



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 07:15 AM UTC

PDB ID : 8I4U / pdb_00008i4u
EMDB ID : EMD-35184
Title : Cryo-EM structure of 5-subunit Smc5/6 hinge region
Authors : Qian, L.; Jun, Z.; Xiang, Z.; Wang, Z.; Tong, C.; Duo, J.; Zhenguo, C.; Wang, L.
Deposited on : 2023-01-21
Resolution : 6.73 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

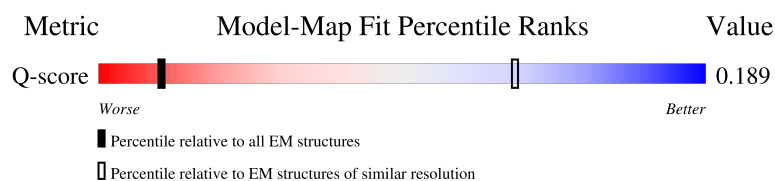
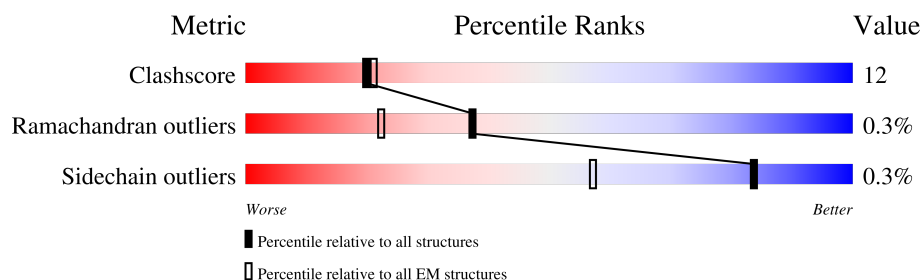
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.73 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	481 (6.23 - 7.23)

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	1093	8% 30% 11% 59%
2	B	1114	7% 30% 11% 59%
3	C	267	10% 54% 19% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18058 atoms, of which 9095 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 Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	453	Total	C	H	N	O	S	0	0
			7487	2297	3811	658	708	13		

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	458	Total	C	H	N	O	S	0	0
			7483	2290	3759	686	736	12		

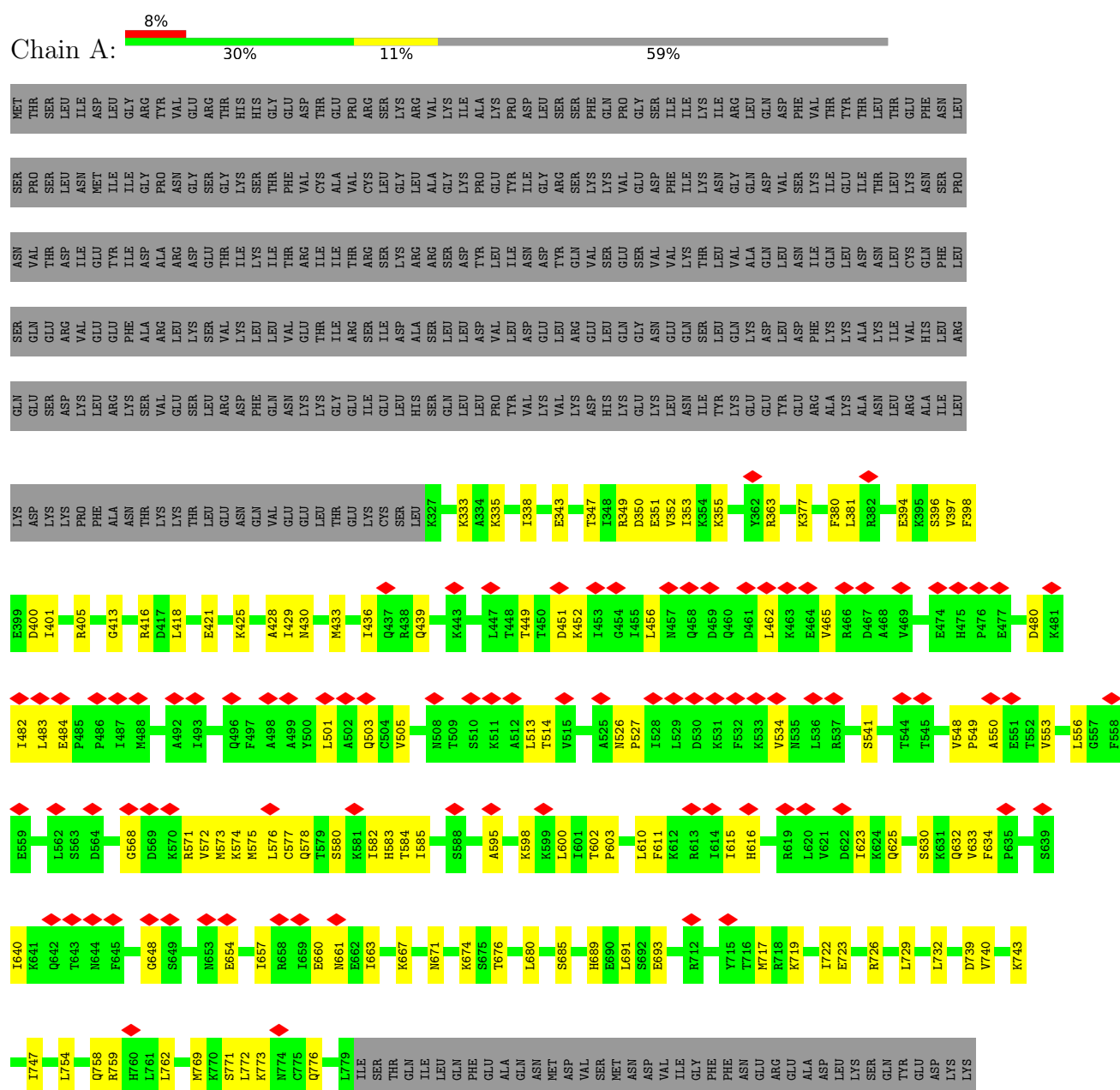
- Molecule 3 is a protein called E3 SUMO-protein ligase MMS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	197	Total	C	H	N	O	S	0	0
			3088	968	1525	260	323	12		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Structural maintenance of chromosomes protein 5

