



wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 06:15 PM EDT

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

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

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A user guide is available at

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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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

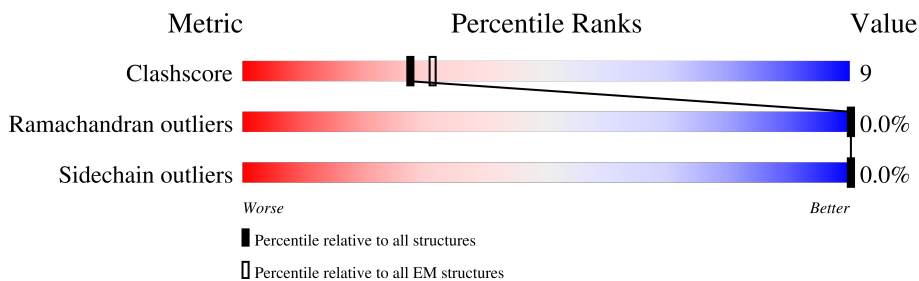
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 24617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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



Mol	Chain	Residues	Atoms					AltConf
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).



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

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

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Mg 2 2	0





Q4549	Q4550	A4551	T4552	I4553	D4554	F4558	Q4559	V4560	K4564	K4574	L4577	I4581	P4586	L4587	T4588	K4594	M4597	T4598	P4599	K4600	K4601	A4602	V4609	Y4610	L4611	I4619	A4627	T4628	K4629	R4638	V4642	E4646	R3611	T3612	S3613	F3614	L3615	D3616	D3617	A3618	F3619	R3620	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	Y3641	D3642	P3643	V3644	P3647	R3654	R3655	T3656	Q3657	G3658	R3659	V3660	L3661	C3665	D3666	Q3667	D3668	P3673	S3680	T3681	P3684	L3692	C3693	S3694	R3695	N3700	F3701	T3702	E3715	V3716	D3725	R3728	Q3735	Q3739	L3742	R3743	Q3744	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	N3771	N3772	L3773	K3774	R3775	E3779	V3780	T3781	R3782	K3783	V3784	E3785	Q3792	T3796	L3802	P3803	M3815	E3816	S3817	I3821	L3824	S3828	Y3836	H3837	R3838	V3839	L3840	D3851	H3852	T3853	L3863	V3871	R3872	R3873	D3879	A3888	R3889	G3897	D3902	L3909	R3910	E3913	T3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3930	E3933	R3937	K3945	D3946	L3947	V3951	P3966	L3973	E3976	E3977	L3992	R4000	L4013	L4025	D4026	L4027	V4031	P4037	M4038	T4039	P4040	H4084	L4058	M4063	T4064	Q4065	S4068	I4069	A4070	I4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	Q4079	A4080	D4081	K4082	A4087	V4088	R4092	M4095	L4096	K4097	M4098	V4099	G4104	V4105	L4106	M4107	Q4108	K4112	L4113	L4116	Q4117	P4118	R4123	L4124	T4127	I4130	R4140	F4147	R4176	A4177	R4178	L4179	Y4180	L4183	Q4191	E4192	R4193	L4194	R4195	S4202	Y4205	E4206	A4215	D4220	L4223	D4224	P4235	L4243	L4246	M4247	I4251	R4255	D4261	T4275	E4281	L4284	V4288	H4291	D4298	Q4299	I4300	R4301	E4302	E4303	S4319	P4324	M4325	N4326	K4342	M4343	L4344	K4345	M4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	E4403	M4404	V4417	K4422	L4423	R4428	Q4429	D4430	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	K4457	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4475	I4486	A4501	K4505	L4511	T4524	V4534	S4535	L4536	E4537	T4547	S4548	R4108	K4112	L4113	L4116	Q4117	P4118	R4123	L4124	T4127	I4130	R4140	F4147	R4176	A4177	R4178	L4179	Y4180	L4183	Q4191	E4192	R4193	L4194	R4195	S4202	Y4205	E4206	A4215	D4220	L4223	D4224	P4235	L4243	L4246	M4247	I4251	R4255	D4261	T4275	E4281	L4284	V4288	H4291	D4298	Q4299	I4300	R4301	E4302	E4303	S4319	P4324	M4325	N4326	K4342	M4343	L4344	K4345	M4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	E4403	M4404	V4417	K4422	L4423	R4428	Q4429	D4430	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	K4457	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4475	I4486	A4501	K4505	L4511	T4524	V4534	S4535	L4536	E4537	T4547	S4548	R3611	T3612	S3613	F3614	L3615	D3616	D3617	A3618	F3619	R3620	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	Y3641	D3642	P3643	V3644	P3647	R3654	R3655	T3656	Q3657	G3658	R3659	V3660	L3661	C3665	D3666	Q3667	D3668	P3673	S3680	T3681	P3684	L3692	C3693	S3694	R3695	N3700	F3701	T3702	E3715	V3716	D3725	R3728	Q3735	Q3739	L3742	R3743	Q3744	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	N3771	N3772	L3773	K3774	R3775	E3779	V3780	T3781	R3782	K3783	V3784	E3785	Q3792	T3796	L3802	P3803	M3815	E3816	S3817	I3821	L3824	S3828	Y3836	H3837	R3838	V3839	L3840	D3851	H3852	T3853	L3863	V3871	R3872	R3873	D3879	A3888	R3889	G3897	D3902	L3909	R3910	E3913	T3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3930	E3933	R3937	K3945	D3946	L3947	V3951	P3966	L3973	E3976	E3977	L3992	R4000	L4013	L4025	D4026	L4027	V4031	P4037	M4038	T4039	P4040	H4084	L4058	M4063	T4064	Q4065	S4068	I4069	A4070	I4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	Q4079	A4080	D4081	K4082	A4087	V4088	R4092	M4095	L4096	K4097	M4098	V4099	G4104	V4105	L4106	M4107	Q4108	K4112	L4113	L4116	Q4117	P4118	R4123	L4124	T4127	I4130	R4140	F4147	R4176	A4177	R4178	L4179	Y4180	L4183	Q4191	E4192	R4193	L4194	R4195	S4202	Y4205	E4206	A4215	D4220	L4223	D4224	P4235	L4243	L4246	M4247	I4251	R4255	D4261	T4275	E4281	L4284	V4288	H4291	D4298	Q4299	I4300	R4301	E4302	E4303	S4319	P4324	M4325	N4326	K4342	M4343	L4344	K4345	M4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	E4403	M4404	V4417	K4422	L4423	R4428	Q4429	D4430	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	K4457	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4475	I4486	A4501	K4505	L4511	T4524	V4534	S4535	L4536	E4537	T4547	S4548	R3611	T3612	S3613	F3614	L3615	D3616	D3617	A3618	F3619	R3620	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	Y3641	D3642	P3643	V3644	P3647	R3654	R3655	T3656	Q3657	G3658	R3659	V3660	L3661	C3665	D3666	Q3667	D3668	P3673	S3680	T3681	P3684	L3692	C3693	S3694	R3695	N3700	F3701	T3702	E3715	V3716	D3725	R3728	Q3735	Q3739	L3742	R3743	Q3744	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	N3771	N3772	L3773	K3774	R3775	E3779	V3780	T3781	R3782	K3783	V3784	E3785	Q3792	T3796	L3802	P3803	M3815	E3816	S3817	I3821	L3824	S3828	Y3836	H3837	R3838	V3839	L3840	D3851	H3852	T3853	L3863	V3871	R3872	R3873	D3879	A3888	R3889	G3897	D3902	L3909	R3910	E3913	T3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3930	E3933	R3937	K3945	D3946	L3947	V3951	P3966	L3973	E3976	E3977	L3992	R4000	L4013	L4025	D4026	L4027	V4031	P4037	M4038	T4039	P4040	H4084	L4058	M4063	T4064	Q4065	S4068	I4069	A4070	I4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	Q4079	A4080	D4081	K4082	A4087	V4088	R4092	M4095	L4096	K4097	M4098	V4099	G4104	V4105	L4106	M4107	Q4108	K4112	L4113	L4116	Q4117	P4118	R4123	L4124	T4127	I4130	R4140	F4147	R4176	A4177	R4178	L4179	Y4180	L4183	Q4191	E4192	R4193	L4194	R4195	S4202	Y4205	E4206	A4215	D4220	L4223	D4224	P4235	L4243	L4246	M4247	I4251	R4255	D4261	T4275	E4281	L4284	V4288	H4291	D4298	Q4299	I4300	R4301	E4302	E4303	S4319	P4324	M4325	N4326	K4342	M4343	L4344	K4345	M4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	E4403	M4404	V4417	K4422	L4423	R4428	Q4429	D4430	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	K4457	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4475	I4486	A4501	K4505	L4511	T4524	V4534	S4535	L4536	E4537	T4547	S4548	R3611	T3612	S3613	F3614	L3615	D3616	D3617	A3618	F3619	R3620	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	Y3641	D3642	P3643	V3644	P3647	R3654	R3655	T3656	Q3657	G3658	R3659	V3660	L3661	C3665	D3666	Q3667	D3668	P3673	S3680	T3681	P3684	L3692	C3693	S3694	R3695	N3700	F3701	T3702	E3715	V3716	D3725	R3728	Q3735	Q3739	L3742	R3743	Q3744	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	N3771	N3772	L3773	K3774	R3775	E3779	V3780	T3781	R3782	K3783	V3784	E3785	Q3792	T3796	L3802	P3803	M3815	E3816	S3817	I3821	L3824	S3828	Y3836	H3837	R3838	V3839	L3840	D3851	H3852	T3853	L3863	V3871	R3872	R3873	D3879	A3888	R3889	G3897	D3902	L3909	R3910	E3913	T3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3930	E3933	R3937	K3945	D3946	L3947	V3951	P3966	L3973	E3976	E3977	L3992	R4000	L4013	L4025	D4026	L4027	V4031	P4037	M4038	T4039	P4040	H4084	L4058	M4063	T4064	Q4065	S4068	I4069	A4070	I4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	Q4079	A4080	D4081	K4082	A4087	V4088	R4092	M4095	L4096	K4097	M4098	V4099	G4104	V4105	L4106	M4107	Q4108	K4112	L4113	L4116	Q4117	P4118	R4123	L4124	T4127	I4130	R4140	F4147	R4176	A4177	R4178	L4179	Y4180	L4183	Q4191	E4192	R4193	L4194	R4195	S4202	Y4205	E4206	A4215	D4220	L4223	D4224	P4235	L4243	L4246	M4247	I4251	R4255	D4261	T4275	E4281	L4284	V4288	H4291	D4298	Q4299	I4300	R4301	E4302	E4303	S4319	P4324	M4325	N4326	K4342	M4343	L4344	K4345	M4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	E4403	M4404	V4417	K4422	L4423	R4428	Q4429	D4430	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	K4457	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4475	I4486	A4501	K4505
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4 Experimental information

