



## wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 10:44 AM EDT

PDB ID : 9BMM / pdb\_00009bmm  
EMDB ID : EMD-44703  
Title : State-4 of the motor domain from full-length human dynein-1 in 5mM AMPPNP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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

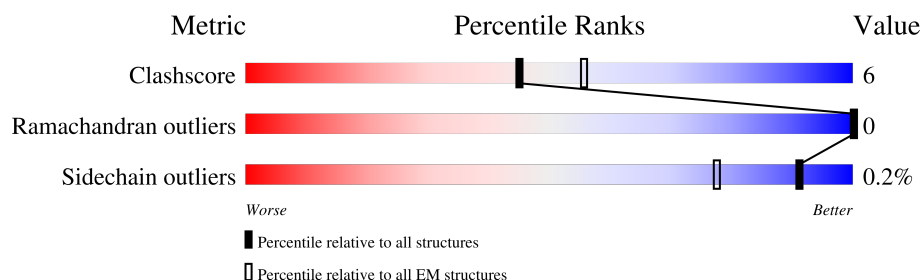
# 1 Overall quality at a glance

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	4646	 52% 10% 38%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23038 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2859	22925	14595	3960	4257	113	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

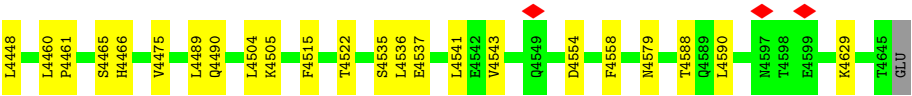
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0





L4312	T4127	L3938	I3760	TYR	LEU	GLN	R2836	R2642	R2451	R2298
S3939	T4130	S3939	L3761	LYS	ALA	GLN	L2837	R2642	C2454	R2298
C3940	I3766	C3940	I3766	GLY	CYS	GLY	V2838	A2651	C2454	G2305
L3941	I3767	L3941	I3767	GLY	GLY	VAL	E2842	A2651	V2469	D2308
F3944	E3776	F3944	E3776	PRO	PRO	ILE	D2847	L2668	M2481	E2313
K3945	E3779	K3945	E3779	THR	LYS	ASP	H2857	M2671	Q2482	L2319
D3946	E3779	D3946	E3779	TRP	TRP	GLN	F2858	Q2677	Q2483	L2319
L3947	D3788	L3947	D3788	ALA	ALA	LYS	K2865	Q2677	Q2484	N2322
K3950	I3789	K3950	I3789	ILE	ILE	VAL	E2864	Q2677	Q2485	N2322
L3961	V3790	L3961	V3790	ALA	ALA	VAL	K2865	Q2677	Q2486	K2323
T3969	I3789	T3969	I3789	GLN	GLN	LYS	E2865	Q2677	Q2487	K2323
L3973	V3810	L3973	V3810	LEU	LEU	GLY	R2869	L2683	I2498	L2325
E3977	S3809	E3977	S3809	ASN	ASN	ASP	Q2869	L2683	I2498	L2325
T3983	S3810	T3983	S3810	TYR	TYR	ILE	Q2869	Q2685	L2502	L2333
L4179	I3811	L4179	I3811	ASP	ASP	ASP	E2903	M2686	L2502	L2333
L4183	M3815	L4183	M3815	ASP	ASP	ARG	E2904	V2687	S2506	F2343
H4187	L3818	H4187	L3818	GLU	GLU	VAL	L2905	V2688	M2510	Q2346
R4195	Y3825	R4195	Y3825	LEU	LEU	ASN	V2906	F2692	I2518	T2355
F3996	I3835	F3996	I3835	LYS	LYS	PHE	I2925	L2703	T2522	C2359
R3997	V3853	R3997	V3853	ARG	ARG	ILE	I2925	L2703	T2522	C2359
M4018	R3854	M4018	R3854	GLU	GLU	THR	I2925	L2703	T2522	C2359
S4019	I3862	S4019	I3862	LEU	LEU	ILE	L2933	D2717	T2522	C2359
T4020	T3863	T4020	T3863	ARG	ARG	ALA	L2933	D2717	T2522	C2359
M4021	T3864	M4021	T3864	ASN	ASN	GLN	I2936	K2721	D2536	G2360
L4027	L3664	L4027	L3664	GLY	GLY	ASN	K2943	P2732	Y2537	M2361
P4037	S3665	P4037	S3665	LEU	LEU	ALA	K2943	P2732	E2538	E2366
M4043	D3666	M4043	D3666	GLN	GLN	VAL	I2961	V2734	S2542	L2369
C4044	I3671	C4044	I3671	LYS	LYS	SER	K2962	V2734	S2542	L2369
D4050	T3681	D4050	T3681	ASP	ASP	ILE	V2963	F2751	W2548	D2388
L4058	S3694	L4058	S3694	ASP	ASP	ILE	H2964	N2752	V2562	E2389
Q4065	R3695	Q4065	R3695	ASP	ASP	LYS	K2965	R2753	V2562	GLY
V4088	L3708	V4088	L3708	ALA	ALA	GLN	K2966	R2763	GLU	ASP
K4237	V3716	K4237	V3716	LYS	LYS	ARG	K2966	R2763	GLU	ASP
T4238	D3723	T4238	D3723	ALA	ALA	ILE	T2967	R2763	GLU	ASP
P4239	L3731	P4239	L3731	LYS	LYS	ARG	T2967	R2763	GLU	ASP
A4242	L3734	A4242	L3734	ASP	ASP	LEU	T2968	N2773	L2572	L2572
L4243	R3741	L4243	R3741	ASN	ASN	VAL	C2969	N2773	D2573	D2573
Y4252	R3743	Y4252	R3743	GLN	GLN	GLU	N2987	E2775	T2574	GLN
G4253	E3746	G4253	E3746	ASN	ASN	VAL	N2987	E2775	ARG	ARG
D4257	V3756	D4257	V3756	GLN	GLN	LYS	D2995	F2784	ARG	ARG
M4258	K3757	M4258	K3757	ILE	ILE	ASN	E2996	F2784	LYS	LYS
E4281	G3758	E4281	G3758	GLU	GLU	TYR	S2997	Y2792	GLY	GLY
K4287	R3759	K4287	R3759	LEU	LEU	MET	N2998	I2793	LYS	LYS
H4291	V3936	H4291	V3936	ALA	ALA	PRO	V2999	Y2794	GLY	GLY
Y4447	R3937	Y4447	R3937	ARG	ARG	ASP	L3000	V2803	ASP	ASP
						VAL	G3003	V2804	GLY	GLY
						GLY	E3006	L2816	GLY	GLY
						LEU	R3007	L2821	ALA	ALA
						ALA	V3017	L2822	ALA	ALA
						SER	L3020	W2825	S2623	S2410
						ILE	M3043	Q2834	P2628	T2422
						GLY	L3044	Q2835	K2633	V2433
						GLN				
						GLN				
						LEU				
						HIS				
						LYS				





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92310	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.145	Depositor
Minimum map value	-1.237	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP

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	0.17	0/23409	0.30	0/31728

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	22925	0	22998	280	0
2	A	81	0	36	3	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23038	0	23046	280	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 6.