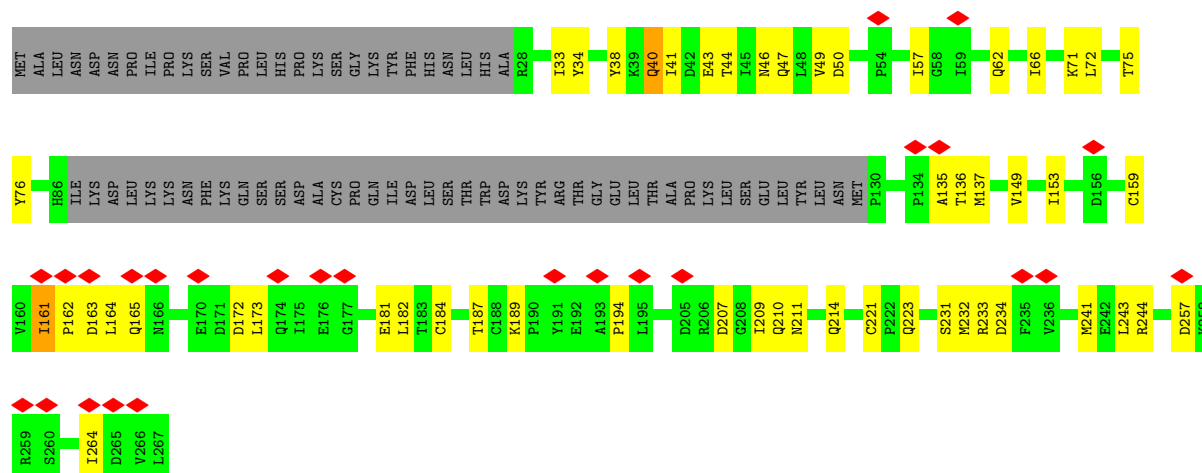


- Molecule 2: Structural maintenance of chromosomes protein 6



R736	A645	S558	Q475	ILE	ASN	SER	ARG	ALA	SER
G759	A646	S559	H476	GLU	GLU	HIS	ASP	ILE	SER
V762	L649	N562	E477	ALA	THR	PHE	GLY	THR	SER
M768	Q650	A563	R478	GLN	LYS	MET	PRO	ILE	ASP
I771	V654	V566	E479	ASP	MET	GLY	SER	GLY	VAL
Q777	M655	N567	R487	ILE	LEU	THR	PHE	LEU	ALA
A659	M656	M568	M491	GLN	GLN	LEU	SER	GLY	THR
A659	M657	P569	K492	ALA	ALA	LEU	SER	ALA	ALA
L660	M658	K570	K493	SER	LYS	GLN	ARG	LYS	ASP
E789	A659	K570	V494	LEU	LEU	GLU	SER	ALA	GLN
E790	L660	D571	E495	THR	THR	ILE	ASN	GLY	ASP
L793	S661	M572	E495	ILE	ILE	GLU	ASN	THR	PHE
K794	L662	R573	D504	ASP	ASP	GLU	GLY	ASN	LEU
I795	R663	L574	T505	VAL	VAL	LEU	GLY	ARG	LEU
E796	D664	F575	T505	ALA	ALA	LEU	GLY	SER	GLU
Q797	S667	R576	M508	HIS	HIS	TYR	SER	GLY	SER
I798	D667	D577	R509	THR	THR	ALA	ASN	LEU	PRO
A799	S667	I578	F510	ASN	ASP	ALA	SER	LEU	SER
E800	G668	M579	D511	VAL	VAL	ILE	ILE	LYS	TYR
E801	Q670	R580	R512	GLU	CYS	ASP	LYS	ASP	GLY
L805	L671	R585	M513	LEU	GLN	ALA	ILE	LEU	LEU
K806	S672	I588	D515	ASN	CYS	HIS	ILE	ILE	LYS
D810	R676	P589	R516	GLU	GLN	ASP	ILE	ARG	LYS
K813	L677	I590	L517	ILE	ASN	TYR	GLN	THR	THR
L816	D678	V591	L518	SER	ILE	ALA	VAL	ALA	ALA
E822	T679	T592	R520	GLY	GLN	PHE	THR	LYS	GLN
Q824	V680	Y593	I521	GLN	GLN	ILE	VAL	ILE	HIS
L829	T681	S596	R524	GLN	GLN	ASN	VAL	HIS	ARG
L830	Y682	A605	K525	LYS	LYS	LEU	SER	LEU	LYS
L831	K685	H606	F528	VAL	VAL	LEU	ASN	ASP	ARG
L832	I686	G607	E529	ARG	ARG	LEU	GLN	GLY	GLY
L833	R687	T611	T530	ASN	ASN	GLY	ALA	GLY	GLY
L834	L688	L612	P531	THR	THR	LEU	ASP	ALA	THR
L835	M691	A615	I533	GLY	GLY	GLY	ALA	GLY	THR
L836	S692	L616	G534	LEU	LEU	GLY	ALA	GLY	THR
L837	M696	E617	P535	GLN	GLN	GLY	ALA	GLY	THR
L838	Q699	F618	L536	GLU	GLU	GLY	ALA	GLY	THR
L839	S619	G537	G537	LYS	LYS	GLY	ALA	GLY	THR
L840	K620	S538	S538	ILE	ILE	GLY	ALA	GLY	THR
L841	P621	L539	L539	GLU	GLU	ARG	ALA	GLY	THR
L842	E622	L539	V540	ARG	ARG	GLY	ALA	GLY	THR
L843	I623	T541	T541	THR	THR	LEU	SER	ILE	THR
L844	R715	I542	F541	ASN	ASN	GLY	THR	ILE	THR
L845	R716	R716	E542	SER	SER	GLN	THR	GLY	THR
L846	D717	R718	R543	GLY	GLY	GLN	GLN	VAL	THR
L847	R718	R718	R543	ASP	ASP	THR	GLN	GLU	THR
L848	Y719	D628	K544	THR	THR	ASP	ASP	ILE	THR
L849	D629	D629	K544	THR	THR	THR	THR	THR	THR

- Molecule 3: E3 SUMO-protein ligase MMS21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99526	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.631	Depositor
Minimum map value	-7.986	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	680.96, 680.96, 680.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.128, 2.128, 2.128	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	0.35	1/3719 (0.0%)	0.57	3/4986 (0.1%)
2	B	0.26	0/3760	0.52	1/5036 (0.0%)
3	C	0.24	0/1589	0.57	0/2156
All	All	0.30	1/9068 (0.0%)	0.55	4/12178 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	MET	C-O	-7.72	1.15	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	SER	N-CA-C	-12.55	98.41	112.72
1	A	717	MET	N-CA-C	-6.19	104.44	111.07
1	A	717	MET	CA-C-O	-5.53	115.02	120.82
2	B	578	ILE	N-CA-C	-5.48	107.03	111.91

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	3676	3811	3810	89	0
2	B	3724	3759	3756	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1563	1525	1524	45	0
All	All	8963	9095	9090	224	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 12.

