



wwPDB EM Validation Summary Report ⓘ

May 25, 2024 – 07:43 AM EDT

PDB ID : 7R6K
EMDB ID : EMD-24280
Title : State E2 nucleolar 60S ribosomal intermediate - Model for Noc2/Noc3 region
Authors : Cruz, V.E.; Sekulski, K.; Peddada, N.; Erzberger, J.P.
Deposited on : 2021-06-22
Resolution : 3.17 Å (reported)
Based on initial model : 6ELZ

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

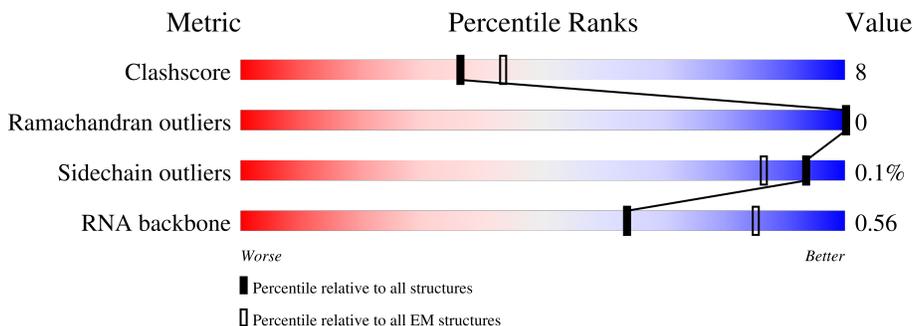
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.17 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	1	152	
2	7	204	
3	8	710	
4	A	291	
5	G	256	
6	I	663	
7	J	427	

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Mol	Chain	Length	Quality of chain
8	N	204	
9	g	121	
10	i	100	
11	l	181	
12	m	807	
13	q	618	
14	r	261	
15	w	841	
16	5	8	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 20543 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	152	3266	1457	597	1060	152	0	0

- Molecule 2 is a protein called 60S ribosomal subunit assembly/export protein LOC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	7	109	888	550	174	164	0	0

- Molecule 3 is a protein called Nucleolar complex protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	8	458	3694	2372	631	678	13	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	108	872	551	149	167	5	0	0

- Molecule 5 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	52	430	280	82	67	1	0	0

- Molecule 6 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	508	4039	2564	680	775	20	0	0

- Molecule 7 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	58	489	315	85	87	2	0	0

- Molecule 8 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	N	92	795	491	168	136	0	0

- Molecule 9 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	g	17	136	86	24	26	0	0

- Molecule 10 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	i	52	417	259	85	72	1	0	0

- Molecule 11 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	l	176	1394	896	244	247	7	0	0

- Molecule 12 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	106	827	511	135	179	2	0	0

- Molecule 13 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	q	177	1347	845	241	253	8	0	0

- Molecule 14 is a protein called Ribosome biogenesis protein NSA2.

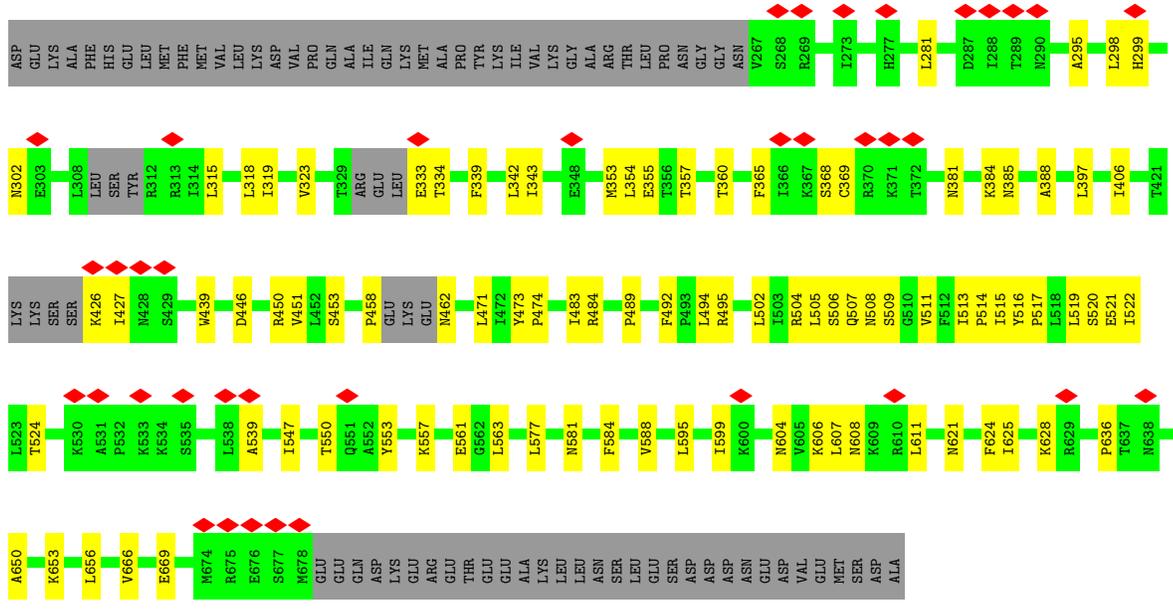
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	r	18	148	92	31	24	1	0	0

- Molecule 15 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

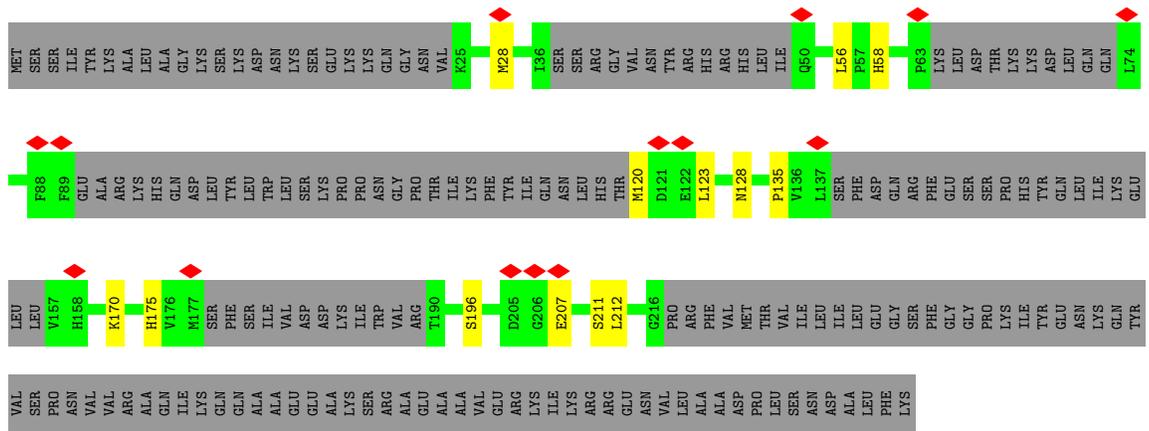
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	w	214	1726	1067	314	339	6	0	0

- Molecule 16 is a protein called RRP17 isoform 1.