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/25022	0.31	0/33900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	24503	0	24573	467	0
2	A	81	0	36	5	0
3	A	31	0	12	1	0
4	A	2	0	0	0	0
All	All	24617	0	24621	467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 467 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4326:ASN:HD22	1:A:4581:ILE:HD13	1.41	0.83
1:A:2665:GLU:HB3	1:A:2668:LEU:HD23	1.63	0.80
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.17	0.77
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.17	0.76
1:A:1511:PRO:HG2	1:A:3659:ARG:HE	1.52	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3035/4646 (65%)	2959 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1510	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2706/4125 (66%)	2705 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3092	ASN

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

Mol	Chain	Res	Type
1	A	2849	ASN
1	A	3869	ASN
1	A	3865	GLN
1	A	4262	GLN
1	A	1894	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
2	ADP	A	4701	-	24,29,29	0.84	0	29,45,45	1.23	3 (10%)
3	ATP	A	4702	4	28,33,33	0.78	0	34,52,52	0.59	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.24	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
2	ADP	A	4703	-	-	4/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	1/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	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	4703	ADP	N3-C2-N1	-3.81	123.50	128.67
2	A	4701	ADP	N3-C2-N1	-3.71	123.64	128.67
2	A	4704	ADP	N3-C2-N1	-3.67	123.69	128.67
2	A	4701	ADP	C4-C5-N7	-2.37	106.83	109.34
3	A	4702	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

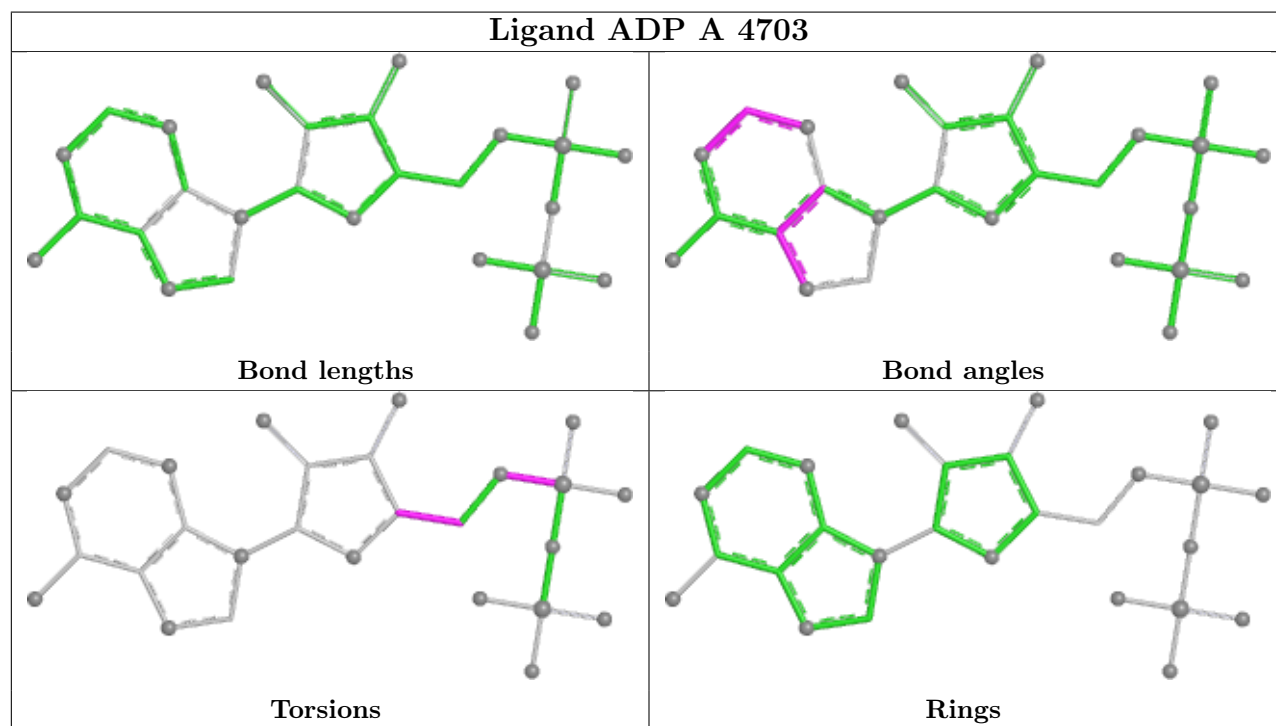
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'

