



wwPDB EM Validation Summary Report ⓘ

Jun 2, 2024 – 07:59 PM EDT

PDB ID : 8D8J
EMDB ID : EMD-27249
Title : Yeast mitochondrial small subunit assembly intermediate (State 1)
Authors : Burnside, C.; Harper, N.; Klinge, S.
Deposited on : 2022-06-08
Resolution : 3.80 Å(reported)
Based on initial model : 5MRC

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:

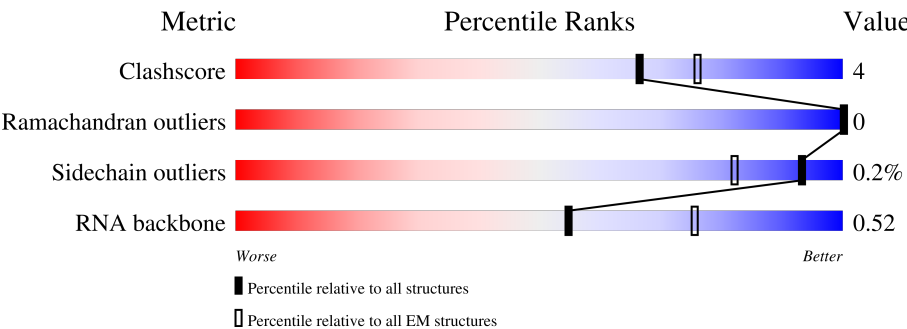
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.80 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	628	<div> <div>13%</div> <div>77%</div> <div>21%</div> </div>
2	5	339	<div> <div>59%</div> <div>69%</div> <div>10%</div> <div>20%</div> </div>
3	d	864	<div> <div>38%</div> <div>76%</div> <div>24%</div> </div>
4	O	286	<div> <div>66%</div> <div>7%</div> <div>27%</div> </div>
5	P	121	<div> <div>6%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
6	Q	237	<div> <div>9%</div> <div>52%</div> <div>8%</div> <div>40%</div> </div>
7	R	138	<div> <div>18%</div> <div>33%</div> <div>8%</div> <div>59%</div> </div>

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Mol	Chain	Length	Quality of chain
8	V	318	
9	2	130	
10	D	486	
11	E	307	
12	F	131	
13	6	345	
14	H	155	
15	a	1713	
16	L	153	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51386 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 Probable S-adenosyl-L-methionine-dependent RNA methyltransferase RSM22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	493	Total	C	N	O	S	0	0
			2448	1458	493	493	4		

- Molecule 2 is a protein called 37S ribosomal protein MRP13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	270	Total	C	N	O	S	0	0
			2199	1426	375	394	4		

- Molecule 3 is a protein called Mitochondrial group I intron splicing factor CCM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	660	Total	C	N	O	S	0	0
			5497	3530	934	999	34		

- Molecule 4 is a protein called 37S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	210	Total	C	N	O	S	0	0
			1724	1079	318	319	8		

- Molecule 5 is a protein called 37S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	115	Total	C	N	O	S	0	0
			913	583	171	157	2		

- Molecule 6 is a protein called 37S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	143	Total	C	N	O	S	0	0
			1172	736	220	215	1		

- Molecule 7 is a protein called 37S ribosomal protein RSM18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	57	Total	C	N	O	S	0	0
			454	280	94	78	2		

- Molecule 8 is a protein called 37S ribosomal protein PET123, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	222	Total	C	N	O	S	0	0
			1787	1136	326	322	3		

- Molecule 9 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 10 is a protein called 37S ribosomal protein NAM9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	308	Total	C	N	O	S	0	0
			2567	1677	452	434	4		

- Molecule 11 is a protein called 37S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	168	Total	C	N	O	S	0	0
			1334	850	243	234	7		

- Molecule 12 is a protein called 37S ribosomal protein MRP17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	131	Total	C	N	O	S	0	0
			1054	671	189	190	4		

- Molecule 13 is a protein called 37S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	250	Total	C	N	O	S	0	0
			2063	1318	374	365	6		

- Molecule 14 is a protein called 37S ribosomal protein S8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	155	Total	C	N	O	S	0	0
			1221	772	218	221	10		

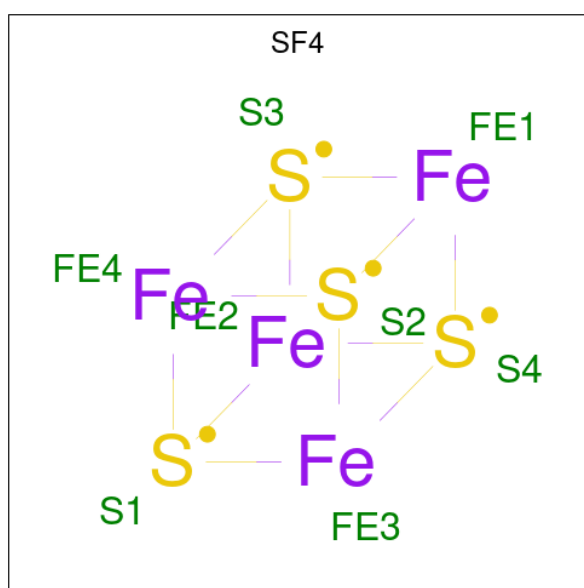
- Molecule 15 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	1183	Total	C	N	O	P	0	0
			25157	11312	4468	8194	1183		

- Molecule 16 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	121	Total	C	N	O	S	0	0
			926	571	190	161	4		

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



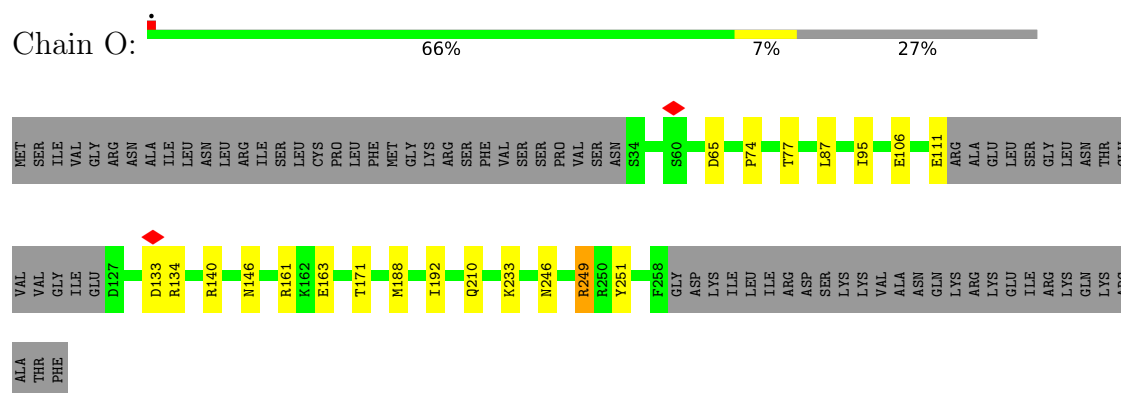
Mol	Chain	Residues	Atoms			AltConf
17	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

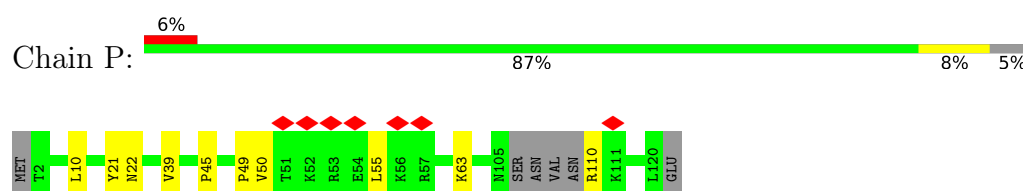
Mol	Chain	Residues	Atoms		AltConf
18	a	29	Total	Mg	0
			29	29	



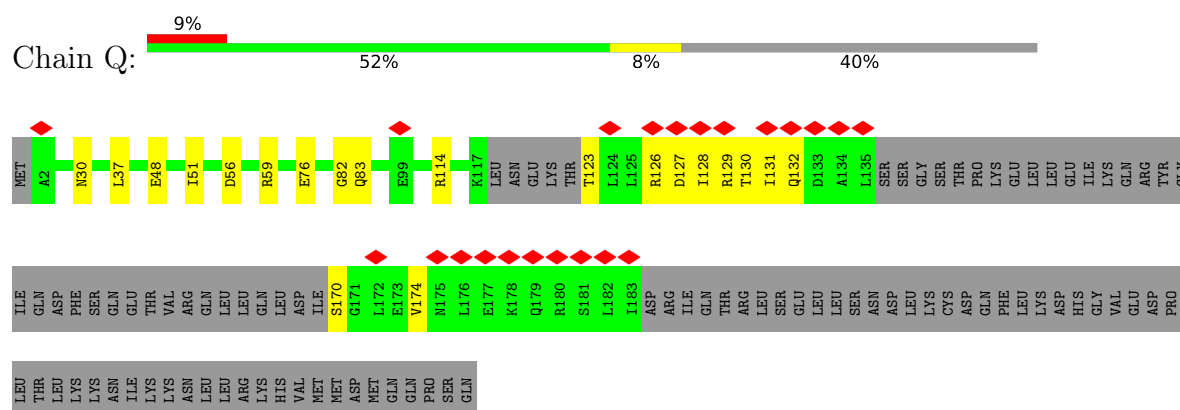
- Molecule 4: 37S ribosomal protein S28, mitochondrial



