



# wwPDB EM Validation Summary Report ⓘ

Jan 6, 2025 – 10:51 AM EST

PDB ID : 9DYH  
EMDB ID : EMD-47304  
Title : BEST2 + glutamate open state  
Authors : Owji, A.P.; Kittredge, A.; Zhang, Y.; Yang, T.  
Deposited on : 2024-10-14  
Resolution : 3.15 Å(reported)  
Based on initial model : 8D1G

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  
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

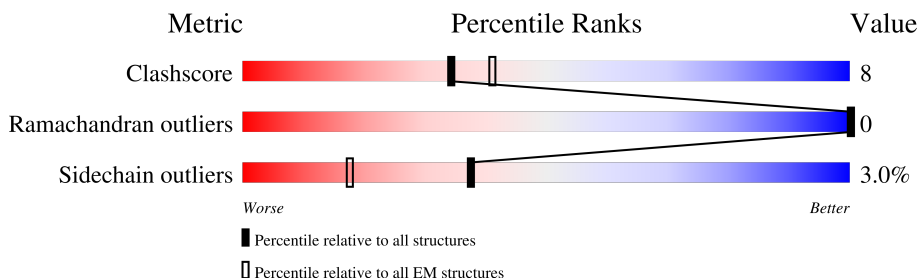
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.15 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  $\geq 3$ , 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	509	<div> <div>7%</div> <div>54%</div> <div>14%</div> <div>32%</div> </div>
1	B	509	<div> <div>7%</div> <div>54%</div> <div>14%</div> <div>32%</div> </div>
1	C	509	<div> <div>7%</div> <div>53%</div> <div>14%</div> <div>32%</div> </div>
1	D	509	<div> <div>8%</div> <div>54%</div> <div>14%</div> <div>32%</div> </div>
1	E	509	<div> <div>8%</div> <div>53%</div> <div>14%</div> <div>32%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14340 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 Bestrophin-2a.

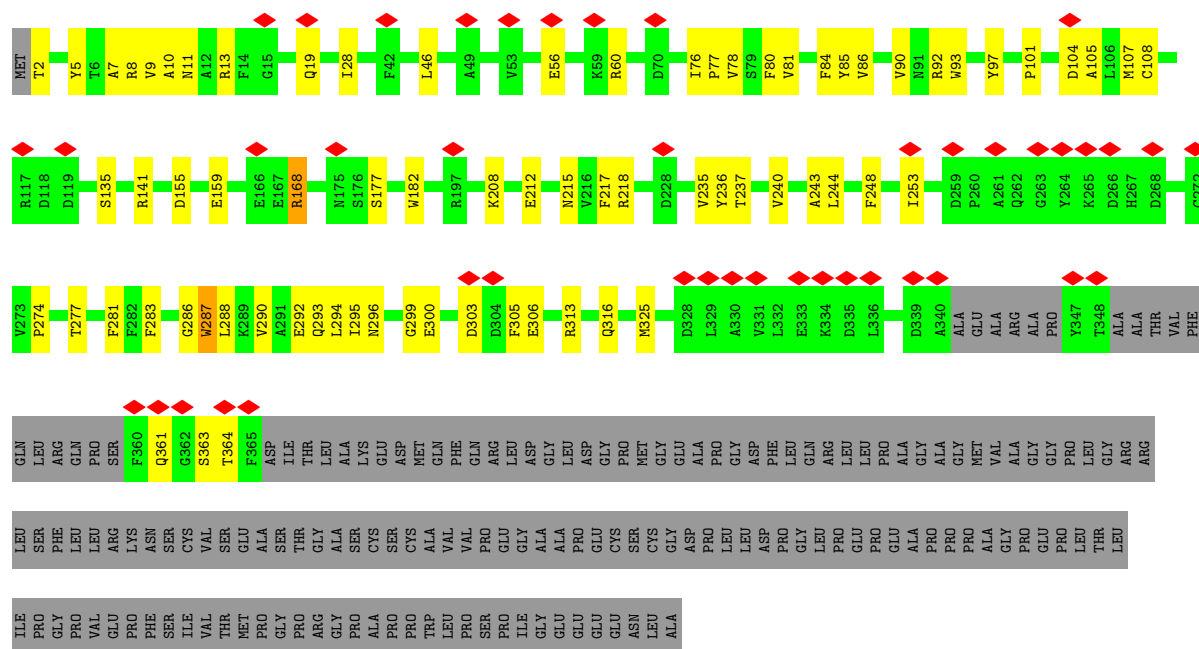
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	347	Total	C	N	O	S	1	0
			2867	1883	471	497	16		
1	E	347	Total	C	N	O	S	1	0
			2867	1883	471	497	16		
1	D	347	Total	C	N	O	S	1	0
			2867	1883	471	497	16		
1	B	347	Total	C	N	O	S	1	0
			2867	1883	471	497	16		
1	C	347	Total	C	N	O	S	1	0
			2867	1883	471	497	16		

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

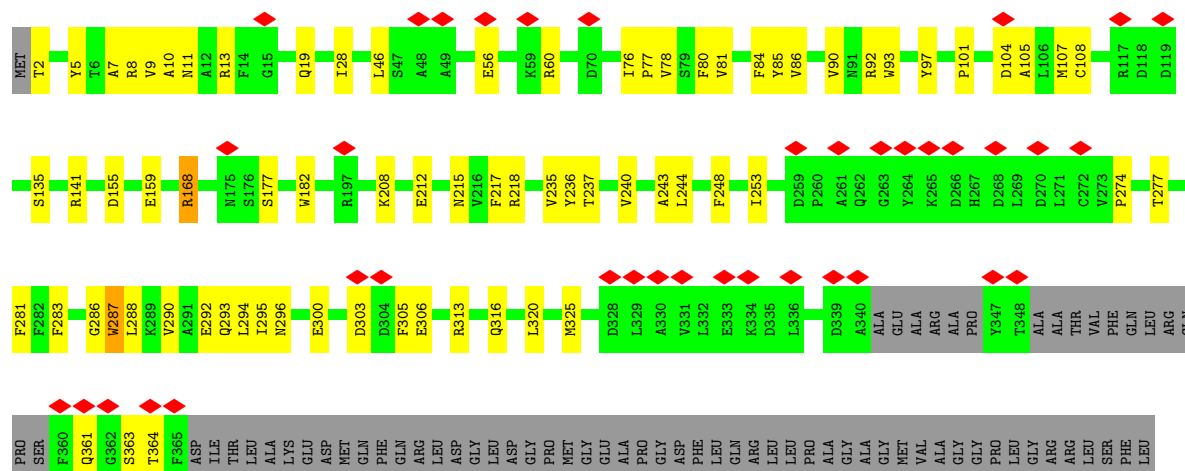
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	E	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	



