



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 12:34 PM EDT

PDB ID : 9BLZ / pdb_00009blz
EMDB ID : EMD-44682
Title : State-1(phi motor) of full-length human dynein-1 in 5mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.20 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

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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

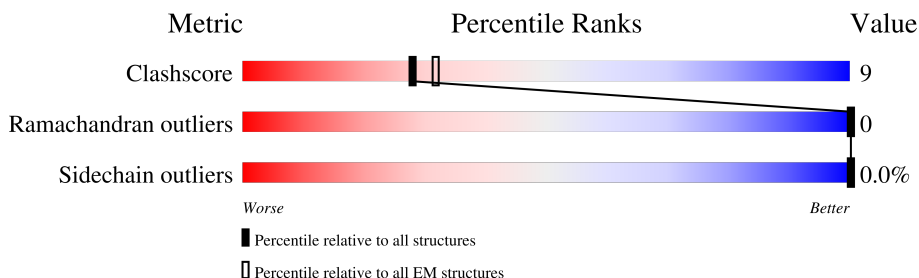
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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>9%</div> <div>48%</div> <div>14%</div> <div>38%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25189 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	2889	23218	14794	4002	4305	117	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			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 2	Mg 2	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	AltConf
5	A	1857	Total O 1857 1857	0



Tyr	Lys	Glu	Glu	Tyr	Val	Val	Leu	Ile	K3207	K3117	S2997	N2860	N2755	V2592	E2484	P2386	L2210	E2116
Leu	Ala	Cys	Gly	K3208	P3118	N2998	I2861	M2755	L2893	Q2485	Q2486	L2893	Q2485	L2893	Q2485	P2387	Y2211	E2117
Leu	Gly	Gly	Val	K3209	L2999	V2999	D2862	R2757	P2596	E2486	E2487	P2596	E2486	P2596	E2487	D2388	Q2212	R2118
Pro	Pro	Thr	Thr	E3210	N3119	L3000	R2863	R2762	Q2598	R2488	R2489	Q2598	R2488	Q2598	R2489	E2389	G2224	G2119
Val	Val	Val	Ala	T3211	D3001	S3002	E2864	R2763	T2804	R2492	R2493	T2804	R2492	T2804	R2493	GLY	A2121	A2120
Leu	Leu	Leu	Leu	V3212	S3003	G3003	E2865	R2773	L2805	Y2493	Y2494	L2805	Y2493	L2805	Y2494	ASP	V2122	A2121
Leu	Leu	Leu	Leu	D3213	F3004	N3014	R2869	M2773	R2610	Y2495	Y2496	R2610	Y2495	R2610	Y2496	GLU	D2123	D2123
Leu	Leu	Leu	Leu	V3214	V3017	V3017	R2870	E2774	R2611	L2498	L2499	R2611	L2498	R2611	L2499	ALA	S2225	P2225
Leu	Leu	Leu	Leu	V3215	L3020	L3020	R2882	E2775	R2612	L2499	L2500	R2612	L2499	R2612	L2500	GLN	S2226	G2227
Leu	Leu	Leu	Leu	E3216	S3040	F3040	P2883	F2776	L2630	G2515	E2516	L2630	G2515	L2630	G2515	ARG	S2228	G2125
Leu	Leu	Leu	Leu	E3217	Q3038	K3039	P2889	R2783	M2621	E2517	E2518	M2621	E2517	M2621	E2518	ARG	G2229	E2126
Leu	Leu	Leu	Leu	Leu	Q3039	K3040	Y2892	R2784	T2626	R2520	R2521	T2626	R2520	T2626	R2521	LYS	K2230	T2127
Leu	Leu	Leu	Leu	Leu	Q3040	F3040	R2897	D2787	L2631	P2525	P2526	L2631	P2525	L2631	P2526	GLY	S2231	A2128
Leu	Leu	Leu	Leu	Leu	Q3041	F3041	L2897	T2788	L2632	P2527	P2528	L2632	P2527	L2632	P2528	LYS	M2232	E2129
Leu	Leu	Leu	Leu	Leu	Q3042	F3042	L2898	Q2789	L2633	P2529	P2530	L2633	P2529	L2633	P2530	ASP	W2233	W2130
Leu	Leu	Leu	Leu	Leu	Q3043	F3043	Y2901	Q2790	L2634	P2531	P2532	L2634	P2531	L2634	P2532	ASP	W2234	W2131
Leu	Leu	Leu	Leu	Leu	Q3044	F3044	L2905	Q2791	L2635	P2533	P2534	L2635	P2533	L2635	P2534	GLY	W2235	W2132
Leu	Leu	Leu	Leu	Leu	Q3045	F3045	L2906	S2795	K2657	P2535	P2536	K2657	P2535	K2657	P2536	GLY	W2236	W2133
Leu	Leu	Leu	Leu	Leu	Q3046	F3046	V2907	P2796	L2661	P2537	P2538	V2907	P2537	L2661	P2538	GLY	W2237	W2134
Leu	Leu	Leu	Leu	Leu	Q3047	F3047	L2908	R2797	E2665	P2539	P2540	L2908	P2539	E2665	P2540	ALA	W2238	W2135
Leu	Leu	Leu	Leu	Leu	Q3048	F3048	L2909	R2801	E2666	P2541	P2542	L2909	P2541	E2666	P2542	ALA	W2239	W2136
Leu	Leu	Leu	Leu	Leu	Q3049	F3049	L2910	W2802	P2668	P2543	P2544	L2910	P2543	P2668	P2544	ALA	W2240	W2137
Leu	Leu	Leu	Leu	Leu	Q3050	F3050	L2911	W2803	P2669	P2545	P2546	L2911	P2545	P2669	P2546	ALA	W2241	W2138
Leu	Leu	Leu	Leu	Leu	Q3051	F3051	L2912	W2804	P2670	P2547	P2548	L2912	P2547	P2670	P2548	ALA	W2242	W2139
Leu	Leu	Leu	Leu	Leu	Q3052	F3052	L2913	W2805	P2671	P2549	P2550	L2913	P2549	P2671	P2550	ALA	W2243	W2140
Leu	Leu	Leu	Leu	Leu	Q3053	F3053	L2914	W2806	P2672	P2551	P2552	L2914	P2551	P2672	P2552	ALA	W2244	W2141
Leu	Leu	Leu	Leu	Leu	Q3054	F3054	L2915	W2807	P2673	P2553	P2554	L2915	P2553	P2673	P2554	ALA	W2245	W2142
Leu	Leu	Leu	Leu	Leu	Q3055	F3055	L2916	W2808	P2674	P2555	P2556	L2916	P2555	P2674	P2556	ALA	W2246	W2143
Leu	Leu	Leu	Leu	Leu	Q3056	F3056	L2917	W2809	P2675	P2557	P2558	L2917	P2557	P2675	P2558	ALA	W2247	W2144
Leu	Leu	Leu	Leu	Leu	Q3057	F3057	L2918	W2810	P2676	P2559	P2560	L2918	P2559	P2676	P2560	ALA	W2248	W2145
Leu	Leu	Leu	Leu	Leu	Q3058	F3058	L2919	W2811	P2677	P2561	P2562	L2919	P2561	P2677	P2562	ALA	W2249	W2146
Leu	Leu	Leu	Leu	Leu	Q3059	F3059	L2920	W2812	P2678	P2563	P2564	L2920	P2563	P2678	P2564	ALA	W2250	W2147
Leu	Leu	Leu	Leu	Leu	Q3060	F3060	L2921	W2813	P2679	P2565	P2566	L2921	P2565	P2679	P2566	ALA	W2251	W2148
Leu	Leu	Leu	Leu	Leu	Q3061	F3061	L2922	W2814	P2680	P2567	P2568	L2922	P2567	P2680	P2568	ALA	W2252	W2149
Leu	Leu	Leu	Leu	Leu	Q3062	F3062	L2923	W2815	P2681	P2569	P2570	L2923	P2569	P2681	P2570	ALA	W2253	W2150
Leu	Leu	Leu	Leu	Leu	Q3063	F3063	L2924	W2816	P2682	P2571	P2572	L2924	P2571	P2682	P2572	ALA	W2254	W2151
Leu	Leu	Leu	Leu	Leu	Q3064	F3064	L2925	W2817	P2683	P2573	P2574	L2925	P2573	P2683	P2574	ALA	W2255	W2152
Leu	Leu	Leu	Leu	Leu	Q3065	F3065	L2926	W2818	P2684	P2575	P2576	L2926	P2575	P2684	P2576	ALA	W2256	W2153
Leu	Leu	Leu	Leu	Leu	Q3066	F3066	L2927	W2819	P2685	P2577	P2578	L2927	P2577	P2685	P2578	ALA	W2257	W2154
Leu	Leu	Leu	Leu	Leu	Q3067	F3067	L2928	W2820	P2686	P2579	P2580	L2928	P2579	P2686	P2580	ALA	W2258	W2155
Leu	Leu	Leu	Leu	Leu	Q3068	F3068	L2929	W2821	P2687	P2581	P2582	L2929	P2581	P2687	P2582	ALA	W2259	W2156
Leu	Leu	Leu	Leu	Leu	Q3069	F3069	L2930	W2822	P2688	P2583	P2584	L2930	P2583	P2688	P2584	ALA	W2260	W2157
Leu	Leu	Leu	Leu	Leu	Q3070	F3070	L2931	W2823	P2689	P2585	P2586	L2931	P2585	P2689	P2586	ALA	W2261	W2158
Leu	Leu	Leu	Leu	Leu	Q3071	F3071	L2932	W2824	P2690	P2587	P2588	L2932	P2587	P2690	P2588	ALA	W2262	W2159
Leu	Leu	Leu	Leu	Leu	Q3072	F3072	L2933	W2825	P2691	P2589	P2590	L2933	P2589	P2691	P2590	ALA	W2263	W2160
Leu	Leu	Leu	Leu	Leu	Q3073	F3073	L2934	W2826	P2692	P2591	P2592	L2934	P2591	P2692	P2592	ALA	W2264	W2161
Leu	Leu	Leu	Leu	Leu	Q3074	F3074	L2935	W2827	P2693	P2593	P2594	L2935	P2593	P2693	P2594	ALA	W2265	W2162
Leu	Leu	Leu	Leu	Leu	Q3075	F3075	L2936	W2828	P2694	P2595	P2596	L2936	P2595	P2694	P2596	ALA	W2266	W2163
Leu	Leu	Leu	Leu	Leu	Q3076	F3076	L2937	W2829	P2695	P2597	P2598	L2937	P2597	P2695	P2598	ALA	W2267	W2164
Leu	Leu	Leu	Leu	Leu	Q3077	F3077	L2938	W2830	P2696	P2599	P2600	L2938	P2599	P2696	P2600	ALA	W2268	W2165
Leu	Leu	Leu	Leu	Leu	Q3078	F3078	L2939	W2831	P2697	P2601	P2602	L2939	P2601	P2697	P2602	ALA	W2269	W2166
Leu	Leu	Leu	Leu	Leu	Q3079	F3079	L2940	W2832	P2698	P2603	P2604	L2940	P2603	P2698	P2604	ALA	W2270	W2167
Leu	Leu	Leu	Leu	Leu	Q3080	F3080	L2941	W2833	P2699	P2605	P2606	L2941	P2605	P2699	P2606	ALA	W2271	W2168
Leu	Leu	Leu	Leu	Leu	Q3081	F3081	L2942	W2834	P2700	P2607	P2608	L2942	P2607	P2700	P2608	ALA	W2272	W2169
Leu	Leu	Leu	Leu	Leu	Q3082	F3082	L2943	W2835	P2701	P2609	P2610	L2943	P2609	P2701	P2610	ALA	W2273	W2170
Leu	Leu	Leu	Leu	Leu	Q3083	F3083	L2944	W2836	P2702	P2611	P2612	L2944	P2611	P2702	P2612	ALA	W2274	W2171
Leu	Leu	Leu	Leu	Leu	Q3084	F3084	L2945	W2837	P2703	P2613	P2614	L2945	P2613	P2703	P2614	ALA	W2275	W2172
Leu	Leu	Leu	Leu	Leu	Q3085	F3085	L2946	W2838	P2704	P2615	P2616	L2946	P2615	P2704	P2616	ALA	W2276	W2173
Leu	Leu	Leu	Leu	Leu	Q3086	F3086	L2947	W2839	P2705	P2617	P2618	L2947	P2617	P2705	P2618	ALA	W2277	W2174
Leu	Leu	Leu	Leu	Leu	Q3087	F3087	L2948	W2840	P2706	P2619	P2620	L2948	P2619	P2706	P2620	ALA	W2278	W2175
Leu	Leu	Leu	Leu	Leu	Q3088	F3088	L2949	W2841	P2707	P2621	P2622	L2949	P2621	P2707	P2622	ALA	W2279	W2176
Leu	Leu	Leu	Leu	Leu	Q3089	F3089	L2950	W2842	P2708	P2623	P2624	L2950	P2623	P2708	P2624	ALA	W2280	W2177
Leu	Leu	Leu	Leu	Leu	Q3090	F3090	L2951	W2843	P2709	P2625	P2626	L2951	P2625	P2709	P2626	ALA	W2281	W2178
Leu	Leu	Leu	Leu	Leu	Q3091	F3091	L2952	W2844	P2710	P2627	P2628	L2952	P2627	P2710	P2628	ALA	W2282	W2179
Leu	Leu	Leu	Leu	Leu	Q3092	F3092	L2953	W2845	P2711	P2629	P2630	L2953	P2629	P2711	P2630	ALA	W2283	W2180
Leu	Leu	Leu	Leu	Leu	Q3093	F3093	L2954	W2846	P2712	P2631	P2632	L2954	P2631	P2712	P2632	ALA	W2284	W2181
Leu	Leu	Leu	Leu	Leu	Q3094	F3094	L2955	W2847	P2713	P2633	P2634	L2955	P2633	P2713	P2634	ALA	W2285	W2182
Leu	Leu	Leu	Leu	Leu	Q3095	F3095	L2956	W2848	P2714	P2635	P2636	L2956	P2635	P2714	P2636	ALA	W2286	W2183
Leu	Leu	Leu	Leu	Leu	Q3096	F3096	L2957	W2849	P2715	P2637	P2638	L2957	P2637	P2715	P2638	ALA	W2287	W2184
Leu	Leu	Leu	Leu	Leu	Q3097	F3097	L2958	W2850	P2716	P2639	P2640	L2958	P2639	P2716	P2640	ALA	W2288	W2185
Leu	Leu	Leu	Leu	Leu	Q3098	F3098	L2959	W2851	P2717	P2641	P2642	L2959	P2641	P2717	P2642	ALA	W2289	W2186
Leu	Leu	Leu	Leu	Leu	Q3099	F3099	L2960	W2852	P2718	P2643	P2644	L2960	P2643	P2718	P2644	ALA	W2290	W2187
Leu	Leu	Leu	Leu	Leu	Q3100	F3100	L2961	W2853	P2719	P2645	P2646	L2961	P2645	P2719	P2646	ALA	W2291	W2188
Leu	Leu	Leu	Leu	Leu	Q3101	F3101	L2962	W2854	P2720	P2647	P2648	L2962	P2647	P2720	P2648	ALA	W2292	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	872840	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)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.322	Depositor
Minimum map value	-0.575	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	183.04001, 183.04001, 183.04001	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.416, 0.416, 0.416	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, ADP, 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	0.27	0/23717	0.49	0/32148

