



## wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 11:42 AM UTC

PDB ID : 9GVG / pdb\_00009gvg  
EMDB ID : EMD-51635  
Title : P116 from Mycoplasma pneumoniae in complex with mild growth suppressor monoclonal antibody  
Authors : Vizarraga, D.; Marcos Silva, M.; Martin Romero, J.; Guerra, P.; Fita, I.; Pinyol, J.  
Deposited on : 2024-09-24  
Resolution : 5.06 Å (reported)  
Based on initial model : 8A9A

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>.

---

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

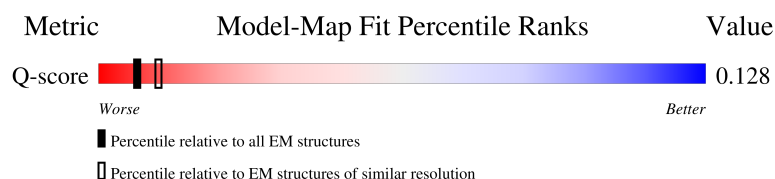
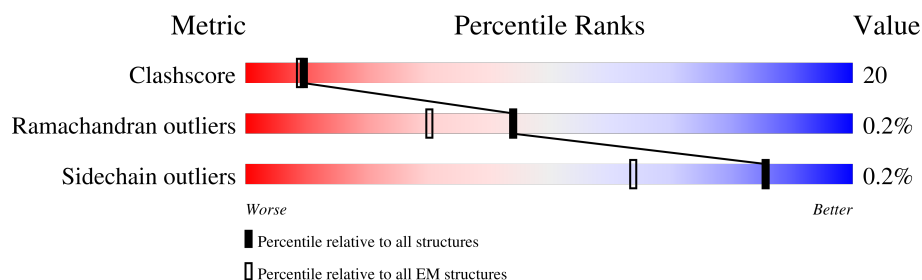
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.06 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	822 ( 4.56 - 5.51 )

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	H	210	<div> <div>20%</div> <div>63%</div> <div>36%</div> </div>
2	L	212	<div> <div>15%</div> <div>67%</div> <div>33%</div> </div>
3	A	809	<div> <div>94%</div> </div>
3	P	809	<div> <div>11%</div> <div>55%</div> <div>44%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10018 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 Heavy chain monoclonal antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	210	Total	C	N	O	S	1	0
			1608	1019	268	314	7		

- Molecule 2 is a protein called Light chain monoclonal antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	212	Total	C	N	O	S	2	0
			1653	1036	277	334	6		

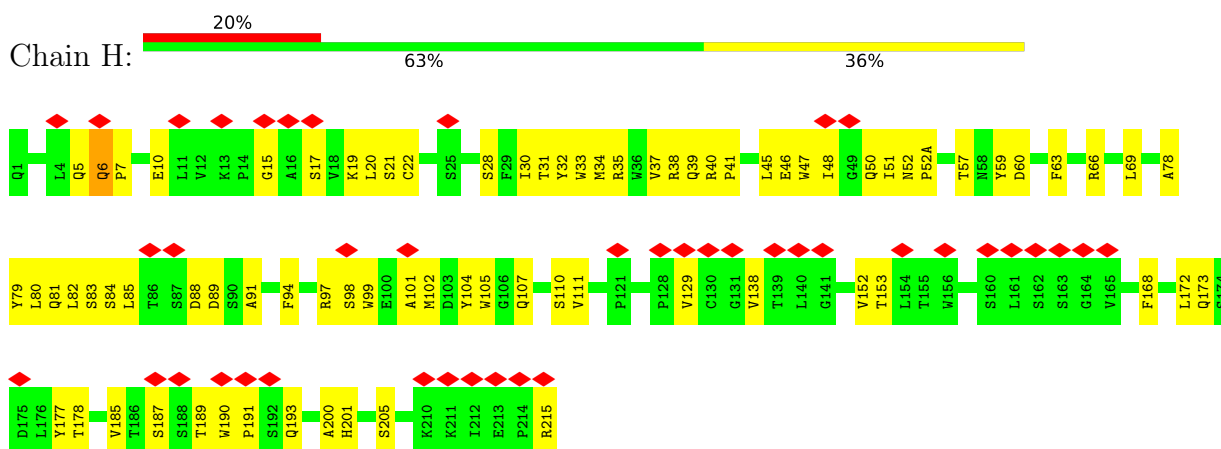
- Molecule 3 is a protein called Uncharacterized protein MG075 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	809	Total	C	N	O	S	0	0
			6386	4120	1027	1231	8		
3	A	47	Total	C	N	O	S	0	0
			371	246	57	67	1		

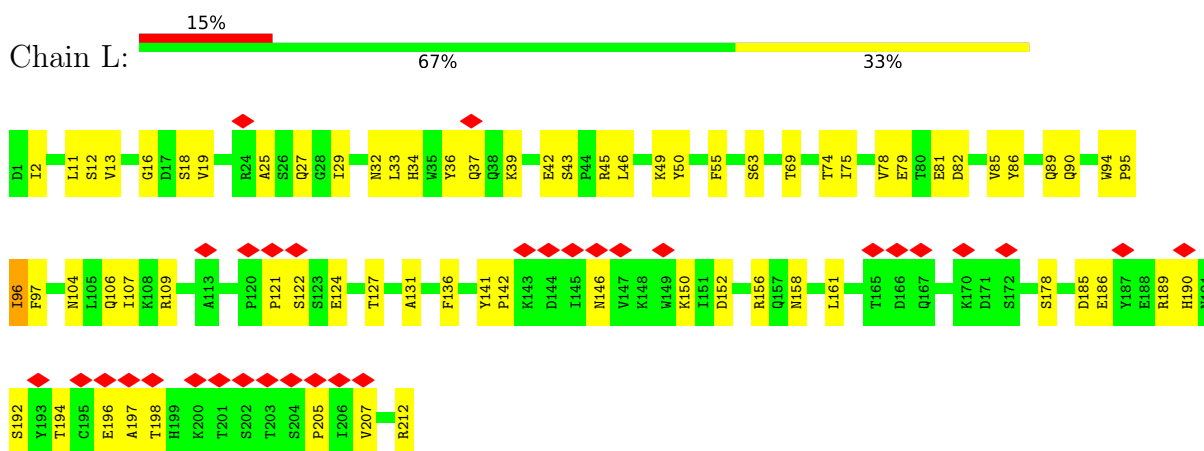
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

