



wwPDB EM Validation Summary Report ⓘ

Jan 29, 2024 – 10:13 AM EST

PDB ID : 8SPU
EMDB ID : EMD-40686
Title : Structure of ESRRB nucleosome bound OCT4 at site c
Authors : Lian, T.; Guan, R.; Bai, Y.
Deposited on : 2023-05-03
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
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) : 2.36

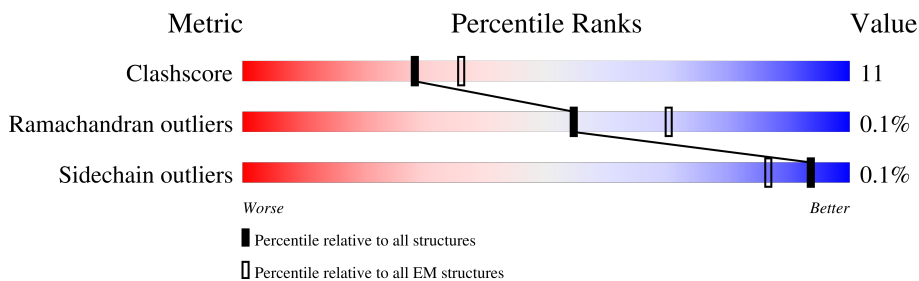
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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

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	J	168	
2	I	168	
3	L	550	
4	A	136	
4	E	136	
5	B	103	
5	F	103	
6	C	129	

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Mol	Chain	Length	Quality of chain
6	G	129	 60% 19% 17%
7	D	126	 64% 10% 25%
7	H	126	 66% 9% 25%
8	K	265	 71% 14% 15%
8	N	265	 63% 22% 15%

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 16181 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 DNA chain called DNA (168-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	J	149	3011	1439	508	915	149	0	0

- Molecule 2 is a DNA chain called DNA (168-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	I	149	3098	1461	615	873	149	0	0

- Molecule 3 is a protein called Maltodextrin-binding protein,POU domain, class 5, transcription factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	75	559	363	93	100	3	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-251	MET	-	initiating methionine	UNP A0A376KDN7
L	-250	LYS	-	expression tag	UNP A0A376KDN7
L	-249	GLU	-	expression tag	UNP A0A376KDN7
L	114	ALA	-	linker	UNP A0A376KDN7
L	115	ALA	-	linker	UNP A0A376KDN7
L	116	ALA	-	linker	UNP A0A376KDN7
L	117	GLN	-	linker	UNP A0A376KDN7
L	118	THR	-	linker	UNP A0A376KDN7
L	119	ASN	-	linker	UNP A0A376KDN7
L	120	ALA	-	linker	UNP A0A376KDN7
L	121	GLY	-	linker	UNP A0A376KDN7
L	122	SER	-	linker	UNP A0A376KDN7
L	123	GLU	-	linker	UNP A0A376KDN7
L	124	ASN	-	linker	UNP A0A376KDN7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	125	LEU	-	linker	UNP A0A376KDN7
L	126	TYR	-	linker	UNP A0A376KDN7
L	127	PHE	-	linker	UNP A0A376KDN7
L	128	GLN	-	linker	UNP A0A376KDN7
L	129	GLY	-	linker	UNP A0A376KDN7
L	130	SER	-	linker	UNP A0A376KDN7
L	131	VAL	-	linker	UNP A0A376KDN7
L	132	ASP	-	linker	UNP A0A376KDN7
L	133	SER	-	linker	UNP A0A376KDN7
L	134	ALA	-	linker	UNP A0A376KDN7
L	135	ALA	-	linker	UNP A0A376KDN7
L	136	ALA	-	linker	UNP A0A376KDN7
L	137	SER	-	linker	UNP A0A376KDN7
L	291	GLU	-	expression tag	UNP Q01860
L	292	PHE	-	expression tag	UNP Q01860
L	293	HIS	-	expression tag	UNP Q01860
L	294	HIS	-	expression tag	UNP Q01860
L	295	HIS	-	expression tag	UNP Q01860
L	296	HIS	-	expression tag	UNP Q01860
L	297	HIS	-	expression tag	UNP Q01860
L	298	HIS	-	expression tag	UNP Q01860

- Molecule 4 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	96	790	499	151	136	4	0	0
4	A	97	801	505	155	137	4	0	0

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	79	633	399	124	109	1	0	0
5	B	82	653	412	127	113	1	0	0

- Molecule 6 is a protein called Histone H2A type 2-C.

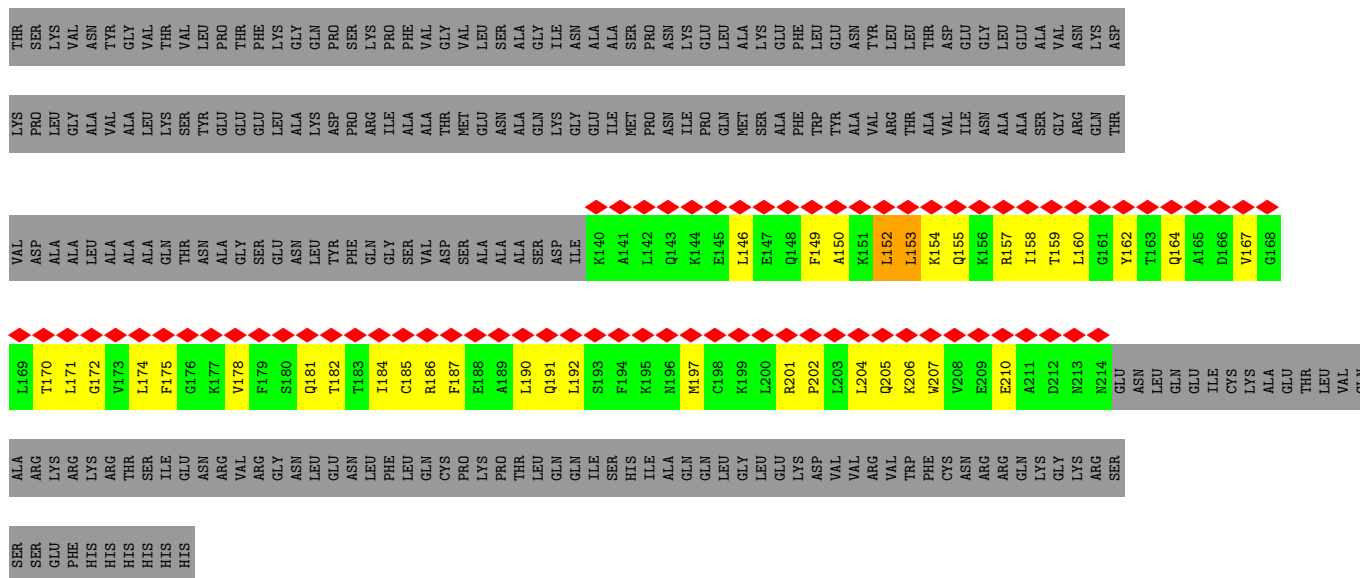
Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	107	Total	C	N	O	S	0	0
			820	518	159	142	1		
6	C	107	Total	C	N	O	S	0	0
			816	515	158	142	1		

- Molecule 7 is a protein called Histone H2B type 2-E.

