



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:52 AM UTC

PDB ID : 9BMC / pdb_00009bmc
EMDB ID : EMD-44695
Title : Post-2 motor domain from full-length human dynein-1 bound to microtubules
in 5mM ADP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

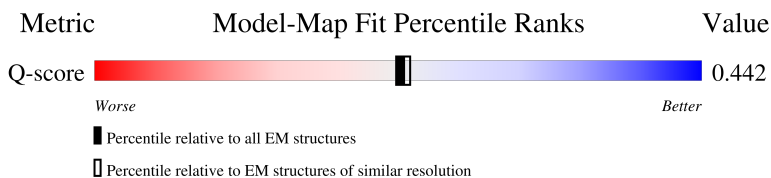
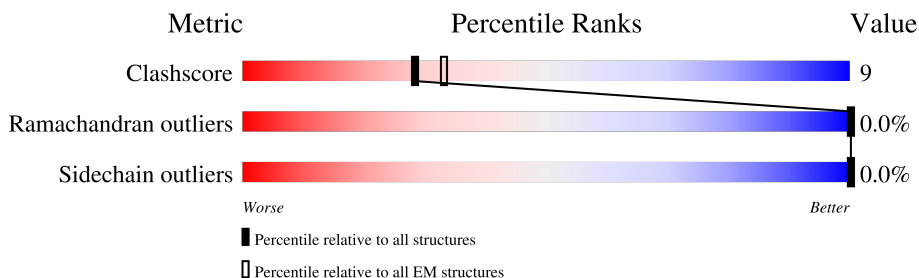
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- 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
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



E3487	Gln	R292	L2508	T2634	Y2748	R2863	T3067	A3162	Gln	Met	Gln	Val	Gln	E3470
E3490	Gln	R293	K2509	F2635	G2749	E2864	M3068	T3168	Gln	Lys	Arg	Arg	Gln	K3471
E3494	Asn	E294	G2515	N2646	T2750	R2865	S3071	M3169	Ala	Asn	Met	Met	Lys	V3472
E3498	Glu	L2295	E2516	L2650	M2755	S2868	S3072	T3172	Lys	Tyr	Ala	Ala	Asn	V3473
E3503	Val	K2297	E2519	A2651	R2756	R2869	E3073	P3173	Lys	Met	Asn	Pro	Pro	R3474
E3503	Pro	W2300	R2519	P2652	L2758	W2876	G3074	R3174	Val	Asn	Pro	Pro	Glu	N3475
E3512	Met	D2304	L2526	W2658	L2759	D2880	L3076	D3178	Met	Pro	Ala	Ala	Met	R3476
E3516	Ile	D2305	P2527	F2662	L2762	D2885	D3077	R3077	Val	Tyr	Val	Val	Ile	A3477
E3519	Asp	G2306	T2528	C2663	R2763	D2885	R3078	A3084	Lys	Arg	Lys	Asp	Lys	L3478
F3520	Leu	V2307	D2536	E2665	E2767	Q2886	A3079	F3086	Leu	Tyr	Leu	Leu	Asp	L3479
W3524	Ala	D2308	W2545	I2666	P2768	Q2886	A3080	N3087	Ala	Trp	Leu	Ala	Ala	K3480
T3530	Ala	W2311	W2556	N2667	L2769	K2898	T3081	E3193	Leu	Glu	Ala	Ala	Lys	S3481
H3534	Leu	L2315	V2557	L2668	M2773	Y2901	A3085	E3196	Gln	Ile	Leu	Ala	Met	L3482
H3535	Lys	D2320	E2558	I2668	F2784	E2902	L3085	E3196	Gln	Gln	Leu	Ala	Lys	A3483
T3540	Glu	D2321	T2559	K2673	D2787	E2903	L3011	H5200	Lys	His	Leu	Ala	Val	S3484
H3544	Val	L2324	H2560	R2678	P2790	L2909	L3012	R3206	Asp	Lys	Val	Ala	Glu	E3485
T3547	Ala	R2332	H2566	V2679	H2791	V2915	G3015	K3207	Thr	Asp	Thr	Thr	Val	R3486
E3551	Ala	L2338	T2571	L2680	Y2792	V2919	P3018	T3208	Lys	Lys	Thr	Thr	Val	
S3554	Ala	W2342	V2575	S2681	Y2793	V2919	F3021	T3211	Gln	Trp	Trp	Trp	Ile	
R3559	Ala	F2343	R2576	T2682	I2794	V2919	E3022	V3215	Val	Lys	Lys	Lys	Ala	
W3562	Ala	Q2346	H2577	T2683	Y2794	V2919	G3023	E3216	Val	Met	Met	Arg	Ala	
L3567	Ala	D2347	L2580	I2684	M2799	V2919	E3023	E3217	Val	Met	Met	Arg	Ala	
P3568	Ala	L2348	L2581	V2687	F2807	V2919	G3024	E3218	Val	Met	Met	Arg	Ala	
C3573	Ala	Y2349	Y2582	E2688	L2816	V2919	L3102	E3219	Val	Met	Met	Arg	Ala	
N3576	Ala	Y2350	T2583	E2688	P2817	V2919	Q3103	E3220	Val	Met	Met	Arg	Ala	
A3577	Ala	R2451	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
I3578	Ala	L2452	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
K3581	Ala	Q2453	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
R3582	Ala	C2454	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
R3585	Ala	S2460	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
I3590	Ala	M2461	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
D3591	Ala	Q2464	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
P3592	Ala	A2465	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
I3600	Ala	N2467	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
M3601	Ala	V2469	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		M2481	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2487	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2492	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		Y2493	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2499	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		W2500	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		D2505	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		S2506	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2397	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2398	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		K2399	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		G2400	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		K2401	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2402	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		D2403	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2404	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		G2405	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2406	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2407	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		A2408	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		A2409	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2413	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		Q2416	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		D2418	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		A2419	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		A2420	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		I2422	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		N2430	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		E2444	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		H2445	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		I2446	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2449	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		T2450	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2451	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2452	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		A2354	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2358	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		W2363	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		F2364	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2369	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		W2373	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2382	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		P2386	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2387	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		G2390	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		F2391	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		D2392	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		Y2493	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		L2499	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		W2500	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		D2505	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		S2506	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	
		R2396	T2583	E2688	P2817	V2919	Q3104	E3221	Val	Met	Met	Arg	Ala	

Q4549	L4395	E4281	Q4108	E3976	S3828	D3725	R3611
Q4550	L4398	L4284	K4112	E3977	Y3836	R3728	T3612
A4551			L4113		H3837		S3613
T4552	E4403	V4288	L4116	L3992	R3838	Q3735	L3615
L4553	M4404		Q4117	R4000	V3839	Q3739	D3616
D4554			P4118		L3840		D3617
F4558	V4417	H4291		L4013	D3851	L3742	A3618
G4559	K4422	D4298	R4123	L4025	H3852	R3743	F3619
V4560	L4423	Q4299	L4124	L4025	T3853	Q3744	R3620
K4564	Q4428	I4300	T4127	L4027	L3863		E3624
R4429	R4301	E4302			V3871		
K4574	E4302	E4303	I4130	V4031	A3872		R3628
L4577	D4430		R4140	P4037	R3873		L3634
T4581	Q4436	S4319	F4147	N4038	E3755		V3635
V4437	C4437	P4324		T4039	V3756		D3637
C4438	E4438	M4325	R4176	P4040	D3879		V3638
E4439	E4439	N4326	A4177	H4054	A3888		Y3641
			R4178	L4058	R3889		D3642
K4442	K4342	K4343	Y4180		G3897		P3644
K4443	M4343	L4344		M4063	D3902		P3647
Q4444	L4344		L4183	Q4065			
T4445	M4346		Q4191	S4068	L3909		R3654
M4446	Q4347		E4192	I4069	R3910		R3655
Y4447	M4348		R4193	A4070	E3913		T3656
L4448	L4349		L4194	I4071	I3914		G3657
R4449	GLU	ASP	R4195	G4072	V3915		G3658
	GLU	GLU		S4073	L3916		R3659
K4457	ASP	LEU	S4202	A4074	S3917		V3660
	LEU	ALA	Y4205	E4075	A3918		L3661
L4460	R4461	TYR	E4206	E4075	G3919		C3665
S4463	V4464	ALA	A4215	F4077	S3920		D3666
S4465	GLU	THR	D4220	N4078	R3923		D3668
H4466	THR	GLU	L4223	Q4079	I3924		P3673
	GLU	LYS	D4224	A4080	Q3925		S3680
V4475	V4475	THR	P4235	D4081	V3929		T3681
I4486	I4486	THR	L4243	K4082	E3930		P3684
A4501	A4501	ASP	L4246	A4087	E3933		L3692
K4505	K4505	SER	M4247	V4088	R3937		C3693
L4511	L4511	THR		R4092	K3945		S3694
T44524	T44524	SER		M4095	D3946		R3695
		ASP		L4096	L3947		N3700
		GLY		K4097			F3701
		ARG		N4098			T3702
W4534	W4534	PRO		V4099			E3715
S4535	S4535	A4375		G4104			V3716
L4536	L4536	H4381		W4105			
E4537	E4537	I4391		L4106			
				M4107			
T4547	T4547						
S4548	S4548						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.446	Depositor
Minimum map value	-0.917	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	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, 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	0.17	0/25022	0.31	0/33900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	24573	467	0
2	A	81	0	36	5	0
3	A	31	0	12	1	0
4	A	2	0	0	0	0
All	All	24617	0	24621	467	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 467 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:4326:ASN:HD22	1:A:4581:ILE:HD13	1.41	0.83
1:A:2665:GLU:HB3	1:A:2668:LEU:HD23	1.63	0.80
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.17	0.77
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.17	0.76
1:A:1511:PRO:HG2	1:A:3659:ARG:HE	1.52	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	3035/4646 (65%)	2959 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1510	SER

