



## wwPDB EM Validation Summary Report ⓘ

Dec 23, 2024 – 04:47 PM JST

PDB ID : 8XMK  
EMDB ID : EMD-38480  
Title : Local refinement of SRCR5-9 domains  
Authors : Xu, H.; Su, X.D.  
Deposited on : 2023-12-27  
Resolution : 3.03 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.40

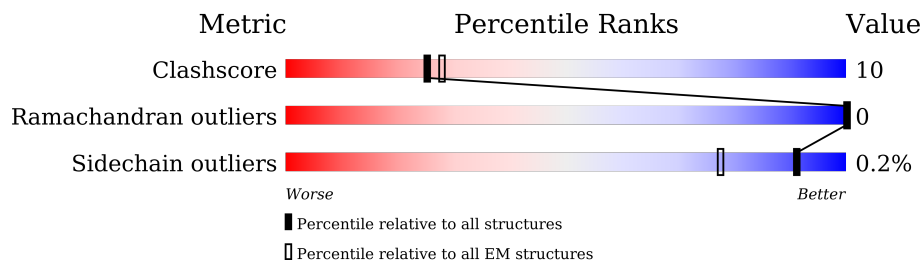
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.03 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  $\geq 3$ , 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	D	1009	
1	E	1009	
1	F	1009	

## 2 Entry composition [i](#)

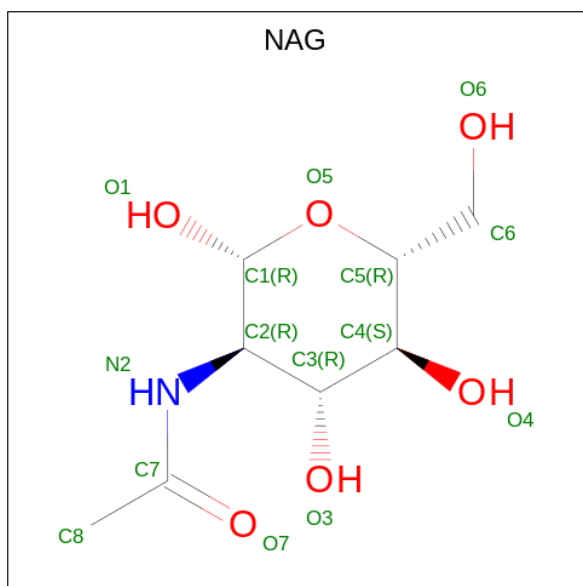
There are 3 unique types of molecules in this entry. The entry contains 11815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	522	Total	C	N	O	S	0	0
			3933	2412	716	761	44		
1	E	509	Total	C	N	O	S	0	0
			3847	2360	698	745	44		
1	F	522	Total	C	N	O	S	0	0
			3934	2412	716	762	44		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	D	6	Total	Ca	0
			6	6	
3	E	5	Total	Ca	0
			5	5	
3	F	6	Total	Ca	0
			6	6	





N994	E995	Y996	E1002	H1006	A1010	R1011	R1012	E1017	H1020	K1021	E1022	D1023	A1024	A1025	V1026	M1027	C1028	T1029	D1030	ILE	SER	VAL	GLN	LYS	THR	PRO	GLN	LYS	ALA	ALA	THR	THR	GLY	ARG	ARG	G951	T952	V953	C954	D955	D956	S957	W958	Q968	Q969	L970	F979	K980	G987	T988	G989	W992	L993	
C835	L839	F842	W847	D871	S879	LEU	ASP	LYS	ALA	MET	S885	P896	P906	S907	T921	I929	R930	T936	S937	C938	E943	I944	W945	S949	W950	G951	T952	V953	C954	D955	D956	S957	W958	Q968	Q969	L970	F979	K980	G987	T988	G989	W992	L993											
GLU	GLU	SER	ALA	ALA	CYS	ILE	GLU	SER	GLY	Q718	L719	G724	C728	A729	V732	W740	V756	C757	R758	A765	S771	G779	G790	S800	H801	C808	R809	H810	K811	E812	V816	I817	C818	M822	S823	L826	T827	S828	ALA	ALA	SER	ARG	GLU	ALA										
V576	C577	S578	R579	I583	G588	R589	T590	E593	V596	K599	L600	L601	W604	G605	S606	H618	V619	V628	M642	W646	R647	C652	H658	M659	V677	A678	I681	L690	S691	S692	CYS	ASN	SER	SER	SER	SER	GLY	PRO	THR	ARG	PRO	THR	ILE	PRO										
CYS	ASP	HIS	TYR	GLU	ALA	LYS	THR	CYS	GLY	S473	P478	R479	L480	V481	C487	R490	V491	D504	S505	D506	L515	C516	R517	V525	S526	I527	G530	E535	A542	E543	E544	G549	S552	H553	L554	R562	T566	C567	S568	H569	S570	R571	D572	V573										
TRP	PHE	ASP	GLY	LEU	ILE	ASP	ASN	SER	ALA	LEU	LEU	CYS	ASN	GLY	THR	THR	VAL	ALA	THR	THR	LYS	ILE	ALA	LEU	THR	ASN	THR	ALA	ALA	GLY	ILE	GLY	ARG	VAL	ASN	ALA	ALA	ARG	LEU	LEU	THR	GLU	ASN	GLY	PHE	GLY	GLY	ARG	LEU	GLU	PRO	ILE		
THR	ARG	GLY	ASN	MET	CYS	SER	GLY	ILE	GLU	ASP	SER	GLU	ALA	LEU	LEU	THR	VAL	ALA	TRP	VAL	CYS	GLY	LYS	ASP	HIS	ASN	ASN	PHE	CYS	ASN	ILE	THR	ALA	HIS	ALA	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432933	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 ( $e^-/\text{\AA}^2$ )	60	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	2.904	Depositor
Minimum map value	-2.426	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA

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	D	0.27	0/4025	0.50	0/5453
1	E	0.27	0/3935	0.49	0/5330
1	F	0.29	0/4026	0.50	0/5454
All	All	0.28	0/11986	0.49	0/16237

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	D	3933	0	3661	82	0
1	E	3847	0	3578	79	0
1	F	3934	0	3661	79	0
2	D	28	0	26	0	0
2	E	28	0	26	0	0
2	F	28	0	26	0	0
3	D	6	0	0	0	0
3	E	5	0	0	0	0
3	F	6	0	0	0	0
All	All	11815	0	10978	233	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 233 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:E:808:CYS:SG	1:F:1021:LYS:NZ	2.62	0.72
1:D:781:ILE:HB	1:D:806:GLN:HG3	1.71	0.72
1:E:779:GLY:O	1:E:810:HIS:NE2	2.20	0.72
1:F:593:GLU:HB2	1:F:681:ILE:HA	1.73	0.70
1:F:779:GLY:O	1:F:810:HIS:NE2	2.21	0.70

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	D	514/1009 (51%)	492 (96%)	22 (4%)	0	100	100
1	E	497/1009 (49%)	480 (97%)	17 (3%)	0	100	100
1	F	514/1009 (51%)	496 (96%)	18 (4%)	0	100	100
All	All	1525/3027 (50%)	1468 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	425/823 (52%)	424 (100%)	1 (0%)	92	96
1	E	419/823 (51%)	419 (100%)	0	100	100
1	F	426/823 (52%)	425 (100%)	1 (0%)	92	96
All	All	1270/2469 (51%)	1268 (100%)	2 (0%)	91	96

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

Mol	Chain	Res	Type
1	D	745	ASP
1	F	811	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	968	GLN
1	F	968	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](#)

Of 23 ligands modelled in this entry, 17 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	F	1101	1	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	E	1101	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	F	1102	1	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	D	1102	1	14,14,15	0.23	0	17,19,21	0.50	0
2	NAG	E	1102	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	D	1101	1	14,14,15	0.20	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1101	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1101	1	-	2/6/23/26	0/1/1/1
2	NAG	F	1102	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1102	1	-	2/6/23/26	0/1/1/1
2	NAG	E	1102	1	-	4/6/23/26	0/1/1/1
2	NAG	D	1101	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1101	NAG	C4-C5-C6-O6
2	E	1102	NAG	O5-C5-C6-O6
2	E	1101	NAG	O5-C5-C6-O6
2	E	1102	NAG	C8-C7-N2-C2
2	E	1102	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

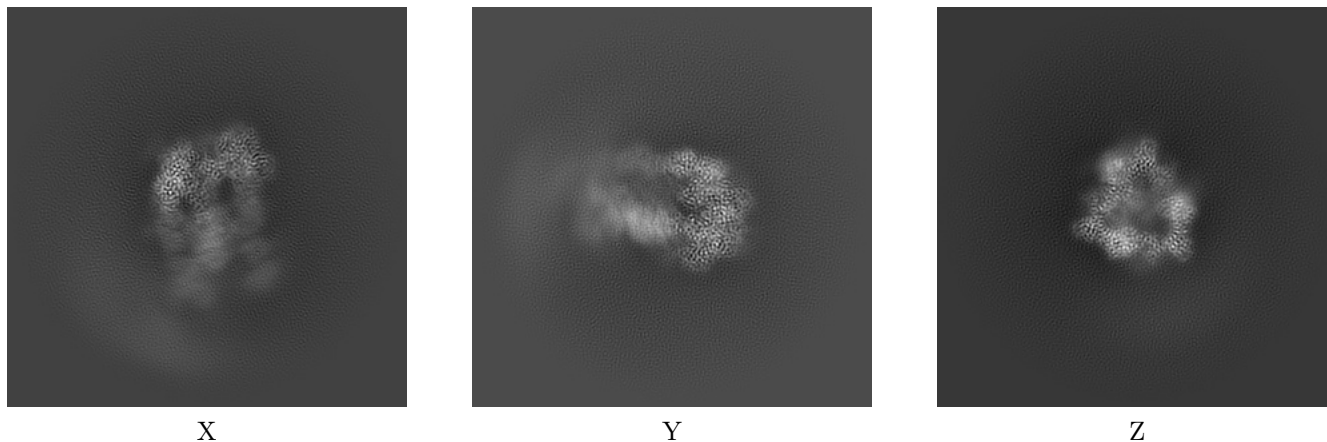
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38480. These allow visual inspection of the internal detail of the map and identification of artifacts.

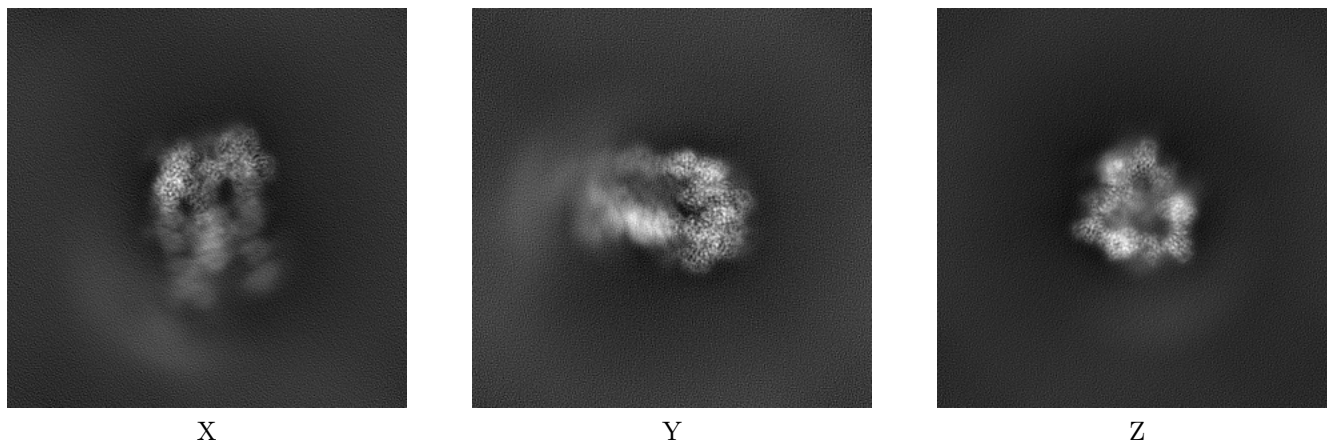
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map



