



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 04:13 pm BST

PDB ID : 9QBG / pdb\_00009qbg  
EMDB ID : EMD-52998  
Title : HER2/ErbB2 extracellular domain (ECD) in extended conformation in complex with trastuzumab (TZB) antibody  
Authors : Gragera, M.; Buschiazzi, A.; Vacca, S.  
Deposited on : 2025-03-02  
Resolution : 3.60 Å(reported)  
Based on initial model : 5MY6

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.dev126  
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) : 2.45.1

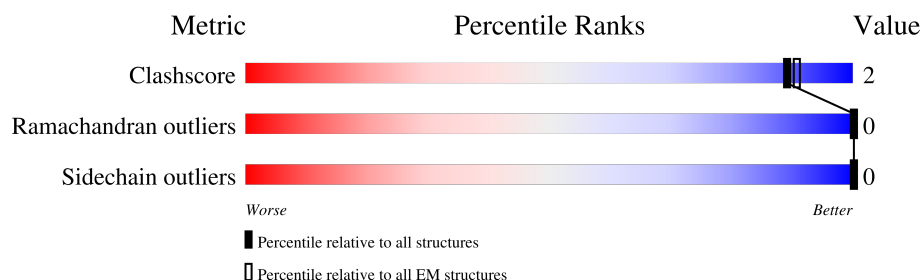
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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	1311	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7684 atoms, of which 3767 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 Receptor tyrosine-protein kinase erbB-2, Green fluorescent protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	508	7684	2437	3767	702	737	41	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P04626
A	-32	LYS	-	expression tag	UNP P04626
A	-31	PHE	-	expression tag	UNP P04626
A	-30	LEU	-	expression tag	UNP P04626
A	-29	VAL	-	expression tag	UNP P04626
A	-28	ASN	-	expression tag	UNP P04626
A	-27	VAL	-	expression tag	UNP P04626
A	-26	ALA	-	expression tag	UNP P04626
A	-25	LEU	-	expression tag	UNP P04626
A	-24	VAL	-	expression tag	UNP P04626
A	-23	PHE	-	expression tag	UNP P04626
A	-22	MET	-	expression tag	UNP P04626
A	-21	VAL	-	expression tag	UNP P04626
A	-20	VAL	-	expression tag	UNP P04626
A	-19	TYR	-	expression tag	UNP P04626
A	-18	ILE	-	expression tag	UNP P04626
A	-17	SER	-	expression tag	UNP P04626
A	-16	TYR	-	expression tag	UNP P04626
A	-15	ILE	-	expression tag	UNP P04626
A	-14	TYR	-	expression tag	UNP P04626
A	-13	ALA	-	expression tag	UNP P04626
A	-12	ASP	-	expression tag	UNP P04626
A	-11	TYR	-	expression tag	UNP P04626
A	-10	LYS	-	expression tag	UNP P04626
A	-9	ASP	-	expression tag	UNP P04626
A	-8	ASP	-	expression tag	UNP P04626
A	-7	ASP	-	expression tag	UNP P04626

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P04626
A	-5	LYS	-	expression tag	UNP P04626
A	-4	HIS	-	expression tag	UNP P04626
A	-3	HIS	-	expression tag	UNP P04626
A	-2	HIS	-	expression tag	UNP P04626
A	-1	HIS	-	expression tag	UNP P04626
A	0	HIS	-	expression tag	UNP P04626
A	1	HIS	-	expression tag	UNP P04626
A	2	HIS	-	expression tag	UNP P04626
A	3	HIS	-	expression tag	UNP P04626
A	4	HIS	-	expression tag	UNP P04626
A	5	HIS	-	expression tag	UNP P04626
A	6	LEU	-	expression tag	UNP P04626
A	7	GLU	-	expression tag	UNP P04626
A	8	VAL	-	expression tag	UNP P04626
A	9	LEU	-	expression tag	UNP P04626
A	10	PHE	-	expression tag	UNP P04626
A	11	GLN	-	expression tag	UNP P04626
A	12	GLY	-	expression tag	UNP P04626
A	13	PRO	-	expression tag	UNP P04626
A	14	TYR	-	expression tag	UNP P04626
A	15	PRO	-	expression tag	UNP P04626
A	16	TYR	-	expression tag	UNP P04626
A	17	ASP	-	expression tag	UNP P04626
A	18	VAL	-	expression tag	UNP P04626
A	19	PRO	-	expression tag	UNP P04626
A	20	ASP	-	expression tag	UNP P04626
A	21	TYR	-	expression tag	UNP P04626
A	22	SER	-	expression tag	UNP P04626
A	789	SER	CYS	engineered mutation	UNP P04626
A	805	SER	CYS	engineered mutation	UNP P04626
A	965	SER	CYS	engineered mutation	UNP P04626
A	1030	LEU	-	linker	UNP P04626
A	1031	GLU	-	linker	UNP P04626
A	1032	VAL	-	linker	UNP P04626
A	1033	LEU	-	linker	UNP P04626
A	1034	PHE	-	linker	UNP P04626
A	1035	GLN	-	linker	UNP P04626
A	1036	GLY	-	linker	UNP P04626
A	1037	PRO	-	linker	UNP P04626
A	1038	GLY	-	linker	UNP P04626
A	1039	SER	-	linker	UNP P04626

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1069	ARG	SER	conflict	UNP P42212
A	1078	ASN	TYR	conflict	UNP P42212
A	1103	LEU	PHE	conflict	UNP P42212
A	1104	THR	SER	conflict	UNP P42212
A	1119	ARG	GLN	conflict	UNP P42212
A	1138	SER	PHE	conflict	UNP P42212
A	1144	THR	ASN	conflict	UNP P42212
A	1184	PHE	TYR	conflict	UNP P42212
A	1192	THR	MET	conflict	UNP P42212
A	1202	ALA	VAL	conflict	UNP P42212
A	1210	VAL	ILE	conflict	UNP P42212
A	1245	VAL	ALA	conflict	UNP P42212



