



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 12:27 PM EDT

PDB ID : 9BMJ / pdb_00009bmj
EMDB ID : EMD-44701
Title : State-1 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

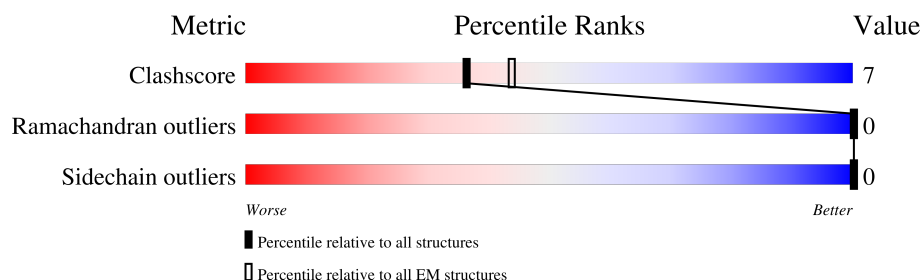
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 ≥ 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 23706 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	2937	23593	15028	4070	4378	117	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).





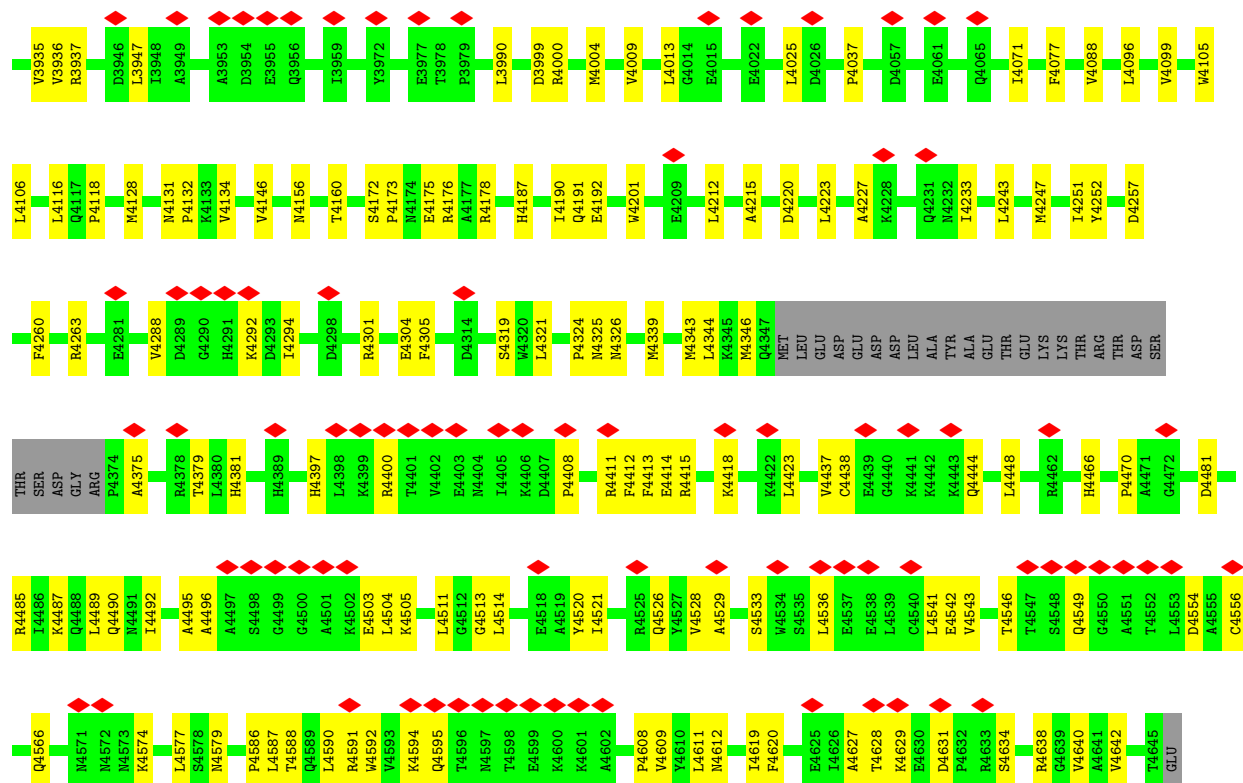
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- 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



Q3830	E3715	S3510	LEU	H3182	E3073	L2920	T2666	Y2517	A2420	V2312
F3831	V3716	Y3516	GLU	L3194	D3077	R2921	N2667	I2518	A2420	E2313
F3832	L3717	A3517	ALA	L3194	D3077	I2922	P2668	I2518	I2422	N2316
L3833	D3723	F3520	ILE	V3203	S3082	L2933	F2708	P2525	N2430	L2319
D3834	V3724	M3524	ARG	L2905	L3085	K2943	C2712	P2527	V2433	V2320
L3835	D3725	R3525	LEU	L3206	L3085	T2944	M2713	T2528	V2433	D2321
Y3836	R3728	R3525	LEU	K3207	C3089	T2945	P2714	A2529	F2441	T2326
V3839	L3731	L3541	GLY	I3208	F3094	A2951	R2726	P2530	E2444	N2342
N3845	N3734	R3544	PRO	K3209	F3094	L2956	R2729	N2531	H2445	F2343
D3862	E3755	T3545	MET	E3210	D3095	L2956	R2729	I2534	I2446	E2344
L3863	V3756	D3546	VAL	T3211	D3096	I2961	H2730	I2534	L2449	L2348
R3870	K3757	T3547	TRP	V3212	S3097	R2965	V2731	E2538	L2452	T2352
V3871	G3758	T3550	ALA	D3213	K3098	K2966	V2732	W2545	R2453	L2353
A3872	R3759	E3551	ILE	V3214	T3099	T2967	V2733	W2548	C2454	V2356
R3873	L3761	L3552	GLN	V3215	E3100	G2969	I2747	A2564	S2457	C2359
G3874	D3762	L3553	LEU	E3216	Q3104	G2969	R2757	P2565	W2461	E2360
M3875	D3763	R3559	ASP	E3217	K3107	D2975	R2763	D2566	A2465	R2361
L3876	D3764	S3566	ASP	R3220	N3119	D2975	R2763	V2569	N2468	F2364
D3879	T3765	E3575	LEU	L3221	D3124	D2995	Q2789	L2572	Q2471	V2368
M3885	I3767	E3575	VAL	L3222	Y3125	V2999	Y2792	D2573	D2478	T2374
V3896	L3770	L3580	ARG	K3225	V3129	L3000	W2802	V2574	M2481	L2382
G3897	E3771	R3582	ILE	S3226	D3130	D3001	E2828	V2576	Q2482	D2388
E3898	K3772	R3582	THR	E3228	D3131	S3002	A2828	R2578	I2483	E2389
E3904	L3773	R3585	VAL	E3228	K3132	G3003	E2842	E2578	L2486	GLY
F3905	K3774	T3597	ASN	E3230	L3133	F3004	E2843	E2578	L2486	GLU
Q3906	R3775	T3597	ASN	E3231	P3134	L3005	R2844	L2581	ASP	ALA
L3909	E3779	I3600	ALA	V3231	Q3135	N3009	E2848	L2581	ALA	GLN
G3911	R3782	R3611	LEU	K3232	F3136	N3009	E2848	Q2482	ARG	ARG
N3912	K3783	E3611	GLN	L3233	P3137	N3014	E2848	Q2482	ARG	LYS
E3913	V3784	D3617	LYS	A3234	K3140	V3017	D2851	L2590	LYS	LYS
I3914	E3785	L3634	ASP	A3236	E3141	L3020	T2852	L2591	GLU	ASP
V3915	E3786	V3638	ASP	A3236	K3142	F3021	E2843	L2592	GLU	ALA
L3916	T3787	Y3638	ALA	N3237	I3143	E3022	E2843	L2593	ALA	ALA
S3917	D3788	V3638	LYS	D3238	V3144	M3030	E2848	L2612	ARG	ARG
A3918	I3789	E3652	ASN	K3239	V3148	M3030	E2848	M2615	ARG	ARG
L3919	M3791	D3666	GLN	L3240	F3149	M3030	E2848	L2620	LYS	LYS
S3920	Q3792	T3666	LYS	K3241	L3154	M3030	E2848	P2622	GLU	GLU
T3921	E3795	T3681	ALA	K3242	R3160	M3030	E2848	S2623	ASP	ASP
Q3922	Q3799	L3692	TYR	MET	R3160	M3030	E2848	T2626	GLY	GLY
R3923	C3808	C3693	VAL	VAL	R3160	M3030	E2848	T2626	GLY	GLY
T3924	S3809	S3694	ASN	ASN	R3160	M3030	E2848	T2626	GLY	GLY
Q3925	R3815	V3696	PRO	GLN	R3160	M3030	E2848	T2626	GLY	GLY
G3926	M3815	L3708	SER	GLU	R3160	M3030	E2848	T2626	GLY	GLY
L3927	L3818	Y3825	TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY
T3928	Y3825		TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY
V3929			TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY
E3930			TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY
Q3931			TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY
A3932			TYR	LYS	R3160	M3030	E2848	T2626	GLY	GLY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130832	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	3.246	Depositor
Minimum map value	-1.755	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	555.52, 555.52, 555.52	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3888, 1.3888, 1.3888	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: ATP, MG, ADP