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	3092	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2849	ASN
1	A	3869	ASN
1	A	3865	GLN
1	A	4262	GLN
1	A	1894	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	32,33,33	0.48	0	48,52,52	0.29	0
2	ADP	A	4704	-	28,29,29	1.36	5 (17%)	43,45,45	1.81	8 (18%)
2	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4701	-	28,29,29	1.38	5 (17%)	43,45,45	1.80	10 (23%)

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	-	1/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	6/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.76	1.47	1.39
2	A	4704	ADP	C5-C4	4.41	1.47	1.39
2	A	4701	ADP	C5-C4	4.41	1.47	1.39
2	A	4703	ADP	C5-C6	2.61	1.48	1.41
2	A	4704	ADP	C5-N7	-2.52	1.34	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.30	118.05	126.72
2	A	4704	ADP	C5-C4-N3	-5.72	118.84	126.72
2	A	4701	ADP	C5-C4-N3	-5.59	119.02	126.72
2	A	4703	ADP	N3-C4-N9	5.15	135.93	127.17
2	A	4704	ADP	N3-C4-N9	4.52	134.85	127.17

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

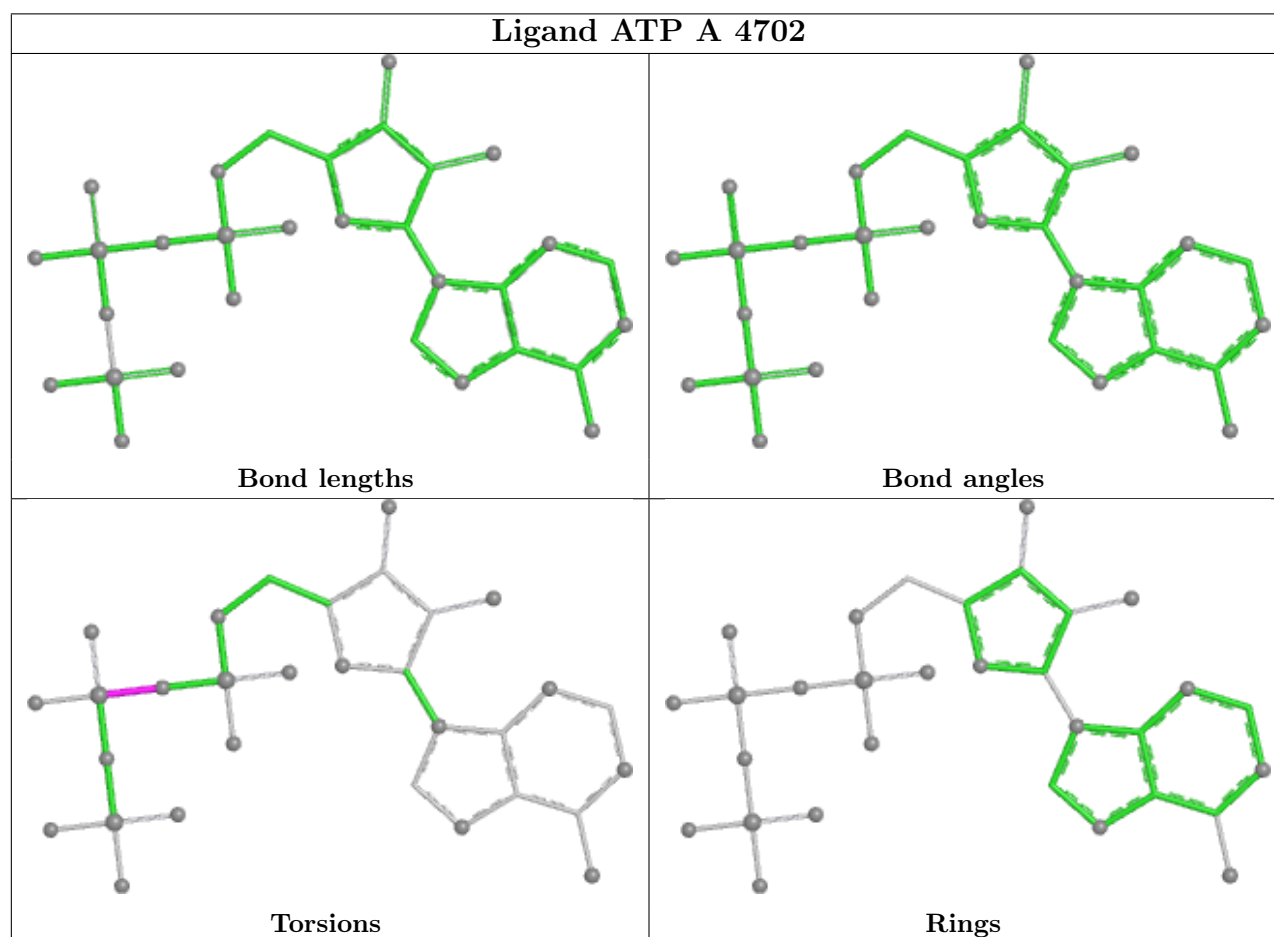
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'