The worst 5 of 280 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.63	0.81
1:A:2115:LYS:HD2	1:A:2118:ARG:HH21	1.46	0.79
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.62	0.79
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.66	0.76
1:A:2834:GLN:NE2	1:A:2847:ASP:OD2	2.21	0.74

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	2851/4646 (61%)	2809 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2532/4125 (61%)	2526 (100%)	6 (0%)	92	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2734	VAL
1	A	3875	MET

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Mol	Chain	Res	Type
1	A	4127	THR
1	A	1991	ASP
1	A	1690	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3952	GLN
1	A	4335	GLN
1	A	4595	GLN
1	A	4508	HIS
1	A	4114	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.78	1 (3%)
3	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.80	1 (2%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	0/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4704	ADP	N3-C2-N1	-3.56	123.83	128.67
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4703	ADP	C4-C5-N7	-2.47	106.72	109.34
3	A	4702	ATP	C5-C6-N6	2.34	123.88	120.31

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

3 monomers are involved in 3 short contacts:

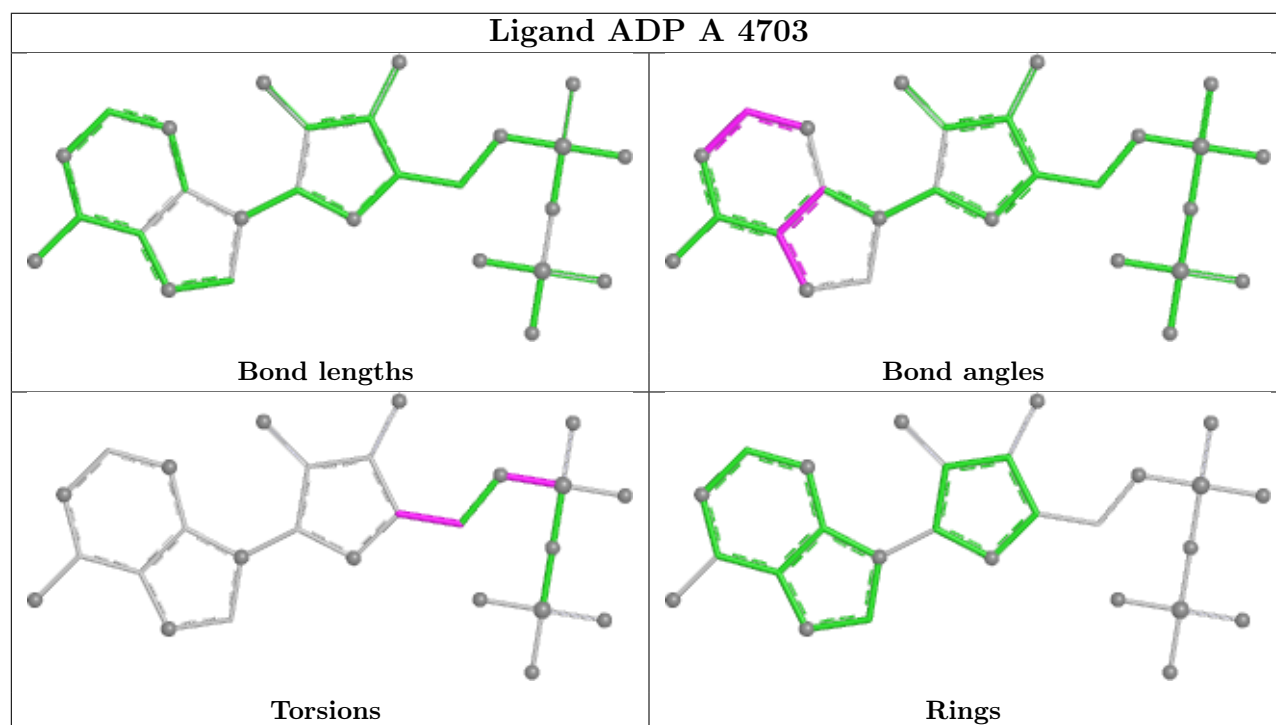
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4703	ADP	1	0

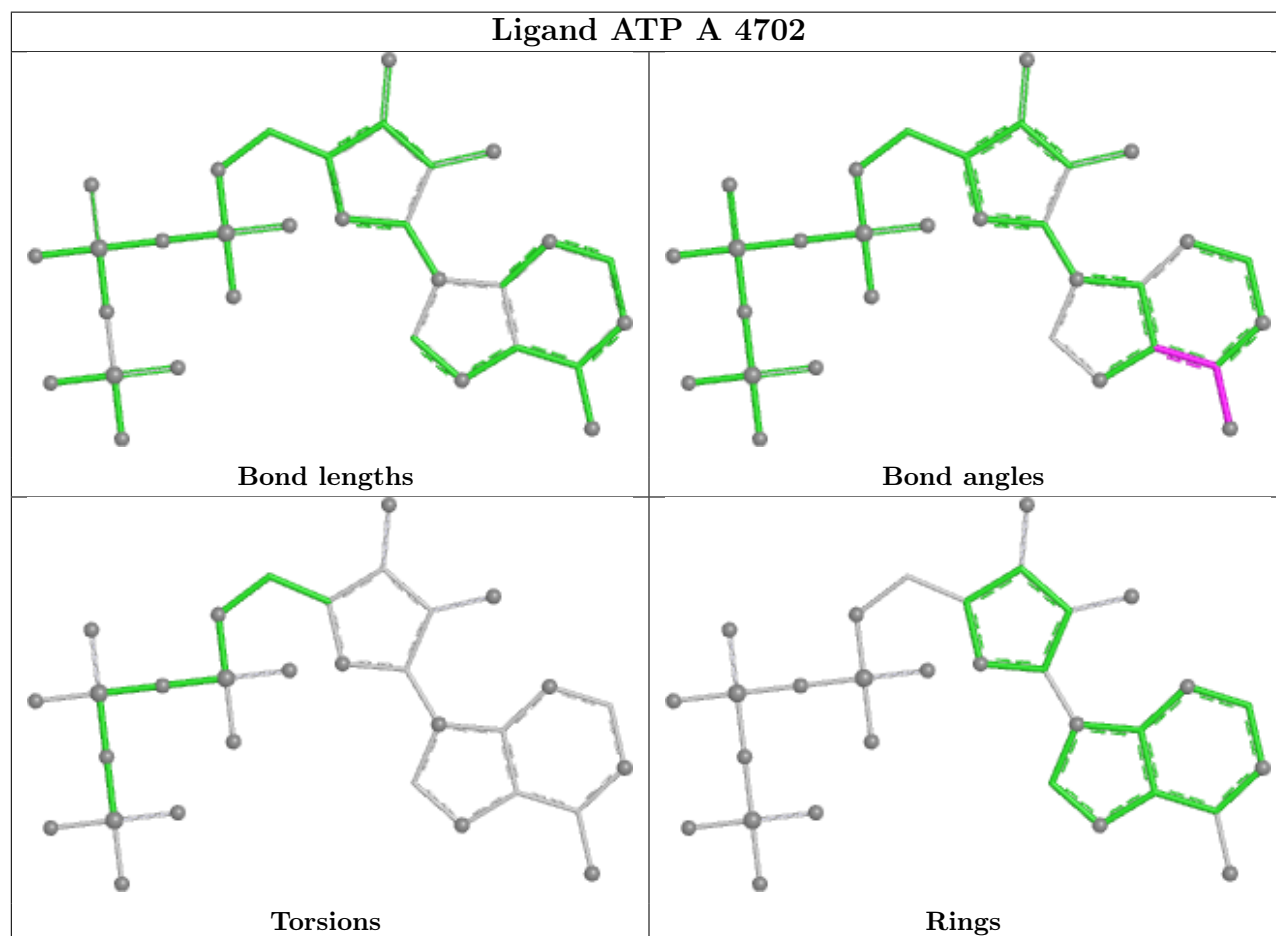
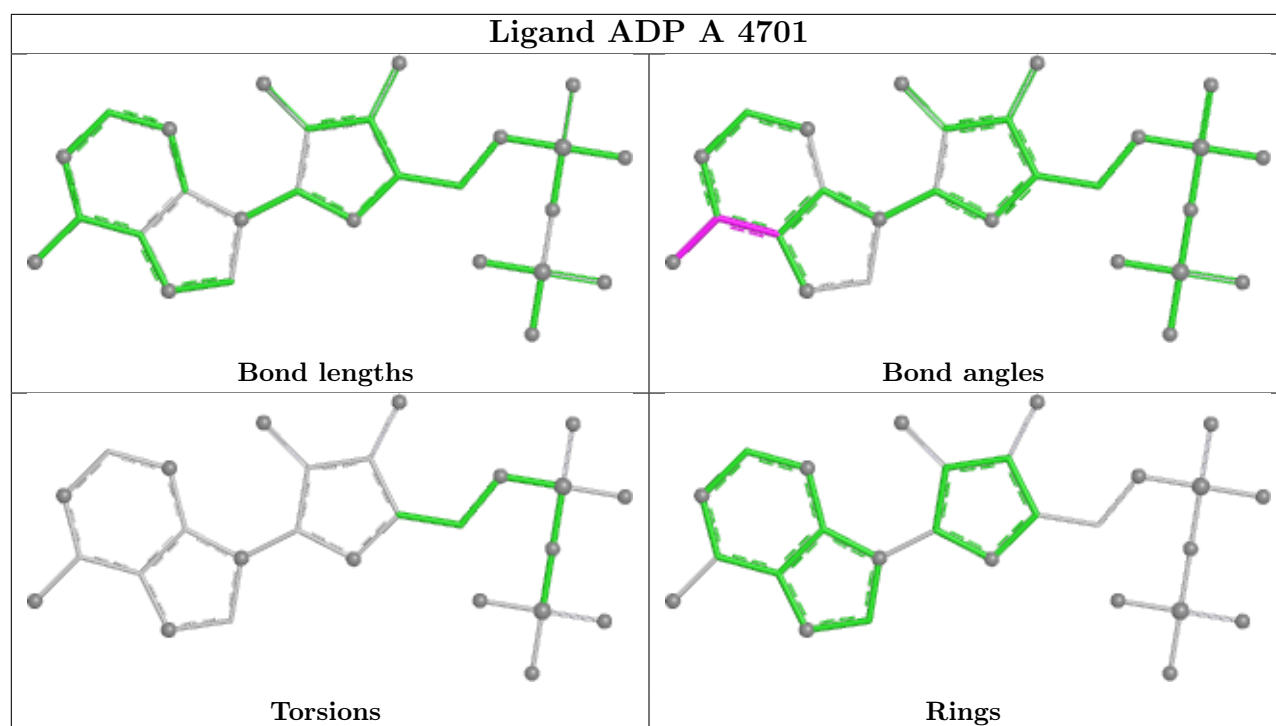
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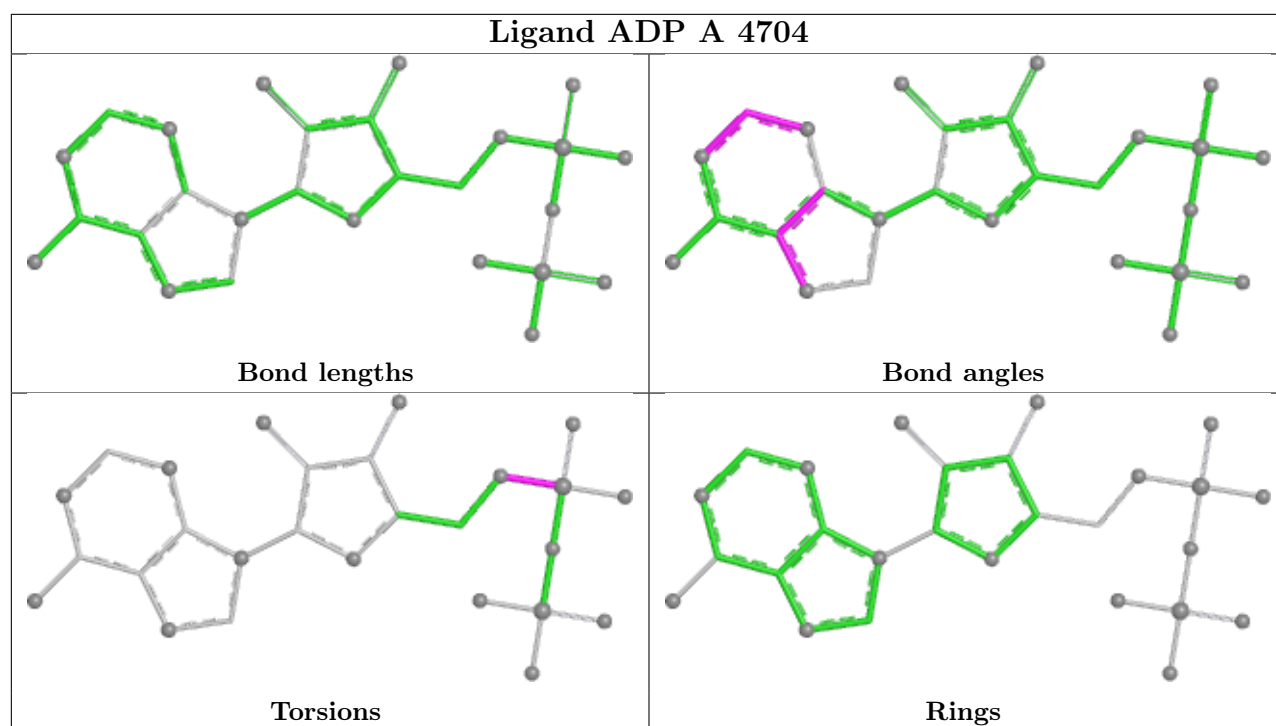
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
2	A	4704	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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.



