



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:04 PM UTC

PDB ID : 9DH9 / pdb_00009dh9
EMDB ID : EMD-46860
Title : State-7-Post-2 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg²⁺
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

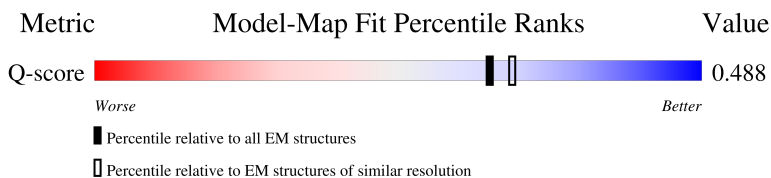
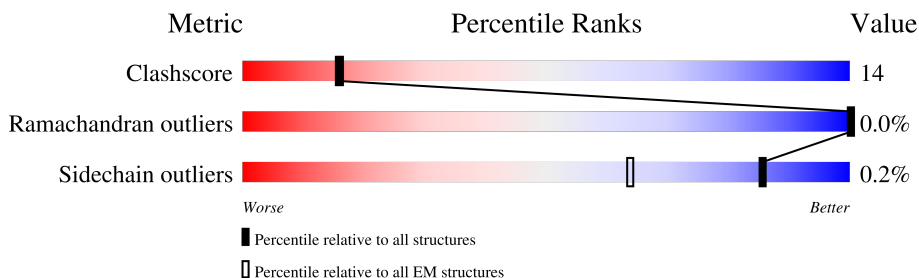
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 5 unique types of molecules in this entry. The entry contains 23113 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.

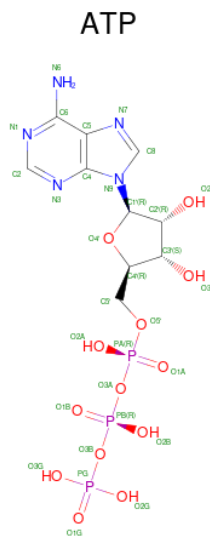
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2858	Total	C	N	O	S	0	0
			22994	14663	3967	4249	115		

- 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).



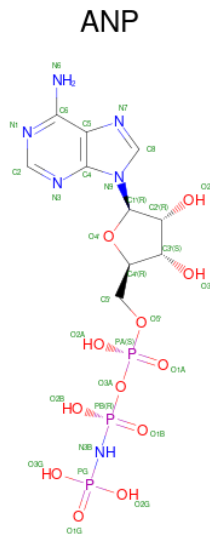
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

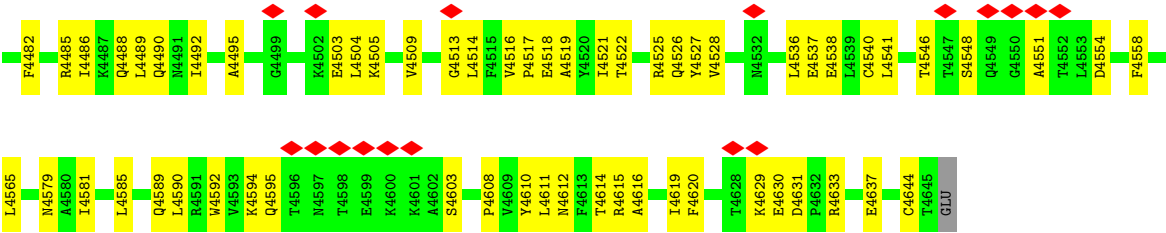
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total 3	Mg 3	0



LYS	P3123	Q3031	L2946	W2845	W2752	T2644	L2532	W2445	P2225	Q2109
GLU	D3124	Q3032	S2947	N2849	R2763	T2644	P2533	T2446	S2226	R2113
ASP	X3125	K3033	R2948	F2858	R2757	Q2654	I2534	G2227	K2227	E2114
LEU	M3126	K3034	F2949	P2859	L2768	W2658	L2635	L2452	K2230	LYS
ASP	P3127	E3035	F2949	P2859	L2768	L2658	L2636	R2453	M2342	GLU
VAL	V3128	E3035	F2949	P2859	L2768	L2658	L2637	C2454	R2231	GLU
GLU	K3132	Q3036	W2954	L2861	L2762	W2660	E2538	S2457	W2234	ARG
GLU	L3133	Q3037	W2954	L2861	L2762	L2661	V2539	L2461	L2238	GLU
PRO	L3133	Q3038	W2954	L2861	L2762	L2661	W2545	H2462	L2238	ALA
ALA	P3134	K3039	L2961	R2863	E2767	C2662	K2561	H2463	R2243	VAL
VAL	Q3135	E3040	K2962	E2864	P2768	C2662	V2562	H2463	L2244	ASP
ILE	Q3136	Q3041	W2963	K2865	F2776	L2668	A2564	Q2464	E2245	GLU
GLU	P3137	L3042	H2964	A2866	F2777	L2668	P2565	A2465	G2246	GLU
VAL	P3137	L3043	R2965	M2867	T2776	V2679	P2566	V2469	E2248	GLU
LYS	R3140	L3044	G2969	S2868	M2779	T2683	V2570	Q2470	D2262	ILE
ASN	E3141	L3045	E2970	R2869	M2780	T2683	Q2471	Q2471	D2262	ASP
ALA	A3142	S3046	E2974	P2870	Q2781	Q2685	Q2472	Q2472	D2262	GLU
ALA	A3142	S3046	E2974	P2870	Q2781	Q2685	Q2472	Q2472	D2262	GLU
VAL	L3143	L3050	D2975	L2871	E2782	Q2685	P2567	Q2473	D2262	GLU
LYS	V3144	L3050	D2975	L2871	E2782	Q2685	V2569	W2473	D2262	GLU
ASP	N3145	L3050	D2975	L2871	E2782	Q2685	P2569	W2473	D2262	GLU
LYS	V3148	V3064	L2976	K2879	R2783	V2687	T2571	F2479	D2262	GLU
LYS	L3154	V3065	L2977	L2889	Q2789	V2687	T2571	F2479	D2262	GLU
GLN	L3154	F3066	R2979	L2889	P2790	V2687	T2571	F2479	D2262	GLU
MET	A3162	T3067	V2979	L2889	H2791	V2687	L2572	F2479	D2262	GLU
LYS	A3162	T3067	V2979	L2889	H2791	V2687	L2572	F2479	D2262	GLU
ASP	G3166	S3070	R2981	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLN	R3167	S3070	R2981	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLN	L3171	S3070	R2981	L2897	L2793	E2704	T2576	F2479	D2262	GLU
ALA	A3184	L2990	E2988	L2897	L2793	E2704	T2576	F2479	D2262	GLU
ASN	N3185	L2990	E2988	L2897	L2793	E2704	T2576	F2479	D2262	GLU
LYS	L3186	F2992	K2991	L2897	L2793	E2704	T2576	F2479	D2262	GLU
LYS	L3186	F2992	K2991	L2897	L2793	E2704	T2576	F2479	D2262	GLU
VAL	K3190	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
MET	R3191	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
SER	S3192	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLN	E3193	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
ALA	E3195	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLU	M3199	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLU	N3202	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
HIS	R3206	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
LEU	K3207	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLN	L3208	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLY	K3209	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
SER	E3210	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
THR	T3211	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
ASP	V3212	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
GLN	D3213	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
MET	Q3214	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
VAL	E3216	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
ILE	E3217	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU
VAL	L3218	L2993	M2994	L2897	L2793	E2704	T2576	F2479	D2262	GLU