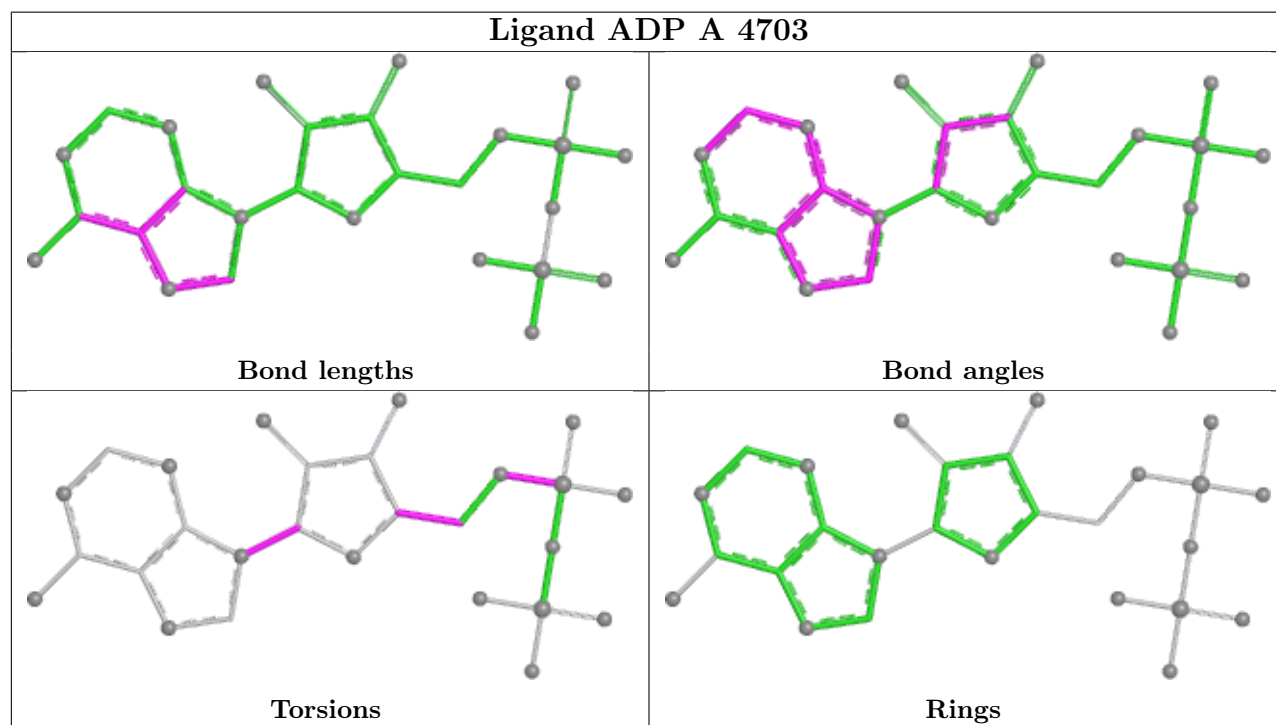
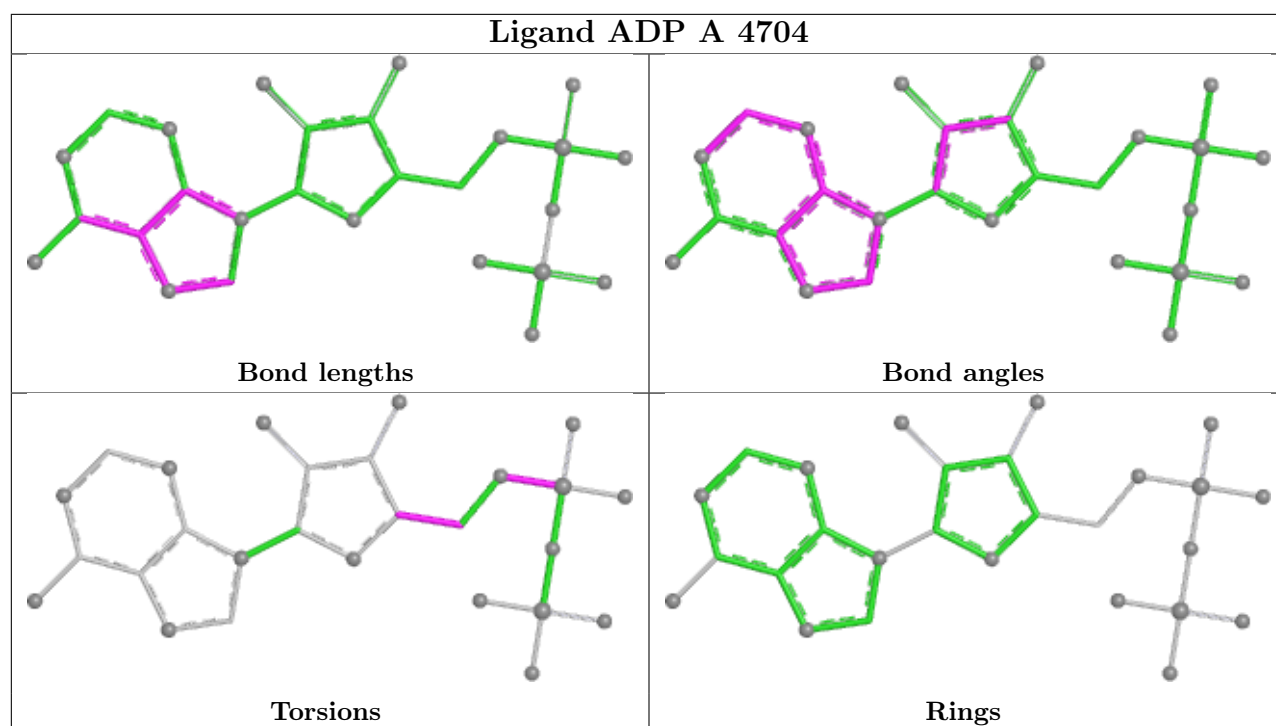
There are no ring outliers.

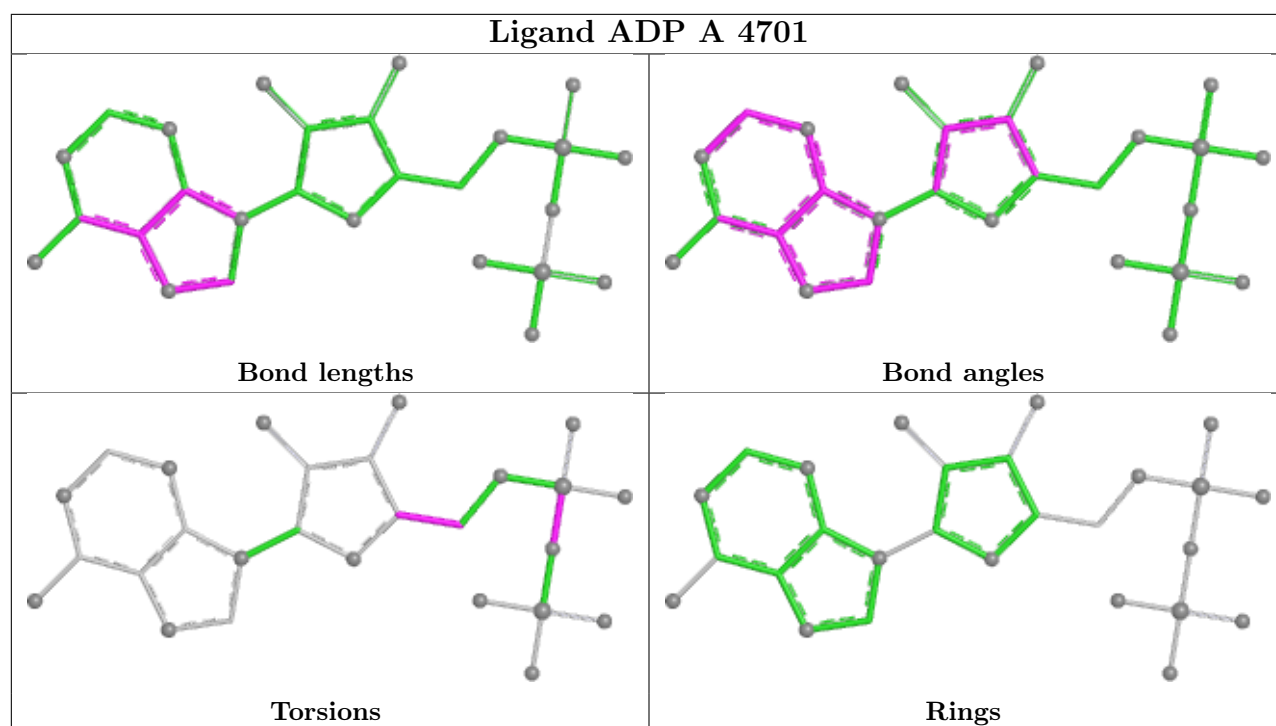
3 monomers are involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

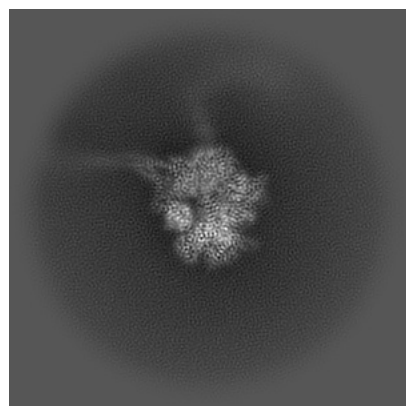
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44695. These allow visual inspection of the internal detail of the map and identification of artifacts.

