



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 11:33 AM EDT

PDB ID : 9BN3 / pdb_00009bn3
EMDB ID : EMD-44720
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class1
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.80 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

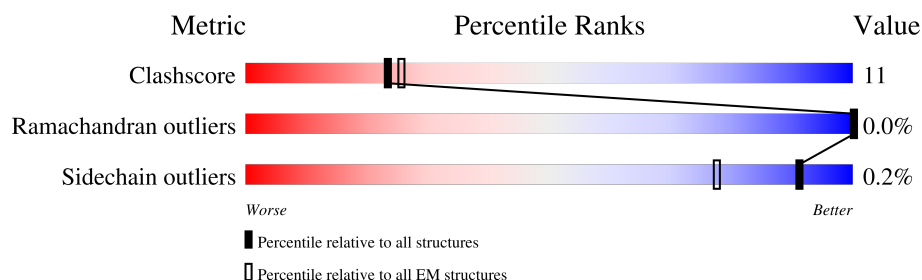
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.

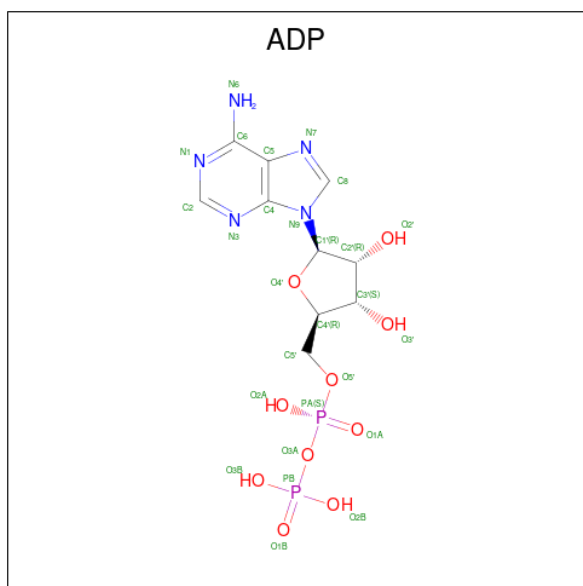
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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:

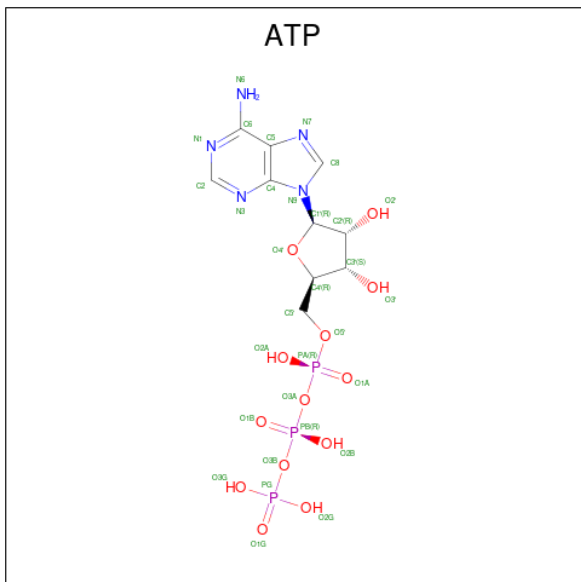
Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

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



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

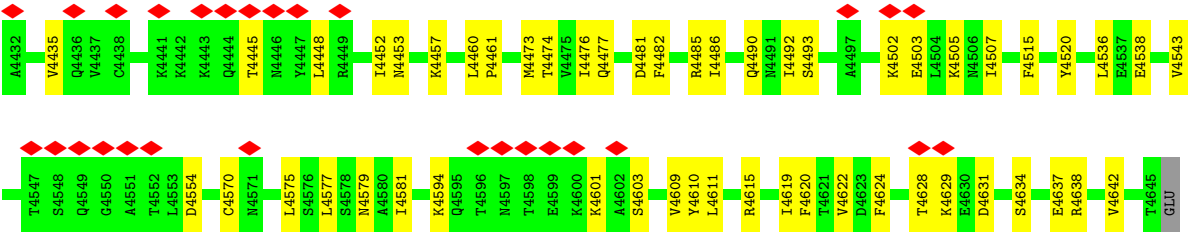
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).





LEU	Q3156	E3073	D2995	D2885	D2787	K2673	L2591	L2449	R2358	Y2265	GLY	ARG
LYS	A3157	G3074	E2996	Q2886	W2802	F2682	V2592	L2450	F2364	D2269	GLU	SER
MET	N3158	L3075	S2997	E2887	W2806	M2686	P2596	R2451	S2365	P2270		ASN
VAL	K3163	K3076	N2998	R2890	L2806	M2697	L2605	C2454	V2368	R2273		K2034
ASP	R3164	D3077	V2999	K2894	A2809	D2697	L2609	S2457	L2369	D2277		L2035
GLN	M3169	R3078	L3000	K2894	L2810	V2701	L2610	L2458	S2370	F2280		F2036
GLU	T3172	A3079	D3001	K2898	T2815	K2702	R2611	L2462	T2374	F2200		K2037
ALA	Y3176	A3080	L3004	E2898	L2816	E2703	P2613	R2467	I2138	K2286		P2044
LYS	E3193	L3084	L3005	E2903	L2817	E2704	D2614	R2465	E2152	V2291		R2045
LYS	L3194	L3085	E3006	E2904	V2818	R2705	D2615	V2469	D2153	R2292		R2046
VAL	F3096	F3086	K3007	D2906	G2820	I2706	W2616	Q2470	L2160	G2293		F2059
MET	E3195	N3087	G3015	V2910	L2821	F2706	V2617	Y2472	E2294	E2294		L2065
SER	E3196	N3092	F3021	N2913	L2822	G2710	F2622	D2478	GLY	R2295		A2066
GLN	Q3197	W3093	E3022	N2913	R2823	R2720	S2623	M2481	ASP	Q2296		K2067
GLU	Q3198	F3094	G3023	L2922	L2824	K2721	S2624	Q2485	GLU	F2165		K2068
ILE	G3095	D3024	D2923	D2923	A2826	R2726	T2626	Q2485	GLN	W2300		L2069
GLU	H3200	D3096	E3025	R2924	A2829	P2731	T2627	Q2485	ALA	V2300		V2070
GLN	L3201	N3201	E3026	L2924	L2830	V2732	P2628	Q2485	ALA	D2306		P2071
LEU	V3203	A3101	Y3026	L2925	R2831	P2732	E2629	Q2485	ARG	E2188		L2075
HIS	G3204	V3105	L3029	Q2928	L2832	V2733	E2629	R2488	ARG	D2195		Q2079
LYS	L3205	M3113	M3030	Q2930	F2833	V2734	L2630	L2498	ARG	E2205		Y2086
GLN	R3206	N3119	T3031	L2933	V2838	Y2735	K2633	L2498	GLY	E2310		L2090
GLU	K3207	N3119	Q3032	L2934	E2839	P2738	T2634	W2500	LYS	W2311		L2093
VAL	L3208	P3123	C3033	L2935	D2840	P2739	T2635	S2501	GLU	V2312		L2097
ILE	K3209	E3210	K3034	L2936	R2844	G2740	D2636	L2502	GLY	Q2209		G2101
ALA	E3210	T3211	E3035	G2937	W2845	E2743	H2637	D2505	ASP	L2315		R2105
LYS	V3212	M3126	G3036	W2938	T2846	S2743	E2640	P2527	GLU	D2320		E2106
GLN	K3213	P3127	A3037	S2939	D2847	I2747	R2643	P2530	ALA	D2321		Q2109
SER	Q3214	V3128	Q3038	T2944	E2849	L2748	G2749	W2531	ALA	L2327		K2104
VAL	V3215	V3129	E3040	R2948	L2850	R2753	H2646	L2532	P2411	E2327		R2105
GLU	E3216	Y3130	G3041	R2948	D2851	R2753	Q2647	P2533	E2412	K2230		E2106
ASP	E3217	D3131	L3042	D2961	T2852	L2756	V2648	L2534	L2413	Q2230		K2105
ASP	L3218	K3132	M3043	K2962	V2853	L2756	V2649	L2535	Q2416	R2231		E2106
LYS	R3219	L3133	L3044	V2963	A2854	R2757	L2650	L2535	R2417	R2332		Q2109
VAL	R3220	P3134	D3045	H2964	L2855	L2758	A2851	W2545	Q2416	L2333		I2111
GLU	ASP	Q3135	S3046	R2965	D2862	L2759	P2852	Q2554	W2423	S2334		K2112
PRO	LEU	P3136	H3047	K2966	R2863	L2762	V2653	Q2554	Q2424	W2338		E2114
ALA	VAL	P3137	E3048	R2966	E2864	A2766	Q2654	D2566	S2429	R2339		LYS
VAL	ARG	S3138	E3049	E2970	K2865	A2766	L2655	D2566	N2430	R2340		GLU
ILE	ILE	R3139	K3052	D2971	E2867	T2770	V2660	V2569	R2341	I2341		GLU
GLN	GLU	E3141	F3054	L2976	S2868	L2661	L2661	R2576	W2342	R2243		ARG
ASN	ASN	R3140	T3053	L2979	R2869	R2773	F2662	H2577	F2343	L2244		GLY
ALA	ALA	V3144	F3053	V2979	R2869	V2774	C2663	R2577	E2344	G2246		GLU
VAL	VAL	S3145	L3055	E2981	I2871	D2774	D2664	H2581	W2345	V2247		ALA
LYS	LYS	C3147	I3059	R2981	R2783	E2783	E2665	L2581	Q2346	E2248		VAL
SER	ASN	V3148	V3065	K2986	S2876	F2784	E2665	W2584	Y2350	K2261		ASP
ALA	ALA	H3151	F3066	N2987	K2879	T2785	L2668	W2584	R2351	G2261		GLU
ALA	ALA	Q3152	T3067	E2988	D2880	Q2786	P2669	P2590	T2352			
ASN	ASN	T3153	M3069	E2988			D2670	L2353	A2354			
ASP	ASP	L3154	P3070	E2988								
LYS	LYS	H3155	S3071	E2988			D2672					

