



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:26 AM EDT

PDB ID : 9BMB / pdb_00009bmb
EMDB ID : EMD-44694
Title : Post-1 motor domain from full-length human dynein-1 bound to microtubules
in 5mM ADP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.60 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

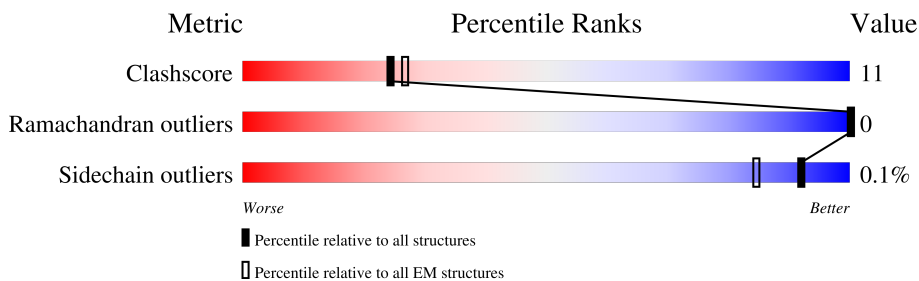
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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>9%</div> <div>48%</div> <div>17%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 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	3043	24503	15606	4234	4541	122	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	2	Total Mg 2 2	0



SER	ALA	MET	H3182	E3073	D2995	R2890	F2784	Y2674	F2479	L2382	L2279	R2179
TYR	VAL	SER	T3183	G3074	E2996	R2894	D2787	G2675	T2583	P2480	F2280	E2180
ASN	LYS	GLN	A3184	L3075	S2997	K2894	T2788	T2682	W2584	P2386	T2281	E2181
GLU	ALA	ILE	K3076	K3077	N2998	L2897	Q2788	T2683	L2585	L2387	R2285	L2182
VAL	LEU	GLN	Q3197	D3077	V2999	L2901	T2790	Q2684	P2590	L2288	V2203	K2203
ASN	SER	GLN	R3078	R3078	E2902	E2901	T2791	Q2685	L2591	D2289	V2204	E2204
ARG	ILE	LEU	A3079	A3079	E2903	E2903	T2792	Q2686	V2592	D2290	E2205	E2205
ALA	CYS	HIS	A3080	A3080	E2904	E2904	T2793	Q2686	L2593	V2291	K2206	V2206
SER	LEU	GLN	T3081	T3081	L2905	L2905	R2797	Q2491	P2596	E2392	V2207	V2207
LEU	LEU	GLN	S3082	S3082	L2906	L2906	E2798	Q2492	S2598	R2292	L2208	L2208
ALA	LEU	GLN	P3083	P3083	E2906	E2906	T2799	Y2493	G2600	G2293	Q2209	Q2209
CYS	GLY	VAL	R3083	R3083	E3007	E3007	T2800	L2499	K2601	E2294	L2210	L2210
GLY	GLU	ILE	R3088	R3088	H3008	H3008	F2807	L2703	L2605	R2396	V2211	V2211
PRO	SER	THR	G3089	G3089	N3009	N3009	E2807	E2704	L2606	Q2397	Q2296	Q2296
MET	THR	ASP	V3090	V3090	L2911	L2911	L2816	R2705	F2606	R2398	T2214	T2214
LYS	ASP	LYS	L3091	L3091	F2912	F2912	T2817	R2706	L2609	K2399	L2220	L2220
TRP	TRP	GLN	H3092	H3092	V2915	V2915	V2818	Q2707	L2610	G2400	L2221	L2221
ALA	LYS	GLN	W3093	W3093	L2920	L2920	L2821	F2708	R2810	K2401	R2222	R2222
ILE	ALA	VAL	F3094	F3094	R2921	R2921	L2822	V2709	P2613	E2402	G2224	G2224
GLN	ARG	LYS	G3095	G3095	L2924	L2924	R2823	C2712	V2617	E2404	G2227	G2227
LEU	LEU	ASP	W3096	W3096	R2925	R2925	A2826	T2716	L2620	G2405	W2311	W2311
ASN	ILE	ASP	W3097	W3097	L2933	L2933	L2830	D2717	L2621	V2312	K2230	K2230
TYR	ILE	LEU	L3102	L3102	L2939	L2939	R2831	Q2718	F2622	E2406	S2231	S2231
ALA	MET	ASP	Y3103	Y3103	K2943	K2943	E2834	R2719	N2629	E2407	N2314	N2314
ASP	ARG	GLU	M3113	M3113	K2964	K2964	Q2834	R2720	L2630	A2408	L2315	L2315
LEU	ASN	VAL	V3122	V3122	V2965	V2965	D2835	L2723	L2631	A2409	V2318	V2318
ILE	PRO	GLN	P3123	P3123	R2966	R2966	R2836	S2724	L2635	M2412	K2242	K2242
LYS	ALA	ASN	D3124	D3124	Y2967	Y2967	E2837	H2725	D2636	L2413	E2242	E2242
VAL	PRO	VAL	G3125	G3125	T2968	T2968	W2838	R2726	R2643	L2324	R2243	R2243
GLU	THR	ILE	Y3125	Y3125	G2969	G2969	E2839	R2729	T2644	L2325	L2244	L2244
LEU	VAL	ALA	Y3130	Y3130	E2970	E2970	E2848	H2730	P2645	T2327	E2248	E2248
GLU	ASN	GLN	D3131	D3131	D2971	D2971	N2849	D2732	N2646	A2419	I2254	I2254
ASN	PHE	ASN	K3132	K3132	F2972	F2972	I2850	P2733	G2647	A2420	A2258	A2258
GLU	SER	ALA	P3136	P3136	E2974	E2974	L2855	V2734	L2650	L2437	D2262	D2262
LEU	GLU	VAL	R3140	R3140	D2975	D2975	D2862	V2735	P2652	L2333	H2263	H2263
ASN	GLN	LYS	E3141	E3141	L2976	L2976	R2863	D2736	L2655	S2334	L2264	L2264
GLU	ILE	ILE	I3143	I3143	V2979	V2979	S2868	D2737	L2656	L2335	Y2265	Y2265
LEU	ILE	ILE	V3150	V3150	E2974	E2974	R2869	L2744	V2660	L2336	L2268	L2268
ASP	ALA	GLN	L3154	L3154	D2975	D2975	R2869	L2747	I2666	L2337	D2269	D2269
ASP	ARG	VAL	A3162	A3162	L2976	L2976	S2868	Q2755	L2667	S2338	P2270	P2270
GLN	VAL	VAL	R3163	R3163	V2979	V2979	R2869	Q2756	L2668	P2339	T2272	T2272
ASP	ARG	ARG	T3168	T3168	R2981	R2981	R2869	R2757	P2669	L2339	R2273	R2273
LYS	LYS	SER	A3170	A3170	E2982	E2982	S2874	E2776	V2569	L2339	E2274	E2274
GLN	ALA	MET	I3171	I3171	S2983	S2983	S2874	E2776	V2569	L2339	E2274	E2274
ASN	ALA	ASN	H3175	H3175	N2987	N2987	S2876	T2778	R2576	Q2346	Q2275	Q2275
PRO	VAL	PRO	D3178	D3178	E2988	E2988	D2885	T2778	R2576	L2348	E2275	E2275
GLN	PRO	ALA			T2990	T2990			H2577	D2347	T2277	T2277
									Q2465	F2343	G2278	G2278
									D2467	M2342		
										L2452		
										R2453		
										L2461		
										L2462		
										H2463		
										Q2464		
										A2354		
										D2277		
										R2358		
										F2364		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139709	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	1.327	Depositor
Minimum map value	-0.840	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: ADP, ATP, MG

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	0.26	0/25022	0.49	0/33900

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	24503	0	24574	518	0
2	A	81	0	36	5	0
3	A	31	0	12	1	0
4	A	2	0	0	0	0
All	All	24617	0	24622	518	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 11.