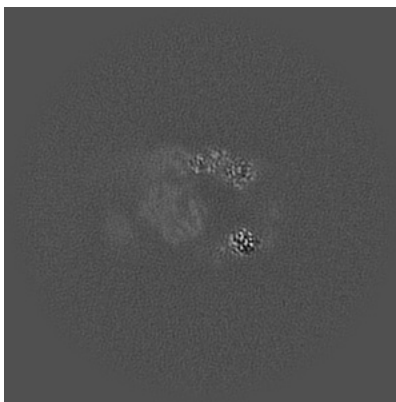
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

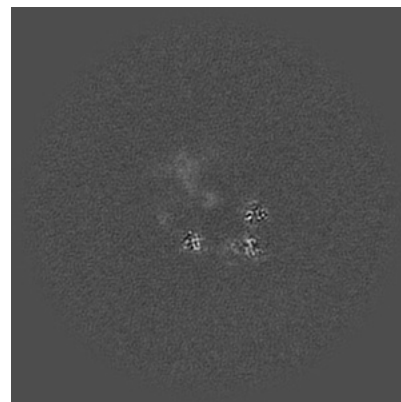
### 6.2.1 Primary map



X Index: 180

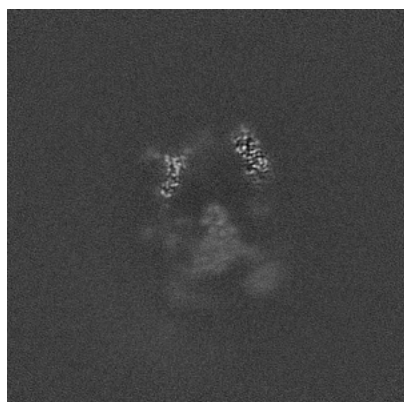


Y Index: 180

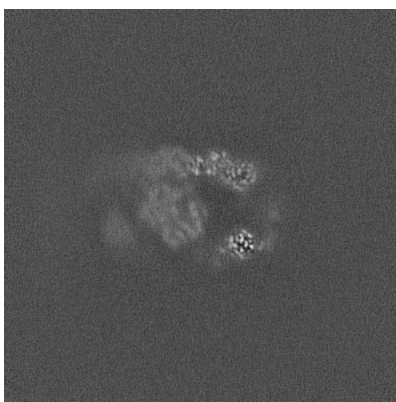


Z Index: 180

### 6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

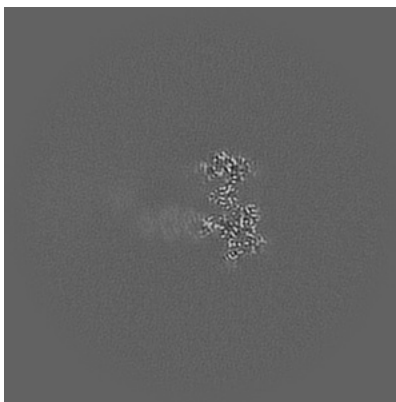
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

