



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 01:15 AM UTC

PDB ID : 9BMD / pdb_00009bmd
EMDB ID : EMD-44696
Title : Motor domain from full-length human dynein-1 bound to microtubules in 5mM AMPPNP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.90 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:

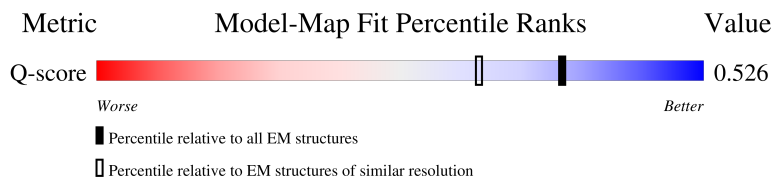
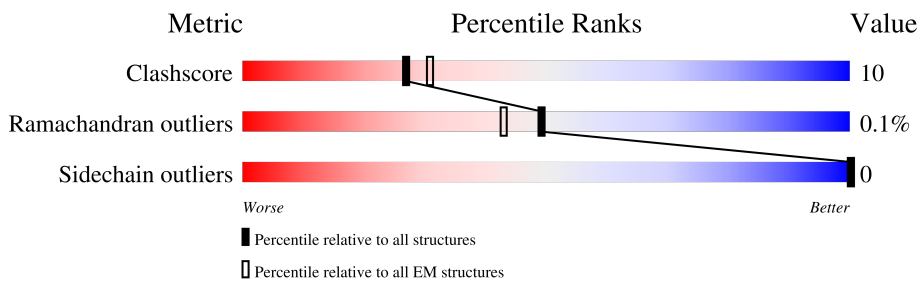
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	<p>21% (red), 49% (green), 17% (yellow), 35% (grey)</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24603 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	3038	24479	15591	4228	4538	122	1	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



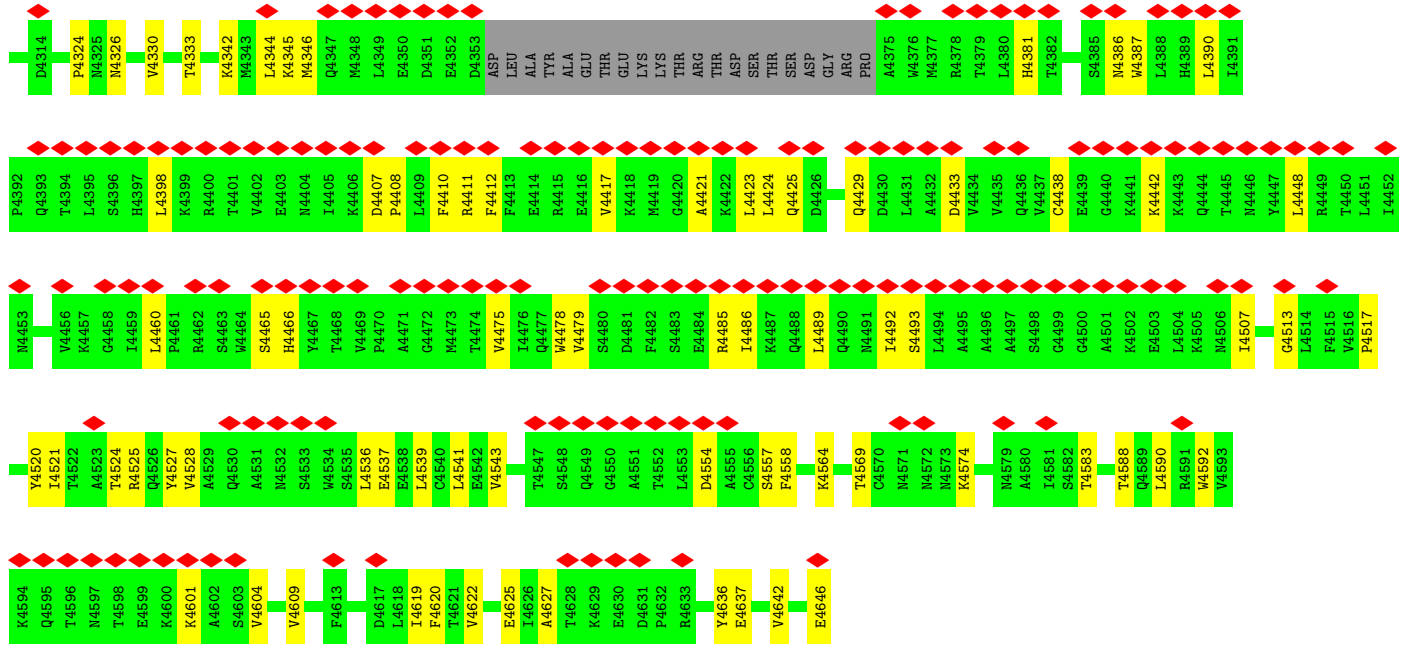
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

K3113	D3114	L3115	E3116	K3117	F3118	N3119	I3120	I3121	F3122	D3123	I3124	K3125	K3126	F3127	V3128	D3131	K3132	L3133	F3134	I3135	F3136	F3137	R3140	E3141	A3142	I3143	V3144	V3148	T3067	N3069	F3070	SER	SER	GLU	GLY	LEU	LYS	ASP	ARG	ALA	A3080	T3081	S3082	R3088	C3088	V3090	L3091	N3092	V3093	T3099	Y3103	E3108	K3112			
L2090	L2093	K2094	L2097	V2103	K2104	E2105	E2106	T2107	Q2108	Q2109	K2110	T2111	K2112	R2113	E2114	K2115	E2116	E2117	R2118	G2119	E2120	A2121	V2122	D2123	E2205	K2206	V2207	L2208	G2125	E2126	T2127	A2128	E2129	N2130	L2131	F2132	E2133	Q2134	E2135	L2136	L2137	I2138	Q2139	S2140	V2141	K2148	L2149	V2150	A2151	D2152	D2153	P2155	L2156	L2157	L2160	L2161
S2162	D2163	V2168	Q2169	Y2170	H2171	K2260	K2261	D2262	T2267	E2174	M2175	R2179	E2180	E2181	E2188	L2191	T2192	D2195	E2196	E2197	M2202	V2203	V2204	E2205	K2206	V2207	L2208	Q2209	E2210	T2211	Q2212	I2213	T2214	Q2215	I2216	N2217	H2218	G2219	L2220	M2221	V2222	G2223	G2227	K2230	S2231	M2232	V2233	A2234	E2235	V2236	E2242	R2243				
L2244	E2245	E2248	R2340	T2341	S2260	K2261	D2262	T2267	L2268	D2269	P2270	N2271	T2272	R2273	E2274	W2275	T2276	D2277	G2278	T2281	H2282	R2285	L2288	D2289	S2290	V2291	R2292	G2293	E2294	L2295	Q2296	K2297	D2306	P2309	E2313	N2314	L2319	D2320	D2321	N2322	K2323	L2324	L2325	T2326	L2327	P2328	N2329	G2330	E2331	R2332	L2333					
S2334	L2335	R2340	T2341	F2342	R2343	E2344	Q2345	Q2346	D2347	L2348	A2351	T2352	L2353	S2357	R2358	C2359	G2360	M2361	V2362	W2363	D2367	V2368	L2369	S2370	T2371	D2372	M2373	L2374	L2382	T2385	P2386	L2387	D2388	E2389	G2390	E2391	D2392	E2393	A2394	Q2395	R2396	R2397	R2398	K2399	G2400	L2401	E2402	D2403	E2404	G2405	E2406	E2407	A2408			
A2409	S2410	P2411	M2412	Q2413	Q2414	I2415	Q2416	R2417	D2418	A2419	A2420	T2428	S2429	N2430	V2433	T2434	L2437	E2438	H2439	A2440	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2449	T2450	R2451	L2452	R2453	C2454	S2460	A2465	C2466	R2467	N2468	Q2471	Y2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	I2483	E2484			
R2485	L2486	R2488	V2493	L2494	V2495	T2498	L2499	L2502	S2503	D2504	Q2505	S2506	R2507	K2508	P2509	L2510	V2511	A2512	E2513	L2514	G2515	E2516	L2517	L2518	R2519	R2520	L2521	T2522	L2523	V2524	P2527	T2528	A2529	P2530	N2531	L2532	P2533	T2534	L2535	L2541	S2542	G2543	E2544	W2545	K2551	Q2554	L2555	E2556	V2557	E2558	T2559					
H2560	K2561	A2564	P2565	D2566	T2571	T2574	H2577	L2581	Q2505	S2506	R2507	K2508	P2509	L2510	V2511	A2512	E2513	L2514	G2515	E2516	L2517	L2518	R2519	R2520	L2521	T2522	L2523	V2524	P2527	T2528	A2529	P2530	N2531	L2532	P2533	T2534	L2535	L2541	S2542	G2543	E2544	W2545	K2551	Q2554	L2555	E2556	V2557	E2558	T2559							
H2560	K2561	A2564	P2565	D2566	T2571	T2574	H2577	L2581	Q2505	S2506	R2507	K2508	P2509	L2510	V2511	A2512	E2513	L2514	G2515	E2516	L2517	L2518	R2519	R2520	L2521	T2522	L2523	V2524	P2527	T2528	A2529	P2530	N2531	L2532	P2533	T2534	L2535	L2541	S2542	G2543	E2544	W2545	K2551	Q2554	L2555	E2556	V2557	E2558	T2559							
R2667	L2668	M2671	D2672	K2673	Y2674	G2675	R2684	T2685	S2686	D2687	V2701	F2708	H2688	K2689	L2690	V2691	P2714	P2718	G2719	R2720	L2723	R2726	F2727	L2728	V2731	P2732	V2733	V2734	Y2735	V2736	D2737	I2747	Y2748	P2636	H2637	R2642	R2643	T2644	P2645	N2646	V2648	L2655	G2656	K2657	F2662	D2664	E2665	T2666								
D2787	T2788	R2797	E2798	M2799	L2883	K2894	A2895	R2896	L2897	K2898	V2899	F2900	Y2901	E2902	E2903	E2904	L2905	D2906	V2907	V2910	E2914	V2915	H2918	V2919	L2920	E2921	L2922	D2923	R2924	I2925	F2926	R2927	Q2928	P2929	Q2930	L2933	L2934	L2935	I2936	G2937	V2938	K2943	L2946	S2947	R2948	F2949	V2950	M2953	L2956							
L2961	K2962	V2963	H2964	K2966	Y2967	T2968	G2969	E2970	F2971	D2972	D2973	E2974	D2975	R2982	K2986	K2989	D2995	E2996	S2997	N2998	V2999	L3000	D3001	S3002	G3003	F3004	L3005	E3006	R3007	M3008	N3009	T3010	L3011	L3012	A3013	N3014	G3015	E3016	V3017	P3018	N3019	N3022	R2948	F2949	V2950	M2953	L2956									
Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	M3043	L3044	S3045	S3046	H3047	E3048	K3052	Q3057	R3060	N3061	V3064	V3065	F3066	M3067	M3068	N3069	F3070	SER	SER	GLU	GLY	LEU	LYS	ASP	ARG	ALA	A3080	T3081	S3082	R3088	C3088	V3090	L3091	N3092	V3093	T3099	Y3103	E3108	K3112							
D3178	A3184	H3188	R3191	S3192	E3193	L3194	E3195	E3196	D3178	A3184	H3188	R3191	S3192	E3193	L3194	E3195	E3196																																							