The worst 5 of 224 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:548:VAL:HG22	1:A:553:VAL:HG11	1.52	0.91
2:B:658:MET:SD	2:B:672:SER:OG	2.34	0.85
3:C:40:GLN:O	3:C:44:THR:HG23	1.83	0.78
2:B:504:ASP:OD1	2:B:512:ARG:NH1	2.20	0.75
2:B:381:ASN:OD1	2:B:382:ALA:N	2.20	0.74

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	451/1093 (41%)	402 (89%)	48 (11%)	1 (0%)	43	78
2	B	456/1114 (41%)	409 (90%)	47 (10%)	0	100	100
3	C	193/267 (72%)	154 (80%)	37 (19%)	2 (1%)	12	48
All	All	1100/2474 (44%)	965 (88%)	132 (12%)	3 (0%)	37	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	GLU
3	C	164	LEU

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Mol	Chain	Res	Type
3	C	161	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	418/1003 (42%)	418 (100%)	0	100	100
2	B	416/1003 (42%)	415 (100%)	1 (0%)	87	87
3	C	184/248 (74%)	182 (99%)	2 (1%)	65	76
All	All	1018/2254 (45%)	1015 (100%)	3 (0%)	84	86

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

Mol	Chain	Res	Type
2	B	530	THR
3	C	40	GLN
3	C	43	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	657	ASN
2	B	670	GLN
3	C	174	GLN
2	B	808	GLN
1	A	653	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

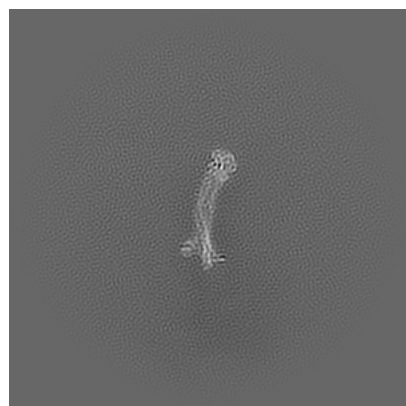
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35184. These allow visual inspection of the internal detail of the map and identification of artifacts.

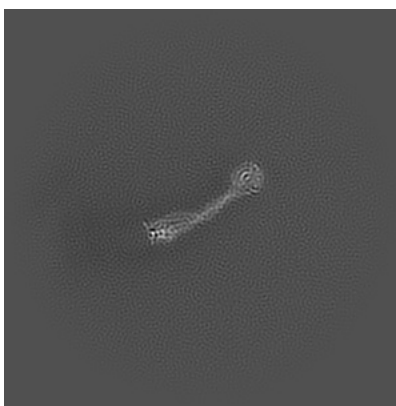
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