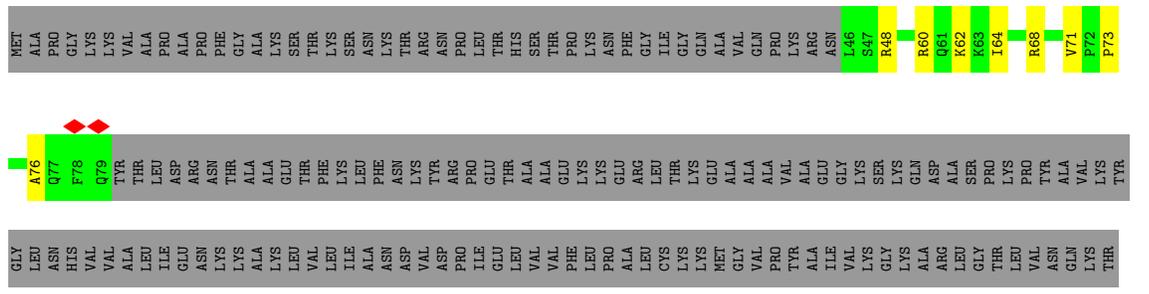
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	5	8	75	46	16	13	0	0



• Molecule 4: Ribosome biogenesis protein BRX1

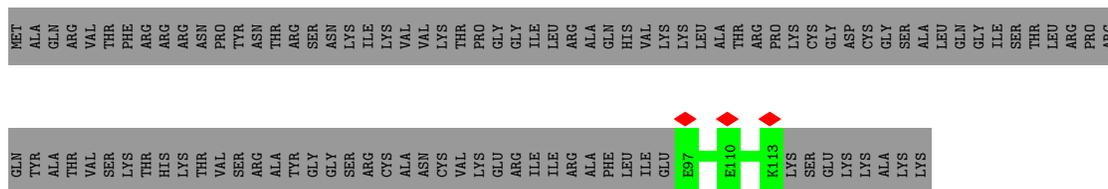


• Molecule 5: 60S ribosomal protein L8-A





• Molecule 9: 60S ribosomal protein L34-A



• Molecule 10: 60S ribosomal protein L36-A



• Molecule 11: 60S ribosome subunit biogenesis protein NIP7



• Molecule 12: Ribosome biogenesis protein ERB1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size (\AA)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.20	0/3645	0.73	0/5653
2	7	0.24	0/895	0.53	0/1194
3	8	0.25	0/3759	0.48	0/5066
4	A	0.27	0/885	0.47	0/1185
5	G	0.25	0/439	0.50	0/586
6	I	0.24	0/4099	0.46	0/5529
7	J	0.26	0/498	0.49	0/661
8	N	0.24	0/803	0.58	0/1064
9	g	0.24	0/135	0.37	0/177
10	i	0.23	0/419	0.54	0/555
11	l	0.26	0/1425	0.51	0/1922
12	m	0.24	0/840	0.45	0/1141
13	q	0.25	0/1367	0.51	0/1852
14	r	0.25	0/150	0.65	0/198
15	w	0.24	0/1748	0.45	0/2329
16	5	0.21	0/75	0.57	0/98
All	All	0.24	0/21182	0.54	0/29210

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 [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	1	3266	0	1649	52	0
2	7	888	0	944	12	0
3	8	3694	0	3806	83	0
4	A	872	0	851	11	0
5	G	430	0	462	8	0
6	I	4039	0	4144	34	0
7	J	489	0	497	17	0
8	N	795	0	813	38	0
9	g	136	0	153	0	0
10	i	417	0	454	0	0
11	l	1394	0	1426	0	0
12	m	827	0	795	0	0
13	q	1347	0	1366	0	0
14	r	148	0	157	0	0
15	w	1726	0	1711	0	0
16	5	75	0	77	1	0
All	All	20543	0	19305	222	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 8.

The worst 5 of 222 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)
3:8:513:ILE:CG2	3:8:515:ILE:HG13	1.61	1.30
8:N:27:VAL:HB	8:N:122:ASN:HD21	1.11	1.15
3:8:607:LEU:HD21	3:8:611:LEU:HD11	1.25	1.10
3:8:513:ILE:HG22	3:8:515:ILE:HG13	1.03	0.99
3:8:607:LEU:CD2	3:8:611:LEU:HD11	1.94	0.95

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	7	105/204 (52%)	97 (92%)	8 (8%)	0	100	100
3	8	446/710 (63%)	420 (94%)	26 (6%)	0	100	100
4	A	96/291 (33%)	91 (95%)	5 (5%)	0	100	100
5	G	48/256 (19%)	48 (100%)	0	0	100	100
6	I	504/663 (76%)	485 (96%)	19 (4%)	0	100	100
7	J	54/427 (13%)	54 (100%)	0	0	100	100
8	N	82/204 (40%)	79 (96%)	3 (4%)	0	100	100
9	g	15/121 (12%)	15 (100%)	0	0	100	100
10	i	50/100 (50%)	50 (100%)	0	0	100	100
11	l	174/181 (96%)	164 (94%)	10 (6%)	0	100	100
12	m	104/807 (13%)	100 (96%)	4 (4%)	0	100	100
13	q	171/618 (28%)	164 (96%)	7 (4%)	0	100	100
14	r	16/261 (6%)	16 (100%)	0	0	100	100
15	w	206/841 (24%)	199 (97%)	7 (3%)	0	100	100
16	5	6/8 (75%)	6 (100%)	0	0	100	100
All	All	2077/5692 (36%)	1988 (96%)	89 (4%)	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	7	97/181 (54%)	97 (100%)	0	100	100
3	8	416/647 (64%)	416 (100%)	0	100	100
4	A	100/263 (38%)	100 (100%)	0	100	100
5	G	45/208 (22%)	45 (100%)	0	100	100
6	I	461/602 (77%)	460 (100%)	1 (0%)	93	98
7	J	54/383 (14%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	N	83/176 (47%)	83 (100%)	0	100	100
9	g	15/103 (15%)	15 (100%)	0	100	100
10	i	43/82 (52%)	43 (100%)	0	100	100
11	l	151/156 (97%)	151 (100%)	0	100	100
12	m	95/723 (13%)	95 (100%)	0	100	100
13	q	148/535 (28%)	148 (100%)	0	100	100
14	r	16/229 (7%)	16 (100%)	0	100	100
15	w	181/745 (24%)	180 (99%)	1 (1%)	86	94
16	5	8/8 (100%)	8 (100%)	0	100	100
All	All	1913/5041 (38%)	1911 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I	284	ARG
15	w	694	ASN

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

Mol	Chain	Res	Type
3	8	621	ASN
8	N	122	ASN
8	N	123	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	139/152 (91%)	30 (21%)	2 (1%)

5 of 30 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	40	A
1	1	42	C
1	1	43	A
1	1	269	G
1	1	277	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	908	G
1	1	2603	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	13

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1558:A	O3'	2408:U	P	104.38
1	1	297:G	O3'	818:C	P	80.85
1	1	926:A	O3'	1538:G	P	29.62
1	1	56:G	O3'	268:A	P	29.31
1	1	896:A	O3'	907:G	P	25.78

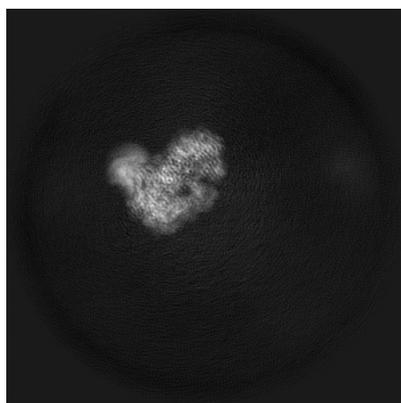
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24280. These allow visual inspection of the internal detail of the map and identification of artifacts.

