



## wwPDB EM Validation Summary Report ⓘ

Apr 21, 2026 – 10:08 am BST

PDB ID : 9H2Q / pdb\_00009h2q  
EMDB ID : EMD-51814  
Title : Stabilized complex of Chlamydia trachomatic efector CT622 in complex with human WD40 domain of ATG16L1  
Authors : Zahradnik, J.; Kolenko, P.  
Deposited on : 2024-10-14  
Resolution : 3.80 Å(reported)  
Based on initial model : .

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.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

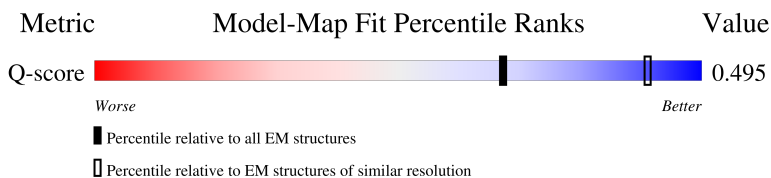
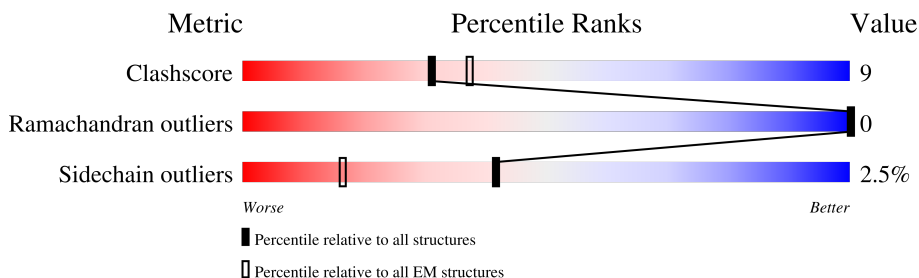
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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	674	 5% 26% 9% 64%
2	B	309	 1% 78% 19% 2%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4102 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 Maltose/maltodextrin-binding periplasmic protein, CHLPN 76 kD protein-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	242	1798	1116	306	368	8	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	HIS	-	expression tag	UNP P0AEY0
A	-21	HIS	-	expression tag	UNP P0AEY0
A	-20	HIS	-	expression tag	UNP P0AEY0
A	-19	HIS	-	expression tag	UNP P0AEY0
A	-18	HIS	-	expression tag	UNP P0AEY0
A	-17	HIS	-	expression tag	UNP P0AEY0
A	353	SER	-	linker	UNP P0AEY0
A	354	LEU	-	linker	UNP P0AEY0
A	355	LEU	-	linker	UNP P0AEY0
A	356	LEU	-	linker	UNP P0AEY0
A	357	ASP	-	linker	UNP P0AEY0
A	358	ASP	-	linker	UNP P0AEY0
A	359	VAL	-	linker	UNP P0AEY0
A	360	ASP	-	linker	UNP P0AEY0
A	456	GLY	SER	engineered mutation	UNP A0A0H2X2S1
A	494	ASP	SER	engineered mutation	UNP A0A0H2X2S1
A	505	ASP	SER	engineered mutation	UNP A0A0H2X2S1
A	512	LEU	ASN	engineered mutation	UNP A0A0H2X2S1
A	532	ASP	ASN	engineered mutation	UNP A0A0H2X2S1
A	559	GLU	ASP	engineered mutation	UNP A0A0H2X2S1
A	564	ILE	THR	engineered mutation	UNP A0A0H2X2S1
A	577	LYS	MET	engineered mutation	UNP A0A0H2X2S1
A	583	ALA	SER	engineered mutation	UNP A0A0H2X2S1
A	599	ASN	ALA	engineered mutation	UNP A0A0H2X2S1
A	608	LYS	GLN	engineered mutation	UNP A0A0H2X2S1
A	619	ARG	SER	engineered mutation	UNP A0A0H2X2S1
A	623	ALA	SER	engineered mutation	UNP A0A0H2X2S1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	626	LEU	ASN	engineered mutation	UNP A0A0H2X2S1
A	629	GLU	ARG	engineered mutation	UNP A0A0H2X2S1
A	633	GLN	ALA	engineered mutation	UNP A0A0H2X2S1

- Molecule 2 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	300	Total	C	N	O	S	0	0
			2304	1440	416	442	6		

There are 47 discrepancies between the modelled and reference sequences:

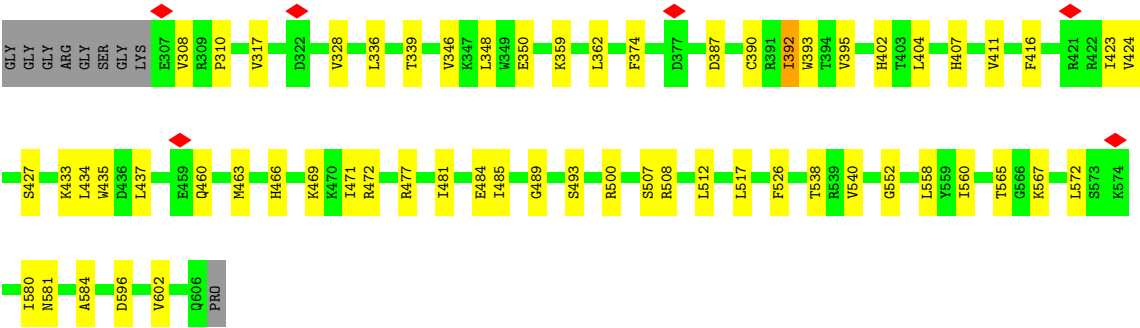
Chain	Residue	Modelled	Actual	Comment	Reference
B	299	GLY	-	expression tag	UNP Q676U5
B	300	GLY	-	expression tag	UNP Q676U5
B	301	GLY	-	expression tag	UNP Q676U5
B	302	ARG	-	expression tag	UNP Q676U5
B	310	PRO	VAL	engineered mutation	UNP Q676U5
B	316	GLN	CYS	engineered mutation	UNP Q676U5
B	333	ASP	GLY	engineered mutation	UNP Q676U5
B	334	GLY	SER	engineered mutation	UNP Q676U5
B	342	ASN	MET	engineered mutation	UNP Q676U5
B	354	GLY	GLU	engineered mutation	UNP Q676U5
B	355	SER	LYS	engineered mutation	UNP Q676U5
B	363	THR	SER	engineered mutation	UNP Q676U5
B	367	GLY	ALA	engineered mutation	UNP Q676U5
B	376	PRO	SER	engineered mutation	UNP Q676U5
B	377	ASP	ALA	engineered mutation	UNP Q676U5
B	379	LYS	SER	engineered mutation	UNP Q676U5
B	388	LYS	PHE	engineered mutation	UNP Q676U5
B	390	CYS	SER	engineered mutation	UNP Q676U5
B	412	TYR	LEU	engineered mutation	UNP Q676U5
B	417	SER	LEU	engineered mutation	UNP Q676U5
B	418	PRO	LEU	engineered mutation	UNP Q676U5
B	420	GLY	ASN	engineered mutation	UNP Q676U5
B	421	ARG	ALA	engineered mutation	UNP Q676U5
B	439	LYS	SER	engineered mutation	UNP Q676U5
B	440	GLY	LYS	engineered mutation	UNP Q676U5
B	441	THR	VAL	engineered mutation	UNP Q676U5
B	452	ALA	CYS	engineered mutation	UNP Q676U5
B	461	SER	CYS	engineered mutation	UNP Q676U5
B	462	ILE	VAL	engineered mutation	UNP Q676U5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	467	HIS	PHE	engineered mutation	UNP Q676U5
B	478	THR	SER	engineered mutation	UNP Q676U5
B	479	GLY	GLU	engineered mutation	UNP Q676U5
B	483	GLN	ARG	engineered mutation	UNP Q676U5
B	485	ILE	MET	engineered mutation	UNP Q676U5
B	488	GLN	LEU	engineered mutation	UNP Q676U5
B	493	SER	ALA	engineered mutation	UNP Q676U5
B	499	ASP	GLU	engineered mutation	UNP Q676U5
B	510	ASN	ASP	engineered mutation	UNP Q676U5
B	511	THR	LEU	engineered mutation	UNP Q676U5
B	514	ILE	VAL	engineered mutation	UNP Q676U5
B	521	SER	ALA	engineered mutation	UNP Q676U5
B	533	SER	CYS	engineered mutation	UNP Q676U5
B	555	ASP	GLU	engineered mutation	UNP Q676U5
B	564	ARG	LEU	engineered mutation	UNP Q676U5
B	575	HIS	GLN	engineered mutation	UNP Q676U5
B	599	GLY	CYS	engineered mutation	UNP Q676U5
B	607	PRO	TYR	engineered mutation	UNP Q676U5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113881	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.686	Depositor
Minimum map value	-0.354	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	261.7856, 261.7856, 261.7856	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0226, 1.0226, 1.0226	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.14	0/1812	0.33	0/2442
2	B	0.13	0/2353	0.33	0/3183
All	All	0.13	0/4165	0.33	0/5625

