



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:46 AM EDT

PDB ID : 9BMU / pdb_00009bmu
EMDB ID : EMD-44711
Title : State-6 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.70 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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<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

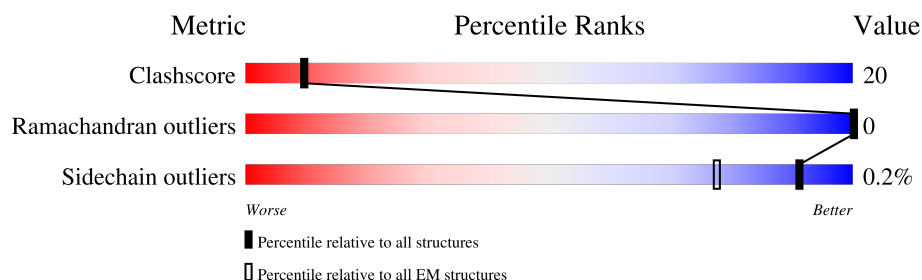
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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>5%</div> <div>35%</div> <div>23%</div> <div>42%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21776 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
1	A	2698	Total	C	N	O	S	0	0
			21664	13799	3740	4014	111		

- 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
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



K3093	T3010	E2841	M2755	P2669	L2591	G2504	M2423	K2349	E2274	D1295	L2075
F3094	L3011	E2842	L2756	D2670	V2592	D2505	Q2424	Y2350	W2275	D2185	R2085
G3095	L3012	R2843	R2757	G2593	G2594	R2507	F2427	T2352	T2276	E2198	R2086
K3096	G3013			G2595	G2596	R2508		L2356	G2278	M2202	R2091
S3098	K3014	D2847	R2763	T2676	T2677	K2509	G2431	S2357	F2279	H2203	K2092
T3099	E3015	L2850	P2768	Q2677	Q2678	R2510	L2432	R2358	F2280	V2204	L2093
E3100	E3016	D2851	L2769	V2679	V2679	R2511	V2433	C2359	T2281	E2205	
A3101	P3017	T2852	T2770	L2680	L2680	A2512	T2434	M2361	V2282	L2208	L2097
	G3019	V2853		S2681	F2606	E2513	K2435	G2360	V2283	L2209	V2103
			M2773	S2682	F2607	E2516	A2436	M2362	L2284	K2104	K2105
V3105	L3020	K2856	M2777	F2683	A2608	V2517	L2437	V2362	R2285	L2210	R2106
G3106	F3021	R2857	T2778	R2684	A2609	T2518	E2438	H2363	T2287	Y2211	
F3109	E3025	Q2685		Q2685	L2609			L2369	I2288	Q2212	E2106
T3110		V2686	Q2781	V2686	L2612	L2521	I2446	S2370	R2107	L2213	R2107
K3113	L3029	E2782	E2782	E2687	P2613		L2449	M2373	R2292	T2214	I2108
K3114	V2950	R2863	E2785	E2688	D2614	V2524	T2450	T2374	G2293	Q2215	
L3115		E2864	Q2786	G2689	M2615	P2525	R2451	F2375	E2294	G2219	K2112
	Q3038		Q2787	Q2691	E2616	P2527	R2452	L2452	Q2296	L2220	E2114
T3121		R2869	D2787	F2692	V2617		G2454	N2377	R2297	M2221	
K3126	L2956	P2870	Q2788	K2702	V2618	T2534	L2455	R2382	R2298	V2223	R2118
P3127	S2957	I2871	Q2789	E2704	G2619	T2535	G2456	R2383	Q2299	W2300	K2121
V3128	V2958	L2872	Q2790	R2705	L2620	D2536	S2457	L2387	W2301	I2301	A2128
V3129	Q2960	S2874	P2790	L2706	S2623	E2538		D2388	V2302	K2330	
V3130	I2961	V2875		Q2707	A2625	W2548	H2463	E2389	D2304	S2231	Q2134
D3131	H2964	W2876		V2709	T2626	P2553	Q2464	GLY	P2309	W2234	I2136
K3132	R2965	Y2878		C2712	P2627	E2558	A2465	ASP	L2315	R2235	
P3133	K2966	W2799		K2721	P2628	H2560	G2466	GLU	L2237	L2237	
P3134	Y2967			L2723	F2635		R2467	ALA	N2316	L2238	
E3141	T2968	W2802		R2722	G2639	A2563	N2468	GLN	L2319	K2239	C2142
A3142	Q2969	F2807		L2726	E2640	V2568	P2480	ARG	D2320	A2240	V2146
I3143	E2970	R2811		F2727	Y2641	V2569	M2481	ARG	D2321	L2241	F2147
G3147	L2976	P2812		R2728	R2642	E2484	Q2482	LYS	E2242	R2243	K2148
V3148	L2980	L2813		L2729	P2645	Q2485	Q2483	GLY	E2244	E2245	L2149
F3149	R2981	E2814		R2730	N2646	L2486	L2485	GLU	L2326	E2248	E2152
T3153	K2989	T2815		V2731	Q2647	T2571	L2487	ASP	P2328	G2249	D2153
L3154	I2990	L2816		P2732		T2572	E2488	GLY	N2329	G2249	I2154
	A2991	E2819		V2733	L2650	T2574	Y2489	GLU	E2331	I2254	P2155
L3161	F2992	I2822		Q2734	A2651	R2576	Q2491	GLU	D2332	D2255	L2156
R3164	I2993	R2823		V2735	P2652	H2577	R2492	ALA	L2333	T2259	D2163
R3167	M2994	A2826		V2736	V2653	E2578	L2493	ALA	P2337	I2263	V2168
T3168	D2995	H2827		Q2654	Q2654		L2494	S2410		H2263	
	N2998	R2827		K2657	K2657	L2581	V2495	P2411		G2266	R2179
T3171	V2999	R2831		W2658	W2658	V2582	Y2496	M2412	R2340		
T3172	L3000	V2910		L2659	L2659	T2583	A2497	L2413	T2341		
H3175	D3001	F2912		V2660	V2660	W2584	L2498	Q2414	M2342		
	S3002	E2914		L2661	L2661	L2585	L2499	I2415	F2343		E2181
T3180	G3003	R2835		F2662	F2662	A2586	W2500	A2420	E2344		K2184
K3087	F3004	L2837		Y2748	Y2748	E2587	S2501	T2421	V2345		V2185
G3089	L3005	V2838		G2749	G2749	E2588	L2502	T2272	Q2346		
V3090	E3006	E2839		T2750	T2750	K2589	L2503	L2422	D2347		
L3091		F2751		L2666	L2666				L2348		E2188
N3092				L2668	L2668						