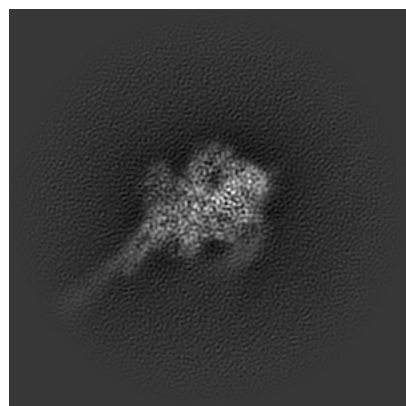
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44703. These allow visual inspection of the internal detail of the map and identification of artifacts.

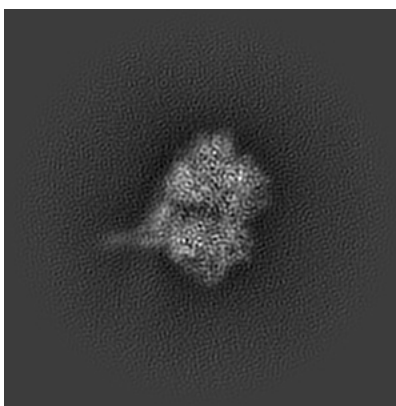
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

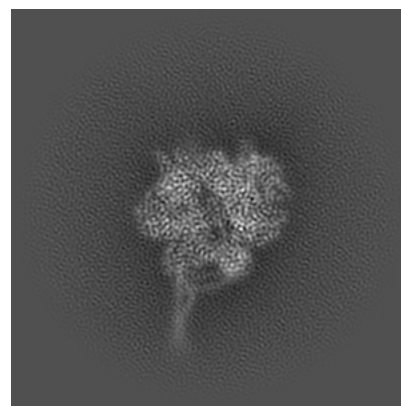
#### 6.1.1 Primary map



X

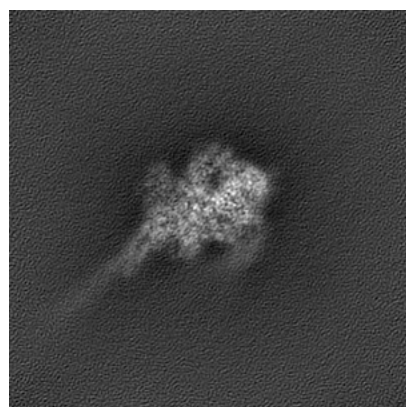


Y

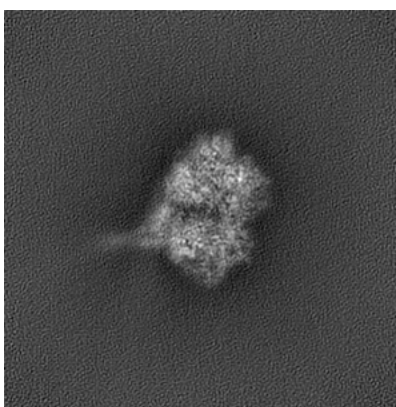


Z

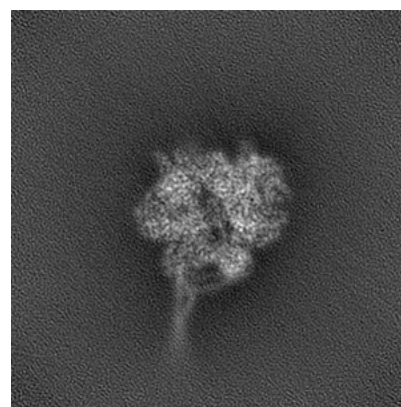
#### 6.1.2 Raw map



X



Y

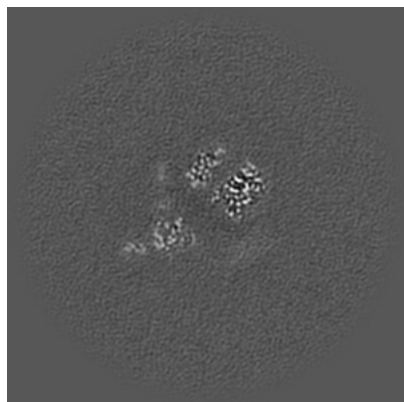


Z

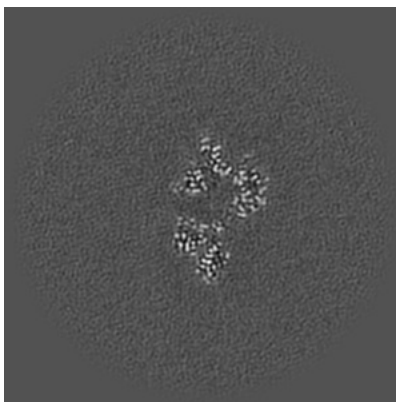
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