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	23218	0	23256	437	0
2	A	81	0	36	7	0
3	A	31	0	12	5	0
4	A	2	0	0	0	0
5	A	1857	0	0	38	0
All	All	25189	0	23304	437	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 9.

The worst 5 of 437 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.56	0.86
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.08	0.85
1:A:4571:ASN:O	1:A:4574:LYS:HB2	1.82	0.80
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.64	0.79
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.18	0.75

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	2881/4646 (62%)	2838 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2567/4125 (62%)	2566 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	1973	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2677	GLN
1	A	3092	ASN
1	A	4477	GLN
1	A	3202	ASN
1	A	4262	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 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	$\# Z > 2$
3	ATP	A	4702	4	28,33,33	0.76	0	34,52,52	0.80	1 (2%)
2	ADP	A	4701	4	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
2	ADP	A	4703	-	24,29,29	0.74	0	29,45,45	0.72	1 (3%)
2	ADP	A	4704	-	24,29,29	0.74	0	29,45,45	0.79	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	4	-	1/18/38/38	0/3/3/3
2	ADP	A	4701	4	-	0/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ATP	C5-C6-N6	2.30	123.82	120.31
2	A	4704	ADP	C5-C6-N6	2.29	123.80	120.31
2	A	4701	ADP	C5-C6-N6	2.24	123.73	120.31
2	A	4703	ADP	C5-C6-N6	2.19	123.64	120.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	O4'-C4'-C5'-O5'