L4182	A4087	F3996	P3899	S3748	L3671	E3598	K3491	ASN	ALA	TYR	ALA	GLU	K3190
L4183	V4088	R3997	T3900	L3749	L3679	E3603	T3492	GLU	ASN	MET	ASN	LYS	R3191
F4186	K4089	P3998	H3907	L3750	S3680	E3604	S3483	VAL	PRO	SER	PRO	LYS	S3192
H4187	S4090	D3999	R3907	Q3751	Y3604	K3605	S3483	GLN	ASN	GLY	ALA	VAL	E3193
A4188	G4091	R4000	F3908	Q3752	Q3820	D3606	T3494	MET	PRO	SER	ALA	VAL	L3194
T4189	R4092	L4001	L3909	A3753	R3682	R3607	F3496	ILE	SER	TYR	VAL	SER	E3195
L4190	M4095	A4003	E3913	H3754	P3684	R3611	Q3499	ARG	ASN	ASN	LYS	GLN	E3196
Q4191	I3914	M4004	I3914	E3755	P3685	T3612	M3500	ASP	TYR	TYR	LEU	GLU	H3199
R4193	V3915	A4005	V3915	V3756	T3685	T3613	K3500	LEU	GLU	GLU	ALA	ILE	H3200
L4194	L3916	H4006	L3916	V3757	V3686	S3613	I3503	ALA	VAL	VAL	GLU	GLN	L3201
R4195	M4007	F4008	S3917	K3757	P3690	F3614	D3506	ALA	ASN	ARG	SER	GLN	H3202
Y4196	A3918	V4009	A3918	G3758	D3691	R3617	R3506	ILE	ASN	ARG	ILE	LEU	V3203
G4200	G3919	T4010	G3919	R3759	L3692	S3617	A3512	ALA	ALA	ALA	CYS	HIS	G3204
W4201	Q3931	T4011	I3833	I3760	C3693	R3620	Y3516	TYR	SER	SER	LEU	GLN	L3205
Y4205	L4013	L4013	D3836	L3761	S3694	R3624	A3517	LYS	LEU	ALA	LEU	GLN	R3206
E4206	V3935	G4014	N3838	D3762	R3695	S3625	F3520	GLY	CYS	GLY	GLY	VAL	K3207
E4207	E4015	E4015	V3839	D3763	V3696	A3626	M3524	TYR	PRO	SER	THR	ILE	I3208
F4207	S4016	F4017	L3840	D3764	T3702	L3627	M3524	VAL	MET	MET	THR	ALA	K3209
L4212	L4018	M4018	L3846	I3766	V3703	R3628	N3540	LEU	LYS	LYS	ASP	GLN	E3210
D4220	K3945	L4027	V3849	I3767	G3704	F3632	N3540	ILE	TRP	TRP	ASP	LYS	T3211
T4221	R3945	T3850	T3850	T3768	S3707	V3635	F3643	SER	ALA	ALA	LYS	MET	V3212
W4222	L3947	D3851	D3851	T3769	S3710	V3636	R3544	GLU	ILE	ALA	GLN	VAL	D3213
A4227	L3948	R3855	R3855	L3770	N3714	D3637	T3545	ALA	ALA	ILE	ARG	VAL	D3214
N4232	A3949	K3950	K3950	E3771	E3715	V3638	D3546	GLN	GLN	SER	GLU	GLY	Q3214
L4233	V3951	V4035	V3951	H3772	V3716	E3639	I3547	ALA	ASN	ILE	ILE	ASP	V3215
P4239	Q3952	L3863	F3864	K3773	G3841	Y3552	Y3552	LYS	ALA	TYR	ILE	LEU	E3216
W4240	A3953	Q3865	Q3865	L3773	V3717	V3640	L3553	ASP	ASP	ALA	MET	ASP	E3217
S4241	D3954	R3870	R3870	K3774	K3718	P3643	S3554	LEU	LEU	GLU	GLY	VAL	L3218
N4242	F3957	V3871	A3872	R3775	D3723	V3644	E3554	ALA	ALA	LEU	ASN	GLU	R3219
L4243	W3960	G3874	R3873	E3776	V3724	L3645	E3558	VAL	LYS	ARG	PHE	PRO	R3220
K4244	L3961	M3875	R3873	A3777	D3725	N3646	R3559	GLU	VAL	VAL	ILE	ALA	ASP
A4248	P3966	L3876	M3876	E3778	E3726	L3649	W3562	ALA	GLU	GLU	THR	ILE	LEU
Q4249	P3971	H3877	H3877	V3780	K3727	N3650	Q3563	LYS	PRO	LEU	ILE	GLU	ARG
S4250	Y3972	D3878	Q3878	T3781	R3728	R3651	L3567	ASN	LEU	VAL	ALA	GLN	SER
T4251	L3973	H3880	H3880	K3782	S3729	E3652	P3568	ASN	ASN	ARG	ASN	GLN	GLU
Y4252	W3974	I3881	I3881	K3783	D3730	V3653	A3569	GLU	GLU	ASN	ALA	LEU	ALA
F4260	S3975	T3882	T3882	V3784	L3731	R3655	D3570	LEU	ALA	LEU	VAL	GLU	GLU
D4261	E3976	F3883	F3883	E3785	L3732	R3656	D3571	LYS	GLU	LYS	SER	VAL	VAL
Q4262	T3981	A3884	A3884	E3786	K3733	T3656	N3576	ILE	ILE	ILE	ILE	LYS	LYS
R4263	T3981	A3888	A3888	T3787	L3734	G3657	L3478	GLU	ASP	GLU	LYS	LYS	ASN
L4264	G3984	R3889	R3889	T3788	Q3735	G3658	R3582	ASP	ASP	ASP	ASP	ALA	ALA
R4271	Q3985	I3890	I3890	D3788	G3736	R3659	K3480	ALA	ALA	ALA	ALA	GLN	ALA
L4272	A3986	K3891	K3891	I3789	E3737	V3660	S3481	ILE	ILE	ALA	ILE	HIS	ASN
R4176	R3989	L3892	L3892	V3790	F3738	L3661	Y3586	LYS	LYS	ARG	ARG	LEU	LYS
A4177	K3893	G3894	G3894	K3791	L3662	T3663	L3482	ASP	GLY	GLY	VAL	VAL	ASP
R4178	T3895	E3894	E3894	Q3792	L3662	L3663	S3483	GLN	ASN	ASN	GLU	GLU	LYS
F4278	E3993	E3898	E3898	E3793	R3740	L3664	A3484	GLN	GLN	GLN	MET	VAL	LEU
F4282	Q4079	L3992	L3992	V3794	R3741	G3665	E3485	LYS	LYS	LYS	LYS	ARG	LYS
K4283	I3993	E3998	E3998	E3795	L3742	D3666	R3486	MET	LYS	LYS	LYS	SER	MET
				T3796	R3743	Q3667	E3487	VAL	VAL	ALA	VAL	VAL	VAL
				V3797	Q3744	D3668	R3488	LYS	LYS	LYS	LYS	LYS	LYS
				Q3799	L3745	T3669	E3489	ASP	ASP	ASP	ASP	ASP	ASP
				Q3800	E3746	D3670	E3490	GLN	GLN	GLN	GLN	GLN	GLN
				A3807	K3747			ALA	ALA	ALA	ALA	ALA	ALA
				S3810									
				I3811									
				T3814									



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93339	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	0.603	Depositor
Minimum map value	-0.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.30	0/22127	0.53	1/29993 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2603	MET	CG-SD-CE	-6.36	90.03	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2229	GLY	Peptide

5.2 Too-close contacts

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	21664	0	21700	848	0
2	A	81	0	36	15	0
3	A	31	0	12	4	0
All	All	21776	0	21748	849	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 20.

The worst 5 of 849 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:2688:GLU:HB2	1:A:2730:HIS:HE1	1.33	0.90
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.58	0.84
1:A:2794:TYR:HE1	1:A:2836:ARG:HH21	1.30	0.80
1:A:2609:LEU:HD23	1:A:2660:VAL:HG21	1.65	0.78
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	1.65	0.78

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	2684/4646 (58%)	2592 (97%)	92 (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	2397/4125 (58%)	2393 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1679	ARG
1	A	2377	ASN
1	A	3474	ARG
1	A	3747	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4466	HIS
1	A	4156	ASN
1	A	3714	ASN
1	A	3650	ASN
1	A	3907	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	-	28,33,33	0.99	2 (7%)	34,52,52	0.65	1 (2%)
2	ADP	A	4703	-	24,29,29	0.83	0	29,45,45	1.33	4 (13%)
2	ADP	A	4704	-	24,29,29	0.81	0	29,45,45	1.28	2 (6%)
2	ADP	A	4701	-	24,29,29	0.86	0	29,45,45	1.32	5 (17%)

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	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	PA-O3A	-2.72	1.56	1.59
3	A	4702	ATP	PB-O3B	-2.64	1.56	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4701	ADP	N3-C2-N1	-3.35	124.12	128.67
2	A	4703	ADP	N3-C2-N1	-3.21	124.32	128.67
2	A	4703	ADP	C4'-O4'-C1'	2.90	112.58	109.92
2	A	4704	ADP	C4-C5-N7	-2.67	106.52	109.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