The worst 5 of 518 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:3618:ALA:O	1:A:3621:LYS:HB3	1.61	0.98
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.48	0.79
1:A:2593:LEU:HD12	1:A:2605:LEU:HD12	1.67	0.75
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.69	0.74
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.70	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	3035/4646 (65%)	2952 (97%)	83 (3%)	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	2706/4125 (66%)	2704 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2671	MET
1	A	2966	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3535	HIS
1	A	3865	GLN
1	A	3869	ASN
1	A	2416	GLN
1	A	1495	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 6 ligands modelled in this entry, 2 are 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	4704	-	24,29,29	0.84	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
2	ADP	A	4701	4	24,29,29	0.89	0	29,45,45	1.20	2 (6%)
3	ATP	A	4702	4	28,33,33	0.72	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	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	4	-	3/12/32/32	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 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.76	123.57	128.67
2	A	4701	ADP	N3-C2-N1	-3.72	123.62	128.67
2	A	4704	ADP	N3-C2-N1	-3.59	123.80	128.67
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4703	ADP	C4-C5-N7	-2.40	106.81	109.34

There are no chirality outliers.

5 of 14 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	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	O4'-C4'-C5'-O5'

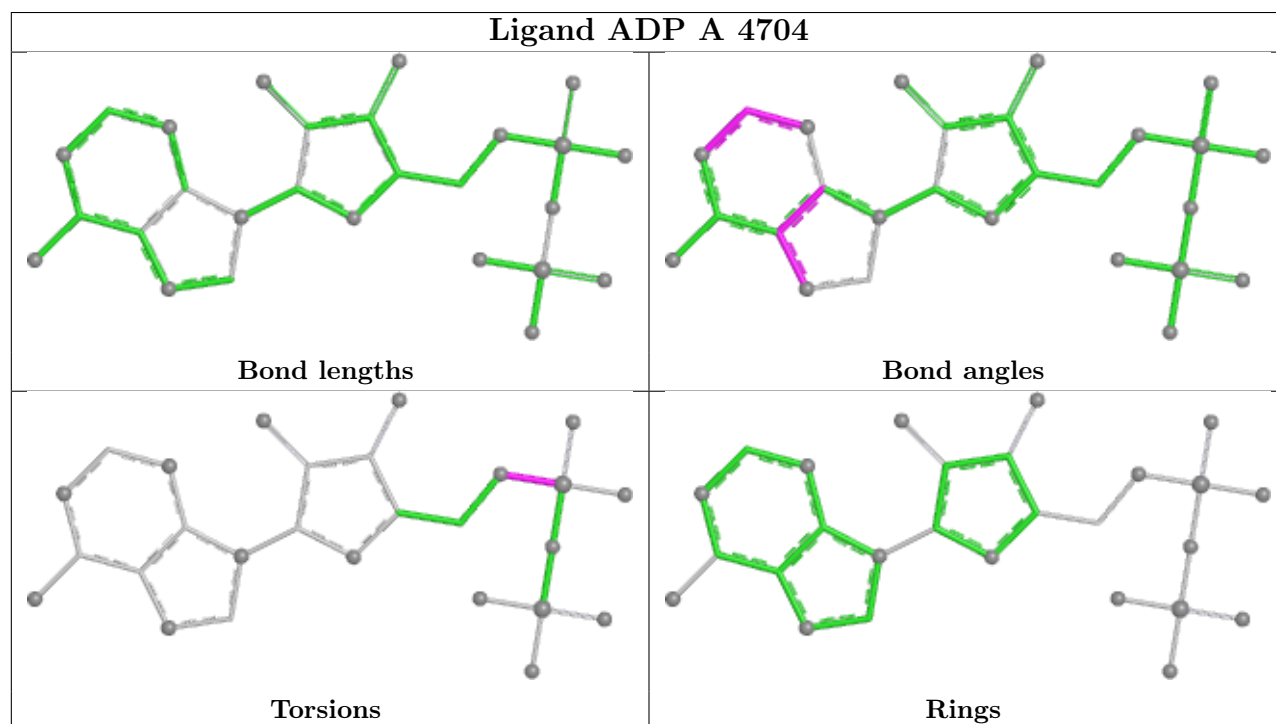
There are no ring outliers.

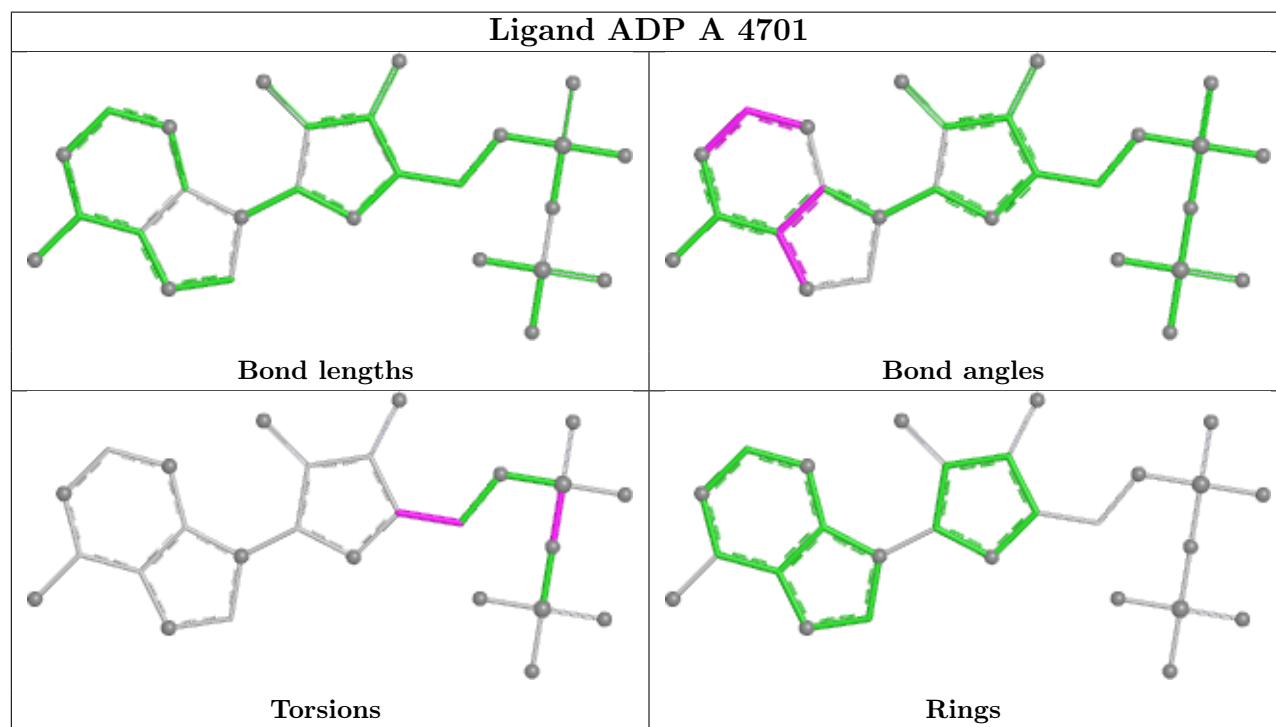
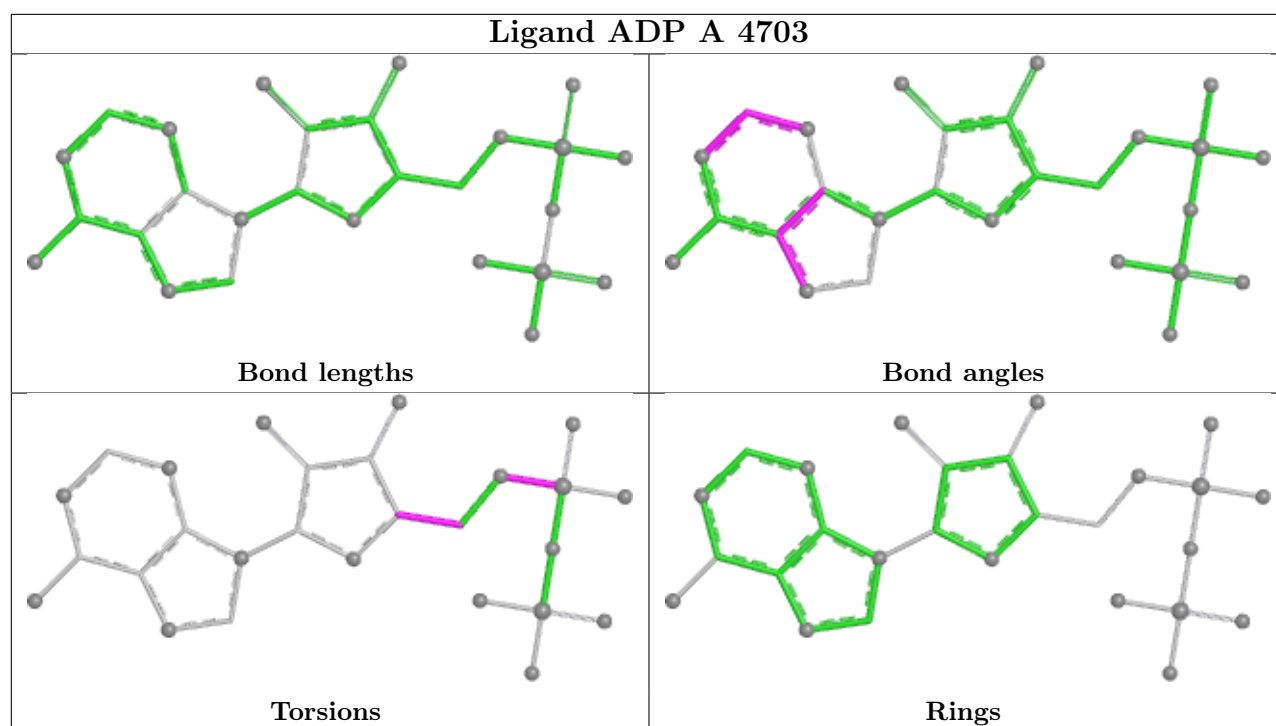
4 monomers are involved in 6 short contacts:

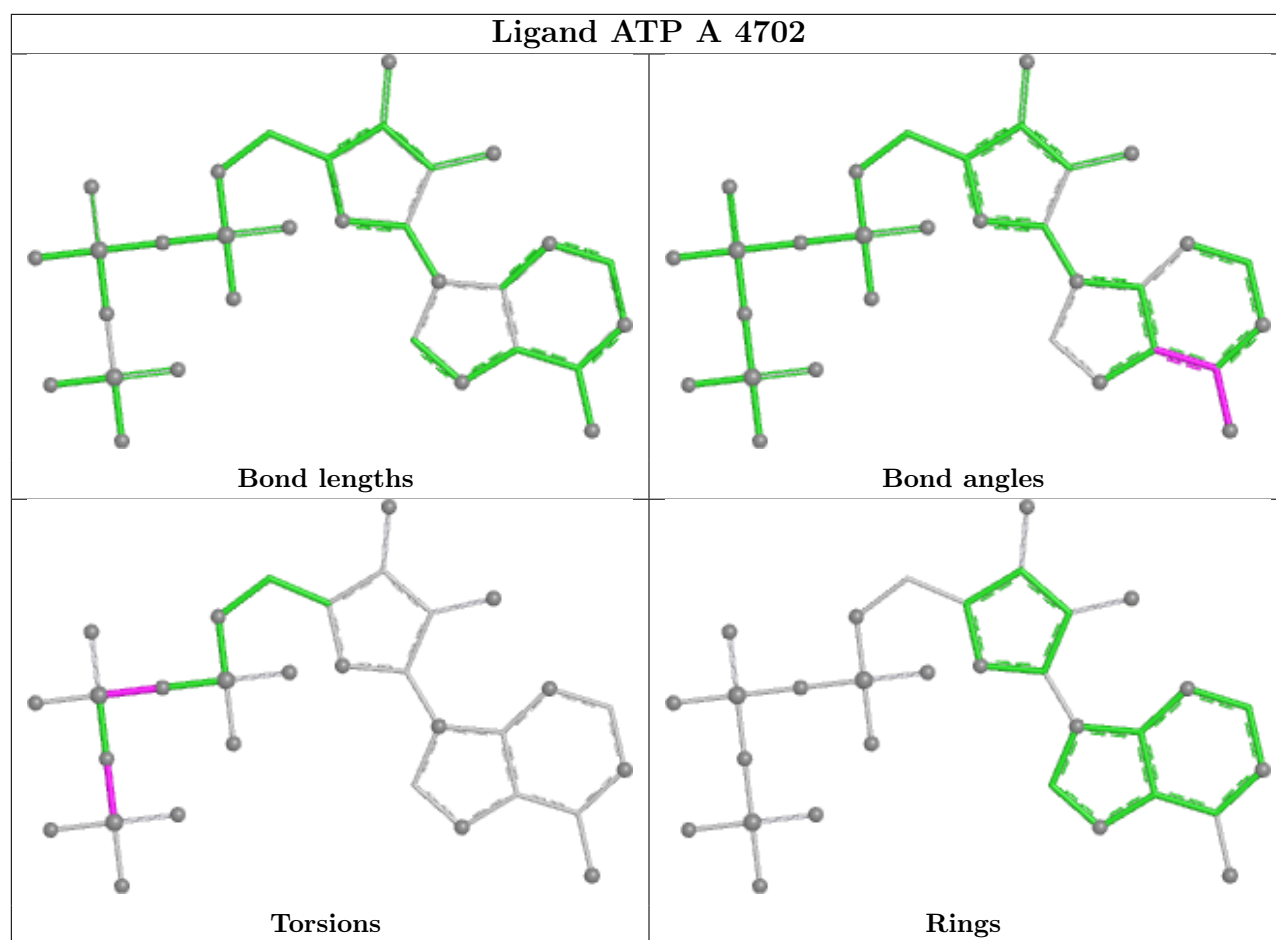
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	2	0
2	A	4703	ADP	1	0
2	A	4701	ADP	2	0
3	A	4702	ATP	1	0

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.

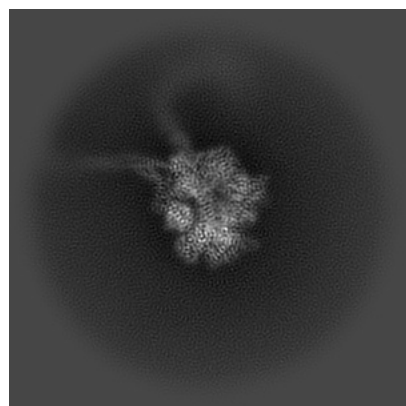
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44694. These allow visual inspection of the internal detail of the map and identification of artifacts.

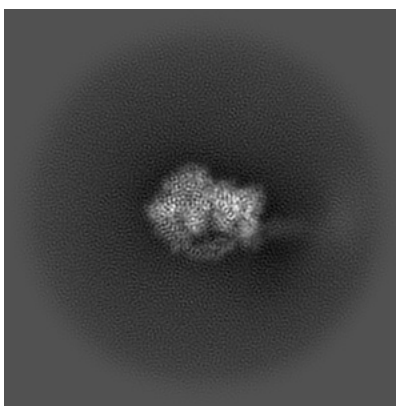
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