GLN	GLY	ASP	ALA	THR	ILE	MET	ASN	GLY	LYS	LEU	THR	GLY	LEU	LYS	PHE	THR	LYS	GLY	LEU	LYS	LEU	PRO	VAL	THR	THR	LEU	THR	TYR	GLY	VAL	GLN	CYS	PHE	SER	ARG	TYR	PRO	ASN	PRO	ASP	ILE	LEU	HIS	MET	LYS	ARG	HIS	LEU	GLU	TYR	PHE	ASP	ALA	ASN	PRO	GLU	GLY	TYR	VAL
GLN	GLU	ARG	THR	ILE	SER	PHE	LYS	ASP	LYS	ASP	THR	GLY	VAL	ASN	THR	TYR	LYS	THR	ARG	ALA	THR	GLY	VAL	LYS	PHE	GLU	VAL	GLY	ASP	THR	LEU	VAL	ASN	ARG	THR	ILE	GLN	GLU	LEU	LYS	GLY	ILE	VAL	ASP	GLN	PHE	LYS	GLU	ASP	GLY	ASN	ILE	ASP	GLY	ASN	THR	TYR	ILE	THR
ALA	ASP	LYS	GLN	LYS	ASN	GLY	ILE	LYS	ALA	PHE	LYS	ILE	ARG	HIS	ASN	VAL	GLU	ASP	GLY	SER	VAL	GLN	LEU	ALA	ASP	HIS	TYR	GLN	GLN	ASN	THR	PRO	ILE	GLY	GLY	PRO	VAL	LEU	LEU	PRO	ASP	ASN	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	VAL	LEU	LYS	ASP	PRO	ASN	GLU		
LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	THR	ALA	ALA	GLY	ILE	THR	HIS	GLY	MET	ASP	GLU	LEU	TYR	LYS																																				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77784	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 ( $e^-/\text{\AA}^2$ )	72.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.644	Depositor
Minimum map value	-0.609	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	260.40002, 260.40002, 260.40002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3020002, 1.3020002, 1.3020002	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	A	1.16	4/4004 (0.1%)	1.33	40/5443 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	HIS	CB-CG	-6.41	1.41	1.50
1	A	303	TYR	CB-CG	-5.58	1.39	1.51
1	A	491	GLN	CG-CD	-5.38	1.38	1.52
1	A	260	HIS	CB-CG	-5.26	1.42	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLY	CA-C-N	7.67	127.85	119.87
1	A	229	GLY	C-N-CA	7.67	127.85	119.87
1	A	488	ASN	CA-C-N	7.63	127.30	119.82
1	A	488	ASN	C-N-CA	7.63	127.30	119.82
1	A	384	ASP	CA-C-N	7.60	127.31	119.56

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	3917	3767	3765	13	0
All	All	3917	3767	3765	13	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 2.

The worst 5 of 13 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:195:CYS:O	1:A:196:SER:C	2.53	0.50
1:A:463:SER:OG	1:A:464:GLY:N	2.45	0.49
1:A:28:GLY:N	1:A:57:GLN:O	2.47	0.47
1:A:533:GLN:OE1	1:A:533:GLN:N	2.48	0.47
1:A:170:LYS:O	1:A:217:ARG:NH2	2.48	0.47

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	502/1311 (38%)	489 (97%)	13 (3%)	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	436/1144 (38%)	436 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	318	HIS

### 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.

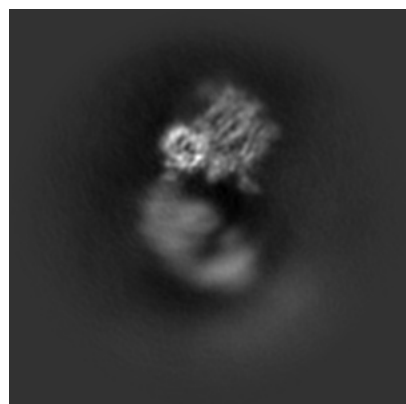
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52998. These allow visual inspection of the internal detail of the map and identification of artifacts.

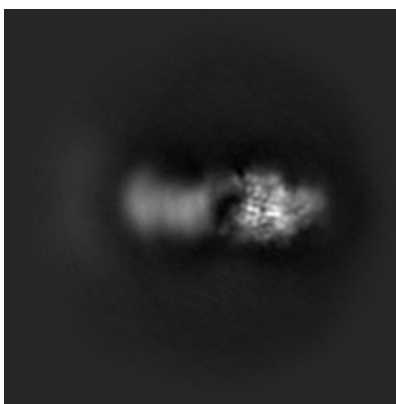
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

