



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 11:12 AM EDT

PDB ID : 9DH7 / pdb\_00009dh7  
EMDB ID : EMD-46858  
Title : State-4 of the motor domain from full-length human dynein-1 in 5mM  
AMPPNP with 5mM Mg<sup>2+</sup>  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 3.40 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.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.42

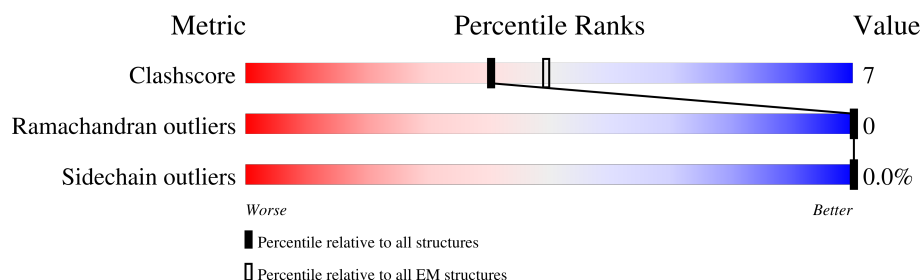
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	

## 2 Entry composition [i](#)

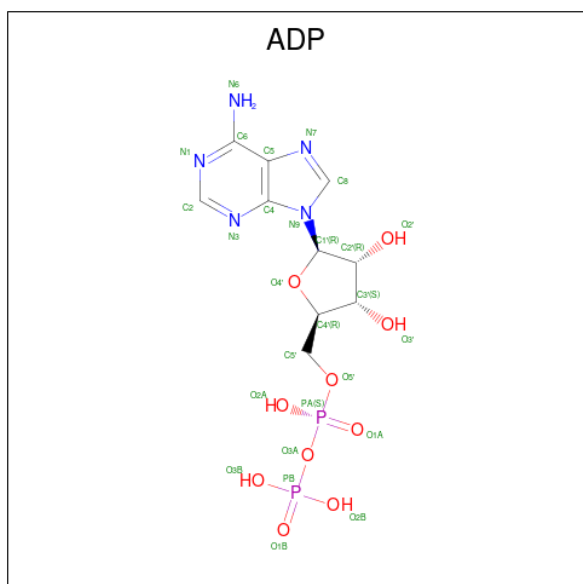
There are 4 unique types of molecules in this entry. The entry contains 23020 atoms, of which 0 are hydrogens and 0 are deuteriums.

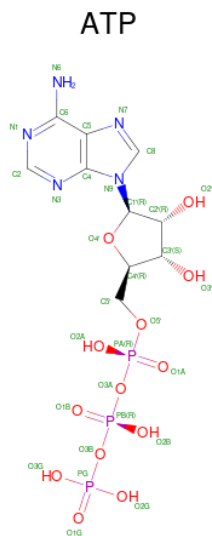
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2857	Total	C	N	O	S	0	0
			22907	14584	3957	4253	113		

- 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
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- 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





D3668	L3547	A3452	MET	V3212	L2905	V2648	Y2617	Q2346	E2188
L3671	L3563	V3453	VAL	D3213	F2912	D2664	T2521	D2347	D2195
T3681	D3557	L3454	TRP	Q3214	N2913	D2670	T2528	L2348	E2198
D3682	R3561	I3455	ILE	V3215	E2914	D2671	D2536	L2382	T2213
R3683	R3561	A3456	ALA	E3216	L2920	Q2677	E2538	D2388	T2216
D3691	P3568	A3457	GLN	R3217	L2925	T2676	D2537	GLU	GLY
L3692	A3569	Q3458	LEU	L3218	L2933	Q2677	E2538	GLY	L2220
C3693	D3570	A3460	ASN	R3219	L2933	V2701	W2548	ASP	W2221
S3694	A3461	A3461	TYR	R3220	L2933	E2704	W2548	GLU	L2224
R3695	I3461	A3462	ALA	D3221	A2951	E2704	K2551	ALA	G2224
L3708	K3462	A3463	GLU	L3222	L2956	D2717	T2555	ARG	R2230
V3716	A3463	A3464	ASN	R3223	K2962	R2726	E2556	ARG	S2231
D3725	A3464	A3465	PHE	I3224	R2962	V2731	E2557	ARG	W2232
D3725	A3465	A3466	ILE	K3225	R2965	P2732	A2564	GLY	K2233
R3728	A3466	A3467	THR	Q3226	K2966	P2732	A2564	LYS	K2234
F3738	A3467	A3468	ILE	Q3227	Y2967	Y2738	V2567	GLU	E2242
Q3739	A3468	A3469	ILE	E3228	E2974	I2747	V2568	GLU	R2243
L3740	A3469	A3470	ASN	E3229	D2975	F2751	P2570	GLY	E2248
R3743	A3470	K3471	GLN	L3230	R2976	R2787	L2571	GLU	K2257
Q3744	K3471	R3474	LYS	K3232	R2978	F2784	D2573	ALA	V2262
Q3745	L3474	S3475	ILE	N3233	E2996	Y2794	V2574	ALA	D2269
E3746	A3477	S3476	LYS	A3234	L3000	W2802	R2576	Q2414	P2270
E3755	L3478	L3478	ALA	A3236	D3001	V2803	R2577	D2418	R2273
V3756	L3478	S3481	ARG	N3237	S3002	V2804	E2578	A2419	S2290
K3757	L3482	L3482	VAL	K3239	L3005	E2808	L2581	A2420	L2295
R3759	R3488	R3488	GLN	L3240	L3005	E2808	P2590	T2421	K2296
L3760	K3491	K3491	LYS	K3241	N3014	E2814	L2593	I2422	K2297
D3762	E3494	E3494	ASN	LYS	G3015	T2815	P2596	V2433	D2304
D3763	T3495	T3495	VAL	VAL	E3016	L2816	T2596	L2437	G2305
D3764	F3496	F3496	ASN	ASP	V3017	P2817	T2604	R2451	D2306
T3765	K3497	K3497	PRO	GLN	F3021	V2818	S2607	S2457	V2307
I3766	N3498	N3498	ALA	ALA	L3020	E2819	L2620	M2461	D2308
K3774	Q3499	Q3499	VAL	GLU	D3024	G2820	N2621	A2465	E2310
R3775	M3500	M3500	TYR	ALA	L3029	A2829	T2627	F2479	V2312
K3777	I3503	I3503	GLU	LYS	L3029	D2840	T2628	E2487	D2321
R3782	S3510	S3510	ILE	LYS	L3042	R2843	P2629	Y2493	R2332
K3783	Y3516	Y3516	VAL	VAL	M3043	L2855	T2634	L2498	N2338
V3784	A3517	A3517	ASN	ILE	H3047	R2863	R2642	R2498	W2342
E3785	R3517	R3517	ARG	GLN	E3048	E2864	R2643	R2507	F2343
R3559	D3521	D3521	LEU	GLN	Y3051	L2872	N2646		
V3660	Q3522	Q3522	ALA	GLN	R3060		G2647		
L3664	Q3523	Q3523	CYS	LEU					
G3665	H3524	H3524	GLY	LEU					
D3666	R3525	R3525	GLU	LYS					
Q3667	H3535	H3535	PRO	VAL					
	R3544	R3544	VAL	ILE					
	T3545	T3545	VAL	ILE					
	D3546	D3546	VAL	ILE					



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20077	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	1.167	Depositor
Minimum map value	-0.523	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	0.27	0/23391	0.48	0/31705

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 [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	22907	0	22979	311	0
2	A	81	0	36	3	0
3	A	31	0	12	2	0
4	A	1	0	0	0	0
All	All	23020	0	23027	311	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 7.

