



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2025 – 08:26 PM JST

PDB ID : 8WJL / pdb_00008wjl
EMDB ID : EMD-37584
Title : Cryo-EM structure of 6-subunit Smc5/6 hinge region
Authors : Li, Q.; Zhang, J.; Zhang, X.; Cheng, T.; Wang, Z.; Jin, D.; Chen, Z.; Wang, L.
Deposited on : 2023-09-26
Resolution : 6.15 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

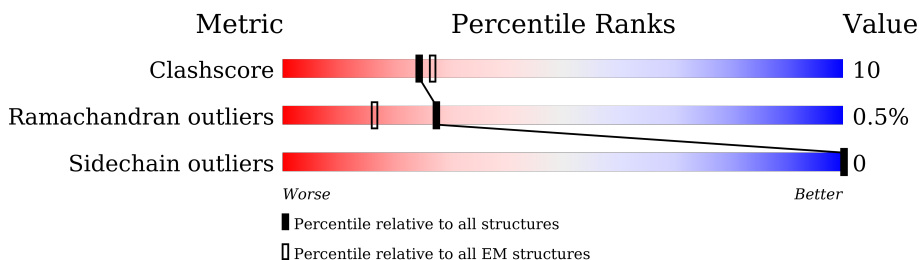
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.15 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	1114	
2	A	1093	
3	C	267	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17995 atoms, of which 9066 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 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	458	Total	C	H	N	O	S	0	0
			7491	2292	3763	686	738	12		

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	454	Total	C	H	N	O	S	0	0
			7500	2302	3818	659	708	13		

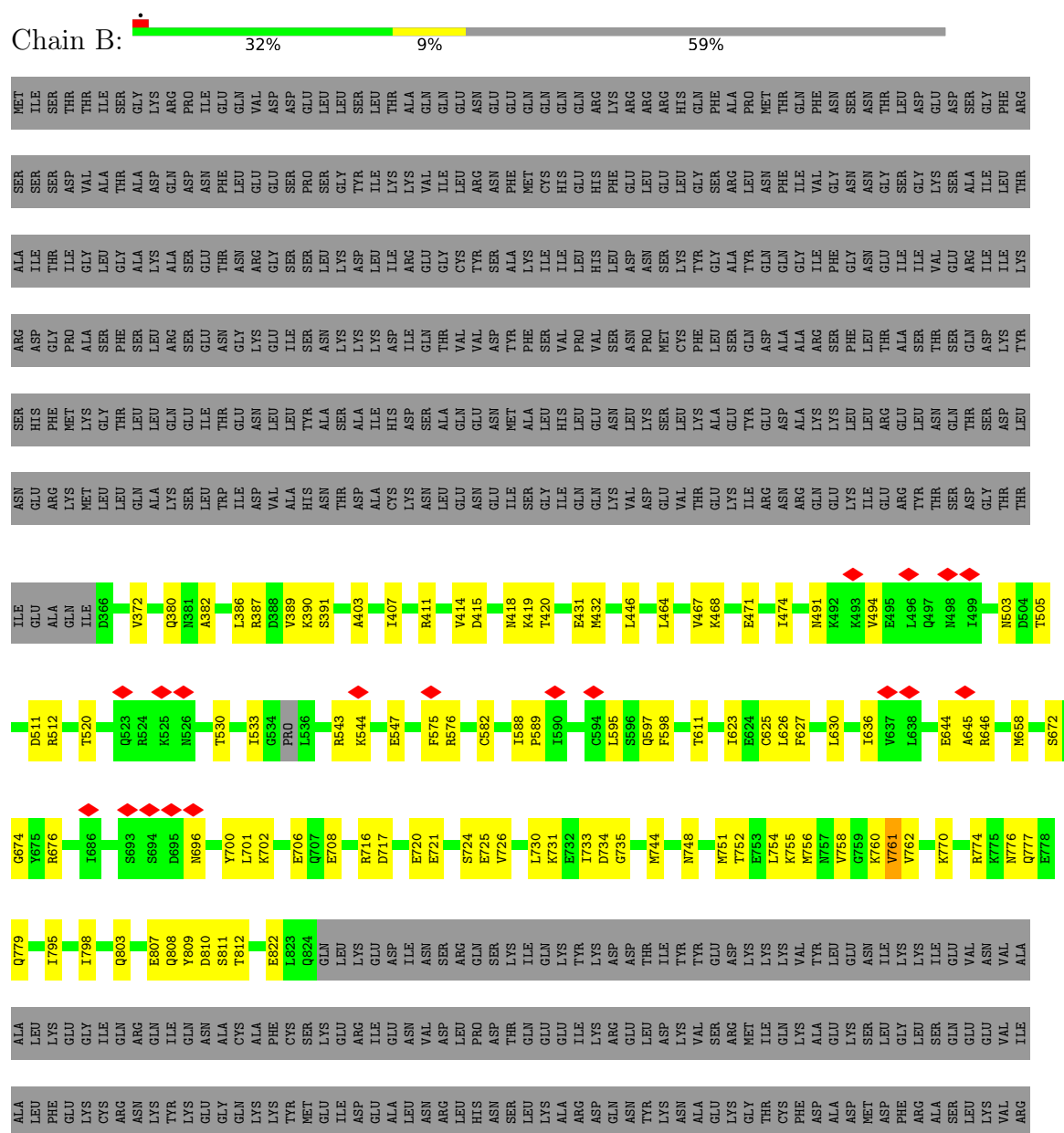
- Molecule 3 is a protein called E3 SUMO-protein ligase MMS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	192	Total	C	H	N	O	S	0	0
			3004	942	1485	250	315	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 6