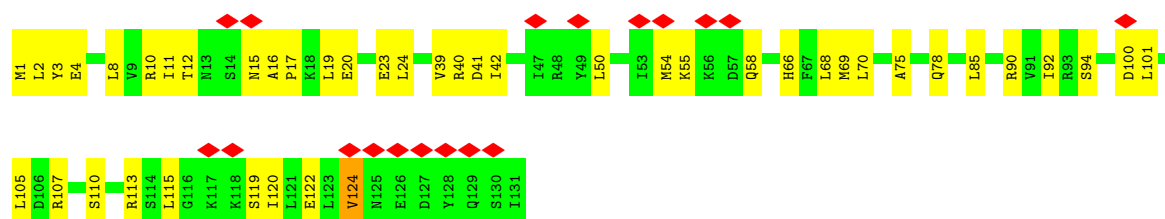
- Molecule 5: 37S ribosomal protein S16, mitochondrial



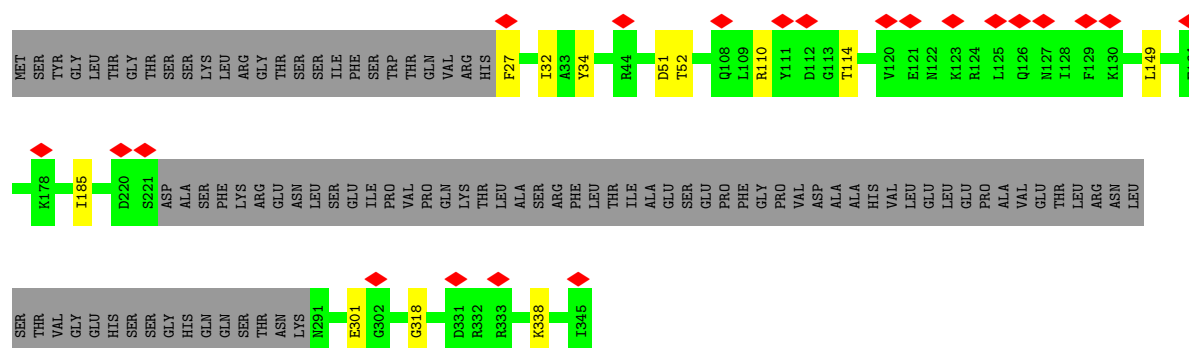
- Molecule 6: 37S ribosomal protein S17, mitochondrial



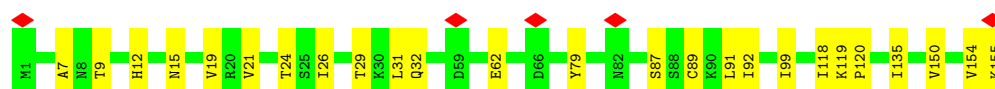
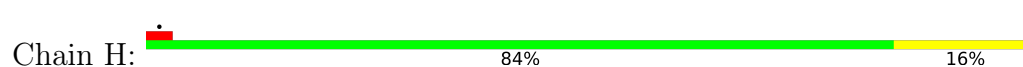
- Molecule 12: 37S ribosomal protein MRP17, mitochondrial



- Molecule 13: 37S ribosomal protein S35, mitochondrial

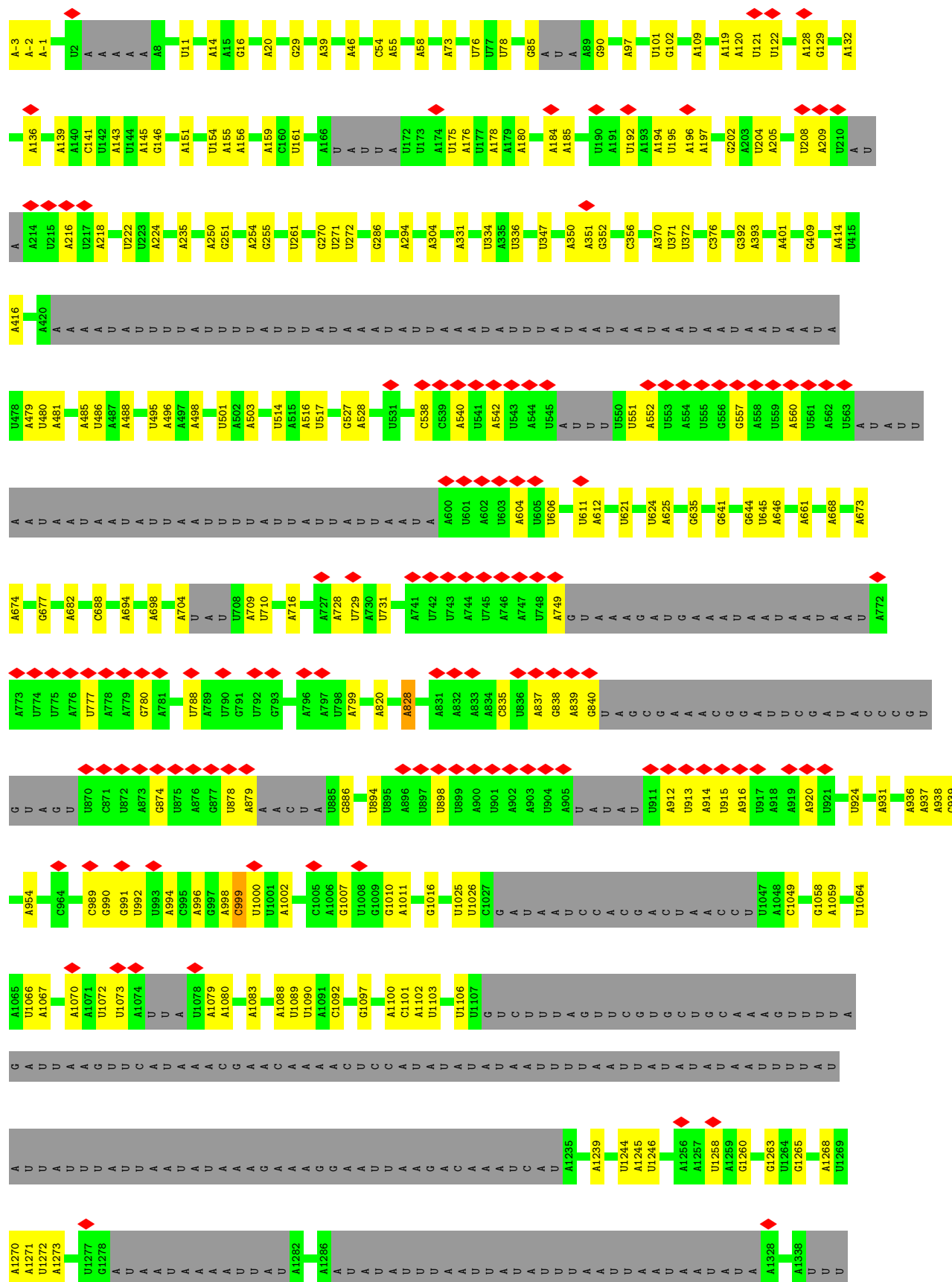


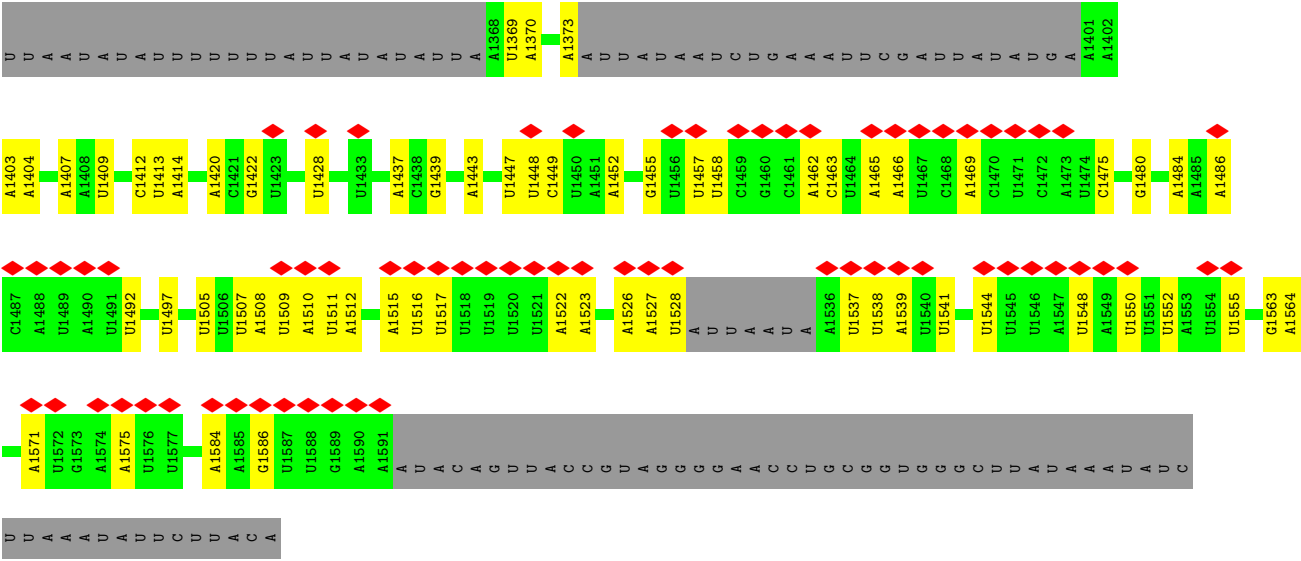
- Molecule 14: 37S ribosomal protein S8, mitochondrial



