



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:31 PM UTC

PDB ID : 9BM7 / pdb_00009bm7
EMDB ID : EMD-44690
Title : State-7b of motor domain from full-length human dynein-1 in 5 mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.58 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

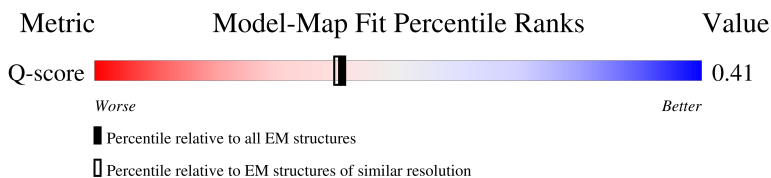
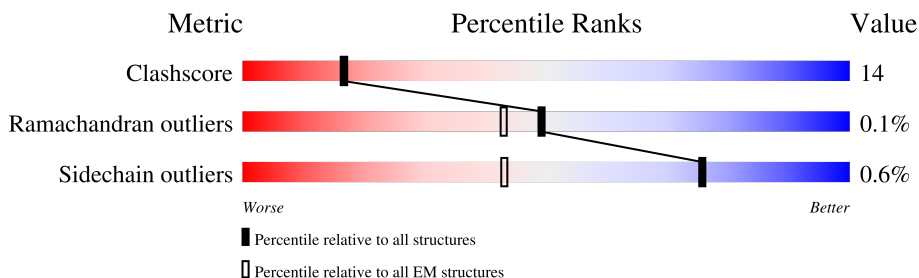
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

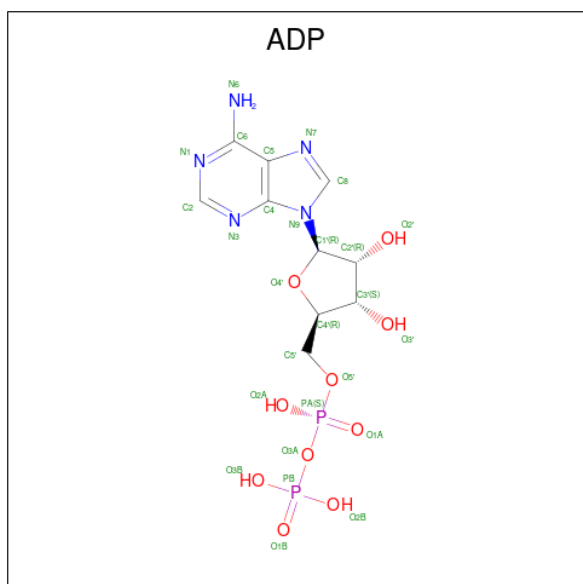
There are 3 unique types of molecules in this entry. The entry contains 21818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

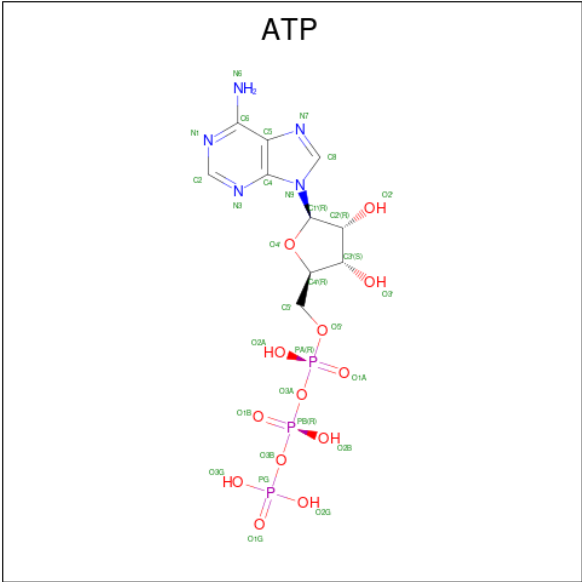
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2703	21702	13828	3748	4016	110	0	0

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

- 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	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	





T4445	N4446	L4451	E4454	R4462	R4485	L4489	L4511	G4512	G4513	L4514	F4515	V4516	P4517	E4537	N4544	Q4549	G4550	A4551	T4552	L4553	F4558	L4565	N4572	N4573	K4574	L4577	M4578	L4579	L4585	Q4595	T4596	N4597	K4600	K4601	A4602	S4603	V4604	V4605	R4615	D4631	P4632															
ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	THR	THR	ASP	SER	SER	ASP	ARG	PRO	A4375	R4378	H4381	L4388	L4388	T4394	L4398	K4399	R4400	K4406	D4407	P4408	L4409	F4410	E4414	L4424	R4428	L4431	A4432	V4435	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444														
GLN	GLU	VAL	ILE	THR	THR	SER	LYS	THR	THR	GLN	ILE	VAL	GLN	LYS	PHE	LYS	VAL	GLU	THR	ILE	VAL	ALA	GLN	ASN	PHE	SER	ALA	GLU	LYS	ILE	SER	LYS	ASN	TYR	ASN	TYR	GLU	ALA	ILE	VAL	GLU	VAL	SER	ILE	CYS	LEU	LEU									
LEU	GLY	PRO	THR	THR	ASP	TRP	LYS	MET	GLN	ILE	VAL	ALA	GLN	LYS	ARG	VAL	GLU	ASN	PHE	ILE	ARG	VAL	PRO	THR	ILE	VAL	ASN	PHE	ALA	GLU	LYS	ILE	SER	LYS	ASN	TYR	ASN	TYR	GLU	ALA	ILE	VAL	GLU	VAL	SER	ILE	CYS	LEU	LEU							
F3520	D3521	M3524	N3540	R3544	T3547	E3551	L3552	D3557	E3558	S3566	D3570	D3571	C3572	T3573	E3575	N3576	L3580	T3581	R3582	R3585	Y3586	P3587	K3588	L3588	P3592	T3600	M3601	N3602	E3603	Y3604	D3606	R3607	K3608	D3617	A3618	F3619	R3620	K3621	N3622	S3623	S3624	S3625	K3626	L3627	M3500	D3506	F3513	Y3516	Y3519							
N3631	P3632	D3637	V3638	S3639	S3640	Y3641	E3652	V3653	K3654	R3655	T3656	G3657	G3658	R3659	V3660	L3661	I3662	T3663	L3664	G3665	D3666	Q3667	D3668	L3671	S3674	L3679	S3680	T3681	R3682	D3683	P3684	T3685	V3686	E3687	D3691	L3692	C3693	V3696	T3697	F3698	V3699	N3700	T3704	R3705	S3706	S3707	N3714									
K3718	A3719	E3720	D3725	R3728	S3729	D3730	L3731	L3732	K3733	L3734	Q3735	G3736	E3737	F3738	Q3739	L3740	R3741	L3742	R3743	Q3744	L3745	D3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	L3760	L3761	D3762	D3763	D3764	T3765	L3766	T3767	T3768	T3769	E3771	N3772	L3773	K3774	R3775	E3776	A3777	A3778	E3779	V3780	T3781
R3782	K3783	V3784	E3785	E3786	T3787	D3788	L3789	V3790	M3791	Q3792	E3793	Y3794	E3795	T3796	V3797	S3798	F3813	T3814	L3818	I3821	L3822	S3828	F3831	F3832	I3835	V3839	L3840	N3843	L3846	D3851	R3855	L3856	T3859	D3862	V3866	R3870	R3873	G3874	M3875	L3876	D3879	A3888														
D3902	H3907	F3908	L3909	R3910	G3911	N3912	E3913	L3914	V3915	L3916	S3917	A3918	T3921	P3922	R3923	T3924	Q3925	G3926	L3927	T3928	V3929	E3930	R3931	A3932	E3933	V3936	R3937	L3938	S3939	T3948	Q3952	F3957	L3961	P3966	E3967	Q3968	T3969	Q3985	R3989	L3990	L3991	R3996	F3997	R4000	L4013											
F4017	M4018	M4021	L4025	D4026	L4027	L4030	V4031	G4032	T4033	E4034	P4037	N4038	L4042	N4063	T4064	Q4065	T4066	S4068	L4069	A4070	L4071	A4074	Q4078	A4080	D4081	K4082	L4083	L4084	N4085	V4088	K4089	S4090	G4091	R4092	V4093	M4094	L4095	L4096	K4097	H4100	M4105	L4106	M4107	Q4108	L4109											
E4110	K4111	L4112	L4113	L4116	Q4117	P4118	H4119	A4120	F4125	L4126	T4127	M4128	K4133	N4137	L4138	L4139	R4140	F4145	V4146	P4149	P4150	K4154	M4157	L4158	P4165	R4168	S4172	P4173	R4176	A4177	R4178	L4179	F4186	H4187	I4190	R4193	G4200	W4201	S4202	K4203	R4204	Y4205														
L4212	R4213	S4214	D4220	L4223	D4224	L4233	S4234	K4237	L4238	P4239	A4242	L4243	A4248	Q4249	S4250	T4251	Y4252	G4253	V4256	D4257	M4258	L4269	E4270	R4271	T4274	T4275	R4276	H4291	P4297	L4312	T4315	W4320	N4326	M4343	L4344	K4345	M4346	Q4347	MET	LEU	GLU	ASP	GLU													
ASP	ASP	ALA	ALA	GLU	THR	LYS	THR	THR	THR	ASP	THR	THR	ARG	GLY	PRO	A4375	R4378	H4381	L4388	L4388	T4394	L4398	K4399	R4400	K4406	D4407	P4408	L4409	F4410	E4414	L4424	R4428	L4431	A4432	V4435	Q4436	V4437	C4438	E4439	K4442	K4443	Q4444														
LEU	GLY	PRO	THR	THR	ASP	TRP	LYS	MET	GLN	ILE	VAL	ALA	GLN	LYS	PHE	LYS	VAL	GLU	THR	ILE	VAL	ALA	GLN	ASN	PHE	ALA	GLU	LYS	ILE	SER	LYS	ASN	TYR	ASN	TYR	GLU	ALA	ILE	VAL	GLU	VAL	SER	ILE	CYS	LEU	LEU										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/22168	0.36	0/30054