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

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	1798	0	1793	39	0
2	B	2304	0	2270	34	0
All	All	4102	0	4063	72	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 9.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HA	1:A:399:MET:HE1	1.67	0.75
1:A:532:ASP:HB3	1:A:535:GLN:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:HD22	1:A:361:ASN:N	1.88	0.69
1:A:542:VAL:HG11	1:A:645:LEU:HD22	1.79	0.64
2:B:346:VAL:HB	2:B:362:LEU:HB2	1.80	0.63

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	232/674 (34%)	224 (97%)	8 (3%)	0	100	100
2	B	298/309 (96%)	287 (96%)	11 (4%)	0	100	100
All	All	530/983 (54%)	511 (96%)	19 (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	A	190/538 (35%)	183 (96%)	7 (4%)	30	54
2	B	252/256 (98%)	248 (98%)	4 (2%)	55	68
All	All	442/794 (56%)	431 (98%)	11 (2%)	42	61

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	308	VAL
2	B	392	ILE
2	B	507	SER
2	B	435	TRP
1	A	559	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	GLN
1	A	556	GLN
1	A	636	GLN
2	B	407	HIS
2	B	510	ASN

### 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 [i](#)

There are no chain breaks in this entry.

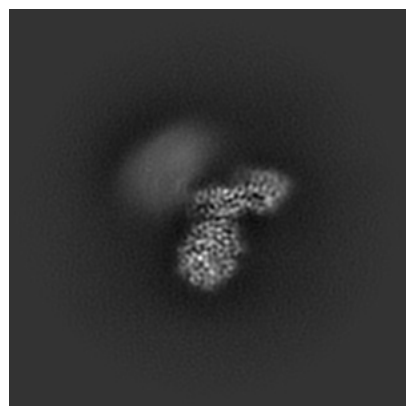
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51814. These allow visual inspection of the internal detail of the map and identification of artifacts.

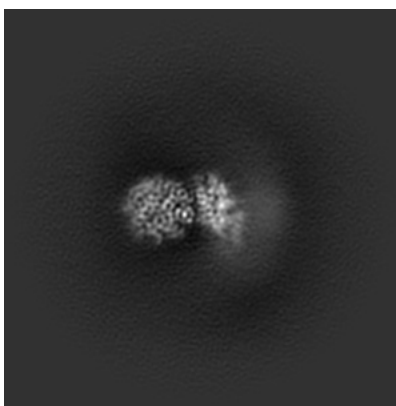
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

