



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:29 AM EDT

PDB ID : 9BMA / pdb_00009bma
EMDB ID : EMD-44693
Title : Motor domain from full-length human dynein-1 bound to microtubules in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.20 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

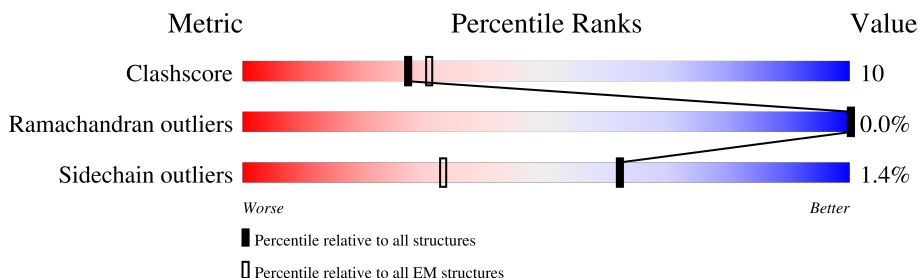
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	<div> <div>8%</div> <div>49%</div> <div>16%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24476 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	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 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
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



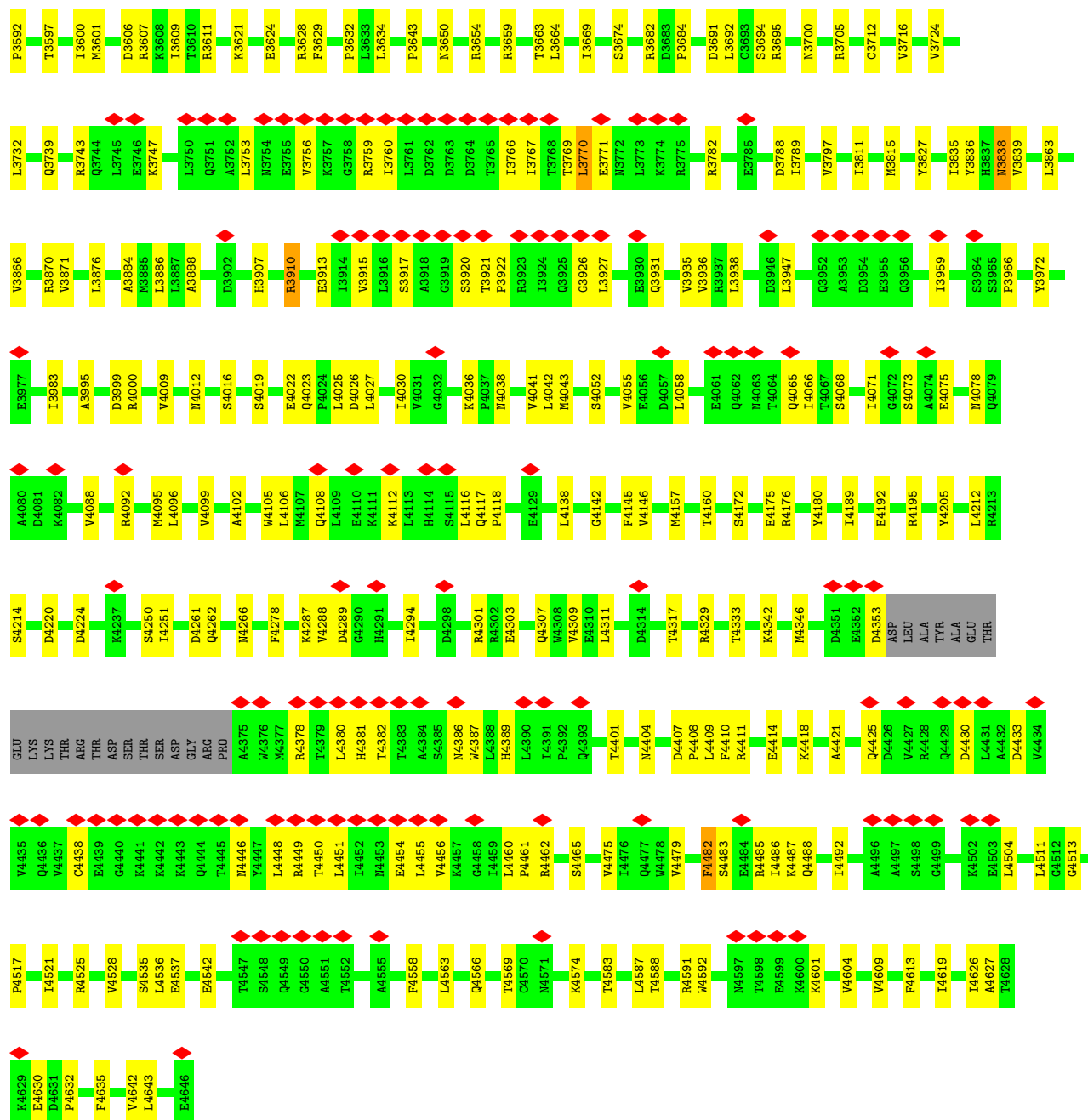
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0

- 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



R3486	E3487	R3488	R3489	E3490	K3491	E3494	T3495	R3498	Q3499	M3500	S3501	S3510	Y3516	F3520	D3521	M3524	Q3538	A3539	M3540	I3541	R3544	I3547	T3550	E3551	Y3552	L3553	D3557	E3558	R3559	W3562	L3567	P3568	D3571	L3572	C3573	N3576	A3577	I3578	R3579	L3580	R3585	D3591	S3483					
ASP	ASN	GLN	GLN	LYS	ALA	ASN	GLU	VAL	GLN	MET	ILE	ASN	GLU	VAL	TYR	LYS	GLU	GLY	GLU	VAL	ILE	TRP	GLN	ALA	ILE	LYS	ASP	ASP	LEU	ALA	VAL	GLU	A3470	K3471	N3472	R3473	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483			
VAL	GLU	VAL	ARG	LYS	SER	ASN	MET	VAL	VAL	ASN	TYR	ILE	VAL	ALA	GLY	THR	LYS	CYS	ALA	SER	LEU	GLY	GLU	GLN	ARG	ILE	ASP	ARG	GLU	ASN	ASN	PRO	THR	ILE	VAL	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN				
LYS	ASP	GLN	GLN	GLU	ALA	GLU	LYS	LYS	PRO	ALA	VAL	VAL	VAL	GLU	GLN	LEU	LYS	GLY	VAL	ILE	THR	THR	TRP	GLN	MET	SER	ILE	VAL	LYS	VAL	GLU	ASN	PRO	ILE	VAL	ILE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN				
A3142	I3143	V3144	T3172	P3173	R3174	H3175	Y3176	L3177	A3184	R3191	L3194	L3201	G3204	L3205	R3206	K3207	T3208	K3209	E3210	T3211	V3212	D3213	Q3214	V3215	E3216	E3217	L3218	R3219	D3220	D3221	LEU	ARG	ILE	LYS	SER	GLN	GLU	ALA	VAL	ASN	ASN	ASP	ASP					
E2902	E2903	E2904	L2905	D2906	P3173	R3174	H3175	Y3176	K3043	E3048	K3052	W3053	Q3057	F3066	T3067	K3068	R3069	P3070	S3071	S3072	K3076	D3077	T3081	W3093	F3094	G3095	D3096	W3097	S3098	Q3104	E3108	R3113	D3114	L3115	E3116	N3119	D3124	Y3125	M3126	P3127	Y3130	D3131	K3132	L3133	P3134	R3140	E3141	
D2636	E2640	Y2641	T2644	W2645	P2646	M2646	G2647	F2662	T2666	N2667	Y2693	R2694	L2703	I2706	C2712	N2713	P2714	P2715	R2720	R2726	F2727	L2728	V2731	Y2735	Y2738	P2739	G2740	P2741	L2744	I2747	Y2748	M2755	L2758	I2759	L2762	R2763	E2767	P2768	E2775									
E2538	I2541	W2545	S2546	P2547	W2548	Q2549	A2550	K2551	V2562	V2569	P2570	L2571	L2572	D2573	T2574	R2575	A2579	L2580	L2581	Y2582	T2583	W2584	E2587	P2590	L2591	G2595	P2596	P2597	G2598	T2602	F2606	L2609	D2614	M2615	E2616	V2617	S2623	S2624	A2625	T2626	E2629	K2633						
E2444	H2445	I2446	L2449	T2450	L2451	L2452	R2453	C2454	M2461	A2465	C2466	R2467	N2468	V2469	Q2470	Y2472	N2473	H2476	P2477	D2478	M2481	Q2482	L2483	E2484	Q2485	V2495	W2500	S2503	K2509	M2510	R2511	E2513	I2518	L2526	P2527	T2528	A2529	P2530	N2531	I2532	P2533	I2534	I2535	D2536	Y2537			
V2366	S2367	R2368	M2361	F2364	S2365	E2366	N2377	F2378	L2379	A2380	R2381	L2382	R2383	S2384	T2385	P2386	L2387	E2389	GLY	GLU	ASP	GLU	ALA	GLN	ARG	ARG	ARG	LYS	GLY	GLU	ASP	GLY	GLU	A2408	A2409	M2412	L2413	Q2414	T2415	Q2416	R2417	L2418	A2419	A2420	T2421	I2422	T2434	E2438
T2267	L2268	D2269	P2270	N2271	T2272	R2273	E2274	V2275	L2279	V2283	T2287	L2288	D2289	S2290	R2292	G2293	E2294	L2295	Q2296	R2297	V2302	F2303	D2304	V2307	D2308	V2311	V2312	E2313	D2320	D2321	N2322	L2323	L2325	E2331	R2332	S2334	L2335	P2336	R2340	I2341	W2342	F2343	E2344	Q2346	L2348			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.091	Depositor
Minimum map value	-0.677	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	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: 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	0.28	0/24908	0.49	1/33751 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3770	LEU	CA-CB-CG	5.16	127.17	115.30