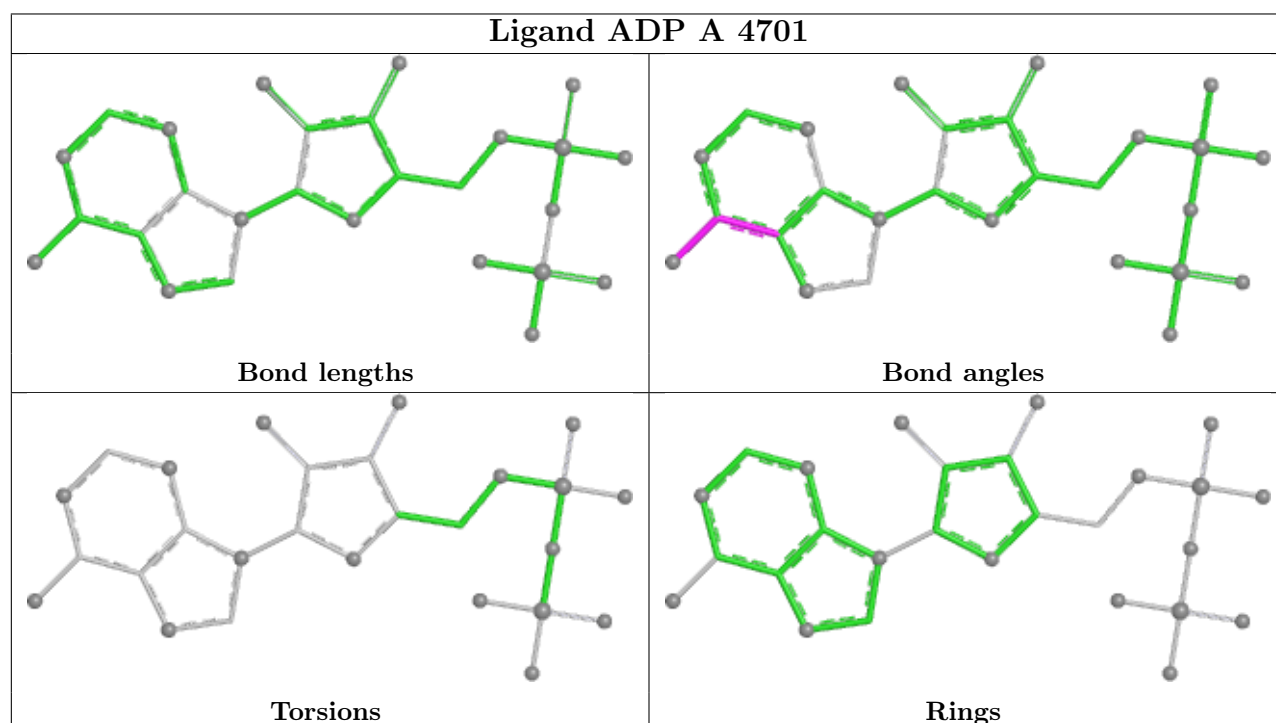
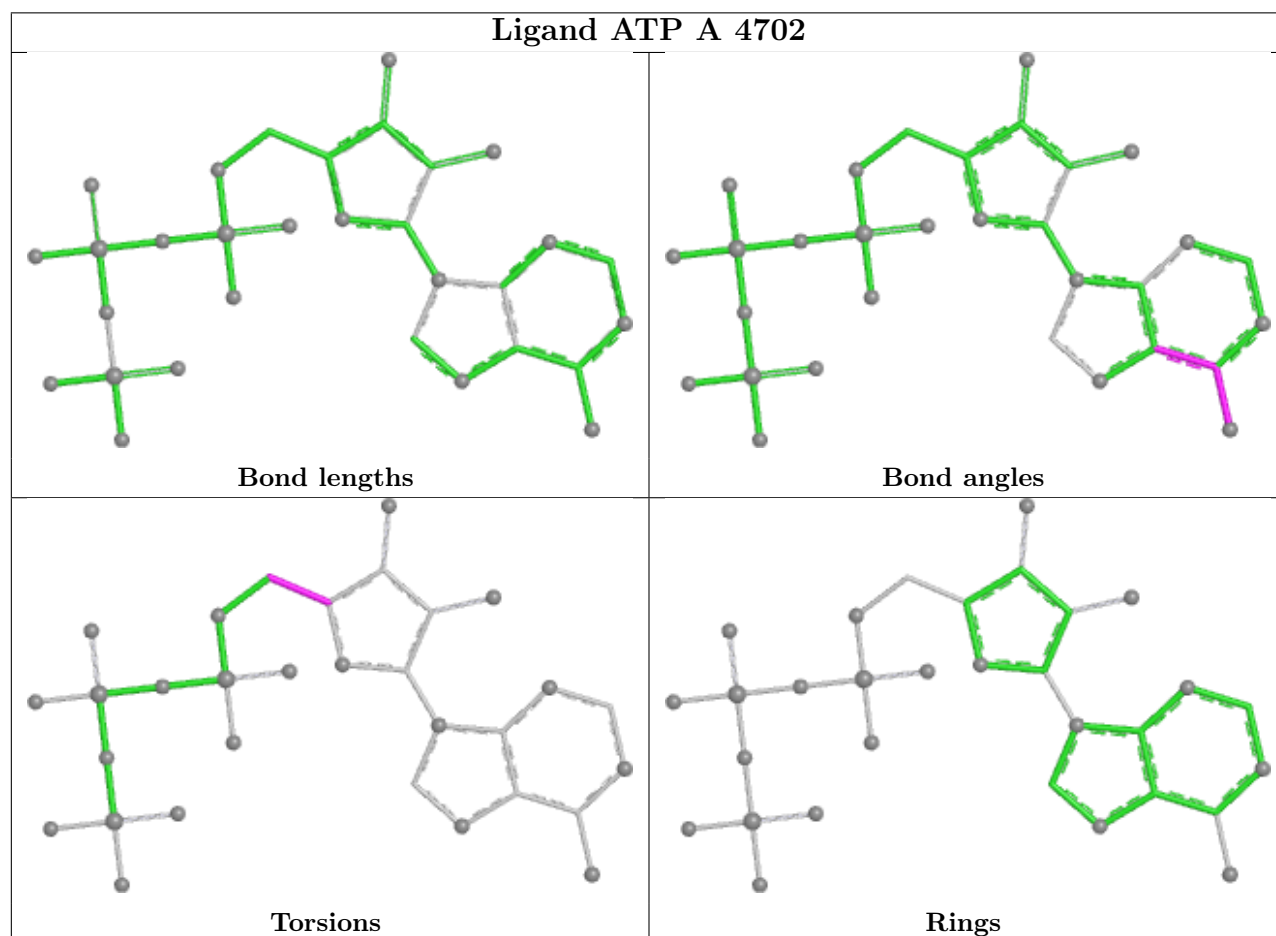
There are no ring outliers.

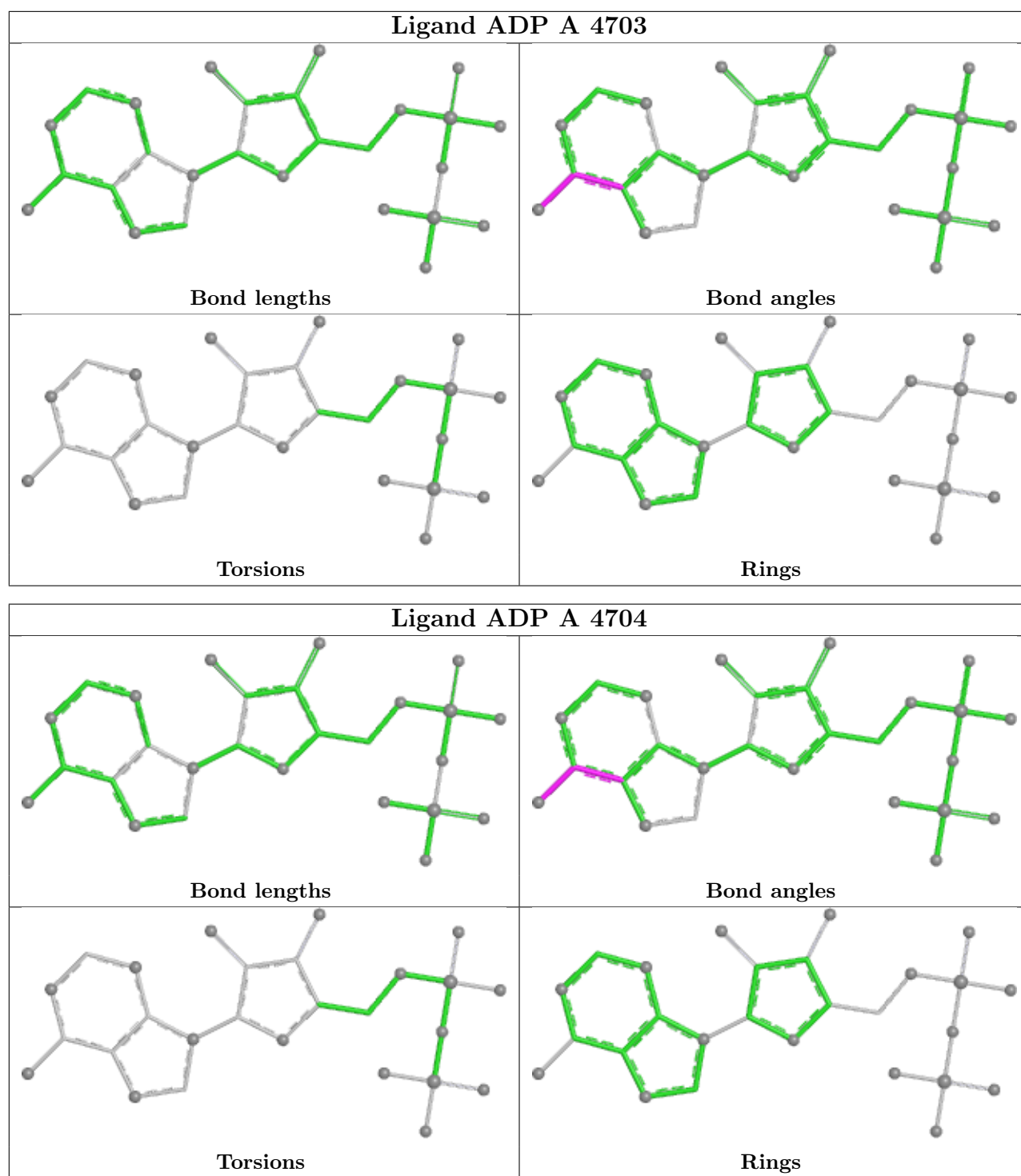
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	5	0
2	A	4701	ADP	4	0
2	A	4703	ADP	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 ⓘ