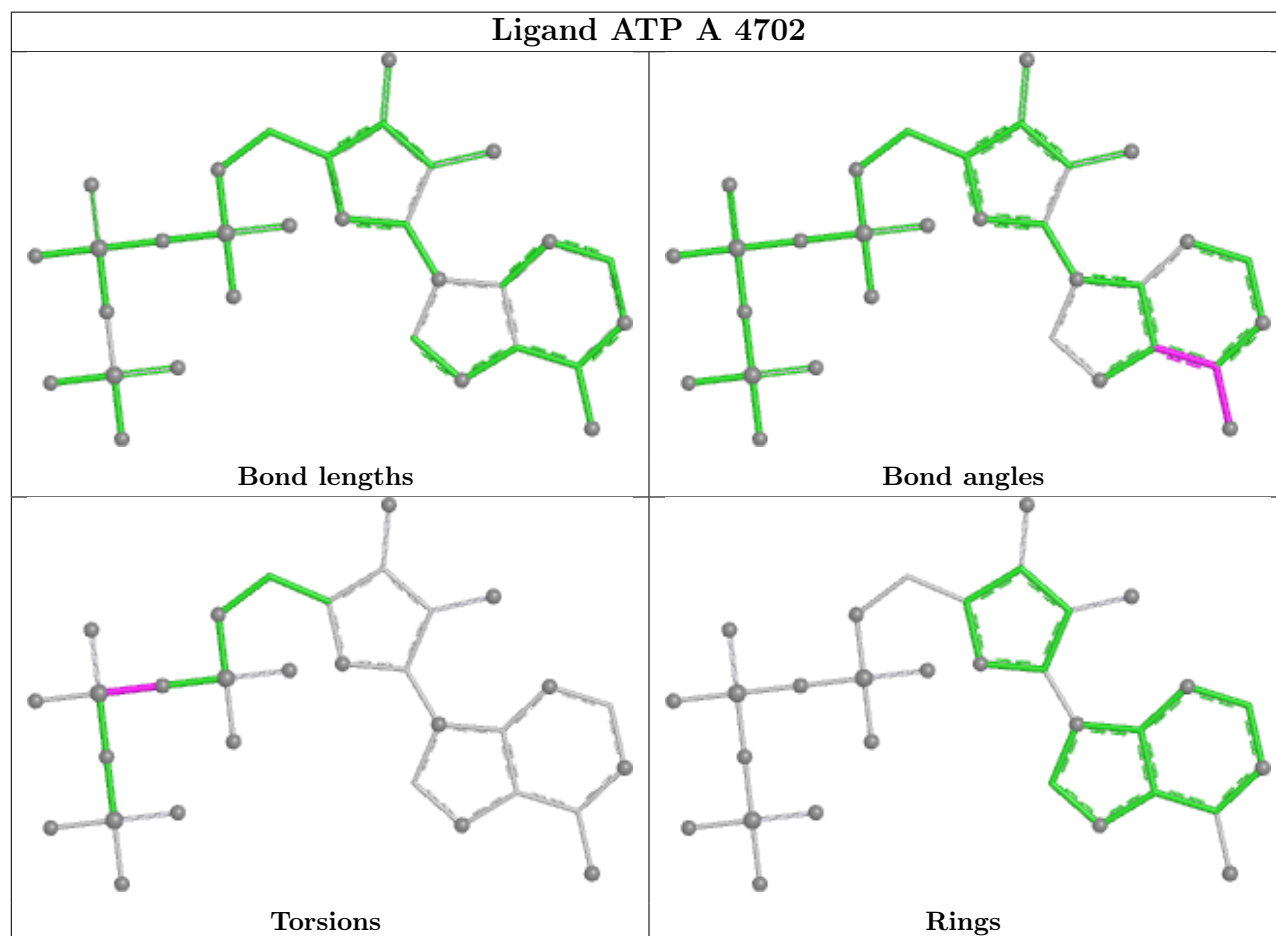
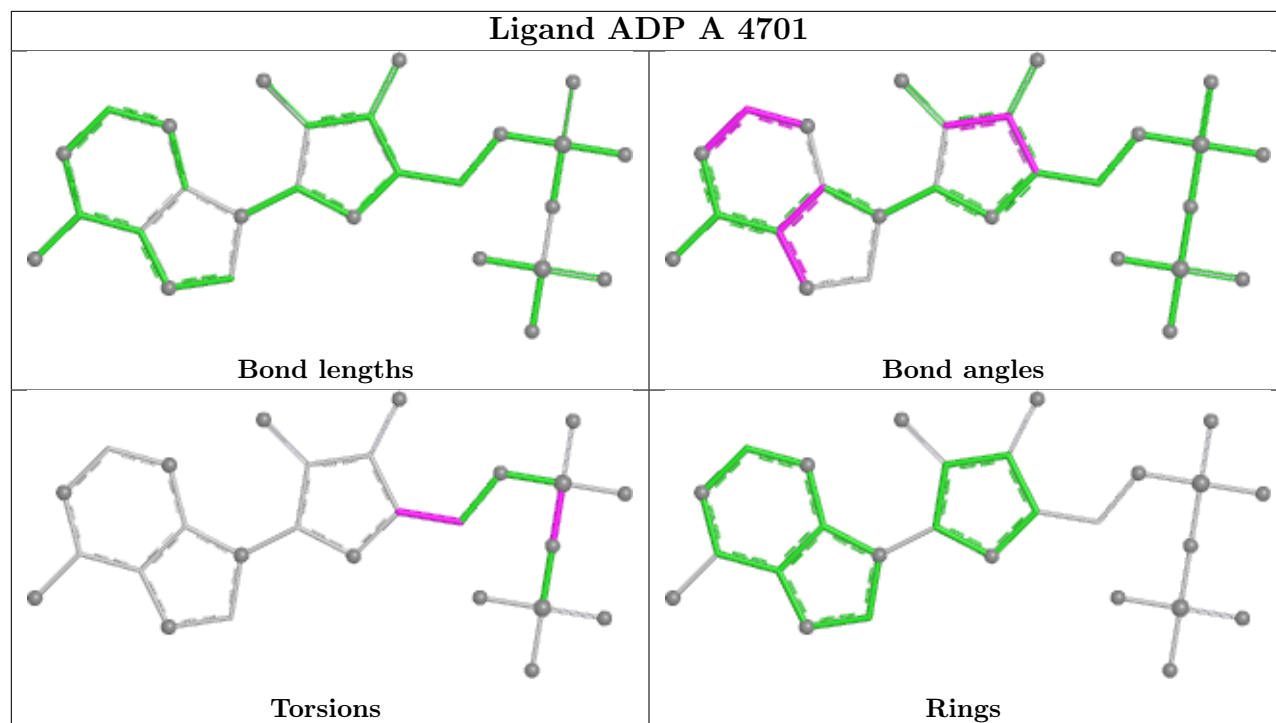
There are no ring outliers.

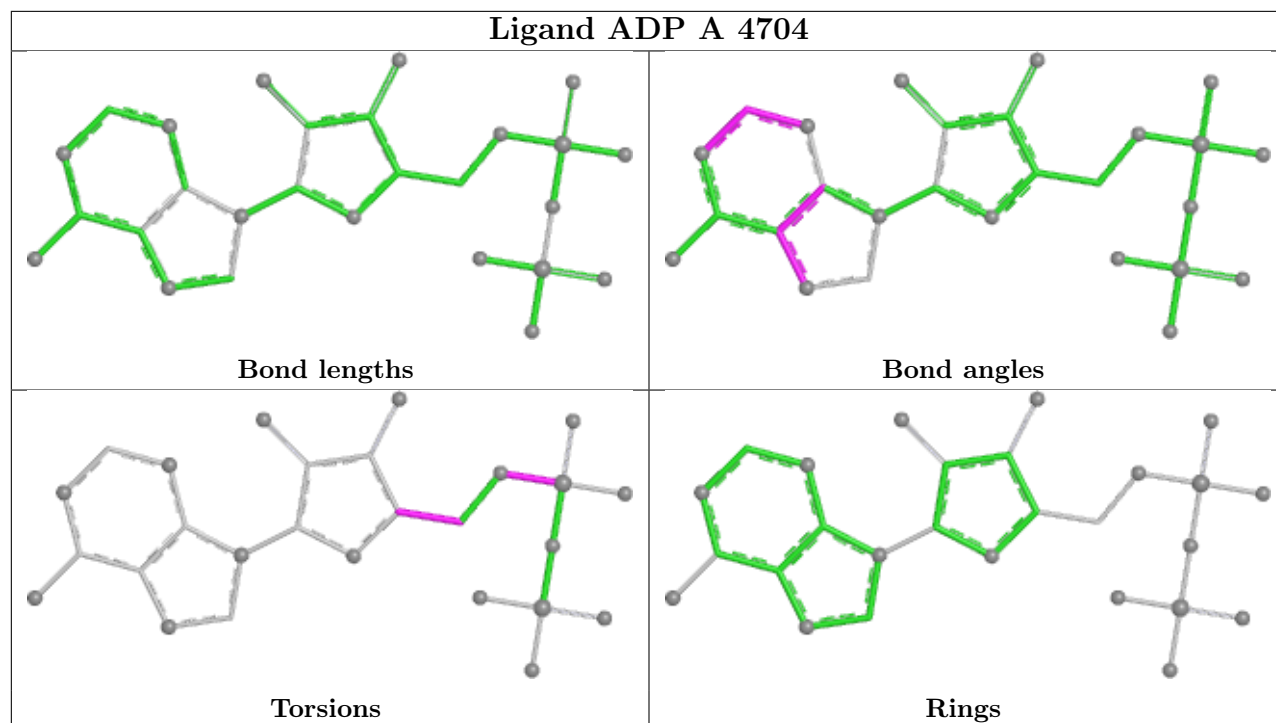
3 monomers are involved in 6 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

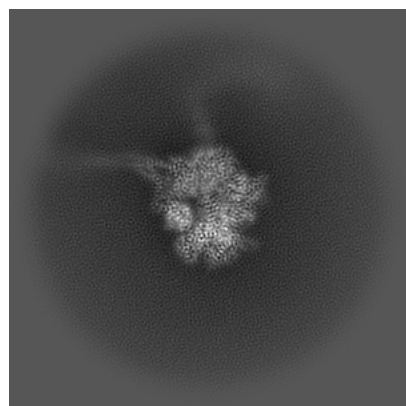
6 Map visualisation [i](#)

