



wwPDB EM Validation Summary Report ⓘ

May 12, 2024 – 09:08 am BST

PDB ID : 6T7A
EMDB ID : EMD-10391
Title : Structure of human Sox11 transcription factor in complex with a nucleosome
Authors : Dodonova, S.O.; Zhu, F.; Dienemann, C.; Taipale, J.; Cramer, P.
Deposited on : 2019-10-21
Resolution : 3.70 Å(reported)
Based on initial model : 6T79

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

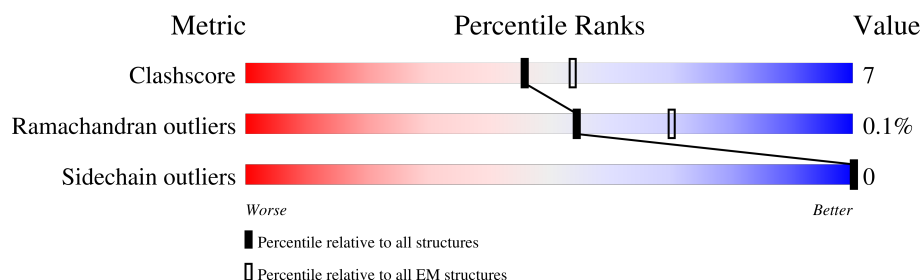
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


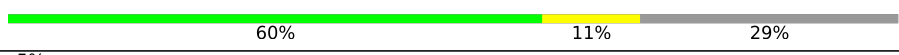

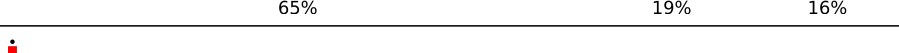




The reported resolution of this entry is 3.70 Å.

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	A	136	
1	E	136	
2	B	103	
2	F	103	
3	C	151	
3	G	151	
4	D	126	
4	H	126	

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Mol	Chain	Length	Quality of chain
5	I	147	 54% 10% 35%
6	J	147	 53% 12% 35%
7	K	109	 14% 71% 29%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10338 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			809	511	157	139	2		
1	E	97	Total	C	N	O	S	0	0
			800	505	155	138	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP Q71DI3
E	110	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	86	Total	C	N	O	S	0	0
			698	440	141	116	1		
2	F	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	106	Total	C	N	O	0	0
			819	517	160	142		
3	G	106	Total	C	N	O	0	0
			819	517	160	142		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	initiating methionine	UNP P04908
C	-20	GLY	-	expression tag	UNP P04908
C	-19	SER	-	expression tag	UNP P04908

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	SER	-	expression tag	UNP P04908
C	-17	HIS	-	expression tag	UNP P04908
C	-16	HIS	-	expression tag	UNP P04908
C	-15	HIS	-	expression tag	UNP P04908
C	-14	HIS	-	expression tag	UNP P04908
C	-13	HIS	-	expression tag	UNP P04908
C	-12	HIS	-	expression tag	UNP P04908
C	-11	GLU	-	expression tag	UNP P04908
C	-10	ASN	-	expression tag	UNP P04908
C	-9	LEU	-	expression tag	UNP P04908
C	-8	TYR	-	expression tag	UNP P04908
C	-7	PHE	-	expression tag	UNP P04908
C	-6	GLN	-	expression tag	UNP P04908
C	-5	SER	-	expression tag	UNP P04908
C	-4	ASN	-	expression tag	UNP P04908
C	-3	ALA	-	expression tag	UNP P04908
C	-2	PRO	-	expression tag	UNP P04908
C	-1	TRP	-	expression tag	UNP P04908
G	-21	MET	-	initiating methionine	UNP P04908
G	-20	GLY	-	expression tag	UNP P04908
G	-19	SER	-	expression tag	UNP P04908
G	-18	SER	-	expression tag	UNP P04908
G	-17	HIS	-	expression tag	UNP P04908
G	-16	HIS	-	expression tag	UNP P04908
G	-15	HIS	-	expression tag	UNP P04908
G	-14	HIS	-	expression tag	UNP P04908
G	-13	HIS	-	expression tag	UNP P04908
G	-12	HIS	-	expression tag	UNP P04908
G	-11	GLU	-	expression tag	UNP P04908
G	-10	ASN	-	expression tag	UNP P04908
G	-9	LEU	-	expression tag	UNP P04908
G	-8	TYR	-	expression tag	UNP P04908
G	-7	PHE	-	expression tag	UNP P04908
G	-6	GLN	-	expression tag	UNP P04908
G	-5	SER	-	expression tag	UNP P04908
G	-4	ASN	-	expression tag	UNP P04908
G	-3	ALA	-	expression tag	UNP P04908
G	-2	PRO	-	expression tag	UNP P04908
G	-1	TRP	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
4	H	95	Total	C	N	O	S	0	0
			744	467	136	139	2		

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	95	Total	C	N	O	P	0	0
			1936	936	303	602	95		

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	95	Total	C	N	O	P	0	0
			1959	933	393	538	95		

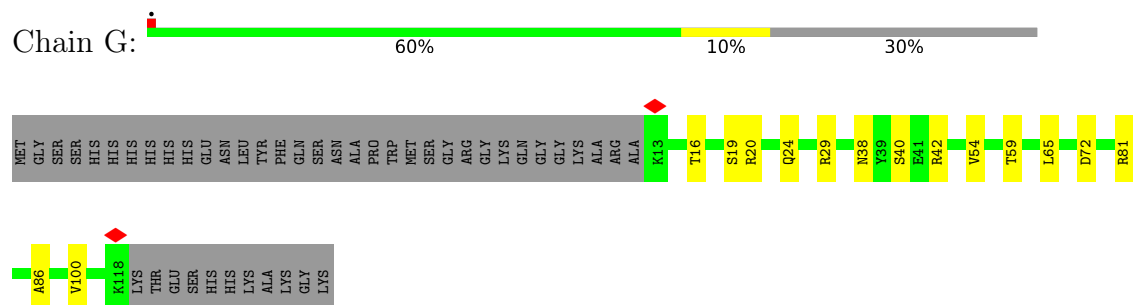
- Molecule 7 is a protein called Transcription factor SOX-11.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	77	Total	C	N	O	0	0
			307	154	77	76		

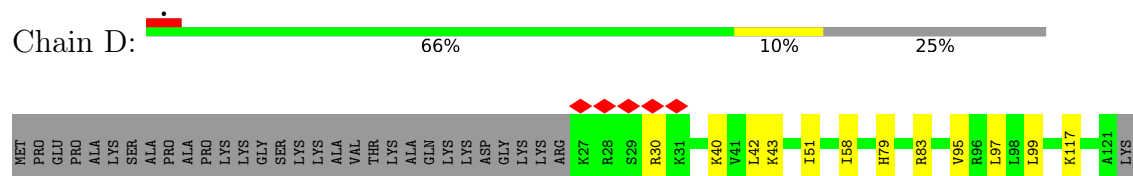
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	30	SER	-	expression tag	UNP P35716
K	31	ASN	-	expression tag	UNP P35716
K	32	ALA	-	expression tag	UNP P35716