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	21702	0	21742	610	0
2	A	54	0	24	7	0
3	A	62	0	24	11	0
All	All	21818	0	21790	610	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 610 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:3151:HIS:HD1	1:A:3516:TYR:HH	0.96	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3660:VAL:HG22	1:A:3671:LEU:HD13	1.60	0.84
1:A:2437:LEU:HD22	1:A:2502:LEU:HD21	1.61	0.81
1:A:1882:THR:HB	1:A:1883:PRO:HD2	1.64	0.79
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.64	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2689/4646 (58%)	2606 (97%)	80 (3%)	3 (0%)	48 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	2387	LEU

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	2401/4125 (58%)	2387 (99%)	14 (1%)	78 79

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2388	ASP
1	A	2452	LEU
1	A	4454	GLU
1	A	3623	LEU
1	A	4315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4012	ASN
1	A	4326	ASN
1	A	4526	GLN
1	A	4389	HIS
1	A	4174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4701	-	28,29,29	0.47	0	43,45,45	0.56	0
2	ADP	A	4704	-	28,29,29	1.38	5 (17%)	43,45,45	1.81	9 (20%)
3	ATP	A	4703	-	32,33,33	0.49	0	48,52,52	0.32	0
3	ATP	A	4702	-	32,33,33	0.55	0	48,52,52	0.60	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
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/16/32/32	0/3/3/3
3	ATP	A	4703	-	-	4/22/38/38	0/3/3/3
3	ATP	A	4702	-	-	6/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.45	1.47	1.39
2	A	4704	ADP	C5-C6	2.58	1.48	1.41
2	A	4704	ADP	C5-N7	-2.49	1.34	1.39
2	A	4704	ADP	C8-N7	2.28	1.36	1.31
2	A	4704	ADP	C4-N9	-2.08	1.33	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C4-N3	-5.69	118.88	126.72
2	A	4704	ADP	N3-C4-N9	4.39	134.63	127.17
2	A	4704	ADP	C2-N3-C4	3.60	120.63	111.83
2	A	4704	ADP	C4-C5-N7	-3.56	106.51	110.58
2	A	4704	ADP	N3-C2-N1	-3.10	123.88	128.58

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

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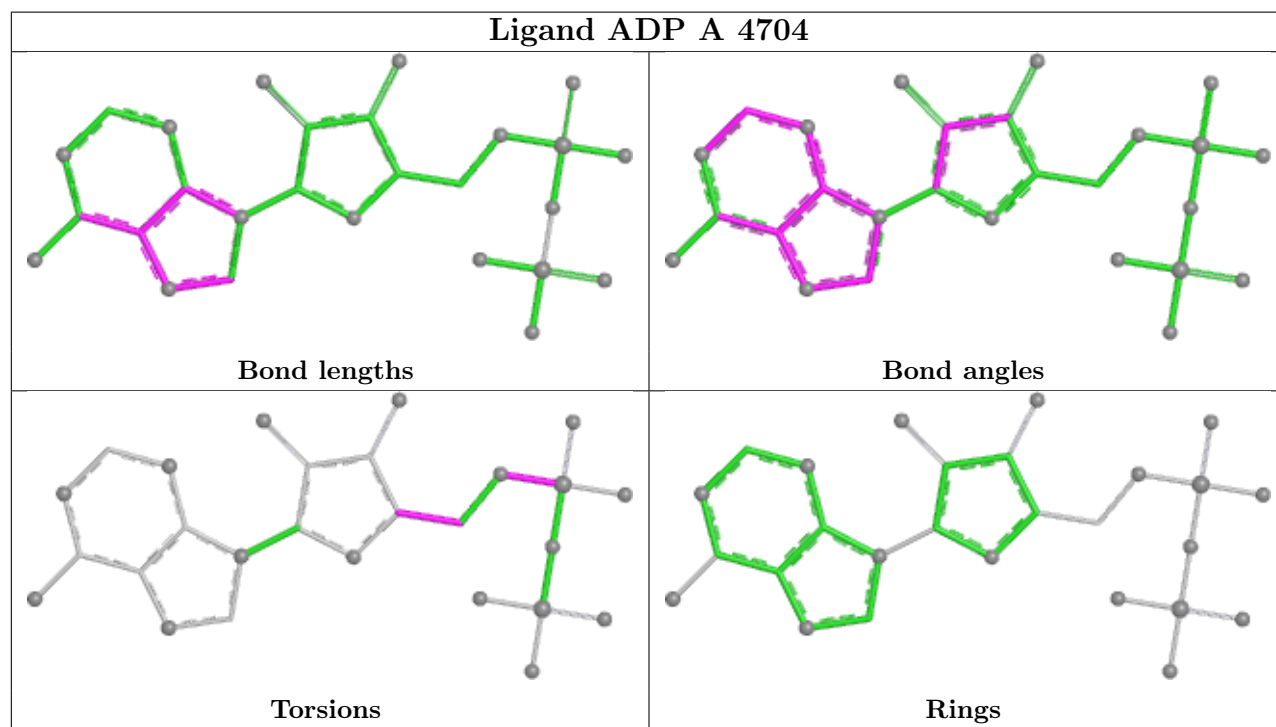
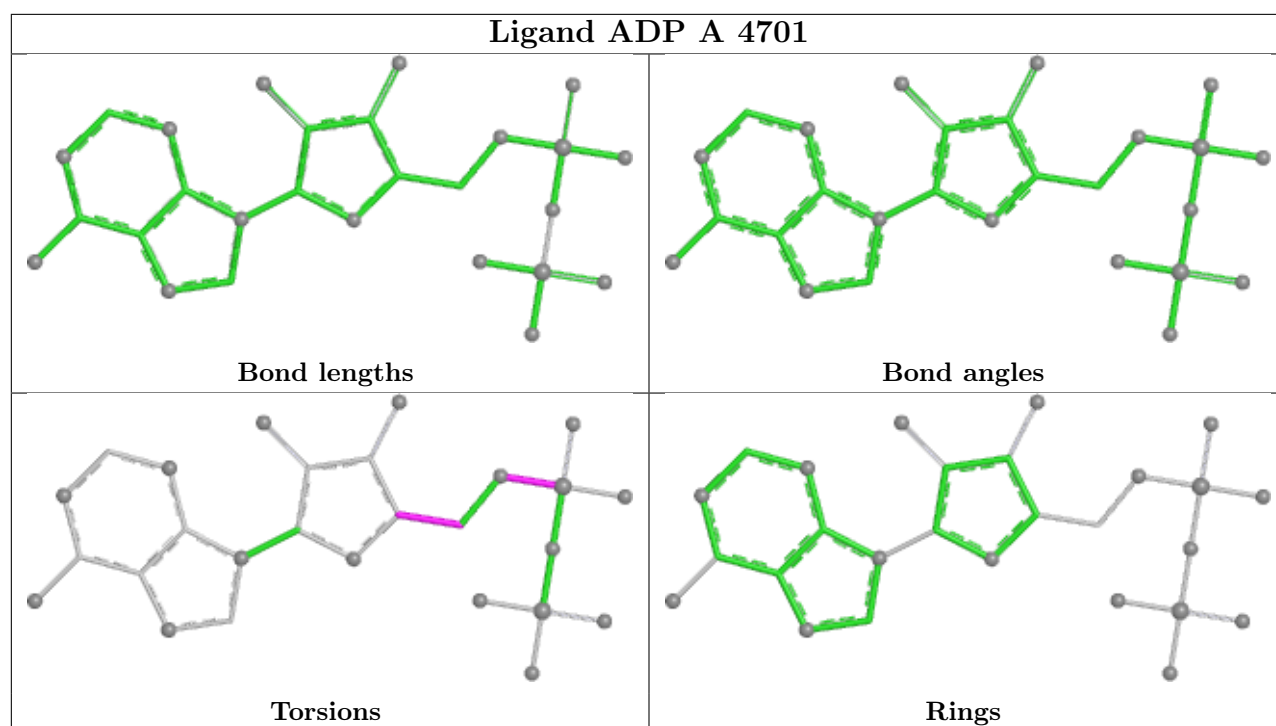
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

