



## wwPDB EM Validation Summary Report ⓘ

May 29, 2025 – 05:05 pm BST

PDB ID : 9F12 / pdb\_00009f12  
EMDB ID : EMD-50122  
Title : CryoEM structure of the F plasmid relaxosome with oriT DNA ss-27\_-3ds-2\_+143 and TraI its TE mode, derived from ss-27\_-3ds-2\_+143-R Locally-refined 3.42 Å Map.  
Authors : Williams, S.M.; Waksman, G.  
Deposited on : 2024-04-17  
Resolution : 3.42 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.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) : 2.43.1

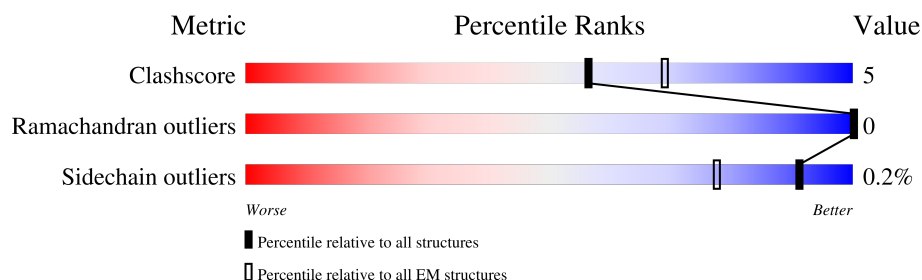
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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	A	170	
2	B	145	
3	C	99	
4	D	94	
5	E	131	
5	F	131	
5	G	131	
6	H	1763	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called T-strand DNA (96-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	P	0	0
			1982	950	367	569	96		

- Molecule 2 is a DNA chain called R-strand DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	85	Total	C	N	O	P	0	0
			1739	841	293	520	85		

- Molecule 3 is a protein called Integration host factor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total	C	N	O	S	0	0
			764	478	142	143	1		

- Molecule 4 is a protein called Integration host factor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			749	467	139	140	3		

- Molecule 5 is a protein called Relaxosome protein TraY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	120	Total	C	N	O	S	0	0
			960	606	179	171	4		
5	G	109	Total	C	N	O	S	0	0
			846	529	157	157	3		
5	E	109	Total	C	N	O	S	0	0
			881	555	165	157	4		

- Molecule 6 is a protein called Multifunctional conjugation protein TraI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	564	Total	C	N	O	S	0	0
			4249	2623	772	834	20		

There are 8 discrepancies between the modelled and reference sequences:

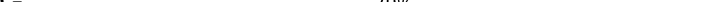
Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	MET	-	initiating methionine	UNP P14565
H	-5	GLU	-	expression tag	UNP P14565
H	-4	PHE	-	expression tag	UNP P14565
H	-3	GLU	-	expression tag	UNP P14565
H	-2	LEU	-	expression tag	UNP P14565
H	-1	GLY	-	expression tag	UNP P14565
H	0	THR	-	expression tag	UNP P14565
H	16	PHE	TYR	engineered mutation	UNP P14565

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	H	1	Total	Mg	0
			1	1	



M1	M13	A29	E40	R44	D47	R51	Y52	T71	W91	F108	Y112	I116	F117	E119	A120	ASP	LYS	GLU	GLU	ASP	ILE	THR	PHE	ASN	THR	LEU
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- Chain G:  8% 79% 5% 17%

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- Chain E:  76% 8% 17%

V11	V14	V22	S30	R35	L45	A58	GLY	ASN	ILE	TVR	G63	L74	T78	L82	K93	I102	N113	SER	GLU	ILE	PHE	ARG	GLU	ALA	ASP	LYS	GLU	GLU	ASP	ILE	THR	PHE	ASN	THR	LEU
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- Chain H:  29% 68%

MET	GLU	PHE	LEU	LEU	GLY	THR	M1	M2	S3	I4		T18	ASP	LVS	ASP	ASN	TVA	TRR	VAL	LEU	GLY	S28	E31	D48	V51	E57	G58	R59	R68	W69	Q70	L82	TR3		M107	V110	D111	F112	A113		Q116	V117	M141	R150	V162	A163	N164		L175
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Category	Item	Value
D	D178	100
	Y213	100
	K220	100
	H221	100
	M226	100
	R237	100
	D248	100
	Q279	100
	T280	100
	L281	100
E	K282	100
	E283	100
	A290	100
	A294	100
	A295	100
	D296	100
	D300	100
	T303	100
	L304	100
	T	THR
PRO		100
GLY		100
PRO		100
ALA		100
SER		100
GLN		100
ASP		100
GLY		100
PRO		100
ASP		100
VAL		100
GLN		100
GLN		100
ALA		100
VAL		100
THR		100
GLN		100
ALA		100
ILE		100
ALA		100
GLY		100
GLY		100
LEU		100
SER		100
GLU		100
ARG	100	
LYS	100	
VAL	100	
GLN	100	

THR	TYR	THR	THR	ASP	ASP	LEU	ALA	ALA	ARG	THR	THR	VAL	GLY	ILE	LEU	PRO	PRO	GLU	ASN	GLY	VAL	ILE	ILE	GLU	ARG	ARG	ALA	ALA	ALA	GLY	ILE	ILE	ASP	GLU	ASP	ALA	ALA	ILE	SER	ARG	ARG	GLU	GLN	LEU	LEU	ILE	ILE	LEU	LEU	PRO	LEU	ASP	ARG	GLU	GLY	GLY	LEU	LEU	PHE	THR	THR	SER	GLY	ILE	ILE	HIS	VAL	VAL	LEU	ASP	GLU	GLU	LEU	SER	SER	VAL	VAL	ARG
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LEU	SER	ARG	ASP	ILE	MET	LYS	GLN	ASN	ARG	ARG	VAL	THR	VAL	HIS	PRO	GLU	LYS	SER	VAL	PRO	ARG	THR	ALA	GLY	TYR	SER	ASP	ALA	ALA	VAL	SER	VAL	LEU	ALA	GLN	ASP	ARG	PRO	SER	LEU	ALA	ILE	VAL	SER	GLY	GLN	GLY	GLY	ALA	ALA	GLY	GLN	ARG	GLU	ARG	VAL	LEU	VAL
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MET	ALA	ARG	GLN	GLY	ARG	GLU	VAL	GLN	ILE	ALA	ALA	ASP	ARG	ARG	SER	GLN	MET	ASN	LYS	GLN	ASP	GLU	LEU	LEU	GLY	GLY	GLY	ARG	ARG	GLN	LEU	LEU	THR	THR	THR	PRO	GLY	SER	THR	VAL	ILE	VAL	ASP	GLN	GLY	GLU	LYS	LEU
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LEU	LYS	GLU	THR	LEU	THR	LEU	LEU	LEU	ASP	GLY	ALA	ALA	ARG	HIS	ASN	VAL	GLN	VAL	LEU	ILE	THR	ASP	SER	GLY	GLN	ARG	THR	GLY	THR	GLY	SER	ALA	ALA	LEU	MET	MET	LYS	ASP	ALA	ALA	GLY	VAL	ASN	THR	THR	TYR	ARG	TRP	GLN	GLY	GLY	GLU	GLN	R566	E573	P574	D575	V578	P580
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L583	K619	L626	T663	D685	E689	R694	S697	A713	E716	V720	V729	V740	M745	V782	S783	D784	F789	R810	S817	L818	D819	T834	VAL	VAL	SER	SER	GLU	GLN	ILE	LYS	THR	ARG	ALA	GLY	GLU	THR	SER	SER	LEU	LEU	THR	ALA
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SER HIS HIS GLN LYS SER ALA LEU THR PRO GLN GLN ALA ILE HIS HIS ALA GLN LEU LEU PRO VAL VAL GLY SER LYS LYS LEU LEU ALA PHE SER MET VAL ASP LEU LEU THR GLU GLU ALA LYS SER SER PHE ALA ALA GLU GLY GLY PHE THR GLU LEU GLY GLY GLU ILE ASN ALA ALA GLN ILE