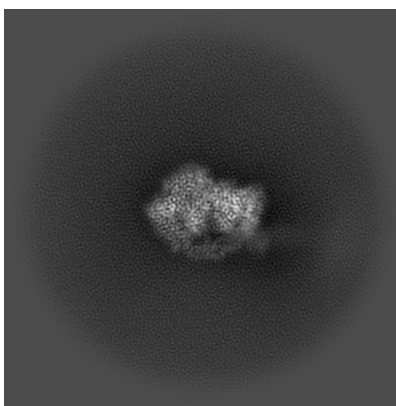
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

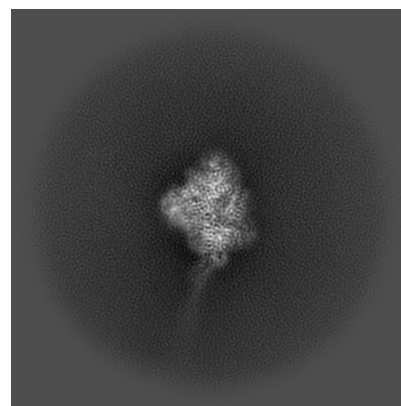
6.1.1 Primary map



X

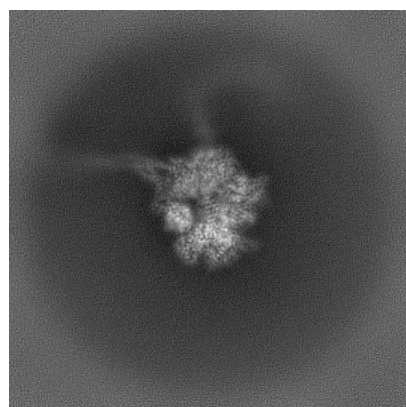


Y

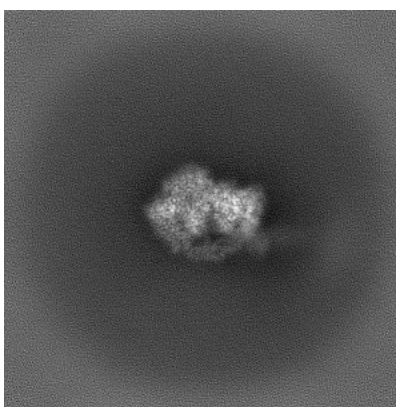


Z

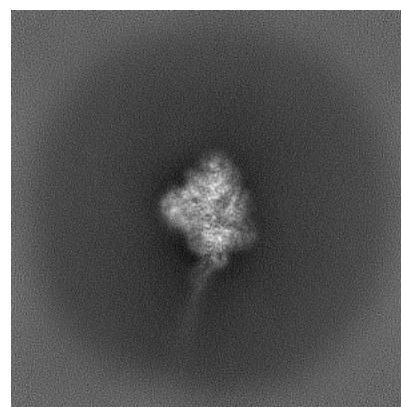
6.1.2 Raw map



X



Y

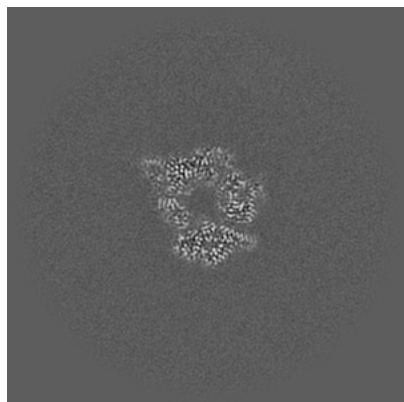


Z

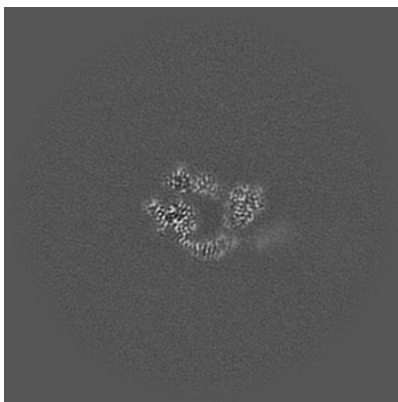
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

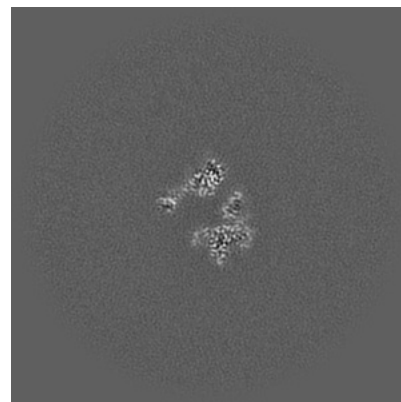
6.2.1 Primary map



X Index: 192

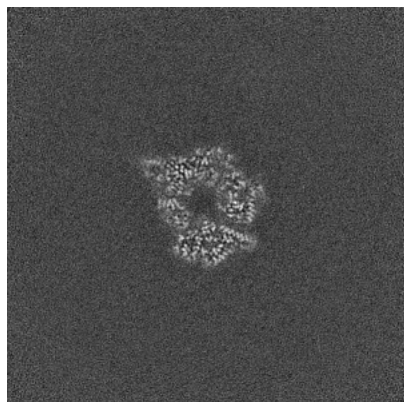


Y Index: 192



Z Index: 192

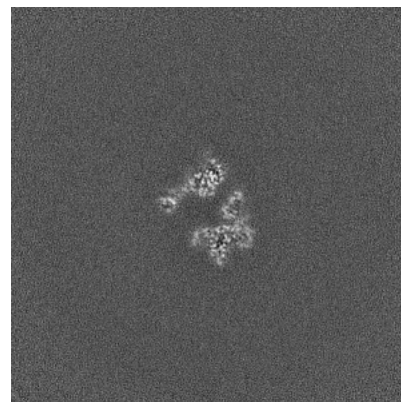
6.2.2 Raw map



X Index: 192



Y Index: 192

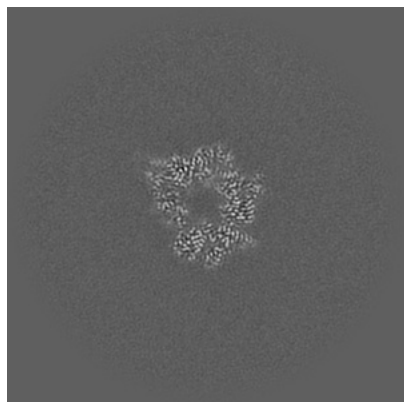


Z Index: 192

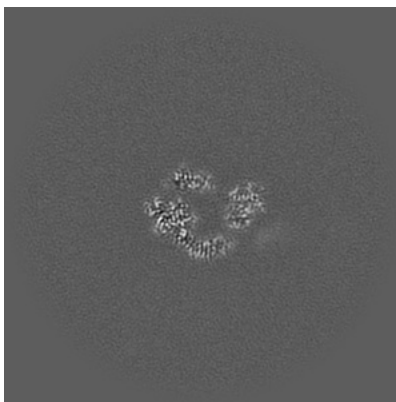
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