There are no chain breaks in this entry.

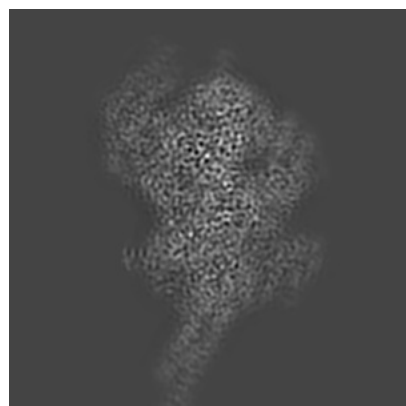
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44682. These allow visual inspection of the internal detail of the map and identification of artifacts.

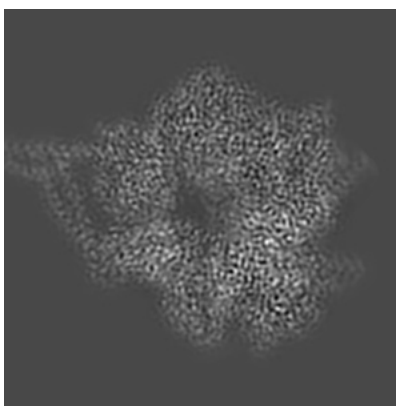
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

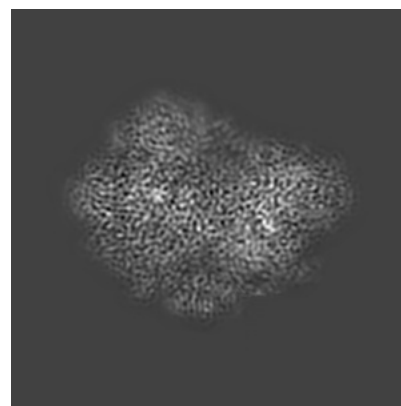
6.1.1 Primary map



X

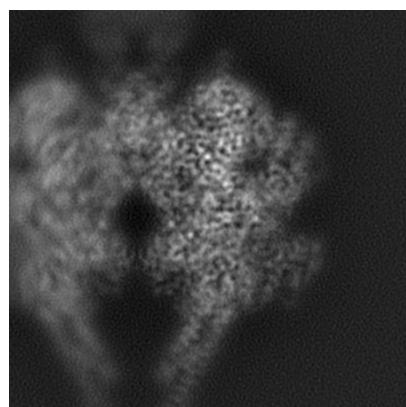


Y

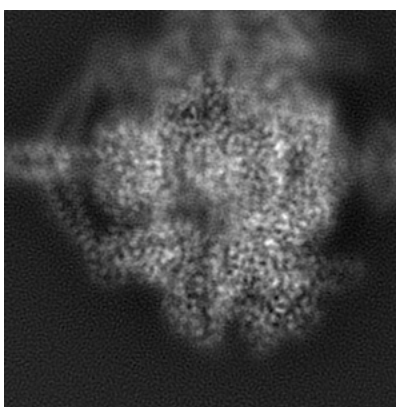


Z

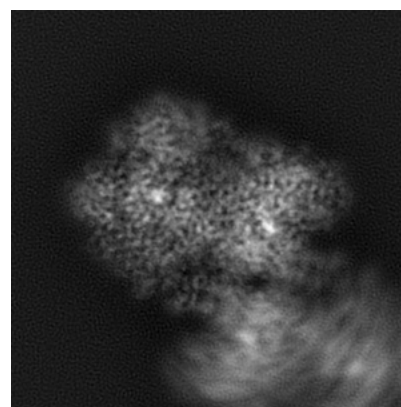
6.1.2 Raw map



X



Y

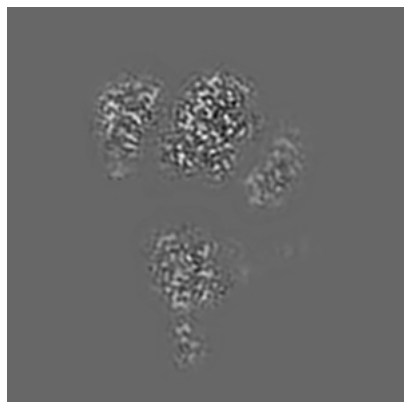


Z

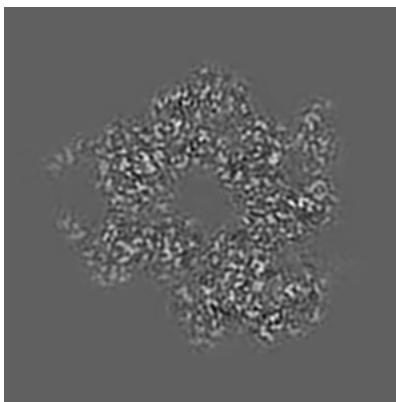
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

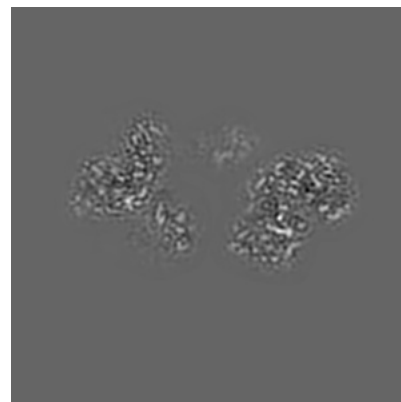
6.2.1 Primary map



X Index: 220

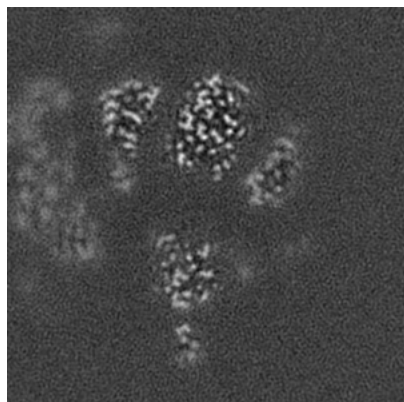


Y Index: 220

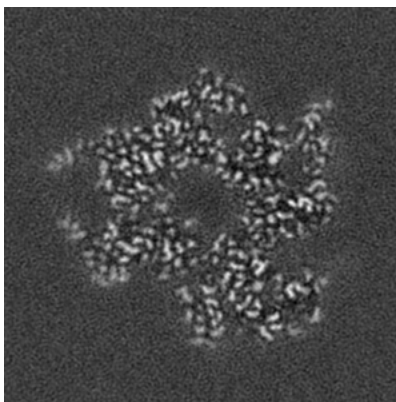


Z Index: 220

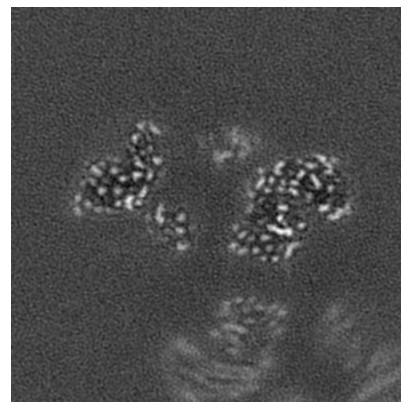
6.2.2 Raw map



X Index: 220



Y Index: 220

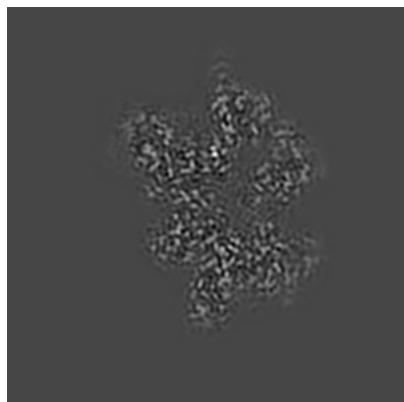


Z Index: 220

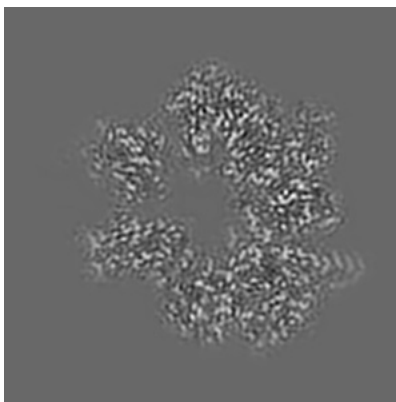
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