ARG GLY ASP LEU TYR VAL ASP VAL LYS GLY TYR GLY THR GLY LEU LEU VAL SER ARG ALA ALA GLY LEU LEU VAL SER ARG ALA ALA LYS SER SER TYR GLU ALA GLU LYS SER SER ILE LEU LEU HIS ARG GLY LYS GLU GLU ALA VAL MET PRO LEU MET GLU MET LEU MET LEU LYS VAL PRO GLY THR SER GLY

[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177743	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 ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.092	Depositor
Minimum map value	-1.581	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.35	Depositor
Map size ( $\text{\AA}$ )	462.0, 462.0, 462.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.825, 0.825, 0.825	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: MG

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	0.28	0/2228	0.49	0/3439
2	B	0.27	0/1946	0.46	0/3002
3	C	0.17	0/775	0.26	0/1036
4	D	0.16	0/763	0.23	0/1021
5	E	0.16	0/895	0.25	0/1198
5	F	0.15	0/977	0.27	0/1312
5	G	0.13	0/860	0.25	0/1161
6	H	0.16	0/4319	0.32	0/5856
All	All	0.20	0/12763	0.37	0/18025

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	A	1982	0	1088	34	0
2	B	1739	0	974	20	0
3	C	764	0	779	6	0
4	D	749	0	756	7	0
5	E	881	0	903	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	960	0	969	11	0
5	G	846	0	812	4	0
6	H	4249	0	4109	30	0
7	H	1	0	0	0	0
All	All	12171	0	10390	106	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 5.

The worst 5 of 106 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)
2:B:46:DA:OP2	3:C:76:ARG:NH1	2.15	0.76
6:H:3:SER:OG	6:H:83:THR:OG1	2.13	0.66
1:A:79:DG:N2	2:B:80:DT:O2	2.29	0.66
2:B:11:DC:H2'	2:B:12:DA:C8	2.31	0.65
2:B:33:DT:H2'	2:B:34:DT:H71	1.83	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	93/99 (94%)	93 (100%)	0	0	100	100
4	D	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
5	E	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
5	F	118/131 (90%)	115 (98%)	3 (2%)	0	100	100
5	G	107/131 (82%)	102 (95%)	5 (5%)	0	100	100
6	H	558/1763 (32%)	540 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1073/2349 (46%)	1044 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	C	82/86 (95%)	82 (100%)	0	100	100
4	D	79/79 (100%)	79 (100%)	0	100	100
5	E	95/116 (82%)	95 (100%)	0	100	100
5	F	101/116 (87%)	101 (100%)	0	100	100
5	G	86/116 (74%)	86 (100%)	0	100	100
6	H	442/1428 (31%)	440 (100%)	2 (0%)	86	92
All	All	885/1941 (46%)	883 (100%)	2 (0%)	91	96

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

Mol	Chain	Res	Type
6	H	663	THR
6	H	782	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	H	76	HIS

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

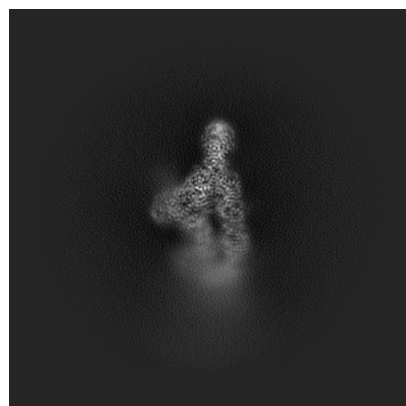
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50122. These allow visual inspection of the internal detail of the map and identification of artifacts.

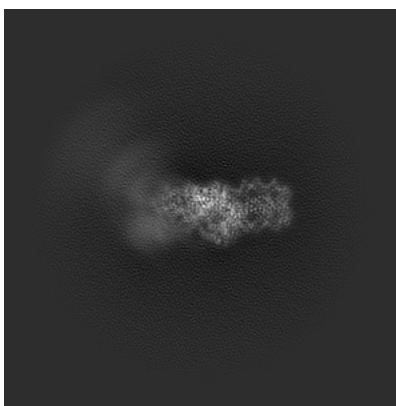
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