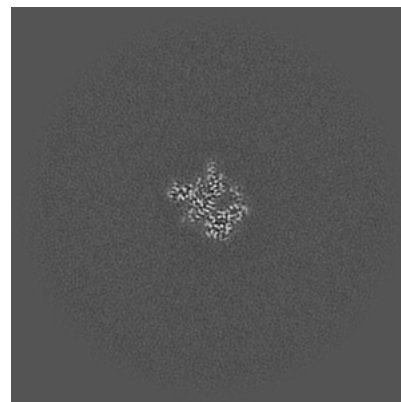
6.3.1 Primary map



X Index: 194

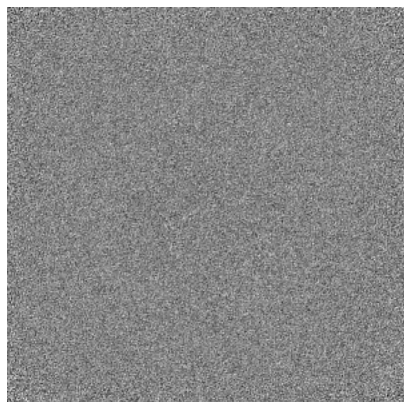


Y Index: 196

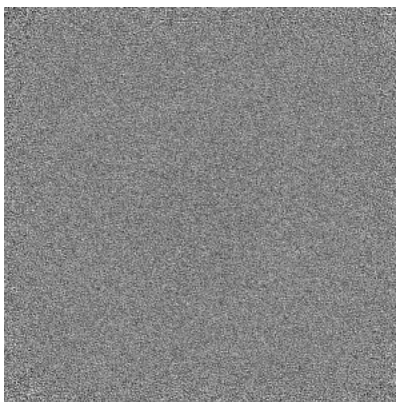


Z Index: 162

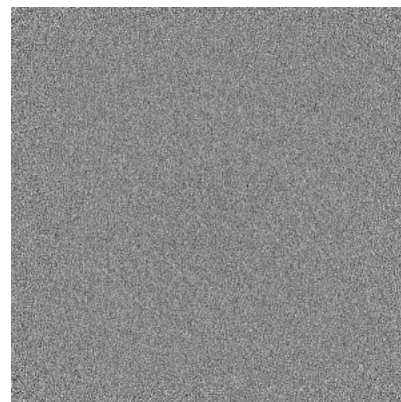
6.3.2 Raw map



X Index: 0



Y Index: 0

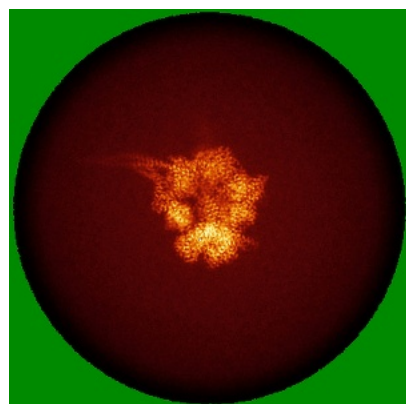


Z Index: 0

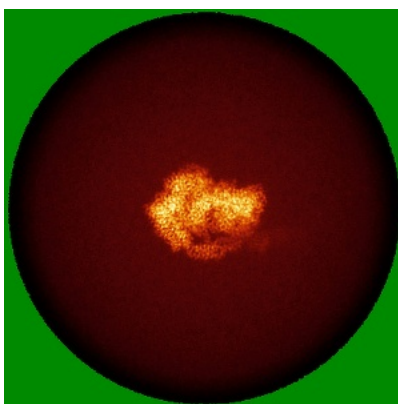
The images above show the largest variance slices of the map in three orthogonal directions.

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

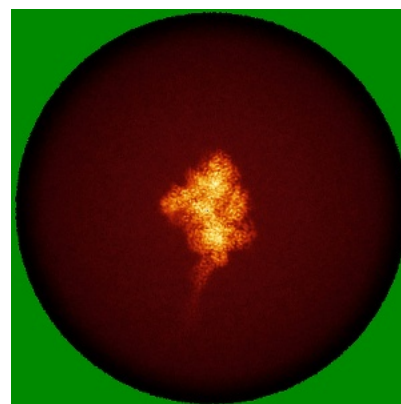
6.4.1 Primary map



X

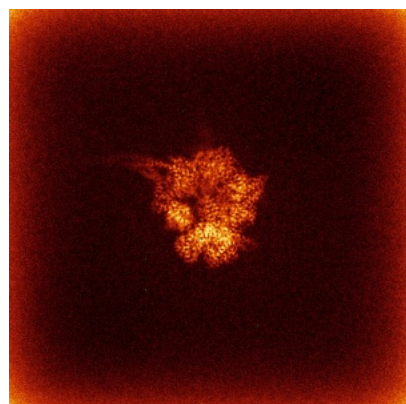


Y

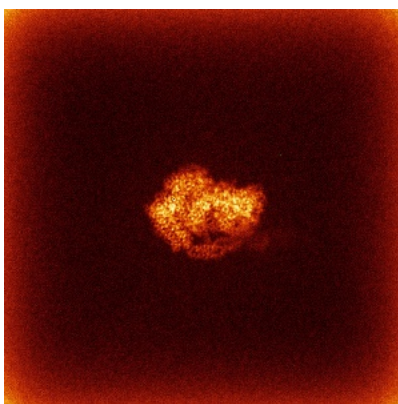


Z

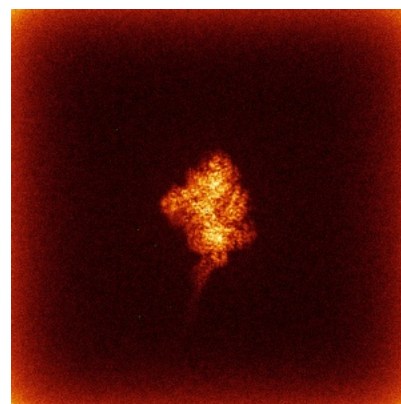
6.4.2 Raw map



X



Y

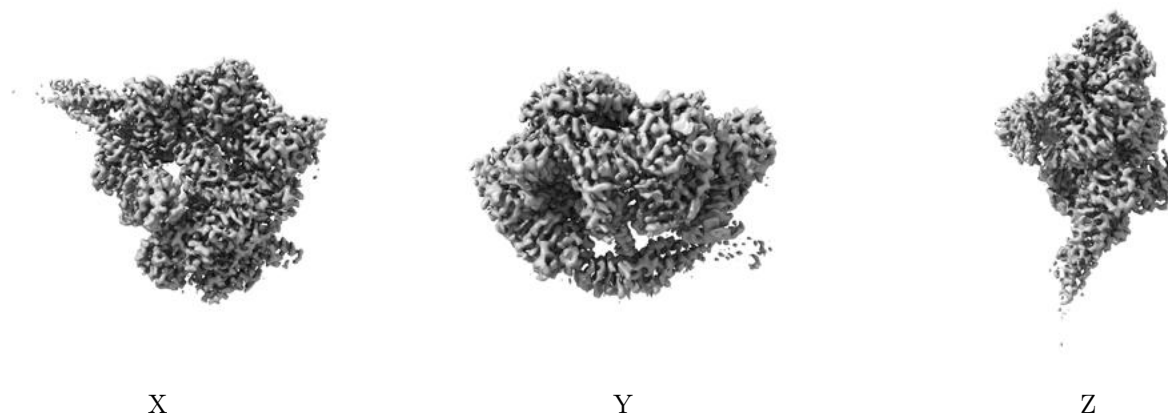


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

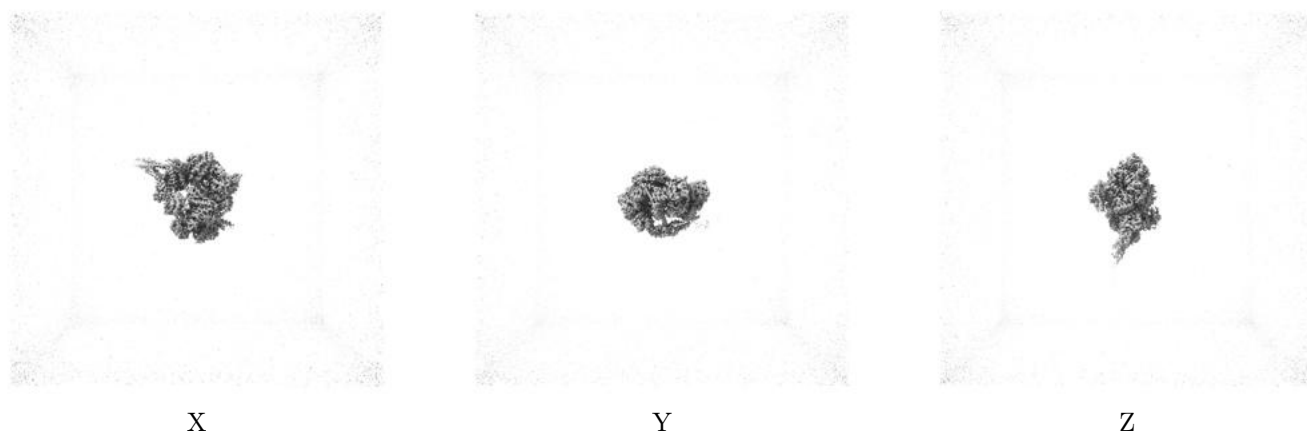
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

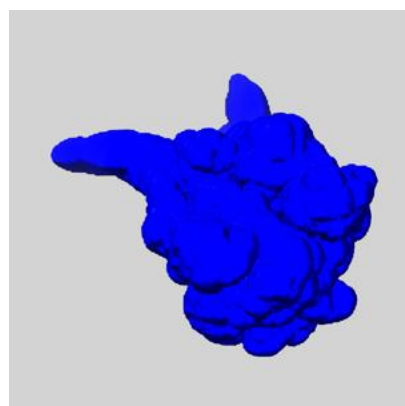
6.6 Mask visualisation [i](#)

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

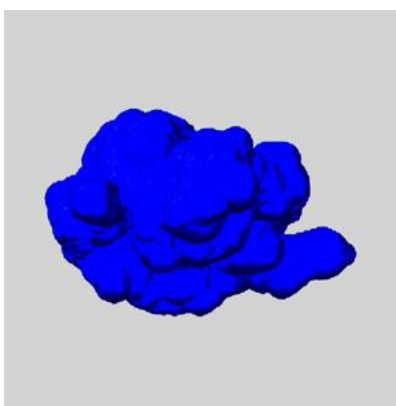
A mask typically either:

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

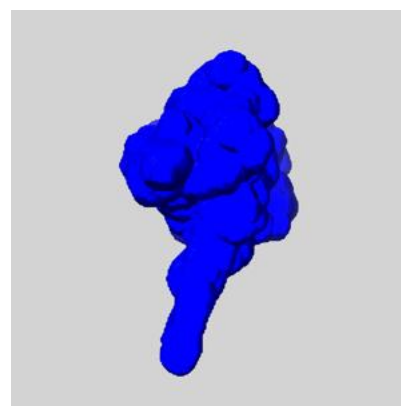
6.6.1 emd_44695_msk_1.map [i](#)



X



Y

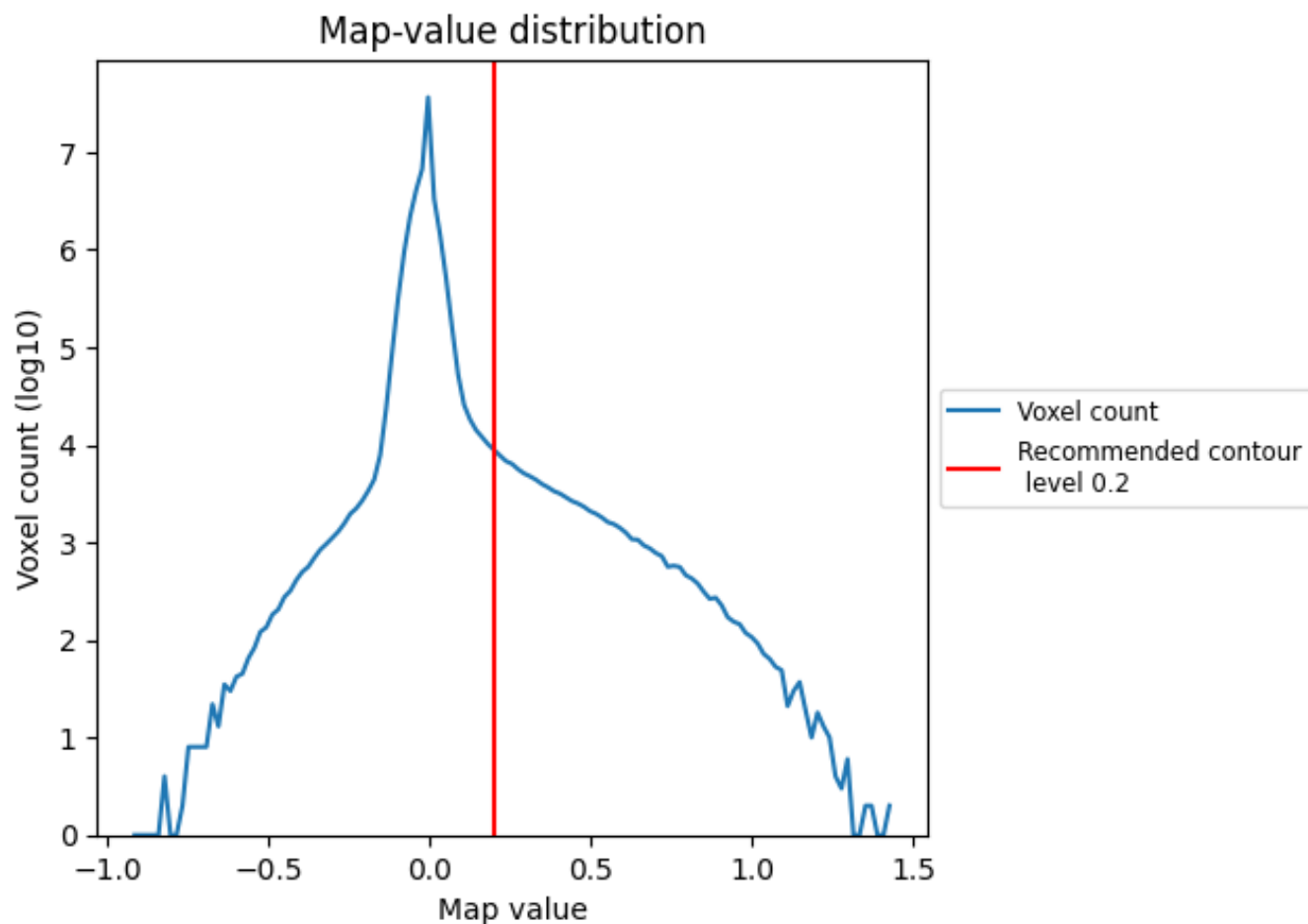


Z

7 Map analysis [i](#)

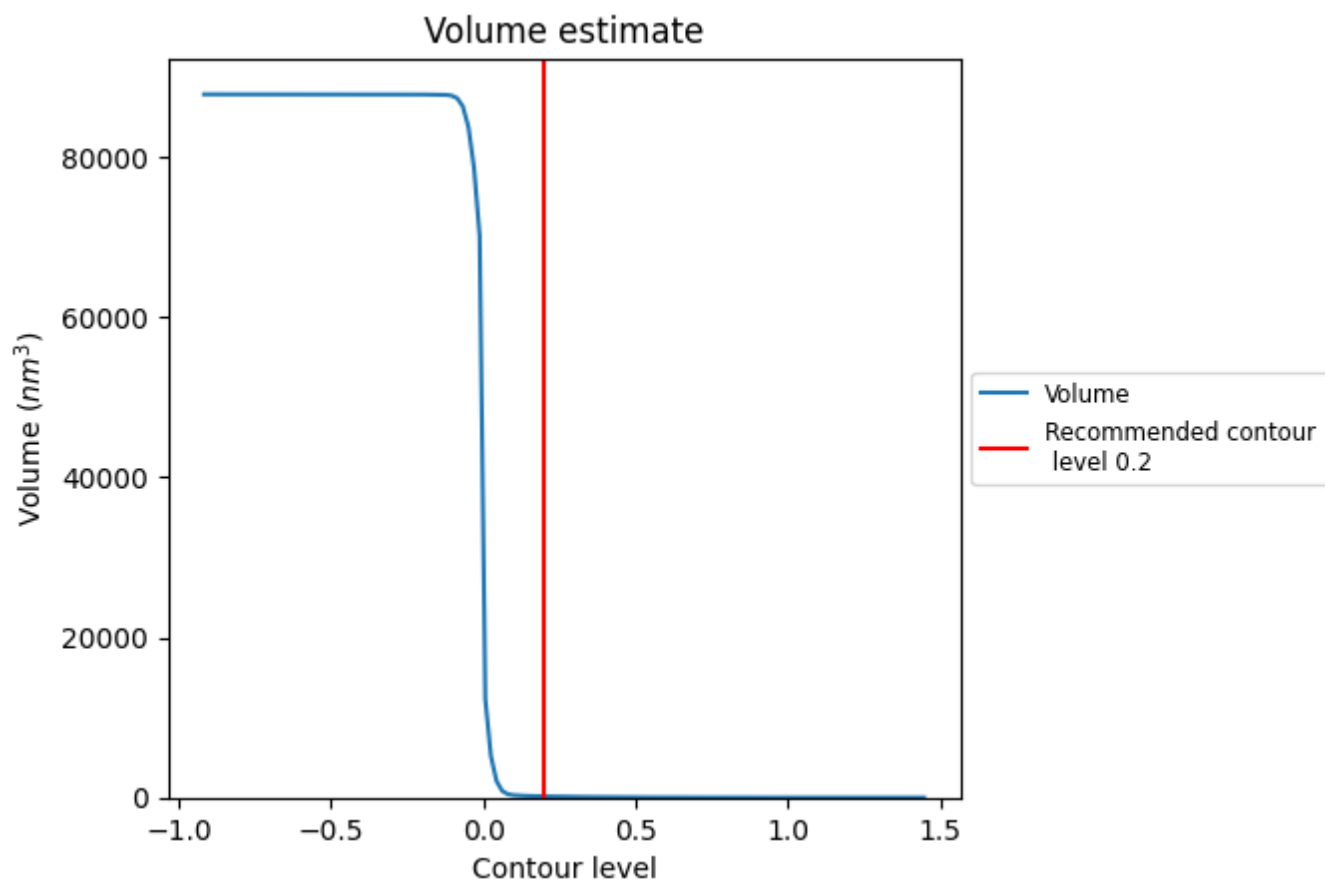
This section contains the results of statistical analysis of the map.

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.

