



## wwPDB EM Validation Summary Report ⓘ

Apr 29, 2025 – 01:40 pm BST

PDB ID : 9GOS / pdb\_00009gos  
EMDB ID : EMD-51499  
Title : CryoEM structure of the native Chlamydomonas reinhardtii Flagella Membrane Glycoprotein 1B.  
Authors : Nievergelt, A.P.; Hoepfner, L.M.; Matrino, F.; Scholz, M.; Foster, H.E.; Rodenfels, J.; von Appen, A.; Hippler, M.; Pigino, G.  
Deposited on : 2024-09-06  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

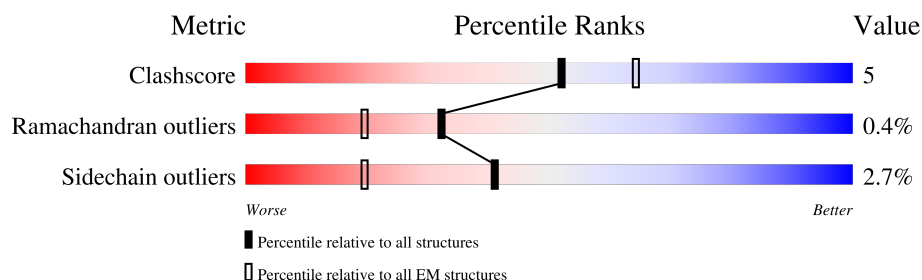
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	4545	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54175 atoms, of which 27330 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 Flagella Membrane Glycoprotein 1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3878	Total	C	H	N	O	S	0	0
			54175	16804	27330	4408	5538	95		



LYS	GLN	PRO	ILE	ASN	LYS	SER	R4059	A3924	I3605	P3336	T3006	T2773	S2420	ASN	CYS	PRO
LYS	SER	ALA	THR	ALA	ASP	PRO	N4060	N3925	V3606	N3337	S3007	T2773	T2439	CYS	THR	GLY
ASN	THR	PHE	ALA	VAL	VAL	PRO	G4061	L3926	V3625	A3340	T3016	L2787	T2439	ILE	THR	CYS
THR	ILE	THR	GLN	THR	THR	SER	S4062	I3932	V3653	V3350	L3017	V2789	K2457	PHE	THR	ALA
ALA	THR	GLN	LEU	ALA	PRO	PRO	A4063	I3945	K3673	L3354	K3022	T2811	L2482	SER	THR	ALA
ALA	THR	GLN	ALA	VAL	VAL	SER	A4064	A3946	D3674	I3378	M3023	L2812	S2496	CYS	THR	THR
ALA	THR	GLN	GLN	THR	THR	THR	A4065	D3947	Q3675	V3377	Y3024	K2849	A2497	GLY	ALA	GLY
ALA	THR	GLN	ALA	ASP	ASP	ALA	A4070	I3950	V3680	I3381	P3030	V2855	N2501	GLY	THR	THR
ALA	THR	GLN	ALA	THR	THR	ASN	C4071	A3951	S3698	I3381	I3033	V2855	R2502	ALA	SER	ALA
ALA	THR	GLN	ALA	VAL	VAL	SER	A4072	V3951	I3381	I3381	L3034	V2855	R2502	VAL	ASP	ALA
ALA	THR	GLN	ALA	THR	THR	ALA	V4073	L3952	T3707	V3390	L3034	V2855	T2524	CYS	ALA	GLY
ALA	THR	GLN	ALA	THR	THR	ARG	A4074	A3953	L3708	C3420	A3035	V2855	N2541	THR	LEU	ALA
ALA	THR	GLN	ALA	THR	THR	GLY	A4075	G3970	C3733	S3424	T3040	V2855	T2560	CYS	GLY	GLY
ALA	THR	GLN	ALA	THR	THR	ALA	D4076	A3971	C3733	I3430	P3041	V2855	D2561	THR	THR	ILE
ALA	THR	GLN	ALA	THR	THR	THR	G4077	D3972	V3748	I3430	V3049	T2882	S2501	SER	GLY	SER
ALA	THR	GLN	ALA	THR	THR	GLY	L4078	I3975	C3754	N3452	V3052	G2893	T2607	GLY	THR	THR
ALA	THR	GLN	ALA	THR	THR	PRO	L4082	L3976	I3765	V3461	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	CYS	A4086	A3977	L3765	V3461	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	ASN	A4087	V3978	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	I3983	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	S3984	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	F3985	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V3986	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	G3987	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4092	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4016	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	L4017	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4018	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	F4019	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	P4020	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4029	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4030	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	T4031	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	I4032	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4033	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4040	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	S4041	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4042	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	L4043	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	T4046	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4047	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4048	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4049	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	D4050	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	C4051	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	N4052	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4053	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4054	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4055	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	V4056	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	I4057	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER
ALA	THR	GLN	ALA	THR	THR	VAL	Y4088	A4058	V3777	A3464	L3075	T2904	T2607	CYS	TYR	SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	583765	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.208	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	488.96, 488.96, 488.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	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	0.15	0/27240	0.35	0/37509

