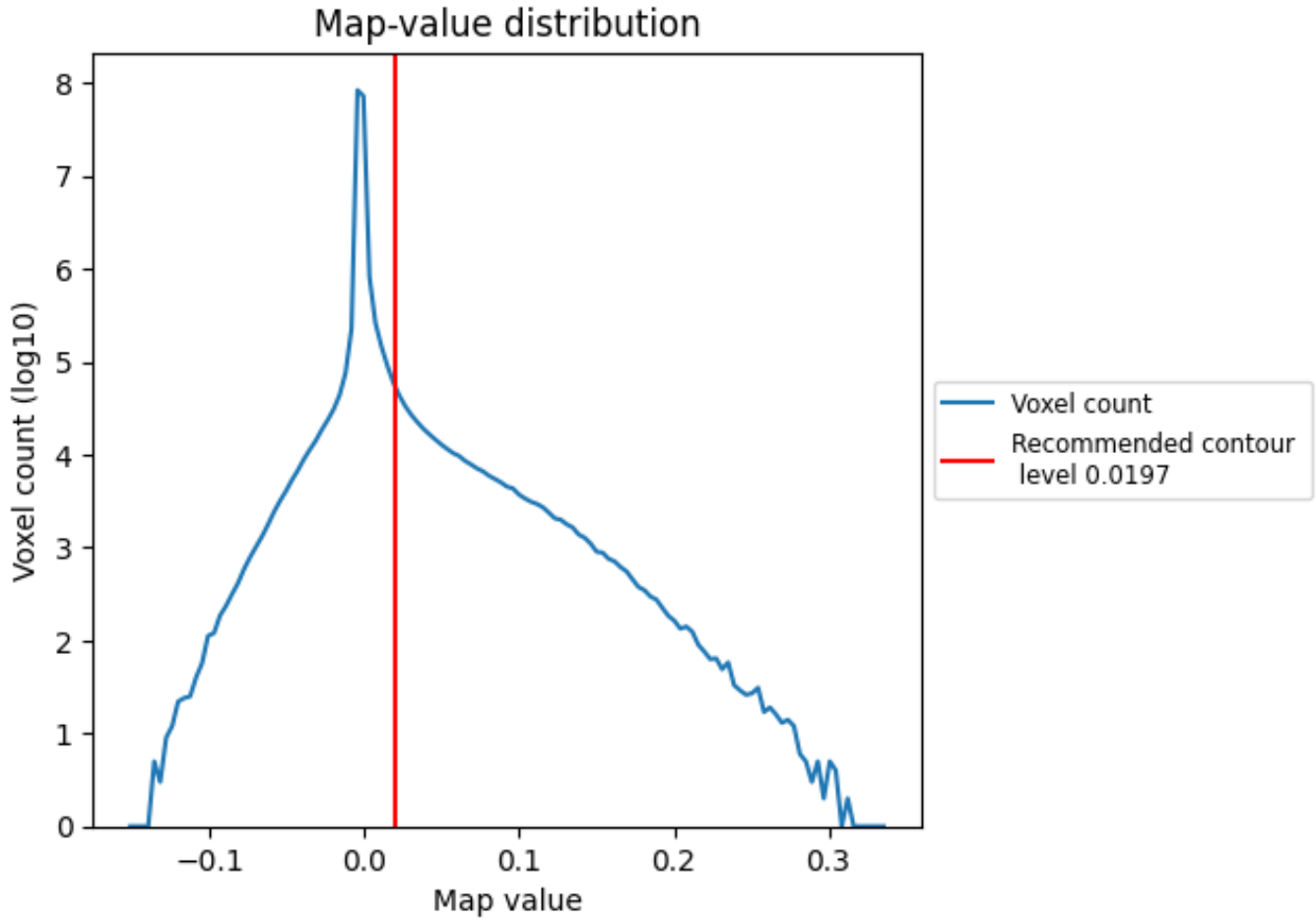


Z

7 Map analysis

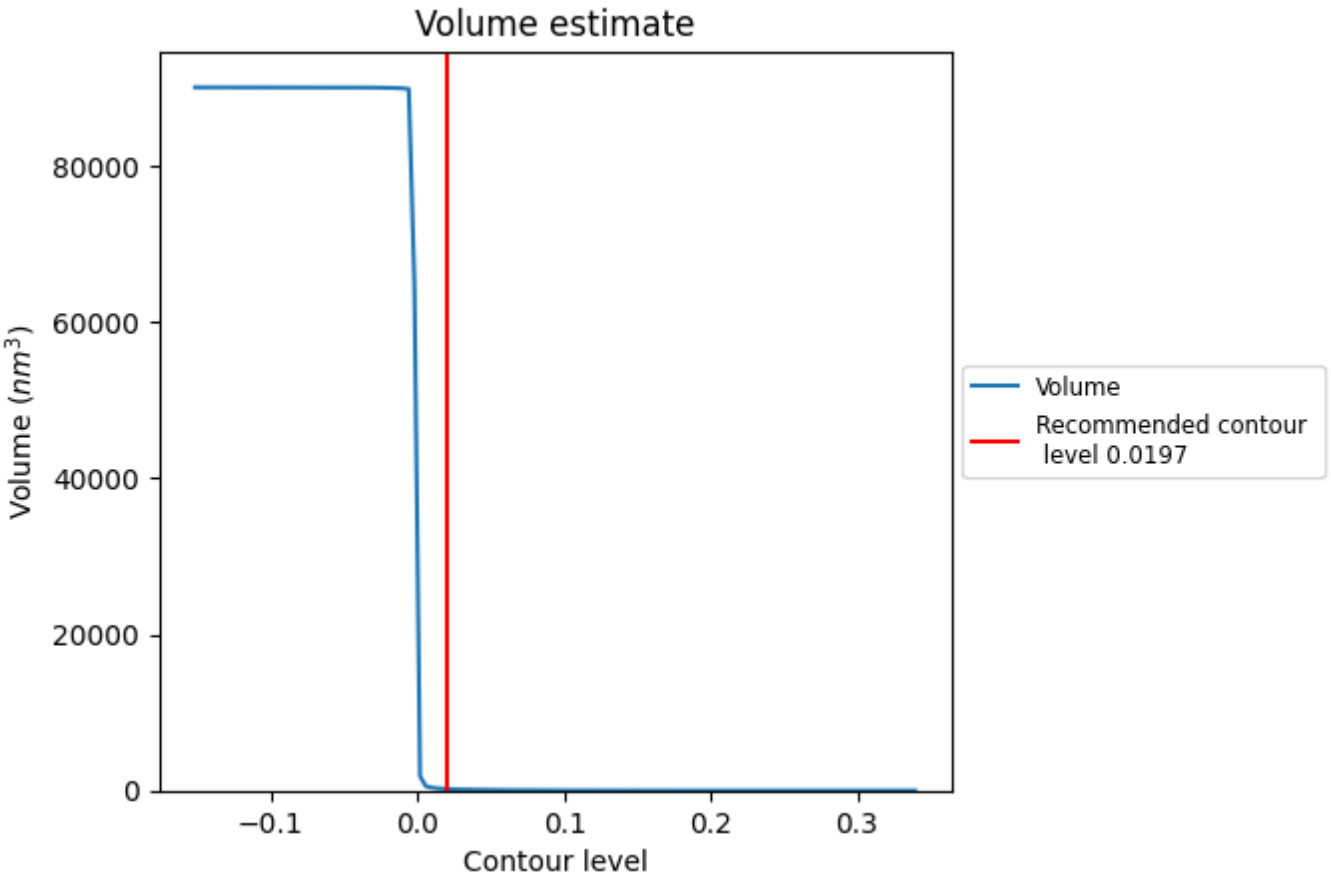
This section contains the results of statistical analysis of the map.

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.