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	24390	0	24462	470	0
2	A	31	0	12	3	0
3	A	54	0	24	3	0
4	A	1	0	0	0	0
All	All	24476	0	24498	471	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 10.

The worst 5 of 471 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:1462:PHE:HB2	1:A:3628:ARG:HD3	1.51	0.91
1:A:1830:ILE:HD11	1:A:1837:GLU:HB2	1.61	0.81
1:A:1650:LEU:HD21	1:A:1698:ILE:HD11	1.64	0.78
1:A:2481:MET:SD	1:A:2485:GLN:NE2	2.57	0.77
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.69	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	3019/4646 (65%)	2950 (98%)	68 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2741	PRO

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	2696/4125 (65%)	2657 (99%)	39 (1%)	62	82

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3838	ASN
1	A	4462	ARG
1	A	3910	ARG
1	A	4052	SER
1	A	4482	PHE

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	2130	ASN
1	A	2377	ASN
1	A	2713	ASN
1	A	2827	HIS
1	A	4012	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
3	ADP	A	4702	-	24,29,29	0.73	0	29,45,45	0.87	2 (6%)
3	ADP	A	4703	-	24,29,29	0.73	0	29,45,45	0.75	1 (3%)
2	ATP	A	4701	4	28,33,33	0.74	0	34,52,52	0.79	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
3	ADP	A	4702	-	-	0/12/32/32	0/3/3/3
3	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
2	ATP	A	4701	4	-	1/18/38/38	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(°)
3	A	4702	ADP	C4'-O4'-C1'	-2.54	107.60	109.92
3	A	4703	ADP	C5-C6-N6	2.30	123.81	120.31
2	A	4701	ATP	C5-C6-N6	2.27	123.76	120.31
3	A	4702	ADP	C5-C6-N6	2.25	123.73	120.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	C4'-C5'-O5'-PA

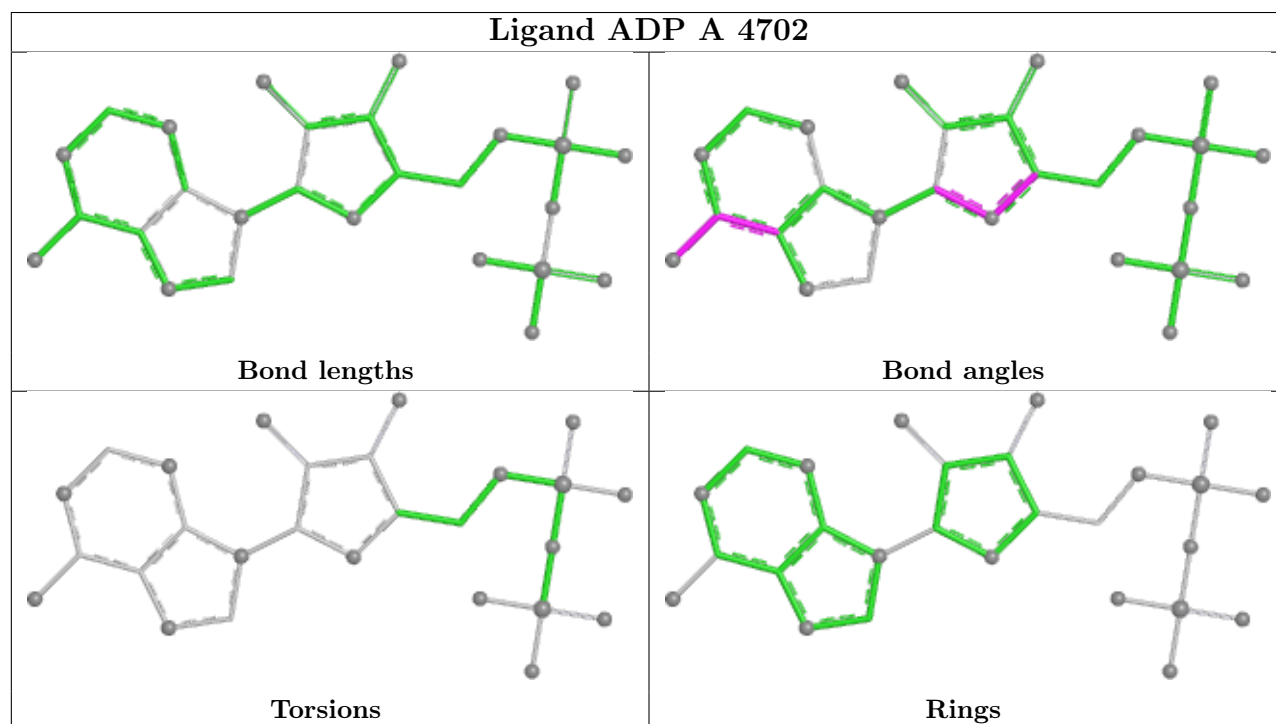
There are no ring outliers.