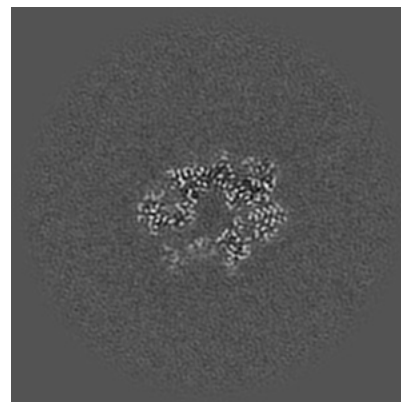
### 6.2.1 Primary map



X Index: 128

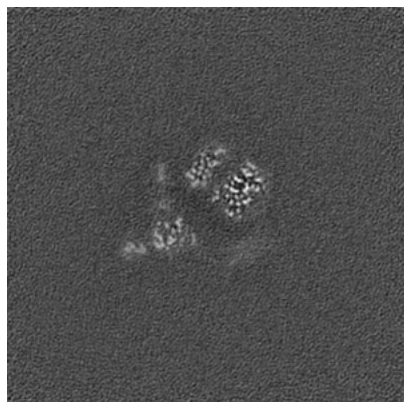


Y Index: 128

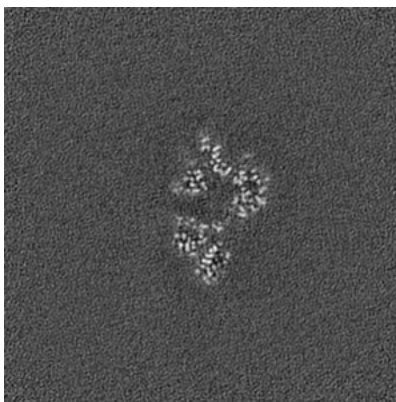


Z Index: 128

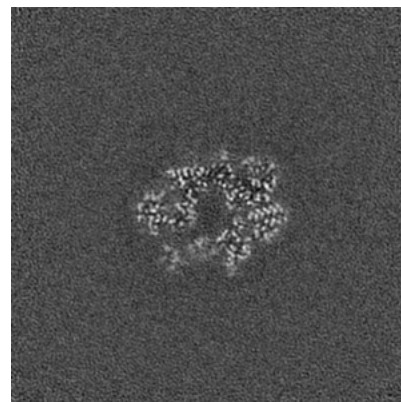
### 6.2.2 Raw map



X Index: 128



Y Index: 128

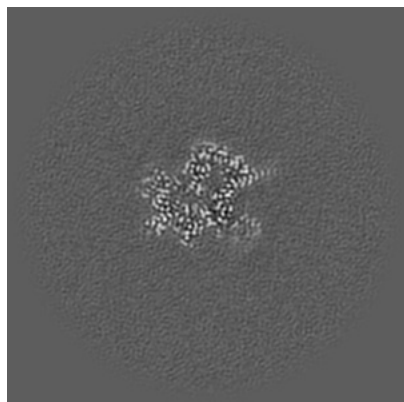


Z Index: 128

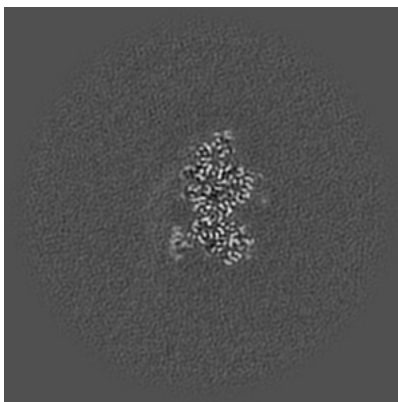
The images above show central slices of the map in three orthogonal directions.