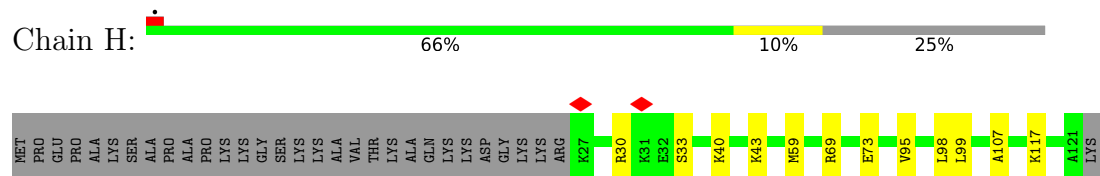
- Molecule 3: Histone H2A type 1-B/E



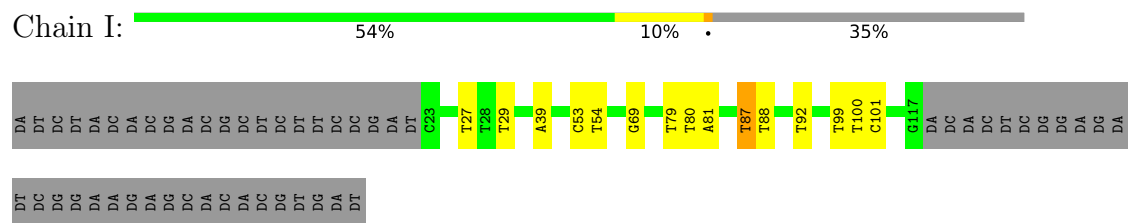
- Molecule 4: Histone H2B type 1-K



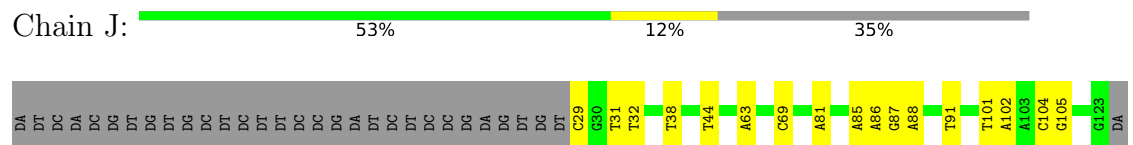
- Molecule 4: Histone H2B type 1-K



- Molecule 5: DNA (147-MER)



- Molecule 6: DNA (147-MER)



SER	ASN	ALA	ALA	LEU	ASP	GLU	SER	ASP	PRO	ASP	TRP	CYS	LYS	THR	ALA	S46	G47	G70	K95	A102	M110	A111	P114	D115	Y116	K117	Y118	R119	P120	R121	K122	LYS	PRO	LYS	MET	ASP	PRO	SER	ALA	LYS	PRO	SER	ALA	SER	GLN	SER	PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202142	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 ($e^-/\text{\AA}^2$)	1.125	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	147.0, 147.0, 147.0	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	A	0.34	0/821	0.46	0/1101
1	E	0.33	0/812	0.48	0/1089
2	B	0.35	0/706	0.52	0/943
2	F	0.38	0/711	0.55	0/948
3	C	0.33	0/829	0.51	0/1118
3	G	0.33	0/829	0.51	0/1118
4	D	0.31	0/755	0.50	0/1014
4	H	0.31	0/755	0.50	0/1014
5	I	0.70	0/2158	1.16	3/3331 (0.1%)
6	J	0.74	0/2210	0.92	0/3406
7	K	0.27	0/306	0.50	0/380
All	All	0.53	0/10892	0.79	3/15462 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	87	DT	P-O3'-C3'	5.30	126.06	119.70
5	I	92	DT	O4'-C4'-C3'	-5.23	102.41	104.50
5	I	88	DT	C3'-C2'-C1'	-5.17	96.29	102.50

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	809	0	851	19	0
1	E	800	0	839	21	0
2	B	698	0	752	23	0
2	F	703	0	753	35	0
3	C	819	0	879	12	0
3	G	819	0	879	20	0
4	D	744	0	769	15	0
4	H	744	0	769	15	0
5	I	1936	0	1094	20	0
6	J	1959	0	1062	14	0
7	K	307	0	75	0	0
All	All	10338	0	8722	123	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 7.

The worst 5 of 123 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:70:LEU:HD11	2:B:26:ILE:CD1	1.69	1.21
1:A:70:LEU:CD1	2:B:26:ILE:HD13	1.75	1.16
1:E:73:GLU:OE1	2:F:25:ASN:HB2	1.36	1.13
1:A:70:LEU:HD11	2:B:26:ILE:HD13	1.30	1.11
1:E:70:LEU:HD11	2:F:26:ILE:HD13	1.36	1.03

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	
1	A	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	84/103 (82%)	84 (100%)	0	0	100	100
2	F	85/103 (82%)	83 (98%)	1 (1%)	1 (1%)	13	48
3	C	104/151 (69%)	101 (97%)	3 (3%)	0	100	100
3	G	104/151 (69%)	101 (97%)	3 (3%)	0	100	100
4	D	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
4	H	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
7	K	75/109 (69%)	73 (97%)	2 (3%)	0	100	100
All	All	829/1141 (73%)	813 (98%)	15 (2%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	29	ILE

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	A	85/110 (77%)	85 (100%)	0	100	100
1	E	84/110 (76%)	84 (100%)	0	100	100
2	B	72/79 (91%)	72 (100%)	0	100	100
2	F	72/79 (91%)	72 (100%)	0	100	100
3	C	84/119 (71%)	84 (100%)	0	100	100
3	G	84/119 (71%)	84 (100%)	0	100	100
4	D	81/105 (77%)	81 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
All	All	643/826 (78%)	643 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12

such sidechains are listed below:

Mol	Chain	Res	Type
1	E	93	GLN
1	E	108	ASN
4	H	79	HIS
1	E	113	HIS
1	A	113	HIS

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.

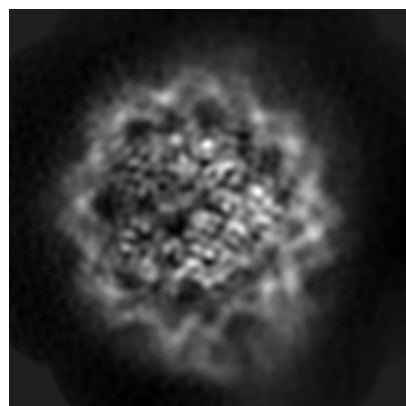
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10391. These allow visual inspection of the internal detail of the map and identification of artifacts.