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
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2640	THR	Peptide
1	A	2893	GLY	Peptide

### 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	26845	27330	27329	283	0
All	All	26845	27330	27329	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 283 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:987:ILE:HD12	1:A:1050:ILE:HD12	1.59	0.84
1:A:839:VAL:HG13	1:A:844:THR:HG21	1.61	0.82
1:A:1984:VAL:HG21	1:A:2010:ILE:HD13	1.68	0.76
1:A:3294:ARG:NH2	1:A:3317:LEU:HD13	2.01	0.75
1:A:2935:VAL:HG11	1:A:2949:LEU:HD22	1.67	0.75

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	3874/4545 (85%)	3543 (92%)	316 (8%)	15 (0%)	30 63

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	VAL
1	A	476	ALA
1	A	2339	ALA
1	A	3465	THR
1	A	4126	VAL

### 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	2939/3422 (86%)	2861 (97%)	78 (3%)	40 67

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2747	TYR
1	A	3754	CYS
1	A	2787	LEU
1	A	3092	SER
1	A	3845	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2458	GLN
1	A	2623	ASN
1	A	3914	GLN
1	A	3045	ASN
1	A	805	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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.

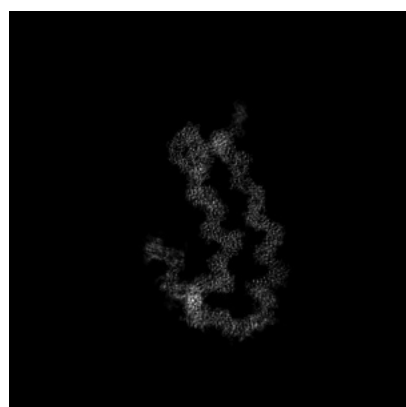
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51499. These allow visual inspection of the internal detail of the map and identification of artifacts.

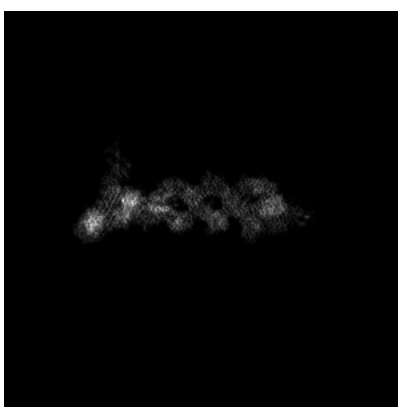
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