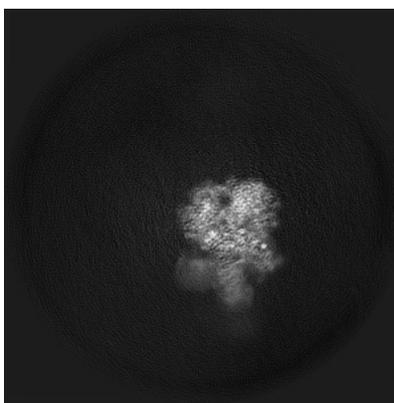
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

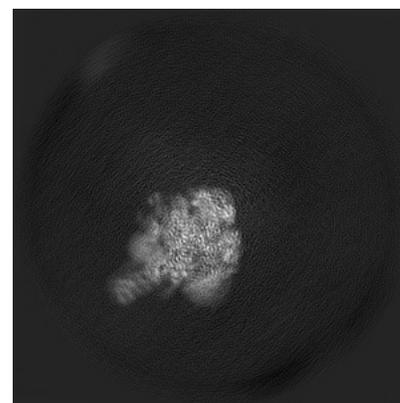
6.1.1 Primary map



X

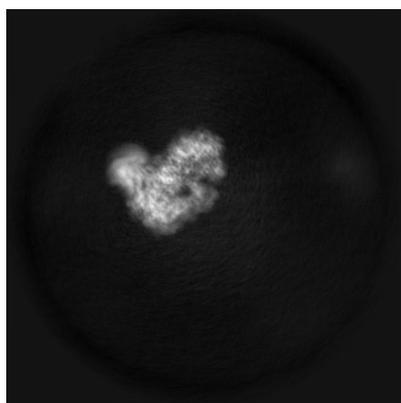


Y

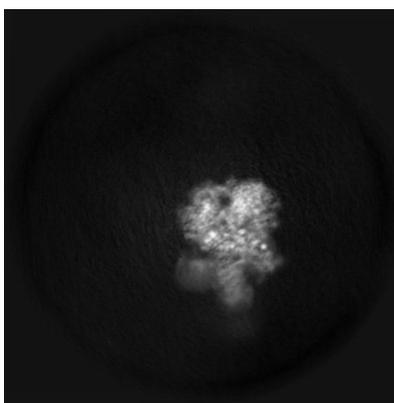


Z

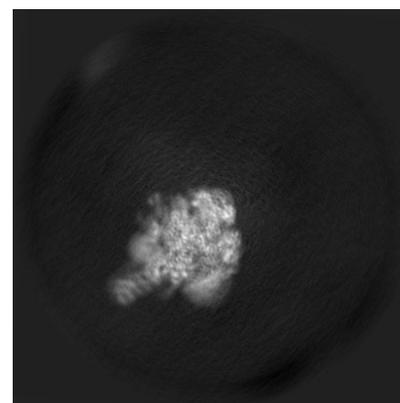
6.1.2 Raw map



X



Y

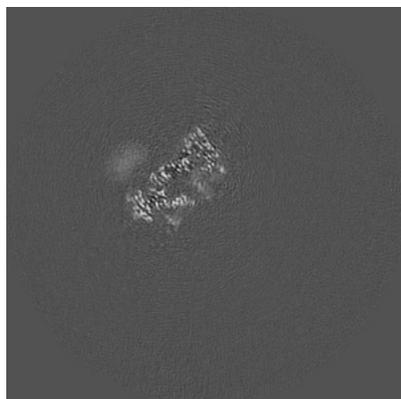


Z

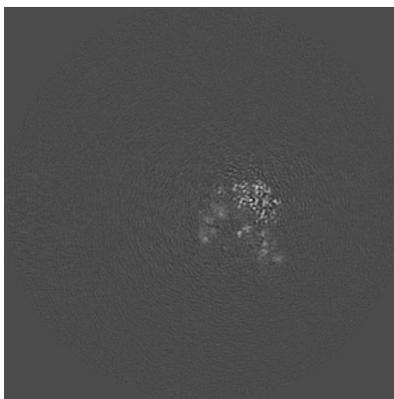
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

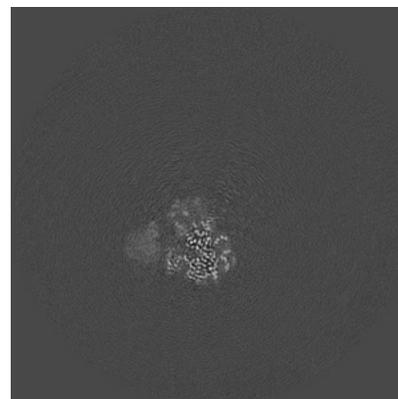
6.2.1 Primary map



X Index: 210

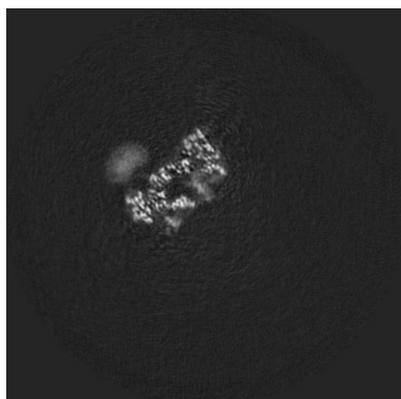


Y Index: 210

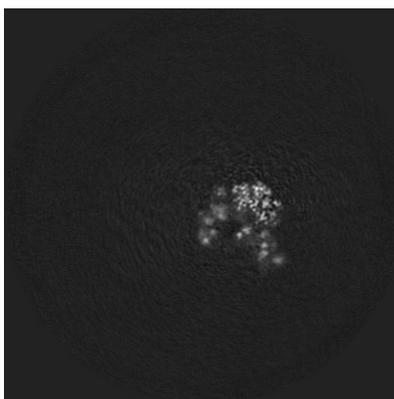


Z Index: 210

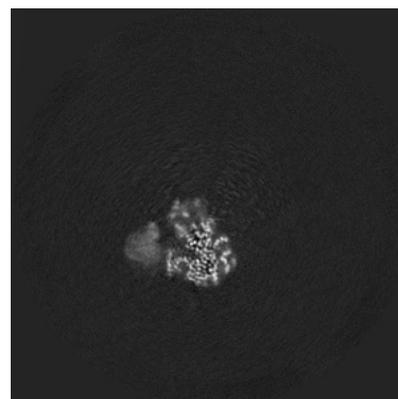
6.2.2 Raw map



X Index: 210



Y Index: 210

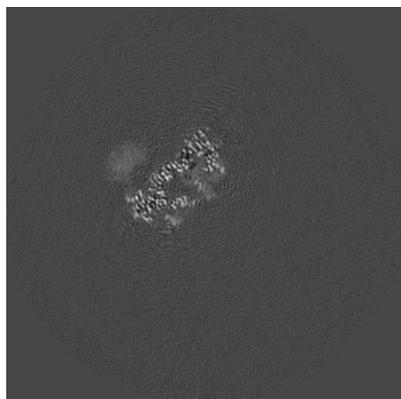


Z Index: 210

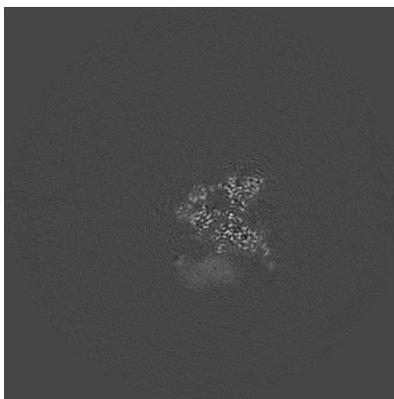
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

