wwPDB EM Validation Summary Report (i)

Apr 1, 2023 – 09:26 am BST

PDB ID	:	8C92
EMDB ID	:	EMD-16499
Title	:	Cryo-EM captures early ribosome assembly in action
Authors	:	Lauer, S.; Nikolay, R.; Qin, B.
Deposited on	:	2023-01-21
Resolution	:	3.79 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 (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 (i)) were used in the production of this report:

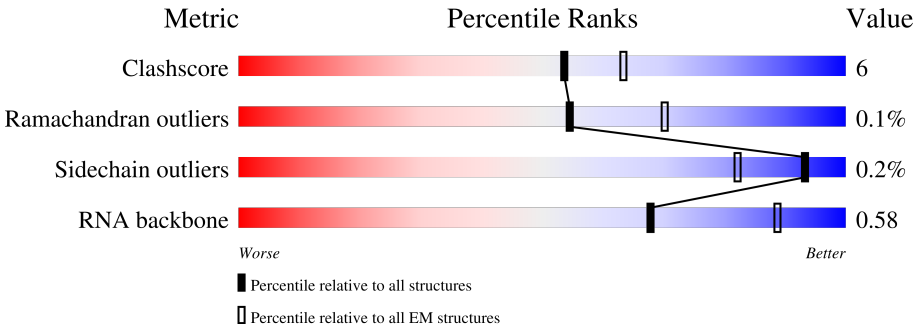
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.79 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.



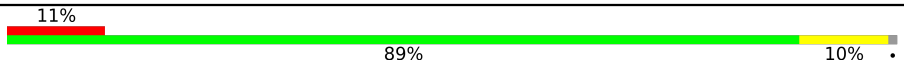
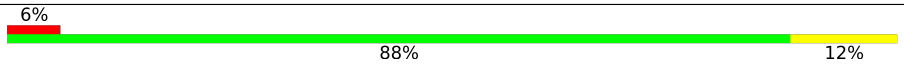
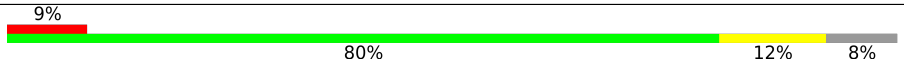
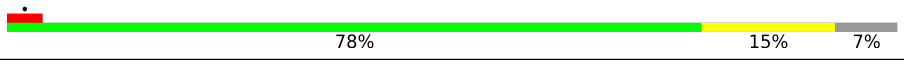
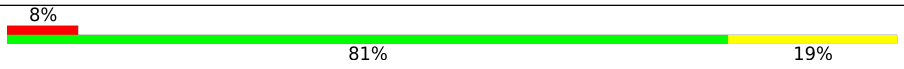
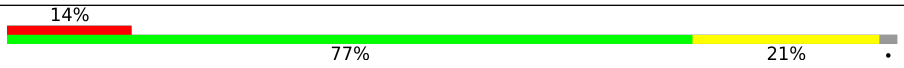
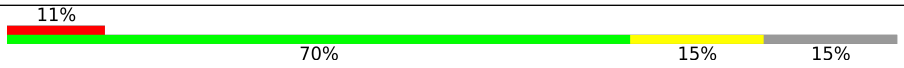
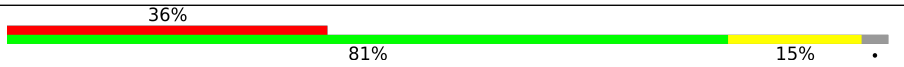
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	2904	8% 43% 19% • 36%
2	D	209	7% 67% 17% 16%
3	E	201	6% 79% 14% 7%
4	J	142	8% 83% 16% •
5	K	123	53% 79% 20% •
6	L	144	47% 62% 13% 24%
7	N	127	• 73% 20% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	P	115	
9	Q	118	
10	R	103	
11	S	110	
12	T	100	
13	U	104	
14	Y	63	
15	0	57	
16	2	46	
17	Z	59	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 53489 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1873	40250	17955	7457	12965	1873	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	175	1306	820	235	247	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	187	1438	904	255	274	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L13.

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

- Molecule 5 is a protein called 50S ribosomal protein L14.

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

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	L	109	778	483	149	146	0	0

- Molecule 7 is a protein called 50S ribosomal protein L17.

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

- Molecule 8 is a protein called 50S ribosomal protein L19.

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

- Molecule 9 is a protein called 50S ribosomal protein L20.

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

- Molecule 10 is a protein called 50S ribosomal protein L21.

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

- Molecule 11 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	101	Total	C	N	O	S	0	0
			789	492	150	145	2		

- Molecule 12 is a protein called 50S ribosomal protein L23.

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

- Molecule 13 is a protein called 50S ribosomal protein L24.

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

- Molecule 14 is a protein called 50S ribosomal protein L29.

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

- Molecule 15 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 16 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	39	Total	C	N	O	S	0	0
			312	187	77	47	1		

- Molecule 17 is a protein called 50S ribosomal protein L30.

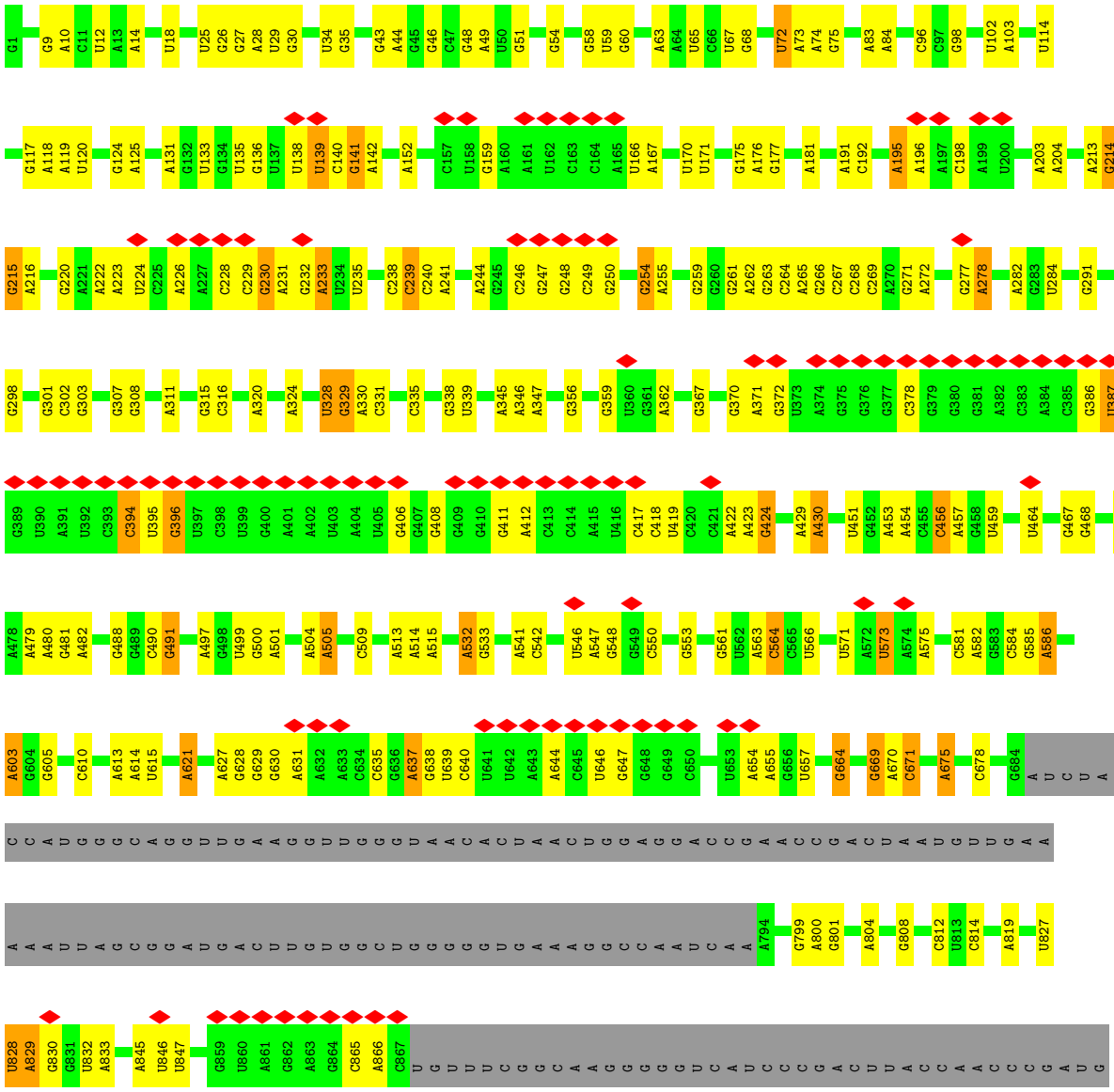
Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