The worst 5 of 311 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:3557:ASP:OD1	1:A:3743:ARG:NH1	2.22	0.73
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.71	0.73
1:A:4225:ASP:O	1:A:4228:LYS:NZ	2.22	0.73
1:A:4267:THR:HG23	1:A:4633:ARG:HD2	1.71	0.71
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.24	0.71

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	2849/4646 (61%)	2808 (99%)	41 (1%)	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	2530/4125 (61%)	2529 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3607	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1856	GLN
1	A	1985	HIS
1	A	2621	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	4701	-	24,29,29	0.74	0	29,45,45	0.75	1 (3%)
2	ADP	A	4703	-	24,29,29	0.72	0	29,45,45	0.73	1 (3%)
3	ATP	A	4702	4	28,33,33	0.74	0	34,52,52	0.79	1 (2%)
2	ADP	A	4704	-	24,29,29	0.75	0	29,45,45	0.74	1 (3%)

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	4701	-	-	1/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	1/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C6-N6	2.30	123.82	120.31
2	A	4704	ADP	C5-C6-N6	2.29	123.81	120.31
2	A	4701	ADP	C5-C6-N6	2.28	123.78	120.31
3	A	4702	ATP	C5-C6-N6	2.25	123.73	120.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	O4'-C4'-C5'-O5'

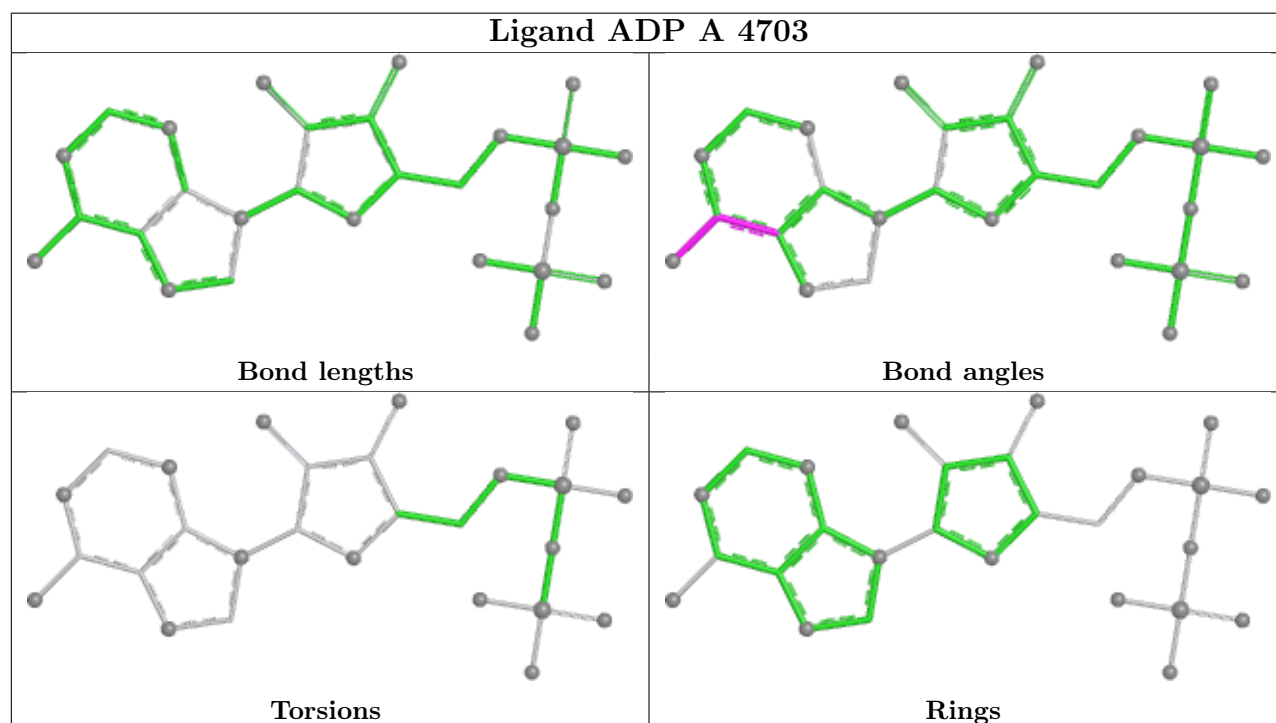
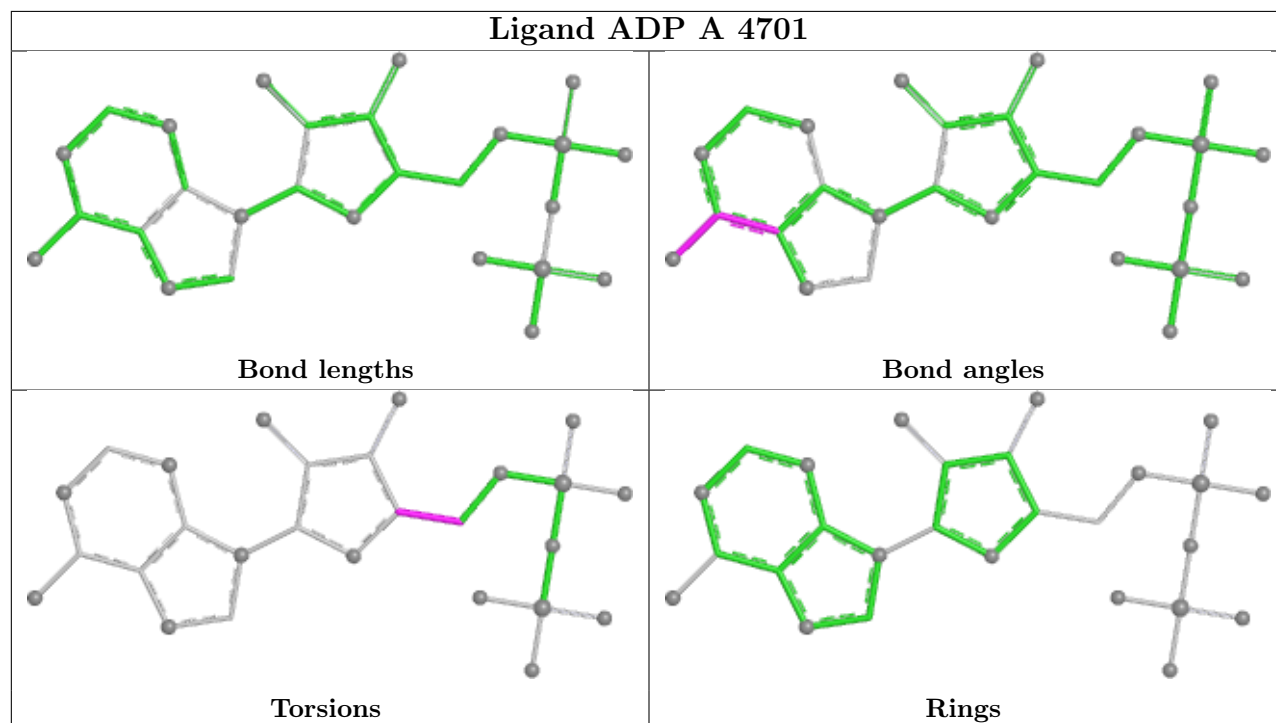
There are no ring outliers.

