



wwPDB EM Validation Summary Report ⓘ

Aug 14, 2025 – 01:42 PM EDT

PDB ID : 9BMV / pdb_00009bmv
EMDB ID : EMD-44712
Title : State-7a-post1 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

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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

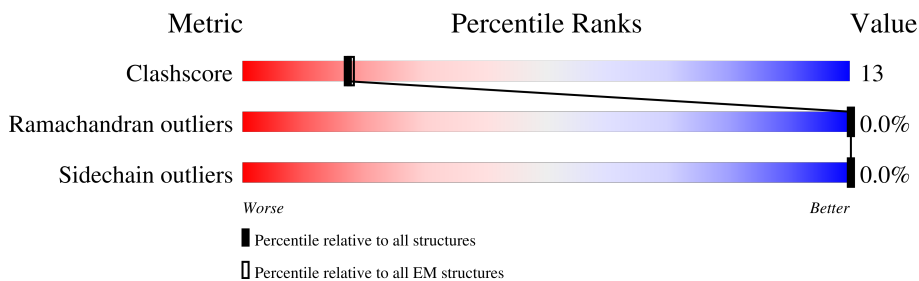
1 Overall quality at a glance

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>9%</div> <div>45%</div> <div>20%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

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



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0



SER	L3115	L3020	F2926	V2838	L2723	R2643	R2519	A2420	L2335	H2252	E2133	G2021
GLN	E3116	F3021	R2927	E2859	R2726	T2644	T2557	A2421	P2336	I2253	E136	TYR
LEU	Y3125	E3022	Q2930	D2840	F2727	P2645	T2552	I2421	P2337	A2258	I2137	ALA
GLU	G3023	E2841	G2931	E2842	L2728	G2647	T2523	I2422	M2338	I2259	L2137	GLY
VAL	D3024	E2843	H2932	R2844	R2729	V2648	V2524	S2429	I2341	K2260	I2138	ARG
LYS	E3025	R2844	L2935	R2844	H2730	V2649	P2527	R2430	M2342	K2261	V2141	S2026
ASN	D3131	L2850	L2935	A2651	H2731	A2651	D2536	K2435	F2343	D2262	V2146	P2029
ALA	L3132	D2851	G2940	P2652	V2732	P2652	F2544	L2437	E2344	H2263	D2030	D2030
ALA	P3134	H2857	K2943	K2657	V2733	K2657	V2545	E2438	Q2346	L2264	L2149	L2035
ASN	R3140	H2857	K2943	K2657	L2744	K2657	V2545	H2439	D2347	Y2265	L2156	L2041
ASP	E3142	H2857	L2946	H2857	I2747	V2660	V2557	Q2442	T2352	D2269	L2156	M2041
LYS	A3142	H2857	L2946	H2857	I2747	L2661	V2557	Q2442	T2352	P2270	L2161	P2044
LEU	I3143	H2857	L2946	H2857	I2747	F2662	T2559	Q2442	L2353	M2271	L2176	M2053
LYS	S3146	H2857	L2946	H2857	I2747	D2663	T2559	R2451	A2354	T2272	E2181	L2054
MET	V3150	H2857	L2946	H2857	I2747	R2664	T2559	L2455	R2358	E2274	C2186	S2056
VAL	L3042	H2857	L2946	H2857	I2747	E2665	T2559	L2455	R2358	W2275	L2191	R2060
LYS	L3043	H2857	L2946	H2857	I2747	L2666	T2559	S2460	F2364	G2277	T2192	L2065
ASP	L3044	H2857	L2946	H2857	I2747	L2667	T2559	M2461	V2368	G2278	W2203	A2066
GLN	D3045	H2857	L2946	H2857	I2747	L2668	T2559	L2462	L2369	L2281	V2204	L2069
GLN	S3046	H2857	L2946	H2857	I2747	P2669	T2559	A2465	D2372	L2284	E2205	L2080
ALA	A3162	H2857	L2946	H2857	I2747	D2670	T2559	M2473	M2373	T2287	K2206	Q2083
GLU	E3049	H2857	L2946	H2857	I2747	M2671	T2559	L2481	P2386	R2292	Q2209	Y2086
ALA	L3050	H2857	L2946	H2857	I2747	D2672	T2559	L2481	P2386	G2293	L2210	L2093
GLU	T3168	H2857	L2946	H2857	I2747	M2672	T2559	L2486	L2387	E2294	L2211	L2094
LYS	M3169	H2857	L2946	H2857	I2747	K2673	T2559	E2487	L2295	Q2296	T2214	R2091
LYS	R3174	H2857	L2946	H2857	I2747	G2675	T2559	R2488	L2295	K2297	L2220	A2092
VAL	T3067	H2857	L2946	H2857	I2747	T2676	T2559	L2490	E2393	R2298	M2221	L2093
MET	D3178	H2857	L2946	H2857	I2747	L2682	T2559	Y2489	A2394	T2301	M2222	K2094
SER	F3179	H2857	L2946	H2857	I2747	I2683	T2559	Q2491	E2393	L2301	G2224	L2097
GLN	I3180	H2857	L2946	H2857	I2747	Q2684	T2559	Y2493	Q2395	D2304	K2230	N2102
ILE	M3199	H2857	L2946	H2857	I2747	Q2685	T2559	L2495	R2396	G2305	V2103	N2103
GLN	H3200	H2857	L2946	H2857	I2747	M2686	T2559	L2495	R2396	D2306	R2104	R2105
GLU	L3075	H2857	L2946	H2857	I2747	E2687	T2559	L2495	R2397	D2307	W2234	K2110
GLN	K3076	H2857	L2946	H2857	I2747	H2688	T2559	L2495	R2398	E2309	R2235	I2111
LEU	S3077	H2857	L2946	H2857	I2747	H2689	T2559	L2495	K2399	E2310	W2236	R2112
HIS	A3079	H2857	L2946	H2857	I2747	R2694	T2559	L2495	G2400	W2311	K2239	R2113
LYS	A3080	H2857	L2946	H2857	I2747	D2697	T2559	L2495	K2401	V2312	A2240	E2114
GLN	P3083	H2857	L2946	H2857	I2747	K2702	T2559	L2495	G2402	E2313	R2242	K2115
VAL	I3208	H2857	L2946	H2857	I2747	L2703	T2559	L2495	K2402	L2315	E2244	E2116
ILE	K3209	H2857	L2946	H2857	I2747	E2704	T2559	L2495	D2403	V2318	E2245	G2119
ASP	E3210	H2857	L2946	H2857	I2747	R2705	T2559	L2495	E2404	K2323	G2246	V2122
LYS	T3211	H2857	L2946	H2857	I2747	Q2706	T2559	L2495	G2405	L2325	E2248	L2131
GLN	V3212	H2857	L2946	H2857	I2747	L2707	T2559	L2495	G2405	E2248	E2248	P2132
MET	D3213	H2857	L2946	H2857	I2747	F2708	T2559	L2495	E2406	E2248	E2248	P2132
SER	Q3214	H2857	L2946	H2857	I2747	V2709	T2559	L2495	E2406	E2248	E2248	P2132
VAL	V3215	H2857	L2946	H2857	I2747	C2712	T2559	L2495	E2406	E2248	E2248	P2132
GLU	E3216	H2857	L2946	H2857	I2747	D2717	T2559	L2495	E2406	E2248	E2248	P2132
ASP	E3217	H2857	L2946	H2857	I2747	P2718	T2559	L2495	E2406	E2248	E2248	P2132
LEU	L3218	H2857	L2946	H2857	I2747	Q2719	T2559	L2495	E2406	E2248	E2248	P2132
LYS	R3219	H2857	L2946	H2857	I2747	R2720	T2559	L2495	E2406	E2248	E2248	P2132
VAL	R3220	H2857	L2946	H2857	I2747	F2634	T2559	L2495	E2406	E2248	E2248	P2132
	D3221	H2857	L2946	H2857	I2747	F2635	T2559	L2495	E2406	E2248	E2248	P2132
	LEU	H2857	L2946	H2857	I2747	F2635	T2559	L2495	E2406	E2248	E2248	P2132
	ARG	H2857	L2946	H2857	I2747	F2635	T2559	L2495	E2406	E2248	E2248	P2132
	ILE	H2857	L2946	H2857	I2747	F2635	T2559	L2495	E2406	E2248	E2248	P2132
	LYS	H2857	L2946	H2857	I2747	F2635	T2559	L2495	E2406	E2248	E2248	P2132