T4333	G4300	V4099	M4004	N3912	V3797	G3736	A3564	K3480	GLU	LYS
G4336	W4201	H4100	M4007	L3916	Y3801	R3655	L3567	S3481	ASP	LYS
V4337	K4204	L4106	L4025	S3917	L3802	T3656	P3569	L3482	ALA	GLN
I4340	F4207	M4107	L4025	S3918	P3803	G3657	A3569	ARG	ILE	HIS
S4341	D4220	Q4108	H4029	G3919	T3806	G3658	D3570	GLY	VAL	VAL
M4342	D4220	L4109	I4030	G3920	T3806	R3659	D3571	LYS	VAL	GLY
K4343	A4227	K4111	T4033	T3921	T3811	R3660	K3581	MET	GLN	VAL
K4345	A4227	K4112	T4033	P3922	Y3812	L3661	L3581	ARG	GLN	VAL
K4346	A4230	L4113	E4034	R3923	L3818	L3662	R3585	LYS	GLN	VAL
M4347	A4230	L4113	P4037	R3923	L3818	T3663	T3586	ASN	ALA	ASN
MET	I4233	L4116	P4040	I3924	T3821	G3665	P3587	TYR	ASN	ALA
LEU	I4233	Q4117	P4040	Q3925	Q3826	D3666	I3590	ASN	ASN	LYS
GLU	I4238	P4118	M4043	Q3926	Q3826	Q3667	D3591	PRO	ALA	ALA
ASP	M4247	H4119	S4045	F3930	L3829	D3668	F3599	TYR	VAL	VAL
ASP	I4251	L4124	V4046	Q3931	L3829	I3669	T3599	ASN	LYS	LYS
ASP	Y4252	F4125	E4056	A3932	T3835	D3670	N3602	TYR	LEU	LEU
ALA	I4264	L4126	D4057	V3935	N3838	E3603	K3497	ALA	ALA	ALA
ALA	I4265	T4127	L4058	V3936	V3839	Y3604	N3498	ILE	ILE	ILE
M4266	M4266	M4128	L4058	R3937	L3840	K3605	Q3499	VAL	VAL	VAL
THR	E4270	K4133	A4060	L3938	E3842	D3606	M3500	ASN	ASN	ASN
GLY	E4270	V4134	A4061	L3938	N3843	R3607	S3501	ARG	ARG	ILE
LYS	F4278	P4135	E4062	P3942	N3844	K3608	T3502	ALA	ALA	CYS
THR	L4284	L4139	T4064	K3945	K3847	I3609	I3503	SER	LEU	LEU
ASP	K4287	R4140	Q4065	D3946	V3849	T3610	C3507	LYS	ALA	LEU
THR	V4289	I4144	S4068	A3949	H3852	R3611	L3508	CYS	GLY	GLY
THR	D4289	F4145	T4069	V3951	T3853	D3691	L3509	TRP	TRP	TRP
ASP	Q4290	V4146	A4070	Q3952	Q3854	C3693	S3510	LYS	LYS	LYS
GLY	H4291	F4147	I4071	A3953	R3855	R3618	I3512	ALA	ALA	ILE
ARG	M4296	E4148	Q4072	A3953	L3856	F3619	F3620	GLU	GLU	GLN
PRO	P4297	K4154	Q4073	D3954	S3857	K3620	M3524	ALA	ALA	ILE
R4375	D4298	R4168	A4074	E3955	I3858	E3624	L3536	GLN	GLN	ARG
R4378	R4302	I4169	E4075	Q3956	F3864	R3628	Q3537	LEU	LEU	SER
H4389	V4306	S4172	F4077	I3959	R3870	F3629	Q3538	TYR	TYR	ILE
Q4393	E4310	P4173	H4078	P3966	V3871	L3633	A3539	ALA	ALA	MET
L4398	E4314	R4174	Q4079	Y3972	R3872	L3634	N3540	ASP	ASP	ARG
K4399	P4318	A4177	D4081	E3976	R3873	V3635	I3541	MET	MET	GLU
E4403	P4318	R4178	A4082	E3977	E3776	D3637	R3544	LYS	LYS	PHE
K4406	L4321	A4179	A4083	E3978	A3777	Y3638	T3545	ARG	ARG	ILE
F4412	P4324	W4185	I4084	P3979	A3778	Y3643	D3546	VAL	VAL	PRO
E4416	N4326	I4189	I4085	A3980	E3779	V3644	E3558	GLU	GLU	THR
L4431	N4326	E4192	T4086	P3981	R3782	L3649	R3559	PRO	PRO	ILE
	V4330	Y4196	K4089	T3982	R3783	E3652	L3560	ALA	ALA	VAL
			R4092	E3785	V3784	V3653	W3562	LEU	LEU	VAL
			M4095	E3786	E3785		R3561	ASN	ASN	ARG
			L4096	T3787	L3732		Q3563	GLY	GLY	VAL
			K4097	D3788	K3733			LEU	LEU	ALA
			N4098	I3789	L3734			GLN	GLN	ALA
				V3790	Q3735			LYS	LYS	GLY
				M3791				LEU	LEU	ILE
				Q3792						
				E3793						
				V3794						
				E3795						
				T3796						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433112	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	2.677	Depositor
Minimum map value	-1.892	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1458, 1.1458, 1.1458	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

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	0.26	1/23533 (0.0%)	0.51	3/31898 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3587	PRO	CG-CD	-6.12	1.30	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3587	PRO	N-CD-CG	-10.98	86.73	103.20
1	A	3587	PRO	CA-CB-CG	-8.39	88.05	104.00
1	A	3587	PRO	CA-N-CD	-5.11	104.34	111.50

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	497	0
2	A	81	0	36	0	0
3	A	31	0	12	1	0
All	All	23152	0	23156	497	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 11.

The worst 5 of 497 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:2423:MET:HE1	1:A:2462:LEU:HD13	1.62	0.81
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.26	0.79
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.63	0.79
1:A:1511:PRO:HG3	1:A:3628:ARG:HE	1.47	0.78
1:A:3209:LYS:HG3	1:A:3486:ARG:HH21	1.48	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	2854/4646 (61%)	2750 (96%)	103 (4%)	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%)	2543 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1729	LYS
1	A	2377	ASN
1	A	3741	ARG
1	A	3937	ARG
1	A	4029	HIS

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	4065	GLN
1	A	4326	ASN
1	A	4117	GLN
1	A	3843	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.28	2 (6%)
2	ADP	A	4704	-	24,29,29	0.86	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.91	0	29,45,45	1.23	3 (10%)
3	ATP	A	4702	-	28,33,33	0.67	0	34,52,52	0.61	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	4701	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.84	123.47	128.67
2	A	4701	ADP	N3-C2-N1	-3.76	123.56	128.67
2	A	4703	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4701	ADP	C4-C5-N7	-2.75	106.43	109.34
2	A	4704	ADP	C4-C5-N7	-2.56	106.63	109.34