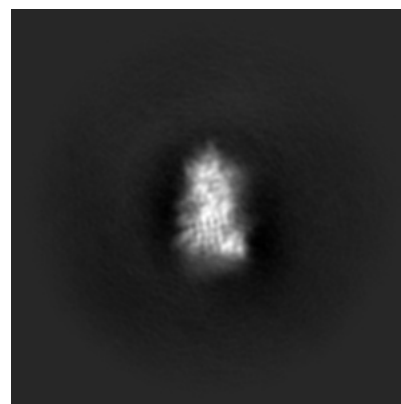
#### 6.1.1 Primary map



X

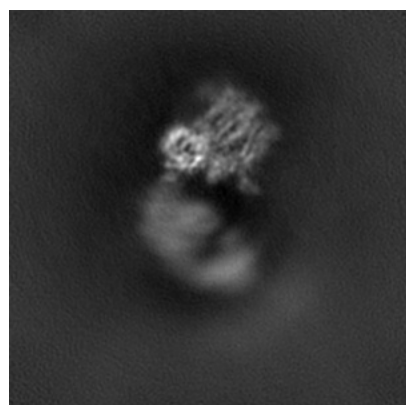


Y

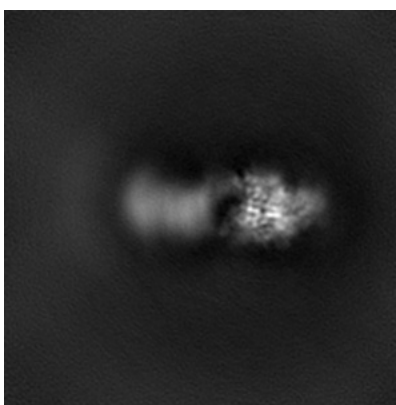


Z

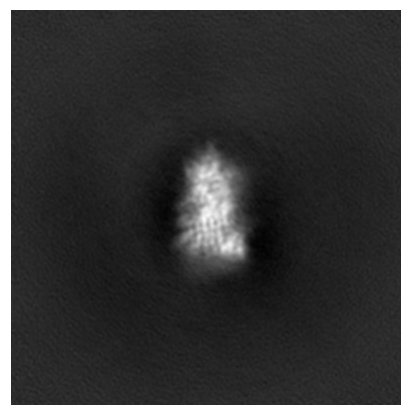
#### 6.1.2 Raw map



X



Y

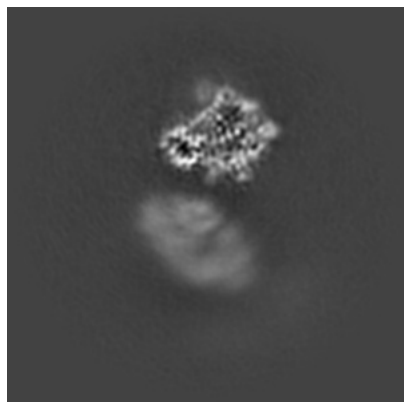


Z

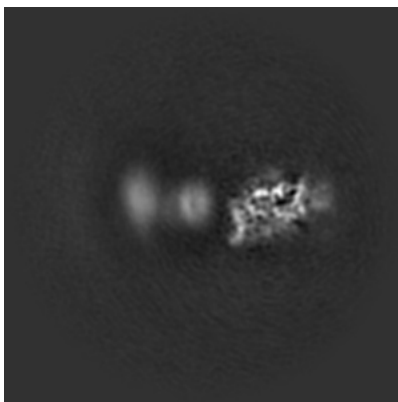
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

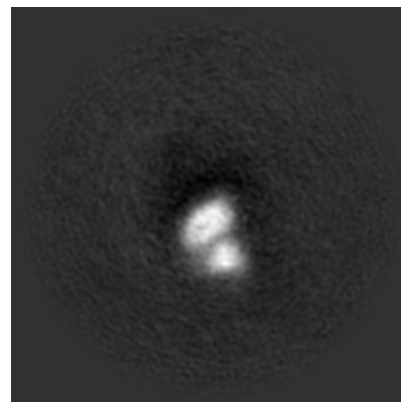
### 6.2.1 Primary map



X Index: 100

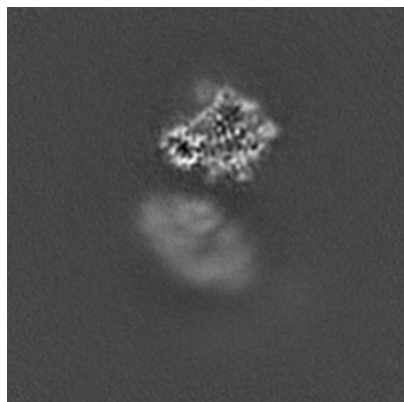


Y Index: 100

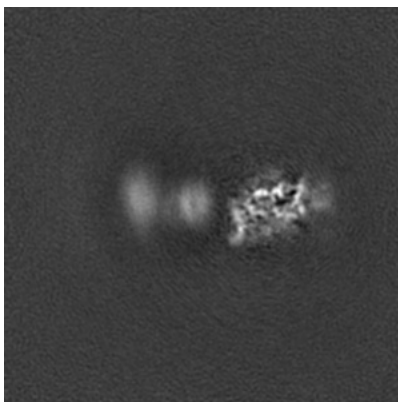


Z Index: 100

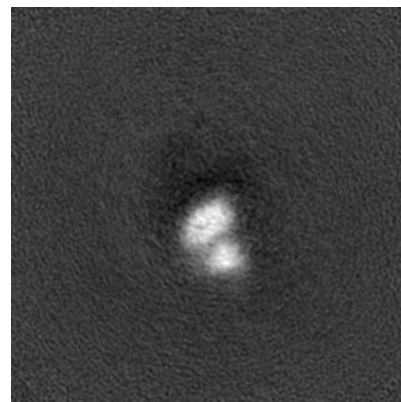
### 6.2.2 Raw map



X Index: 100



Y Index: 100

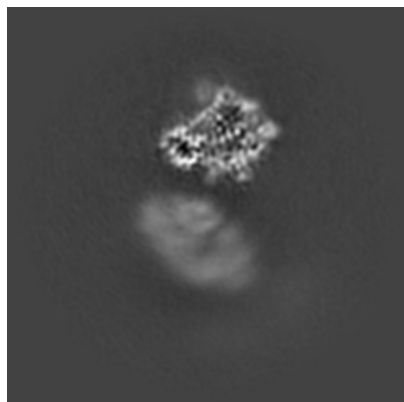


Z Index: 100

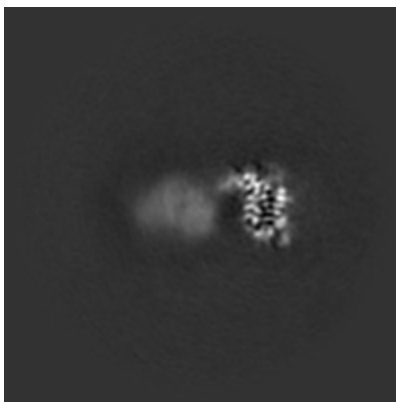
The images above show central slices of the map in three orthogonal directions.