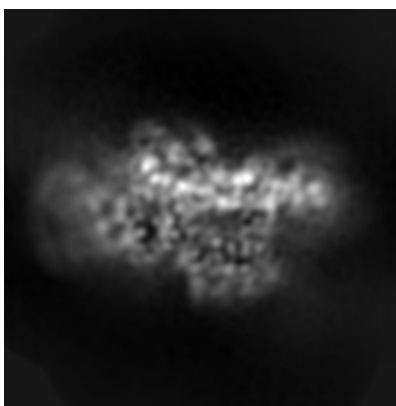
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

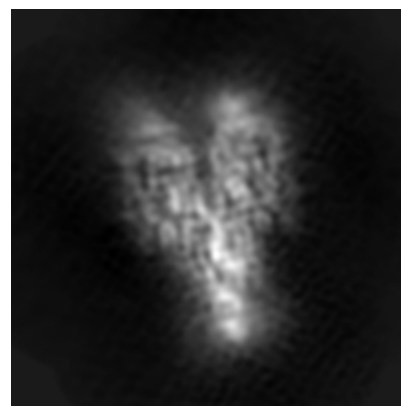
6.1.1 Primary map



X

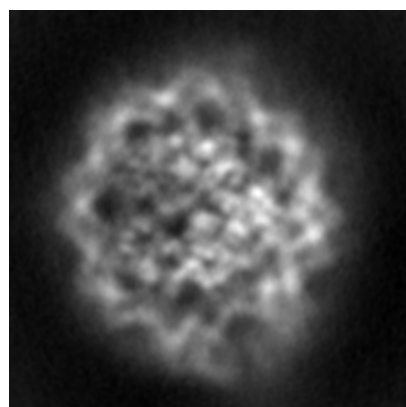


Y

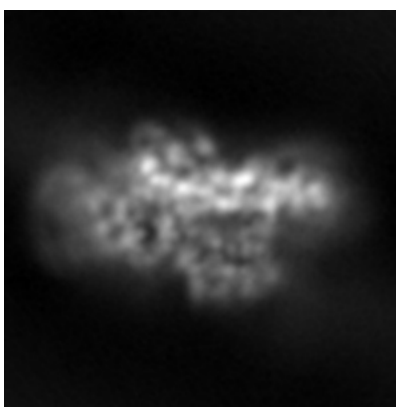


Z

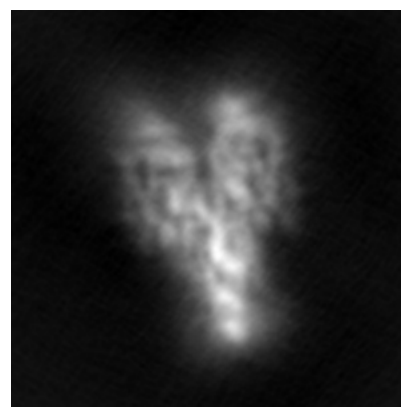
6.1.2 Raw map



X



Y

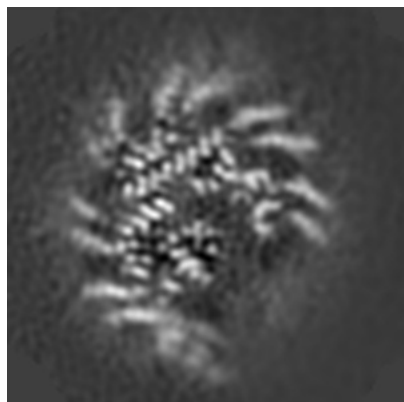


Z

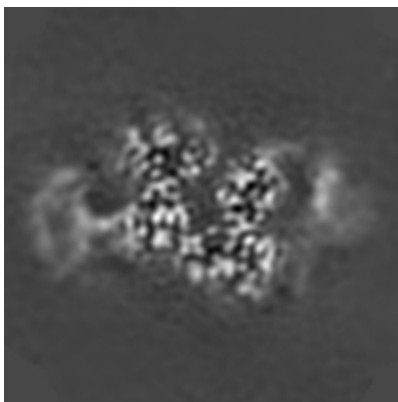
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

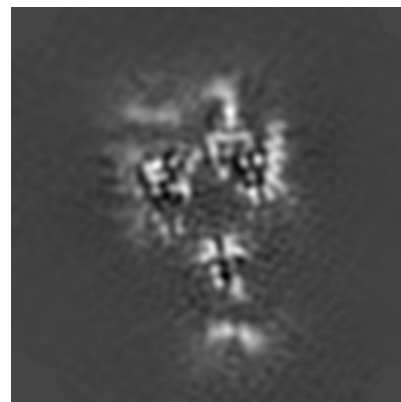
6.2.1 Primary map



X Index: 70

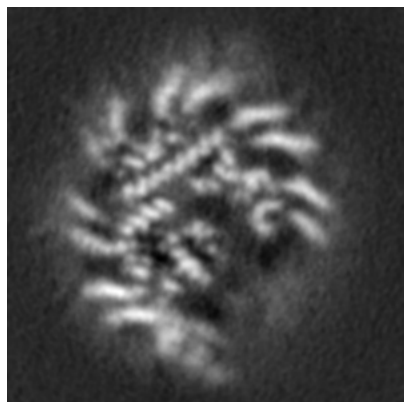


Y Index: 70

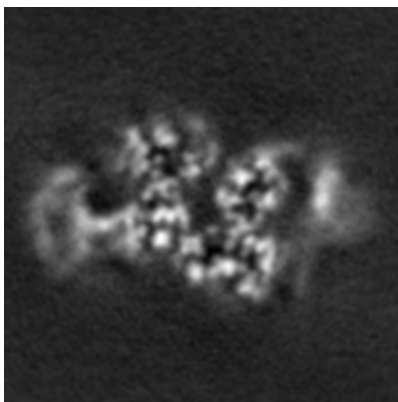


Z Index: 70

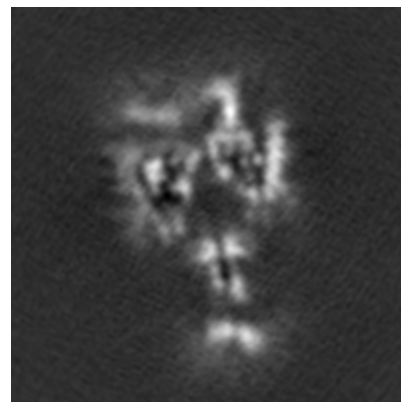
6.2.2 Raw map



X Index: 70



Y Index: 70

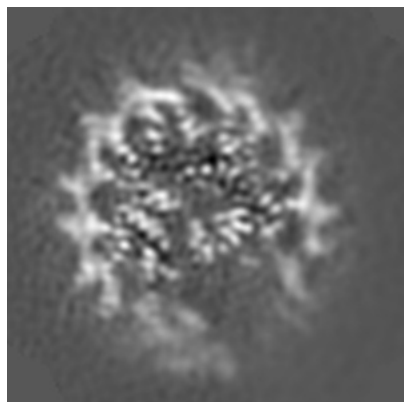


Z Index: 70

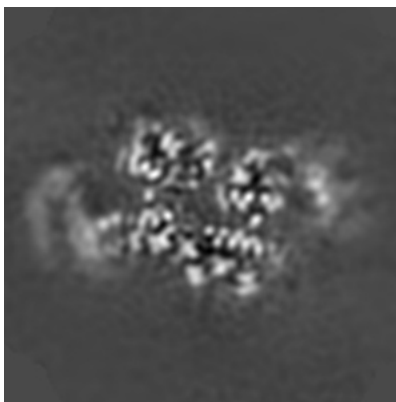
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