L4344	I4405	L4243	V4134	F4017	I3924	F3831	G3736	N3631	R3549	ARG
K4346	K4406	K4244	P4136	M4018	Q3926	F3832	E3737	V3635	T3550	SER
Q4347	F4410		L4027	L4027	L3927		F3738	Q3636	Y3552	ILE
		M4247	R4140		T3928	I3835	Q3739		L3553	ALA
	LEU	A4248		I4030	V3929	V3839	R3743	E3639	ASP	MET
	GLU		R4143	V4035	Q3930			S3640	MET	GLU
ASP	ASP	G4253	I4144	V4036	Q3931			Y3641	LEU	ASN
GLU	GLU	G4254	F4145	K4036	Q3932			D3642	LYS	PHE
ASP	ASP	R4255	V4146	P4037	E3933			F3643	ARG	ILE
ASP	ASP	V4256	F4147	M4043	A3934			V3644	VAL	PRO
LEU	LEU	D4257			I3935			L3645	GLU	THR
ALA	ALA	N4258	T4160		V3936				ALA	ILE
TYR	TYR			S4052	R3937				PRO	THR
L4423	K4422	D4261	R4168					V3653	LEU	VAL
L4424	L4424	Q4262	I4169	V4055	D3946			R3654	ARG	ASN
Q4425	Q4425	R4263		E4056	L3947			R3655	LEU	ASN
D4426	D4426	L4264	S4172	D4057	I3948				GLU	SER
V4427	V4427	GLU	P4173	L4058				T3656	GLU	ALA
R4428	R4428	L4269	N4174	L4058	R3870			G3657	LEU	GLU
Q4429	Q4429		E4175	A3953				G3658	LYS	GLU
D4430	D4430	L4272		I4066	A3954			R3659	LEU	SER
L4431	L4431		R4178	T4067	D3954				GLU	ASP
A4432	A4432	T4275	L4179	S4068	E3955			L3479	ASP	ALA
D4433	D4433	R4276		I4071	Q3956			K3480	ASP	ALA
V4434	V4434	S4277		G4072	F3957			T3578	ARG	ARG
S4435	S4435	F4278	L4182	A4072				R3579	LYS	GLU
Q4436	Q4436		W4185	S4073	L3961			L3580	ASP	GLU
V4437	V4437	E4281	F4186	A4074	D3962			K3581	ASN	LYS
C4438	C4438		H4187	E4075				R3582	GLN	MET
E4439	E4439	L4284	A4188	P3966				F3583	GLN	LYS
			I4189	Q4079				R3486	LYS	ASN
			I4190		V3970			E3487	ALA	TYR
			Q4191	K4082				R3488	GLU	PRO
			E4192	A4083	E3976			W3489	VAL	SER
			R4193	I4084	F3977			E3490	GLU	ASN
			L4194		T3978			K3491	GLN	PRO
			R4195	A4087					MET	SER
				V4088	P3979			E3494	ILE	TYR
				K4089	T3981			T3495	ASN	ASN
			Q4200		A3980				ARG	ARG
			W4201	K4089	E3898			I3600	ASP	TYR
			S4202	R4092	P3899			M3601	LEU	GLU
			K4203		T3982			N3602	GLU	ILE
				W4093	I3983			S3501	ALA	VAL
				W4095	G3984			T3502	ALA	VAL
			D4211		Q3985				SER	ASN
			L4212	M4095				D3606	ILE	ARG
			D4217	L4096	H3988			R3607	ALA	ALA
				K4097	R3989				ARG	SER
			L4223	N4098	L3990			R3611	TYR	LEU
				V4099				A3517	ALA	ALA
				L4100	R3997			G3518	LYS	CYS
			T4226	L4101	E3913			F3519	GLU	GLY
				K4111	I3914			F3614	TYR	ALA
			R4230		V3915			D3521	TYR	PRO
			Q4231		L3916			L3615	ALA	MET
					S3917			E3624	VAL	VAL
			D4236		A3918			Q3523	LEU	VAL
					A4005			R3524	ILE	TRP
			P4239		H4006			L3627	SER	ALA
			W4240		V4009			R3628	GLU	ILE
									ALA	ALA
			I4340		L4013			Q3537		
								N3540		
								I3547		
								A3548		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.822	Depositor
Minimum map value	-0.817	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/23487	0.45	5/31835 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2533	PRO	CA-N-CD	-7.84	101.03	112.00
1	A	2718	PRO	CA-N-CD	-5.99	103.62	112.00
1	A	3125	TYR	CA-C-N	5.68	128.55	123.10
1	A	3125	TYR	C-N-CA	5.68	128.55	123.10
1	A	2859	PRO	CA-N-CD	-5.55	104.24	112.00

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	22994	0	23053	664	0
2	A	54	0	24	5	0
3	A	31	0	12	2	0
4	A	31	0	13	4	0
5	A	3	0	0	0	0
All	All	23113	0	23102	666	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 14.

The worst 5 of 666 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:3933:GLU:OE1	1:A:3937:ARG:NH1	2.03	0.92
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.54	0.88
1:A:3522:GLN:HE21	1:A:3572:LEU:HB2	1.41	0.86
1:A:2346:GLN:HB2	1:A:2726:ARG:HD3	1.58	0.85
1:A:1512:TYR:HE1	1:A:3659:ARG:HH22	1.28	0.81

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	2844/4646 (61%)	2751 (97%)	92 (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	2544/4125 (62%)	2538 (100%)	6 (0%)	87 85

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3540	ASN
1	A	3978	THR
1	A	4391	ILE
1	A	2901	TYR
1	A	2572	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3104	GLN
1	A	4566	GLN
1	A	3538	GLN
1	A	4117	GLN
1	A	3188	HIS

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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	4702	5	32,33,33	0.32	0	48,52,52	0.28	0
2	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
2	ADP	A	4701	5	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
4	ANP	A	4703	5	33,33,33	0.94	4 (12%)	45,52,52	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	5	-	7/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4701	5	-	2/16/32/32	0/3/3/3
4	ANP	A	4703	5	-	3/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.61	1.47	1.39
2	A	4704	ADP	C5-C4	4.60	1.47	1.39
2	A	4701	ADP	C5-C6	2.70	1.48	1.41
2	A	4704	ADP	C5-C6	2.70	1.48	1.41
4	A	4703	ANP	PB-O3A	-2.53	1.55	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-6.24	118.13	126.72
2	A	4704	ADP	C5-C4-N3	-5.78	118.76	126.72
2	A	4701	ADP	N3-C4-N9	4.71	135.17	127.17
2	A	4704	ADP	N3-C4-N9	4.54	134.88	127.17
2	A	4701	ADP	C2-N3-C4	3.95	121.49	111.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