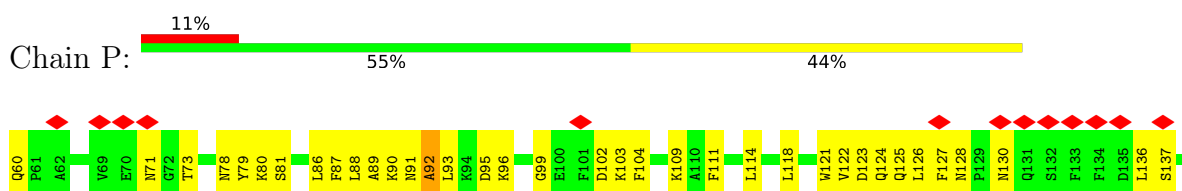
- Molecule 1: Heavy chain monoclonal antibody



- Molecule 2: Light chain monoclonal antibody



- Molecule 3: Uncharacterized protein MG075 homolog





ARG	ALA	ILE	K660	LYS	ILE	GLY	ALA
VAL	ILE	THR		ASN	PHE		LEU
ILE	ASN	THR	Y664	THR	LYS	PHE	SER
PRO	GLN	GLY	K665	GLU	ASN	ASP	PRO
PHE	GLN	GLY	K666	ASN	GLU	LEU	LEU
ALA	VAL	SER	K667	VAL	LEU	PHE	ILE
PHE	LYS	PHE	K668	GLU	LEU	GLY	GLU
VAL	LEU	ASP	D669	LEU	ASN	GLU	GLU
ASP	SER	ILE	K670	GLU	ARG	ALA	LEU
GLY	GLN	LYS	Y671	GLU	SER	ASP	LEU
PHE	SER	TYR	I672	THR	VAL	PHE	THR
GLY	PHE	GLY	K673	THR	GLU	VAL	GLN
ILE	PHE	GLY	E674	THR	VAL	ASP	LYS
GLN	ASN	GLU	G675	THR	ALA	LYS	ASP
LEU	VAL	ASN	G676	LEU	LYS	ILE	THR
LYS	TRP	LEU		LYS	ALA	ALA	TYR
ALA	THR	ASN	Y679	VAL	GLU	GLU	VAL
VAL	ASN	VAL		LYS	ALA	PHE	PHE
ASP	MET	LEU	V686	LYS	LYS	LEU	ASP
	PHE	PRO	P687	LEU	ASP	LEU	LEU
	ASP	ALA		THR	THR	THR	ILE
	SER	TYR		VAL	LYS	LYS	GLN
	ILE	TYR	E891	GLU	GLY	ARG	LYS
	THR	SER	S892	THR	ALA	THR	HIS
	LYS	LEU	I693	LYS	THR	VAL	LYS
	GLN	ILE	E694	VAL	ASP	LYS	GLY
	ILE	ASN	N695	GLU	TYR	ASN	ILE
	PHE	SER	T696	LEU	LYS	GLY	LEU
	GLN	GLU	F697	GLY	LYS	GLU	THR
	LYS	ILE	K698	ASN	GLU	LYS	ASN
	LYS	GLY	S699	PHE	GLN	ILE	LEU
	TYR	TYR	A700	GLU	ALA	GLU	LEU
	GLN	ILE		LYS	LYS	THR	LYS
	PHE	ILE	ASP	LYS	ALA	LYS	ASN
	LYS	ILE	LYS	ASN	LEU	ASP	PHE
	VAL	GLY	THR	GLY	LYS	SER	LEU
	ASN	VAL	LYS	LEU	LYS	LEU	ALA
	ILE	THR	ILE	ILE	PHE	VAL	PHE
	VAL	THR	THR	ALA	LYS	THR	GLN
	PHE	ILE	ASP	MET	HIS	SER	LYS
	ALA	ASP	LEU	GLU	ILE	LEU	THR
	ARG	ALA	PHE	LEU	GLY	LYS	SER
	ASN	THR	GLY	PHE	GLU	ASP	PRO
	GLU	LYS	MET	LEU	ASN	LEU	GLY
	ASP	VAL	THR	PRO	THR	LEU	PHE
	ASN	LYS	LEU	ASP	LEU	GLY	THR
	THR	VAL	PHE	THR	SER	GLU	ASP
	SER	GLU	GLY	LYS	LYS	LYS	GLN
	ARG	LEU	ASN	ASP	THR	VAL	VAL
	LEU	LYS	ASP	LEU	ASN	ALA	ALA
	GLU	ASN	LEU	GLU	LEU	ALA	ILE
	LEU	LYS	SER	THR	ASP	LEU	PHE
	ASP	GLU	THR	THR	LYS	GLY	THR
	ILE	TYR	VAL	THR	ILE	ASP	GLU
	LYS	LYS	GLY	LYS	THR	LEU	LEU
	SER	GLY	GLU	LYS	THR	LEU	PHE
	ASP	LYS	THR	L654	LYS	LEU	ASN
	PRO	LYS	GLY	K656	THR	LEU	ASN
	GLU	LYS	ASP	L657	GLY	LEU	ASN
	GLN	PRO	THR	L658	GLU	ASP	GLU
			F659	VAL	VAL	THR	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	412947	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	7.24	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.212	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	244.79999, 244.79999, 244.79999	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.48, 0.48, 0.48	Depositor

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	H	0.16	0/1653	0.44	0/2259
2	L	0.13	0/1699	0.39	0/2310
3	A	0.15	0/381	0.53	1/508 (0.2%)
3	P	0.15	0/6497	0.43	0/8756
All	All	0.15	0/10230	0.43	1/13833 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	691	GLU	N-CA-C	-6.10	107.66	114.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	94	TRP	Peptide
2	L	95	PRO	Peptide
2	L	96	ILE	Peptide



## 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	H	1608	0	1575	74	0
2	L	1653	0	1585	44	0
3	A	371	0	370	15	0
3	P	6386	0	6434	273	0
All	All	10018	0	9964	397	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 20.

