



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:20 AM EDT

PDB ID : 9BN5 / pdb_00009bn5
EMDB ID : EMD-44722
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATPVi condition, class1
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.30 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.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

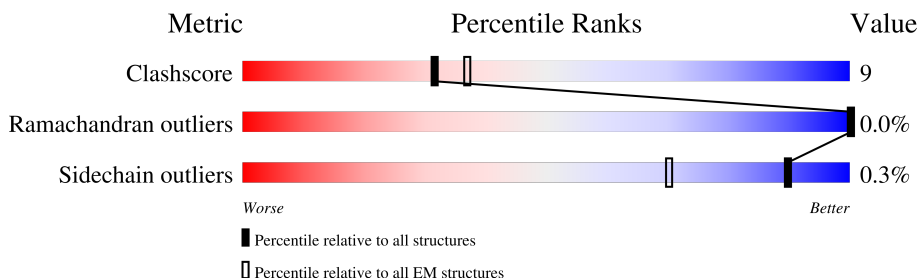
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23152 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.

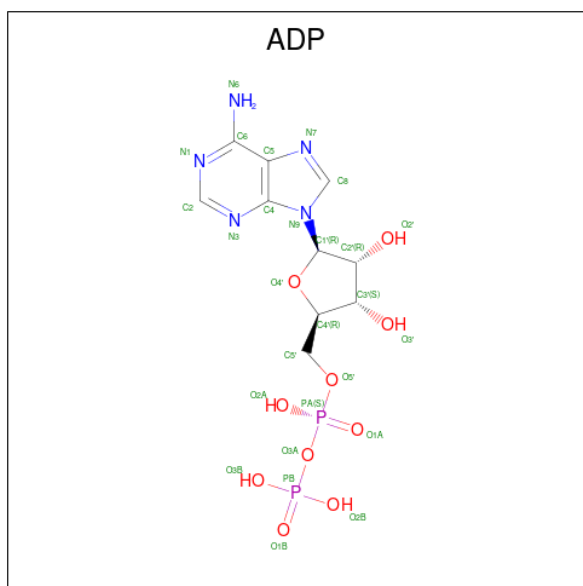
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2866	Total	C	N	O	S	0	0
			23040	14688	3978	4259	115		

There is a discrepancy between the modelled and reference sequences:

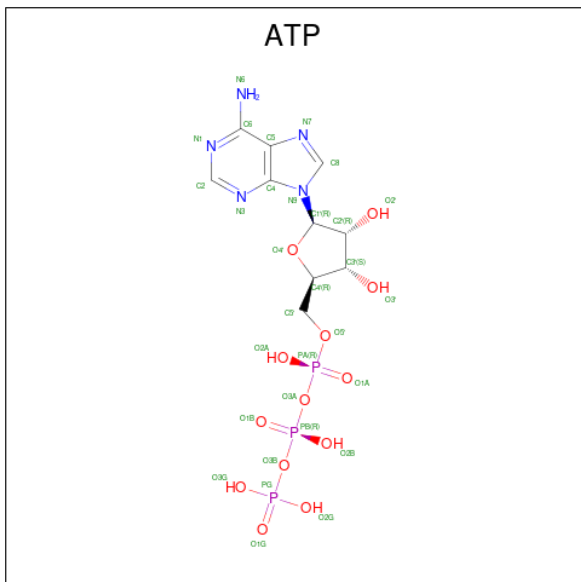
Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (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).





T3476	L2237	N2361	Q2485	L2620	V2733	L2837	V2963	E3049	L3154	ALA	LEU
A3477	L2238	N2377	L2486	N2621	V2734	V2838	K2966	W3053	N3158	ASN	GLN
L3478	R2239	L2382	E2487	F2622	P2741	E2839	D2973	W3059	N3163	ASP	LYS
L3479	E2242	R2383	R2488	T2626	A2742	E2842	L2976	I3059	R3164	LYS	LYS
K3480	R2243	L2389	R2492	T2627	T2745	R2844	L2977	V3065	R3167	VAL	HIS
K3481	L2244	D2246	Y2493	Q2746	T2747	R2849	R2978	N3069	T3168	LEU	VAL
L3482	E2245	V2247	W2500	P2628	I2747	I2850	V2979	V3072	M3169	LYS	ASP
S3483	G2246	ASP	D2505	E2629	N2752	D2851	C2985	E3073	K3172	ASP	GLN
A3484	V2247	GLU	R2519	L2632	M2755	T2852	K2986	E3076	Y3176	GLN	ARG
A3485	I2254	ASP	R2520	L2633	L2756	L2854	L2990	K3076	A3184	ALA	LYS
R3486	D2262	GLU	I2521	F2635	L2757	L2855	A2991	D3077	E3193	GLU	ALA
E3487	Y2265	ALA	T2527	D2636	L2758	D2861	F2992	T3081	E3194	LYS	LYS
R3488	G2266	GLN	T2528	C2639	I2759	I2862	I2993	S3082	E3195	VAL	VAL
W3489	D2269	ARG	A2529	E2640	P2760	R2863	M2994	L3091	E3196	ALA	ALA
E3490	W2275	ARG	P2530	Y2641	R2763	R2864	D2995	N3092	Q3197	VAL	VAL
K3491	L2279	LYS	N2531	R2642	A2766	K2865	N2998	V3093	Q3198	LYS	LYS
E3494	L2279	GLY	I2532	R2643	T2770	K2866	V2999	F3094	M3199	GLU	ALA
T3495	R2285	GLY	L2532	L2650	V2774	E2867	D3001	G3095	N3202	ILE	LEU
Q3499	Y2290	GLU	T2535	V2653	V2774	S2868	S3002	D3096	V3203	GLN	GLU
T3502	W2291	ALA	V2539	Q2654	Q2781	K2869	L3005	E3100	G3204	GLN	GLN
I3503	R2293	ALA	S2542	L2655	E2782	L2871	E3006	A3101	L3205	HIS	ILE
S3510	E2294	L2413	W2545	V2660	R2783	L2877	R3007	L3102	R3206	LYS	LYS
I3514	L2295	Q2416	K2551	E2665	Y2792	S2878	M3008	V3103	K3207	GLN	LEU
Y3516	Q2296	A2420	Q2554	T2666	Y2794	K2879	G3015	Q3104	I3208	GLY	GLY
F3520	V2307	Q2438	Q2554	L2668	R2801	V2884	F3021	K3112	K3209	ILE	ILE
D3521	D2308	H2439	E2559	L2669	W2802	L2911	D3024	M3113	E3210	ALA	THR
Q3522	P2309	F2441	T2559	D2671	E2802	F2912	E3025	D3114	T3211	ASP	THR
M3524	E2310	Q2442	H2560	K2672	F2807	L2922	Y3026	K3117	V3212	LYS	LYS
Q3537	W2311	D2448	V2567	D2673	R2811	L2933	L3029	I3121	Q3213	VAL	VAL
O3538	V2312	L2449	V2568	M2686	P2812	L2934	M3030	V3122	E3216	LYS	GLY
N3540	E2313	S2457	V2569	D2687	L2813	L2937	Q3032	P3123	E3217	ASP	ASP
R3544	L2319	R2467	R2576	L2703	E2814	G2937	C3033	D3124	E3218	LEU	LEU
L3553	D2320	R2471	L2581	E2704	T2815	V2938	K3034	Y3125	R3219	ASP	LYS
D3557	D2321	Y2472	P2590	R2705	V2818	L2943	E3035	M3126	R3220	VAL	VAL
E3558	R2339	S2457	L2592	I2706	E2819	L2948	G3036	P3130	ASP	GLU	ASP
R3559	R2340	R2467	V2592	Q2707	E2822	R2948	A3037	D3131	LEU	PRO	LEU
L3560	W2342	R2471	L2593	Q2710	R2823	K2943	Q3038	K3132	ILE	ALA	LYS
L3567	F2343	Y2472	M2603	C2712	R2823	R2948	K3039	L3133	LYS	ILE	GLY
C3573	E2345	Q2471	P2606	A2711	A2826	R2948	E3040	P3134	GLN	VAL	ALA
T3574	V2345	F2479	P2606	C2712	A2829	K2948	E3041	Q3135	ASN	GLN	ASN
E3575	W2345	P2481	R2610	Q2719	F2833	S2957	L3042	F3136	LEU	GLU	GLU
I3578	T2352	M2481	E2616	K2721	R2836	T2960	M3043	P3137	VAL	VAL	ALA
M3579			V2617	V2731		T2961	L3044	H3139	LYS	LYS	ALA