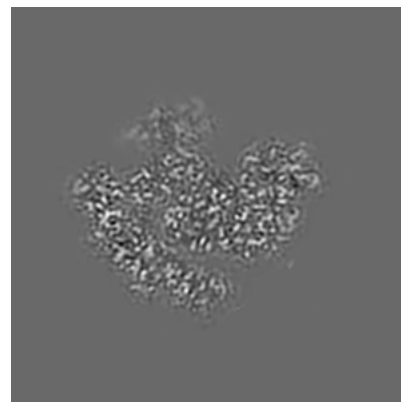
6.3.1 Primary map



X Index: 166

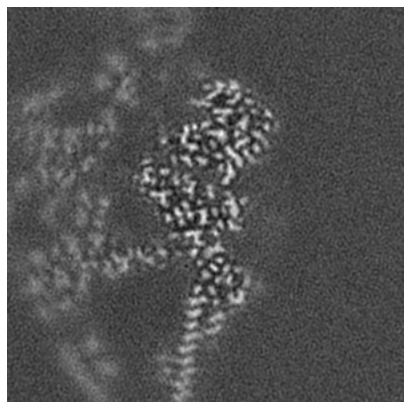


Y Index: 238

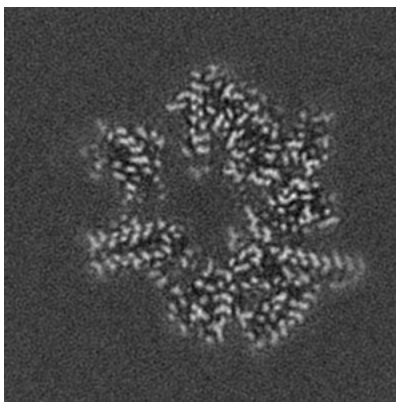


Z Index: 296

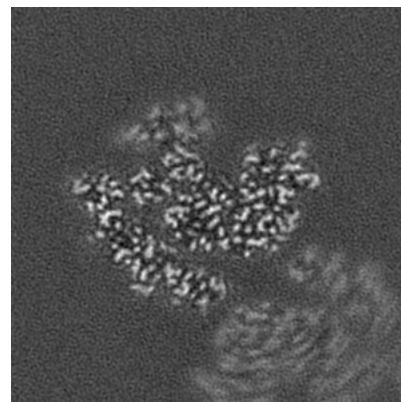
6.3.2 Raw map



X Index: 286



Y Index: 238

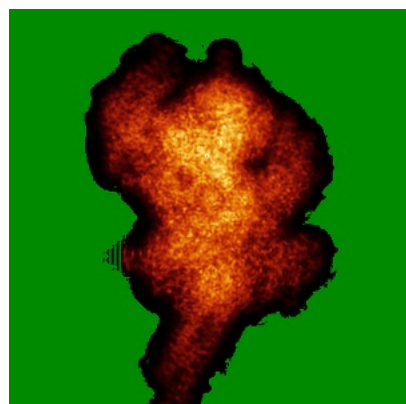


Z Index: 296

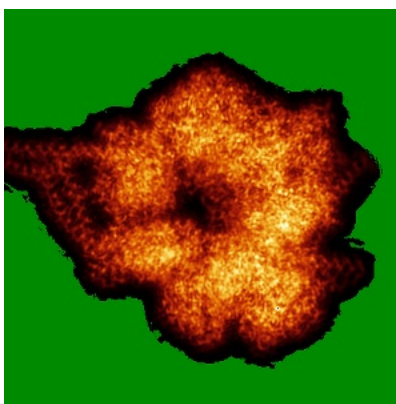
The images above show the largest variance slices of the map in three orthogonal directions.

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

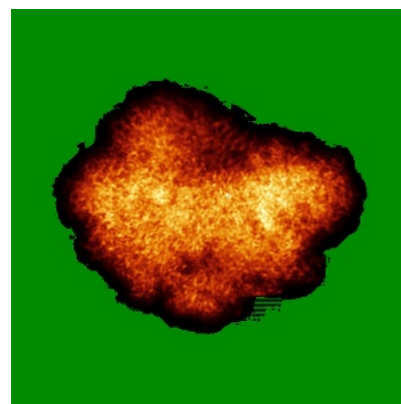
6.4.1 Primary map



X

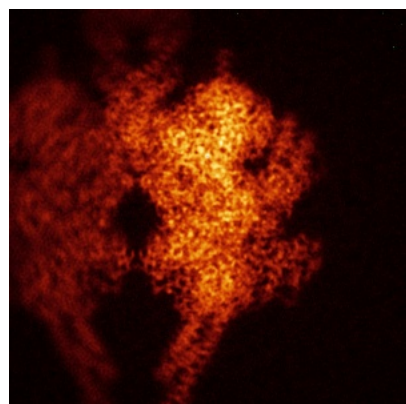


Y

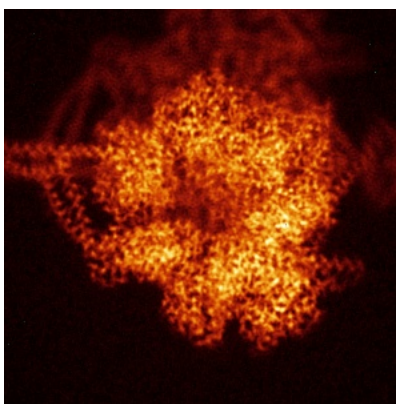


Z

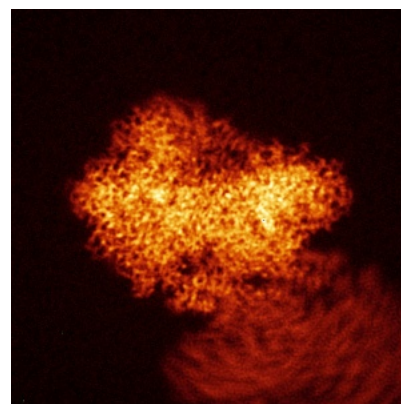
6.4.2 Raw map



X



Y

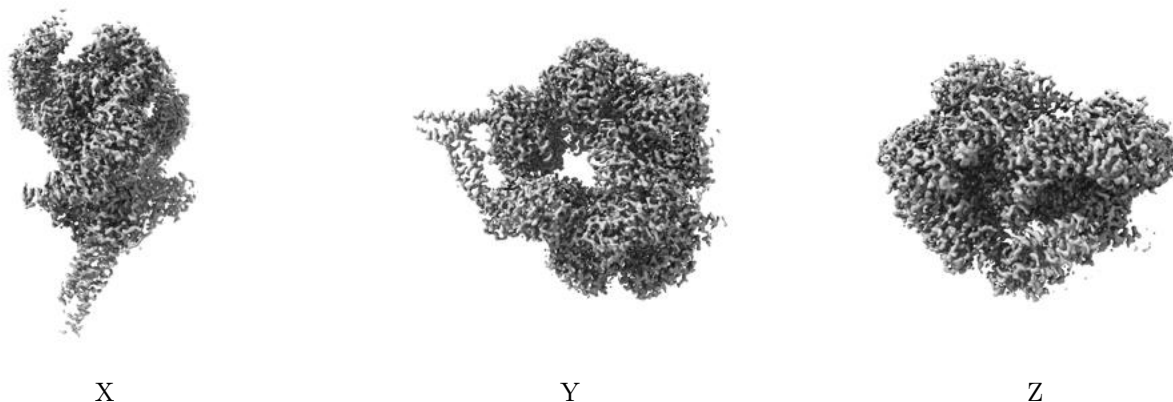


Z

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.