GLN
ASN
ASN
SER
ASN
PHE
TYR
ASN

- Molecule 2: Structural maintenance of chromosomes protein 5

Chain A:  31% 10% 58%

GLN
GLU
SER
ASP
LYS
LEU
ARG
LYS
SER
VAL
GLU
SER
LEU
ARG
ASP
PHE
GLN
ASN
LYS
LYS
GLY
GLU
ILE
GLU
LEU
LEU
PRO
TYR
VAL
LYS
VAL
LYS
ASP
HIS
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GLU
LYS
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ASN
ILE
TYR
LYS
GLU
TYR
GLU
ARG
ALA
ALA
ASN
LEU
ARG
ALA
ILE
PHE

LYS	LYS	LYS	LYS	PRO	PHE	ALA	ASN	LYS	LYS	THR	THR	LEU	GLU	ASN	GLN	VAL	GLU	GLU	LEU	THR	GLU	LYS	CYS	SER	L326	F331	K335	T338	N339	E340	T341	F342	E343	K344	L345	T347	L348	E351	V352	L353	N359	E360	L369	Q370	A371	T372	T373	T374	S375	T376
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Q389	E394	K395	S396	V397	F398	E399	D400	D401	D402	D403	K404	R405	K406	E407	I408	I409		L418		I422		A428	I429	M430	H431	E432		L447	T448	T449		D459	Q460		E474	H475	P476	E477		L482	L483	E484	P485	P486	I487	L488	M488	T489	V490		A495		L513	T514		Y521	K522	L523	
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[illegible]

M632	M633	M634	H706	H709	R712	R713	K714	K715	K716	R726	E727	A736	V740	S741	K742	K743	L754	K773	K774	K775	K776	L779	ILE	SER	THR	GLN	GLN	ILE	ILE	LEU	GLN	PHE	GLU	ALA	ALA	GLN	ASN	ASN	NET	ASP	VAL	SER	SER	NET	ASN	ASP
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VAL	ILE	GLY	PHE	PHE	ASN	GLU	ARG	GLU	ALA	ASP	LYS	SER	GLN	TYR	GLU	ASP	LYS	LYS	PHE	PHE	VAL	VAL	GLY	GLU	MET	ARG	THR	ASP	PRO	GLU	PHE	GLN	SER	TRP	MET	ARG	GLU	ILE	SER	ARG	SER	TYR	ASP	GLN	ASP	THR	THR	LYS	GLU	LYS	LEU	ASN	LYS	VAL	ALA	GLU	LYS	TYR	GLU	GLU	GLU
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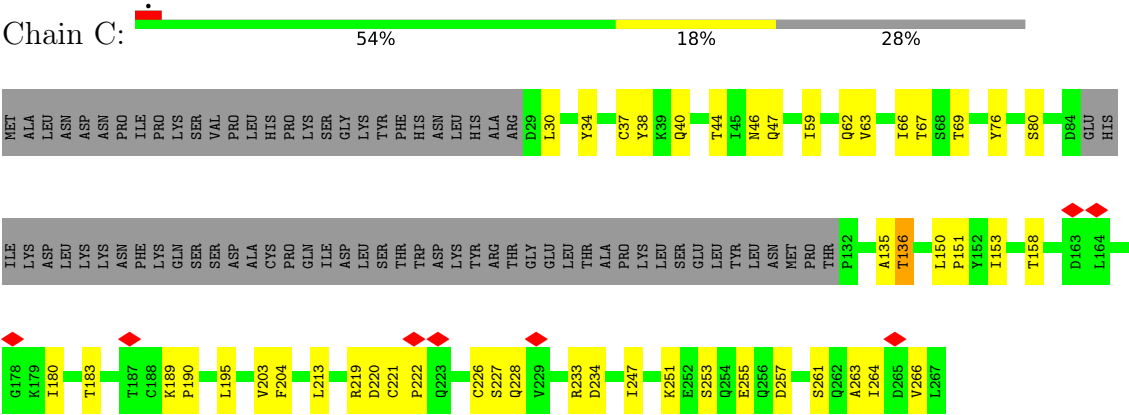
GLY	ASN	PHE	ASN	LEU	SER	PHE	VAL	GLN	ASP	LEU	ASP	LYS	LEU	GLU	SER	GLU	ILE	ALA	LEU	VAL	ASN	ASN	HIS	ASP	GLU	SER	GLU	ALA	ALA	VAL	THR	THR	ILE	LEU	LEU	ASP	ASP	GLN	VAL	THR	VAL	ALA	ALA	GLU	LEU	LEU	GLU	LEU	GLY
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LYS	GLU	ASP	HIS	ALA	VAL	LEU	GLU	PRO	LYS	LEU	ASP	ASP	ILE	VAL	LYS	ILE	SER	ALA	ARG	PHE	ASN	ASN	VAL	GLY	SER	ALA	GLY	VAL	ARG	ARG	LEU	PHE	ASN	ASN	VAL	GLY	SER	ALA	GLU	TRP	LYS	ILE	GLU	ILE	MET	VAL	LYS	PHE	ARG	ASP	ASN	ALA	ALA	PRO	LEU
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LYS LYS LEU LEU ASP SER HIS THR GLN SER SER GLY GLY GLU ARG ALA VAL VAL SER SER THR VAL VAL LEU TYR MET MET ILE ALA ALA LEU GLN GLU PHE THR THR SER SER ALA PRO PHE ARG ARG VAL VAL VAL ASP ASP GLU GLU ILE ASN ASN GLN GLY MET ASP SER ARG ASN ASN GLU ARG ILE VAL HIS LYS LYS ALA ALA MET VAL VAL ASN ASN CYS ALA ALA

GLU	ASN	THR	SER	GLN	TYR	PHE	LEU	LEU	ILE	THR	THR	LYS	LEU	LEU	GLY	GLY	HIS	TYR	HIS	GLU	LYS	ARG	MET	ILE	CYS	HIS	VAL	LEU	THR	ILE	PRO	PRO	ASN	SER	SER	GLU	ASP	PRO	ASP	LYS	THR	THR	SER	ASN	TYR	SER	ASP	PHE
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● 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	179509	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 (6k x 4k)	Depositor
Maximum map value	7.263	Depositor
Minimum map value	-4.323	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	680.96, 680.96, 680.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	B	0.14	0/3762	0.40	0/5036
2	A	0.14	0/3725	0.43	0/4994
3	C	0.18	0/1543	0.48	0/2093
All	All	0.15	0/9030	0.43	0/12123

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	B	3728	3763	3761	67	0
2	A	3682	3818	3816	98	0
3	C	1519	1485	1484	42	0
All	All	8929	9066	9061	188	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 10.