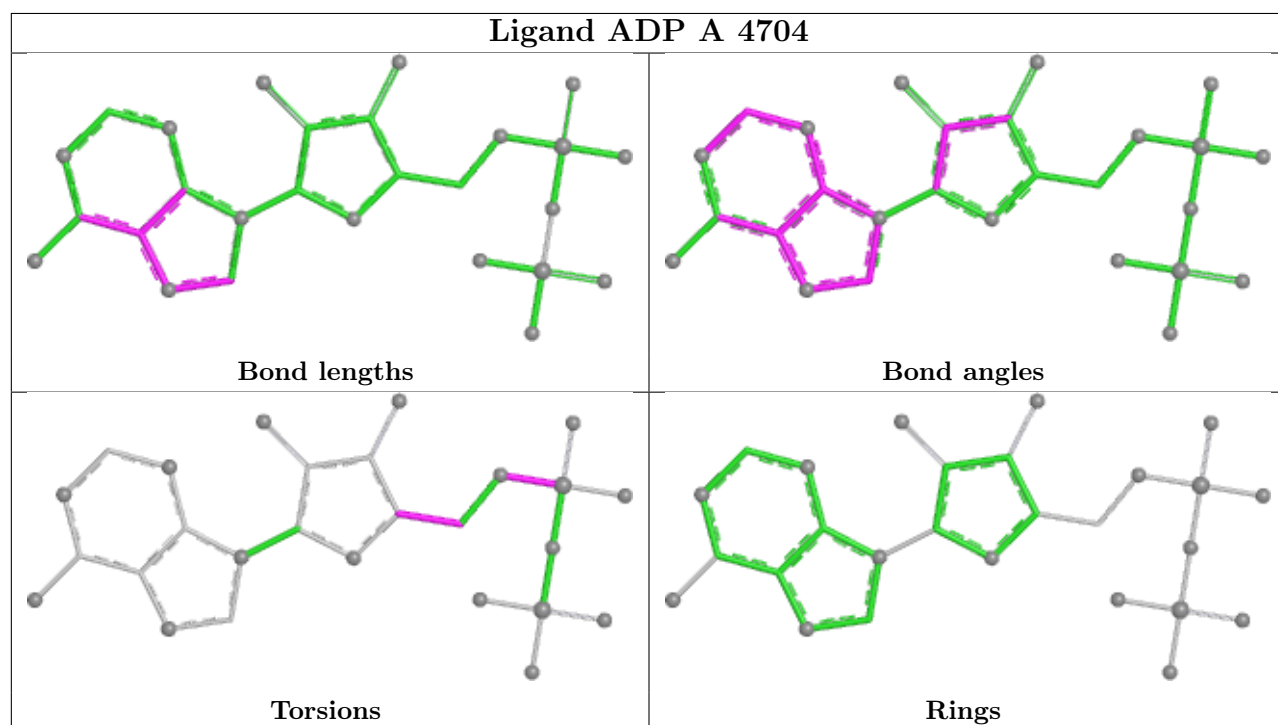
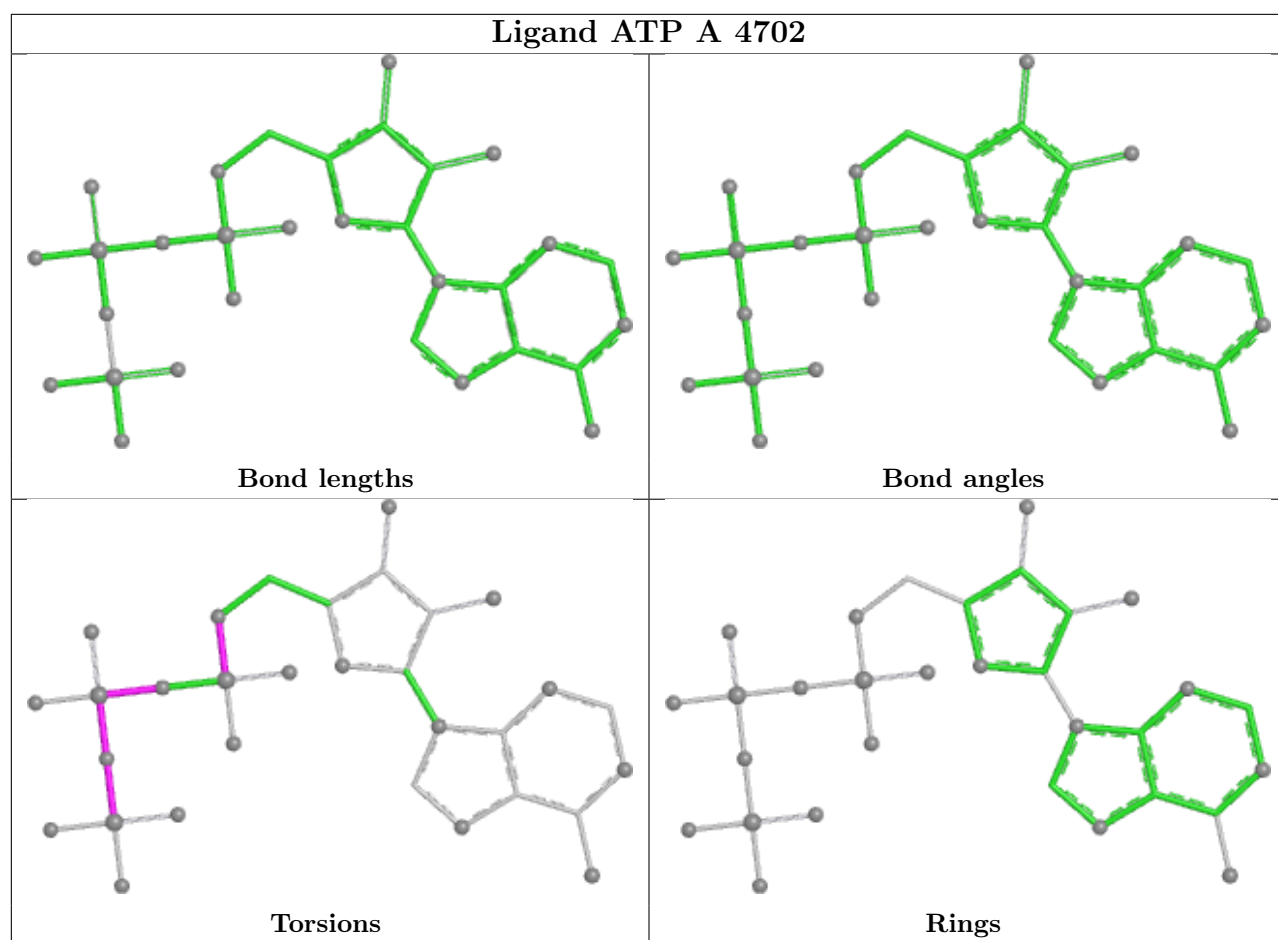
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	PB-O3B-PG-O3G
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O3A

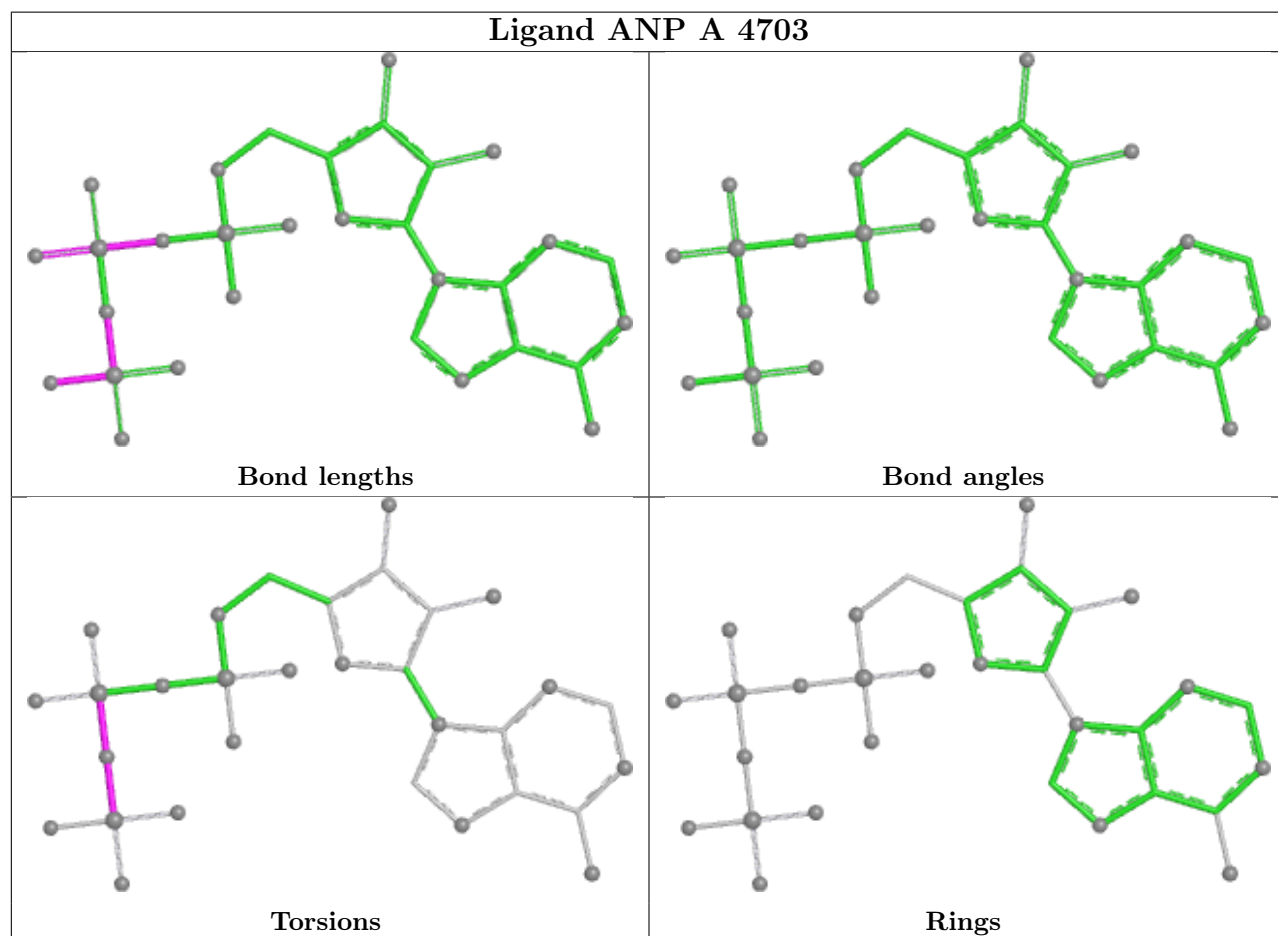
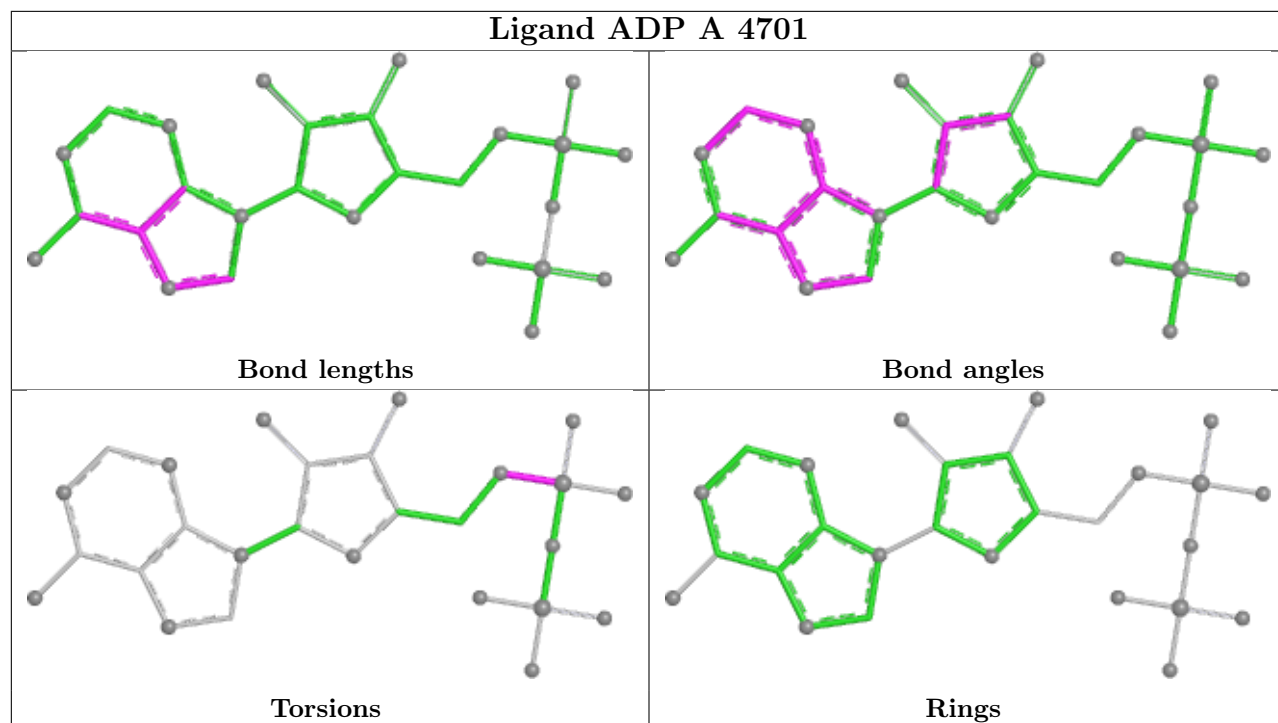
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	2	0
2	A	4704	ADP	1	0
2	A	4701	ADP	4	0
4	A	4703	ANP	4	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.