M4597	T4598	E4599	K4600	V4604	L4607	P4608	V4609	M4612	I4619	F4620	D4623	F4624	A4627	E4630	F4635	E4637	R4638	V4640	V4641	V4642	E4646																													
S4485	H4486	P4470	A4471	G4472	M4473	T4474	V4475	I4476	Q4477	H4478	V4479	S4480	D4481	F4482	S4483	E4484	R4485	I4486	S4493	A4496	A4501	L4504	L4511	E4518	V4528	L4541	Q4549	D4554	A4555	C4556	S4557	V4560	K4564	K4574	L4577	S4578	N4579	L4590	R4591	V4592	Q4595	T4596								
THR	ARG	THR	ASP	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	P4392	Q4393	T4394	L4395	L4398	K4399	R4400	T4401	N4404	L4405	P4408	L4409	F4410	R4411	F4412	F4413	E4414	V4417	L4423	M4428	C4438	K4441	K4442	K4443	Q4444	T4445	M4446	R4449	E4454	L4460	P4461	V4464						
R4230	L4243	M4247	A4248	I4251	Y4252	F4260	L4269	S4277	E4281	F4282	K4287	G4290	H4291	I4294	I4300	E4304	W4320	L4321	R4324	W4325	W4326	L4332	K4342	M4343	L4344	K4345	M4346	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS								
K4089	M4095	L4096	K4097	H4098	V4099	W4105	L4106	M4107	Q4108	E4110	L4113	P4118	R4123	L4124	W4131	L4138	L4139	R4140	F4145	E4148	R4168	S4172	P4173	E4175	R4176	L4183	F4186	H4187	A4188	I4189	I4190	R4193	A4215	C4216	D4217	T4218	V4219	D4220	A4227											
E3930	Q3931	E3932	E3933	R3937	Q3952	P3966	V3970	L3973	E3977	P3982	I3983	Q3984	Q3985	R3989	L3992	F3996	D3999	R4000	L4001	L4002	H4006	M4012	L4025	D4026	L4027	I4030	V4031	P4037	M4038	T4039	P4040	L4042	M4043	C4044	S4045	V4046	D4050	A4051	I4071											
I3835	V3839	L3840	N3845	D3851	H3852	T3853	Q3854	R3855	T3858	L3863	F3864	Q3865	V3866	N3869	R3870	V3871	A3872	R3873	G3874	M3875	H3880	F3883	L3886	L3887	A3888	R3889	I3890	K3891	L3892	D3902	A3903	Q3906	L3909	R3910	E3913	I3914	V3915	L3916	S3917	A3918	G3919	I3811	T3814	L3818	I3821	L3824	S3828	F3831		
E3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	Q3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	A3778	E3779	V3780	T3781	R3782	V3784	E3785	E3786	T3787	D3788	S3809	S3810	I3811	T3814	L3818	I3821	L3824	S3828	F3831
L3649	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	G3658	R3659	I3662	T3663	L3664	G3665	D3666	Q3667	P3673	L3679	S3680	T3681	T3685	P3689	P3690	D3691	L3692	C3693	S3694	R3695	F3698	V3699	N3700	F3701	R3704	R3705	L3708	E3720	D3723	F3629	G3630	N3631	P3632	V3635	V3638	E3639	V3648	R3741	L3742	R3743	Q3744	L3745
R3561	W3562	L3567	T3574	E3575	N3576	A3577	L3578	M3579	R3582	R3585	L3588	D3591	Q3595	S3483	A3484	E3485	R3486	E3487	R3488	W3489	T3492	T3502	L3508	L3509	S3510	A3511	I3514	A3515	Y3516	A3517	G3518	Y3519	F3520	M3524	R3525	W3532	L3536	F3543	R3544	T3545	D3546	R3549	L3553	D3557	E3558					
LEU	LYS	ARG	VAL	GLU	PRO	THR	ILE	GLU	ALA	GLN	ASN	PHE	SER	ALA	VAL	GLY	SER	LEU	GLN	LYS	ILE	LEU	GLU	ARG	GLN	LYS	ASP	ASP	TRP	LYS	GLN	ILE	ALA	GLN	ALA	ARG	LEU	SER	ASN	TYR	ILE	ALA	ASP	MET						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47280	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	0.717	Depositor
Minimum map value	-0.337	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/25022	0.34	0/33900

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1567	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24503	0	24574	659	0
2	A	81	0	36	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	3	0
4	A	1	0	0	0	0
All	All	24616	0	24622	659	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 13.

The worst 5 of 659 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:4189:ILE:HD11	1:A:4321:LEU:HA	1.55	0.88
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.61	0.81
1:A:1551:PHE:HA	1:A:1557:ILE:HD11	1.63	0.80
1:A:3178:ASP:HB2	1:A:3585:ARG:HH21	1.48	0.78
1:A:1632:VAL:HB	1:A:1657:MET:HE1	1.66	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	3035/4646 (65%)	2956 (97%)	78 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1511	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2706/4125 (66%)	2705 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	1567	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2475	ASN
1	A	2786	GLN
1	A	4191	GLN
1	A	2698	GLN
1	A	3032	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.26	3 (10%)
3	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.61	1 (2%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.29	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	5/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.62	123.76	128.67
2	A	4704	ADP	N3-C2-N1	-3.57	123.83	128.67
2	A	4701	ADP	N3-C2-N1	-3.54	123.86	128.67
2	A	4704	ADP	C4-C5-N7	-2.53	106.67	109.34
2	A	4701	ADP	C4-C5-N7	-2.48	106.72	109.34