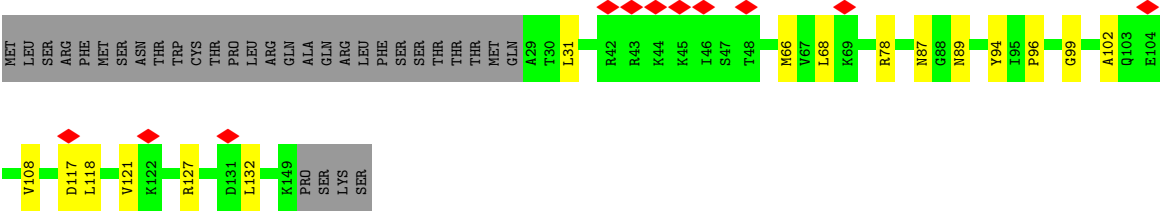
- Molecule 15: 15S ribosomal RNA







● Molecule 16: uS12m



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19720	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 ($e^-/\text{\AA}^2$)	61.73	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	27.063	Depositor
Minimum map value	-10.443	Depositor
Average map value	0.028	Depositor
Map value standard deviation	1.069	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	422.80002, 422.80002, 422.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	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, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.25	0/2447	0.48	0/3404
2	5	0.27	0/2249	0.49	0/3040
3	d	0.28	0/5612	0.52	0/7552
4	O	0.30	0/1746	0.58	0/2335
5	P	0.29	0/928	0.60	0/1252
6	Q	0.29	0/1181	0.59	0/1571
7	R	0.29	0/459	0.75	0/613
8	V	0.28	0/1813	0.55	0/2421
9	2	0.27	0/852	0.53	0/1142
10	D	0.29	0/2642	0.52	0/3561
11	E	0.29	0/1356	0.59	0/1812
12	F	0.29	0/1067	0.62	0/1430
13	6	0.29	0/2113	0.52	0/2845
14	H	0.30	0/1240	0.55	0/1670
15	a	0.34	0/28166	0.81	3/43793 (0.0%)
16	L	0.28	0/940	0.64	0/1261
All	All	0.31	0/54811	0.71	3/79702 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	999	C	C6-N1-C2	-5.99	117.90	120.30
15	a	392	G	C8-N9-C4	-5.35	104.26	106.40
15	a	828	A	N7-C8-N9	5.28	116.44	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F	124	VAL	Peptide

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	0	2448	0	1079	4	0
2	5	2199	0	2246	21	0
3	d	5497	0	5513	0	0
4	O	1724	0	1761	16	0
5	P	913	0	977	7	0
6	Q	1172	0	1226	13	0
7	R	454	0	480	7	0
8	V	1787	0	1915	18	0
9	2	833	0	839	4	0
10	D	2567	0	2630	15	0
11	E	1334	0	1392	20	0
12	F	1054	0	1129	31	0
13	6	2063	0	2095	9	0
14	H	1221	0	1289	16	0
15	a	25157	0	12624	0	0
16	L	926	0	980	13	0
17	0	8	0	0	0	0
18	a	29	0	0	0	0
All	All	51386	0	38175	178	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 4.

The worst 5 of 178 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)
11:E:219:ASP:OD1	14:H:119:LYS:NZ	2.07	0.86
4:O:65:ASP:OD1	4:O:251:TYR:OH	1.98	0.82
12:F:100:ASP:O	12:F:107:ARG:NH1	2.14	0.81
4:O:140:ARG:O	4:O:146:ASN:ND2	2.16	0.79
4:O:134:ARG:NH2	8:V:203:TYR:O	2.15	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	485/628 (77%)	466 (96%)	19 (4%)	0	100	100
2	5	264/339 (78%)	261 (99%)	3 (1%)	0	100	100
3	d	652/864 (76%)	643 (99%)	9 (1%)	0	100	100
4	O	206/286 (72%)	203 (98%)	3 (2%)	0	100	100
5	P	111/121 (92%)	110 (99%)	1 (1%)	0	100	100
6	Q	137/237 (58%)	135 (98%)	2 (2%)	0	100	100
7	R	55/138 (40%)	53 (96%)	2 (4%)	0	100	100
8	V	220/318 (69%)	215 (98%)	5 (2%)	0	100	100
9	2	97/130 (75%)	95 (98%)	2 (2%)	0	100	100
10	D	302/486 (62%)	297 (98%)	5 (2%)	0	100	100
11	E	166/307 (54%)	162 (98%)	4 (2%)	0	100	100
12	F	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
13	6	246/345 (71%)	243 (99%)	3 (1%)	0	100	100
14	H	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
16	L	119/153 (78%)	114 (96%)	5 (4%)	0	100	100
All	All	3342/4638 (72%)	3270 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	7/564 (1%)	7 (100%)	0	100	100
2	5	239/303 (79%)	237 (99%)	2 (1%)	81	89
3	d	610/803 (76%)	609 (100%)	1 (0%)	93	97
4	O	183/250 (73%)	182 (100%)	1 (0%)	88	94
5	P	100/106 (94%)	100 (100%)	0	100	100
6	Q	127/218 (58%)	126 (99%)	1 (1%)	81	89
7	R	48/121 (40%)	47 (98%)	1 (2%)	53	74
8	V	200/287 (70%)	200 (100%)	0	100	100
9	2	90/117 (77%)	90 (100%)	0	100	100
10	D	277/437 (63%)	277 (100%)	0	100	100
11	E	141/266 (53%)	141 (100%)	0	100	100
12	F	120/120 (100%)	120 (100%)	0	100	100
13	6	229/312 (73%)	229 (100%)	0	100	100
14	H	142/142 (100%)	142 (100%)	0	100	100
16	L	100/131 (76%)	100 (100%)	0	100	100
All	All	2613/4177 (63%)	2607 (100%)	6 (0%)	93	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	O	249	ARG
6	Q	129	ARG
7	R	108	ARG
2	5	221	ARG
2	5	197	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
8	V	60	HIS
8	V	204	HIS
9	2	92	HIS
9	2	96	ASN
13	6	46	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	a	1161/1713 (67%)	290 (24%)	0

5 of 290 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	a	-7	A
15	a	-5	G
15	a	-4	G
15	a	-3	A
15	a	-2	A

There are no RNA pucker outliers to report.

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](#)

Of 30 ligands modelled in this entry, 29 are monoatomic - leaving 1 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	$\# Z > 2$
17	SF4	0	701	1	0,12,12	-	-	-		

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
17	SF4	0	701	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

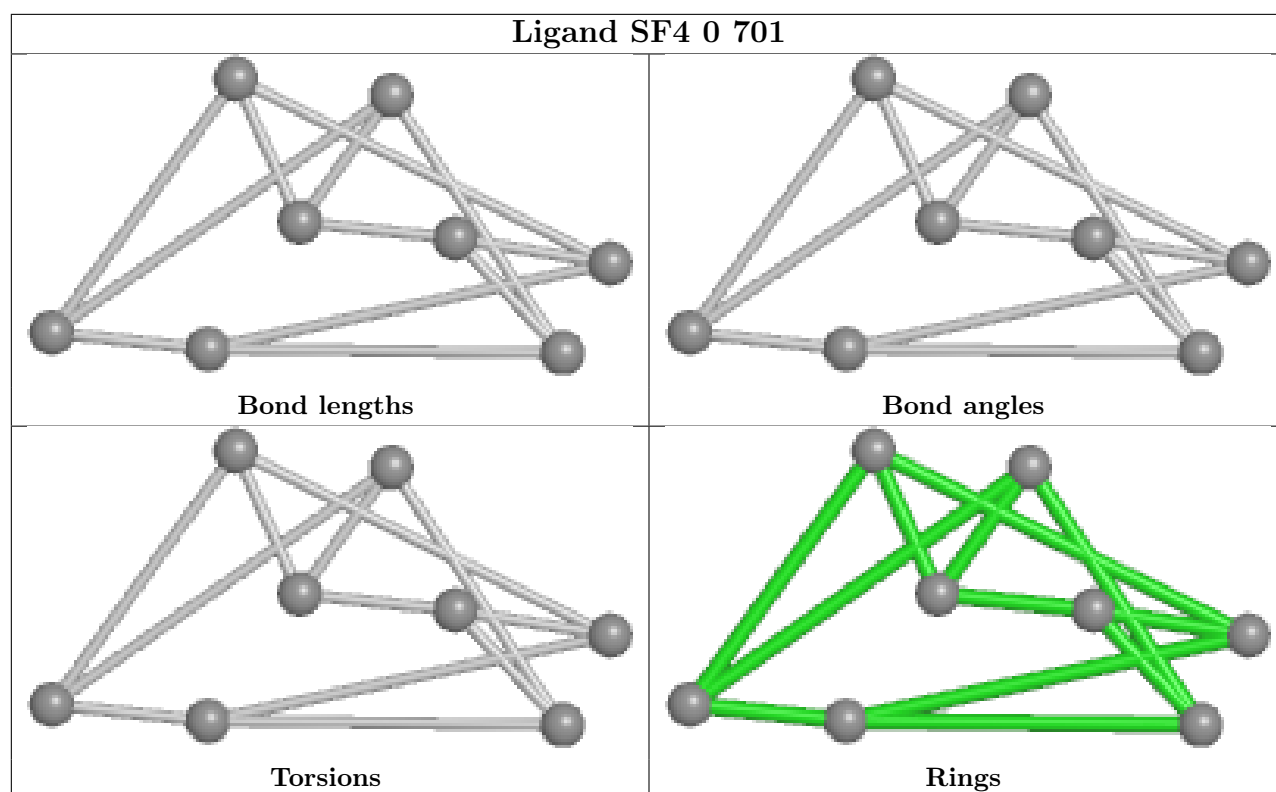
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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.