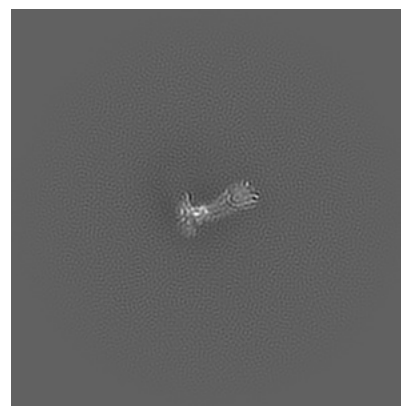
6.1.1 Primary map



X



Y



Z

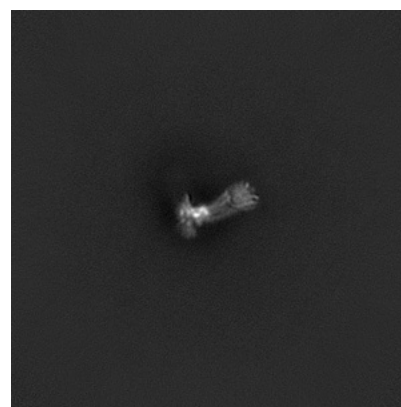
6.1.2 Raw map



X



Y

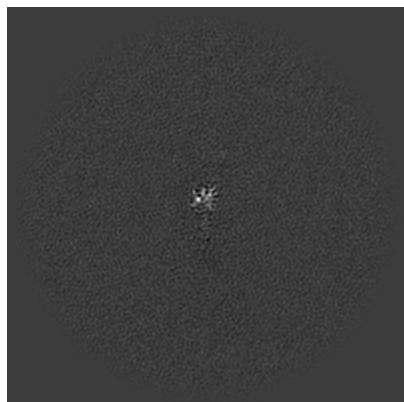


Z

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

6.2 Central slices [i](#)

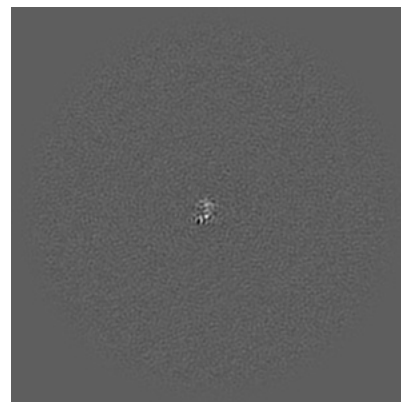
6.2.1 Primary map



X Index: 160

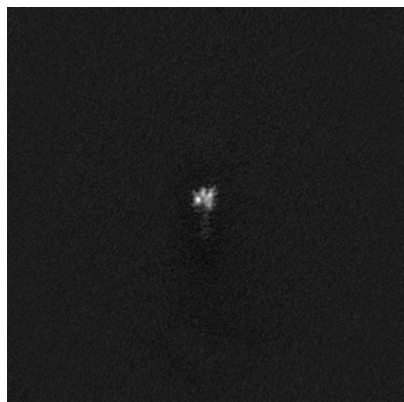


Y Index: 160



Z Index: 160

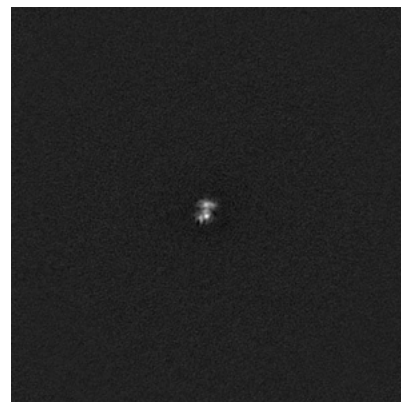
6.2.2 Raw map



X Index: 160



Y Index: 160

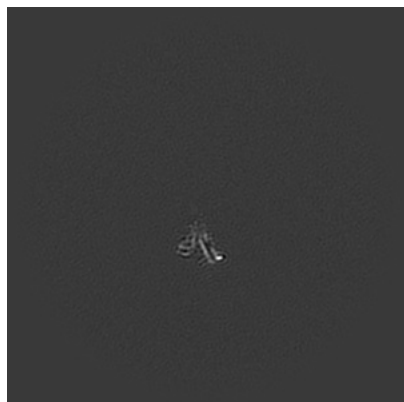


Z Index: 160

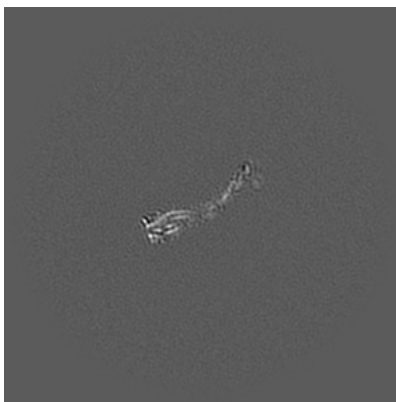
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

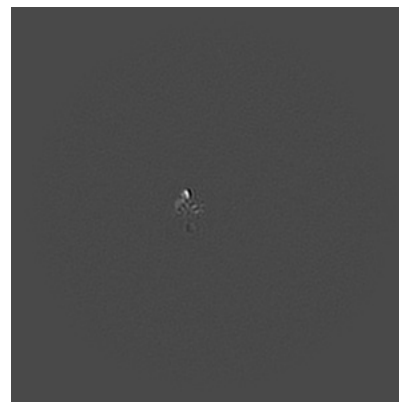
6.3.1 Primary map



X Index: 141

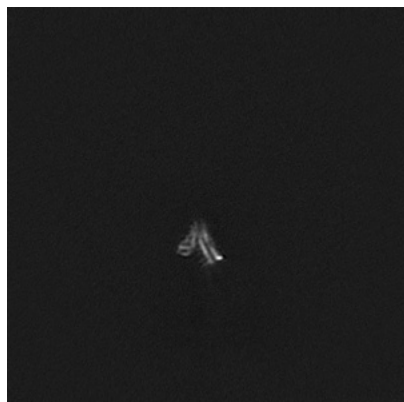


Y Index: 159



Z Index: 119

6.3.2 Raw map



X Index: 141



Y Index: 159



Z Index: 119

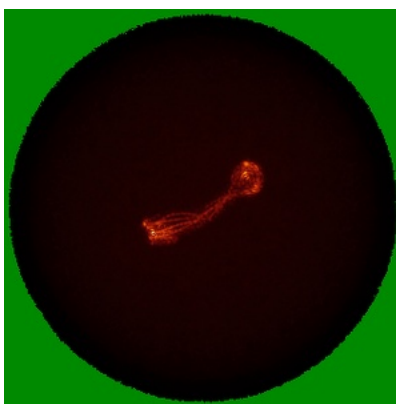
The images above show the largest variance slices of the map in three orthogonal directions.

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

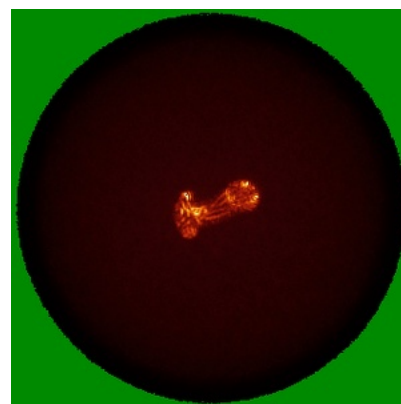
6.4.1 Primary map



X

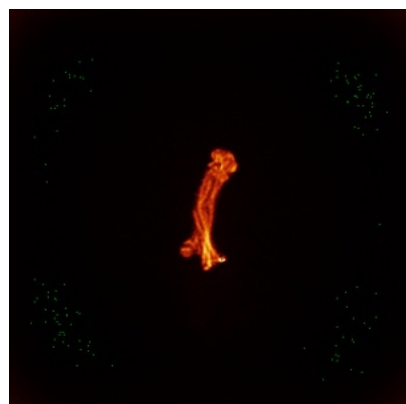


Y

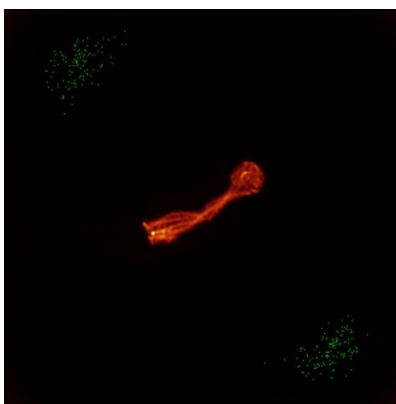


Z

6.4.2 Raw map



X



Y

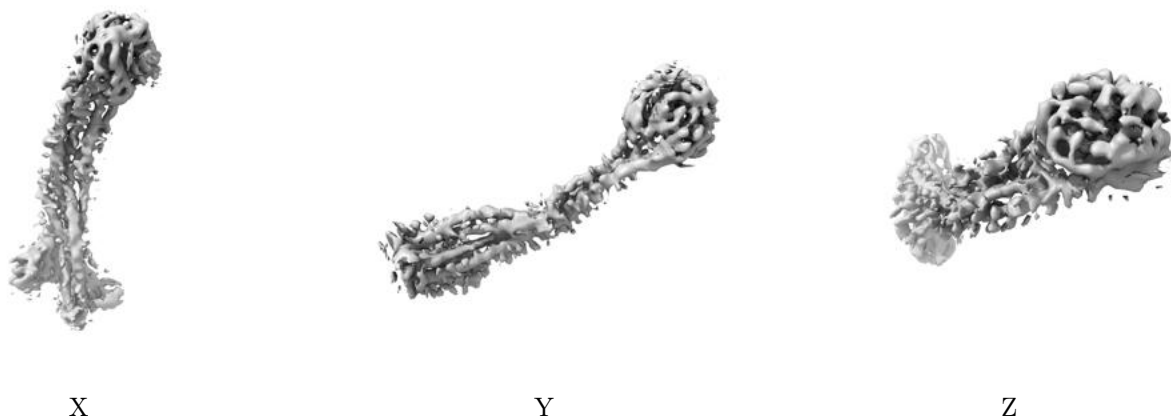


Z

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.