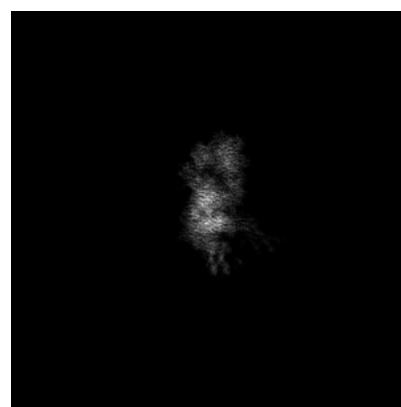
#### 6.1.1 Primary map



X



Y

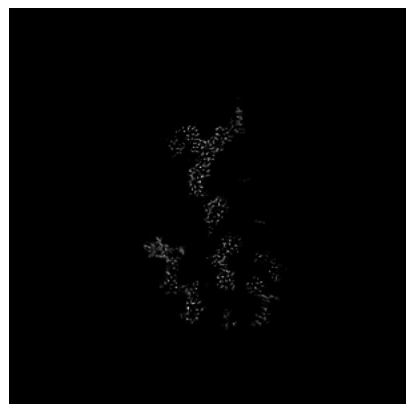


Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 256



Y Index: 256

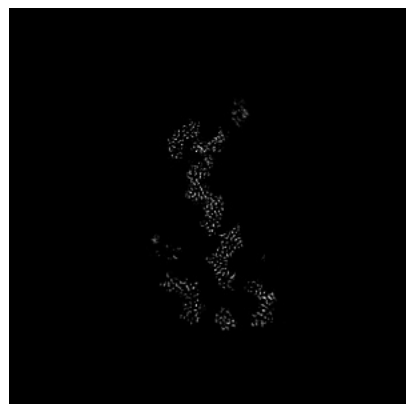


Z Index: 256

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: 251



Y Index: 244

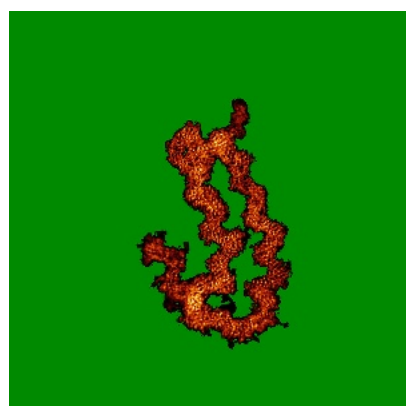


Z Index: 156

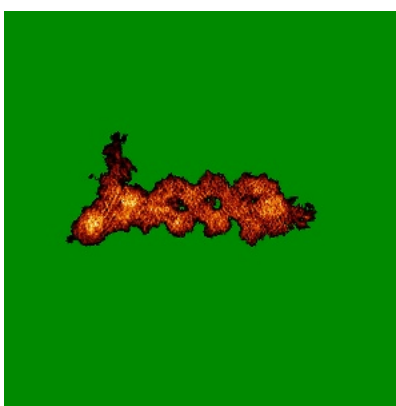
The images above show the largest variance slices of the map in three orthogonal directions.

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

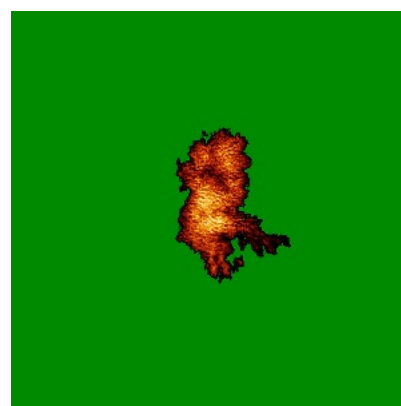
### 6.4.1 Primary map



X



Y



Z

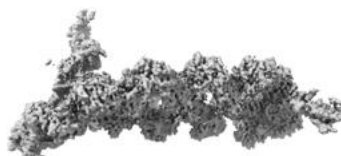
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