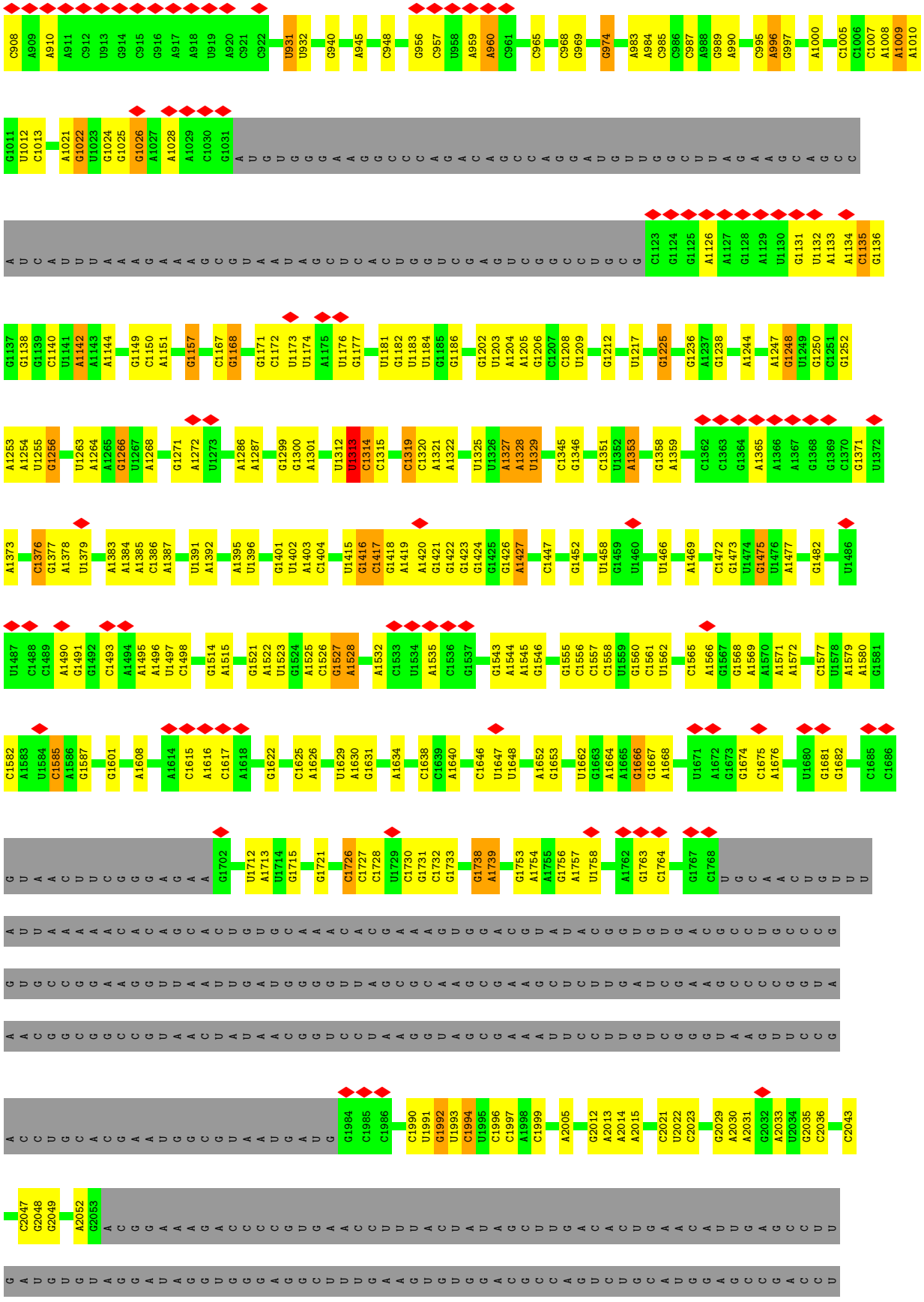
3 Residue-property plots (i)

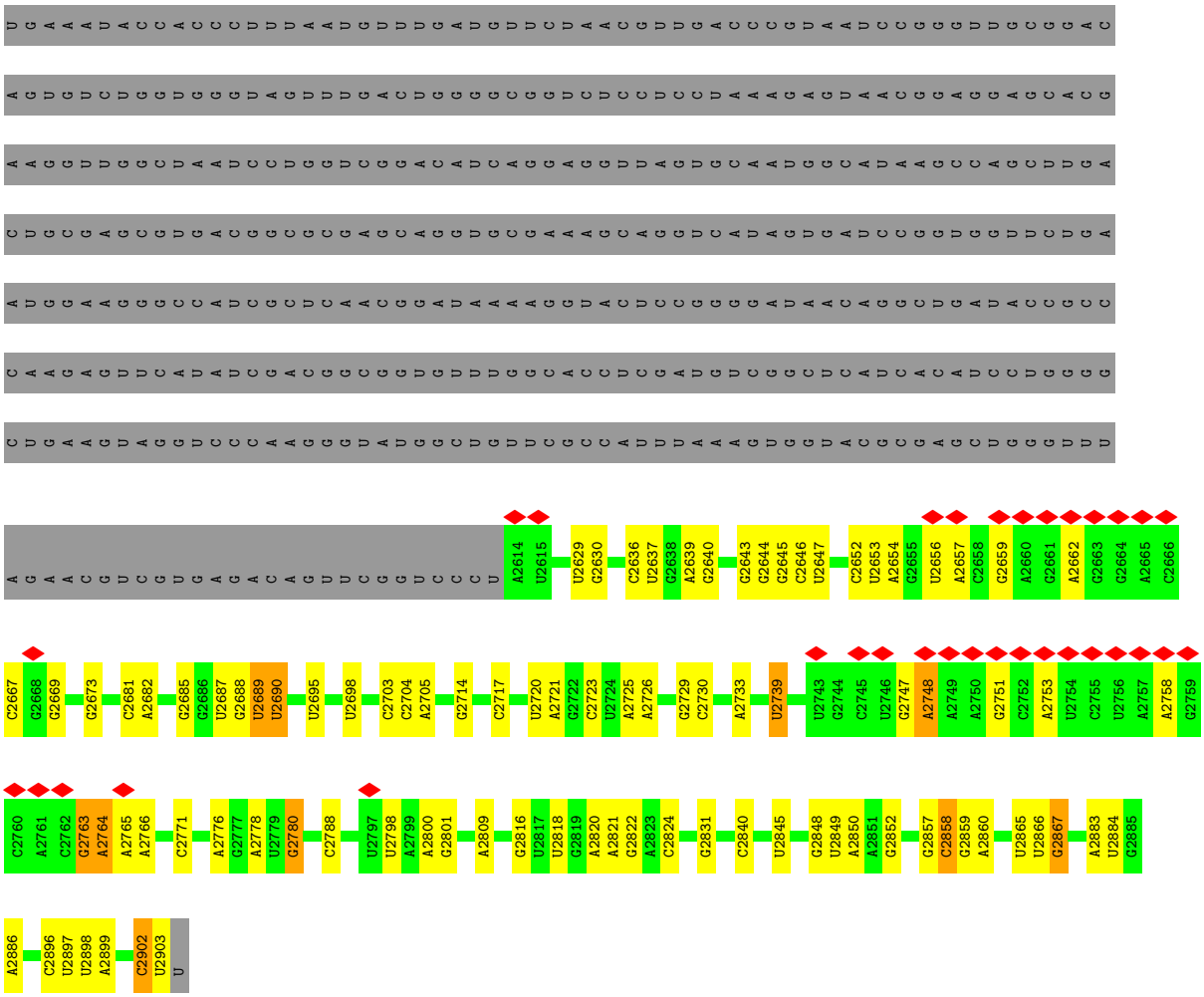
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA

Chain A:

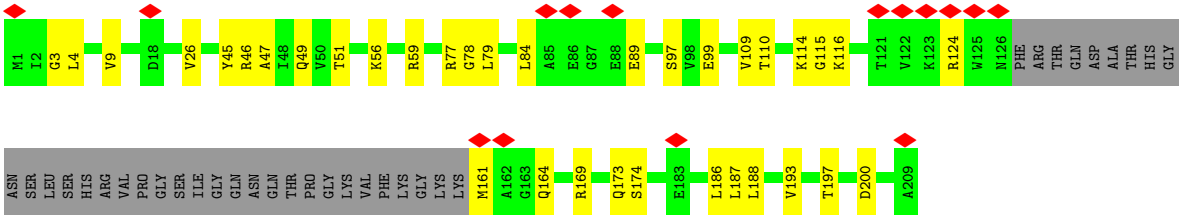






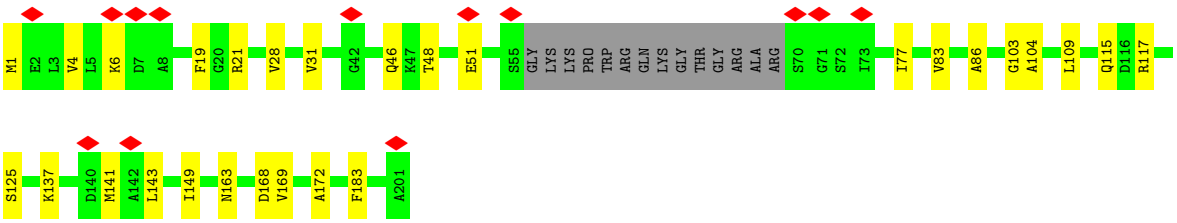
• Molecule 2: 50S ribosomal protein L3

Chain D:



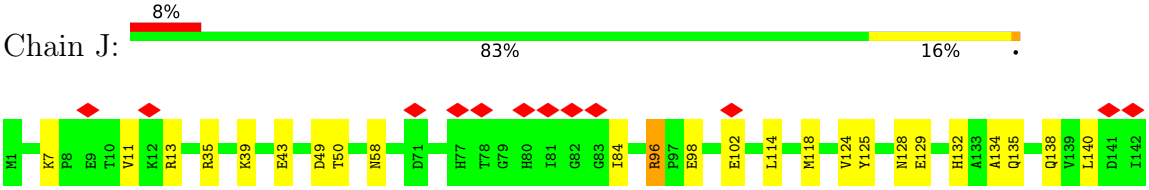
• Molecule 3: 50S ribosomal protein L4

Chain E:



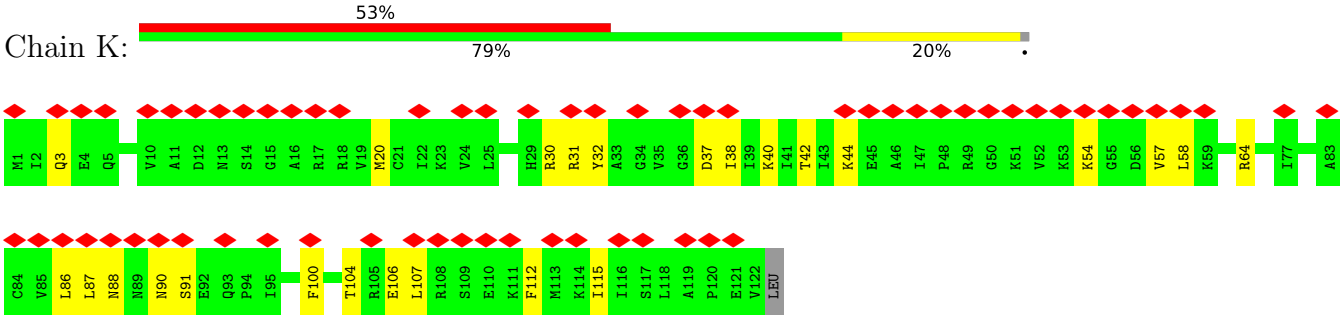
• Molecule 4: 50S ribosomal protein L13

Chain J:



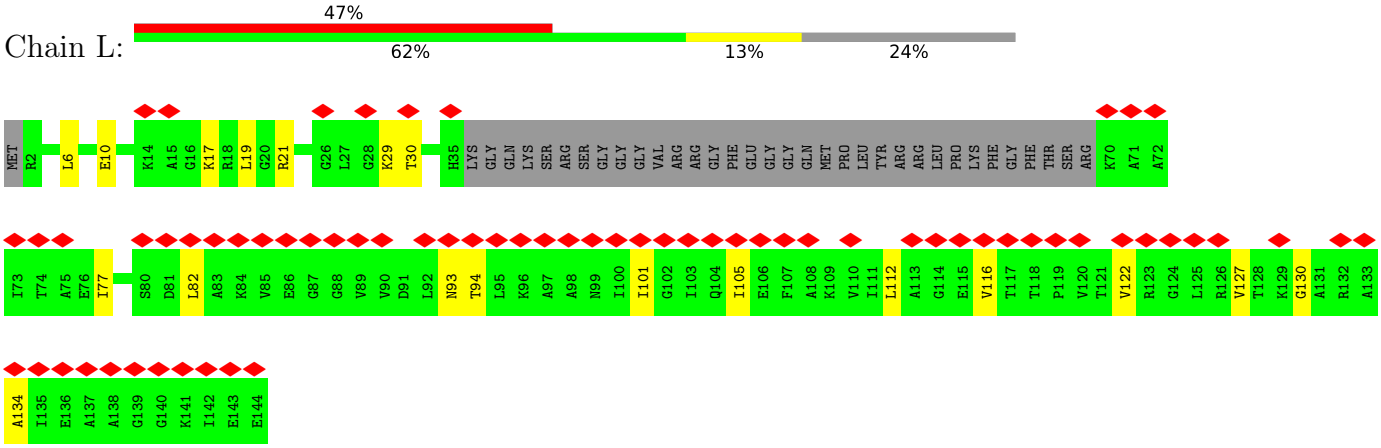
• Molecule 5: 50S ribosomal protein L14

Chain K:



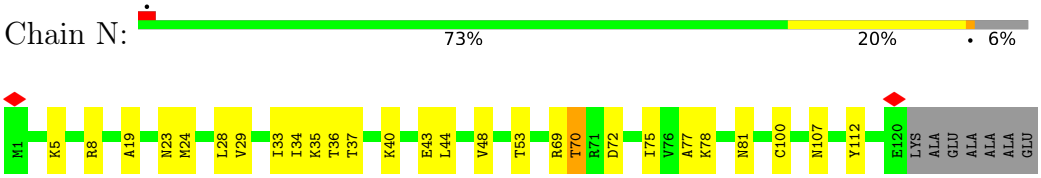
• Molecule 6: 50S ribosomal protein L15

Chain L:



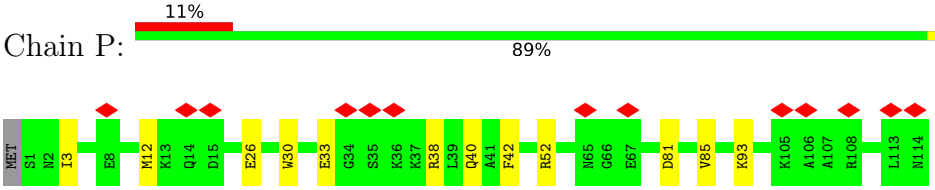
• Molecule 7: 50S ribosomal protein L17

Chain N:



• Molecule 8: 50S ribosomal protein L19

Chain P:

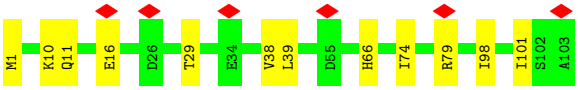


• Molecule 9: 50S ribosomal protein L20

Chain Q:

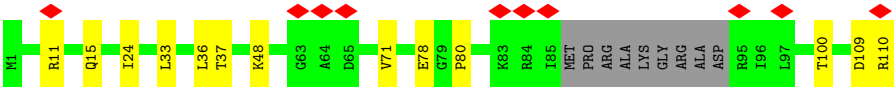
• Molecule 10: 50S ribosomal protein L21

Chain R:



• Molecule 11: 50S ribosomal protein L22

Chain S:

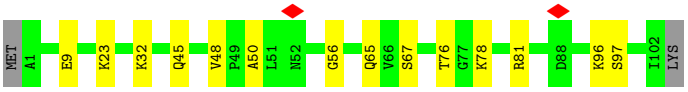


• Molecule 12: 50S ribosomal protein L23

Chain T:

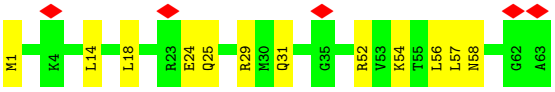
• Molecule 13: 50S ribosomal protein L24

Chain U:



• Molecule 14: 50S ribosomal protein L29

Chain Y:

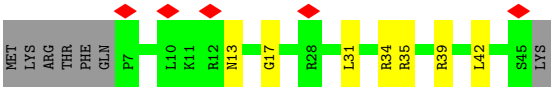


• Molecule 15: 50S ribosomal protein L32

Chain 0:

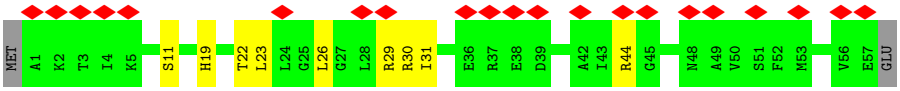
• Molecule 16: 50S ribosomal protein L34

Chain 2:



• Molecule 17: 50S ribosomal protein L30

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17988	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.836	Depositor
Minimum map value	-0.682	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.18	1/45087 (0.0%)	0.72	6/70332 (0.0%)
2	D	0.24	0/1320	0.51	0/1776
3	E	0.24	0/1453	0.47	0/1956
4	J	0.25	0/1152	0.50	0/1551
5	K	0.24	0/947	0.53	0/1268
6	L	0.24	0/780	0.54	0/1041
7	N	0.25	0/973	0.61	0/1301
8	P	0.24	0/929	0.55	0/1242
9	Q	0.25	0/960	0.51	0/1278
10	R	0.26	0/829	0.54	0/1107
11	S	0.24	0/794	0.50	0/1062
12	T	0.24	0/744	0.51	0/994
13	U	0.26	0/787	0.49	0/1051
14	Y	0.25	0/510	0.52	0/677
15	0	0.24	0/450	0.54	0/599
16	2	0.23	0/314	0.65	0/413
17	Z	0.24	0/443	0.55	0/593
All	All	0.19	1/58472 (0.0%)	0.68	6/88241 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	U	C1'-N1	5.92	1.57	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2771	C	N3-C2-O2	-6.13	117.61	121.90
1	A	1313	U	C2-N1-C1'	5.79	124.65	117.70
1	A	635	C	N3-C2-O2	-5.76	117.87	121.90
1	A	1319	C	N1-C2-O2	5.31	122.08	118.90
1	A	1675	C	C2-N1-C1'	5.22	124.54	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	40250	0	20252	304	0
2	D	1306	0	1355	26	0
3	E	1438	0	1494	17	0
4	J	1129	0	1162	19	0
5	K	938	0	1012	16	0
6	L	778	0	841	16	0
7	N	960	0	1000	23	0
8	P	917	0	965	9	0
9	Q	947	0	1022	16	0
10	R	816	0	839	10	0
11	S	789	0	849	9	0
12	T	738	0	807	11	0
13	U	779	0	834	8	0
14	Y	509	0	543	9	0
15	0	444	0	461	13	0
16	2	312	0	344	6	0
17	Z	439	0	485	6	0
All	All	53489	0	34265	456	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 456 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:G:O2'	1:A:215:G:O4'	1.87	0.90
1:A:395:U:O2'	1:A:396:G:N7	2.06	0.88
1:A:320:A:N3	3:E:163:ASN:ND2	2.23	0.87
1:A:1521:G:OP2	1:A:1522:A:O2'	1.92	0.86
1:A:475:C:O2	1:A:479:A:N6	2.09	0.85

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	171/209 (82%)	166 (97%)	5 (3%)	0	100	100
3	E	183/201 (91%)	178 (97%)	5 (3%)	0	100	100
4	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
5	K	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
6	L	105/144 (73%)	93 (89%)	12 (11%)	0	100	100
7	N	118/127 (93%)	109 (92%)	8 (7%)	1 (1%)	19	57
8	P	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
9	Q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
10	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
11	S	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
12	T	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
13	U	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
14	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
15	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
16	2	37/46 (80%)	35 (95%)	2 (5%)	0	100	100
17	Z	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
All	All	1660/1821 (91%)	1584 (95%)	75 (4%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	70	THR

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	136/164 (83%)	136 (100%)	0	100 100
3	E	155/165 (94%)	154 (99%)	1 (1%)	86 92
4	J	116/116 (100%)	115 (99%)	1 (1%)	78 88
5	K	103/104 (99%)	103 (100%)	0	100 100
6	L	76/103 (74%)	76 (100%)	0	100 100
7	N	100/103 (97%)	100 (100%)	0	100 100
8	P	99/100 (99%)	99 (100%)	0	100 100
9	Q	89/90 (99%)	89 (100%)	0	100 100
10	R	84/84 (100%)	84 (100%)	0	100 100
11	S	87/93 (94%)	87 (100%)	0	100 100
12	T	80/84 (95%)	80 (100%)	0	100 100
13	U	83/85 (98%)	83 (100%)	0	100 100
14	Y	55/55 (100%)	55 (100%)	0	100 100
15	0	47/48 (98%)	47 (100%)	0	100 100
16	2	31/38 (82%)	31 (100%)	0	100 100
17	Z	47/49 (96%)	46 (98%)	1 (2%)	53 74
All	All	1388/1481 (94%)	1385 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	1	MET
4	J	96	ARG
17	Z	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	67	HIS
10	R	82	HIS
11	S	15	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1866/2904 (64%)	284 (15%)	8 (0%)

5 of 284 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	25	U
1	A	27	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2858	C
1	A	2763	G
1	A	1420	A
1	A	1313	U
1	A	1738	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

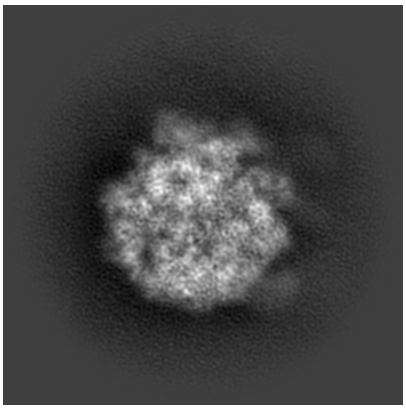
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16499. These allow visual inspection of the internal detail of the map and identification of artifacts.

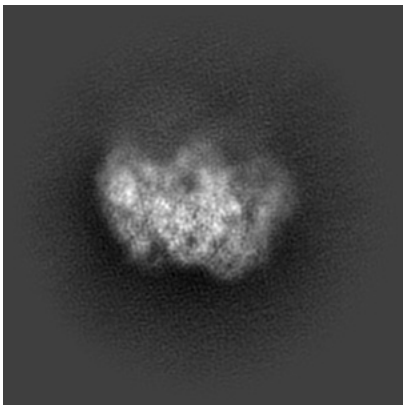
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

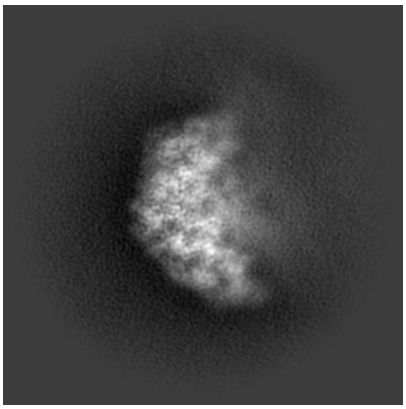
6.1.1 Primary map



X

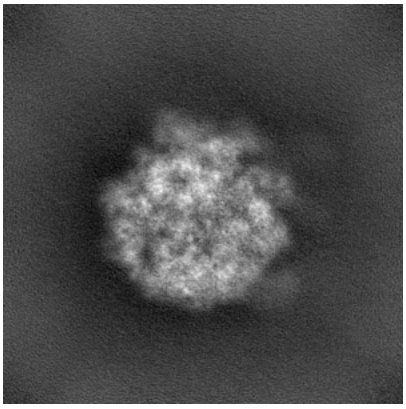


Y

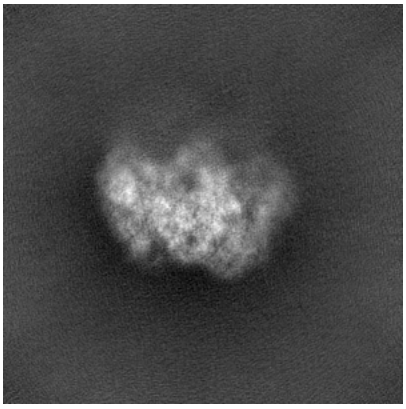


Z

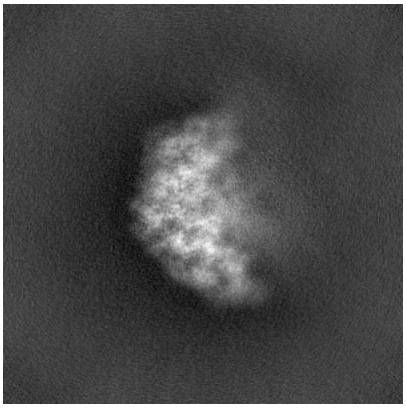
6.1.2 Raw map



X



Y

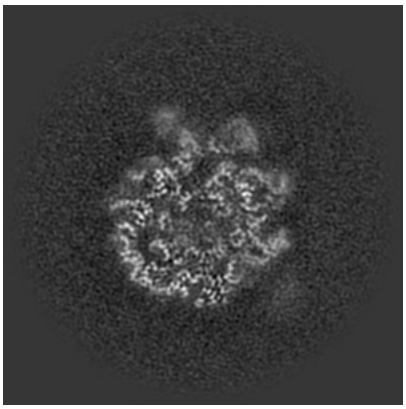


Z

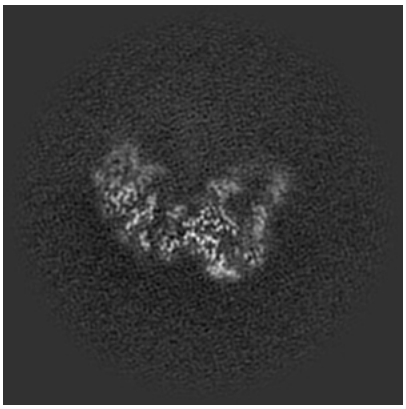
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