E4503	R3585	P3690	K3774	V3915	R3989	N4085	E4192	E4310	L4390	E4503
I4507	L3588	D3691	R3775	L3916	L3990	N4085	R4193	D4310	I4391	I4507
V4528	N3602	R3695	E3776	S3917	R3997	K4089	Y4196	D4314	P4392	V4528
L4536	E3603	V3696	A3777	A3918	D3998	S4090	L4199	P4318	Q4393	L4536
T4547	Y3604	T3697	A3778	G3919	R4000	G4091	G4200	L4321	T4394	T4547
S4548	K3605	F3698	R3782	S3920	M4004	R4092	W4201	G4322	L4398	S4548
Q4549	D3606	T3704	E3785	T3921	M4012	M4095	E4206	L4323	R4400	Q4549
G4550	R3607	S3707	E3786	R3922	N4015	V4099	F4207	P4324	R4400	G4550
A4551	F3614	L3708	T3787	I3924	E4015	H4100	D4211	M4325	E4403	A4551
T4552	D3617	R3721	D3788	Q3925	L4025	L4101	D4220	M4326	F4412	T4552
L4553	L3623	D3725	I3789	G3926	L4025	A4102	A4227	E4327	E4414	L4553
D4554	R3628	E3726	M3791	L3927	I4030	L4106	A4227	R4328	R4415	D4554
S4557	L3633	D3730	V3790	T3928	T4033	M4107	R4230	K4342	R4428	S4557
L4577	L3633	L3731	Q3792	Q3931	E4034	Q4108	I4233	M4343	Q4429	L4577
I4581	D3637	L3732	E3795	A3932	P4037	L4109	K4237	K4345	D4433	I4581
W4592	V3638	G3736	P3803	S3936	P4040	L4111	L4246	Q4347	V4437	W4592
K4594	P3643	E3737	T3806	R3937	M4043	L4112	M4247	LEU	C4438	K4594
M4597	V3644	Q3739	L3829	L3938	V4046	L4113	L4246	LEU	C4438	M4597
T4598	N3645	F3738	Y3836	S3939	P4047	L4114	L4247	GLU	E4439	T4598
E4599	N3646	Q3740	Y3837	P3942	Q4048	S4115	L4272	ASP	K4443	E4599
K4600	V3647	L3740	R3837	A3943	Y4049	Q4117	L4276	GLU	Q4441	K4600
K4601	L3649	R3742	R3837	F3944	D4050	P4118	R4276	THR	K4442	K4601
A4602	N3650	Q3743	N3838	K3945	H4054	P4118	S4277	THR	Q4443	A4602
S4603	R3651	Q3744	V3839	D3946	D4057	F4122	E4281	THR	Q4444	S4603
R4615	E3652	L3745	Q3842	A3949	L4058	R4123	E4281	THR	R4448	R4615
T4628	R3655	E3746	N3843	Q3950	A4059	L4124	E4281	THR	I4452	T4628
K4629	T3656	K3747	L3846	V3951	A4060	L4125	E4281	THR	M4453	K4629
E4630	Q3657	S3748	K3847	Q3952	E4061	L4126	E4281	THR	E4454	E4630
D4631	Q3658	L3749	G3948	A3953	Q4062	T4127	E4281	THR	L4455	D4631
E4637	R3659	L3750	H3852	E3955	Q4065	M4128	E4281	THR	V4456	E4637
R4638	V3660	Q3751	H3852	E3955	Q4065	M4128	E4281	THR	K4457	R4638
Q4639	L3661	Q3752	R3855	Q3956	Q4065	M4128	E4281	THR	G4458	Q4639
T4645	L3662	A3752	A3872	L3959	I4069	K4133	E4281	THR	I4459	T4645
GLU	T3663	S3754	R3873	W3860	A4070	V4134	E4281	THR	L4460	GLU
	L3664	N3754	R3873	L3961	G4072	V4145	E4281	THR	P4461	
	Q3665	E3755	R3873	L3961	S4073	V4146	E4281	THR	T4474	
	D3666	V3756	L3876	D3962	A4074	F4147	E4281	THR	V4475	
	I3669	K3757	H3877	S3963	A4074	E4148	E4281	THR	I4476	
	D3670	G3758	H3880	S3965	G4075	K4154	E4281	THR	D4481	
	S3674	R3759	A3888	P3966	F4077	M4157	E4281	THR	F4482	
	I3677	L3761	A3888	E3967	N4078	I4169	E4281	THR	S4493	
	F3678	D3762	G3897	L3973	G4076	S4172	E4281	THR	S4498	
	L3679	D3763	E3898	L3973	F4077	F4173	E4281	THR	K4502	
	E3687	D3764	L3909	E3976	N4078	N4174	E4281	THR		
	F3688	T3765	R3910	E3977	N4078	F4173	E4281	THR		
	P3689	I3766	Q3911	E3977	N4078	N4174	E4281	THR		
		I3767	R3912	E3977	N4078	N4174	E4281	THR		
		T3768	N3912	E3977	N4078	N4174	E4281	THR		
		T3769	G3984	E3977	N4078	N4174	E4281	THR		
		L3770	Q3985	E3977	N4078	N4174	E4281	THR		
		E3771		E3977	N4078	N4174	E4281	THR		
		N3772		E3977	N4078	N4174	E4281	THR		
		L3773		E3977	N4078	N4174	E4281	THR		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112474	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	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.816	Depositor
Minimum map value	-1.230	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	411.48, 411.48, 411.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.143, 1.143, 1.143	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/23533	0.49	0/31898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23040	0	23108	394	0
2	A	81	0	36	3	0
3	A	31	0	12	8	0
All	All	23152	0	23156	394	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 394 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:2742:ALA:O	1:A:2746:GLN:OE1	1.62	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.54	0.89
1:A:4037:PRO:HG2	1:A:4117:GLN:HE21	1.41	0.86
1:A:2603:MET:HE2	1:A:2603:MET:HA	1.60	0.83
1:A:3514:ILE:HG13	1:A:3579:MET:HG2	1.61	0.80

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	2854/4646 (61%)	2759 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	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	2548/4125 (62%)	2540 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4174	ASN
1	A	3937	ARG
1	A	2912	PHE
1	A	2910	VAL
1	A	3741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3880	HIS
1	A	3985	GLN
1	A	4326	ASN
1	A	4012	ASN
1	A	3843	ASN

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](#)

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
2	ADP	A	4704	-	24,29,29	0.73	0	29,45,45	0.77	1 (3%)
2	ADP	A	4701	-	24,29,29	0.75	0	29,45,45	0.78	1 (3%)
2	ADP	A	4703	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
3	ATP	A	4702	-	28,33,33	0.74	0	34,52,52	0.76	1 (2%)

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	4704	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C6-N6	2.31	123.83	120.31
3	A	4702	ATP	C5-C6-N6	2.30	123.81	120.31
2	A	4704	ADP	C5-C6-N6	2.22	123.69	120.31
2	A	4701	ADP	C5-C6-N6	2.16	123.61	120.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	C5'-O5'-PA-O2A
2	A	4703	ADP	O4'-C4'-C5'-O5'

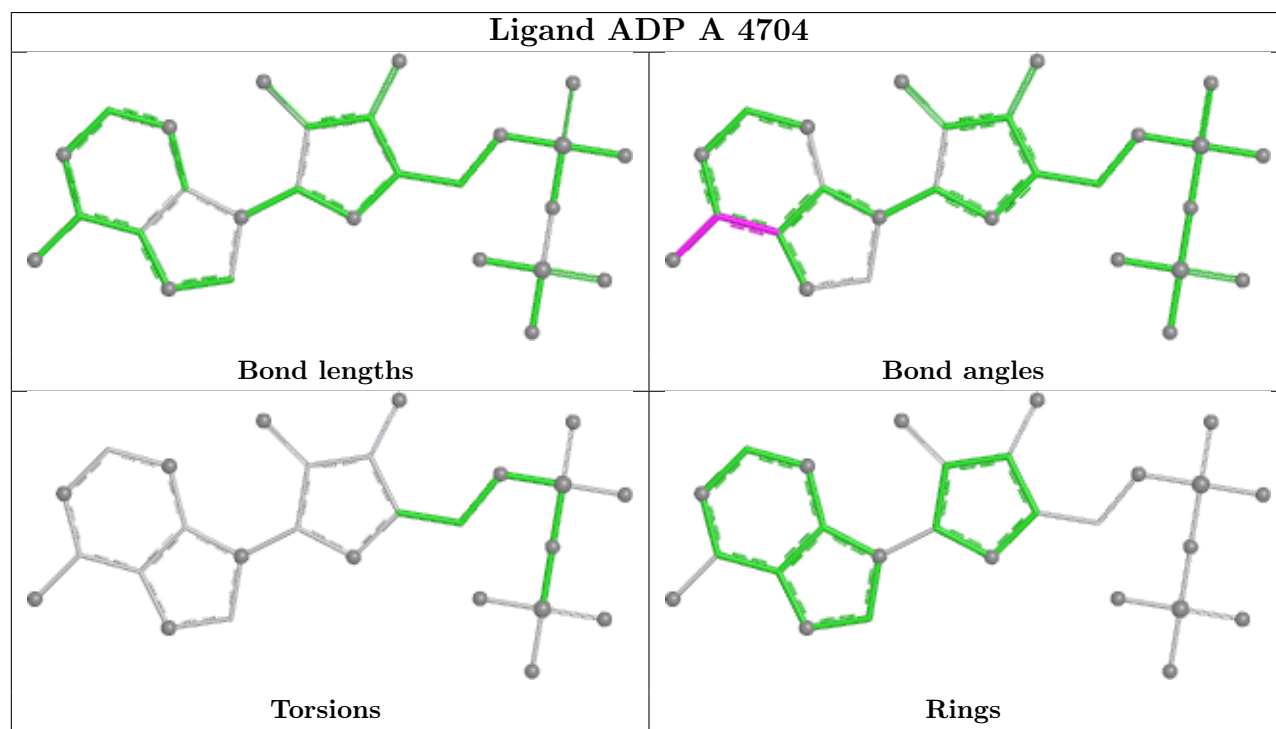
There are no ring outliers.