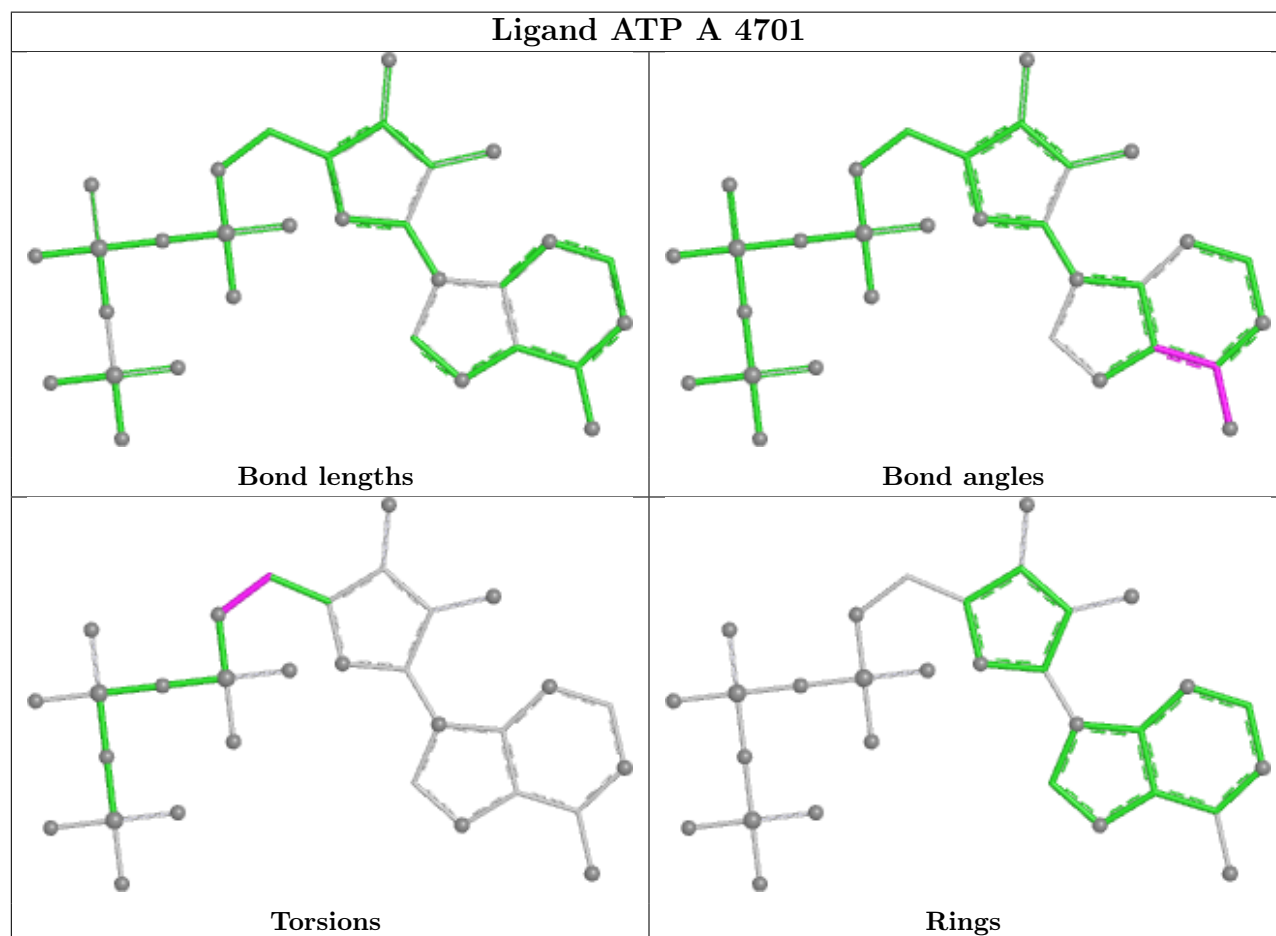
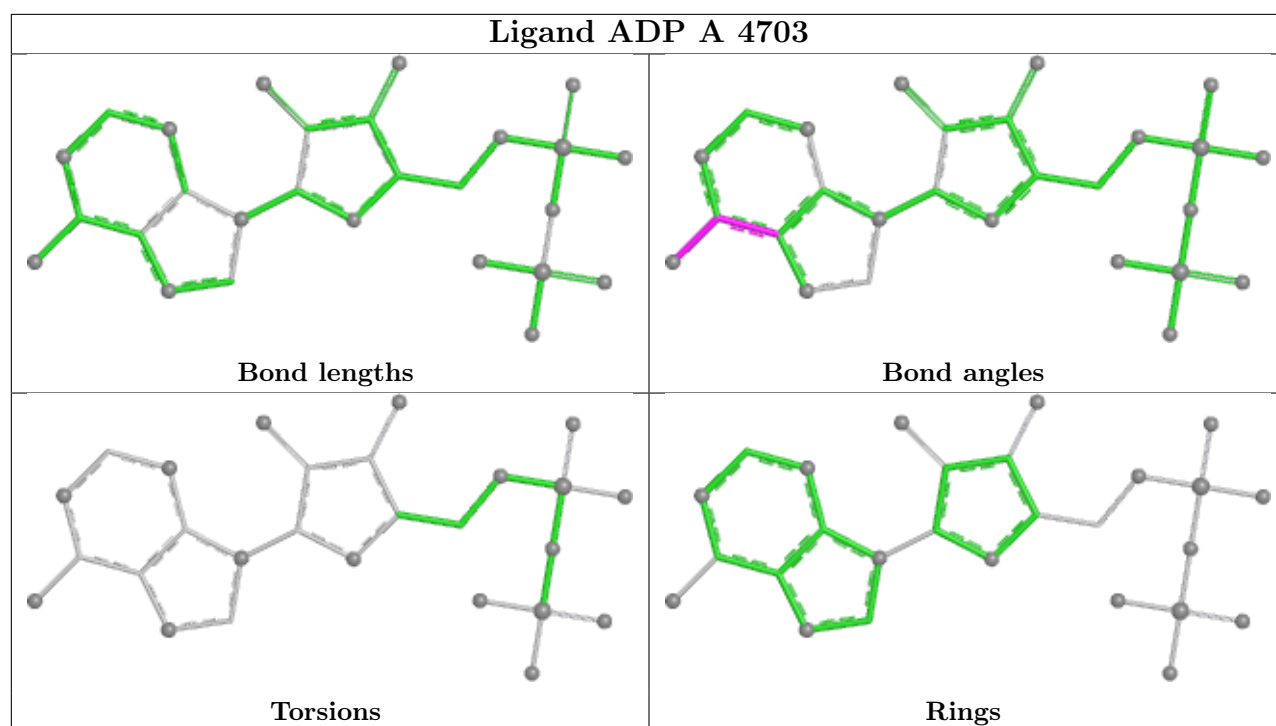
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ADP	2	0
3	A	4703	ADP	1	0
2	A	4701	ATP	3	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.

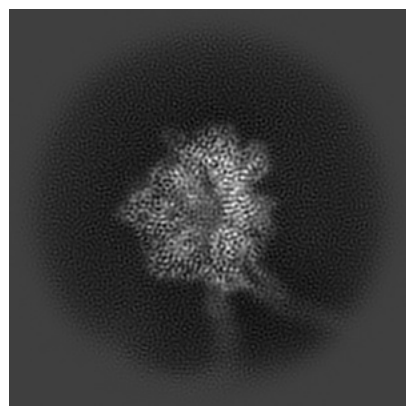
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44693. These allow visual inspection of the internal detail of the map and identification of artifacts.

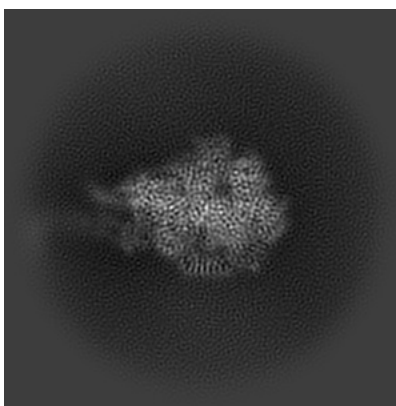
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