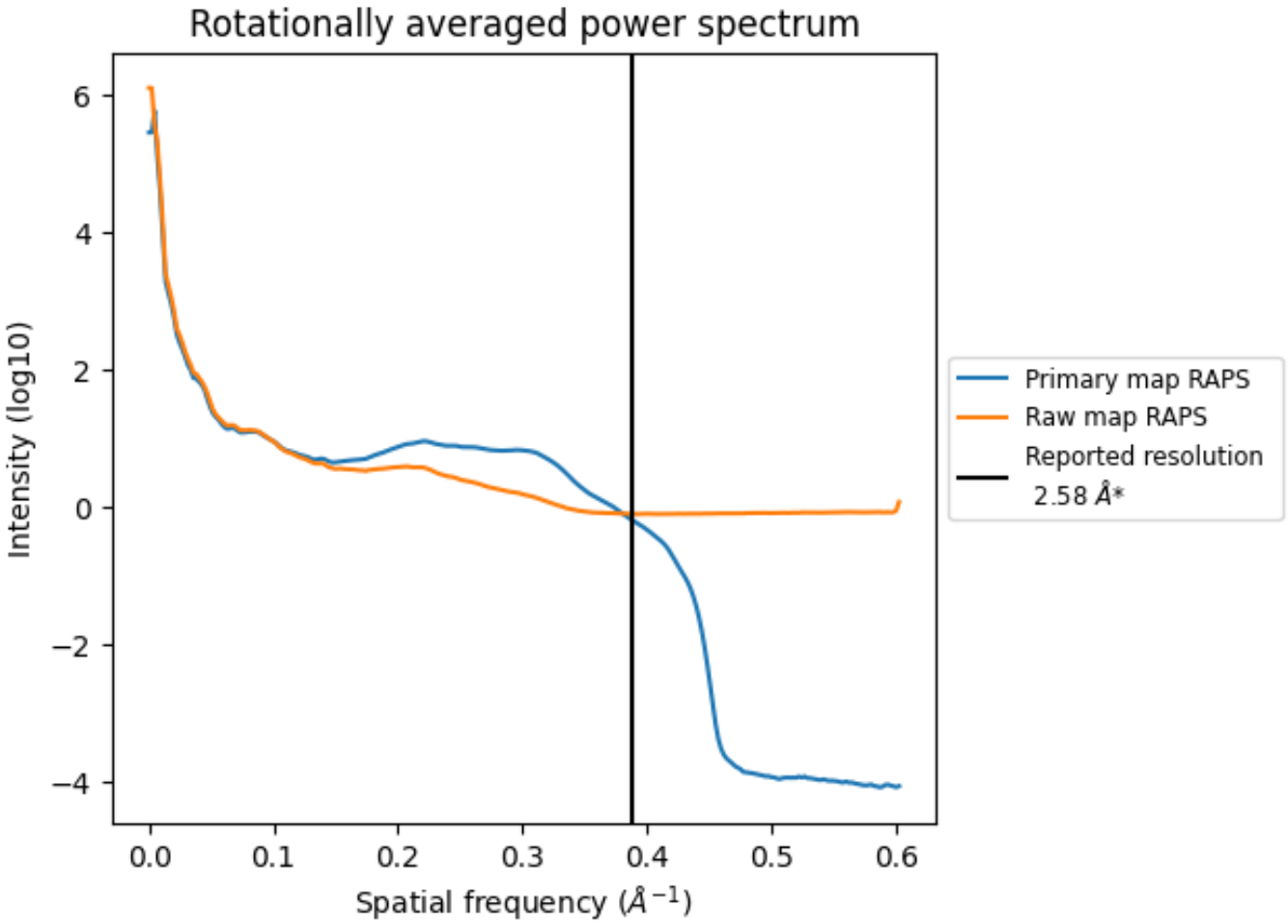
7.2 Volume estimate (i)



The volume at the recommended contour level is 202 nm^3; this corresponds to an approximate mass of 183 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)