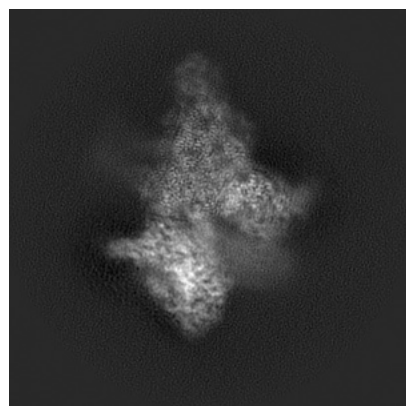
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27249. These allow visual inspection of the internal detail of the map and identification of artifacts.

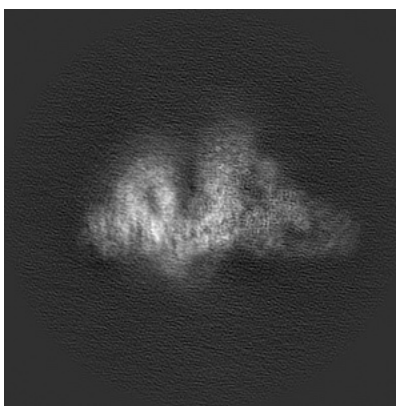
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

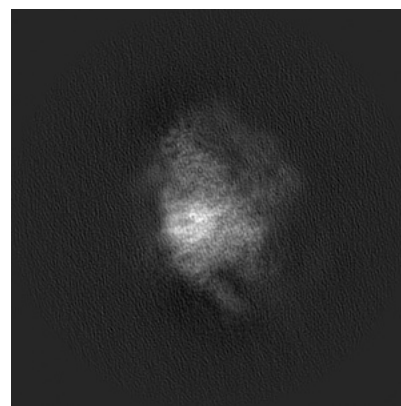
6.1.1 Primary map



X

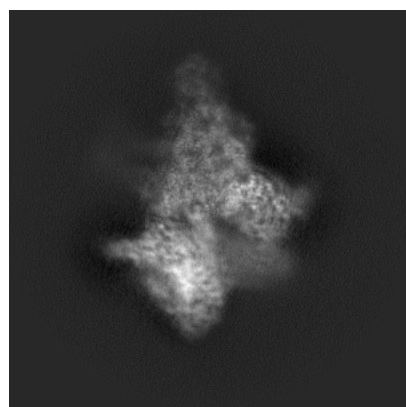


Y

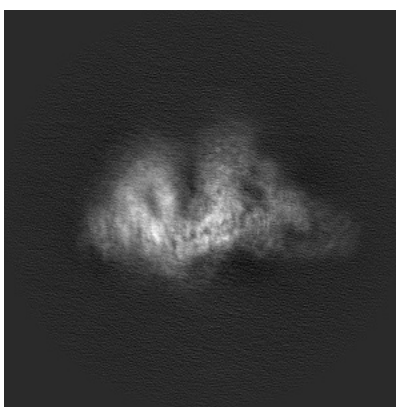


Z

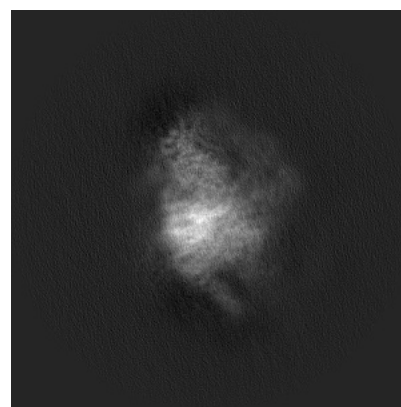
6.1.2 Raw map



X



Y

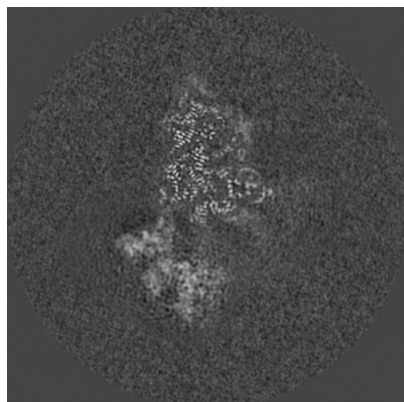


Z

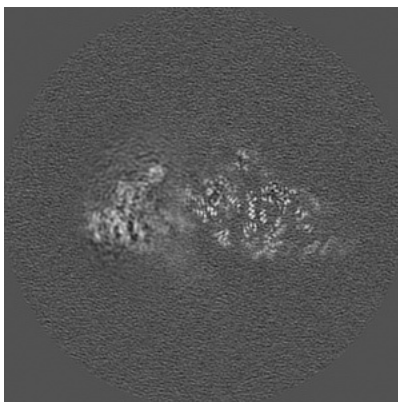
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

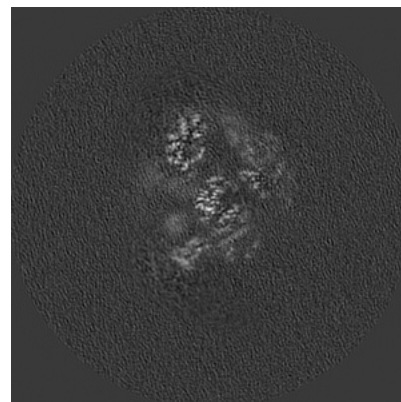
6.2.1 Primary map



X Index: 200

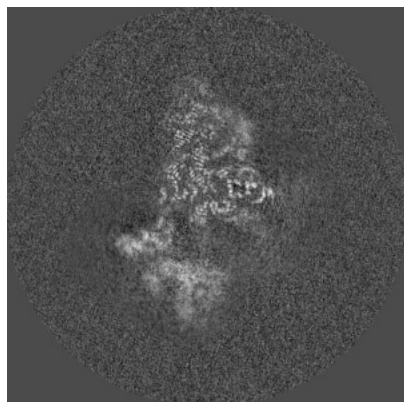


Y Index: 200

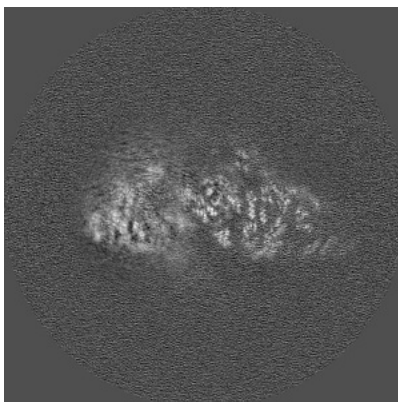


Z Index: 200

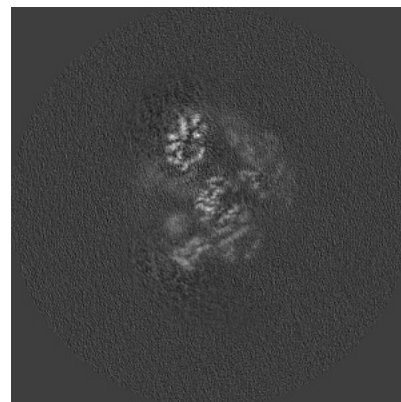
6.2.2 Raw map



X Index: 200



Y Index: 200

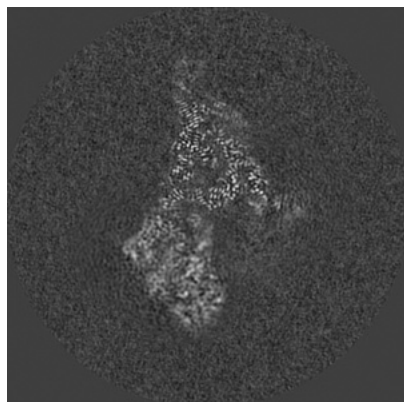


Z Index: 200

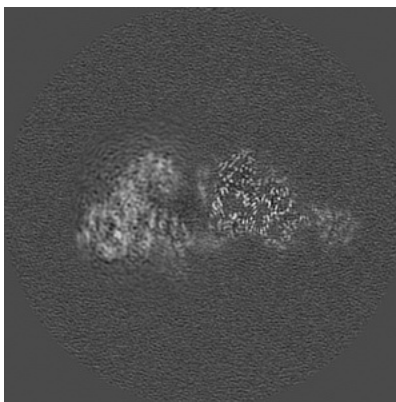
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