- Molecule 1: Bestrophin-2a



- Molecule 1: Bestrophin-2a



LEU	ARG	ASN	SER	CYS	VAL	SER	GLU	ALA	SER	THR	GLY	ALA	SER	CYS	SER	VAL	VAL	PRO	GLU	GLY	ALA	ALA	PRO	GLU	CYS	SER	CYS	GLY	ASP	ASP	PRO	LEU	LEU	ASP	PRO	GLY	GLY	LEU	PRO	GLU	GLU	PRO	PRO	GLY	GLY	PRO	GLY	PRO			
VAL	GLU	PHE	ASN	ILE	VAL	THR	MET	PRO	GLY	ARG	GLY	ALA	PRO	ALA	PRO	TRP	LEU	SER	PRO	ILE	GLY	GLU	GLU	GLU	GLU	ASN	SER	LEU	ALA																						

● Molecule 1: Bestrophin-2a



ASN	SER	ILE	VAL	THR	MET	GLU	GLY	PRO	ARG	GLY	ALA	CYS	GLU	ASP	MET	GLN	PHE	GLN	ARG	LEU	GLY	ASP	GLY	ALA	ALA	CYS	GLU	ASP	PRO	GLU	ILE	GLY	GLU	GLU	GLU	ASN	LEU	ALA						
Q361	G362	S363	T364	F365	ASP	ILE	THR	THR	LEU	ALA	LYS	GLU	ASP	MET	GLN	PHE	GLN	ARG	LEU	ASP	GLY	PRO	PRO	GLY	ASP	PRO	GLY	ASP	PRO	GLY	LEU	THR	LEU	ILE	PRO	GLY	VAL	GLU	PRO					
W287	L288	K289	V290	A291	Q293	L294	I295	N296		G299	E300	D301	D302	D303	F304	V305	E306		R313	Q316	L320	M325	D328	L329	A330	V331	L332	E333	K334	D335	L336	D339	A340	ALA	GLU	ALA	ARG	ALA						
S135	R141	D155	E159	R165	R168	S177	W182	K208	E212	N215	V216	F217	R218	V235	Y236	T237	V240	A243	L244	F248	I253	D259	P260	Q261	Q262	G263	Y264	K265	D266	H267	D268	C272	V273	P274	T277	F281	F282	F283	G286					
MET	T2	Y5	T6	A7	R8	V9	A10	N11	A12	R13	F14	G15	Q19	I28	L46	A49	E56	G57	Q58	R59	R60	D70	I76	P77	V78	S79	F80	V81	F84	Y85	V86	V90	N91	R92	W93	Y97	P101	D104	A105	L106	M107	C108	D118	D119

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.423	Depositor
Minimum map value	-1.551	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 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	A	0.64	0/2947	0.67	0/3997
1	B	0.64	0/2947	0.67	0/3997
1	C	0.64	0/2947	0.67	0/3997
1	D	0.64	0/2947	0.67	0/3997
1	E	0.64	0/2947	0.67	0/3997
All	All	0.64	0/14735	0.67	0/19985

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	2867	0	2833	63	0
1	B	2867	0	2833	64	0
1	C	2867	0	2833	64	0
1	D	2867	0	2833	63	0
1	E	2867	0	2833	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	14340	0	14165	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 8.

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:E:237:THR:OG1	1:D:5:TYR:OH	1.99	0.80
1:A:5:TYR:OH	1:B:237:THR:OG1	2.00	0.78
1:B:5:TYR:OH	1:C:237:THR:OG1	2.01	0.76
1:A:237:THR:OG1	1:E:5:TYR:OH	2.01	0.75
1:D:237:THR:OG1	1:C:5:TYR:OH	2.02	0.71

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	342/509 (67%)	336 (98%)	6 (2%)	0	100	100
1	B	342/509 (67%)	336 (98%)	6 (2%)	0	100	100
1	C	342/509 (67%)	336 (98%)	6 (2%)	0	100	100
1	D	342/509 (67%)	336 (98%)	6 (2%)	0	100	100
1	E	342/509 (67%)	336 (98%)	6 (2%)	0	100	100
All	All	1710/2545 (67%)	1680 (98%)	30 (2%)	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	A	304/428 (71%)	295 (97%)	9 (3%)	36	63
1	B	304/428 (71%)	295 (97%)	9 (3%)	36	63
1	C	304/428 (71%)	295 (97%)	9 (3%)	36	63
1	D	304/428 (71%)	295 (97%)	9 (3%)	36	63
1	E	304/428 (71%)	295 (97%)	9 (3%)	36	63
All	All	1520/2140 (71%)	1475 (97%)	45 (3%)	37	63

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	SER
1	B	316	GLN
1	B	159	GLU
1	B	293	GLN
1	C	135	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	GLN
1	C	316	GLN
1	C	361	GLN
1	E	361	GLN
1	D	316	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 5 ligands modelled in this entry, 5 are 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.

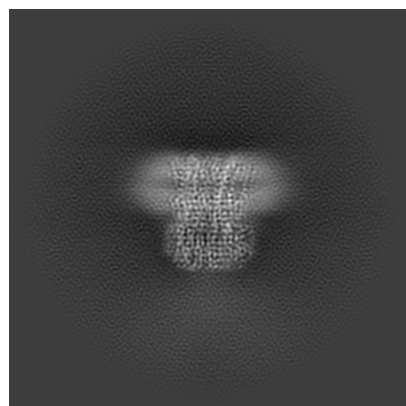
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47304. These allow visual inspection of the internal detail of the map and identification of artifacts.

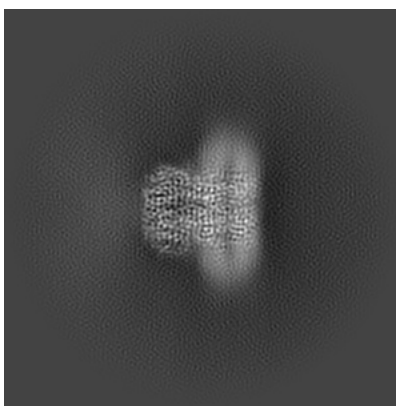
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