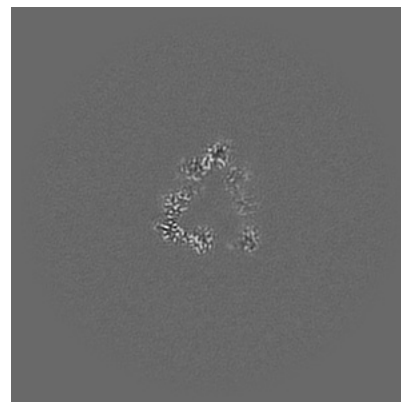
### 6.3.1 Primary map



X Index: 159



Y Index: 150

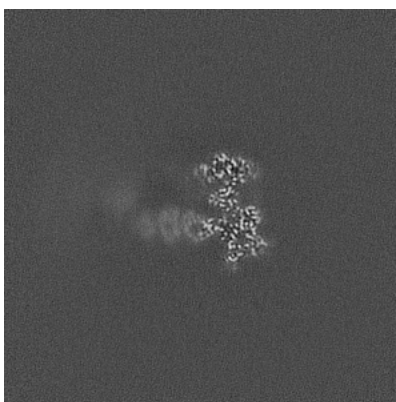


Z Index: 218

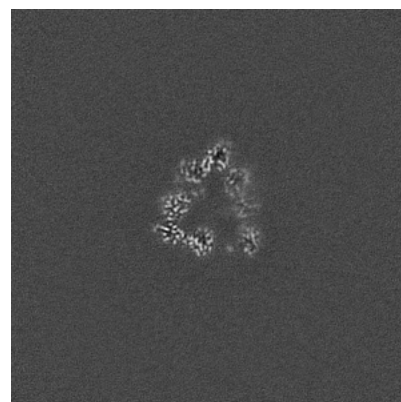
### 6.3.2 Raw map



X Index: 159



Y Index: 150



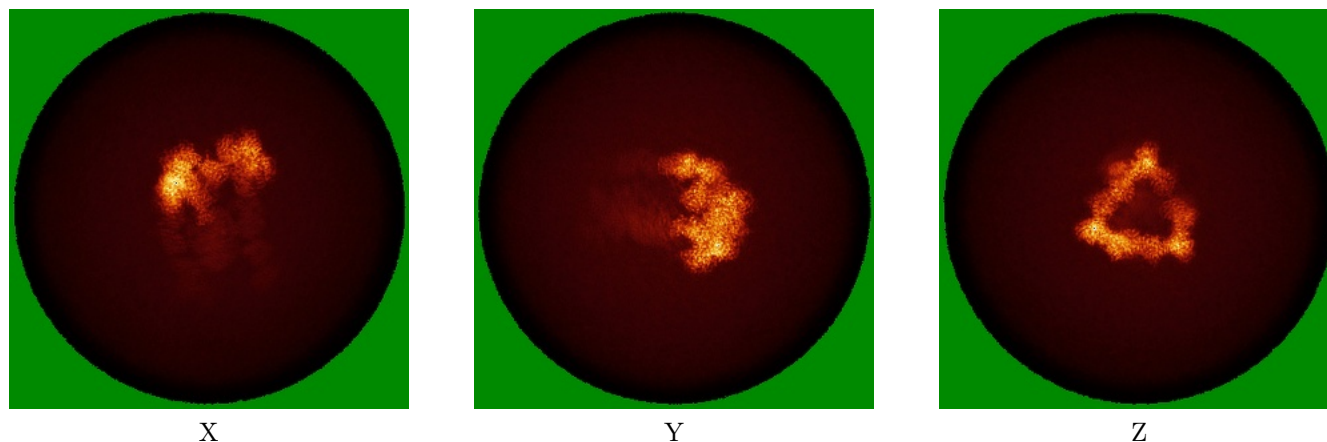
Z Index: 218

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

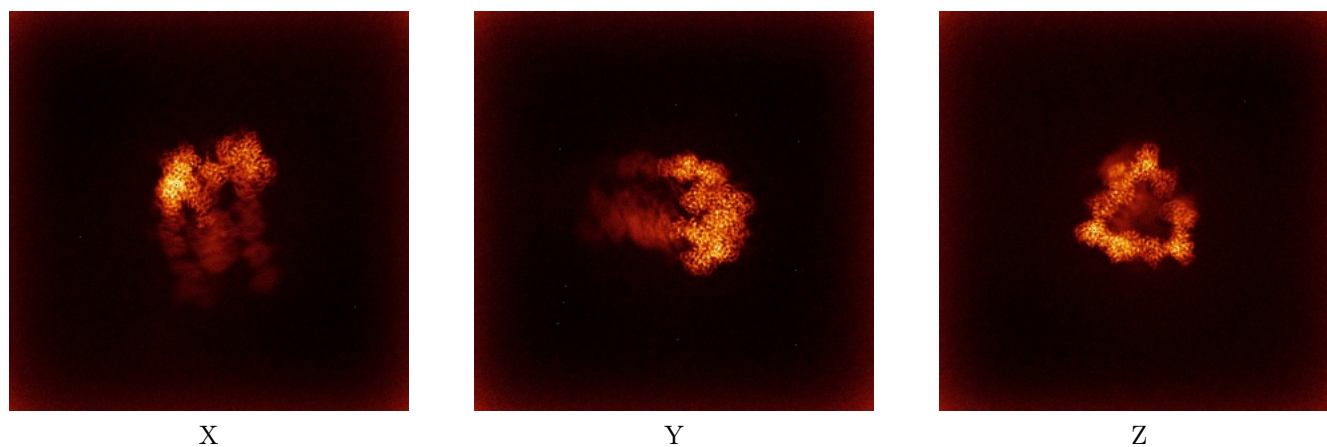


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

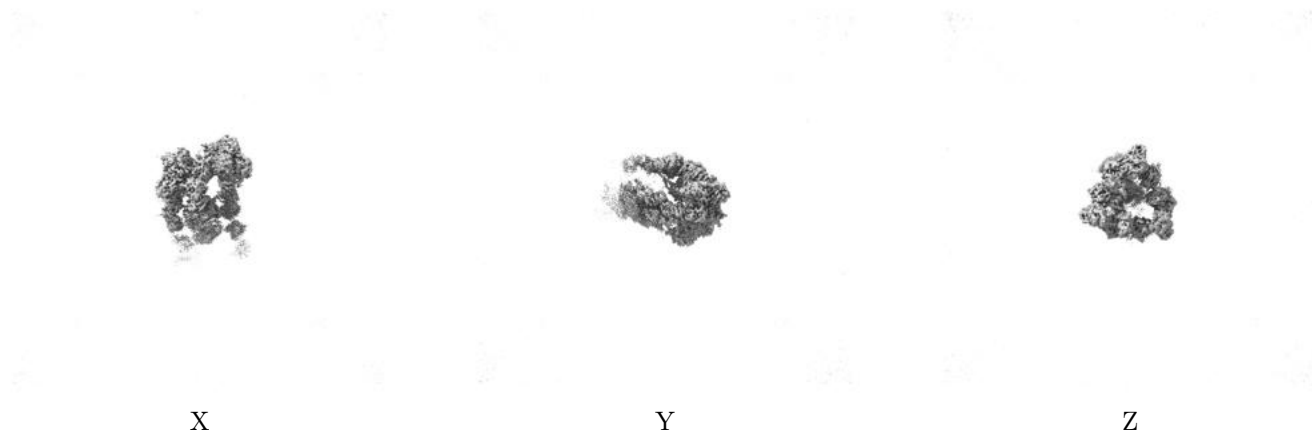
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