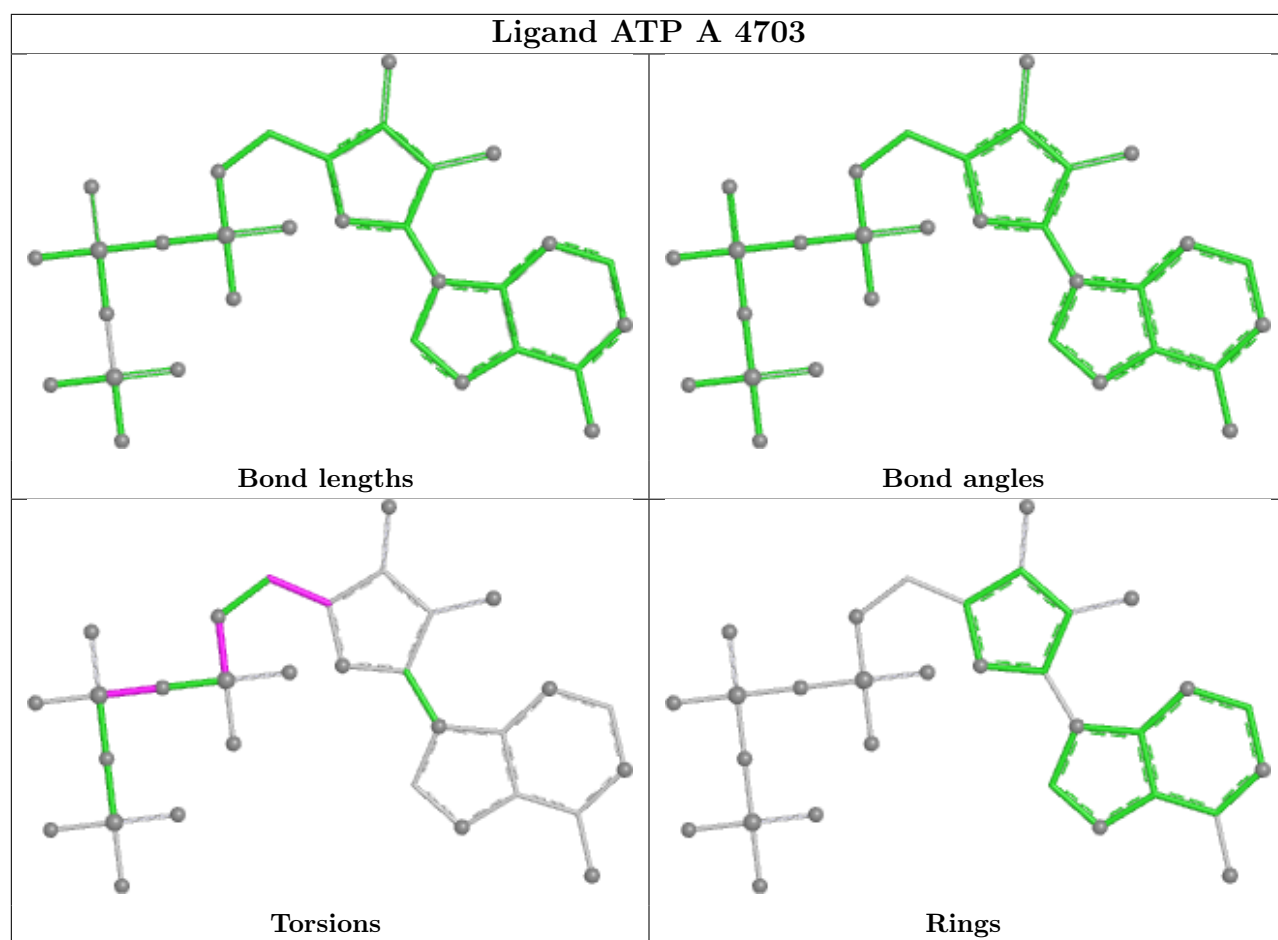
There are no ring outliers.

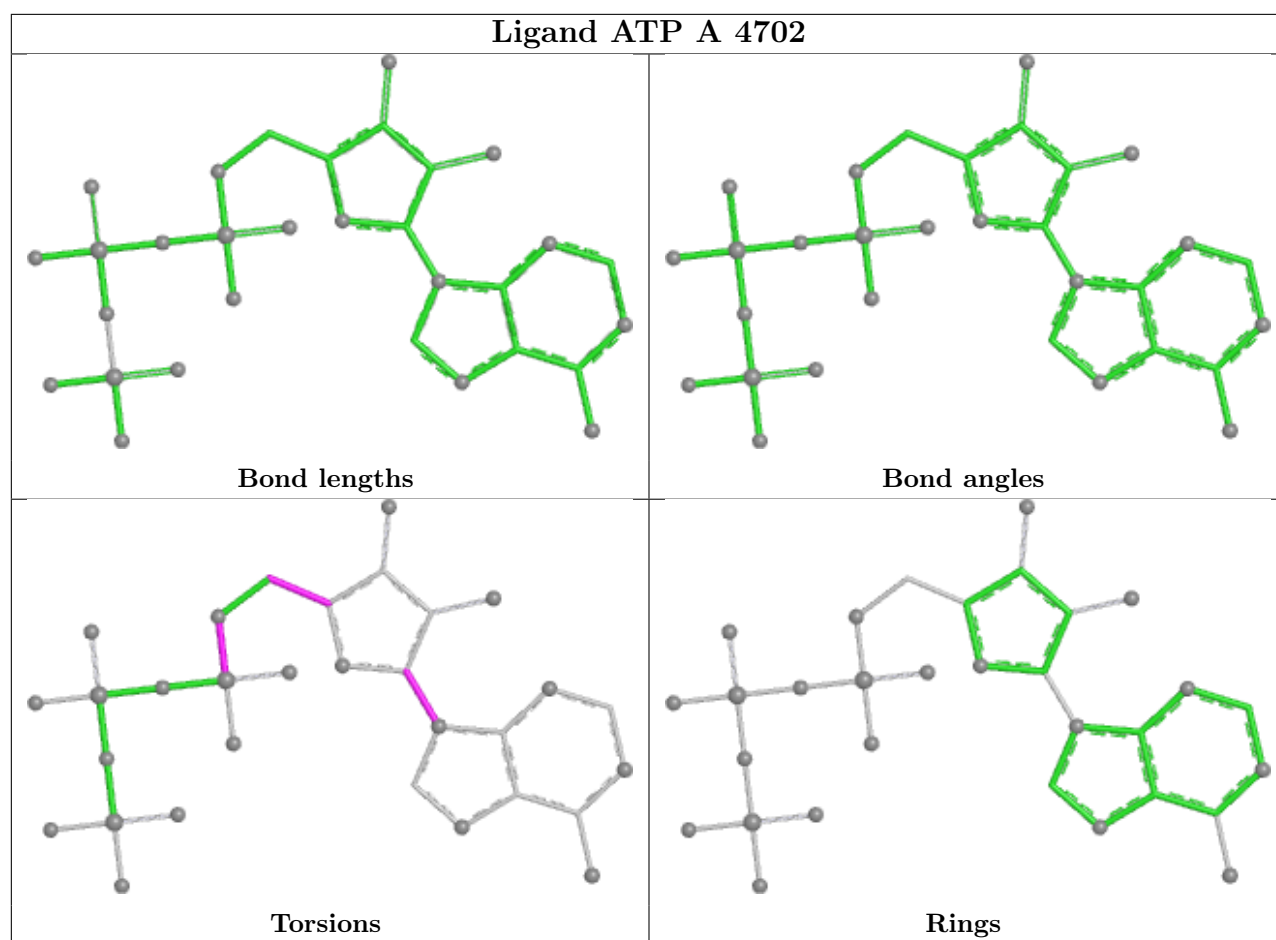
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	5	0
2	A	4704	ADP	2	0
3	A	4703	ATP	4	0
3	A	4702	ATP	7	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.