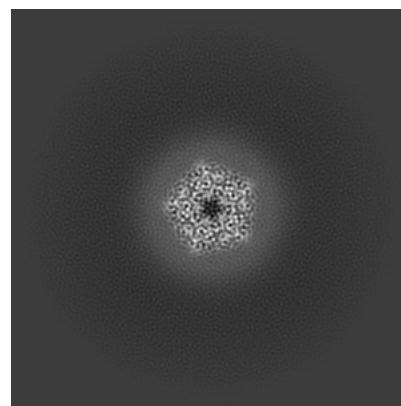
#### 6.1.1 Primary map



X

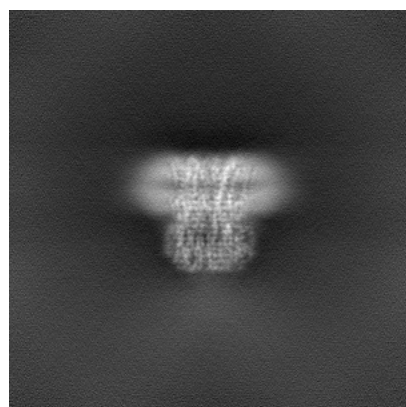


Y

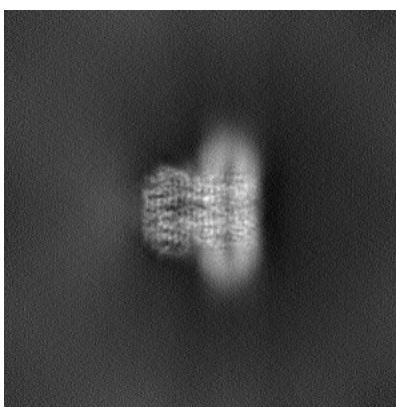


Z

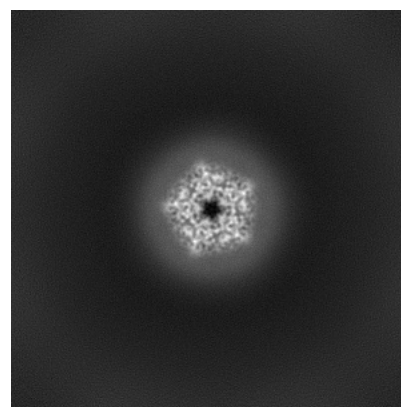
#### 6.1.2 Raw map



X



Y

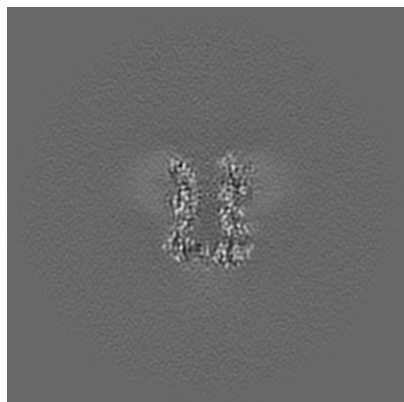


Z

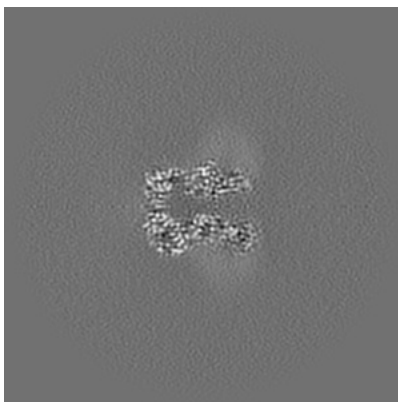
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

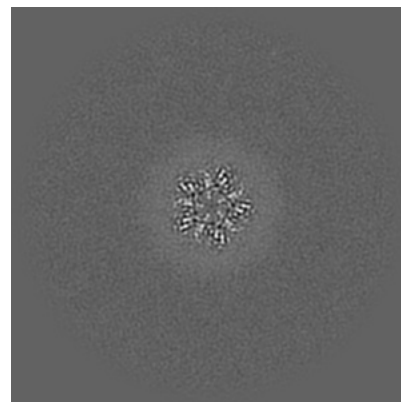
### 6.2.1 Primary map



X Index: 200

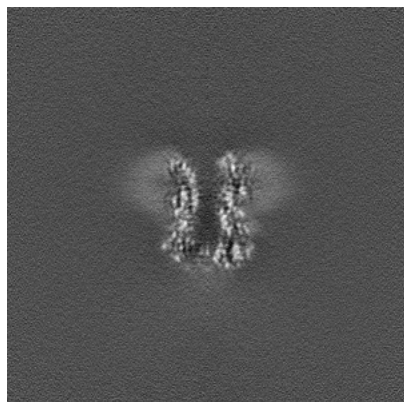


Y Index: 200

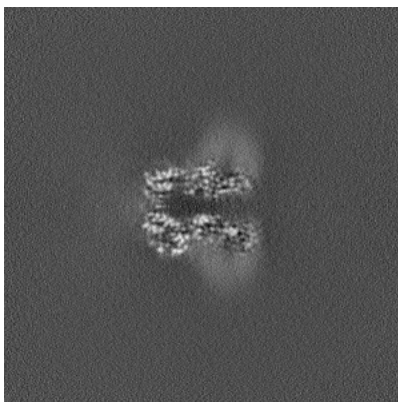


Z Index: 200

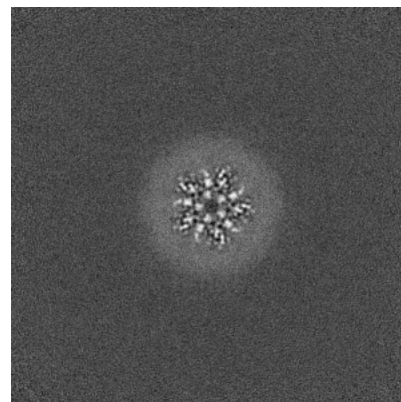
### 6.2.2 Raw map



X Index: 200



Y Index: 200

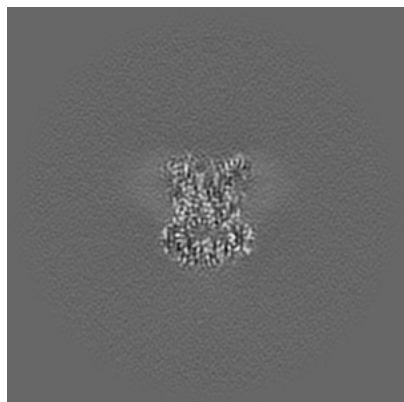


Z Index: 200

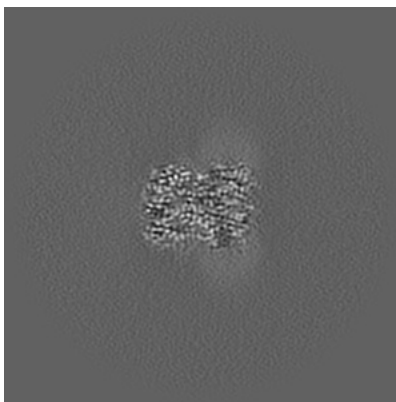
The images above show central slices of the map in three orthogonal directions.