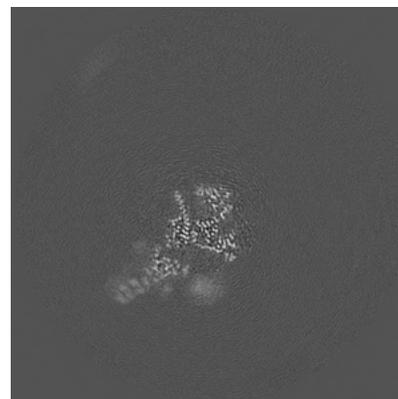
6.3.1 Primary map



X Index: 209

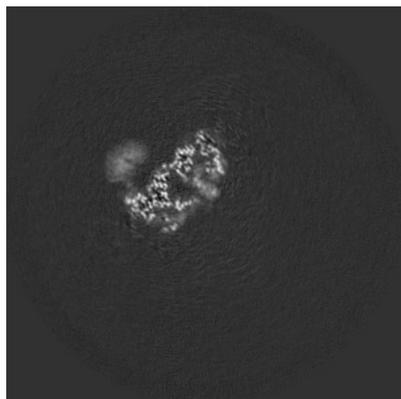


Y Index: 174

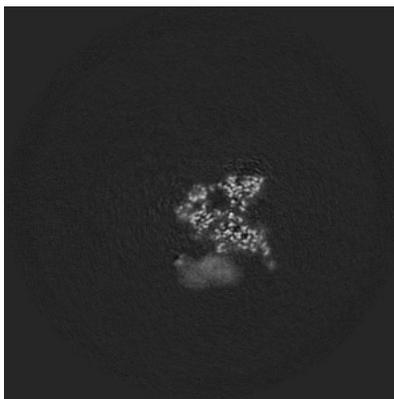


Z Index: 250

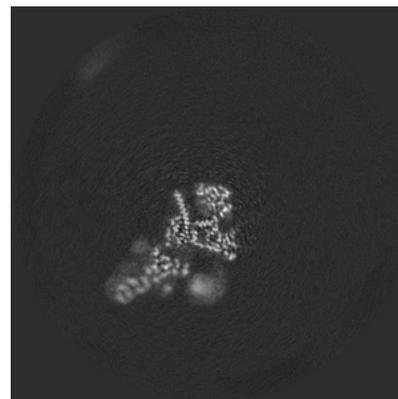
6.3.2 Raw map



X Index: 206



Y Index: 174

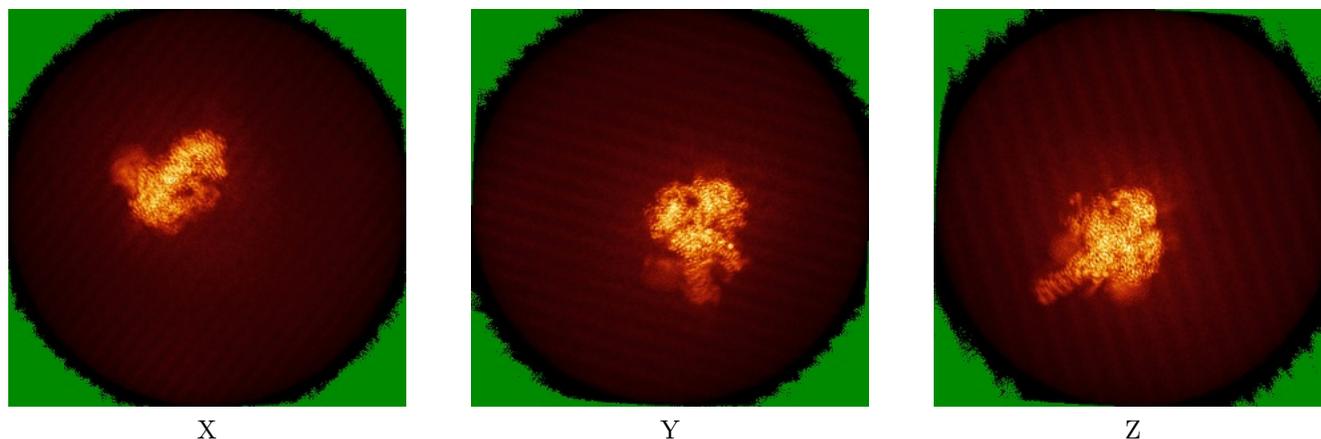


Z Index: 249

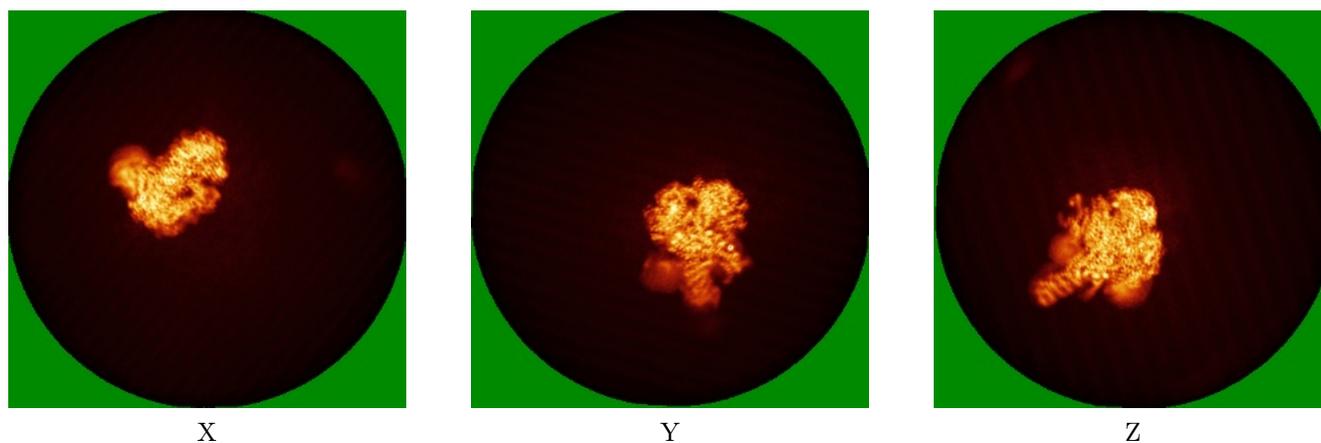
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