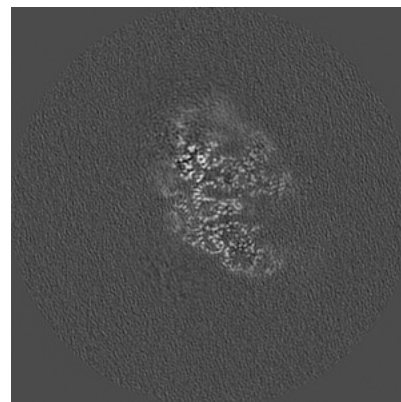
6.3.1 Primary map



X Index: 188

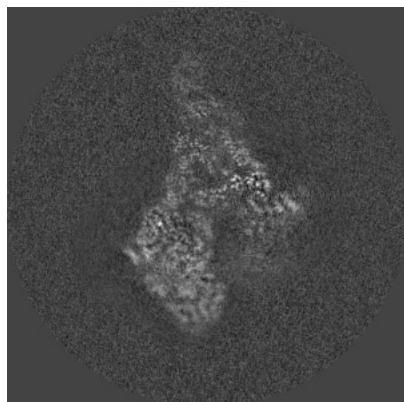


Y Index: 177

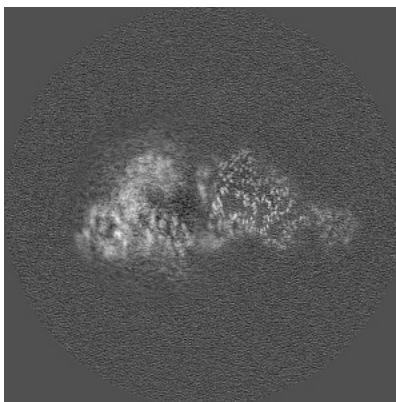


Z Index: 216

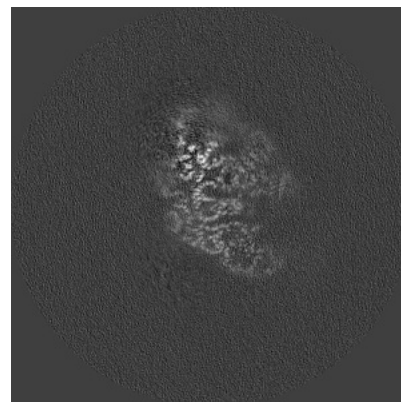
6.3.2 Raw map



X Index: 184



Y Index: 177

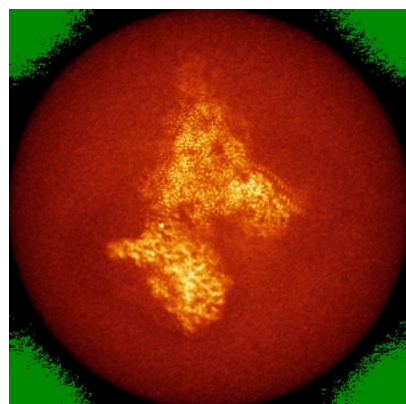


Z Index: 216

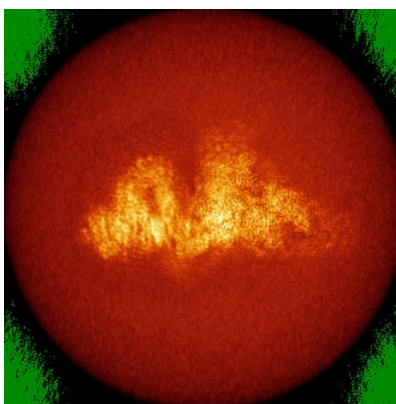
The images above show the largest variance slices of the map in three orthogonal directions.

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

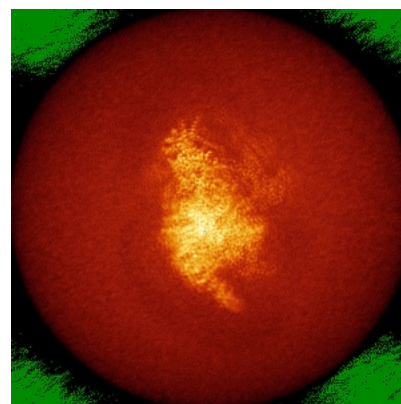
6.4.1 Primary map



X

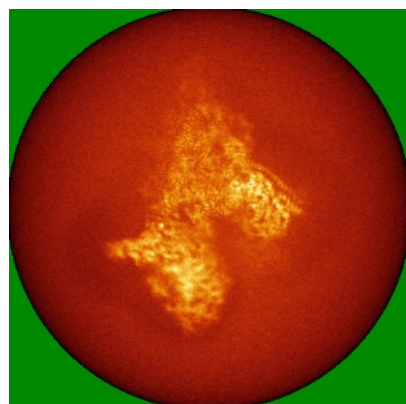


Y

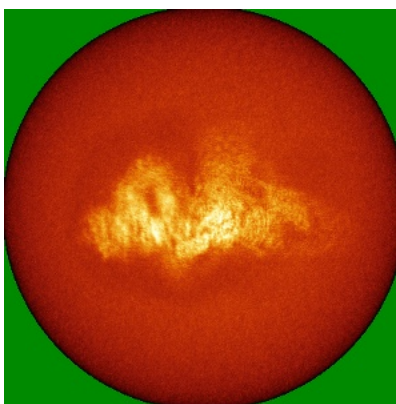


Z

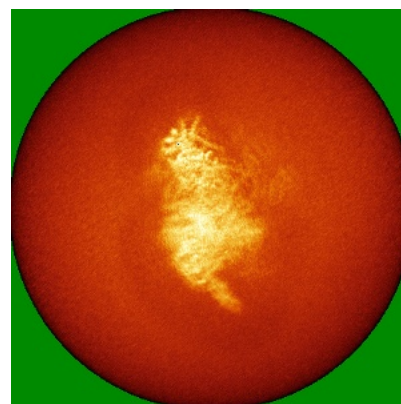
6.4.2 Raw map



X



Y

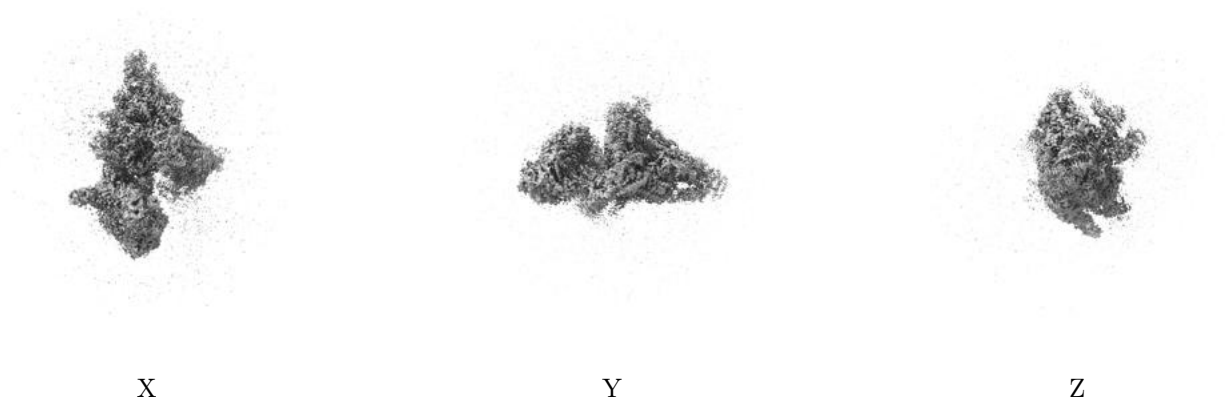


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

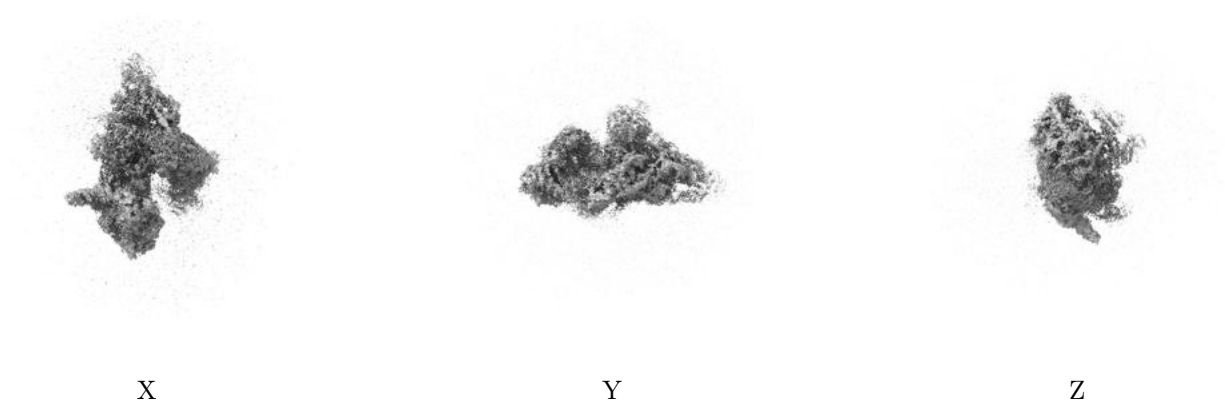
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