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

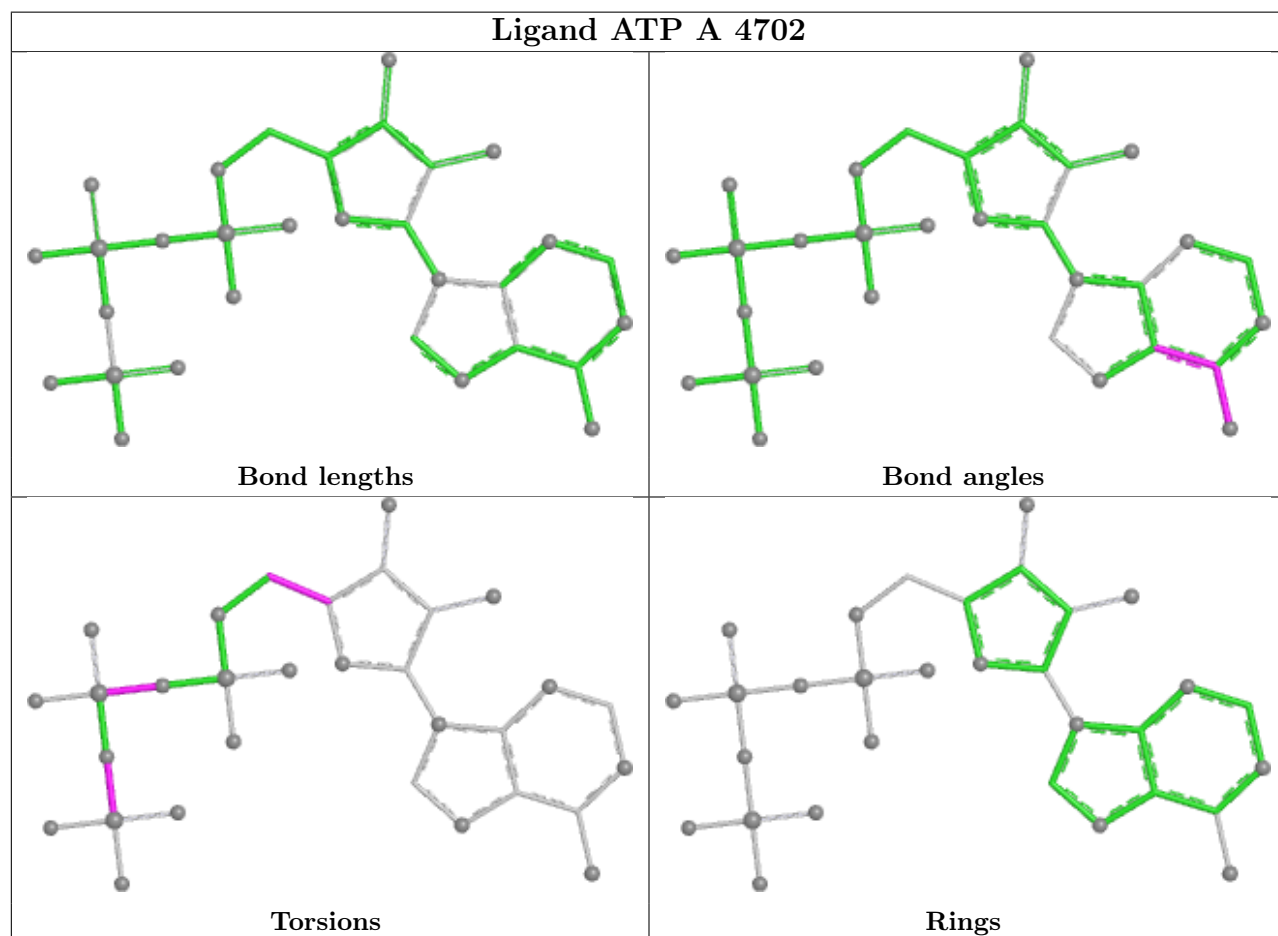
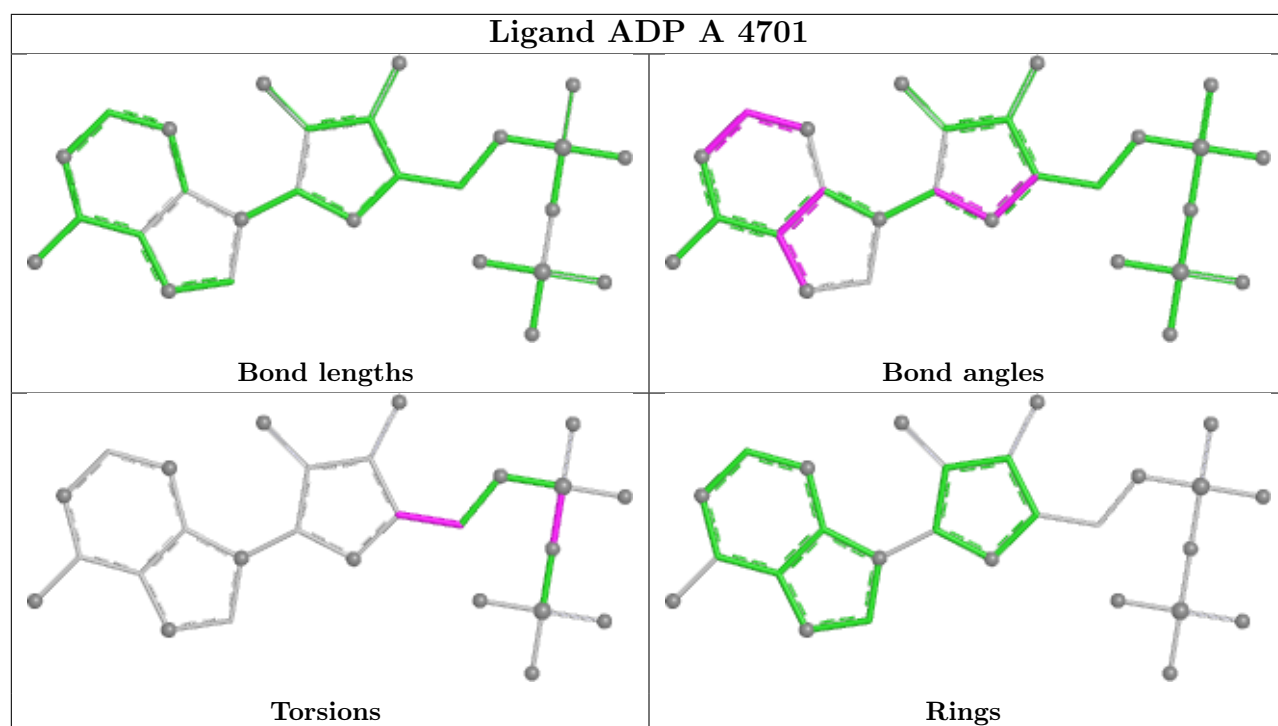
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O3G

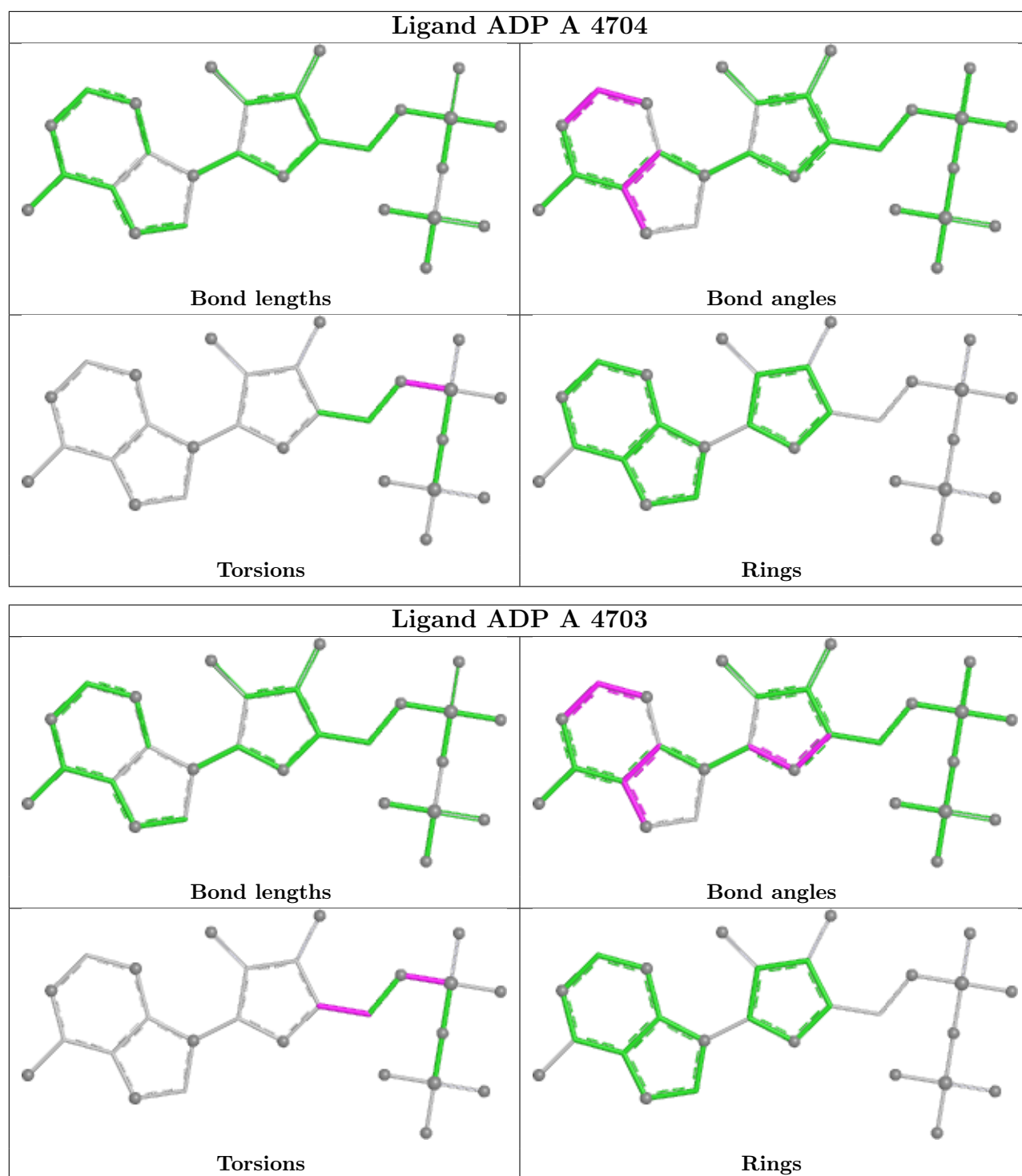
There are no ring outliers.

4 monomers are involved in 12 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

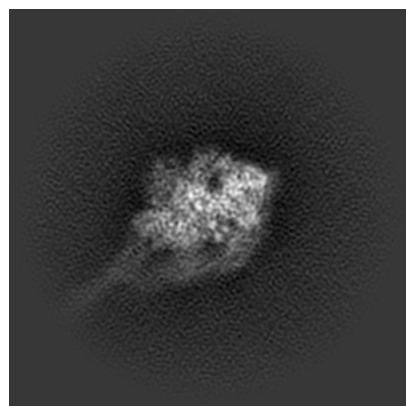
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44712. These allow visual inspection of the internal detail of the map and identification of artifacts.

