



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:23 AM UTC

PDB ID : 9BMN / pdb_00009bmn
EMDB ID : EMD-44704
Title : State-5 of motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

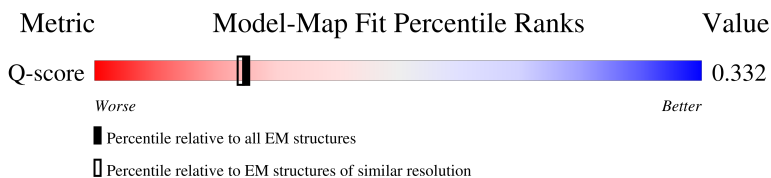
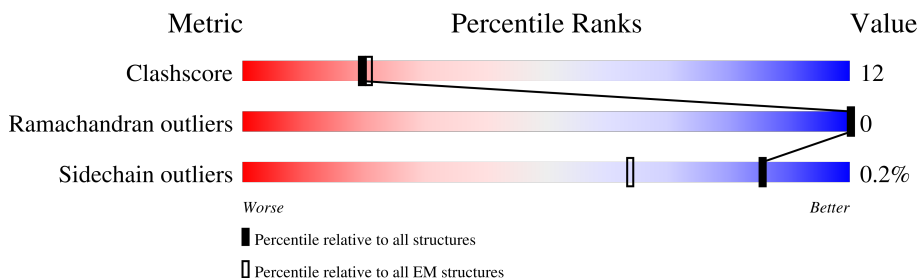
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	<p>9% 42% 16% 42%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21867 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	2711	21755	13852	3757	4035	111	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
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).