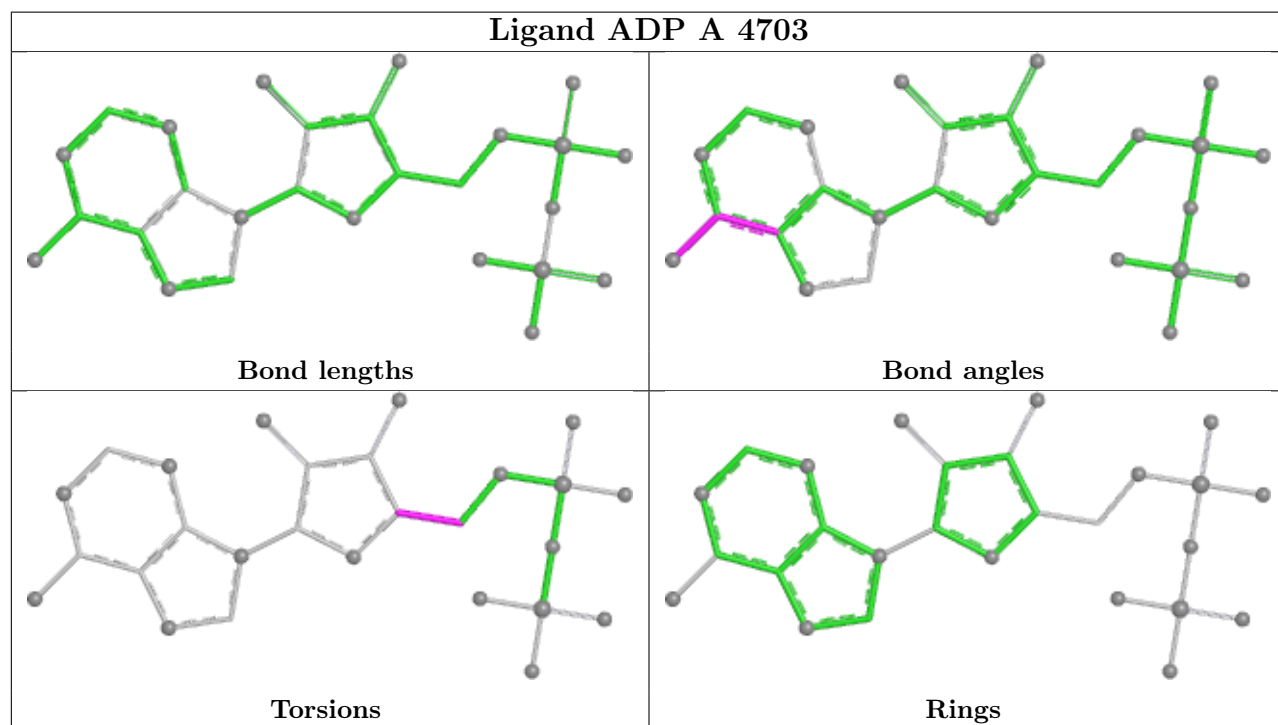
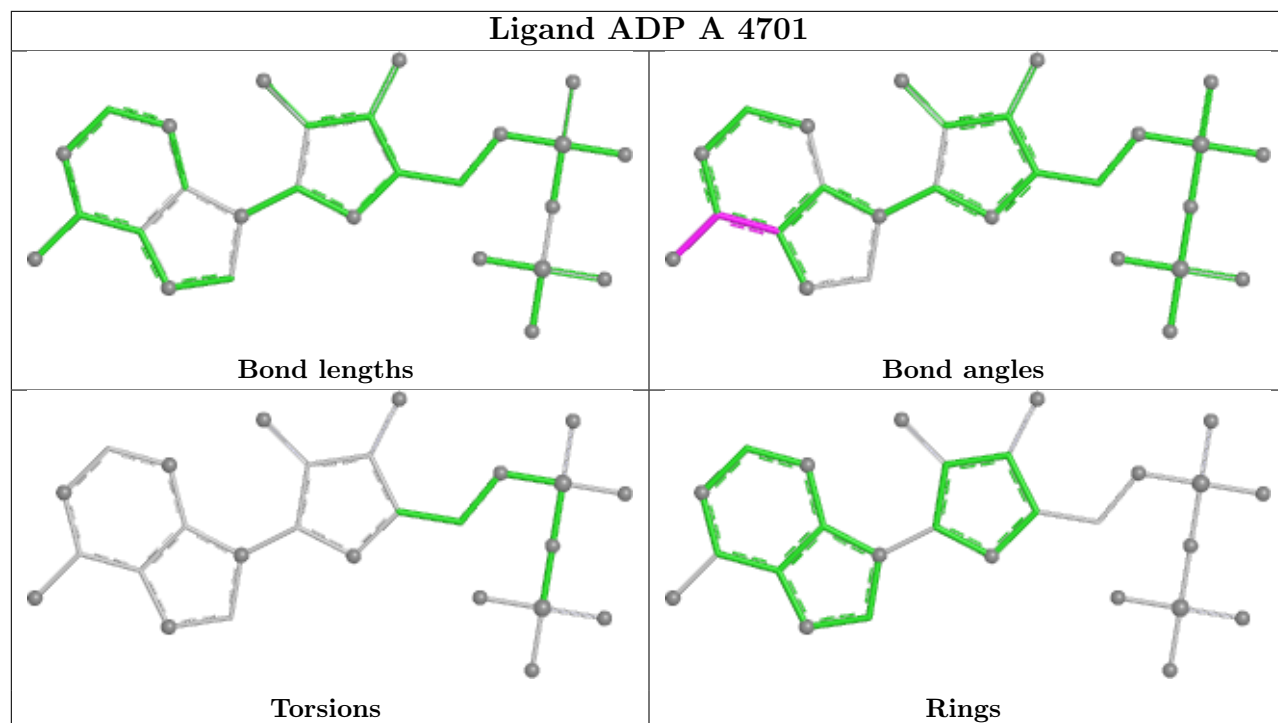
2 monomers are involved in 11 short contacts:

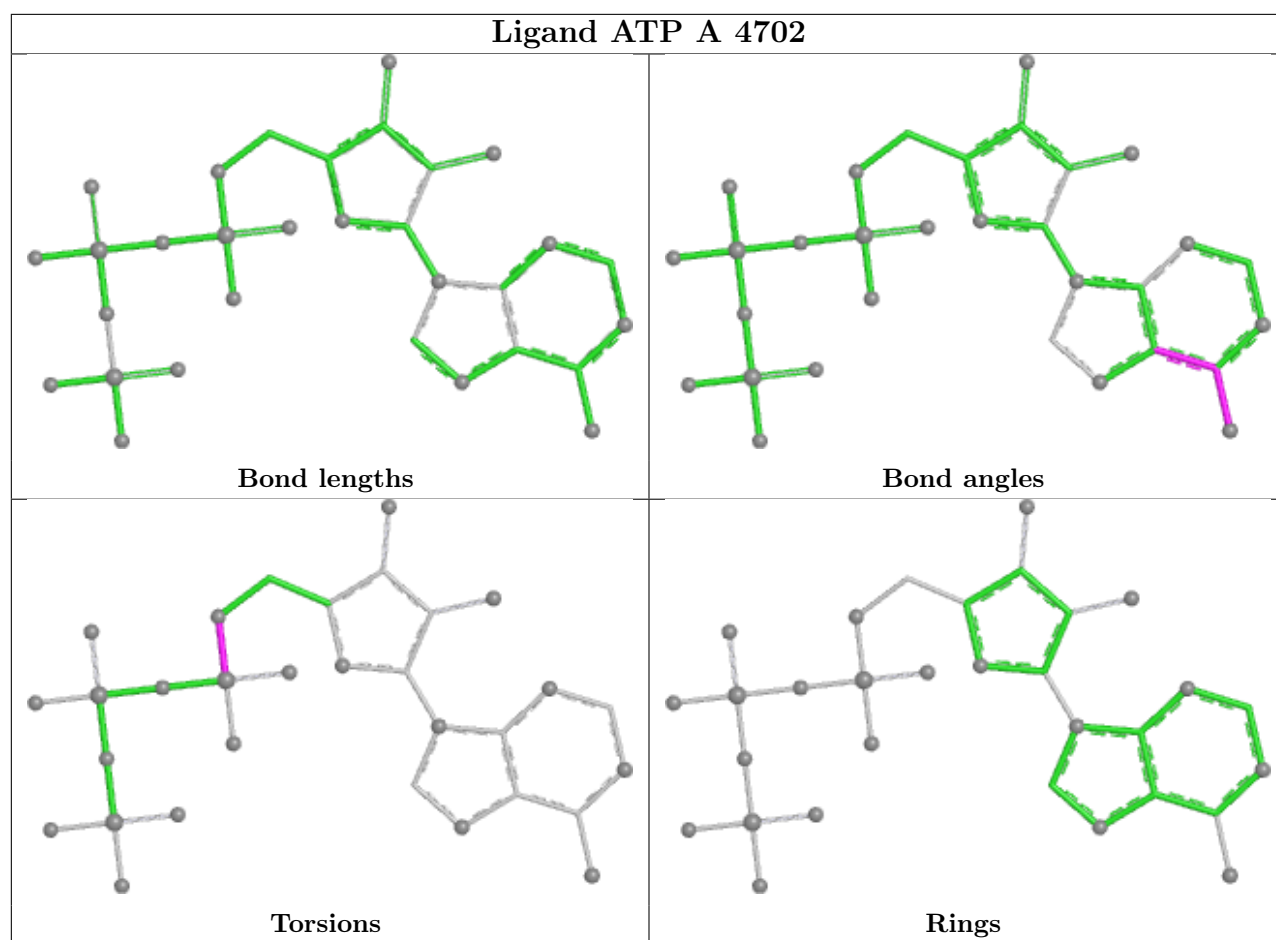
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	0
3	A	4702	ATP	8	0

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.