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	0.25	0/24093	0.47	0/32651

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	23593	0	23659	354	0
2	A	81	0	36	2	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	23706	0	23707	354	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 354 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:2220:LEU:HB2	1:A:2342:MET:HG2	1.68	0.75
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.70	0.73
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.72	0.71
1:A:4437:VAL:HG21	1:A:4448:LEU:HD21	1.71	0.71
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.73	0.70

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	2929/4646 (63%)	2881 (98%)	48 (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	2605/4125 (63%)	2605 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1973	GLN
1	A	2707	GLN
1	A	3009	ASN
1	A	3014	ASN
1	A	4397	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	4701	-	24,29,29	0.86	0	29,45,45	1.35	3 (10%)
2	ADP	A	4703	-	24,29,29	0.86	0	29,45,45	1.22	2 (6%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.19	2 (6%)
3	ATP	A	4702	4	28,33,33	0.67	0	34,52,52	0.59	1 (2%)

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	N3-C2-N1	-3.82	123.49	128.67
2	A	4703	ADP	N3-C2-N1	-3.75	123.58	128.67
2	A	4704	ADP	N3-C2-N1	-3.63	123.74	128.67
2	A	4704	ADP	C4-C5-N7	-2.62	106.57	109.34
2	A	4701	ADP	C4-C5-N7	-2.59	106.60	109.34

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'

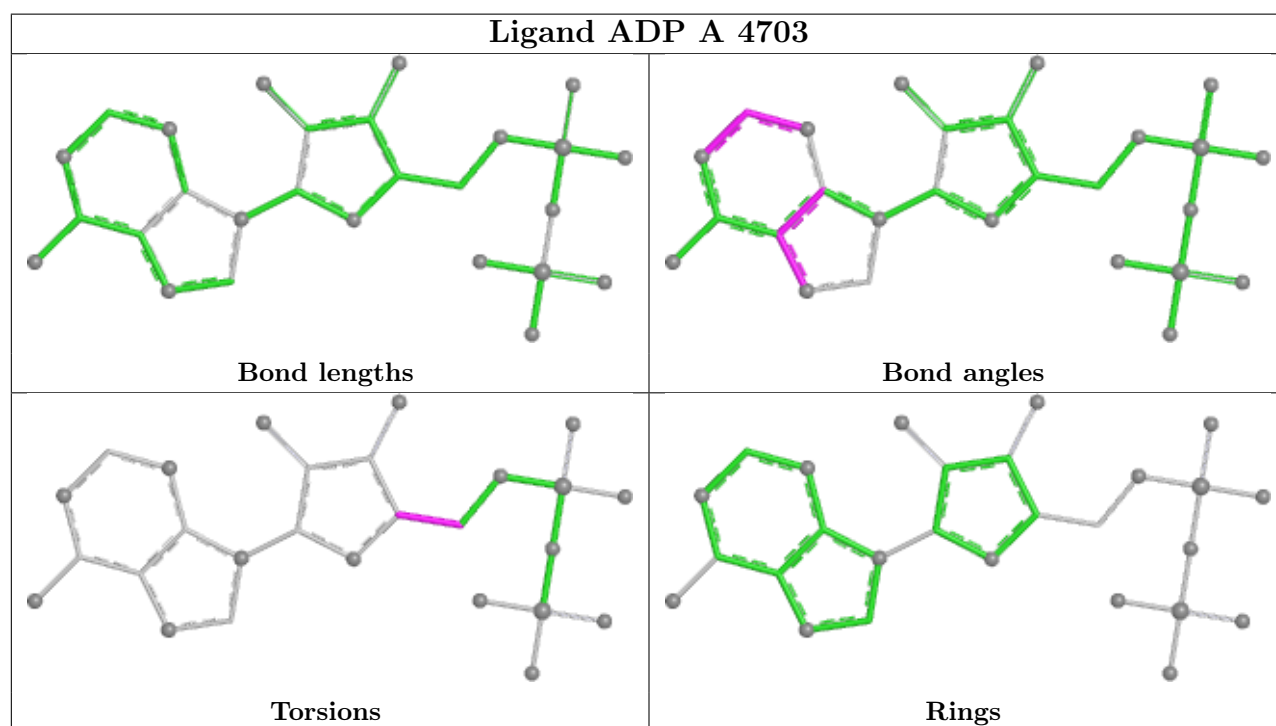
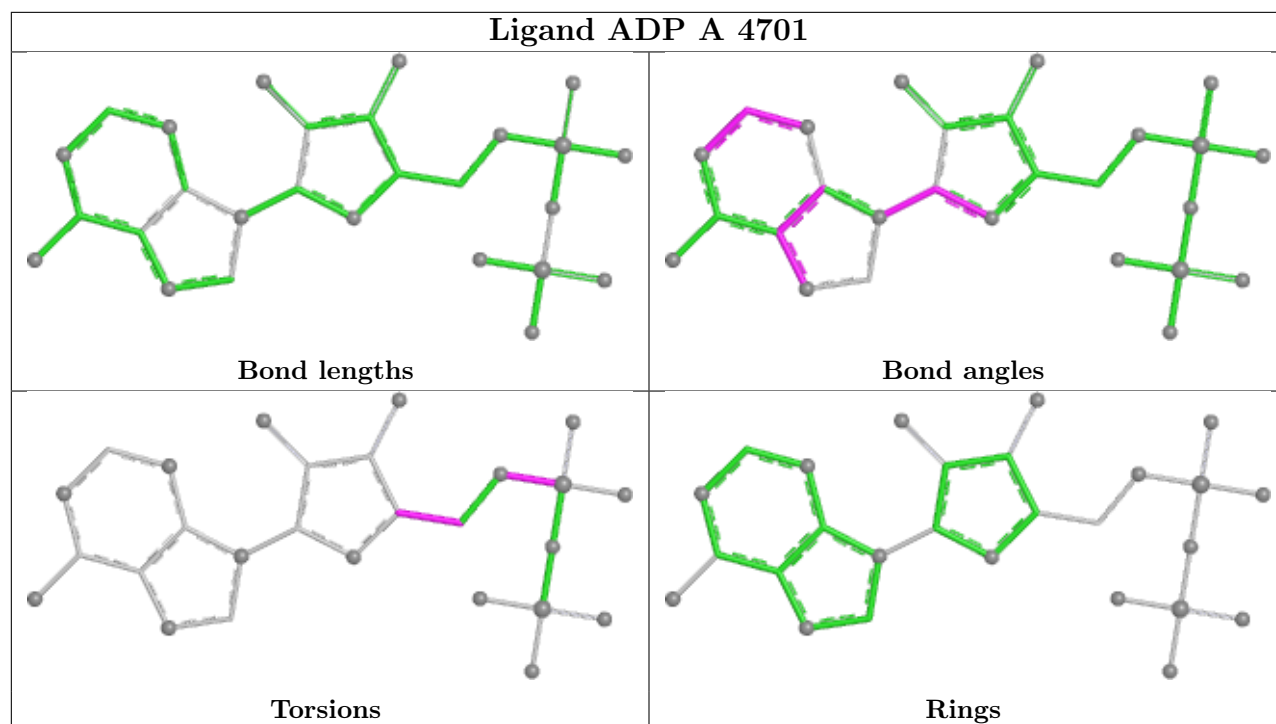
There are no ring outliers.