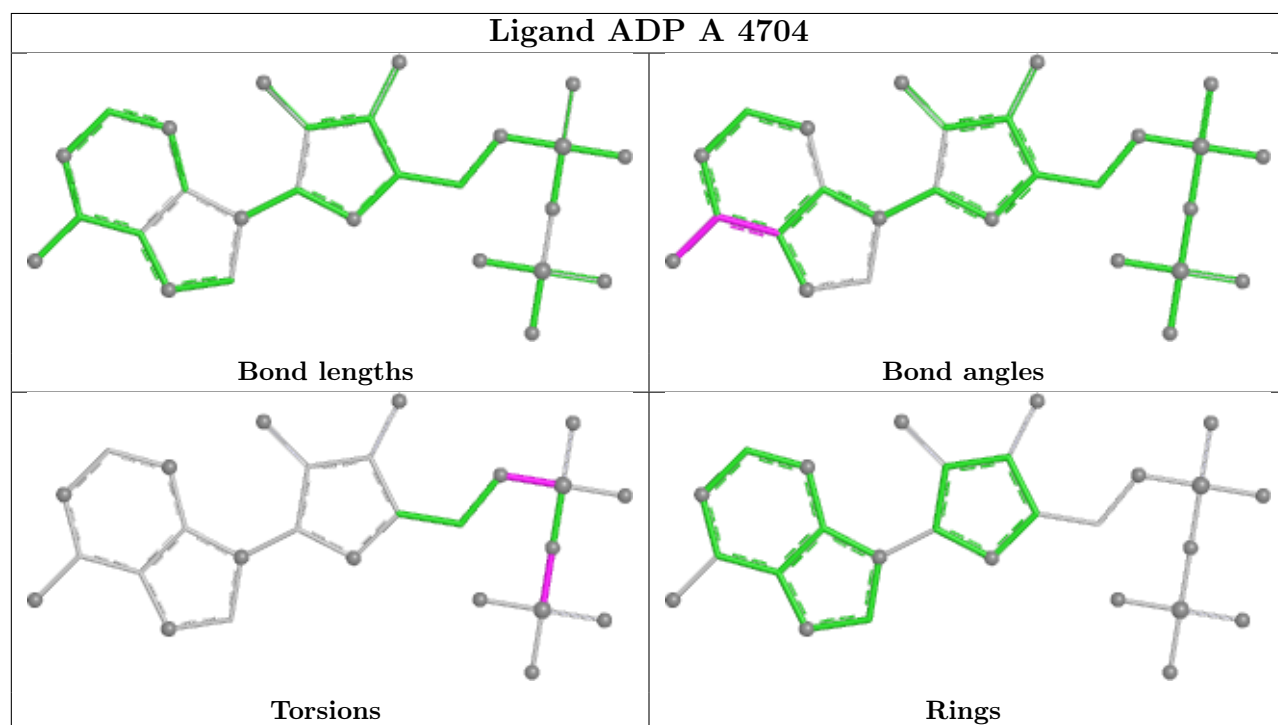
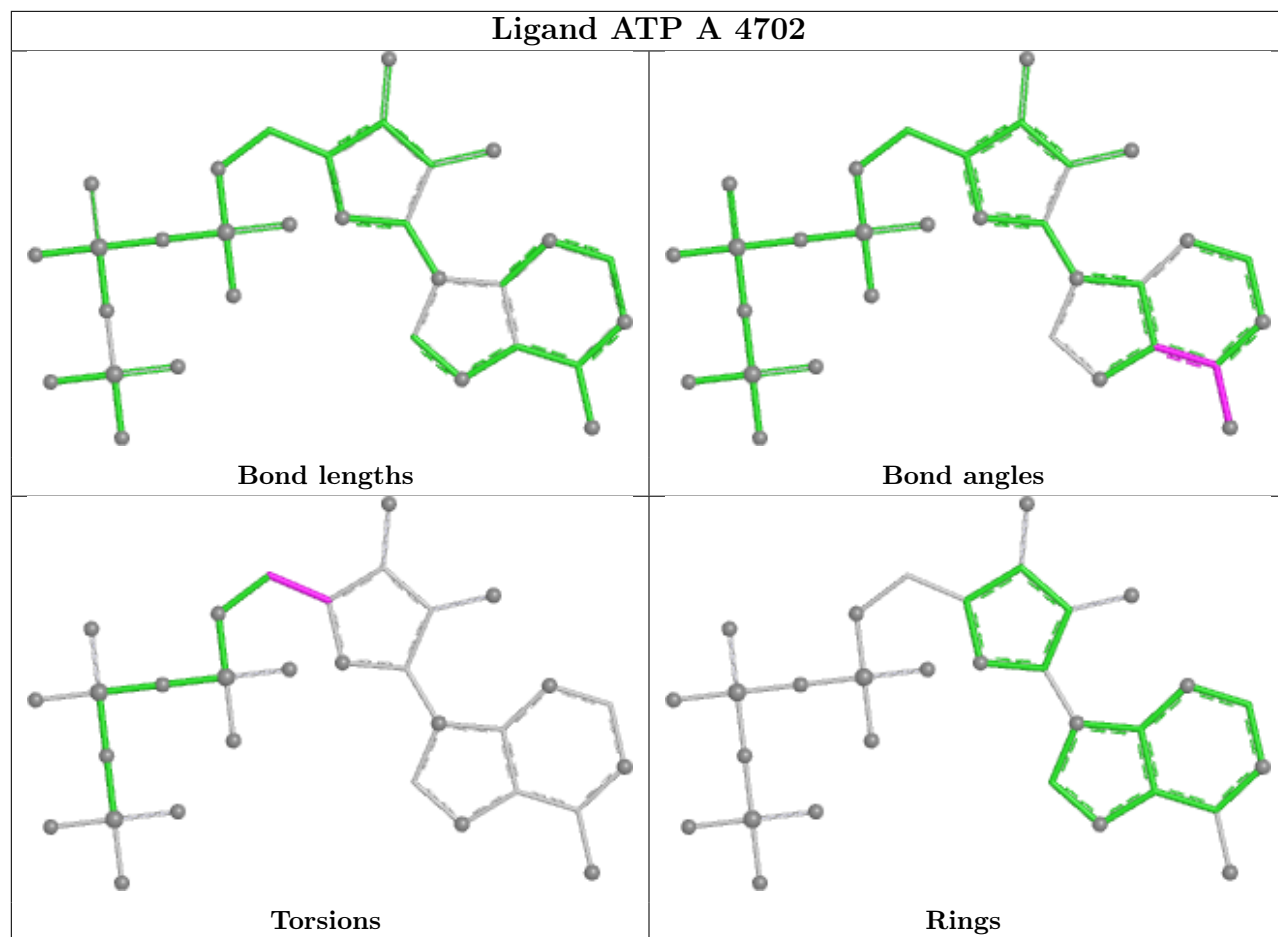
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	0
3	A	4702	ATP	2	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.

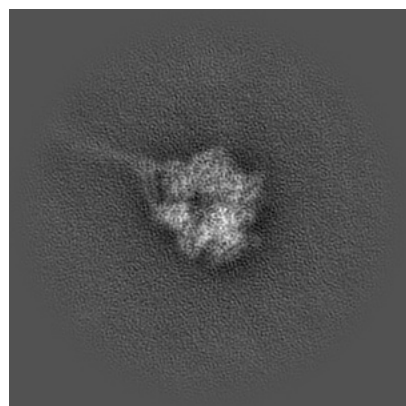
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46858. These allow visual inspection of the internal detail of the map and identification of artifacts.

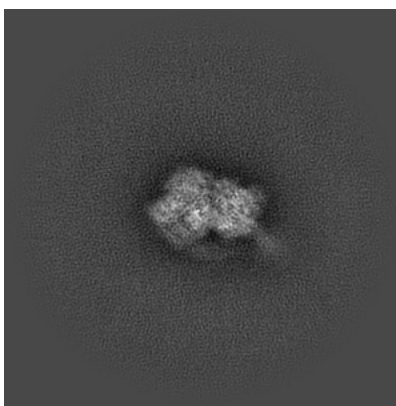
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