The worst 5 of 188 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:C:183:THR:OG1	3:C:189:LYS:O	1.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:713:LYS:O	2:A:716:THR:OG1	1.95	0.83
1:B:611:THR:OG1	1:B:636:ILE:O	1.95	0.82
3:C:66:ILE:O	3:C:69:THR:OG1	1.98	0.82
2:A:394:GLU:OE1	2:A:397:VAL:N	2.14	0.80

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	B	454/1114 (41%)	415 (91%)	38 (8%)	1 (0%)	44	78
2	A	452/1093 (41%)	409 (90%)	40 (9%)	3 (1%)	19	57
3	C	188/267 (70%)	160 (85%)	27 (14%)	1 (0%)	25	65
All	All	1094/2474 (44%)	984 (90%)	105 (10%)	5 (0%)	27	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	761	VAL
2	A	650	ILE
2	A	346	ASN
2	A	775	CYS
3	C	136	THR

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	
1	B	417/1003 (42%)	417 (100%)	0	100	100
2	A	418/1003 (42%)	418 (100%)	0	100	100
3	C	179/248 (72%)	179 (100%)	0	100	100
All	All	1014/2254 (45%)	1014 (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 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	431	HIS
3	C	165	GLN
3	C	174	GLN
1	B	457	ASN
1	B	400	GLN

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 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 ⓘ

There are no chain breaks in this entry.

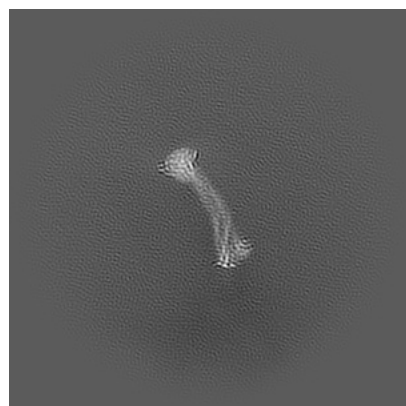
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37584. These allow visual inspection of the internal detail of the map and identification of artifacts.

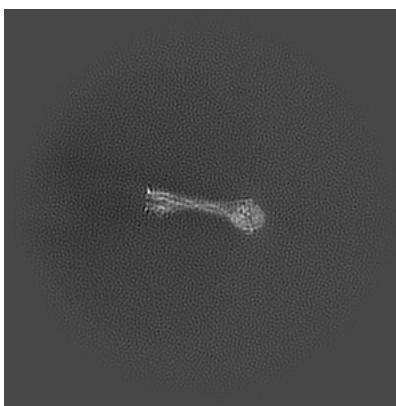
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

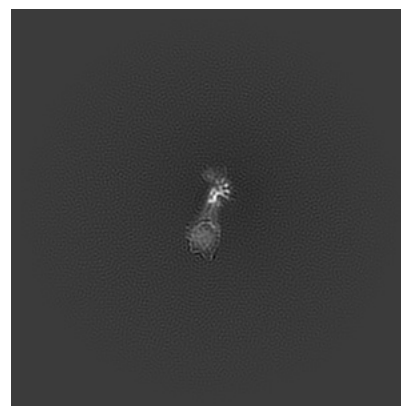
6.1.1 Primary map



X



Y



Z

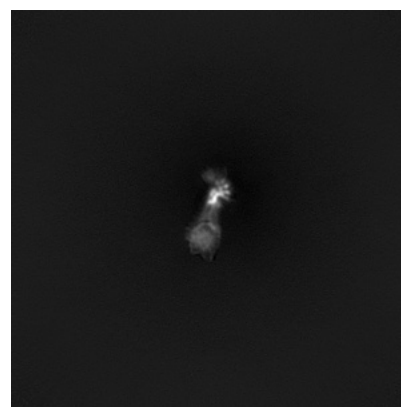
6.1.2 Raw map



X



Y



Z

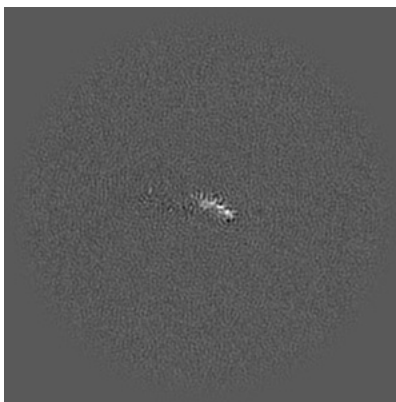
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