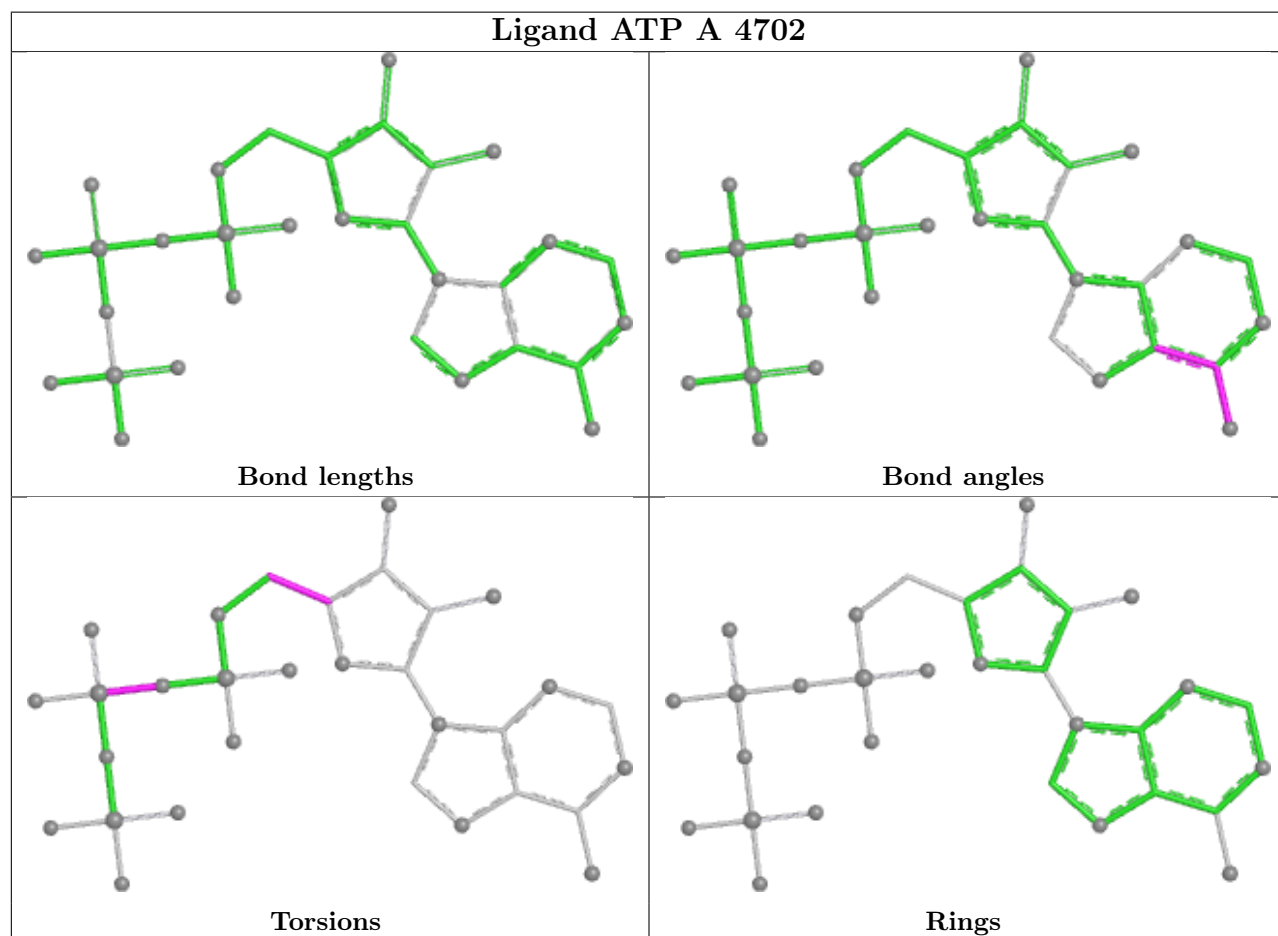
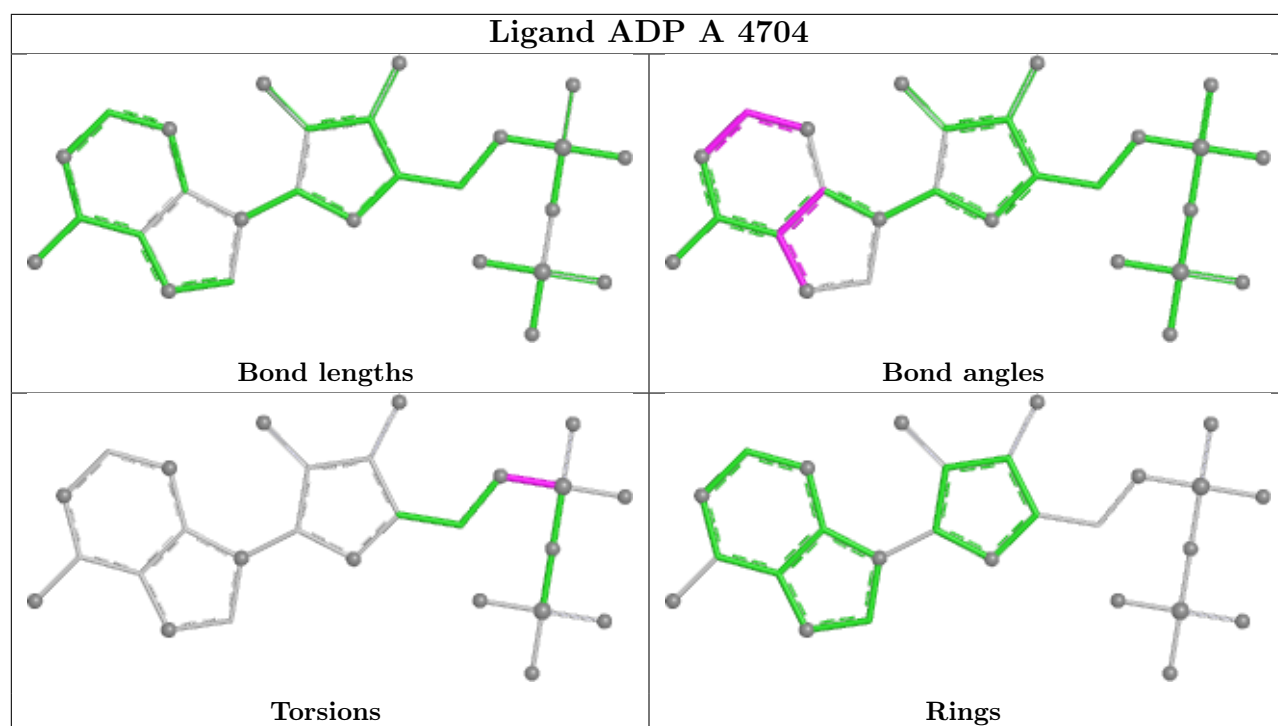
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	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.

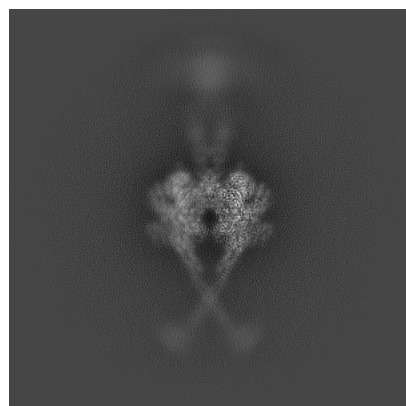
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44701. These allow visual inspection of the internal detail of the map and identification of artifacts.