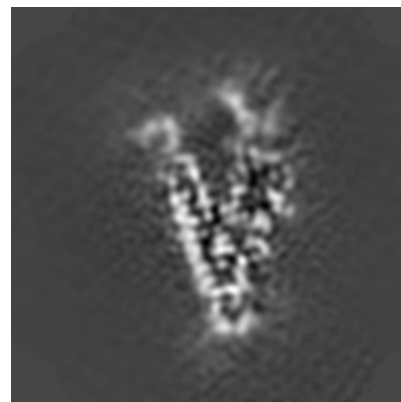
6.3.1 Primary map



X Index: 77

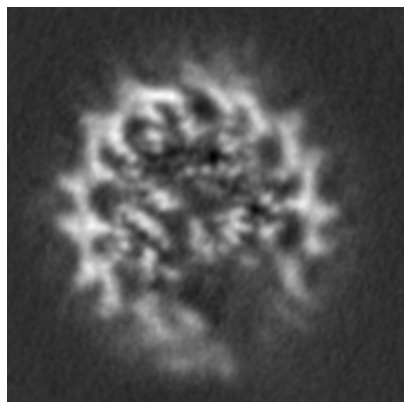


Y Index: 73

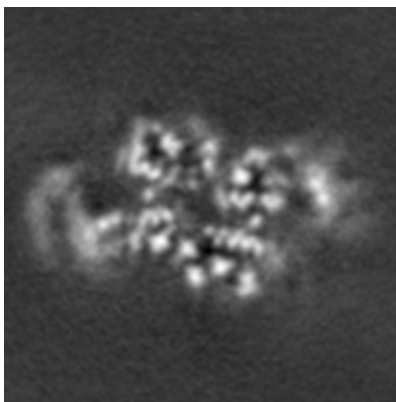


Z Index: 56

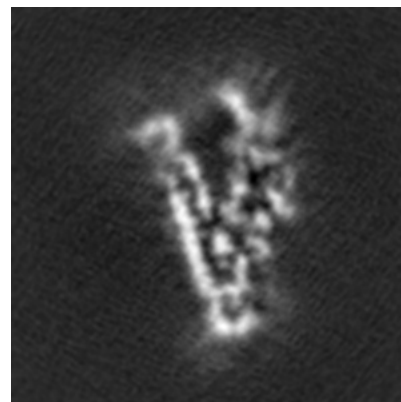
6.3.2 Raw map



X Index: 77



Y Index: 73

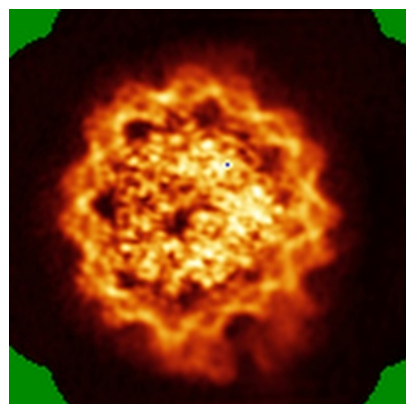


Z Index: 56

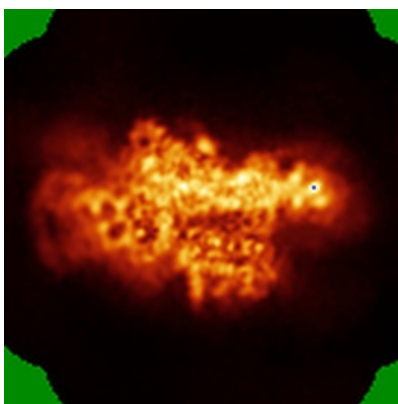
The images above show the largest variance slices of the map in three orthogonal directions.