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

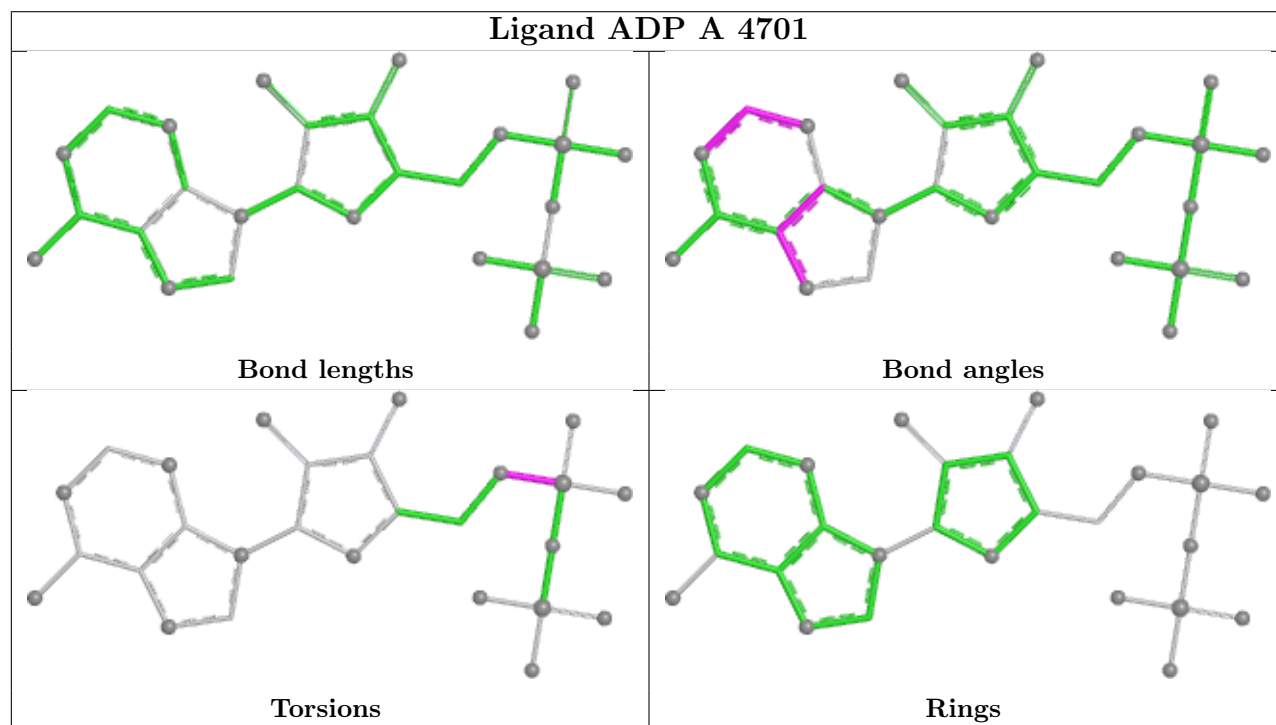
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'

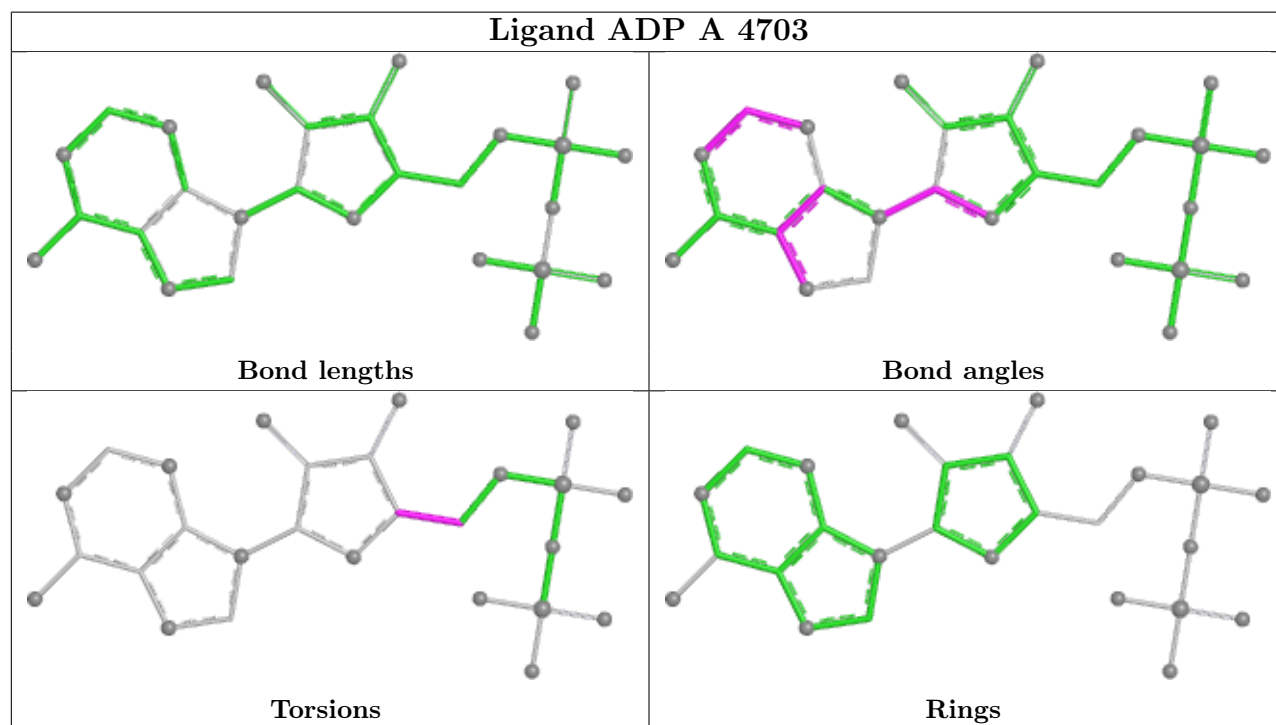
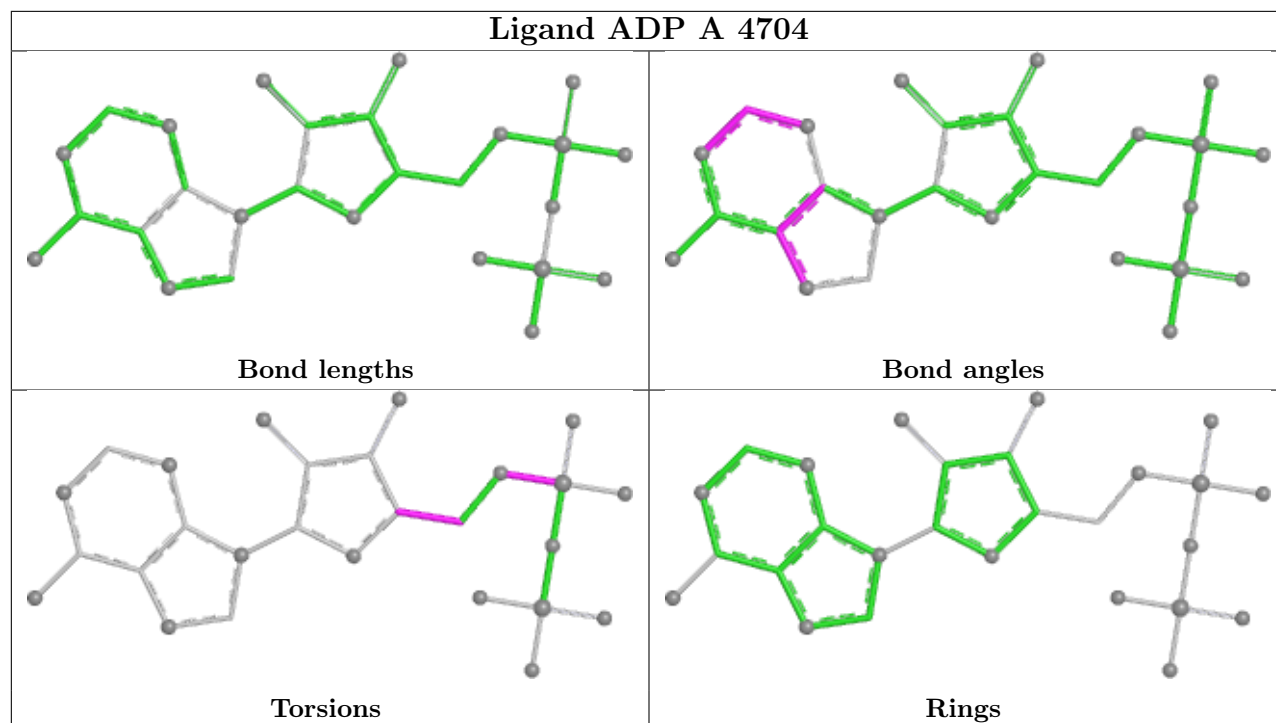
There are no ring outliers.