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241362	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	1.441	Depositor
Minimum map value	-0.841	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ATP, ANP, 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	0.18	0/25000	0.33	0/33870

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	24479	0	24538	487	0
2	A	27	0	12	2	0
3	A	31	0	12	2	0
4	A	62	0	26	3	0
5	A	4	0	0	0	0
All	All	24603	0	24588	487	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 487 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:2598:GLY:H	4:A:4703:ANP:HNB1	1.23	0.82
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.64	0.80
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.68	0.75
1:A:1397:ASN:O	1:A:1401:ILE:HD12	1.91	0.70
1:A:2506:SER:HB3	1:A:2510:MET:HB2	1.71	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	3029/4646 (65%)	2974 (98%)	53 (2%)	2 (0%)	48 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4292	LYS
1	A	4130	ILE

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	2704/4125 (66%)	2704 (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. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3772	ASN
1	A	4174	ASN
1	A	3799	GLN
1	A	4054	HIS
1	A	2215	GLN

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 8 ligands modelled in this entry, 4 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	$\# Z > 2$
4	ANP	A	4704	5	33,33,33	2.29	5 (15%)	45,52,52	1.20	3 (6%)
4	ANP	A	4703	5	33,33,33	2.28	5 (15%)	45,52,52	1.17	3 (6%)
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
3	ATP	A	4702	5	32,33,33	0.38	0	48,52,52	0.27	0

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
4	ANP	A	4704	5	-	8/18/38/38	0/3/3/3
4	ANP	A	4703	5	-	4/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4704	ANP	PB-O3A	8.86	1.70	1.59
4	A	4703	ANP	PB-O3A	8.78	1.70	1.59
4	A	4703	ANP	PG-N3B	6.25	1.79	1.63
4	A	4704	ANP	PG-N3B	6.20	1.79	1.63
4	A	4704	ANP	PG-O1G	4.70	1.53	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.80	118.74	126.72
4	A	4703	ANP	O2B-PB-O1B	4.89	120.35	109.87
4	A	4704	ANP	O2B-PB-O1B	4.81	120.17	109.87
2	A	4701	ADP	N3-C4-N9	4.60	135.00	127.17
4	A	4704	ANP	O1G-PG-N3B	-4.10	105.73	111.77

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

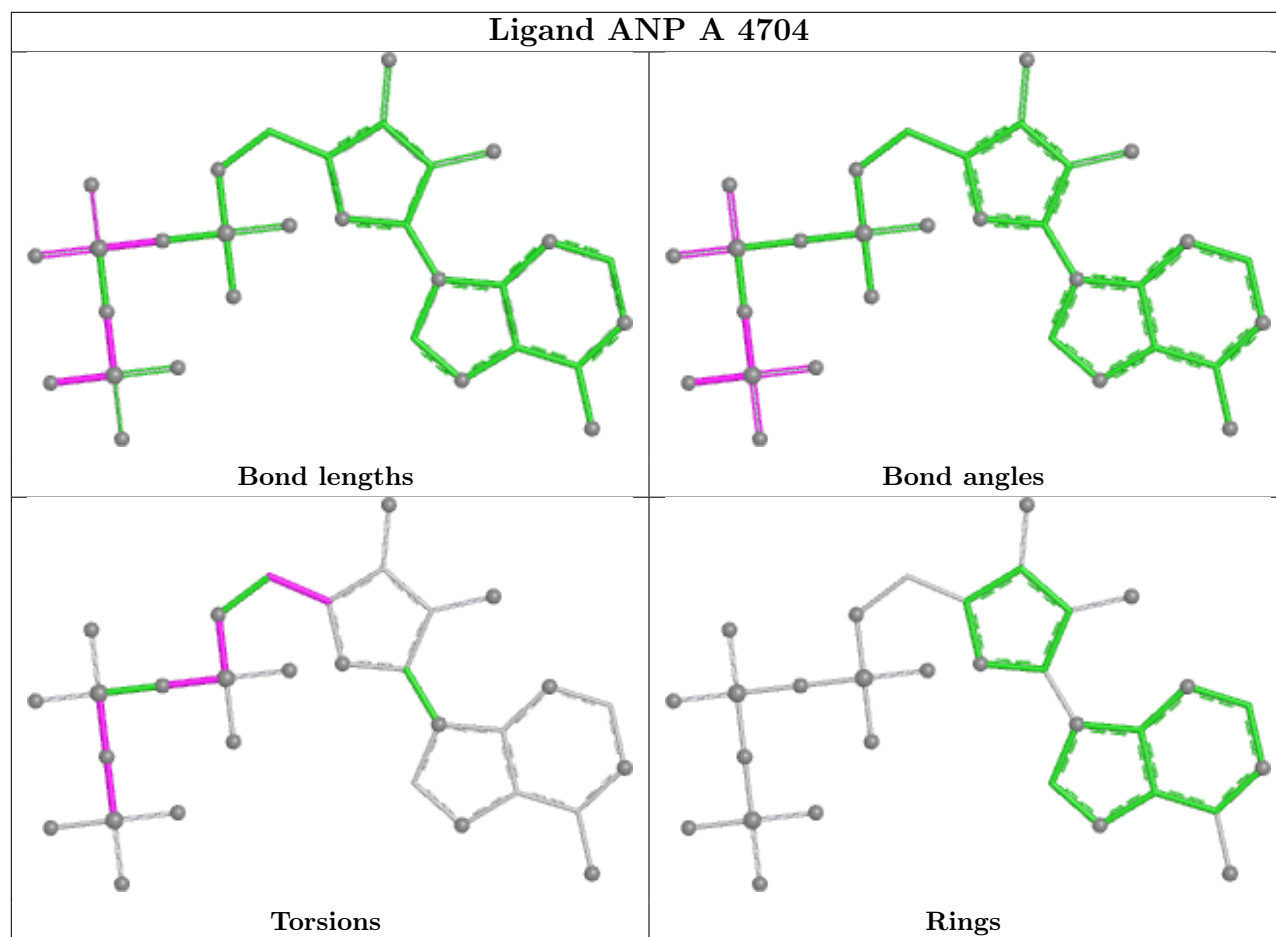
Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4704	ANP	PB-N3B-PG-O1G
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	C5'-O5'-PA-O2A