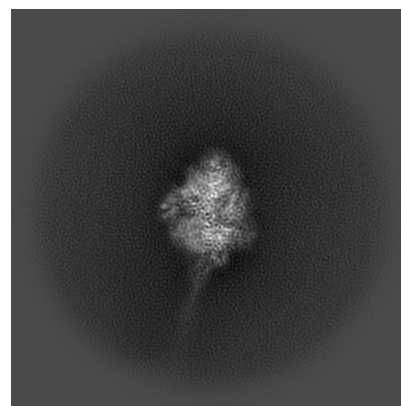
6.1.1 Primary map



X

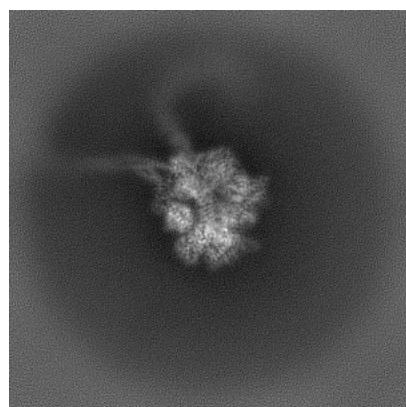


Y

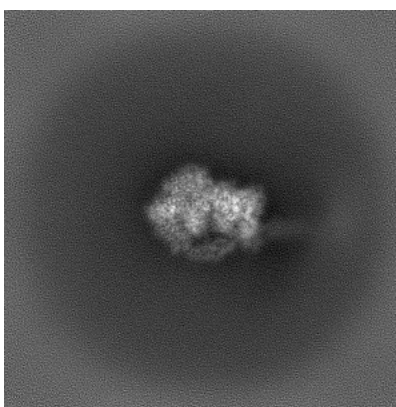


Z

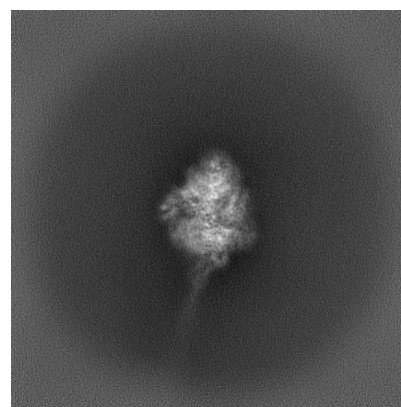
6.1.2 Raw map



X



Y

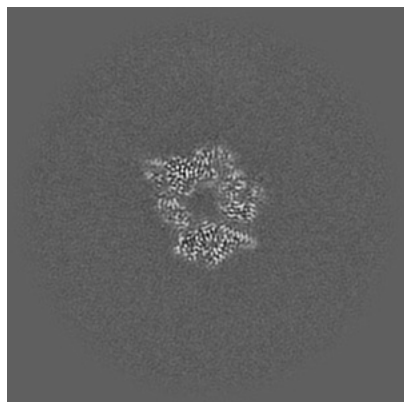


Z

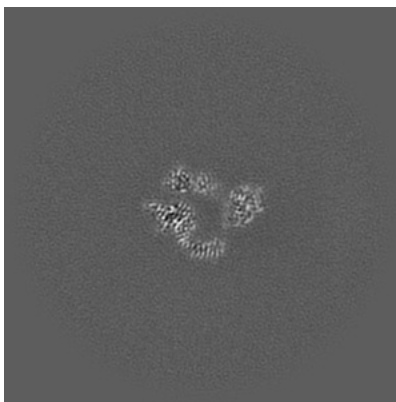
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

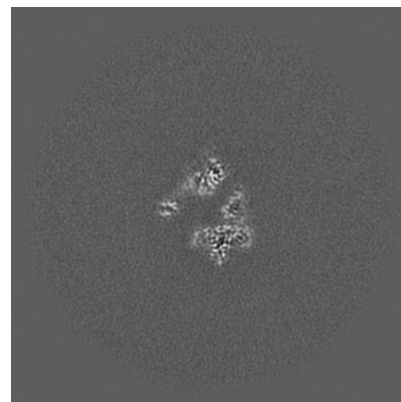
6.2.1 Primary map



X Index: 192

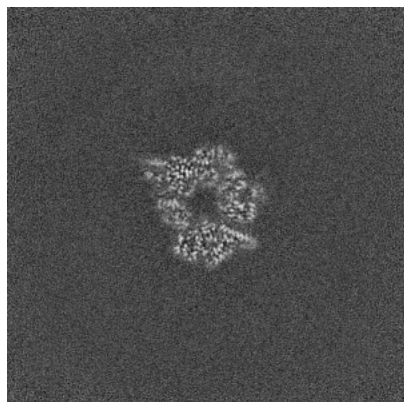


Y Index: 192

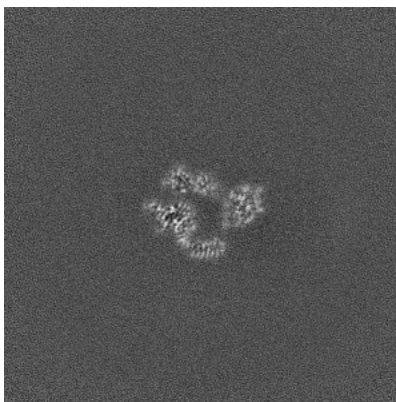


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

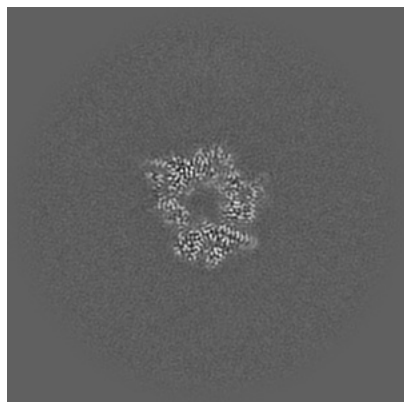


Z Index: 192

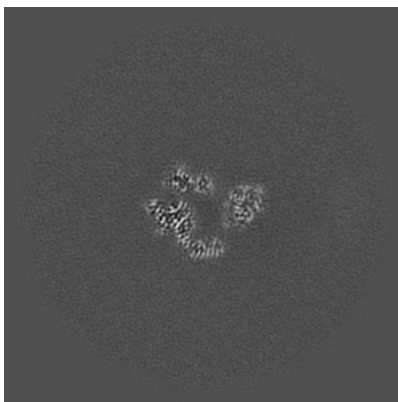
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

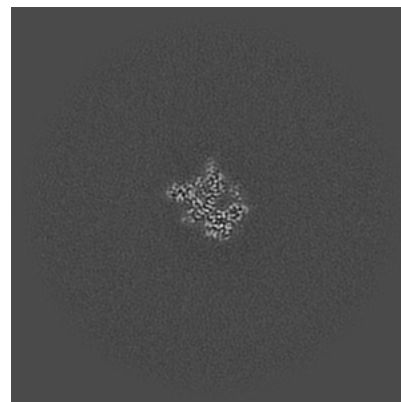
6.3.1 Primary map



X Index: 193

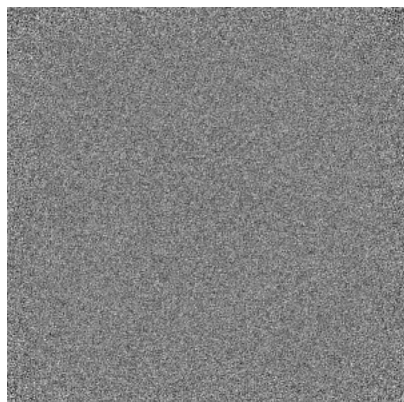


Y Index: 193

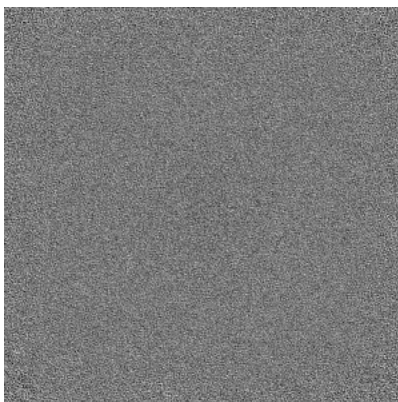


Z Index: 162

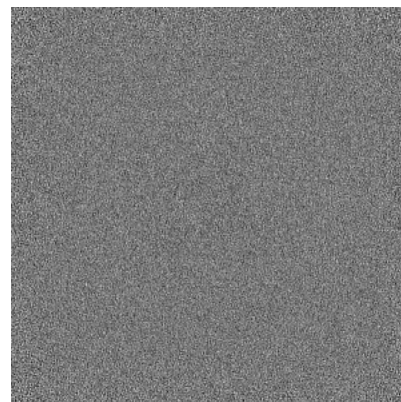
6.3.2 Raw map



X Index: 0



Y Index: 0

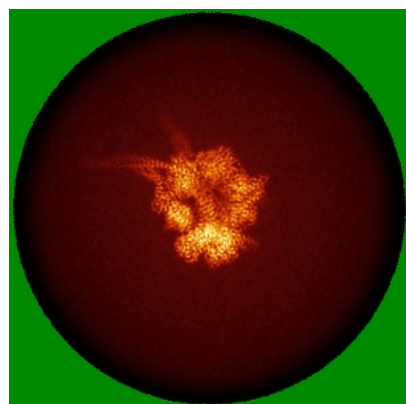


Z Index: 0

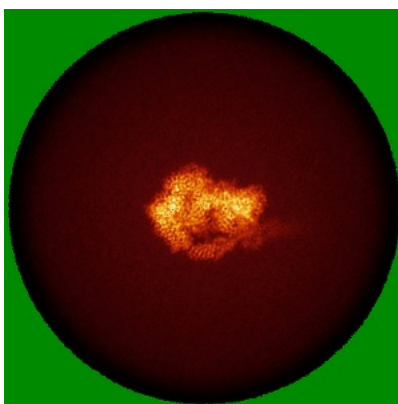
The images above show the largest variance slices of the map in three orthogonal directions.