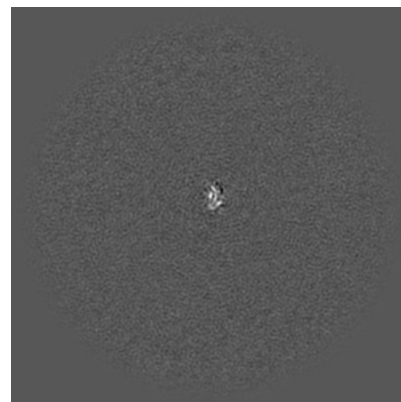
6.2.1 Primary map



X Index: 160

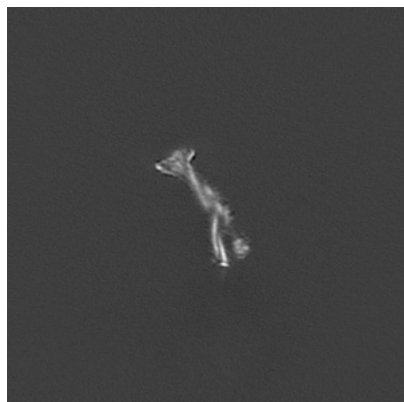


Y Index: 160



Z Index: 160

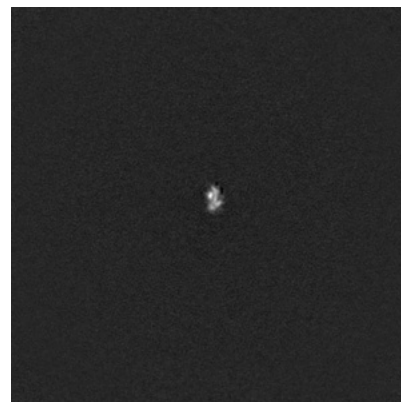
6.2.2 Raw map



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](#)

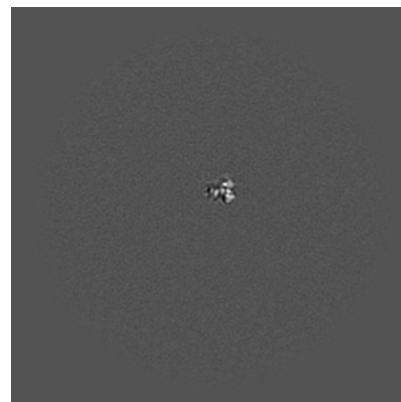
6.3.1 Primary map



X Index: 160

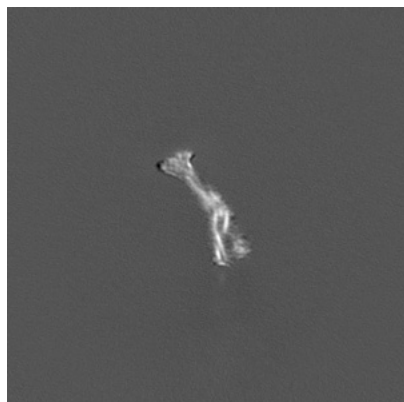


Y Index: 173



Z Index: 115

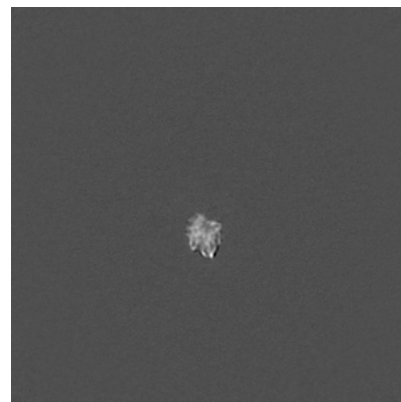
6.3.2 Raw map



X Index: 162



Y Index: 173

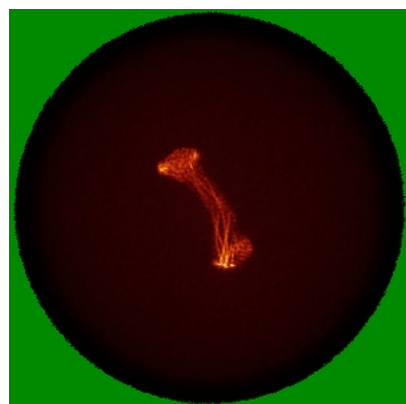


Z Index: 191

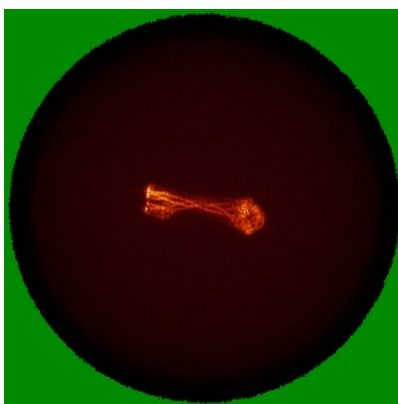
The images above show the largest variance slices of the map in three orthogonal directions.