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

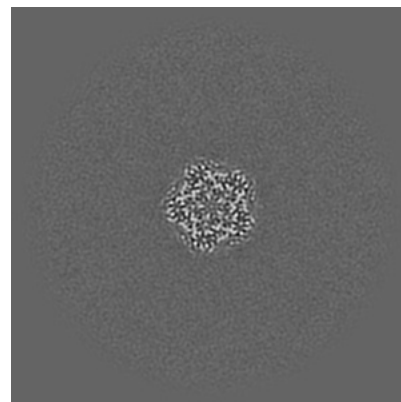
### 6.3.1 Primary map



X Index: 186

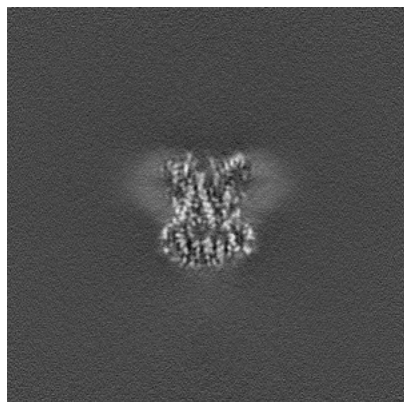


Y Index: 216

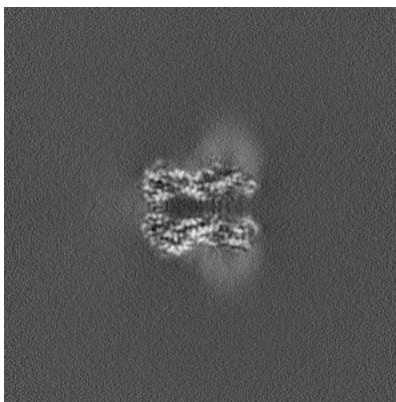


Z Index: 160

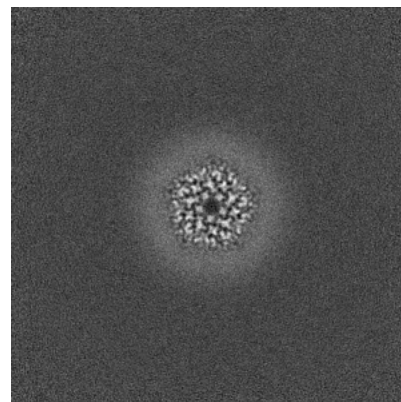
### 6.3.2 Raw map



X Index: 186



Y Index: 205



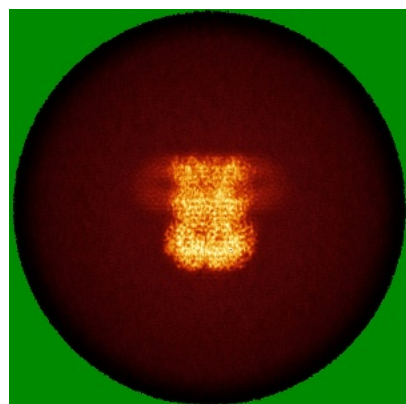
Z Index: 207

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

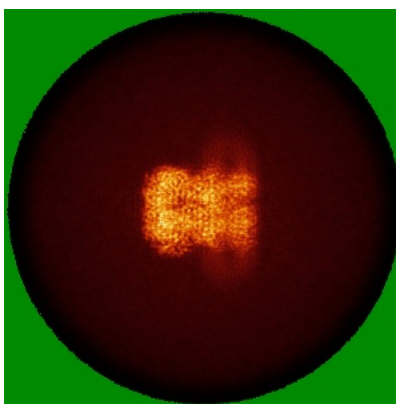


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