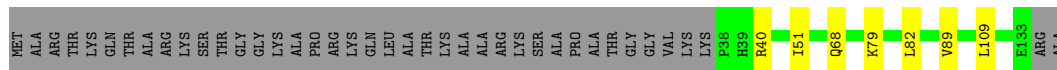
Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	95	Total	C	N	O	S	0	0
			736	462	132	140	2		
7	D	95	Total	C	N	O	S	0	0
			736	462	132	140	2		

- Molecule 8 is a protein called ScFv.

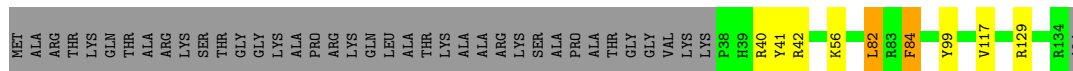
Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	226	Total	C	N	O	S	0	0
			1759	1109	285	357	8		
8	K	226	Total	C	N	O	S	0	0
			1769	1115	289	357	8		



● Molecule 4: Histone H3.1



● Molecule 4: Histone H3.1



● Molecule 5: Histone H4

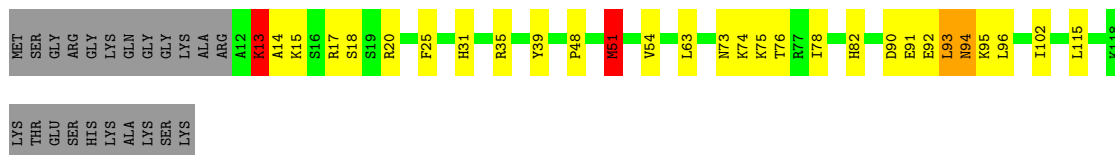


● Molecule 5: Histone H4



● Molecule 6: Histone H2A type 2-C

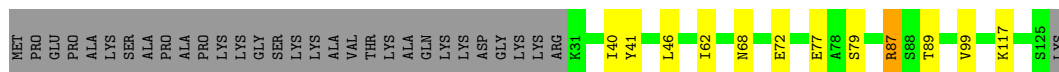




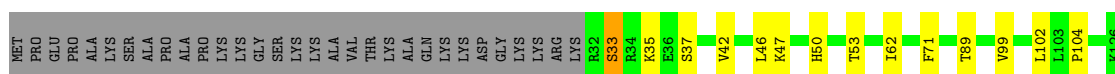
• Molecule 6: Histone H2A type 2-C



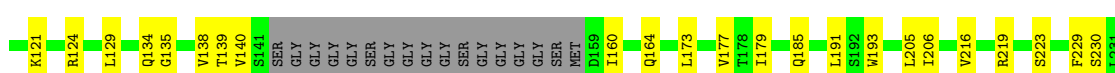
• Molecule 7: Histone H2B type 2-E



• Molecule 7: Histone H2B type 2-E



• Molecule 8: ScFv



• Molecule 8: ScFv



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110991	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 ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.513	Depositor
Minimum map value	-0.606	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	253.44, 253.44, 253.44	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.056, 1.056, 1.056	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	J	0.58	0/3361	0.99	0/5177
2	I	0.58	0/3491	0.84	0/5394
3	L	0.26	0/567	0.71	3/769 (0.4%)
4	A	0.59	2/813 (0.2%)	0.64	1/1090 (0.1%)
4	E	0.47	0/802	0.58	0/1076
5	B	0.31	0/660	0.65	1/883 (0.1%)
5	F	0.79	4/640 (0.6%)	0.75	3/857 (0.4%)
6	C	0.43	1/826 (0.1%)	0.59	0/1114
6	G	0.91	8/830 (1.0%)	0.87	4/1118 (0.4%)
7	D	0.29	0/747	0.61	2/1005 (0.2%)
7	H	0.43	1/747 (0.1%)	0.56	0/1005
8	K	0.31	0/1811	0.59	1/2454 (0.0%)
8	N	0.32	0/1801	0.62	2/2443 (0.1%)
All	All	0.53	16/17096 (0.1%)	0.77	17/24385 (0.1%)

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
6	G	0	2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	51	MET	C-O	-9.74	1.04	1.23
5	F	90	LEU	C-O	-9.27	1.05	1.23
6	G	93	LEU	C-O	-8.39	1.07	1.23
6	G	94	ASN	C-O	-7.48	1.09	1.23
6	C	16	SER	CB-OG	-6.91	1.33	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	51	MET	CB-CG-SD	-9.82	82.92	112.40
3	L	153	LEU	CA-CB-CG	9.77	137.76	115.30
3	L	152	LEU	CA-CB-CG	7.82	133.28	115.30
6	G	51	MET	CG-SD-CE	-7.52	88.16	100.20
7	D	102	LEU	CA-CB-CG	7.30	132.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	51	MET	Mainchain
6	G	92	GLU	Mainchain

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	J	3011	0	1685	71	0
2	I	3098	0	1664	64	0
3	L	559	0	533	42	0
4	A	801	0	839	19	0
4	E	790	0	826	11	0
5	B	653	0	696	11	0
5	F	633	0	673	5	0
6	C	816	0	869	18	0
6	G	820	0	880	32	0
7	D	736	0	749	13	0
7	H	736	0	749	13	0
8	K	1769	0	1708	28	0
8	N	1759	0	1686	38	0
All	All	16181	0	13557	312	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 11.

The worst 5 of 312 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:J:11:DT:H71	3:L:186:ARG:NH2	1.25	1.43
1:J:11:DT:C7	3:L:186:ARG:HH22	1.29	1.42
1:J:11:DT:C7	3:L:186:ARG:NH2	1.87	1.31
6:G:13:LYS:HG3	6:G:14:ALA:N	1.44	1.18
1:J:11:DT:H73	3:L:186:ARG:HH22	1.02	1.13

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	
3	L	73/550 (13%)	73 (100%)	0	0	100	100
4	A	95/136 (70%)	95 (100%)	0	0	100	100
4	E	94/136 (69%)	94 (100%)	0	0	100	100
5	B	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
5	F	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
6	C	105/129 (81%)	100 (95%)	5 (5%)	0	100	100
6	G	105/129 (81%)	96 (91%)	8 (8%)	1 (1%)	15	44
7	D	93/126 (74%)	87 (94%)	6 (6%)	0	100	100
7	H	93/126 (74%)	90 (97%)	3 (3%)	0	100	100
8	K	222/265 (84%)	208 (94%)	14 (6%)	0	100	100
8	N	222/265 (84%)	210 (95%)	12 (5%)	0	100	100
All	All	1259/2068 (61%)	1203 (96%)	55 (4%)	1 (0%)	54	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	13	LYS

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	
3	L	52/452 (12%)	52 (100%)	0	100	100
4	A	85/111 (77%)	85 (100%)	0	100	100
4	E	84/111 (76%)	84 (100%)	0	100	100
5	B	67/79 (85%)	67 (100%)	0	100	100
5	F	65/79 (82%)	65 (100%)	0	100	100
6	C	82/99 (83%)	82 (100%)	0	100	100
6	G	83/99 (84%)	83 (100%)	0	100	100
7	D	80/106 (76%)	80 (100%)	0	100	100
7	H	80/106 (76%)	80 (100%)	0	100	100
8	K	199/224 (89%)	198 (100%)	1 (0%)	88	96
8	N	197/224 (88%)	197 (100%)	0	100	100
All	All	1074/1690 (64%)	1073 (100%)	1 (0%)	93	98

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

Mol	Chain	Res	Type
8	K	57	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	94	ASN
6	C	31	HIS
8	K	196	GLN
6	C	73	ASN
6	G	73	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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.