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

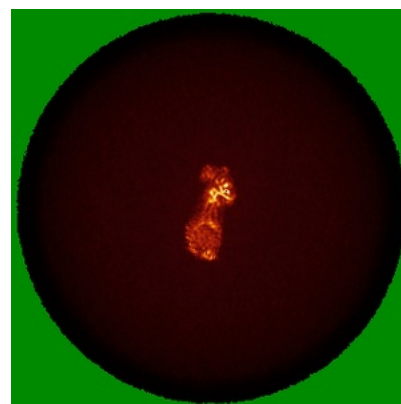
6.4.1 Primary map



X



Y

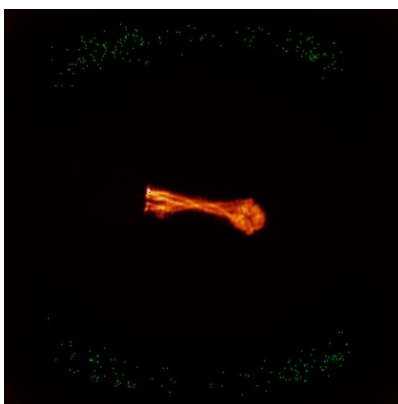


Z

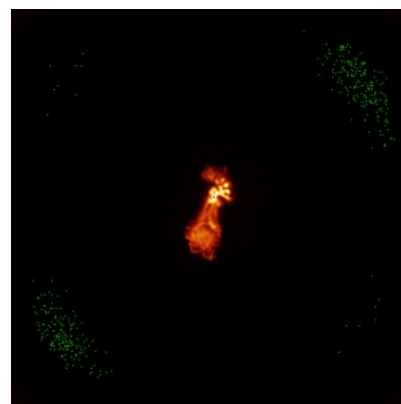
6.4.2 Raw map



X



Y

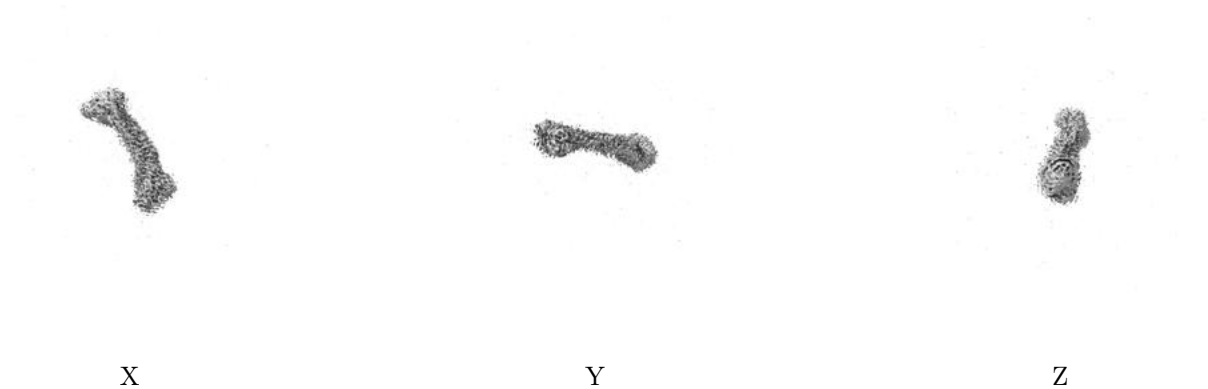


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

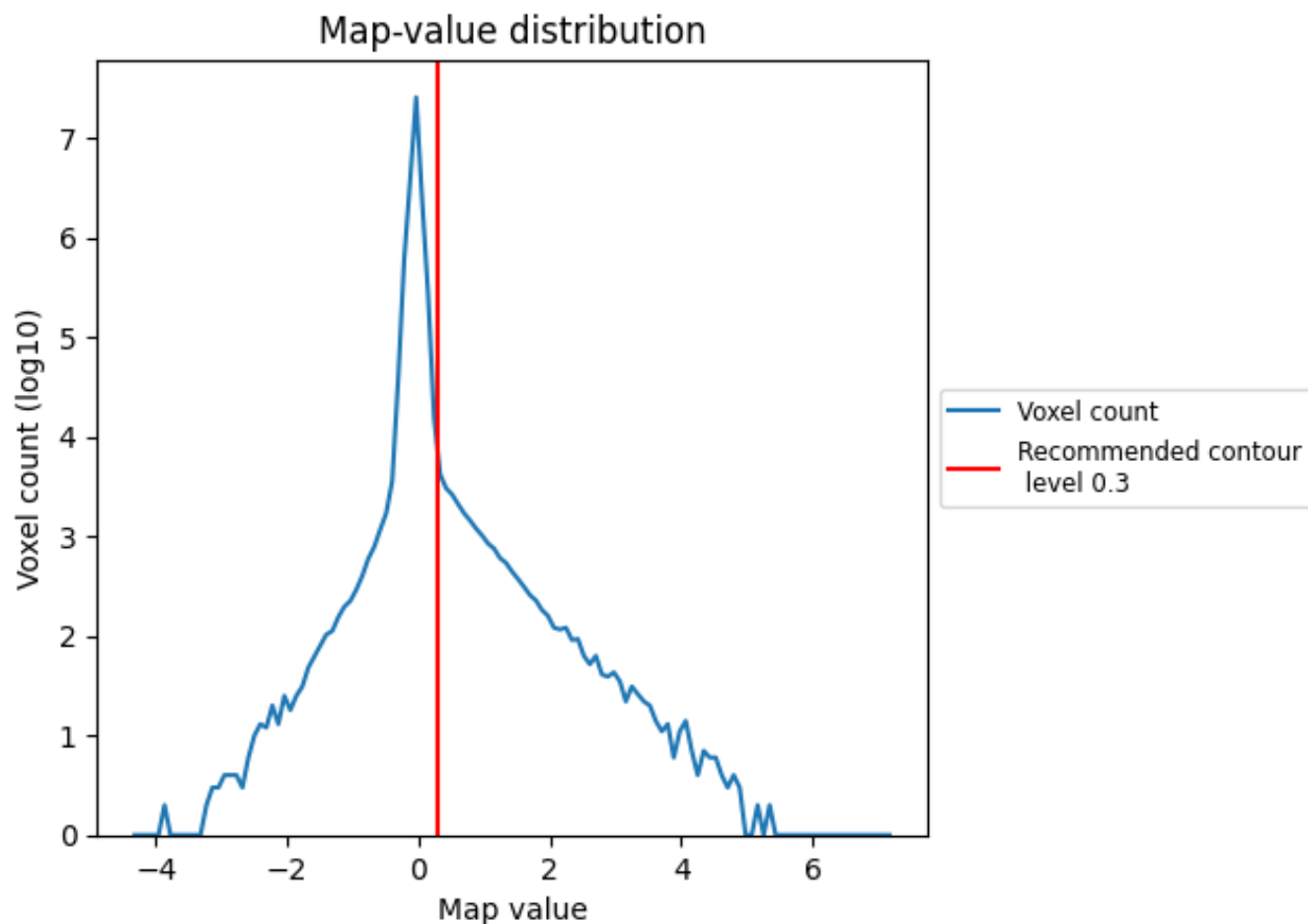
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