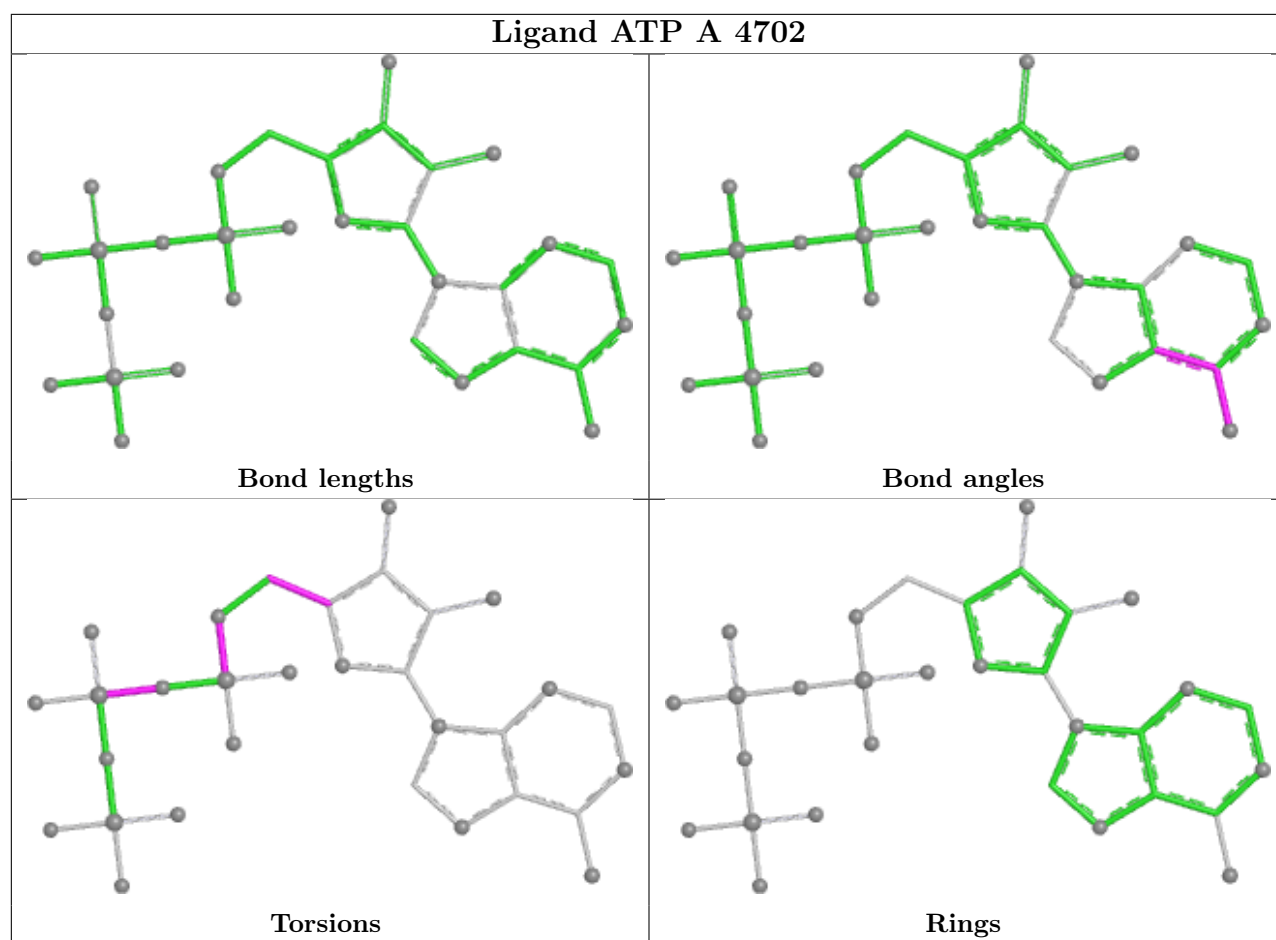
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	1	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.

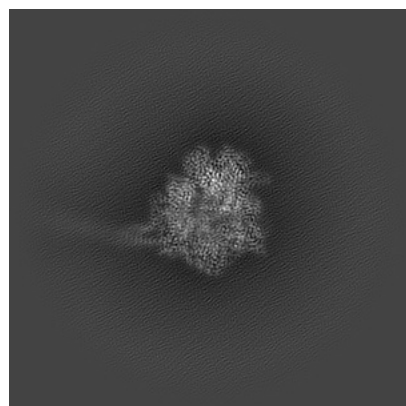
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44720. These allow visual inspection of the internal detail of the map and identification of artifacts.

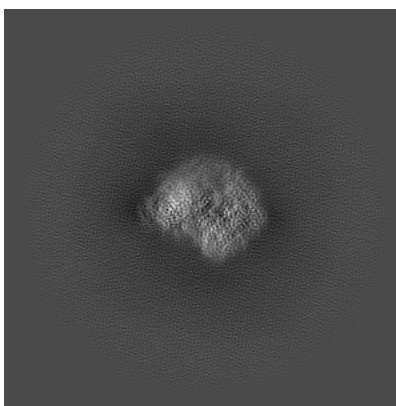
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

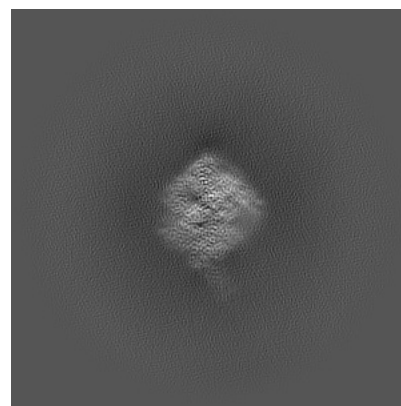
6.1.1 Primary map



X

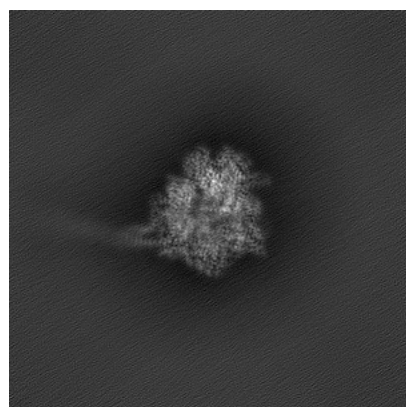


Y

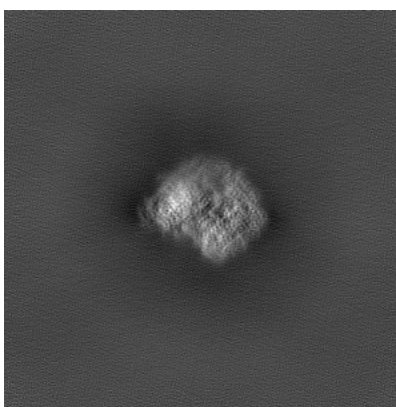


Z

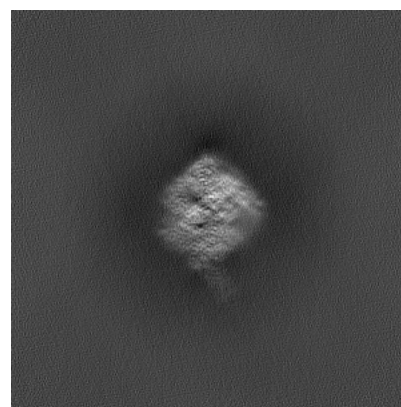
6.1.2 Raw map



X



Y

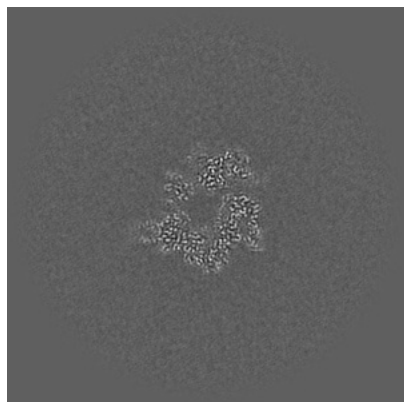


Z

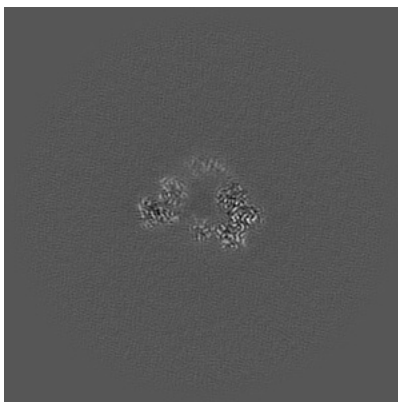
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