L4665	L4666	L4667	L4668	L4669	L4670	L4671	L4672	L4673	L4674	L4675	L4676	L4677	L4678	L4679	L4680	L4681	L4682	L4683	L4684	L4685	L4686	L4687	L4688	L4689	L4690	L4691	L4692	L4693	L4694	L4695	L4696	L4697	L4698	L4699	L4700	L4701	L4702	L4703	L4704	L4705	L4706	L4707	L4708	L4709	L4710	L4711	L4712	L4713	L4714	L4715	L4716	L4717	L4718	L4719	L4720	L4721	L4722	L4723	L4724	L4725	L4726	L4727	L4728	L4729	L4730	L4731	L4732	L4733	L4734	L4735	L4736	L4737	L4738	L4739	L4740	L4741	L4742	L4743	L4744	L4745	L4746	L4747	L4748	L4749	L4750	L4751	L4752	L4753	L4754	L4755	L4756	L4757	L4758	L4759	L4760	L4761	L4762	L4763	L4764	L4765	L4766	L4767			
V4456	K4457	I4458	I4459	L4460	P4461	P4462	H4463	H4464	H4465	H4466	H4467	H4468	H4469	H4470	H4471	H4472	H4473	H4474	H4475	H4476	H4477	H4478	H4479	H4480	H4481	H4482	H4483	H4484	H4485	H4486	H4487	H4488	H4489	H4490	H4491	H4492	H4493	H4494	H4495	H4496	H4497	H4498	H4499	H4500	H4501	H4502	H4503	H4504	H4505	H4506	H4507	H4508	H4509	H4510	H4511	H4512	H4513	H4514	H4515	H4516	H4517	H4518	H4519	H4520	H4521	H4522	H4523	H4524	H4525	H4526	H4527	H4528	H4529	H4530	H4531	H4532	H4533	H4534	H4535	H4536	H4537	H4538	H4539	H4540	H4541	H4542	H4543	H4544	H4545	H4546	H4547	H4548	H4549	H4550	H4551	H4552	H4553	H4554	H4555	H4556	H4557	H4558	H4559	H4560	H4561
P4374	H4377	L4380	H4381	T4382	T4383	H4387	K4399	R4400	F4411	F4412	F4413	E4414	R4415	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	Q4444	T4445	H4446	Y4447	L4448	R4449	T4452	H4453	E4454	L4455																																																																									
K4237	Y4252	G4253	D4257	M4258	E4259	F4260	D4261	F4268	S4277	F4282	V4288	D4289	G4290	H4291	K4292	D4293	M4296	P4297	R4302	E4304	F4305	V4306	Q4307	V4308	V4309	E4310	L4311	P4318	S4319	M4325	M4326	G4336	M4339	L4340	M4343	M4346	Q4347	ASP	LEU	GLU	ASP																																																																
M4107	P4118	N3974	L4124	M4128	M4131	P4132	K4133	P4135	F4145	F4147	E4148	P4149	P4150	T4160	V4166	S4167	R4168	K4171	S4172	P4173	R4176	A4177	R4178	L4179	F4186	E4192	R4195	Y4205	E4209	D4211	L4212	R4213	D4220	L4223	D4224	A4227	T4233	S4234																																																																			
P3971	T3972	N3973	E3976	E3977	A3980	L3983	L3987	L3992	F3996	R4000	T4011	N4012	L4013	F4017	L4020	M4021	E4022	Q4023	L4027	L4030	R4031	P4037	P4040	M4043	G4053	H4054	V4055	L4058	H4063	S4068	A4083	V3951	Q3952	F3957	W3960	P3966																																																																					
Q3854	R3855	L3856	I3859	L3863	F3864	A3867	R3873	T3882	L3886	V3896	G3897	E3898	L3909	R3910	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3933	A3934	V3935	V3936	F3944	K3945	D3946	L3947	K3950	V3951	Q3952																																																																				