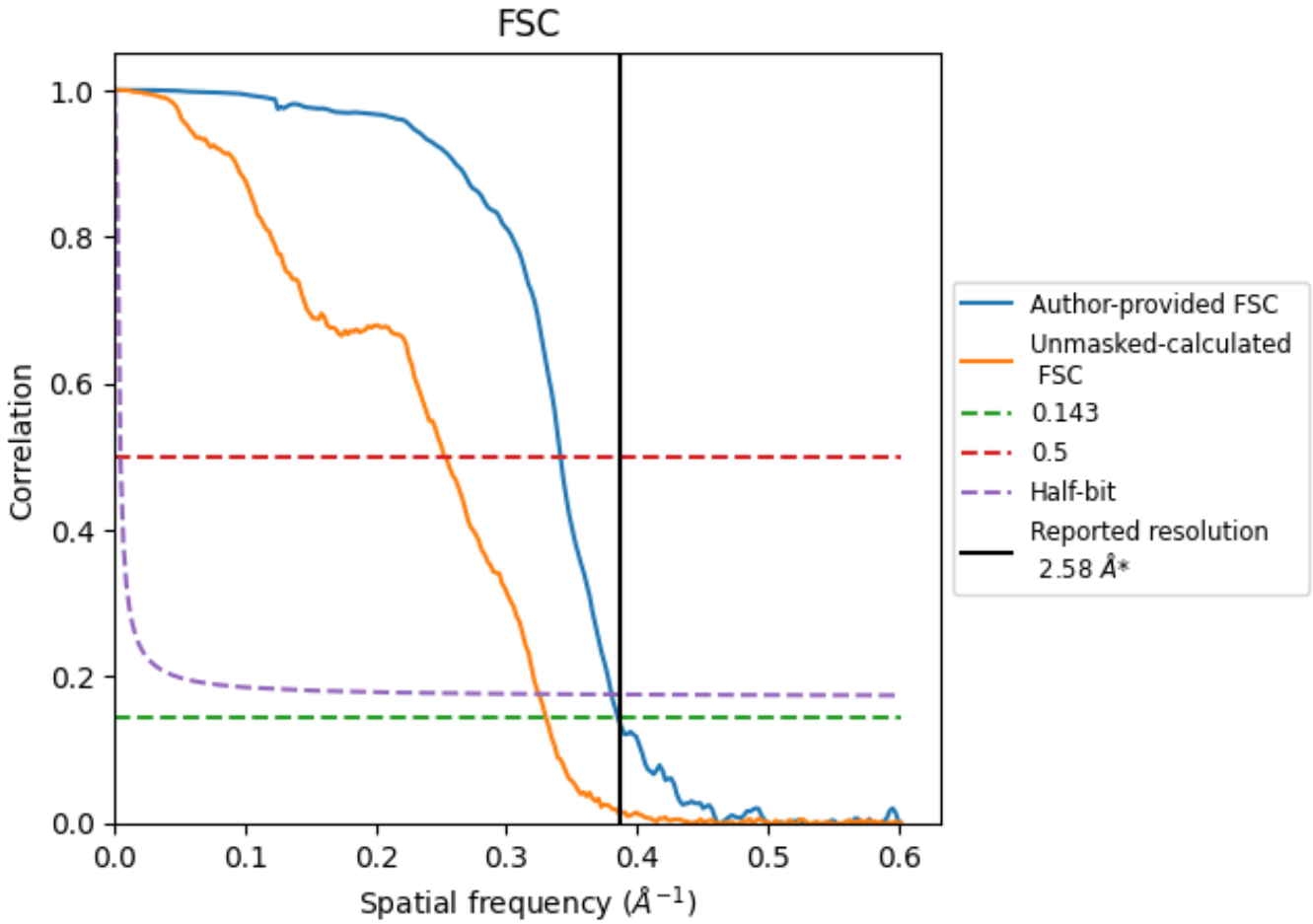


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

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 0.388 Å^{-1}

8.2 Resolution estimates (i)

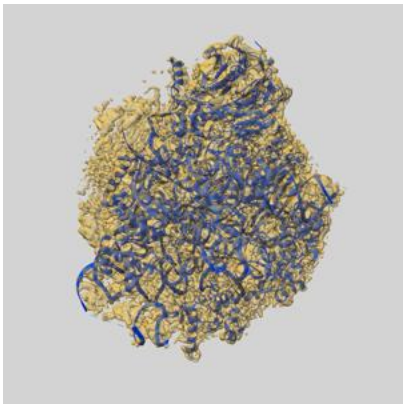
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.59	2.93	2.63
Unmasked-calculated*	3.03	3.96	3.08

*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 3.03 differs from the reported value 2.58 by more than 10 %

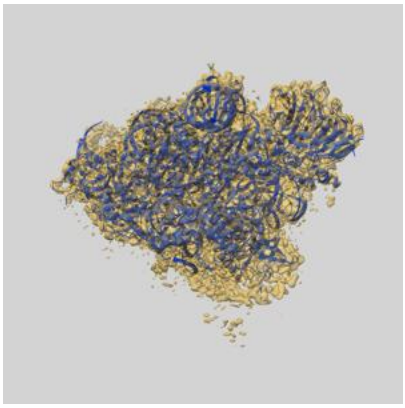
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14003 and PDB model 7QIY. Per-residue inclusion information can be found in section 3 on page 10.

