



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 11:06 AM EDT

PDB ID : 9BN1 / pdb_00009bn1
EMDB ID : EMD-44718
Title : State-8 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.80 Å(reported)

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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

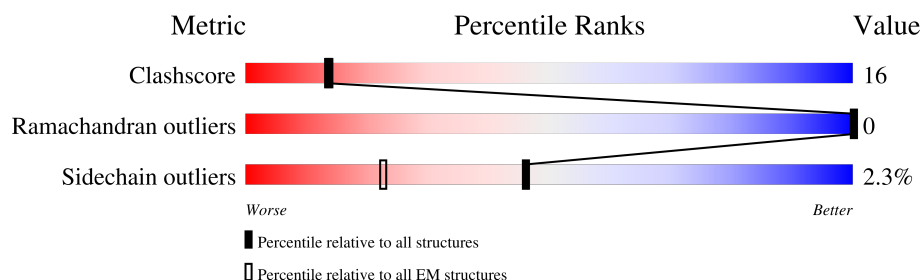
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 4 unique types of molecules in this entry. The entry contains 24476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 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
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

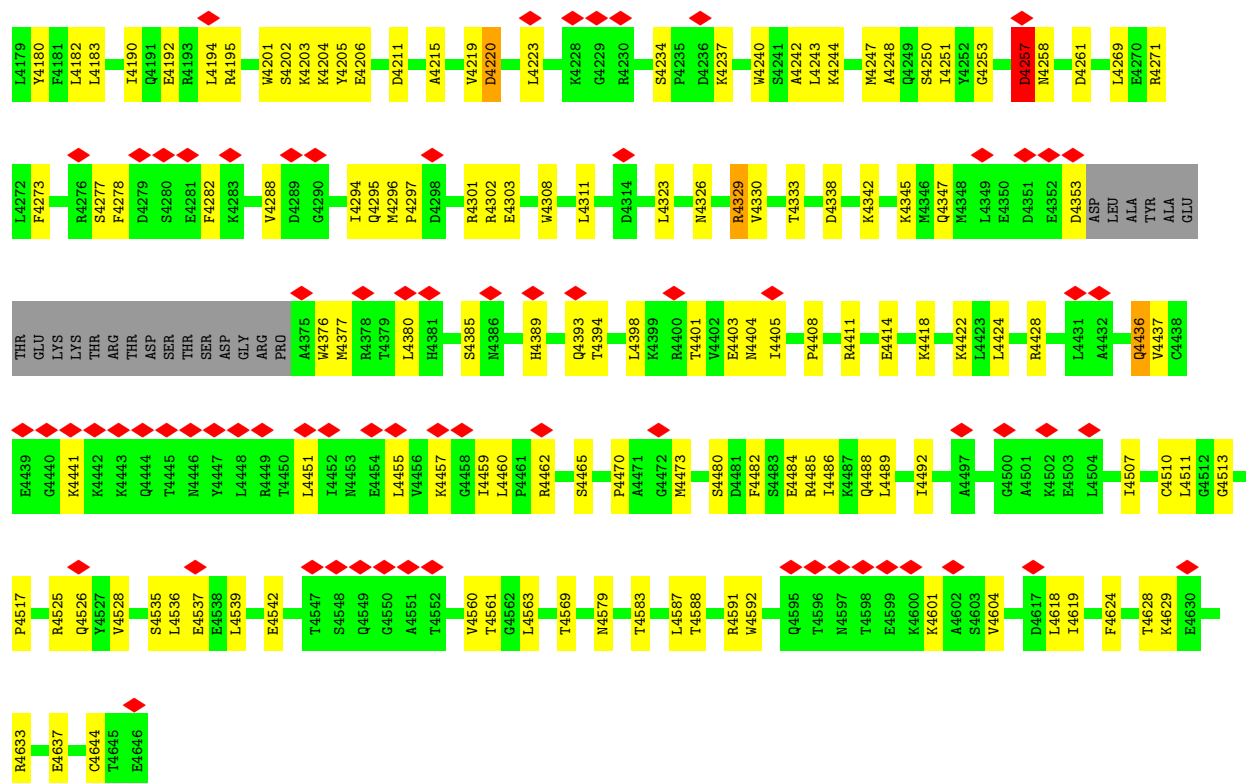
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



E3100	F2992	T2882	M2779	Q2677	P2596	L2508	L2413	S2334	T2287	N2145	V2070	K1992
A3101	D2995	P2883	D2787	R2678	P2597	K2509	Q2414	L2335	L2286	V2146	P2071	T1993
L3102	E2996	L2889	H2791	V2679	G2598	M2510	T2415	P2147	L2269	P2147	F2072	S1994
V3106	S2997	R2890	Y2792	I2683	T2602	R2511	R2416	L2149	P2270	C2076	L2076	A1995
G3106	N2998	D2891	Y2796	R2684	M2603	E2513	D2418	E2152	P2271	D2077	D2077	P1996
K3107	V2999	V2892	S2795	V2687	F2606	L2514	A2419	V2164	T2272	E2078	E2078	I1997
T3110	L3000	T2893	R2797	Y2693	L2609	G2515	T2421	Q2169	R2273	Q2079	Q2079	E2000
S3111	D3001	K2894	E2798	R2694	D2614	I2518	T2422	Y2170	E2274	L2080	L2080	L2001
K3112	F3004	E2902	W2802	Q2698	M2615	L2526	F2427	D2347	D2277	F2088	F2088	L2002
D3113	L3005	E2903	E2816	Q2698	E2616	P2527	K2435	K2349	G2278	G2089	G2089	N2003
L3115	E3006	E2904	V2617	L2703	V2617	T2528	E2438	T2352	L2279	L2090	L2090	Q2004
E3116	T3010	D2905	F2807	E2704	F2622	N2531	H2439	L2353	L2279	R2091	R2091	Q2005
L3011	L3012	D2906	E2808	R2705	S2623	E2536	Q2442	A2354	T2281	A2092	A2092	F2010
P3117	T3011	V2907	R2811	E2706	S2624	Y2537	E2443	E2365	T2281	K2094	K2094	A2013
P3118	L3012	V2910	E2815	Q2707	E2629	D2536	Q2443	R2366	E2294	V2096	V2096	N2019
N3119	V3017	L2916	L2816	C2712	E2630	Y2537	E2444	W2363	L2295	L2097	L2097	P2020
V3120	G3023	L2920	P2817	P2715	L2631	E2538	E2445	F2364	K2297	G2101	G2101	G2021
T3121	D3024	R2927	V2818	T2716	L2632	K2541	H2445	S2365	K2297	K2104	K2104	T19
V3122	C3033	C2937	E2819	T2717	K2633	W2545	L2449	E2366	L2298	R2107	R2107	ALA
K3125	K3034	L2934	Q2820	D2717	T2634	W2548	T2450	L2374	L2299	L2108	L2108	GLY
K3126	E3040	T2936	L2821	R2726	F2635	W2568	R2451	P2375	Q2299	Q2109	Q2109	ARG
P3127	G3041	G2937	E2825	R2726	D2636	K2561	L2452	R2376	K2206	K2110	K2110	W2027
V3128	L3042	G2940	W2829	V2731	R2642	Q2564	R2453	R2377	V2207	L2028	L2028	L2028
V3129	M3043	C2941	A2829	P2732	K2643	Q2564	L2455	L2379	W2300	Q2029	Q2029	D2030
D3130	M3044	C2942	E2837	T2733	T2644	E2568	L2458	L2382	L2210	R2113	R2113	D2031
L3133	L3044	K2943	E2838	V2738	E2647	T2569	F2459	R2383	T2214	E2116	E2116	L2032
F3134	D3045	L2946	E2839	Y2738	L2650	H2560	L2462	S2384	H2218	R2117	R2117	K2033
Q3135	E3048	S2947	E2841	T2744	A2651	K2561	H2463	L2385	G2219	G2119	G2119	F2036
R3139	W3053	R2948	W2845	T2745	P2852	V2568	Q2464	P2386	D2306	E2120	E2120	R2037
R3140	F3054	M2953	W2849	Q2746	V2853	V2569	A2465	E2389	D2307	G2125	G2125	S2038
A3142	Q3057	Q2958	N2849	I2747	L2655	P2570	C2466	GLY	D2308	A2121	A2121	L2039
L3143	V2958	V2958	E2853	T2750	Q2656	L2571	Y2472	ASP	V2222	V2122	V2122	K2043
V3144	V2958	V2958	V2853	F2751	K2657	L2572	W2475	GLU	G2224	D2123	D2123	F2044
S3145	V3065	L2961	A2854	Q2752	W2658	D2573	Q2482	ALA	G2229	E2124	E2124	D2045
S3146	F3066	K2962	L2855	N2752	L2659	T2574	L2483	GLN	K2230	G2126	G2126	R2046
C3147	V2963	V2963	K2856	M2755	V2660	V2575	Q2482	ARG	S2231	I2127	I2127	Q2047
V3148	H2964	H2964	H2857	L2756	L2661	R2576	L2483	ARG	W2232	A2128	A2128	L2048
F3149	R2965	R2965	E2863	R2757	F2662	E2578	T2498	ARG	A2233	N2129	N2129	I2049
V3150	E3073	Q2969	E2864	P2760	D2664	A2579	Y2493	LYS	R2234	N2130	N2130	Q2051
V3151	G3074	E2970	E2864	R2763	L2666	L2580	L2494	GLY	R2235	L2131	L2131	V2052
Q3152	D3077	V2979	R2869	A2766	N2667	L2581	V2495	ASP	L2237	F2132	F2132	W2053
N3158	R3078	V2979	E2873	Q2766	L2668	T2583	W2500	GLY	L2244	E2133	E2133	L2054
G3166	T3081	S2983	Y2873	T2770	D2672	W2584	S2503	GLY	L2244	Q2136	Q2136	V2055
R3167	C2984	C2984	S2874	T2770	K2673	W2584	D2504	GLY	G2249	E2136	E2136	S2056
T3168	F3086	N2986	K2879	E2775	V2674	L2585	Q2504	GLU	I2137	I2137	I2137	Q2057
K3169	F3094	N2987	D2880	E2775	G2675	P2590	D2505	GLU	K2257	E2143	E2143	R2060
T3172	F3096	N2987	Y2881	E2775	T2676	L2591	D2505	A2408		T2144	T2144	L2065
P3173	D3096	W3097										L2069
R3174	W3097											