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

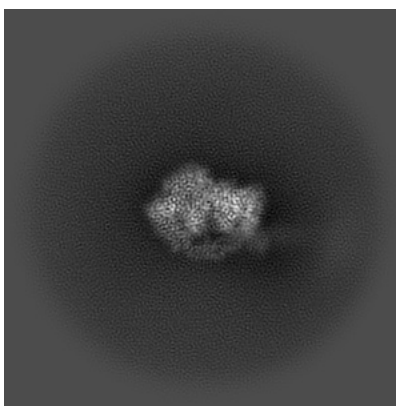
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

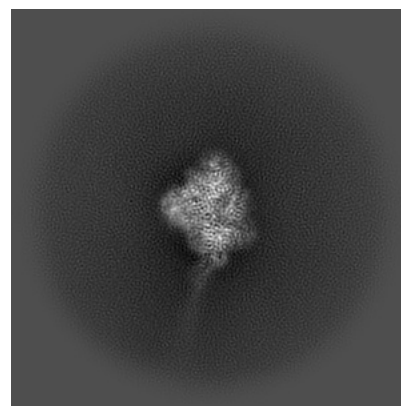
6.1.1 Primary map



X

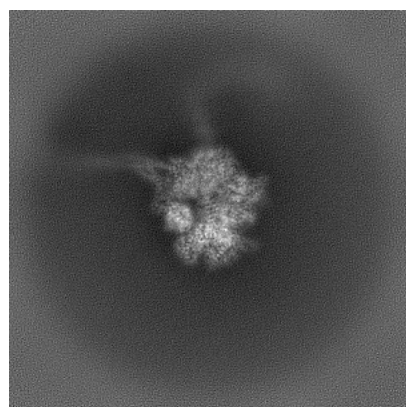


Y

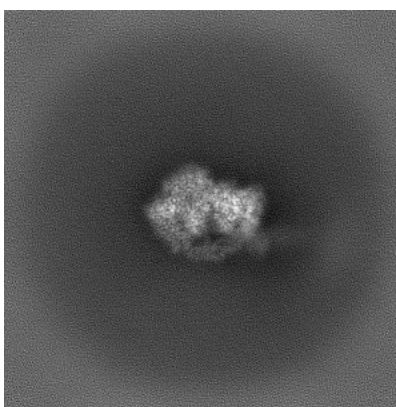


Z

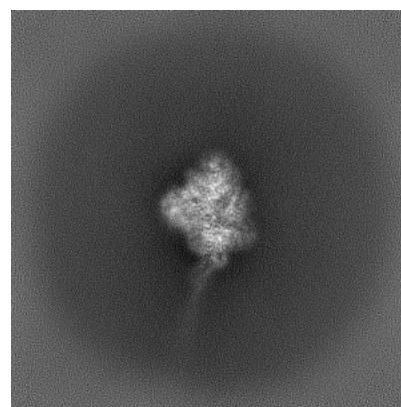
6.1.2 Raw map



X



Y

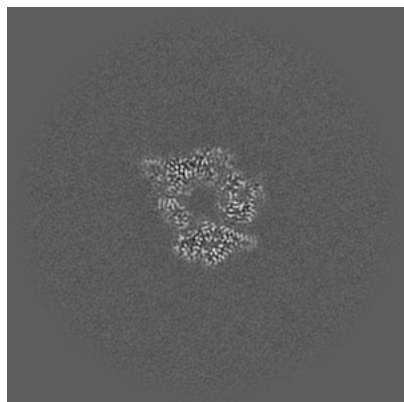


Z

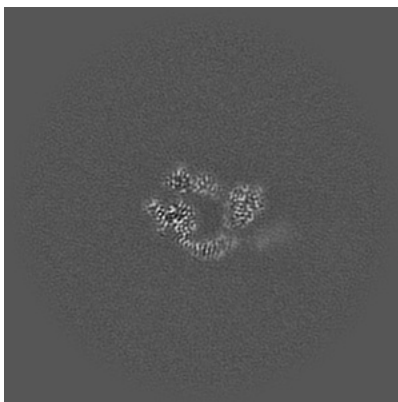
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

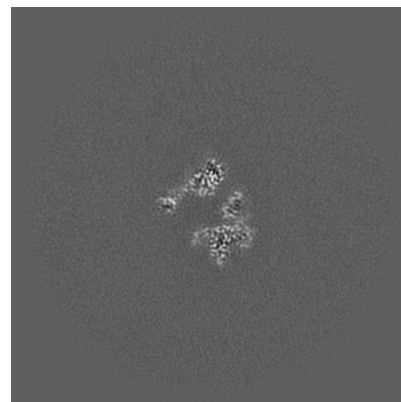
6.2.1 Primary map



X Index: 192

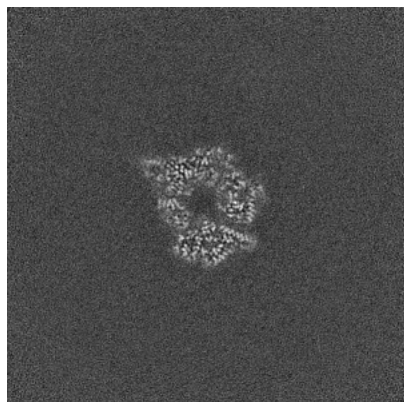


Y Index: 192



Z Index: 192

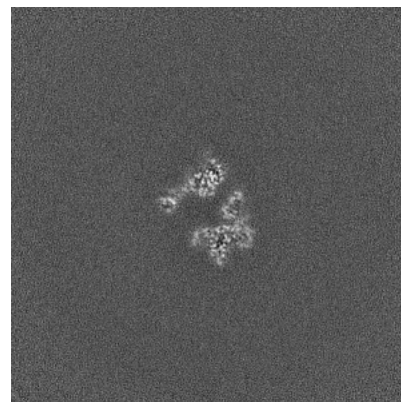
6.2.2 Raw map



X Index: 192



Y Index: 192

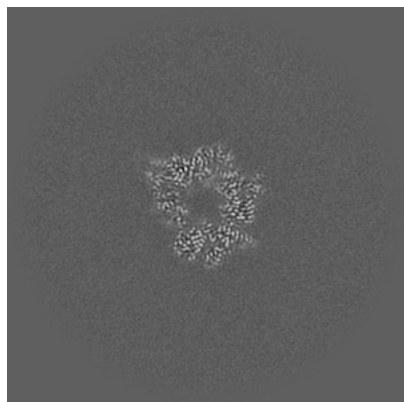


Z Index: 192

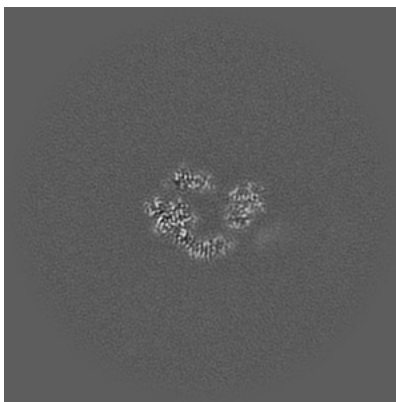
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