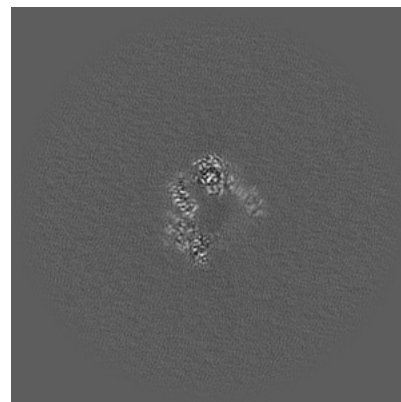
6.2.1 Primary map



X Index: 180

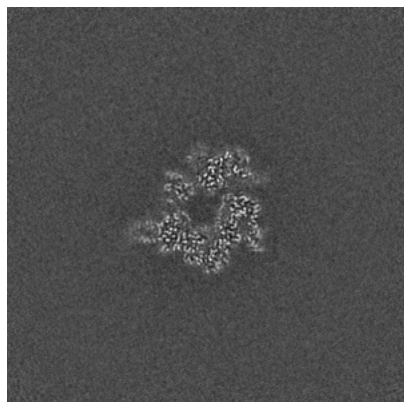


Y Index: 180

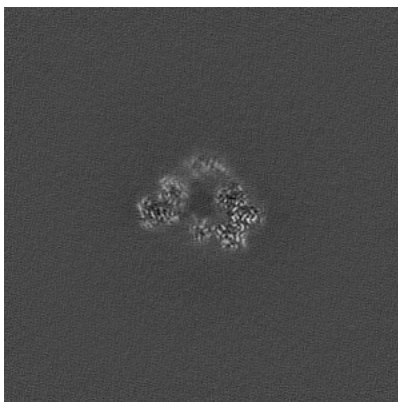


Z Index: 180

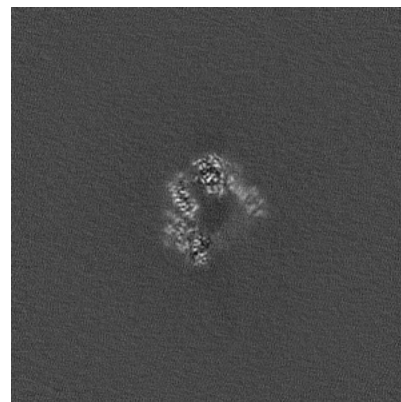
6.2.2 Raw map



X Index: 180



Y Index: 180

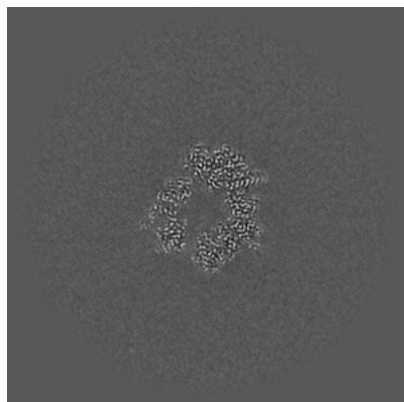


Z Index: 180

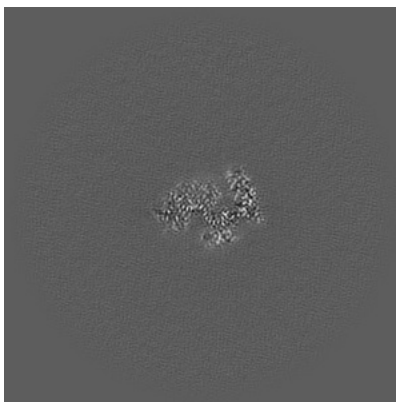
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

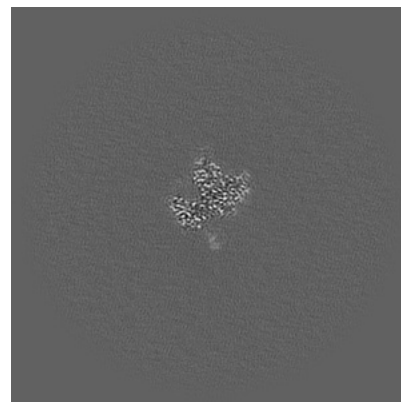
6.3.1 Primary map



X Index: 174

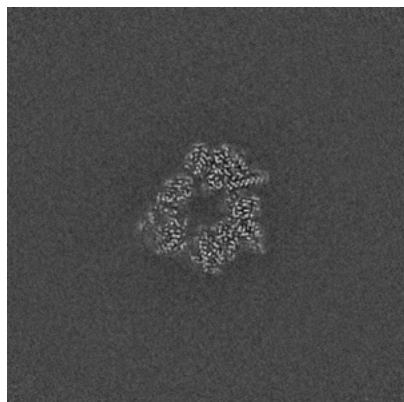


Y Index: 202

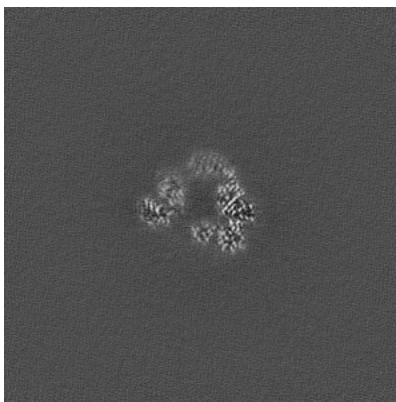


Z Index: 209

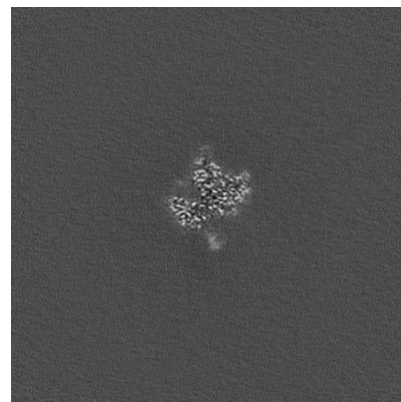
6.3.2 Raw map



X Index: 175



Y Index: 183

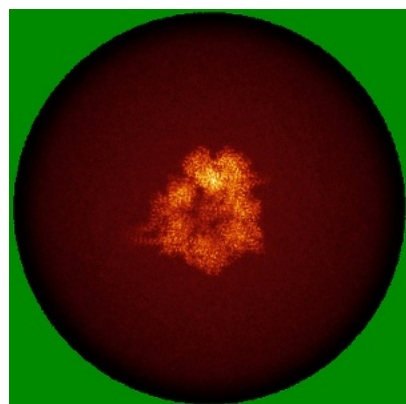


Z Index: 209

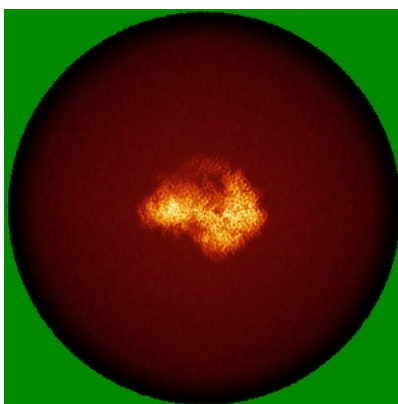
The images above show the largest variance slices of the map in three orthogonal directions.

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

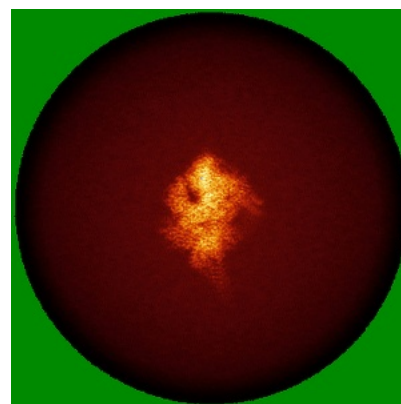
6.4.1 Primary map



X

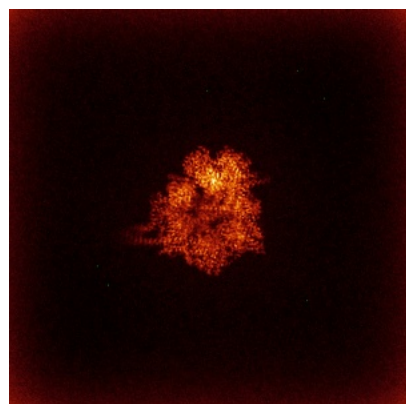


Y

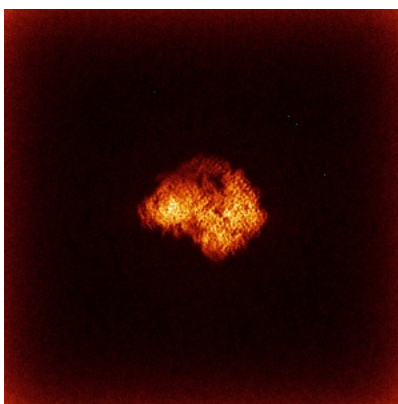


Z

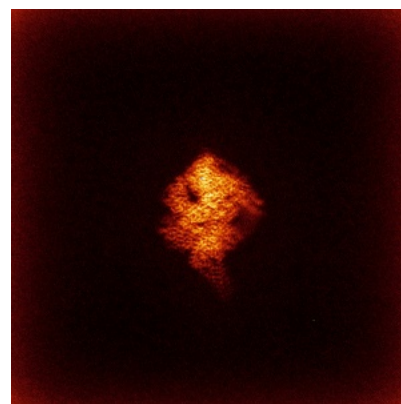
6.4.2 Raw map



X



Y

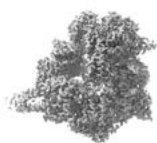


Z

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



X



Y



Z

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



X



Y



Z

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.