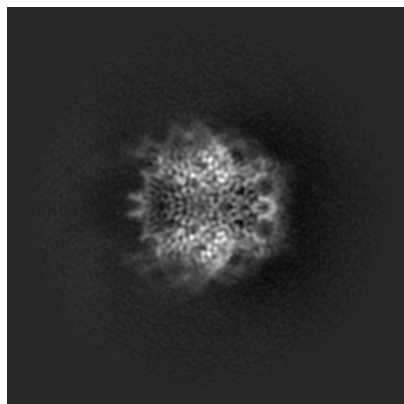
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40686. These allow visual inspection of the internal detail of the map and identification of artifacts.

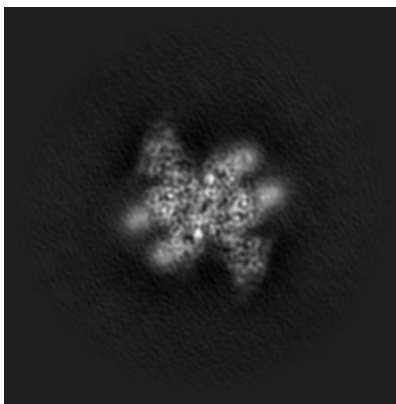
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

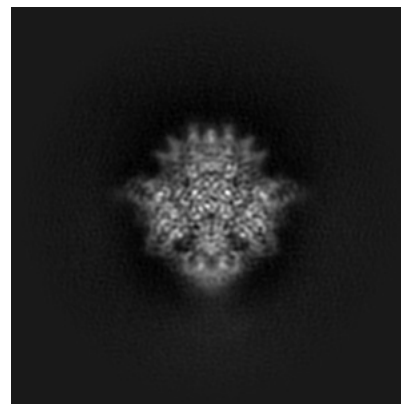
6.1.1 Primary map



X

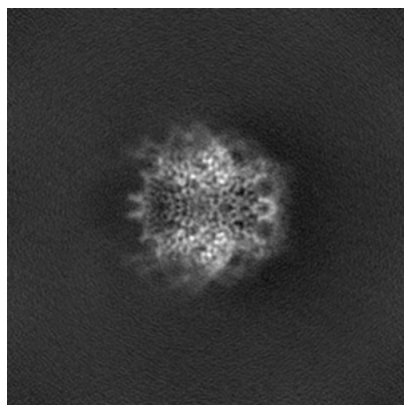


Y

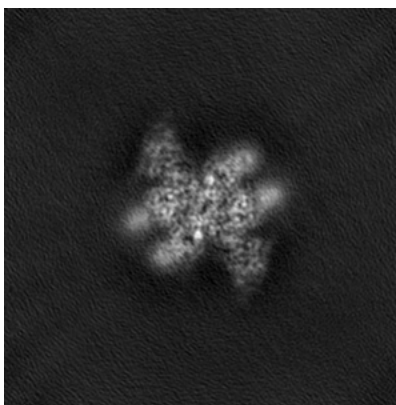


Z

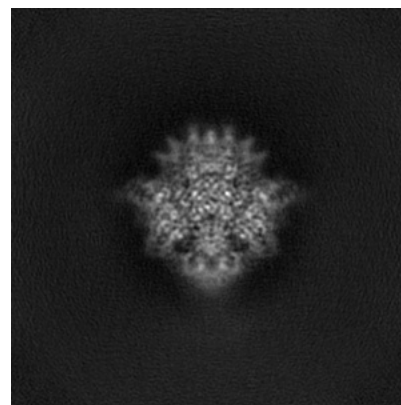
6.1.2 Raw map



X



Y

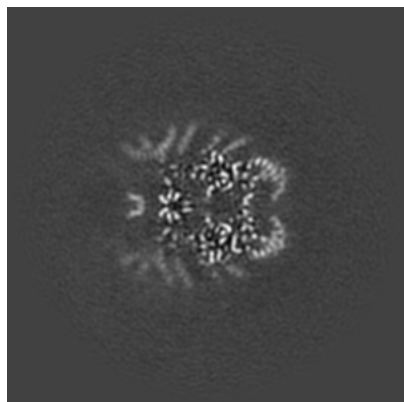


Z

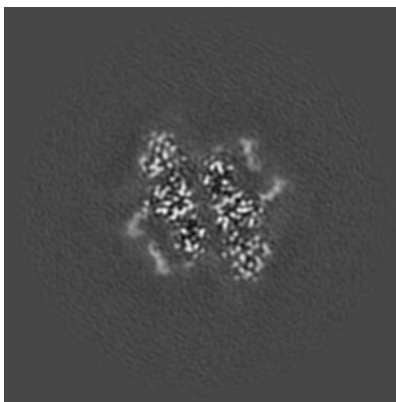
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