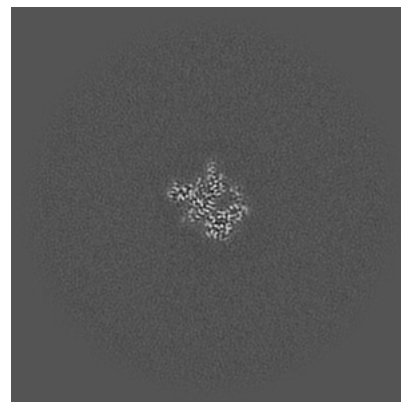
6.3.1 Primary map



X Index: 194

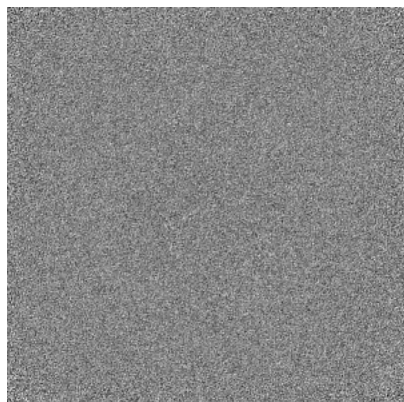


Y Index: 196

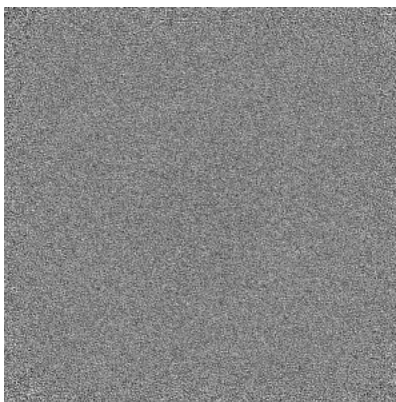


Z Index: 162

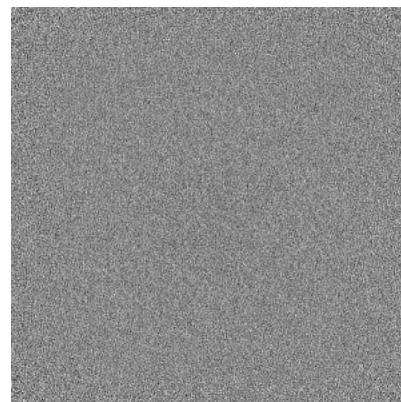
6.3.2 Raw map



X Index: 0



Y Index: 0

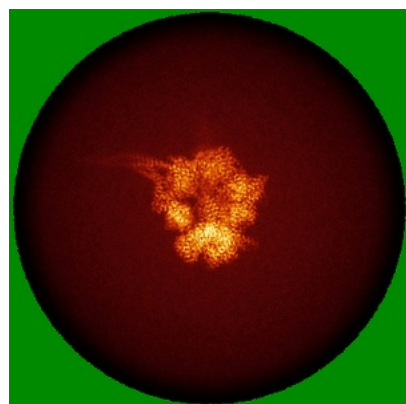


Z Index: 0

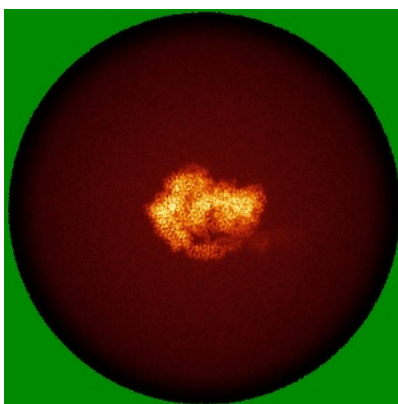
The images above show the largest variance slices of the map in three orthogonal directions.

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

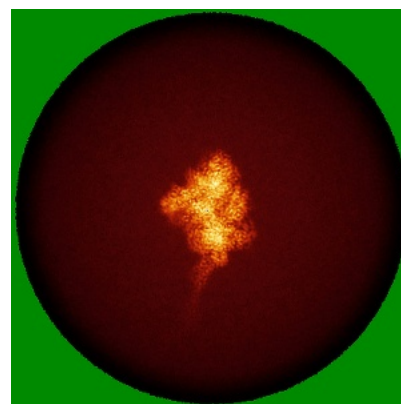
6.4.1 Primary map



X

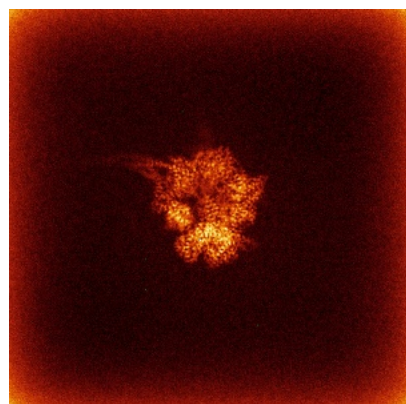


Y

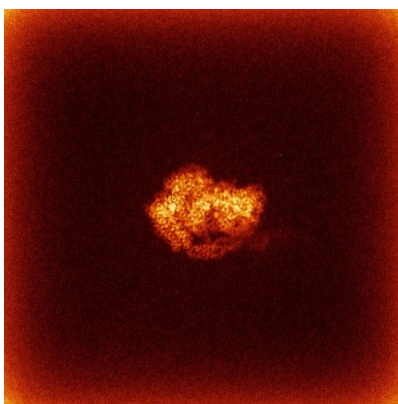


Z

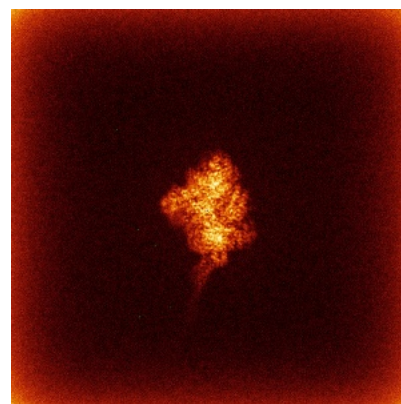
6.4.2 Raw map



X



Y

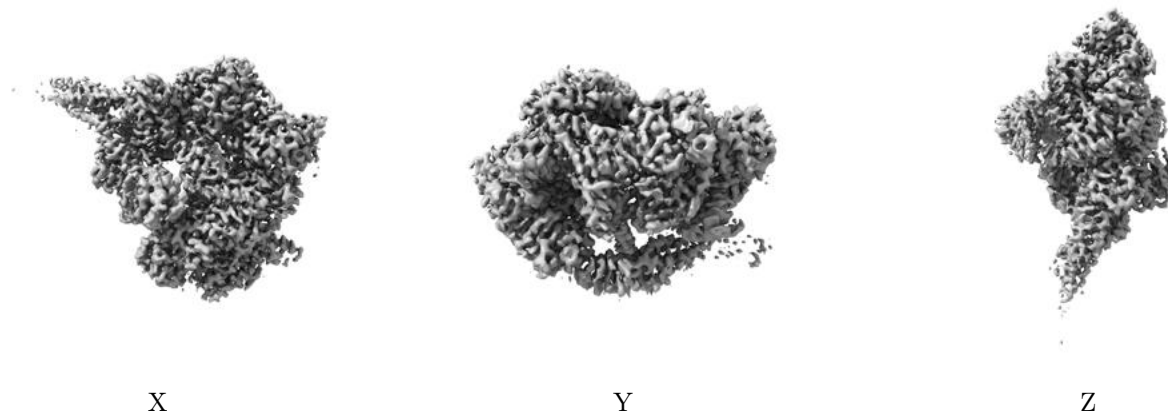


Z

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

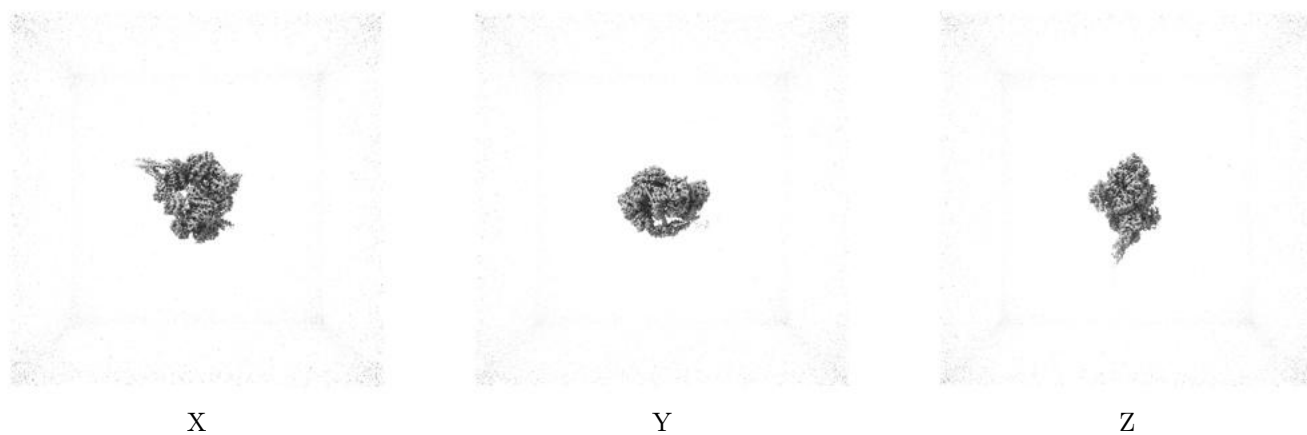
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

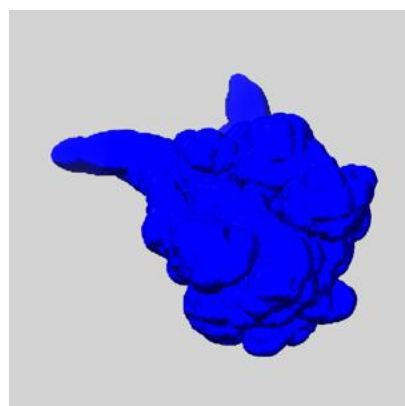
6.6 Mask visualisation [i](#)