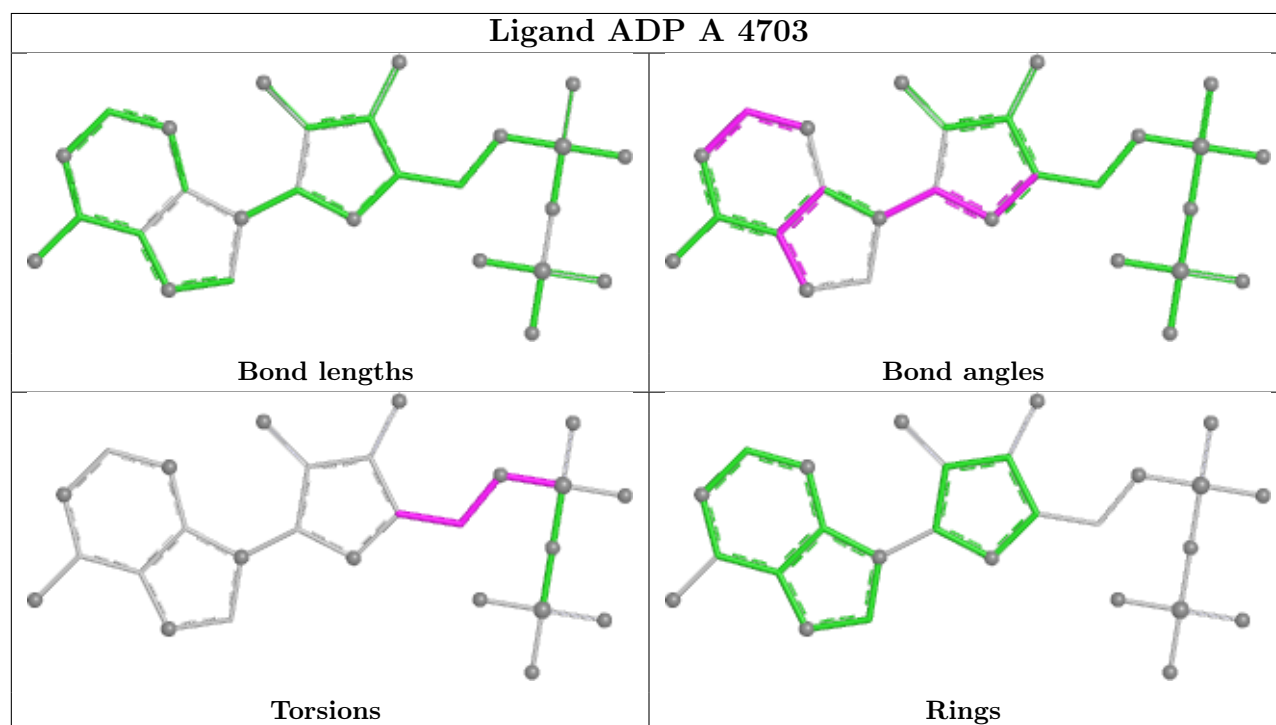
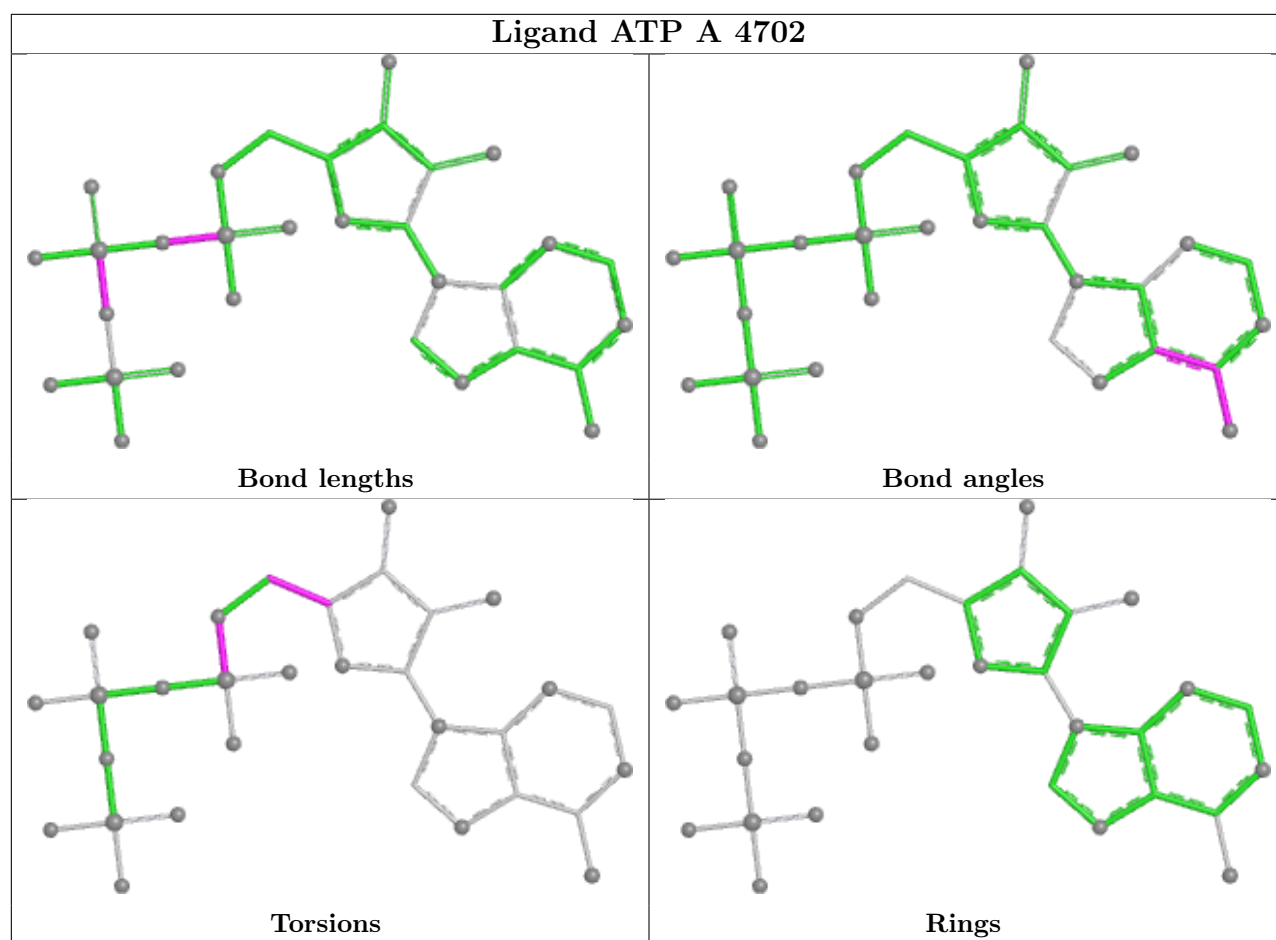
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

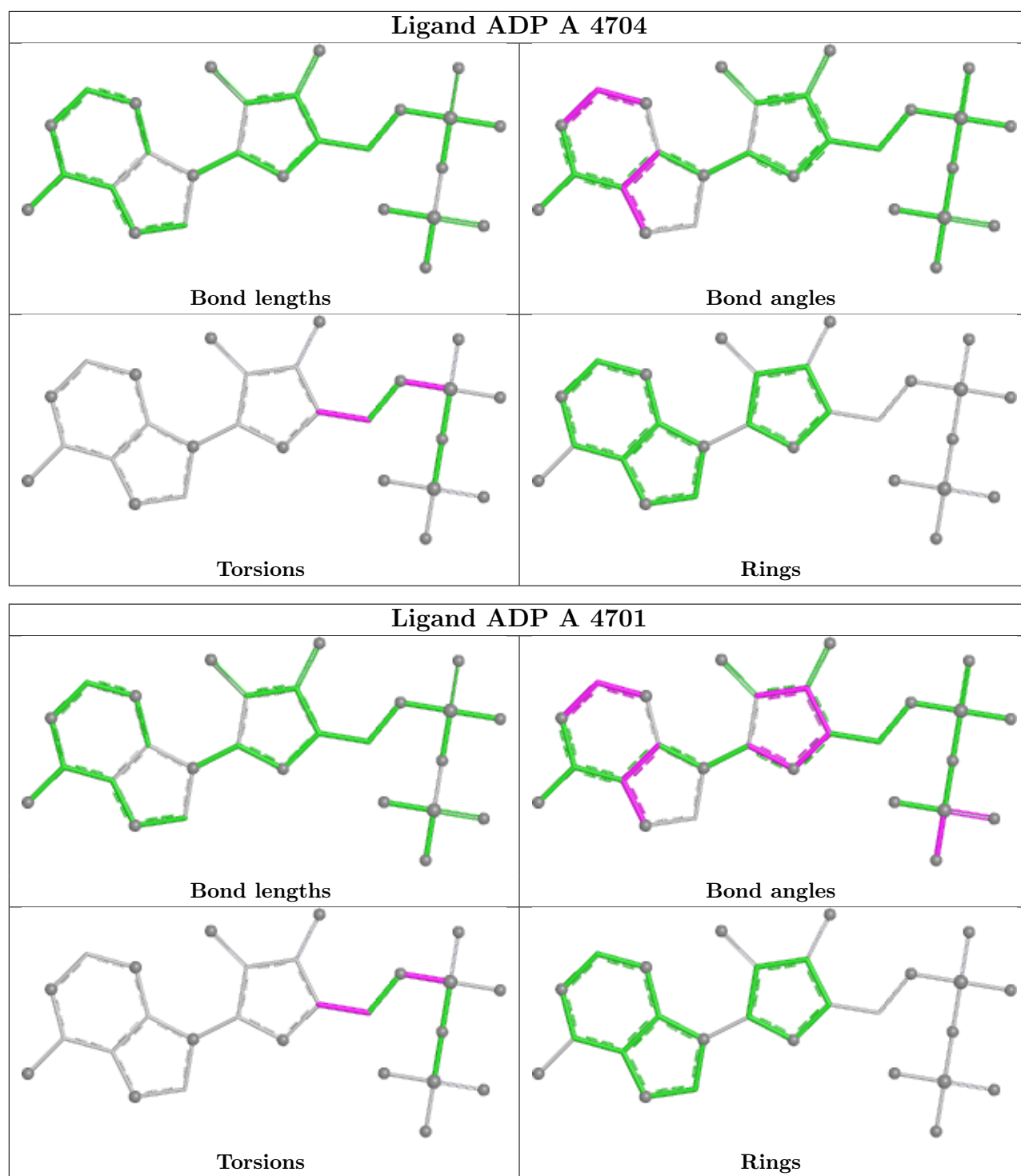
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	4	0
2	A	4703	ADP	7	0
2	A	4704	ADP	3	0
2	A	4701	ADP	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

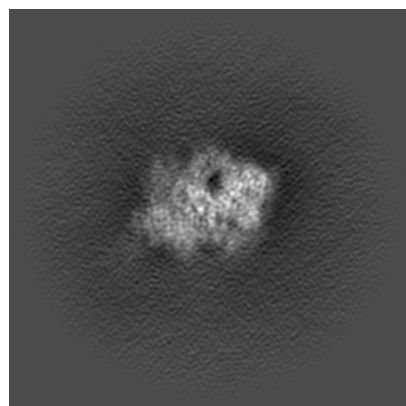
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44711. These allow visual inspection of the internal detail of the map and identification of artifacts.