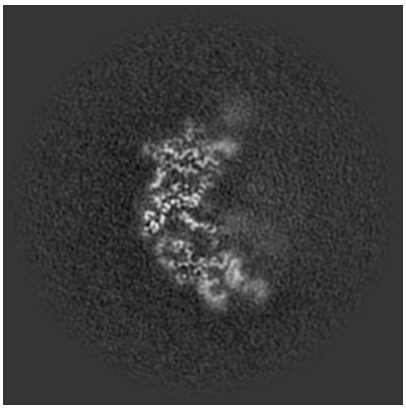
6.2.1 Primary map



X Index: 150

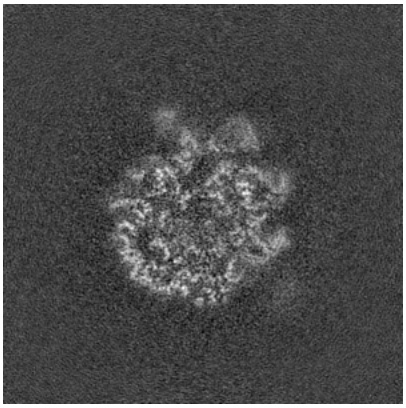


Y Index: 150

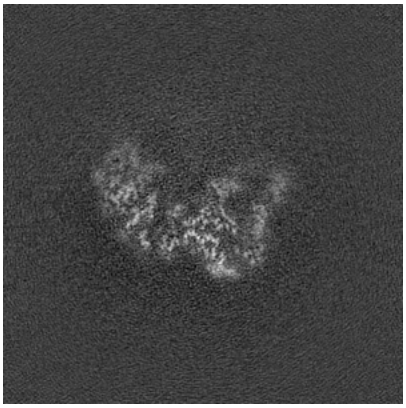


Z Index: 150

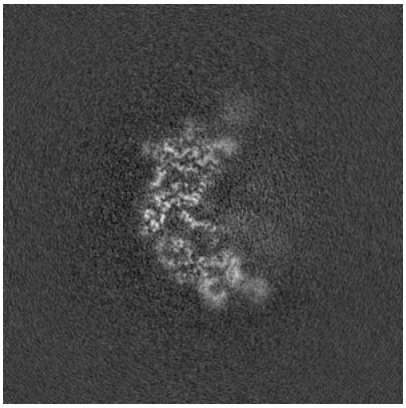
6.2.2 Raw map



X Index: 150



Y Index: 150

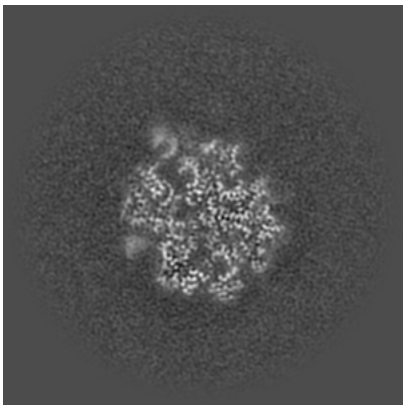


Z Index: 150

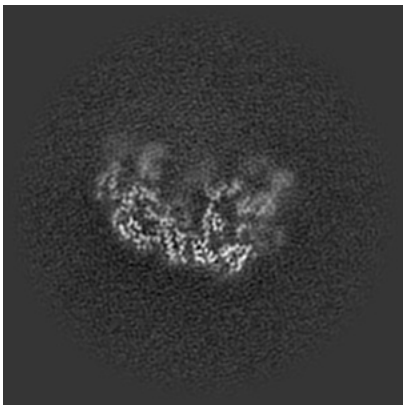
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

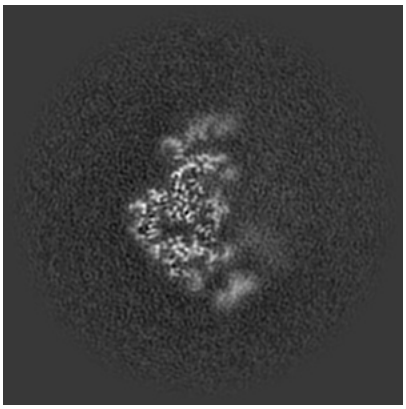
6.3.1 Primary map



X Index: 134

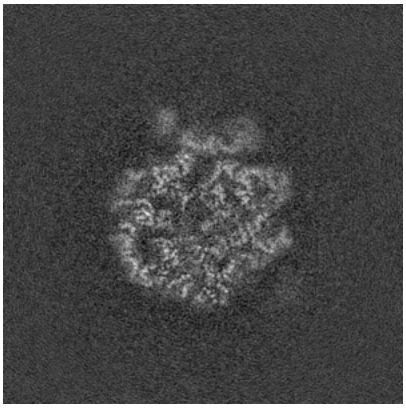


Y Index: 140

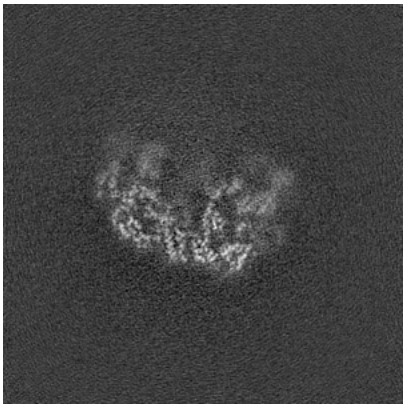


Z Index: 162

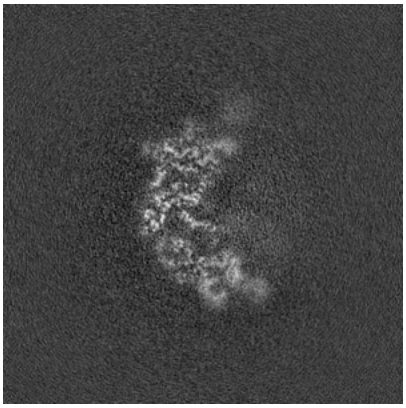
6.3.2 Raw map



X Index: 148



Y Index: 140

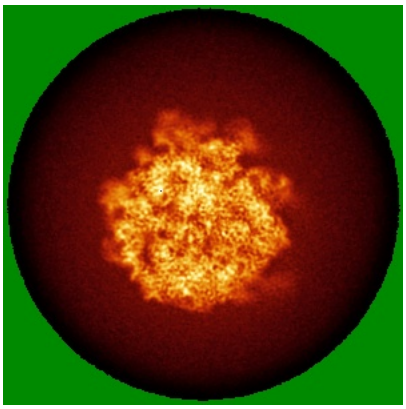


Z Index: 150

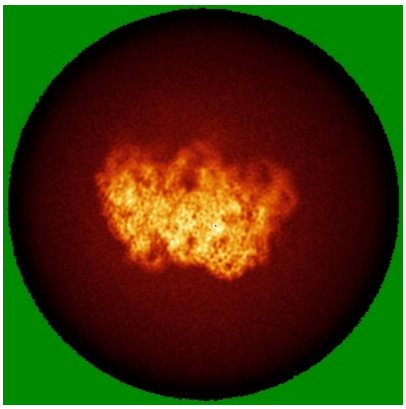
The images above show the largest variance slices of the map in three orthogonal directions.

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

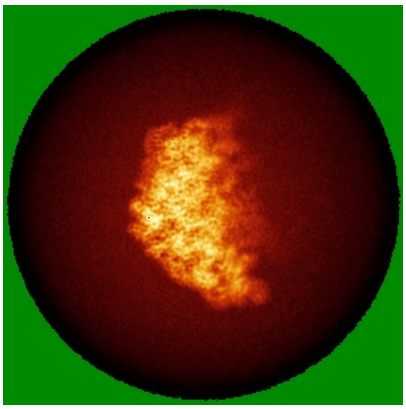
6.4.1 Primary map



X

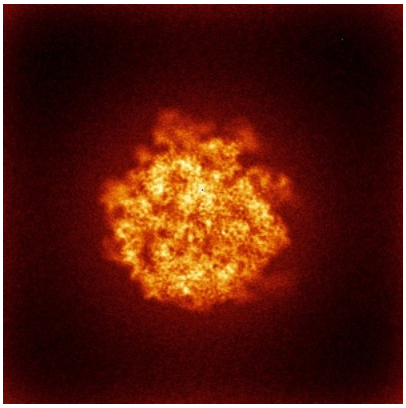


Y

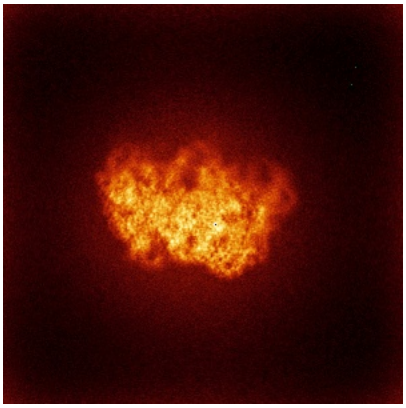


Z

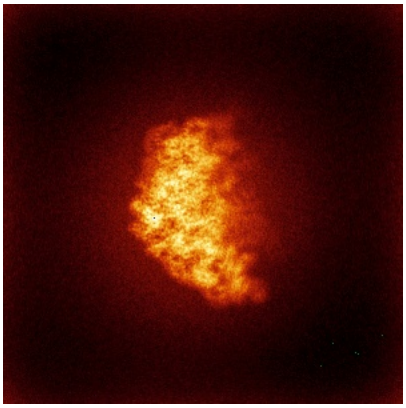
6.4.2 Raw map



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.