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

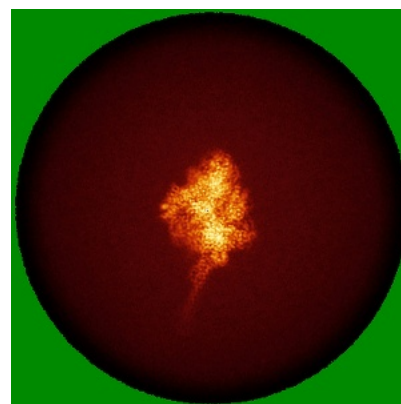
6.4.1 Primary map



X

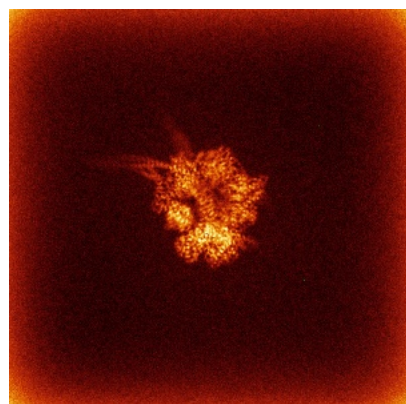


Y

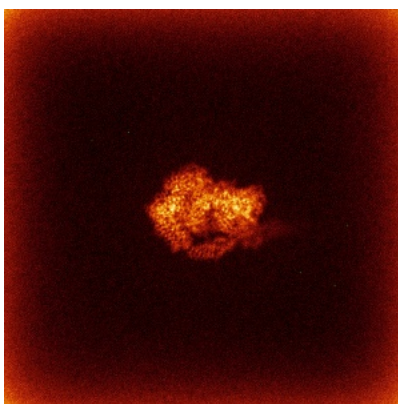


Z

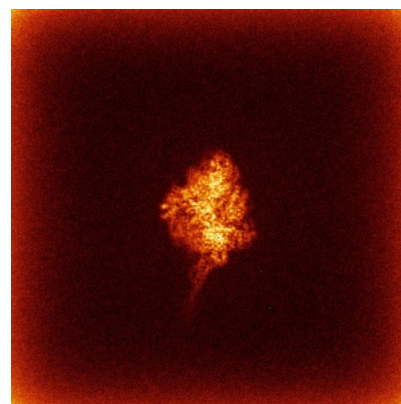
6.4.2 Raw map



X



Y

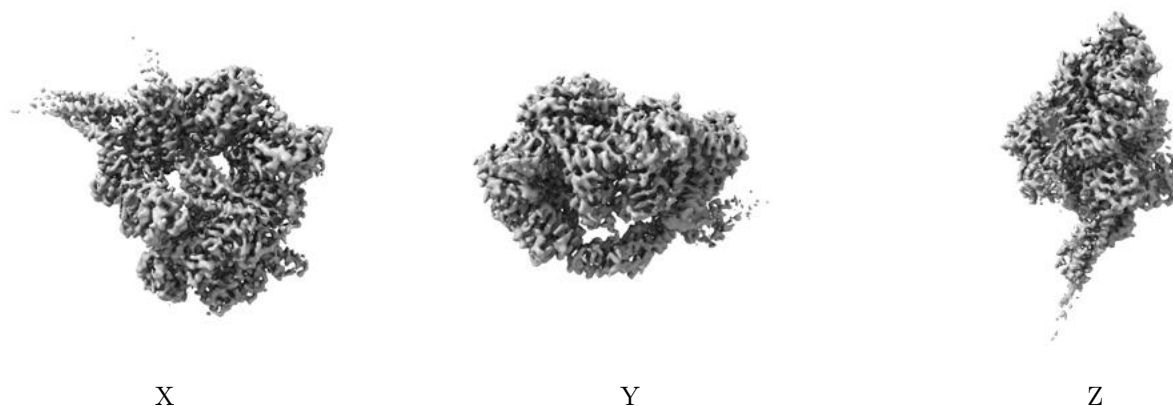


Z

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.

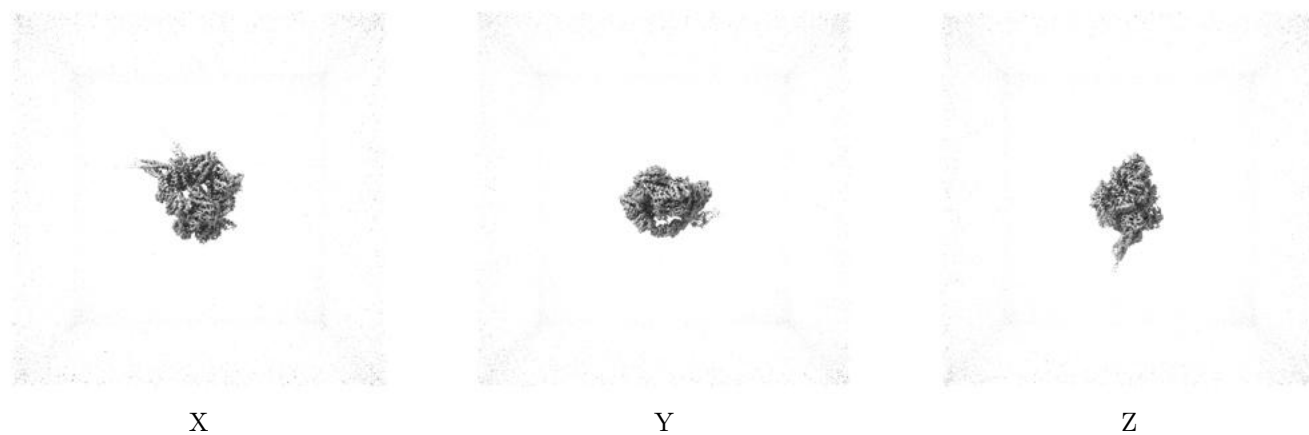
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

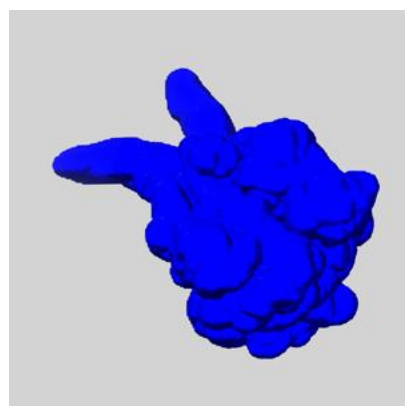
6.6 Mask visualisation [i](#)

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

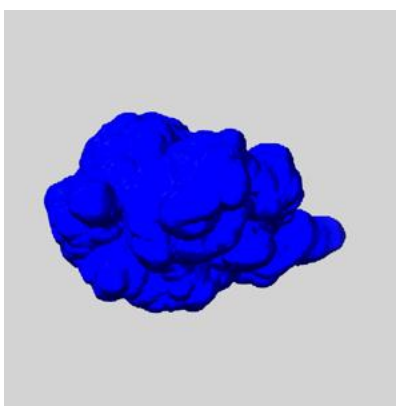
A mask typically either:

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

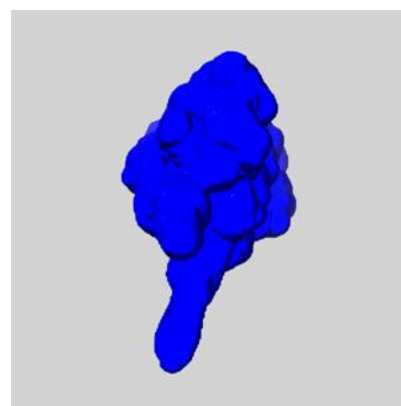
6.6.1 emd_44694_msk_1.map [i](#)