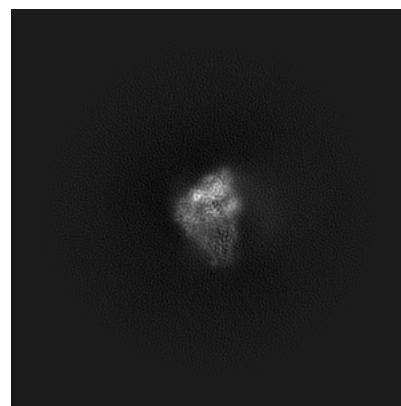
#### 6.1.1 Primary map



X

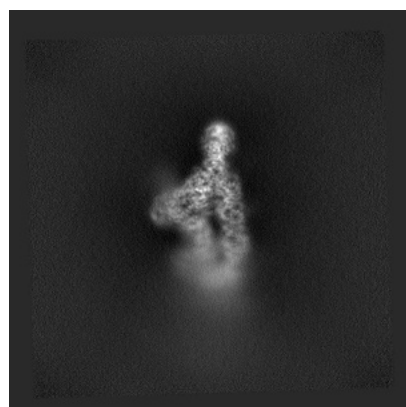


Y

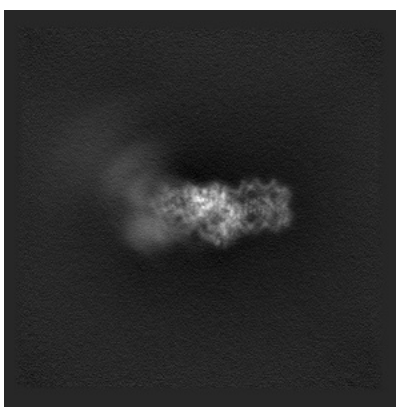


Z

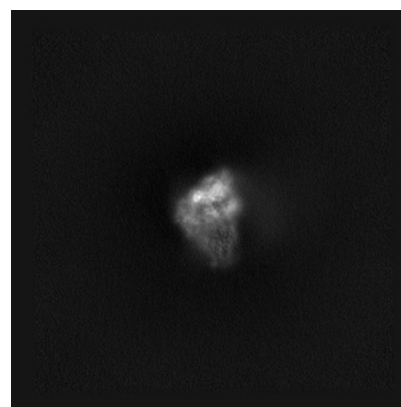
#### 6.1.2 Raw map



X



Y

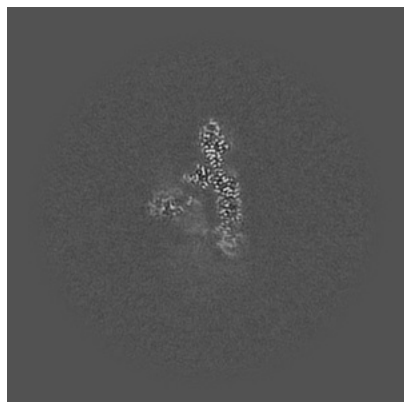


Z

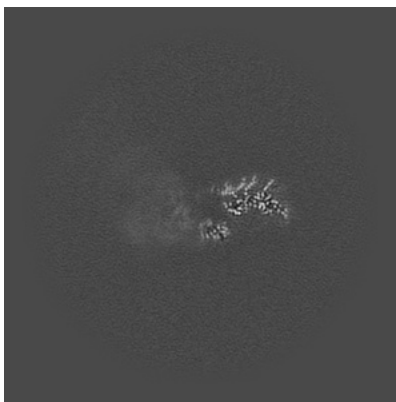
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

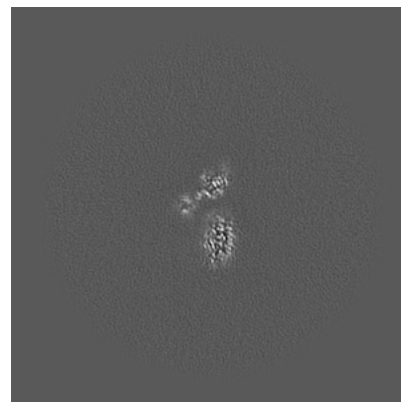
### 6.2.1 Primary map



X Index: 280

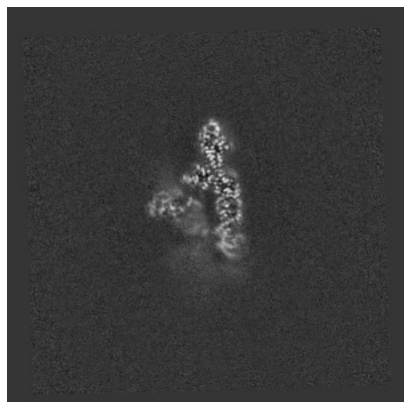


Y Index: 280

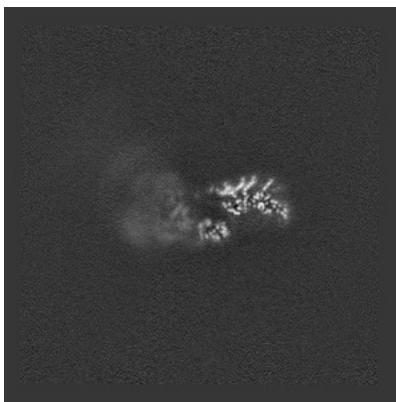


Z Index: 280

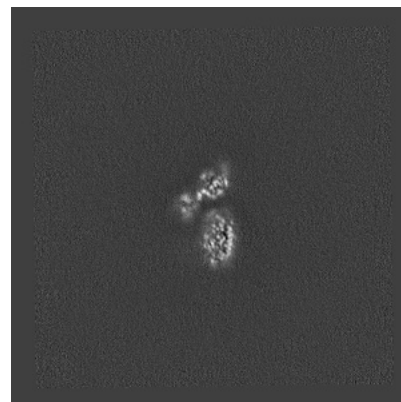
### 6.2.2 Raw map



X Index: 280



Y Index: 280

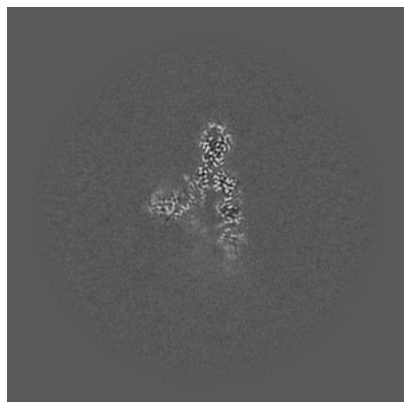


Z Index: 280

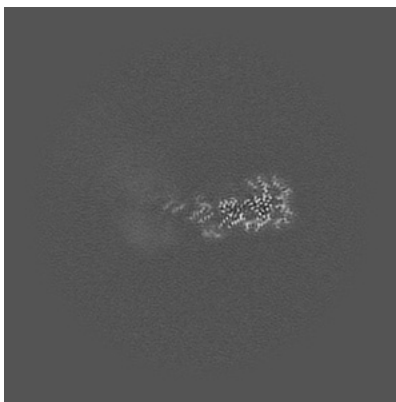
The images above show central slices of the map in three orthogonal directions.