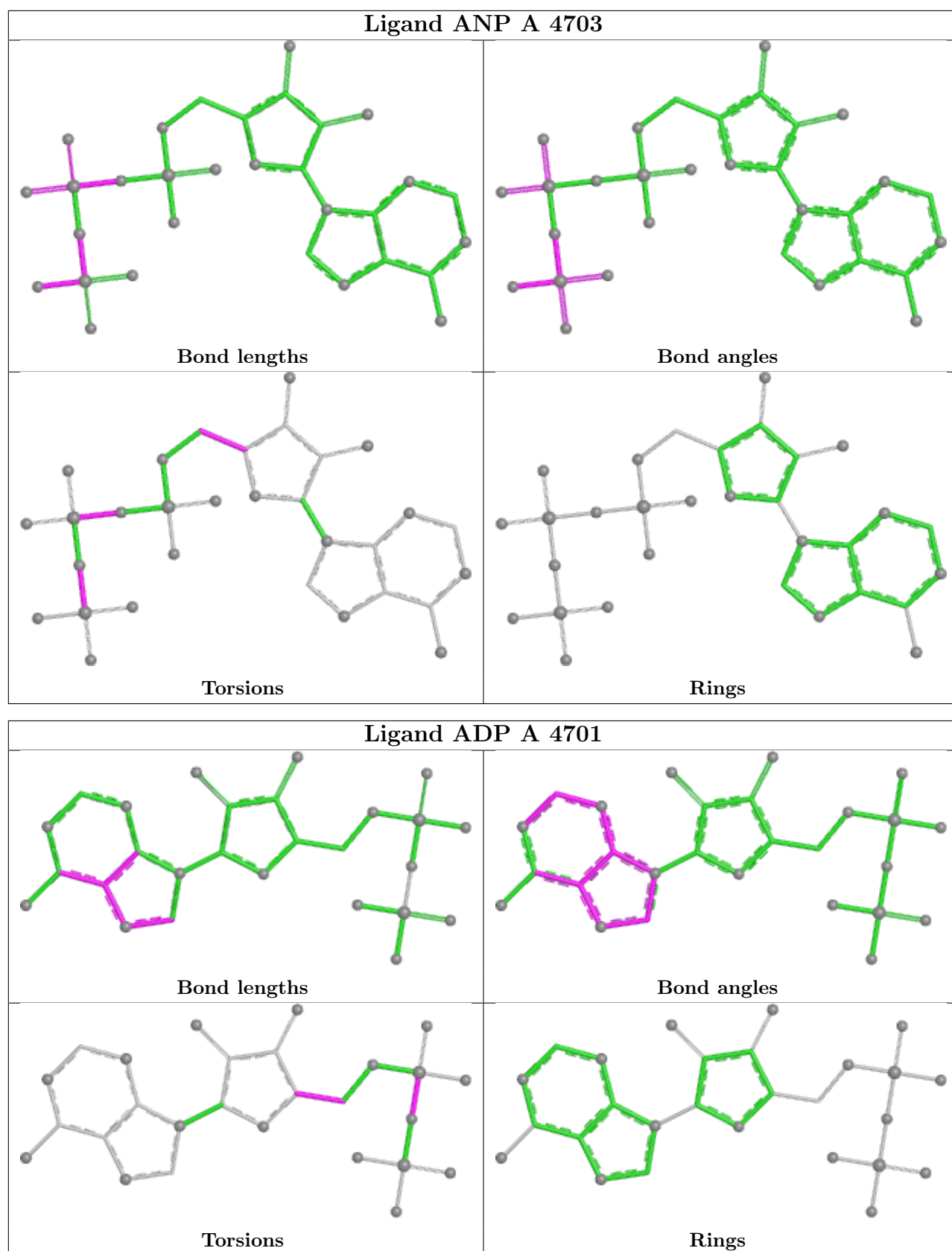
There are no ring outliers.

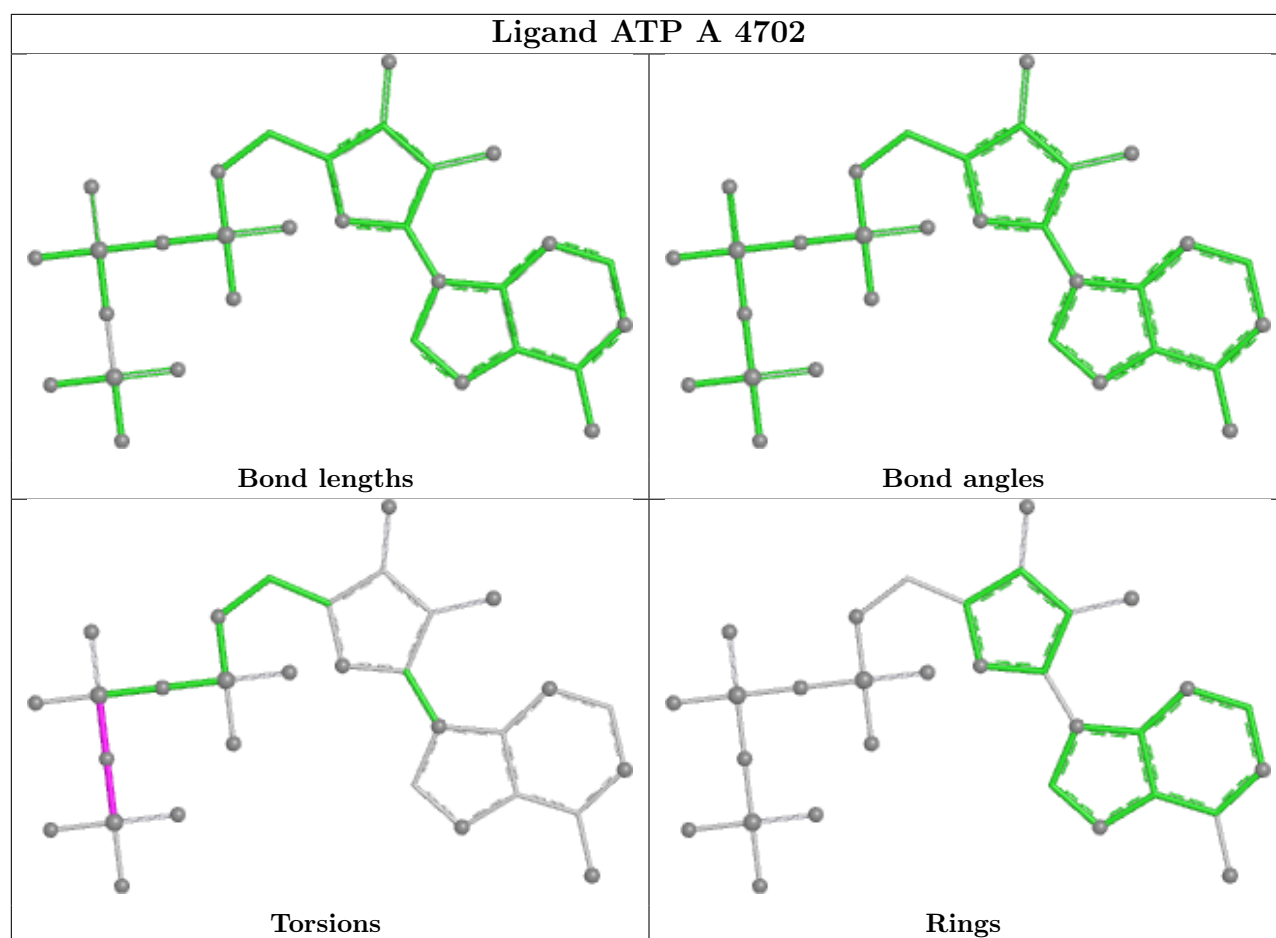
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	3	0
2	A	4701	ADP	2	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.

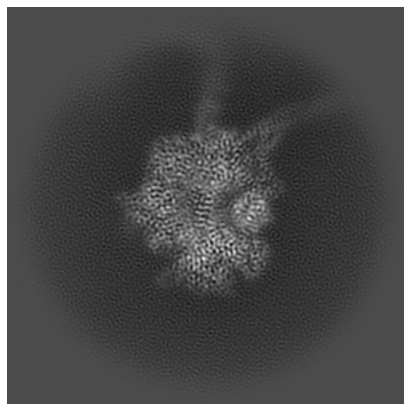
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44696. These allow visual inspection of the internal detail of the map and identification of artifacts.