X



Y

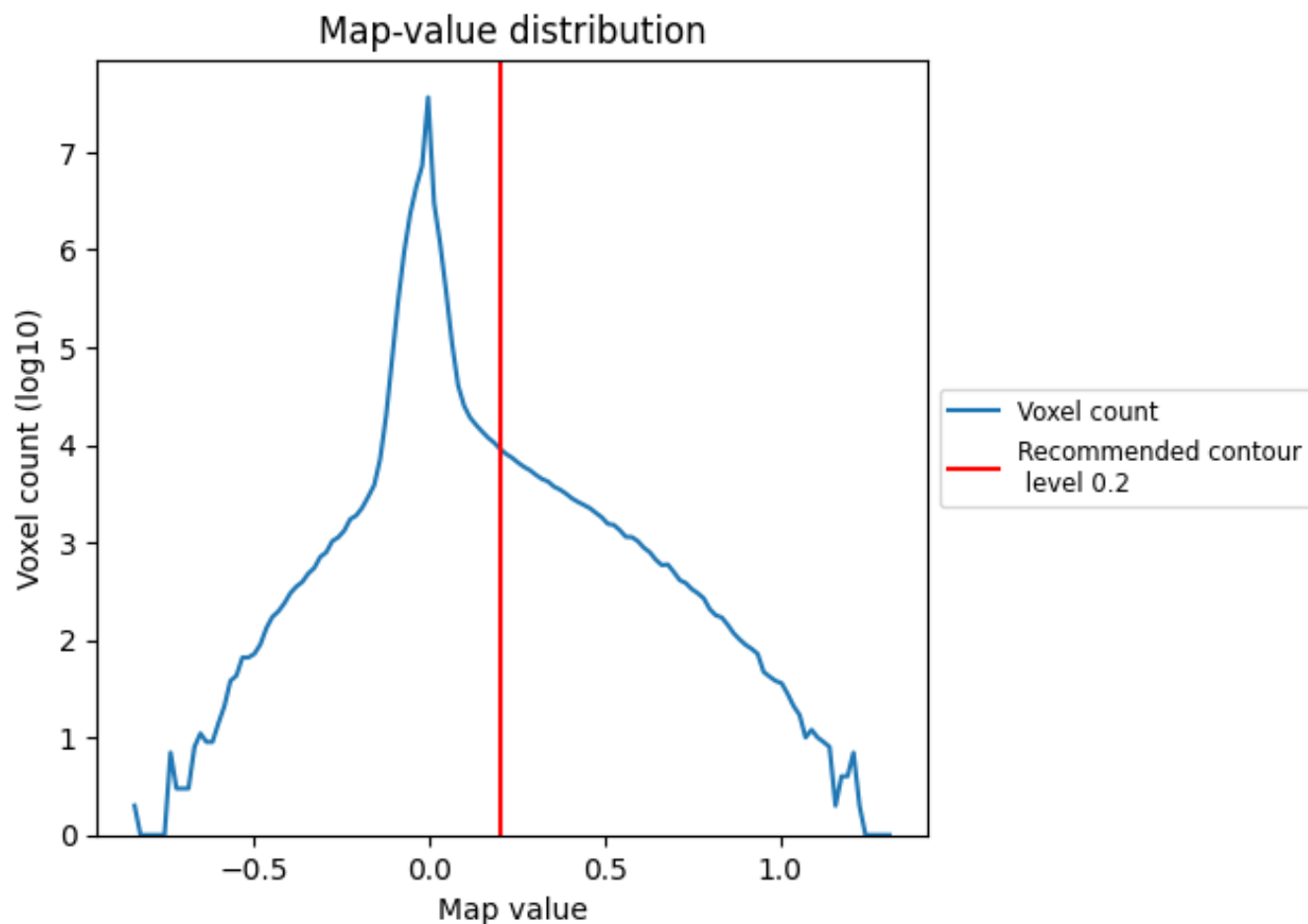


Z

7 Map analysis [i](#)

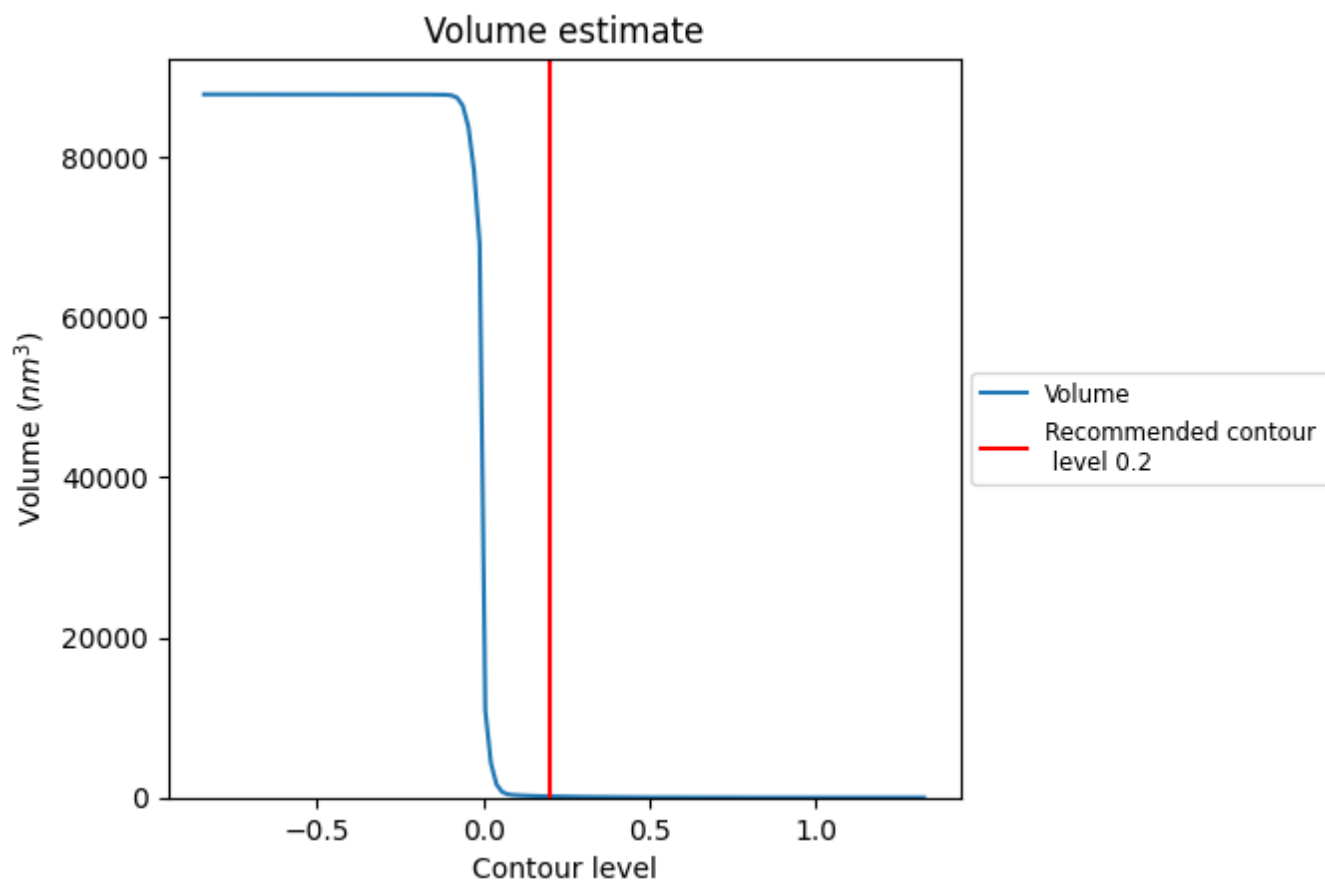
This section contains the results of statistical analysis of the map.

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.