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

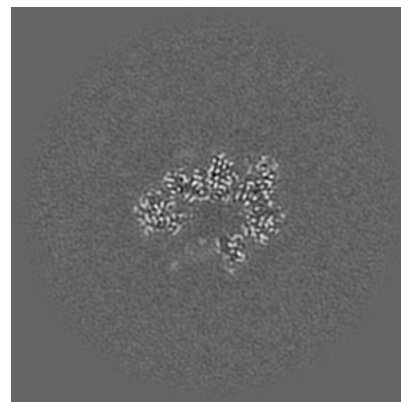
### 6.3.1 Primary map



X Index: 146

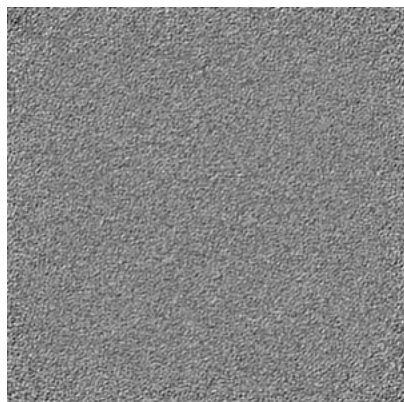


Y Index: 143

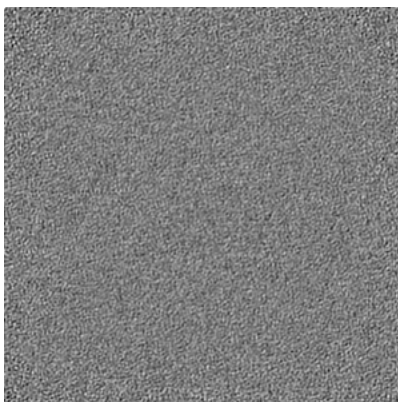


Z Index: 131

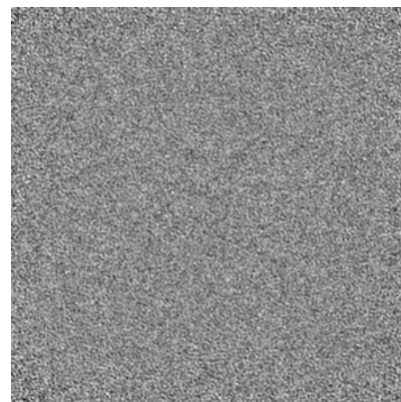
### 6.3.2 Raw map



X Index: 0



Y Index: 0



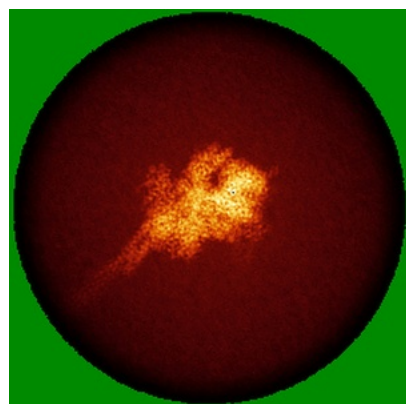
Z Index: 0

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

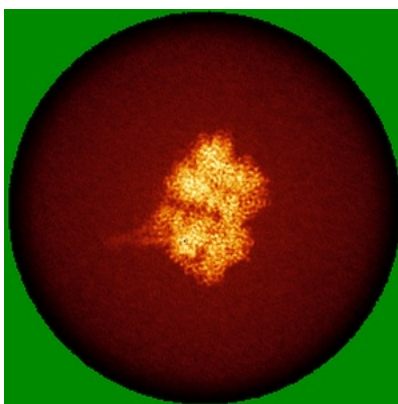


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

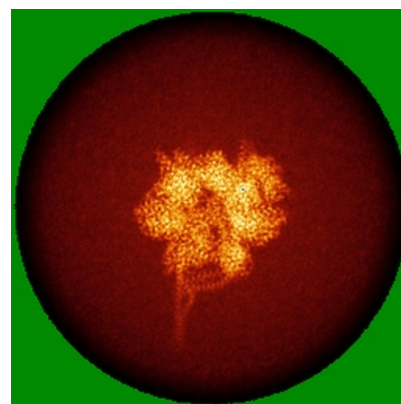
### 6.4.1 Primary map



X

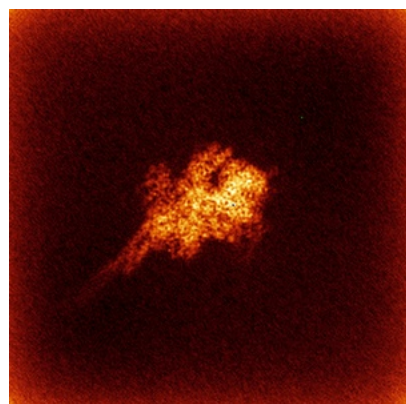


Y

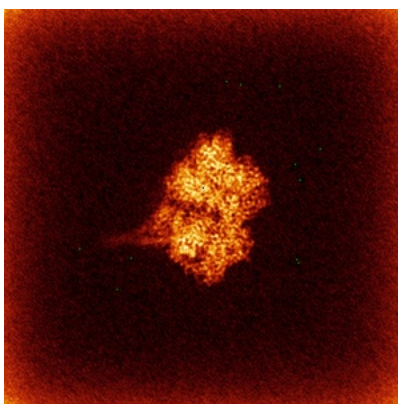


Z

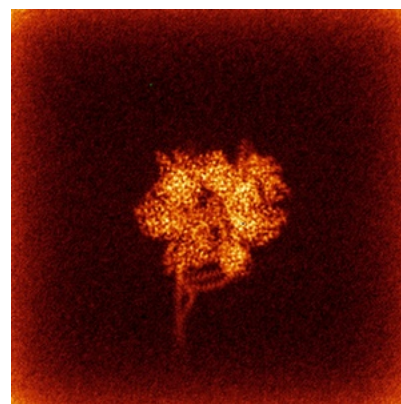
### 6.4.2 Raw map



X



Y

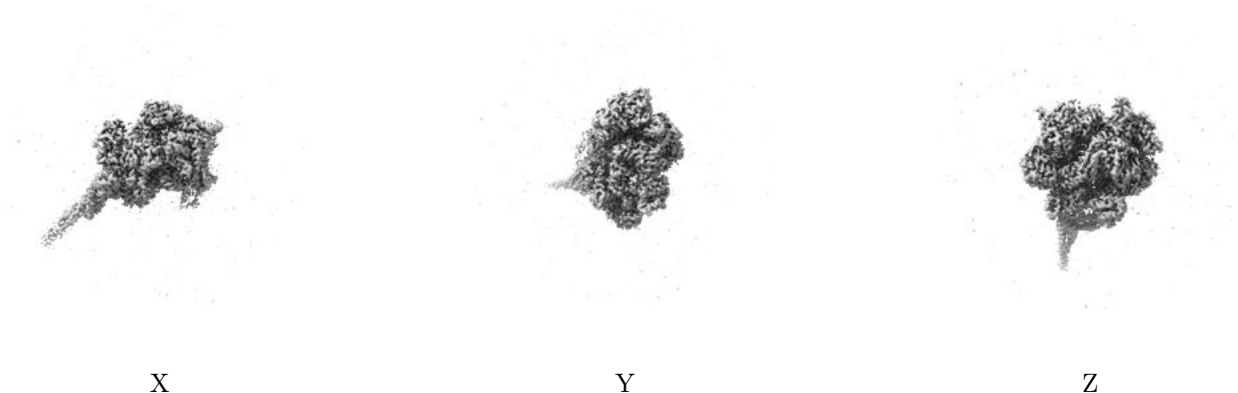


Z

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.

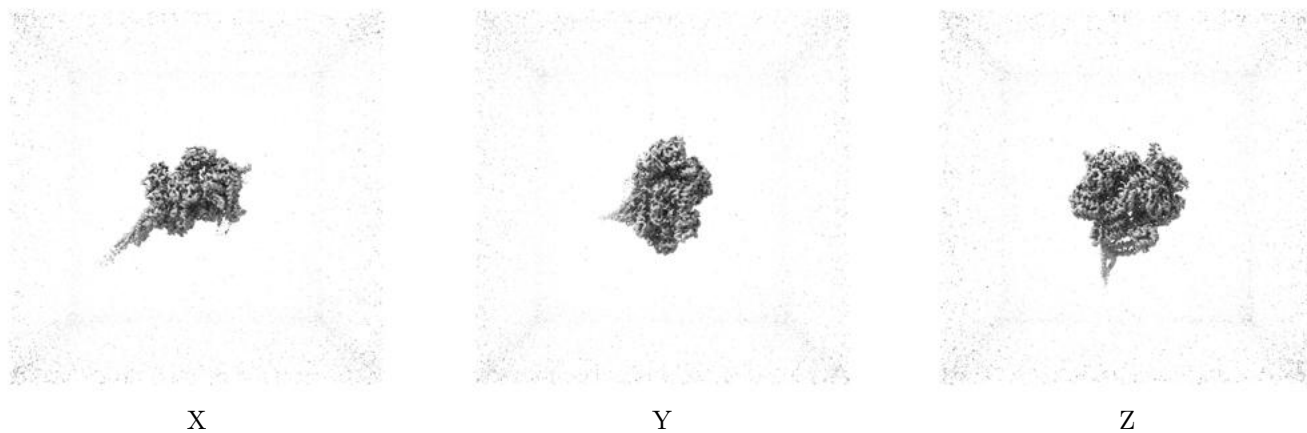
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

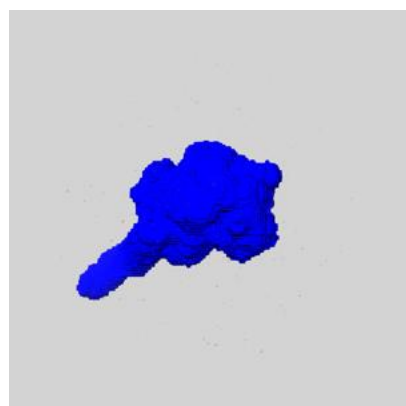
## 6.6 Mask visualisation [i](#)

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

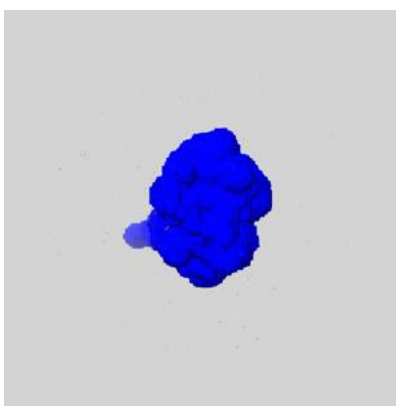
A mask typically either:

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

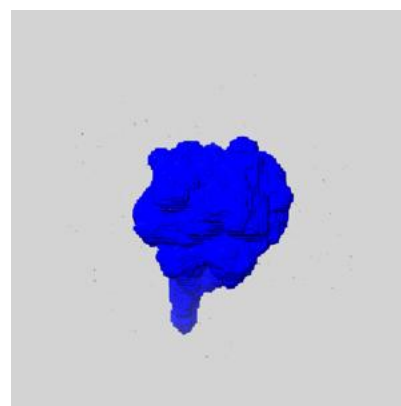
### 6.6.1 emd\_44703\_msk\_1.map [i](#)