T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	A3777	A3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	V3786	E3786	T3787	D3788	L3789	V3790	M3791	Q3792	E3793	V3794	E3795	T3796	V3797	S3798	Q3799	Q3800	T3801	C3808	I3811	S3817	L3818	K3819	Q3826	L3833	D3834	L3835	Y3836	V3839	L3840	Y3841	E3842	N3843	L3846	D3851																																																							
Q3854	R3855	L3856	I3859	L3863	F3864	A3867	R3873	T3882	L3886	V3896	G3897	E3898	L3909	R3910	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	R3923	I3924	Q3925	V3929	E3933	A3934	V3935	V3936	F3944	K3945	D3946	L3947	K3950	V3951	Q3952																																																																				
T3897	F3898	V3899	N3700	F3701	T3702	N3703	T3704	S3707	L3634	V3635	V3638	E3639	S3640	Y3641	D3642	P3643	V3644	L3645	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	G3658	R3659	V3660	L3661	I3662	T3663	L3664	G3665	D3666	D3667	D3668	I3669	D3670	L3671	S3674	L3679	S3680	T3681	E3687	F3688	P3689	P3690	L3692	C3693	S3694	V3695																																																					
L3615	D3616	D3617	R3620	R3628	F3629	L3634	V3635	F3650	M3652	R3653	L3653	R3655	T3656	G3657	G3658	R3659	V3660	L3661	I3662	T3663	L3664	G3665	D3666	D3667	D3668	I3669	D3670	L3671	S3674	L3679	S3680	T3681	E3687	F3688	P3689	P3690	L3692	C3693	S3694	V3695																																																																	
H3500	S3501	T3502	D3506	L3509	S3510	Y3516	F3520	M3524	R3525	Q3526	F3529	W3532	R3544	T3545	D3546	R3549	L3553	E3558	D3570	N3576	R3579	L3580	R3581	F3582	F3583	N3584	L3588	P3592	E3598	F3599	M3601	D3606	R3607	K3608	E3609	T3610	R3611	T3612	S3613	F3614																																																																	
LEU	GLU	ALA	SER	ILE	ALA	ARG	TYR	LYS	GLY	PRO	MET	VAL	LEU	ILE	TRP	ALA	ILE	ALA	GLN	ALA	LEU	ASN	TYR	LYS	ALA	ASP	ASP	LEU	ALA	LEU	ALA	VAL	GLU	VAL	GLU	ASP	ASP	ALA	LEU	VAL	GLU	GLN	MET	ILE	ARG	ASP																																																											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.938	Depositor
Minimum map value	-0.536	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality [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	0.15	0/22220	0.34	3/30121 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2812	PRO	CA-N-CD	-8.91	99.53	112.00
1	A	1848	PRO	CA-N-CD	-6.16	103.37	112.00
1	A	2020	PRO	CA-N-CD	-5.02	104.98	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	21755	0	21789	545	0
2	A	81	0	36	11	0
3	A	31	0	12	1	0
All	All	21867	0	21837	545	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 12.