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

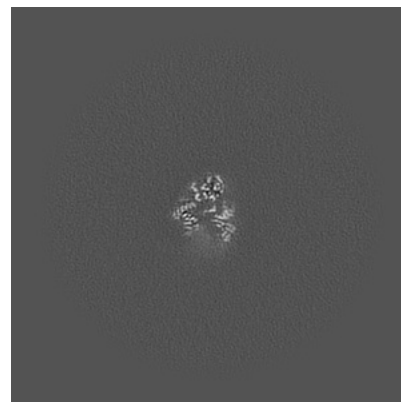
### 6.3.1 Primary map



X Index: 284

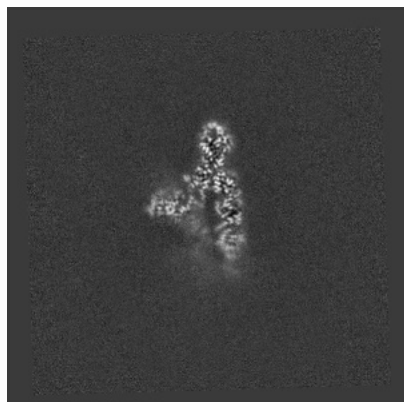


Y Index: 294

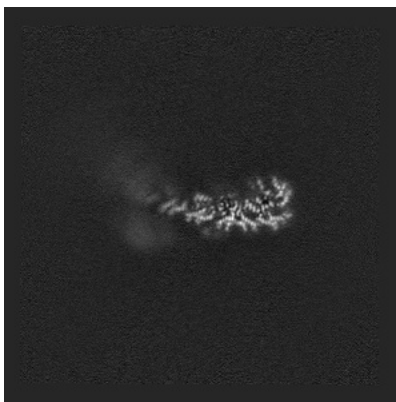


Z Index: 308

### 6.3.2 Raw map



X Index: 283



Y Index: 298



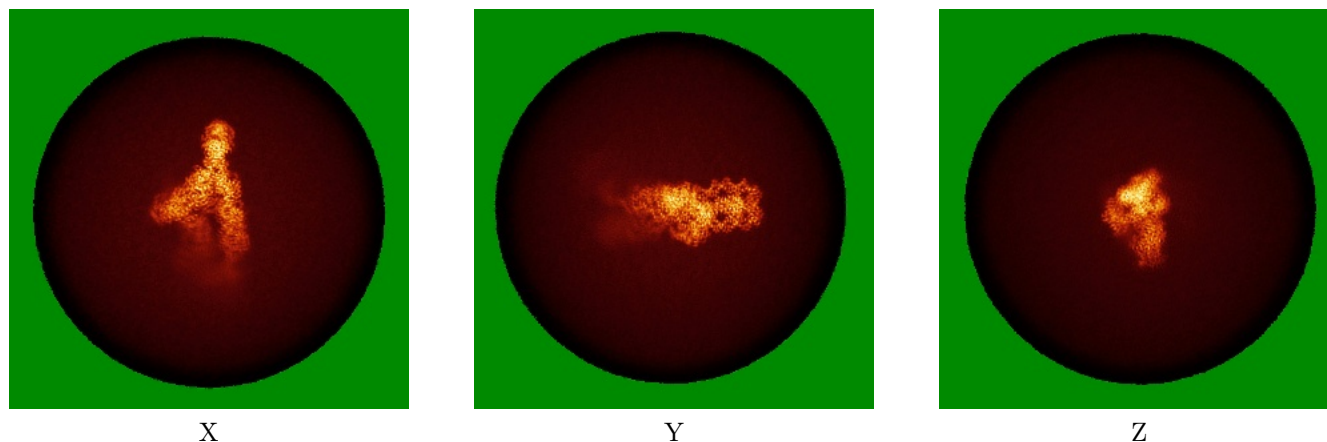
Z Index: 307

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

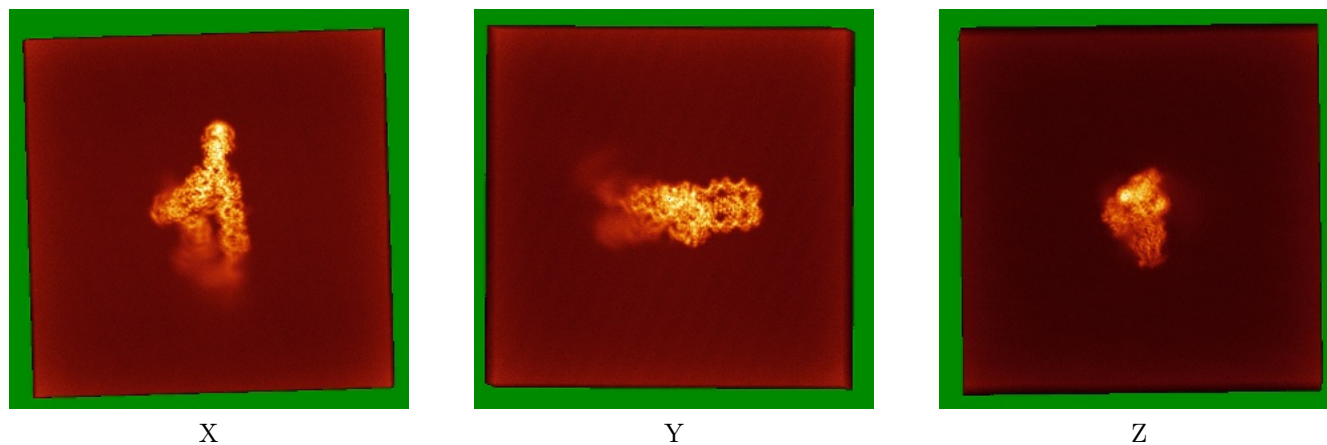


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map

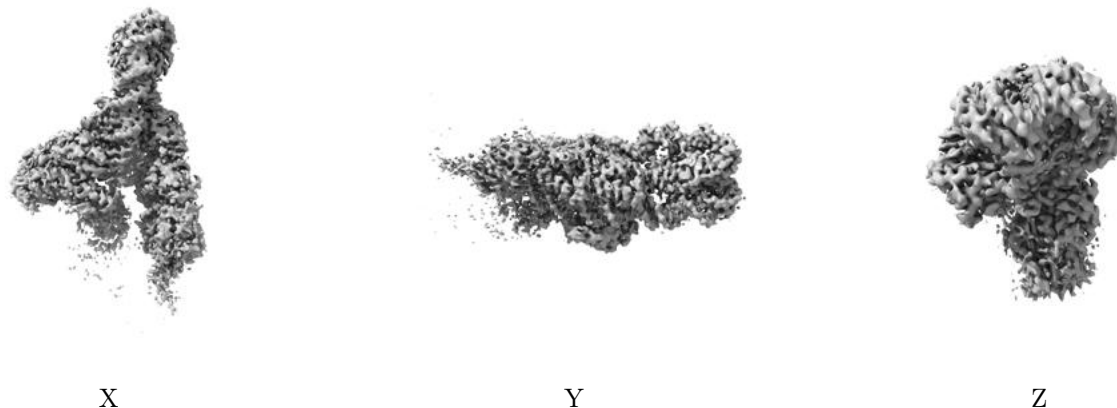


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



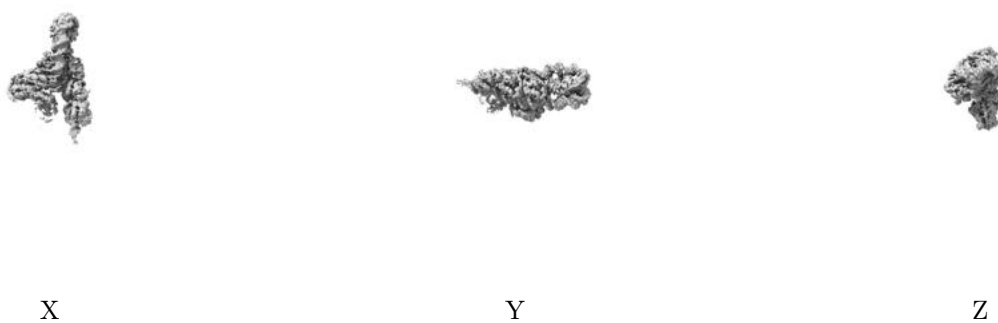
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