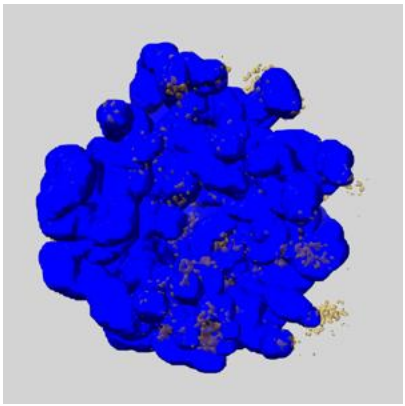
6.6 Mask visualisation (i)

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

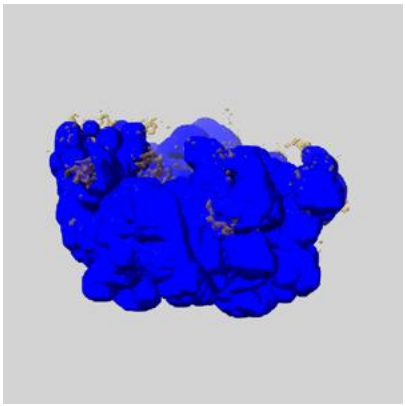
A mask typically either:

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

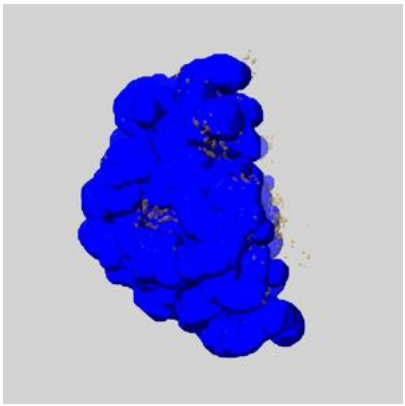
6.6.1 emd_16499_msk_1.map (i)



X



Y

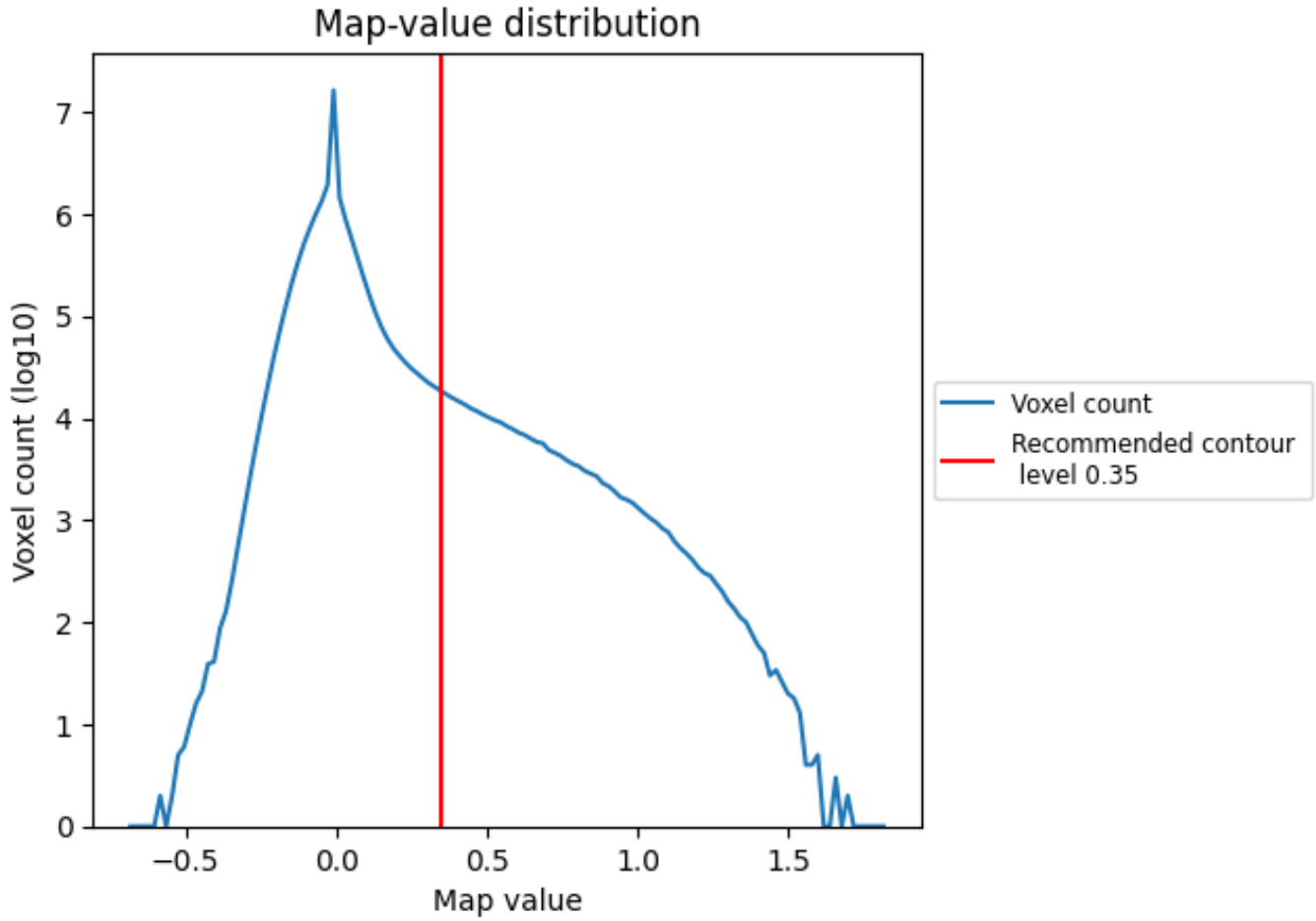


Z

7 Map analysis

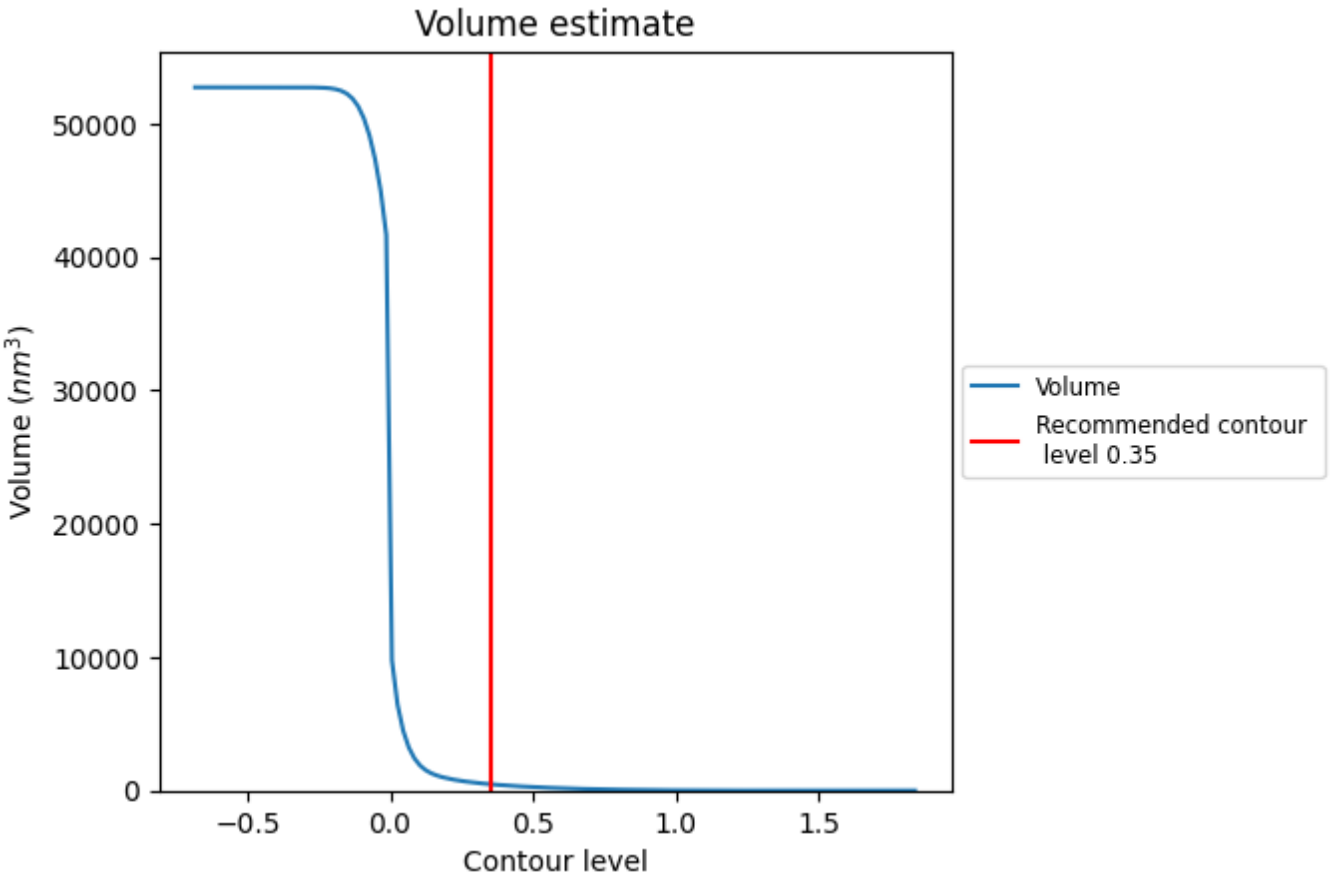
This section contains the results of statistical analysis of the map.