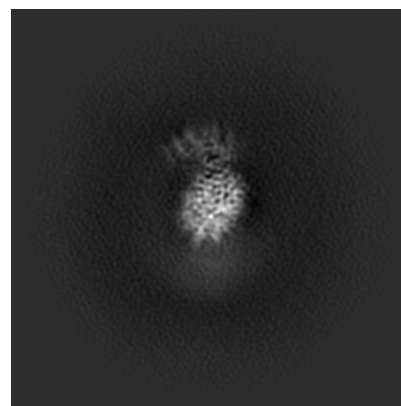
#### 6.1.1 Primary map



X

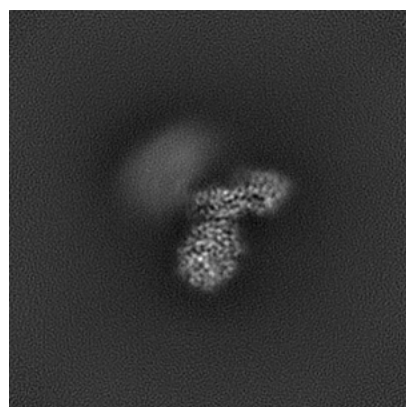


Y

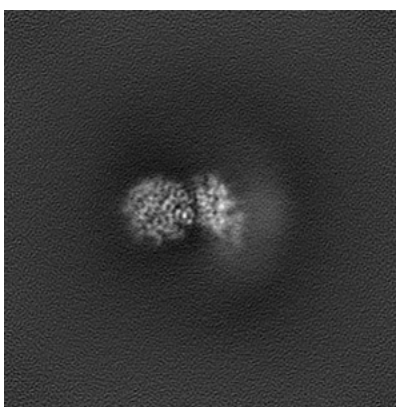


Z

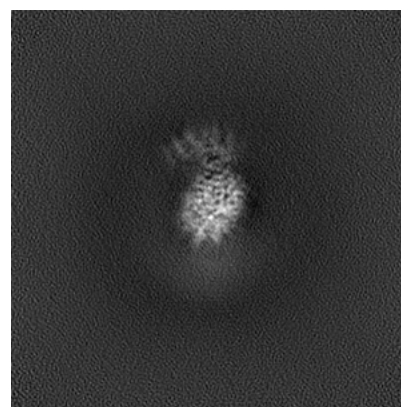
#### 6.1.2 Raw map



X



Y

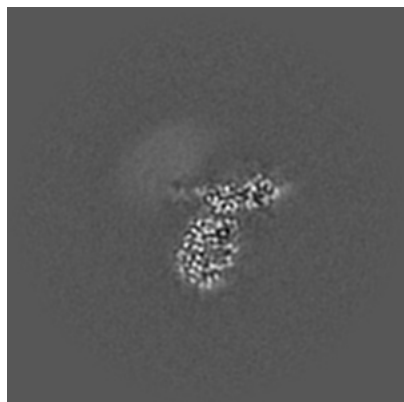


Z

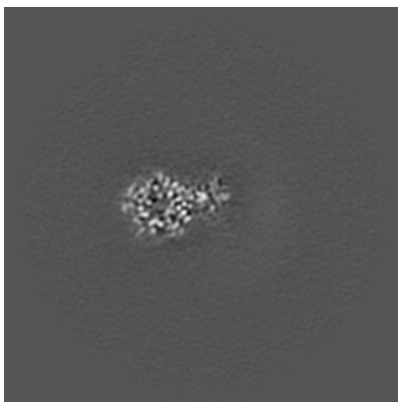
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

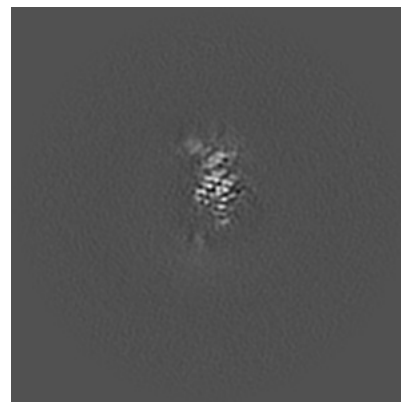
### 6.2.1 Primary map



X Index: 128

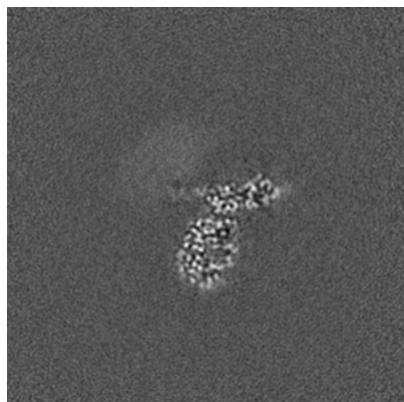


Y Index: 128

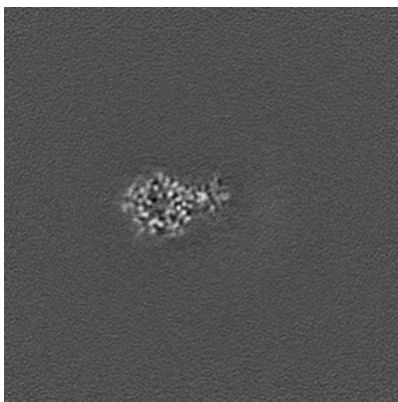


Z Index: 128

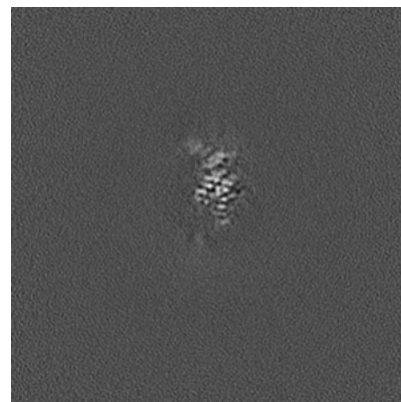
### 6.2.2 Raw map



X Index: 128



Y Index: 128

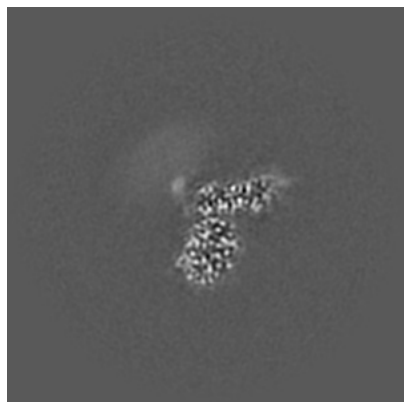


Z Index: 128

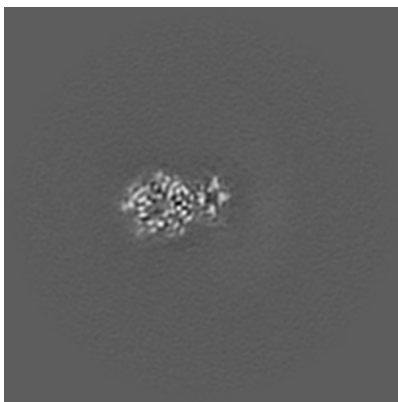
The images above show central slices of the map in three orthogonal directions.