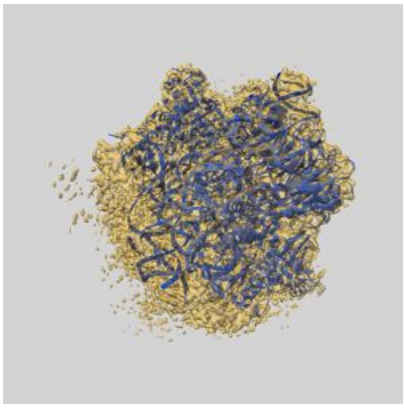
9.1 Map-model overlay



X



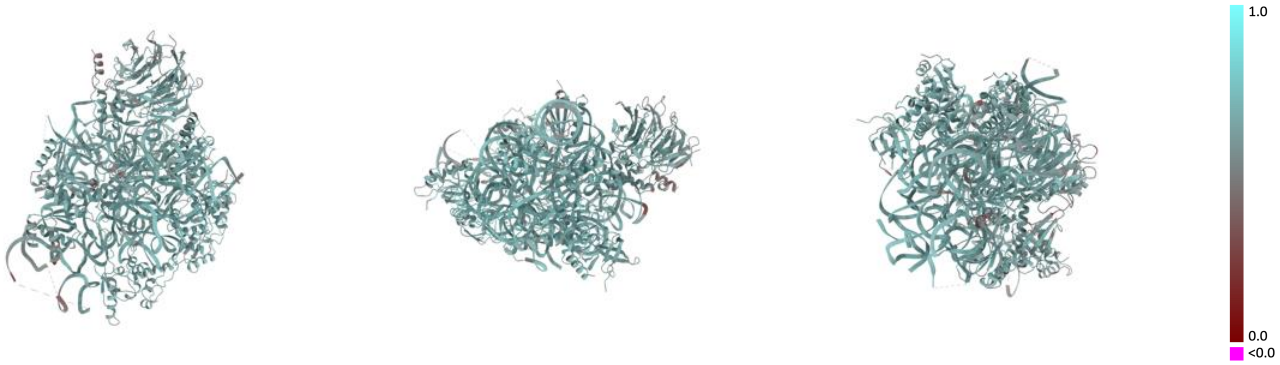
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0197 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.

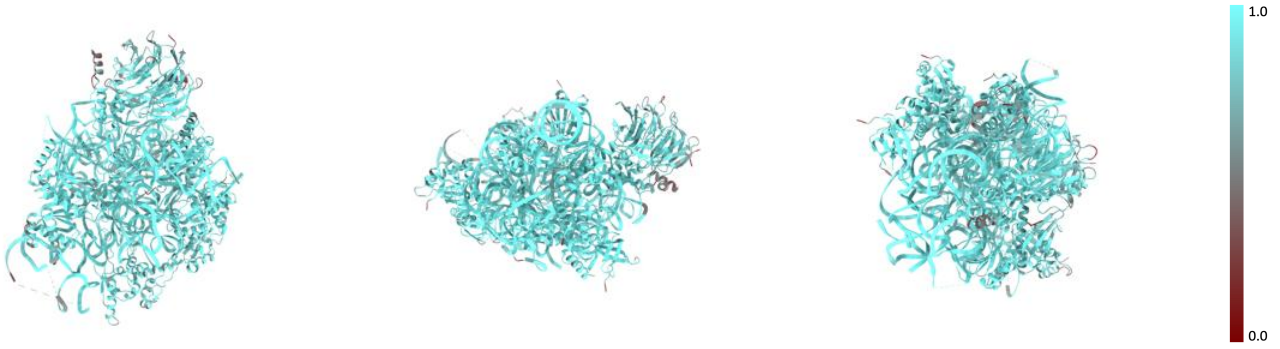
9.2 Q-score mapped to coordinate model (i)



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.