X



Y

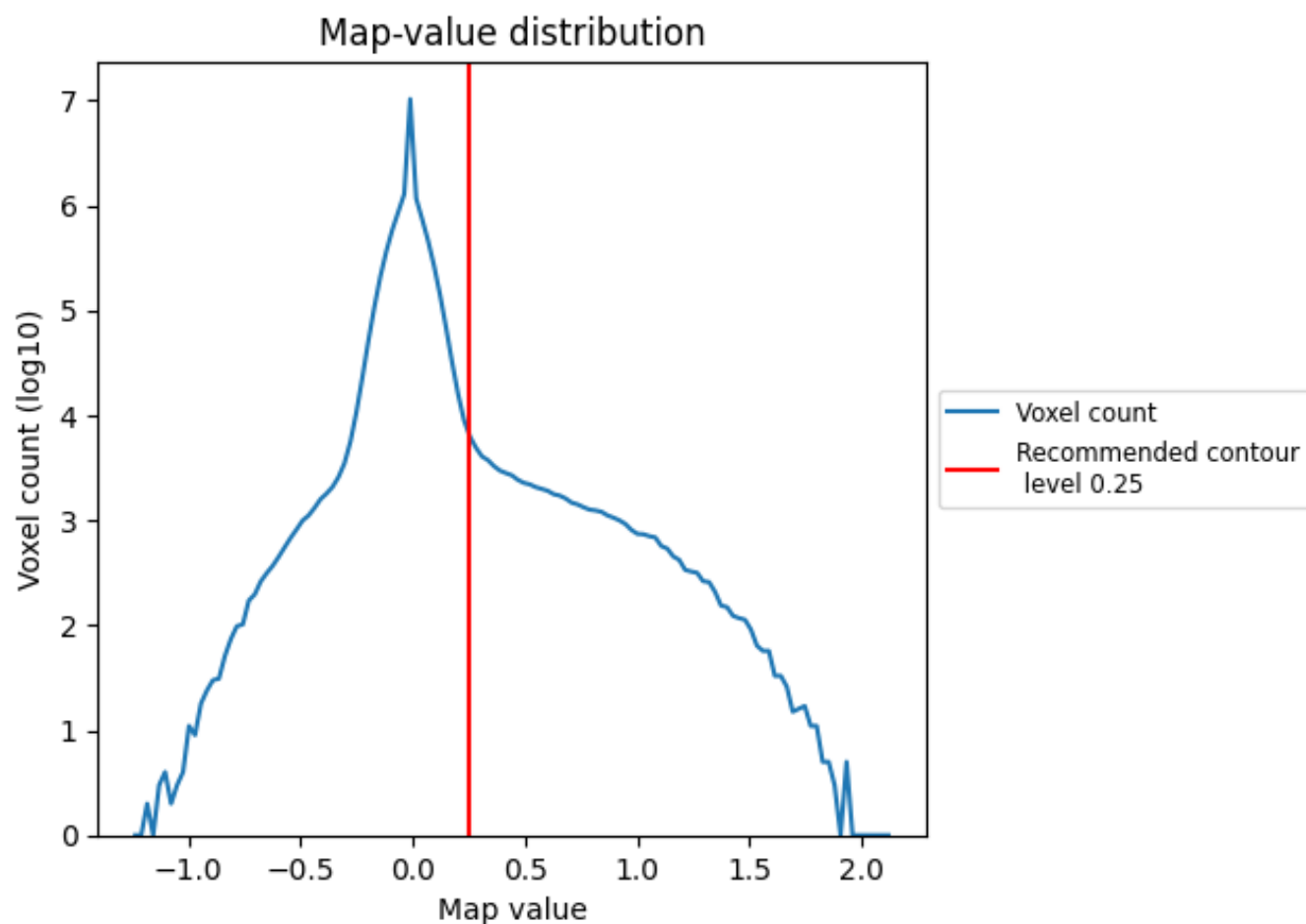


Z

## 7 Map analysis [i](#)

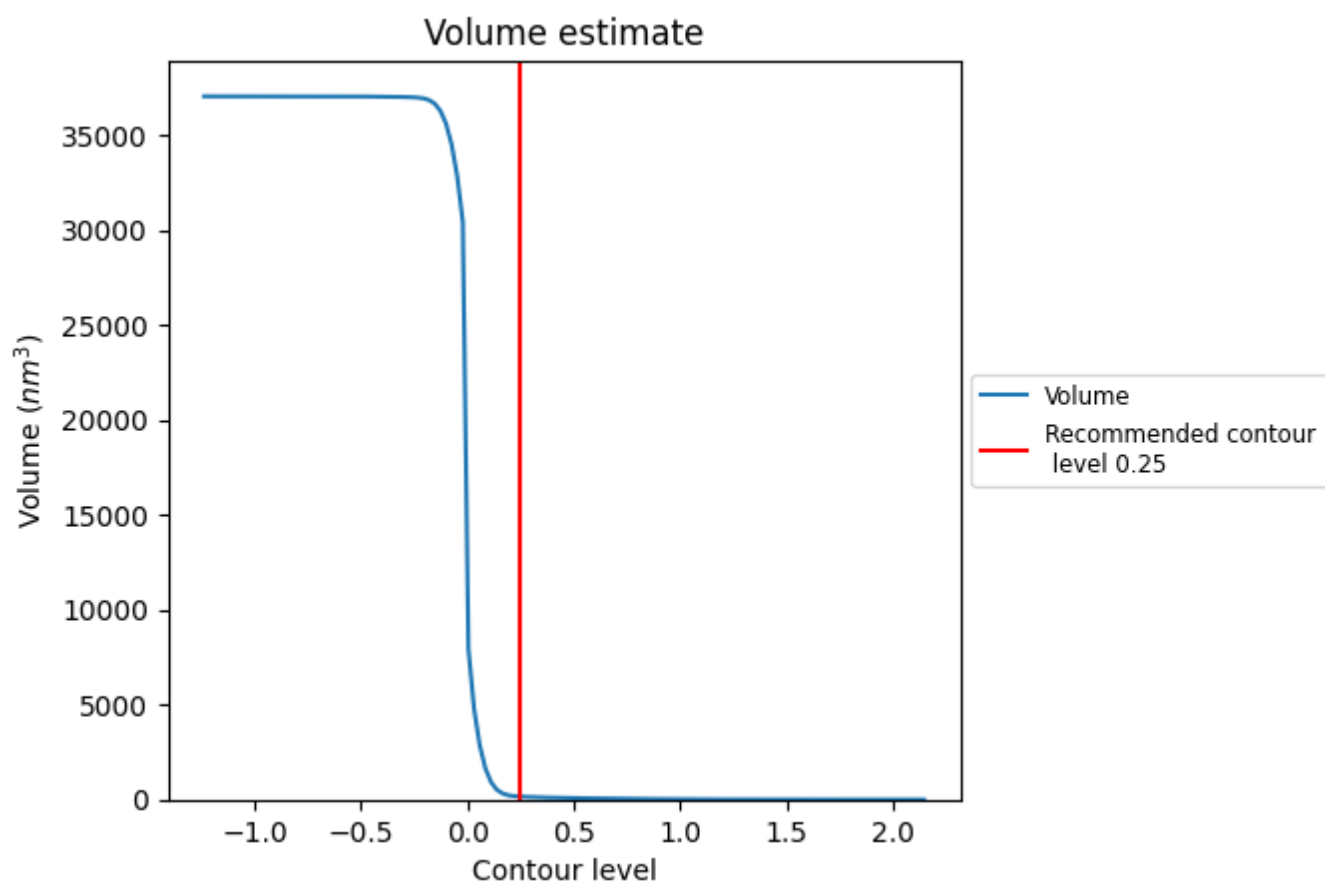
This section contains the results of statistical analysis of the map.