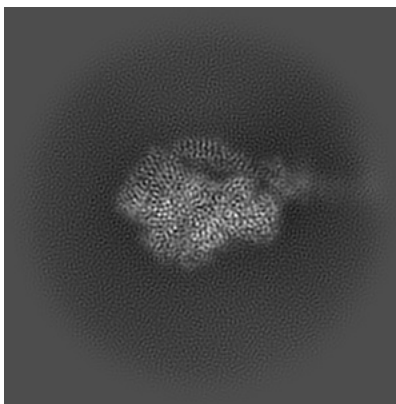
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

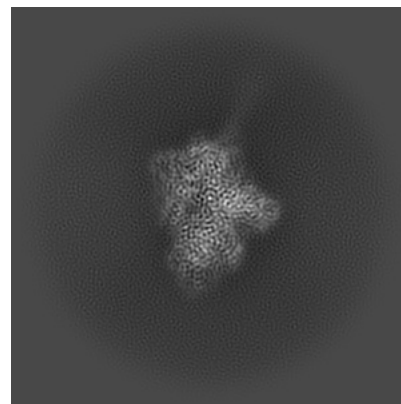
6.1.1 Primary map



X

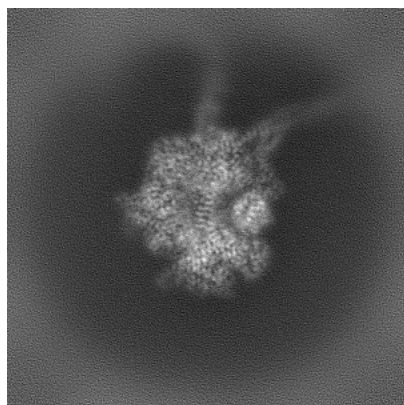


Y

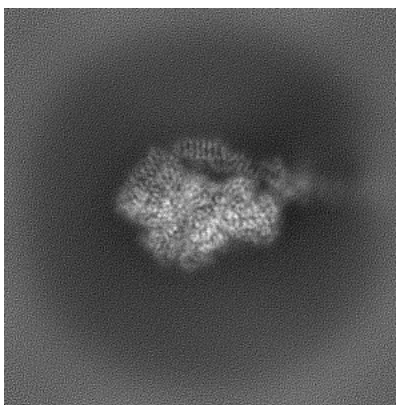


Z

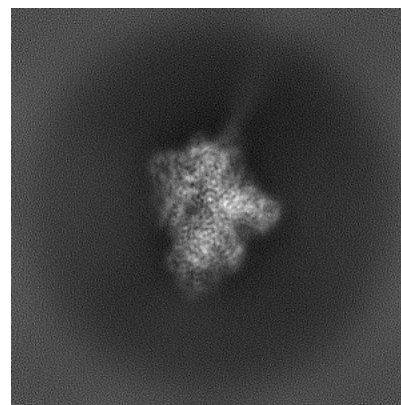
6.1.2 Raw map



X



Y

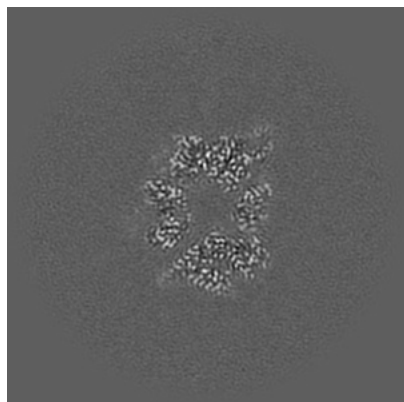


Z

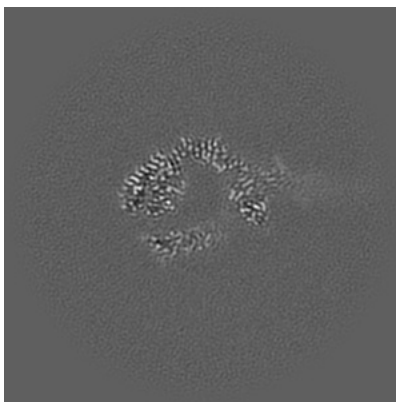
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

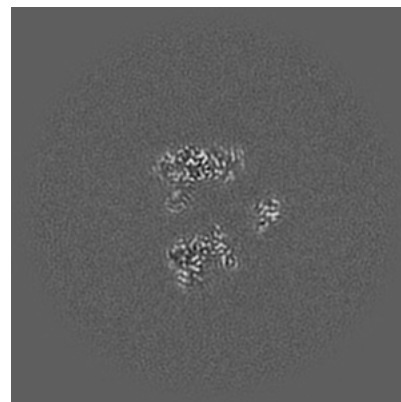
6.2.1 Primary map



X Index: 192

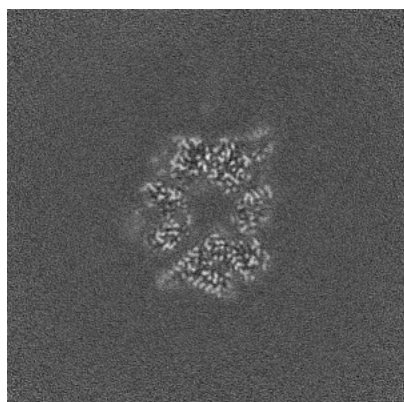


Y Index: 192

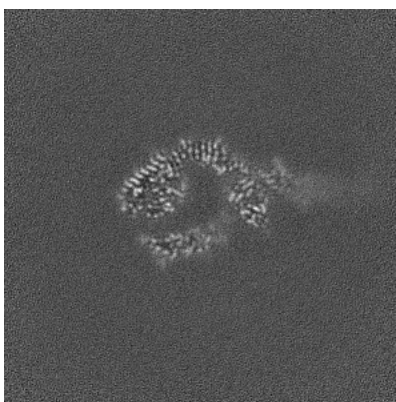


Z Index: 192

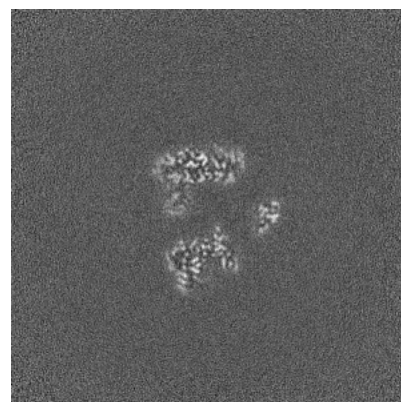
6.2.2 Raw map



X Index: 192



Y Index: 192

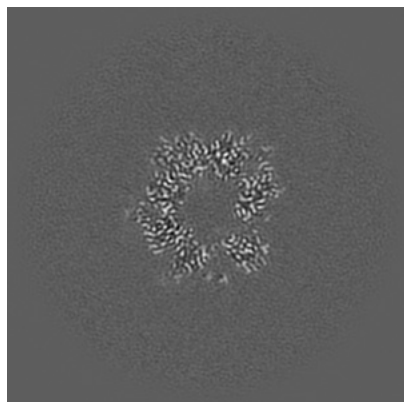


Z Index: 192

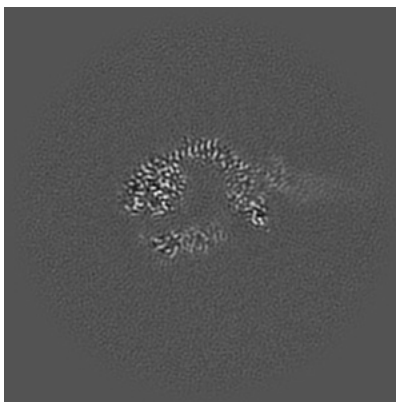
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