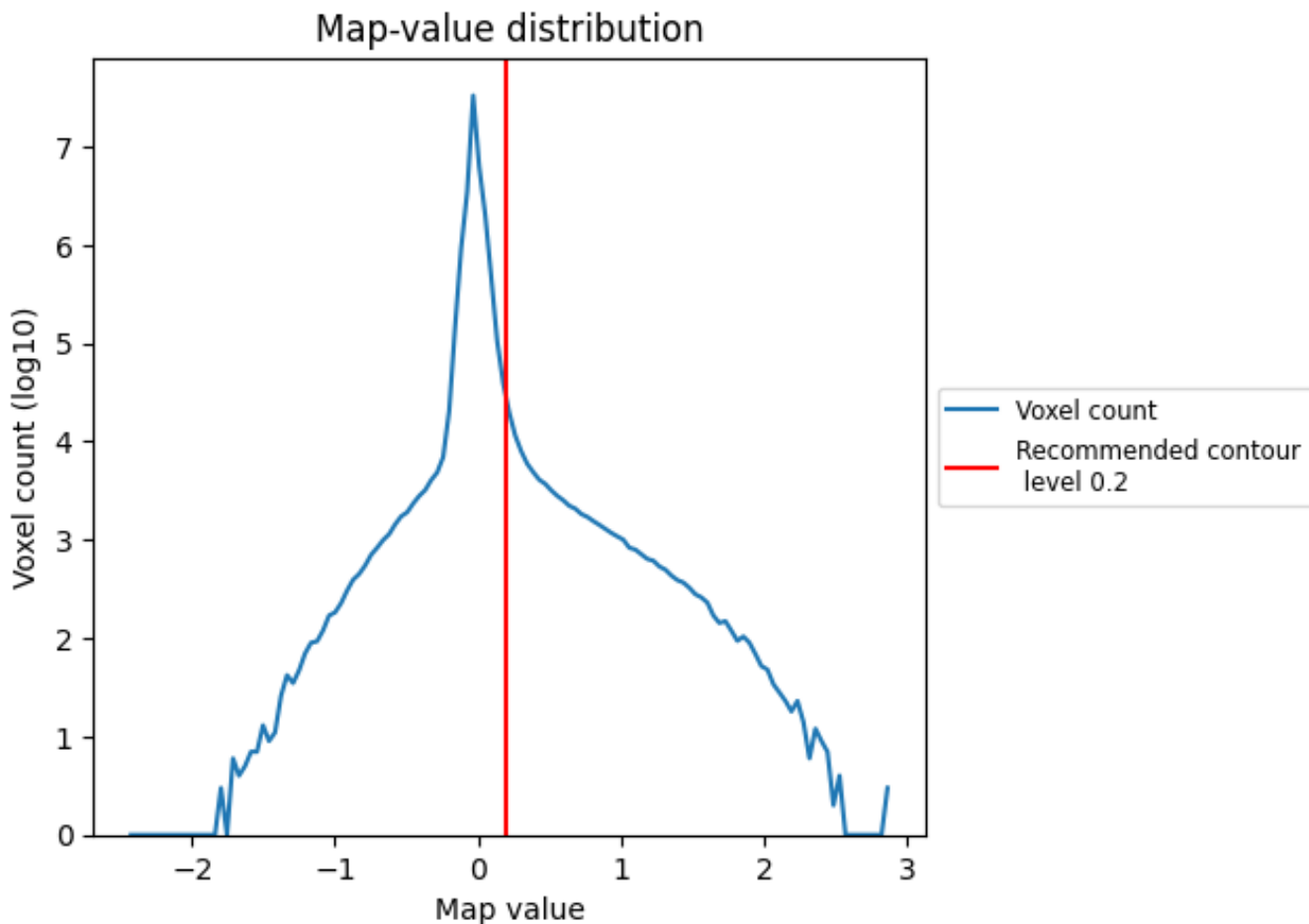
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

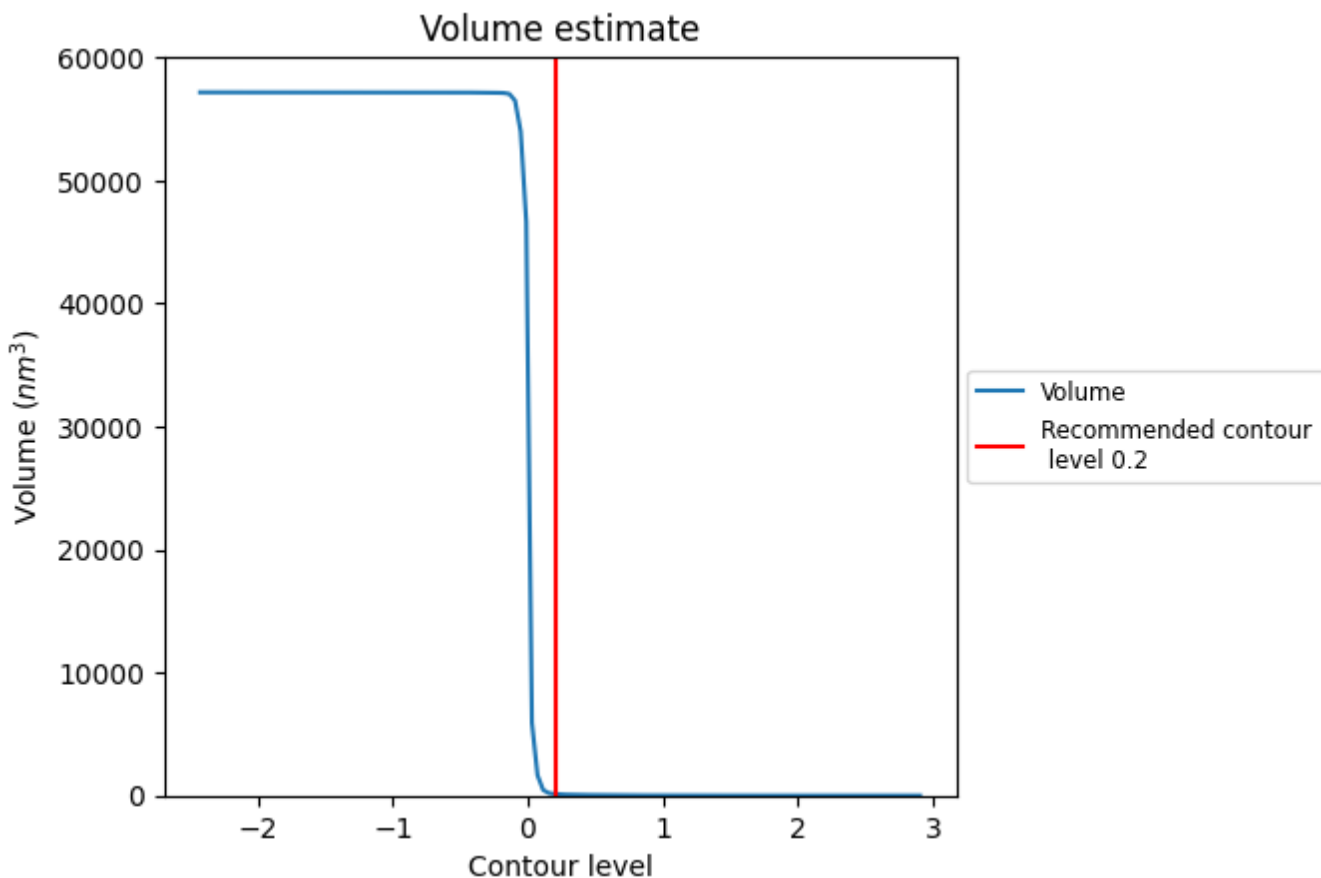
This section contains the results of statistical analysis of the map.