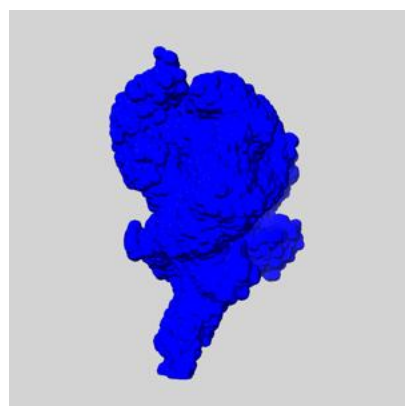
6.6 Mask visualisation [i](#)

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

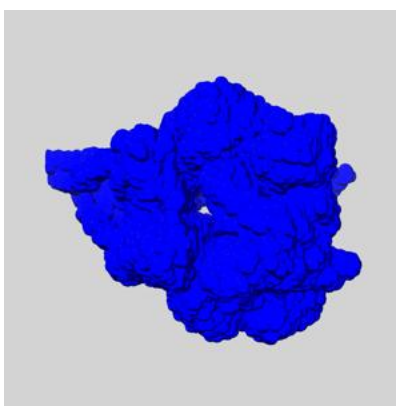
A mask typically either:

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

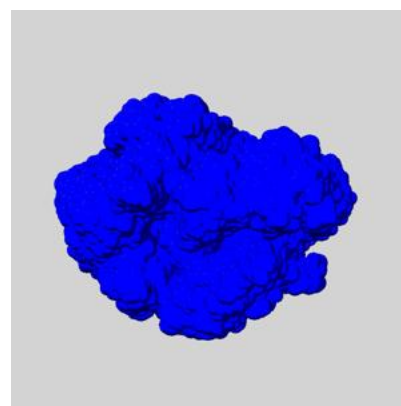
6.6.1 emd_44682_msk_1.map [i](#)



X



Y

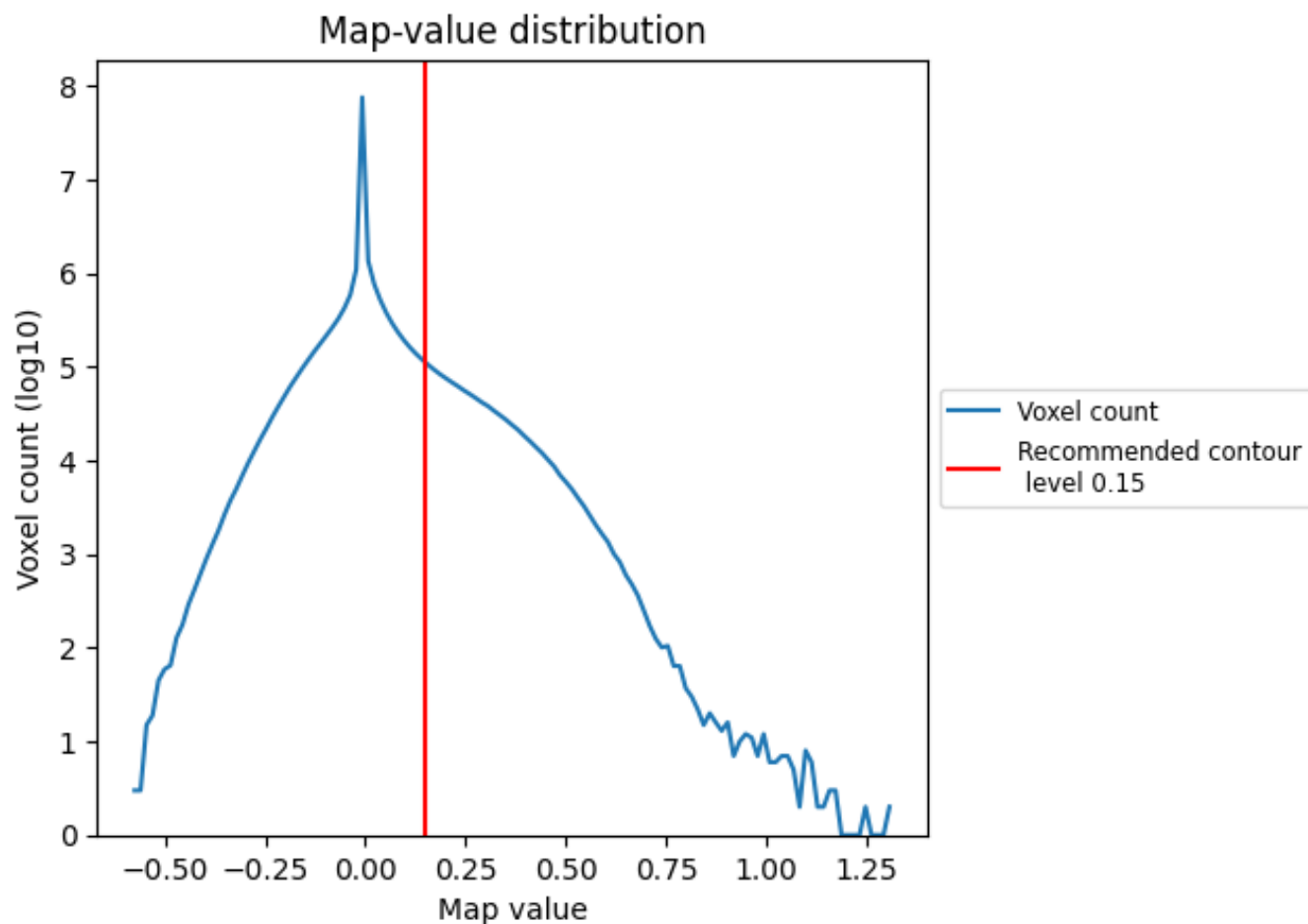


Z

7 Map analysis [i](#)

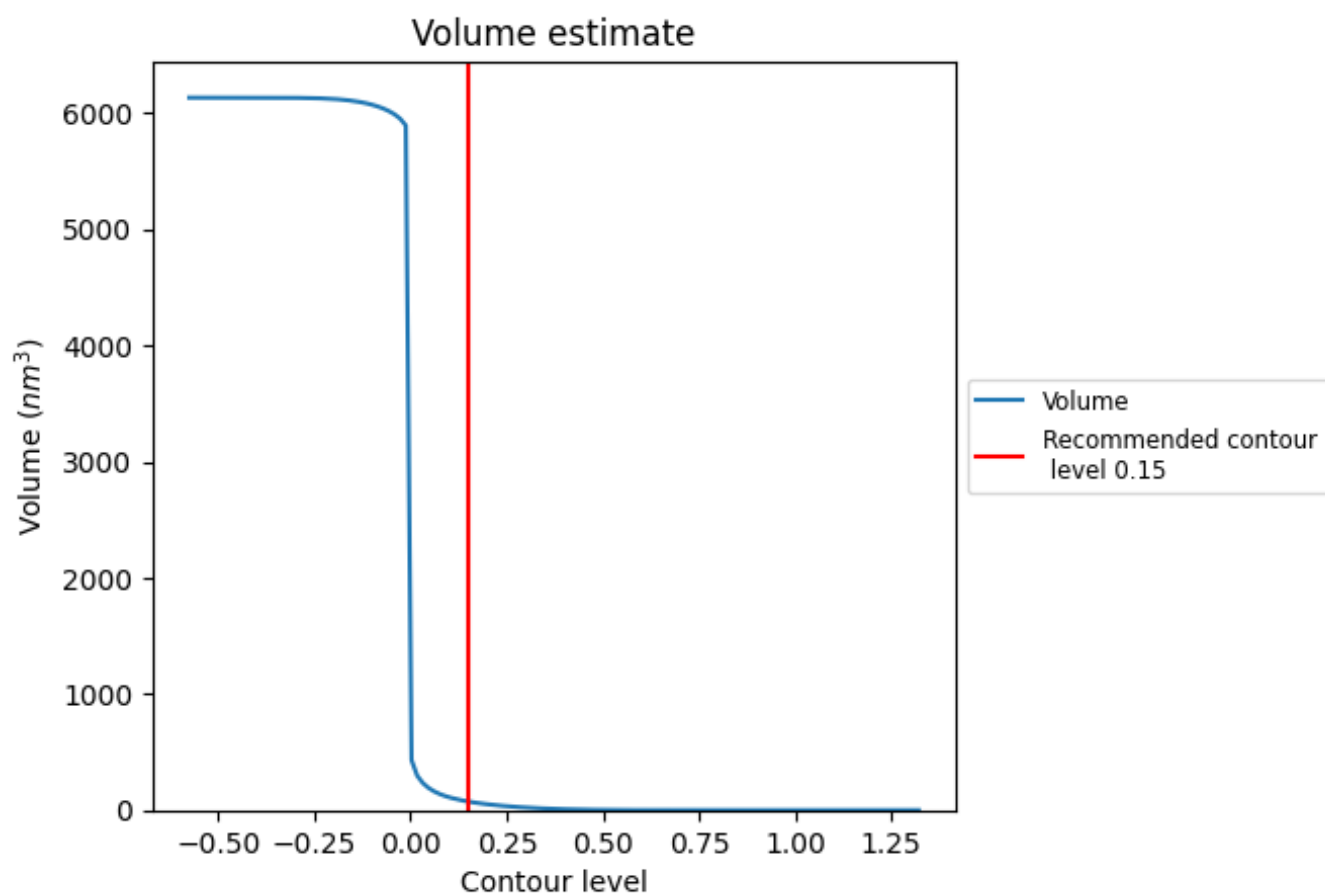
This section contains the results of statistical analysis of the map.