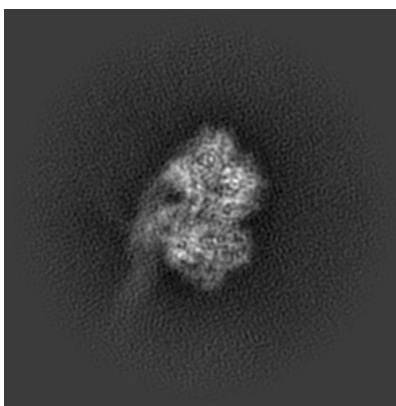
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

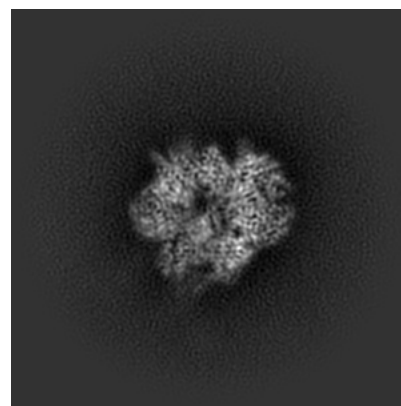
6.1.1 Primary map



X

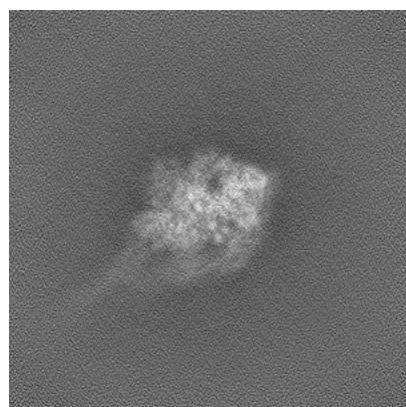


Y

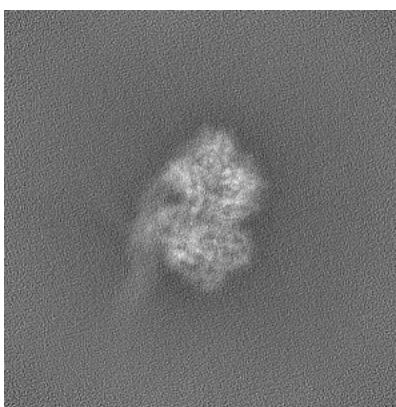


Z

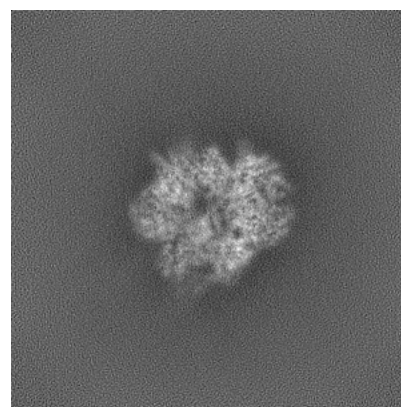
6.1.2 Raw map



X



Y

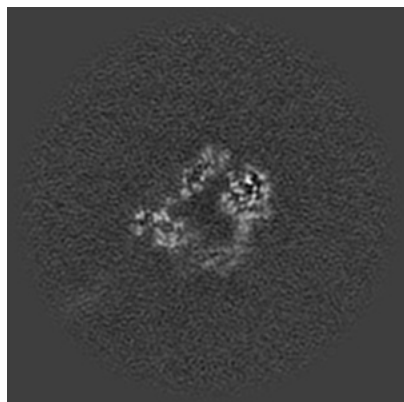


Z

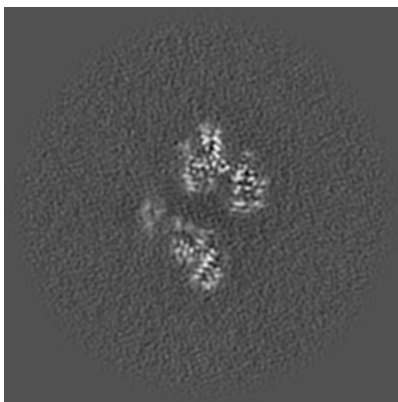
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

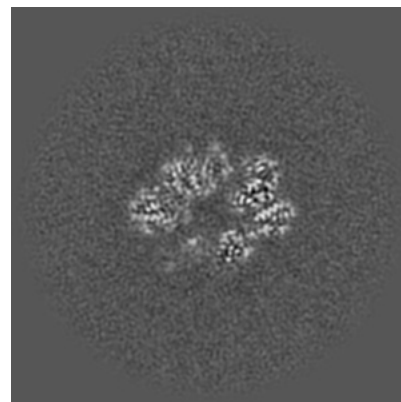
6.2.1 Primary map



X Index: 160

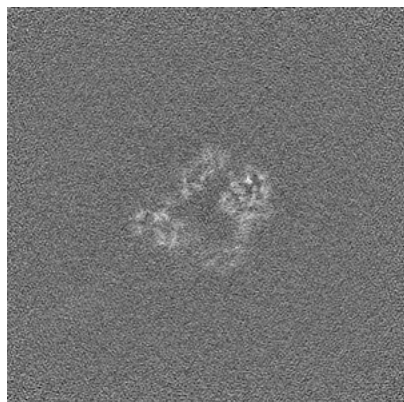


Y Index: 160

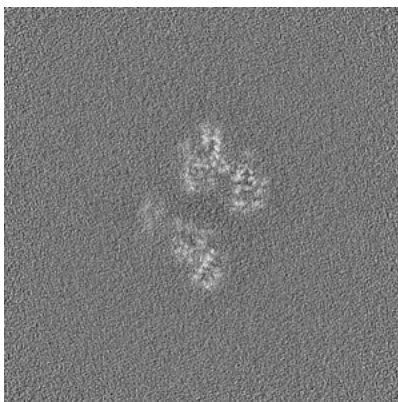


Z Index: 160

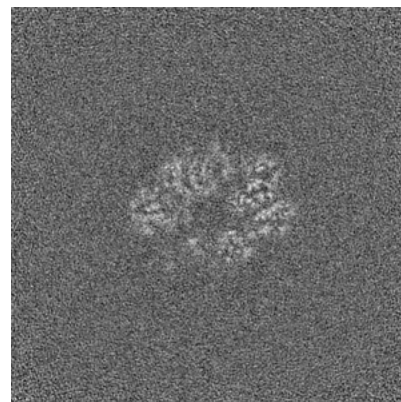
6.2.2 Raw map



X Index: 160



Y Index: 160

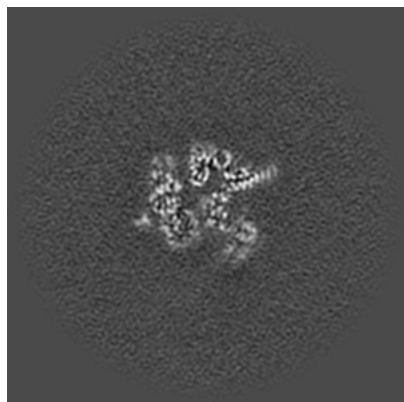


Z Index: 160

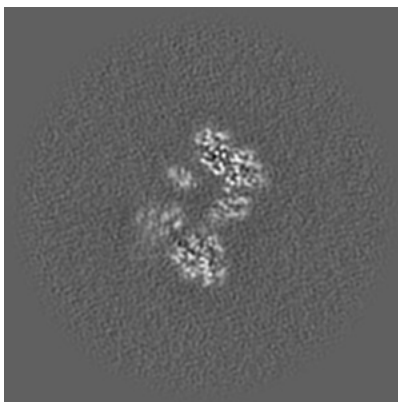
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