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

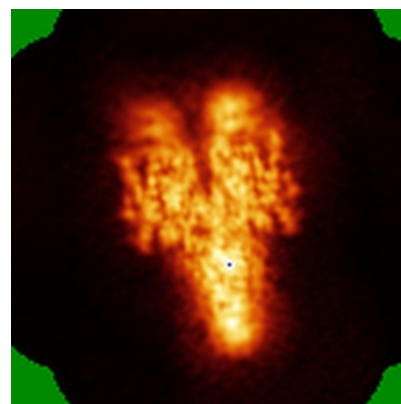
6.4.1 Primary map



X

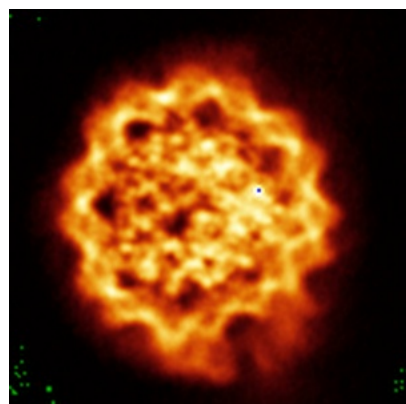


Y

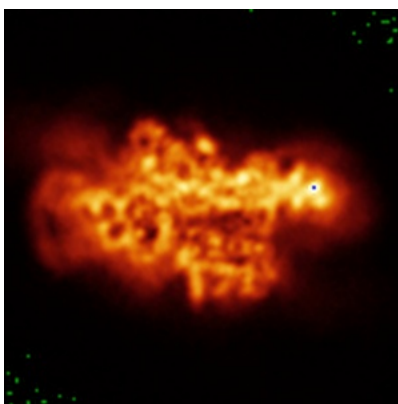


Z

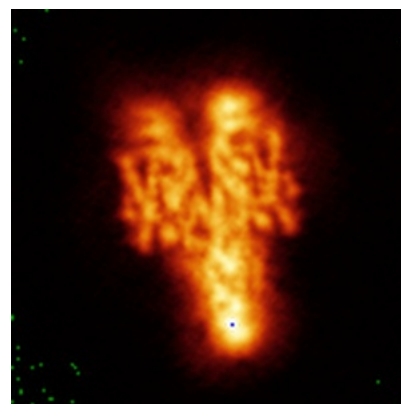
6.4.2 Raw map



X



Y

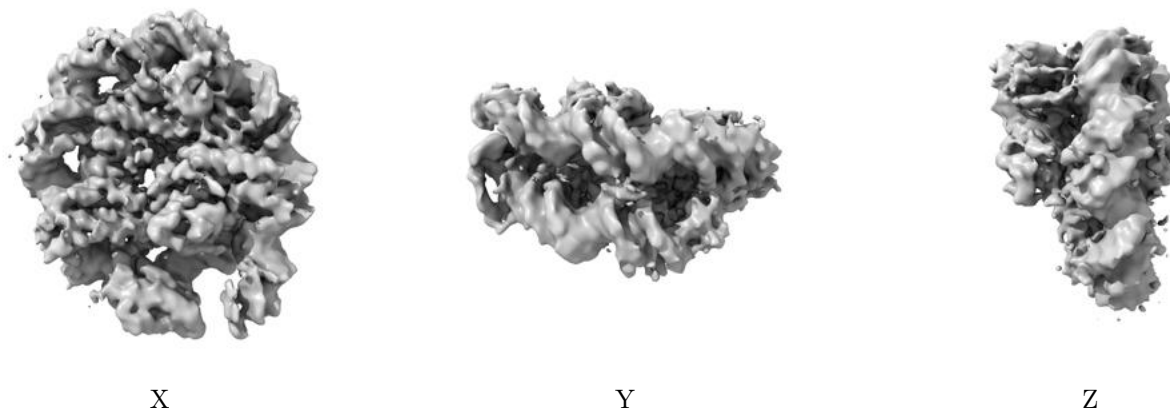


Z

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.

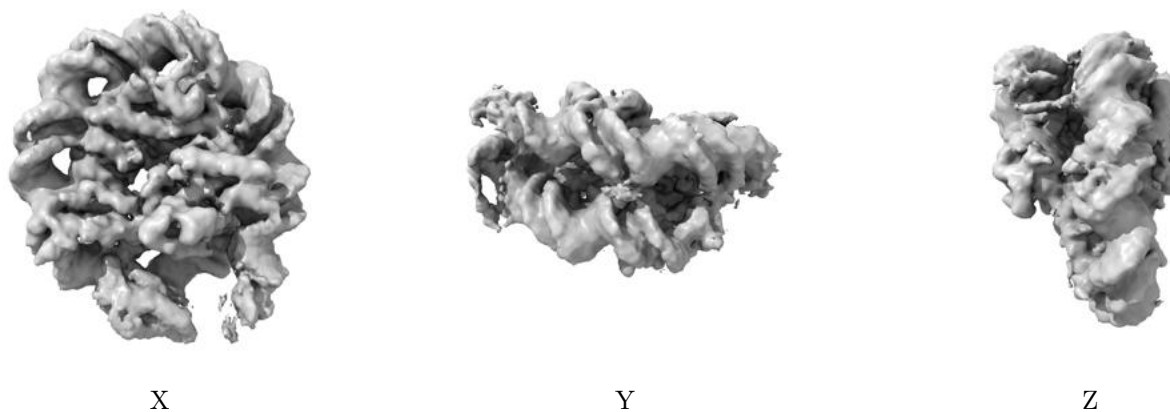
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

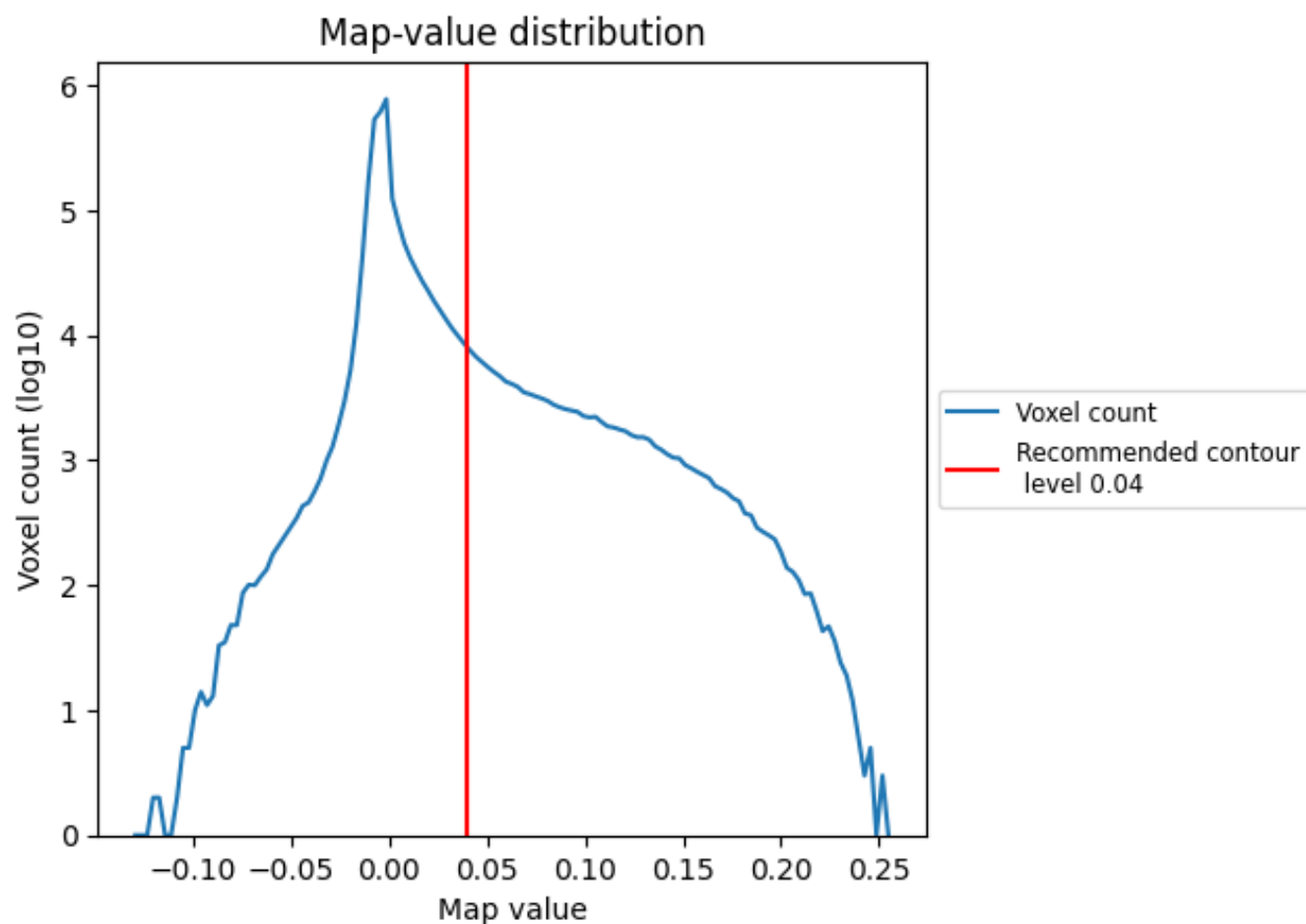
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