### 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.

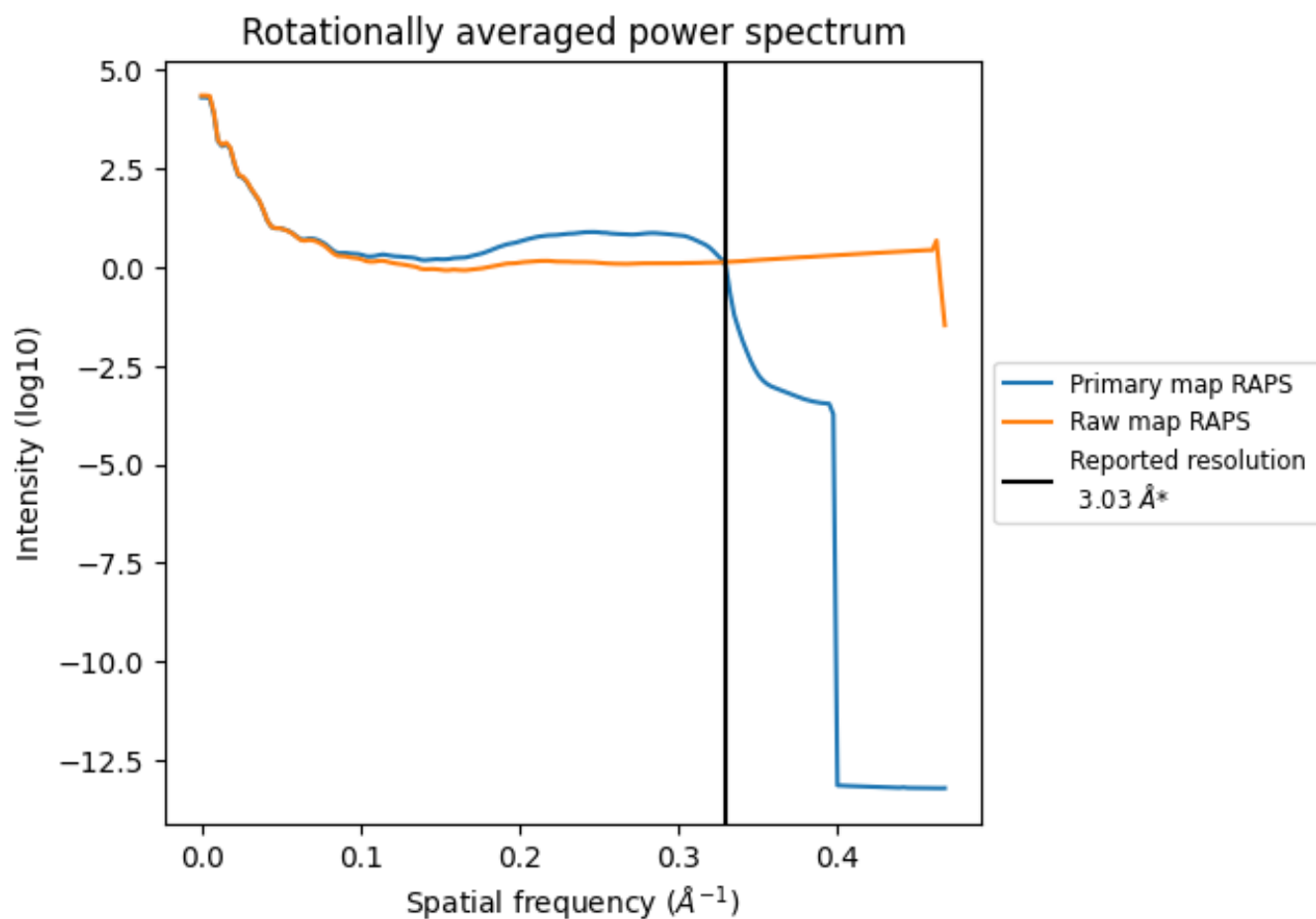
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm<sup>3</sup>; this corresponds to an approximate mass of 115 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](#)