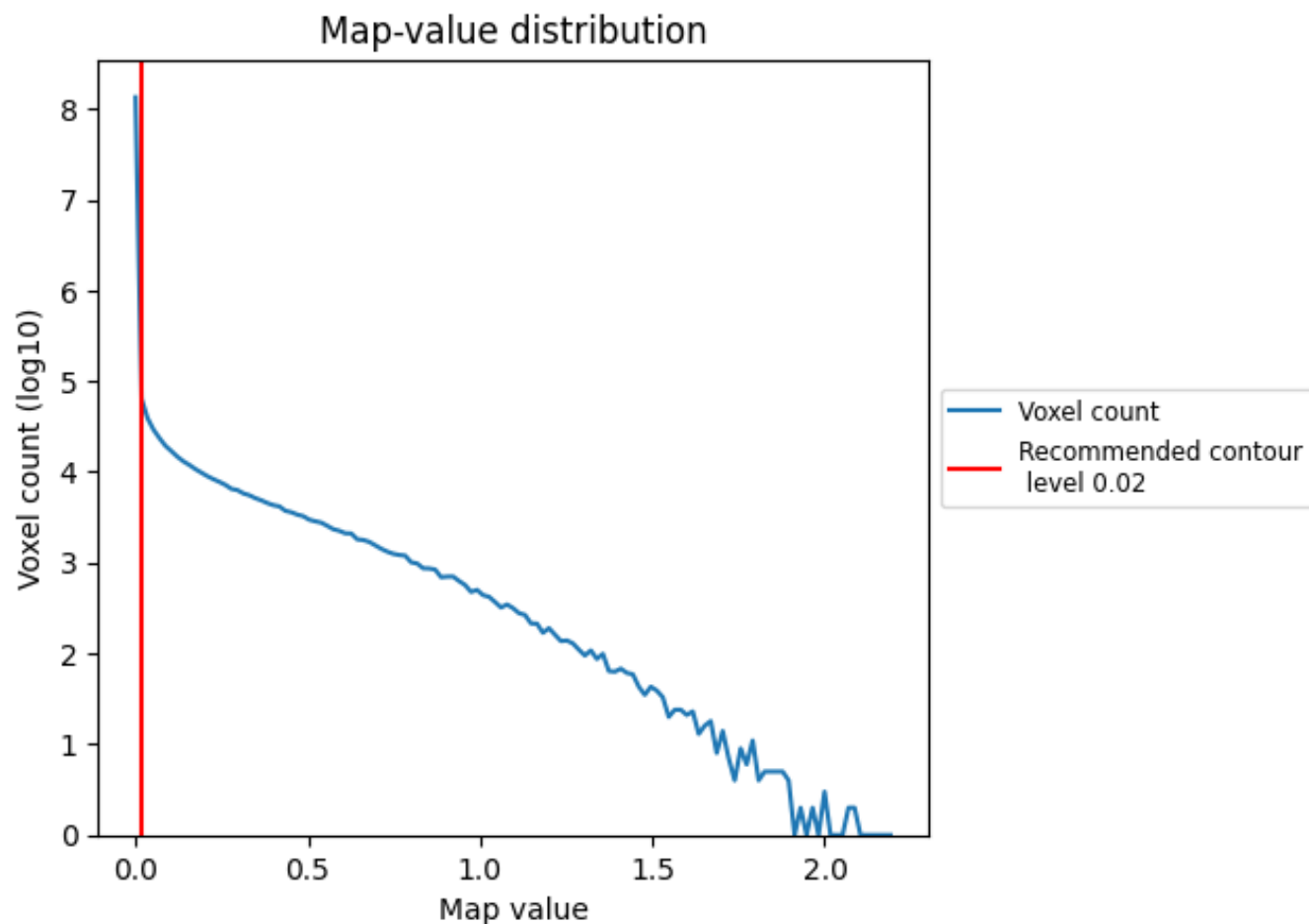
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