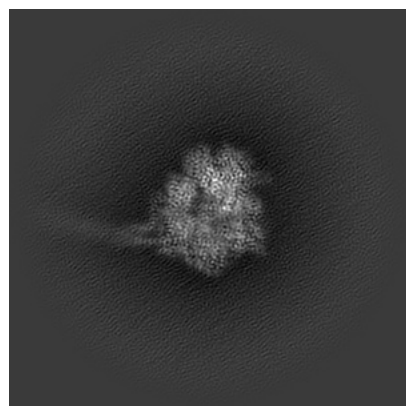
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44722. These allow visual inspection of the internal detail of the map and identification of artifacts.

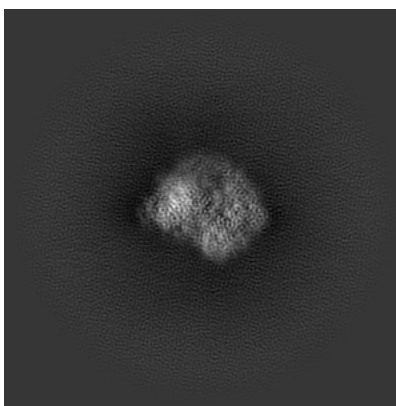
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

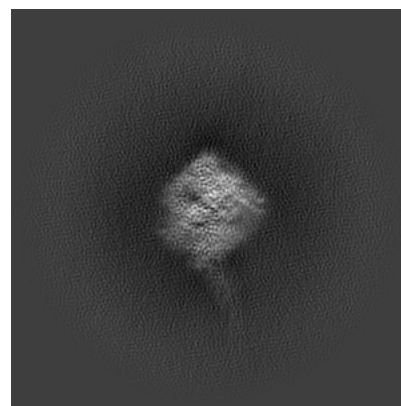
6.1.1 Primary map



X

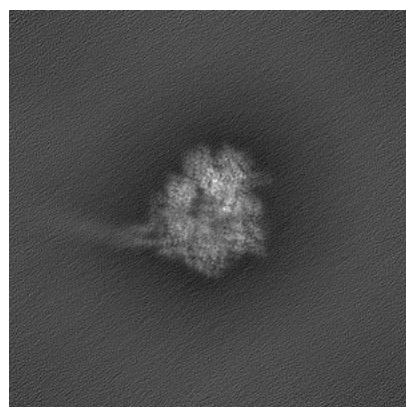


Y

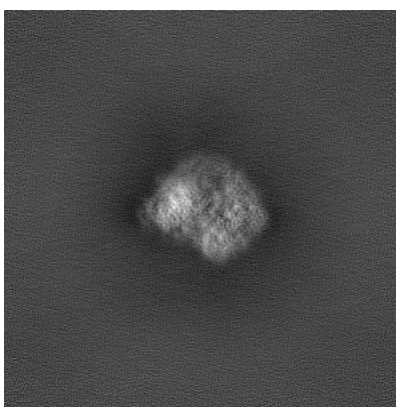


Z

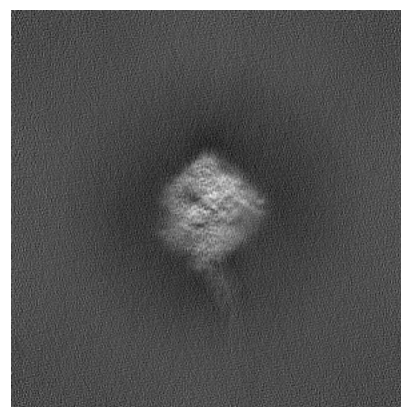
6.1.2 Raw map



X



Y

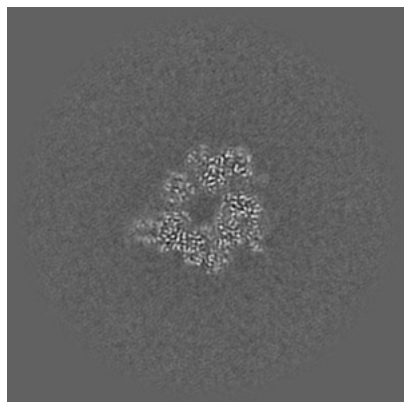


Z

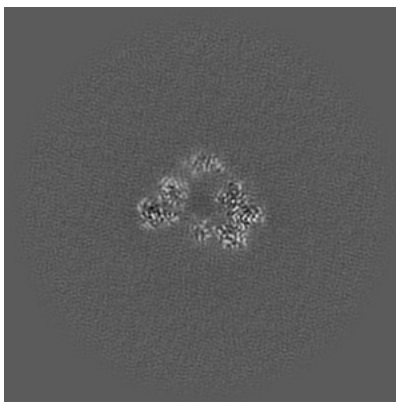
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

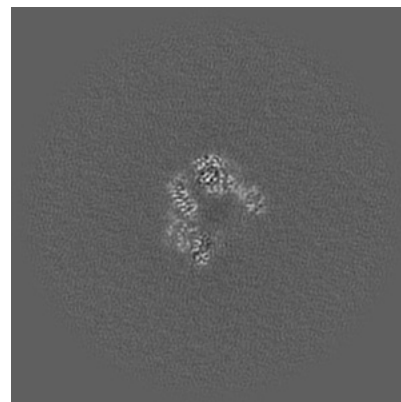
6.2.1 Primary map



X Index: 180

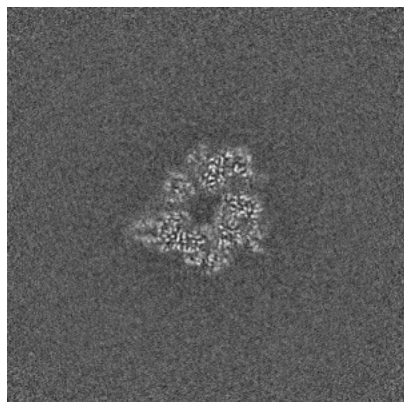


Y Index: 180

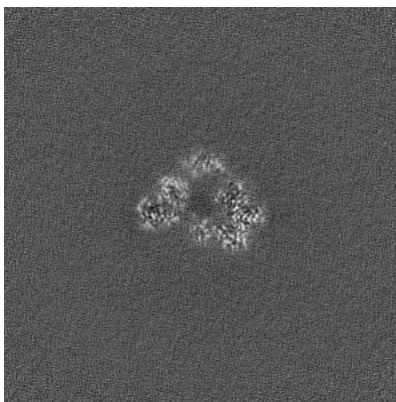


Z Index: 180

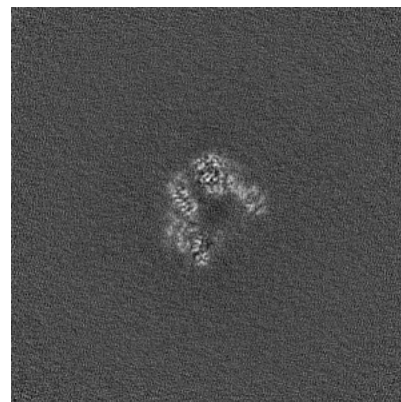
6.2.2 Raw map



X Index: 180



Y Index: 180

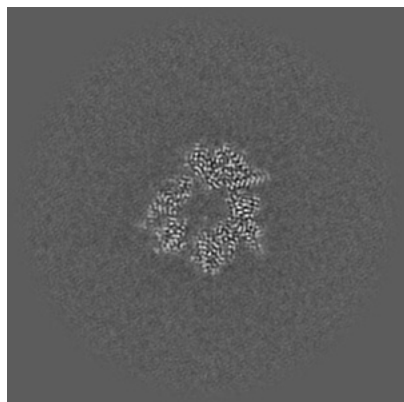


Z Index: 180

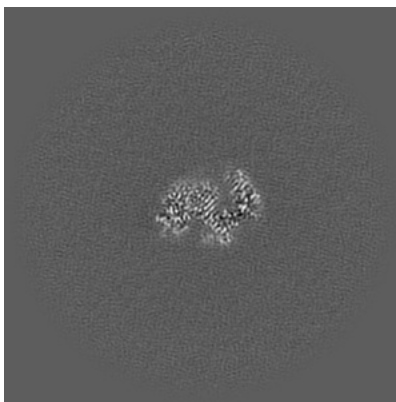
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