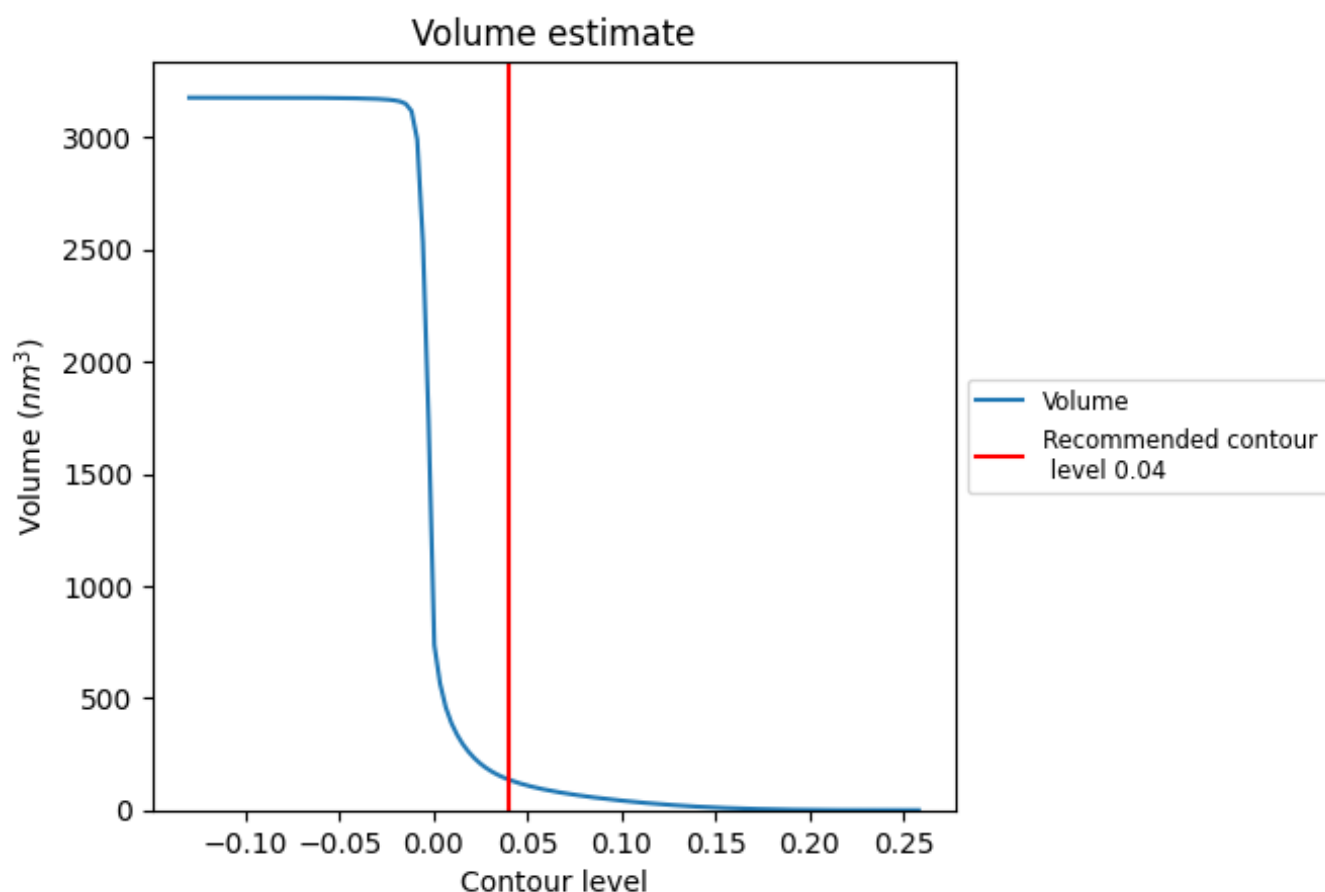
This section contains the results of statistical analysis of the map.

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.

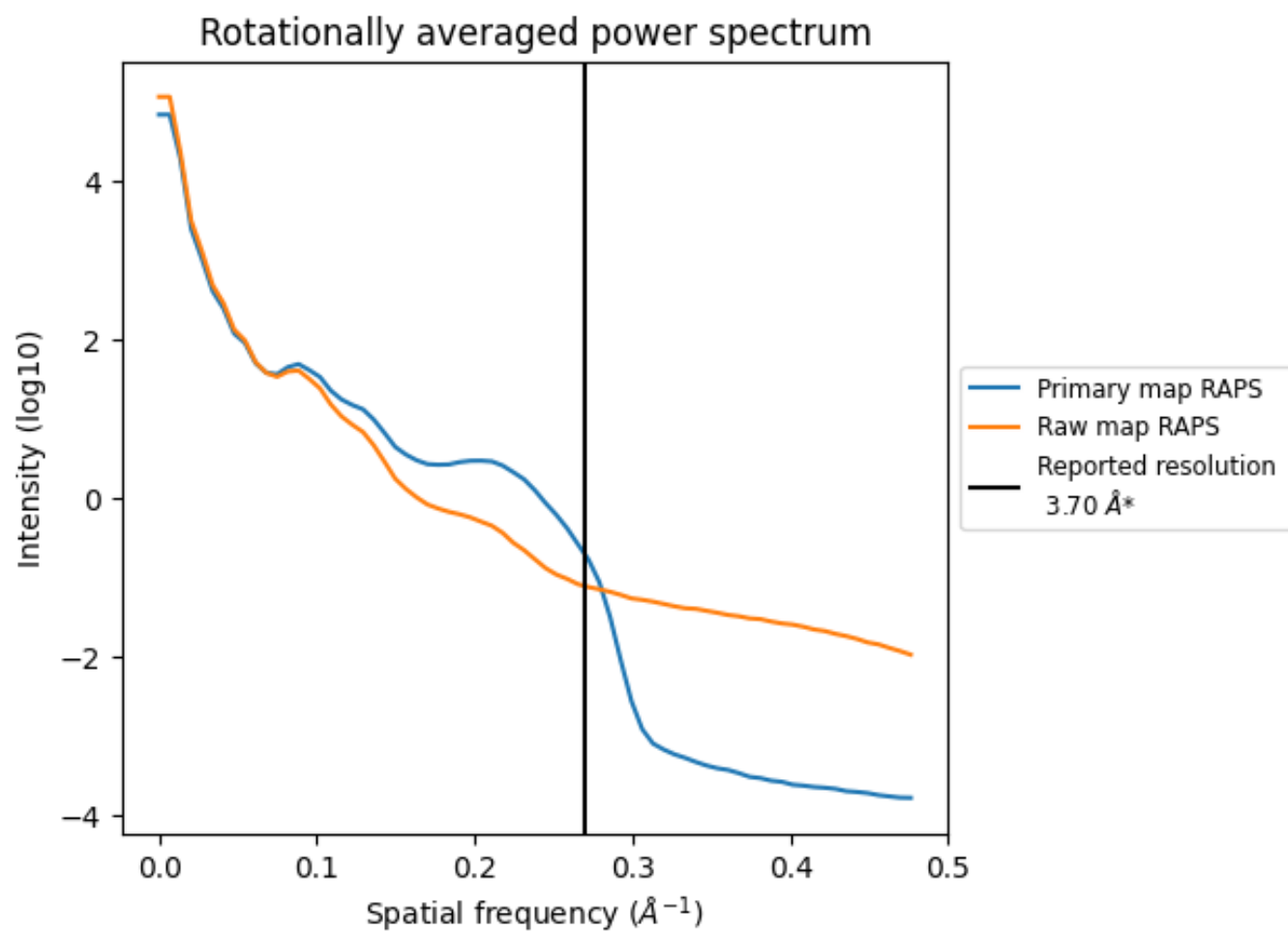
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm^3 ; this corresponds to an approximate mass of 123 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 ⓘ