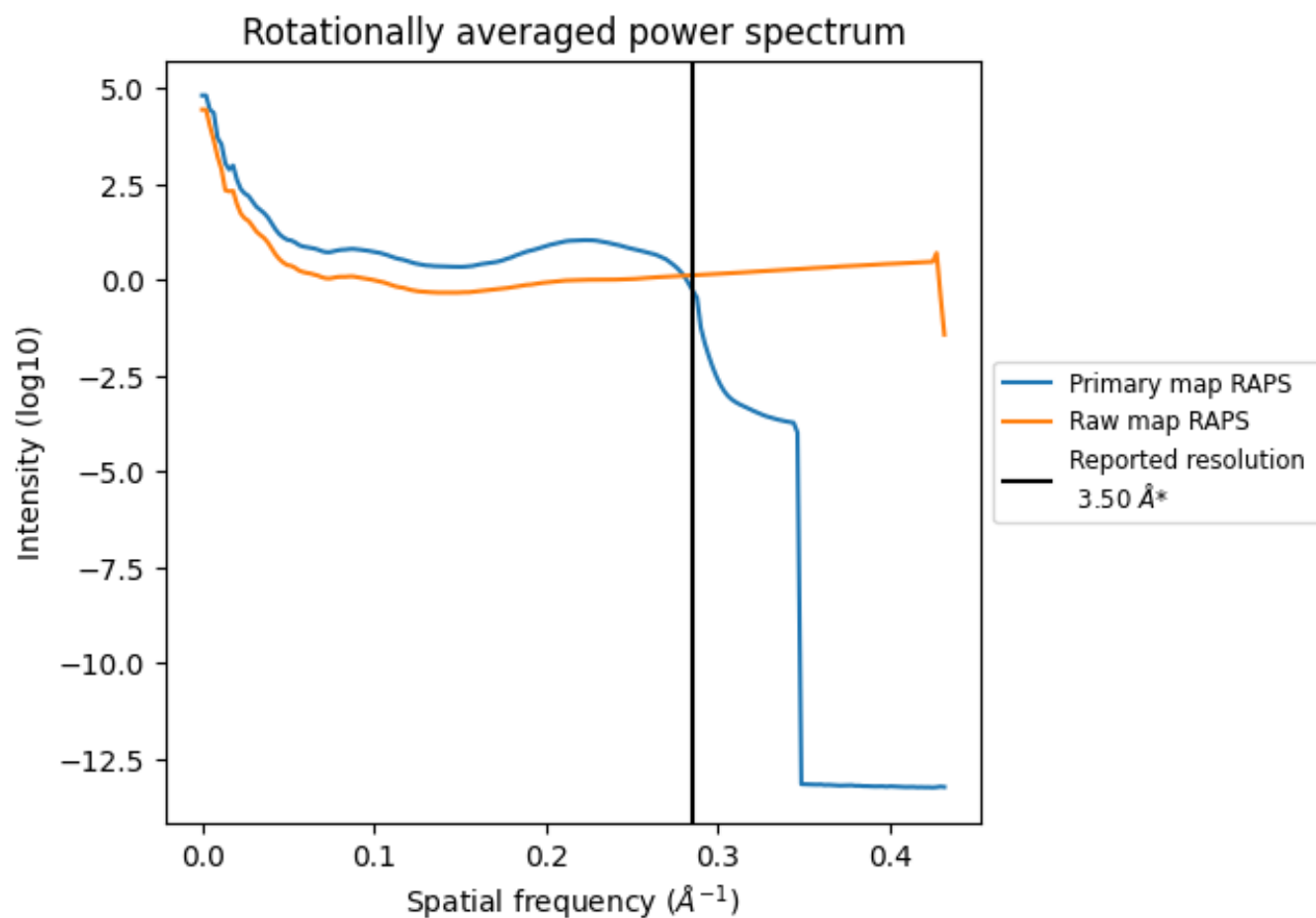
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 135 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 ⓘ

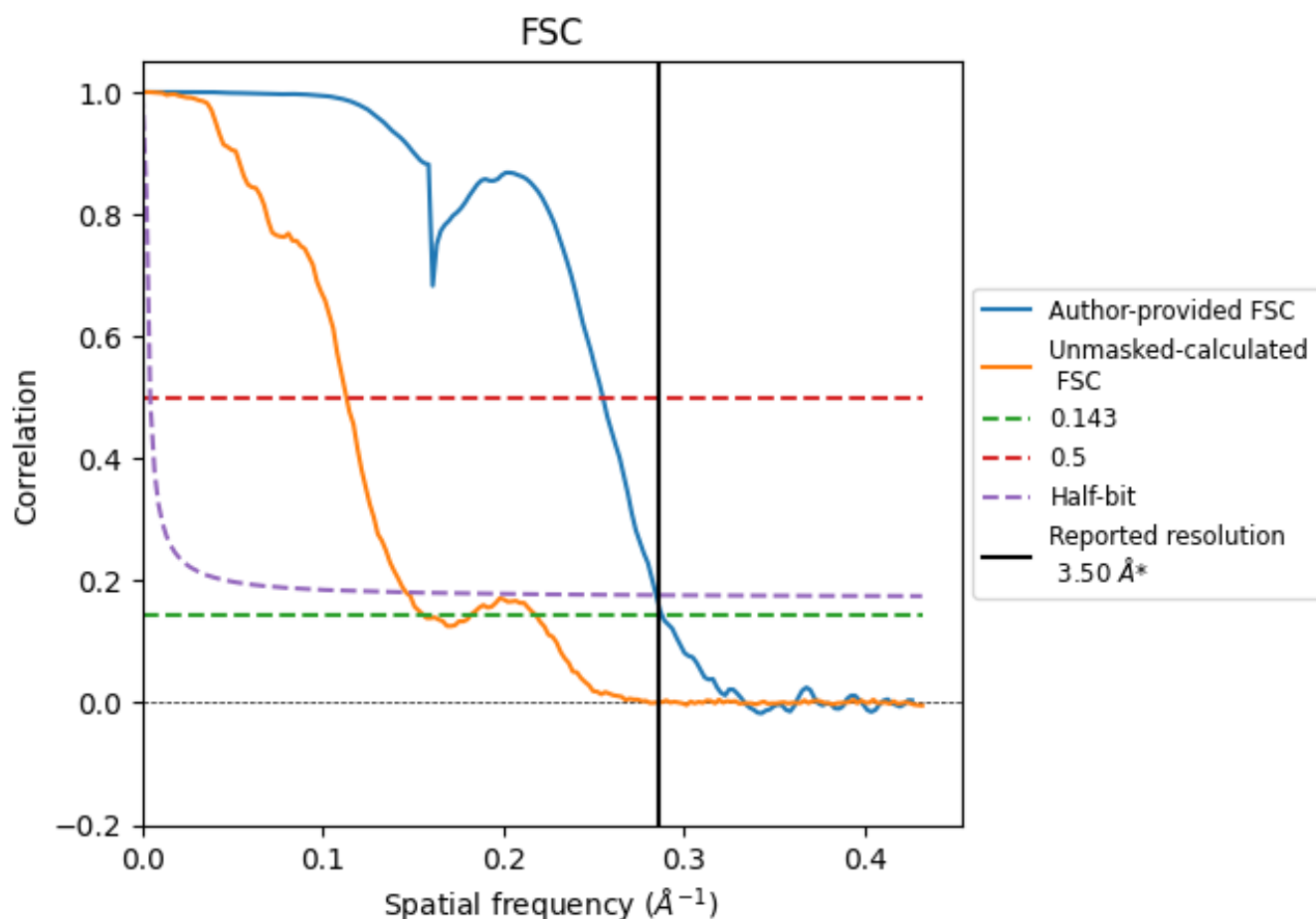


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

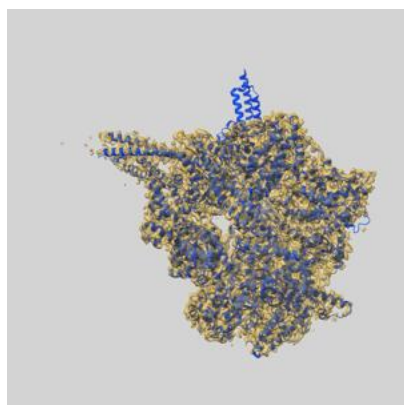
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.92	3.51
Unmasked-calculated*	6.41	8.83	6.84

*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 6.41 differs from the reported value 3.5 by more than 10 %