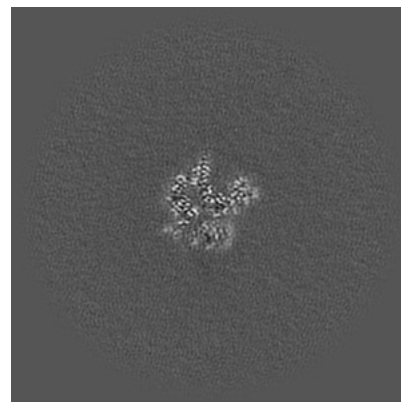
6.3.1 Primary map



X Index: 174

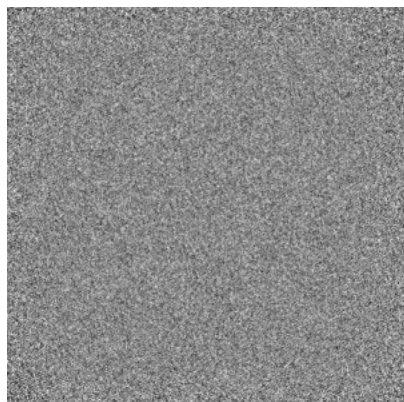


Y Index: 206

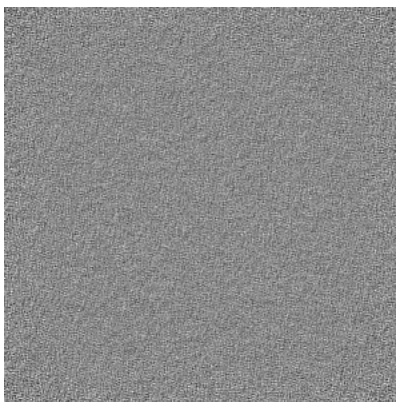


Z Index: 201

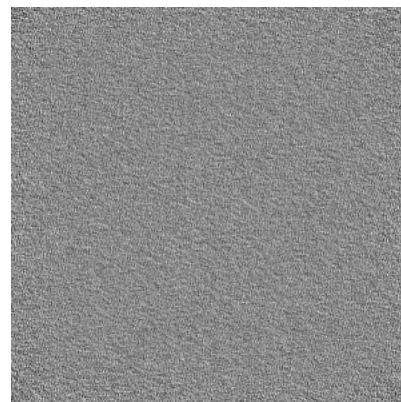
6.3.2 Raw map



X Index: 0



Y Index: 0

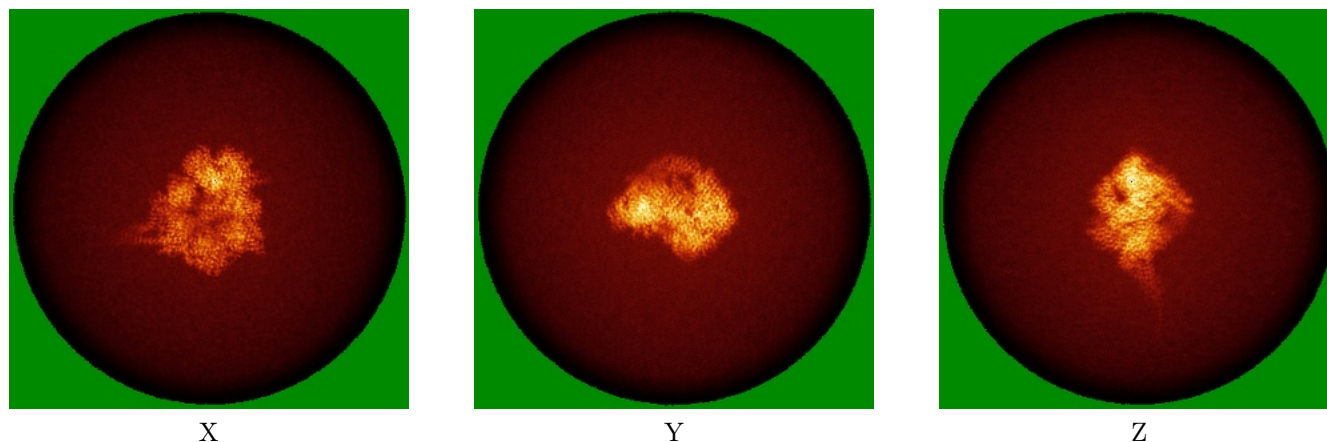


Z Index: 0

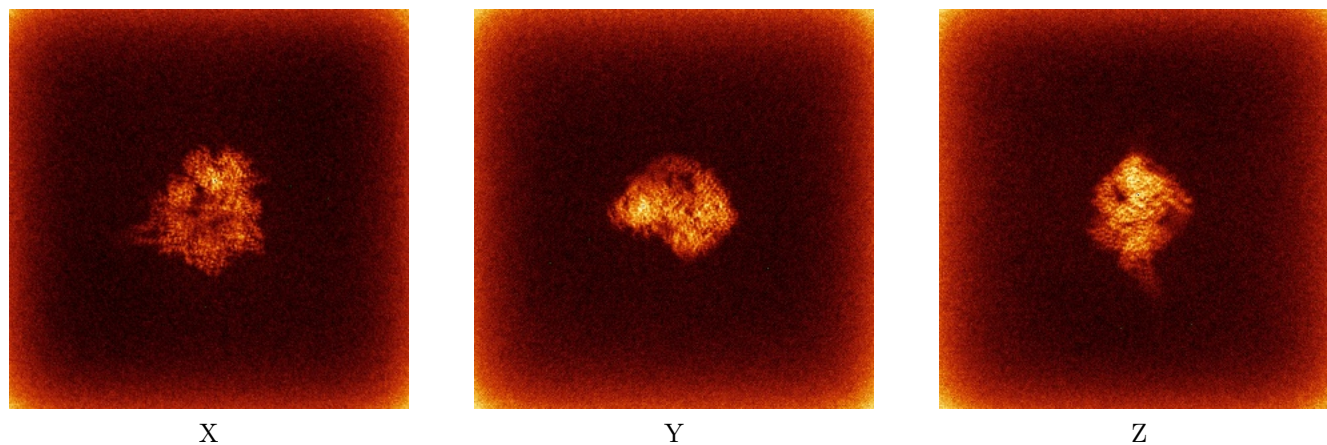
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



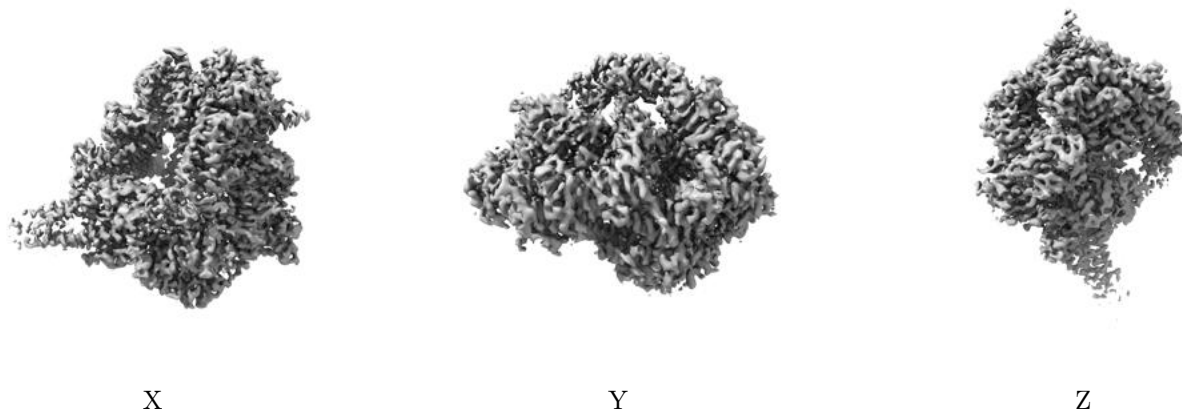
6.4.2 Raw map



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

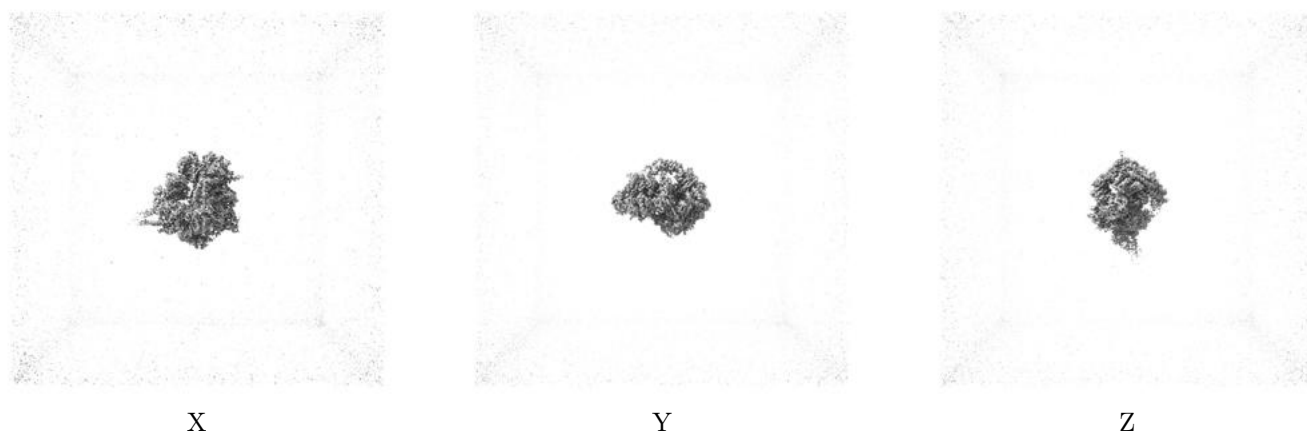
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