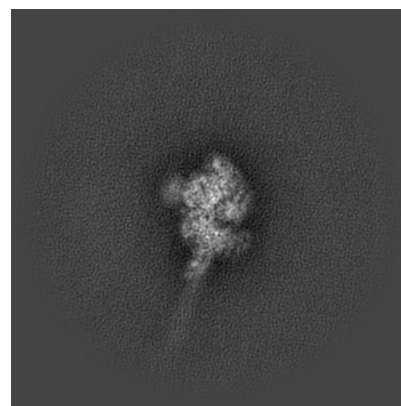
#### 6.1.1 Primary map



X

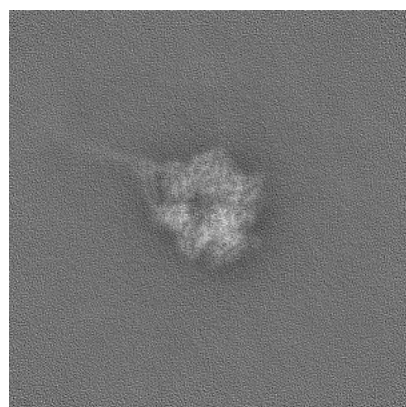


Y

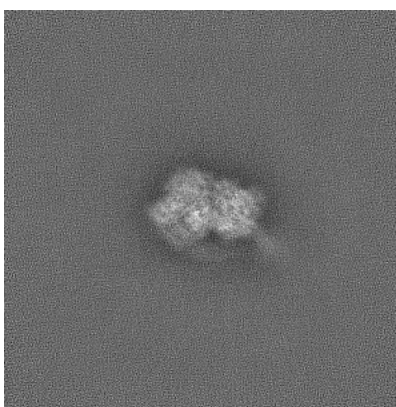


Z

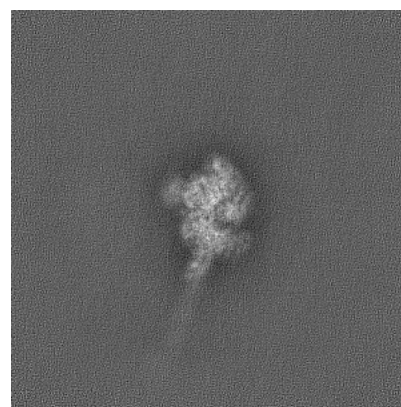
#### 6.1.2 Raw map



X



Y

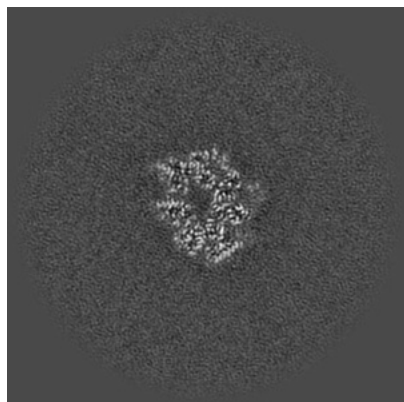


Z

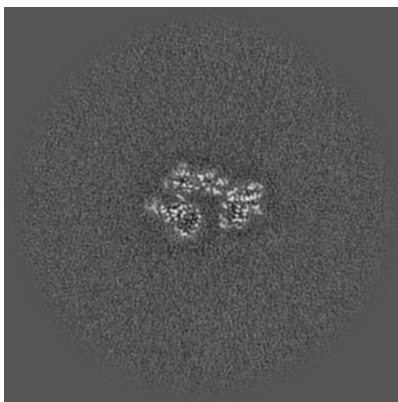
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

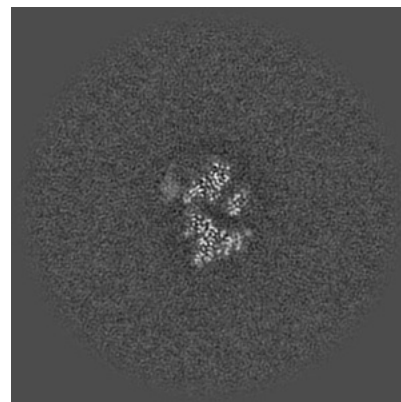
### 6.2.1 Primary map



X Index: 192

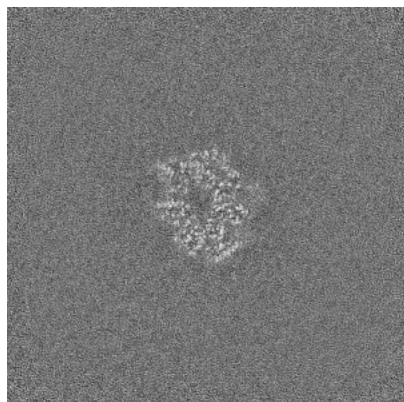


Y Index: 192

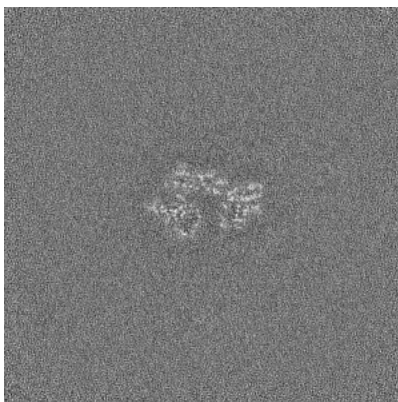


Z Index: 192

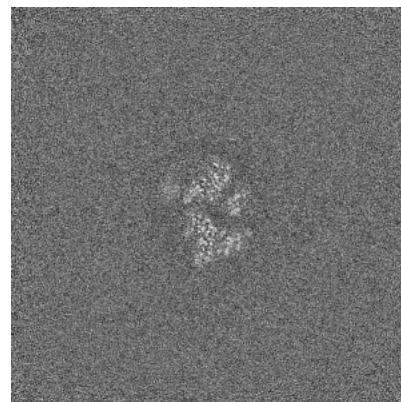
### 6.2.2 Raw map



X Index: 192



Y Index: 192

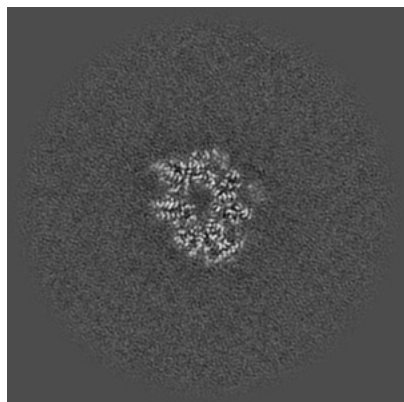


Z Index: 192

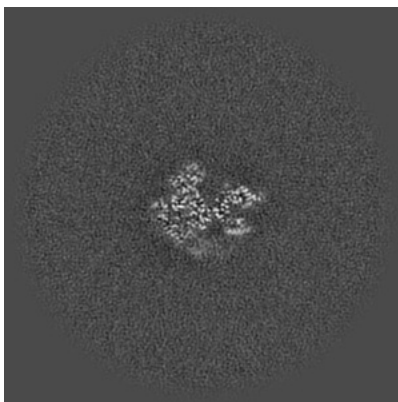
The images above show central slices of the map in three orthogonal directions.

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

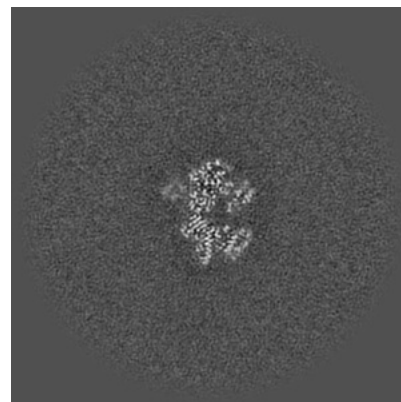
### 6.3.1 Primary map



X Index: 191

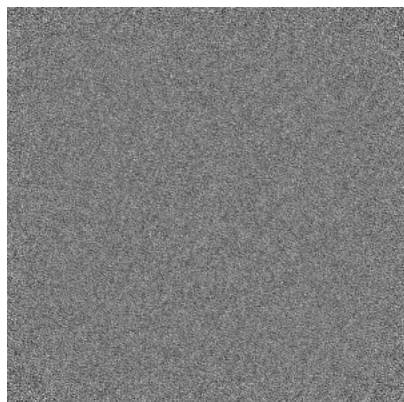


Y Index: 206

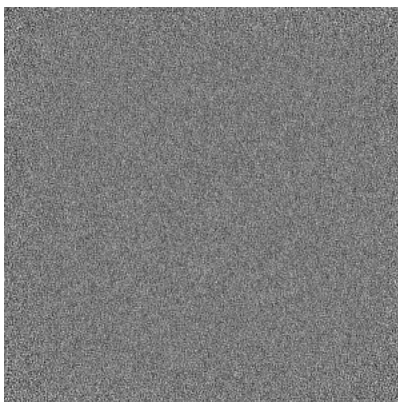


Z Index: 184

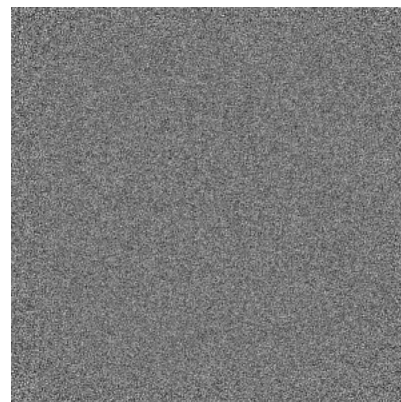
### 6.3.2 Raw map



X Index: 0



Y Index: 0

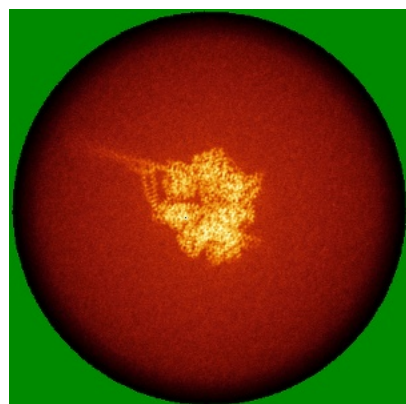


Z Index: 0

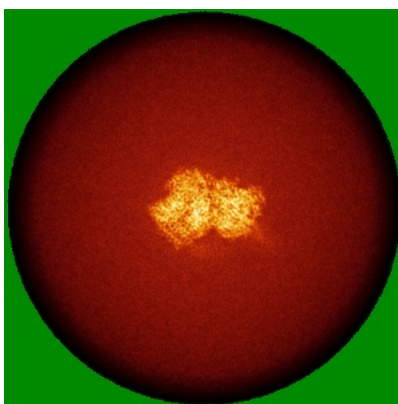
The images above show the largest variance slices of the map in three orthogonal directions.