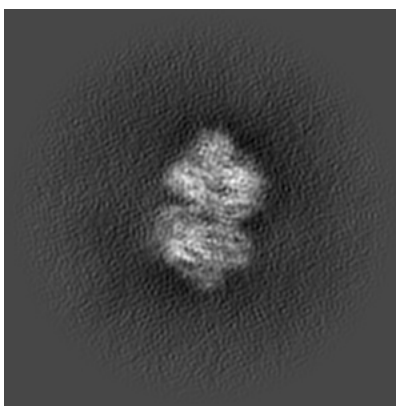
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

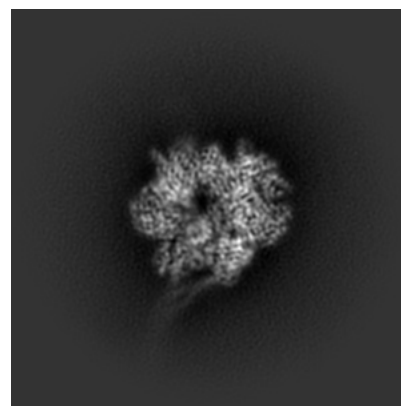
6.1.1 Primary map



X

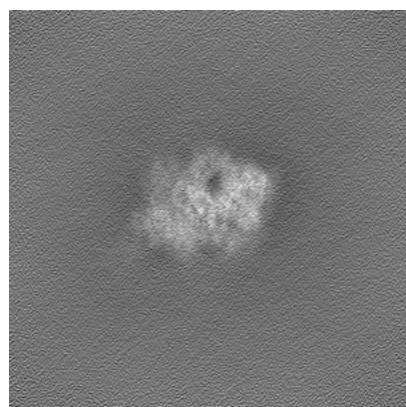


Y

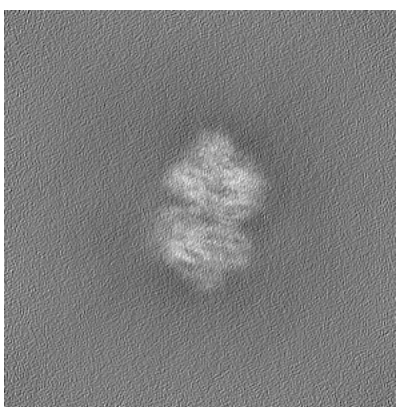


Z

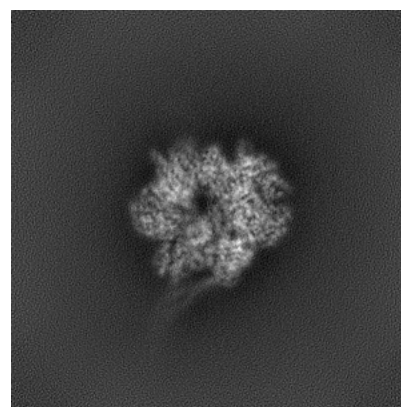
6.1.2 Raw map



X



Y

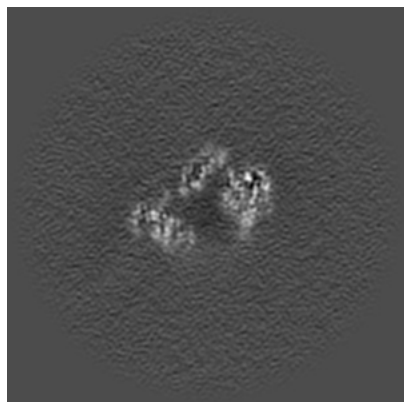


Z

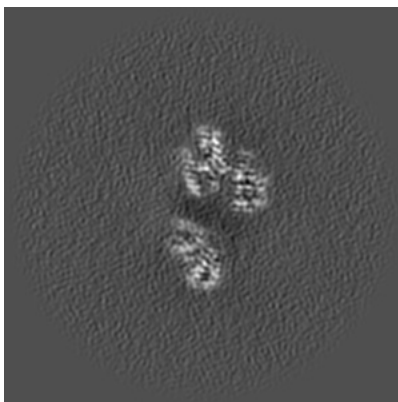
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

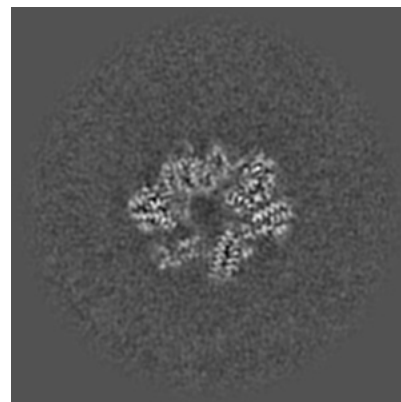
6.2.1 Primary map



X Index: 160

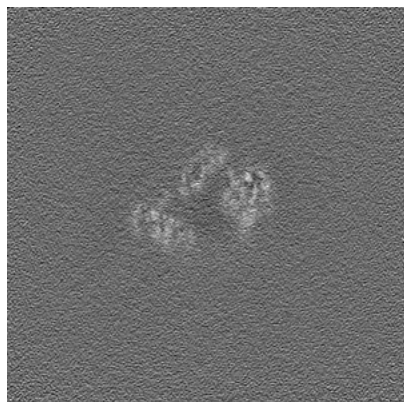


Y Index: 160

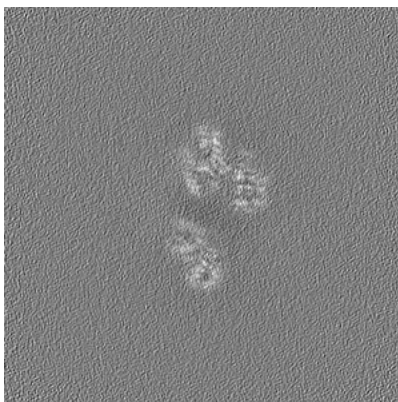


Z Index: 160

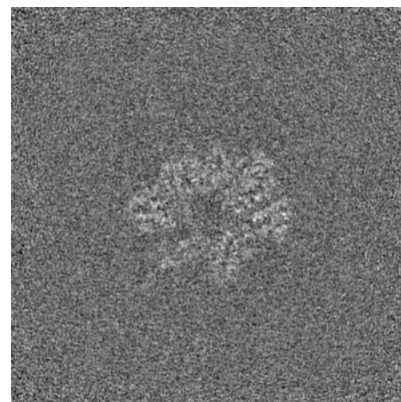
6.2.2 Raw map



X Index: 160



Y Index: 160

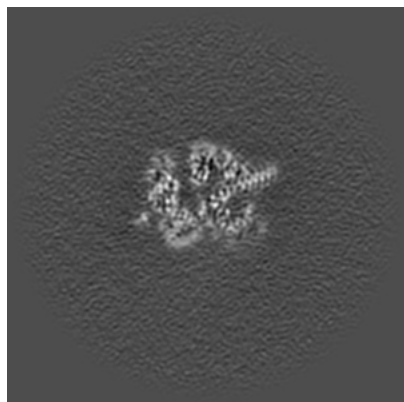


Z Index: 160

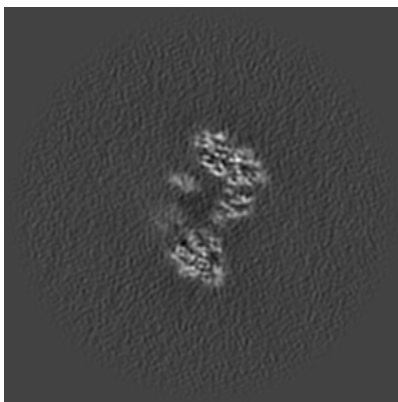
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