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.

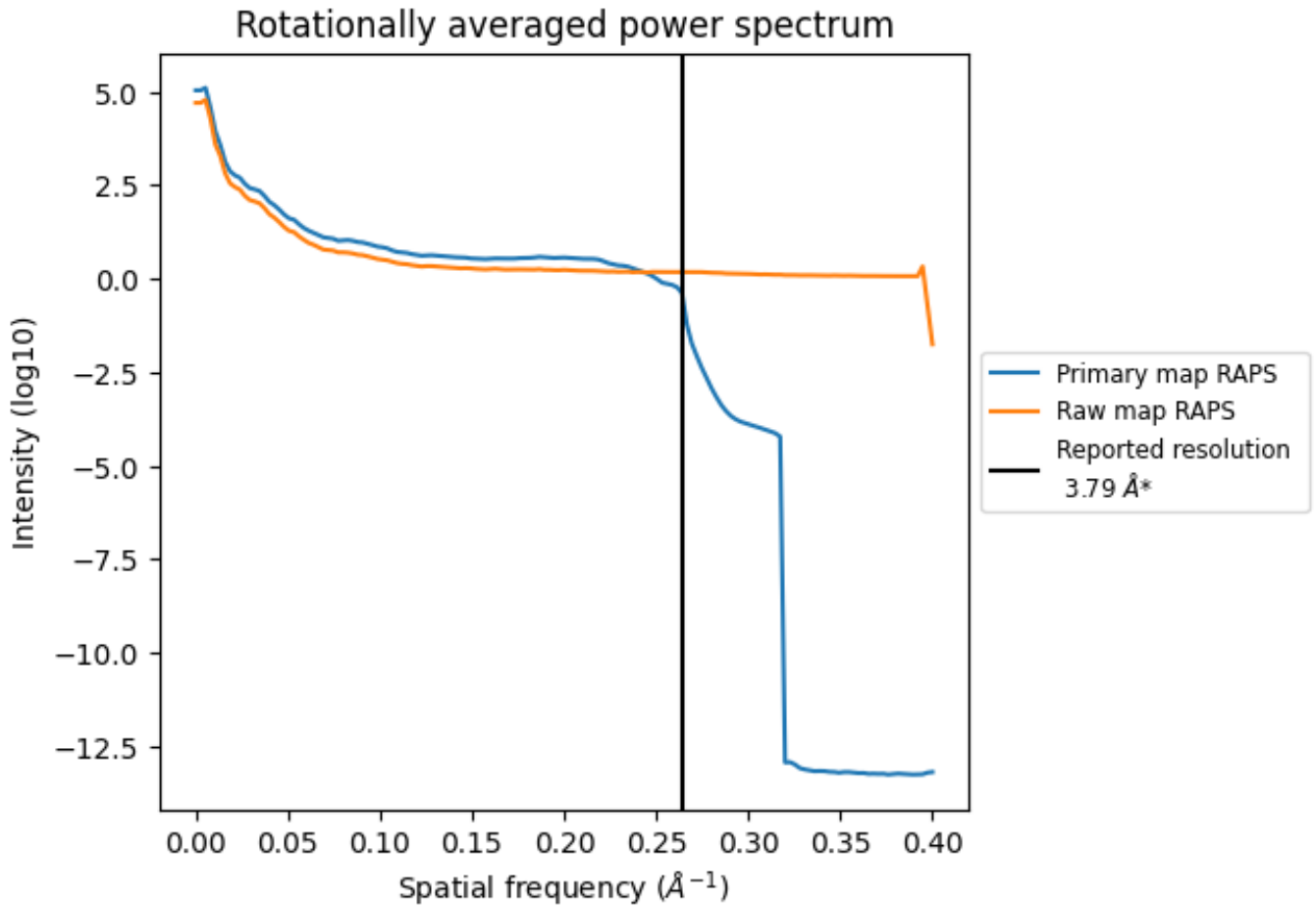
7.2 Volume estimate (i)



The volume at the recommended contour level is 476 nm^3; this corresponds to an approximate mass of 430 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)

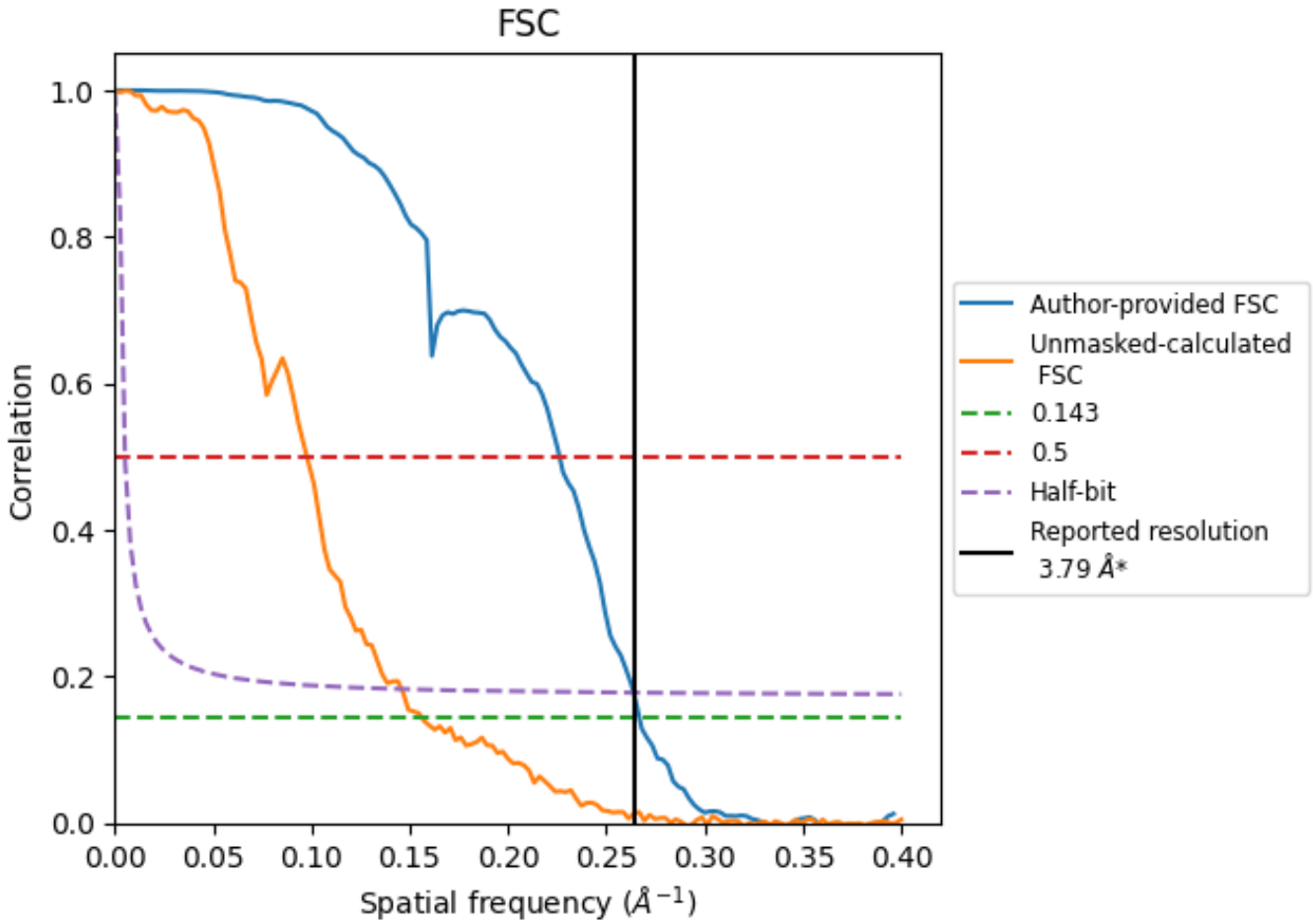


*Reported resolution corresponds to spatial frequency of 0.264 Å^{-1}

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 0.264 Å^{-1}

8.2 Resolution estimates (i)

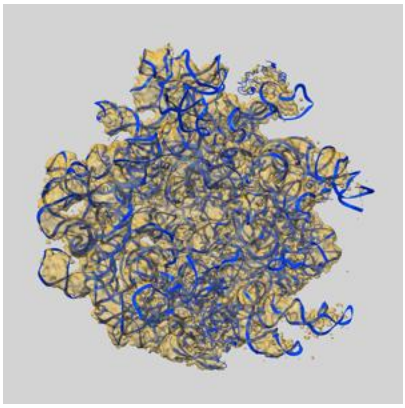
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	3.75	4.42	3.79
Unmasked-calculated*	6.40	10.24	6.86

*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 6.40 differs from the reported value 3.79 by more than 10 %

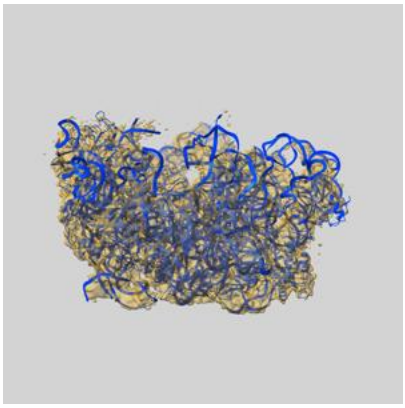
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16499 and PDB model 8C92. Per-residue inclusion information can be found in section 3 on page 7.