### 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](#)

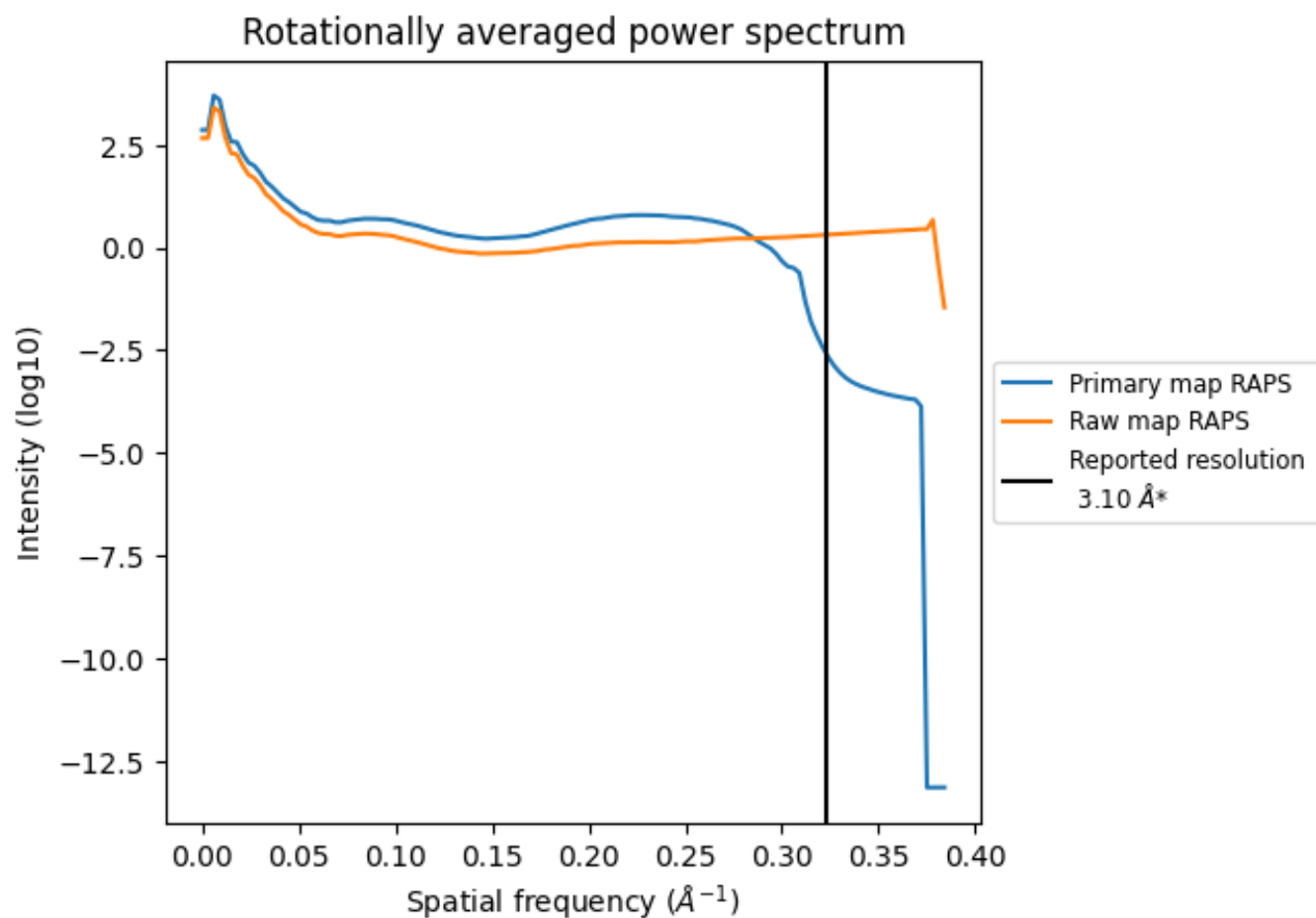


The volume at the recommended contour level is 156 nm<sup>3</sup>; this corresponds to an approximate mass of 141 kDa.

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 ⓘ

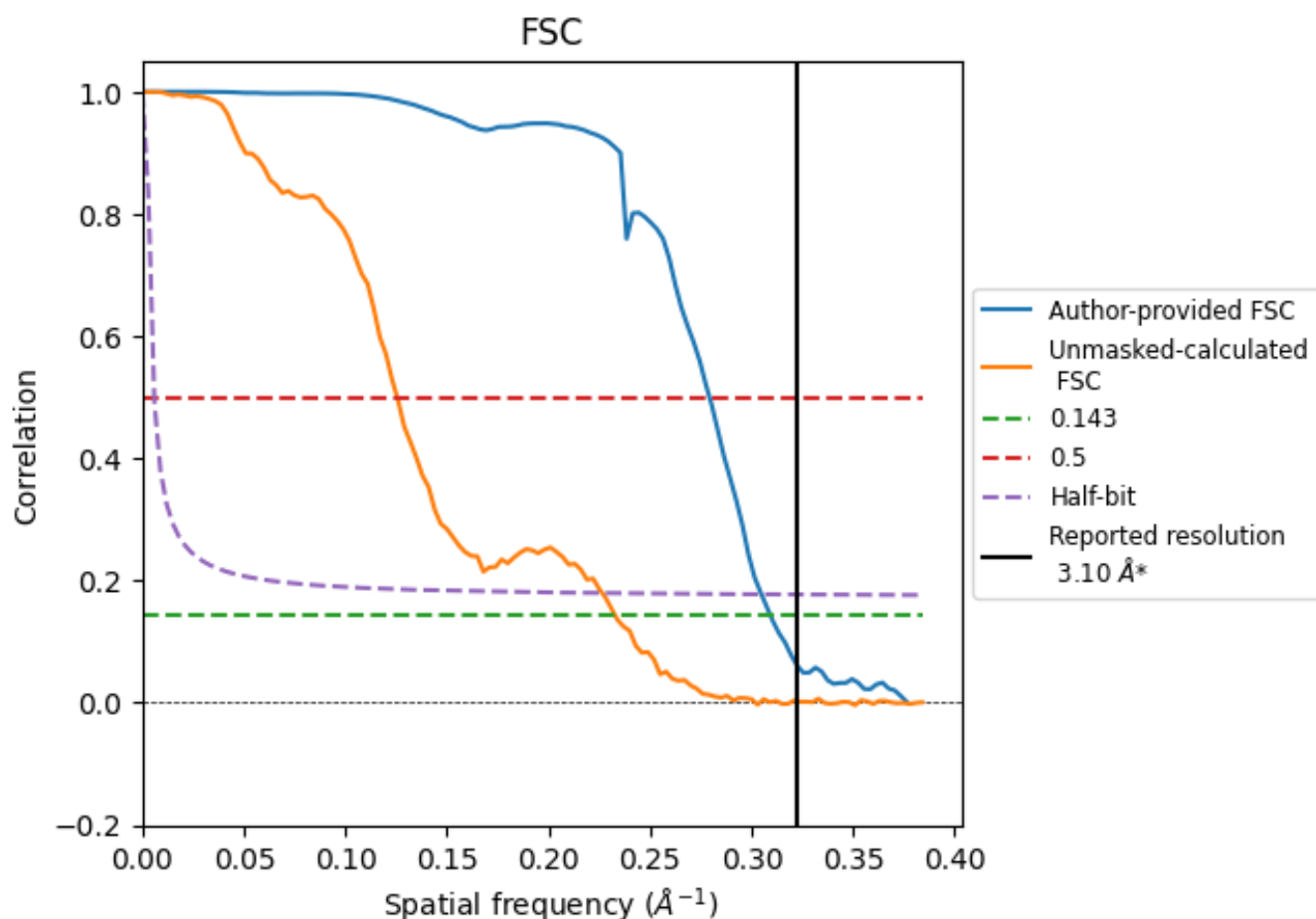


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [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  $0.323 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

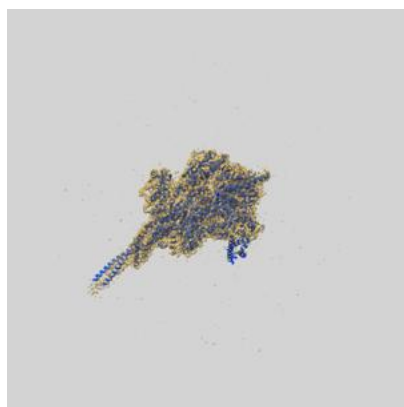
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.23	3.58	3.28
Unmasked-calculated*	4.30	7.97	4.42

\*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 4.30 differs from the reported value 3.1 by more than 10 %

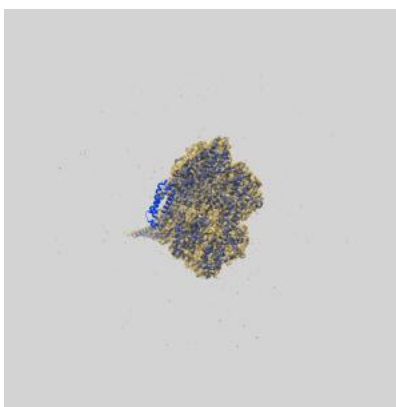
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44703 and PDB model 9BMM. Per-residue inclusion information can be found in section [3](#) on page [5](#).