P4103	H4029	D3946	R3870	I3789	S3729	V3644	L3567	R3488	GLN
C4104	I4030	L3947	R3870	V3790	D3730	L3645	P3568	W3489	LYS
W4105	E4034	I3948	R3873	M3791	L3731	P3646	A3569	E3490	ALA
M4107	E3950	G3874	G3874	K3792	L3732	P3647	D3570	K3491	ASN
Q4108	N4038	V3951	M3875	E3793	K3733	L3648	P3571	T3492	LYS
L4109		Q3952		V3794	L3734	L3649	L3572	S3493	VAL
E4110	L4042	D3953	D3879	E3795	K3735	N3650	C3573	S3494	GLN
K4111	M4043	D3954	H3880	T3796	Q3736	E3652	A3577	E3494	MET
K4112		E3955	I3881	V3797	L3737	V3653	L3578	F3496	ILE
L4113		Q3956	T3882	Q3800	E3737	R3654	M3579	T3497	ARG
L4116	A4051	F3957	L3886	Q3801	F3738	R3655	L3580	T3498	GLY
Q4117	G4053	G3958	L3887	Y3801	Q3739	T3656	K3581	N3498	ILE
P4118	G4053	L3959	L3887	L3804	L3740	G3657	R3582	Q3499	GLU
H4119	H4054	L3959	A3883		L3741	G3658	P3583		ALA
A4120	D4057	E3967	R3889	A3807	R3742	R3659	R3584	I3503	ILE
C4121	L4058	V3970	K3891	S3810	L3743	V3660	R3585	A3504	ARG
R4122	A4059	P3971	L3890	I3811	Q3744	L3661	Y3586	G3505	ALA
R4123	A4060	L3972	L3892	F3812	L3745	I3662	P3587	L3509	LYS
L4124	E4061	L3973	L3892	F3813	E3746	L3663	L3588	S3510	GLY
T4127	Q4062	W3974	T3900	T3814	K3747	L3664	D3591	A3511	GLU
M4128	S3975	S3975	Y3901	M3815	S3748	G3665	P3592	I3514	TYR
E4129	N4063	E3976	A3902	K3819	L3749	Q3667	G3594	A3517	PRO
		E3977	A3903		L3750	D3668	M3601	F3520	THR
K4133	I4066	A3980	Q3906	Y3825	Q3751	L3671	Y3604	D3521	VAL
V4134	T4067	A3980	H3907	Q3826	A3752		K3605	G3518	LEU
L4138	S4068	T3983	R3910	S3827	L3753	I3677	D3606	Y3519	TRP
L4139	I4071	G3984	G3811	L3828	K3754	F3676	R3607	I3521	ILE
R4140	S4073	Q3985	N3912	L3829	E3755	L3679	K3608	G3520	GLN
A4141	A4074	I3987	E3913	F3831	V3756	D3683	I3609	A3524	ALA
C4142	A4075	H3988	I3914	I3835	K3757	P3684	T3612	W3632	LYS
R4143	G4076	L3990	V3915	H3836	G3758	V3685	L3536	L3537	ASP
T4144	F4077	L3991	H3837	H3837	R3759	V3686	Q3537	Q3537	ARG
F4145	Q4078	L3992	N3838	N3838	I3760	E3687	I3541	LEU	ASN
E4148	Q4079	D3999	V3839	V3839	L3761		A3540	ASN	GLY
V4153	A4080		A3918	E3842	D3762	D3691	Q3542	ARG	ILE
N4156	D4081	A4003	G3919		D3763	L3692	R3543	THR	VAL
F4161	A4083	M4004	S3920	N3845	D3764	C3693	F3544	GLU	PRO
I4164	I4084	A4005	T3921	L3846	T3765	R3695	I3547	LEU	ILE
P4165	T4086	H4006	P3922	K3847	L3766	V3696	A3548	VAL	ALA
V4166	A4088	L4013	I3924	G3848	L3767	V3699	R3549	ALA	VAL
	K4089	G4014	Q3925		T3768		T3550	LEU	LYS
L4169	S4090	E4015	G3926	D3851	T3769	V3703	E3551	GLU	SER
G4091	G4091	S4016	L3927	H3852	L3770	T3704	Y3552	ILE	ILE
K4170	R4092	F4017	E3930	Q3854	E3771	R3705	L3553	LYS	LYS
S4172	W4093	M4021	E3933	T3856	N3772	V3716	A3477	ASP	ALA
P4173	V4094	E4022	E3933	L3856	L3773		L3478	ASP	ALA
M4174	M4095	Q4023	V3936	I3859	K3774	R3721	L3479	ASP	ALA
E4175	L4096	P4024	R3937	T3860	R3775	V3724	K3480	GLN	GLN
R4176	K4097	L4025	L3938	K3861	E3776	D3725	S3481	ASN	ASN
A4177	N4098	D4026	S3939	D3862	A3777	E3726	L3482	LEU	LYS
R4178	H4099	L4027	C3940	V3866	A3777	R3727	S3483	VAL	VAL
	H4100	T4028	F3944		A3778	K3728	A3485	LYS	LYS
L4101	L4101		K3945		E3779		R3486	VAL	VAL
A4102	A4102				V3780		E3487	ASP	GLN
					T3781				
					K3782				
					K3783				
					V3784				
					E3785				
					E3786				
					T3787				
					D3788				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50945	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	0.817	Depositor
Minimum map value	-0.311	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	0.27	0/24908	0.53	4/33751 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2002	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	4257	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	1429	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	3479	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1603	ARG	Sidechain

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	24390	0	24462	767	0
2	A	31	0	12	2	0
3	A	54	0	24	5	0
4	A	1	0	0	0	0
All	All	24476	0	24498	767	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 16.

The worst 5 of 767 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:2667:ASN:HD22	1:A:2712:CYS:HB2	1.35	0.91
1:A:1550:ILE:HG23	1:A:1638:LEU:HD21	1.51	0.90
1:A:3206:ARG:HH12	1:A:3209:LYS:HD3	1.35	0.89
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.42	0.83
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	1.63	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	3019/4646 (65%)	2946 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2696/4125 (65%)	2634 (98%)	62 (2%)	45 63

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3125	TYR
1	A	4329	ARG
1	A	3606	ASP
1	A	4311	LEU
1	A	4465	SER

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	2707	GLN
1	A	2752	ASN
1	A	4404	ASN
1	A	2857	HIS
1	A	2299	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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	ADP	A	4702	-	24,29,29	0.86	0	29,45,45	1.27	2 (6%)
2	ATP	A	4701	4	28,33,33	0.88	1 (3%)	34,52,52	0.65	1 (2%)
3	ADP	A	4703	-	24,29,29	0.85	0	29,45,45	1.19	2 (6%)

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	ADP	A	4702	-	-	0/12/32/32	0/3/3/3
2	ATP	A	4701	4	-	4/18/38/38	0/3/3/3
3	ADP	A	4703	-	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ATP	PA-O3A	-2.70	1.56	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	N3-C2-N1	-3.75	123.58	128.67
3	A	4703	ADP	N3-C2-N1	-3.64	123.73	128.67
3	A	4703	ADP	C4-C5-N7	-2.56	106.63	109.34
3	A	4702	ADP	C4-C5-N7	-2.32	106.88	109.34
2	A	4701	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