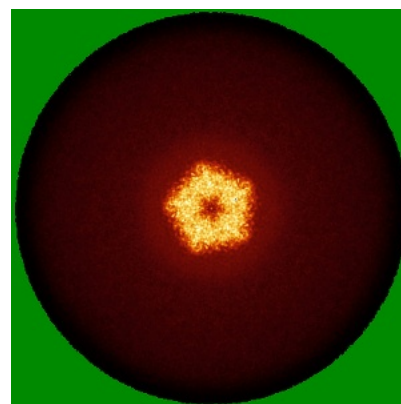
### 6.4.1 Primary map



X

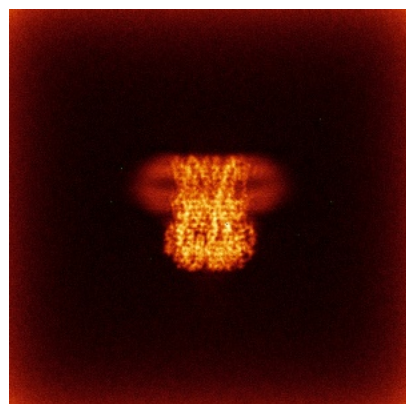


Y

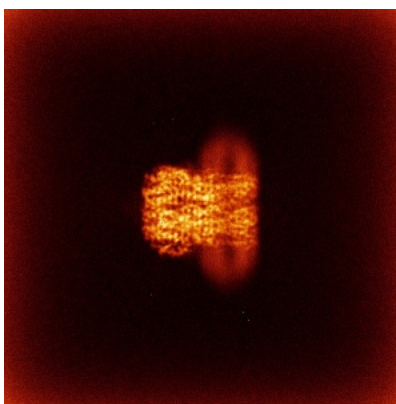


Z

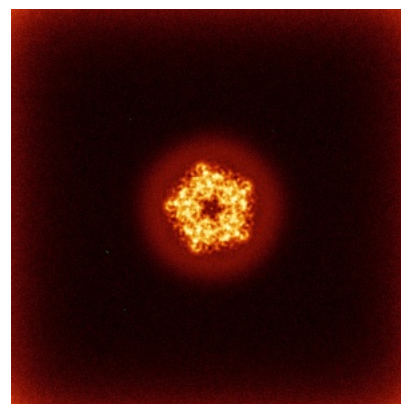
### 6.4.2 Raw map



X



Y

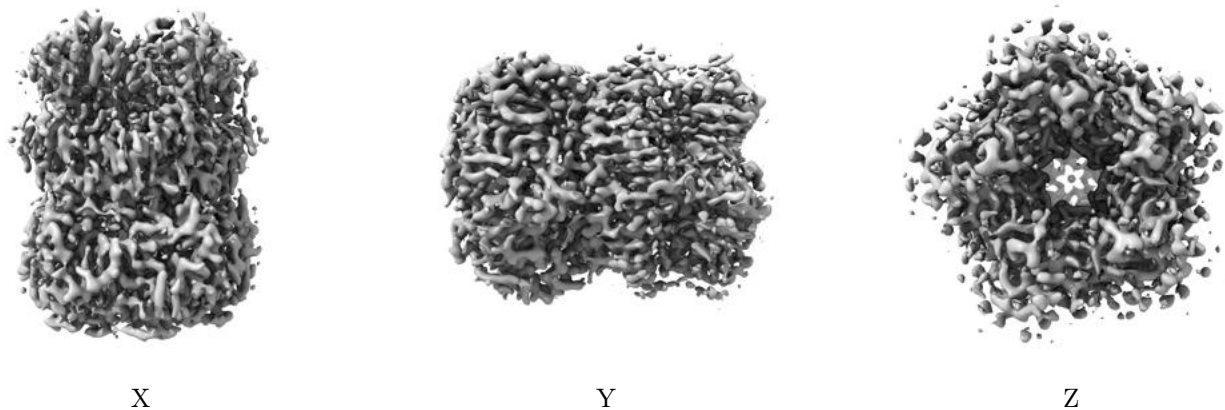


Z

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

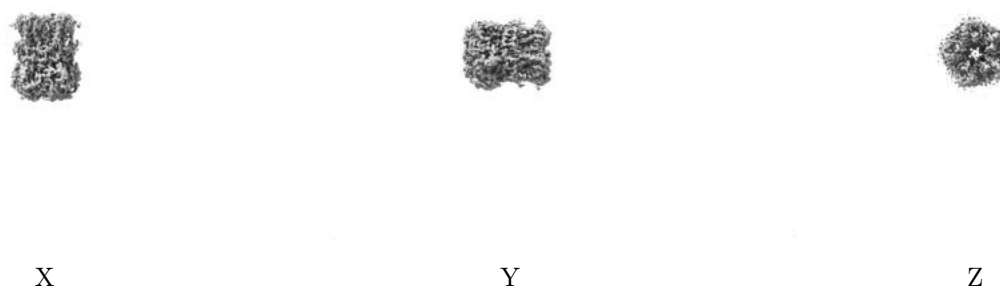
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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](#)

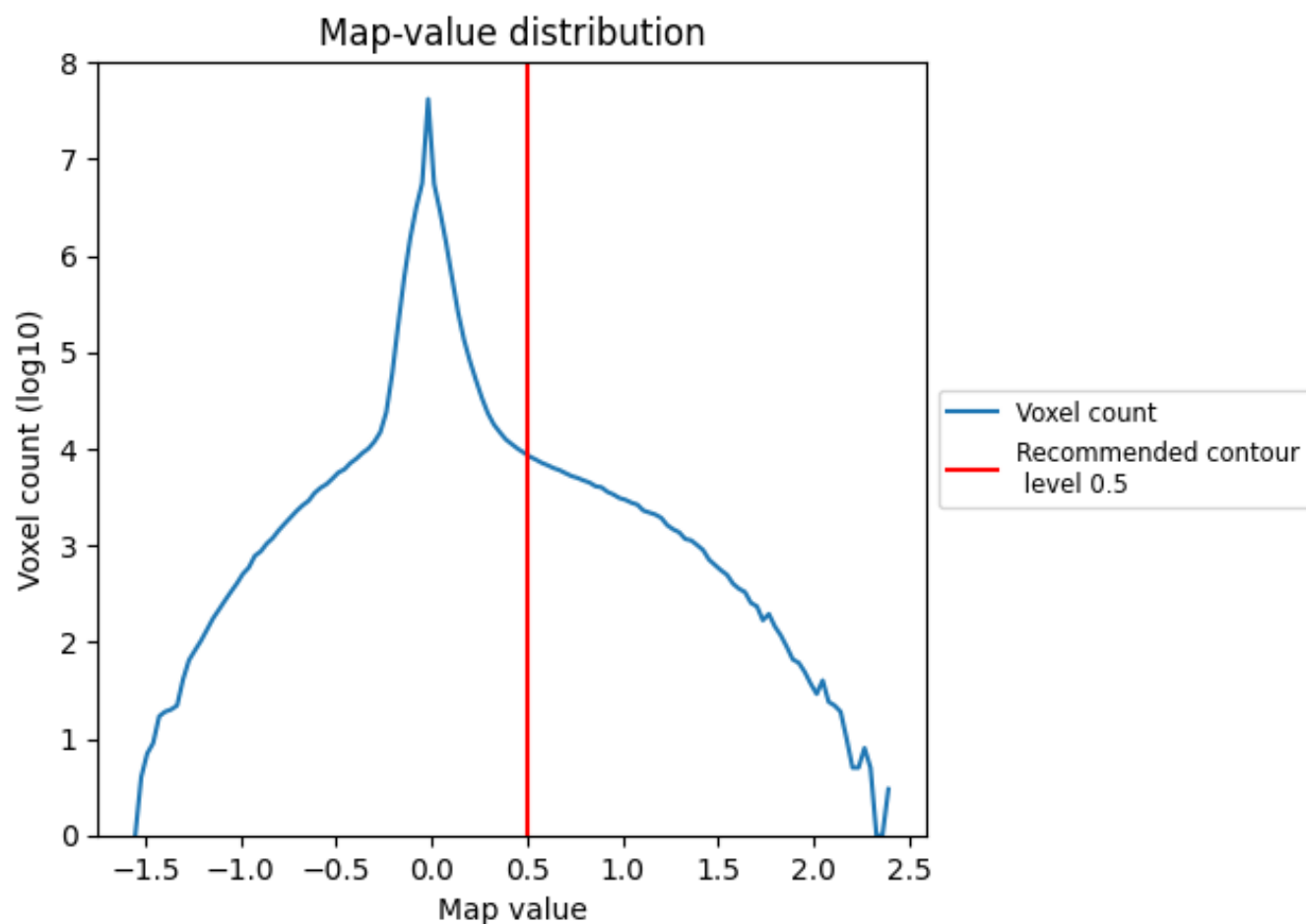
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