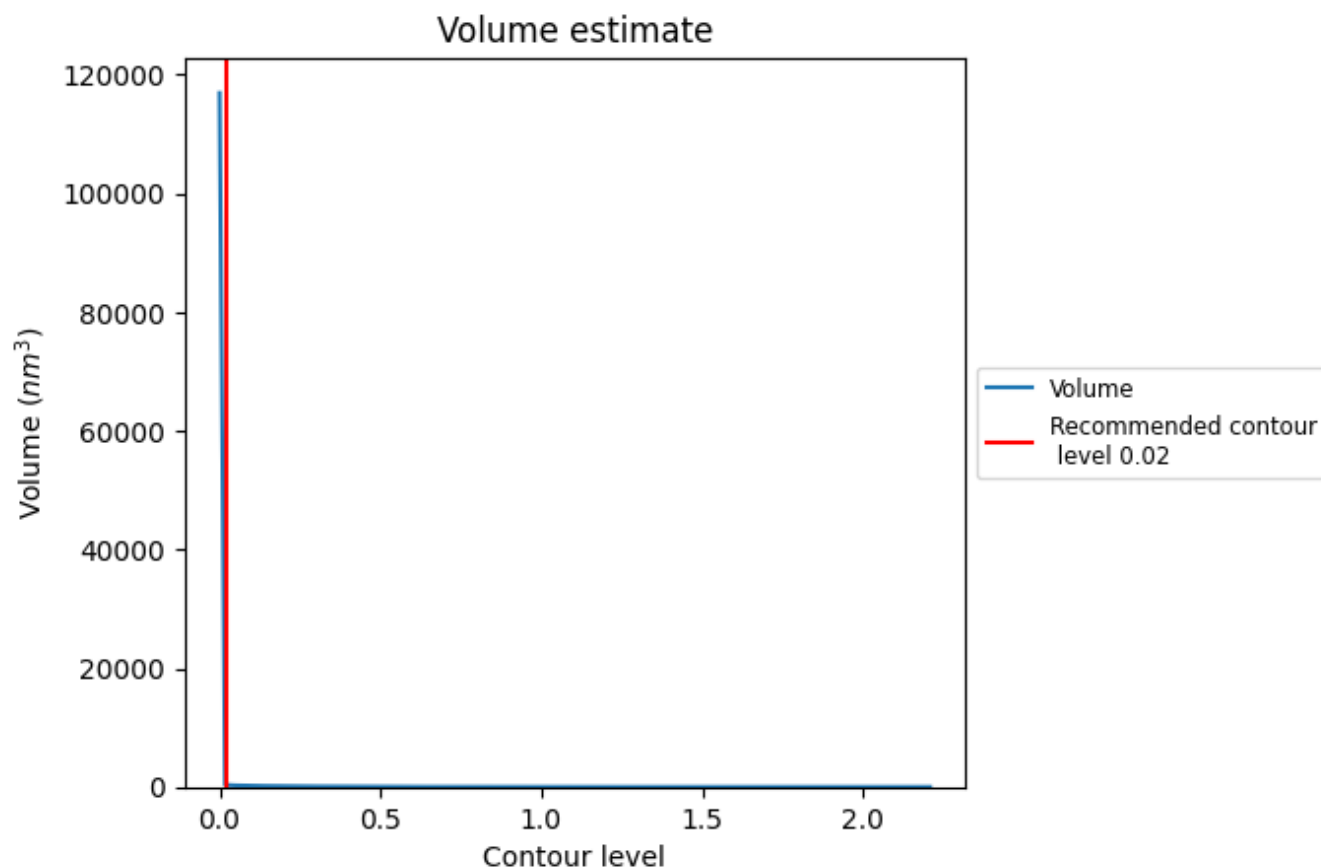
This section contains the results of statistical analysis of the map.