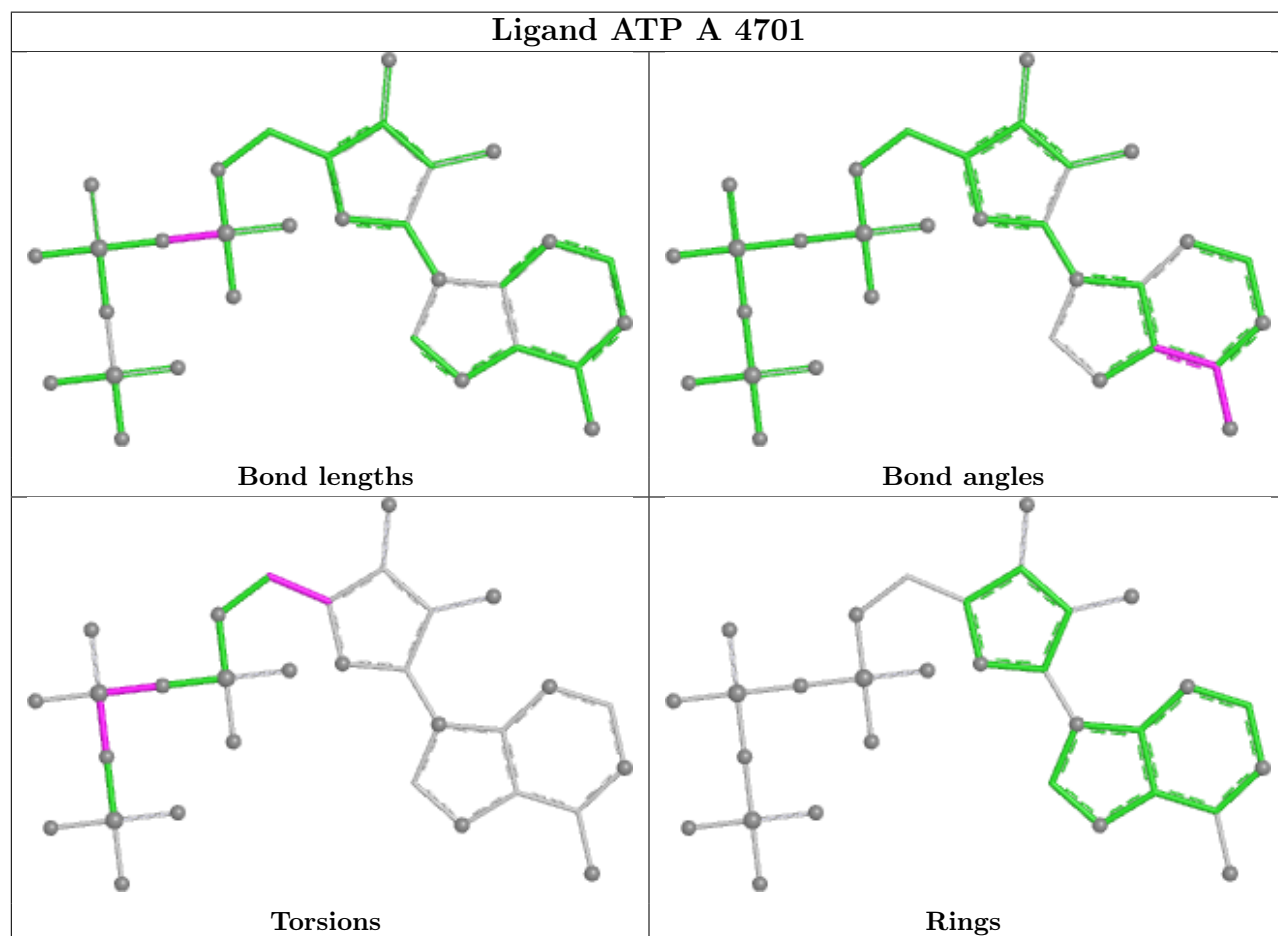
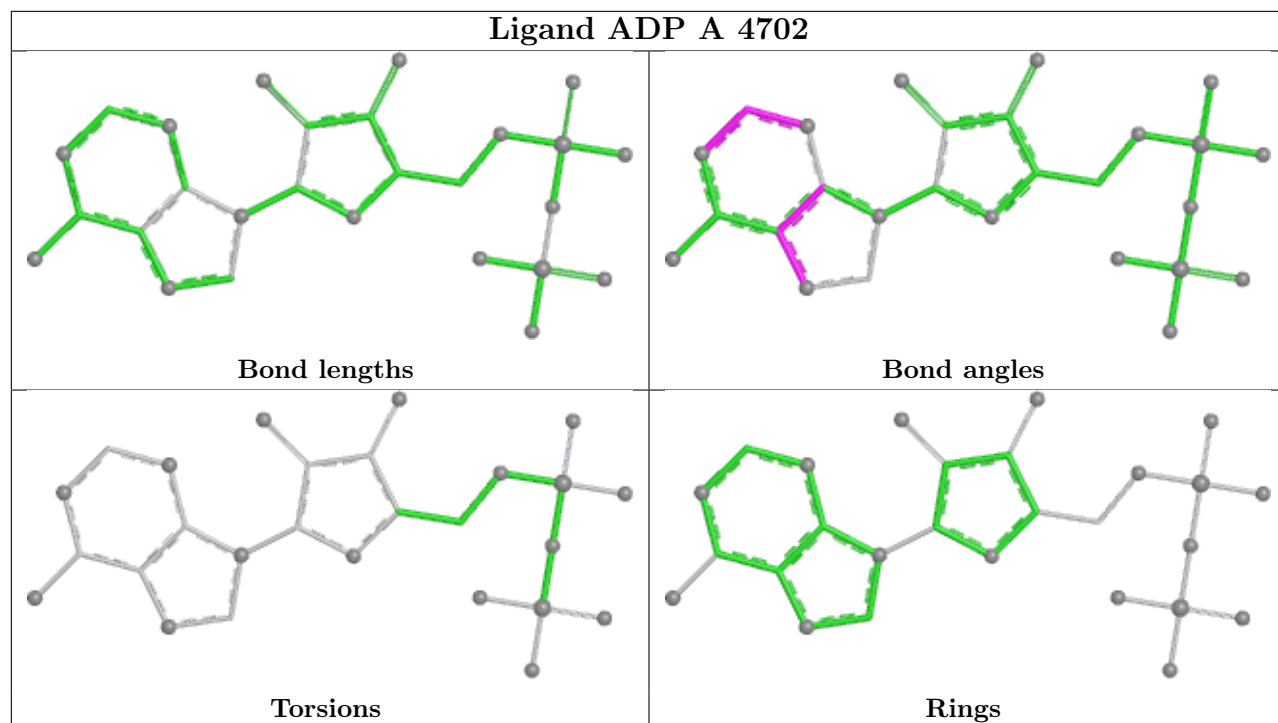
Mol	Chain	Res	Type	Atoms
2	A	4701	ATP	O4'-C4'-C5'-O5'
2	A	4701	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4701	ATP	PG-O3B-PB-O2B
2	A	4701	ATP	PA-O3A-PB-O1B

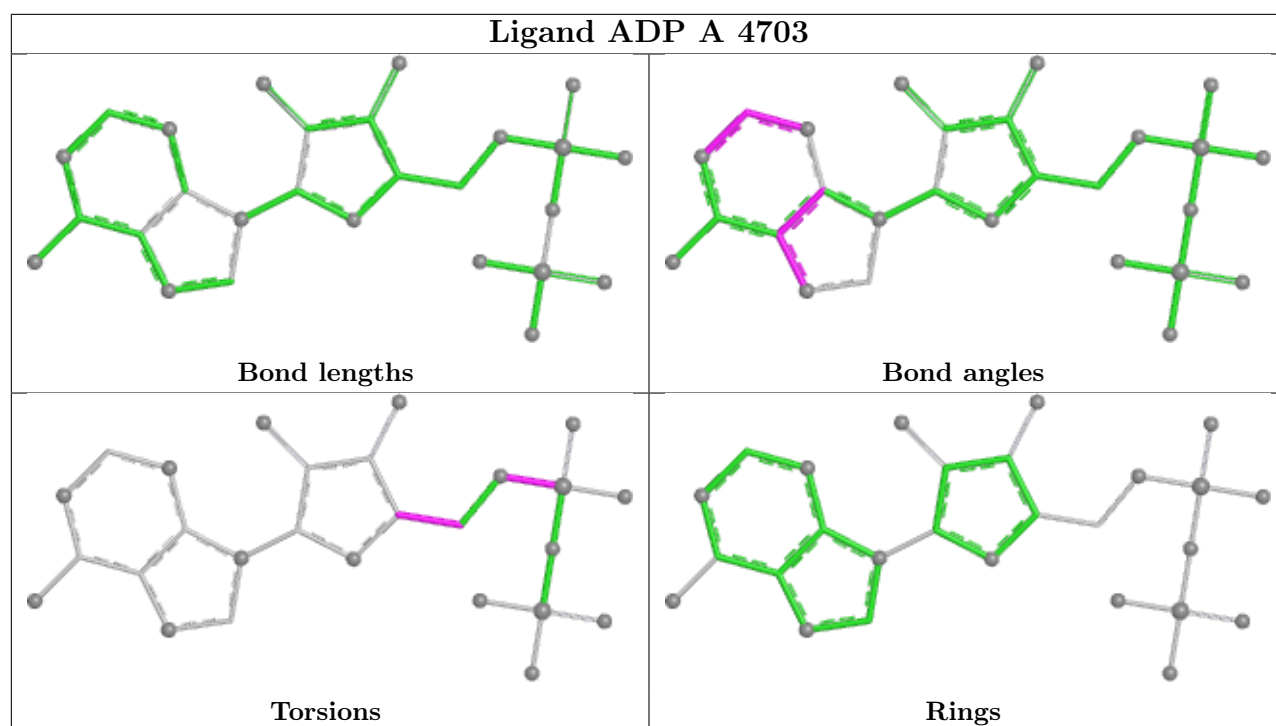
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ADP	3	0
2	A	4701	ATP	2	0
3	A	4703	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.