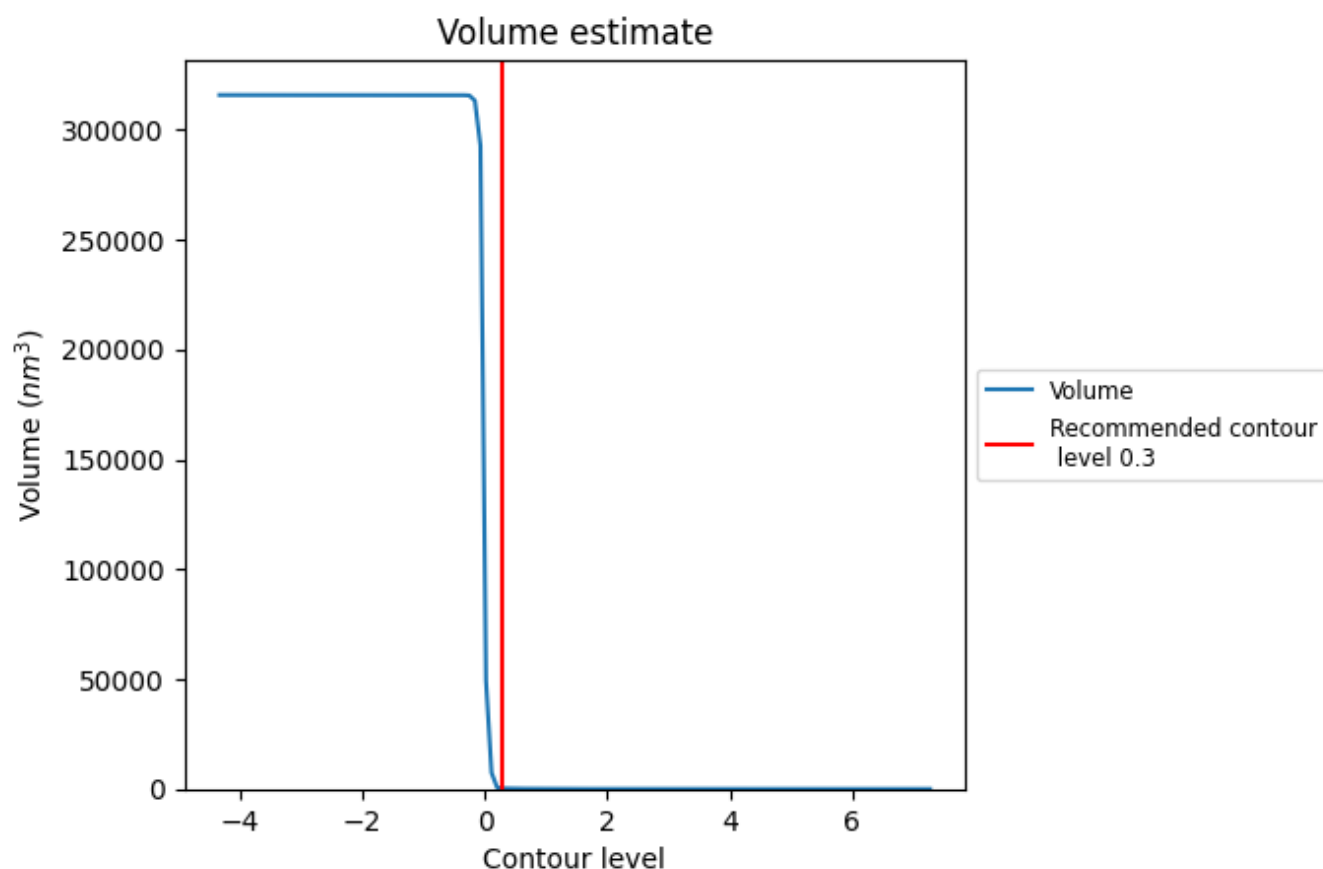
This section contains the results of statistical analysis of the map.

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.

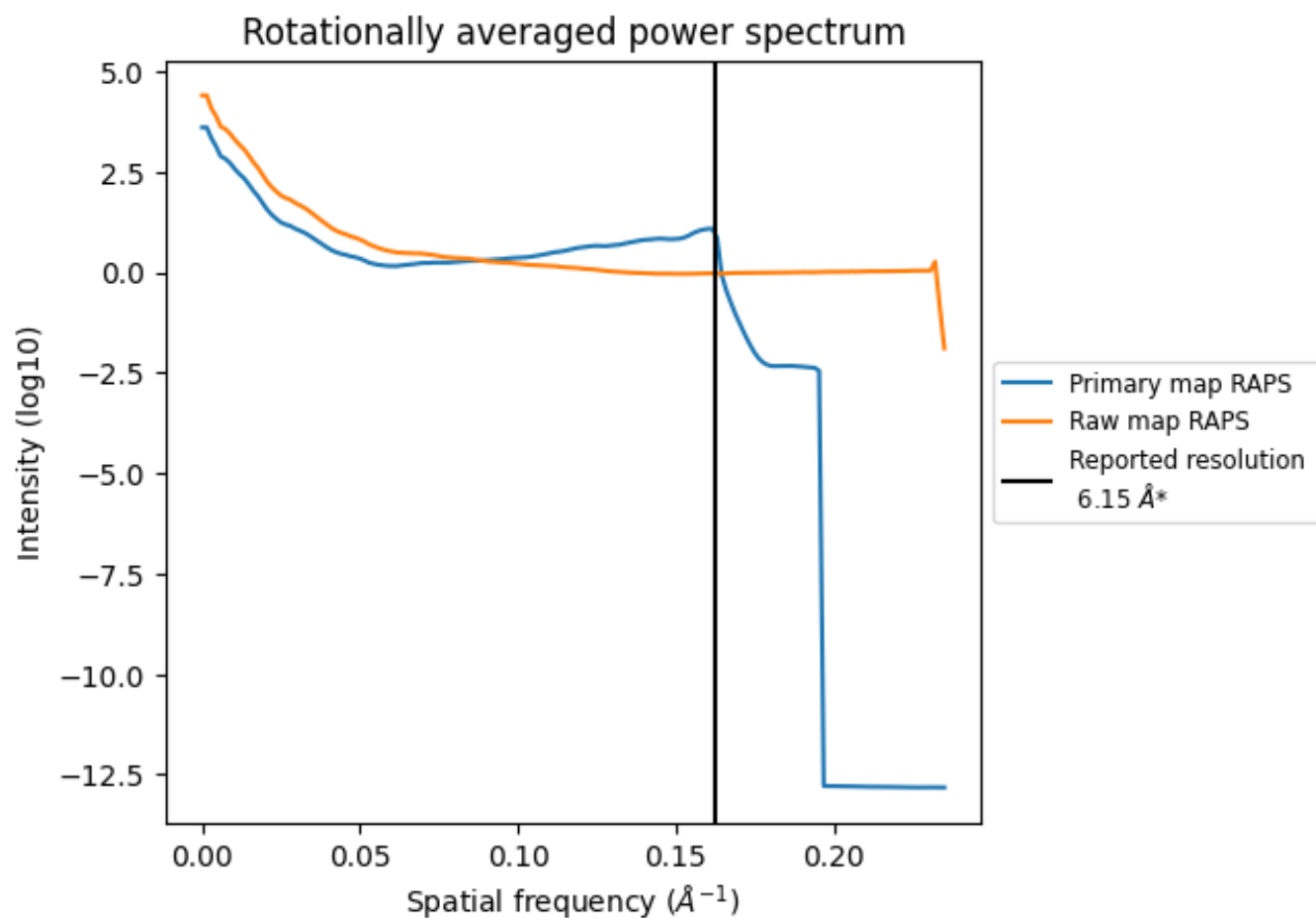
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm³; this corresponds to an approximate mass of 222 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 ⓘ