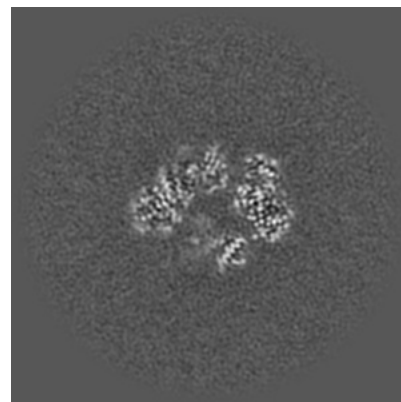
6.3.1 Primary map



X Index: 182

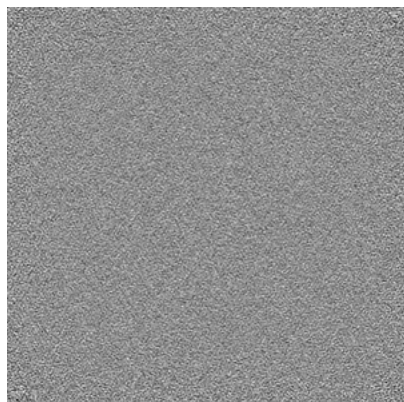


Y Index: 150

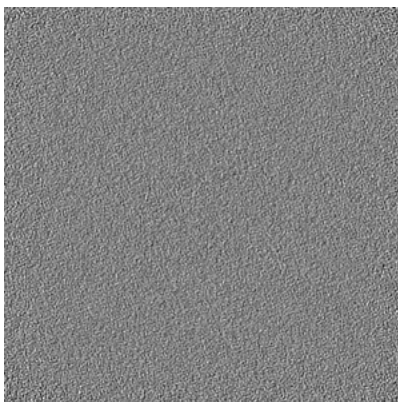


Z Index: 165

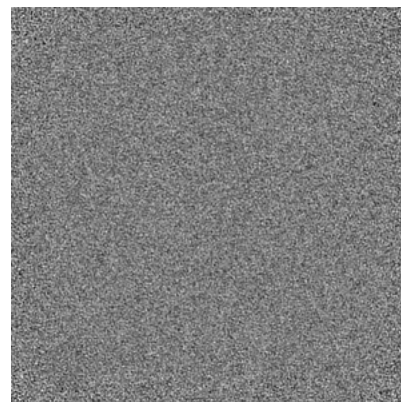
6.3.2 Raw map



X Index: 0



Y Index: 0

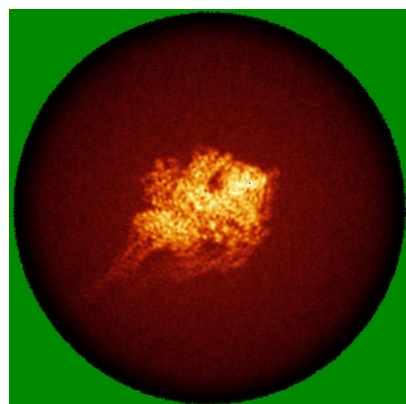


Z Index: 0

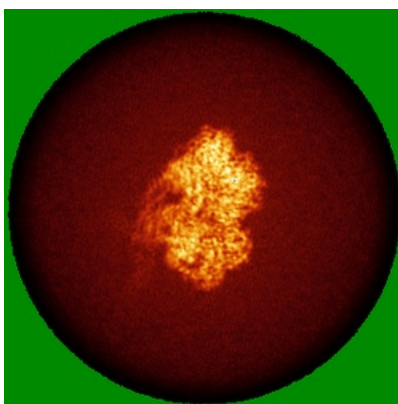
The images above show the largest variance slices of the map in three orthogonal directions.

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

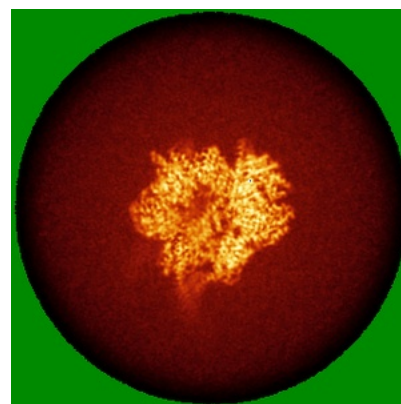
6.4.1 Primary map



X

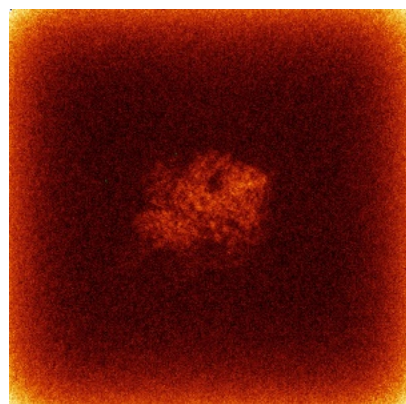


Y

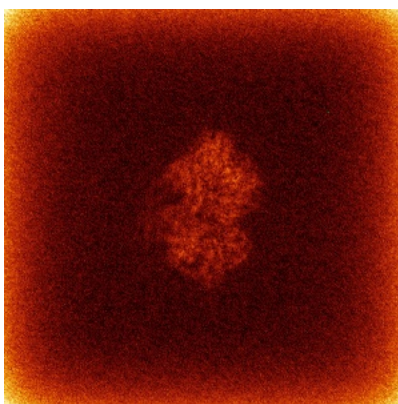


Z

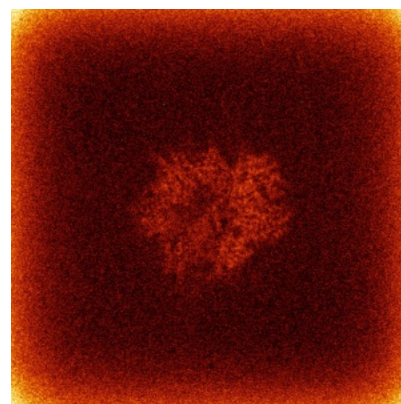
6.4.2 Raw map



X



Y

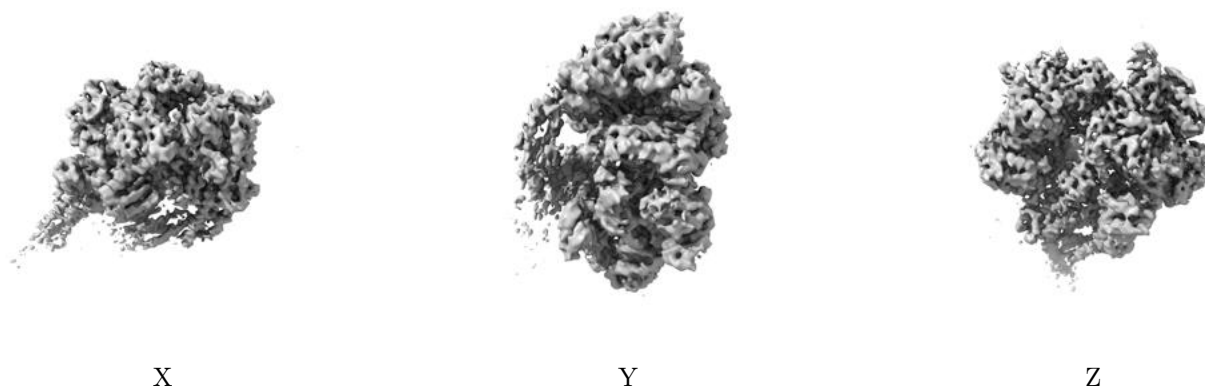


Z

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.

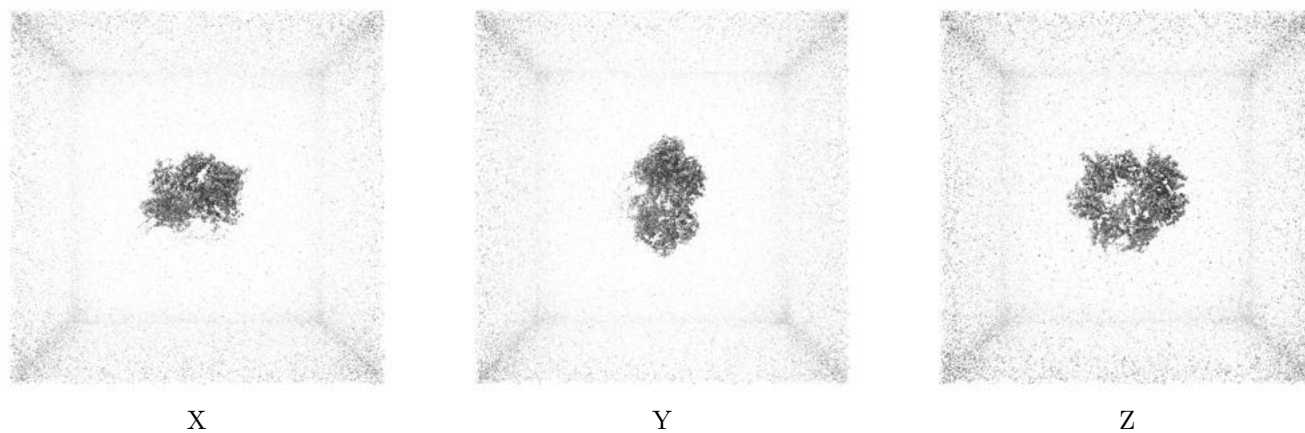
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

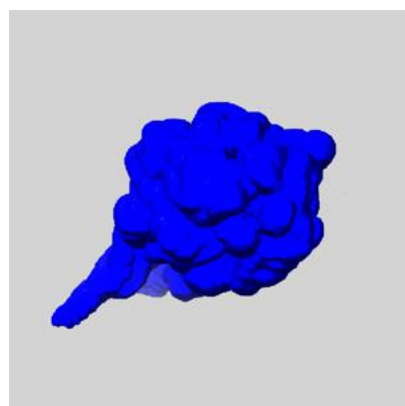
6.6 Mask visualisation [i](#)