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

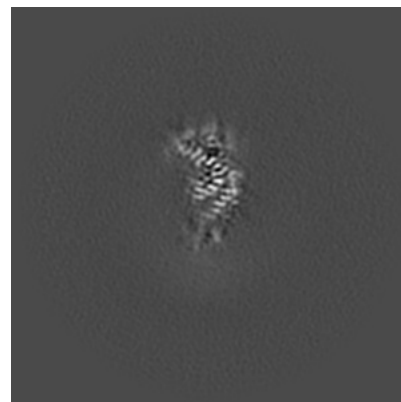
### 6.3.1 Primary map



X Index: 132

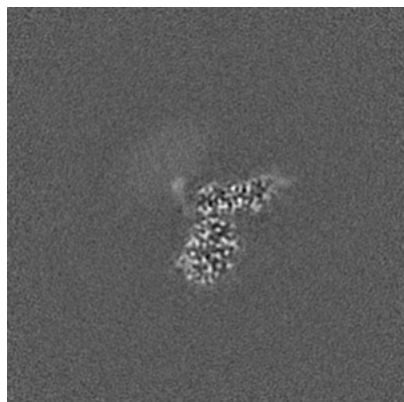


Y Index: 129

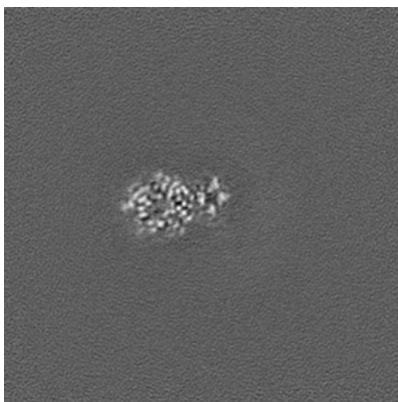


Z Index: 139

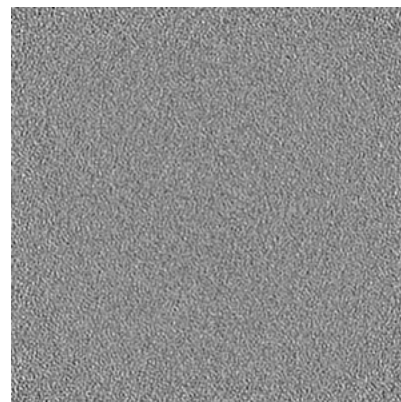
### 6.3.2 Raw map



X Index: 132



Y Index: 129



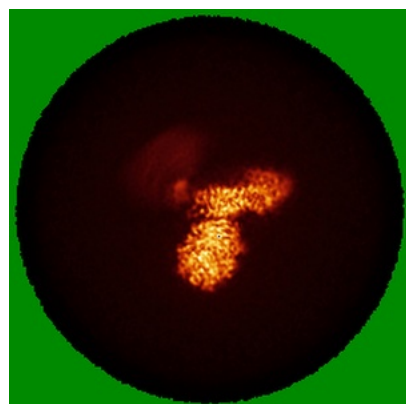
Z Index: 255

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

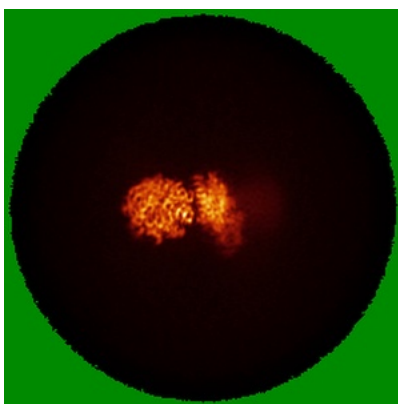


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

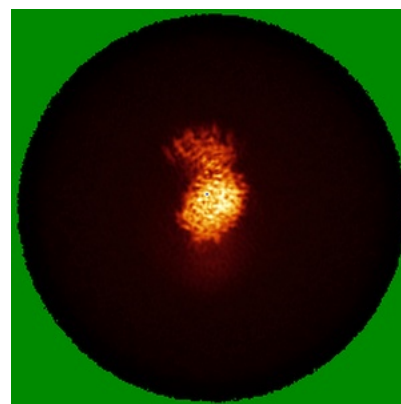
### 6.4.1 Primary map



X

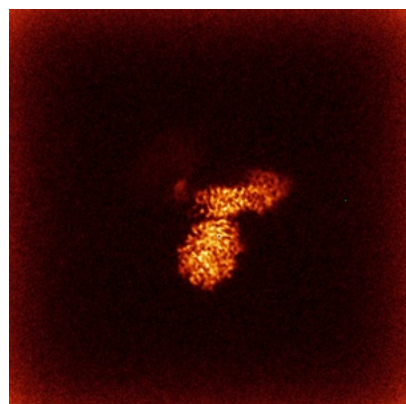


Y

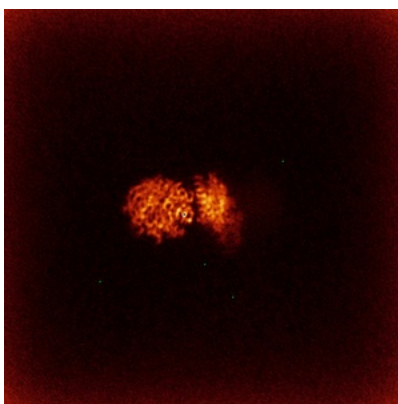


Z

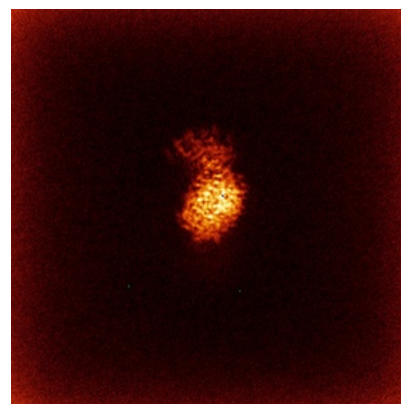
### 6.4.2 Raw map



X



Y

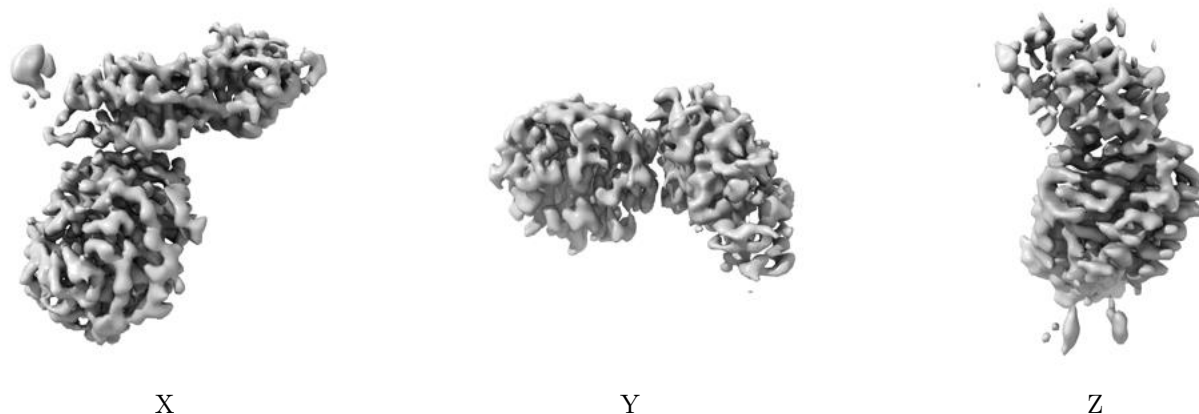


Z

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.

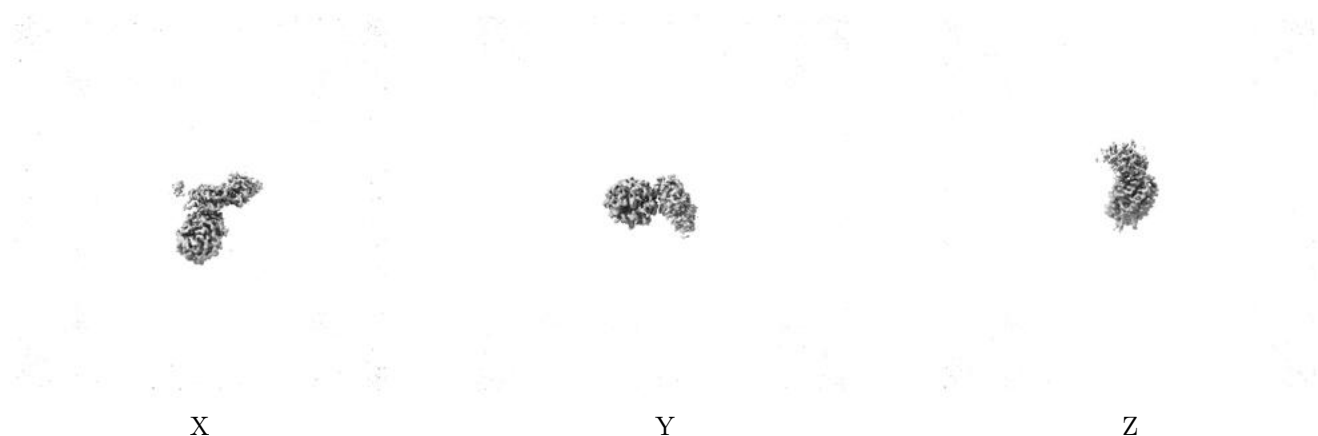
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.