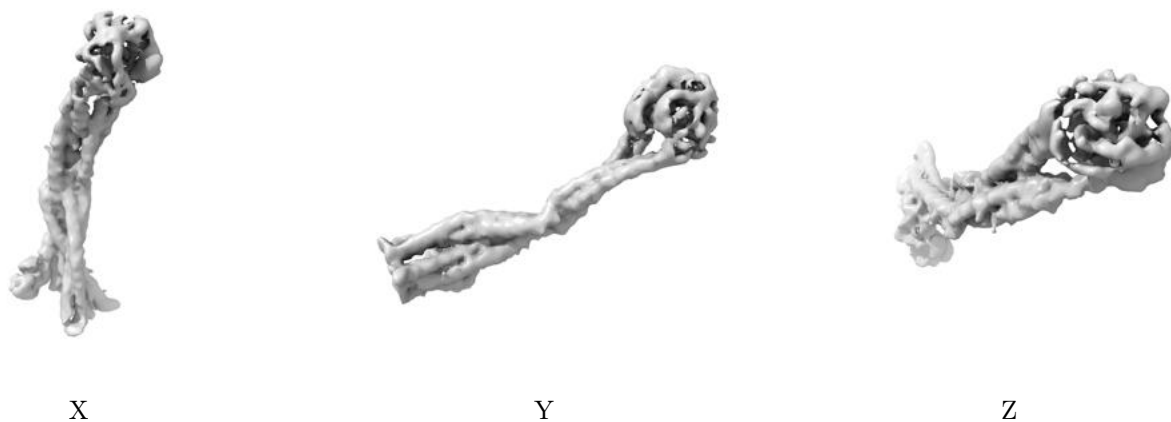
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

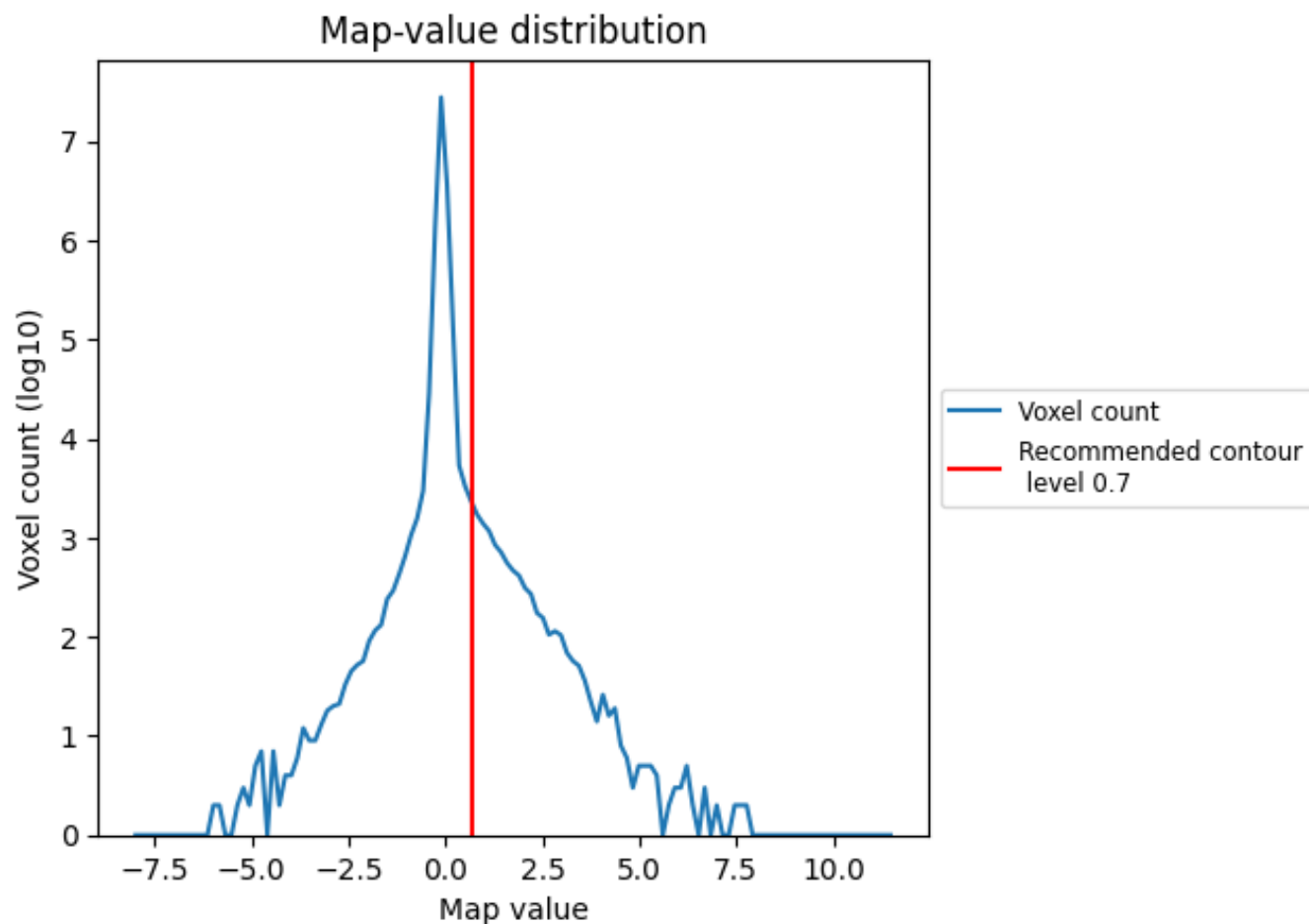
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