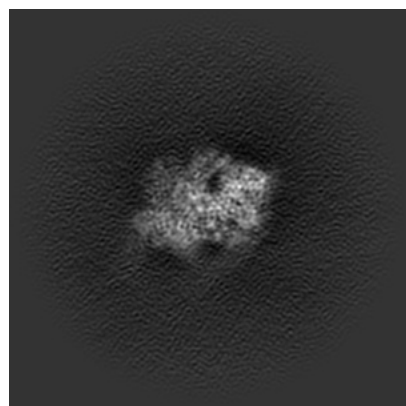
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44690. These allow visual inspection of the internal detail of the map and identification of artifacts.

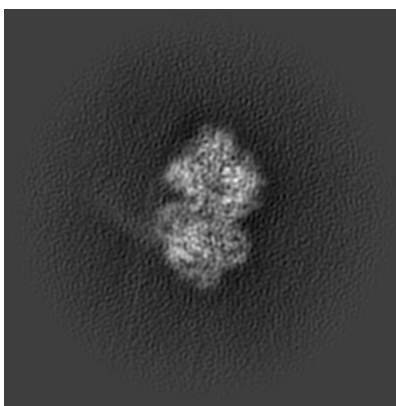
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

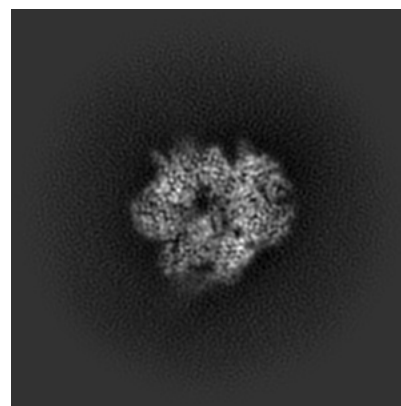
6.1.1 Primary map



X

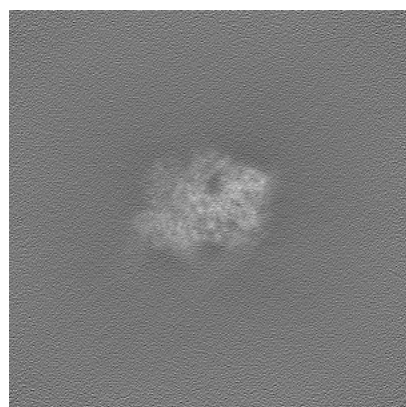


Y

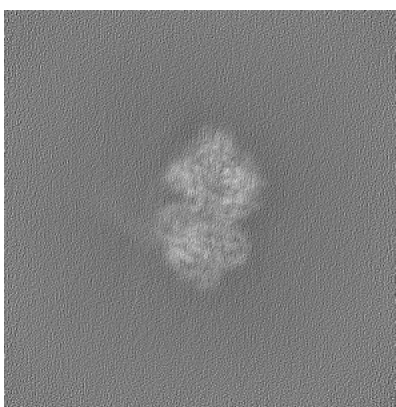


Z

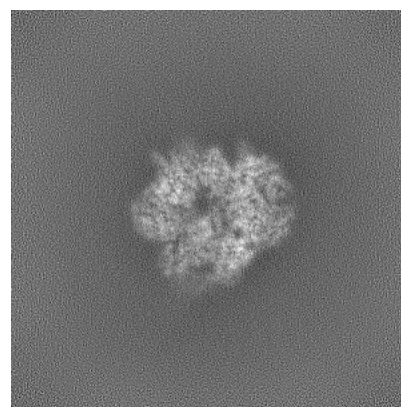
6.1.2 Raw map



X



Y

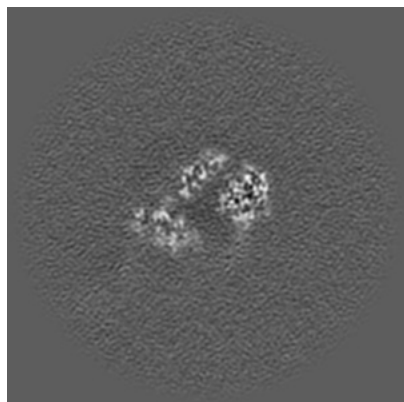


Z

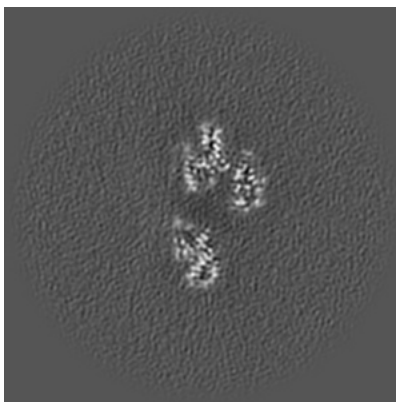
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

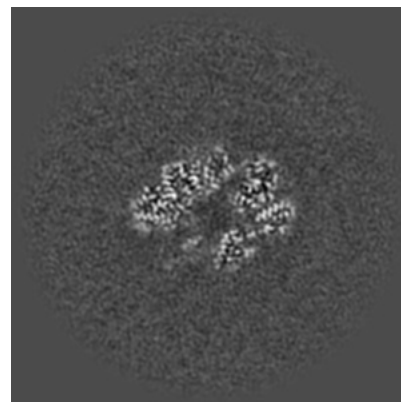
6.2.1 Primary map



X Index: 200

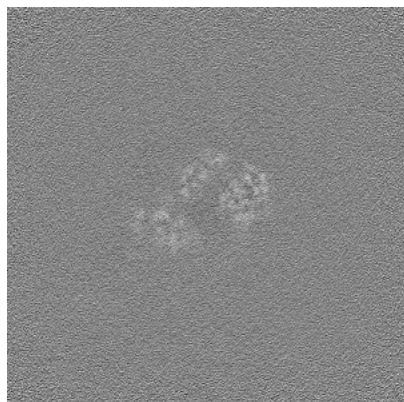


Y Index: 200

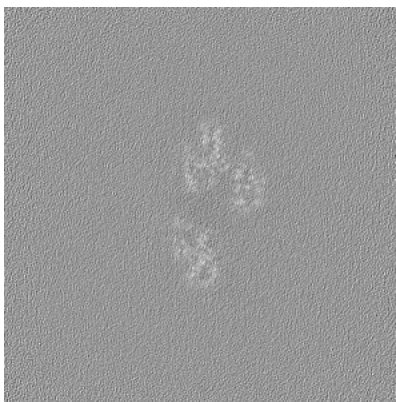


Z Index: 200

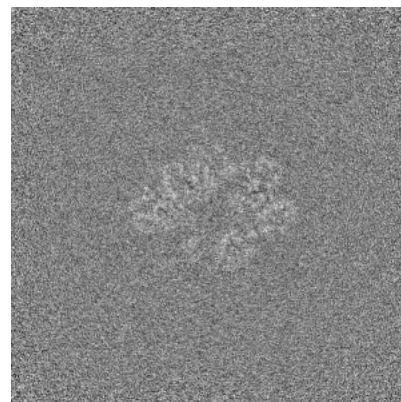
6.2.2 Raw map



X Index: 200



Y Index: 200

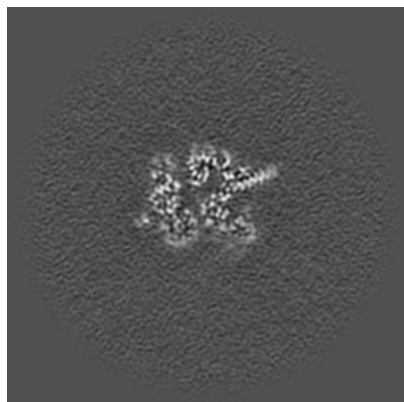


Z Index: 200

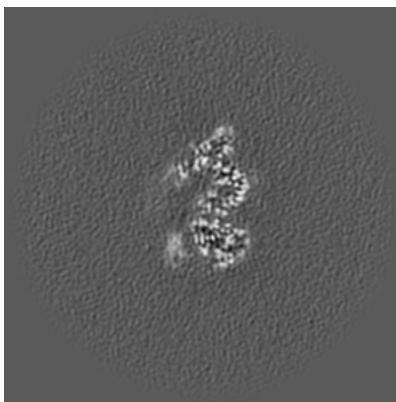
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