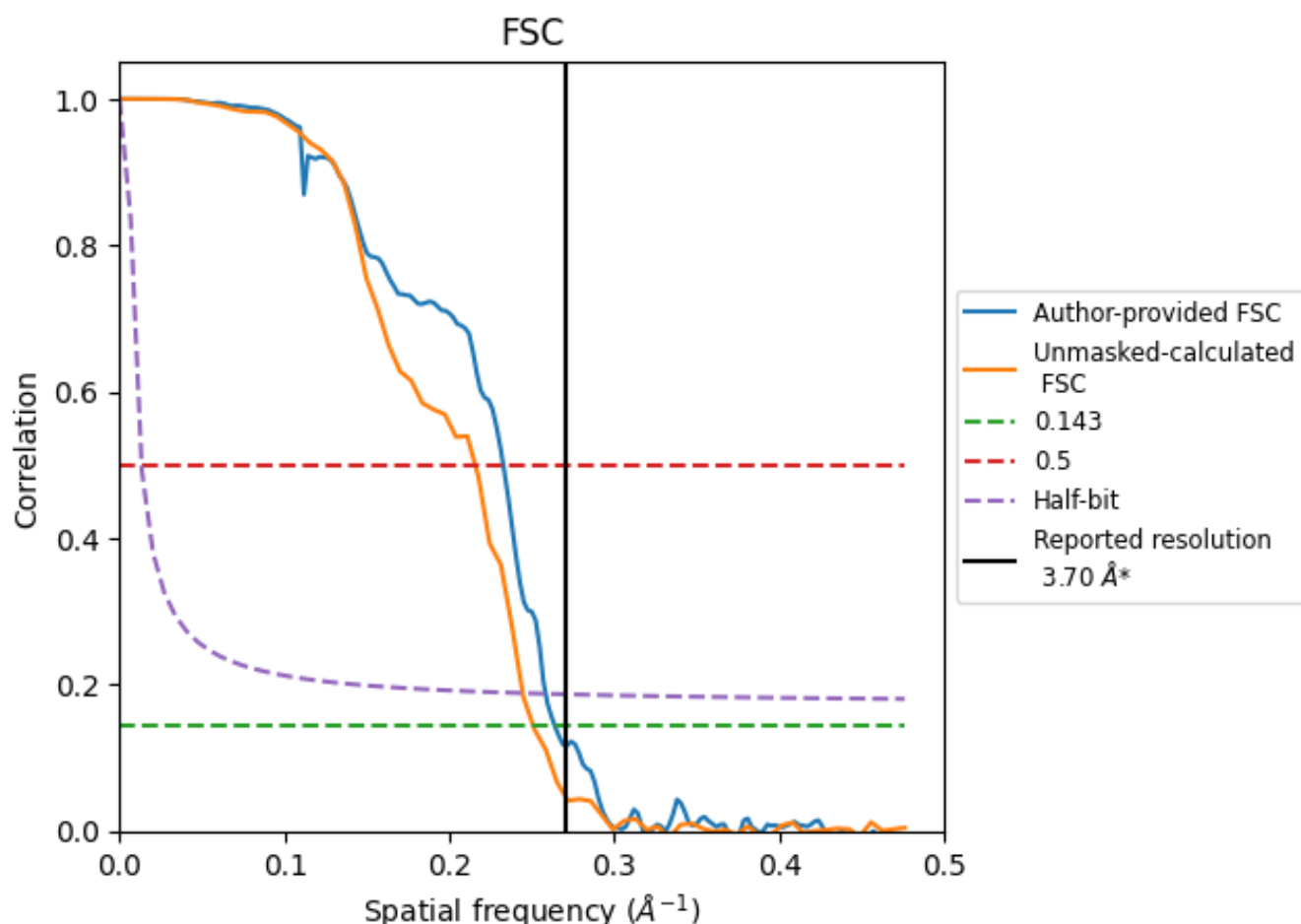


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

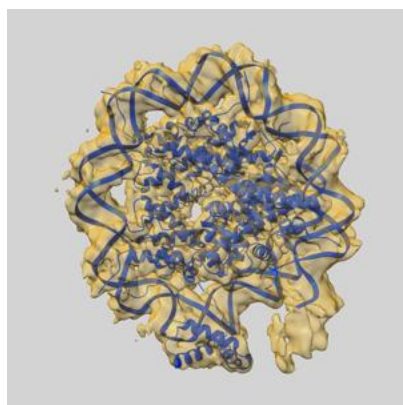
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.79	4.30	3.86
Unmasked-calculated*	3.99	4.64	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

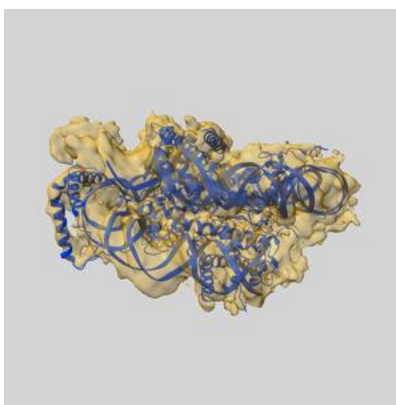
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10391 and PDB model 6T7A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