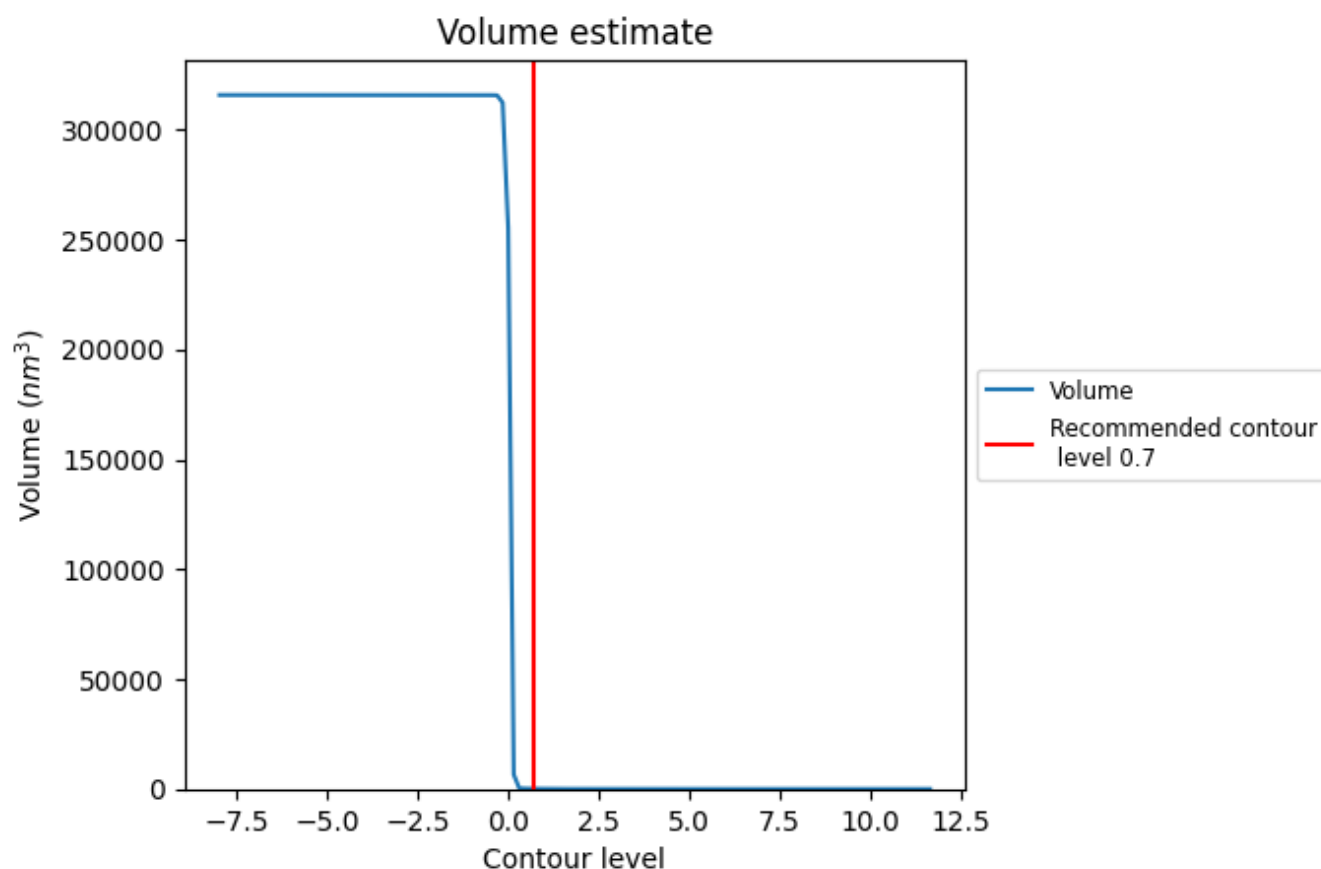
This section contains the results of statistical analysis of the map.

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.

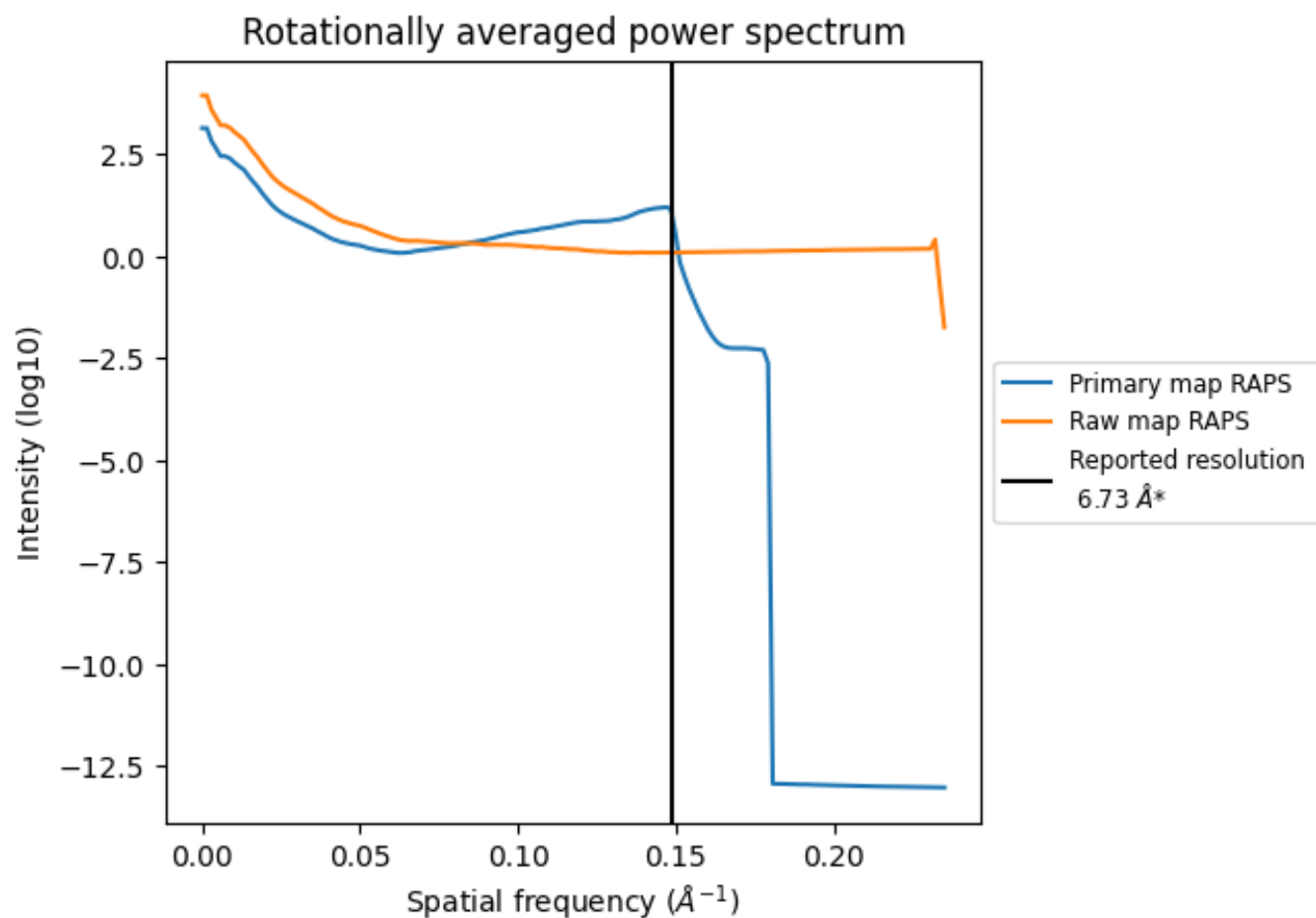
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm^3 ; this corresponds to an approximate mass of 93 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 ⓘ