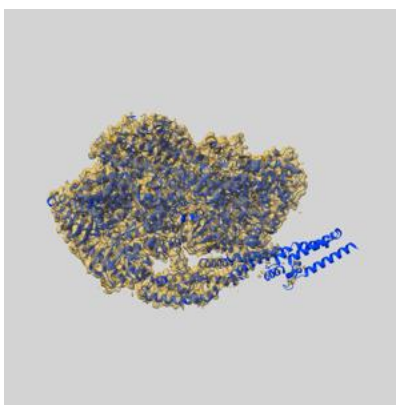
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44695 and PDB model 9BMC. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

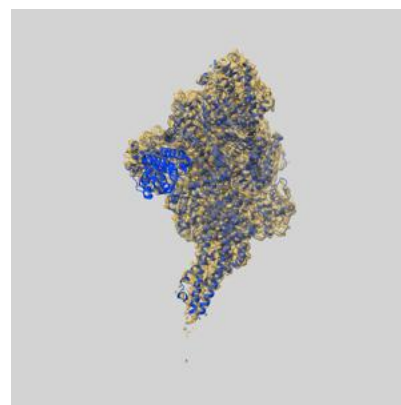
9.1 Map-model overlay [i](#)



X



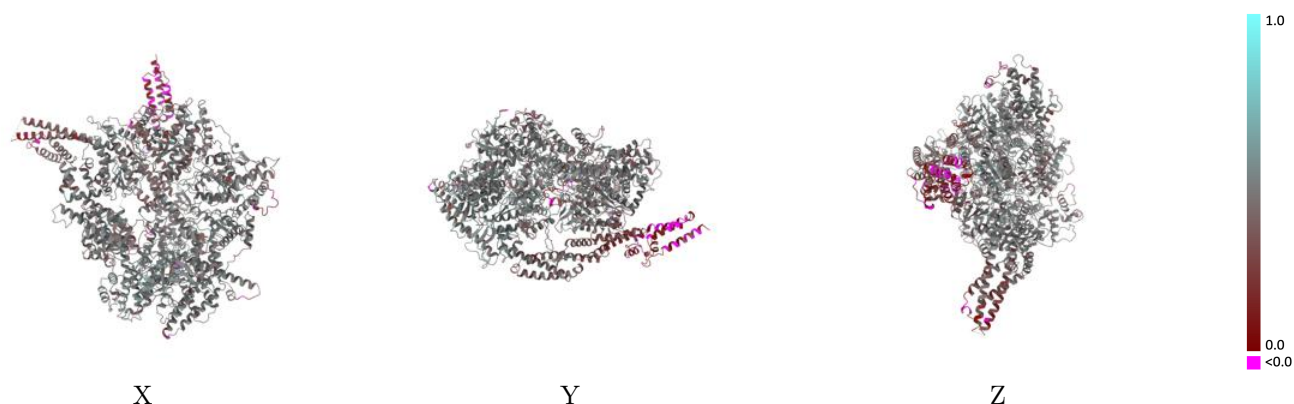
Y



Z

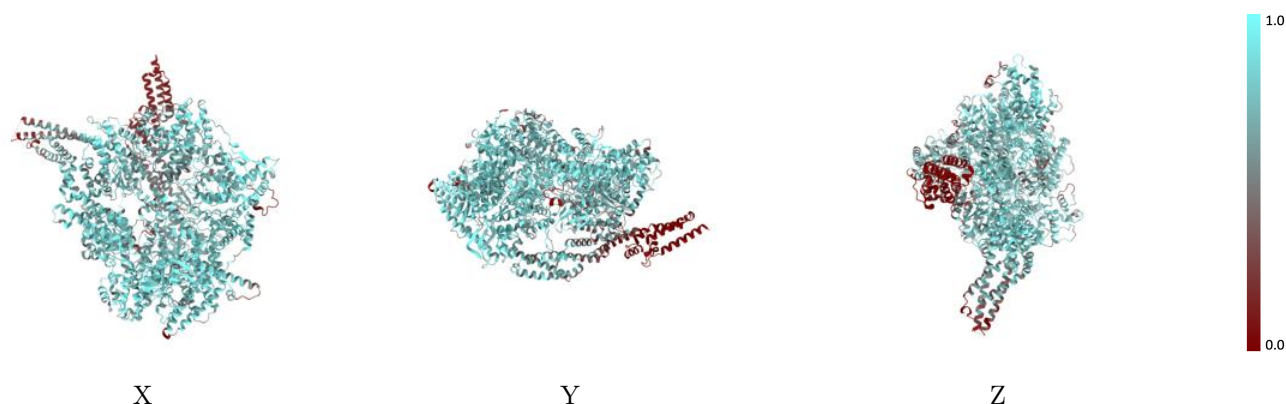
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



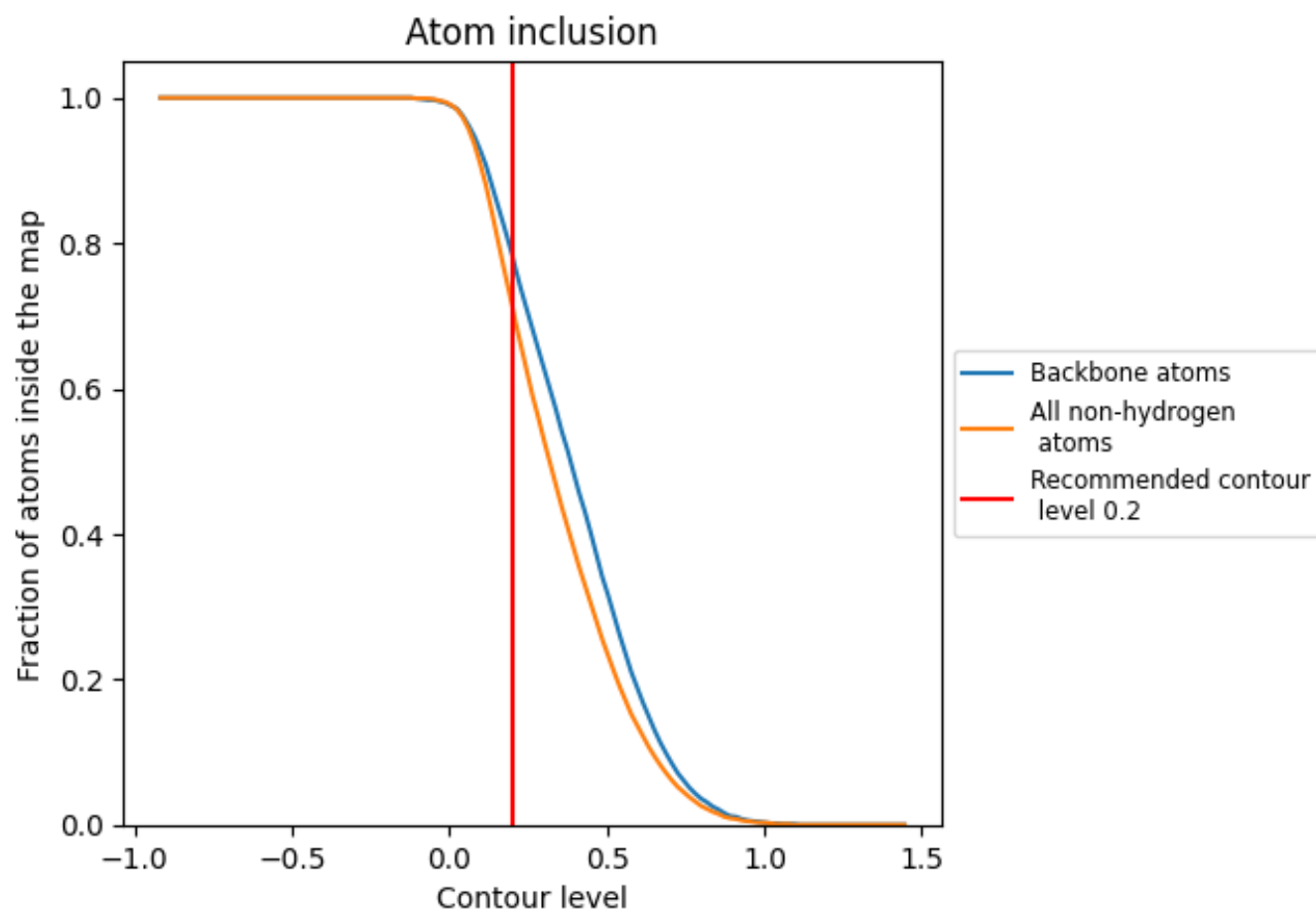
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.4420
A	0.7140	0.4420