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

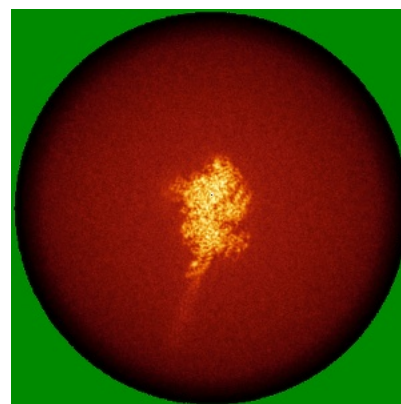
### 6.4.1 Primary map



X

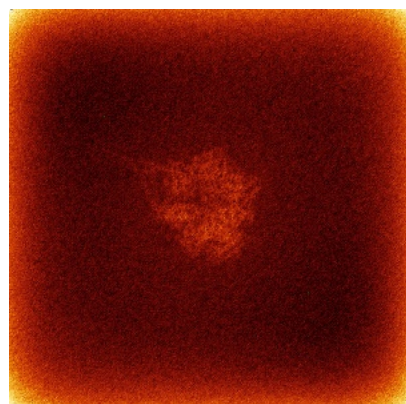


Y

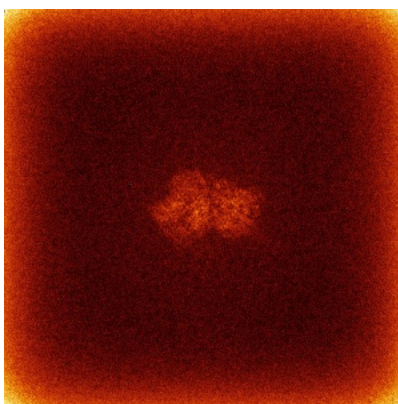


Z

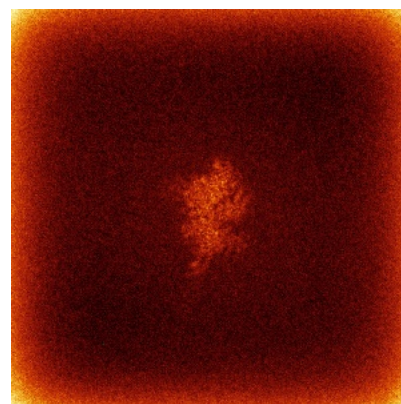
### 6.4.2 Raw map



X



Y

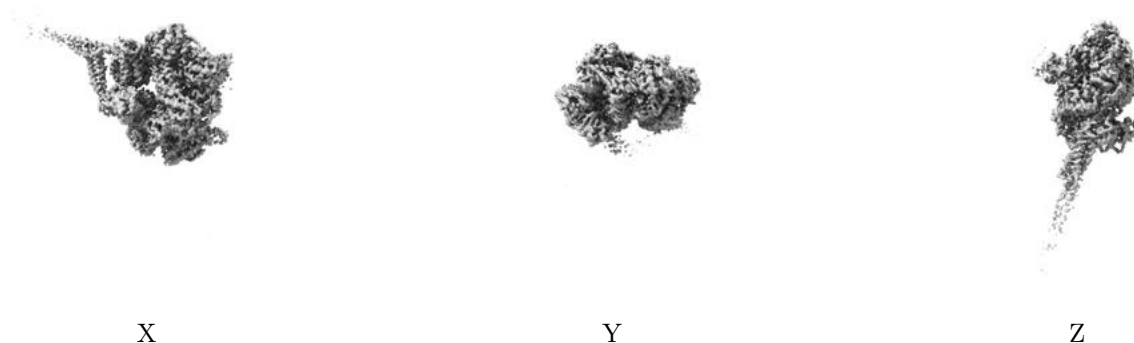


Z

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.

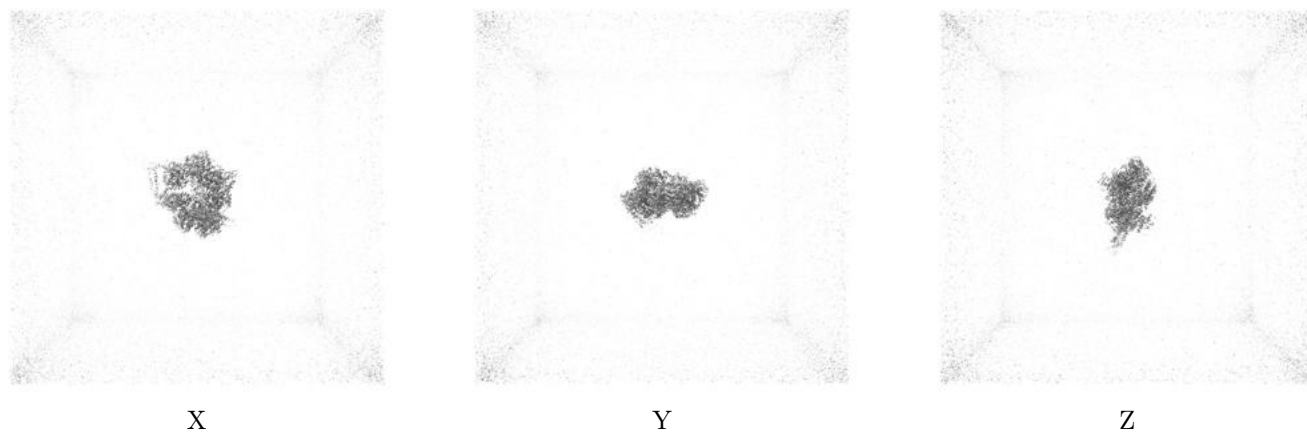
## 6.5 Orthogonal surface views [i](#)

### 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.

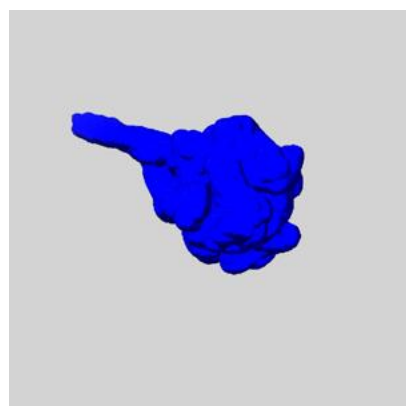
## 6.6 Mask visualisation [i](#)

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

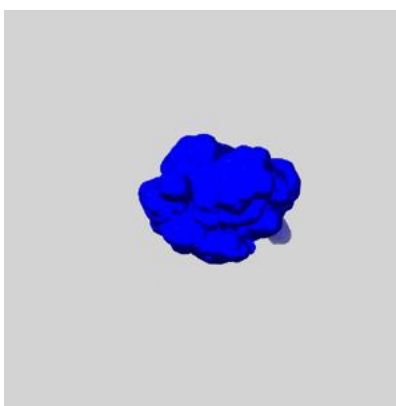
A mask typically either:

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

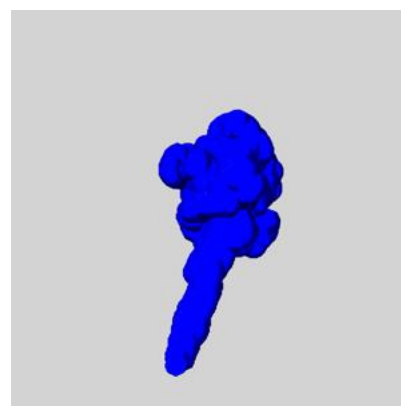
### 6.6.1 emd\_46858\_msk\_1.map [i](#)