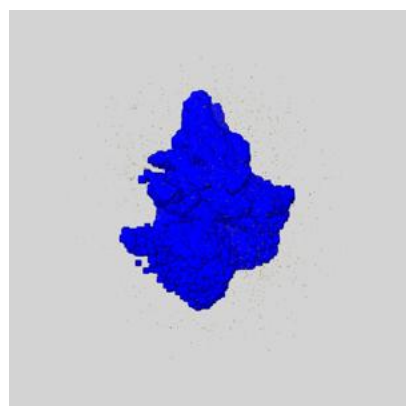
6.6 Mask visualisation [i](#)

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

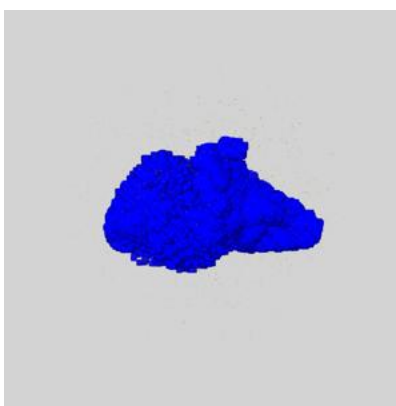
A mask typically either:

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

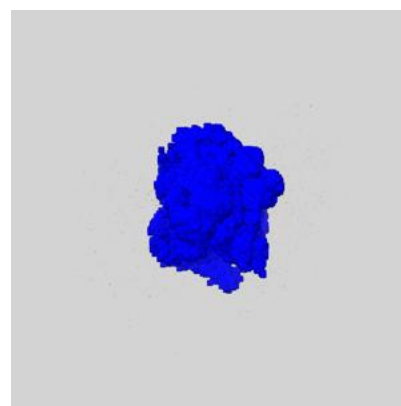
6.6.1 emd_27249_msk_1.map [i](#)



X



Y

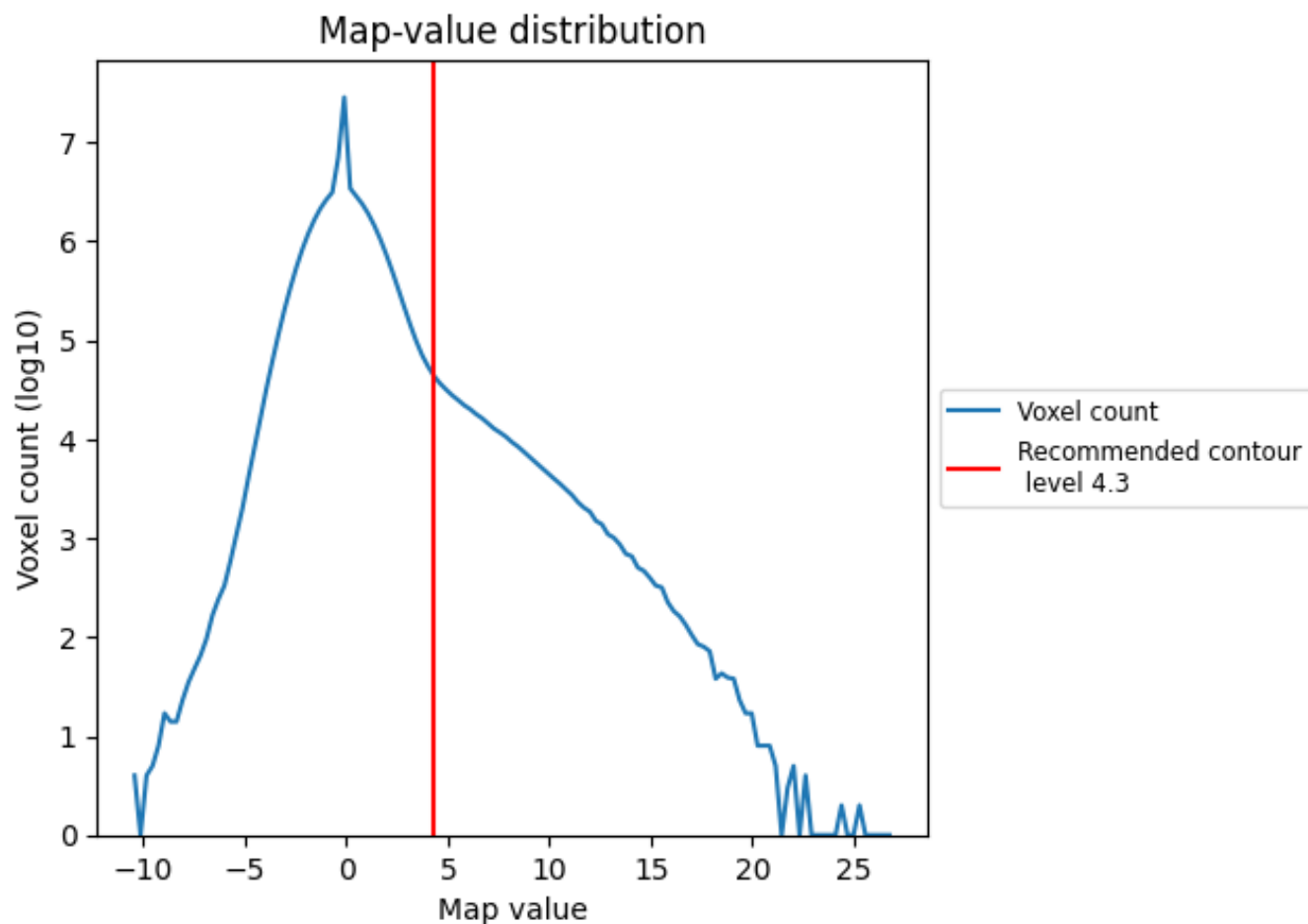


Z

7 Map analysis [i](#)

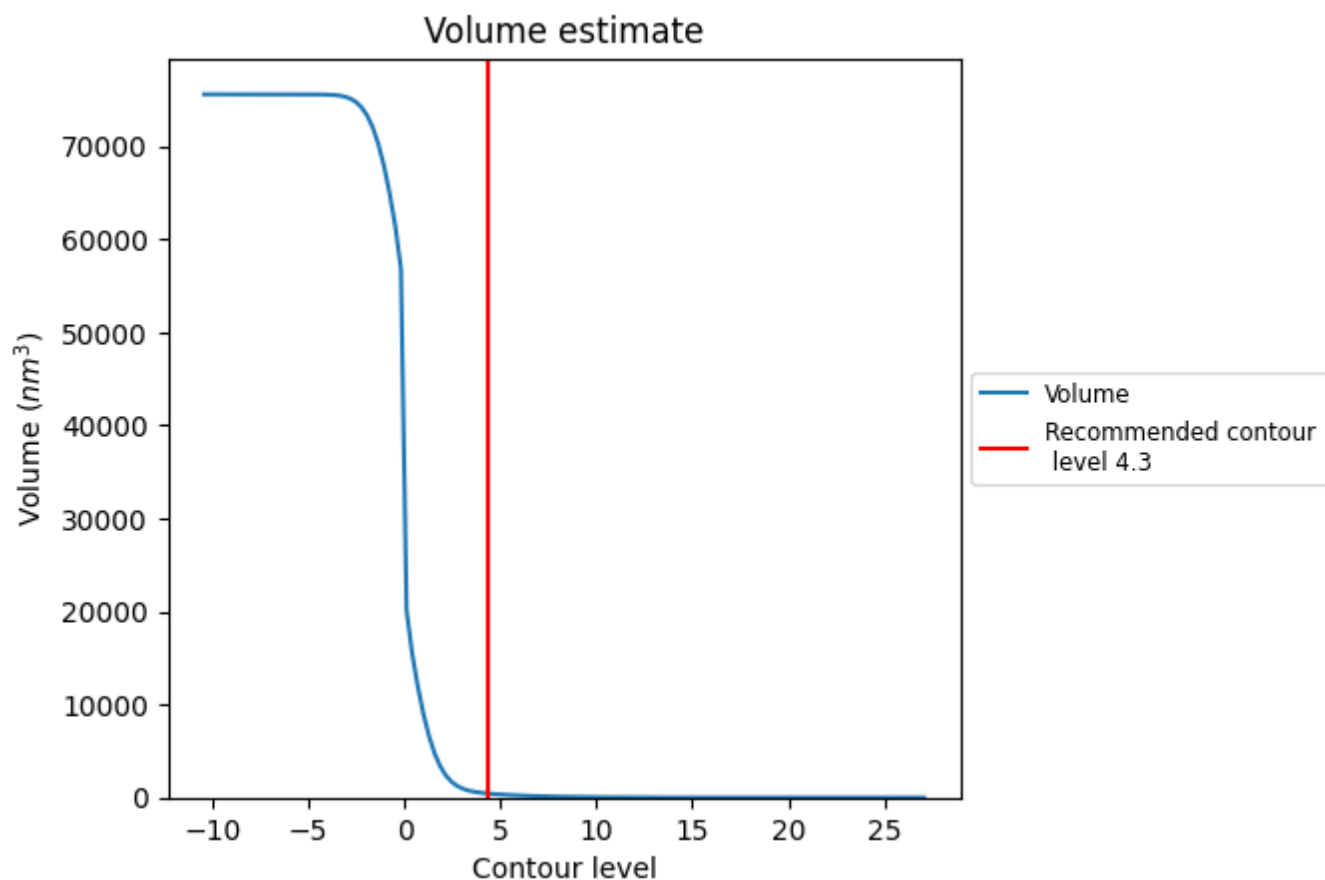
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