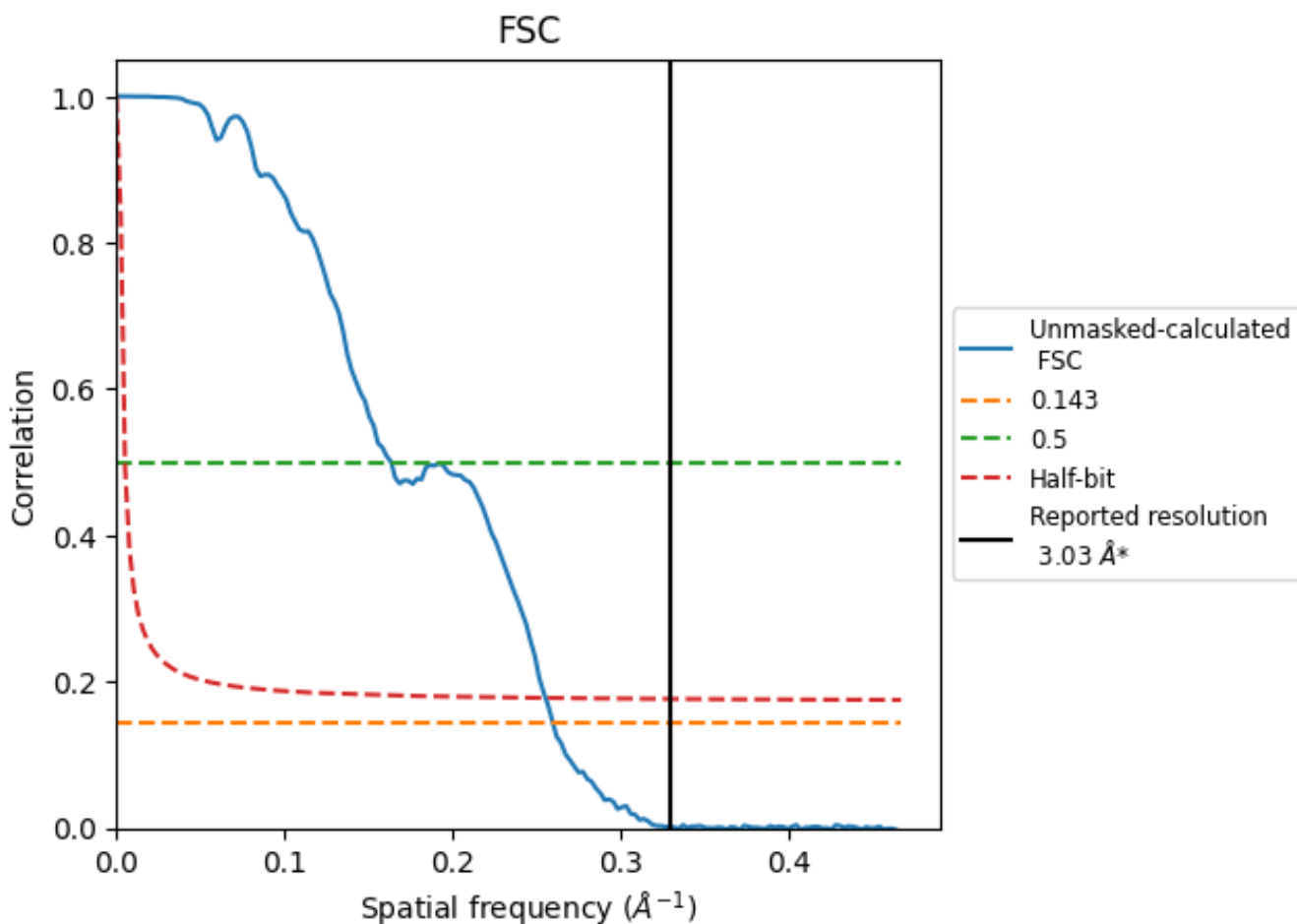


\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>

## 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 0.330  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

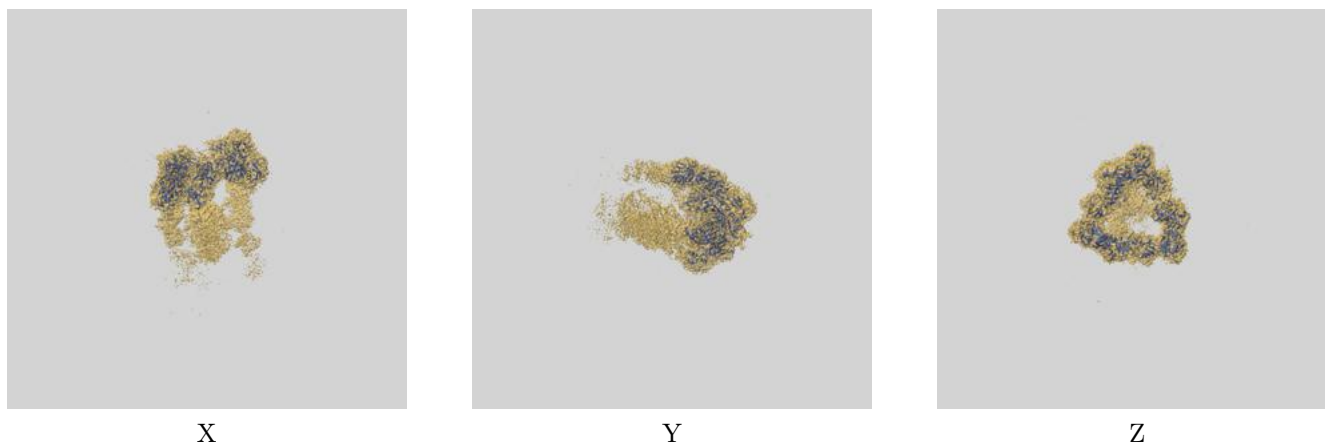
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.11	3.91

\*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 3.85 differs from the reported value 3.03 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38480 and PDB model 8XMK. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