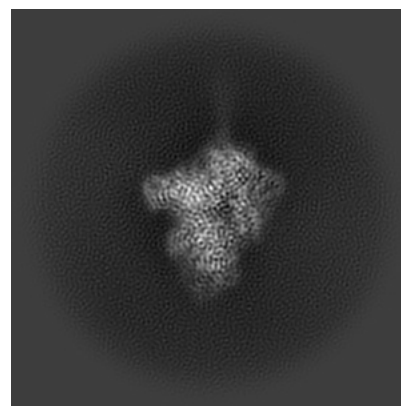
6.1.1 Primary map



X

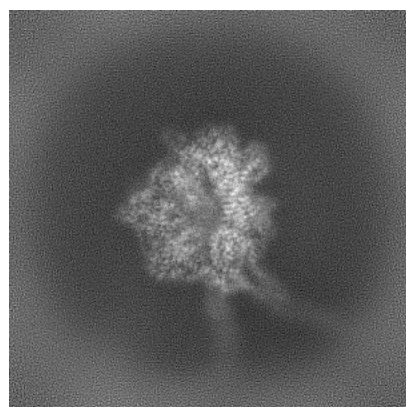


Y

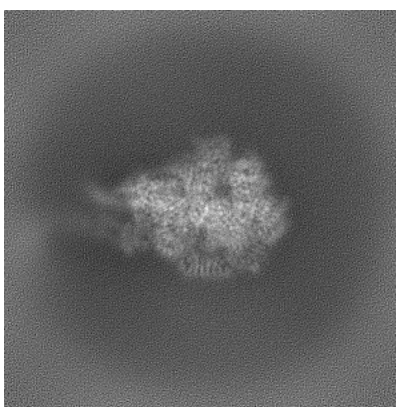


Z

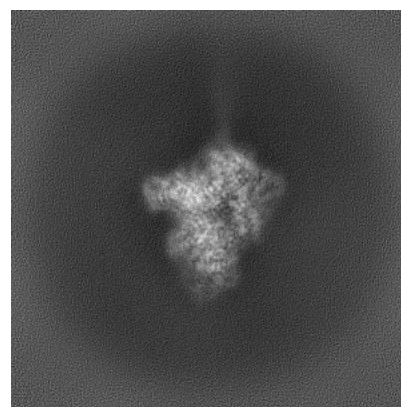
6.1.2 Raw map



X



Y

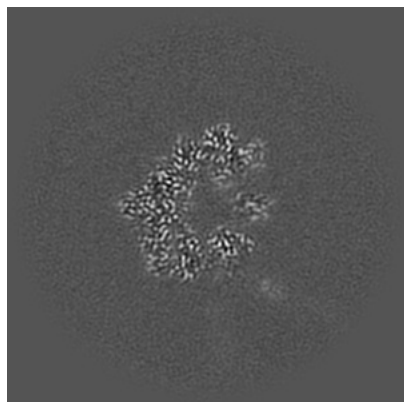


Z

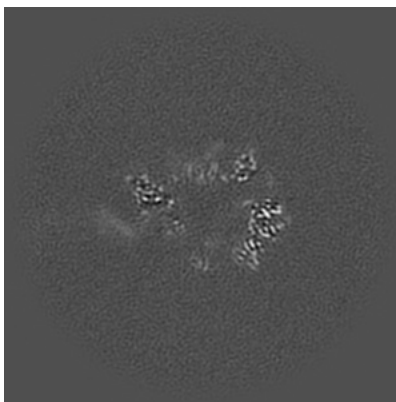
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

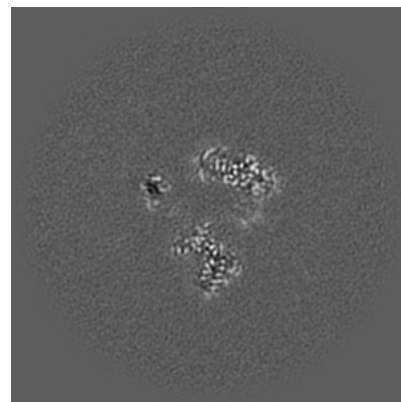
6.2.1 Primary map



X Index: 192

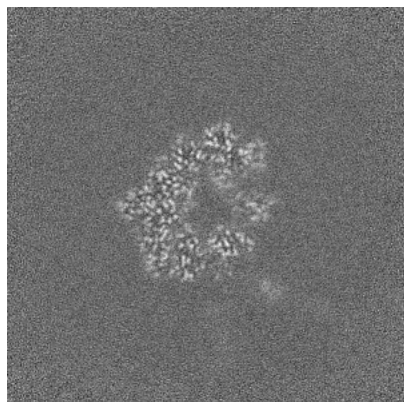


Y Index: 192

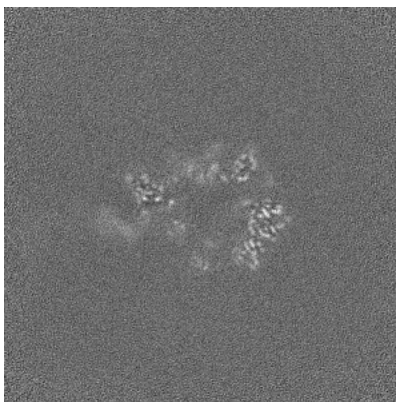


Z Index: 192

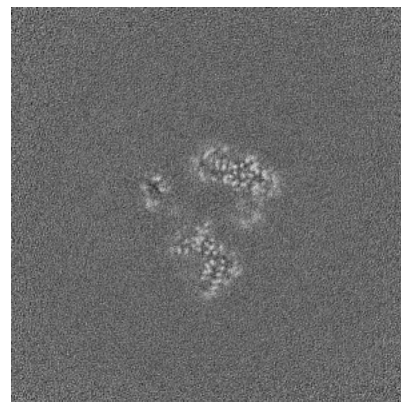
6.2.2 Raw map



X Index: 192



Y Index: 192

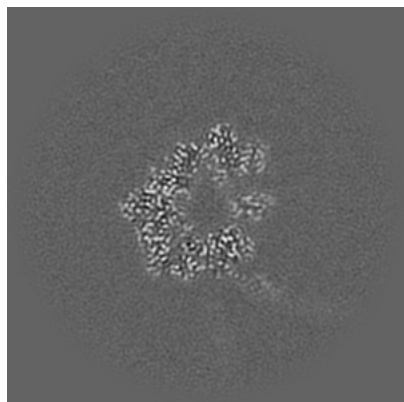


Z Index: 192

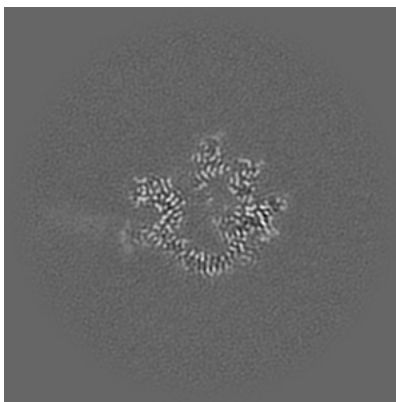
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

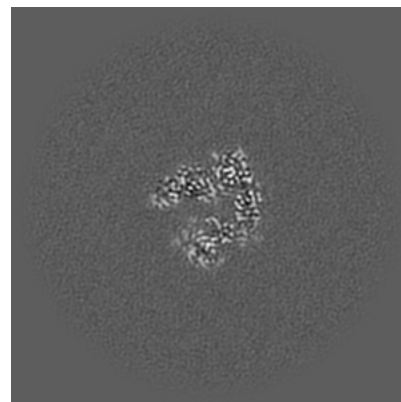
6.3.1 Primary map



X Index: 194

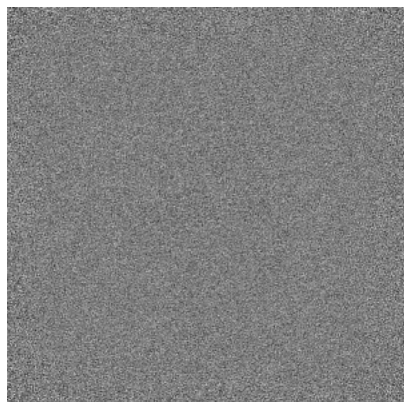


Y Index: 213

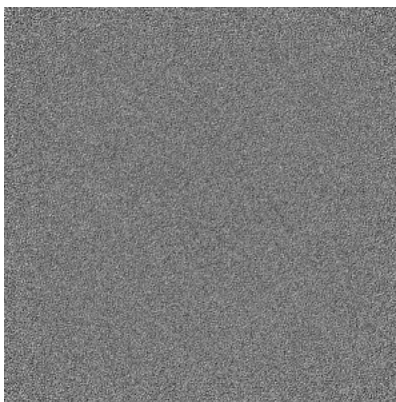


Z Index: 226

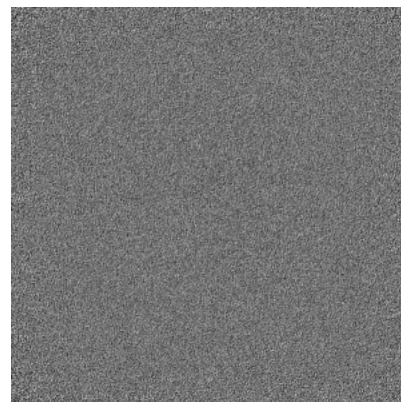
6.3.2 Raw map



X Index: 0



Y Index: 0

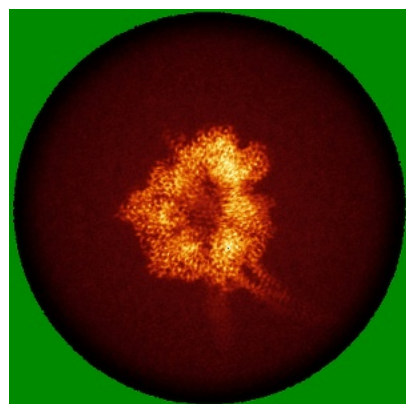


Z Index: 0

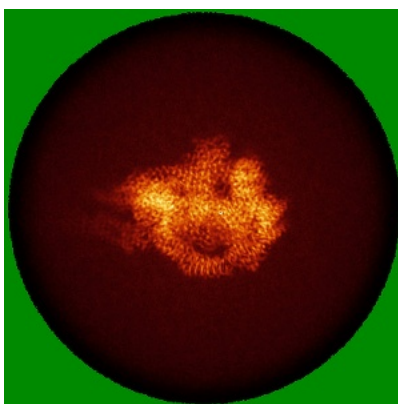
The images above show the largest variance slices of the map in three orthogonal directions.