X



Y

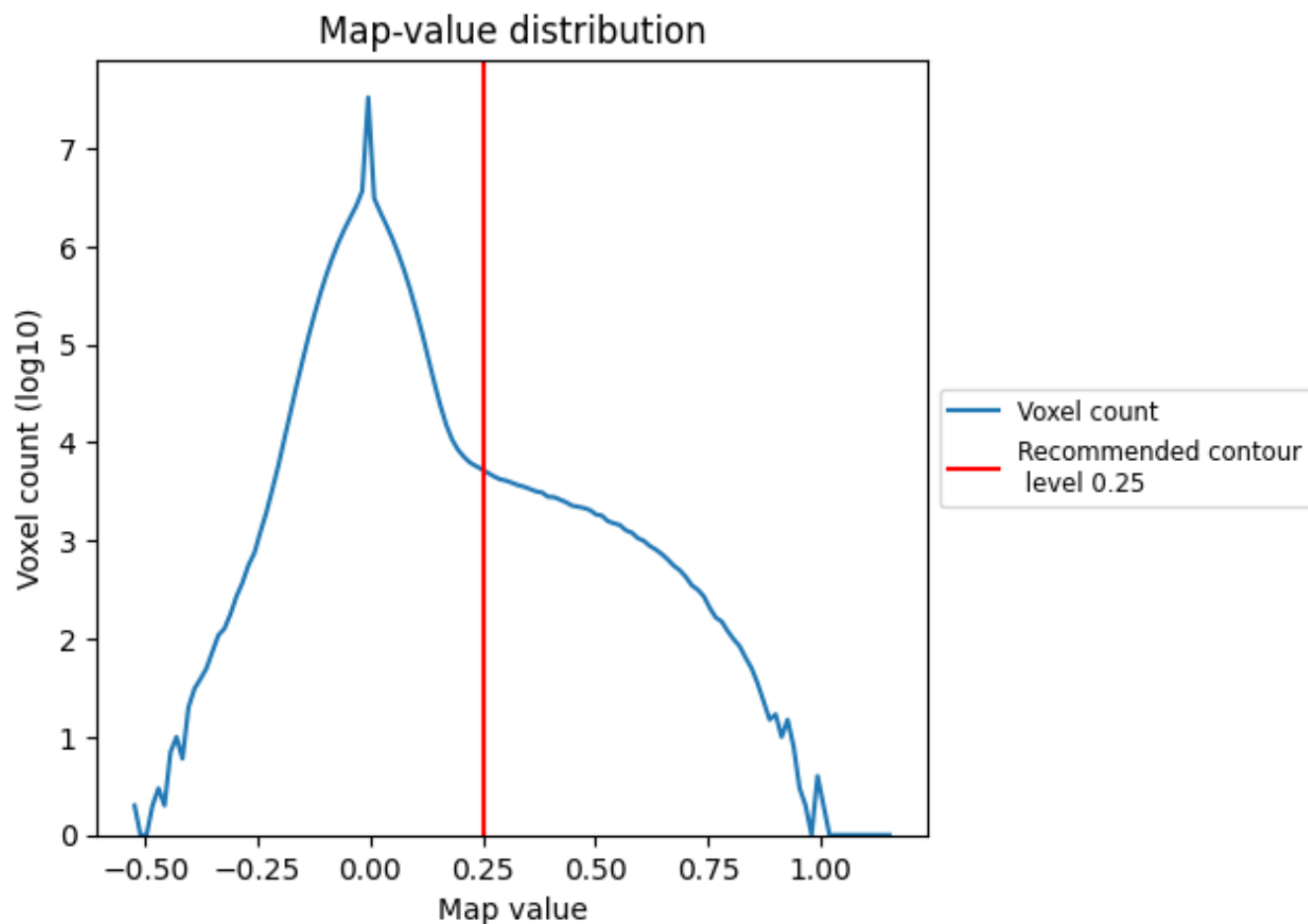


Z

## 7 Map analysis [i](#)

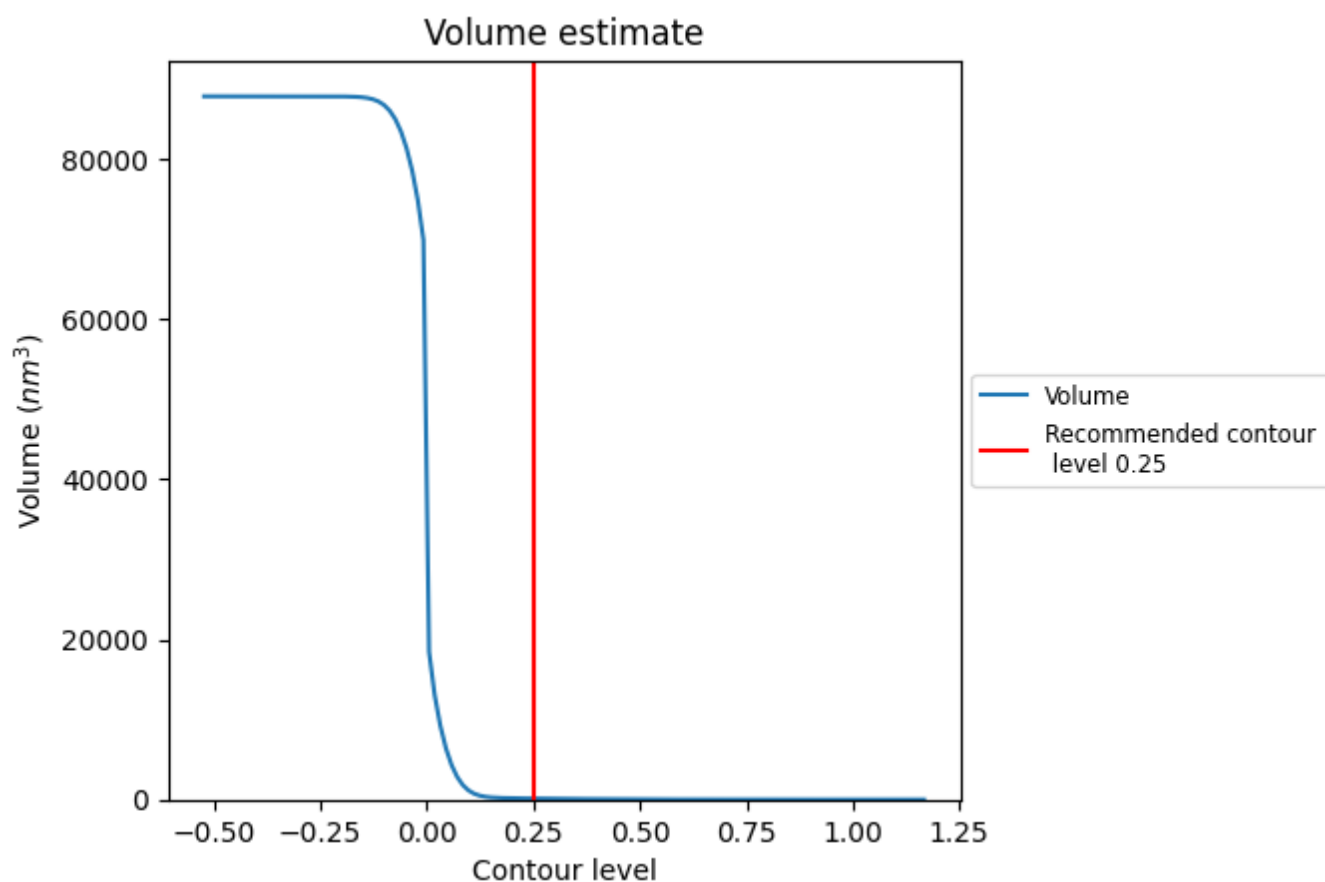
This section contains the results of statistical analysis of the map.