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

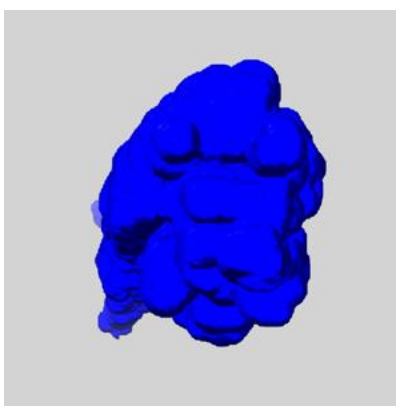
A mask typically either:

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

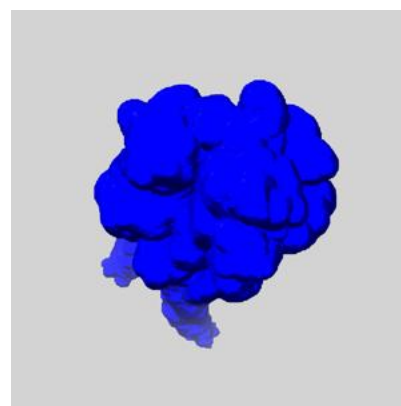
6.6.1 emd_44712_msk_1.map [i](#)



X



Y

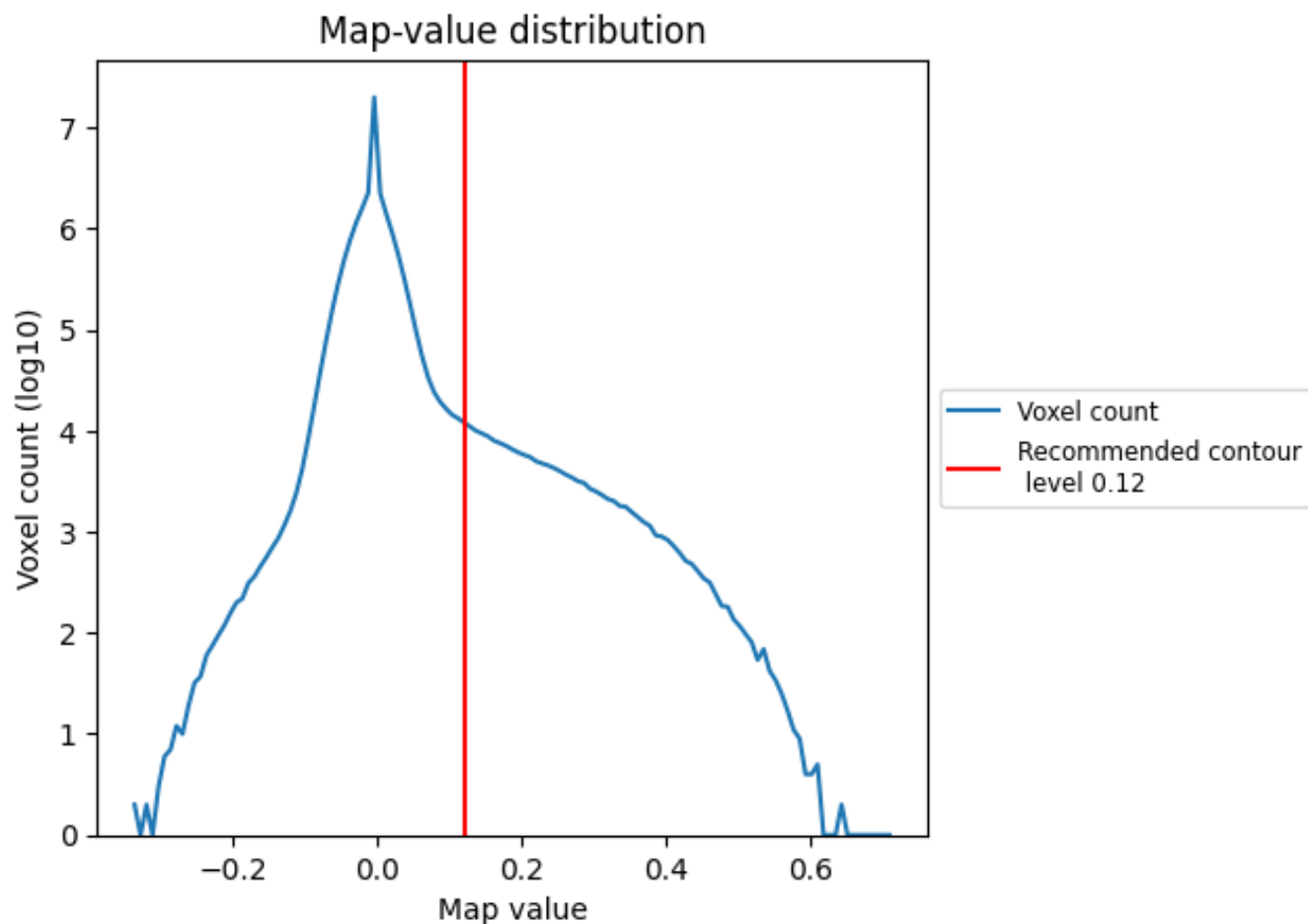


Z

7 Map analysis [i](#)

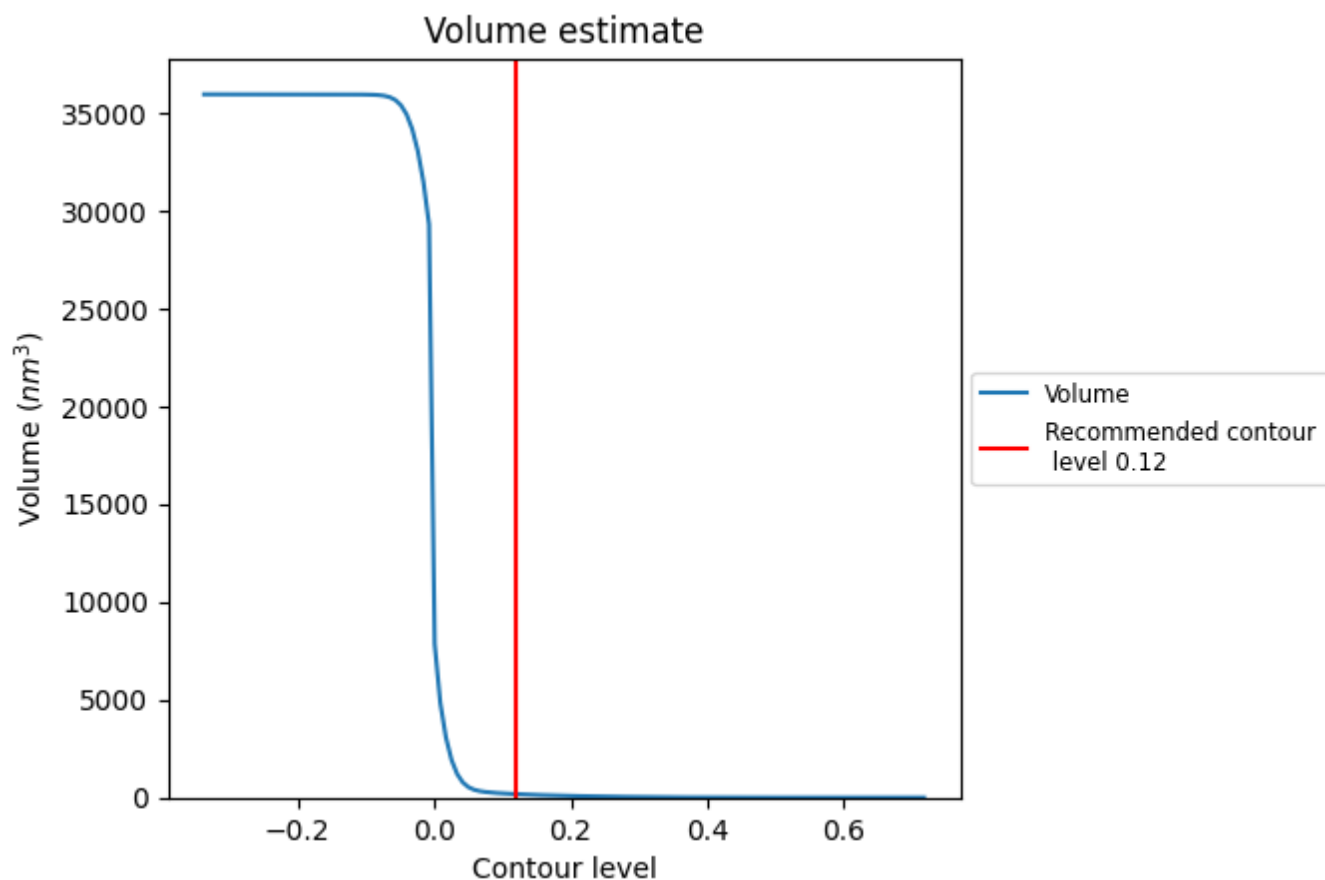
This section contains the results of statistical analysis of the map.