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

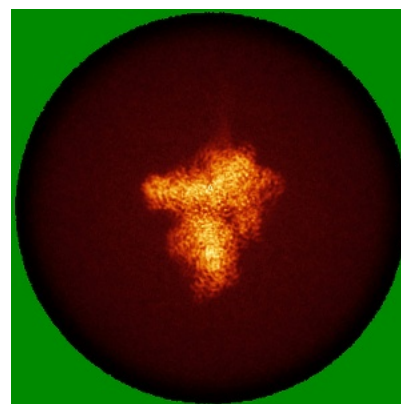
6.4.1 Primary map



X

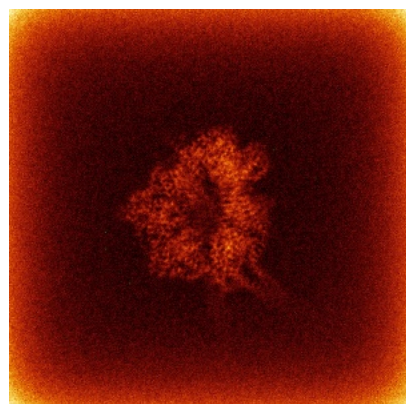


Y

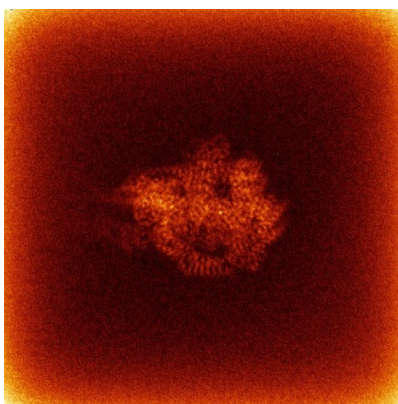


Z

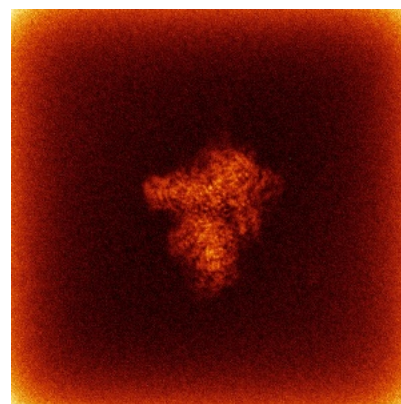
6.4.2 Raw map



X



Y

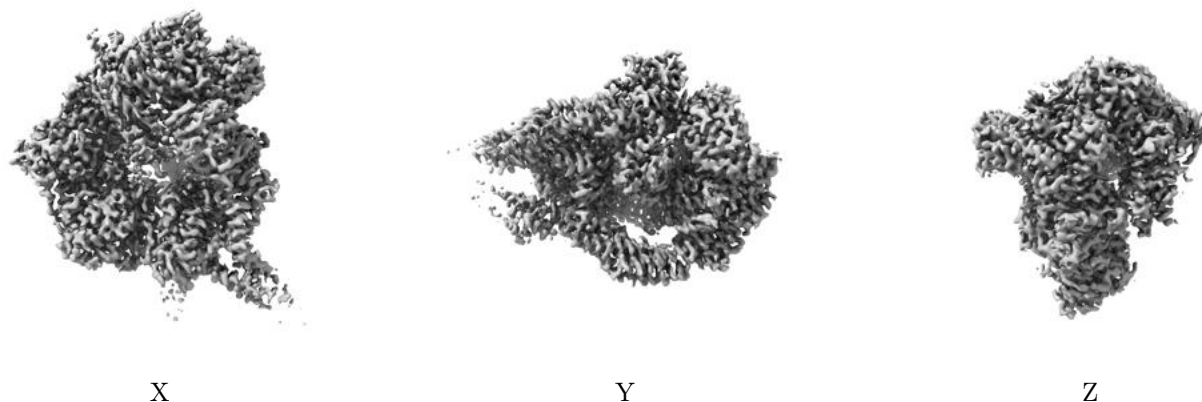


Z

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.

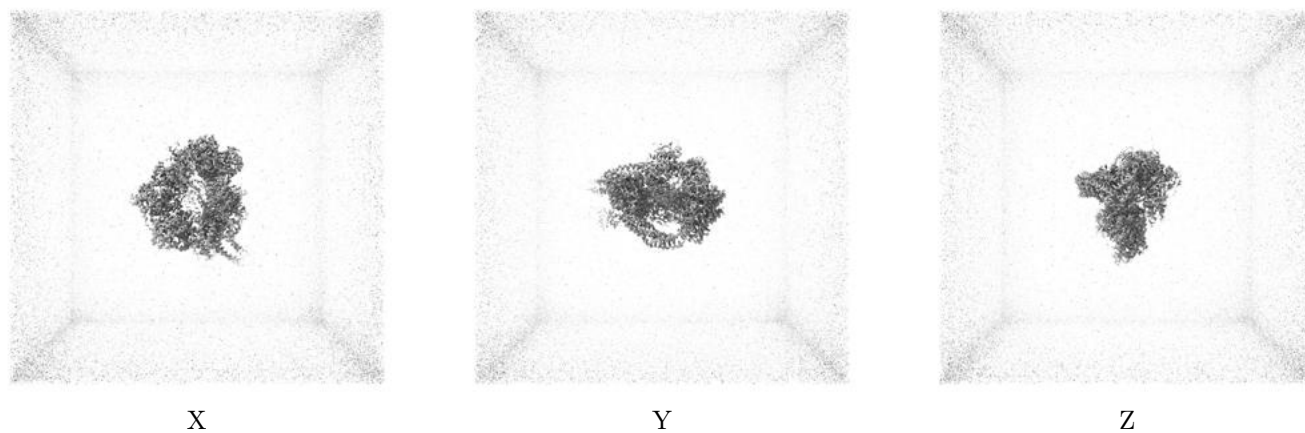
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

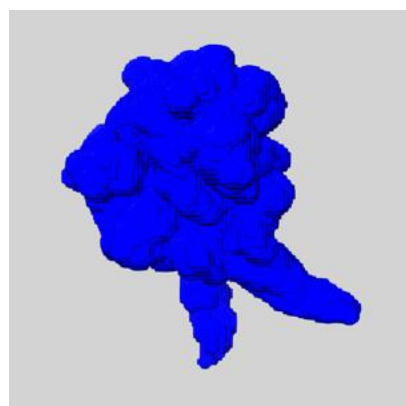
6.6 Mask visualisation [i](#)

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

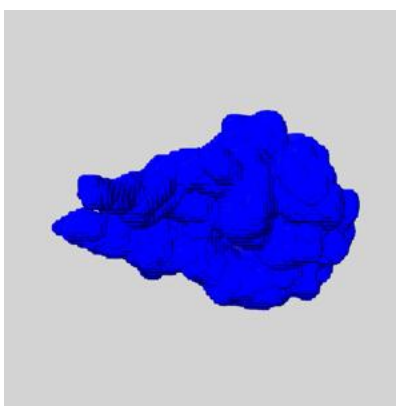
A mask typically either:

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

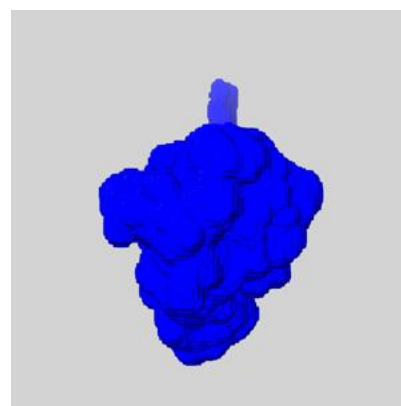
6.6.1 emd_44693_msk_1.map [i](#)