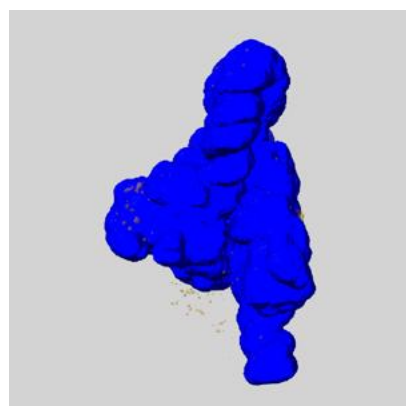
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

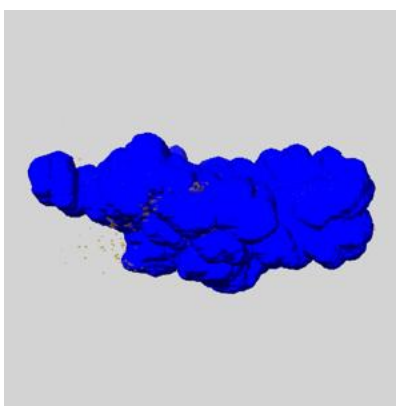
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

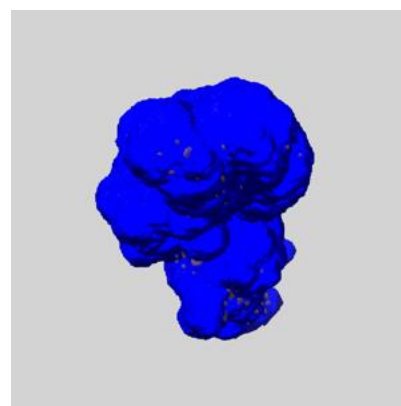
### 6.6.1 emd\_50122\_msk\_1.map [i](#)