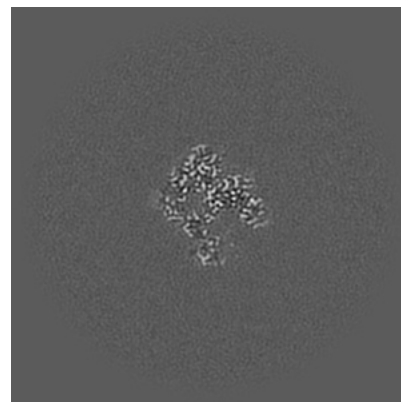
6.3.1 Primary map



X Index: 184

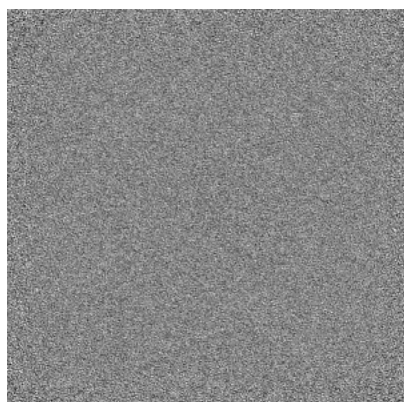


Y Index: 194

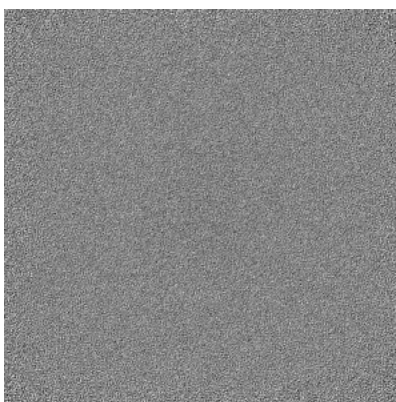


Z Index: 154

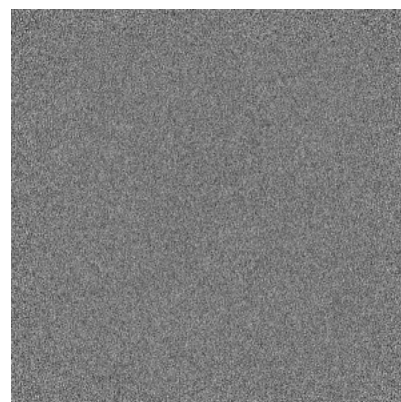
6.3.2 Raw map



X Index: 0



Y Index: 0

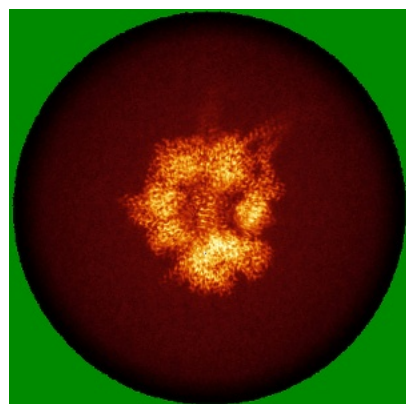


Z Index: 0

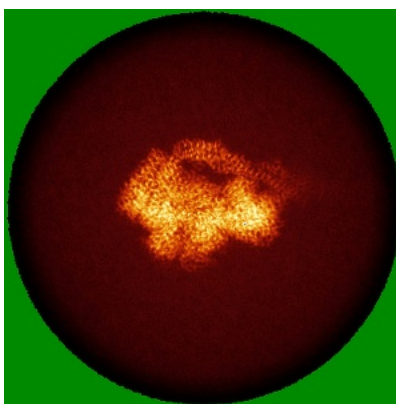
The images above show the largest variance slices of the map in three orthogonal directions.

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

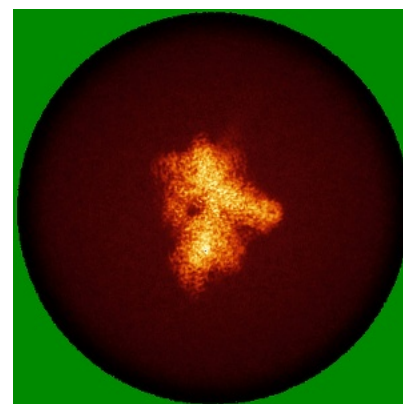
6.4.1 Primary map



X

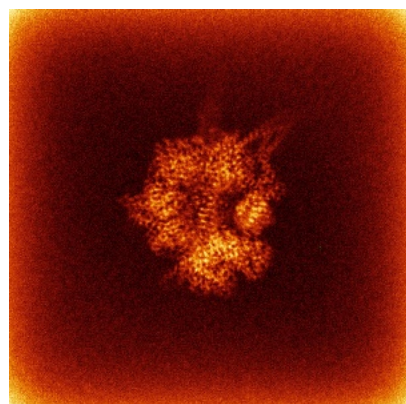


Y

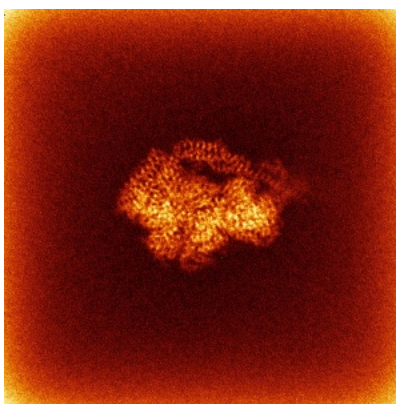


Z

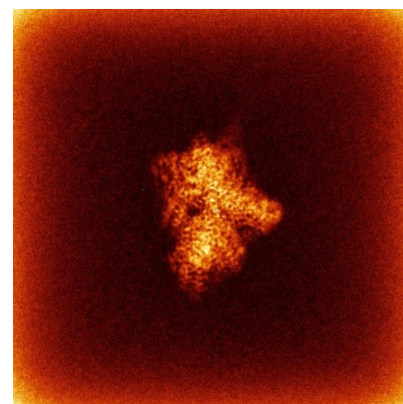
6.4.2 Raw map



X



Y

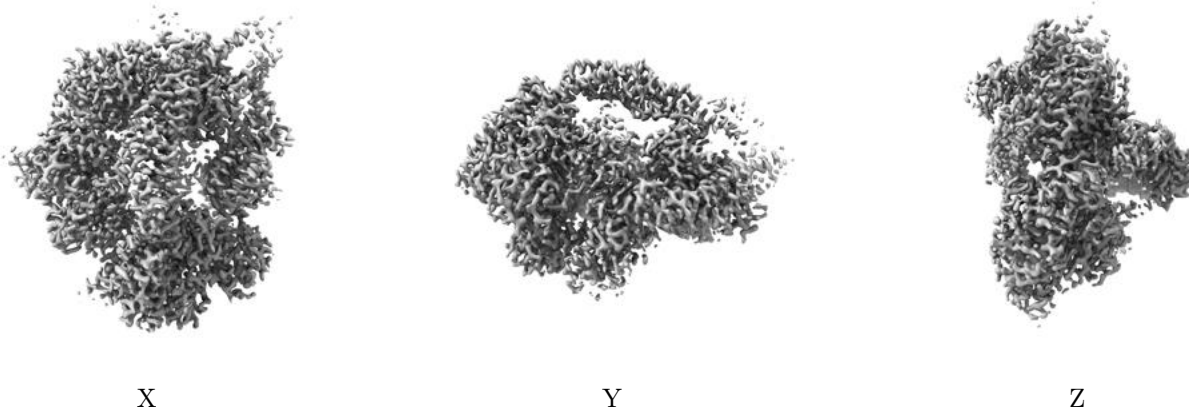


Z

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.

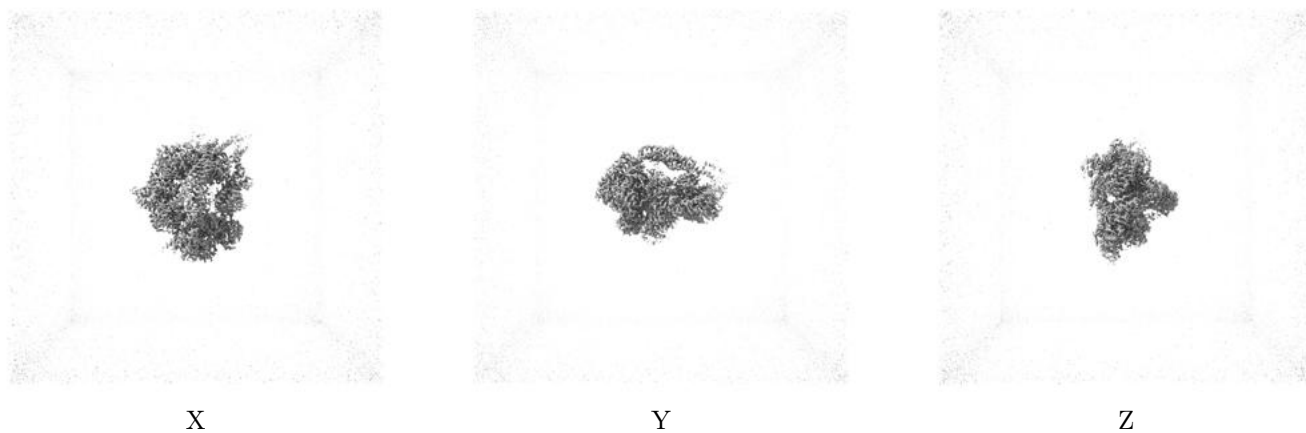
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

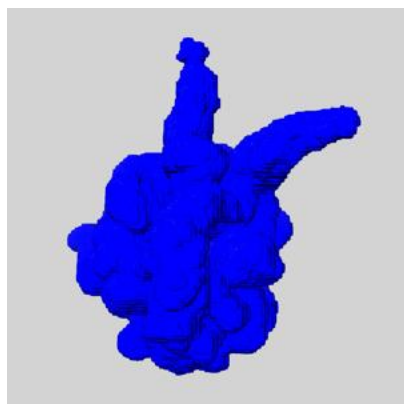
6.6 Mask visualisation [i](#)