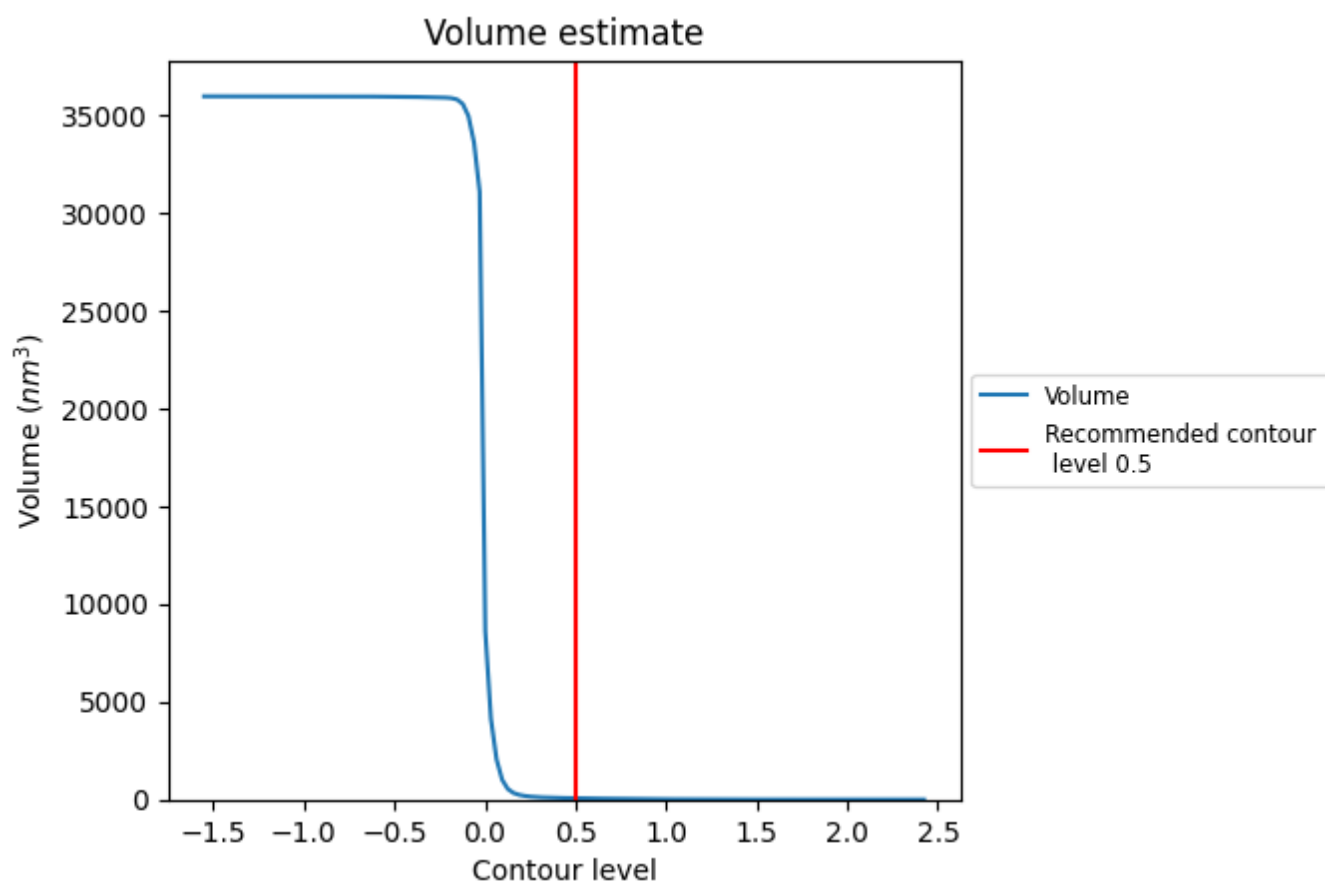
This section contains the results of statistical analysis of the map.

### 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.

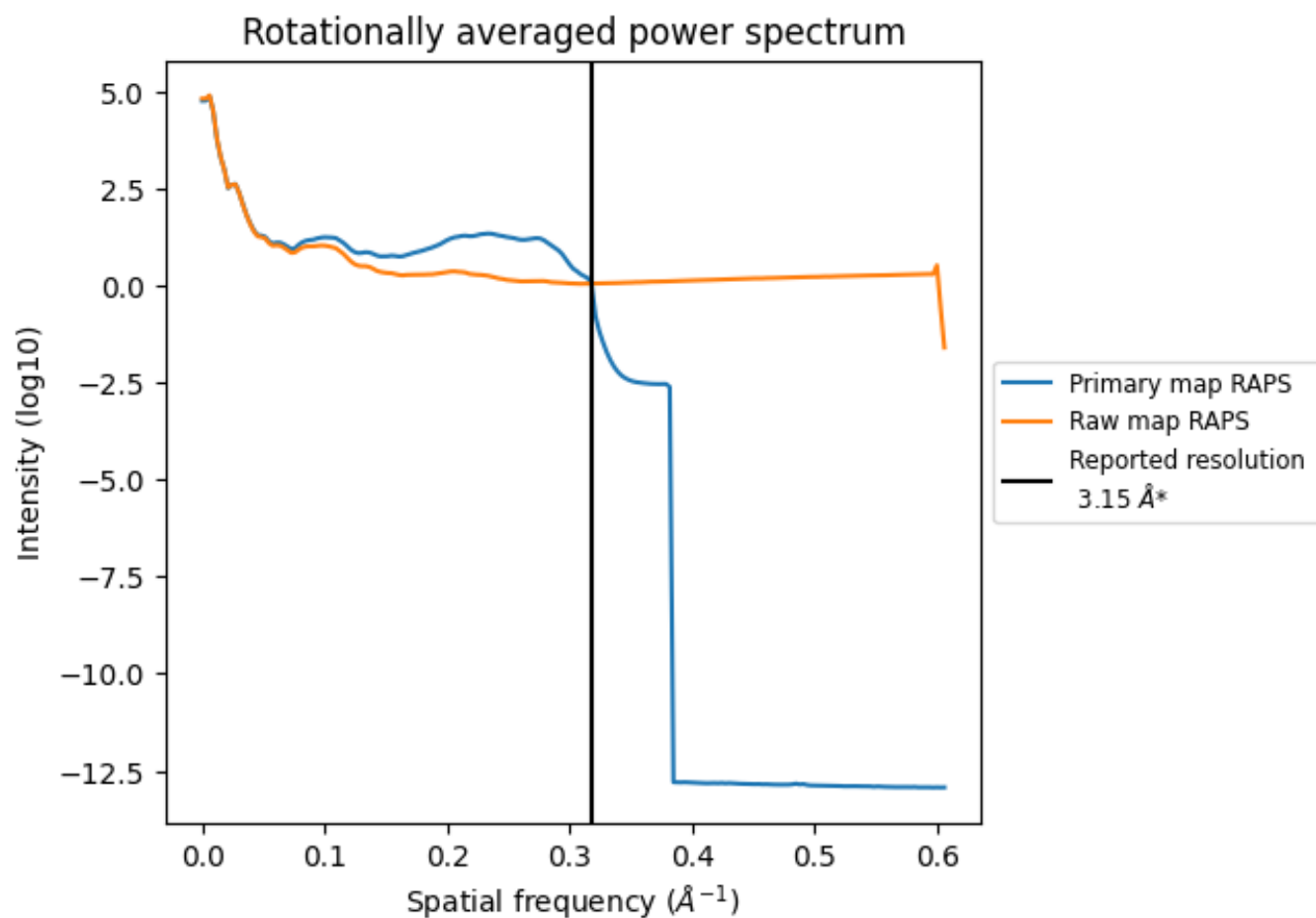
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 61 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](#)