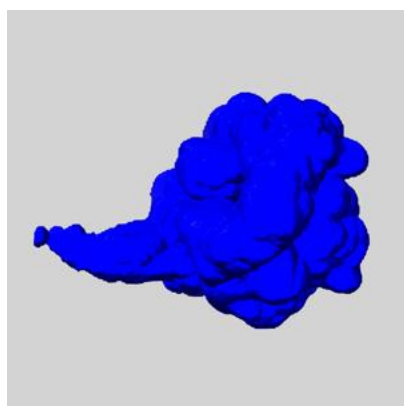
6.6 Mask visualisation [i](#)

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

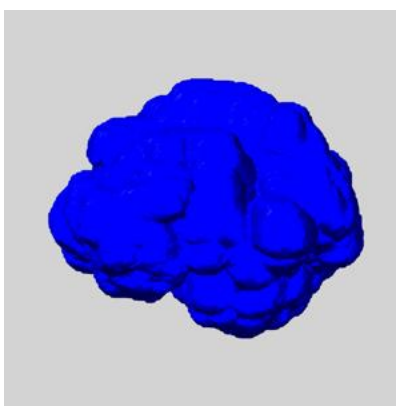
A mask typically either:

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

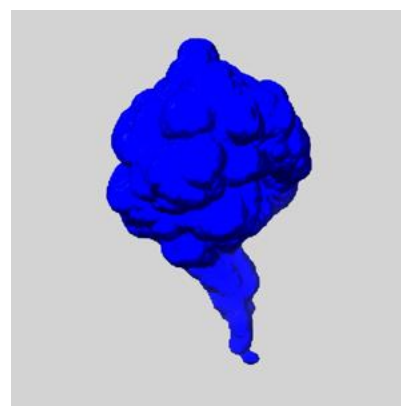
6.6.1 emd_44722_msk_1.map [i](#)



X



Y

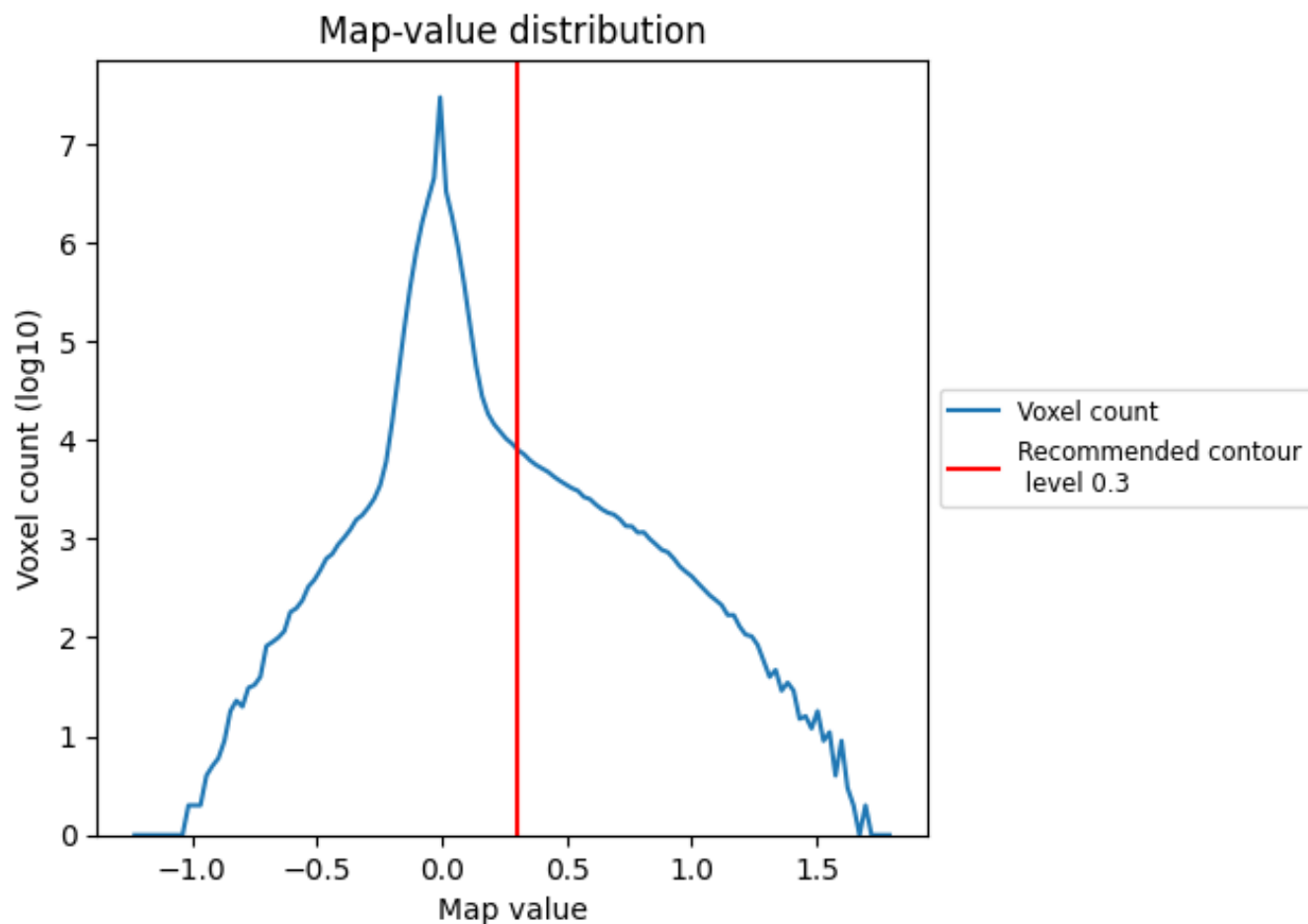


Z

7 Map analysis [i](#)

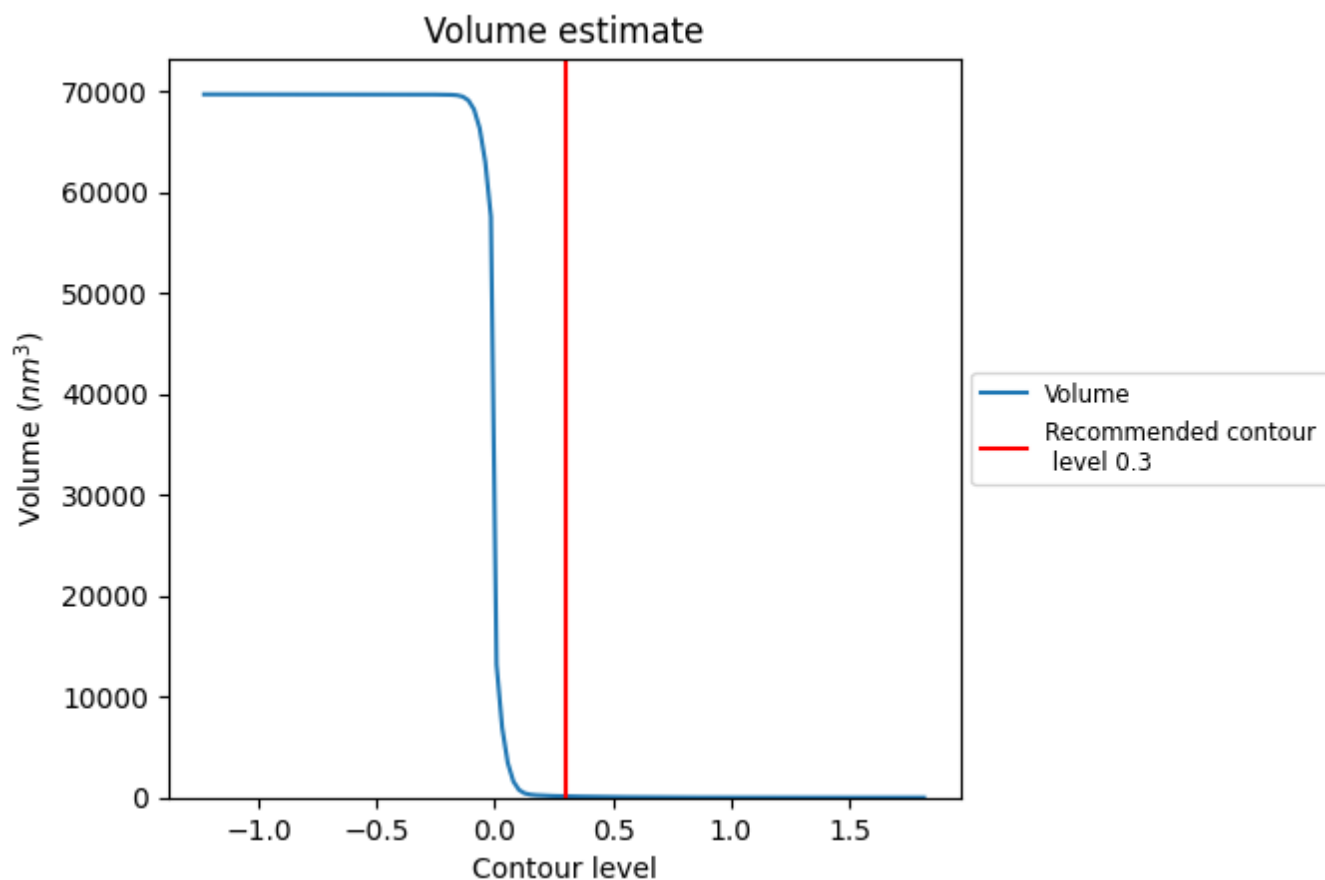
This section contains the results of statistical analysis of the map.