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

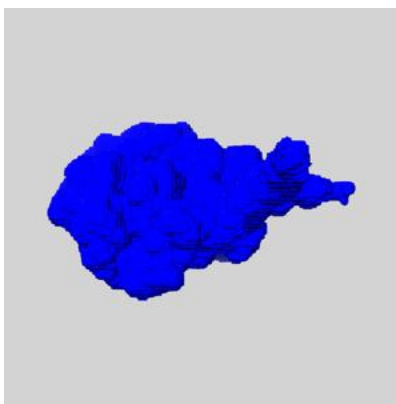
A mask typically either:

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

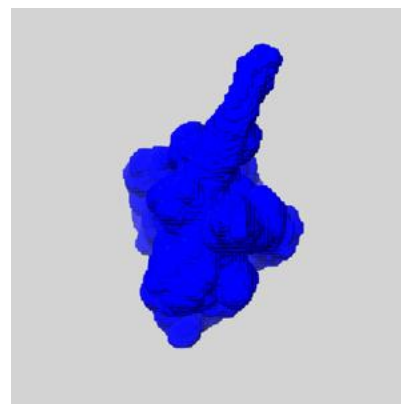
6.6.1 emd_44696_msk_1.map [i](#)



X



Y

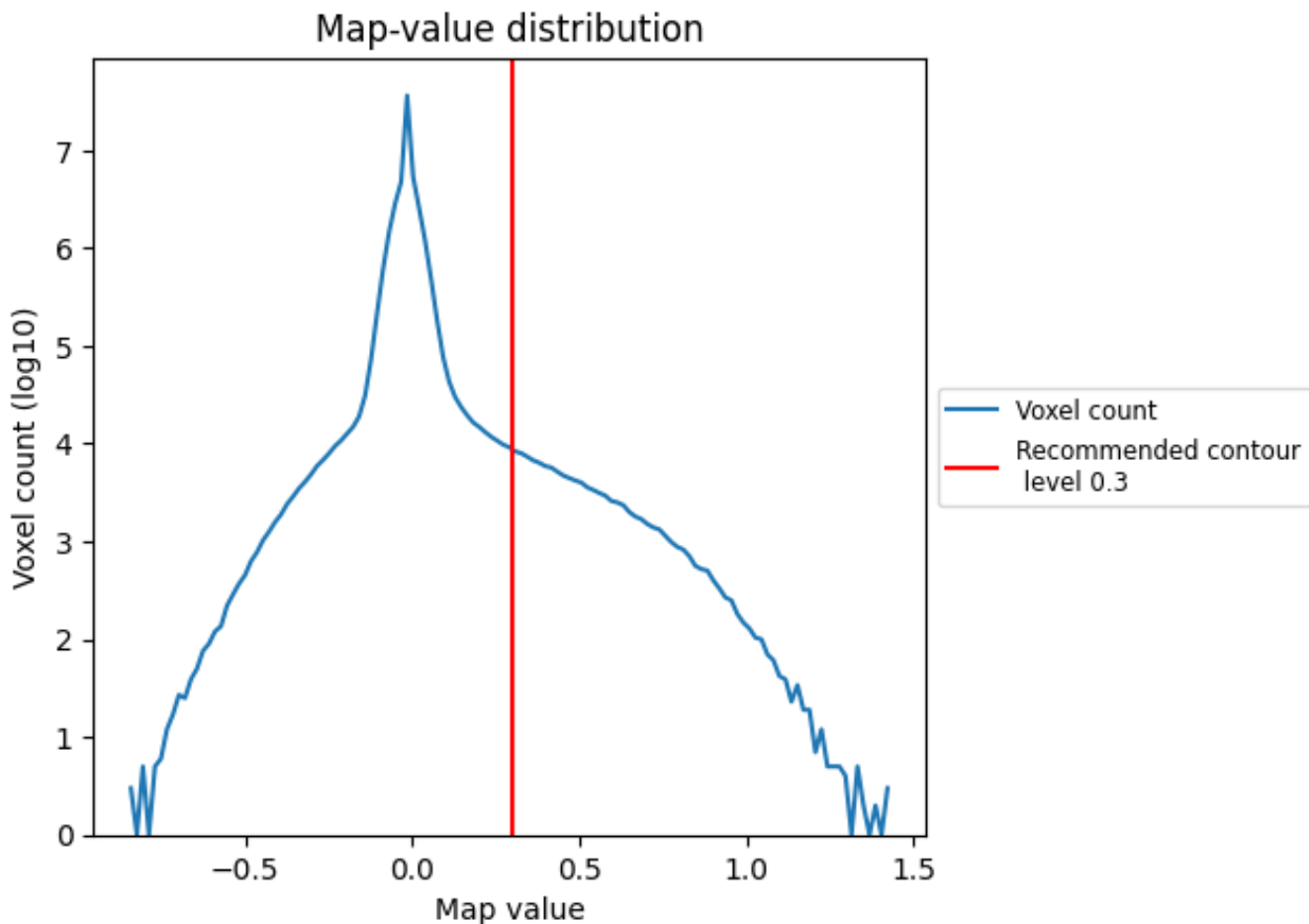


Z

7 Map analysis [i](#)

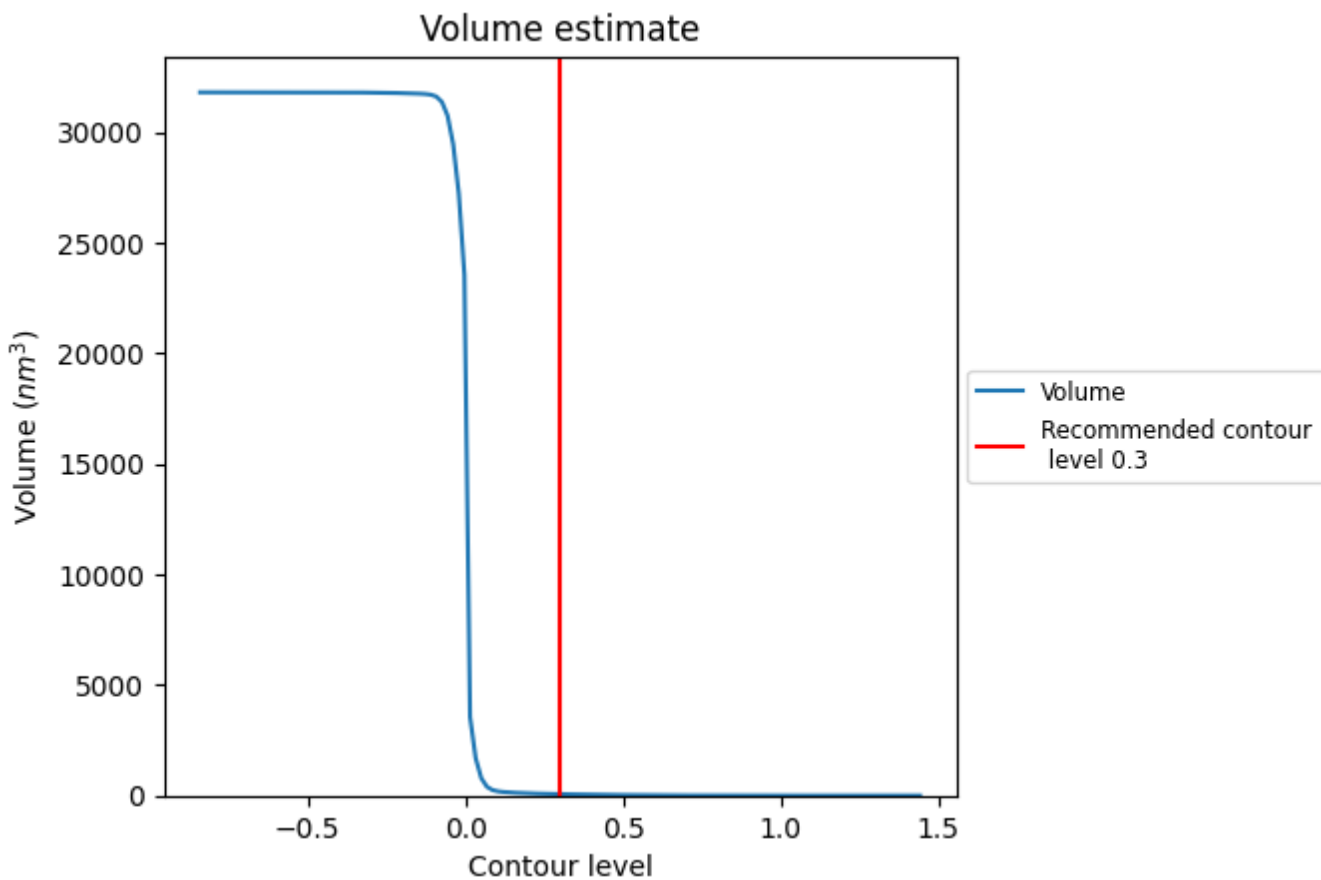
This section contains the results of statistical analysis of the map.