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

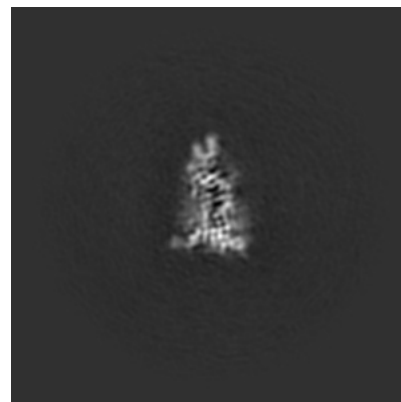
### 6.3.1 Primary map



X Index: 100

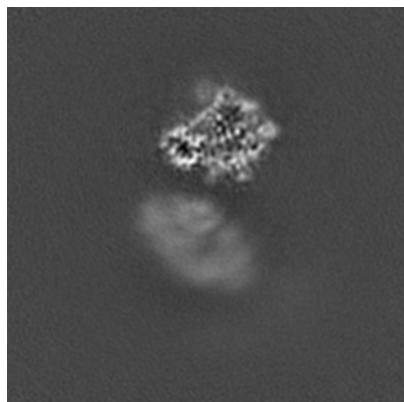


Y Index: 85

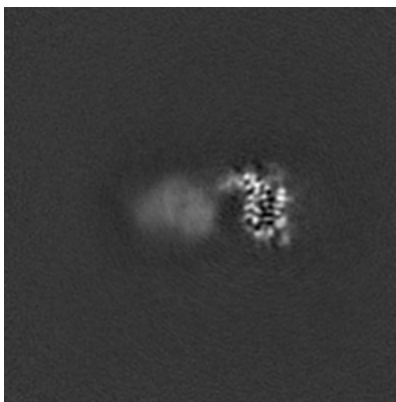


Z Index: 137

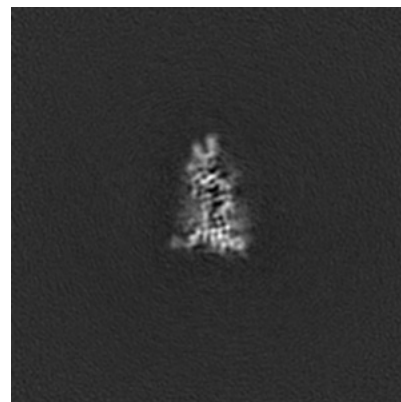
### 6.3.2 Raw map



X Index: 100



Y Index: 85

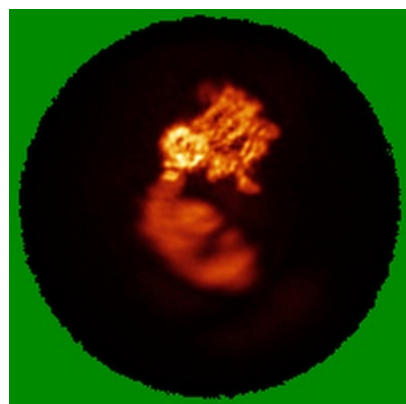


Z Index: 137

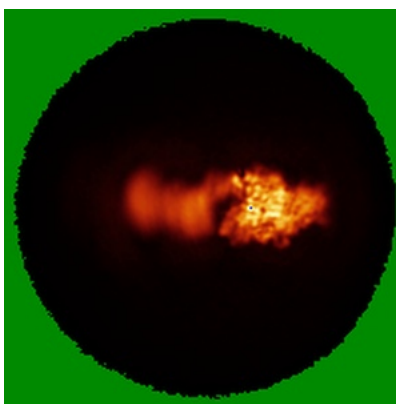
The images above show the largest variance slices of the map in three orthogonal directions.

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

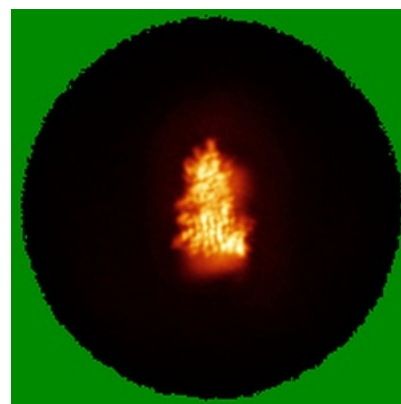
### 6.4.1 Primary map



X

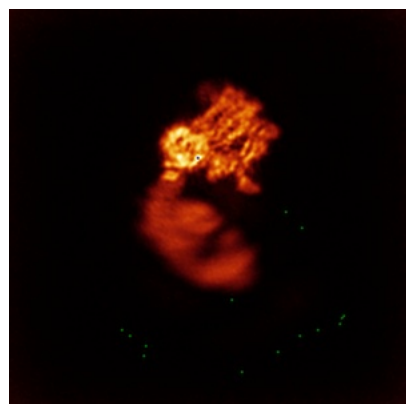


Y

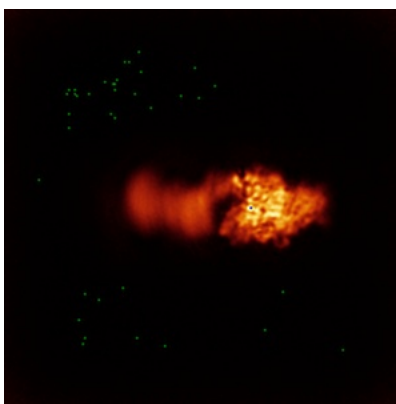


Z

### 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.

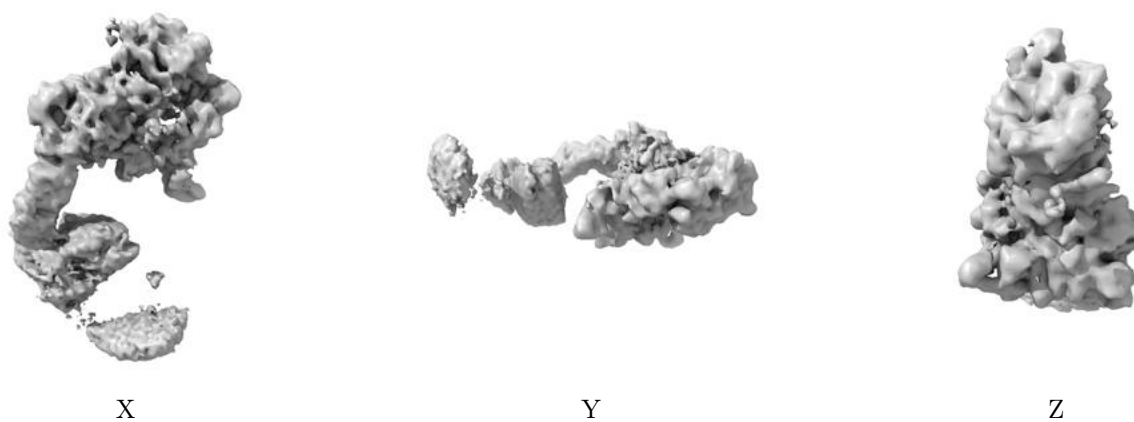
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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



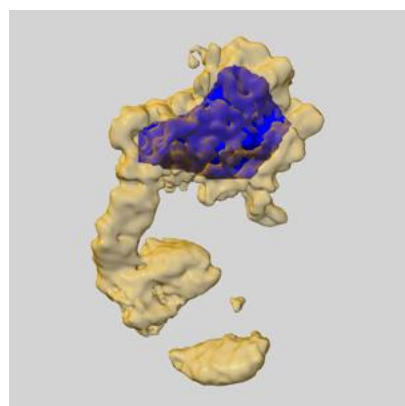
## 6.6 Mask visualisation [i](#)

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

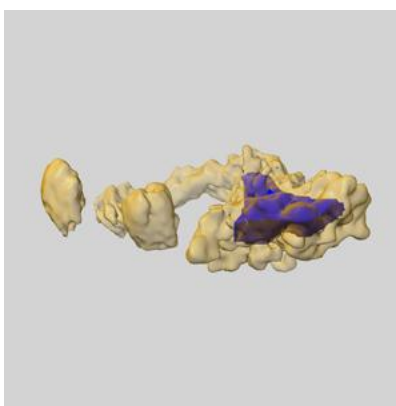
A mask typically either:

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

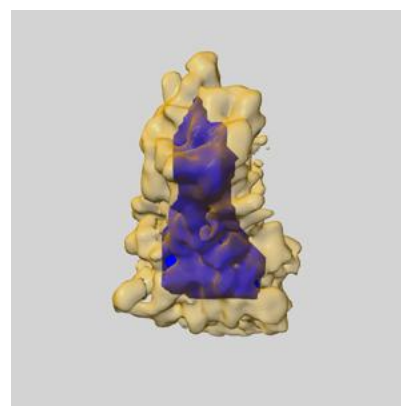
### 6.6.1 emd\_52998\_msk\_1.map [i](#)



X



Y

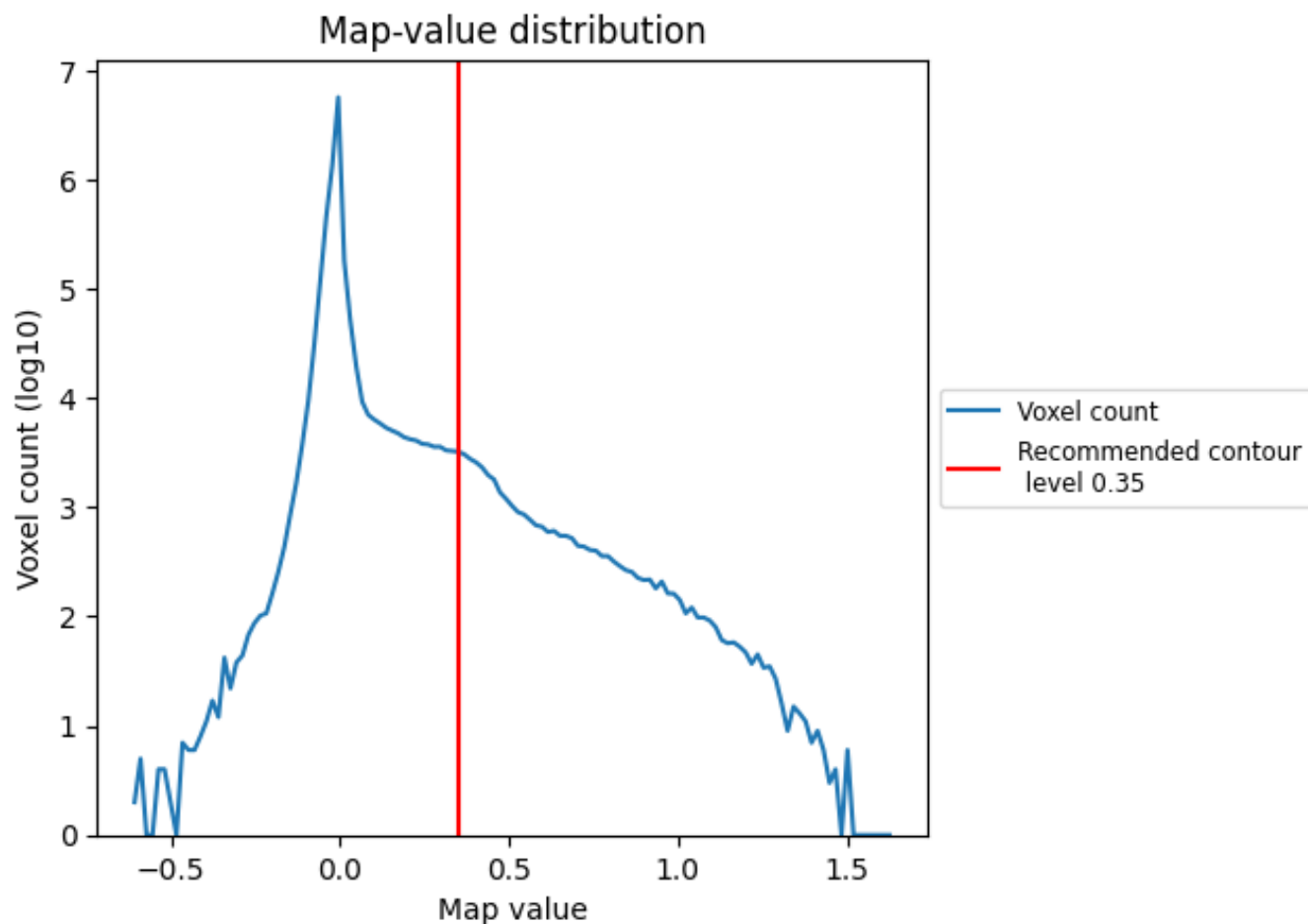


Z

## 7 Map analysis [i](#)

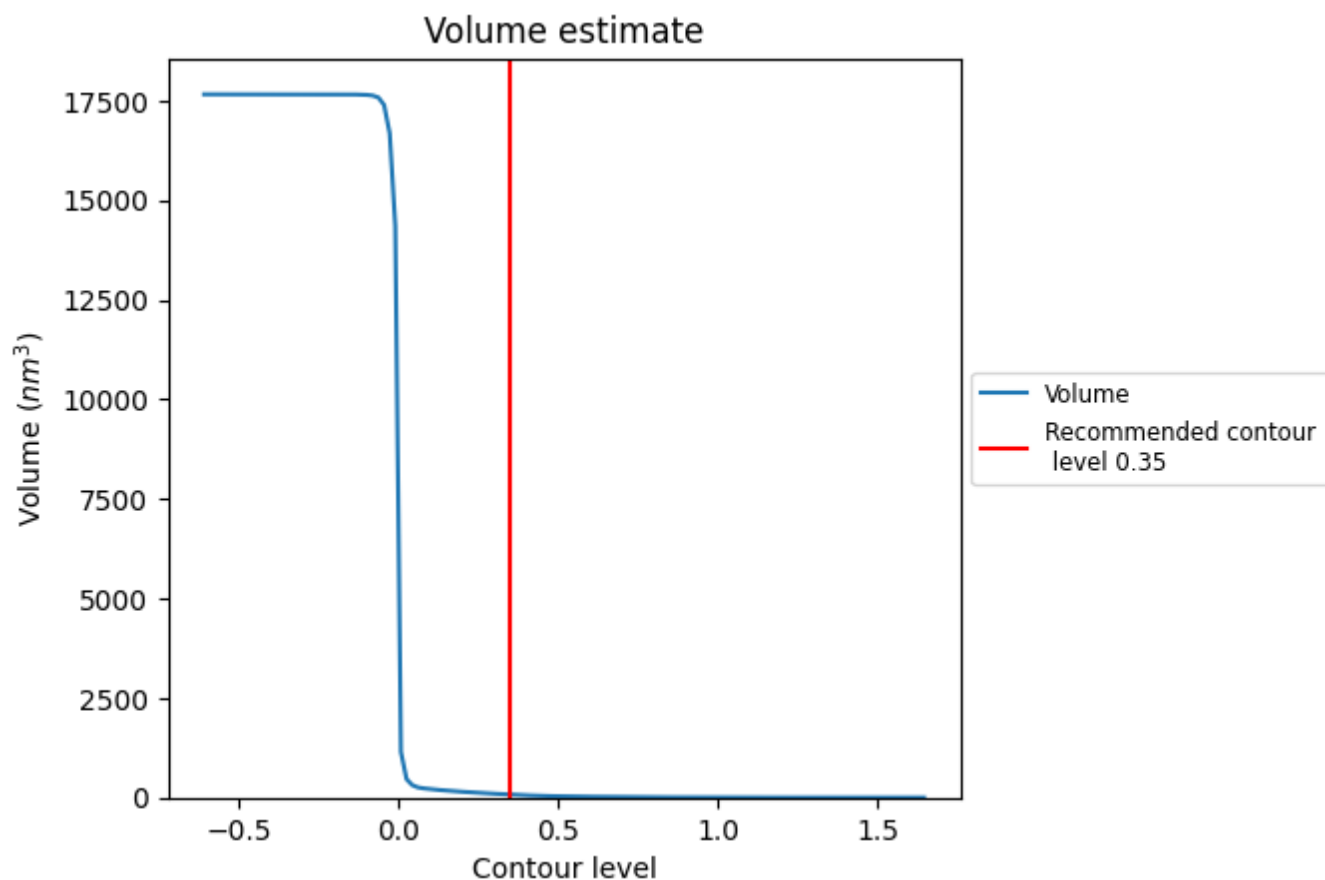
This section contains the results of statistical analysis of the map.