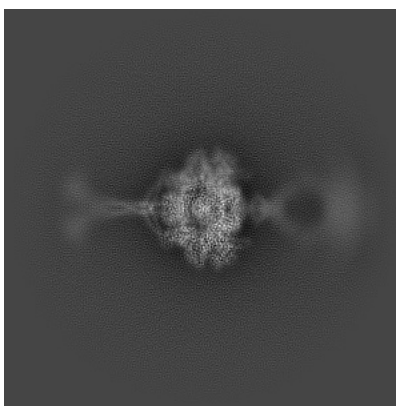
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

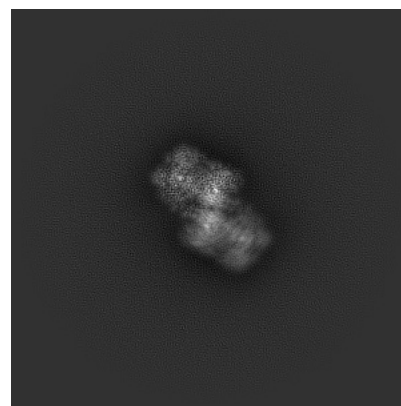
6.1.1 Primary map



X

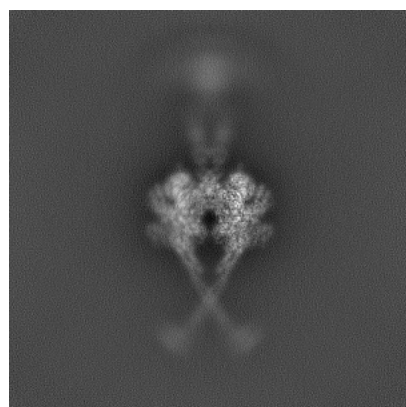


Y

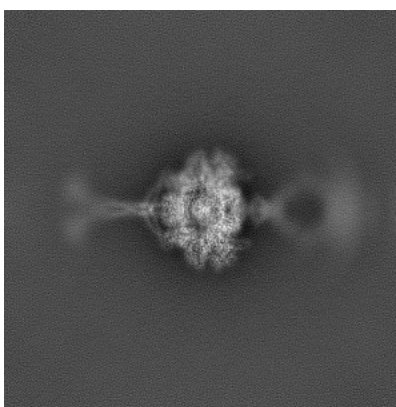


Z

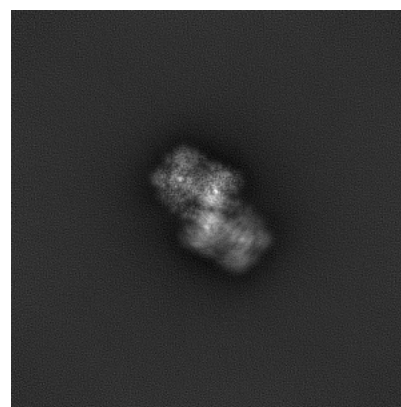
6.1.2 Raw map



X



Y

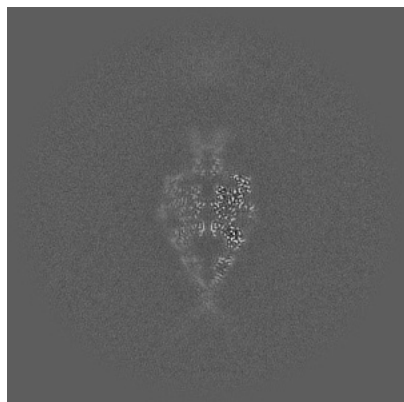


Z

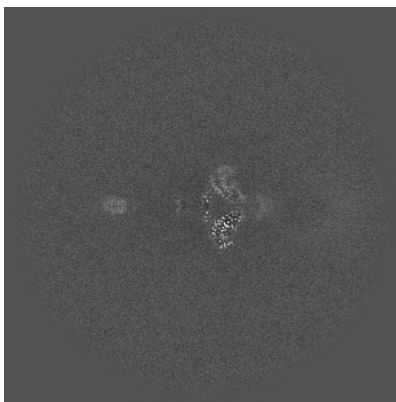
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

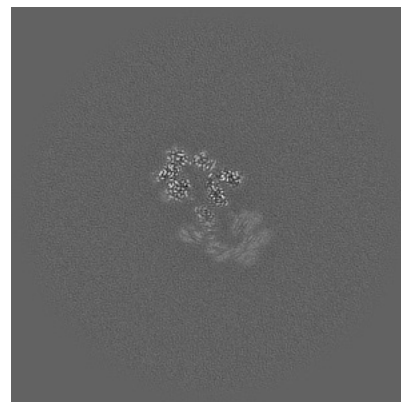
6.2.1 Primary map



X Index: 200

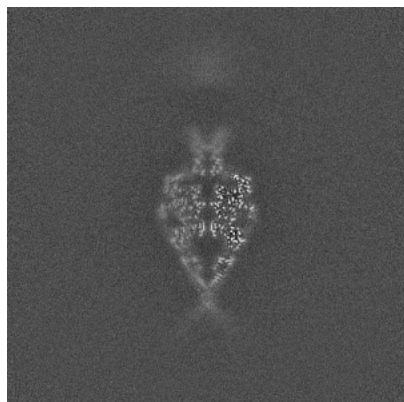


Y Index: 200

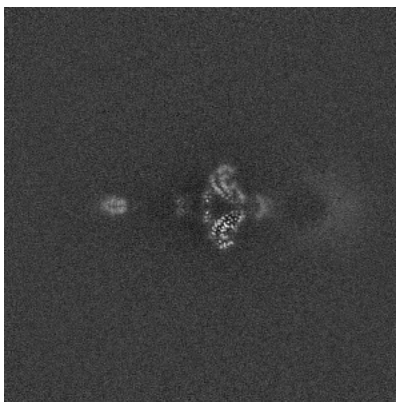


Z Index: 200

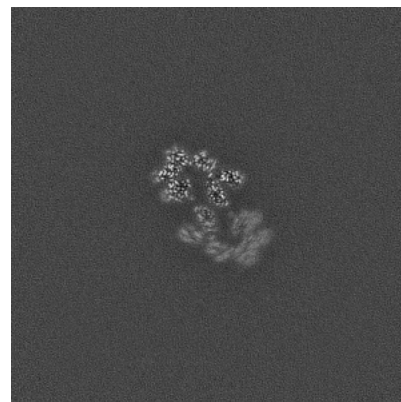
6.2.2 Raw map



X Index: 200



Y Index: 200

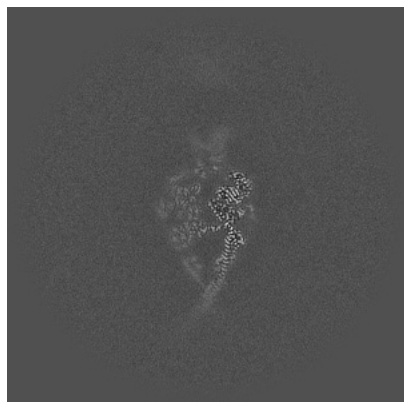


Z Index: 200

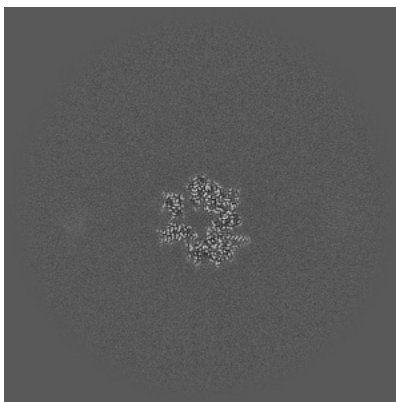
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