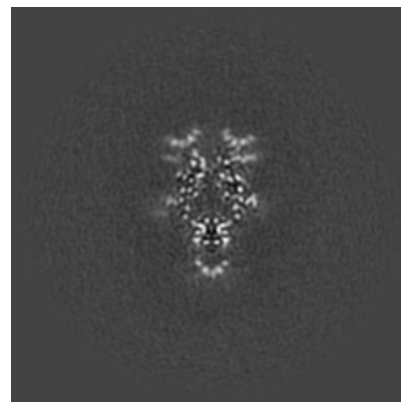
6.2.1 Primary map



X Index: 120

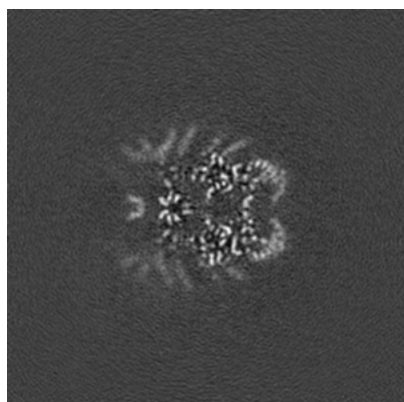


Y Index: 120

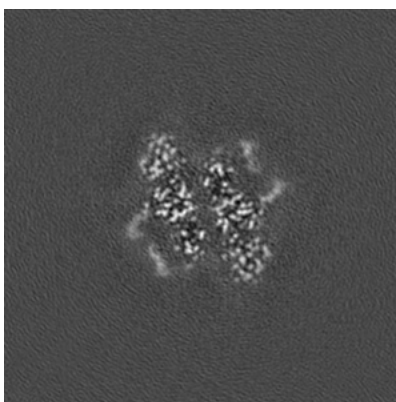


Z Index: 120

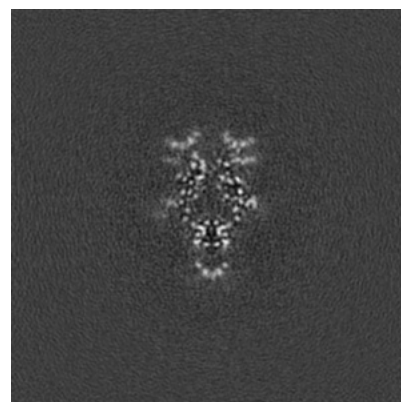
6.2.2 Raw map



X Index: 120



Y Index: 120

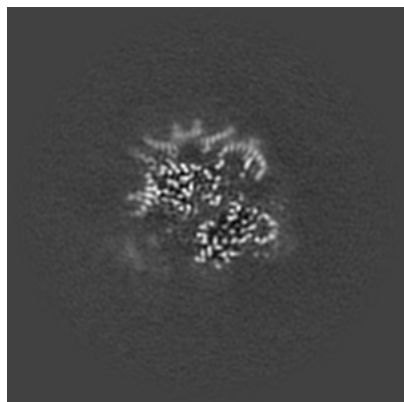


Z Index: 120

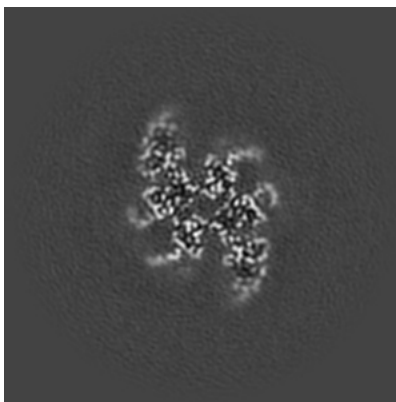
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

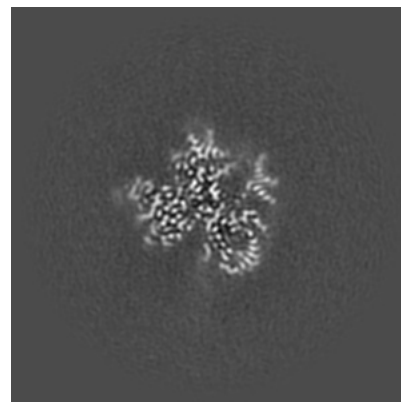
6.3.1 Primary map



X Index: 126

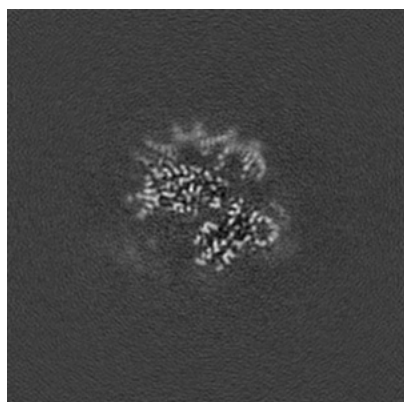


Y Index: 127

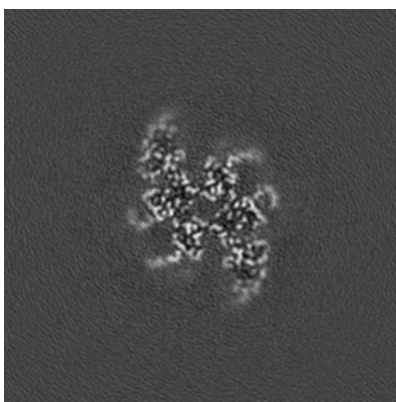


Z Index: 139

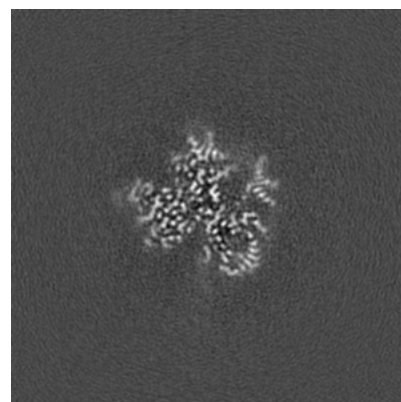
6.3.2 Raw map



X Index: 127



Y Index: 127

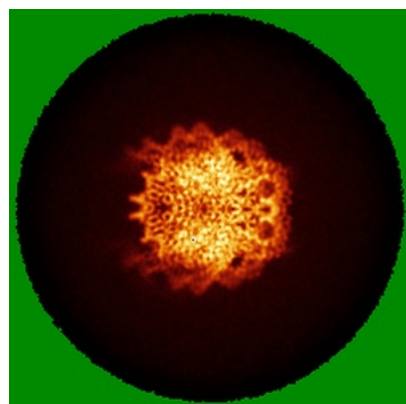


Z Index: 139

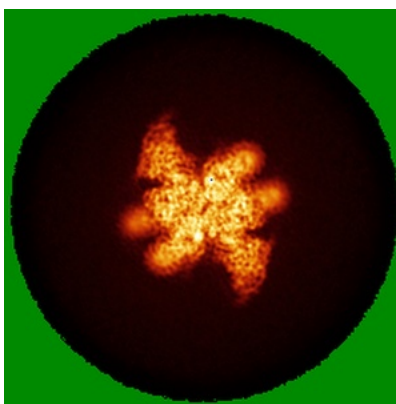
The images above show the largest variance slices of the map in three orthogonal directions.

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

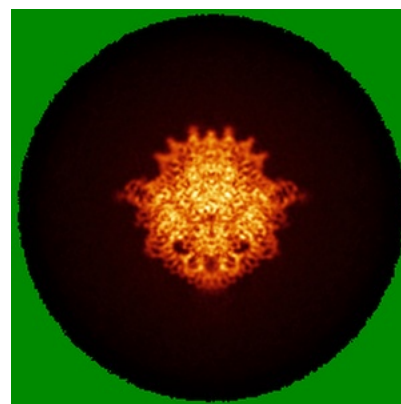
6.4.1 Primary map



X

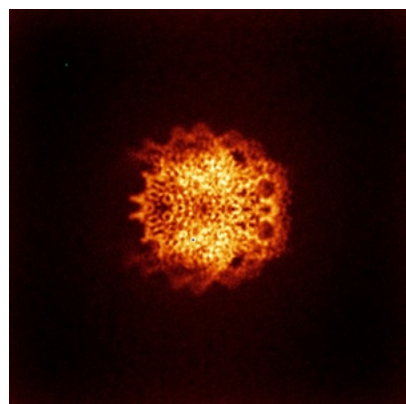


Y

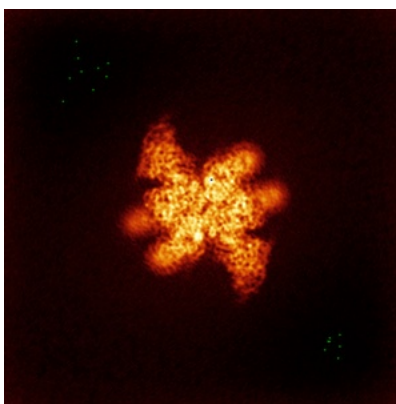


Z

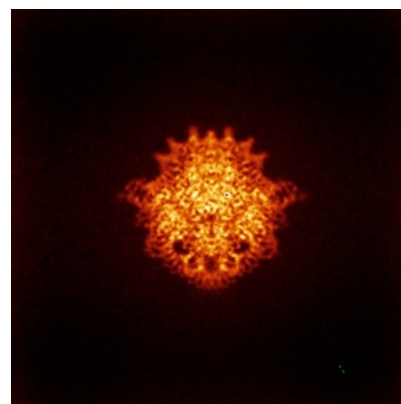
6.4.2 Raw map



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.