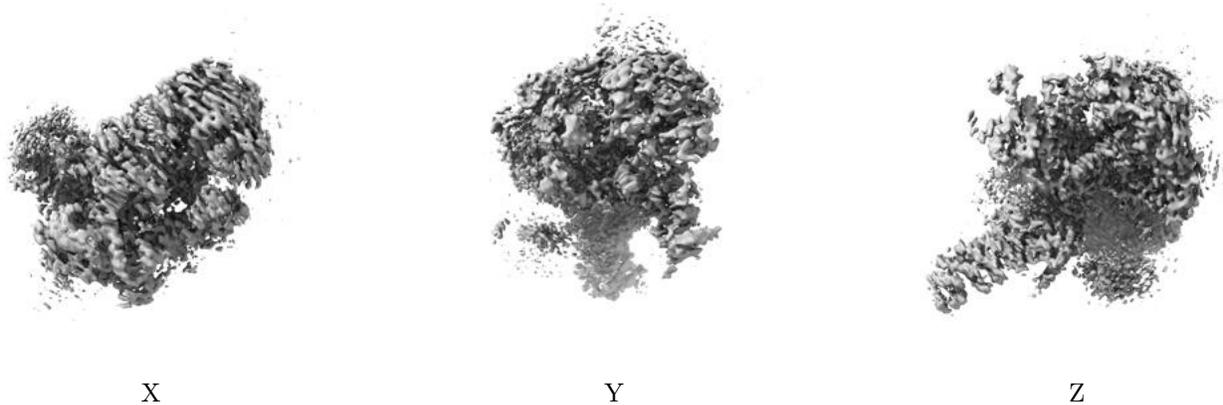
6.4.2 Raw map



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.

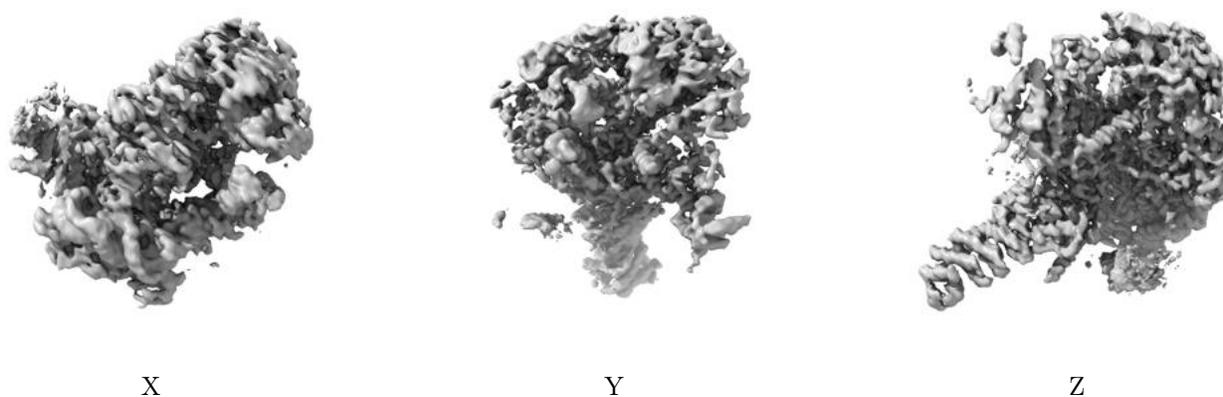
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. 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.

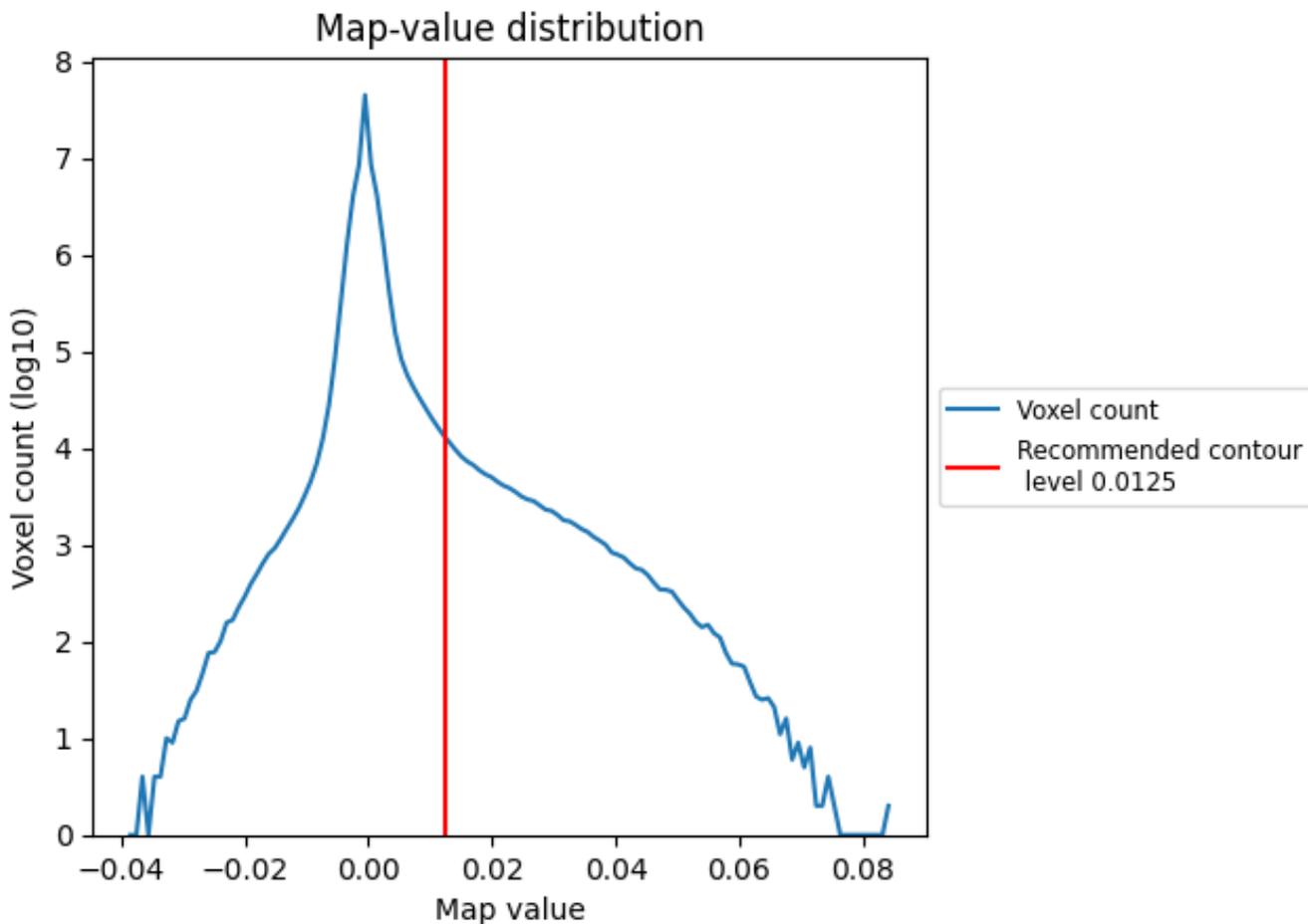
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