The worst 5 of 397 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:505:LYS:HB3	3:P:510:ILE:HG13	1.57	0.85
1:H:47:TRP:HB2	2:L:96:ILE:HD12	1.60	0.83
3:P:537:ASP:HA	3:P:541:PHE:HB2	1.59	0.82
3:P:748:LEU:HB2	3:P:762:GLN:HE21	1.43	0.82
3:P:367:ASN:HA	3:P:370:LYS:HZ3	1.46	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	H	207/210 (99%)	186 (90%)	20 (10%)	1 (0%)	24	63
2	L	212/212 (100%)	200 (94%)	12 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	45/809 (6%)	37 (82%)	8 (18%)	0	100	100
3	P	807/809 (100%)	693 (86%)	113 (14%)	1 (0%)	48	83
All	All	1271/2040 (62%)	1116 (88%)	153 (12%)	2 (0%)	44	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
3	P	92	ALA

### 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	
1	H	183/182 (100%)	181 (99%)	2 (1%)	65	74
2	L	193/191 (101%)	191 (99%)	2 (1%)	68	76
3	A	37/716 (5%)	37 (100%)	0	100	100
3	P	700/716 (98%)	700 (100%)	0	100	100
All	All	1113/1805 (62%)	1109 (100%)	4 (0%)	85	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	152[A]	VAL
1	H	152[B]	VAL
2	L	33[A]	LEU
2	L	33[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	449	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	P	815	GLN
3	P	91	ASN
3	P	119	GLN
3	P	167	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	131:GLY	C	138:VAL	N	6.40

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51635. These allow visual inspection of the internal detail of the map and identification of artifacts.

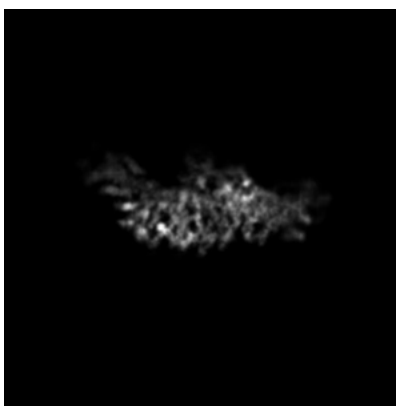
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