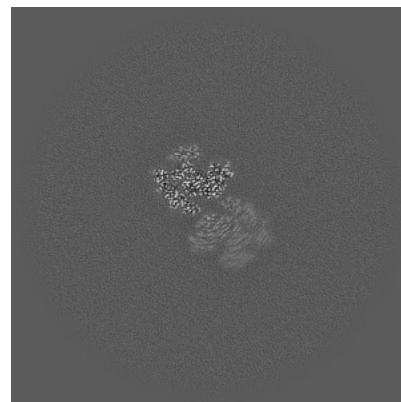
6.3.1 Primary map



X Index: 203



Y Index: 230

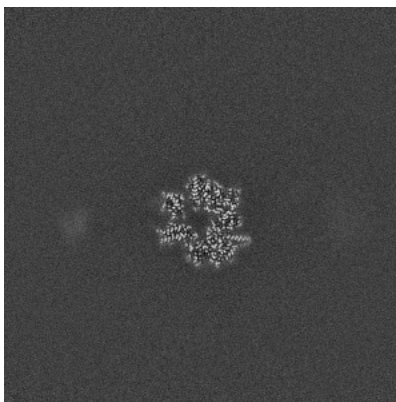


Z Index: 216

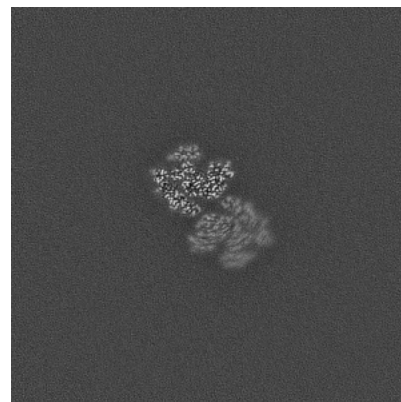
6.3.2 Raw map



X Index: 203



Y Index: 230

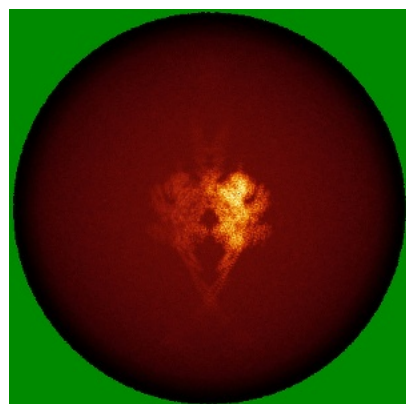


Z Index: 216

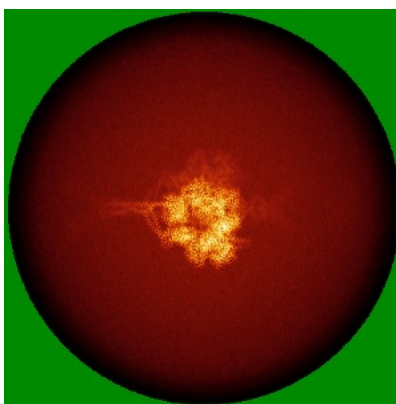
The images above show the largest variance slices of the map in three orthogonal directions.

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

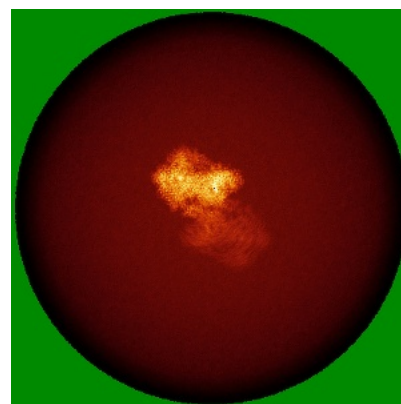
6.4.1 Primary map



X

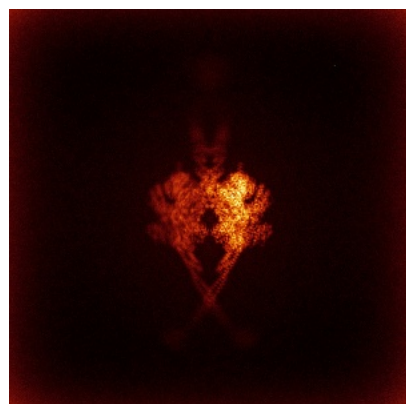


Y

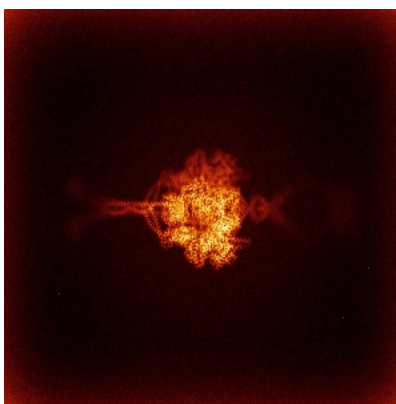


Z

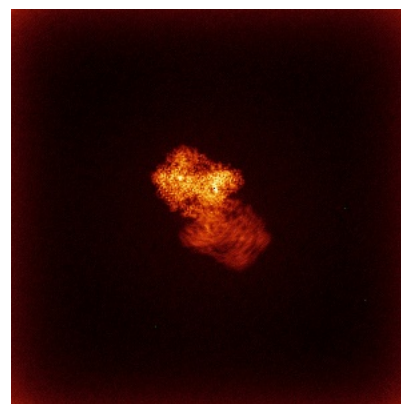
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



X



Y



Z

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.

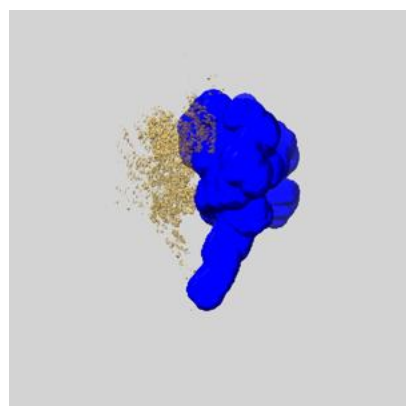
6.6 Mask visualisation [i](#)

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

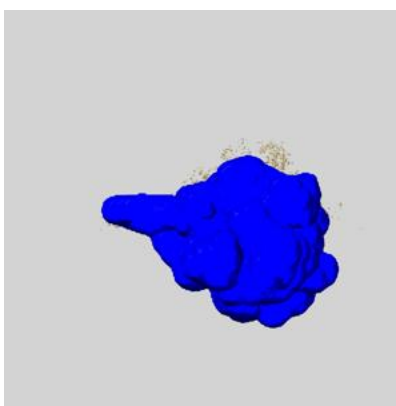
A mask typically either:

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

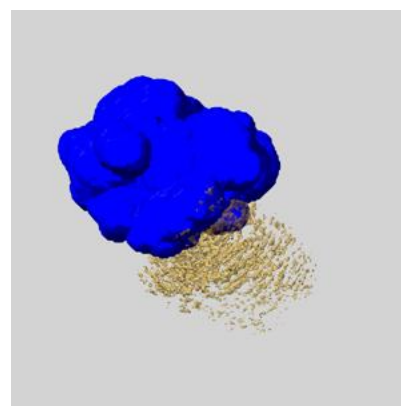
6.6.1 emd_44701_msk_1.map [i](#)