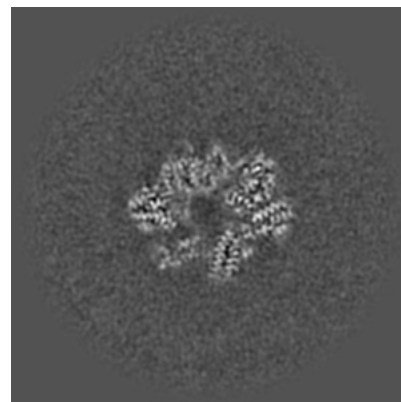
6.3.1 Primary map



X Index: 182

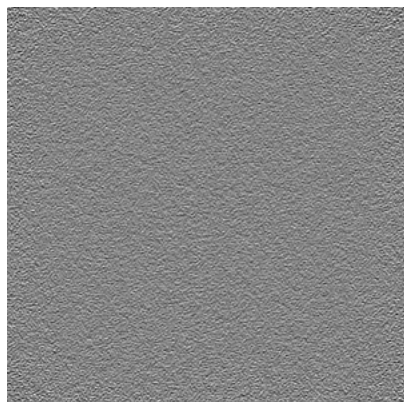


Y Index: 150

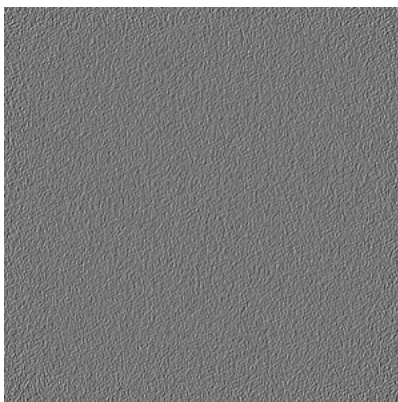


Z Index: 160

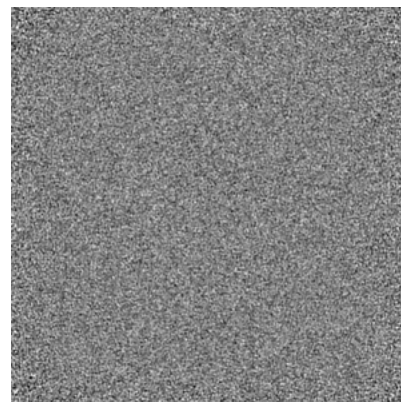
6.3.2 Raw map



X Index: 0



Y Index: 0

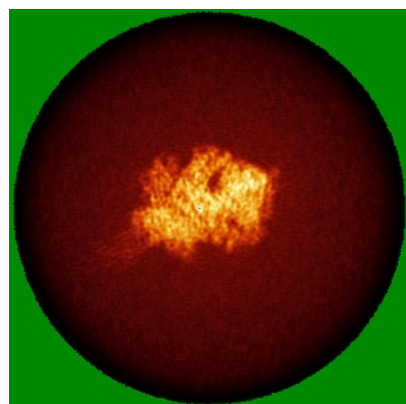


Z Index: 0

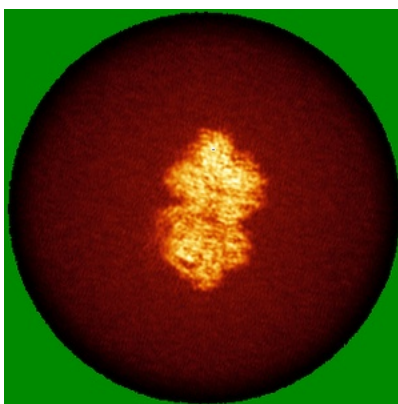
The images above show the largest variance slices of the map in three orthogonal directions.

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

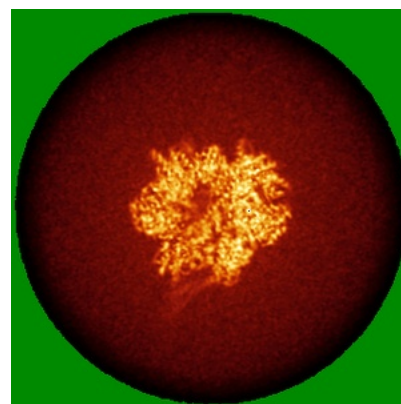
6.4.1 Primary map



X

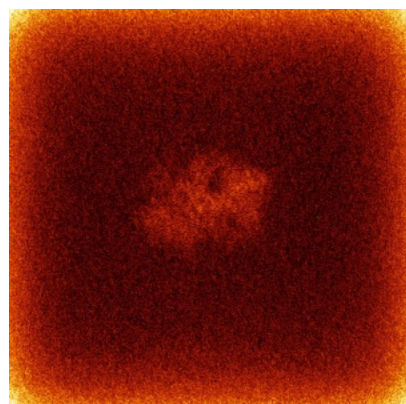


Y

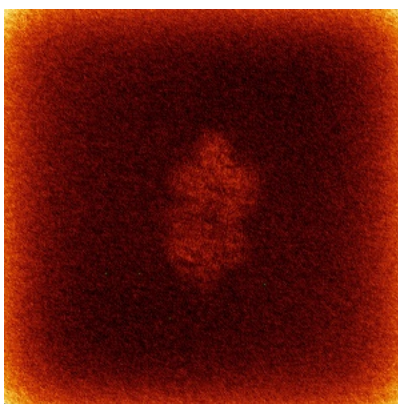


Z

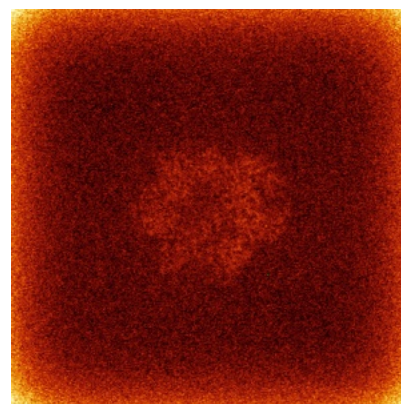
6.4.2 Raw map



X



Y

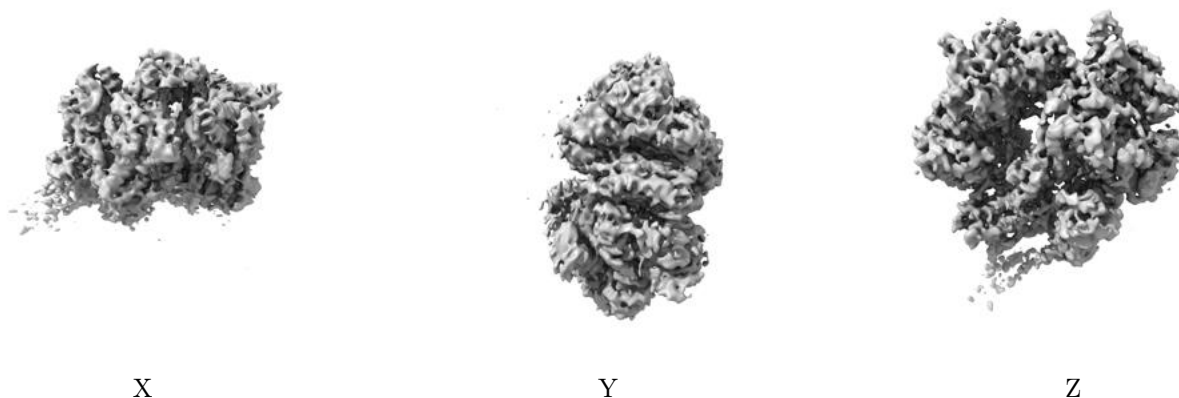


Z

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.

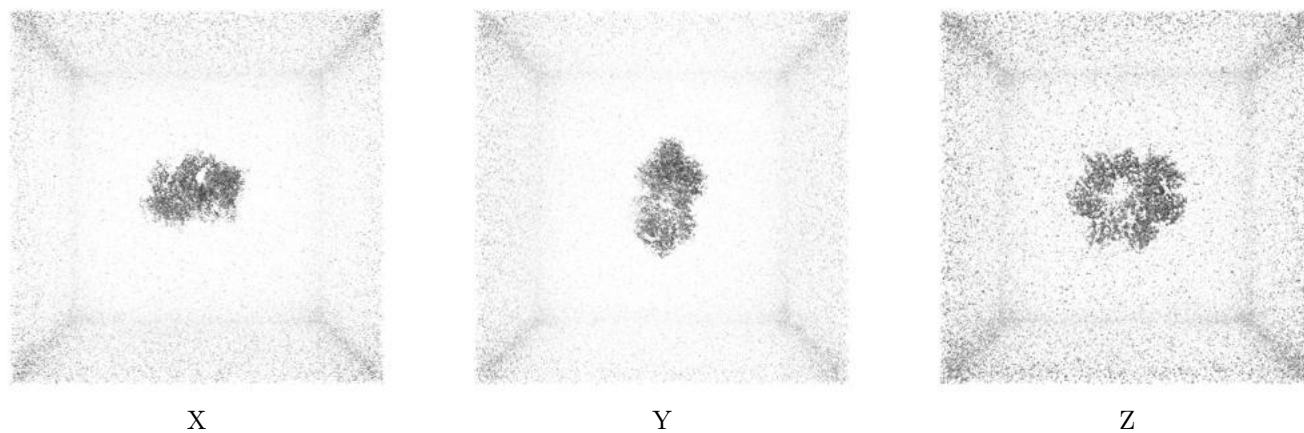
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