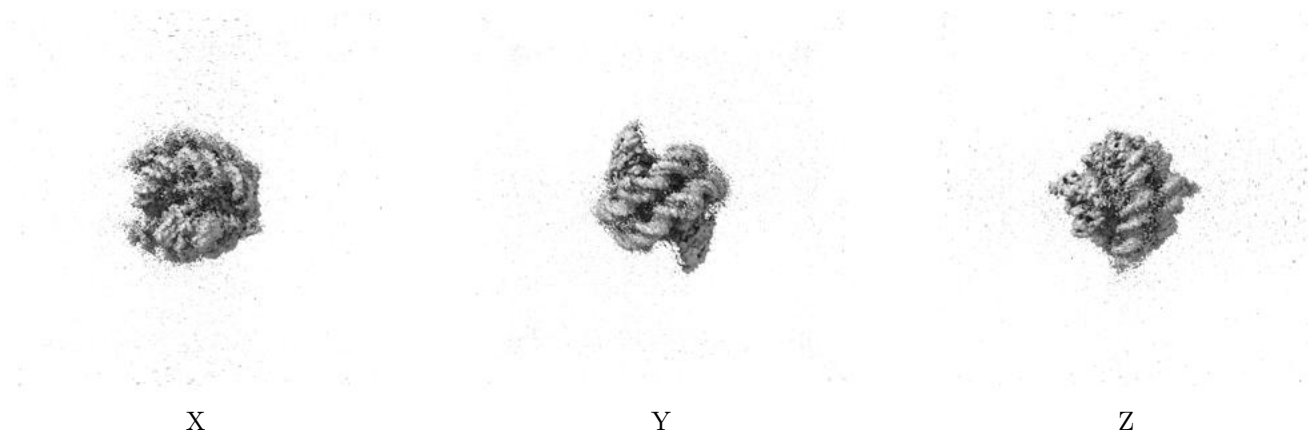
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

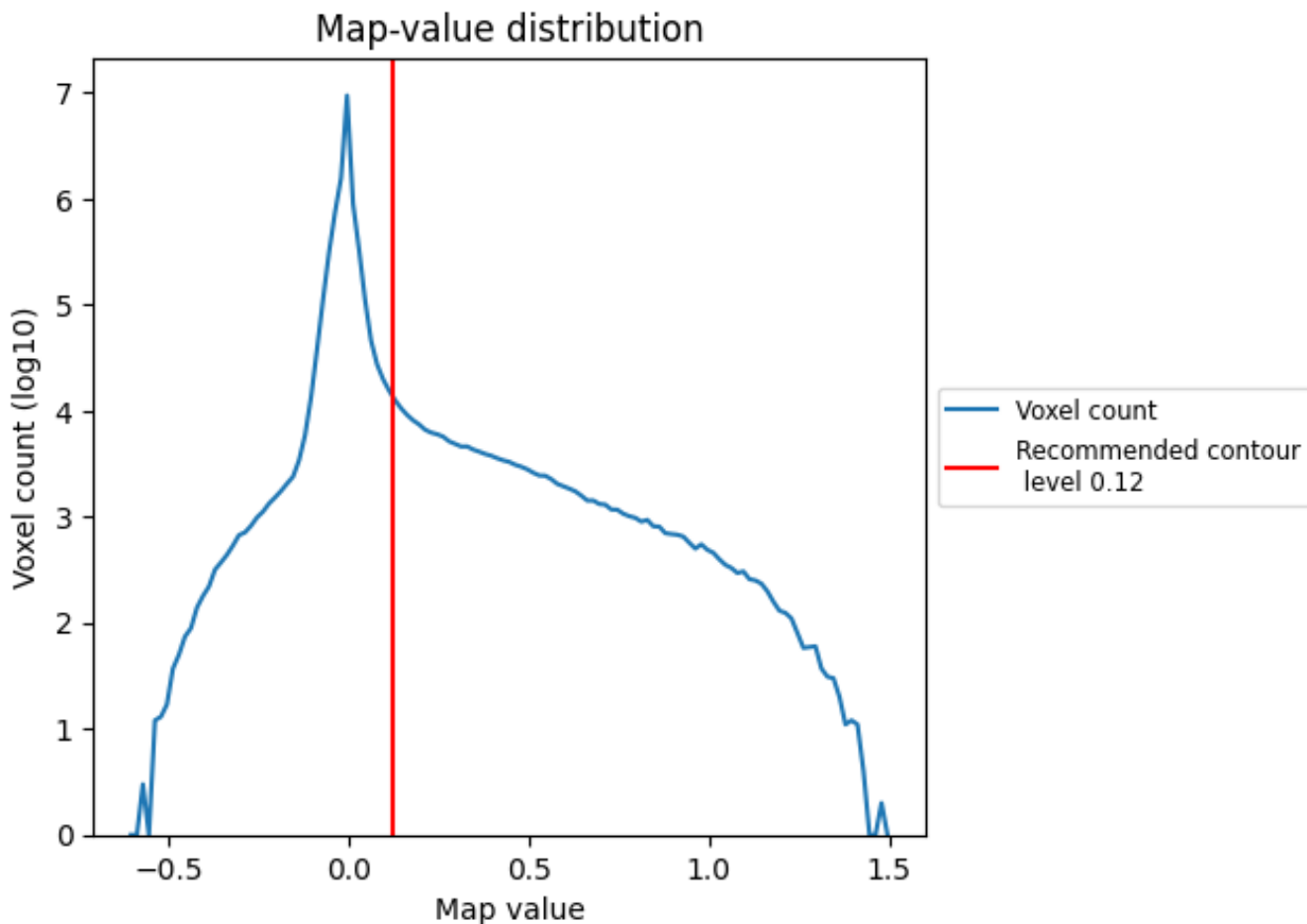
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