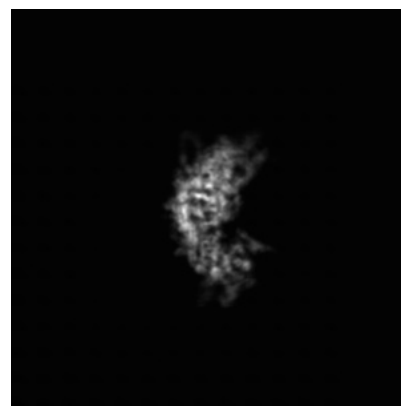
#### 6.1.1 Primary map



X

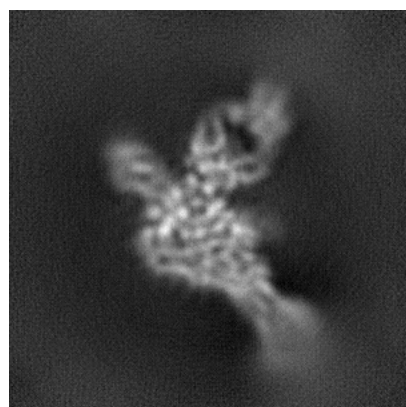


Y

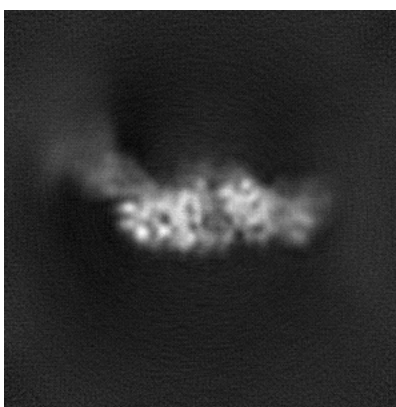


Z

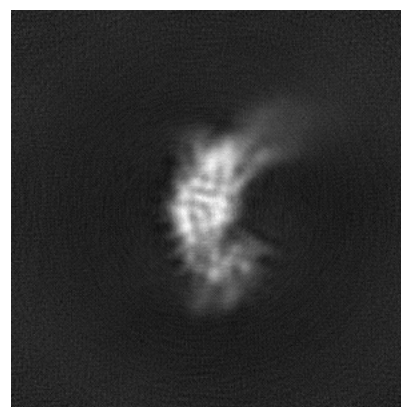
#### 6.1.2 Raw map



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: 255

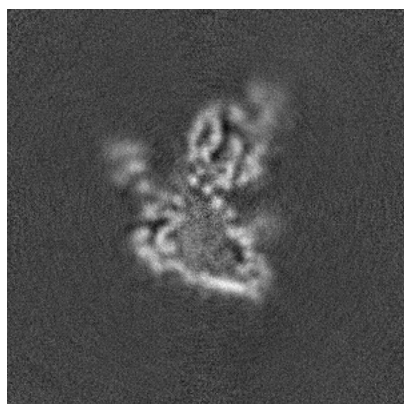


Y Index: 255

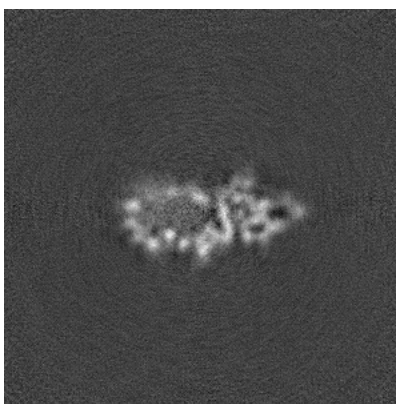


Z Index: 255

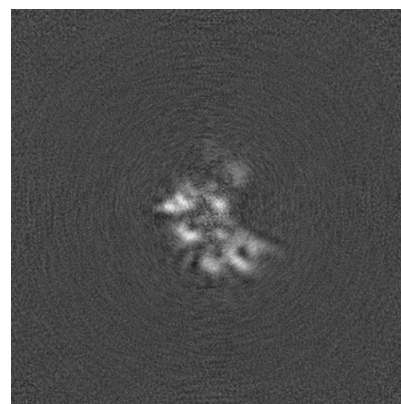
### 6.2.2 Raw map



X Index: 255



Y Index: 255



Z Index: 255

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: 259

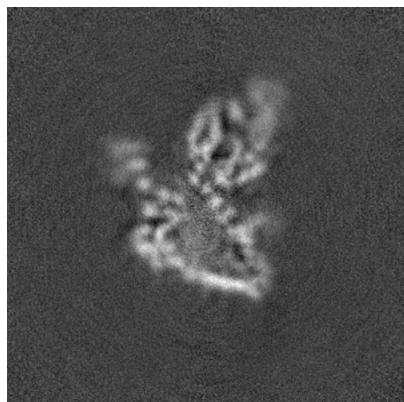


Y Index: 270

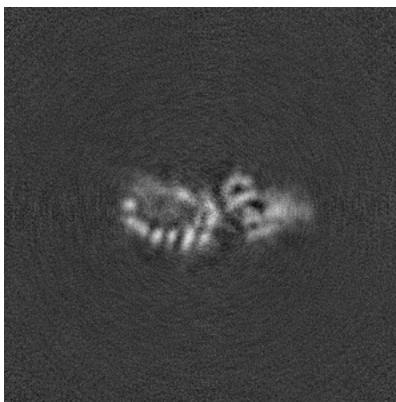


Z Index: 248

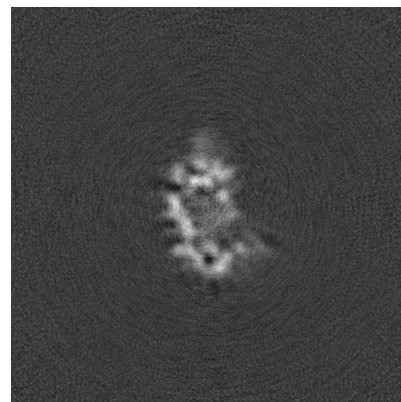
### 6.3.2 Raw map



X Index: 258



Y Index: 268

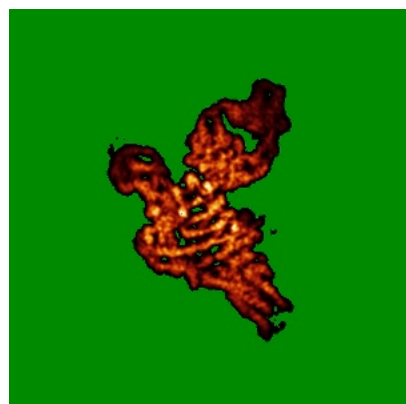


Z Index: 228

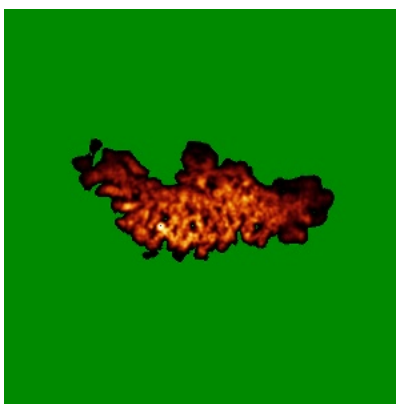
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

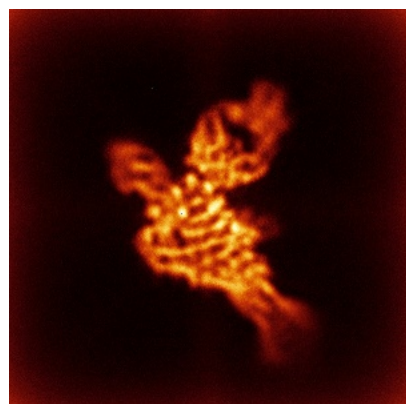


Y

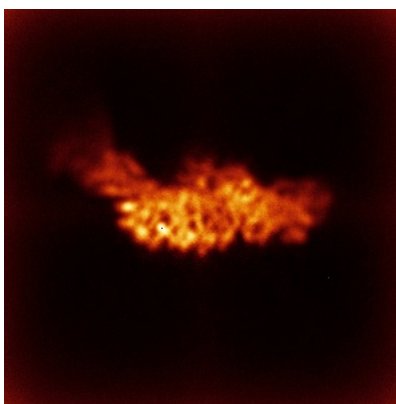


Z

### 6.4.2 Raw map



X



Y



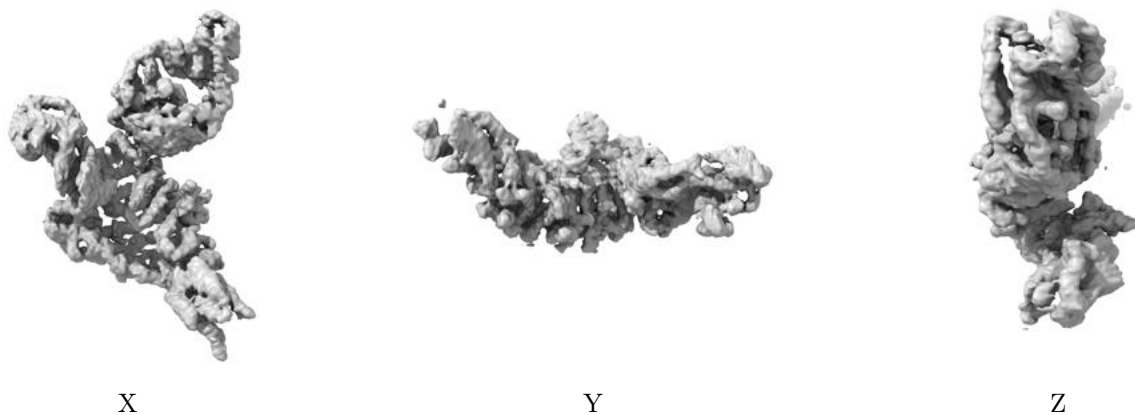
Z

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.



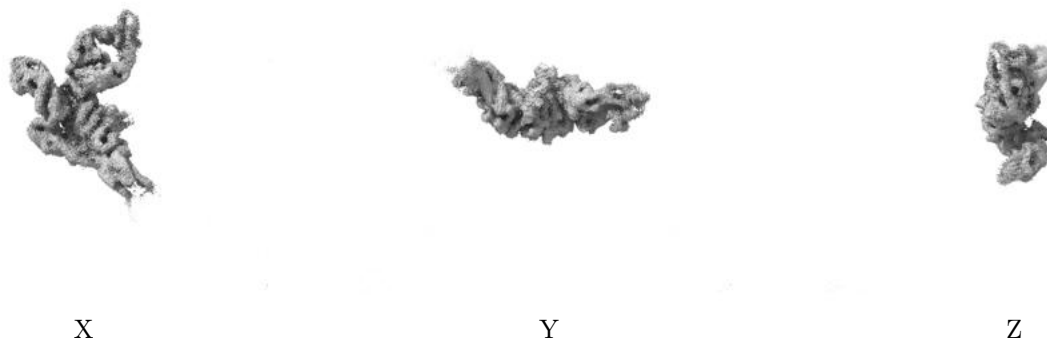
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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](#)