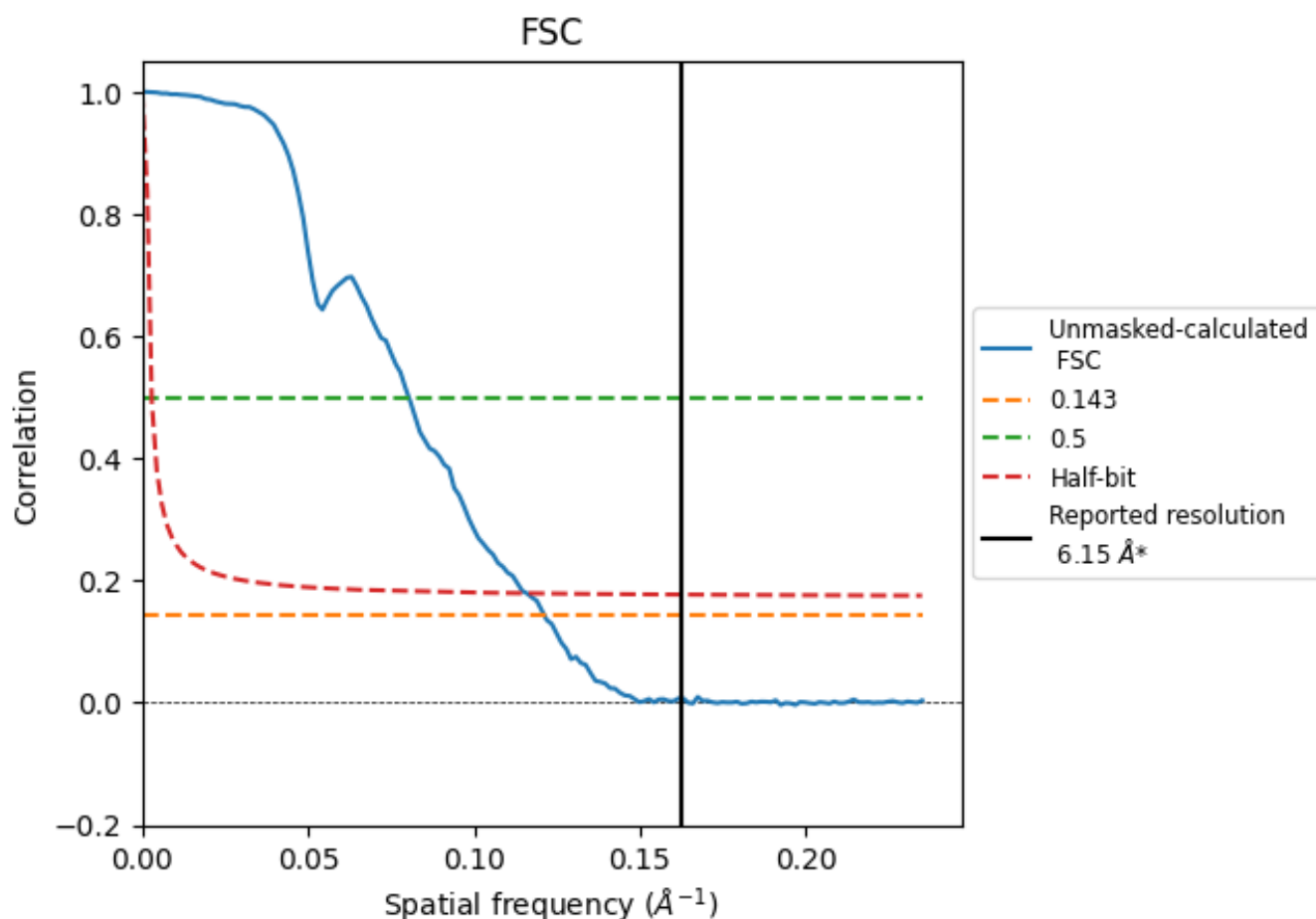


*Reported resolution corresponds to spatial frequency of 0.163 Å⁻¹

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 0.163 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.25	12.45	8.63

*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 8.25 differs from the reported value 6.15 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37584 and PDB model 8WJL. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