The worst 5 of 545 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:3662:ILE:HD11	1:A:3671:LEU:HB2	1.54	0.88
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.56	0.86
1:A:3661:LEU:HD11	1:A:3668:ASP:HB3	1.61	0.83
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	1.66	0.78
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.67	0.77

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	2699/4646 (58%)	2641 (98%)	58 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2407/4125 (58%)	2401 (100%)	6 (0%)	87 87

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

Mol	Chain	Res	Type
1	A	3795	GLU
1	A	4124	LEU
1	A	4628	THR
1	A	1964	GLU
1	A	1931	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3047	HIS
1	A	4488	GLN
1	A	3535	HIS
1	A	4114	HIS
1	A	3214	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](#)

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
3	ATP	A	4702	-	32,33,33	0.40	0	48,52,52	0.29	0
2	ADP	A	4701	-	28,29,29	1.38	4 (14%)	43,45,45	1.91	8 (18%)
2	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	8 (18%)
2	ADP	A	4704	-	28,29,29	1.38	4 (14%)	43,45,45	1.79	8 (18%)

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	-	-	3/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	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	4703	ADP	C5-C4	4.69	1.47	1.39
2	A	4701	ADP	C5-C4	4.63	1.47	1.39
2	A	4704	ADP	C5-C4	4.47	1.47	1.39
2	A	4703	ADP	C5-C6	2.64	1.48	1.41
2	A	4704	ADP	C5-C6	2.58	1.48	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.12	118.29	126.72
2	A	4701	ADP	C5-C4-N3	-6.08	118.34	126.72
2	A	4704	ADP	C5-C4-N3	-5.63	118.97	126.72
2	A	4703	ADP	N3-C4-N9	4.97	135.62	127.17
2	A	4701	ADP	N3-C4-N9	4.90	135.50	127.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	O4'-C1'-N9-C8
2	A	4701	ADP	O4'-C1'-N9-C4

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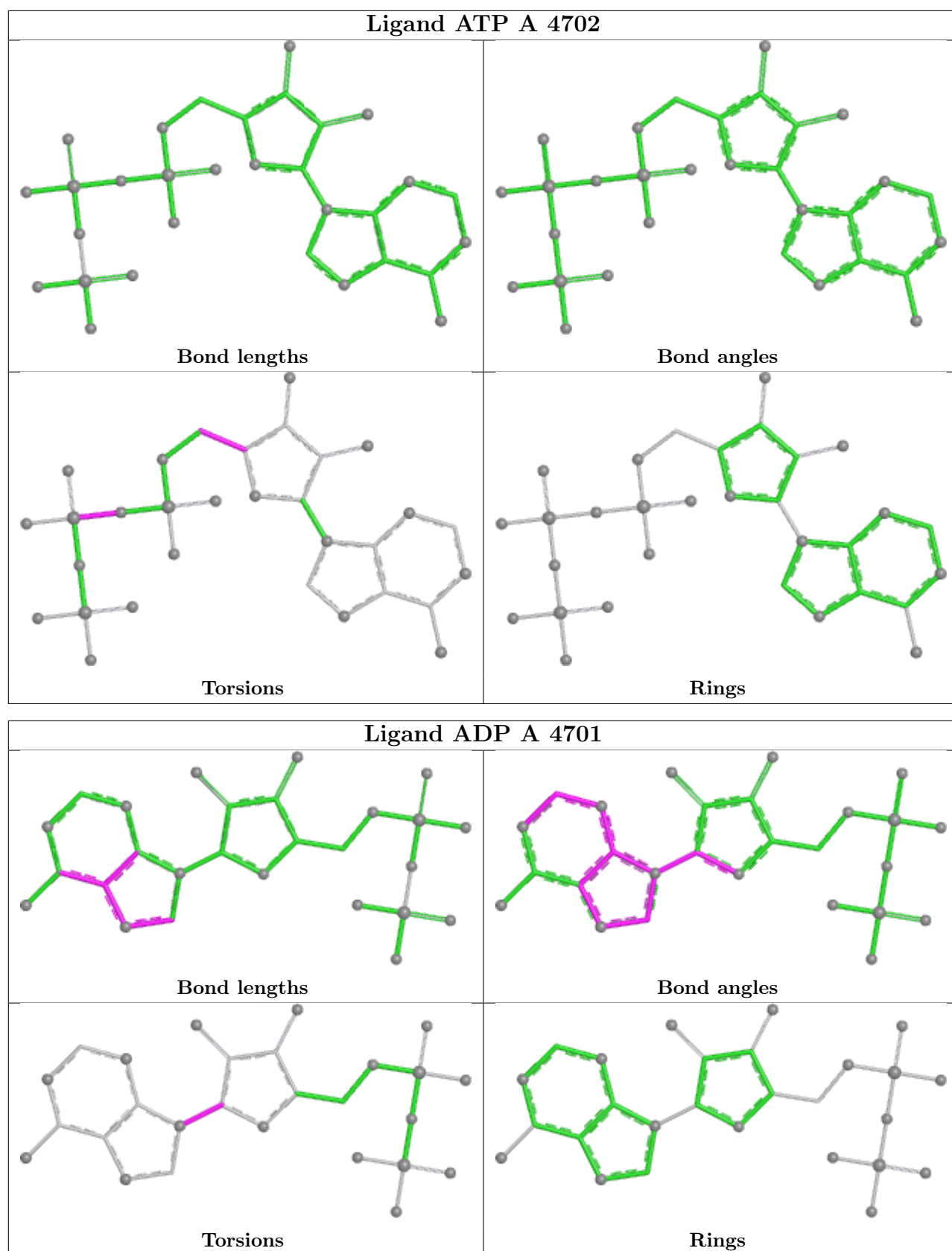
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A