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.

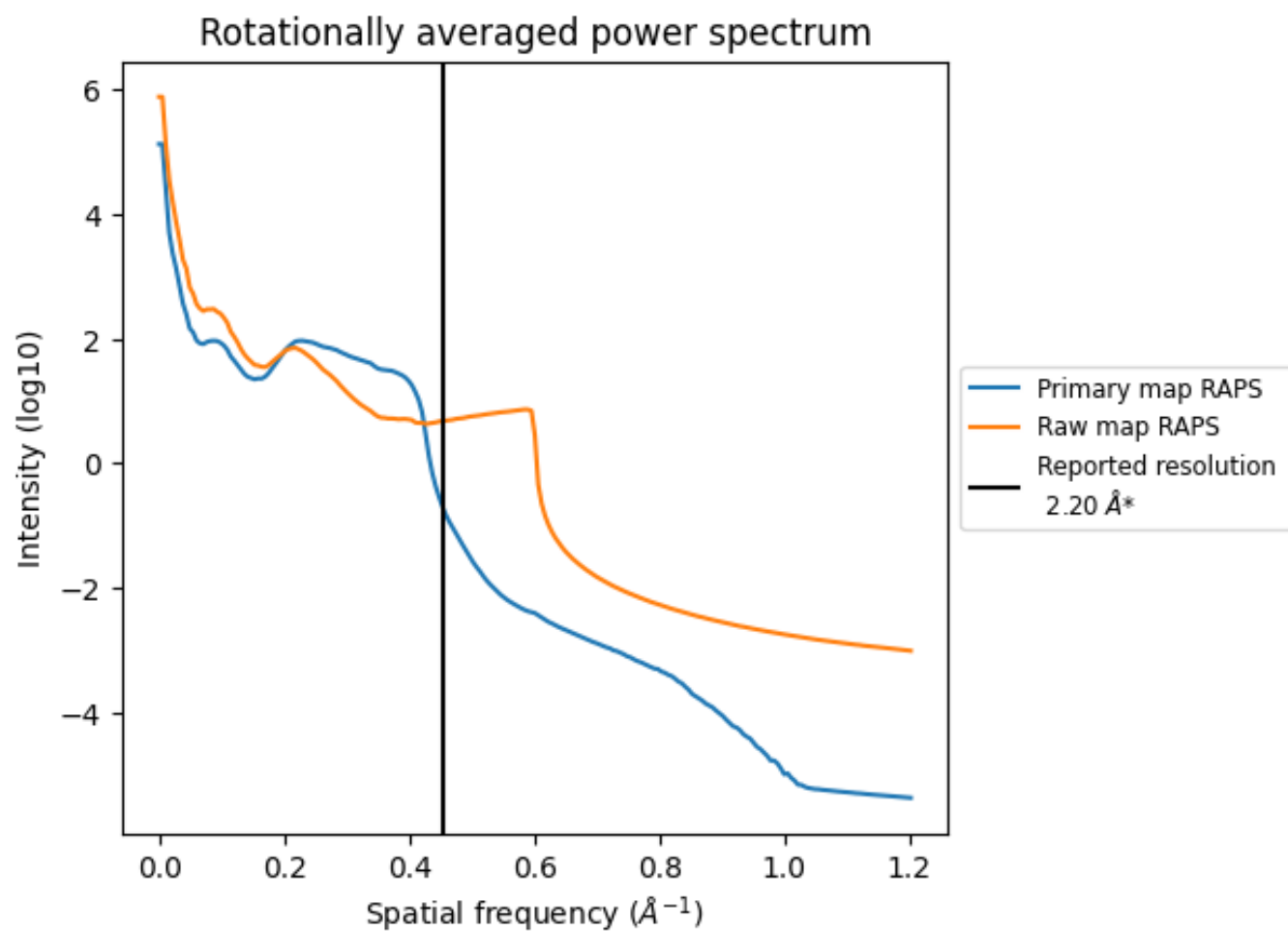
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 ⓘ

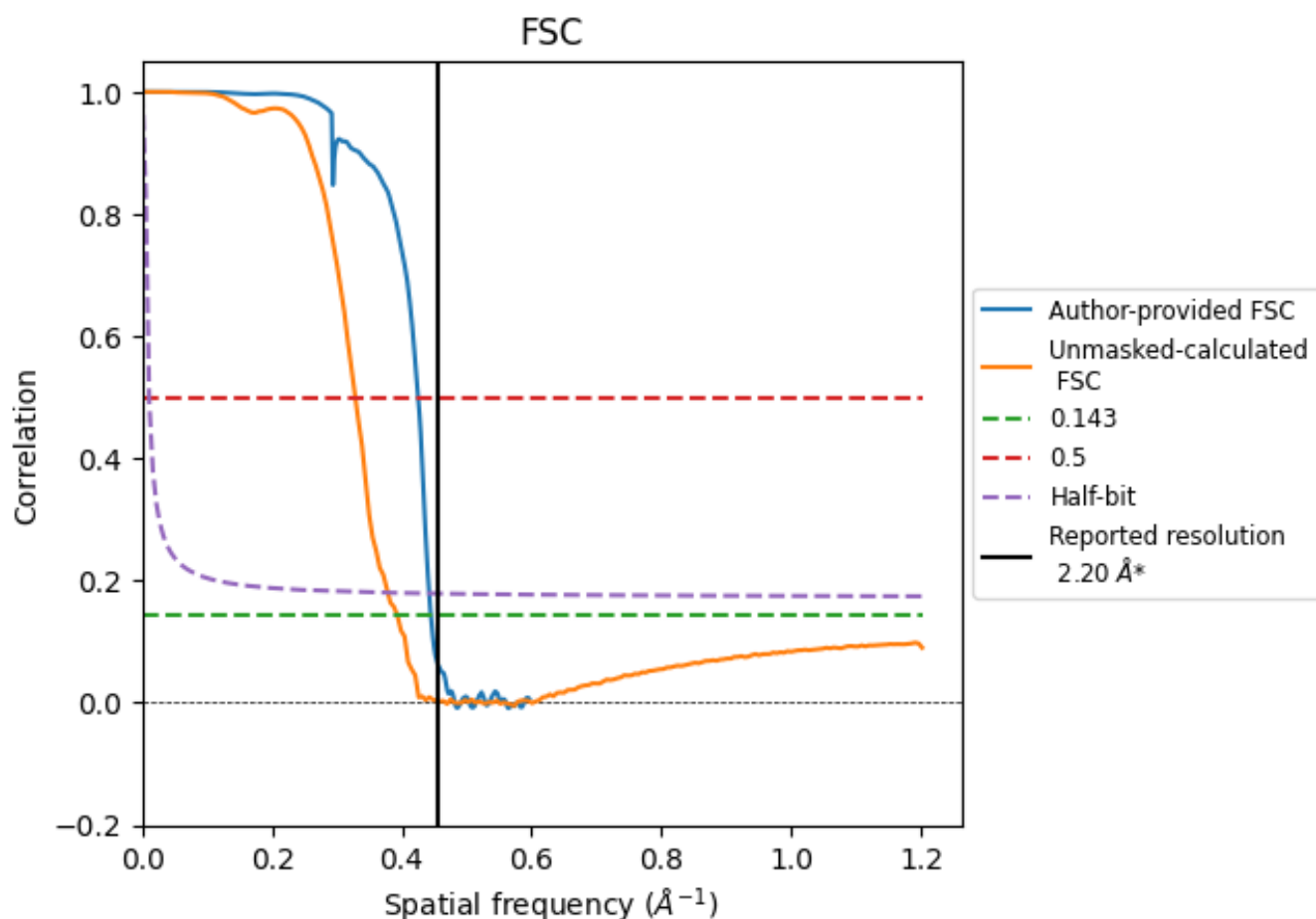


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

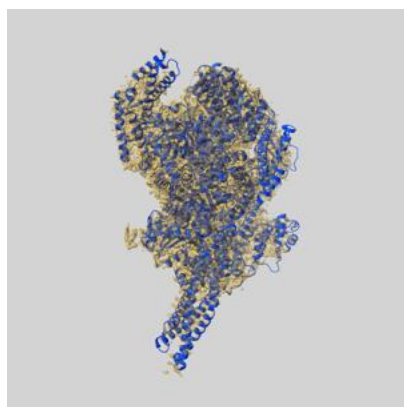
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.25	2.35	2.26
Unmasked-calculated*	2.54	3.05	2.64