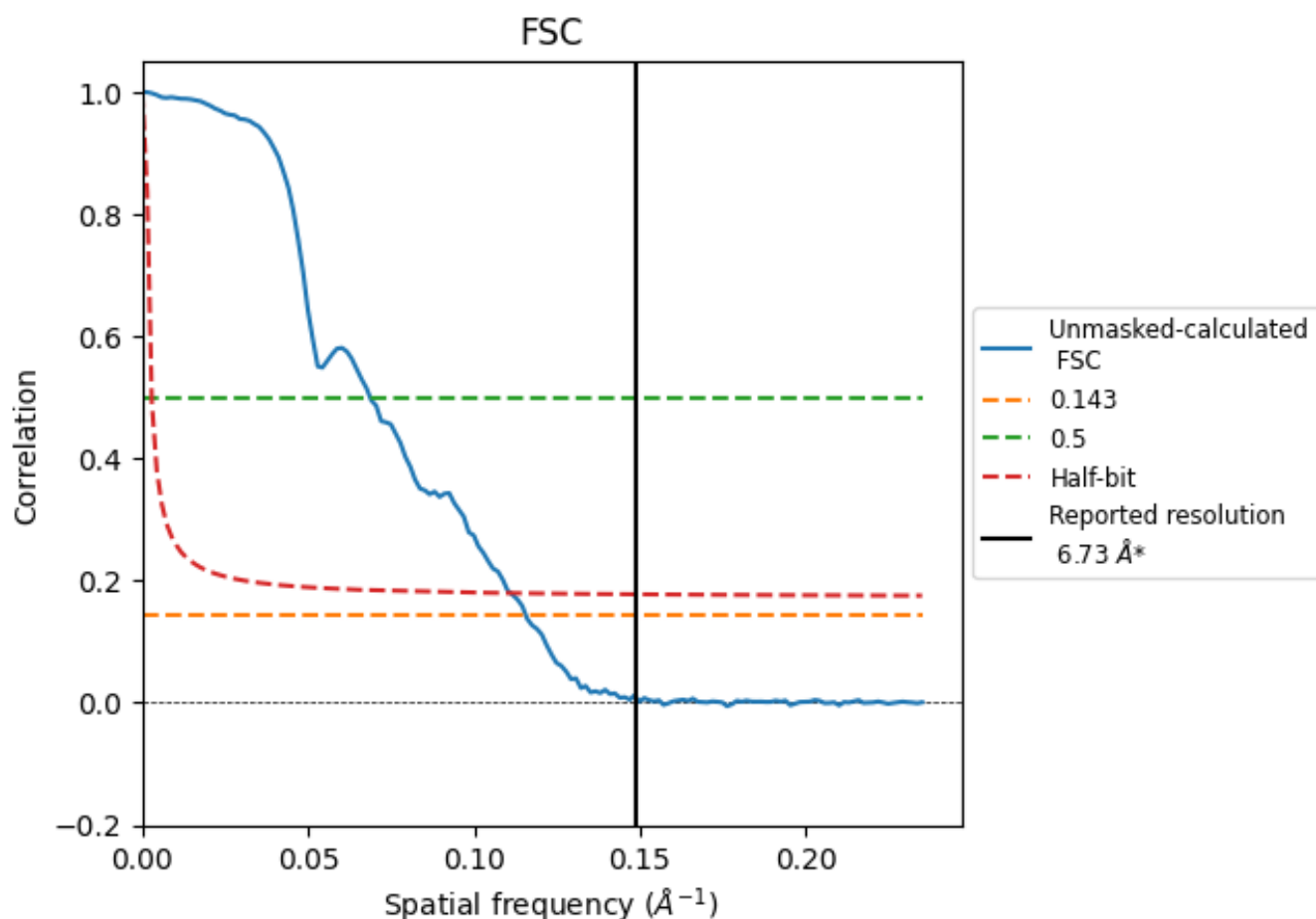


*Reported resolution corresponds to spatial frequency of 0.149 $\text{\AA}^{-1}$

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 0.149 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

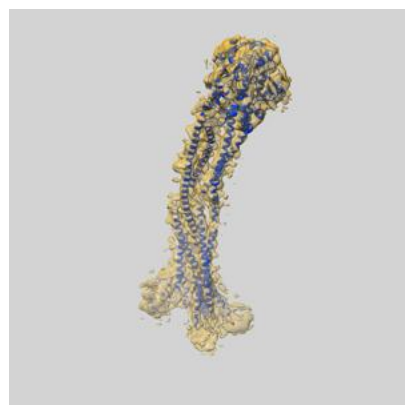
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.65	14.58	9.01

*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 8.65 differs from the reported value 6.73 by more than 10 %

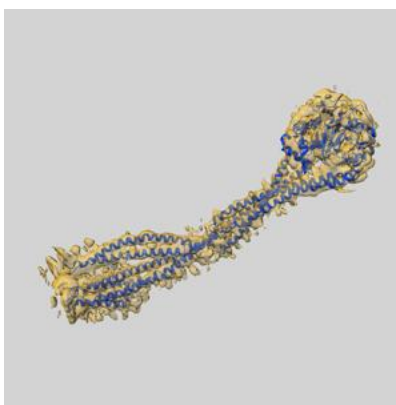
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35184 and PDB model 8I4U. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

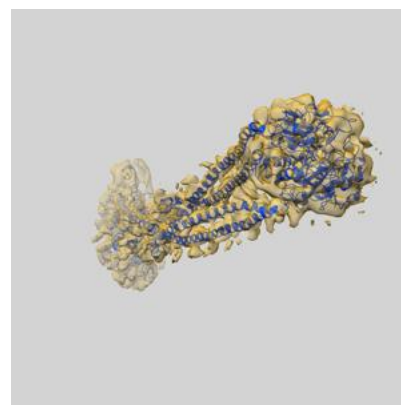
9.1 Map-model overlay [i](#)