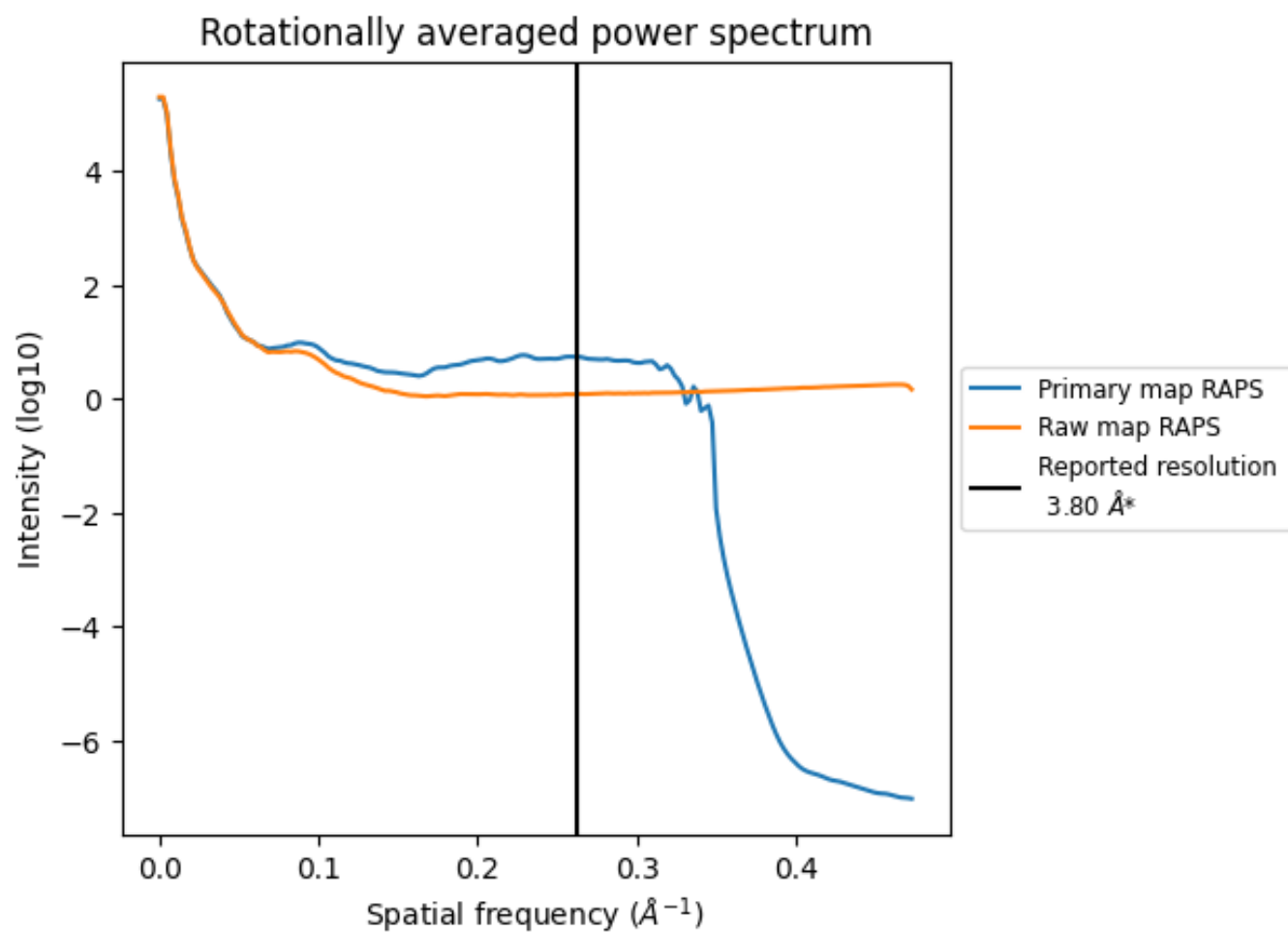
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 397 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

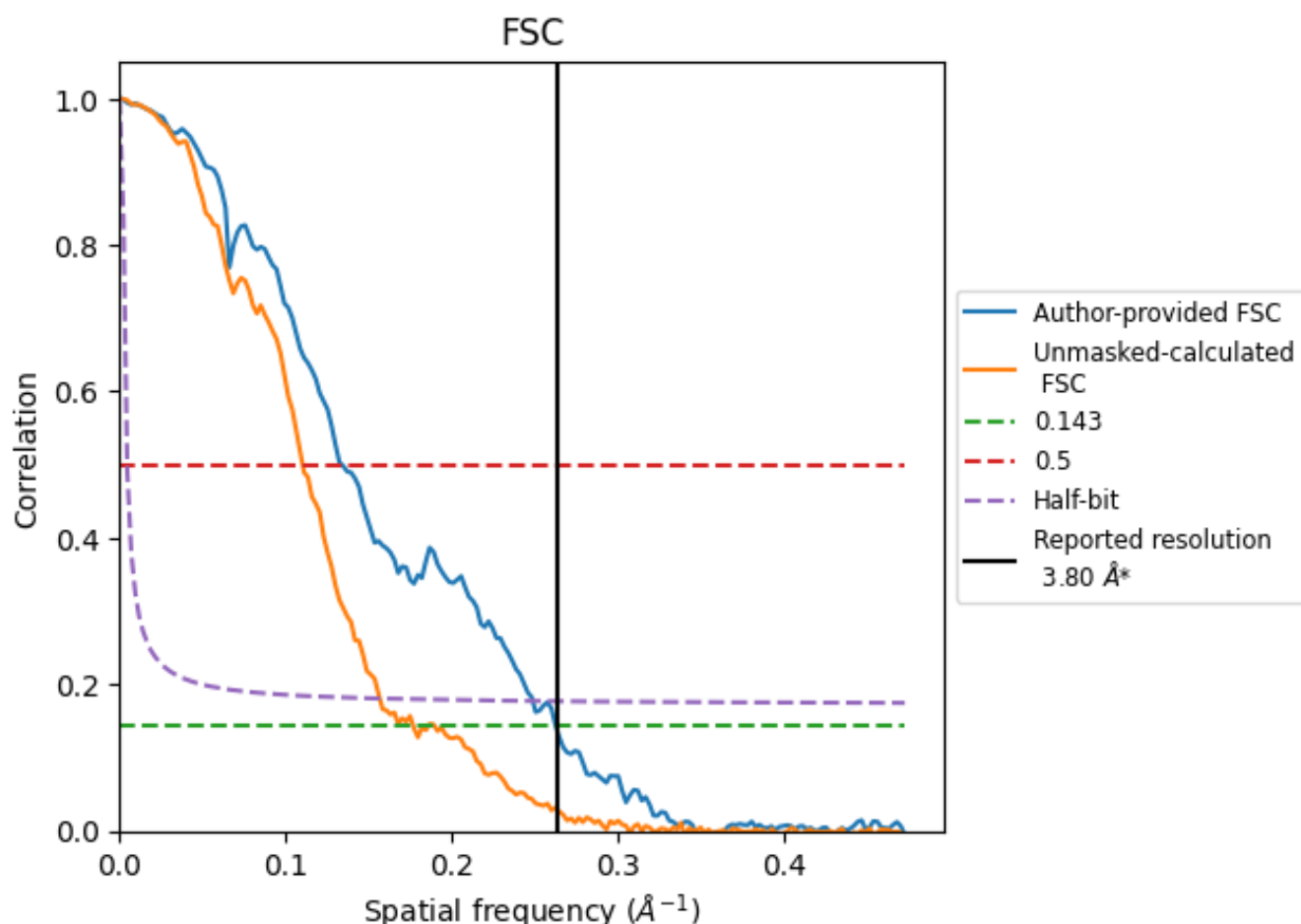


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

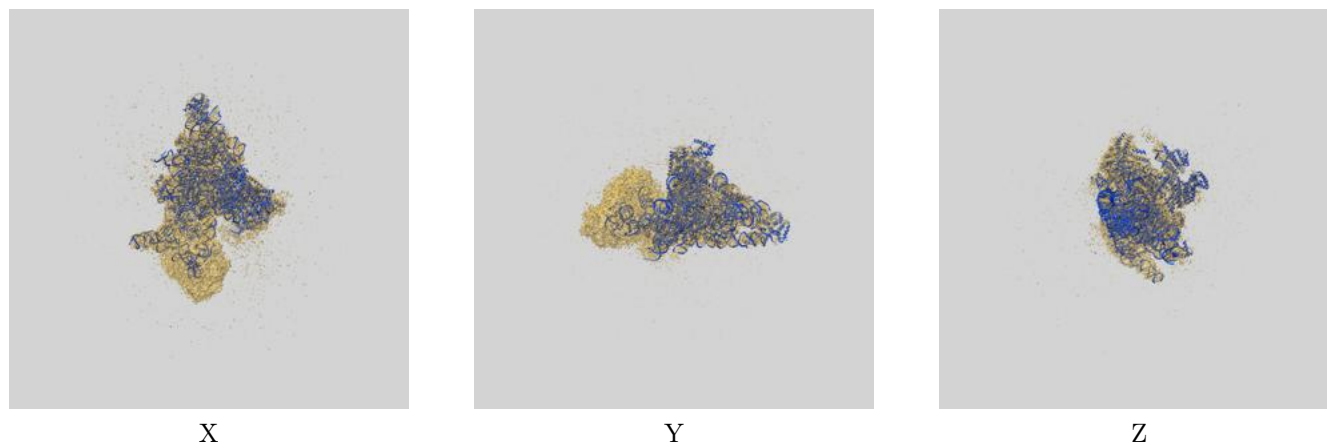
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	7.47	4.02
Unmasked-calculated*	5.65	9.07	6.38