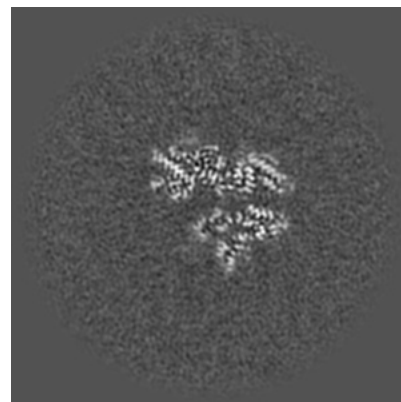
6.3.1 Primary map



X Index: 229

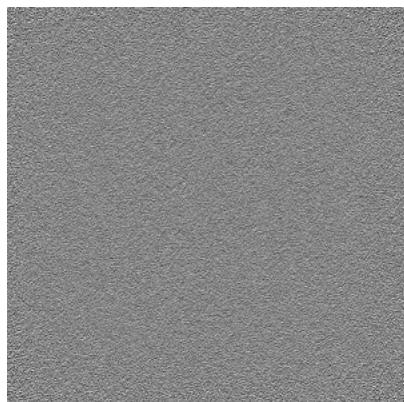


Y Index: 224

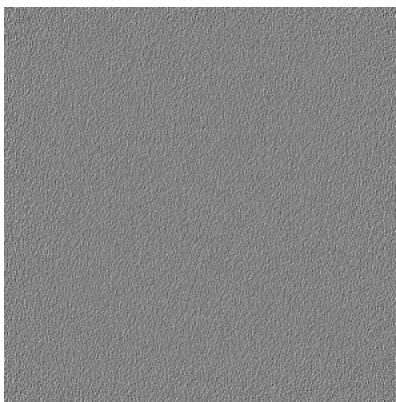


Z Index: 222

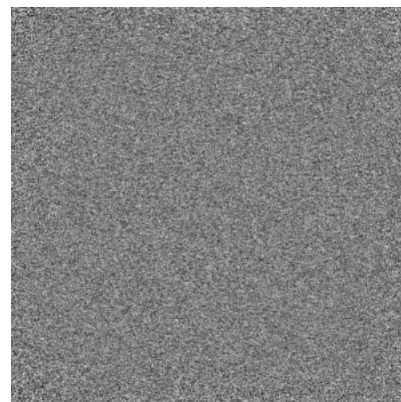
6.3.2 Raw map



X Index: 0



Y Index: 0

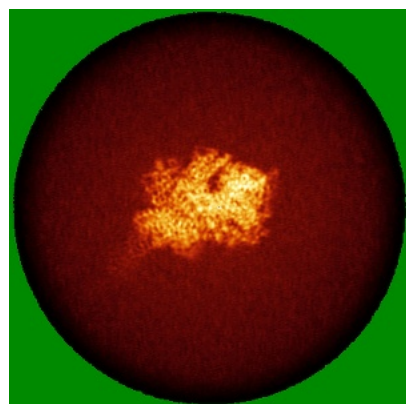


Z Index: 0

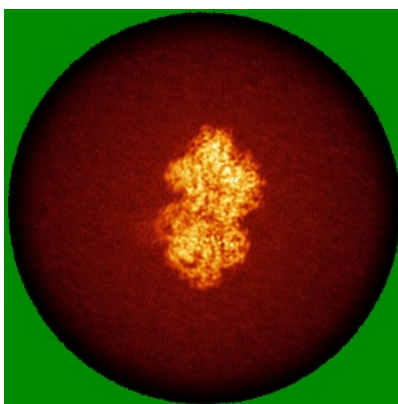
The images above show the largest variance slices of the map in three orthogonal directions.

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

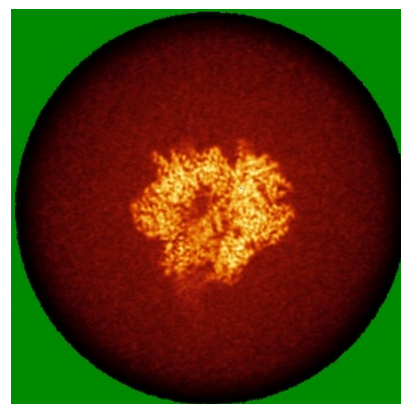
6.4.1 Primary map



X

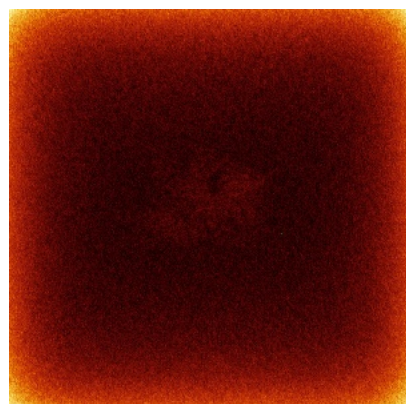


Y

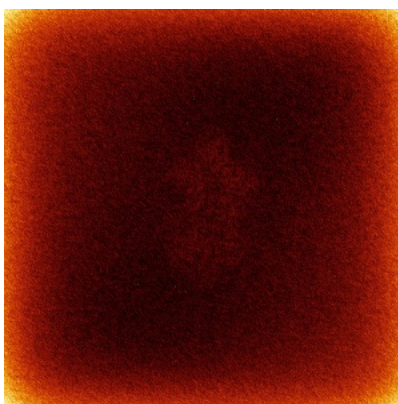


Z

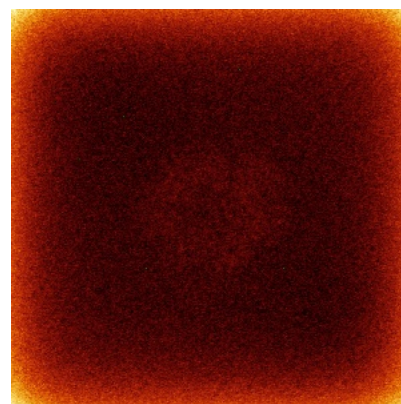
6.4.2 Raw map



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.

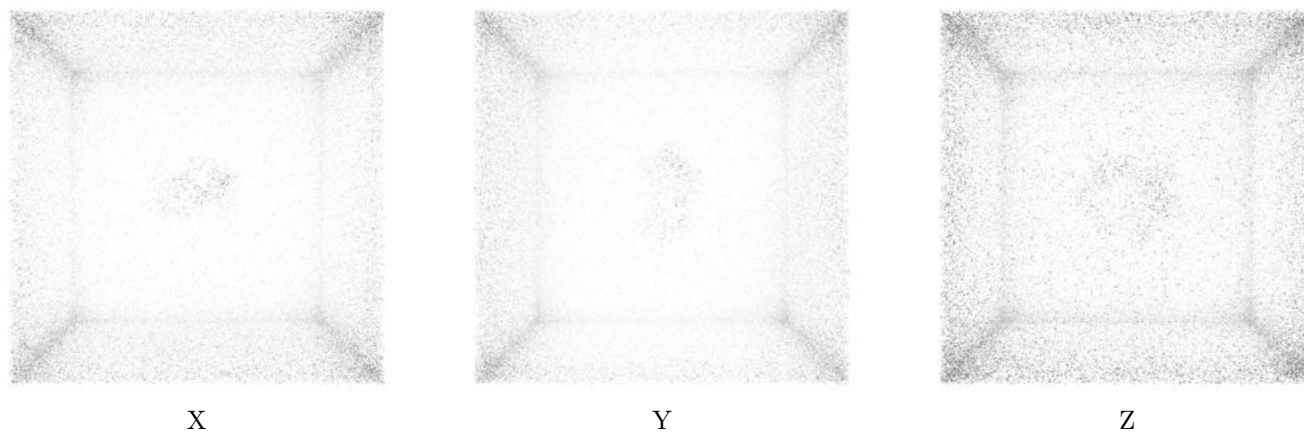
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

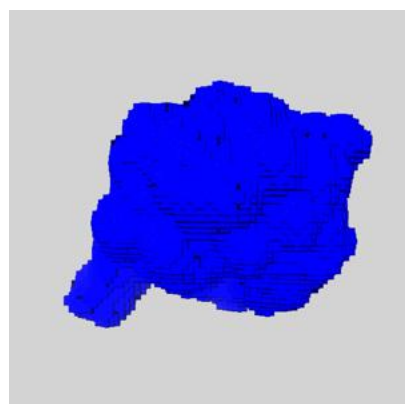
6.6 Mask visualisation [i](#)