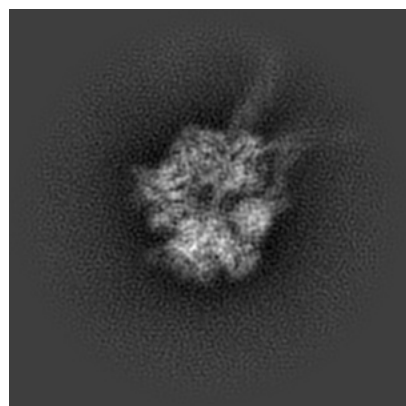
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44718. These allow visual inspection of the internal detail of the map and identification of artifacts.

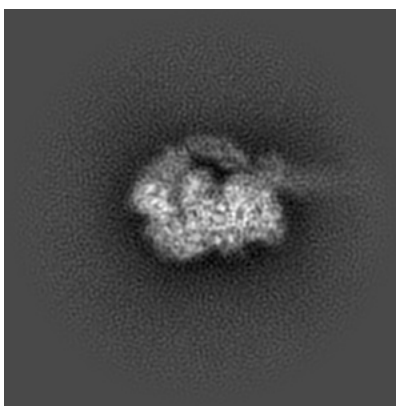
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

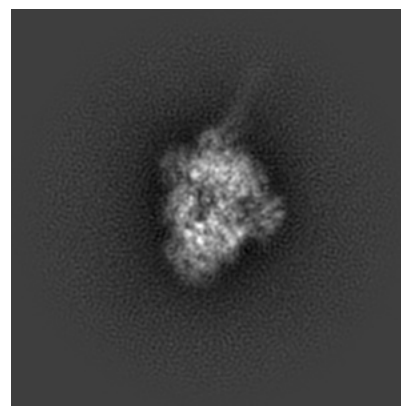
6.1.1 Primary map



X

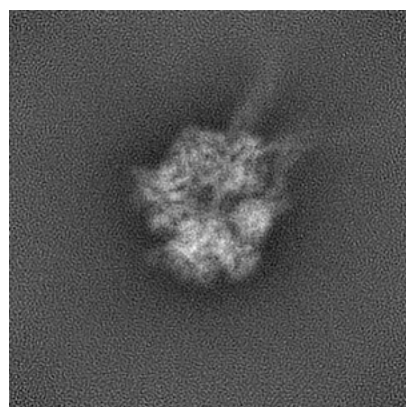


Y

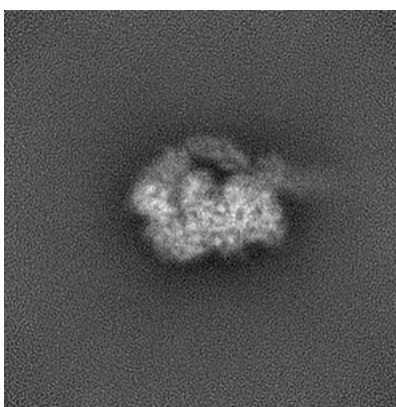


Z

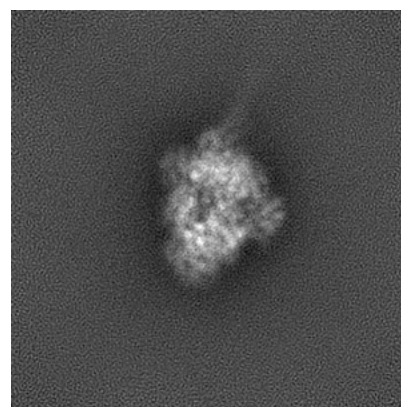
6.1.2 Raw map



X



Y

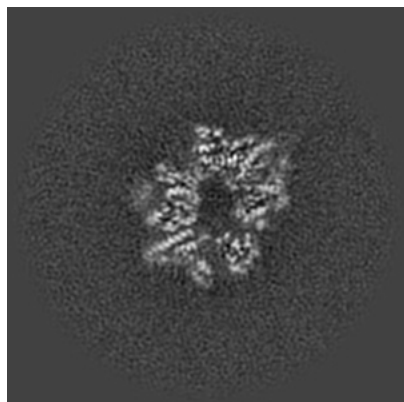


Z

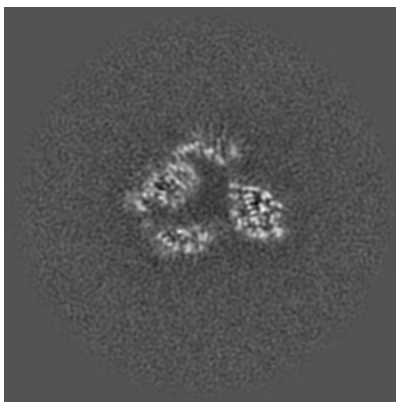
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

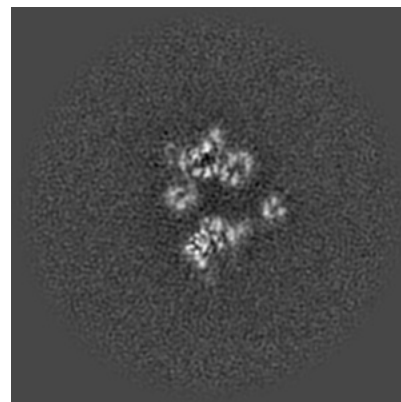
6.2.1 Primary map



X Index: 128

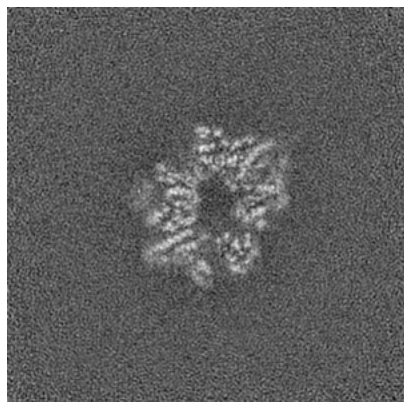


Y Index: 128

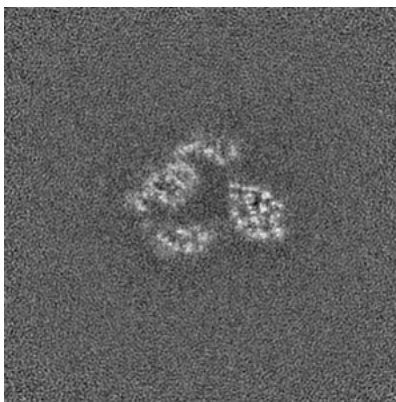


Z Index: 128

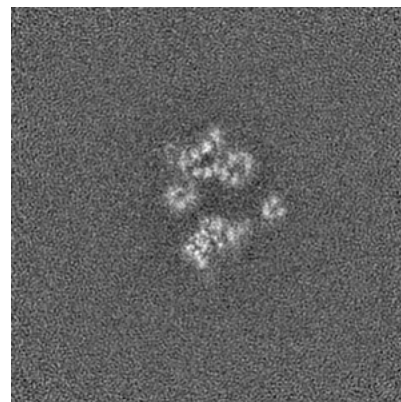
6.2.2 Raw map



X Index: 128



Y Index: 128

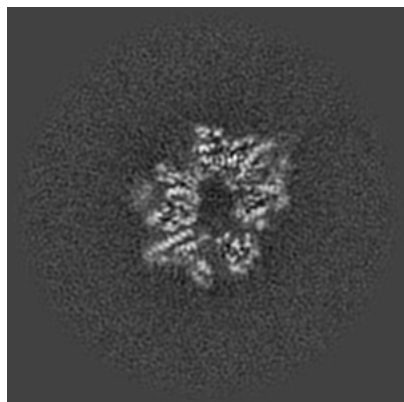


Z Index: 128

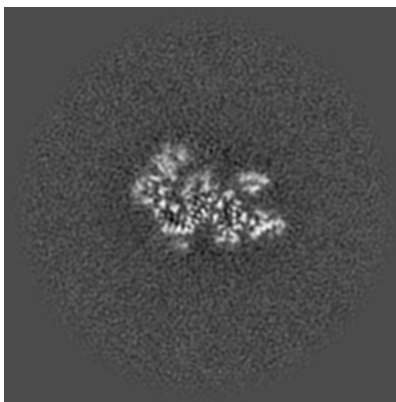
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