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.

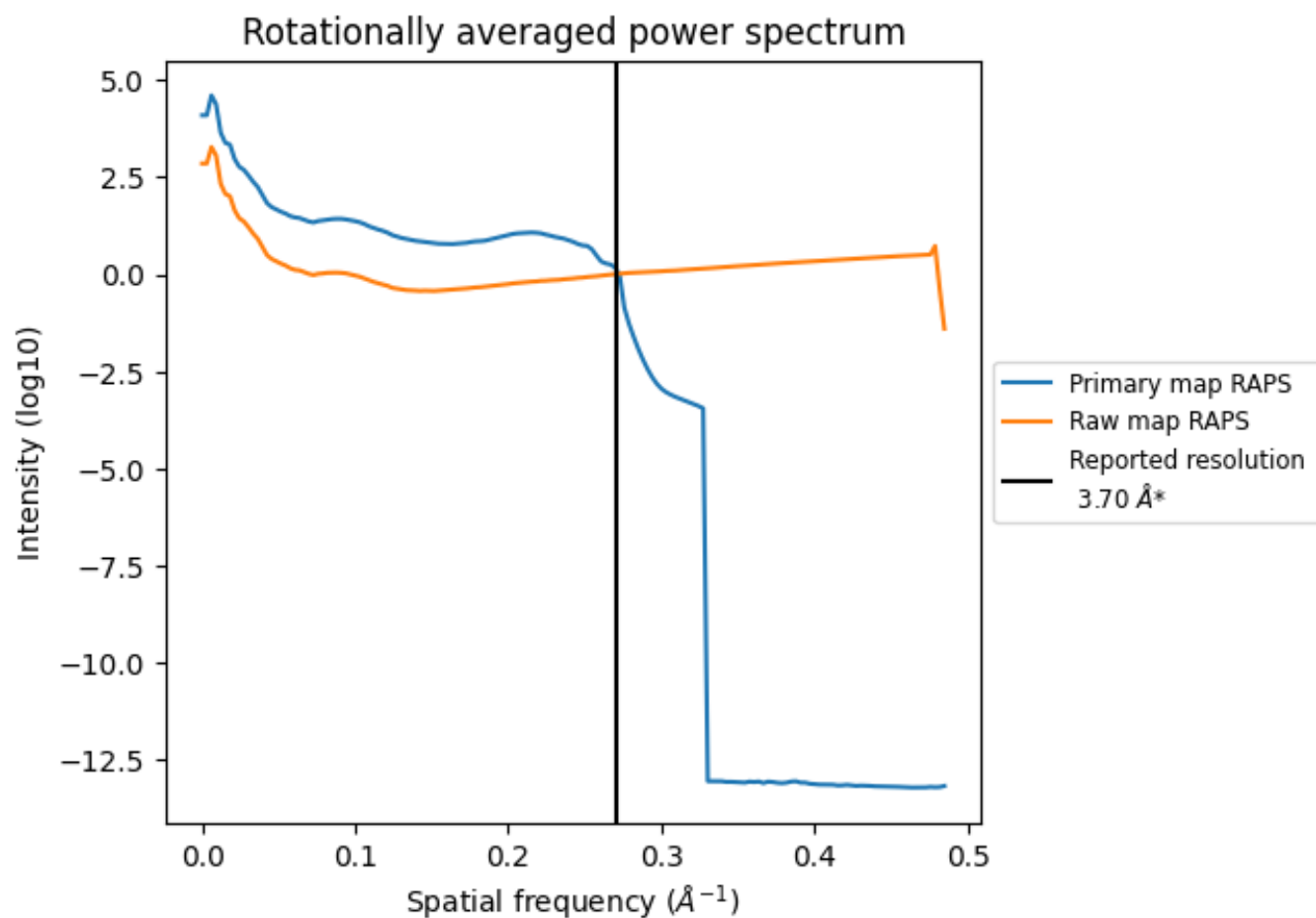
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 159 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 ⓘ

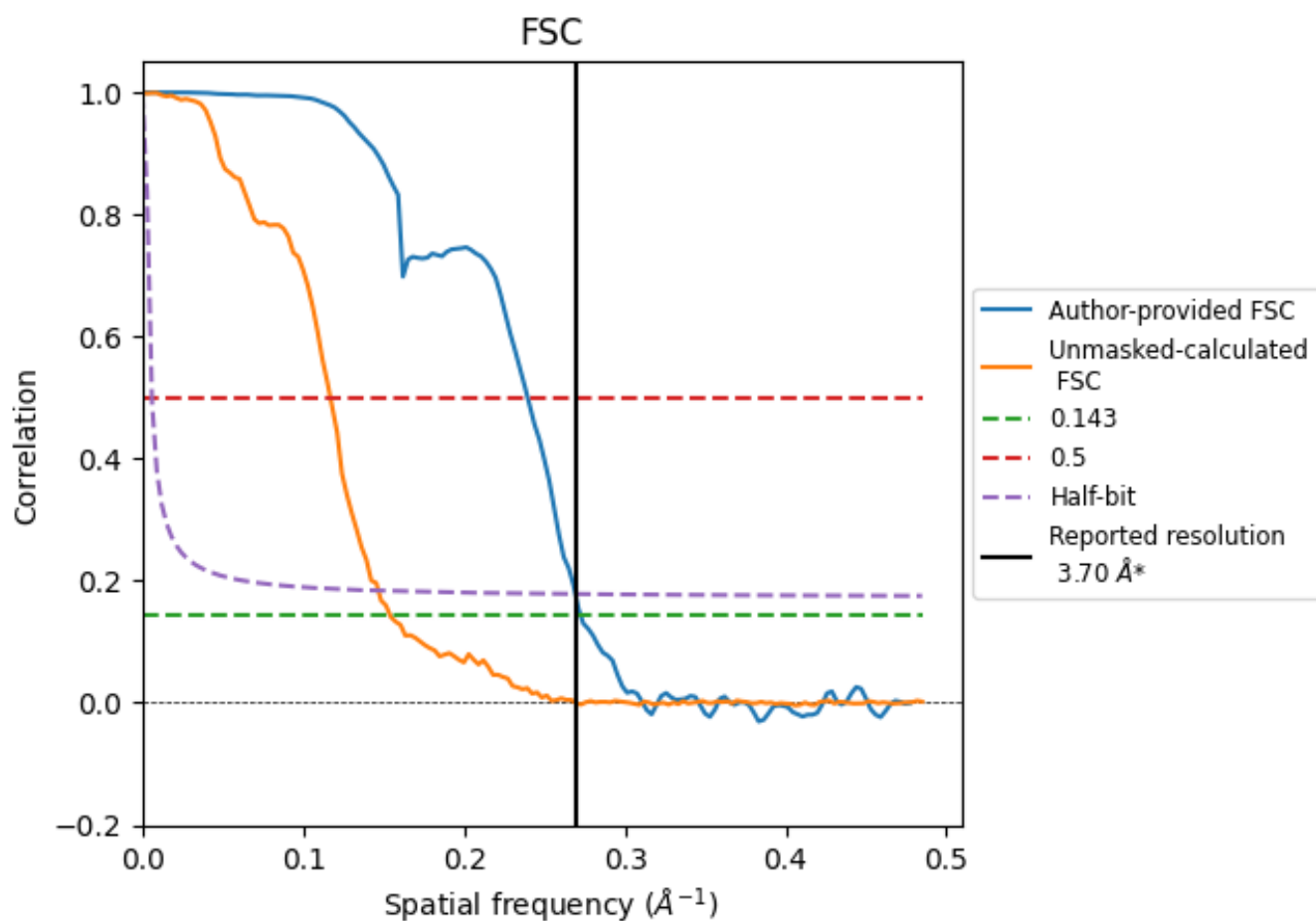


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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](#)

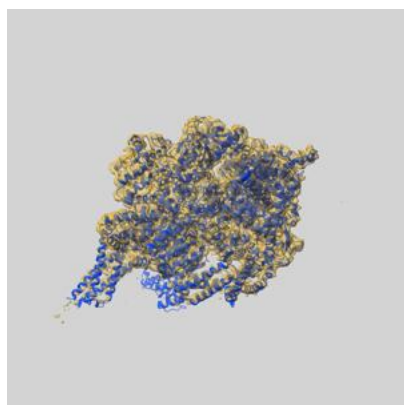
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.17	3.71
Unmasked-calculated*	6.49	8.55	6.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.49 differs from the reported value 3.7 by more than 10 %