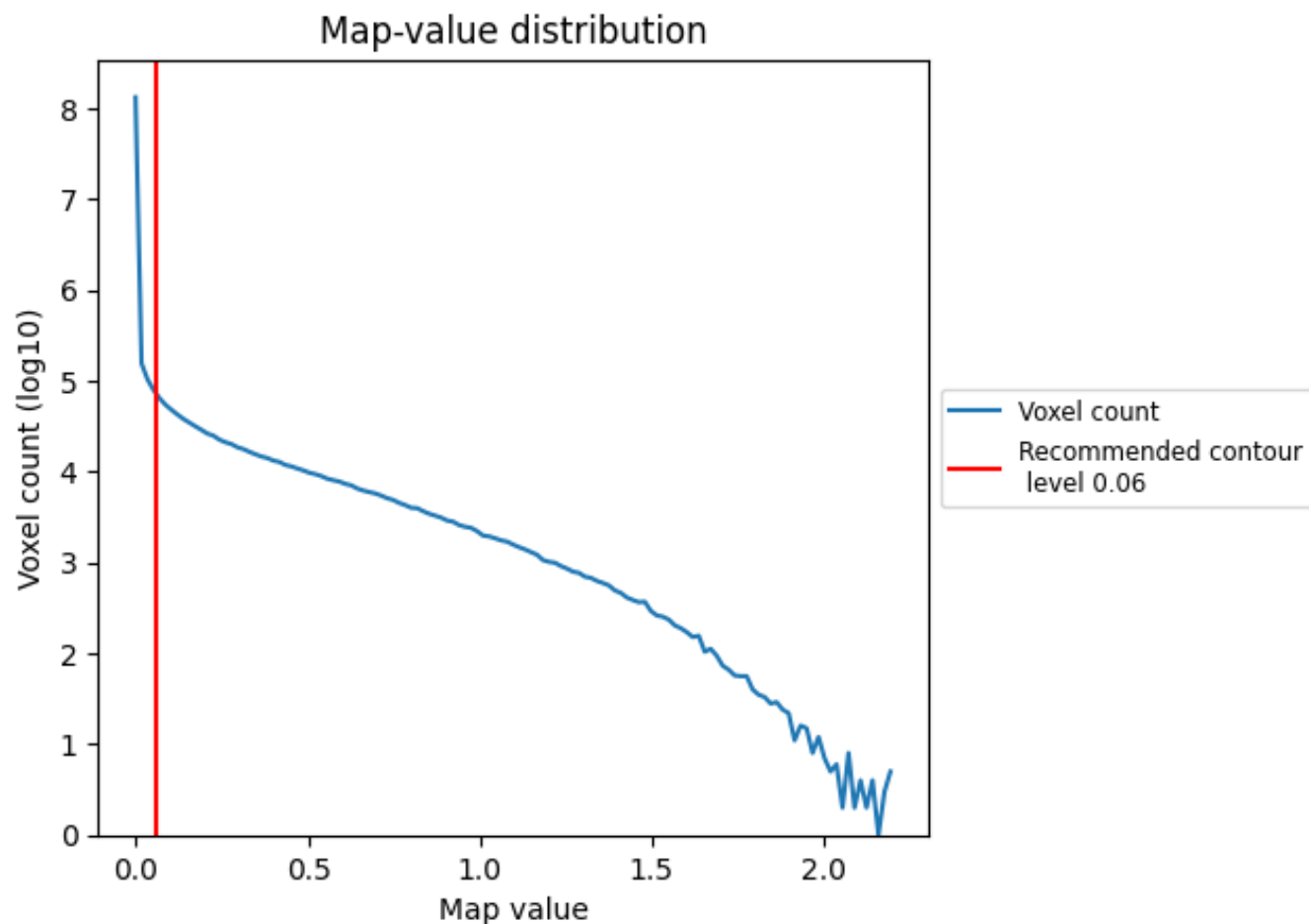
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

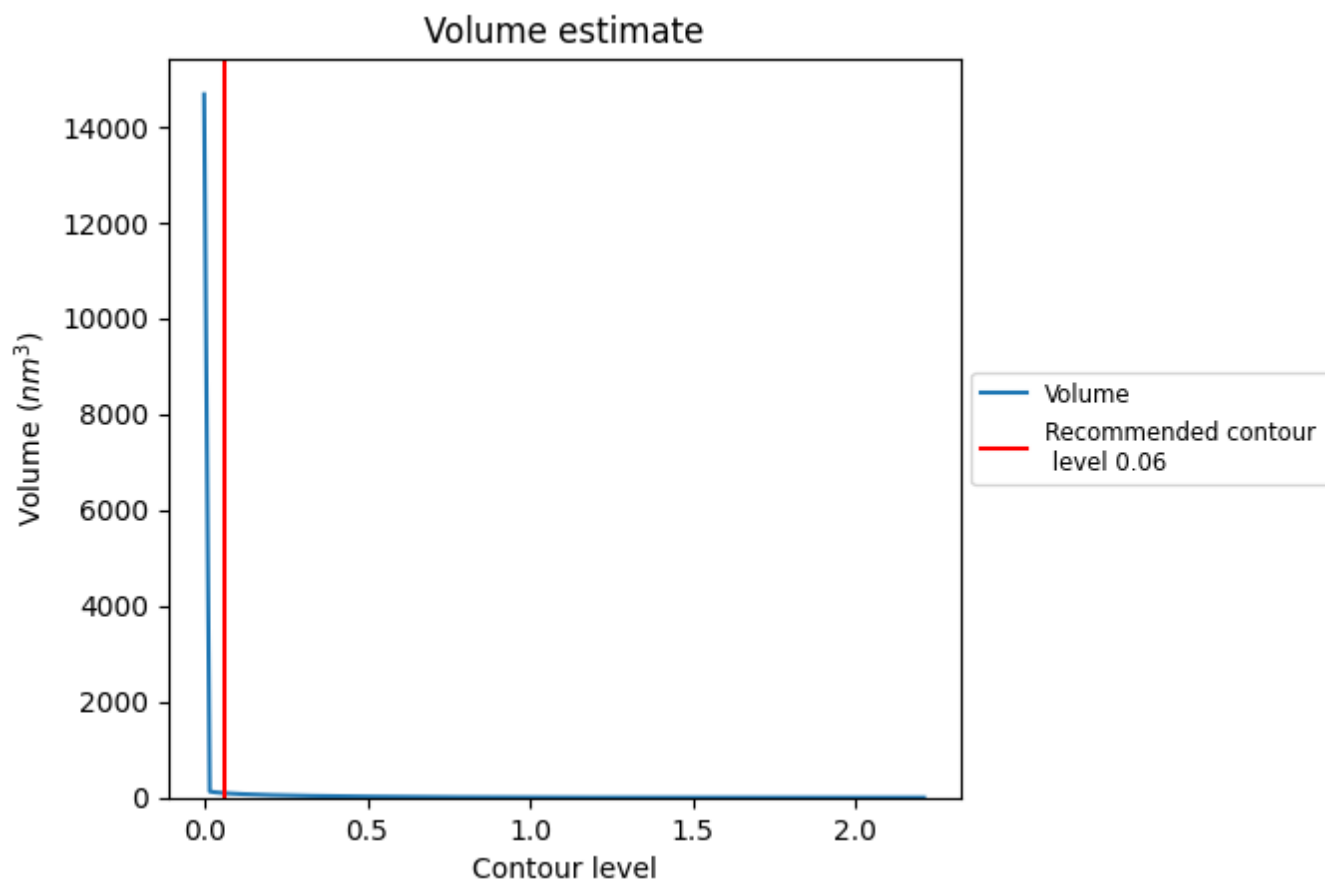
This section contains the results of statistical analysis of the map.