X



Y

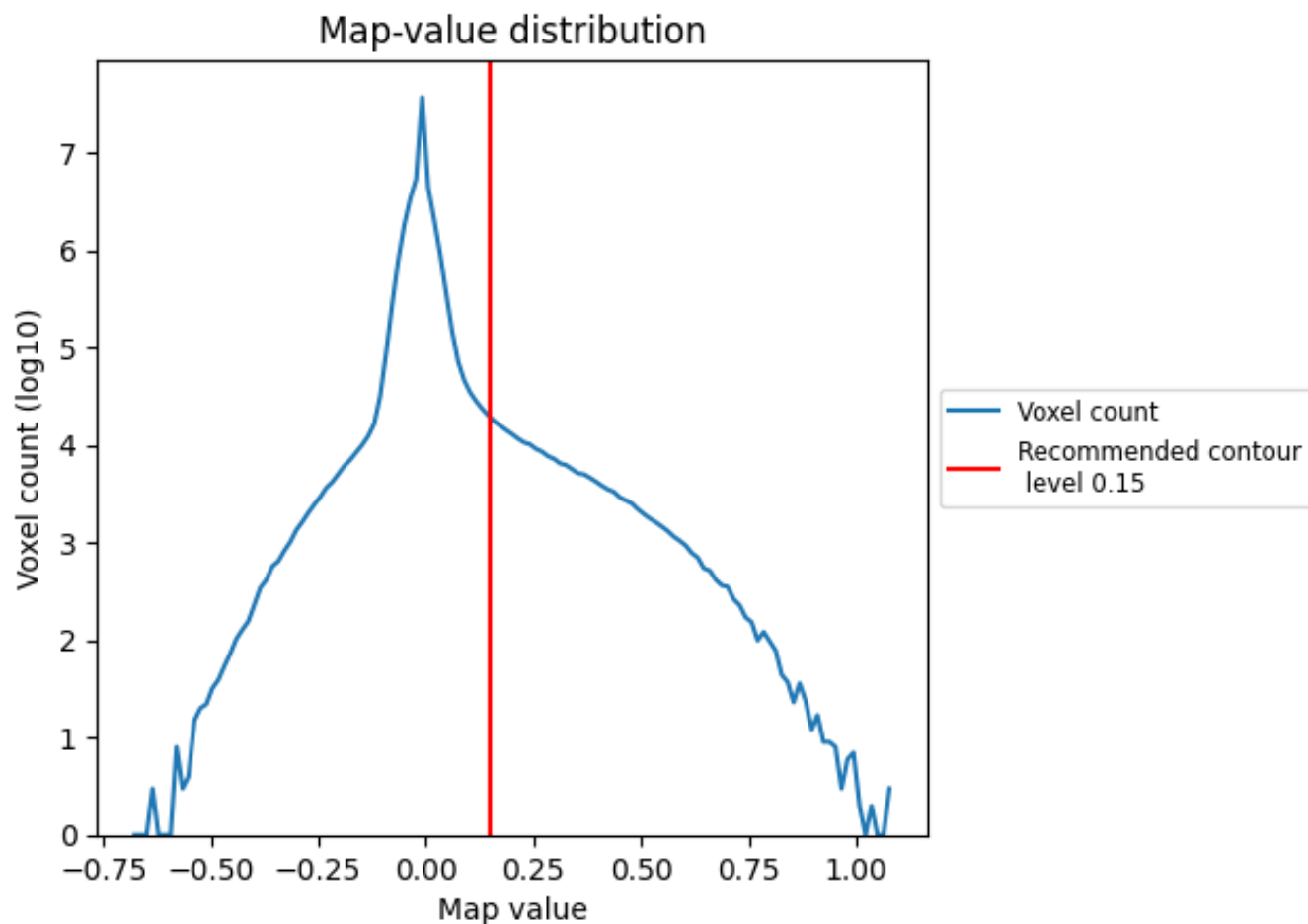


Z

7 Map analysis [i](#)

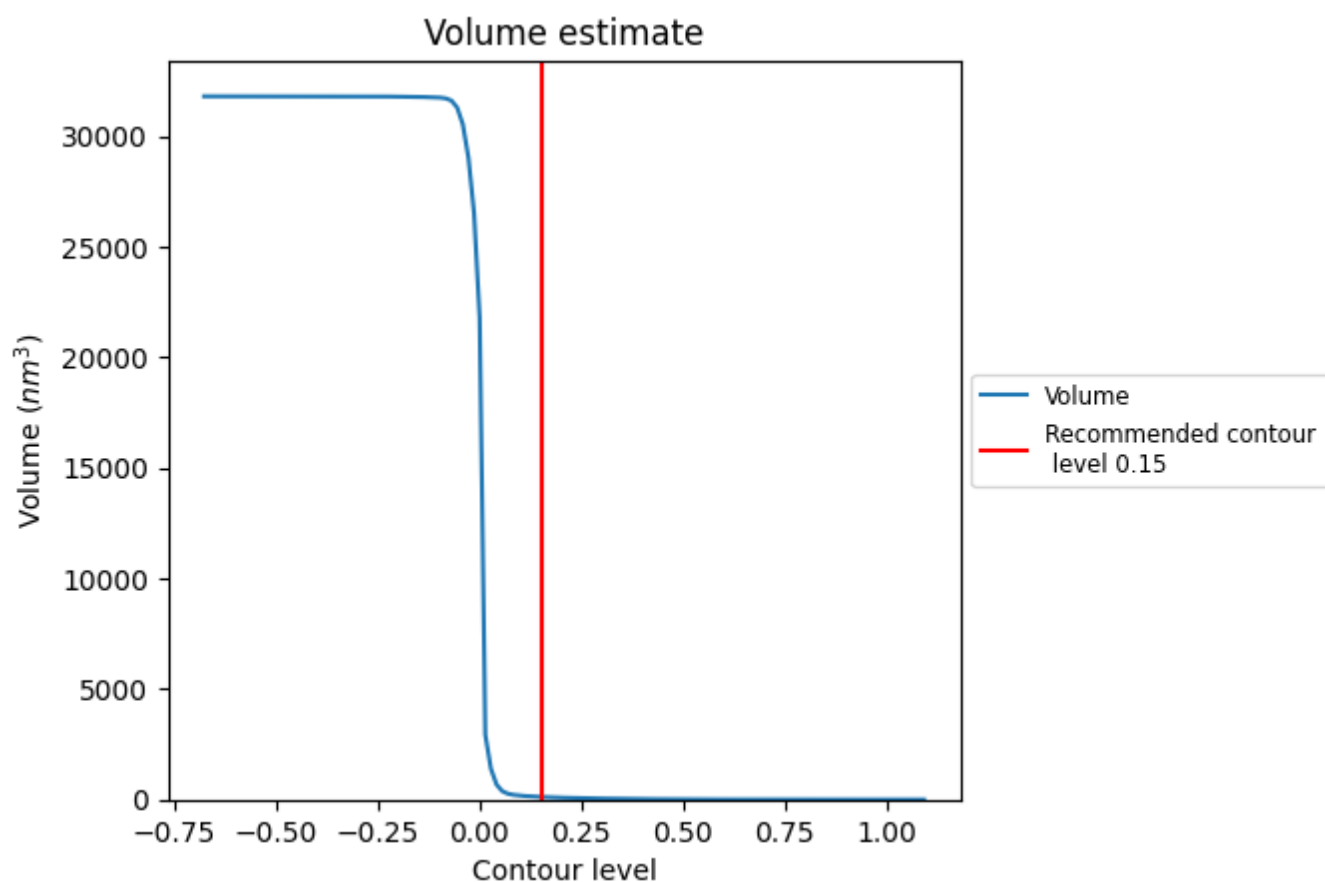
This section contains the results of statistical analysis of the map.

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.