X



Y

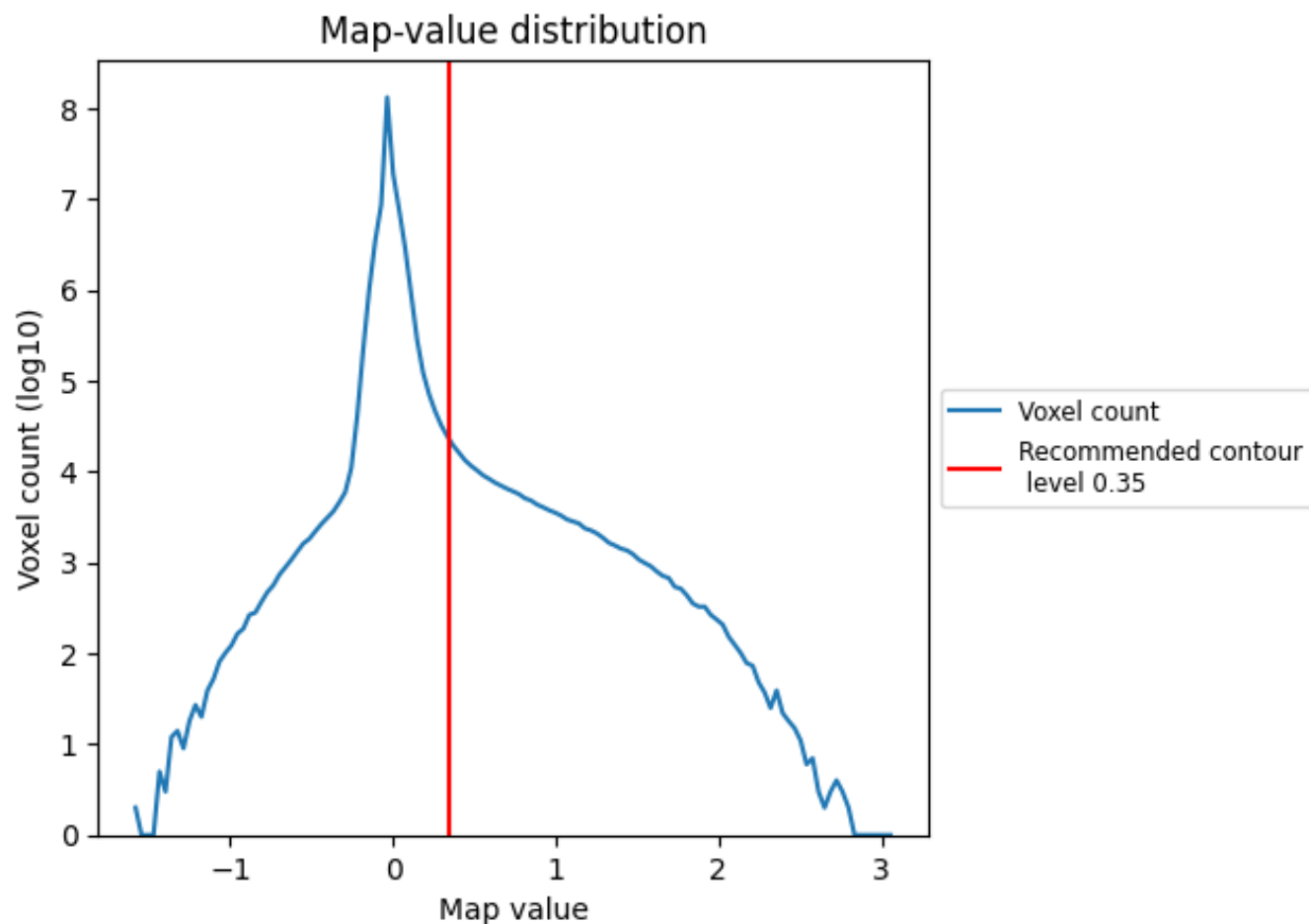


Z

## 7 Map analysis [i](#)

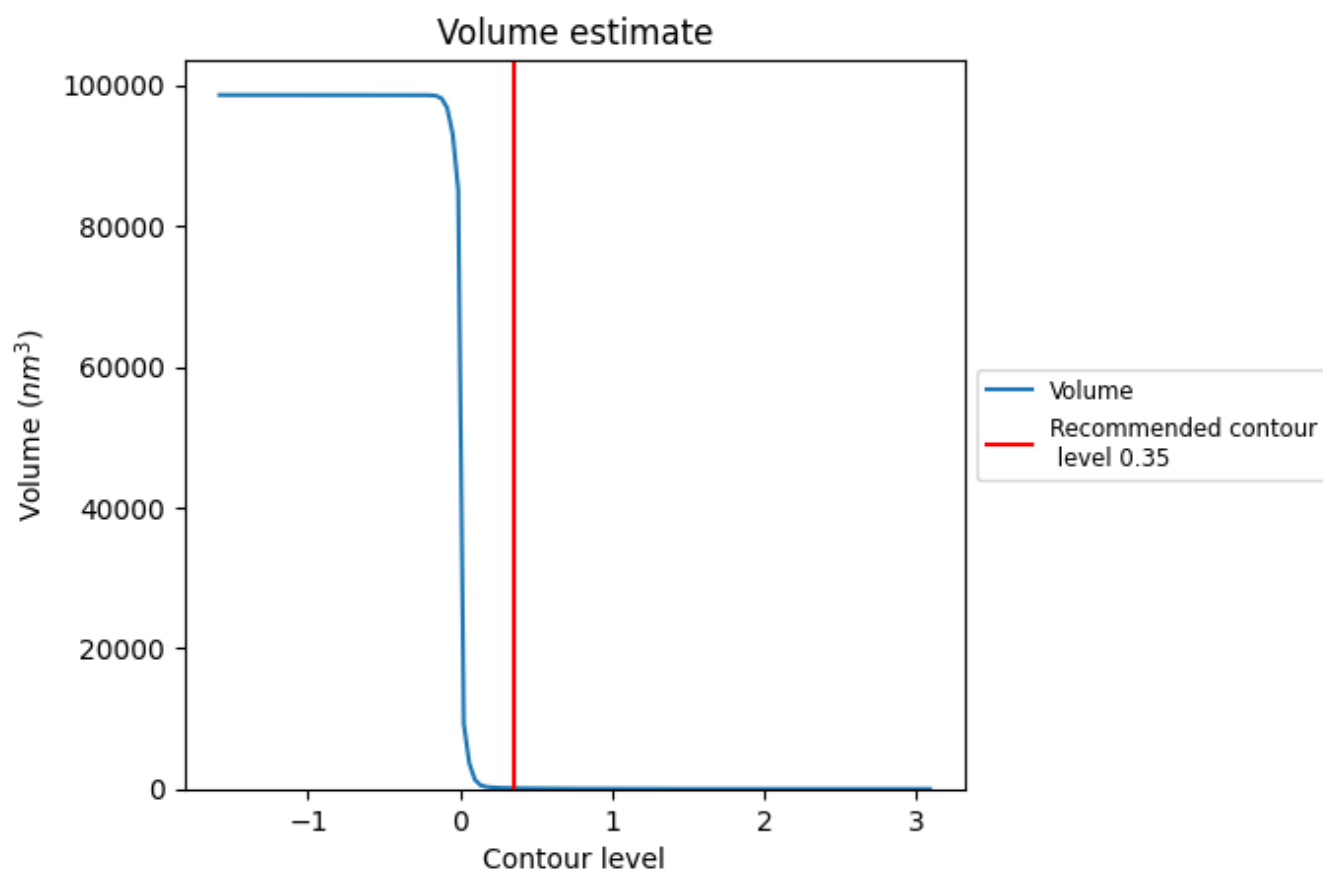
This section contains the results of statistical analysis of the map.

### 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.

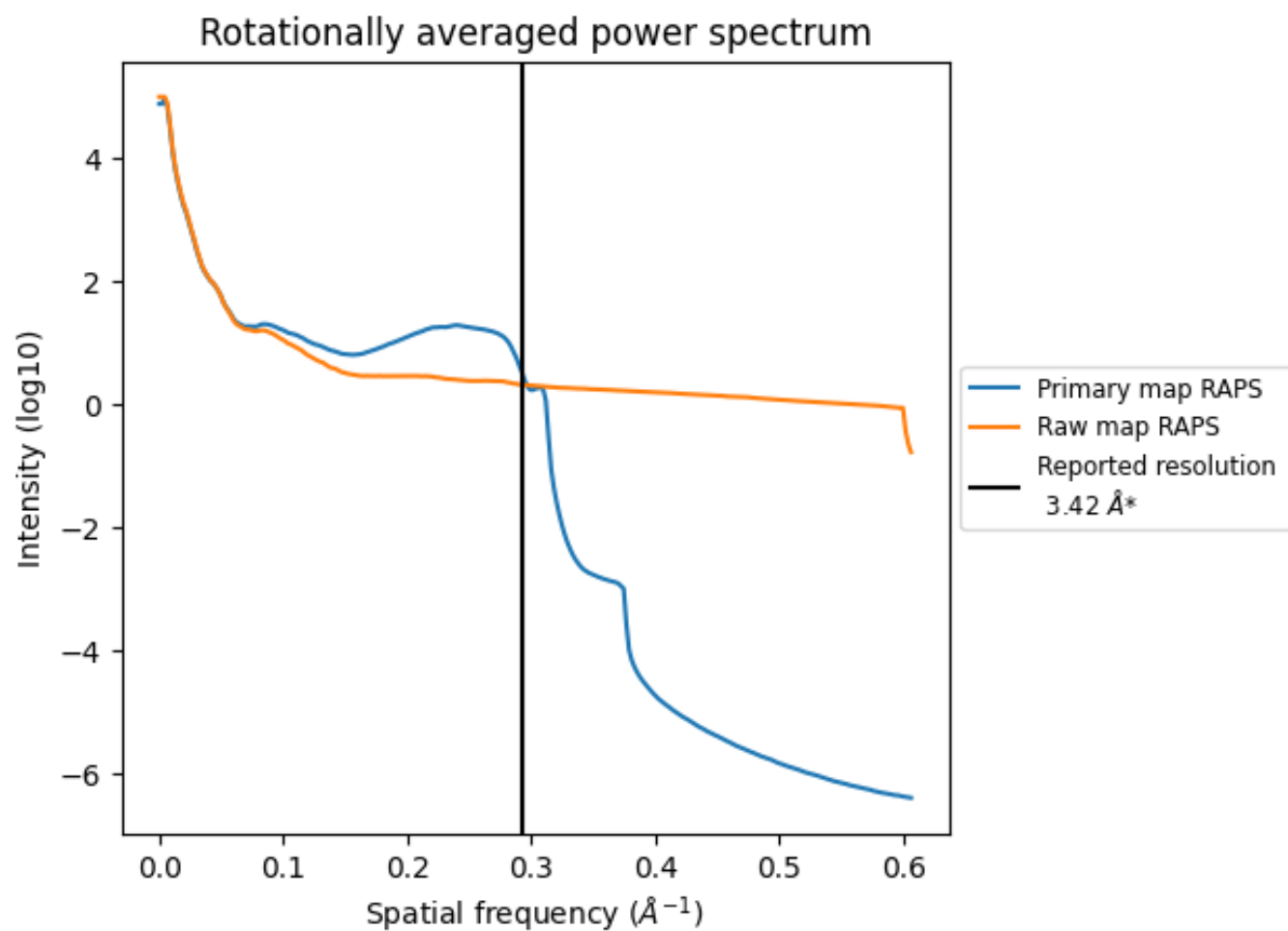
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110  $\text{nm}^3$ ; this corresponds to an approximate mass of 99 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 ⓘ