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.

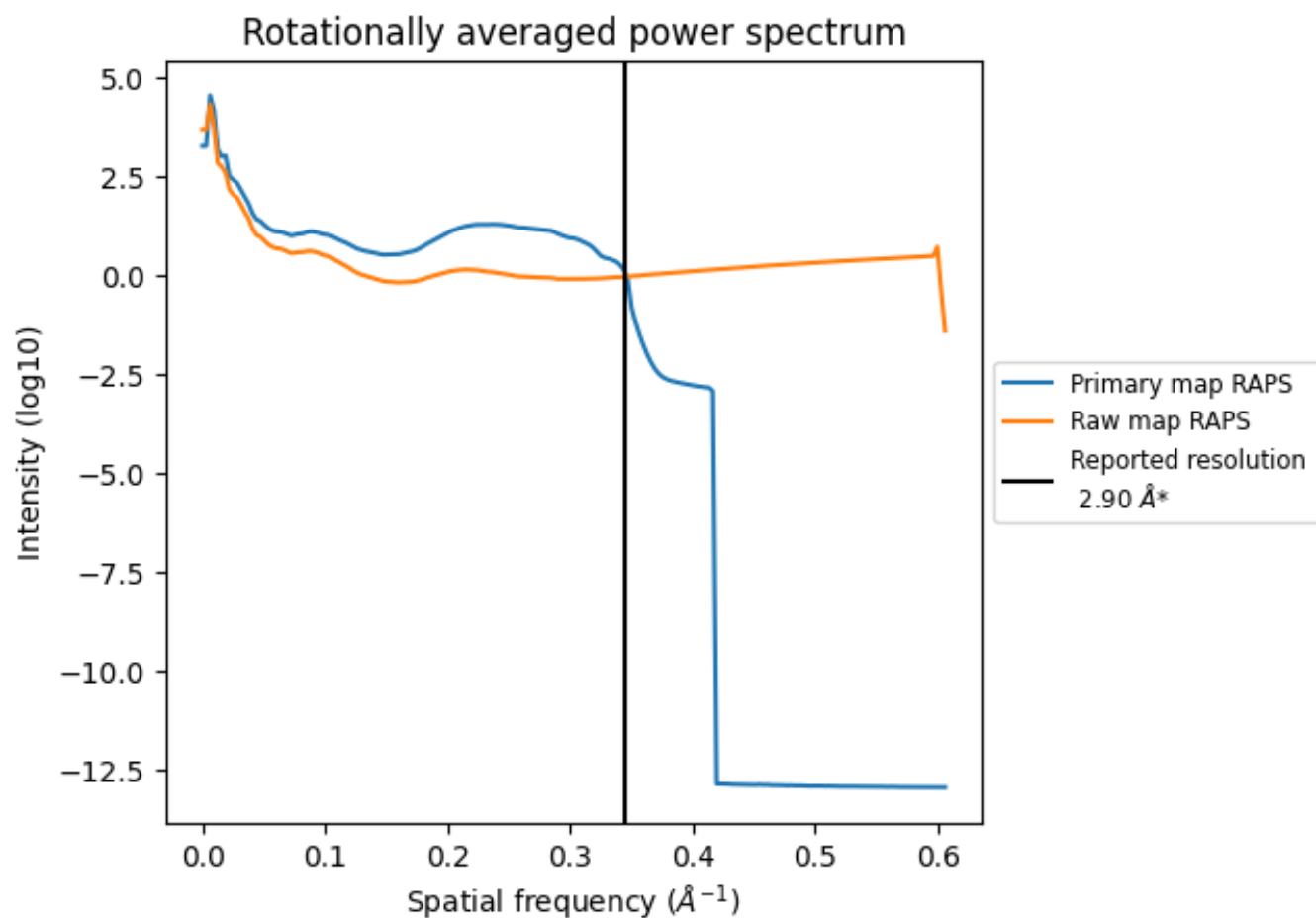
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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](#)

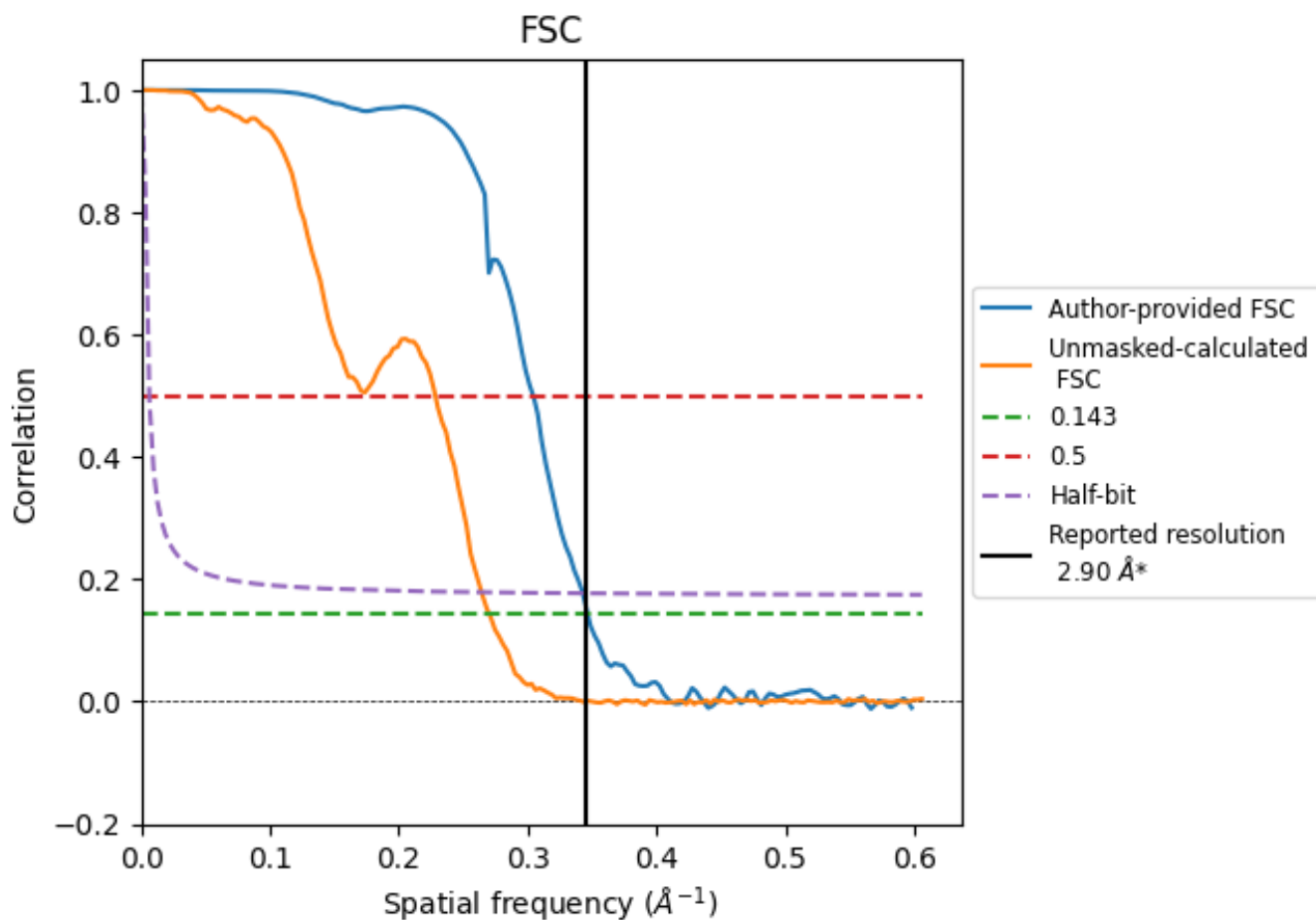


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345\AA^{-1}

8.2 Resolution estimates [i](#)

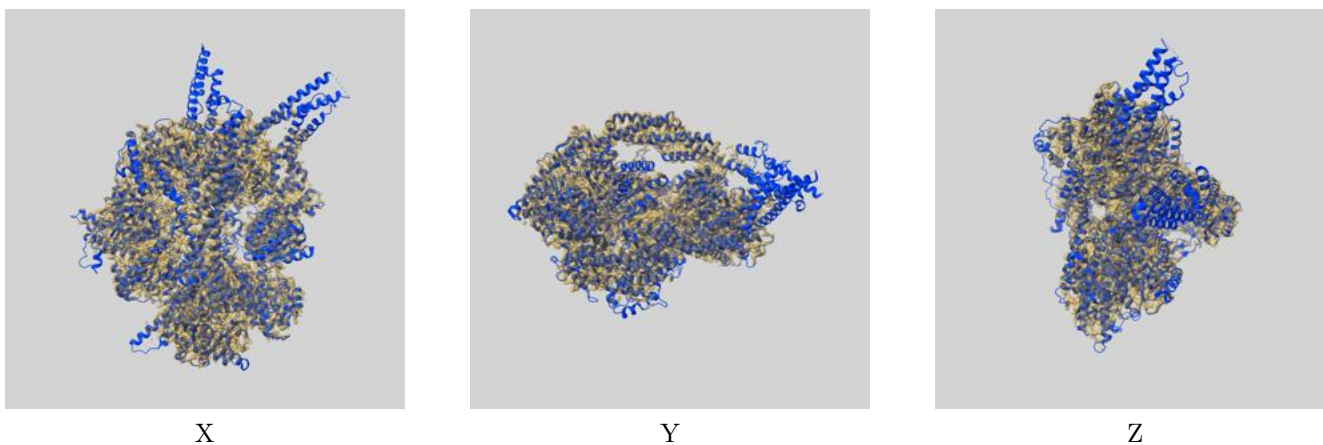
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.29	2.92
Unmasked-calculated*	3.70	4.38	3.79