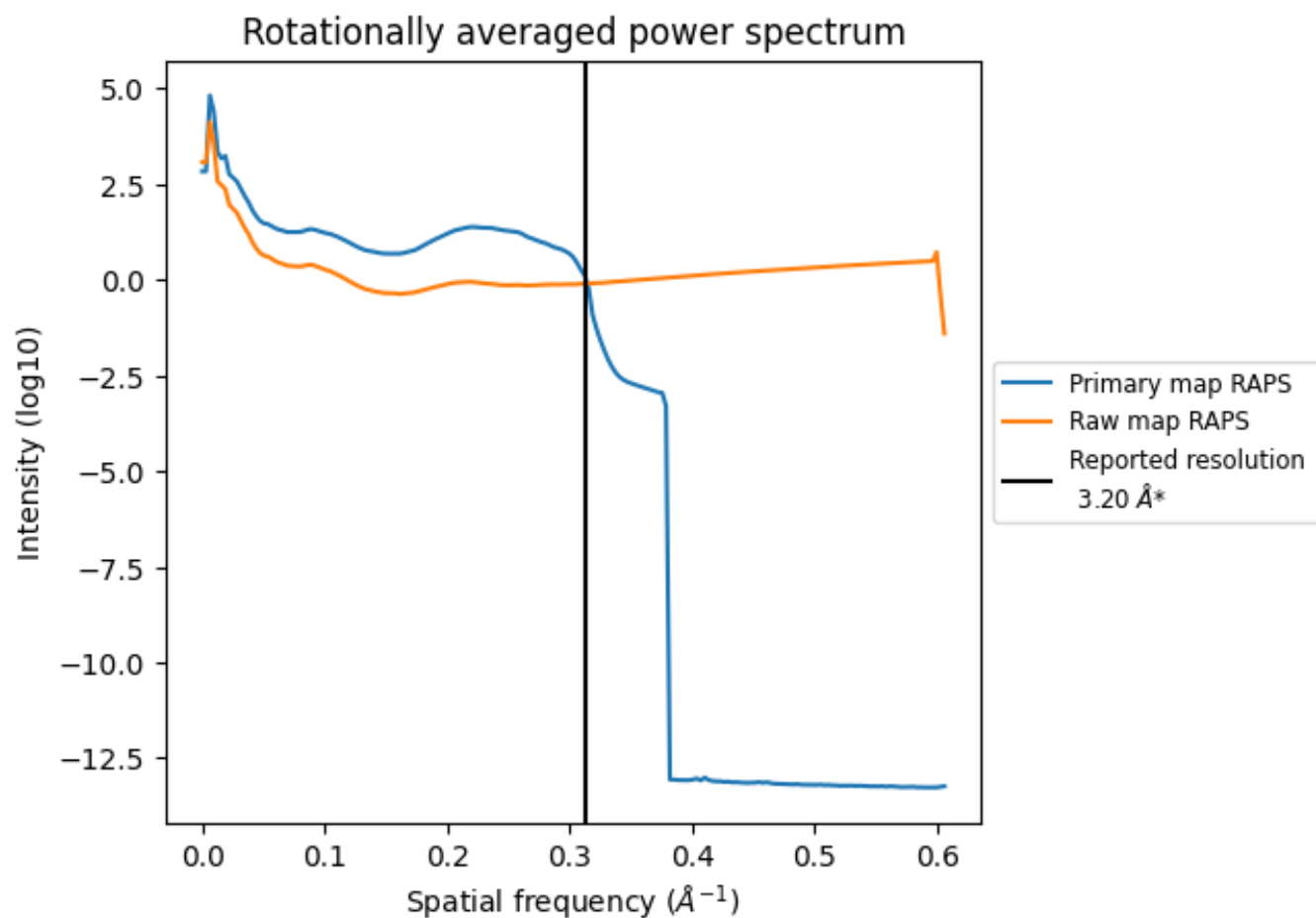
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm^3 ; this corresponds to an approximate mass of 107 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 [i](#)

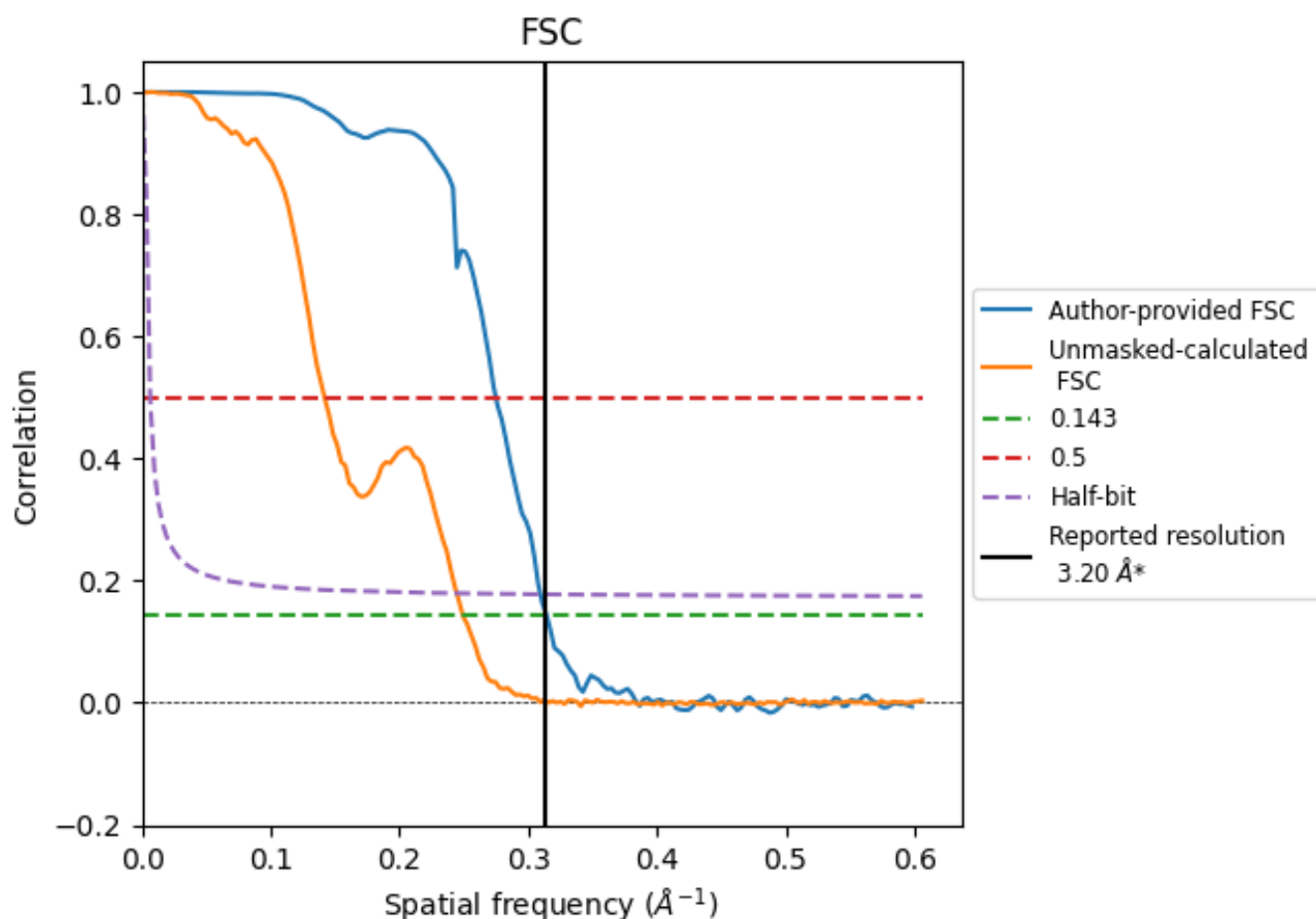


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

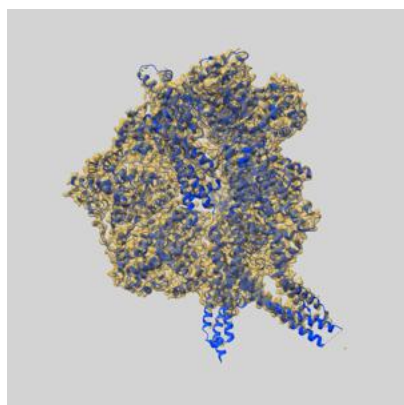
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.64	3.23
Unmasked-calculated*	4.01	7.06	4.09

*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 4.01 differs from the reported value 3.2 by more than 10 %

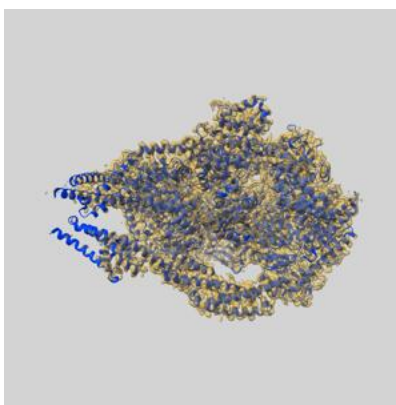
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44693 and PDB model 9BMA. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