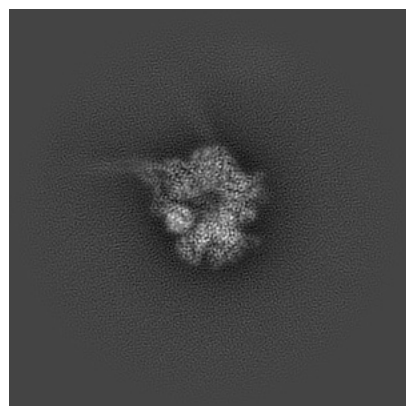
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46860. These allow visual inspection of the internal detail of the map and identification of artifacts.

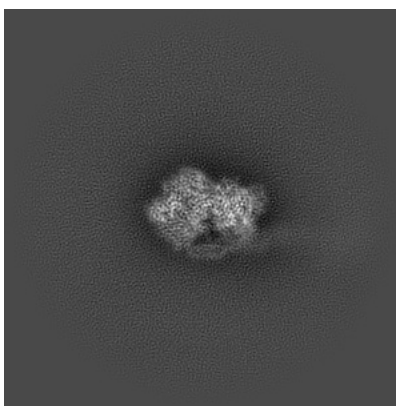
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

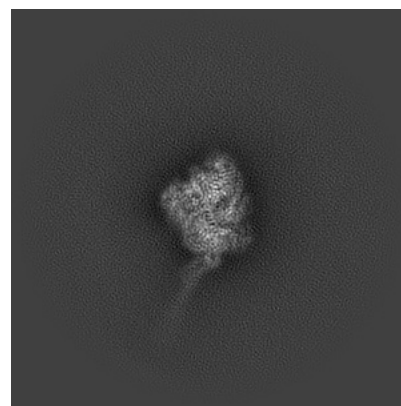
6.1.1 Primary map



X

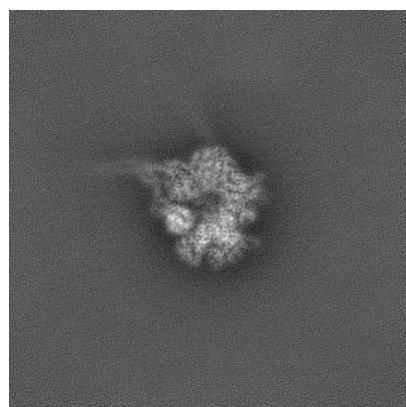


Y

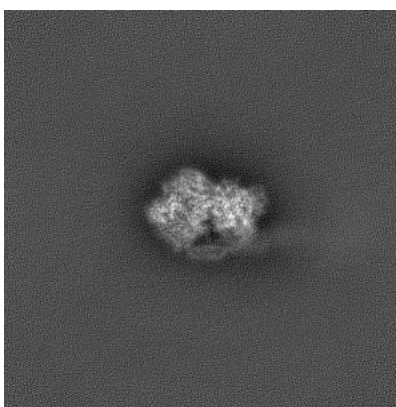


Z

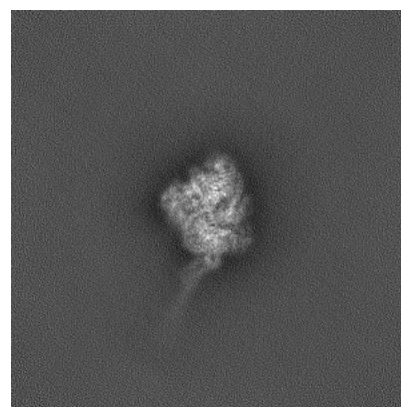
6.1.2 Raw map



X



Y

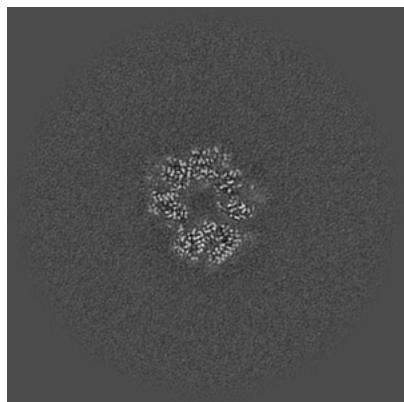


Z

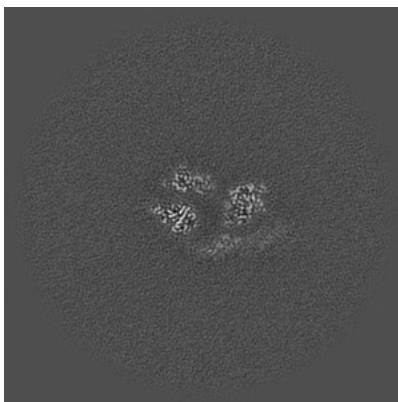
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

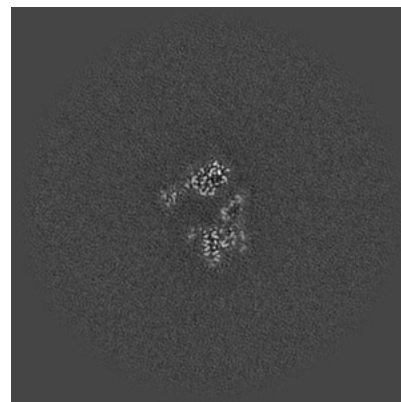
6.2.1 Primary map



X Index: 192

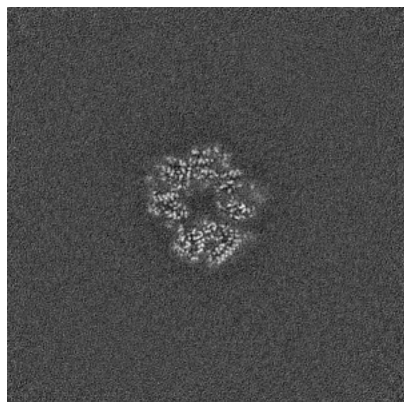


Y Index: 192

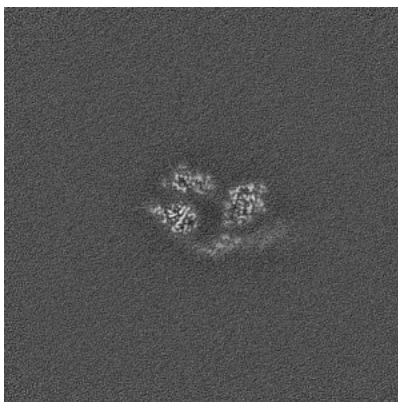


Z Index: 192

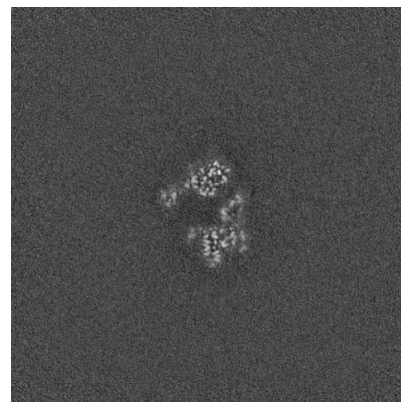
6.2.2 Raw map



X Index: 192



Y Index: 192

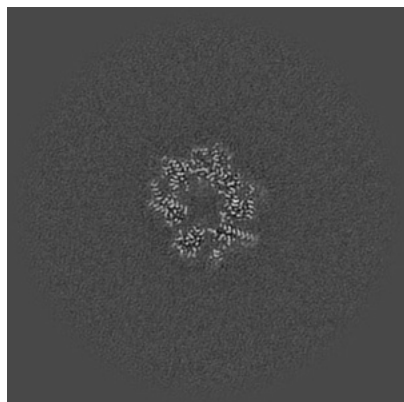


Z Index: 192

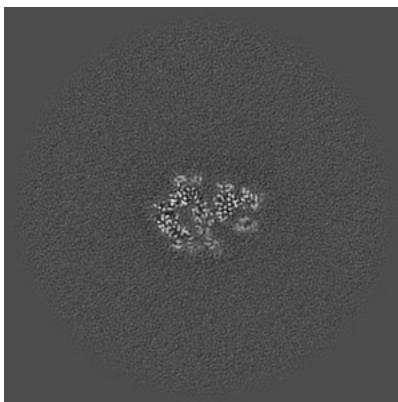
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