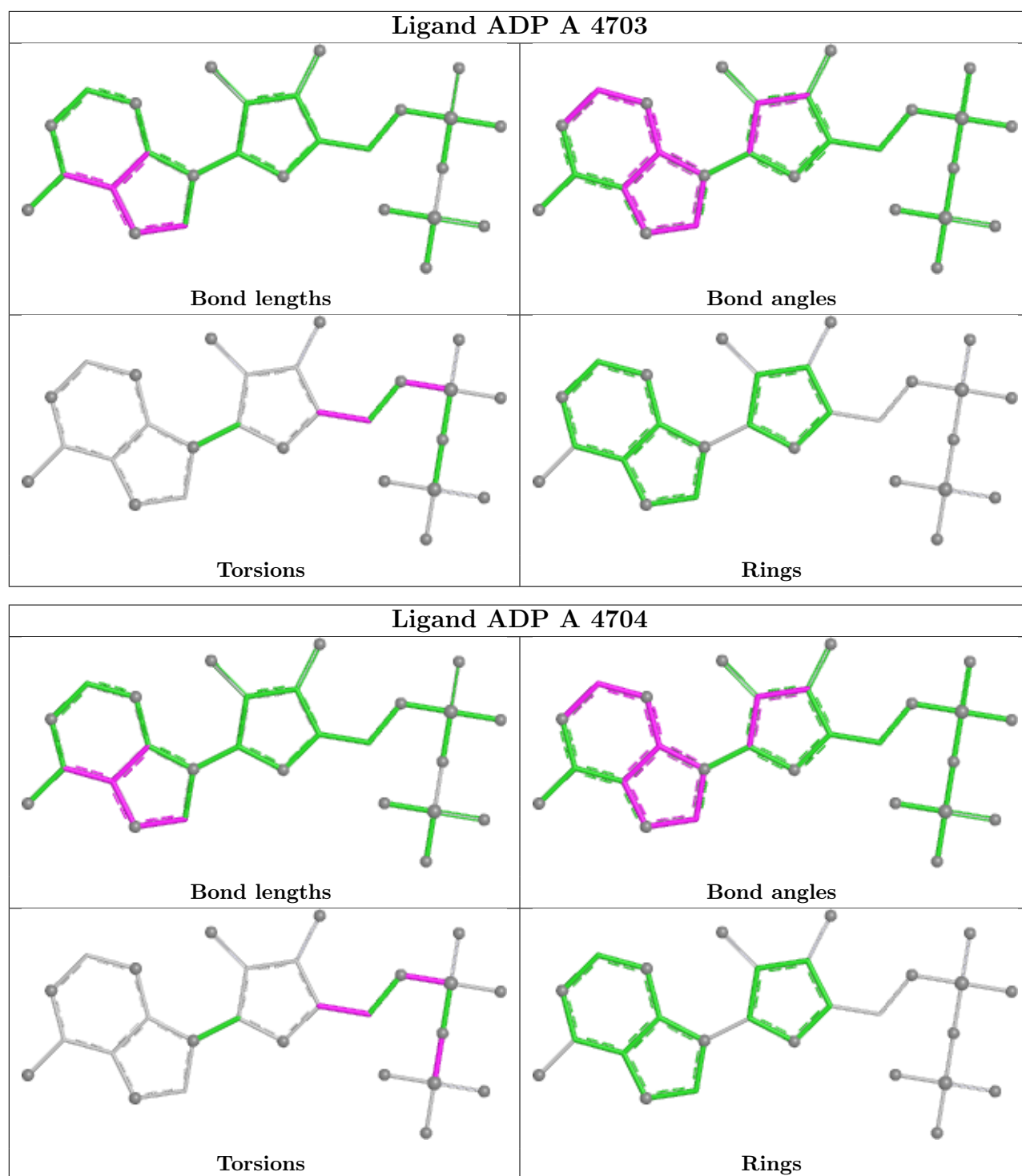
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	1	0
2	A	4701	ADP	7	0
2	A	4703	ADP	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