### 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.

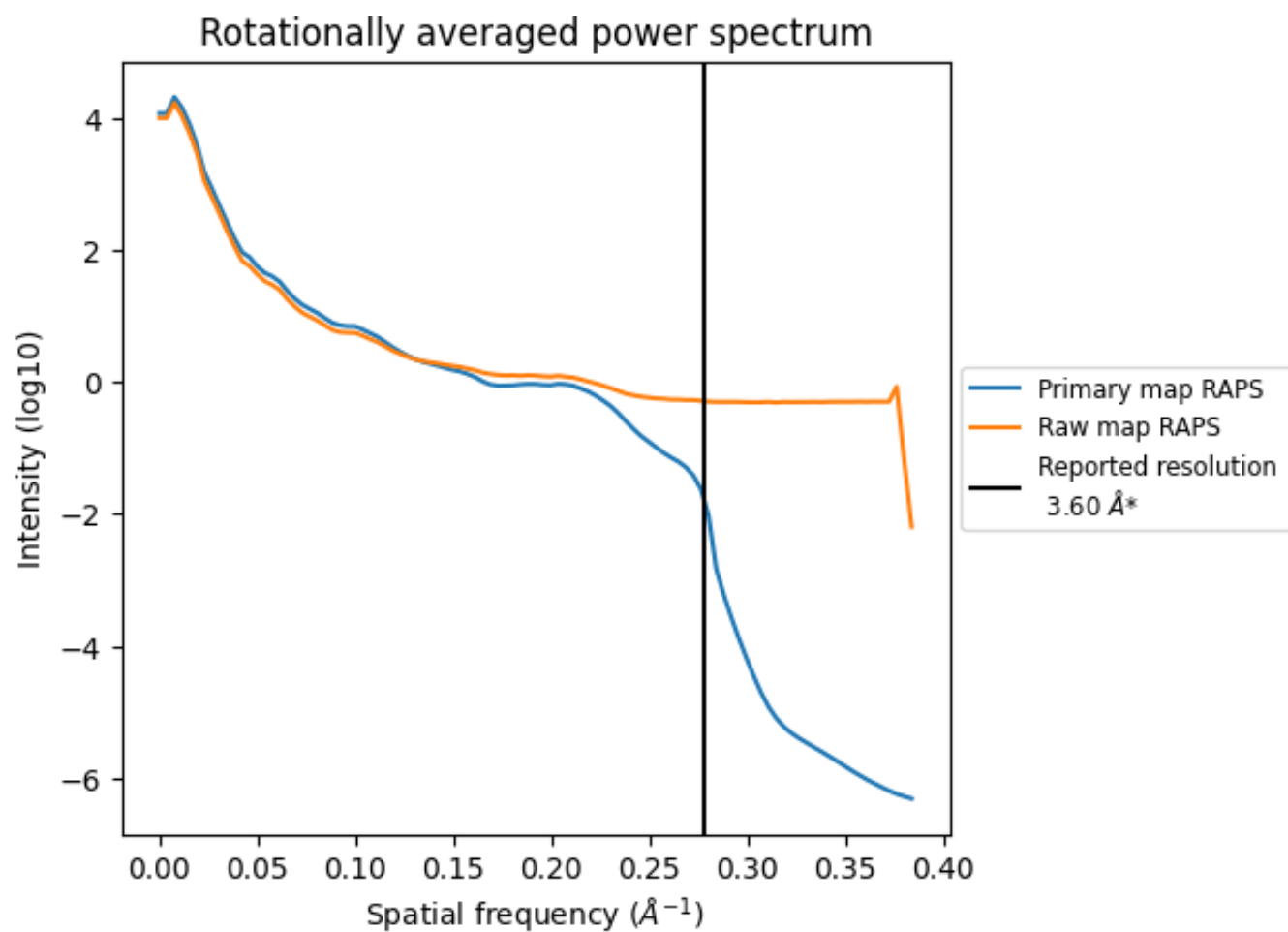
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm<sup>3</sup>; this corresponds to an approximate mass of 68 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 ⓘ