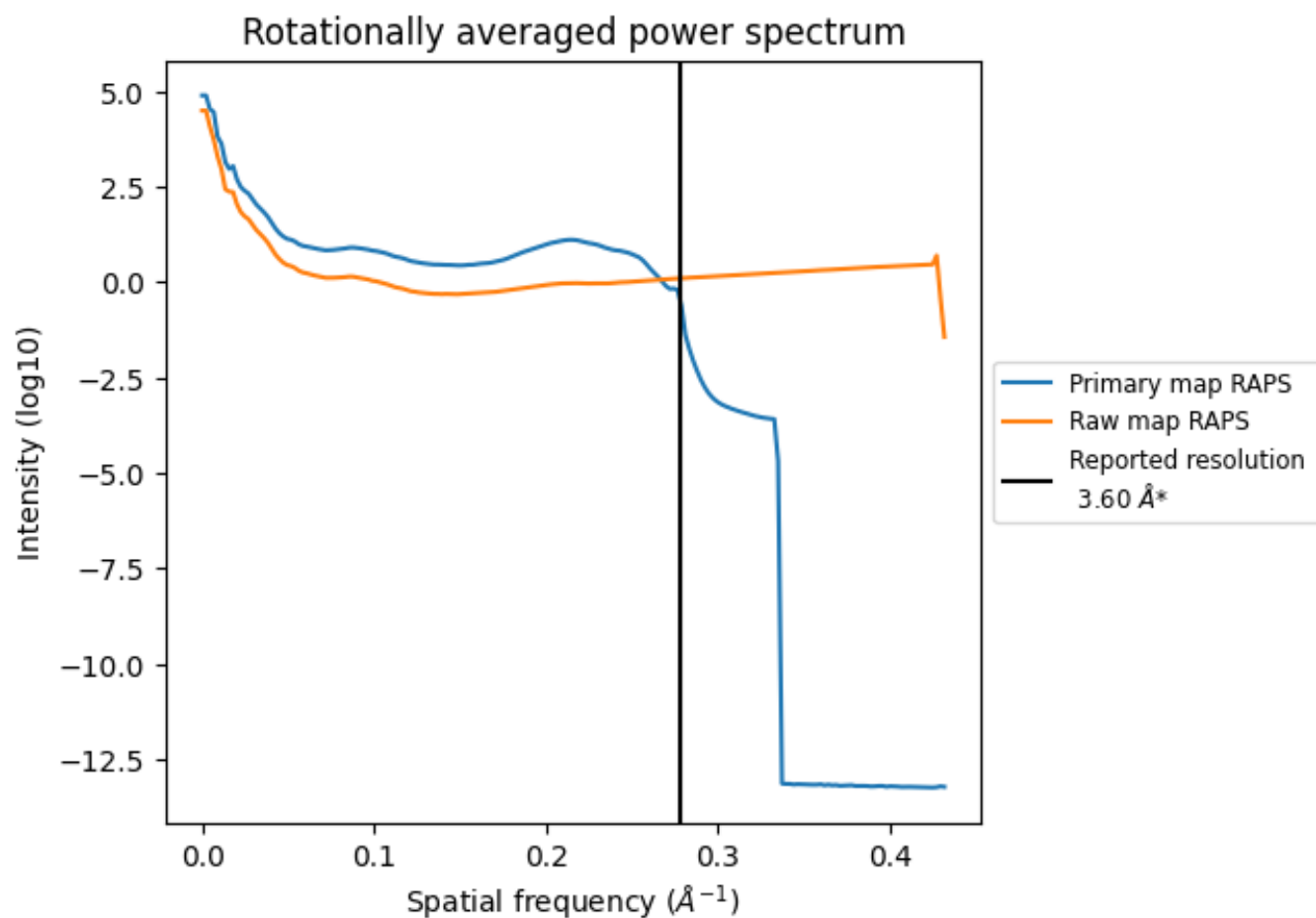
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

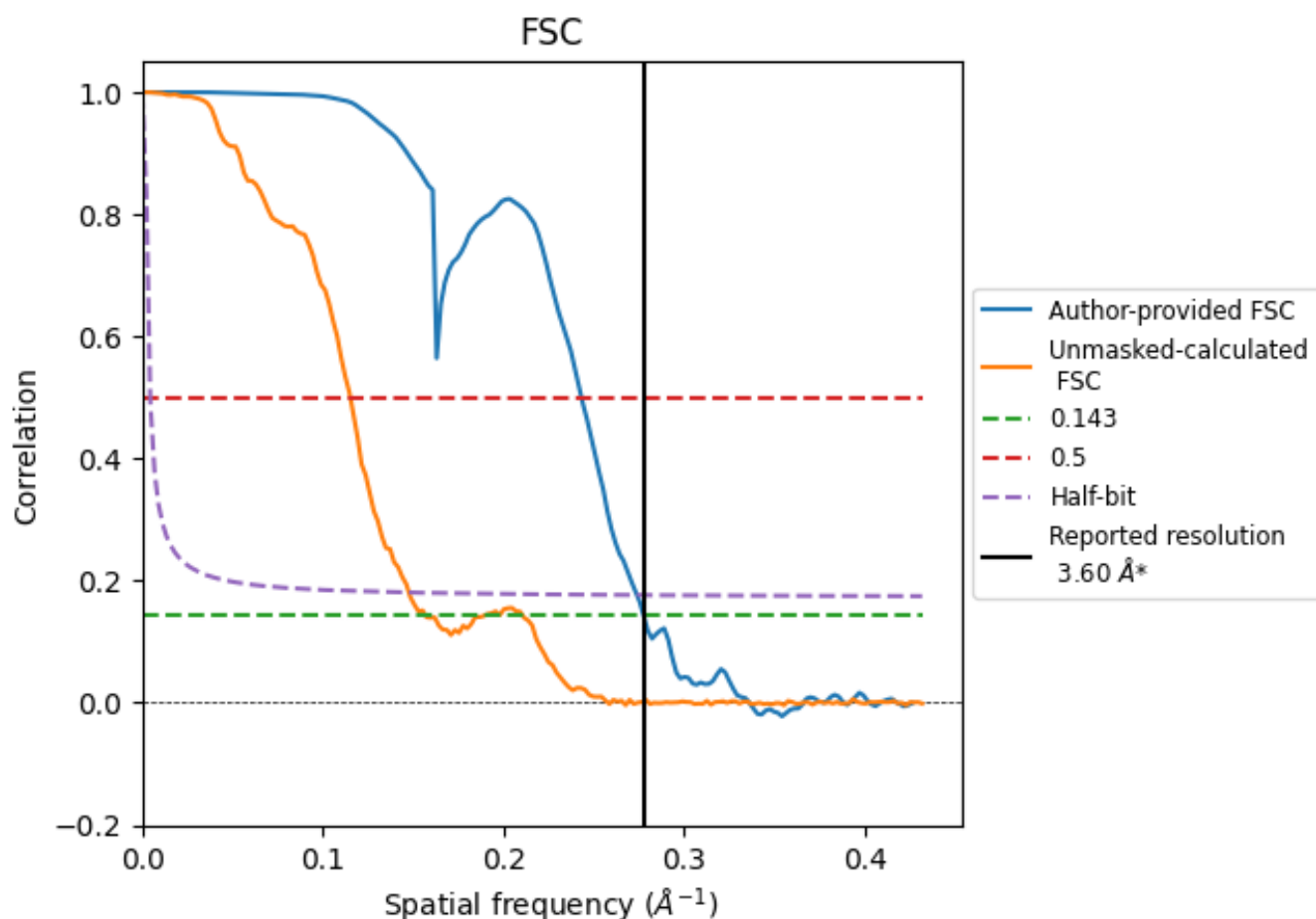


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

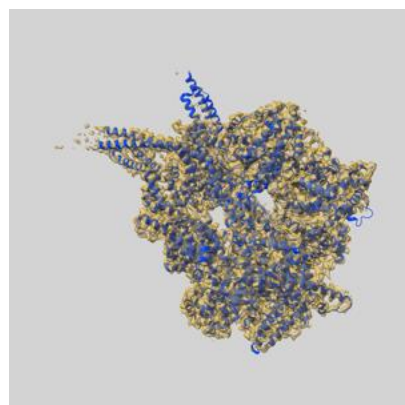
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.11	3.65
Unmasked-calculated*	6.37	8.67	6.77

*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 6.37 differs from the reported value 3.6 by more than 10 %

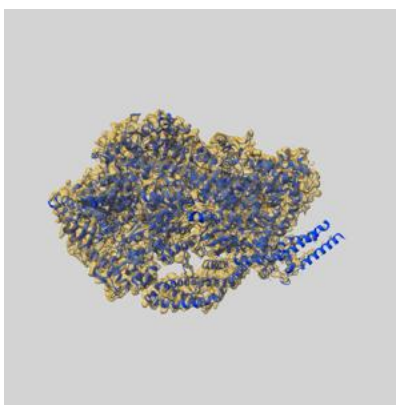
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44694 and PDB model 9BMB. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