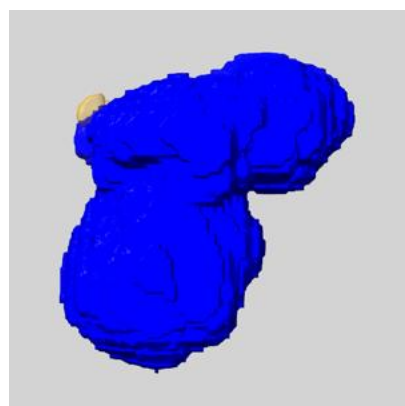
## 6.6 Mask visualisation [i](#)

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

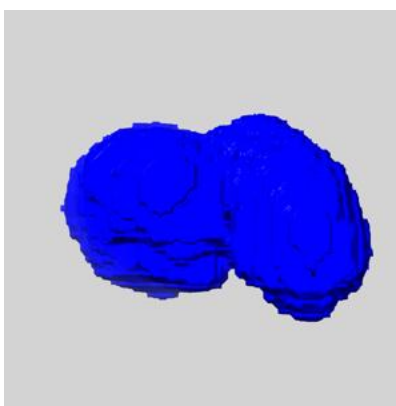
A mask typically either:

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

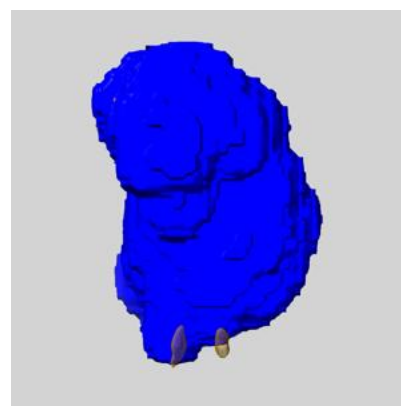
### 6.6.1 emd\_51814\_msk\_1.map [i](#)