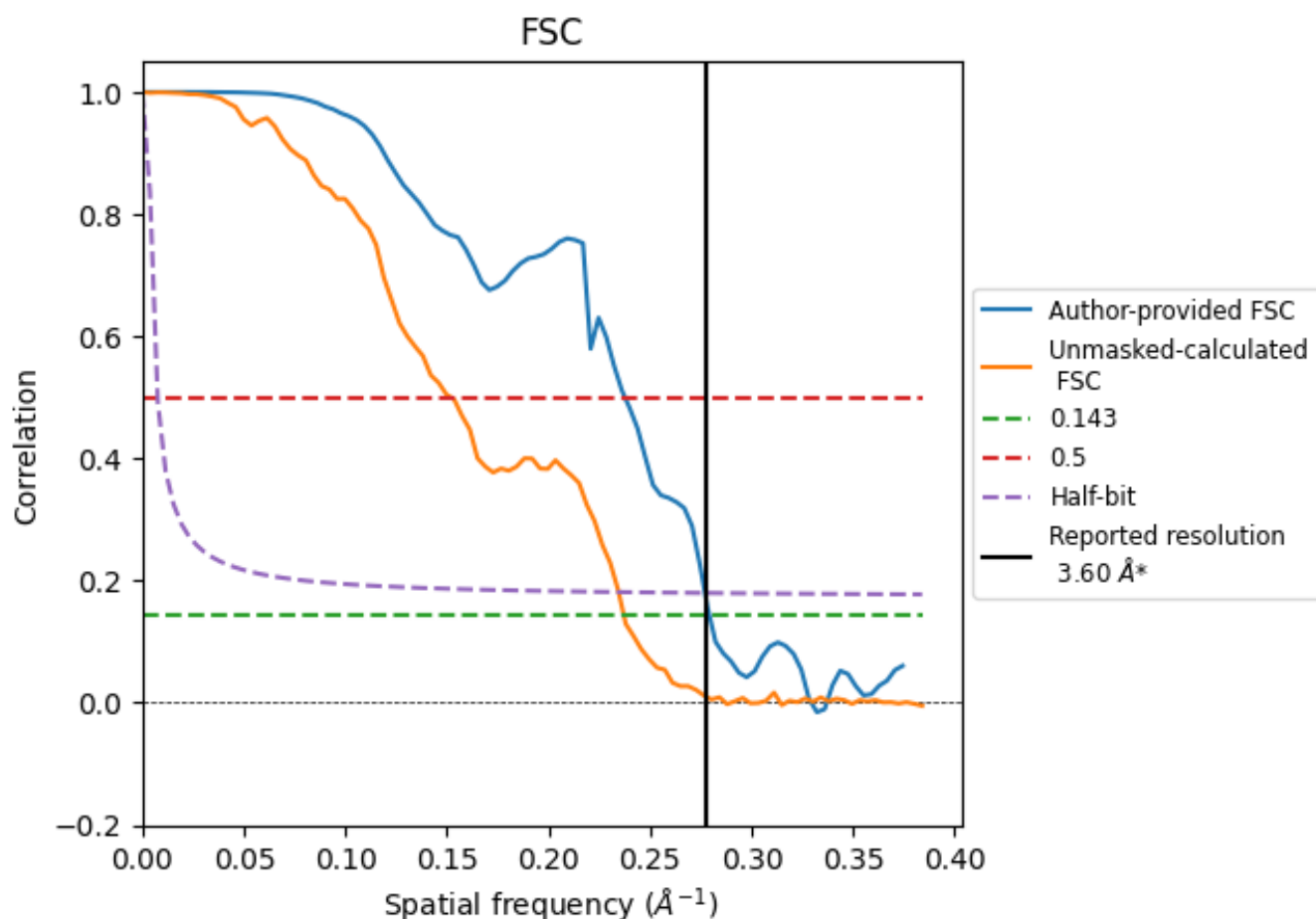


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

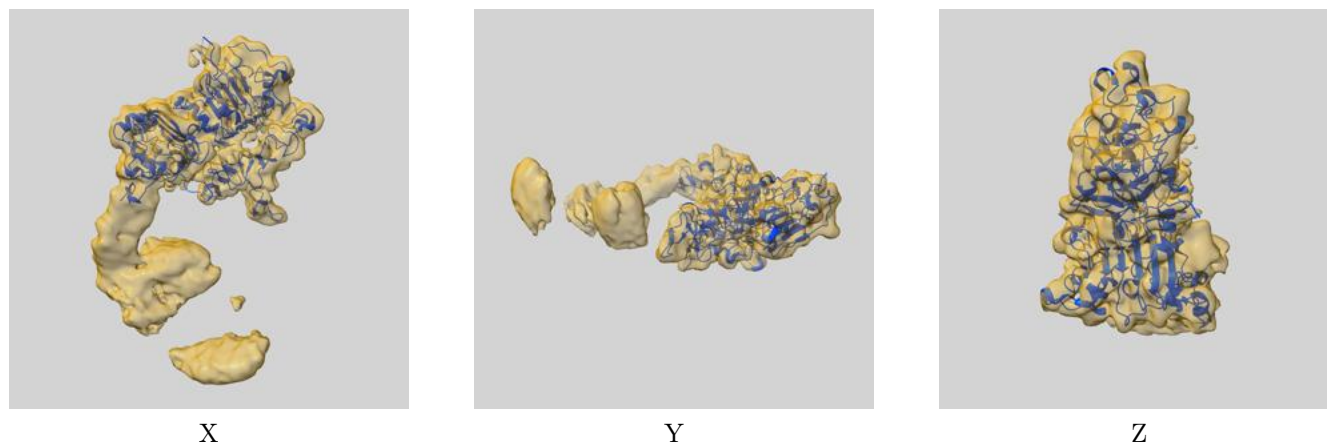
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.21	3.61
Unmasked-calculated*	4.22	6.58	4.26

\*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 4.22 differs from the reported value 3.6 by more than 10 %

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

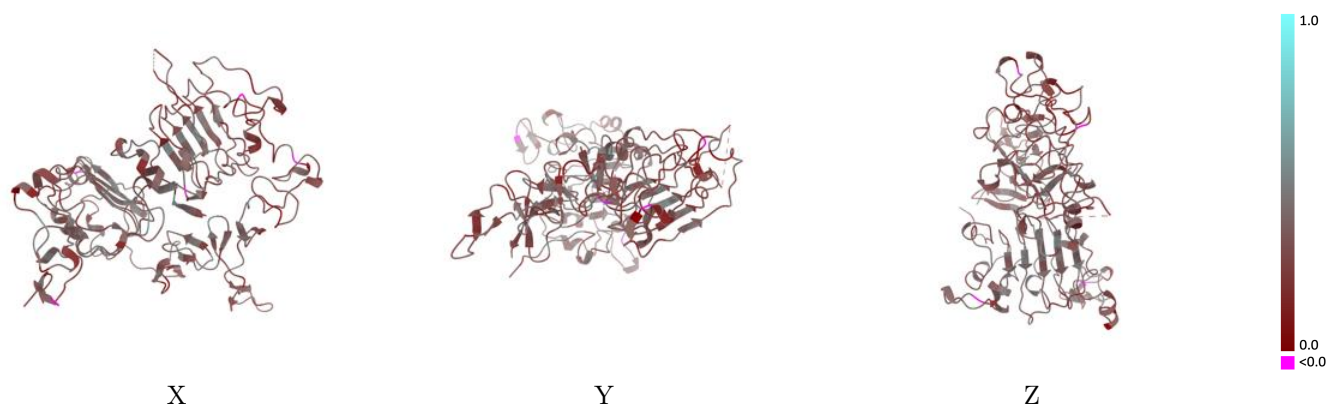
This section contains information regarding the fit between EMDB map EMD-52998 and PDB model 9QBG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