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.

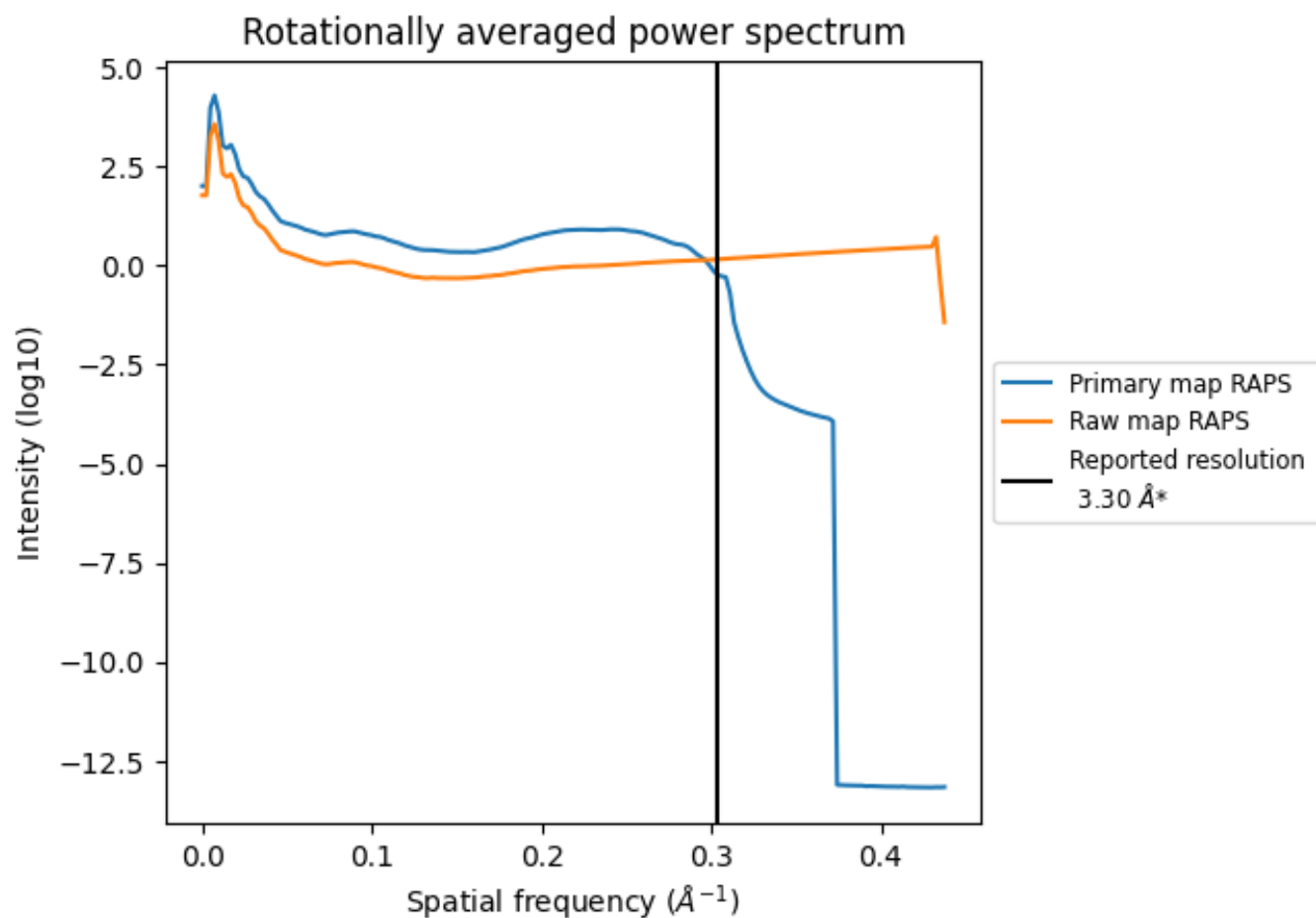
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 114 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 ⓘ

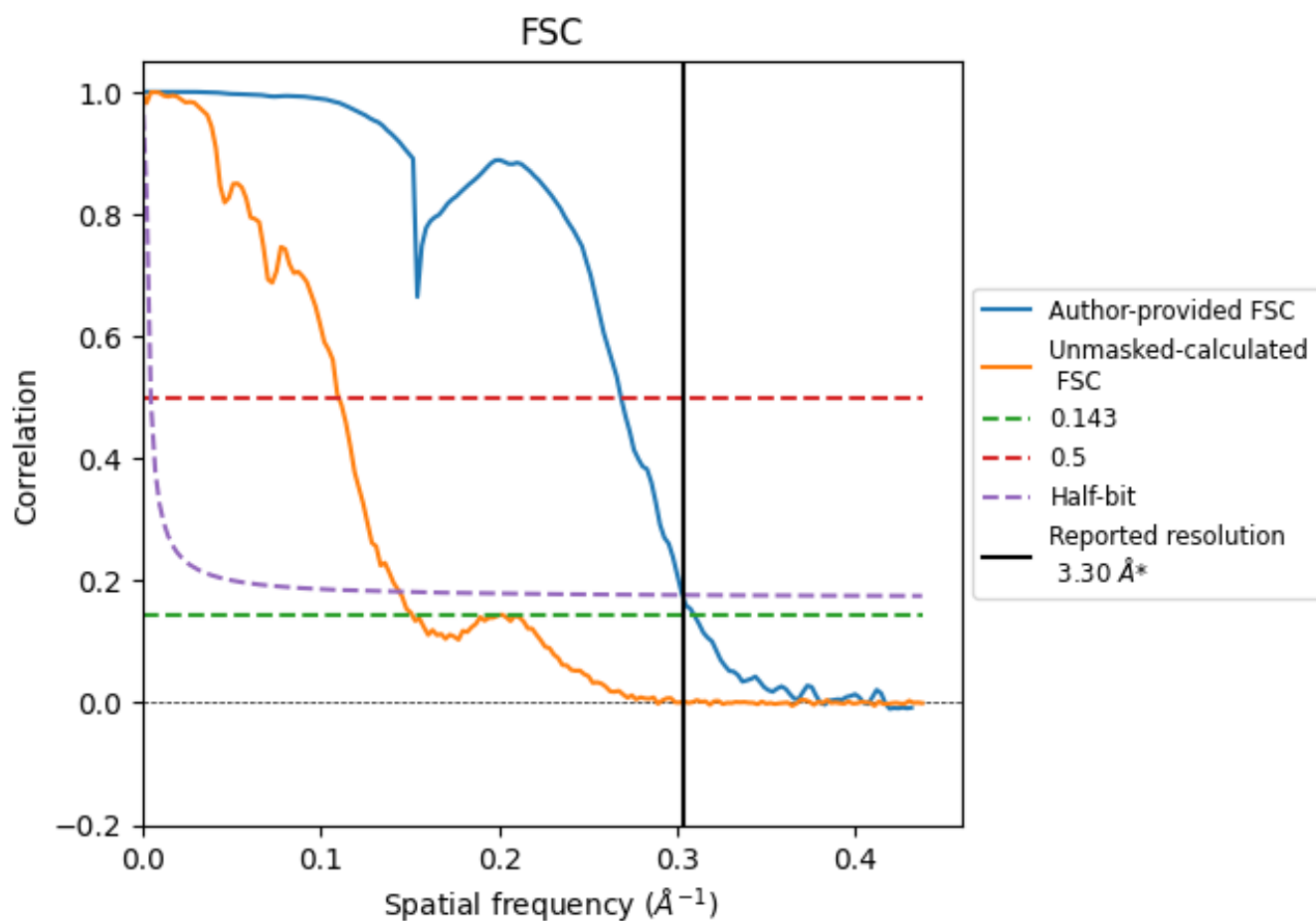


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

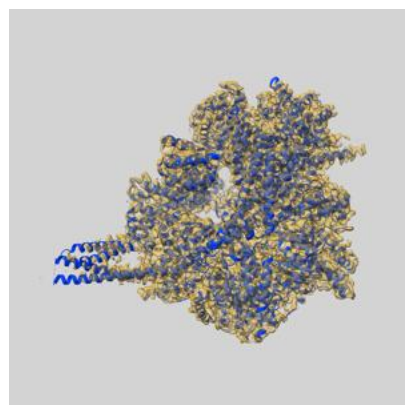
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.23	3.72	3.30
Unmasked-calculated*	6.61	9.08	6.93