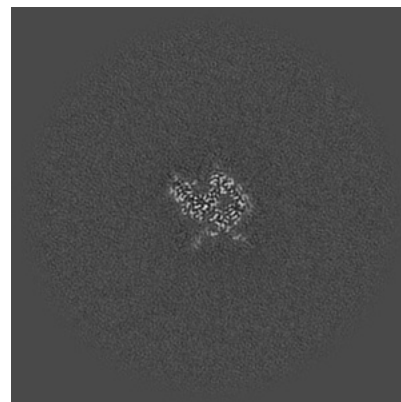
6.3.1 Primary map



X Index: 196

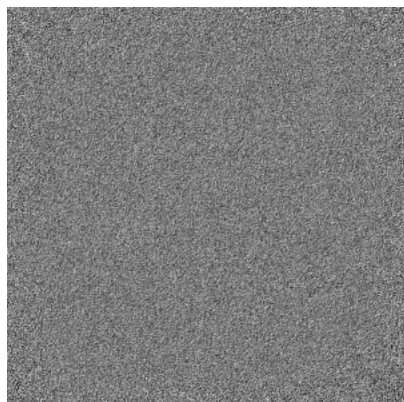


Y Index: 209

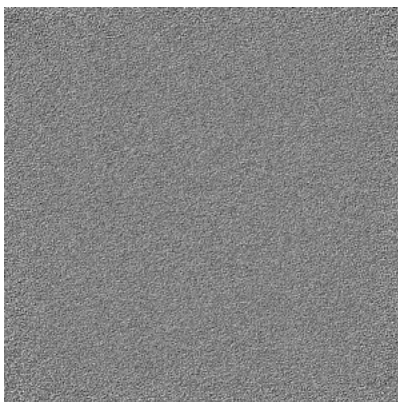


Z Index: 169

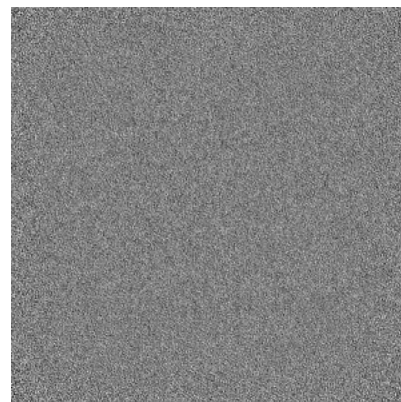
6.3.2 Raw map



X Index: 0



Y Index: 0

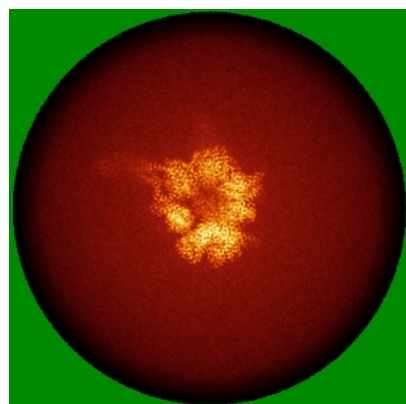


Z Index: 0

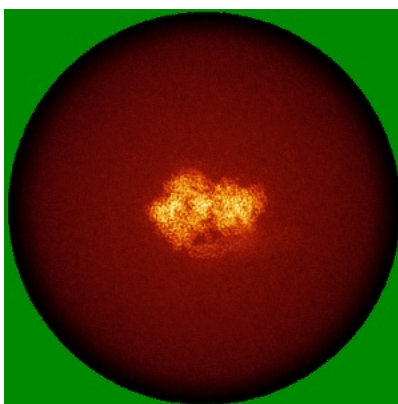
The images above show the largest variance slices of the map in three orthogonal directions.

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

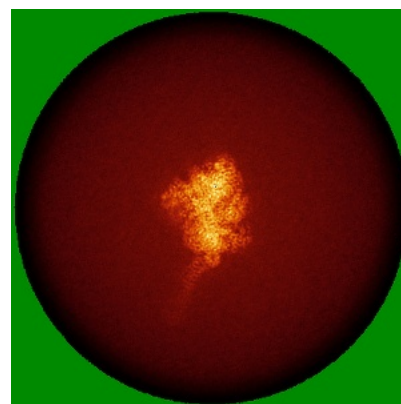
6.4.1 Primary map



X

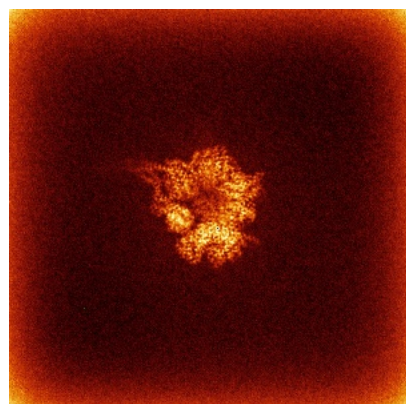


Y

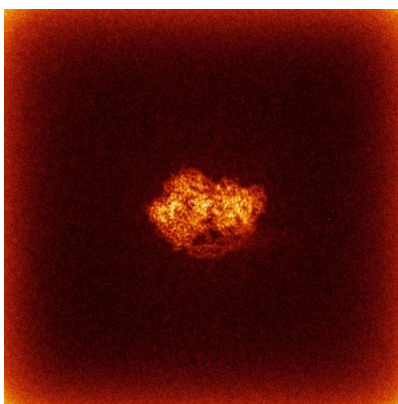


Z

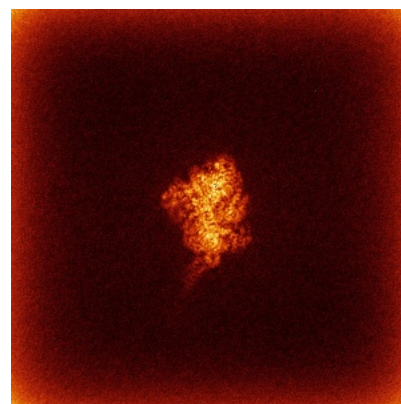
6.4.2 Raw map



X



Y

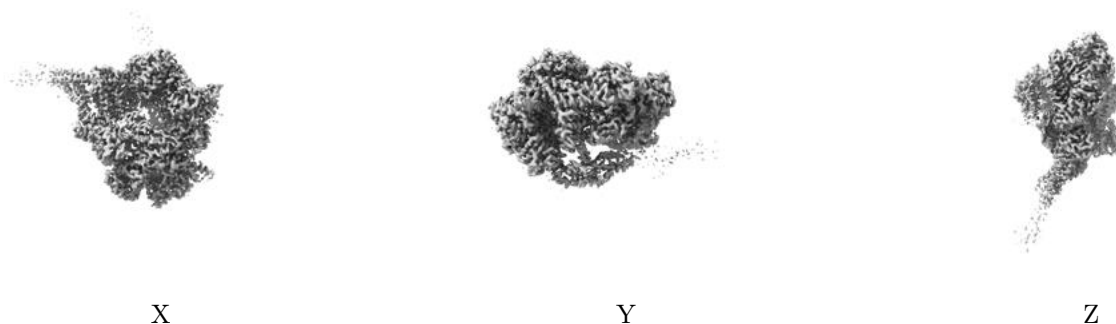


Z

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 0.3. 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.