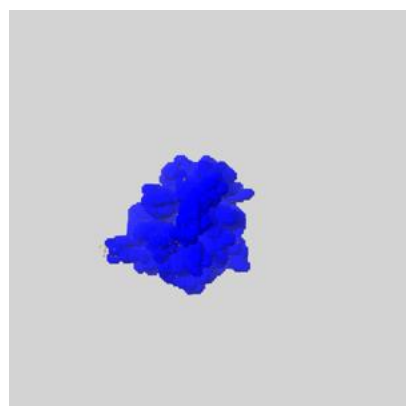
6.6 Mask visualisation [i](#)

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

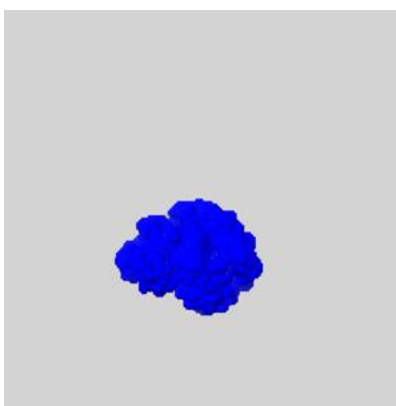
A mask typically either:

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

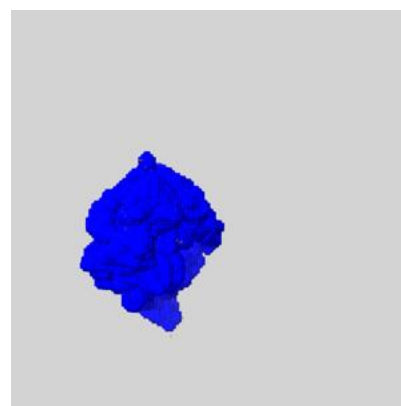
6.6.1 emd_44720_msk_1.map [i](#)



X



Y

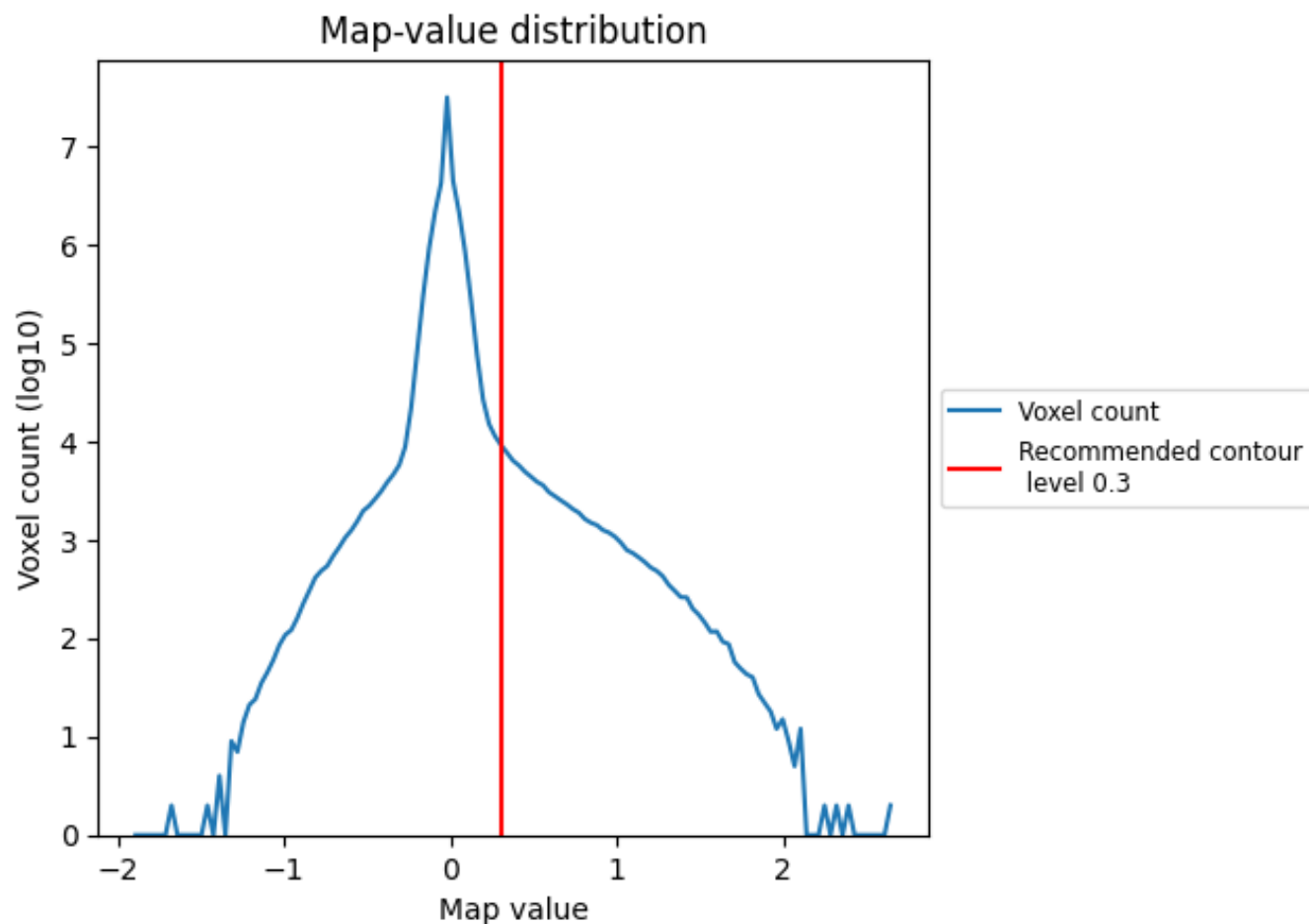


Z

7 Map analysis [i](#)

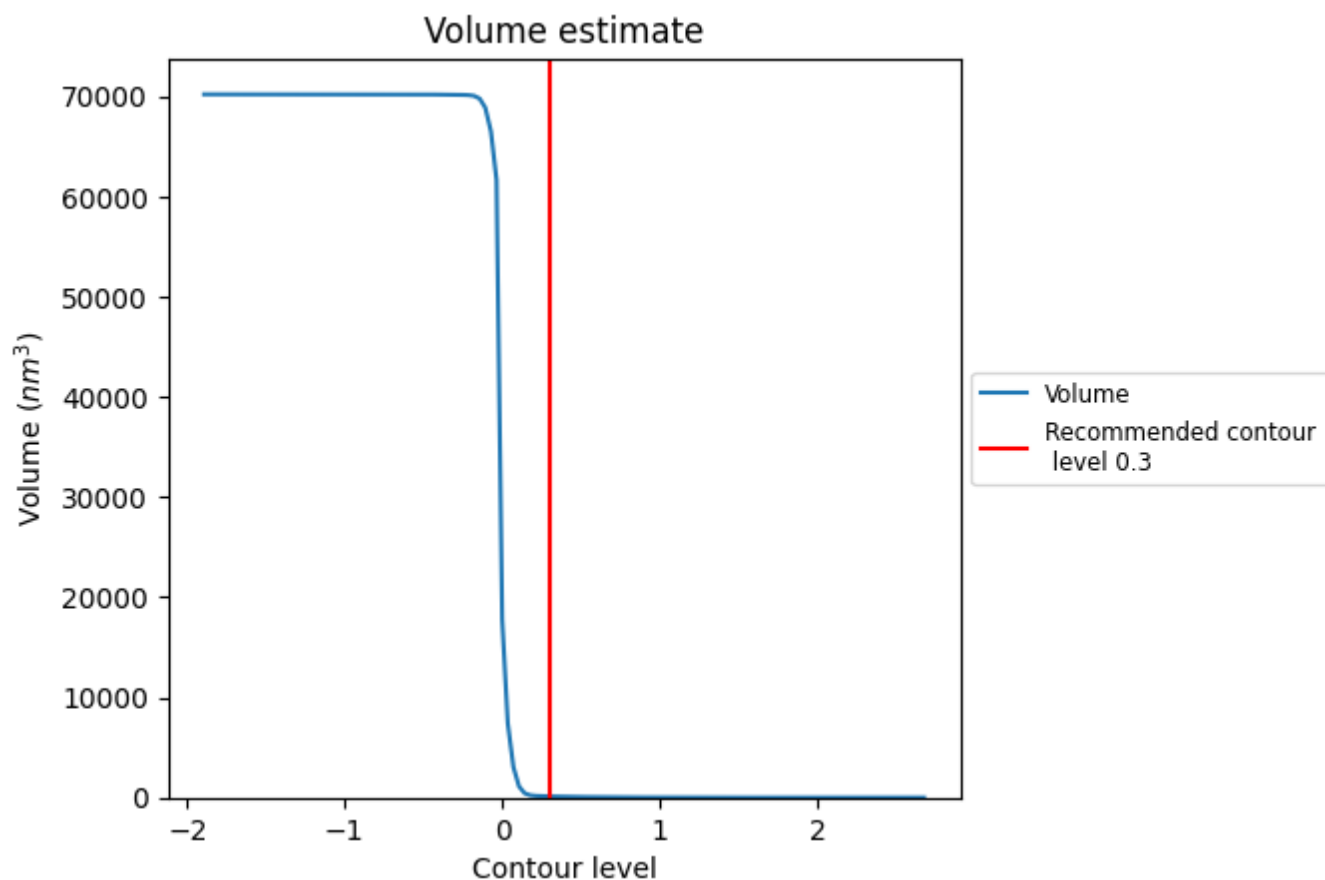
This section contains the results of statistical analysis of the map.