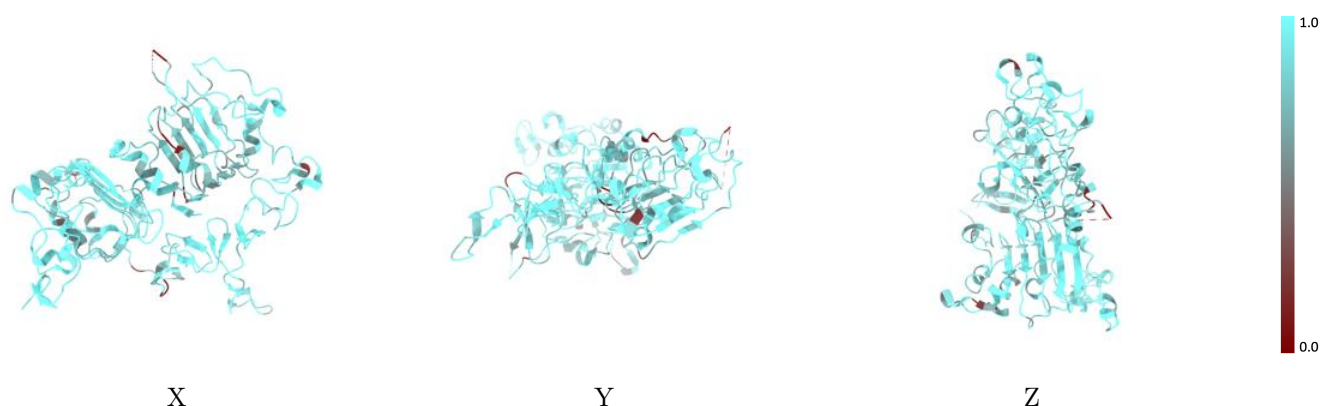
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

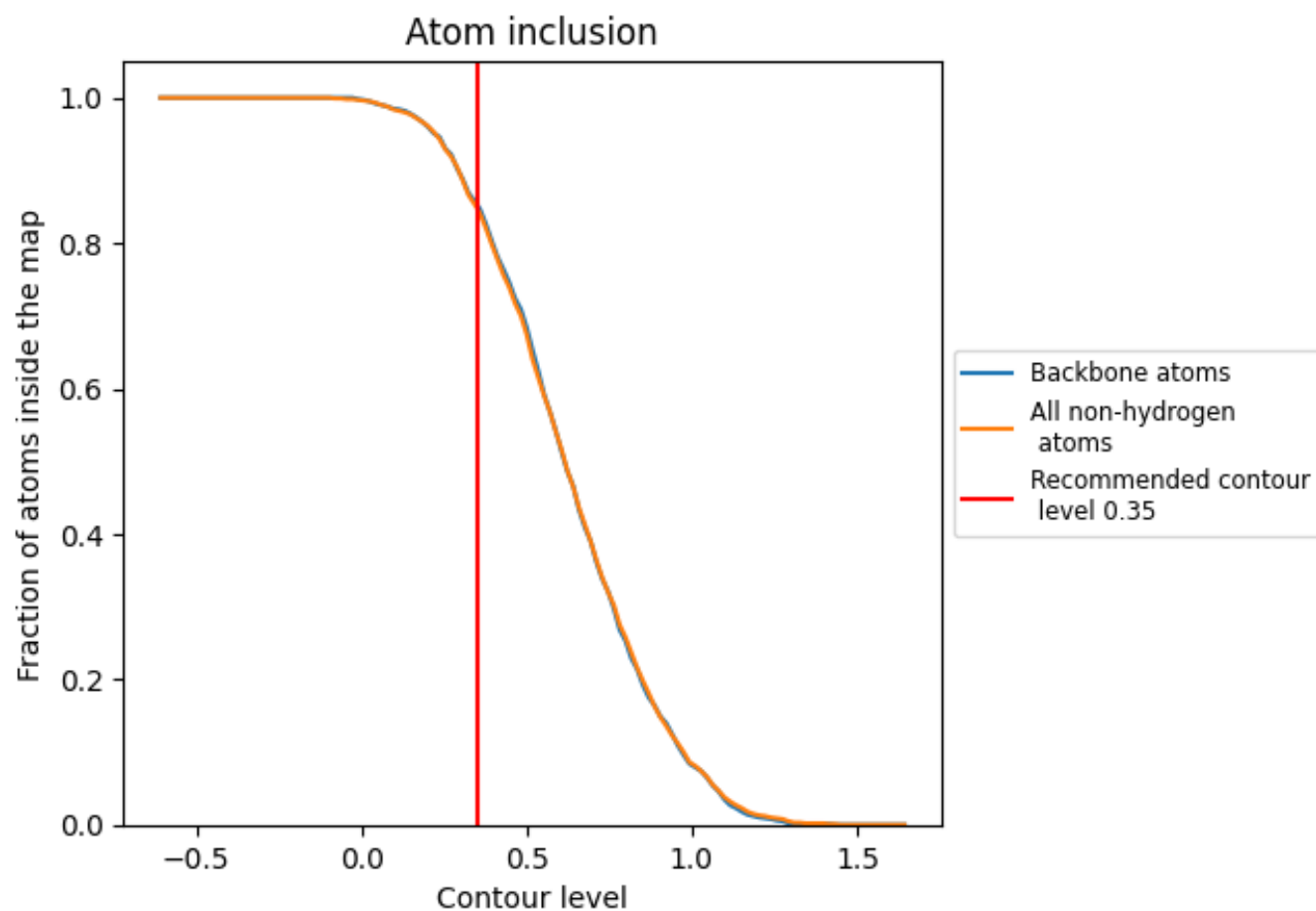
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 85% of all backbone atoms, 85% 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></div> 0.8480	<div><div></div></div> 0.3230
A	<div><div></div></div> 0.8590	<div><div></div></div> 0.3230