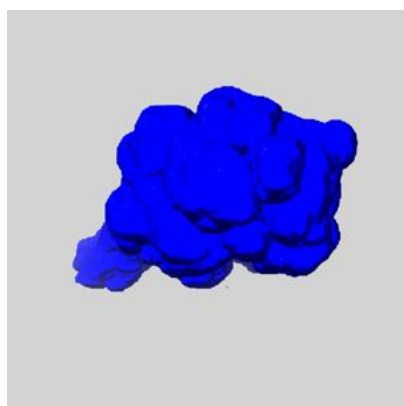
6.6 Mask visualisation [i](#)

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

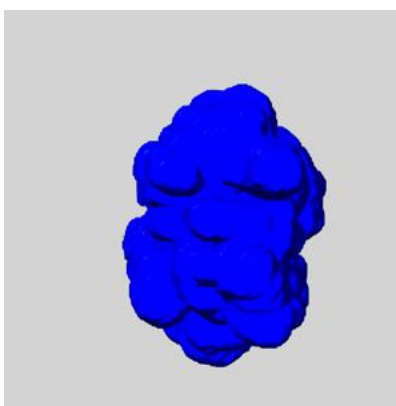
A mask typically either:

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

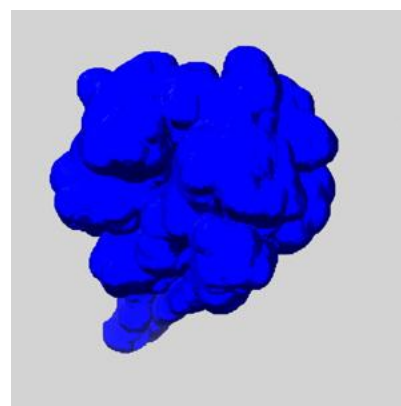
6.6.1 emd_44711_msk_1.map [i](#)



X



Y

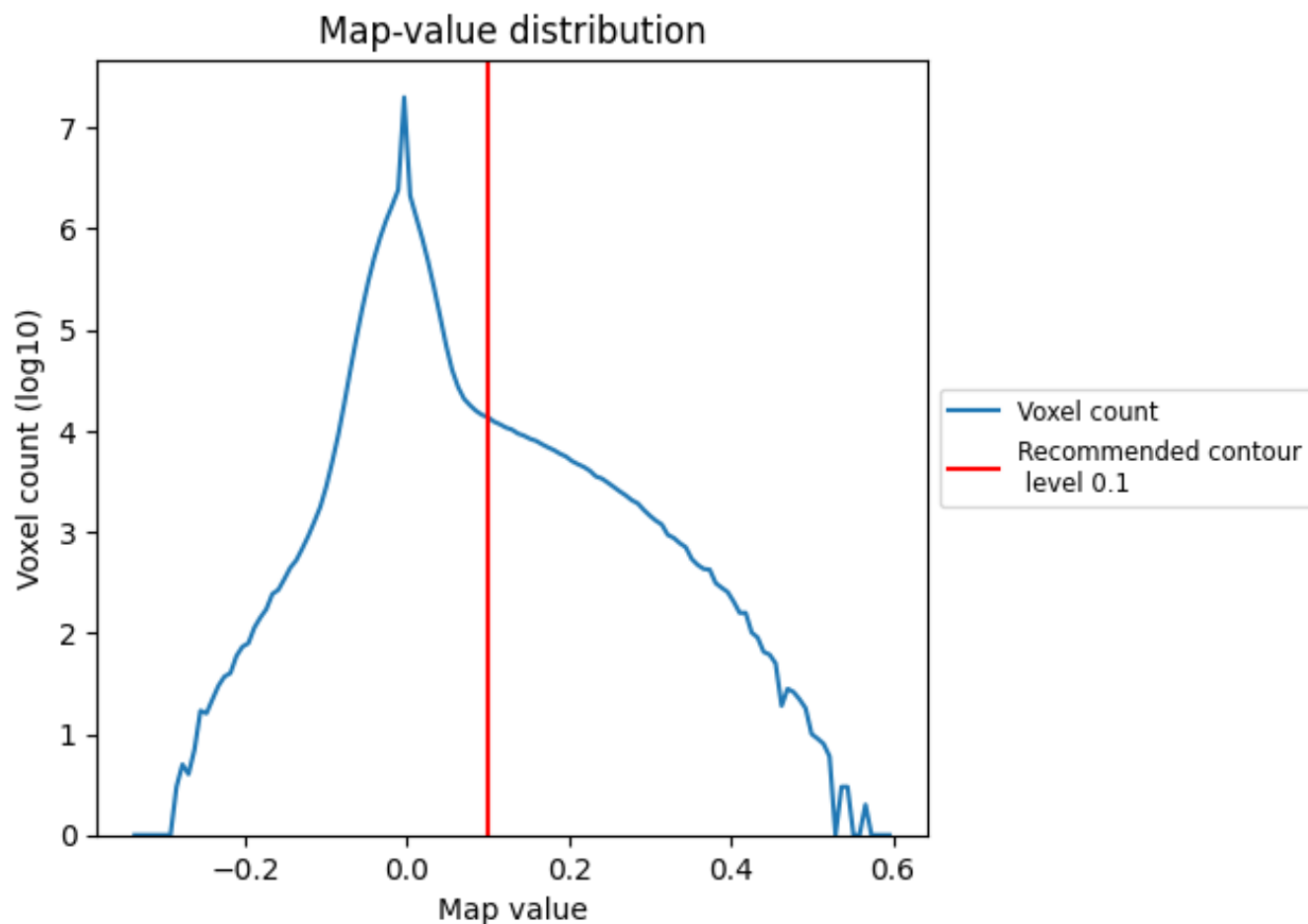


Z

7 Map analysis [i](#)

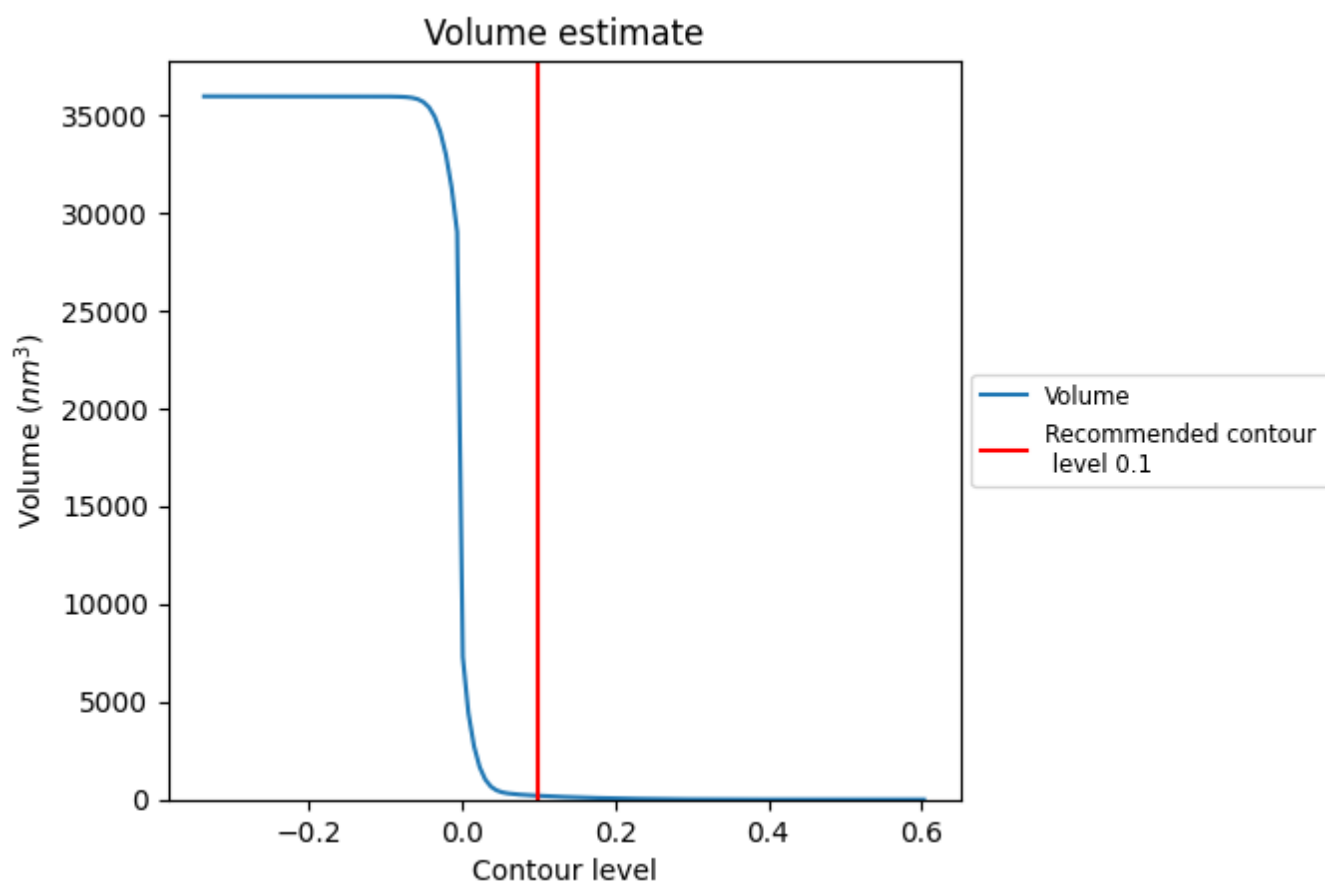
This section contains the results of statistical analysis of the map.