*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 3.70 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

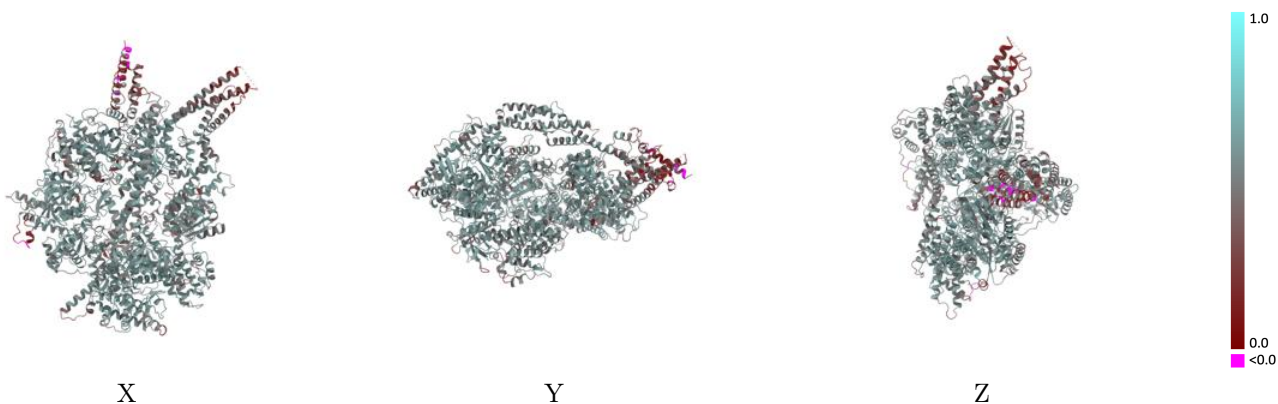
This section contains information regarding the fit between EMDB map EMD-44696 and PDB model 9BMD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



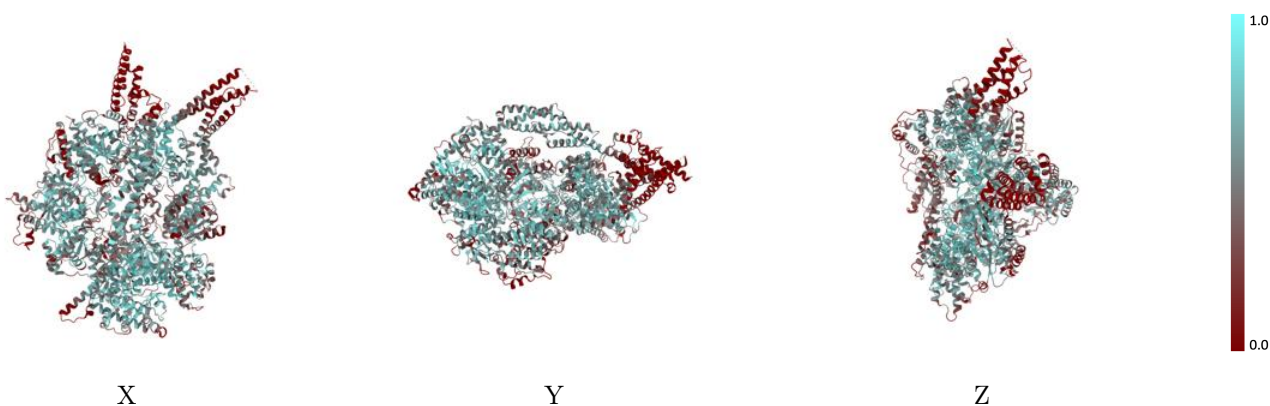
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



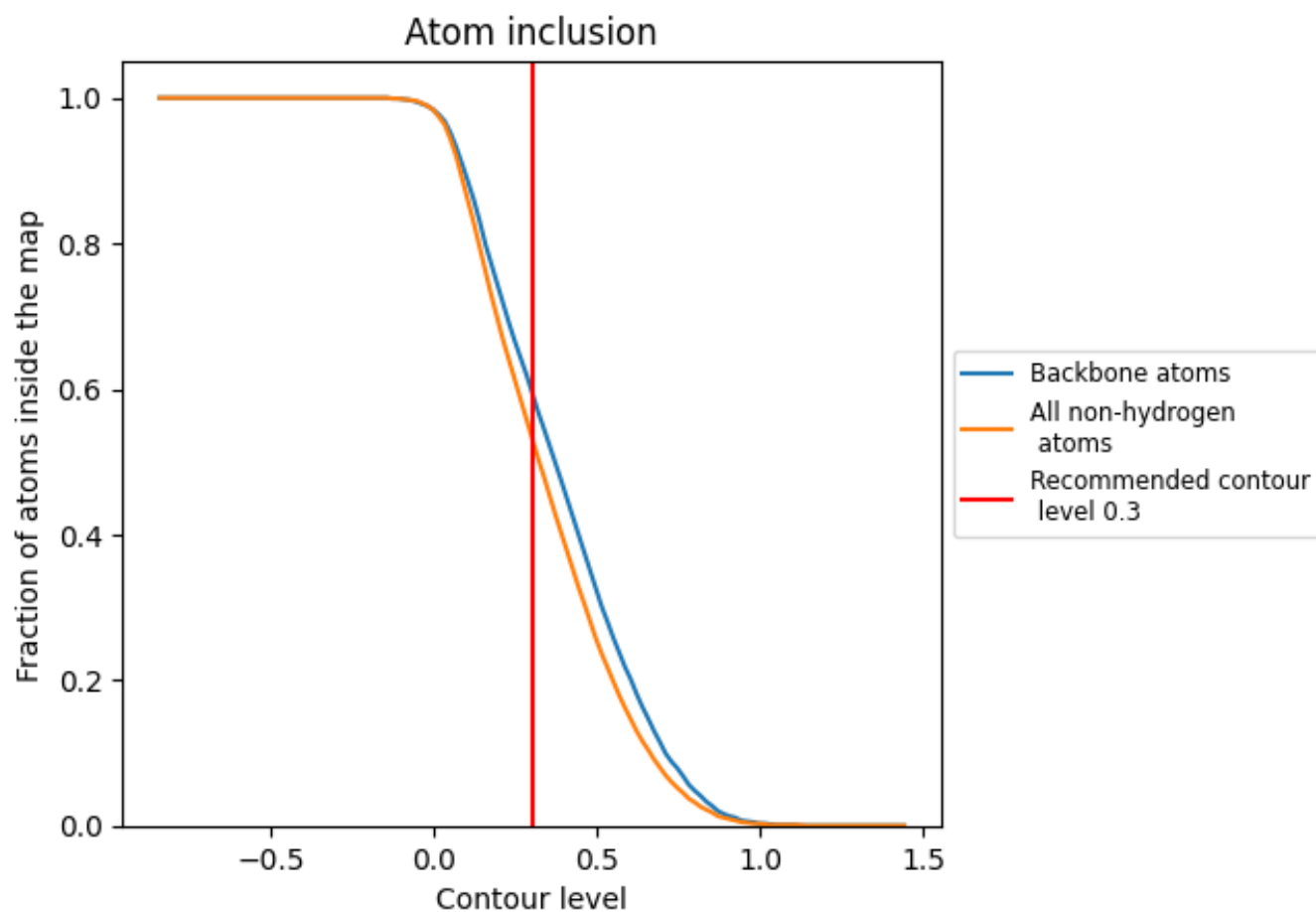
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.5330	■ 0.5260
A	■ 0.5330	■ 0.5260