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

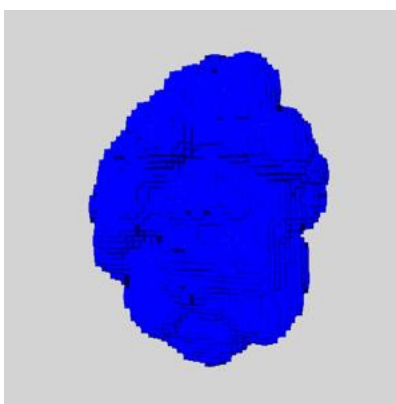
A mask typically either:

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

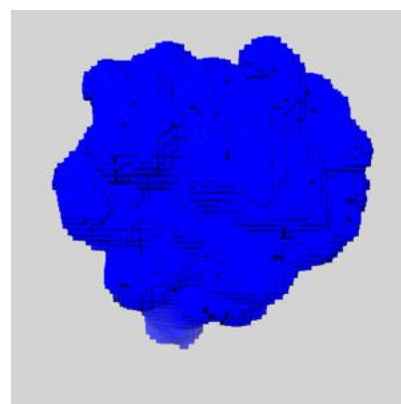
6.6.1 emd_44690_msk_1.map [i](#)



X



Y

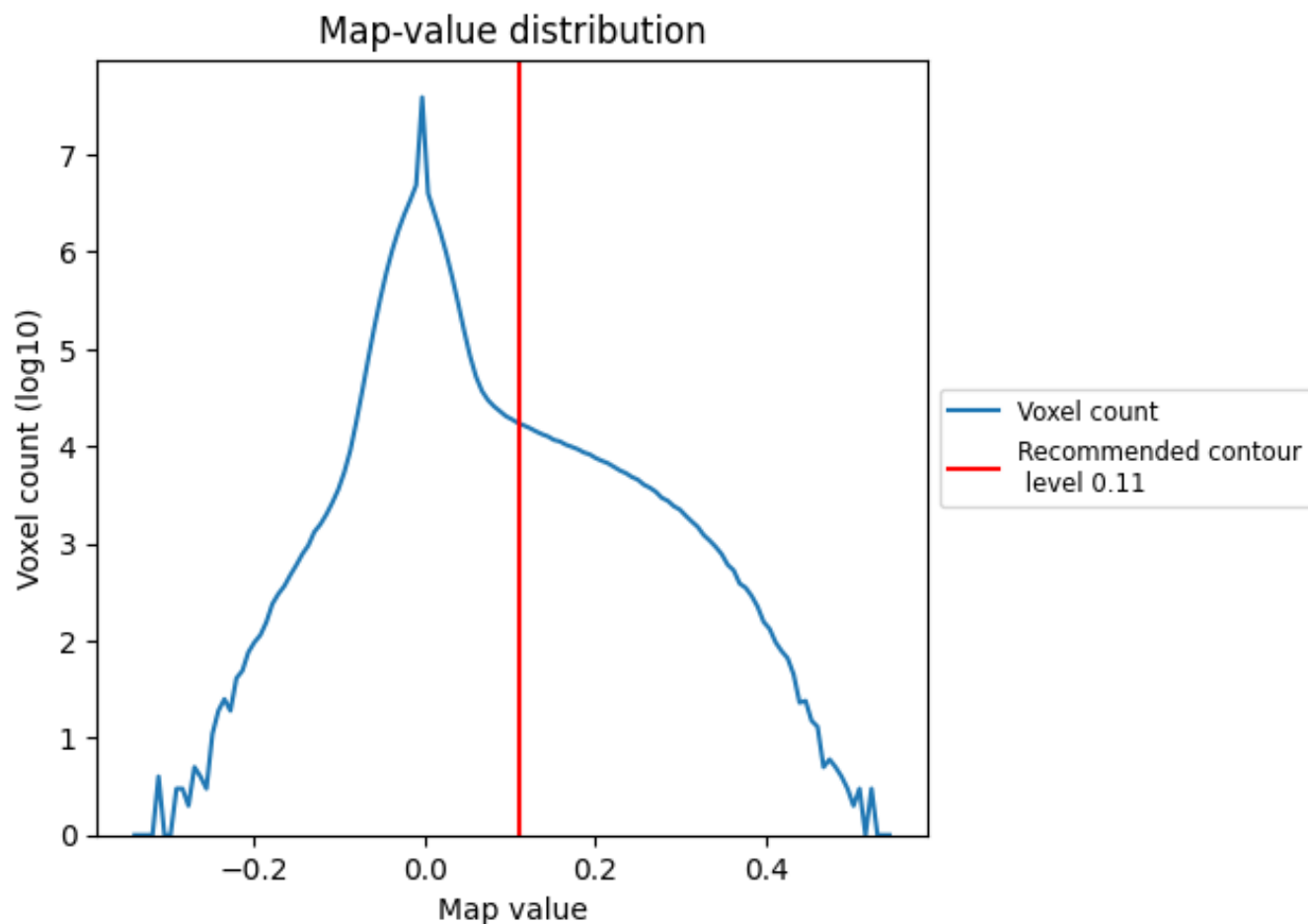


Z

7 Map analysis [i](#)

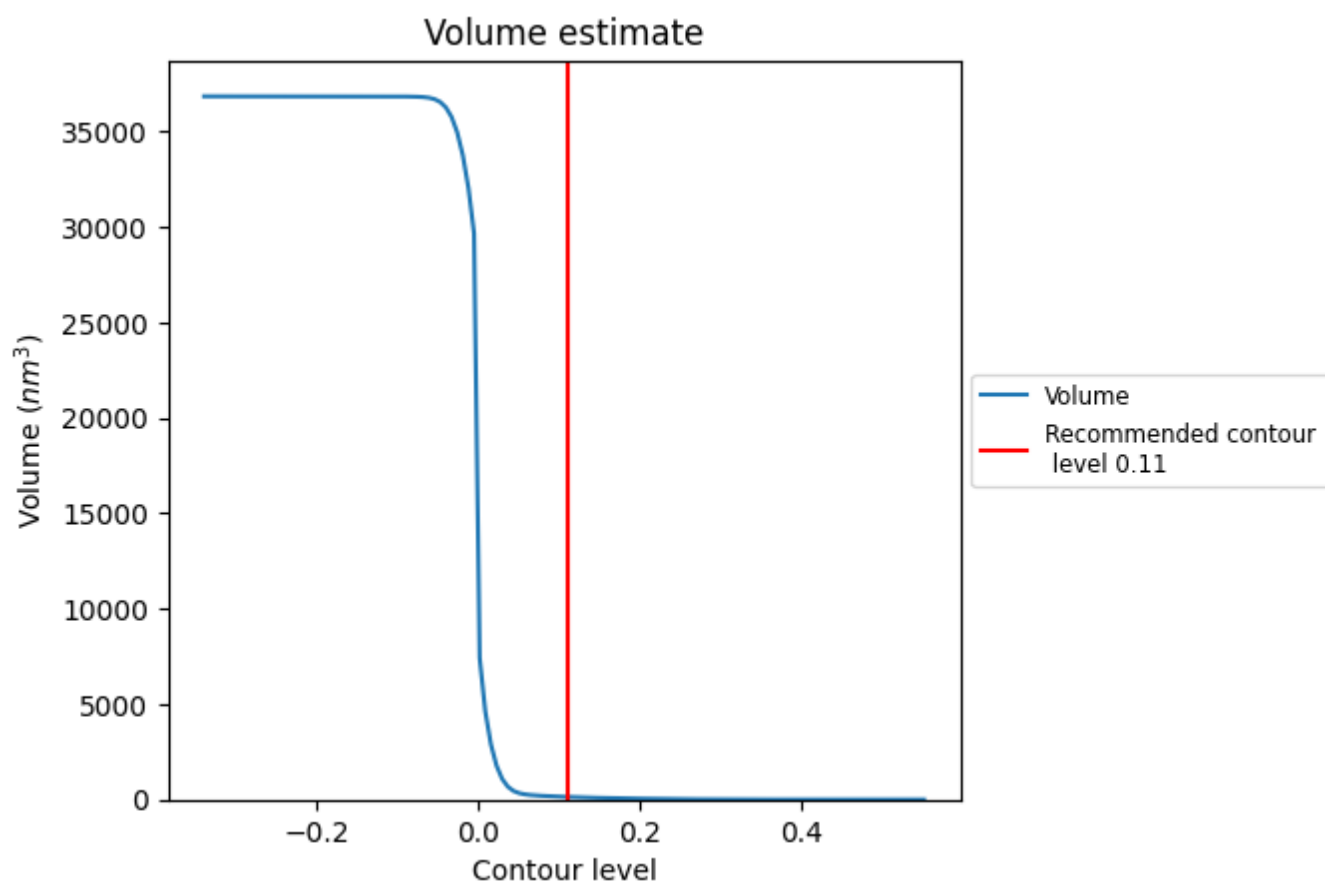
This section contains the results of statistical analysis of the map.