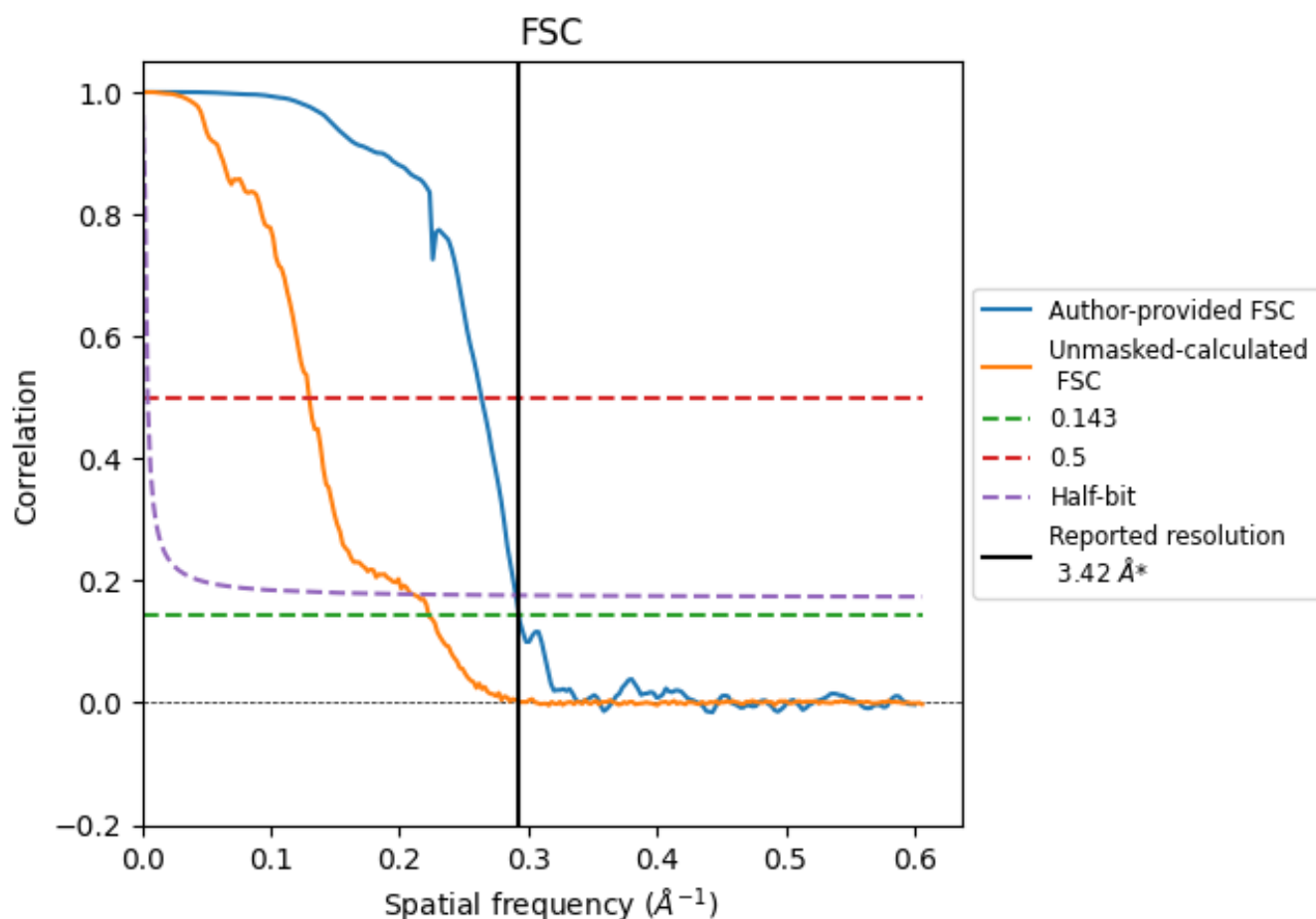


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 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 0.292 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

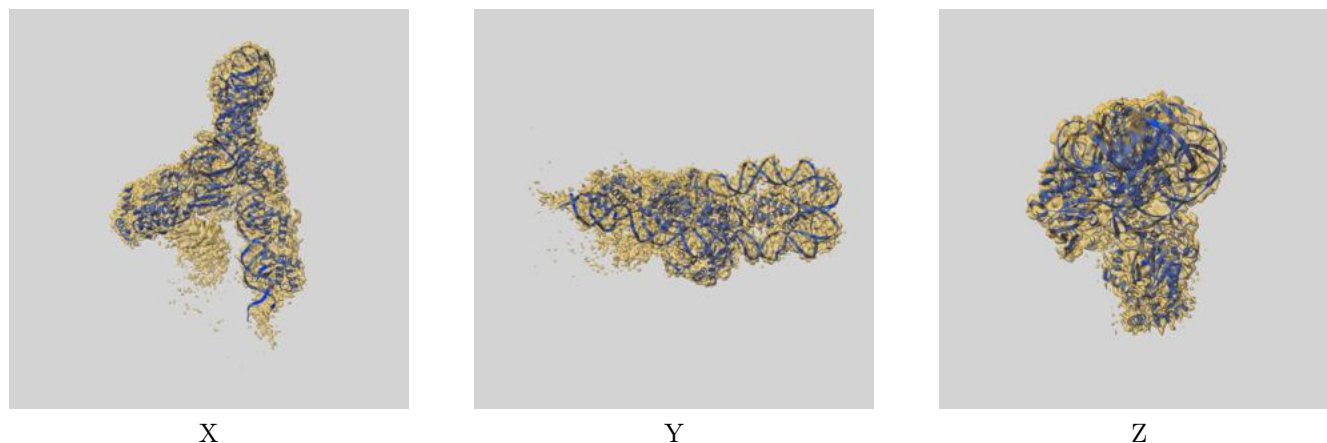
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.79	3.44
Unmasked-calculated*	4.49	7.71	4.76

\*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 4.49 differs from the reported value 3.42 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-50122 and PDB model 9F12. 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 0.35 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.