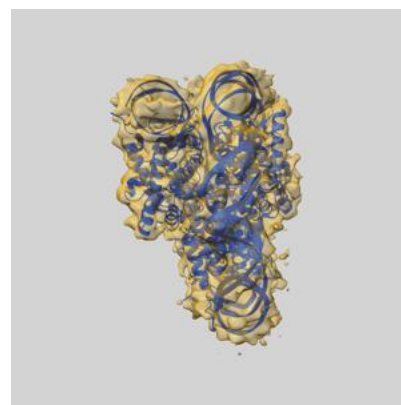
9.1 Map-model overlay [i](#)



X



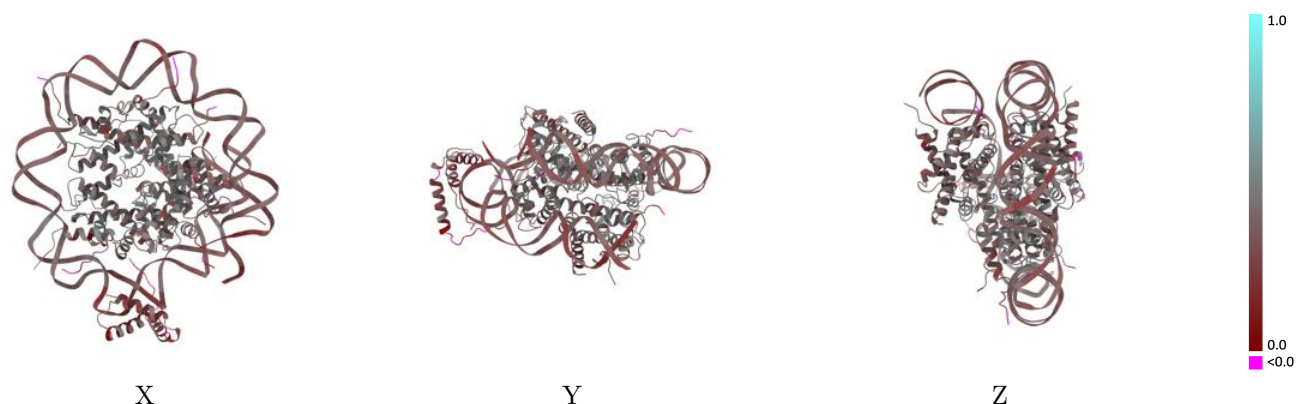
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)



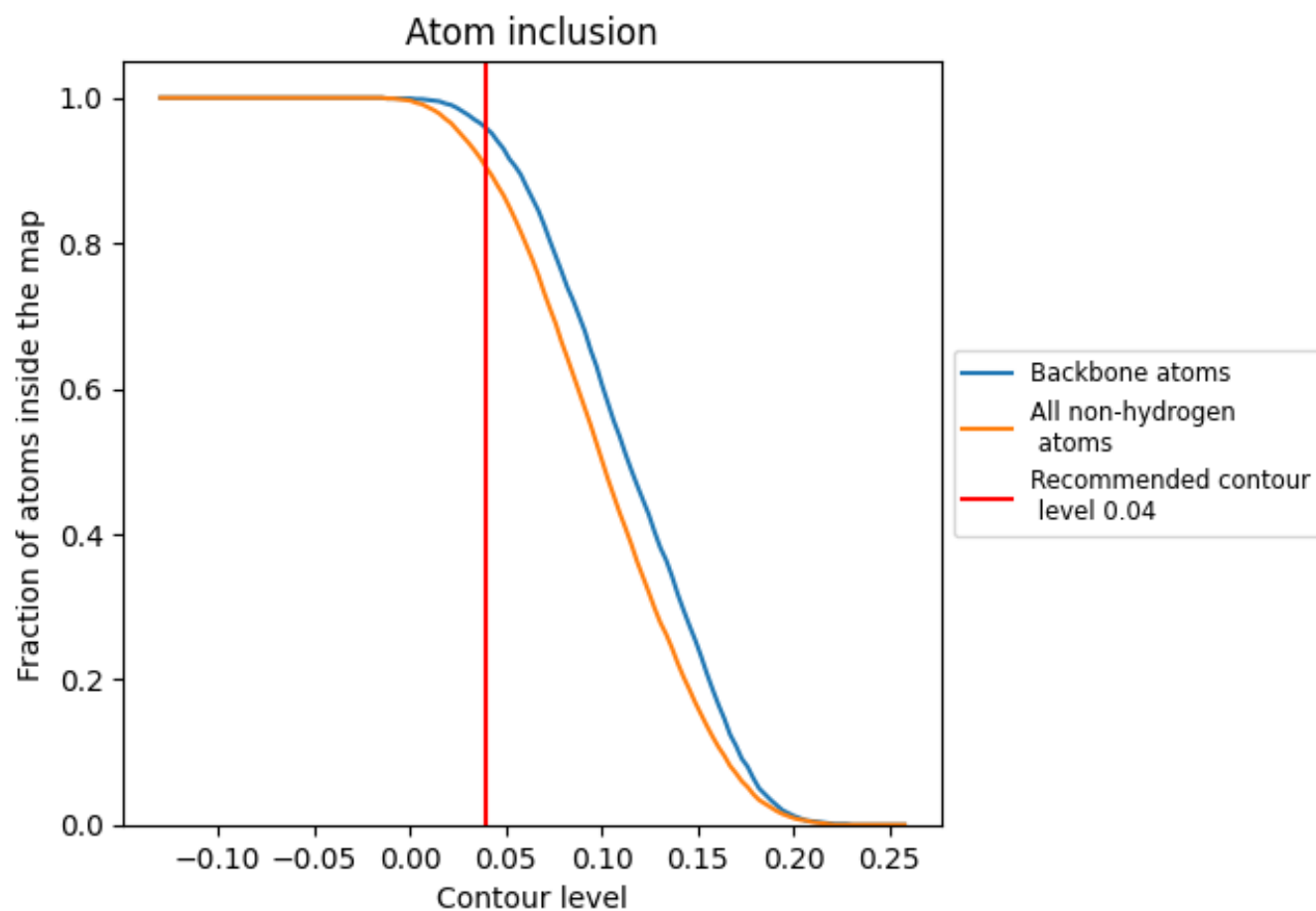
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9040	<div></div> 0.3700
A	<div></div> 0.8830	<div></div> 0.4160
B	<div></div> 0.8680	<div></div> 0.4070
C	<div></div> 0.8730	<div></div> 0.4130
D	<div></div> 0.8520	<div></div> 0.3890
E	<div></div> 0.9000	<div></div> 0.4200
F	<div></div> 0.8230	<div></div> 0.3770
G	<div></div> 0.8460	<div></div> 0.4040
H	<div></div> 0.8700	<div></div> 0.3840
I	<div></div> 0.9770	<div></div> 0.3350
J	<div></div> 0.9720	<div></div> 0.3290
K	<div></div> 0.7650	<div></div> 0.2270

1.0

0.0

<0.0