### 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.

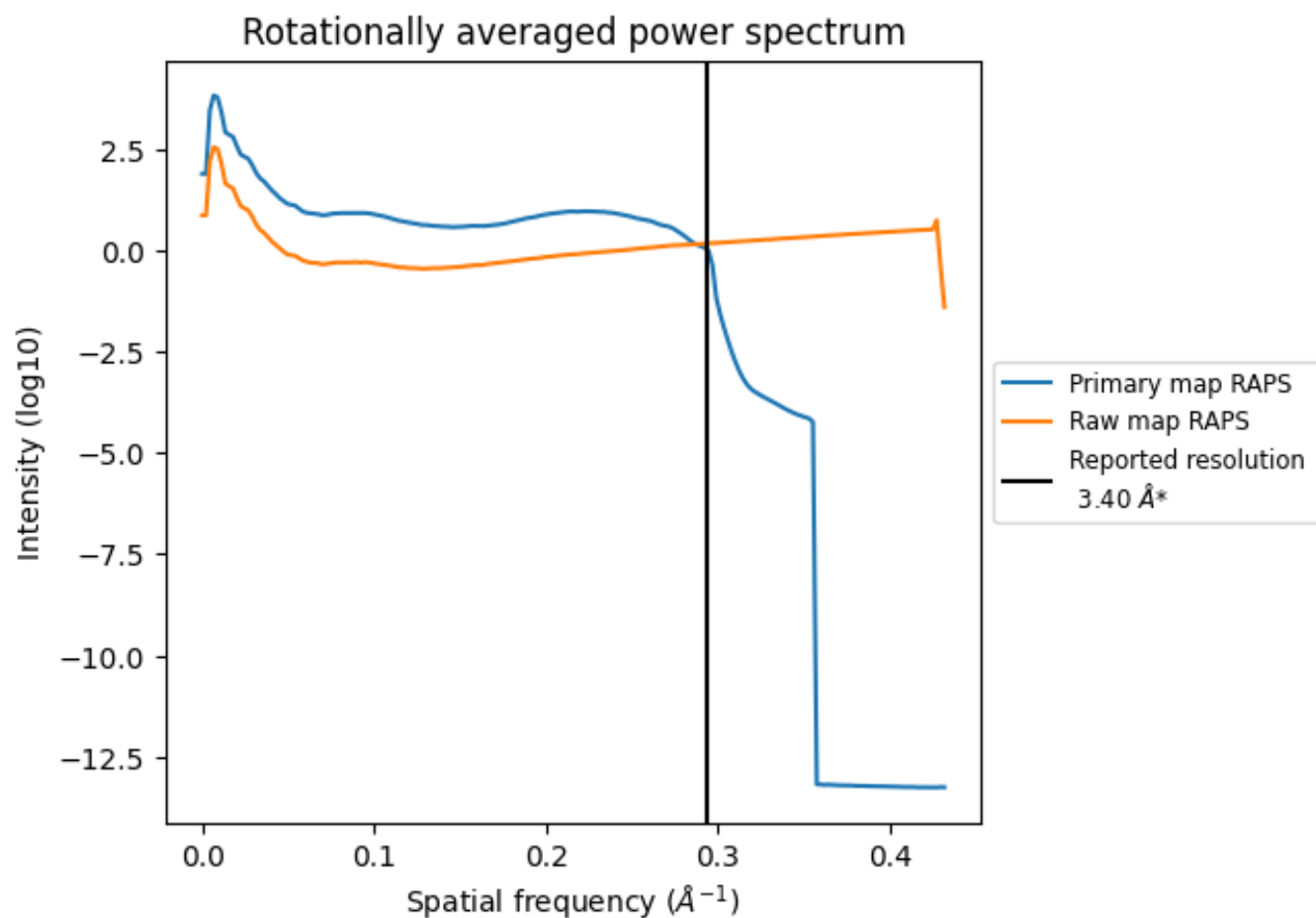
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm<sup>3</sup>; this corresponds to an approximate mass of 115 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 ⓘ

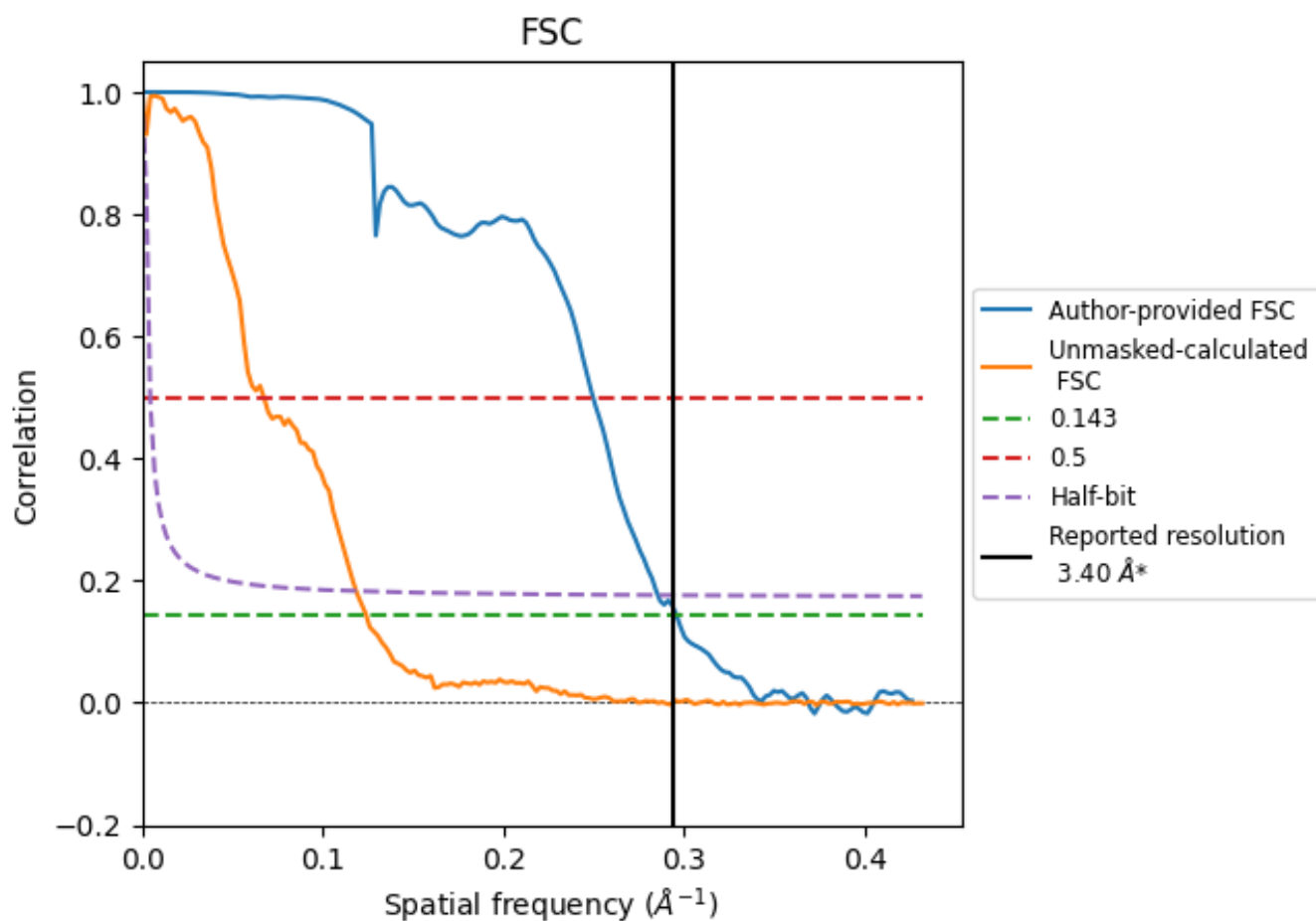


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

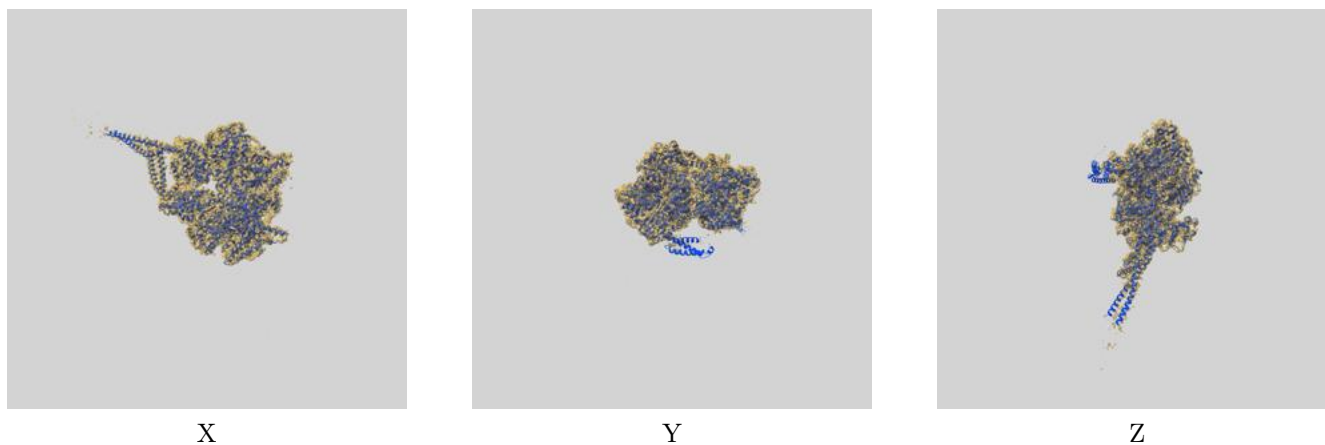
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	4.00	3.50
Unmasked-calculated*	8.06	14.84	8.43