X



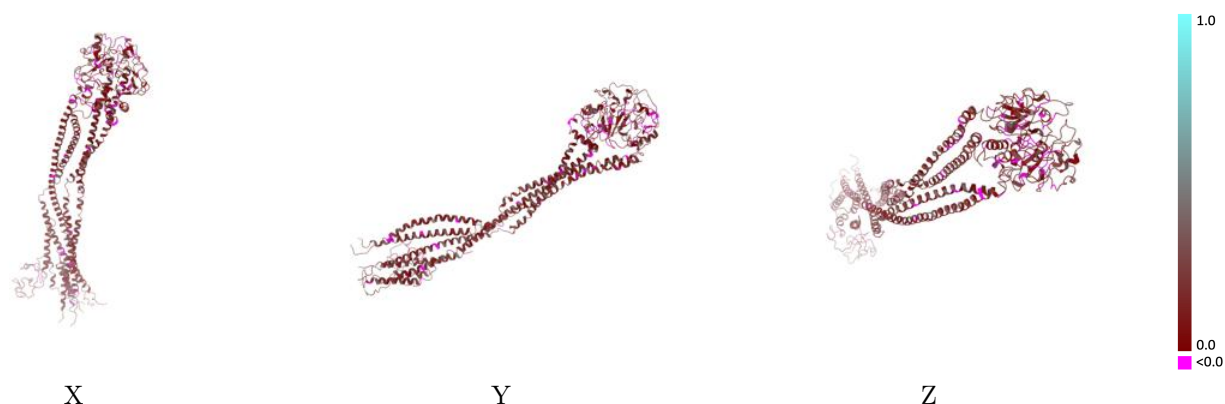
Y



Z

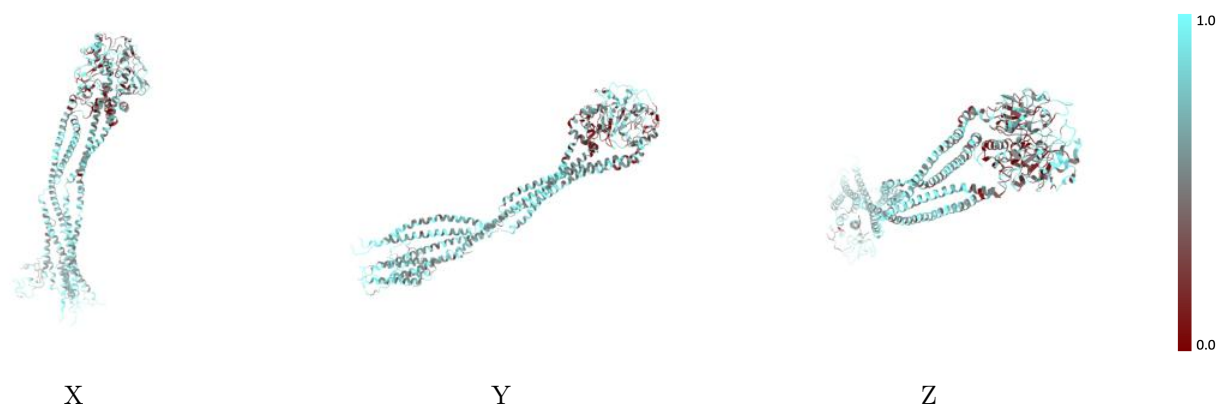
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



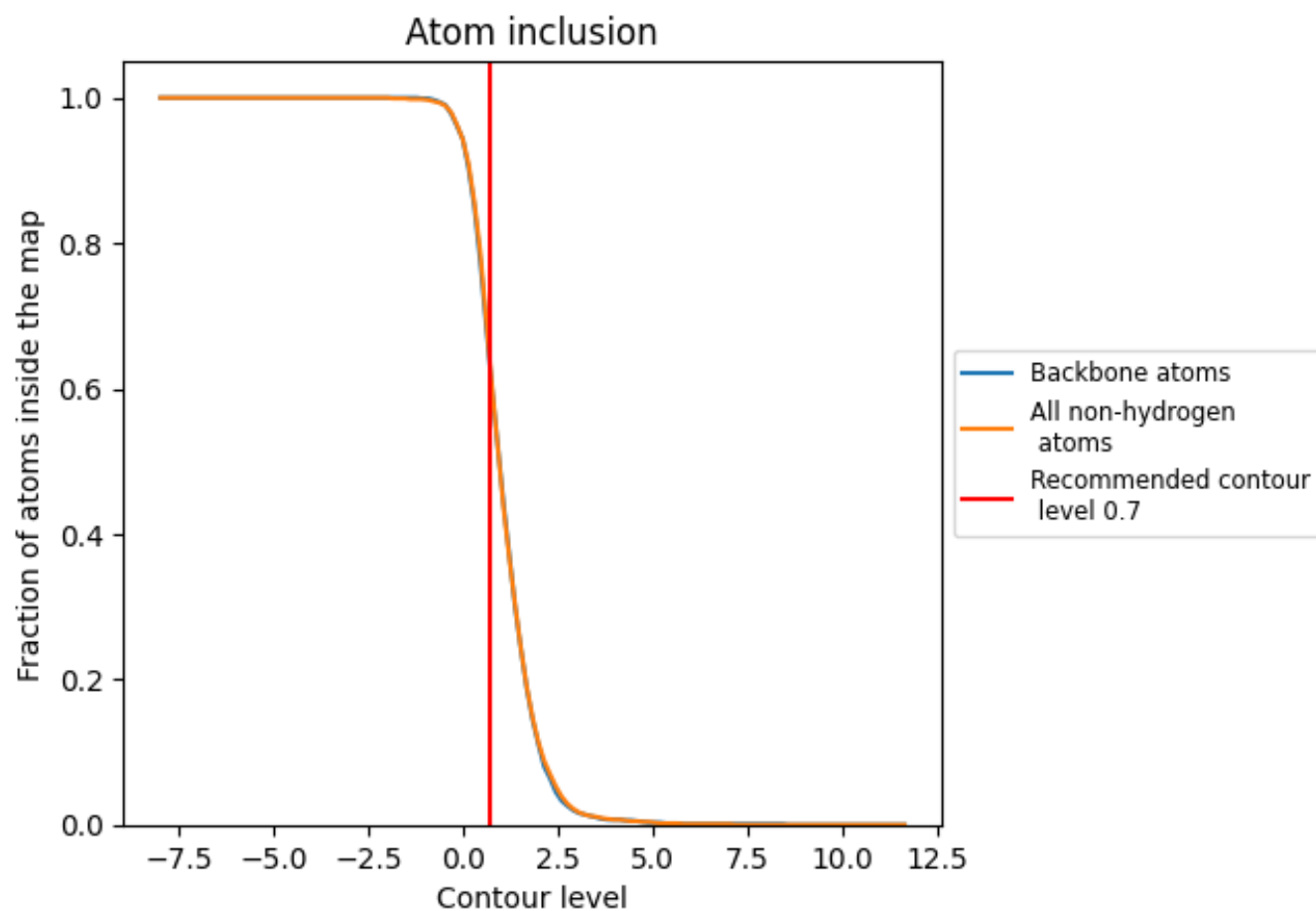
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.1890
A	0.6170	0.1790
B	0.6490	0.1880
C	0.6950	0.2120