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.

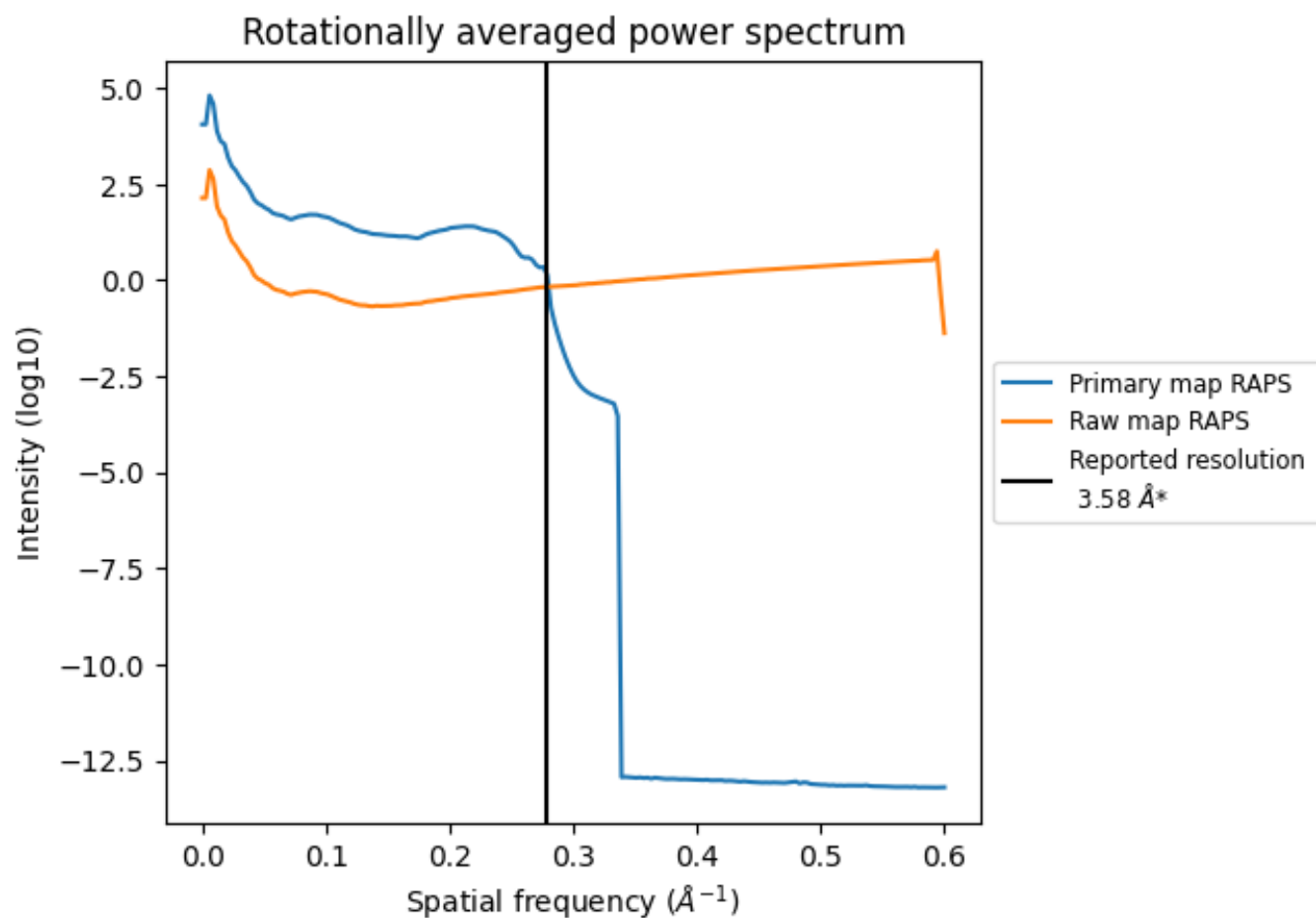
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 124 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 ⓘ

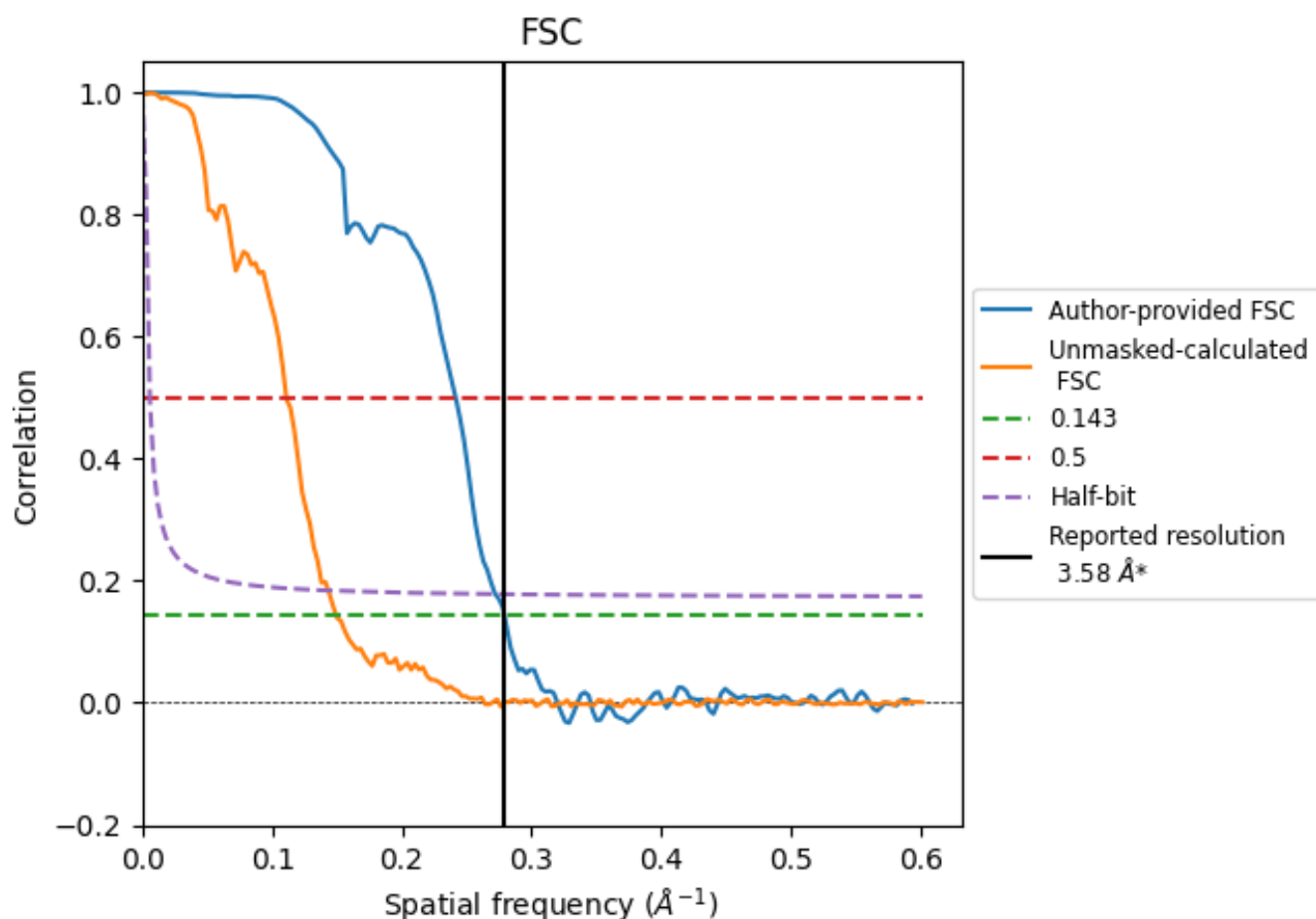


*Reported resolution corresponds to spatial frequency of 0.279 $\text{\AA}^{-1}$

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

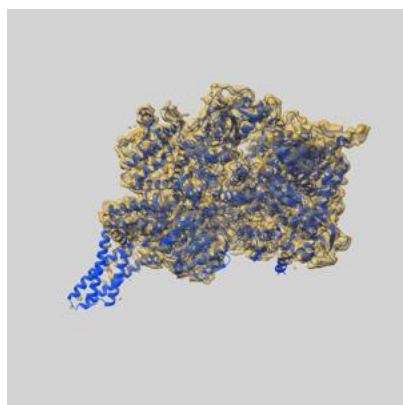
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.14	3.68
Unmasked-calculated*	6.68	9.01	6.97

*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 6.68 differs from the reported value 3.58 by more than 10 %