### 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.

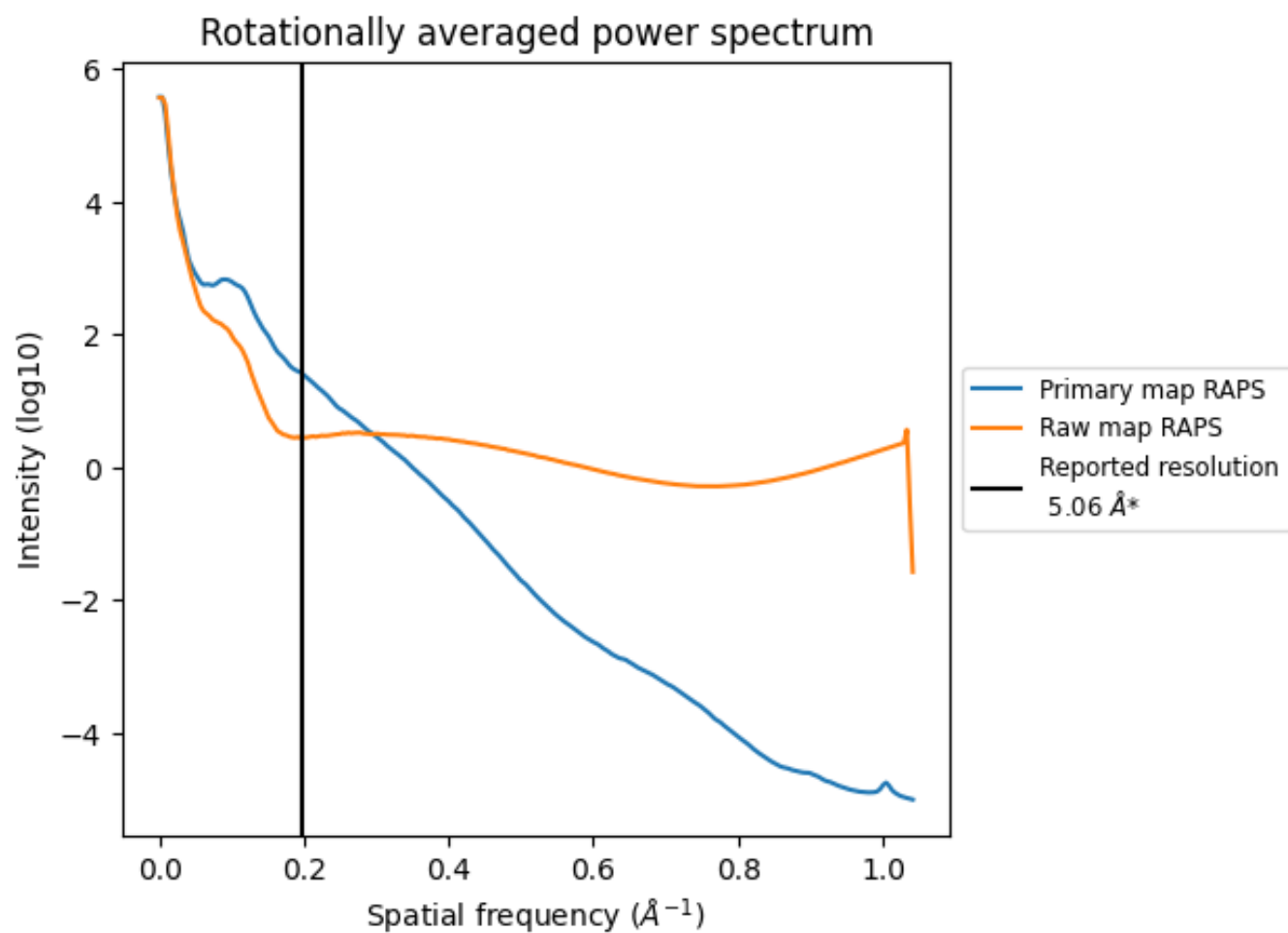
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93  $\text{nm}^3$ ; this corresponds to an approximate mass of 84 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 ⓘ