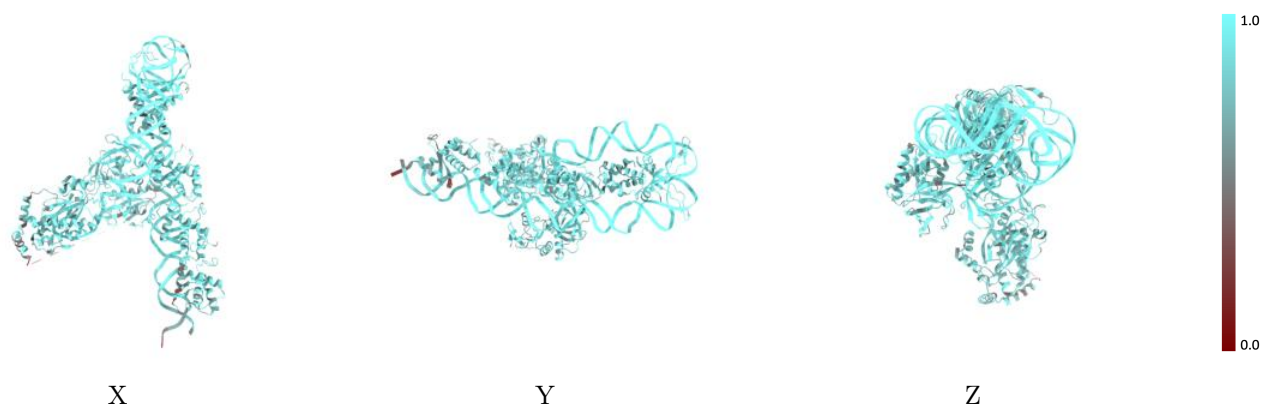


## 9.2 Q-score mapped to coordinate model [i](#)



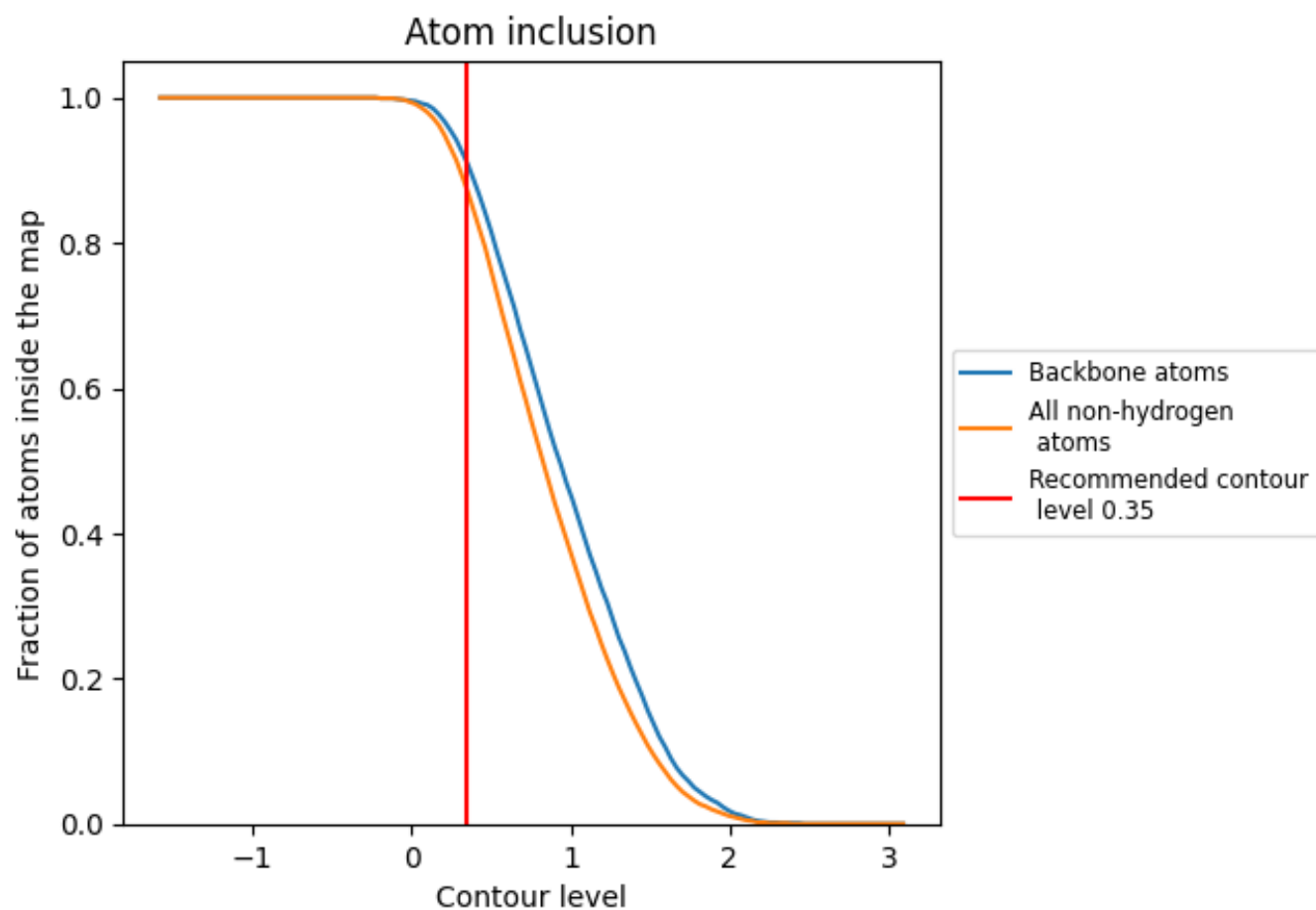
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8730</div>	<div><div></div>0.4760</div>
A	<div><div></div>0.9290</div>	<div><div></div>0.4720</div>
B	<div><div></div>0.9400</div>	<div><div></div>0.4770</div>
C	<div><div></div>0.8860</div>	<div><div></div>0.5190</div>
D	<div><div></div>0.8770</div>	<div><div></div>0.5110</div>
E	<div><div></div>0.8920</div>	<div><div></div>0.5240</div>
F	<div><div></div>0.8710</div>	<div><div></div>0.5000</div>
G	<div><div></div>0.7530</div>	<div><div></div>0.3840</div>
H	<div><div></div>0.8350</div>	<div><div></div>0.4660</div>

1.0

0.0

<0.0