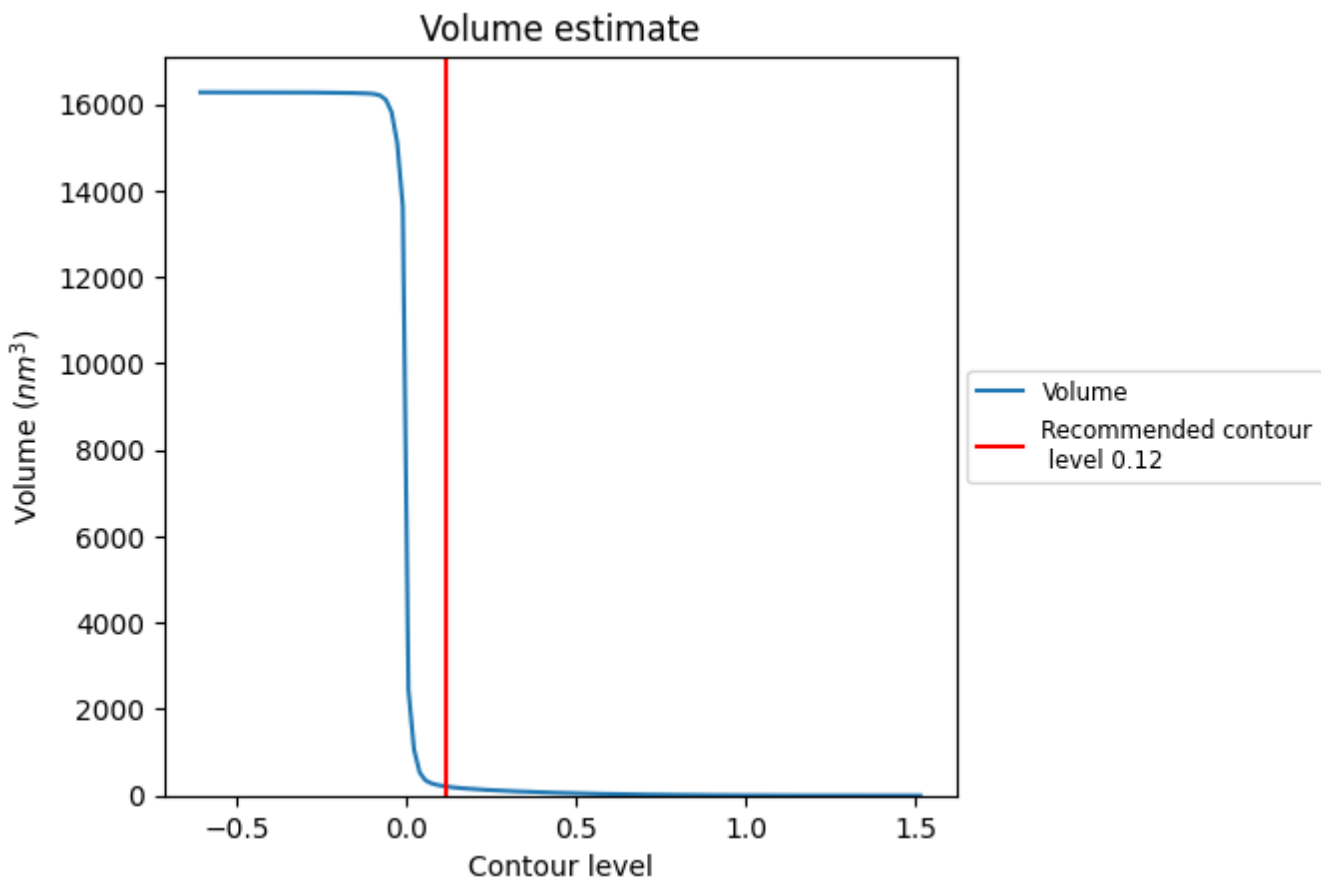
This section contains the results of statistical analysis of the map.

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.

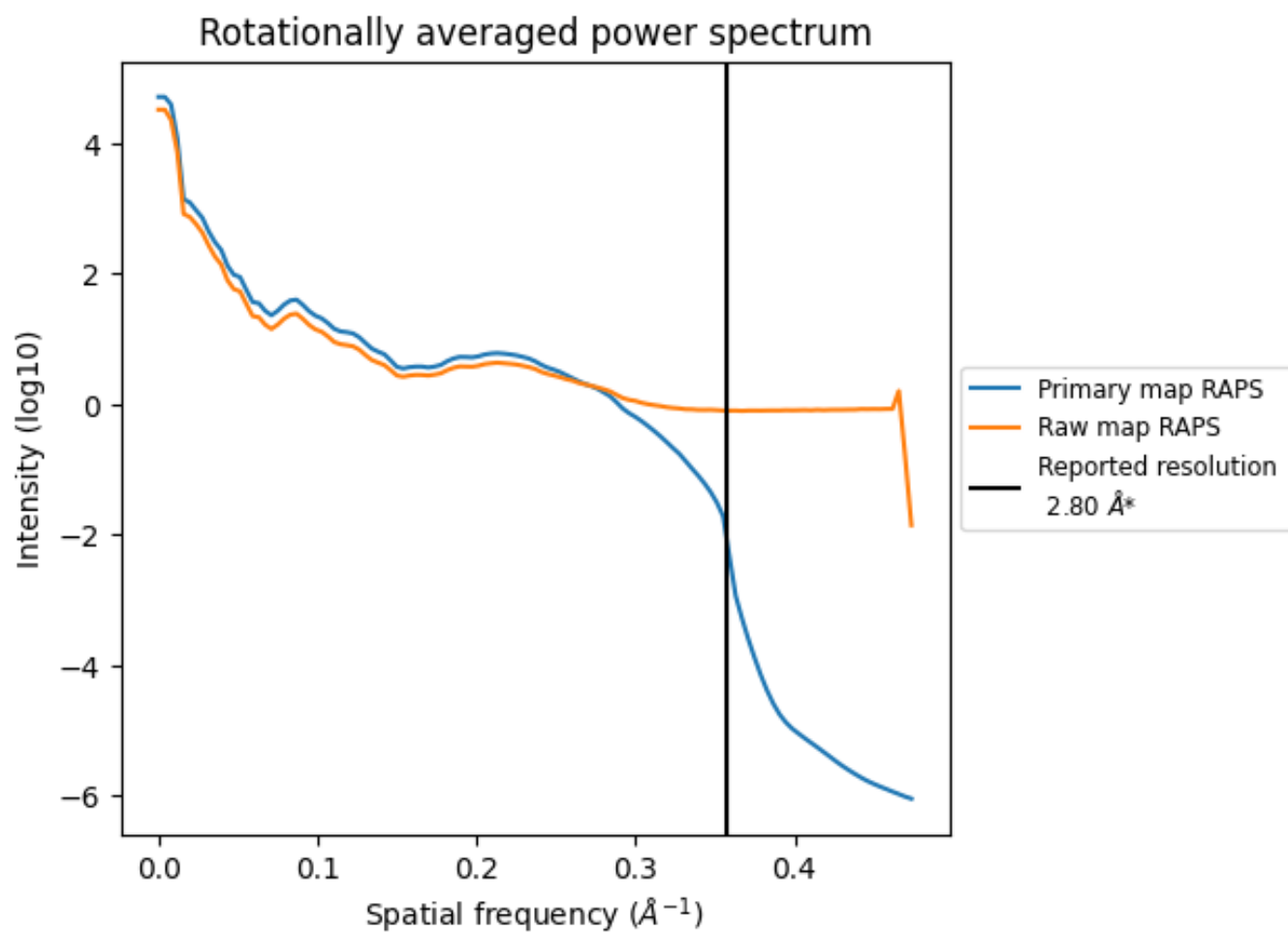
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm^3 ; this corresponds to an approximate mass of 188 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