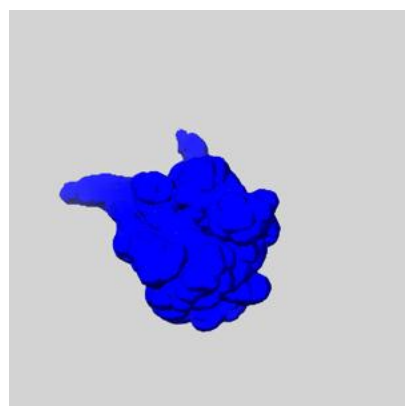
6.6 Mask visualisation [i](#)

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

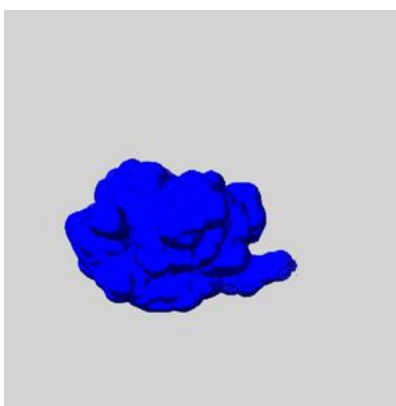
A mask typically either:

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

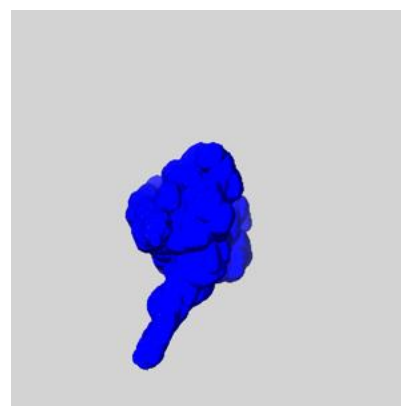
6.6.1 emd_46860_msk_1.map [i](#)



X



Y

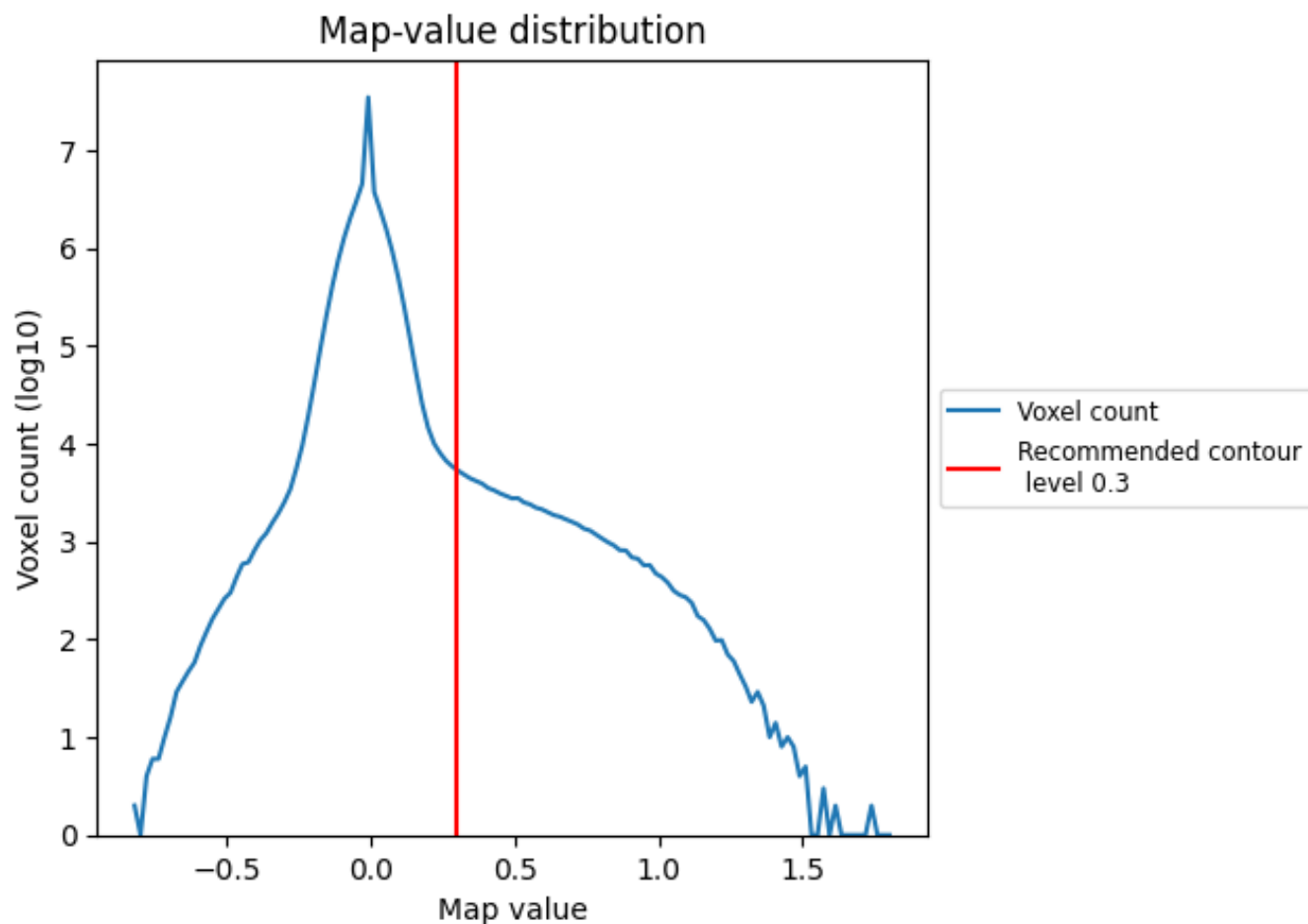


Z

7 Map analysis [i](#)

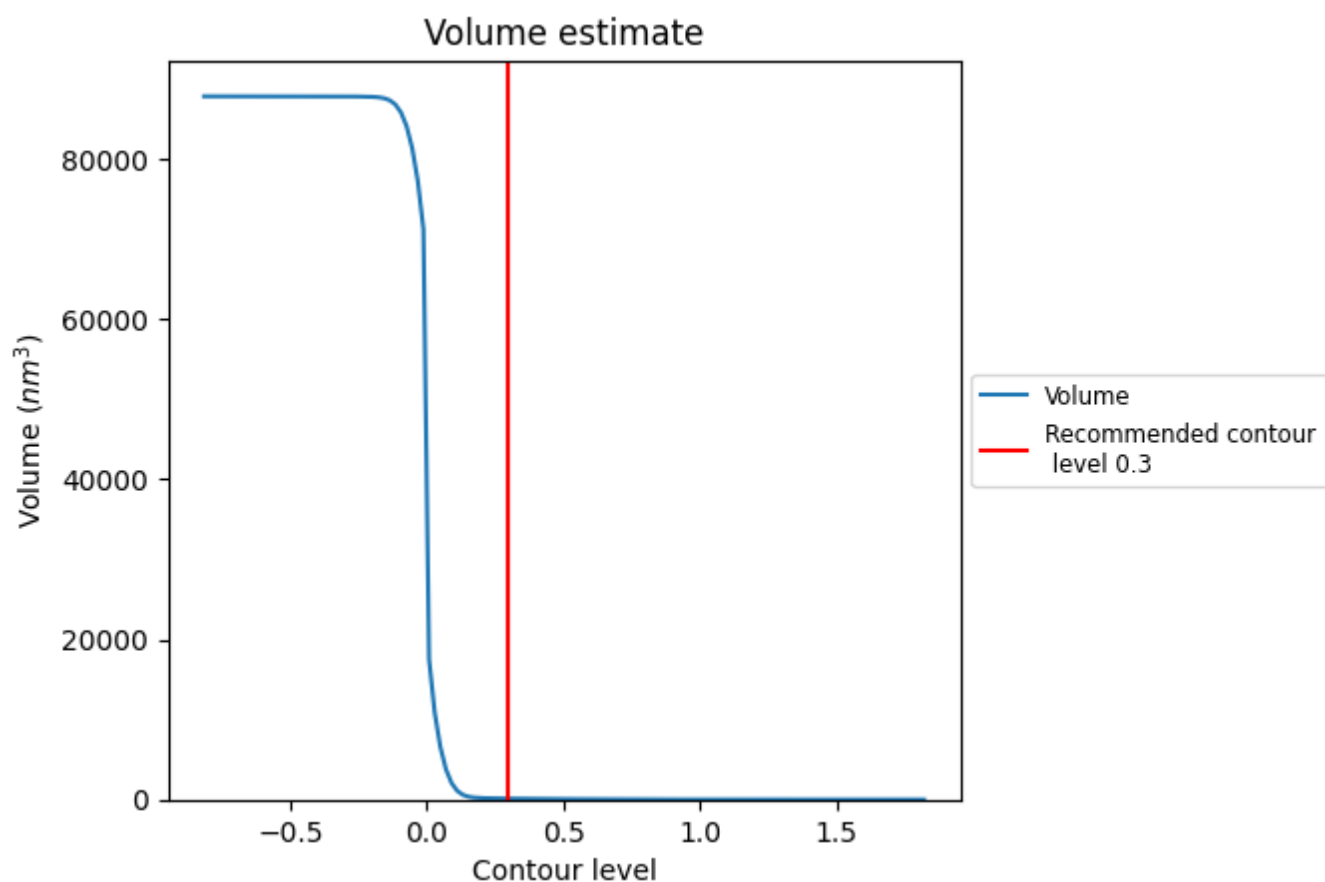
This section contains the results of statistical analysis of the map.