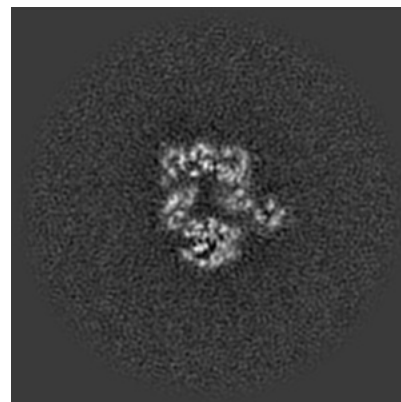
6.3.1 Primary map



X Index: 128

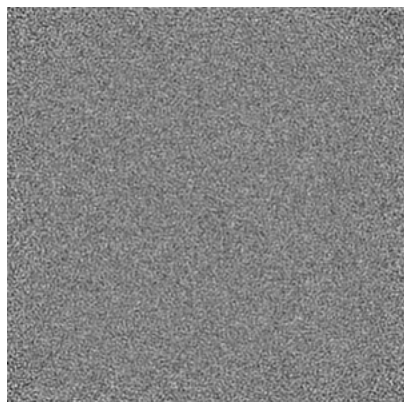


Y Index: 111

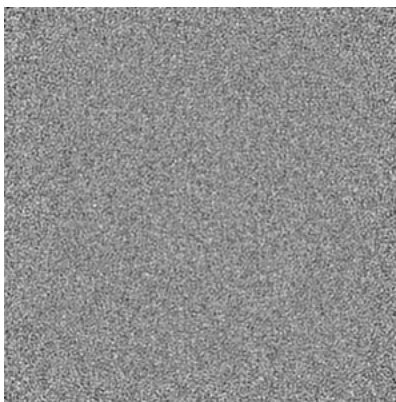


Z Index: 119

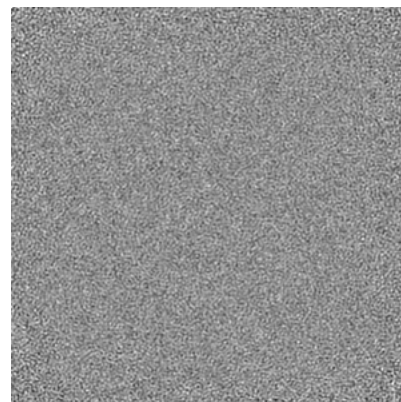
6.3.2 Raw map



X Index: 0



Y Index: 0

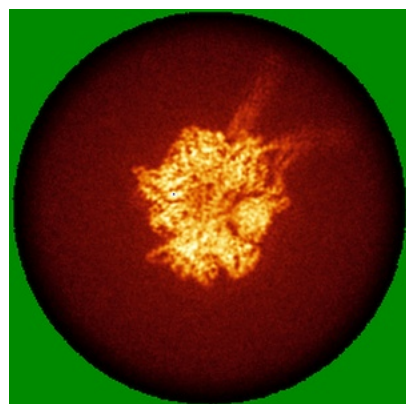


Z Index: 0

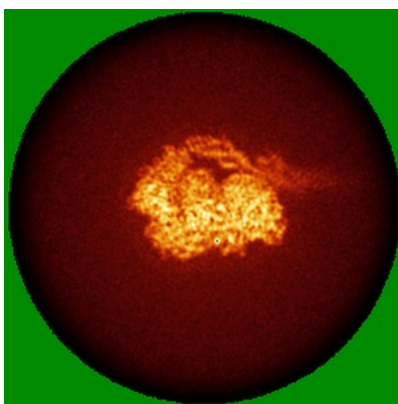
The images above show the largest variance slices of the map in three orthogonal directions.

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

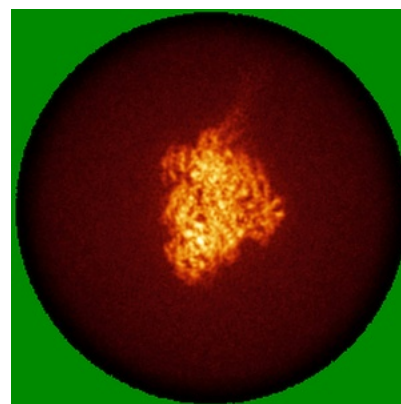
6.4.1 Primary map



X

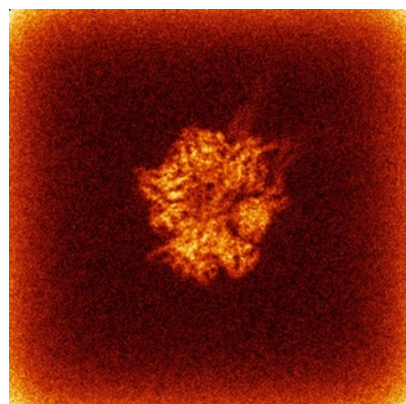


Y

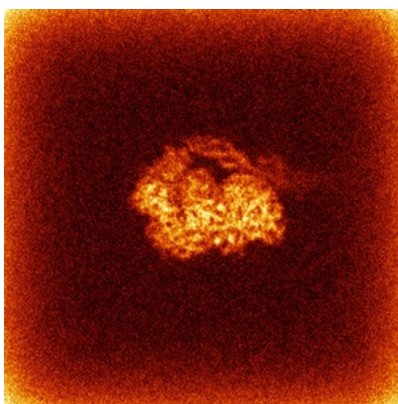


Z

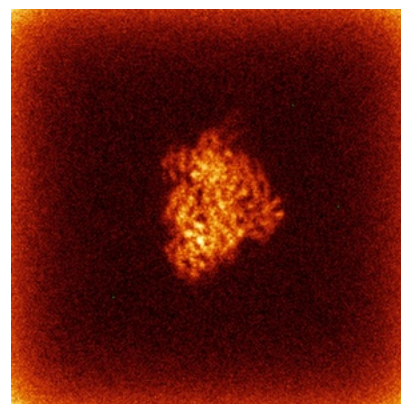
6.4.2 Raw map



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.

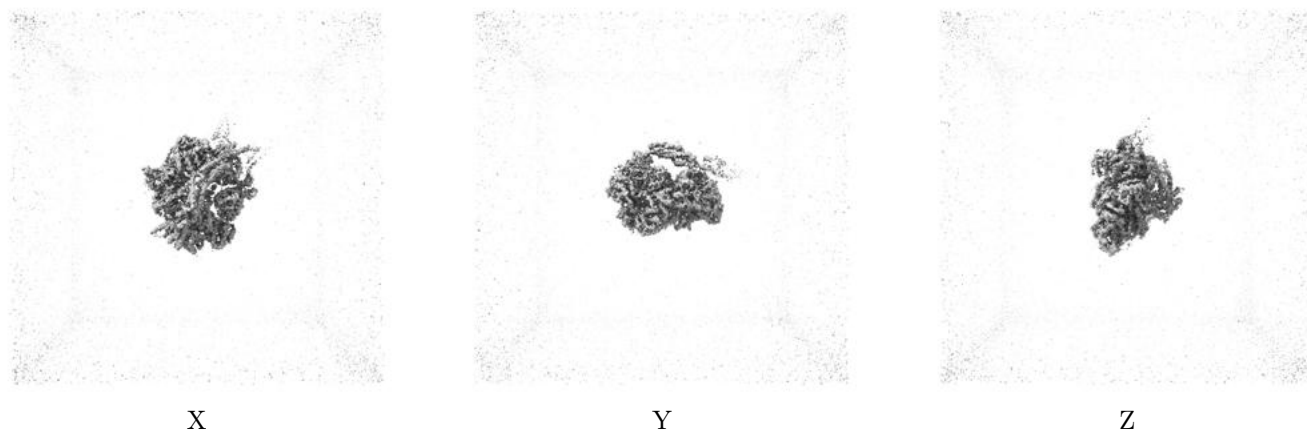
6.5 Orthogonal surface views [i](#)

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.