X



Y

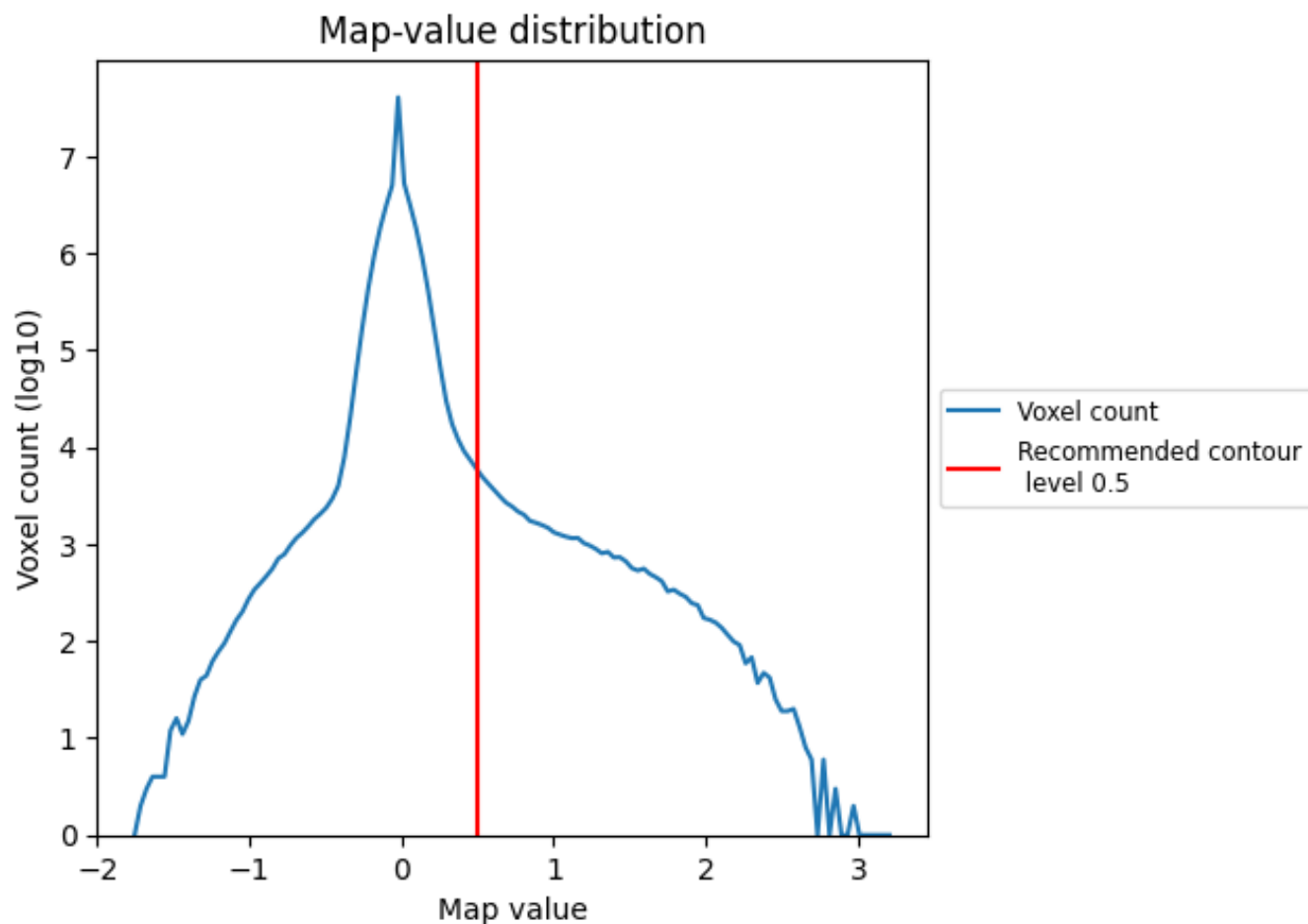


Z

7 Map analysis [i](#)

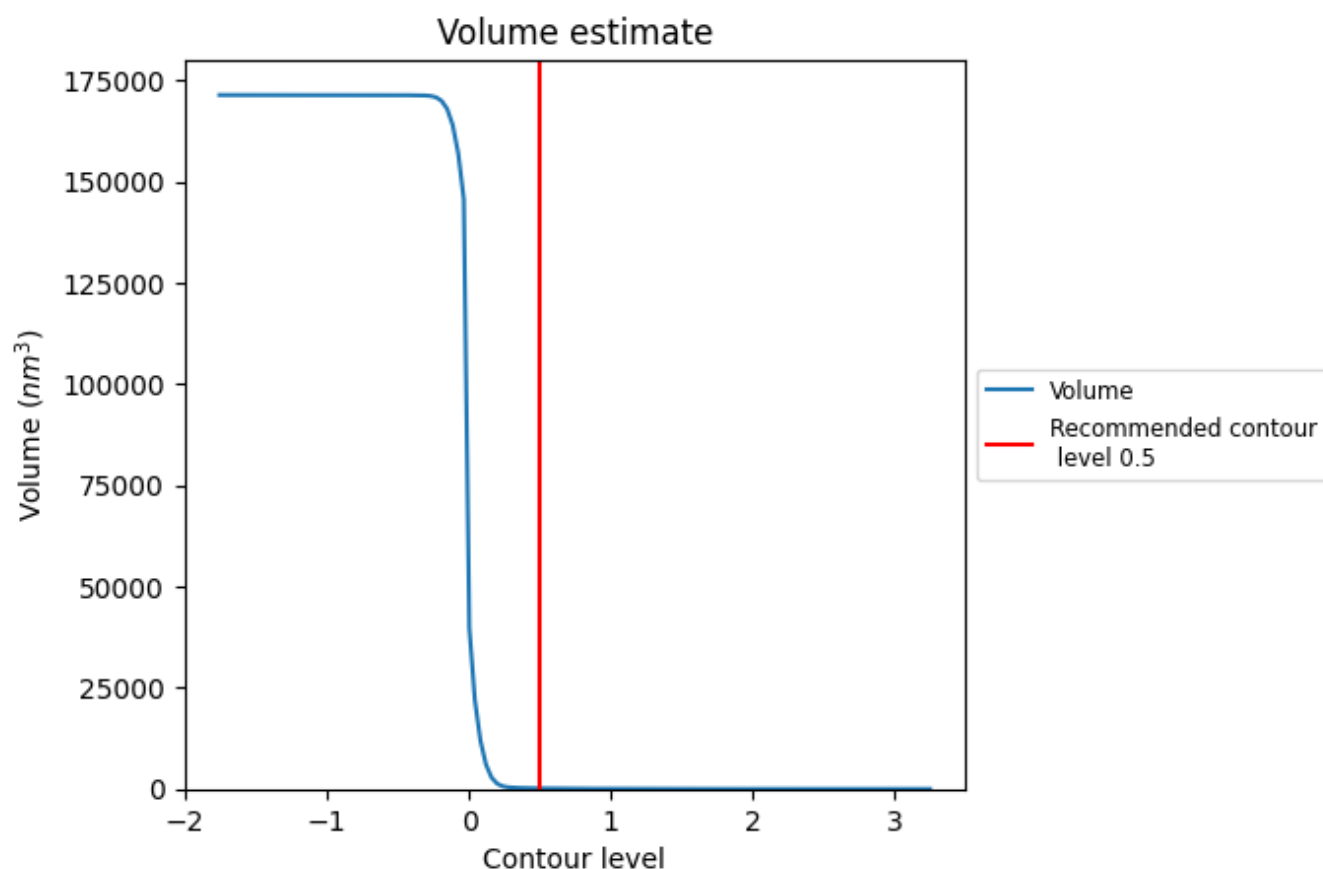
This section contains the results of statistical analysis of the map.

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.