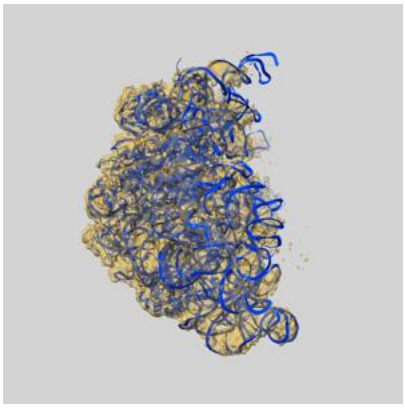
9.1 Map-model overlay



X



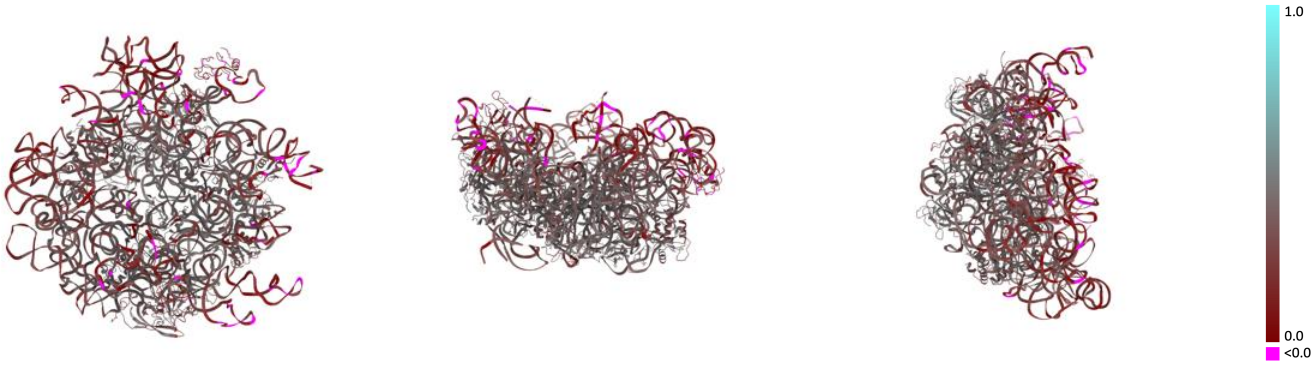
Y



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.

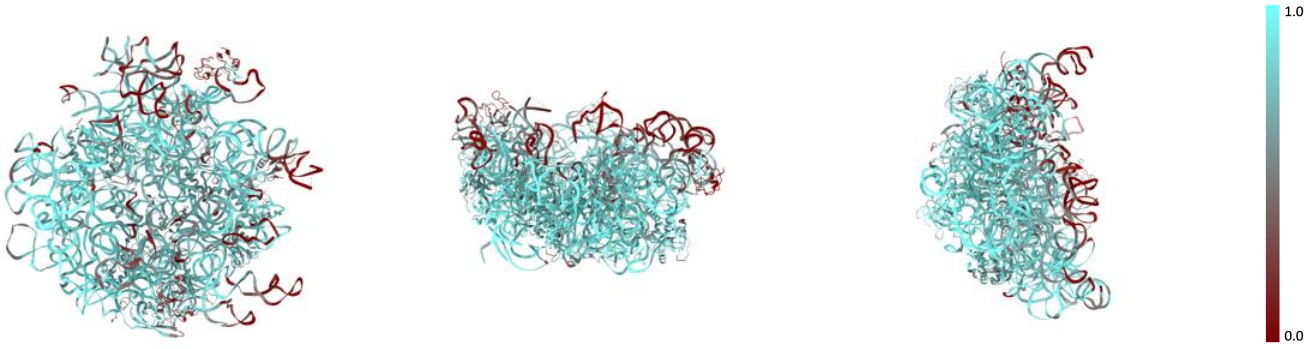
9.2 Q-score mapped to coordinate model



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.

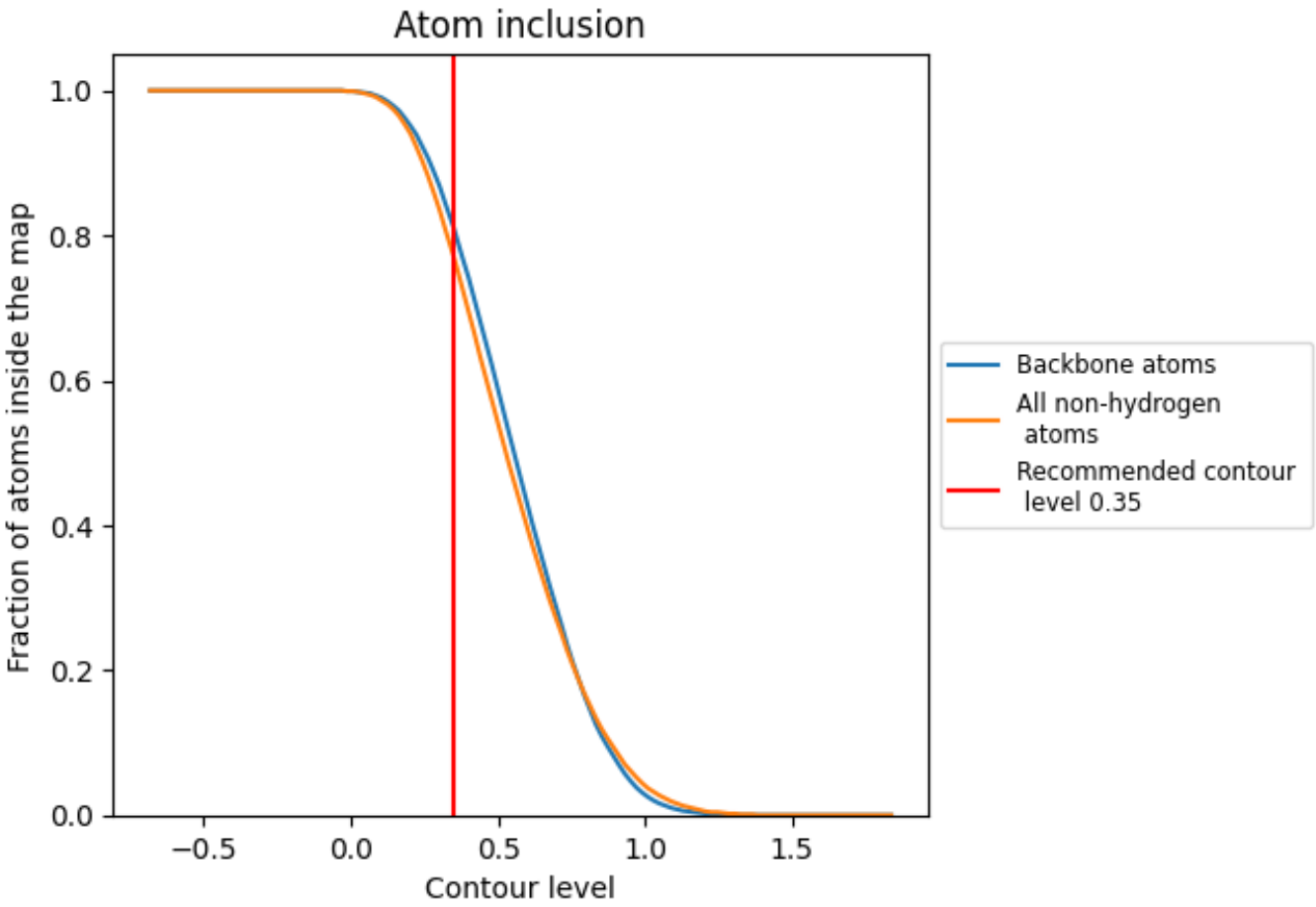
9.3 Atom inclusion mapped to coordinate model



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, 81% of all backbone atoms, 77% 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	0.7700	0.3340
0	0.6940	0.4390
2	0.6950	0.4220
A	0.7930	0.3170
D	0.7430	0.4200
E	0.7580	0.3920
J	0.7700	0.3990
K	0.3690	0.2670
L	0.3080	0.2240
N	0.8360	0.4320
P	0.7140	0.3770
Q	0.8290	0.4180
R	0.7380	0.4170
S	0.7230	0.4290
T	0.7480	0.4170
U	0.8450	0.4310
Y	0.7730	0.3600
Z	0.4610	0.3470