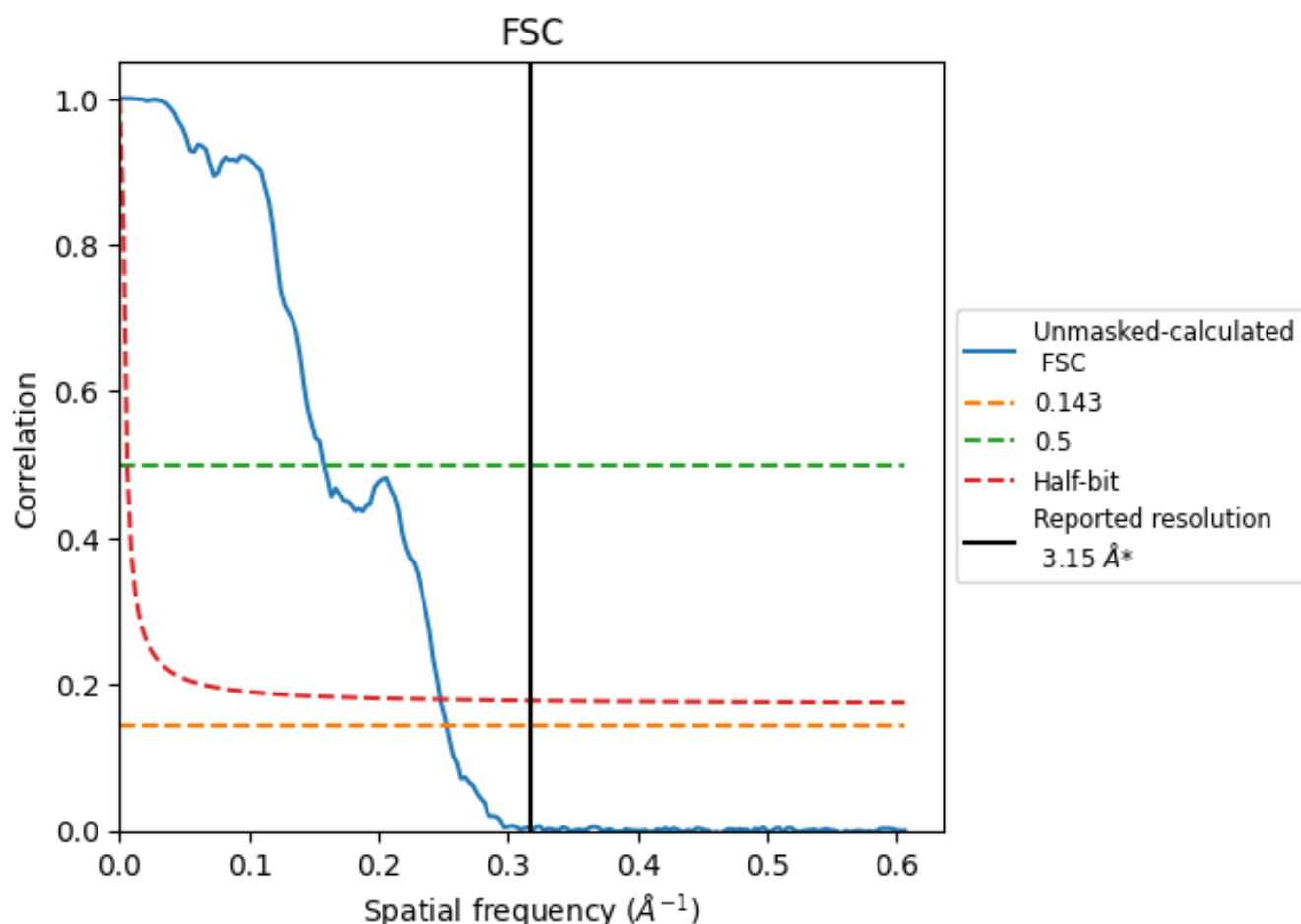


\*Reported resolution corresponds to spatial frequency of 0.317  $\text{\AA}^{-1}$

## 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 0.317 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

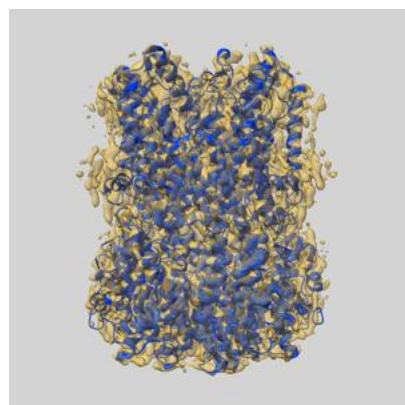
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	6.34	4.03

\*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 3.96 differs from the reported value 3.15 by more than 10 %

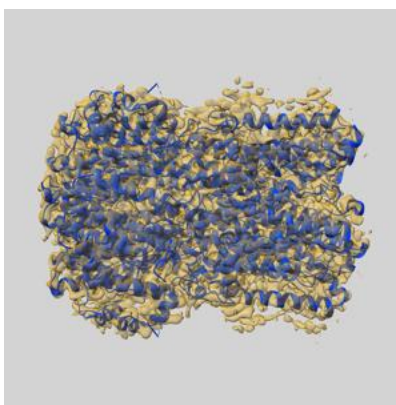
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47304 and PDB model 9DYH. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

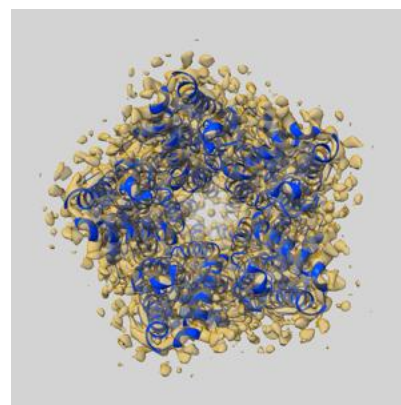
### 9.1 Map-model overlay [i](#)