*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 5.65 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

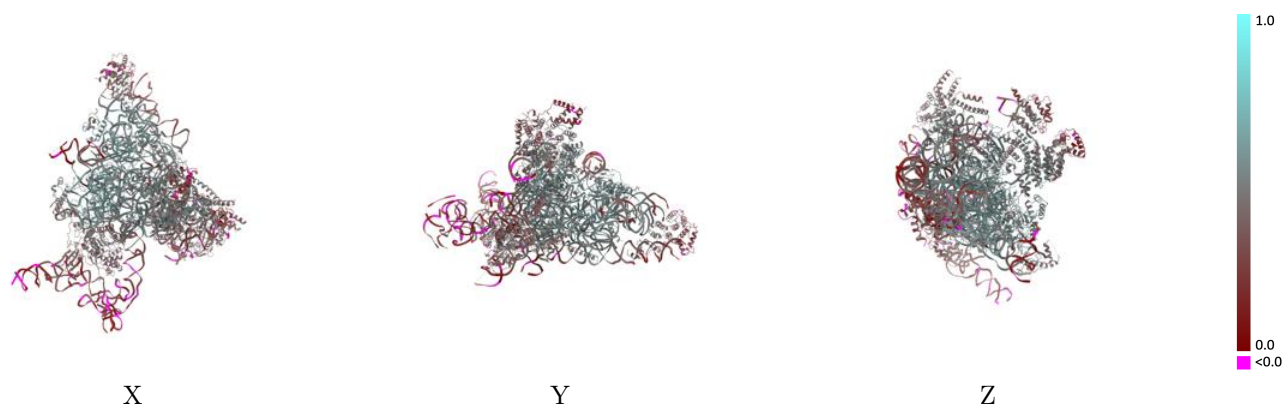
This section contains information regarding the fit between EMDB map EMD-27249 and PDB model 8D8J. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



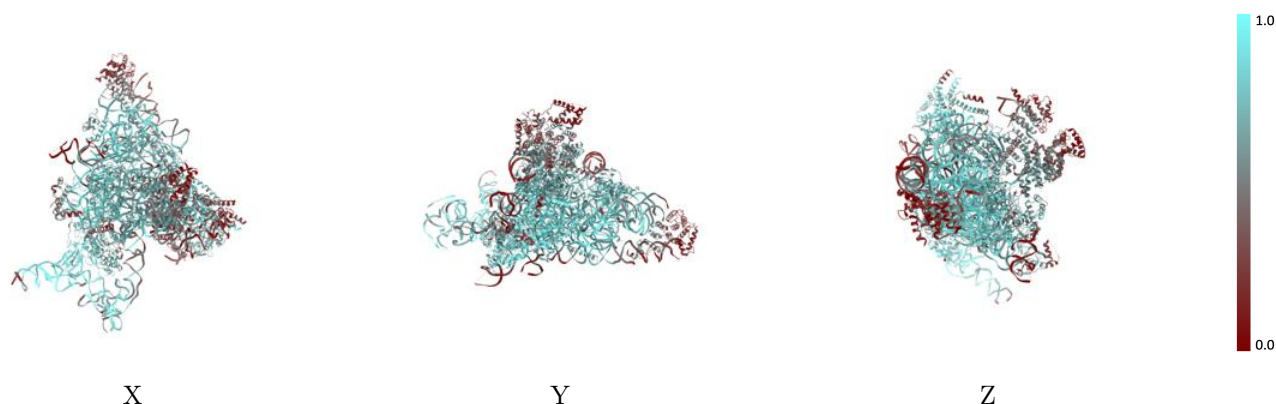
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



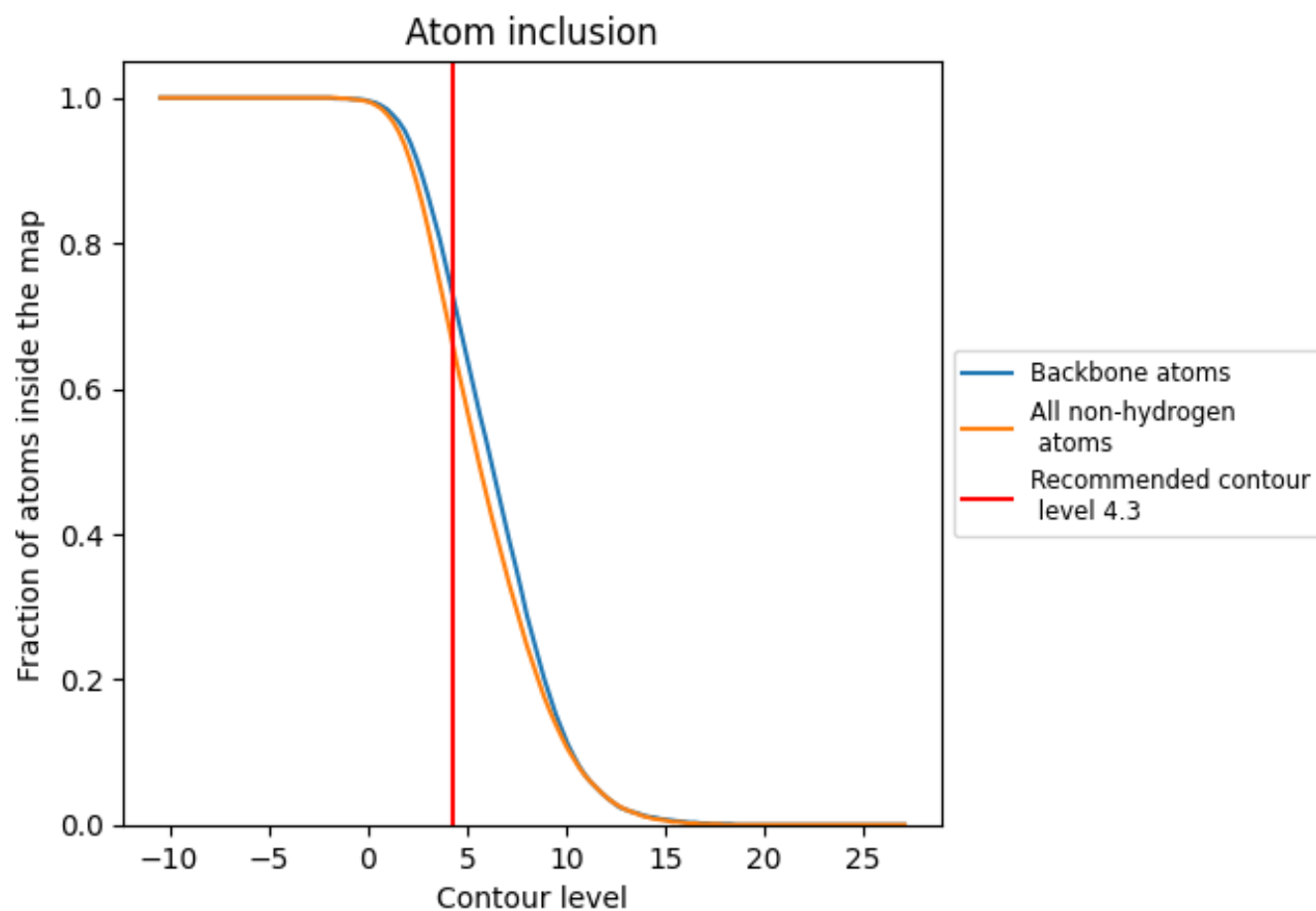
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.3).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.4250
0	 0.7450	 0.3530
2	 0.6990	 0.5360
5	 0.2640	 0.3280
6	 0.6910	 0.5520
D	 0.6950	 0.5470
E	 0.7130	 0.5090
F	 0.6620	 0.3840
H	 0.7150	 0.5390
L	 0.6560	 0.5490
O	 0.8210	 0.4800
P	 0.7420	 0.5580
Q	 0.6760	 0.4770
R	 0.5110	 0.3720
V	 0.6300	 0.4810
a	 0.7150	 0.3910
d	 0.4150	 0.4060