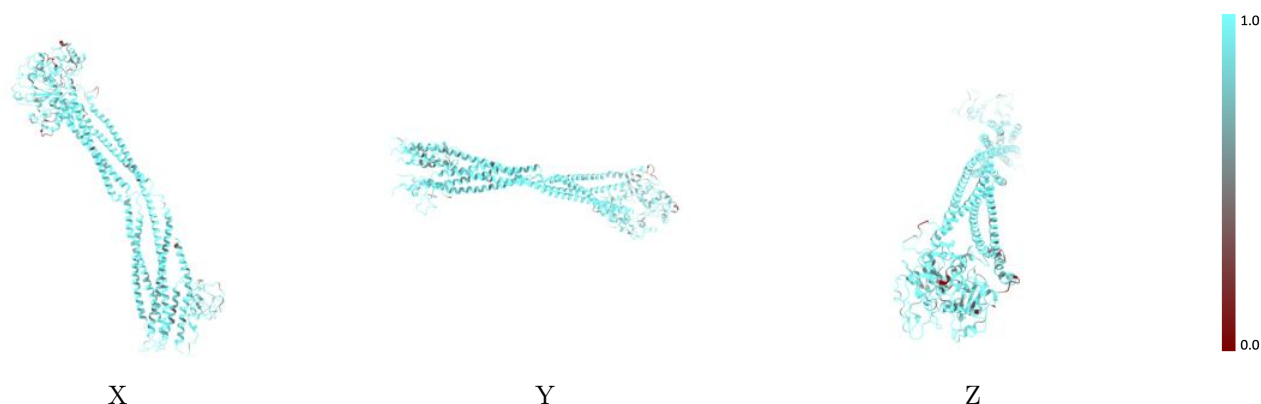
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



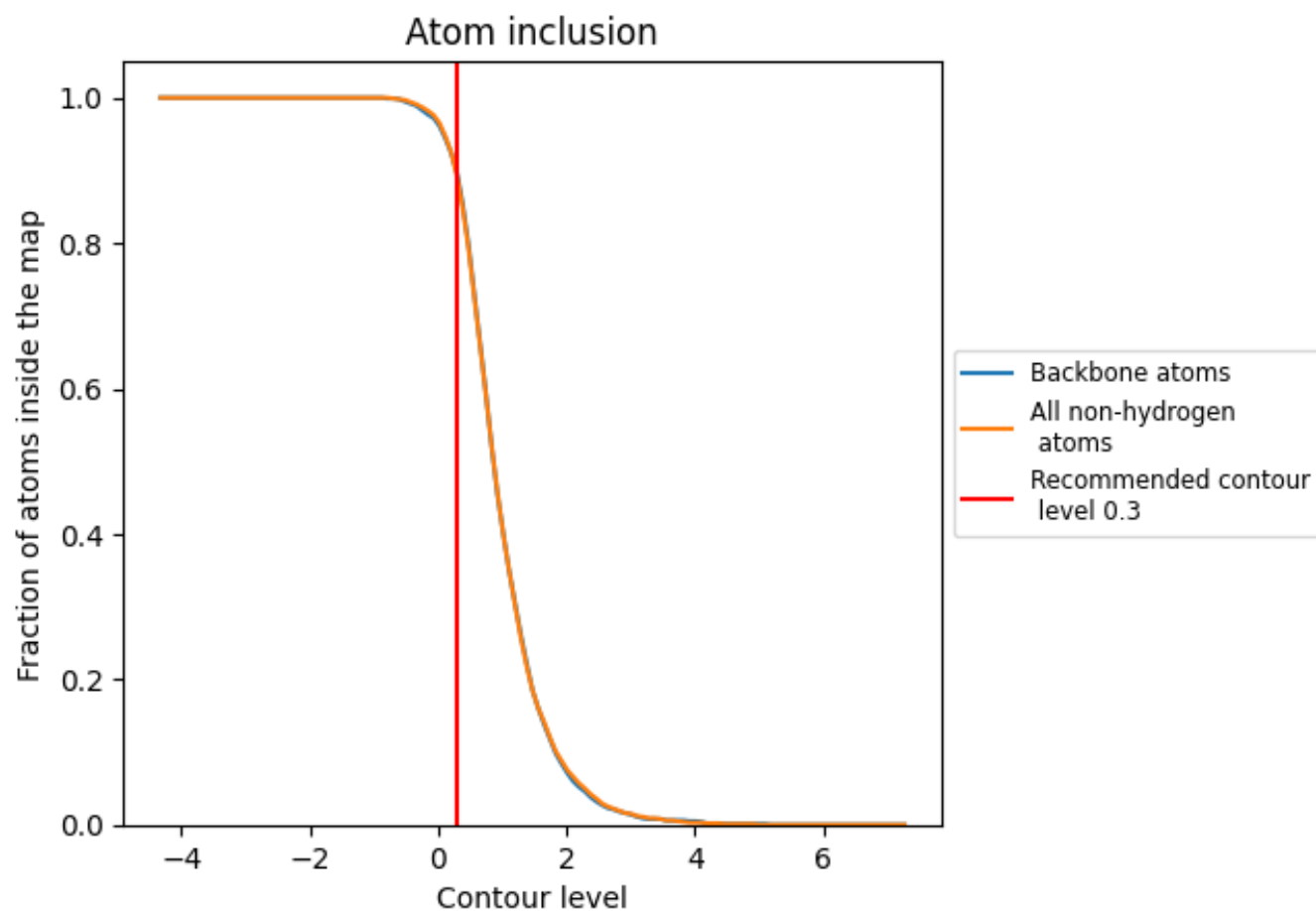
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8900	<div></div> 0.1890
A	<div></div> 0.9050	<div></div> 0.1870
B	<div></div> 0.8880	<div></div> 0.1870
C	<div></div> 0.8720	<div></div> 0.2020