### 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.

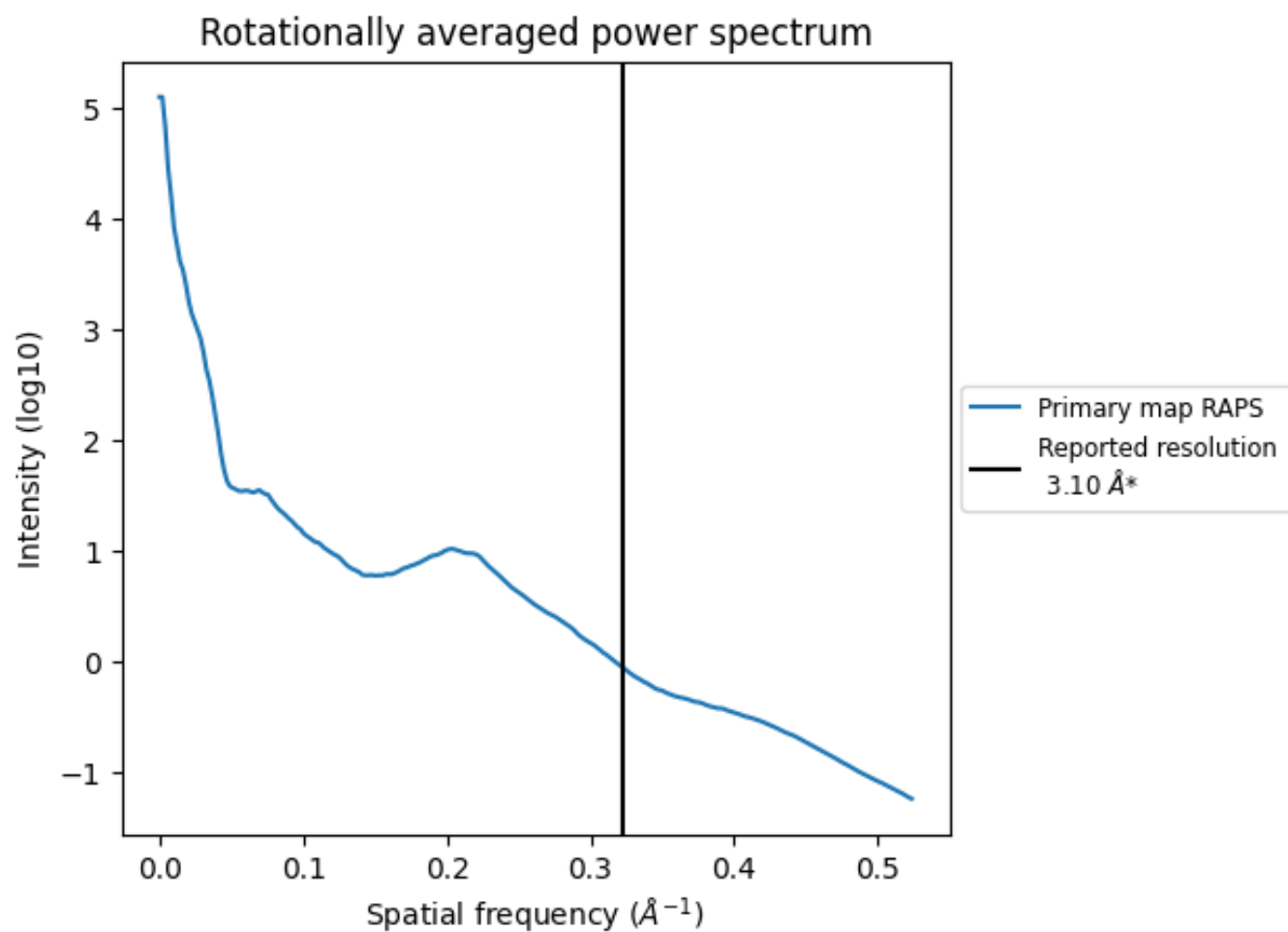
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334  $\text{nm}^3$ ; this corresponds to an approximate mass of 302 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 0.323 Å<sup>-1</sup>



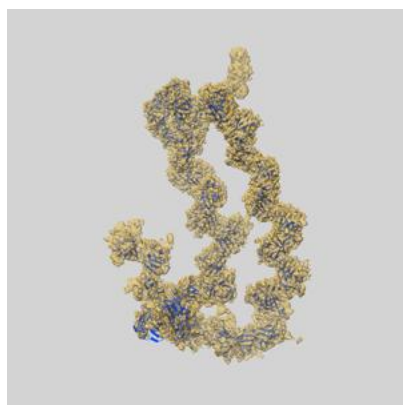
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

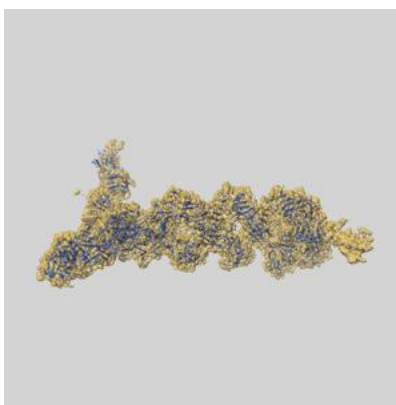
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51499 and PDB model 9GOS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