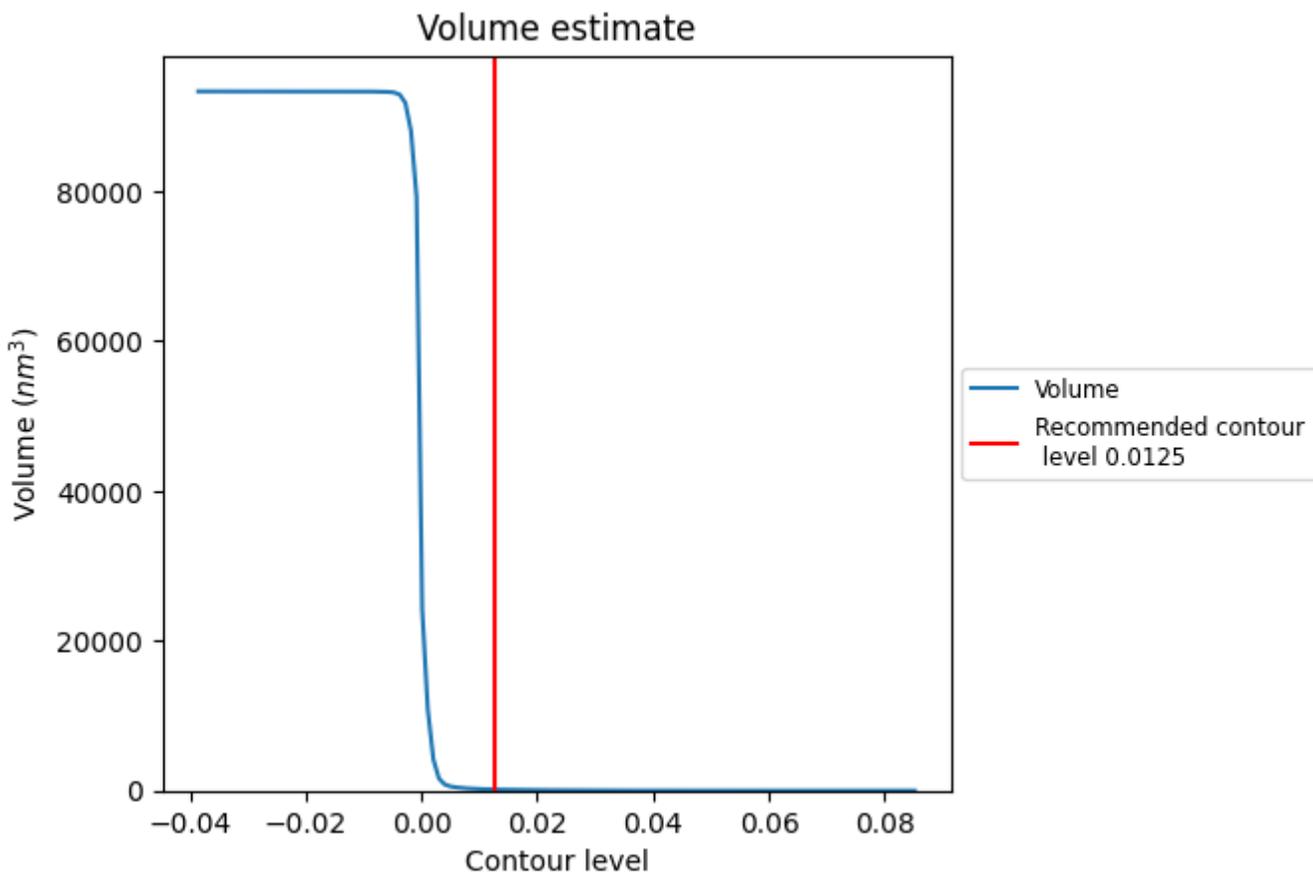
This section contains the results of statistical analysis of the map.

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.

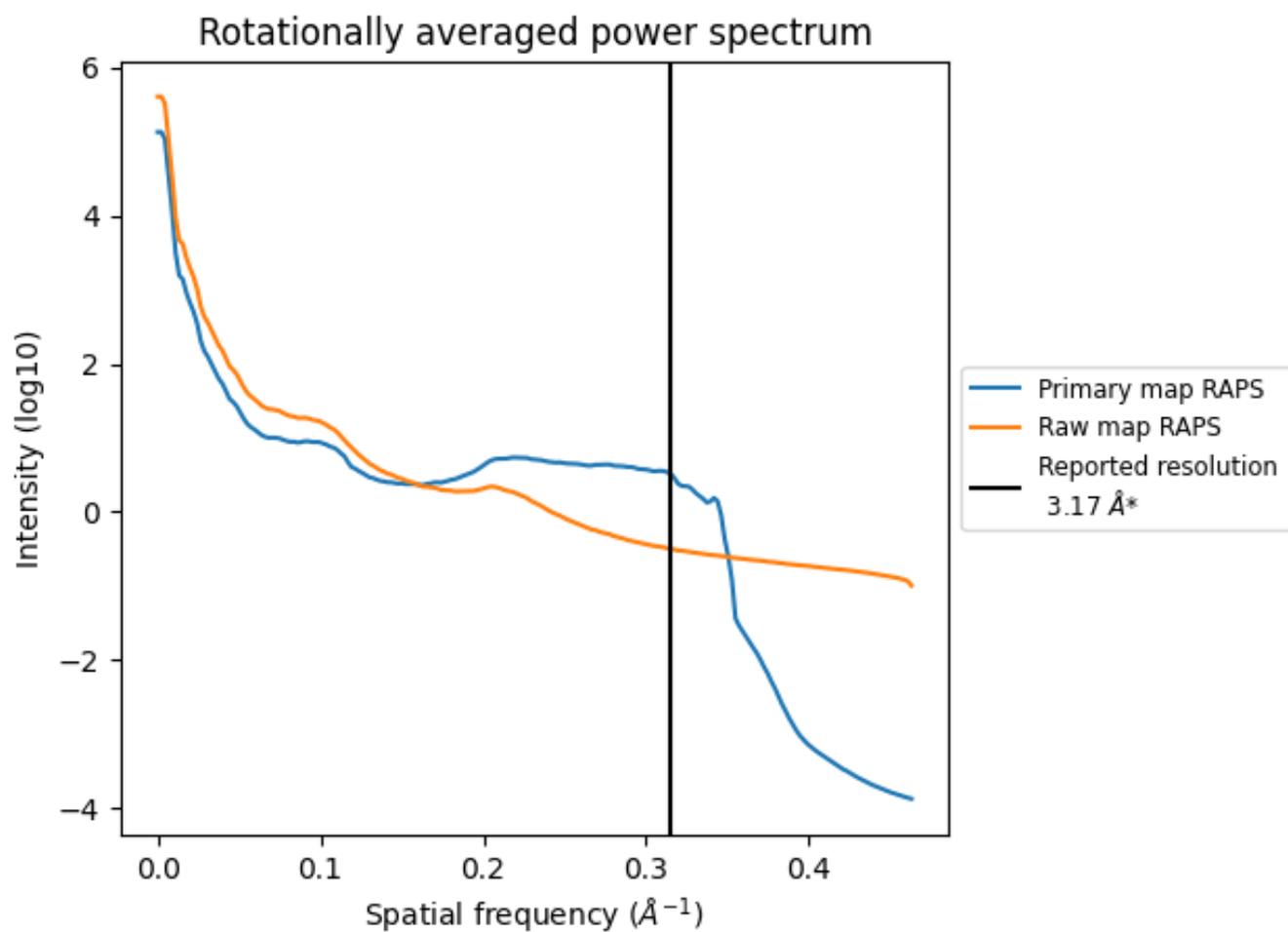
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 138 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](#)