*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 2.54 differs from the reported value 2.2 by more than 10 %

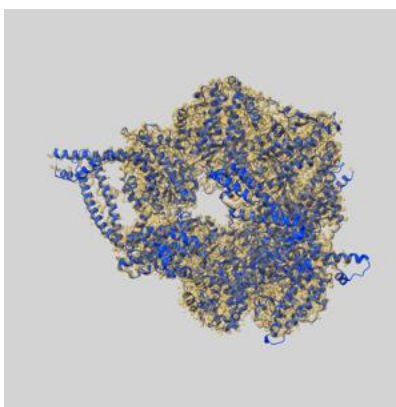
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44682 and PDB model 9BLZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

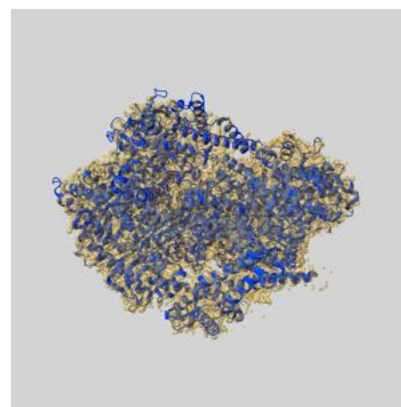
9.1 Map-model overlay [i](#)



X



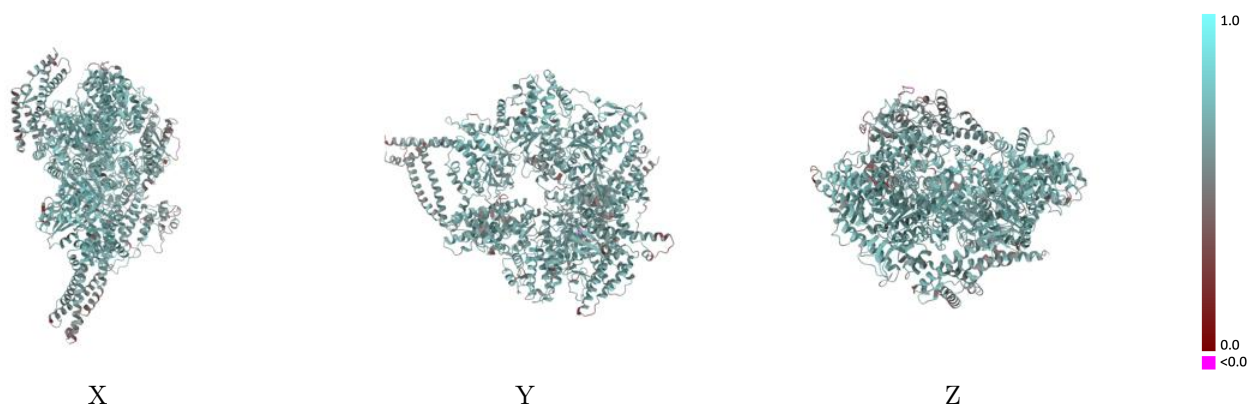
Y



Z

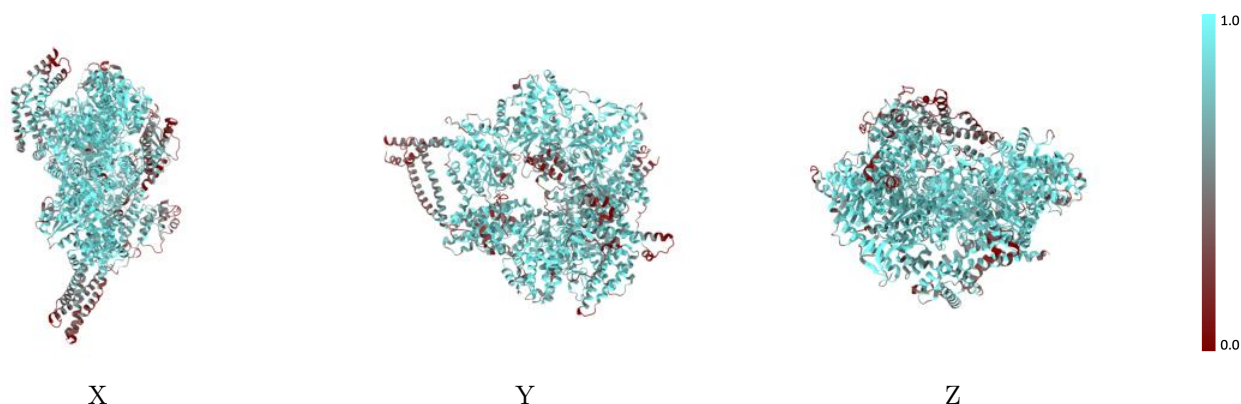
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



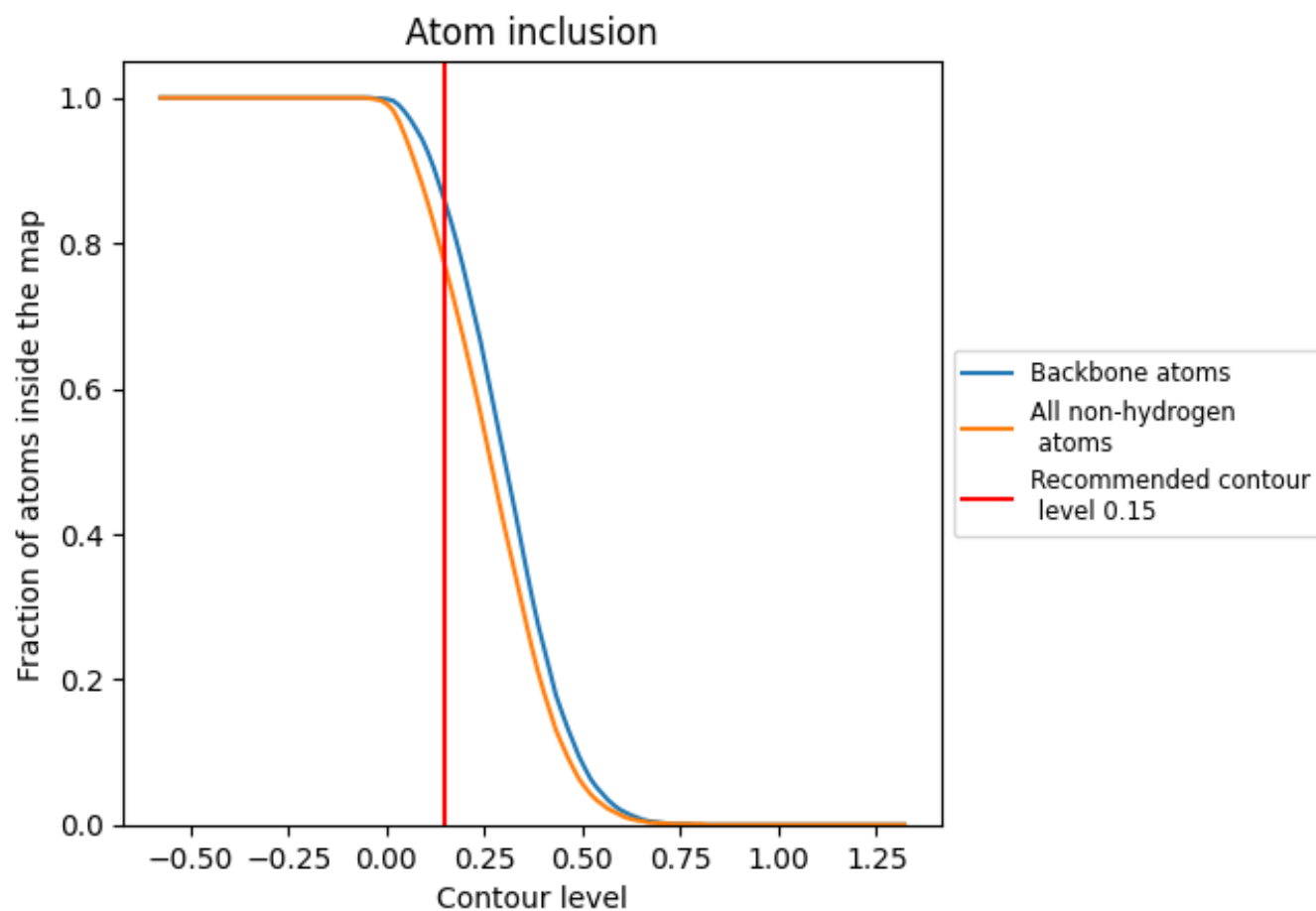
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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> 0.7690	<div></div> 0.6370
A	<div></div> 0.7690	<div></div> 0.6370