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.

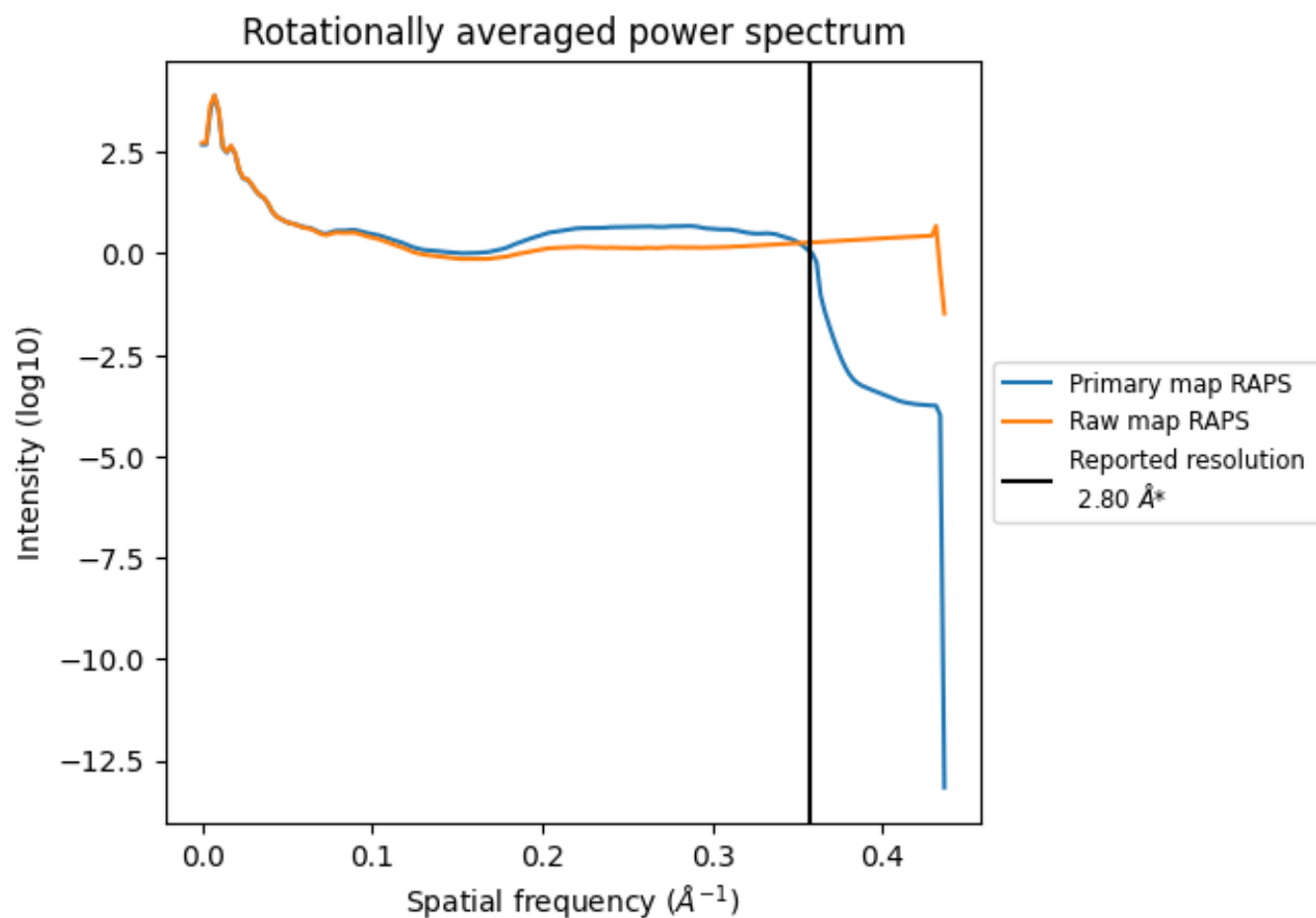
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

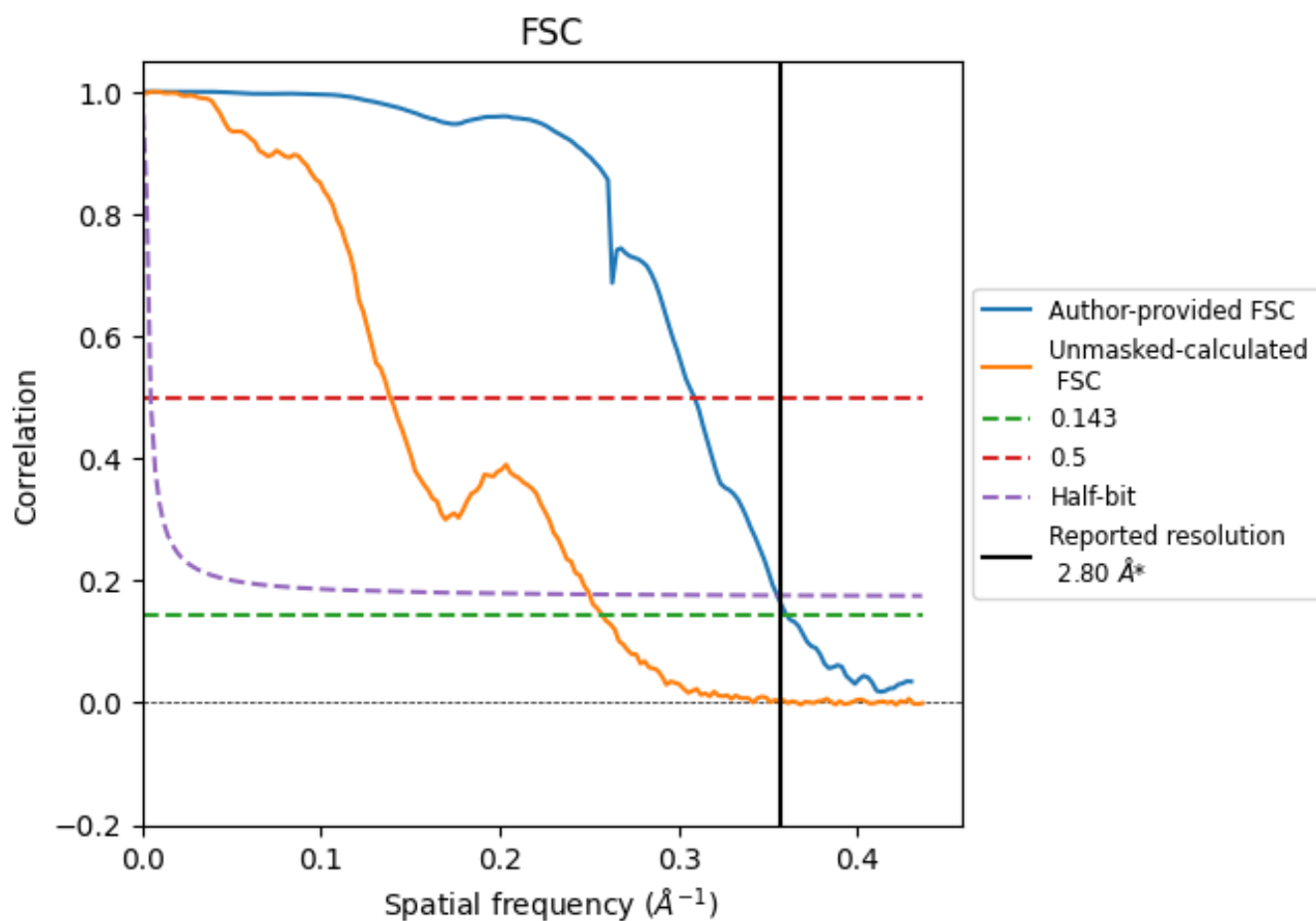


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

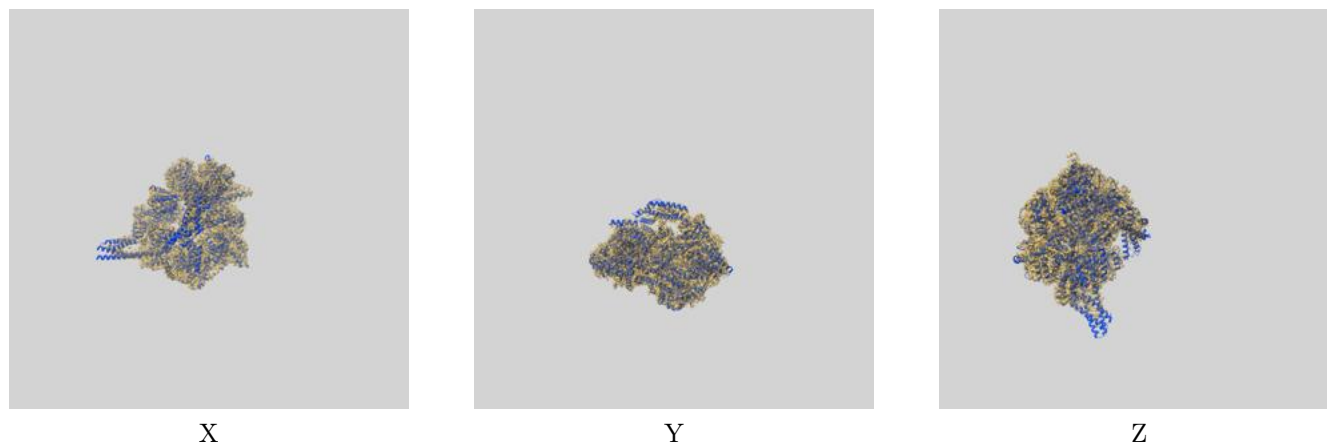
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.24	2.81
Unmasked-calculated*	3.89	7.21	4.00