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.

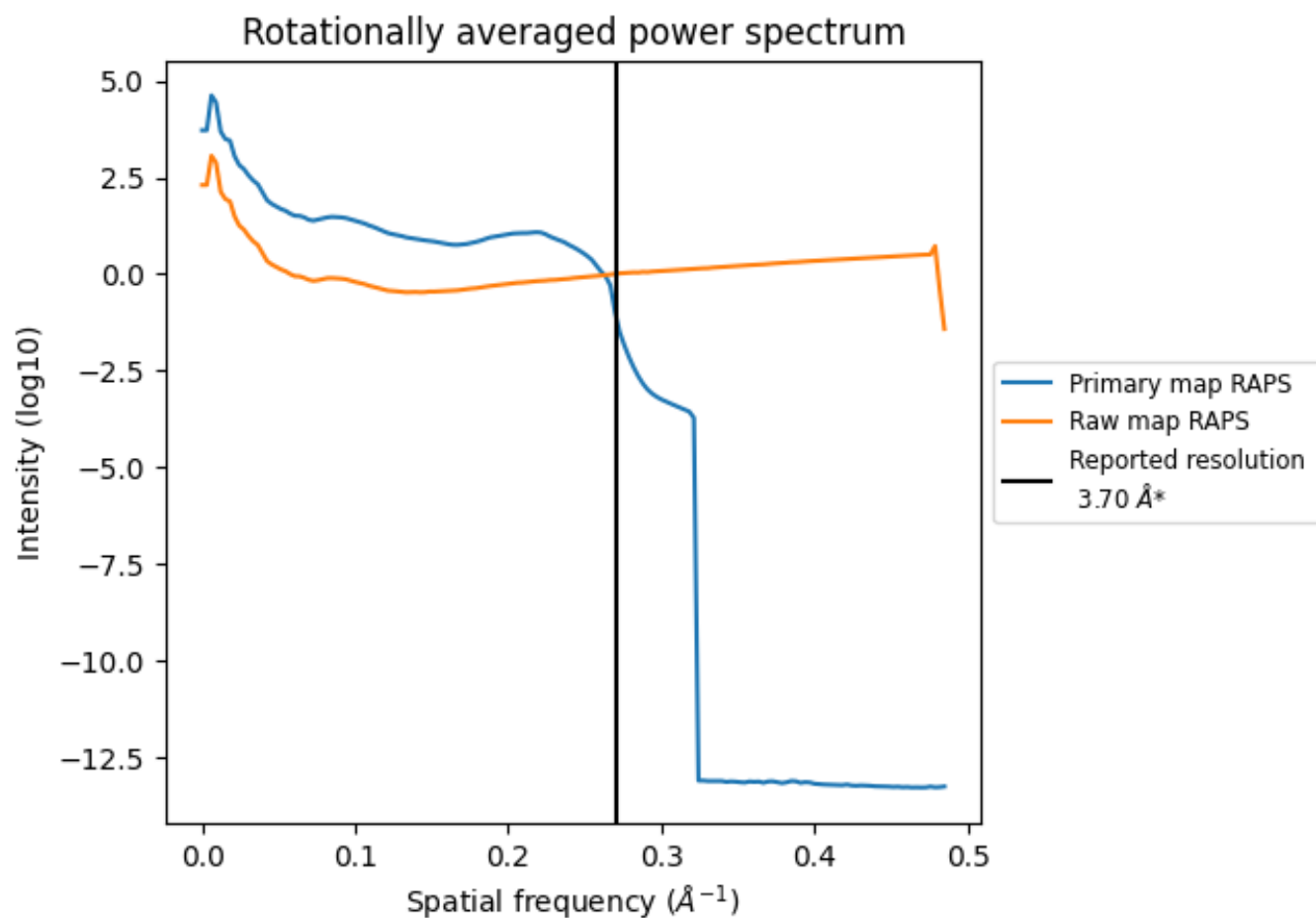
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

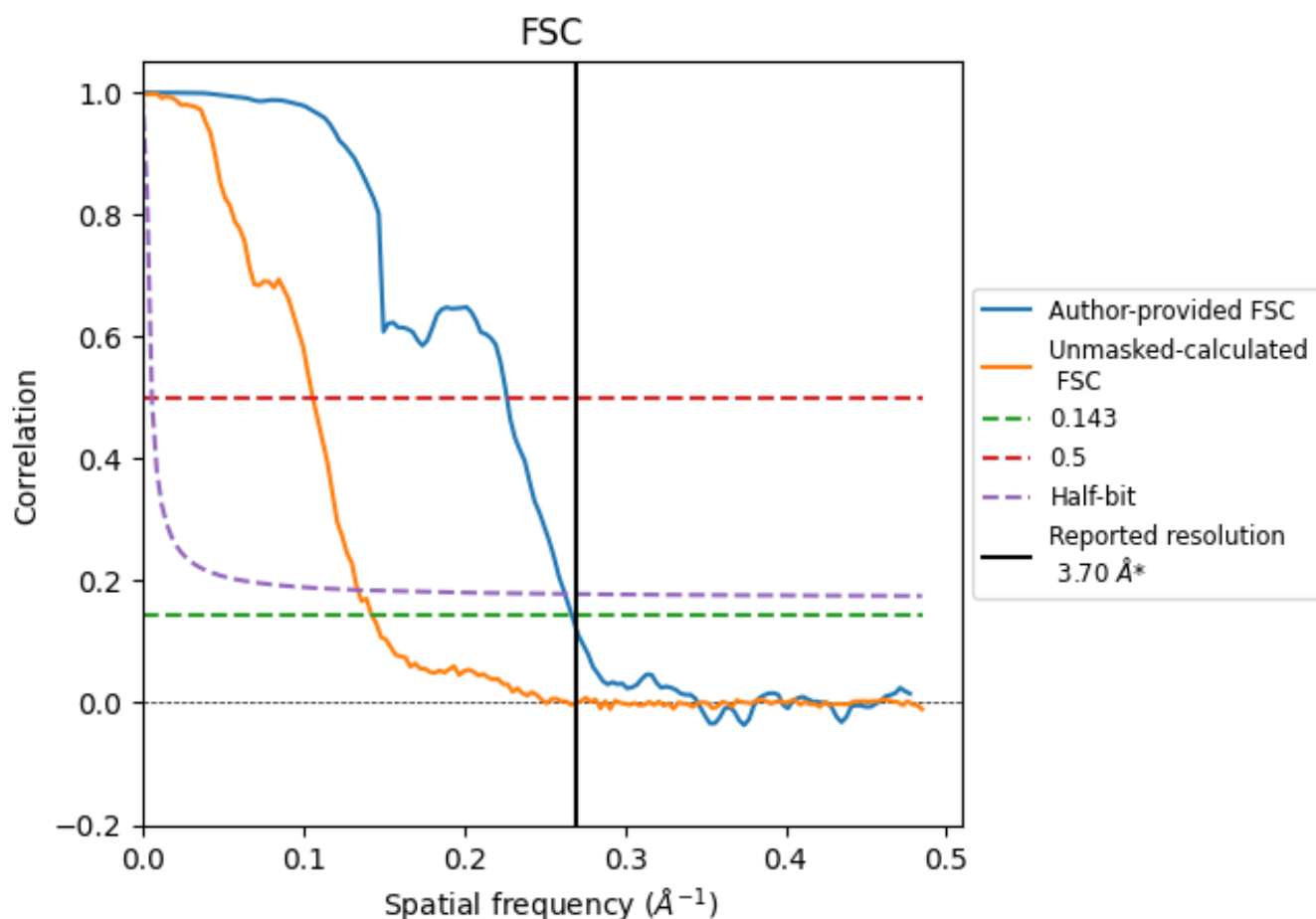


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

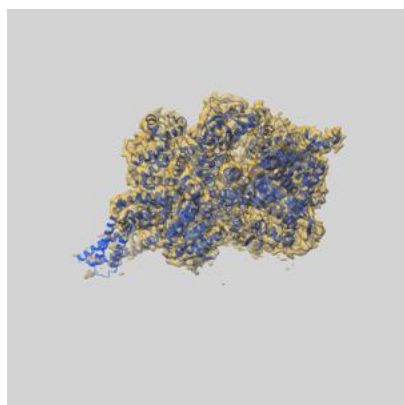
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.41	3.81
Unmasked-calculated*	7.00	9.43	7.46