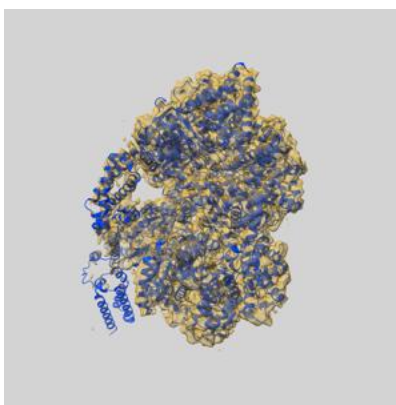
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44712 and PDB model 9BMV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

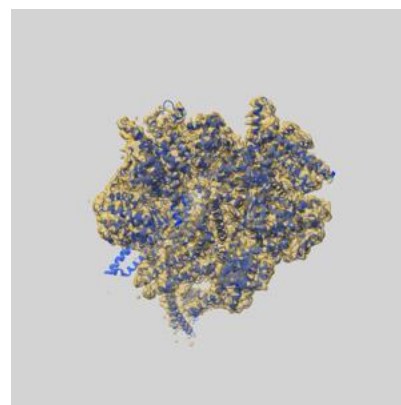
9.1 Map-model overlay [i](#)



X



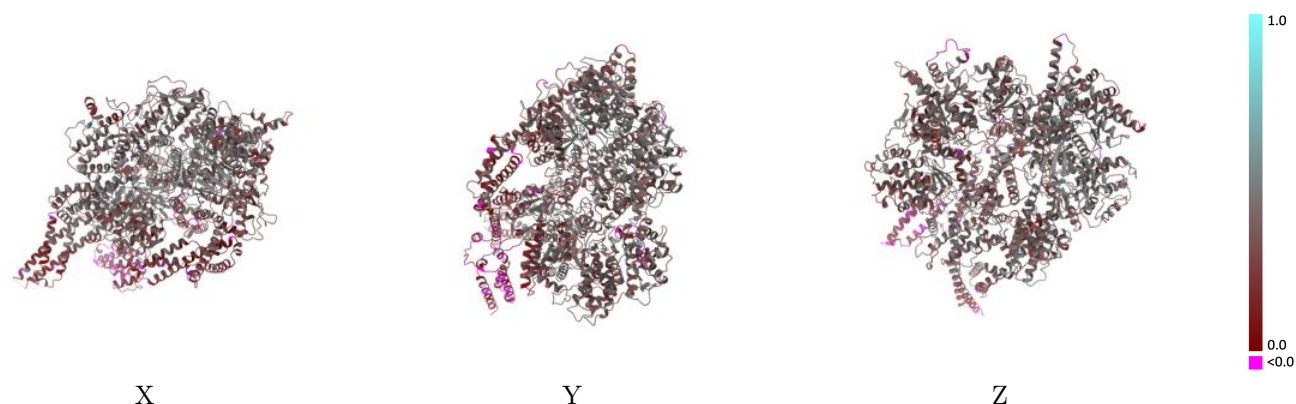
Y



Z

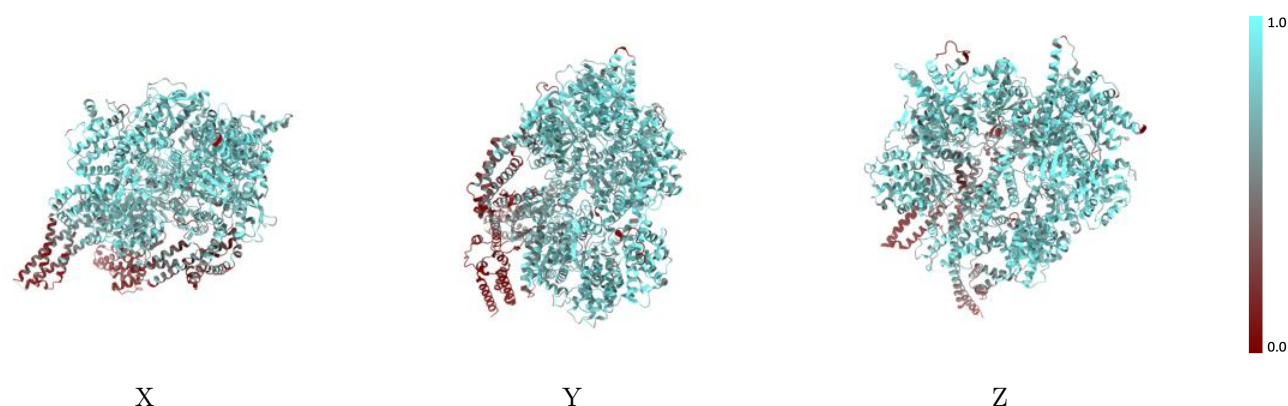
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



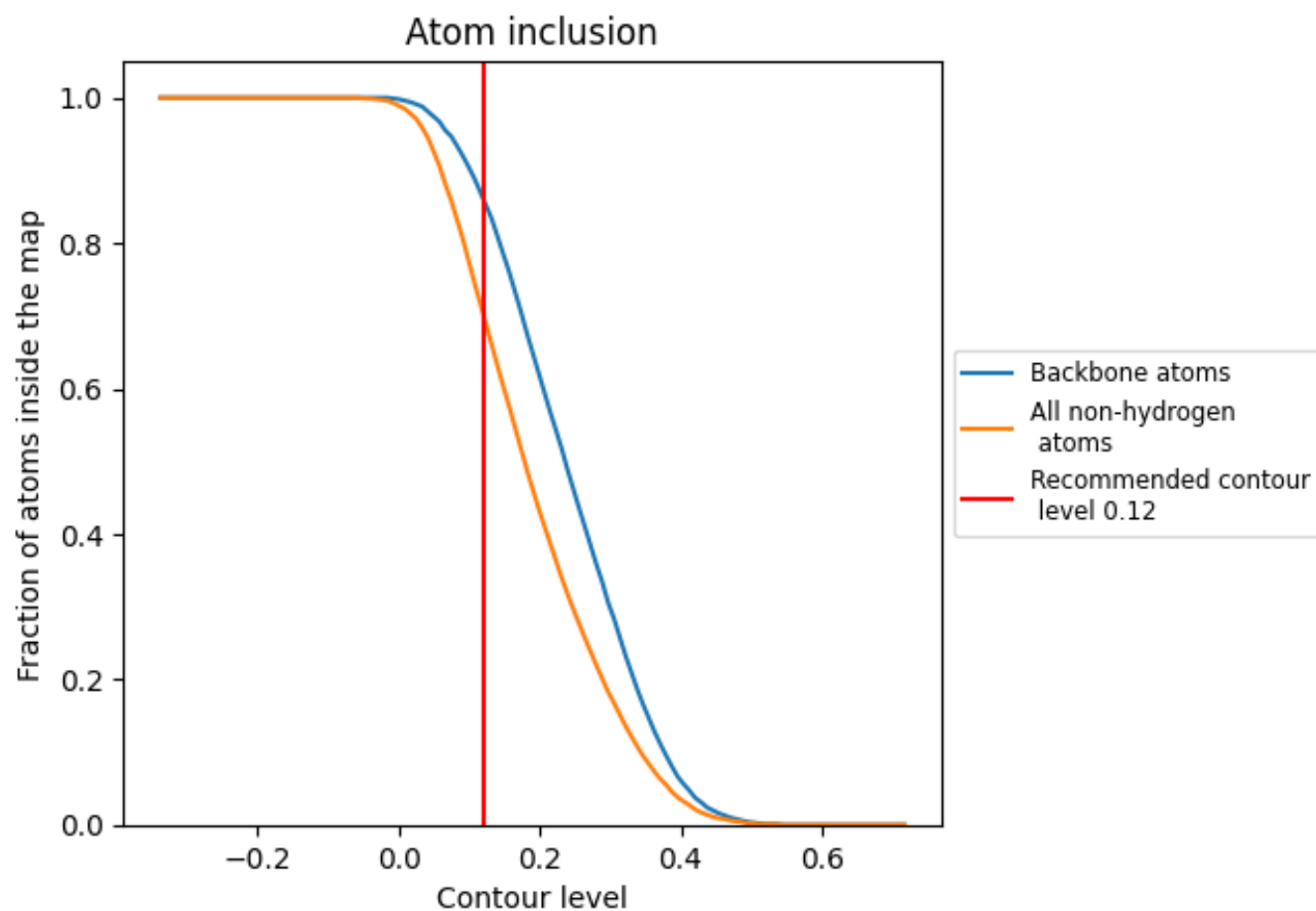
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7030	<div></div> 0.3600
A	<div></div> 0.7030	<div></div> 0.3600