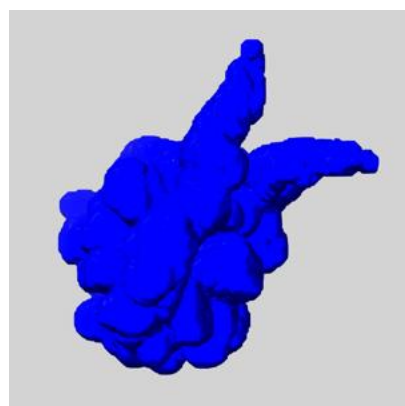
6.6 Mask visualisation [i](#)

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

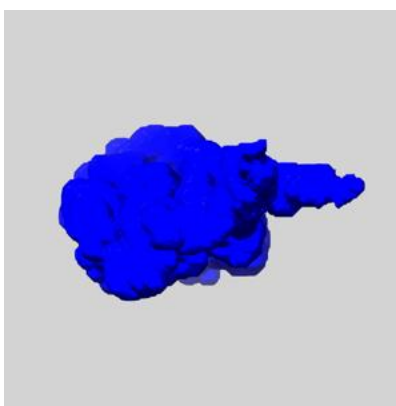
A mask typically either:

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

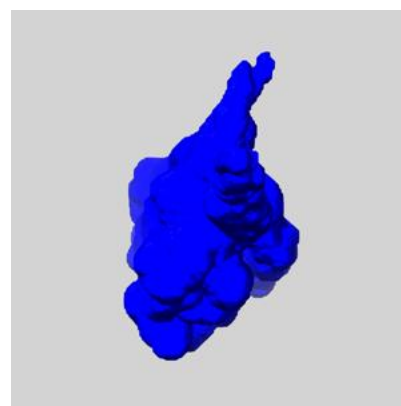
6.6.1 emd_44718_msk_1.map [i](#)



X



Y

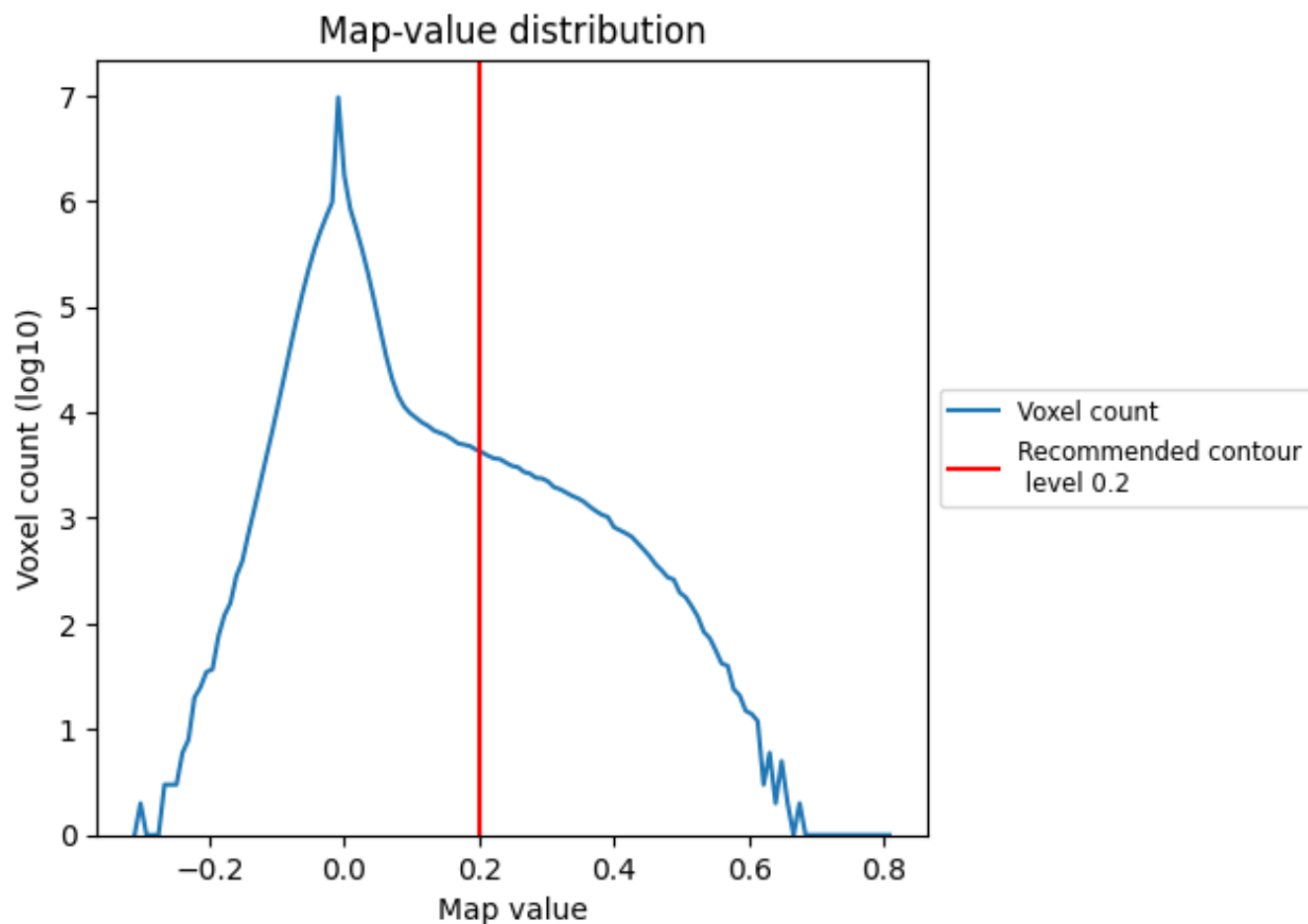


Z

7 Map analysis [i](#)

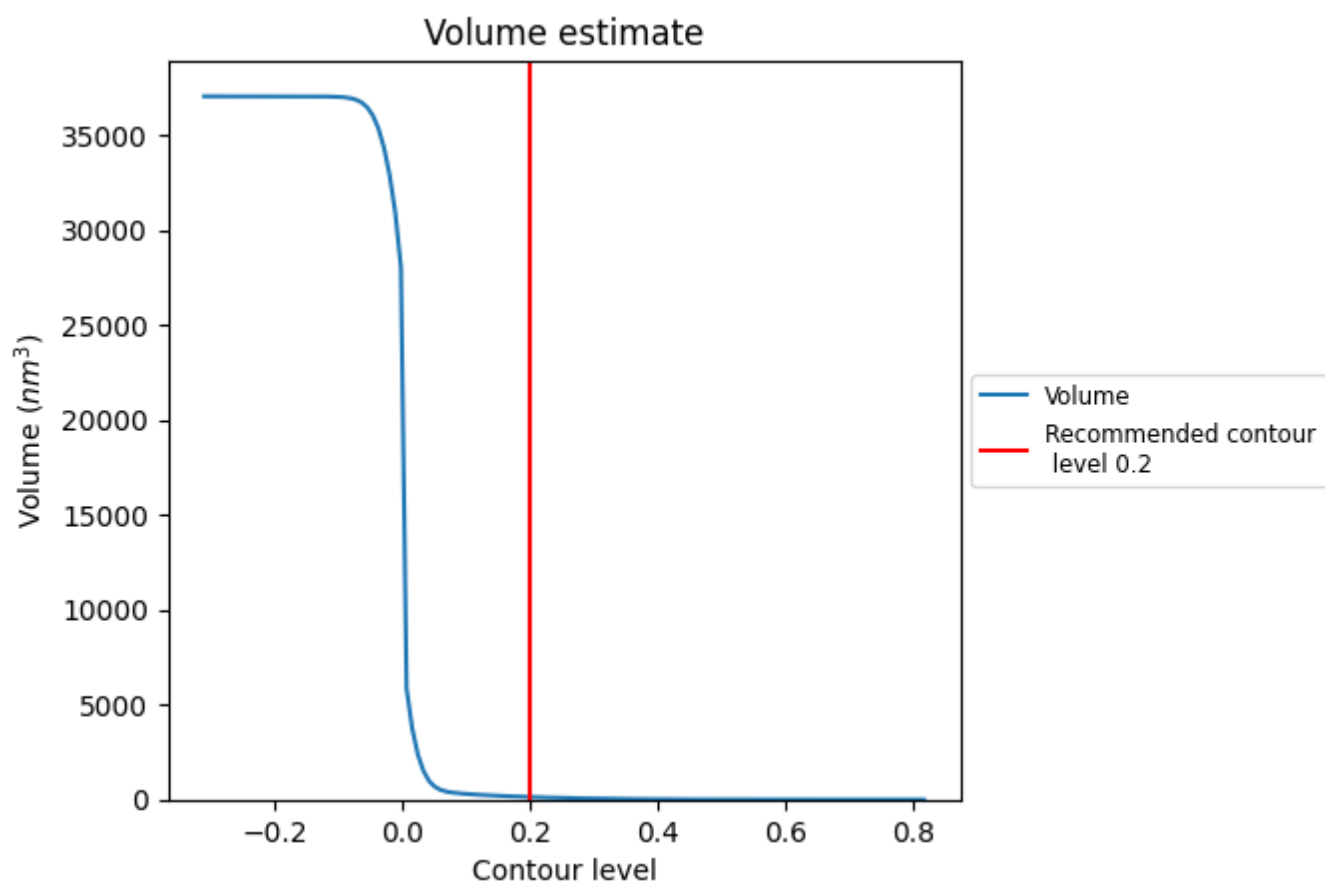
This section contains the results of statistical analysis of the map.