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

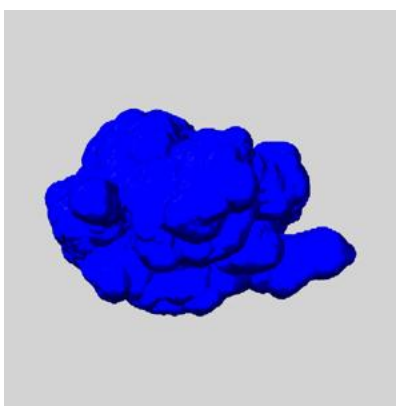
A mask typically either:

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

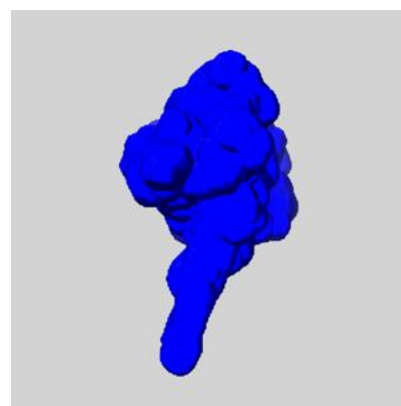
6.6.1 emd_44695_msk_1.map [i](#)



X



Y

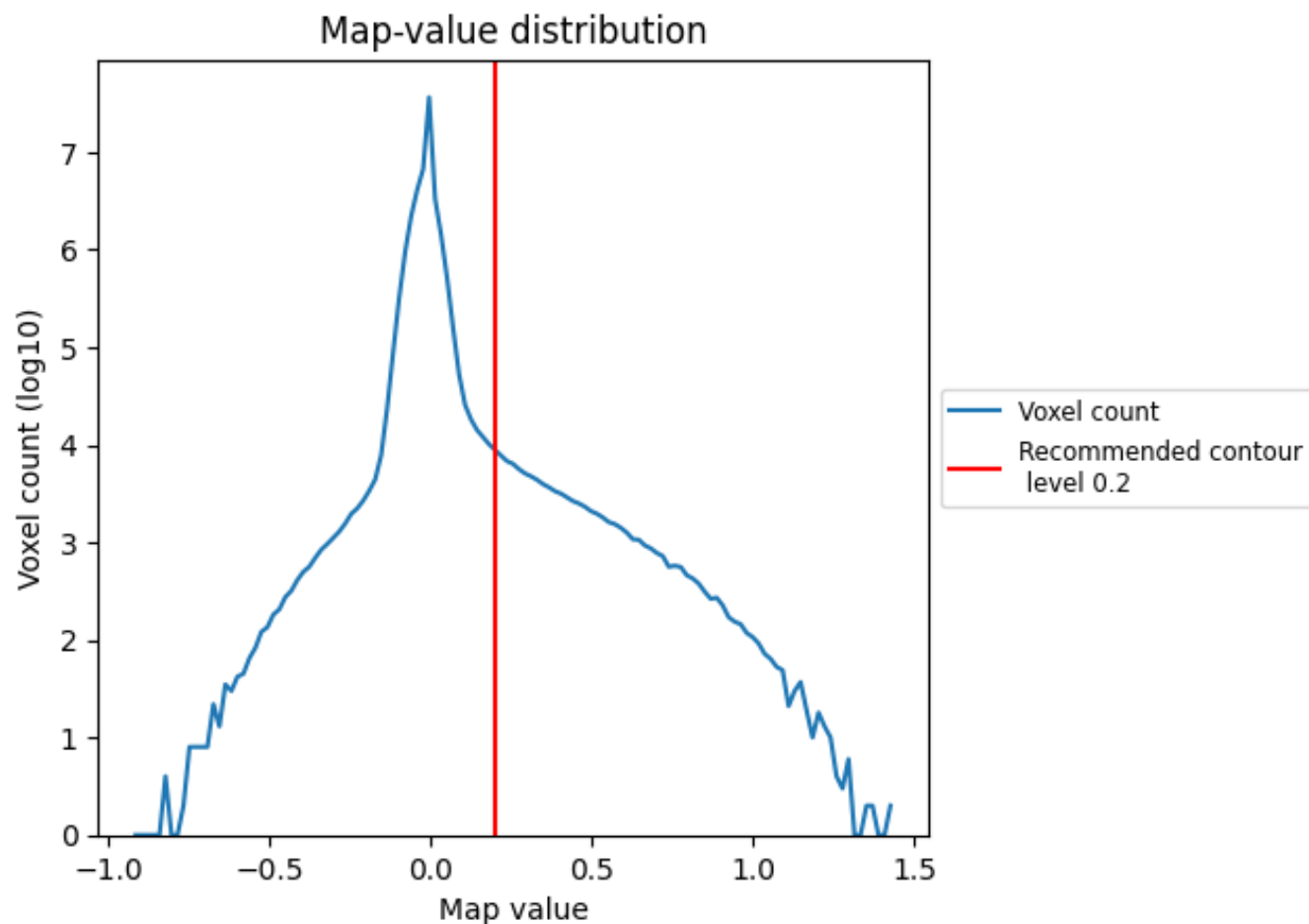


Z

7 Map analysis [i](#)

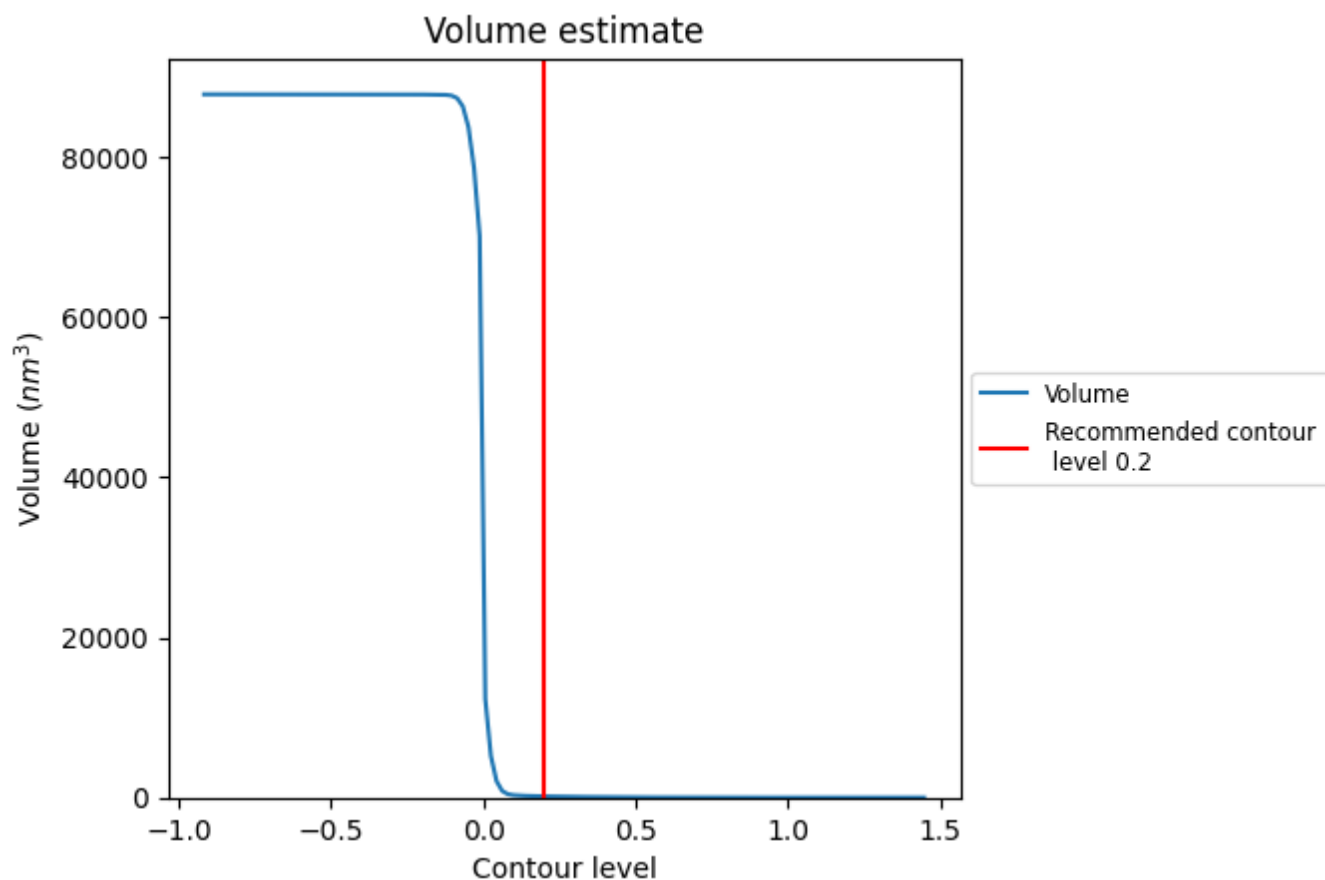
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