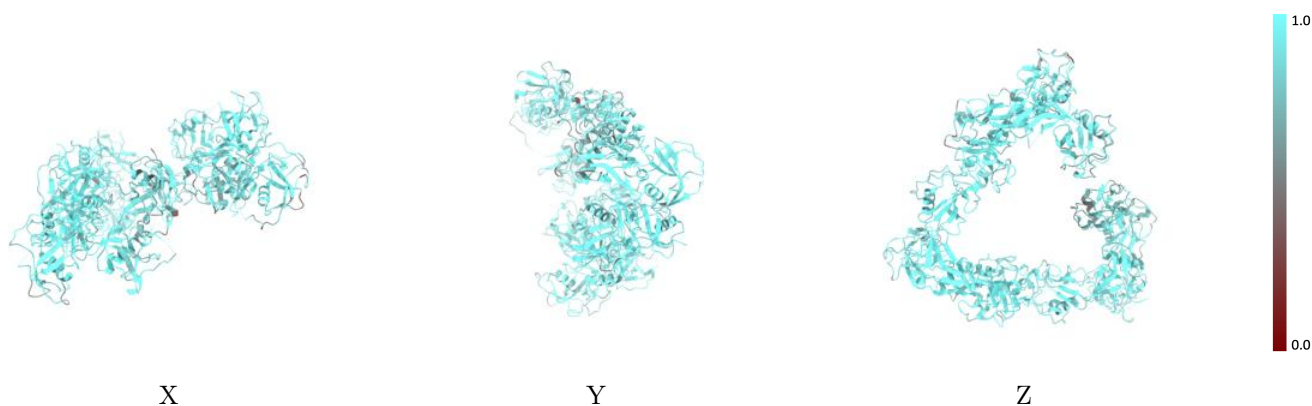


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



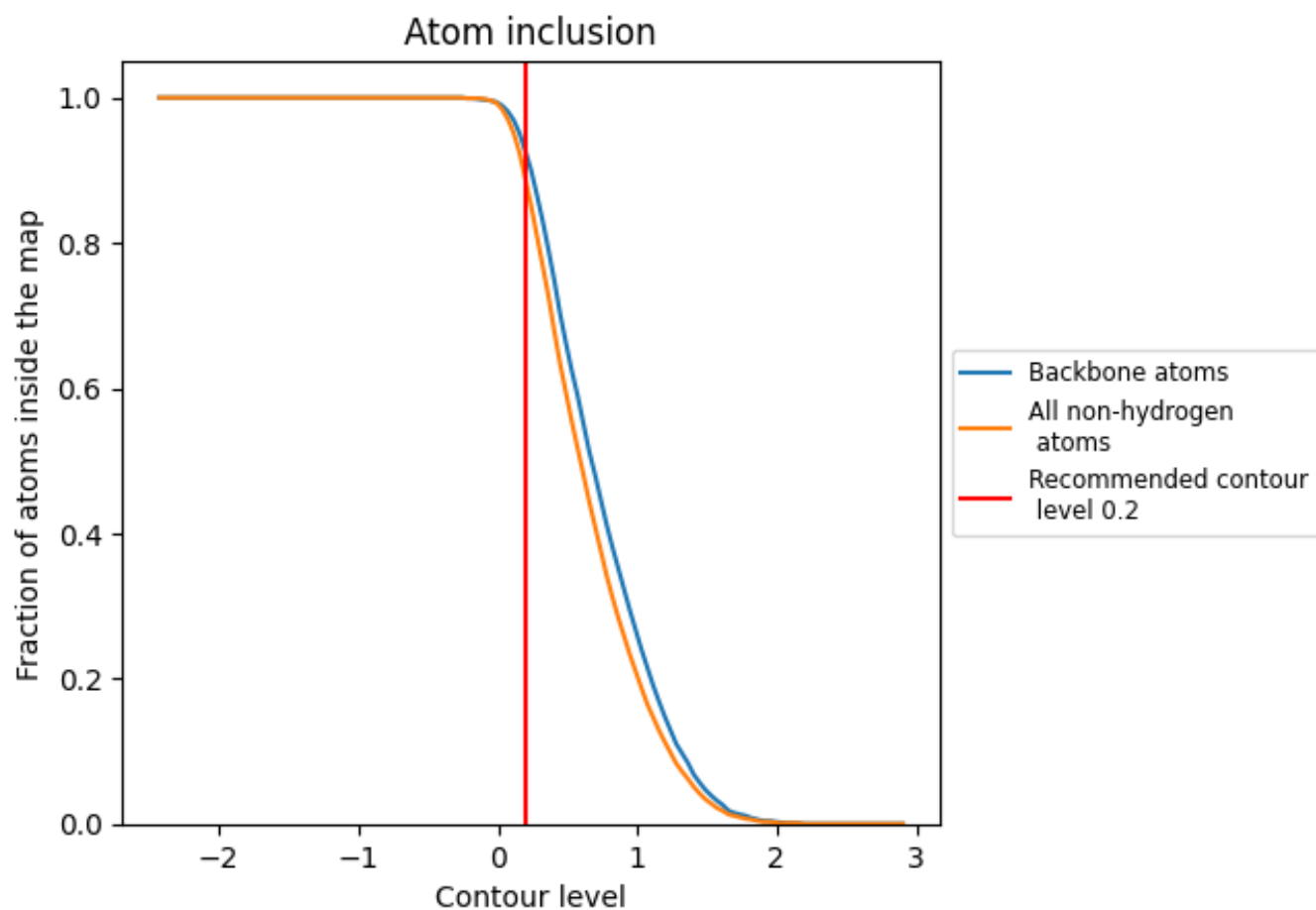
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).




## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.5290
D	 0.8730	 0.5140
E	 0.8630	 0.5160
F	 0.9210	 0.5570