There are no chain breaks in this entry.

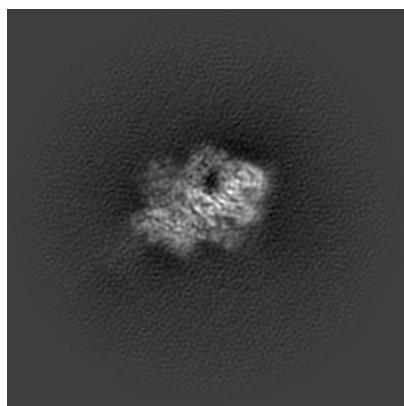
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44704. These allow visual inspection of the internal detail of the map and identification of artifacts.

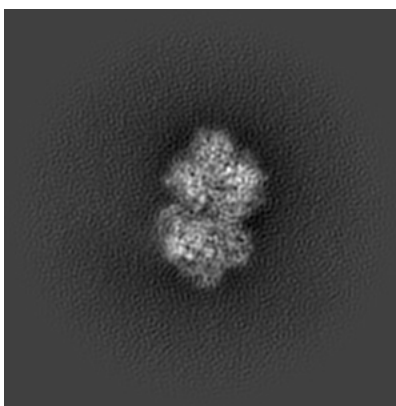
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

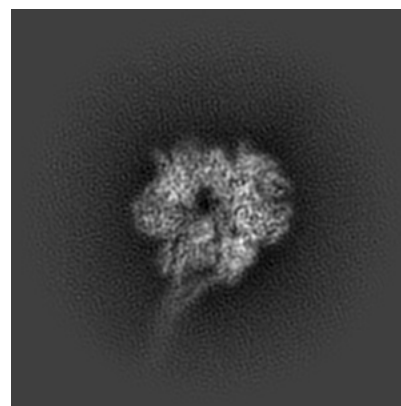
6.1.1 Primary map



X

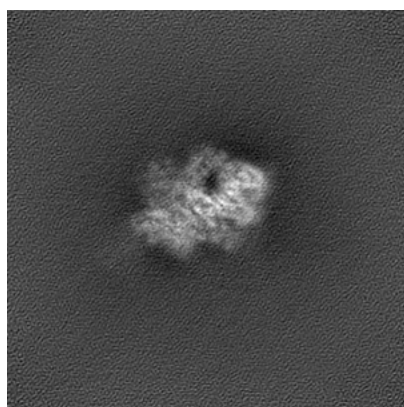


Y

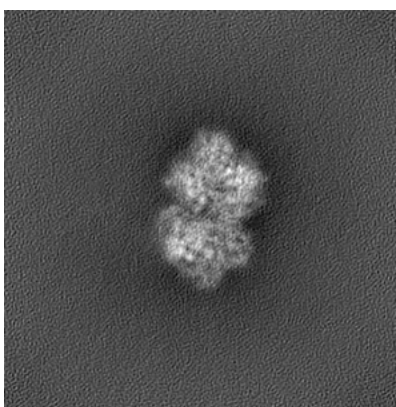


Z

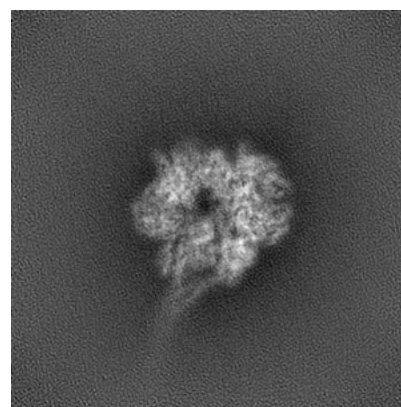
6.1.2 Raw map



X



Y

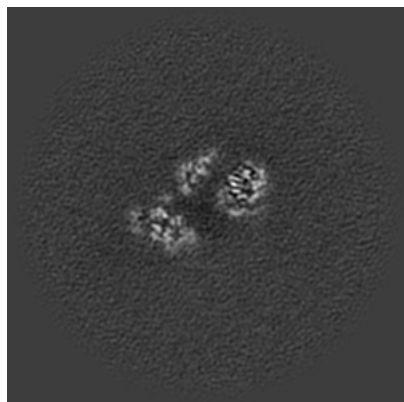


Z

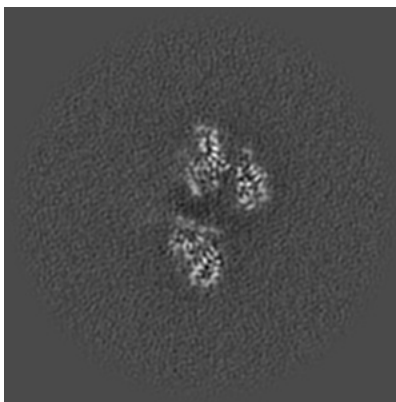
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