*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 6.61 differs from the reported value 3.3 by more than 10 %

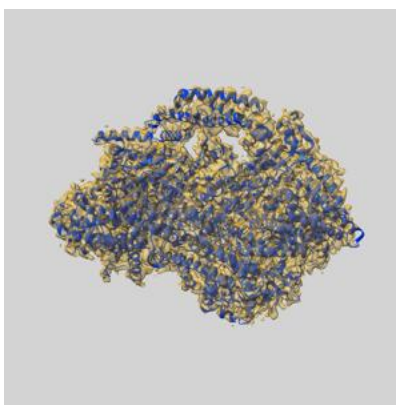
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44722 and PDB model 9BN5. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

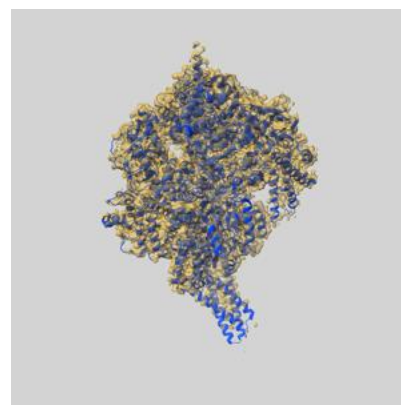
9.1 Map-model overlay [i](#)



X



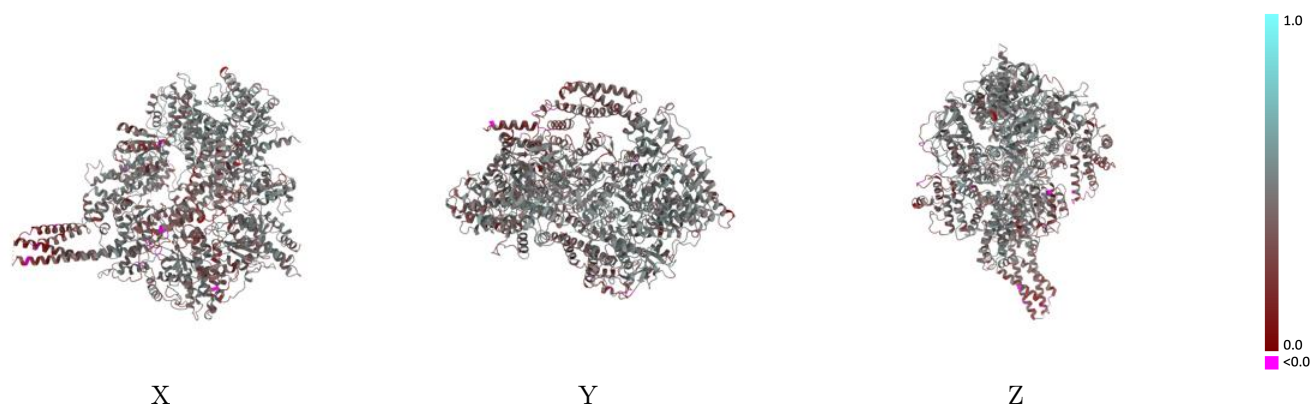
Y



Z

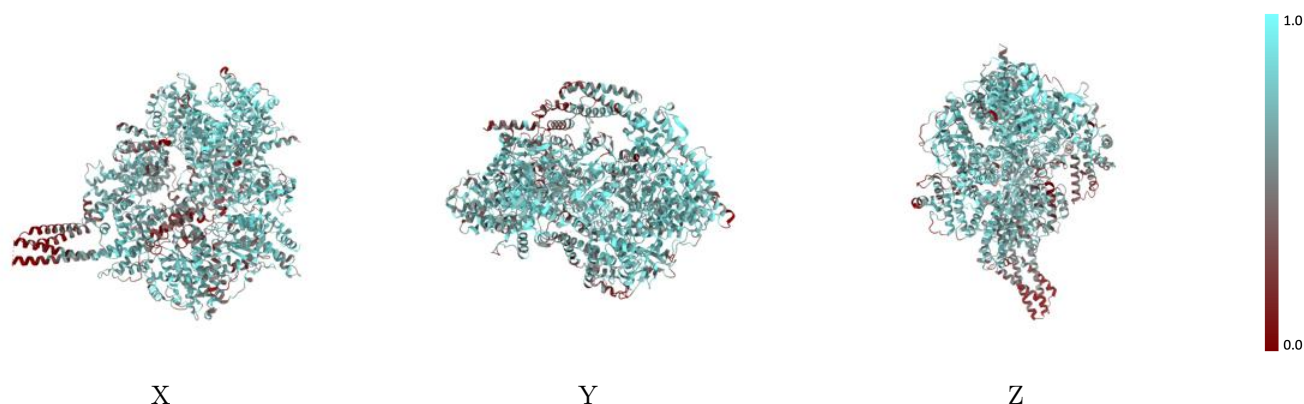
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



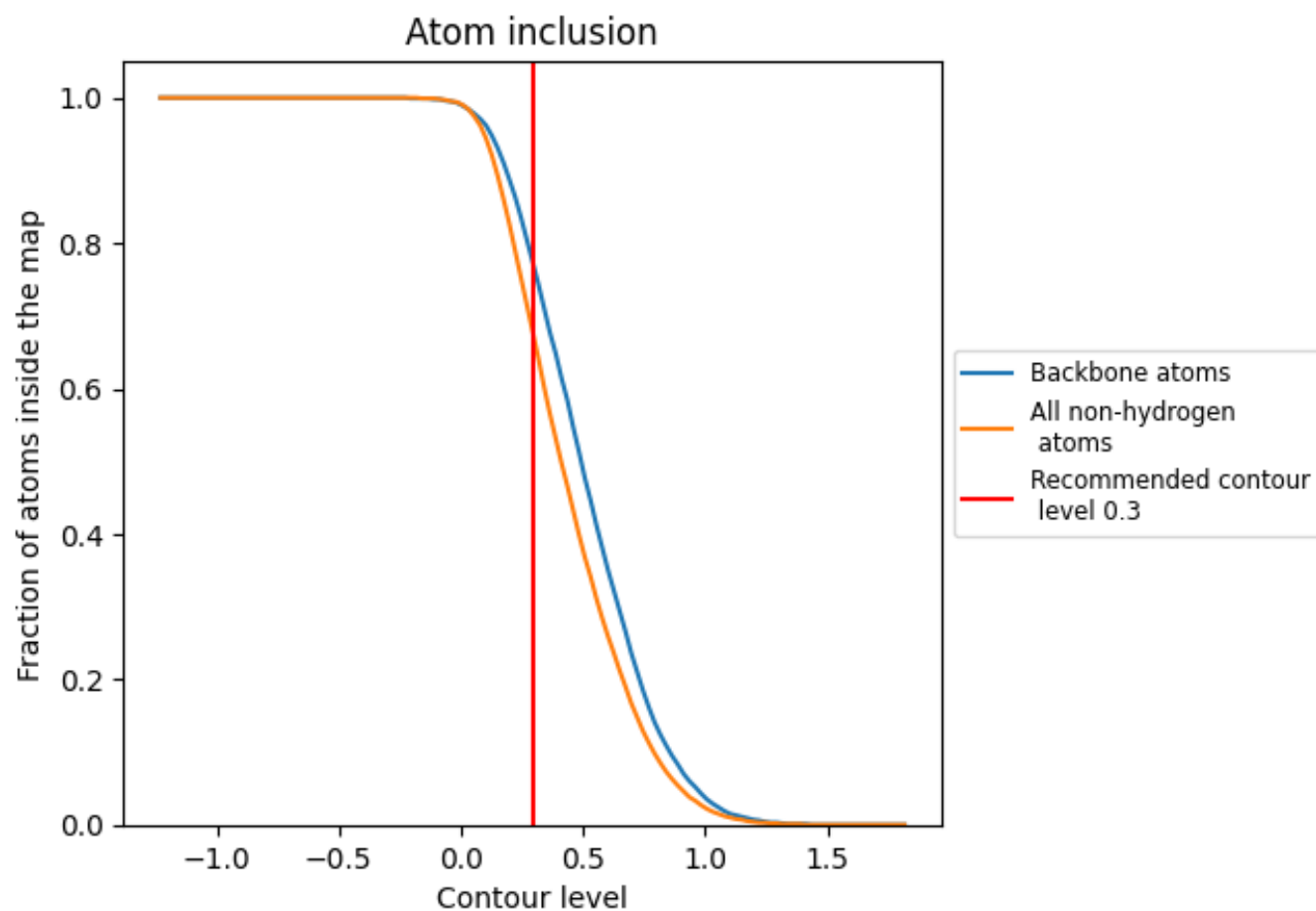
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6680	<div></div> 0.4310
A	<div></div> 0.6680	<div></div> 0.4310