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.

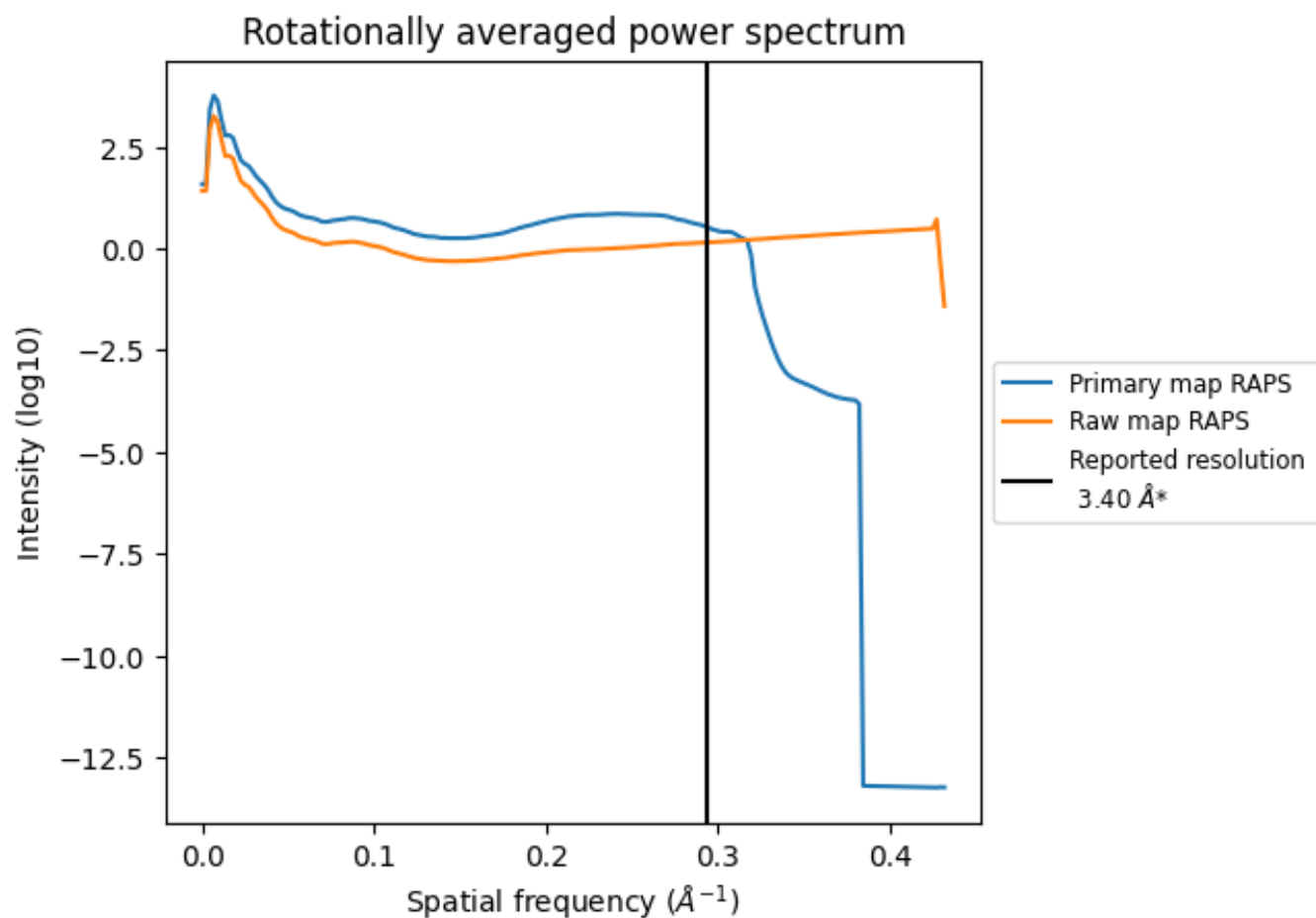
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 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 ⓘ

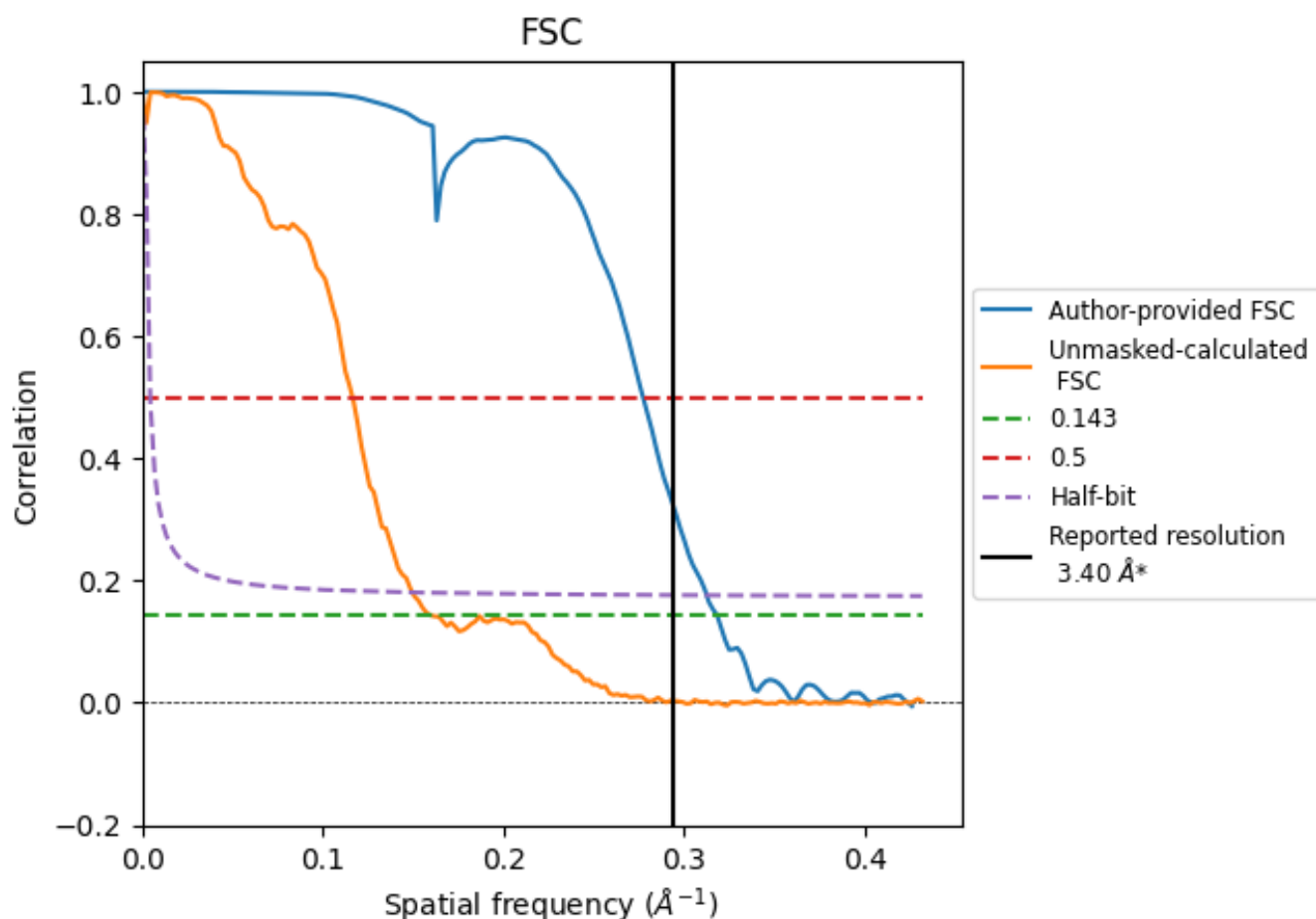


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

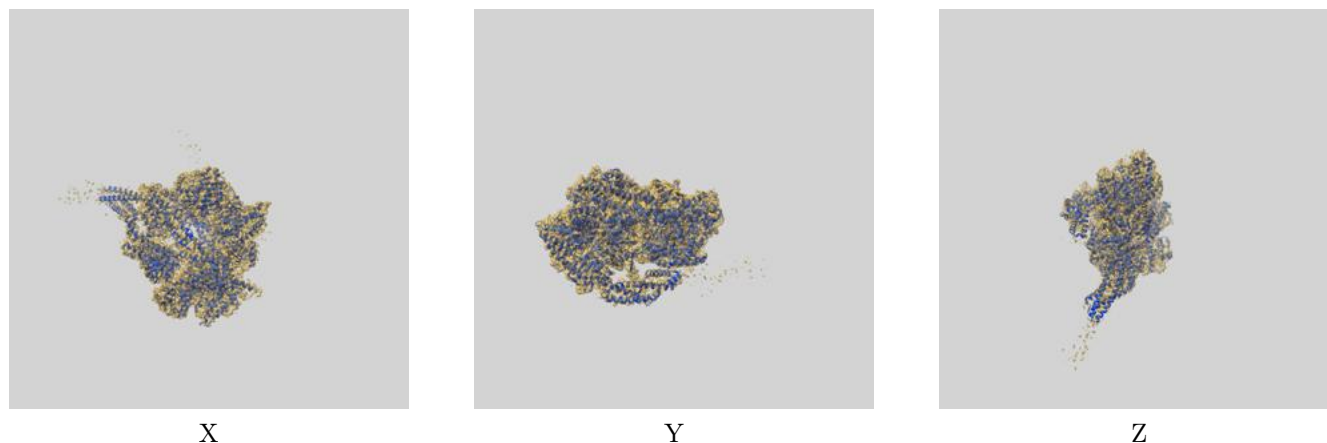
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.14	3.60	3.20
Unmasked-calculated*	6.27	8.58	6.68