*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 3.89 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

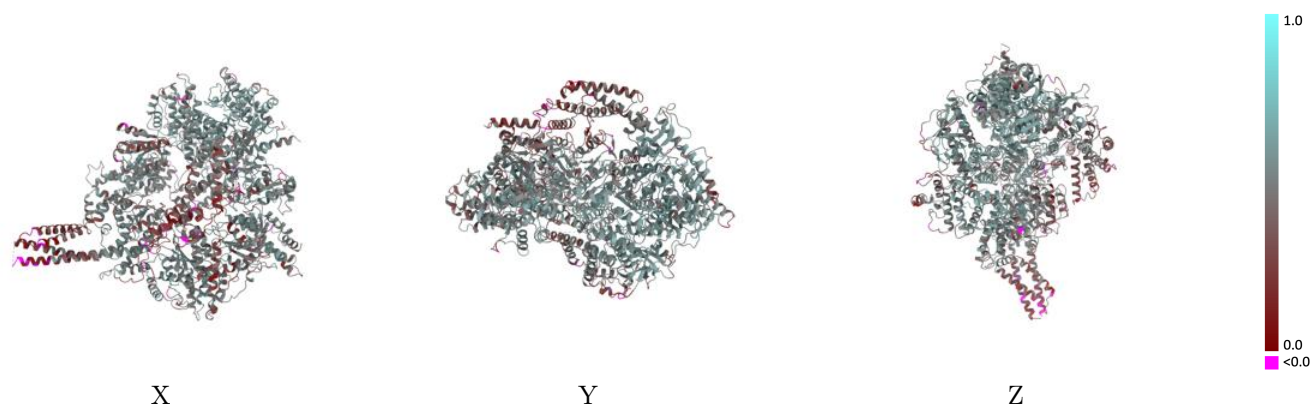
This section contains information regarding the fit between EMDB map EMD-44720 and PDB model 9BN3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



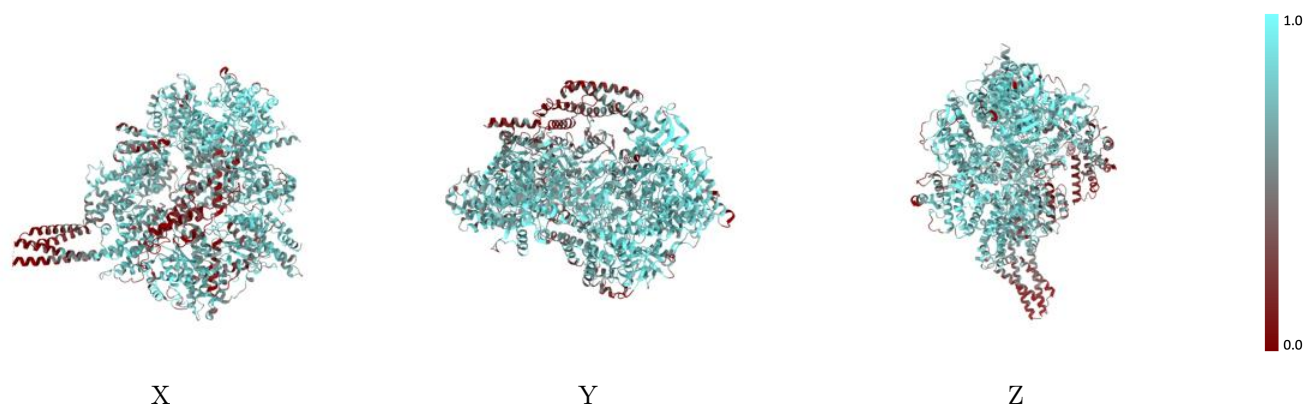
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



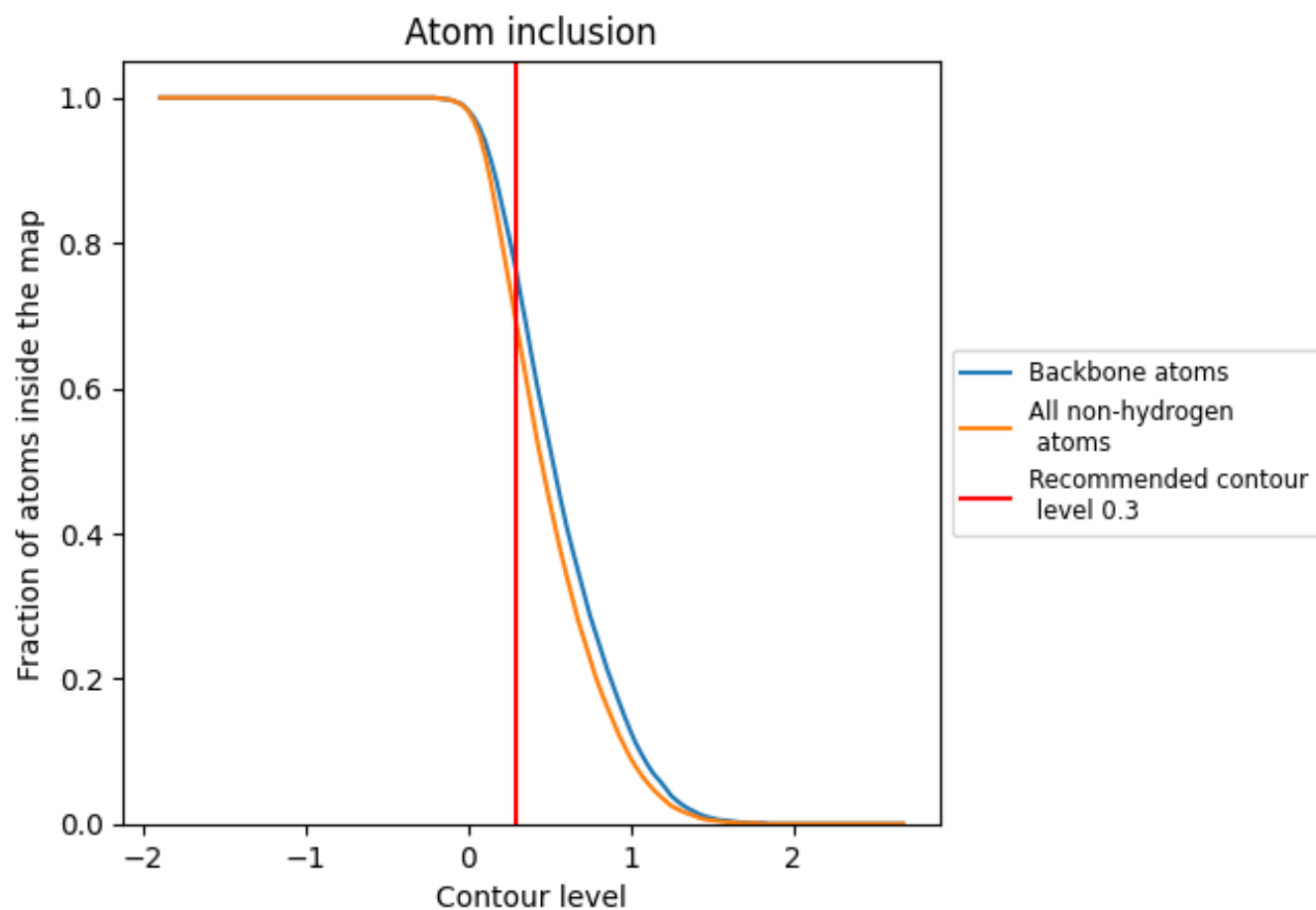
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 69% 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> 0.6880	<div></div> 0.4770
A	<div></div> 0.6880	<div></div> 0.4770