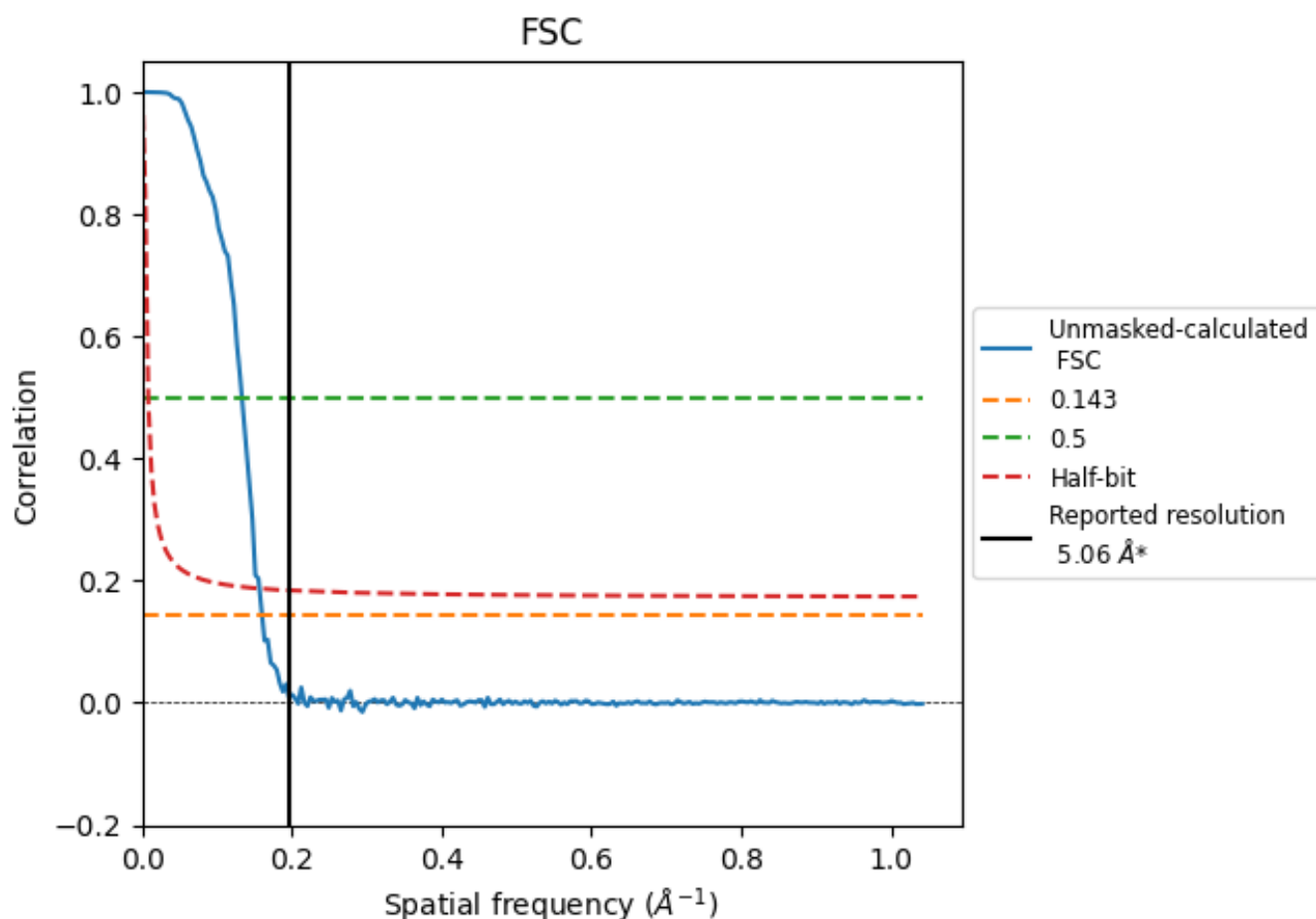


\*Reported resolution corresponds to spatial frequency of 0.198 Å⁻¹

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.198 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

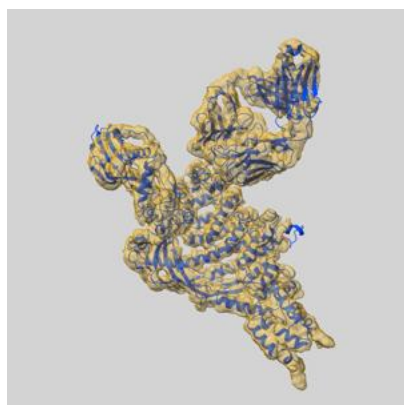
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.25	7.51	6.39

\*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 6.25 differs from the reported value 5.06 by more than 10 %

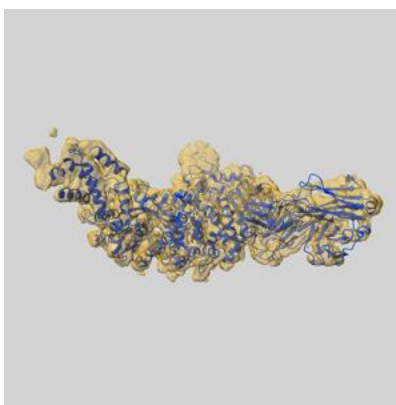
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51635 and PDB model 9GVG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

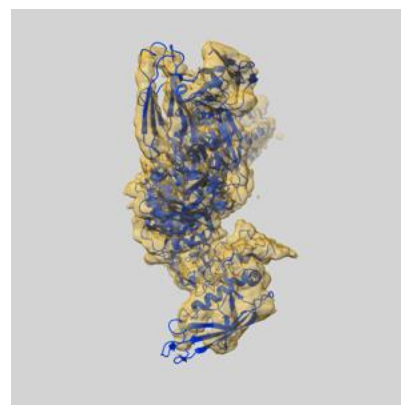
### 9.1 Map-model overlay [i](#)