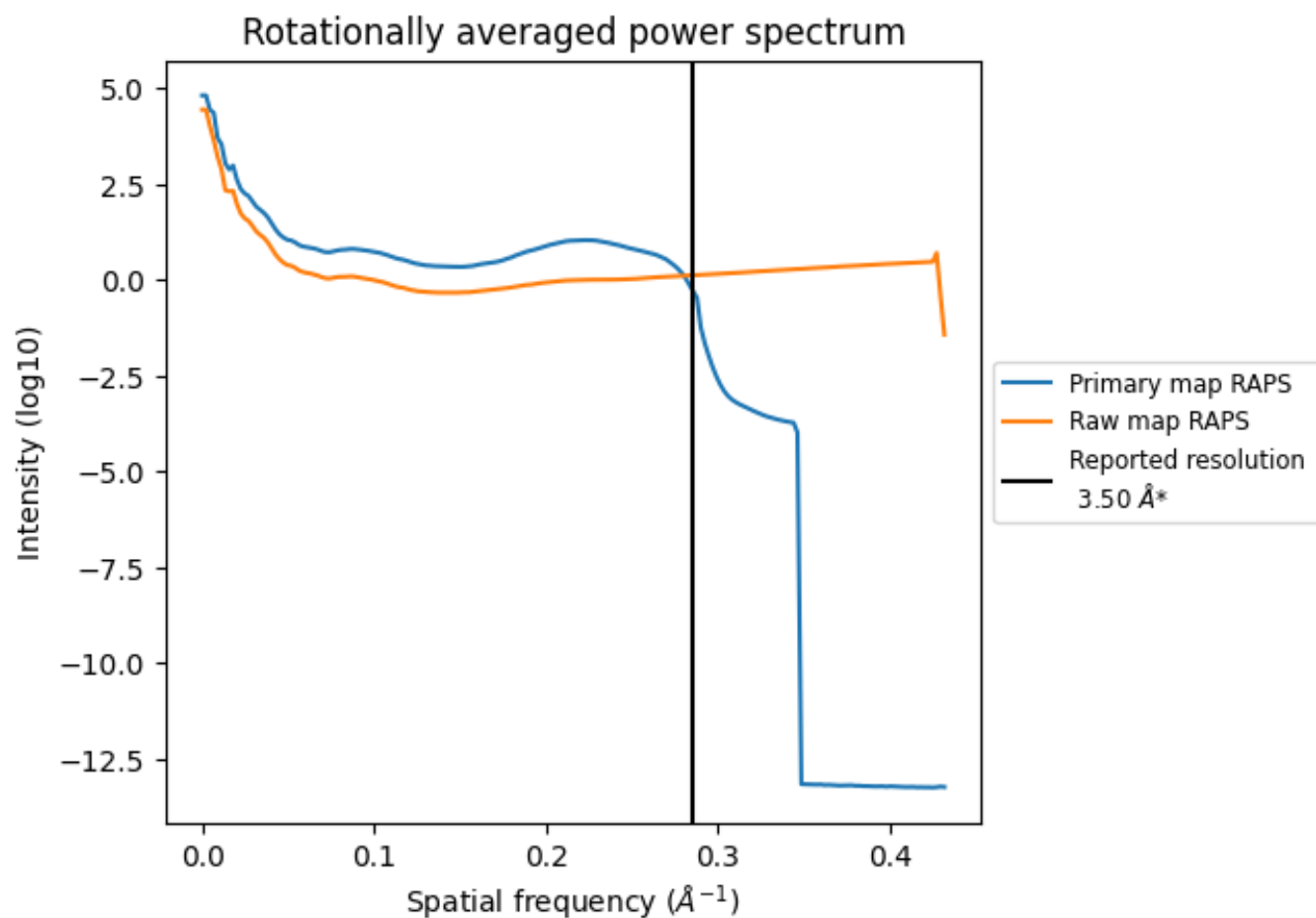
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

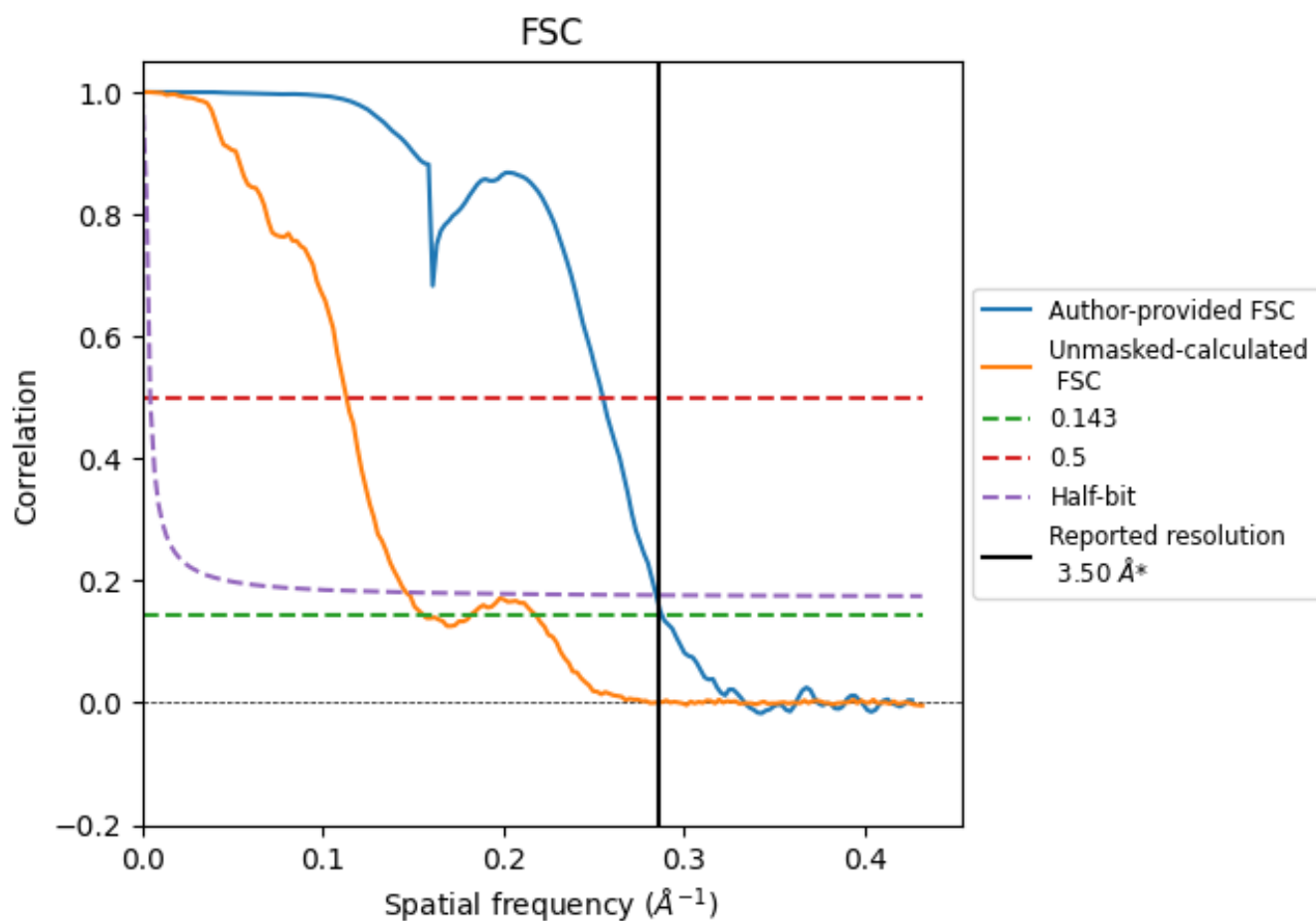


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

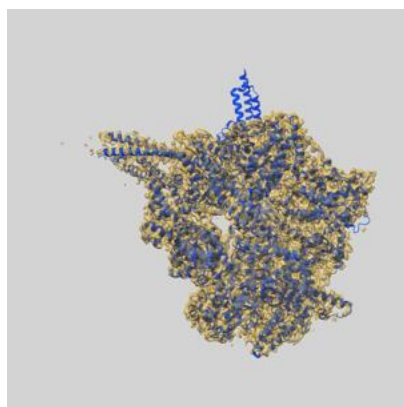
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.92	3.51
Unmasked-calculated*	6.41	8.83	6.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 3.5 by more than 10 %