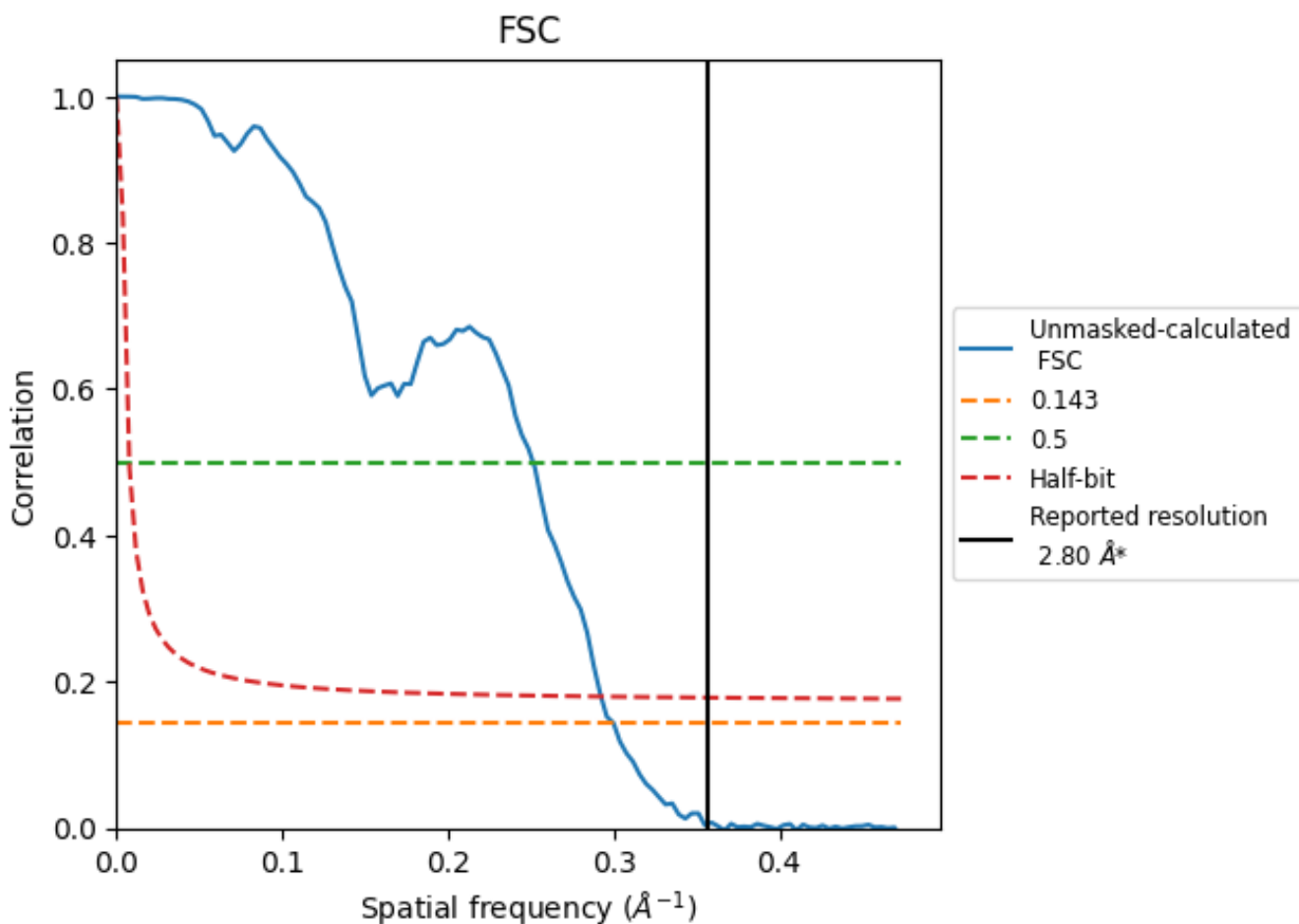


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

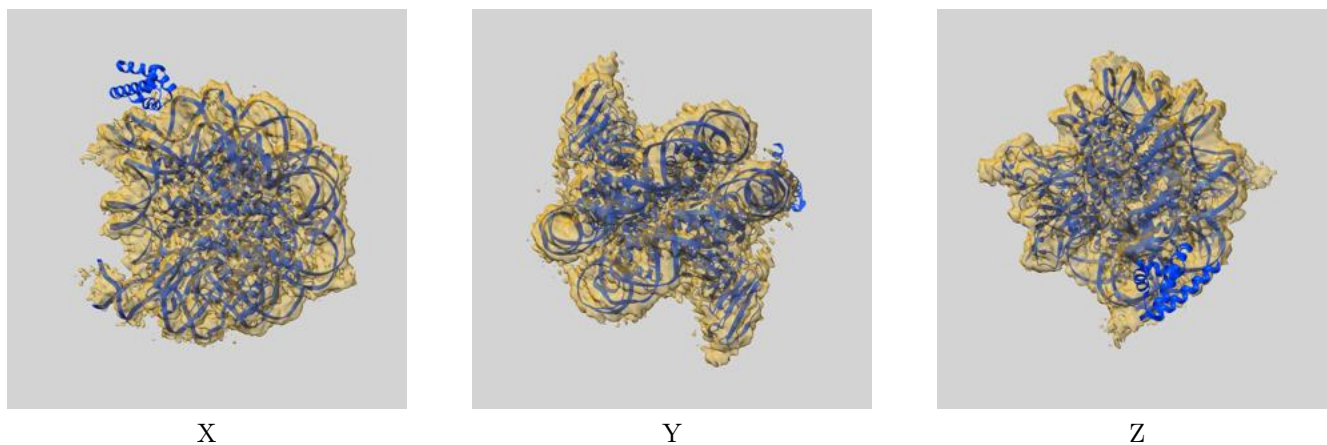
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.33	3.98	3.42

*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 3.33 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