X



Y

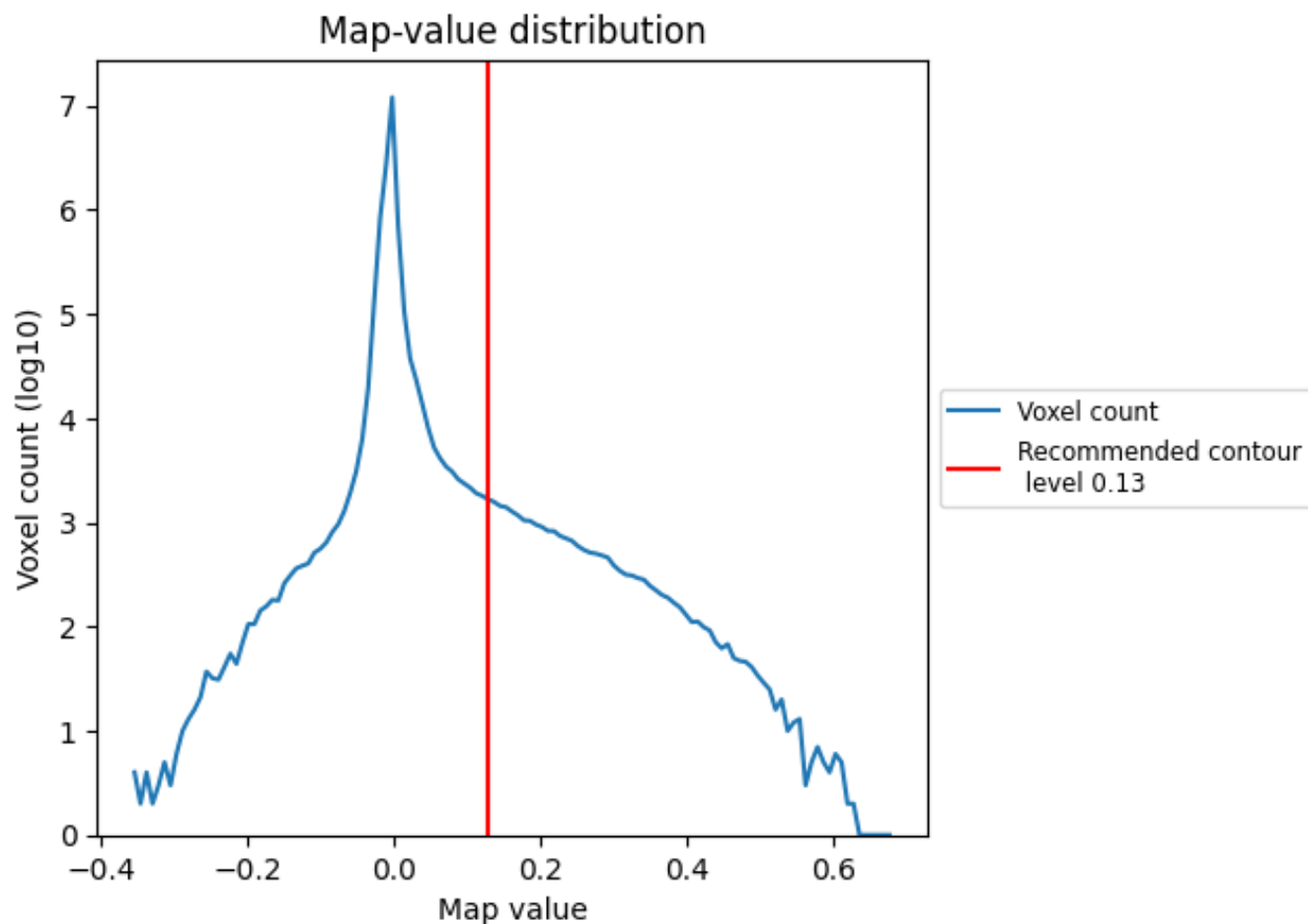


Z

## 7 Map analysis [i](#)

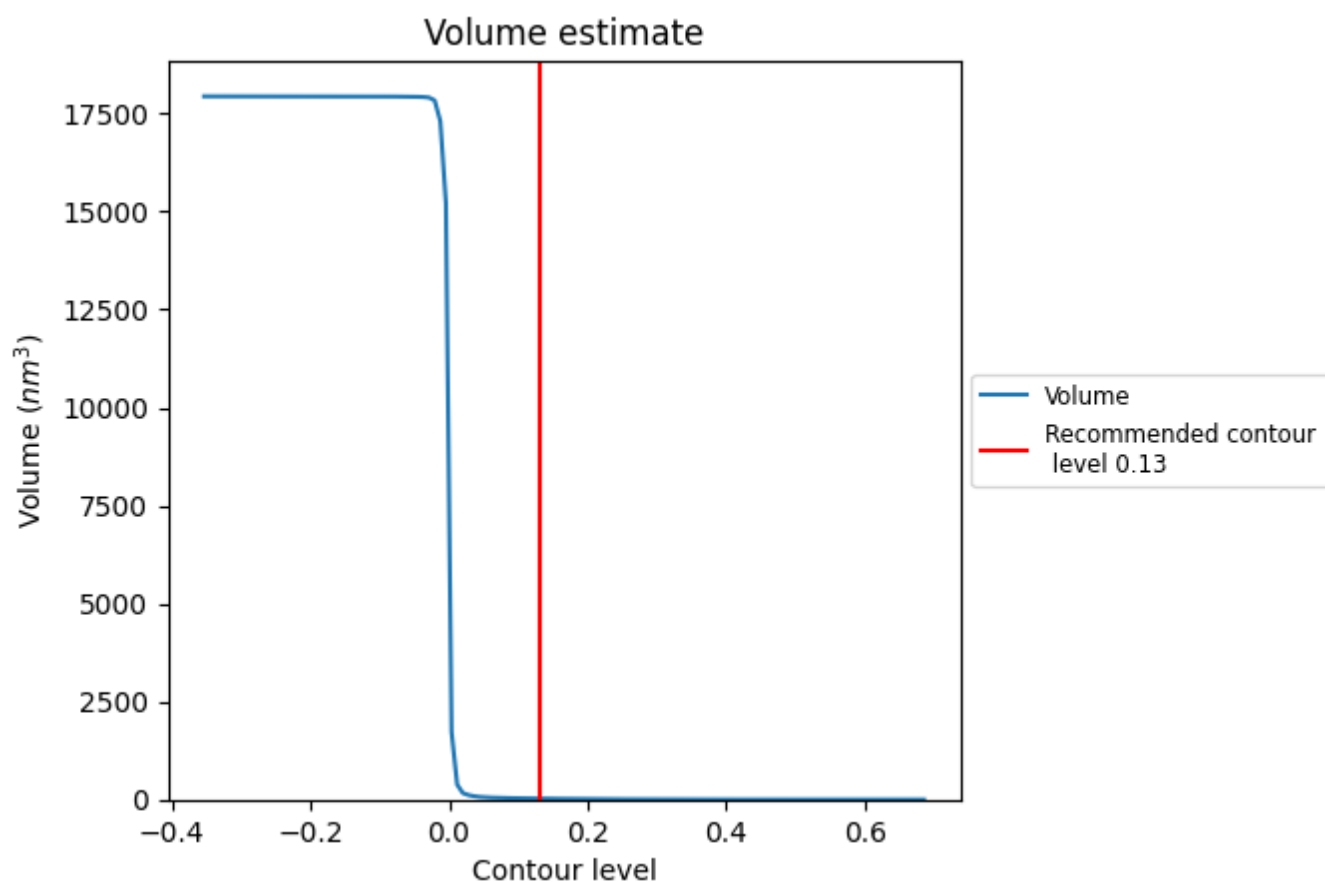
This section contains the results of statistical analysis of the map.

### 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.

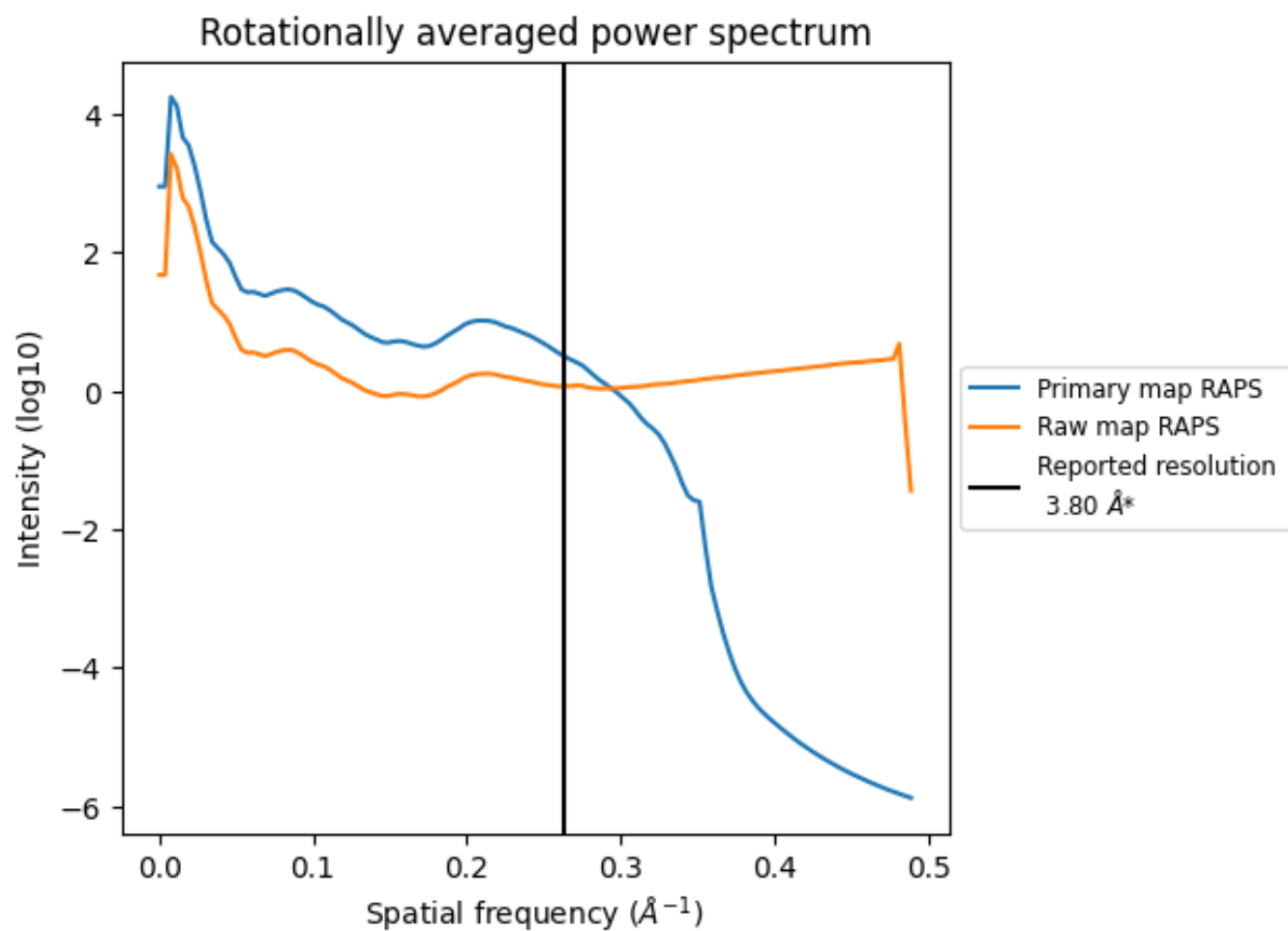
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25  $\text{nm}^3$ ; this corresponds to an approximate mass of 23 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 ⓘ