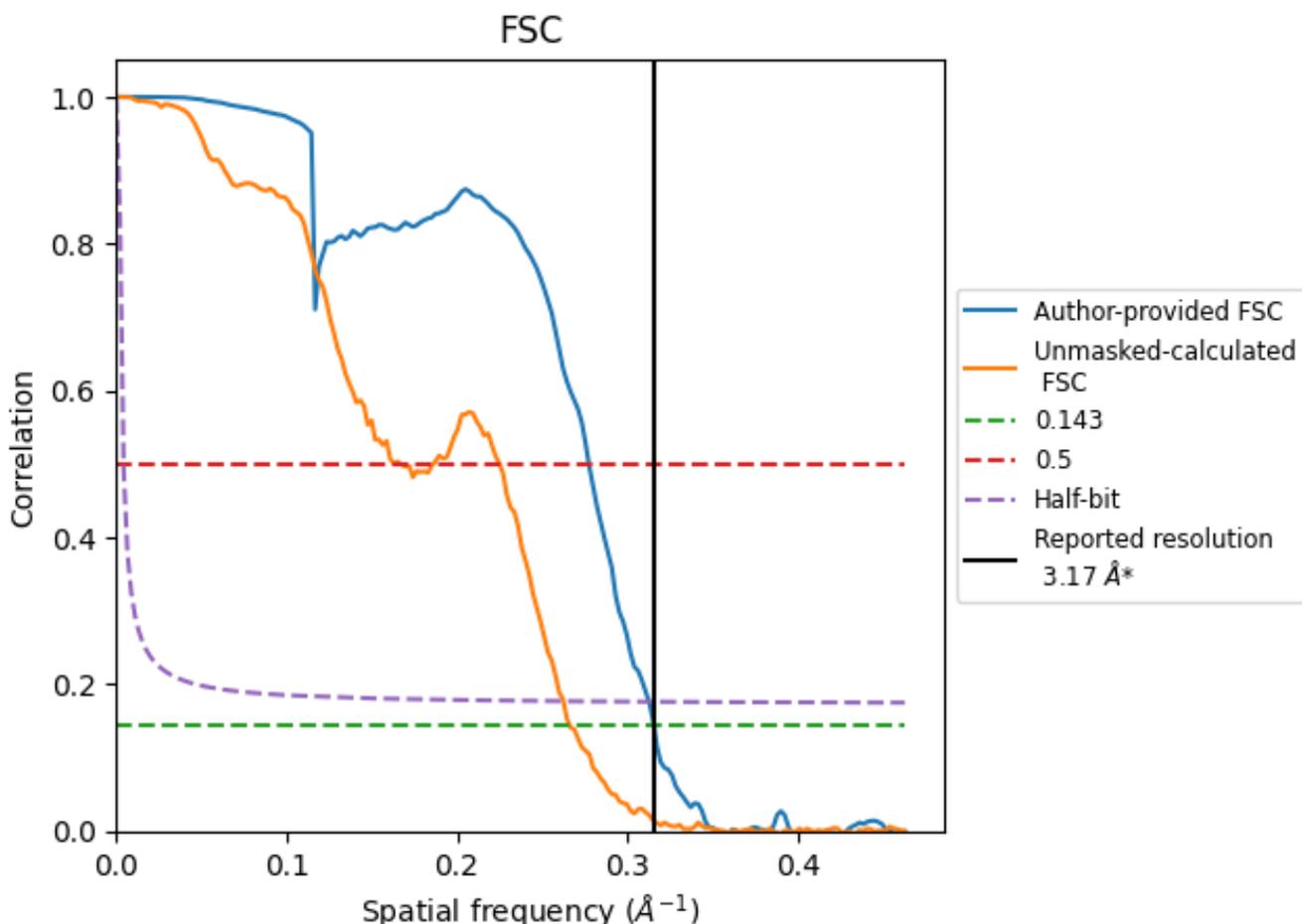


*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

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 0.315 Å⁻¹

8.2 Resolution estimates [i](#)

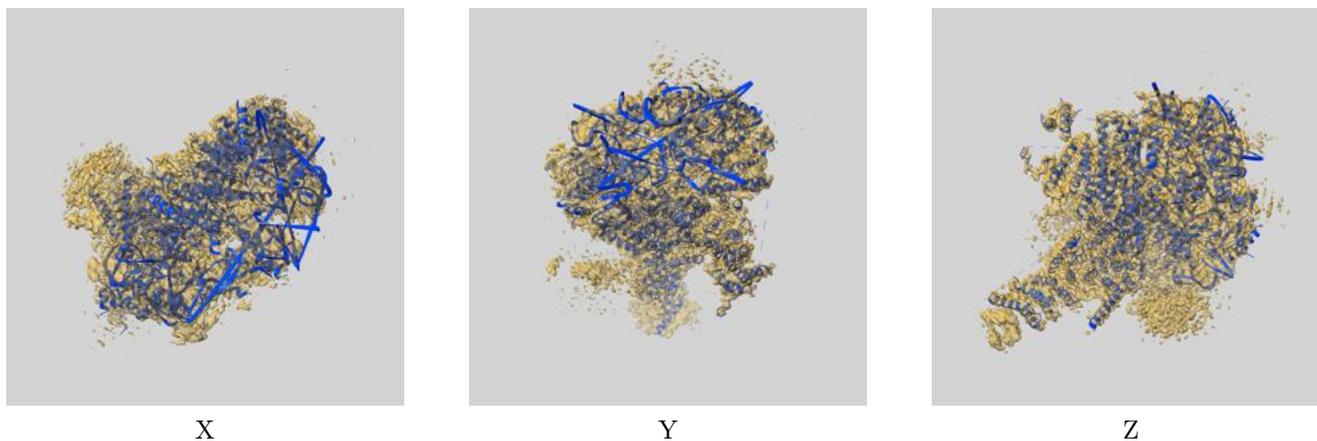
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.60	3.20
Unmasked-calculated*	3.76	6.00	3.81

*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 3.76 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