X



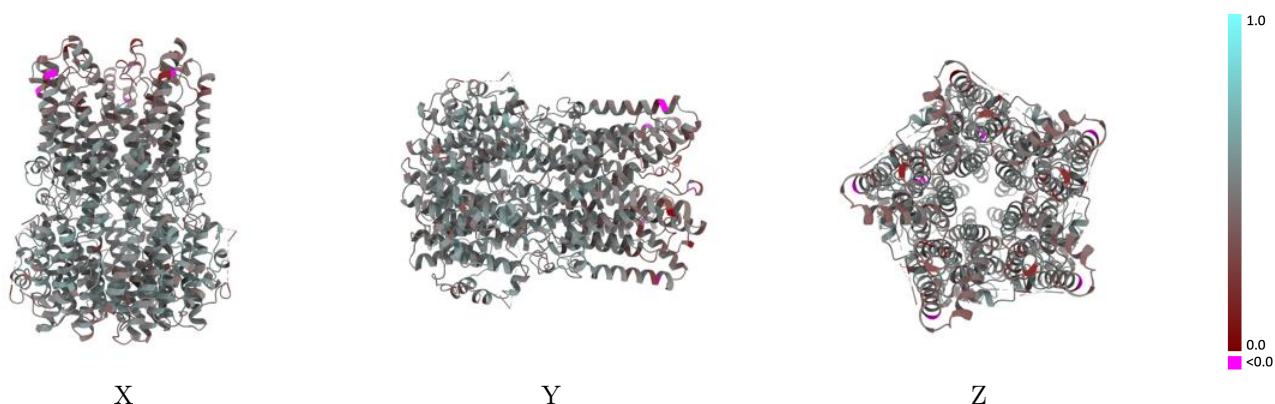
Y



Z

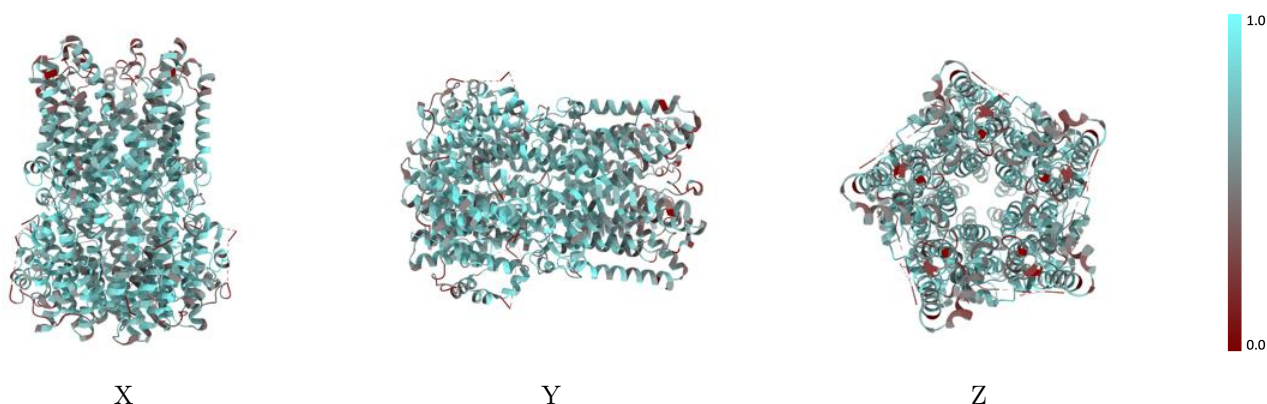
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



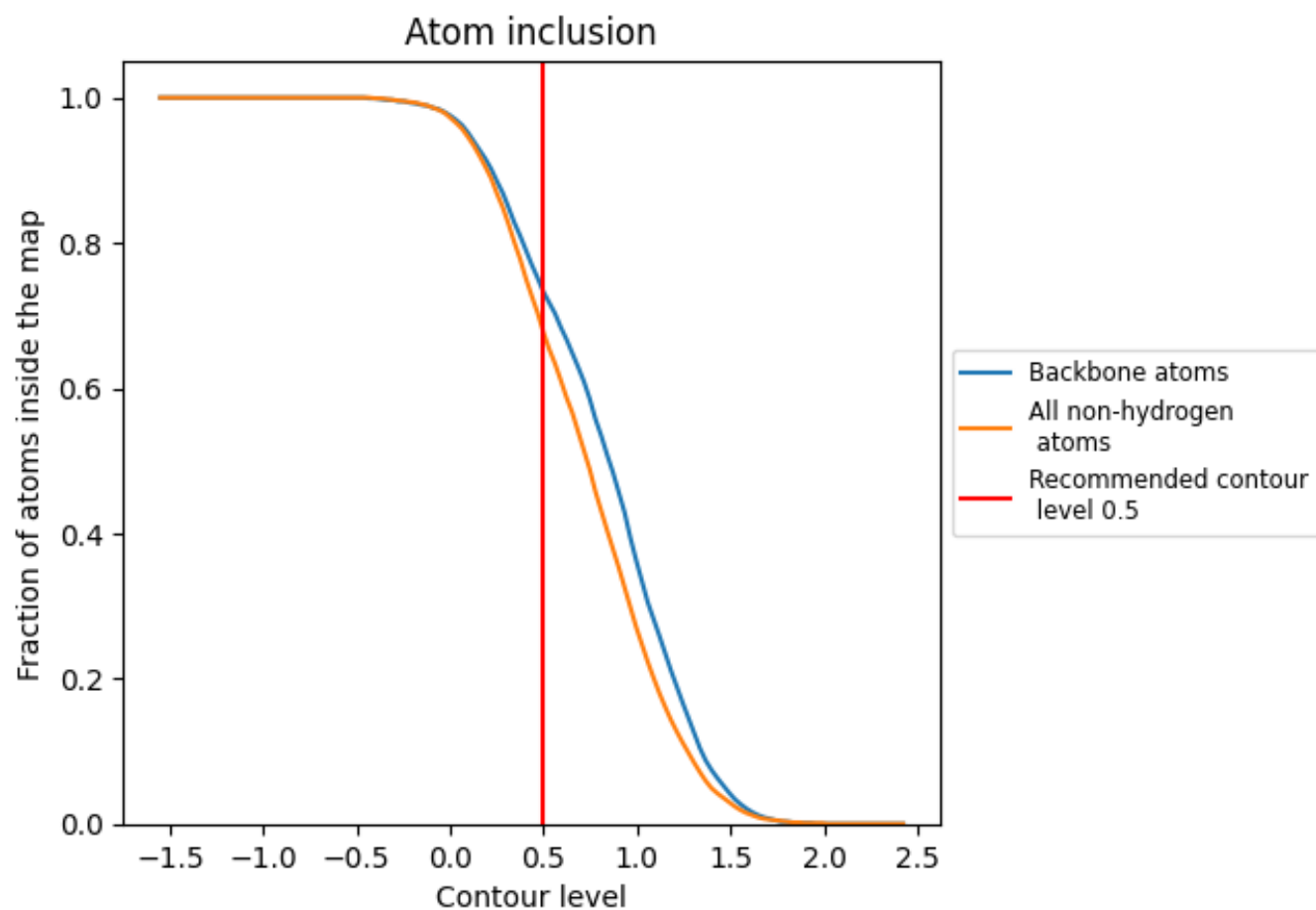
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6760	<div></div> 0.4760
A	<div></div> 0.6780	<div></div> 0.4740
B	<div></div> 0.6790	<div></div> 0.4780
C	<div></div> 0.6720	<div></div> 0.4760
D	<div></div> 0.6780	<div></div> 0.4760
E	<div></div> 0.6760	<div></div> 0.4760