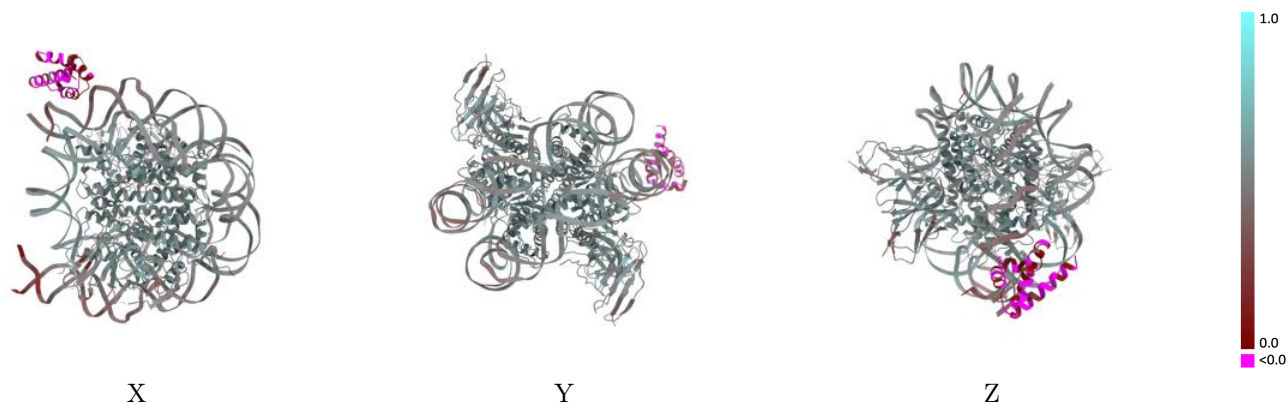
This section contains information regarding the fit between EMDB map EMD-40686 and PDB model 8SPU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



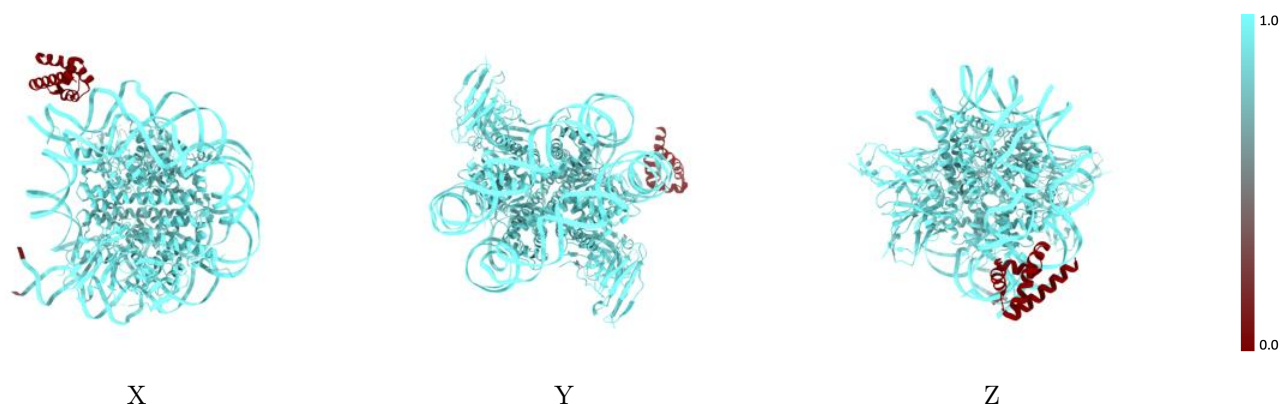
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



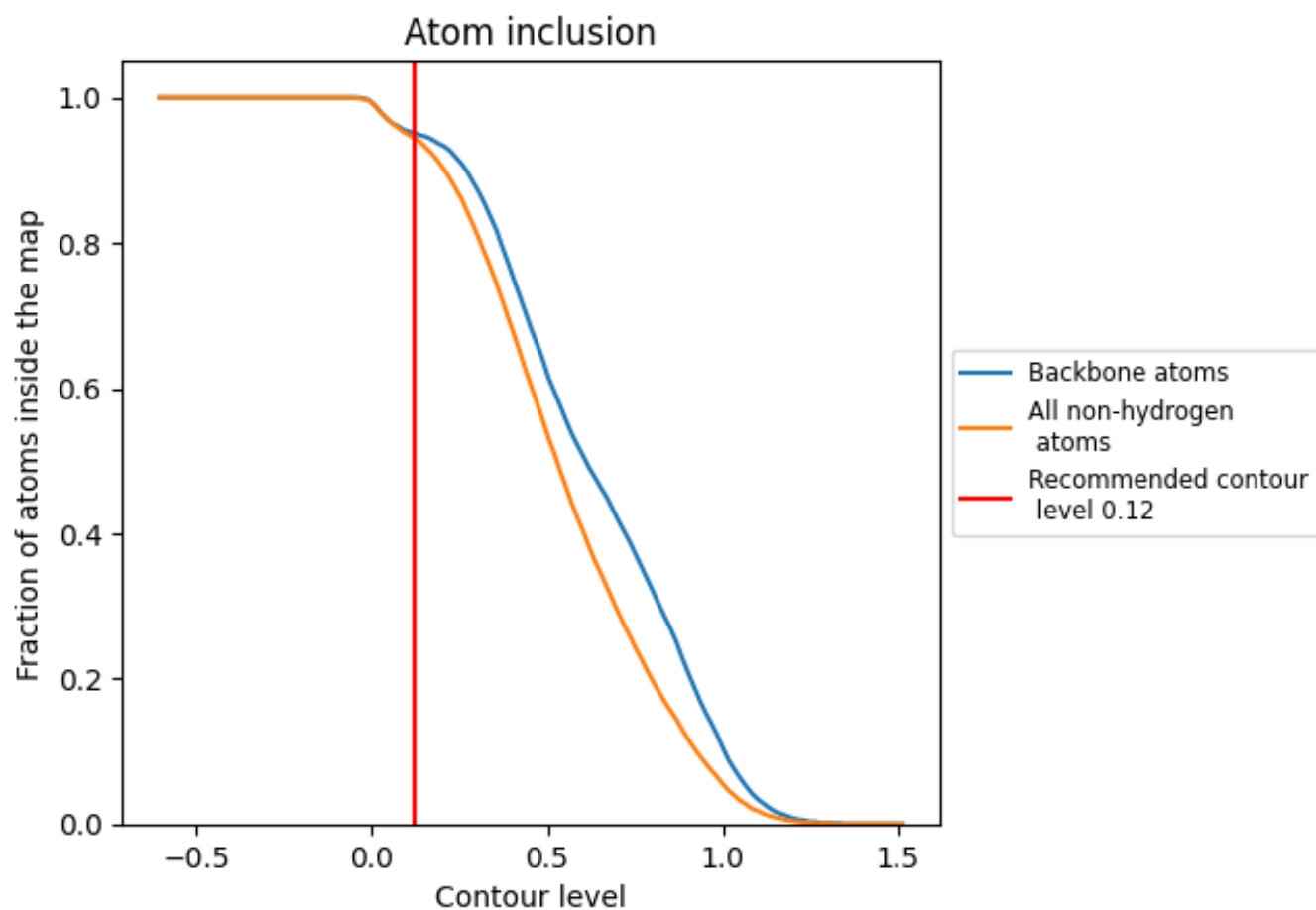
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.4960
A	 0.9770	 0.5550
B	 0.9790	 0.5560
C	 0.9790	 0.5600
D	 0.9750	 0.5460
E	 0.9800	 0.5490
F	 0.9930	 0.5680
G	 0.9700	 0.5480
H	 0.9750	 0.5450
I	 0.9870	 0.4780
J	 0.9870	 0.4840
K	 0.9680	 0.5030
L	 0.0020	 0.0110
N	 0.9620	 0.5020