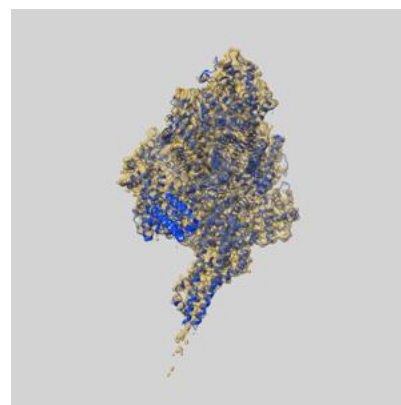
9.1 Map-model overlay [i](#)



X



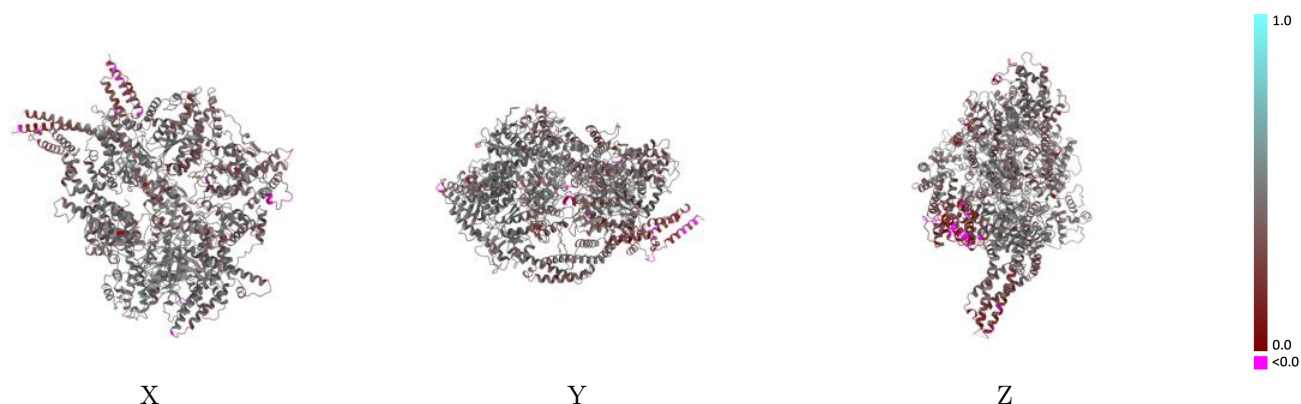
Y



Z

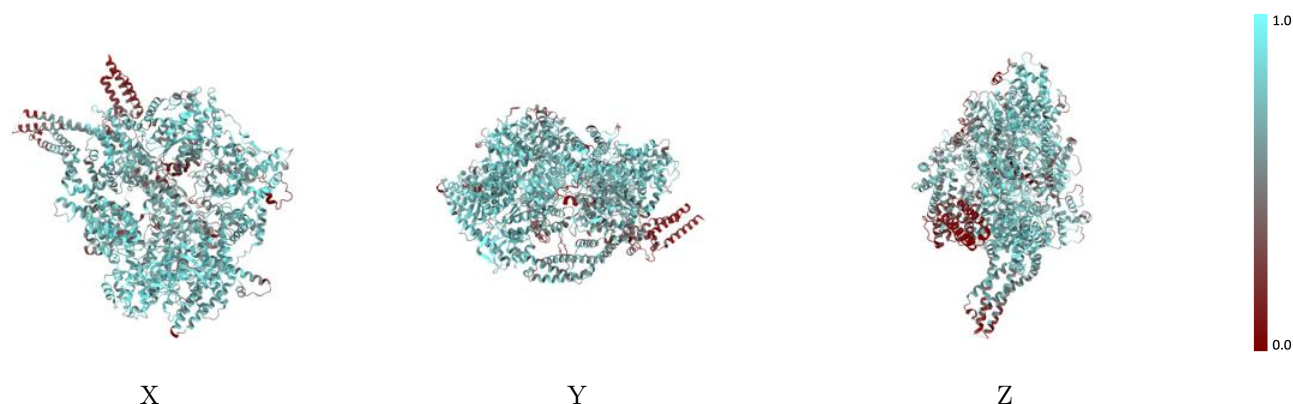
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



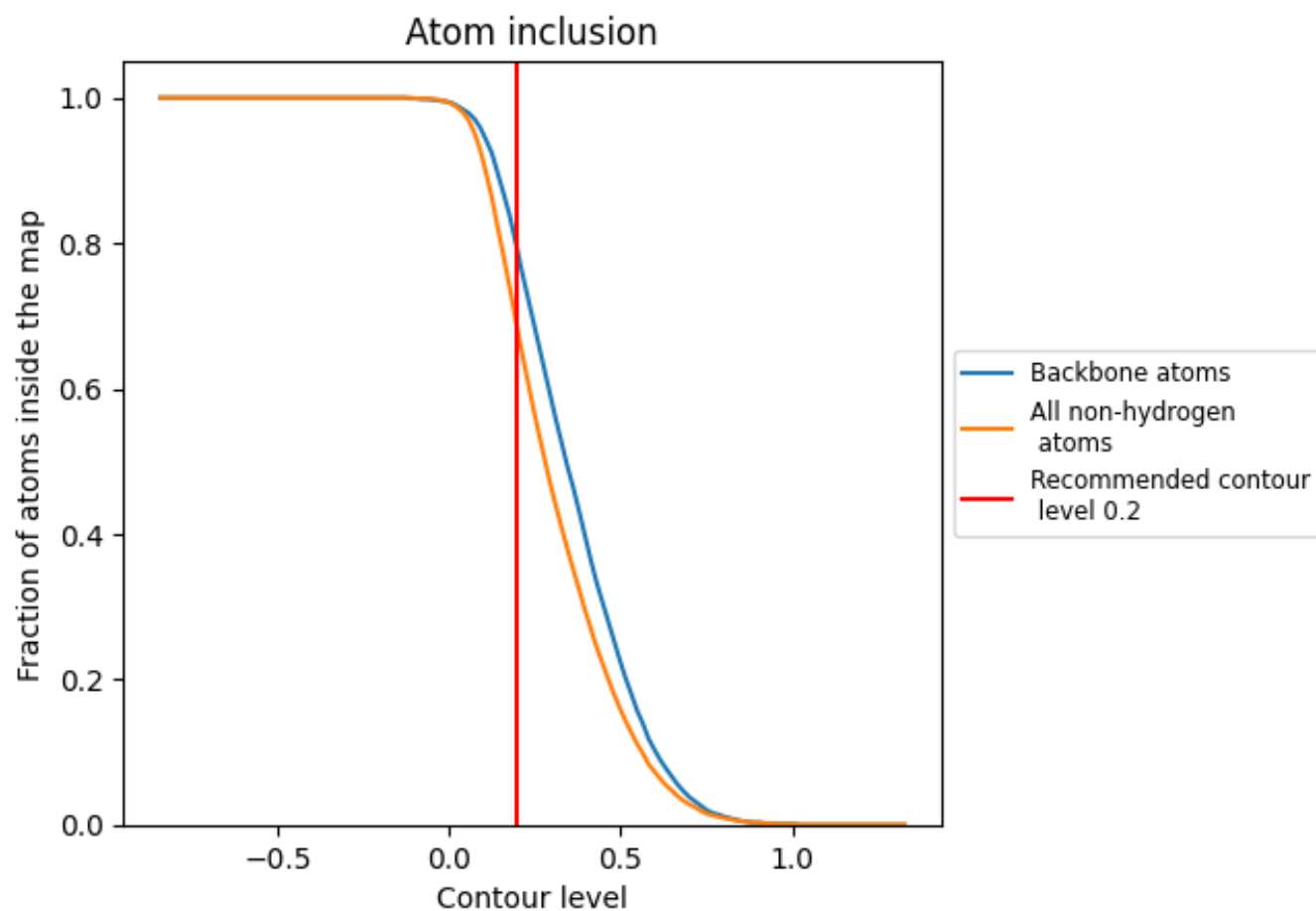
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6810	<div></div> 0.4140
A	<div></div> 0.6810	<div></div> 0.4140