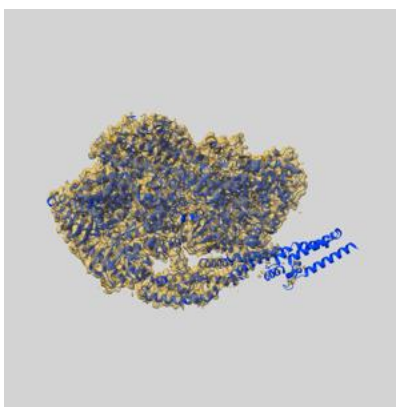
9 Map-model fit [i](#)

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

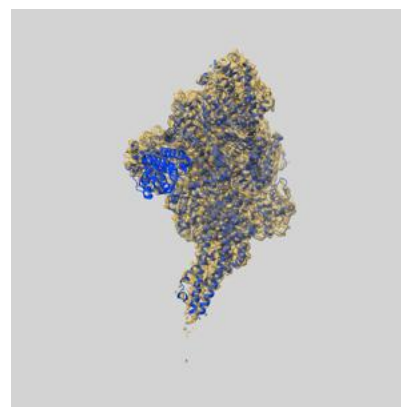
9.1 Map-model overlay [i](#)



X



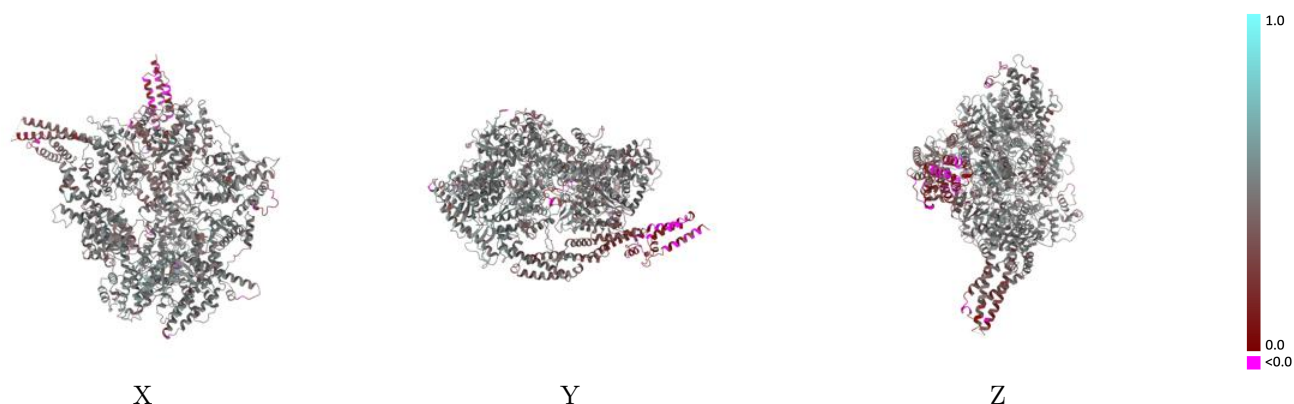
Y



Z

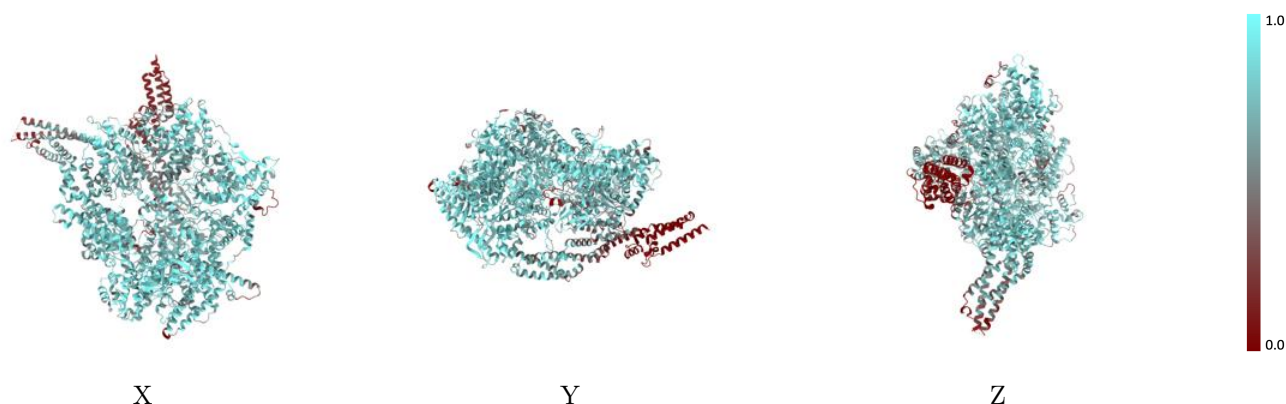
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



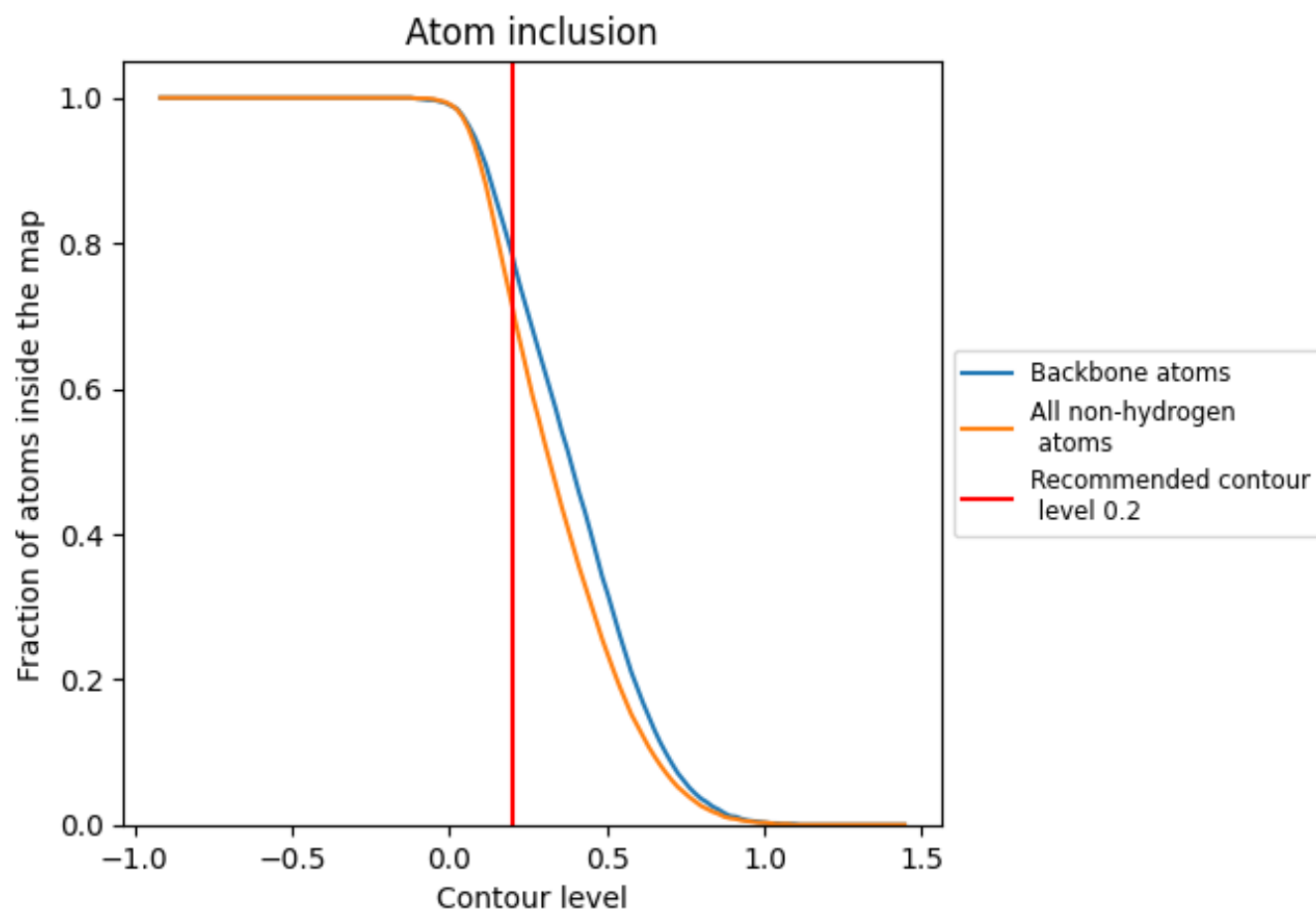
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	<div></div> 0.7140	<div></div> 0.4420
A	<div></div> 0.7140	<div></div> 0.4420