X



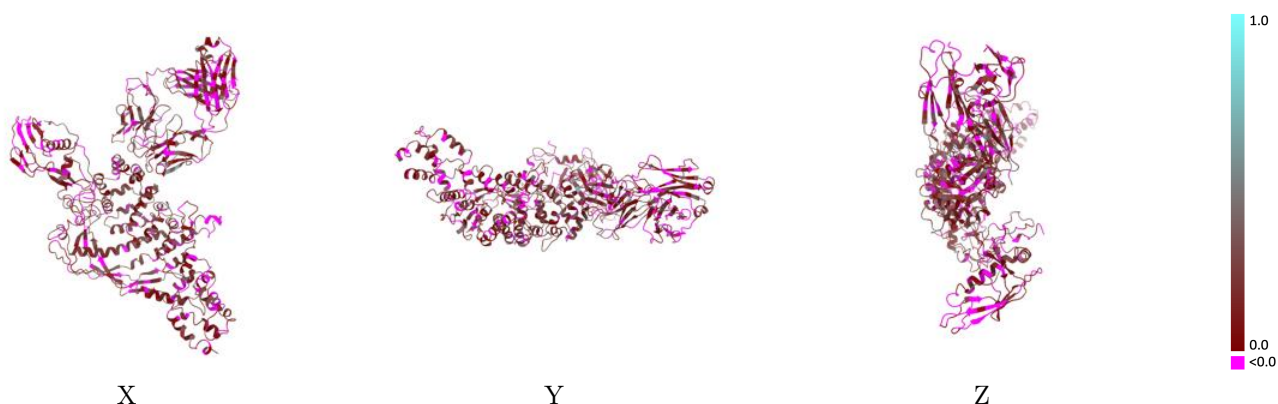
Y



Z

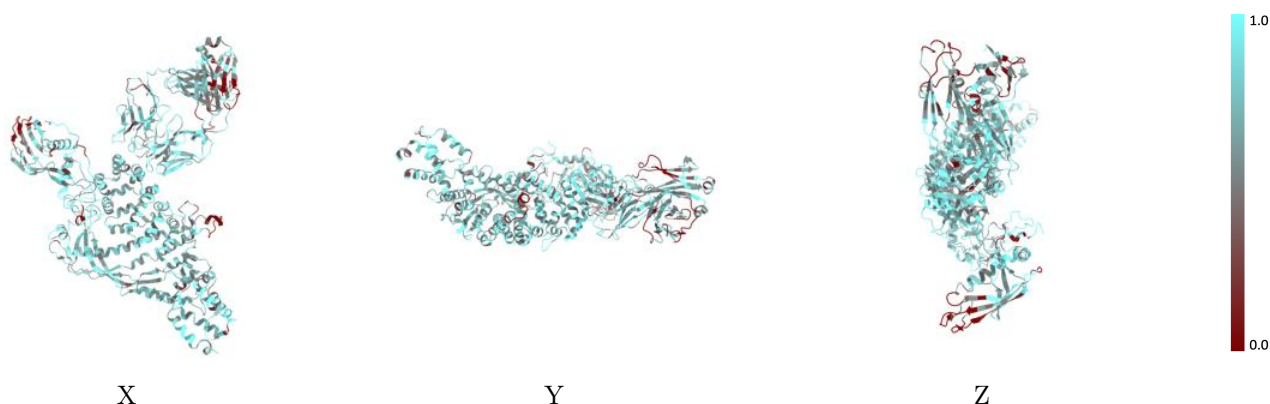
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



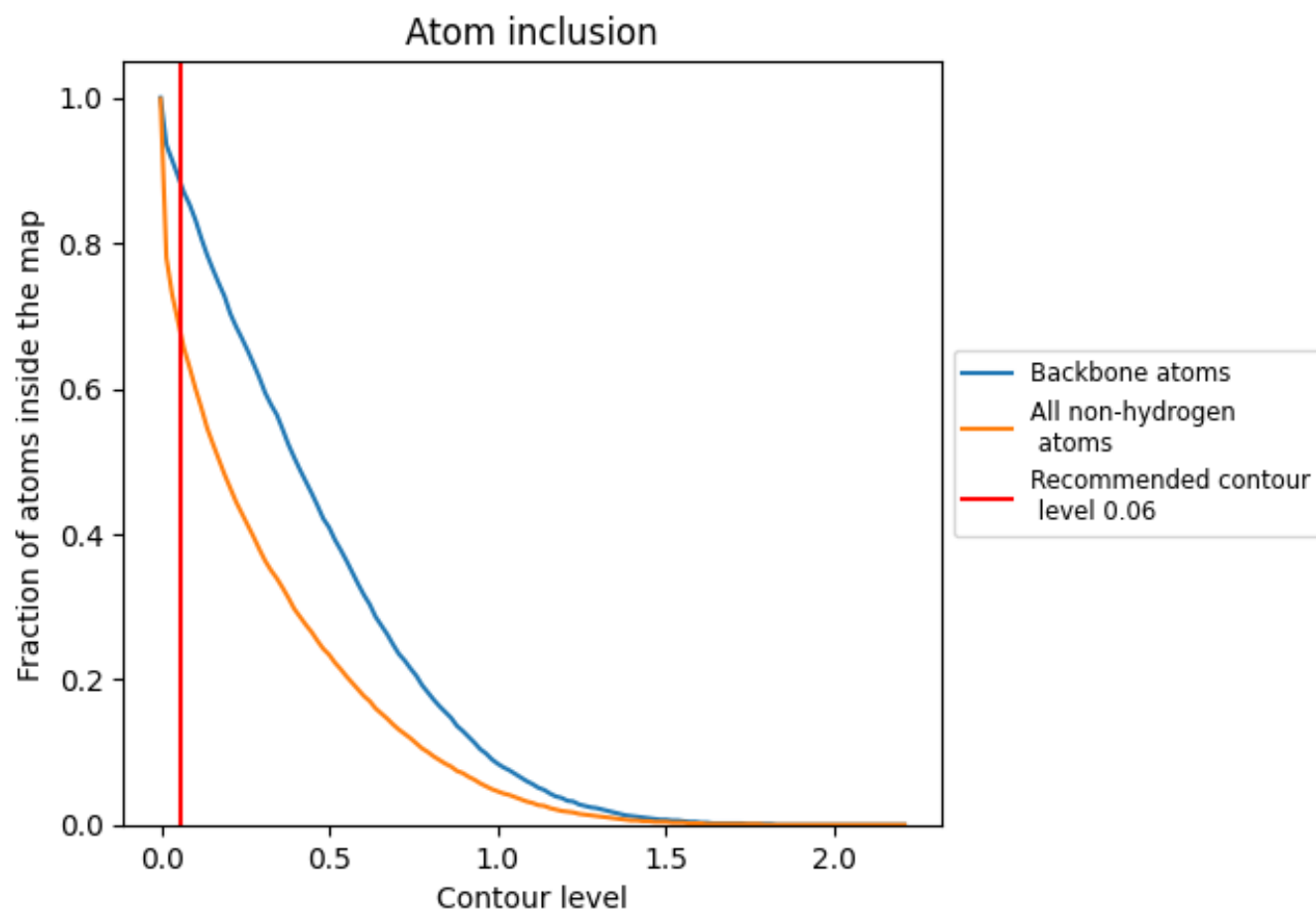
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 67% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6710	<div></div> 0.1280
A	<div></div> 0.7060	<div></div> 0.1150
H	<div></div> 0.6480	<div></div> 0.1230
L	<div></div> 0.6400	<div></div> 0.1280
P	<div></div> 0.6830	<div></div> 0.1300