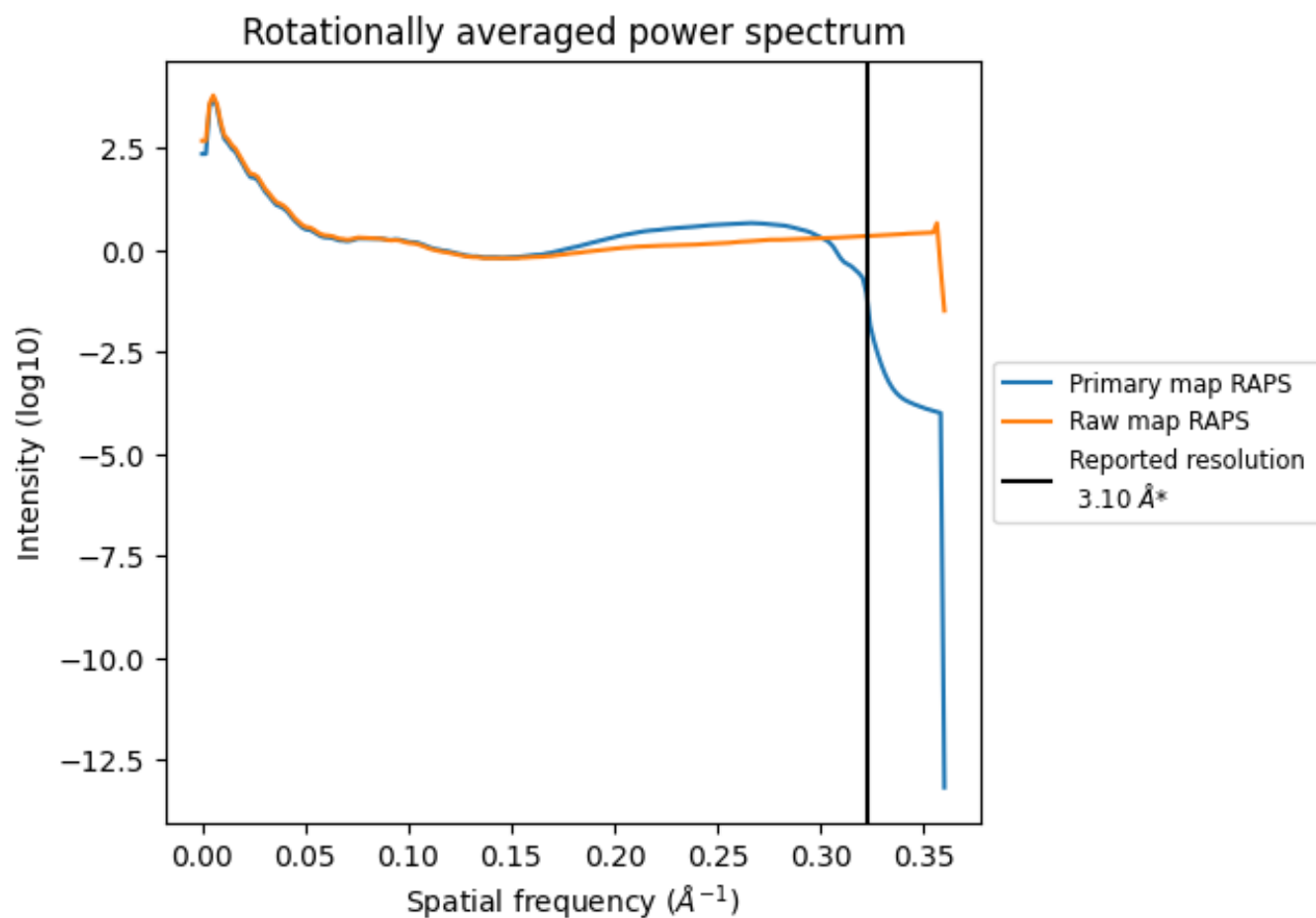
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm^3 ; this corresponds to an approximate mass of 133 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 ⓘ

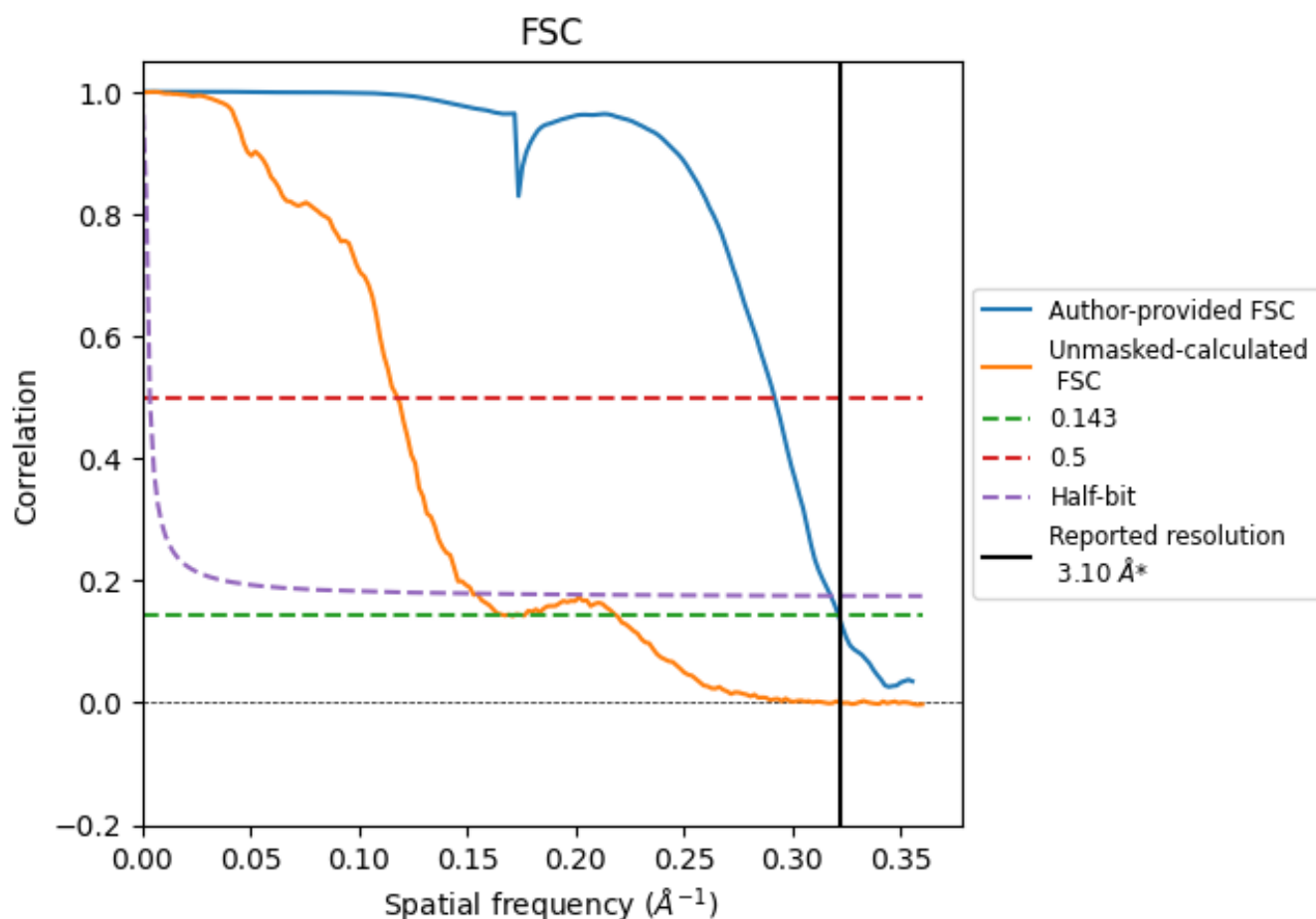


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

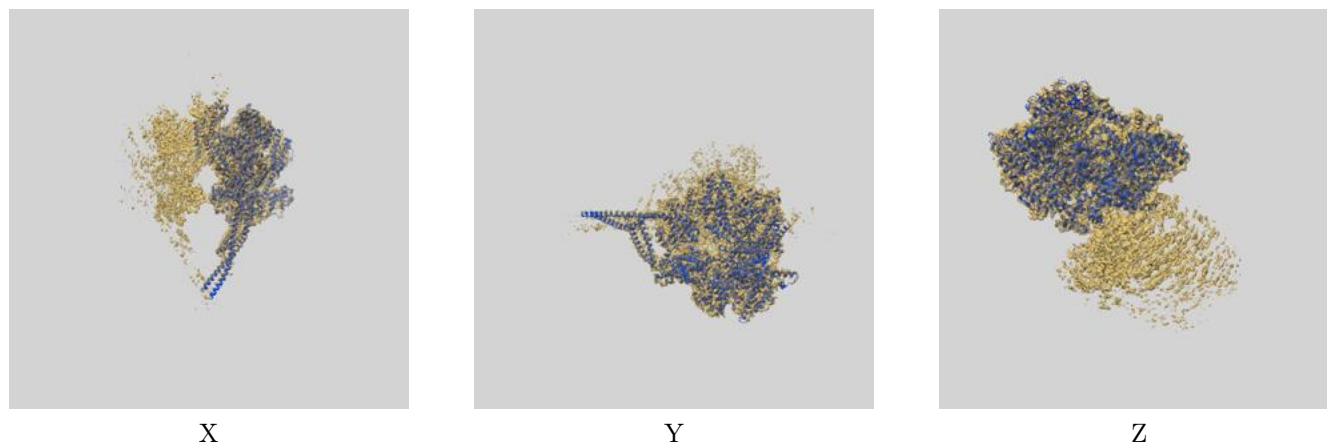
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.43	3.15
Unmasked-calculated*	5.99	8.50	6.55