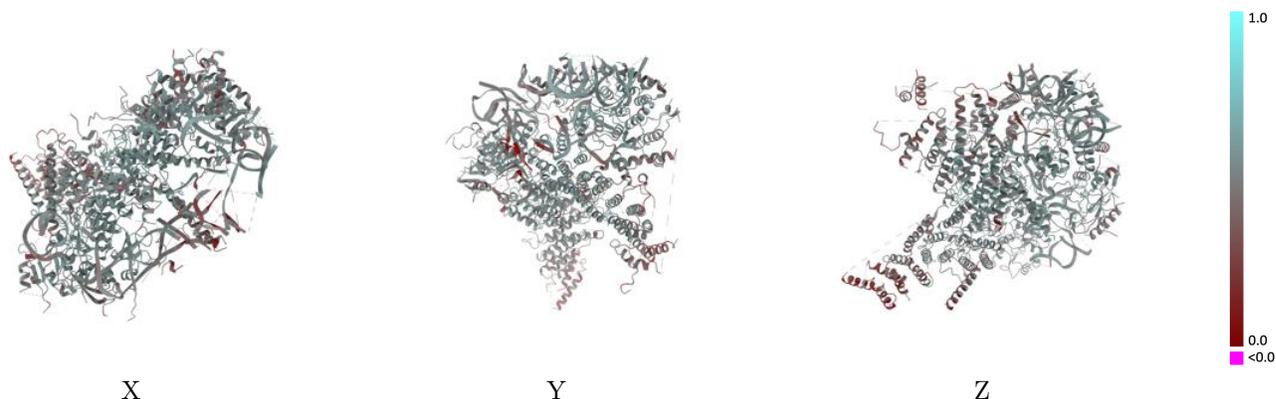
This section contains information regarding the fit between EMDB map EMD-24280 and PDB model 7R6K. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



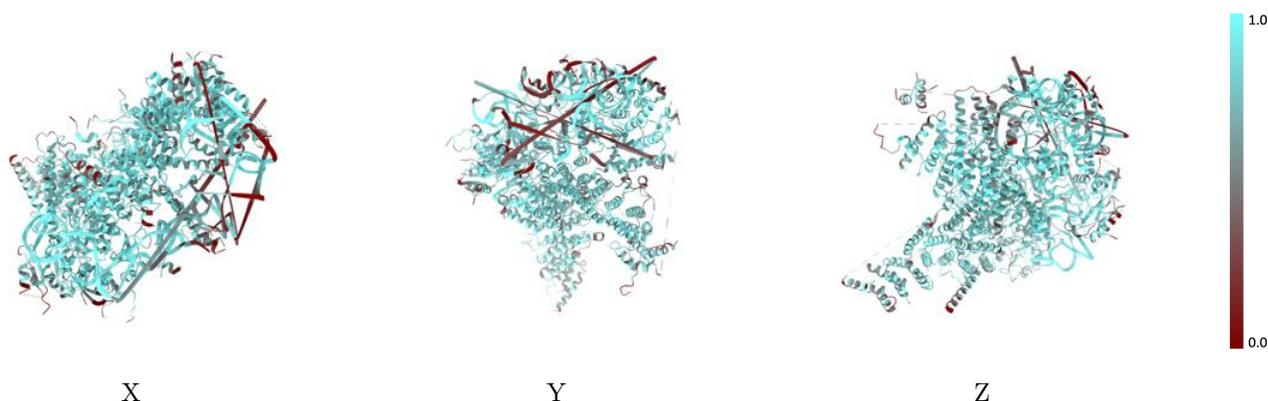
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



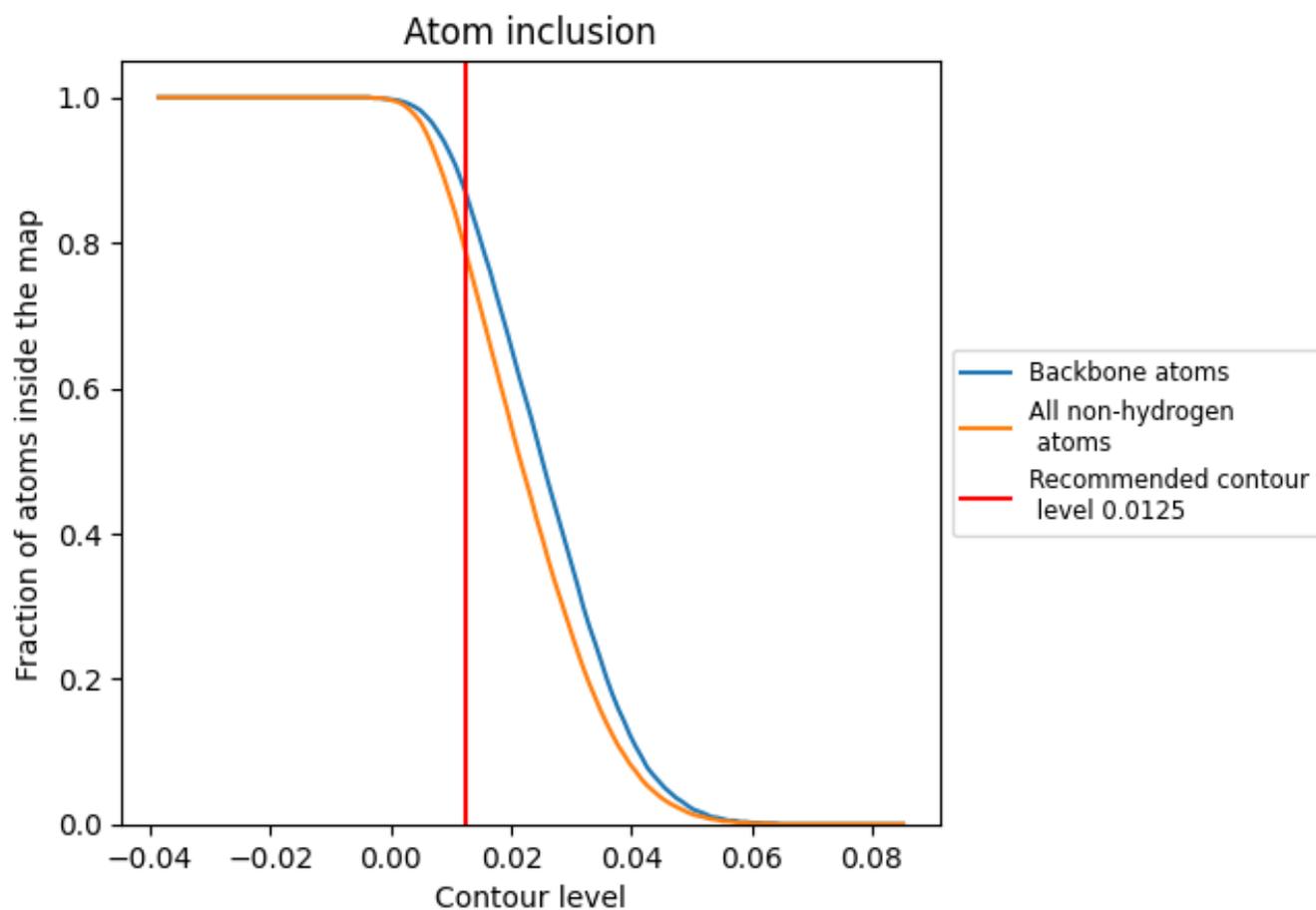
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.4950
1	 0.7640	 0.4800
5	 0.4140	 0.3540
7	 0.7930	 0.5160
8	 0.7540	 0.4390
A	 0.7500	 0.5150
G	 0.7150	 0.4810
I	 0.8500	 0.5180
J	 0.6650	 0.4900
N	 0.7950	 0.5200
g	 0.5510	 0.3640
i	 0.7670	 0.5070
l	 0.8890	 0.5490
m	 0.8840	 0.5490
q	 0.7590	 0.5160
r	 0.7360	 0.4520
w	 0.7440	 0.4890