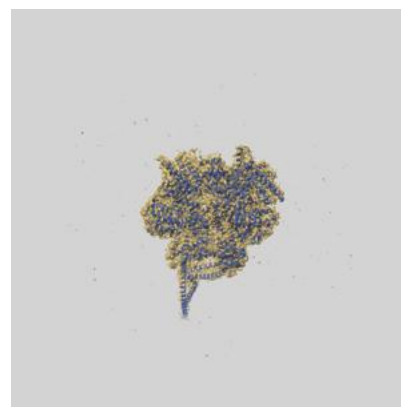
### 9.1 Map-model overlay [i](#)



X



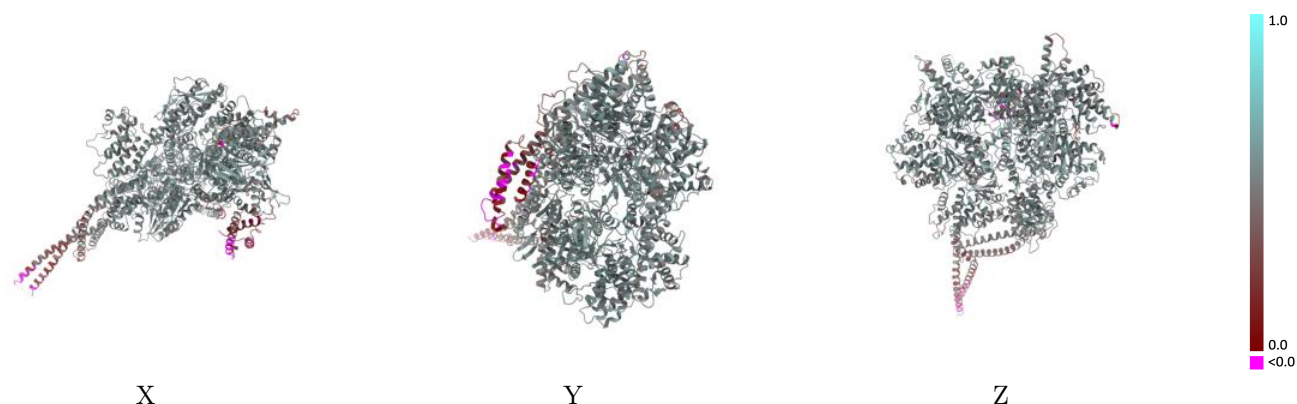
Y



Z

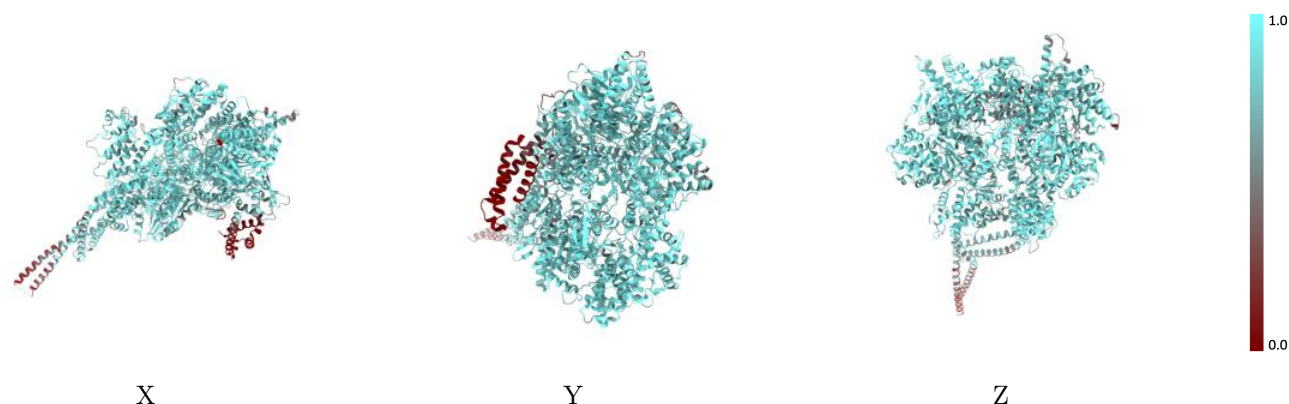
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



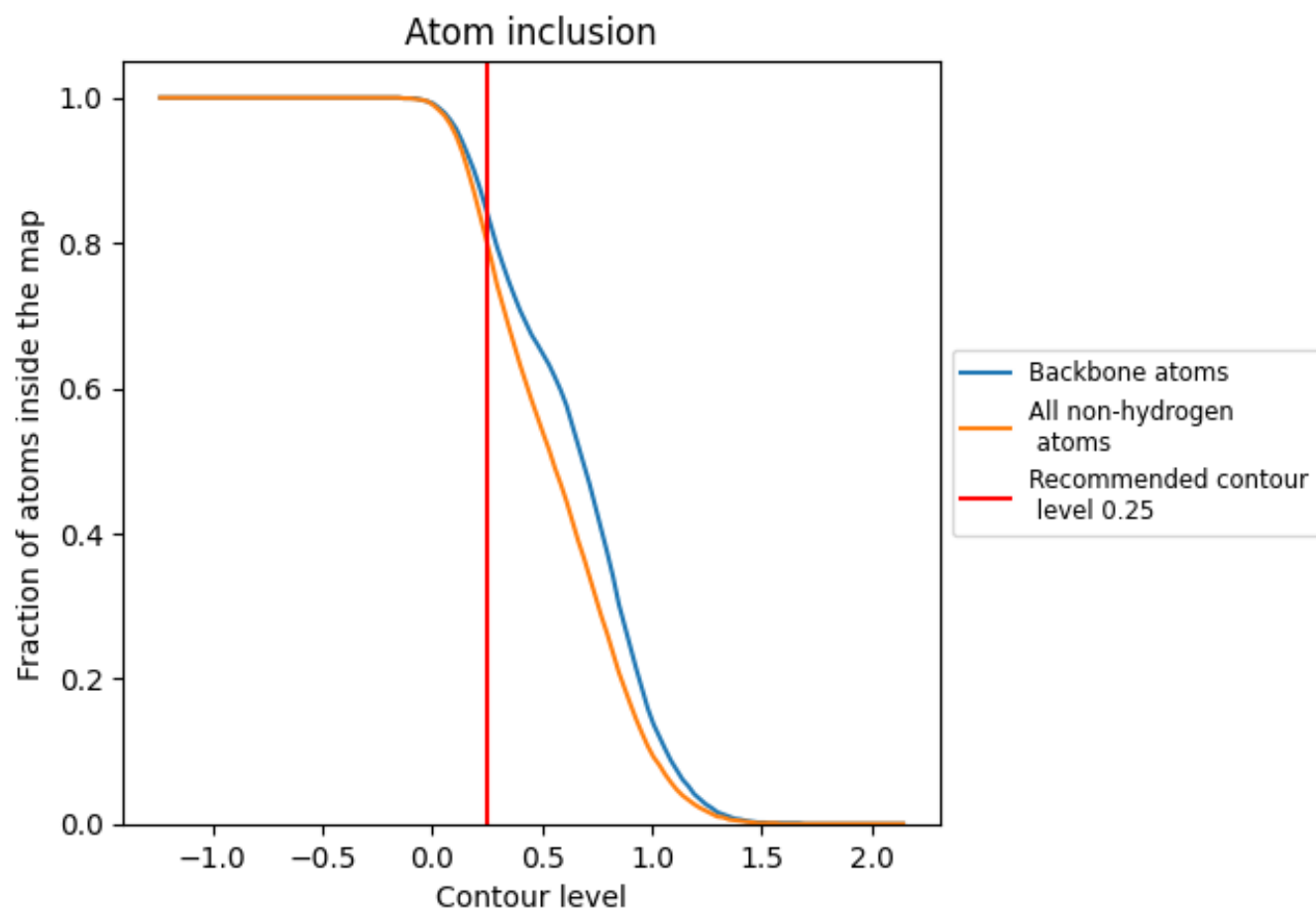
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8000	<div><div></div></div> 0.4970
A	<div><div></div></div> 0.8000	<div><div></div></div> 0.4970