*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 6.27 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

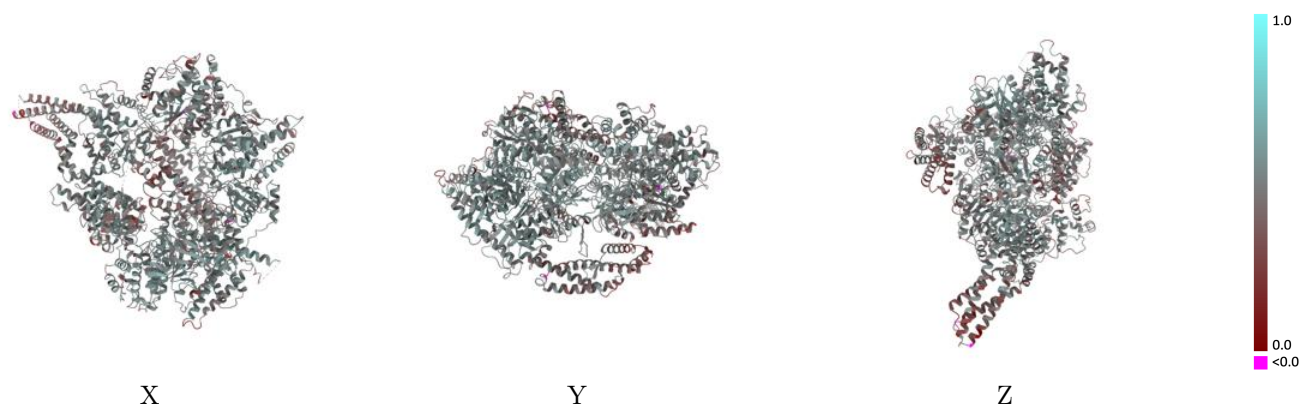
This section contains information regarding the fit between EMDB map EMD-46860 and PDB model 9DH9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



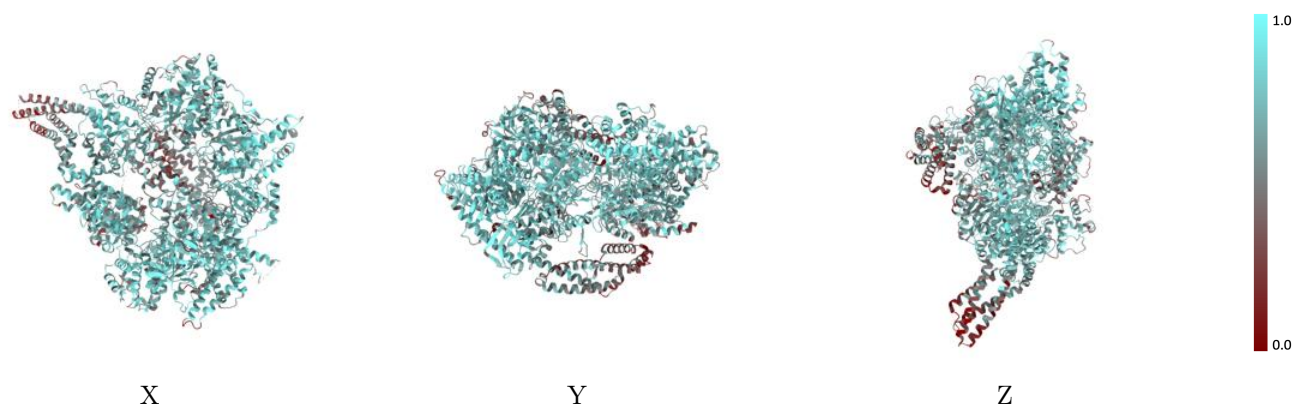
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



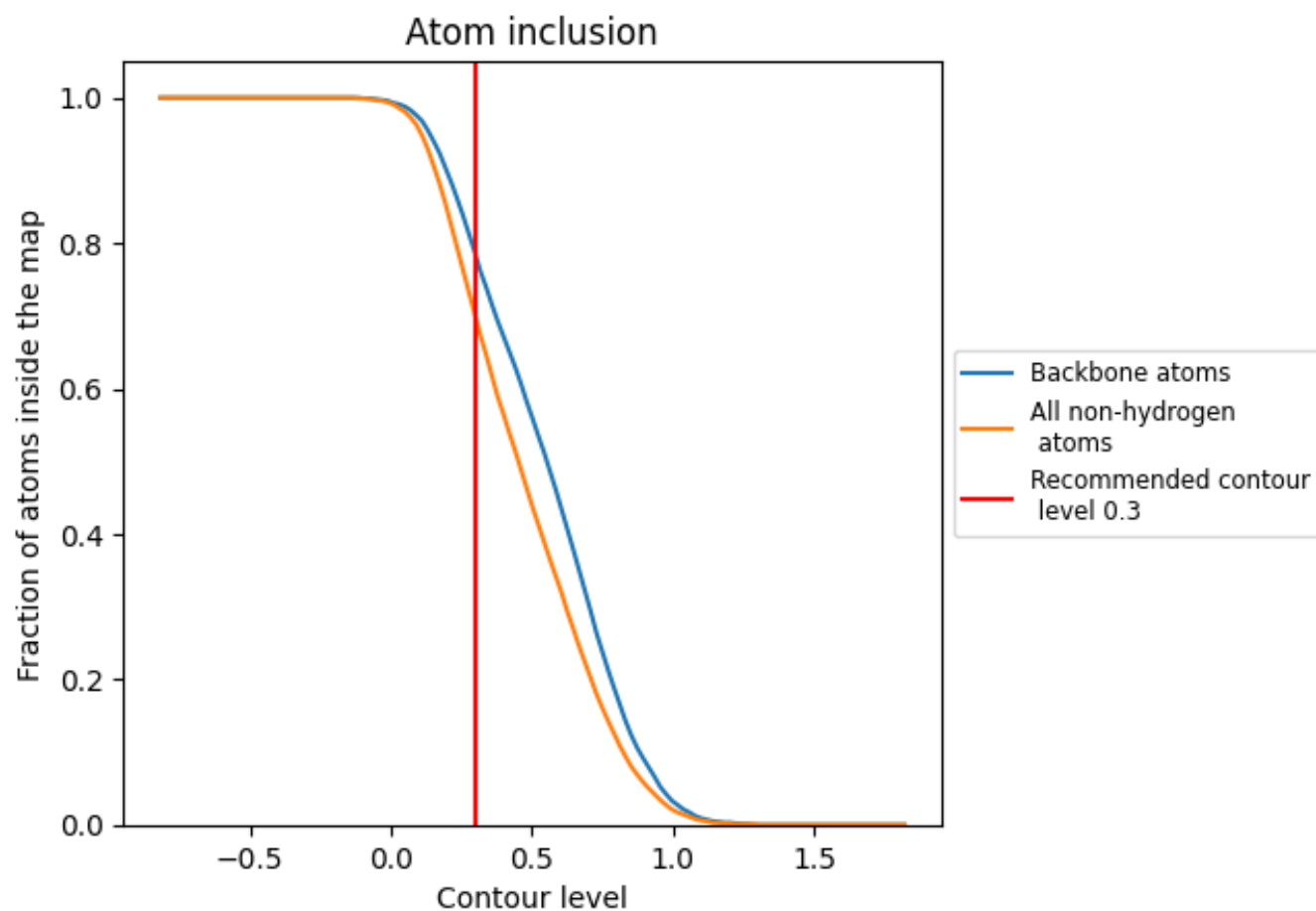
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7000	0.4880
A	0.7000	0.4880