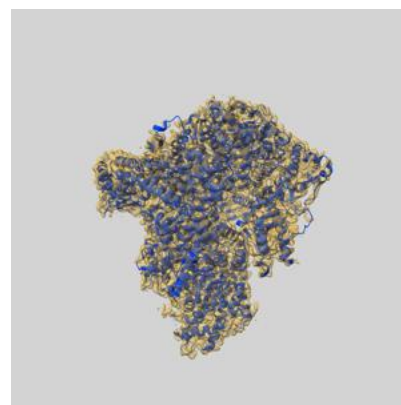
9.1 Map-model overlay [i](#)



X



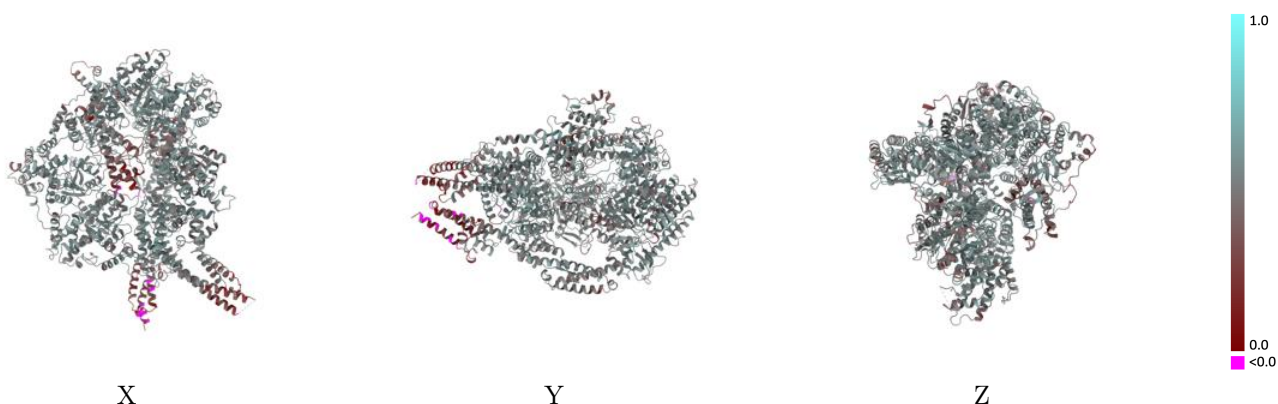
Y



Z

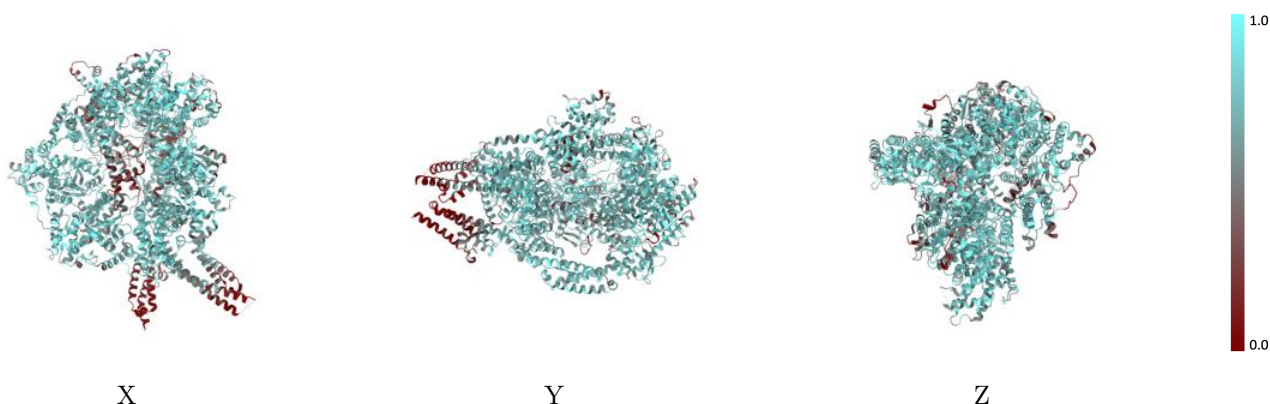
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



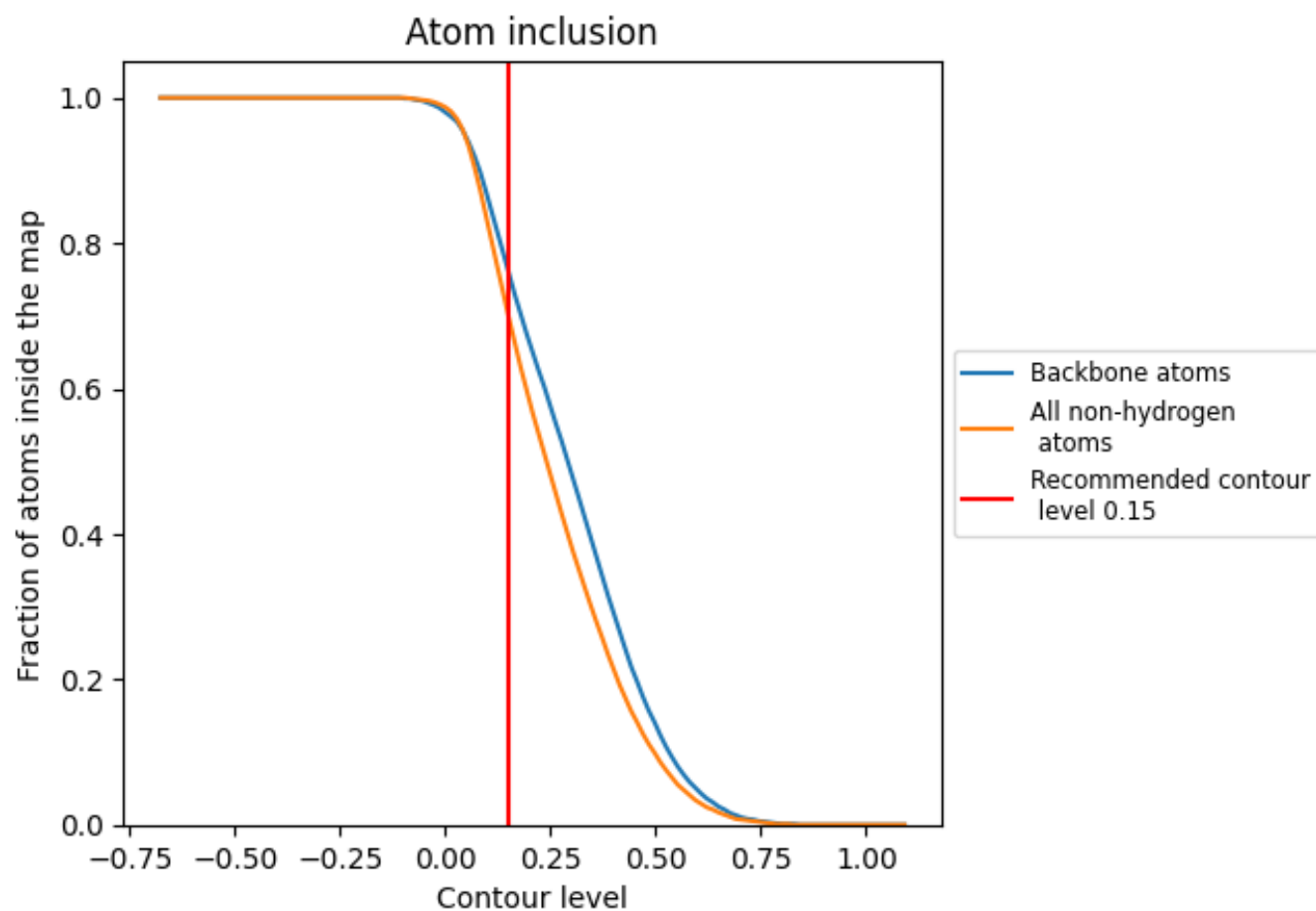
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6990	<div></div> 0.4900
A	<div></div> 0.7000	<div></div> 0.4900