*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 7.00 differs from the reported value 3.7 by more than 10 %

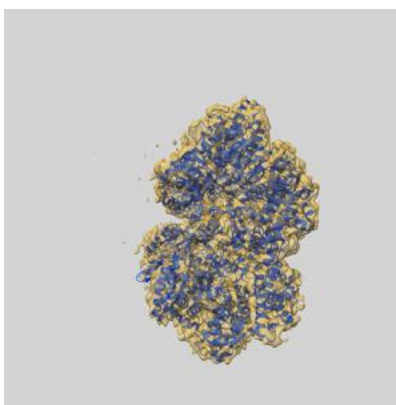
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44711 and PDB model 9BMU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

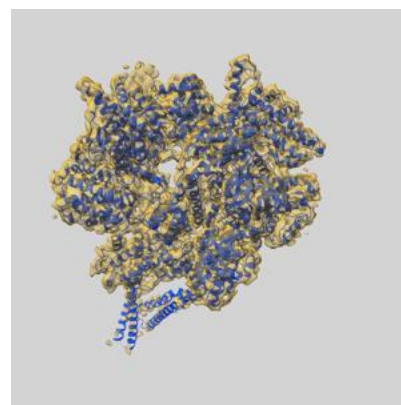
9.1 Map-model overlay [i](#)



X



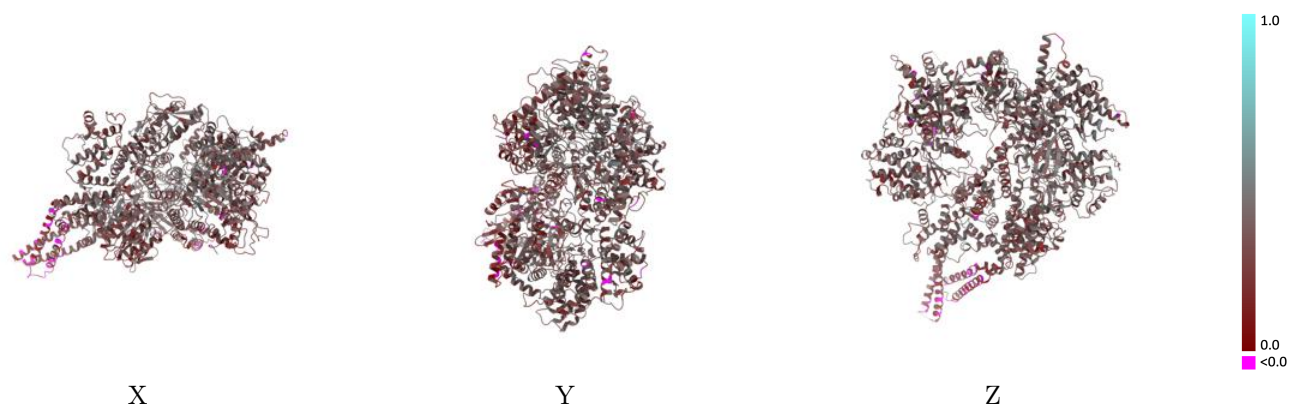
Y



Z

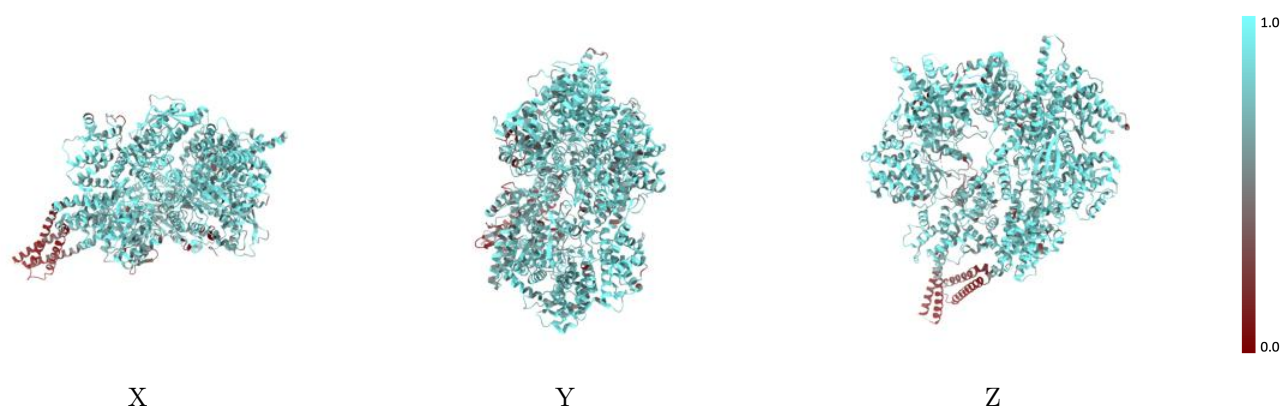
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



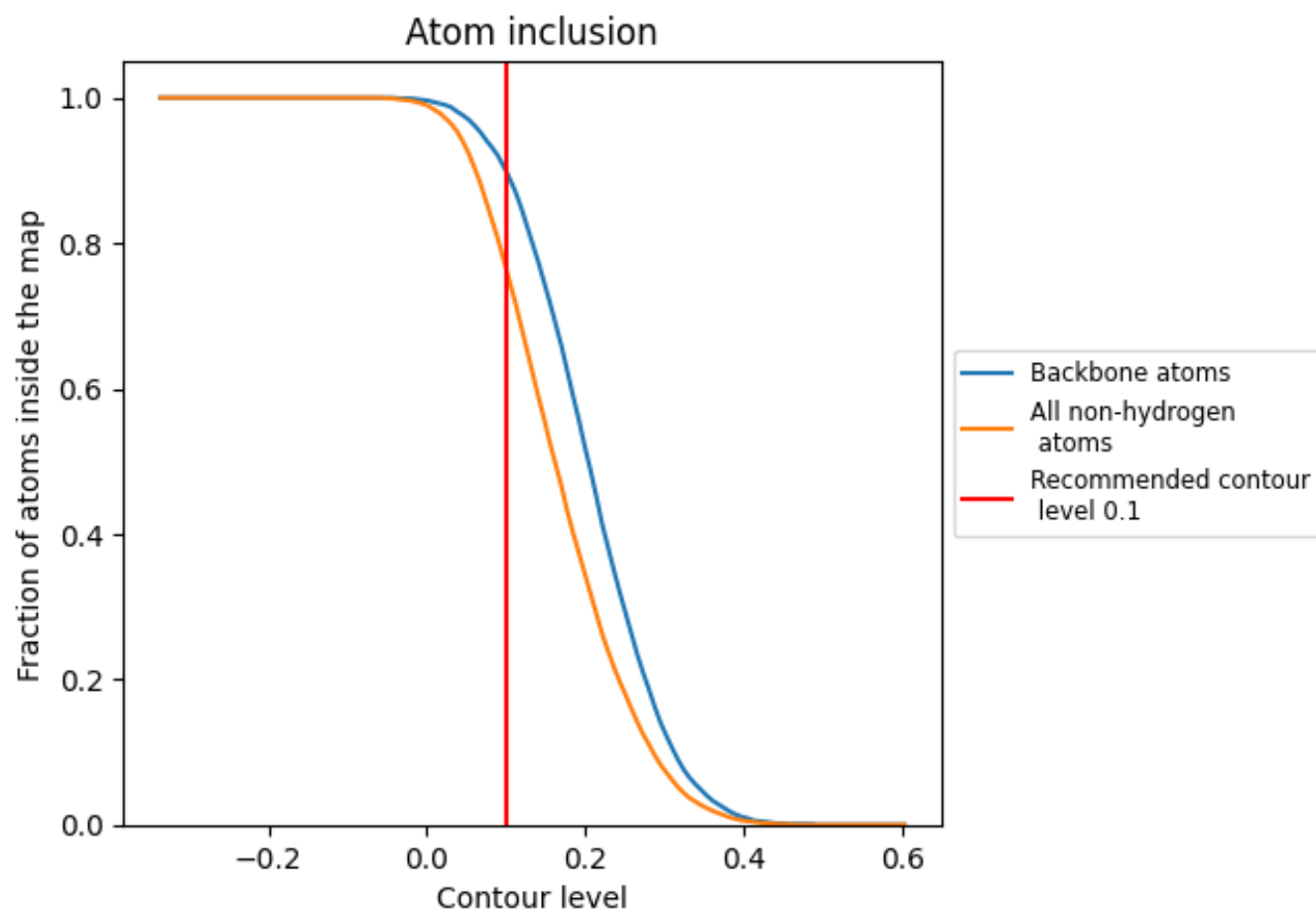
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7650	<div></div> 0.3330
A	<div></div> 0.7650	<div></div> 0.3330