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

9 Map-model fit [i](#)

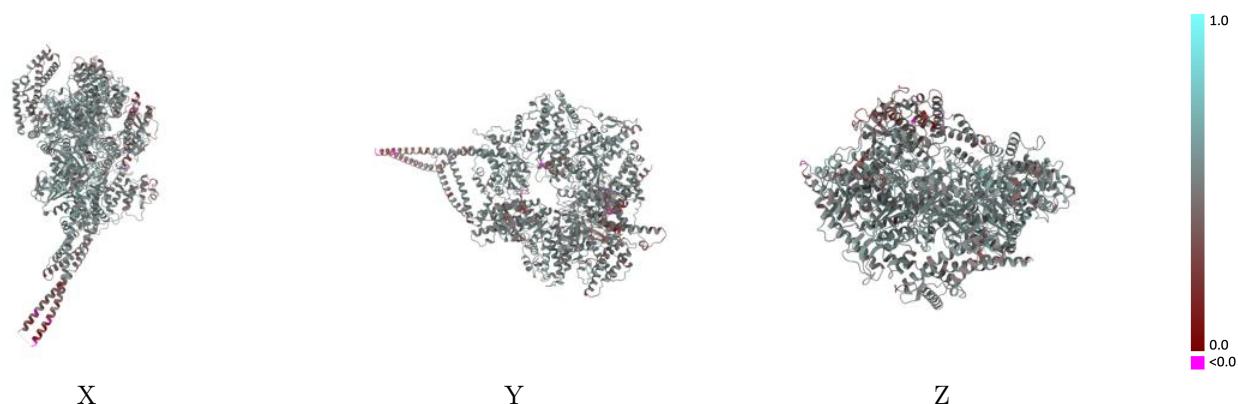
This section contains information regarding the fit between EMDB map EMD-44701 and PDB model 9BMJ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



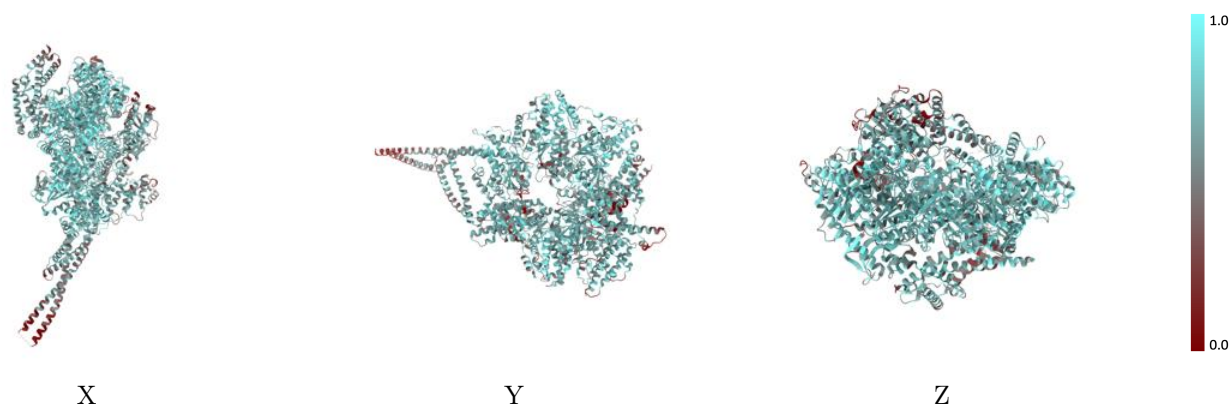
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



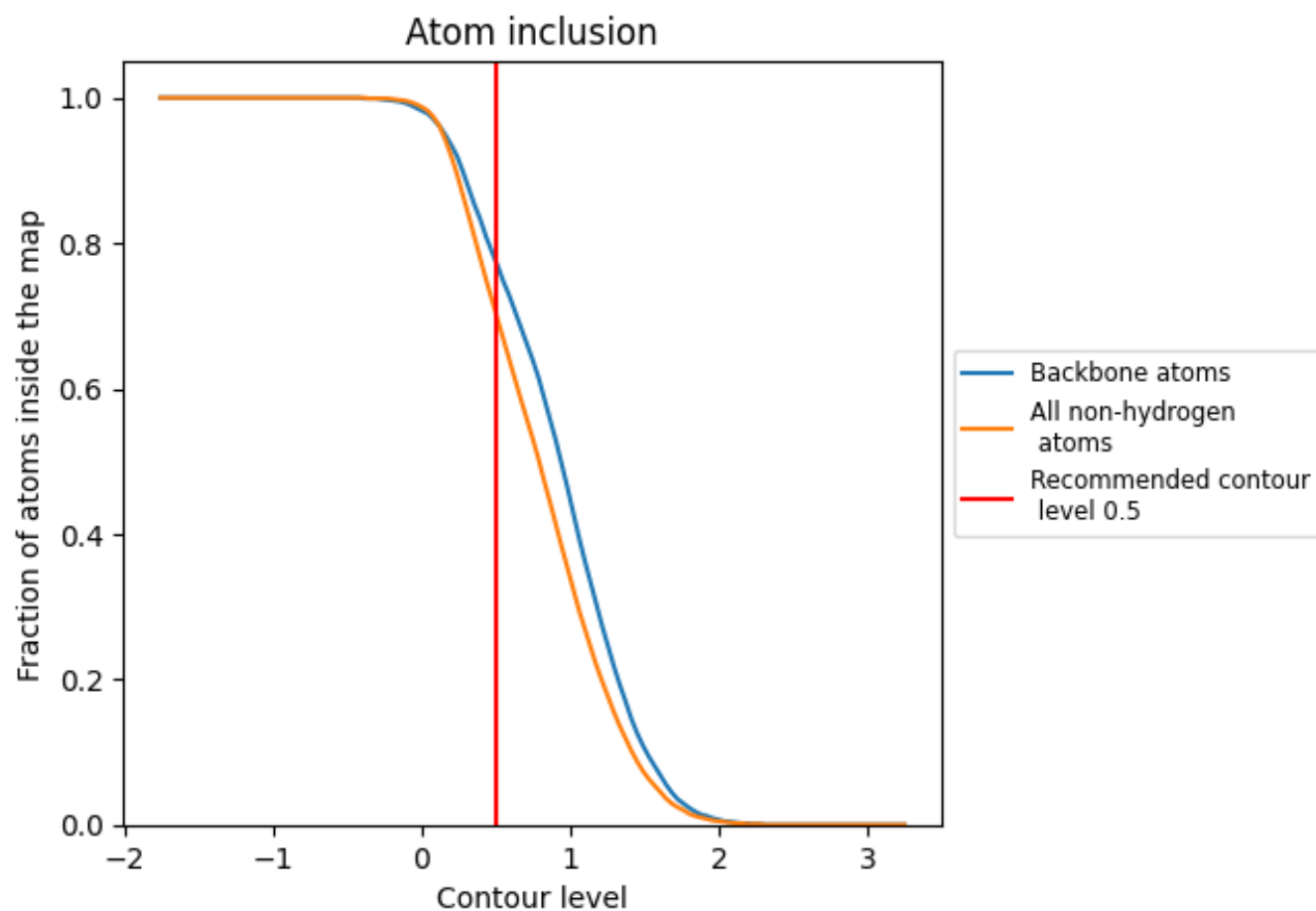
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7030	<div></div> 0.5070
A	<div></div> 0.7030	<div></div> 0.5070