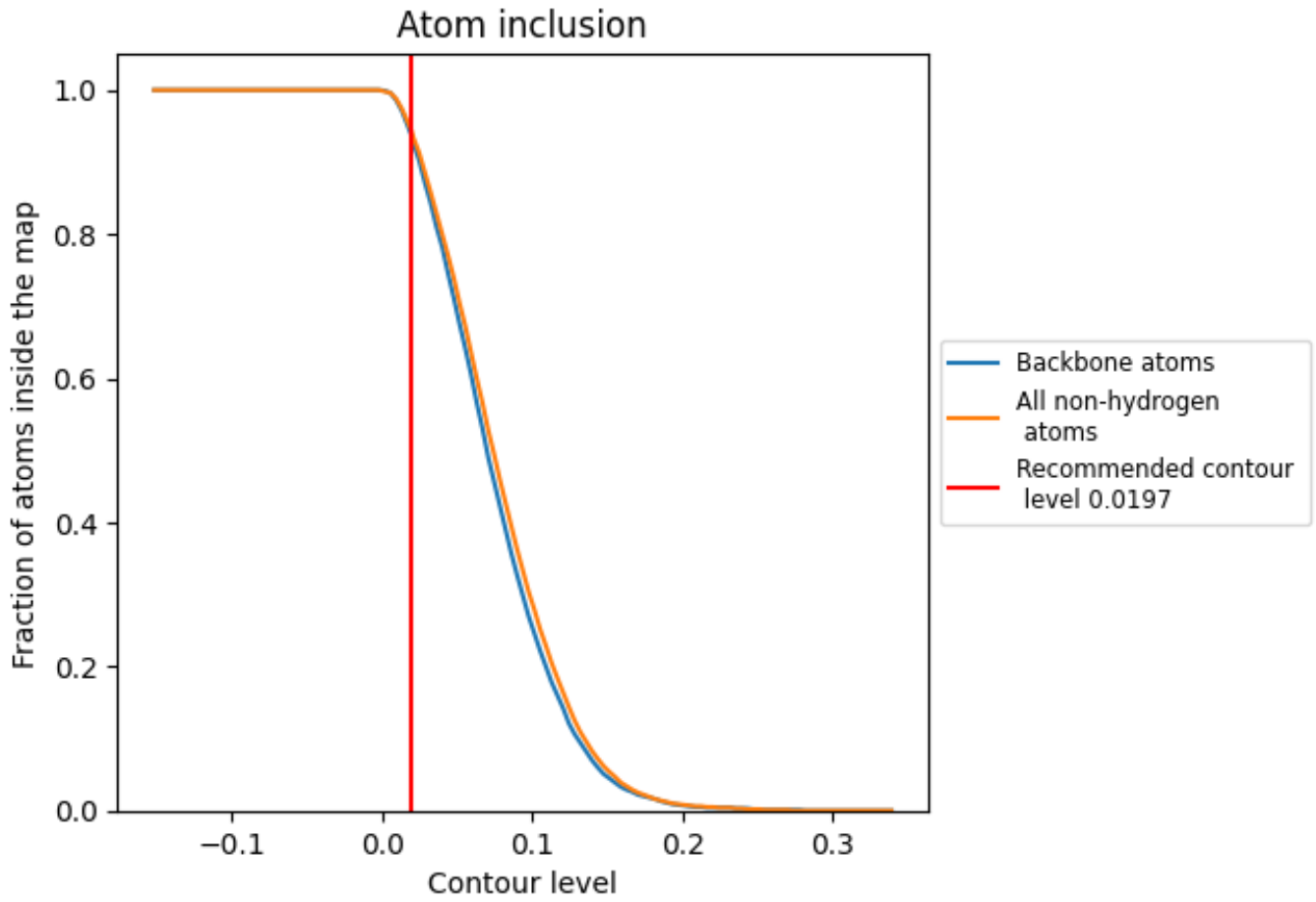
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0197).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.0197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9440	0.6460
2	0.9830	0.6660
D	0.9210	0.6180
E	0.9620	0.6660
F	0.8730	0.5910
G	0.9050	0.6360
H	0.9740	0.6730
I	0.8830	0.5990
J	0.9350	0.6540
K	0.9640	0.6780
L	0.9090	0.6220
M	0.9000	0.6040
N	0.9720	0.6800
O	0.8260	0.5880
P	0.8960	0.6250
Q	0.9700	0.6570
R	0.9680	0.6420