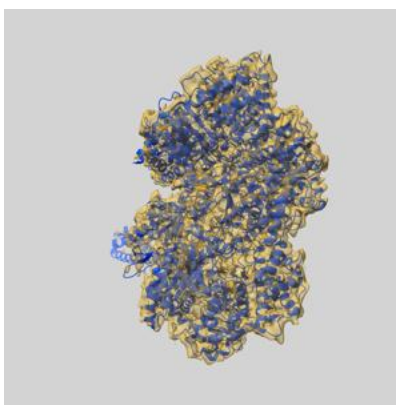
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44690 and PDB model 9BM7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

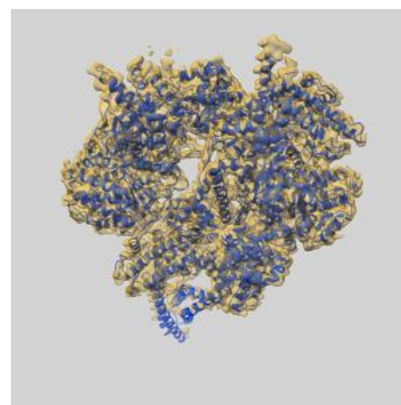
9.1 Map-model overlay [i](#)



X



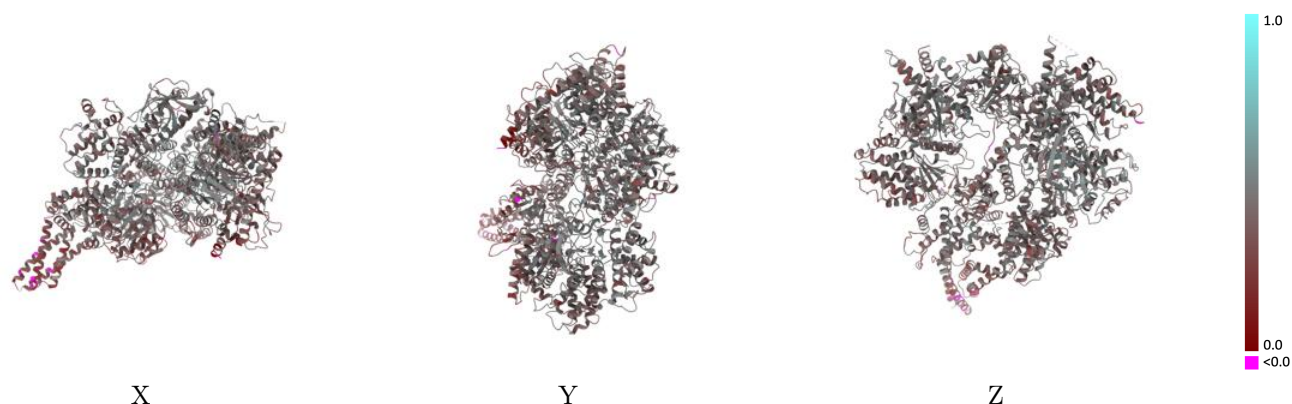
Y



Z

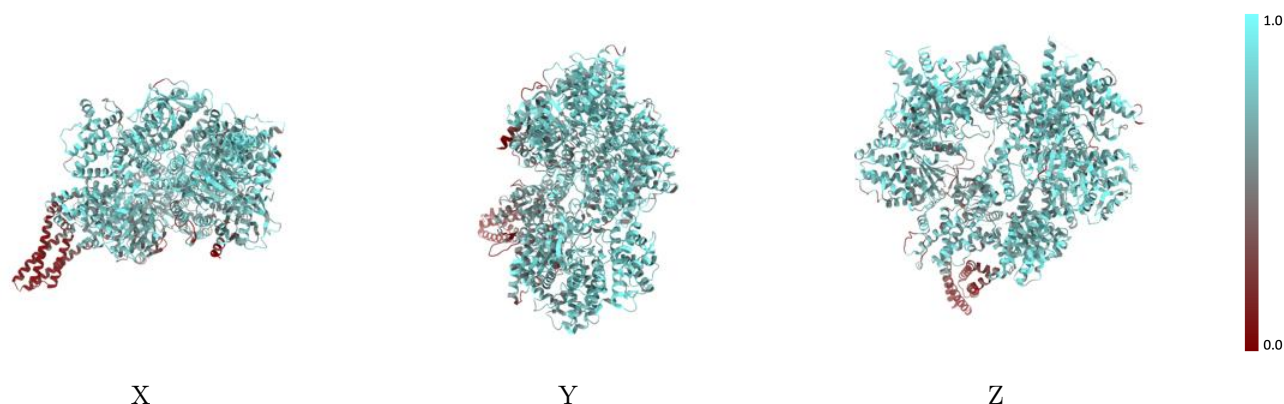
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



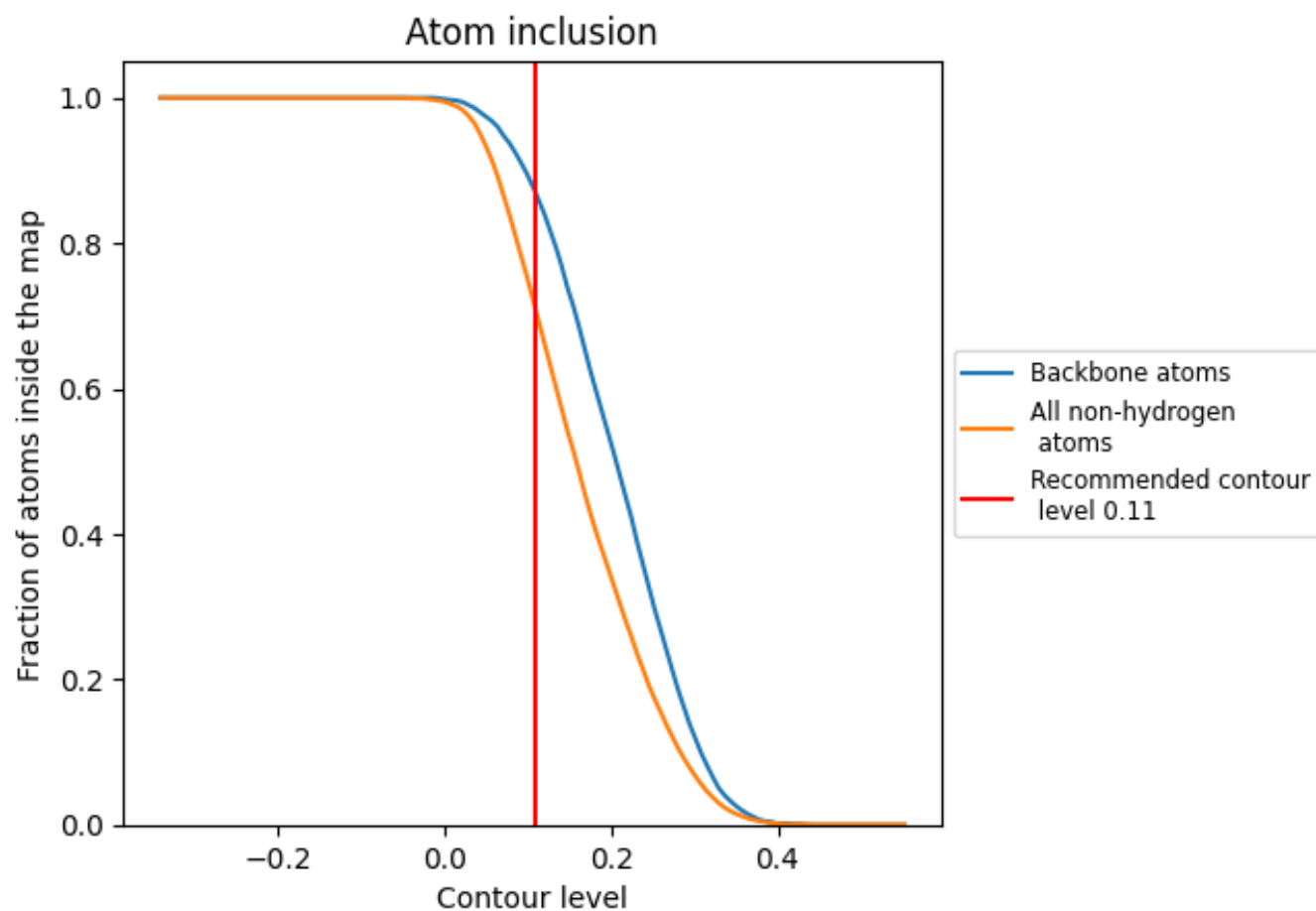
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4100
A	0.7080	0.4100