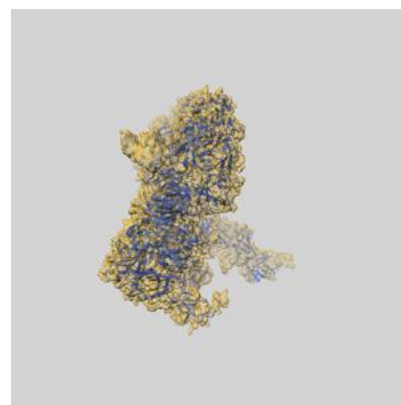
### 9.1 Map-model overlay [i](#)



X



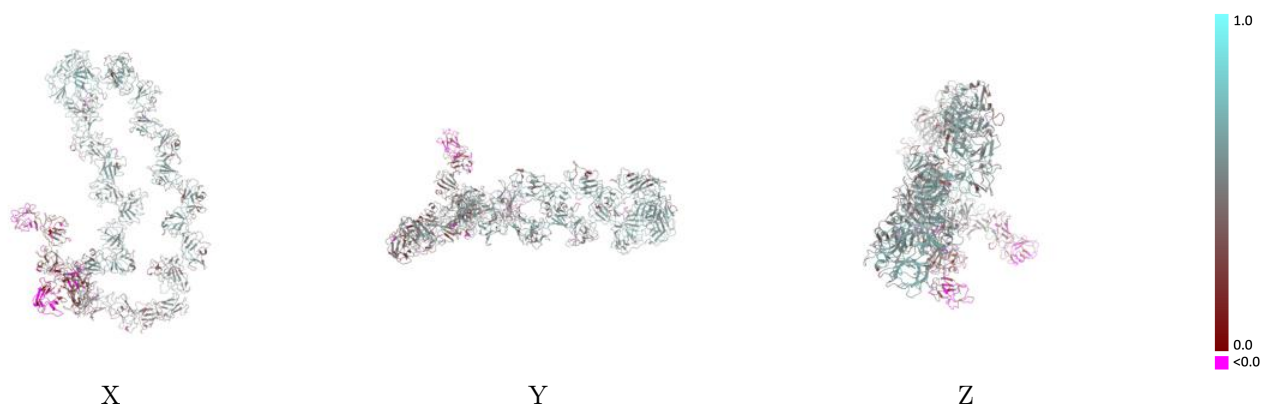
Y



Z

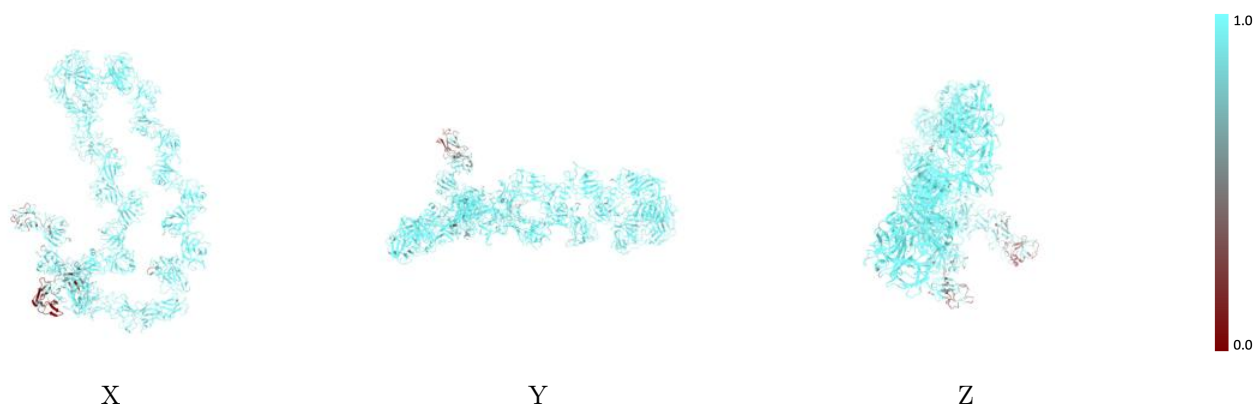
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