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.

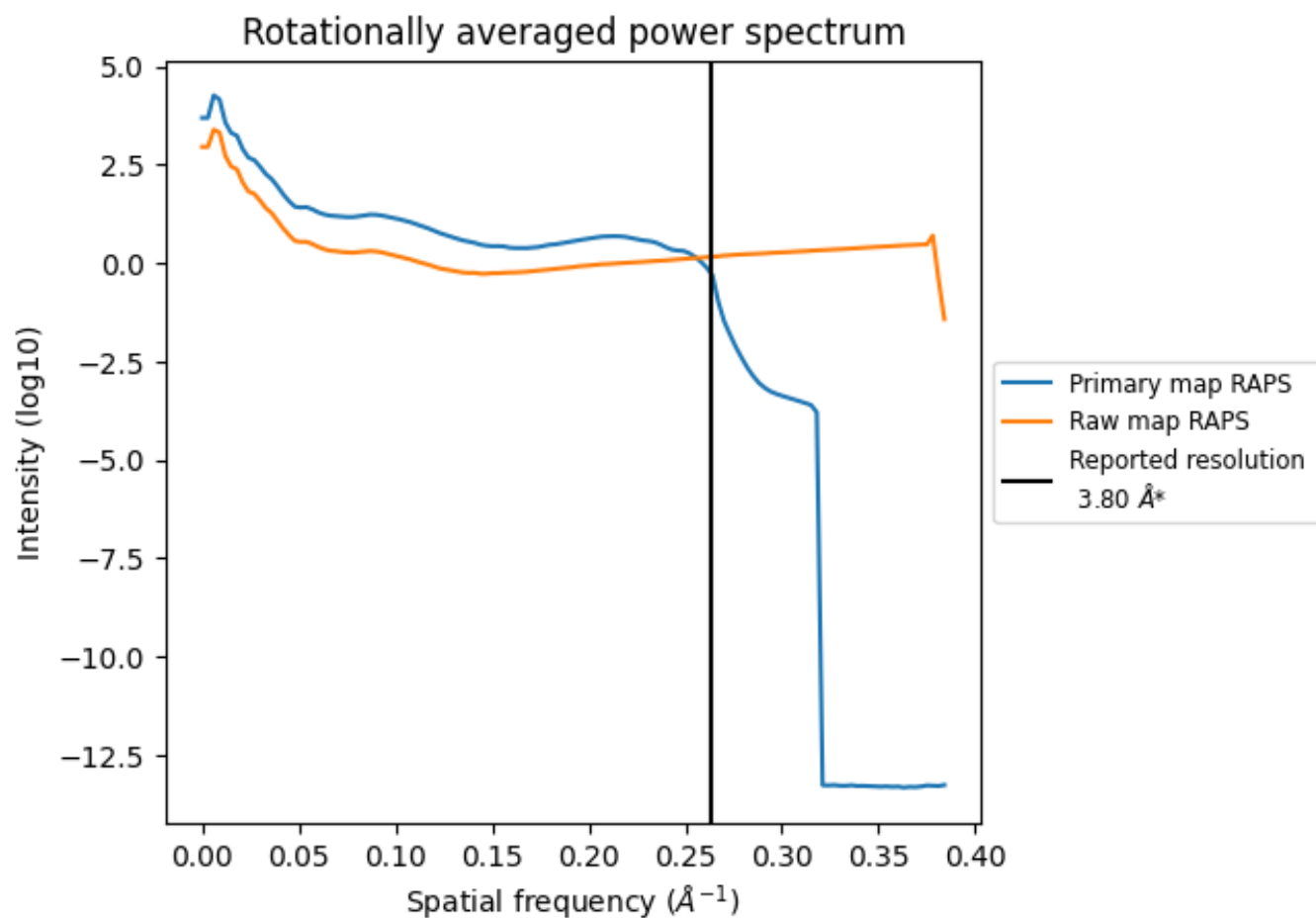
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm^3 ; this corresponds to an approximate mass of 121 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 ⓘ

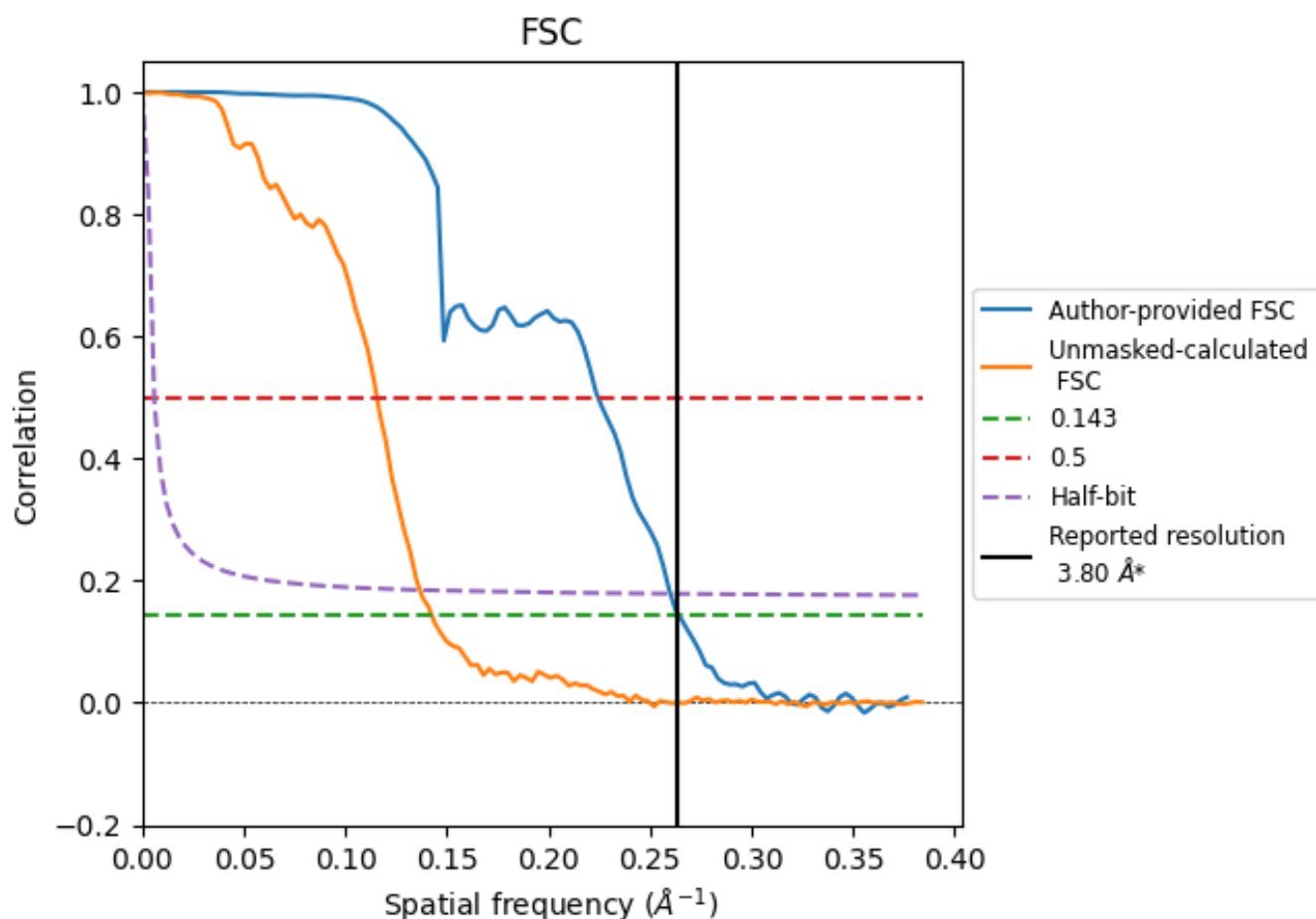


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

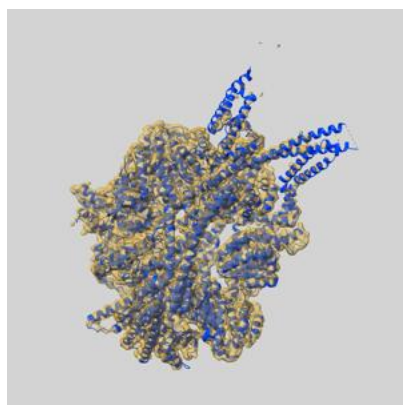
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.46	3.84
Unmasked-calculated*	7.01	8.65	7.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.01 differs from the reported value 3.8 by more than 10 %