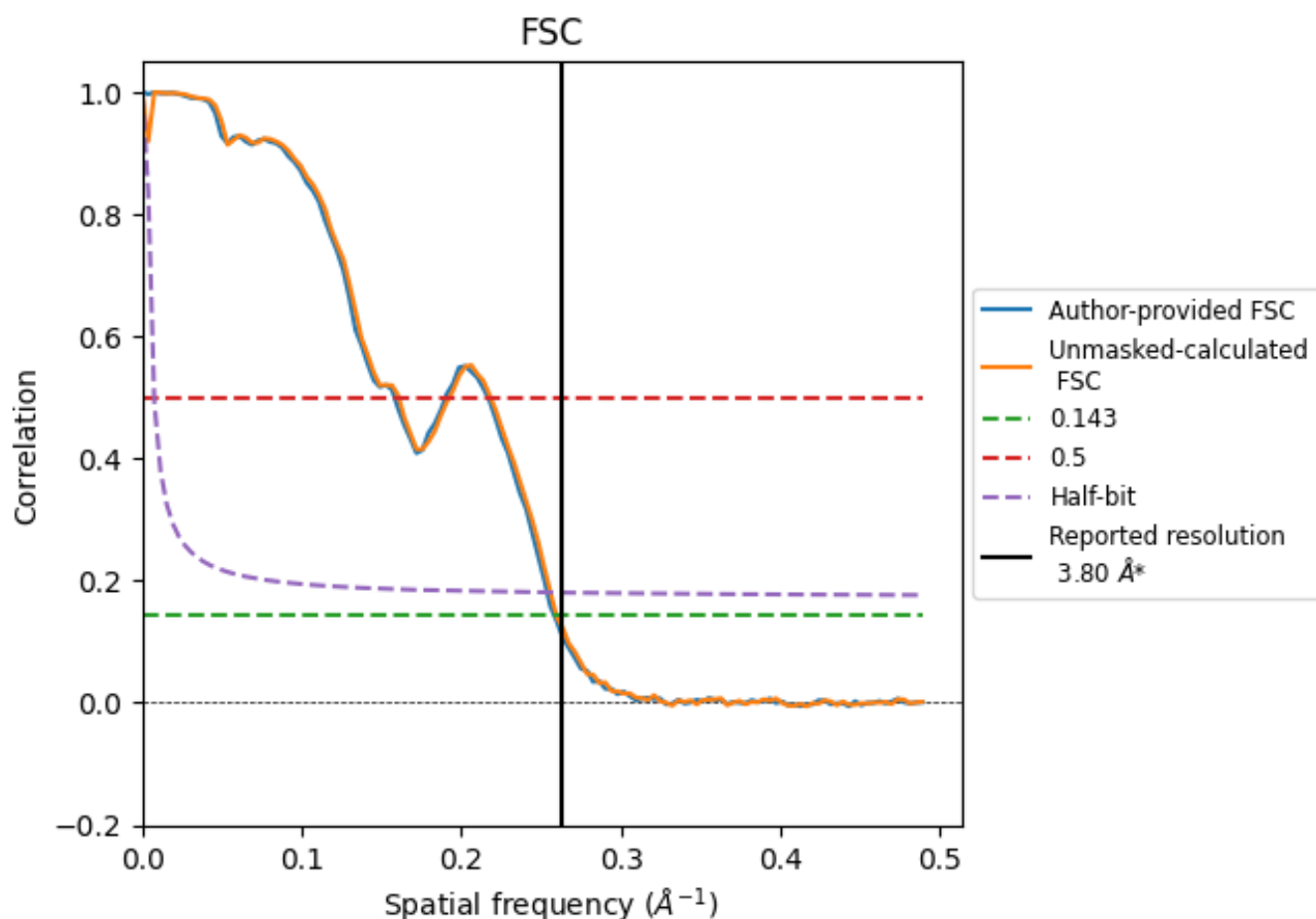


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

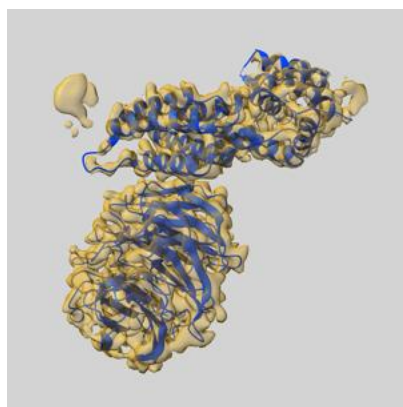
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.87	6.32	3.94
Unmasked-calculated*	3.85	6.22	3.91

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

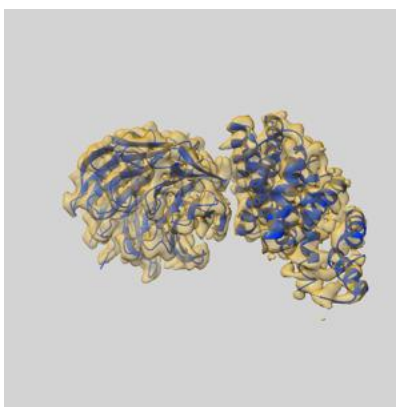
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51814 and PDB model 9H2Q. Per-residue inclusion information can be found in section [3](#) on page [6](#).

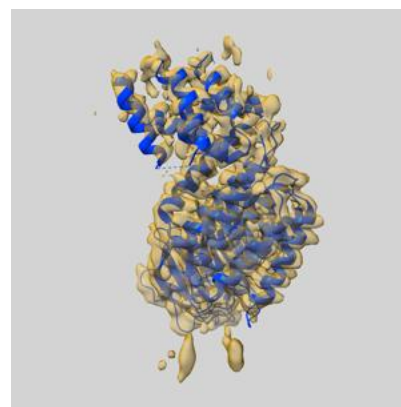
### 9.1 Map-model overlay [i](#)