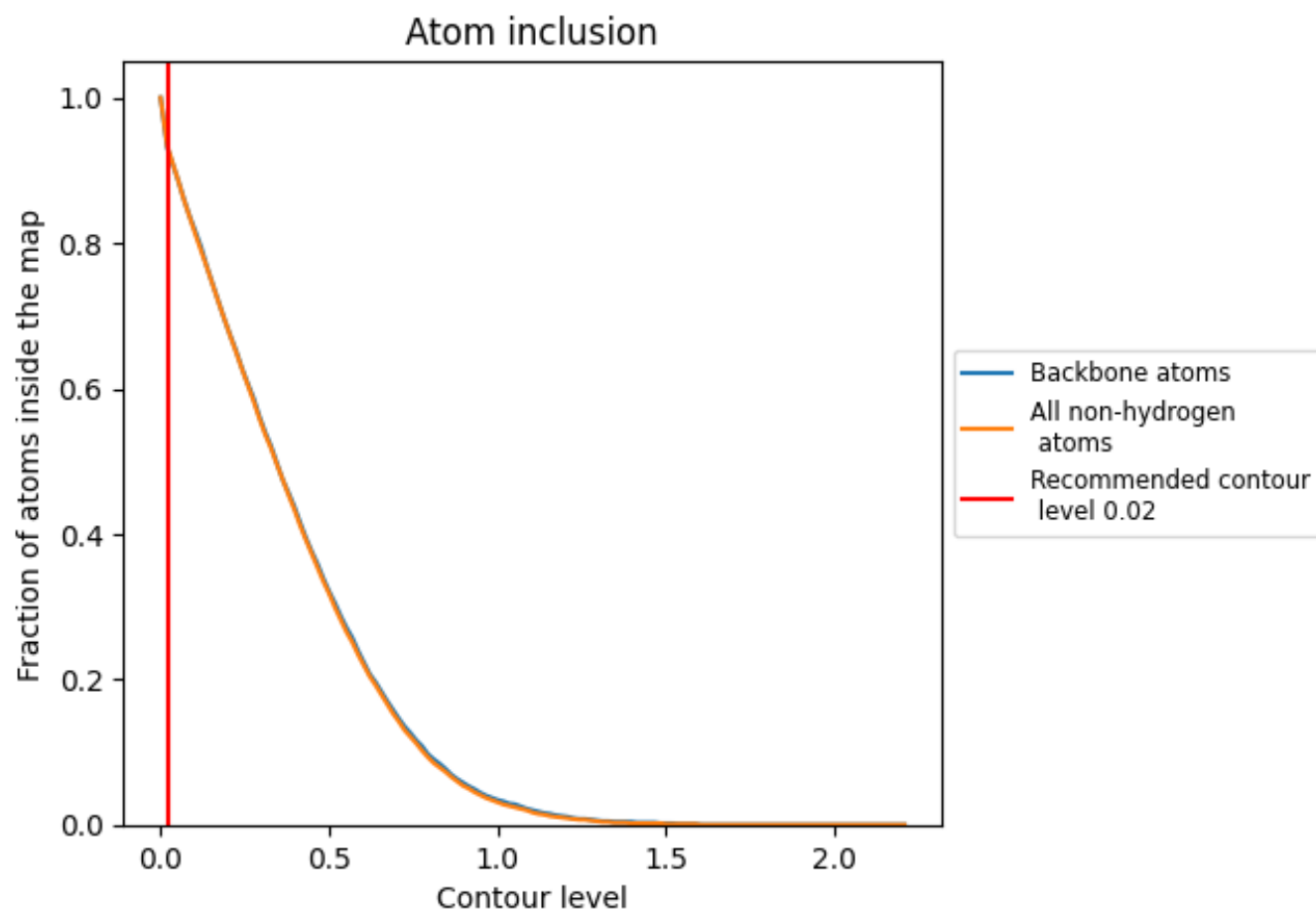
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9330	<div><div></div></div> 0.4580
A	<div><div></div></div> 0.9310	<div><div></div></div> 0.4580