\*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 8.06 differs from the reported value 3.4 by more than 10 %

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

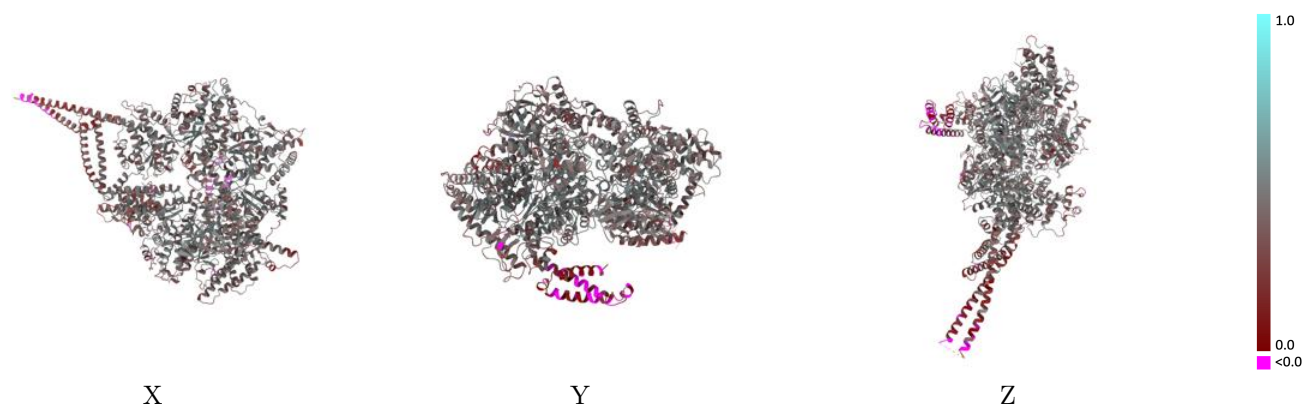
This section contains information regarding the fit between EMDB map EMD-46858 and PDB model 9DH7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



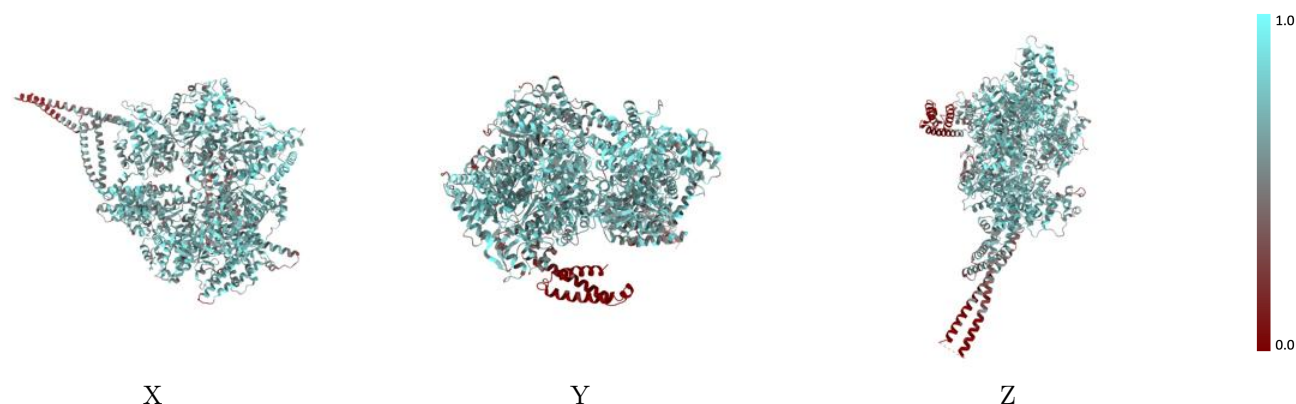
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



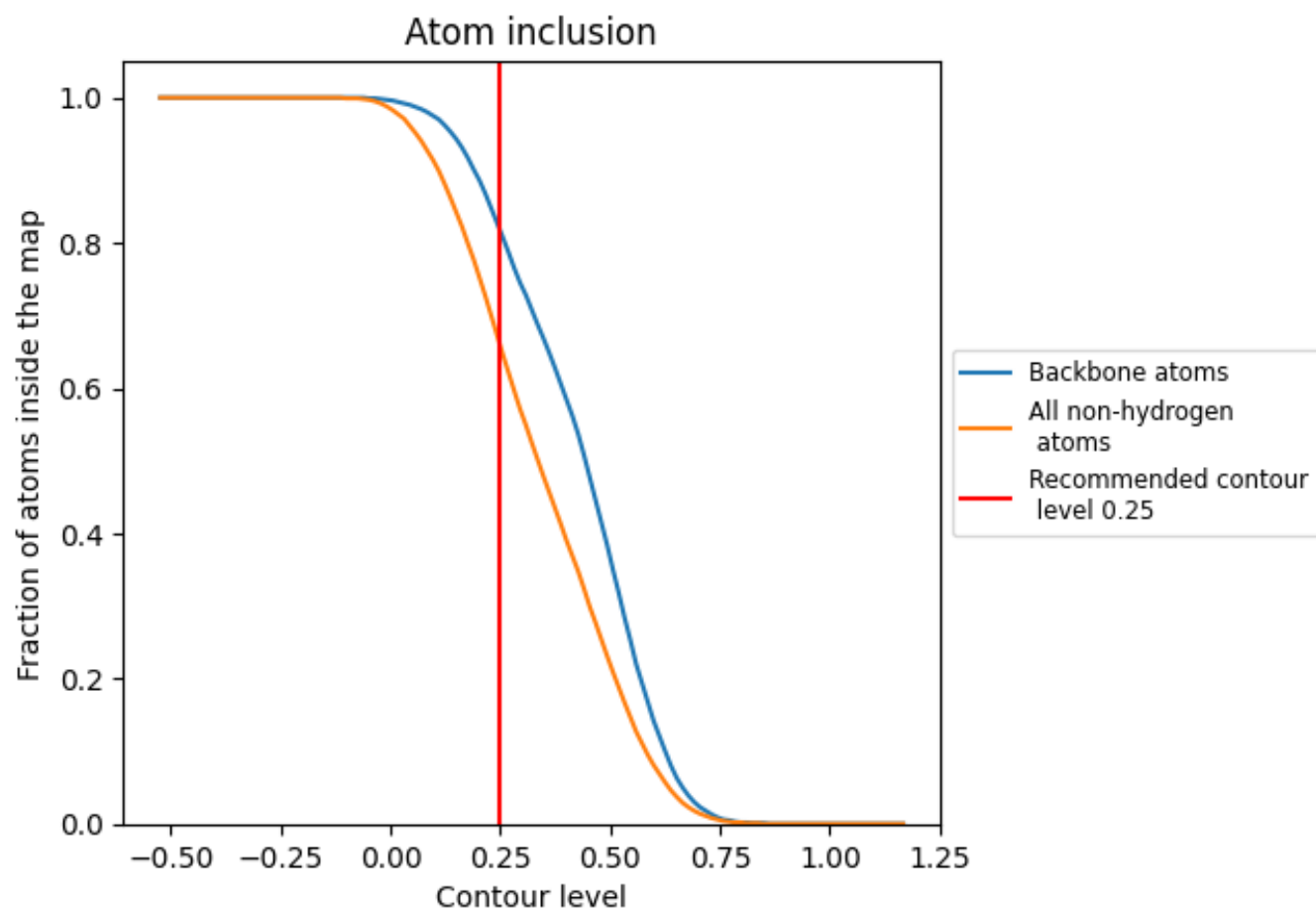
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 82% of all backbone atoms, 66% 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> 0.6580	<div></div> 0.4120
A	<div></div> 0.6580	<div></div> 0.4120