X



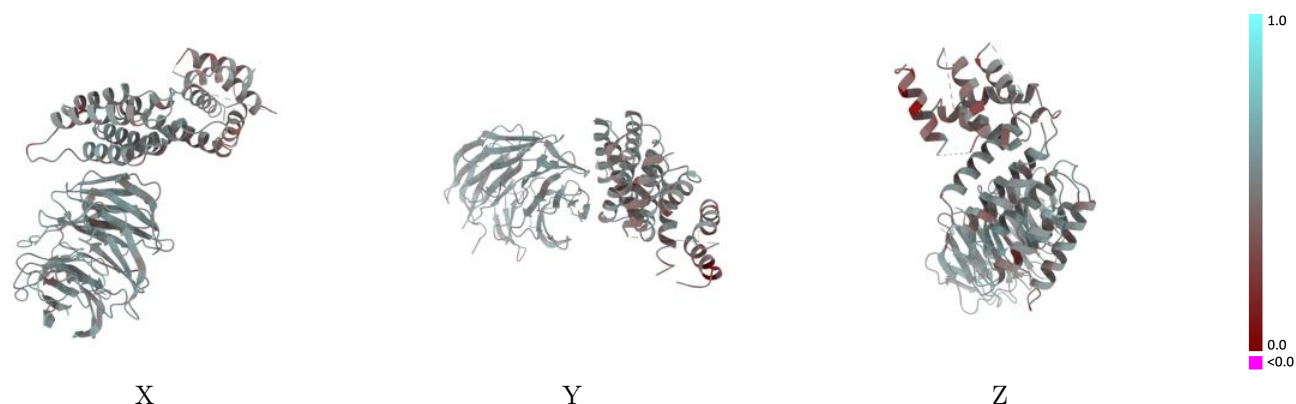
Y



Z

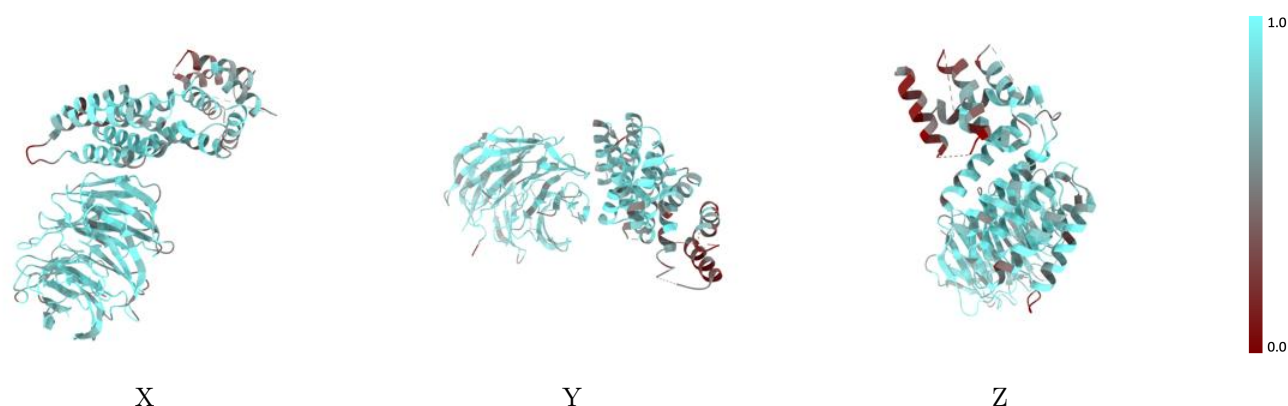
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

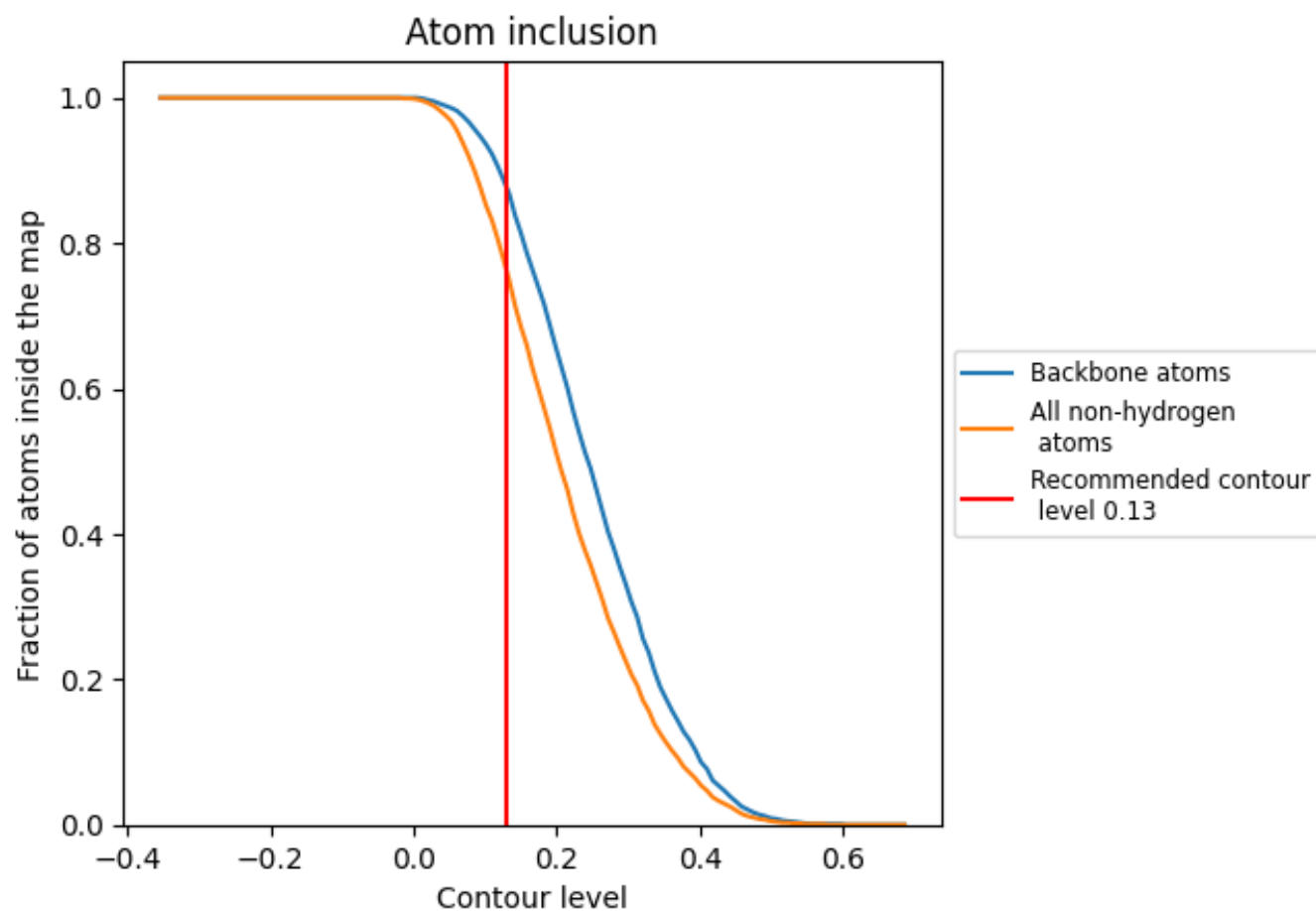
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.13).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7610	<div></div> 0.4950
A	<div></div> 0.6870	<div></div> 0.4610
B	<div></div> 0.8200	<div></div> 0.5220