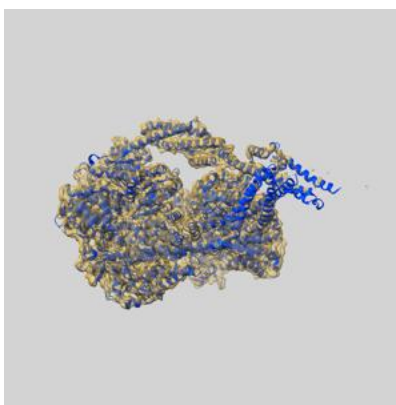
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44718 and PDB model 9BN1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

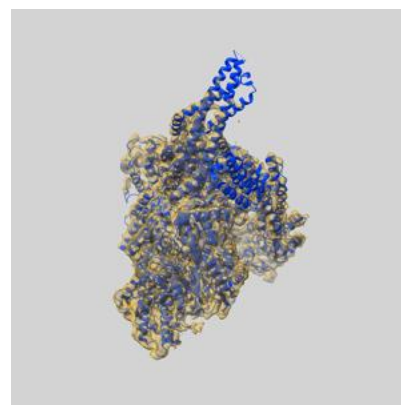
9.1 Map-model overlay [i](#)



X



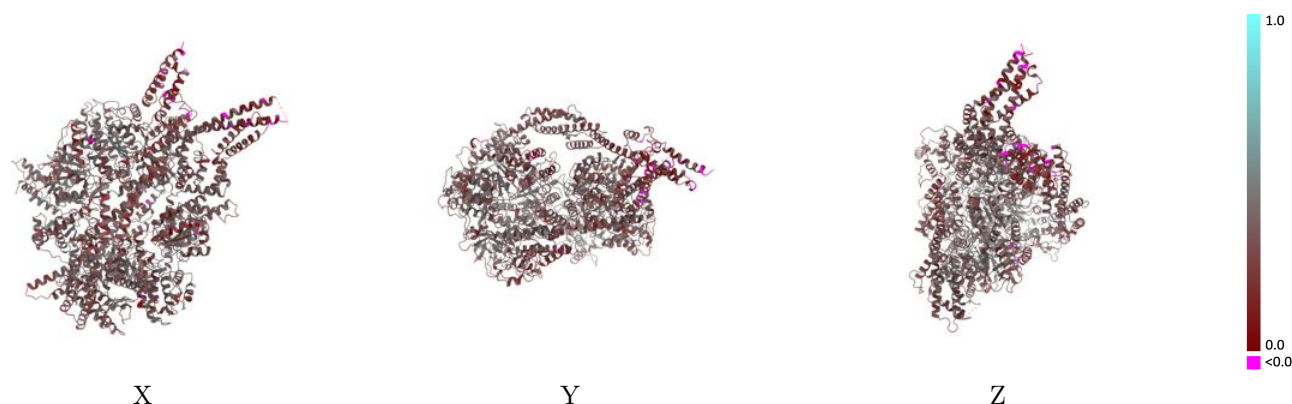
Y



Z

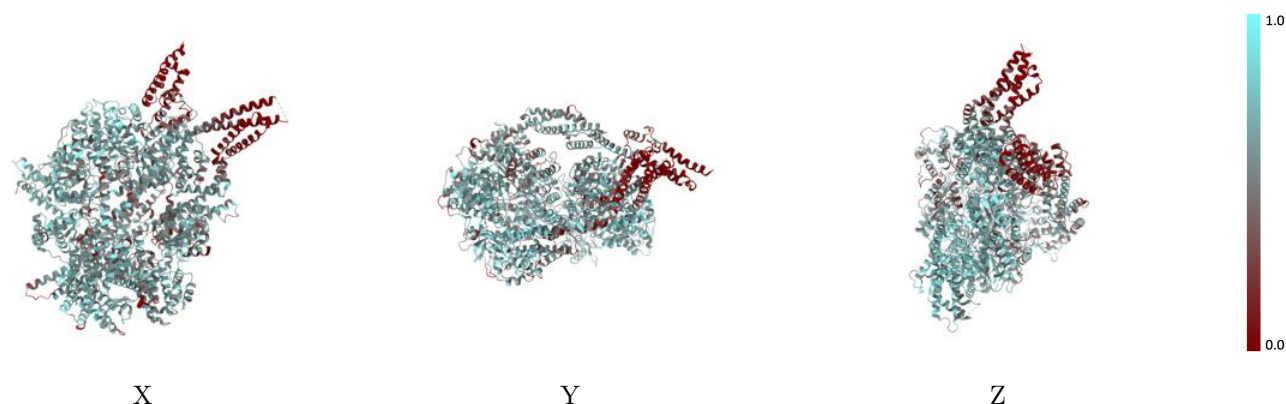
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



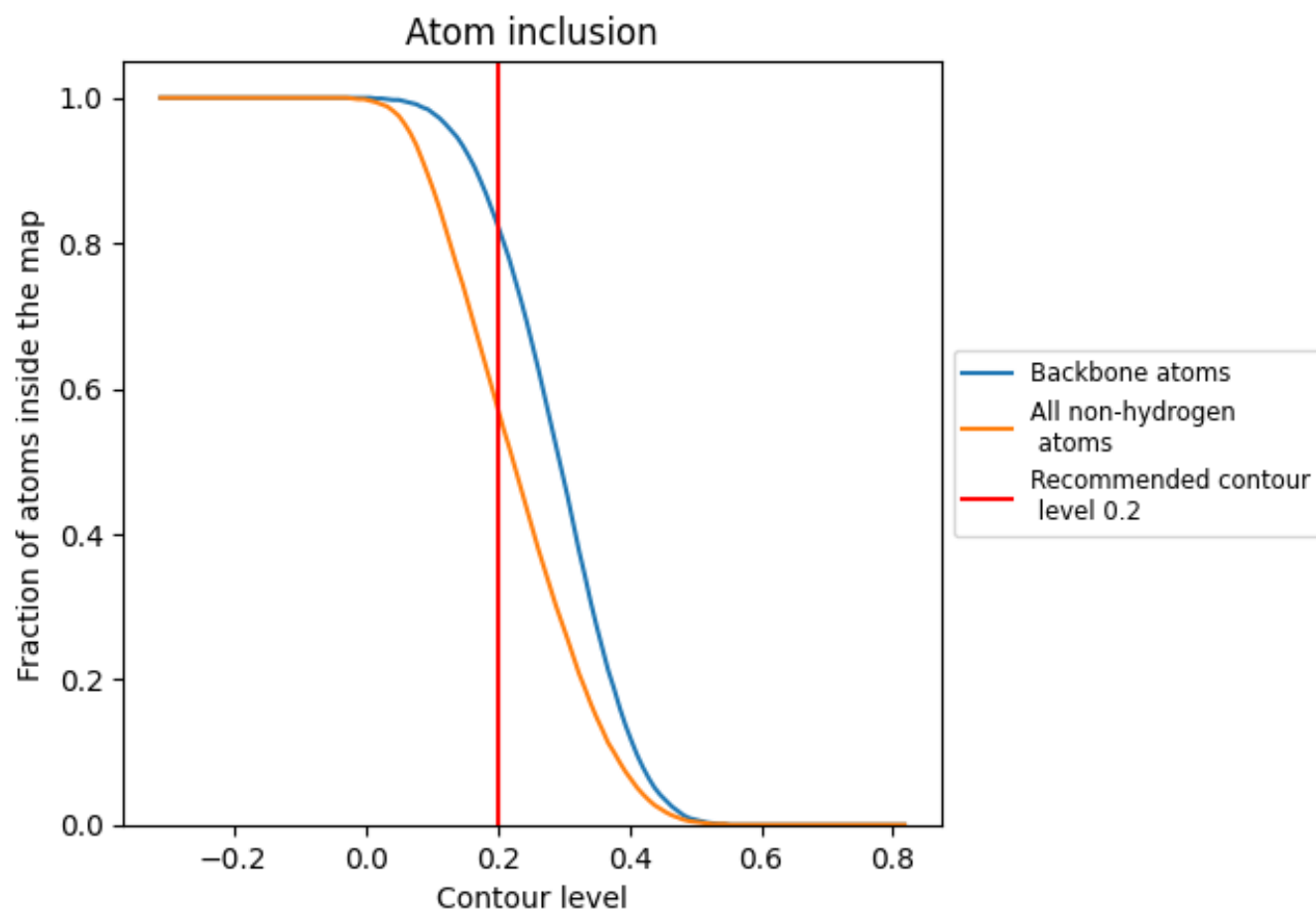
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 57% 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	<div></div> 0.5750	<div></div> 0.3490
A	<div></div> 0.5750	<div></div> 0.3490