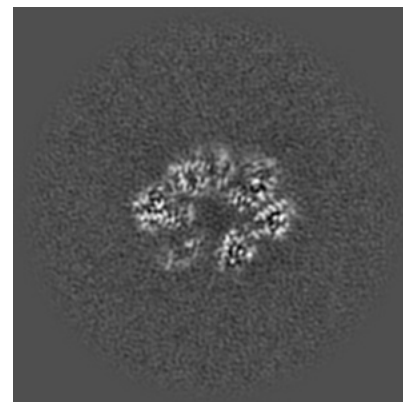
6.2.1 Primary map



X Index: 128

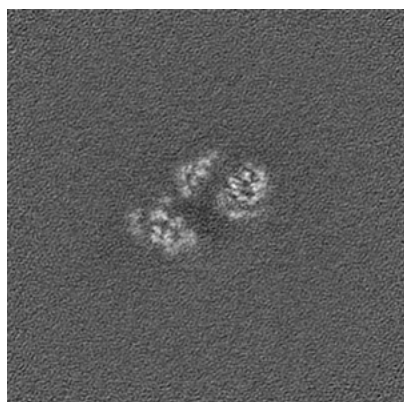


Y Index: 128

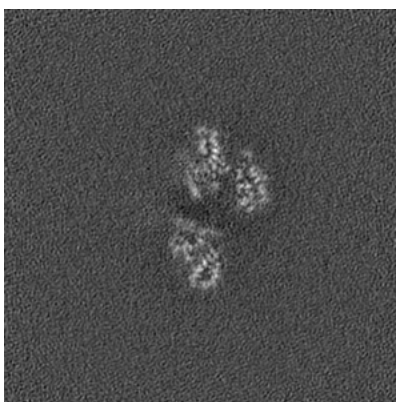


Z Index: 128

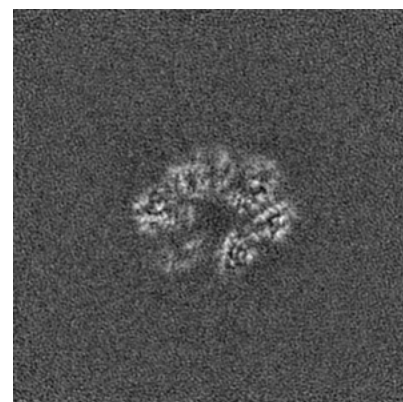
6.2.2 Raw map



X Index: 128



Y Index: 128

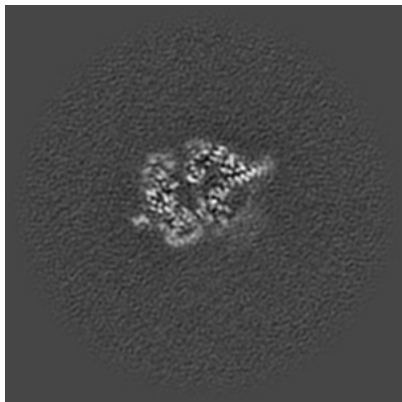


Z Index: 128

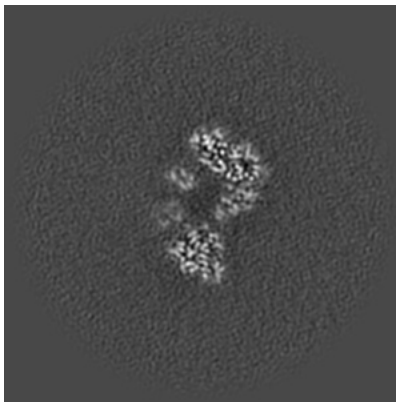
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

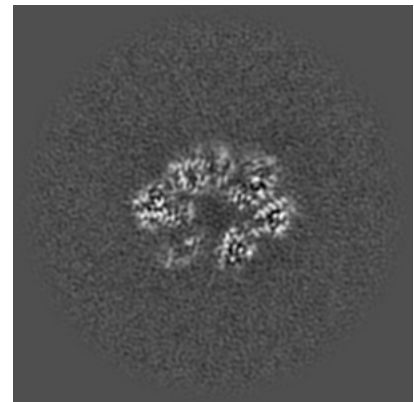
6.3.1 Primary map



X Index: 146

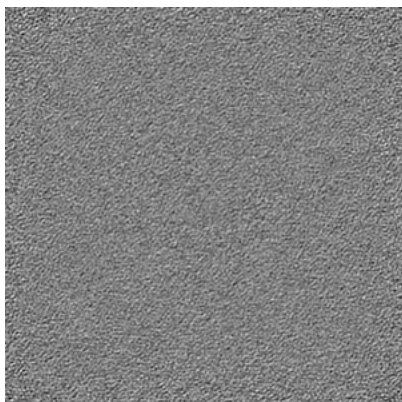


Y Index: 120

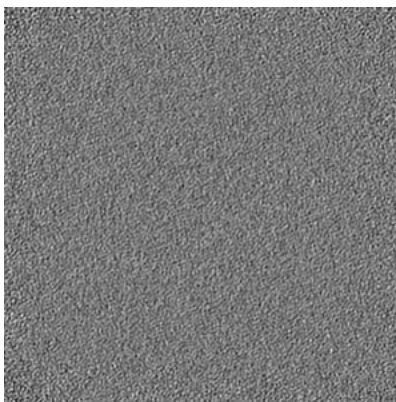


Z Index: 128

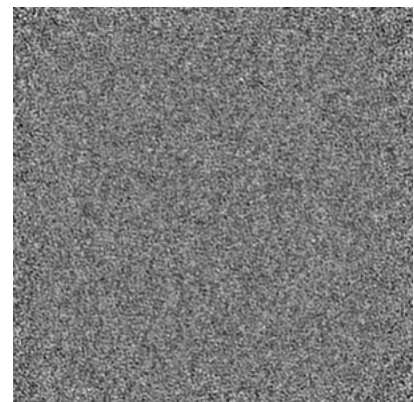
6.3.2 Raw map



X Index: 0



Y Index: 0

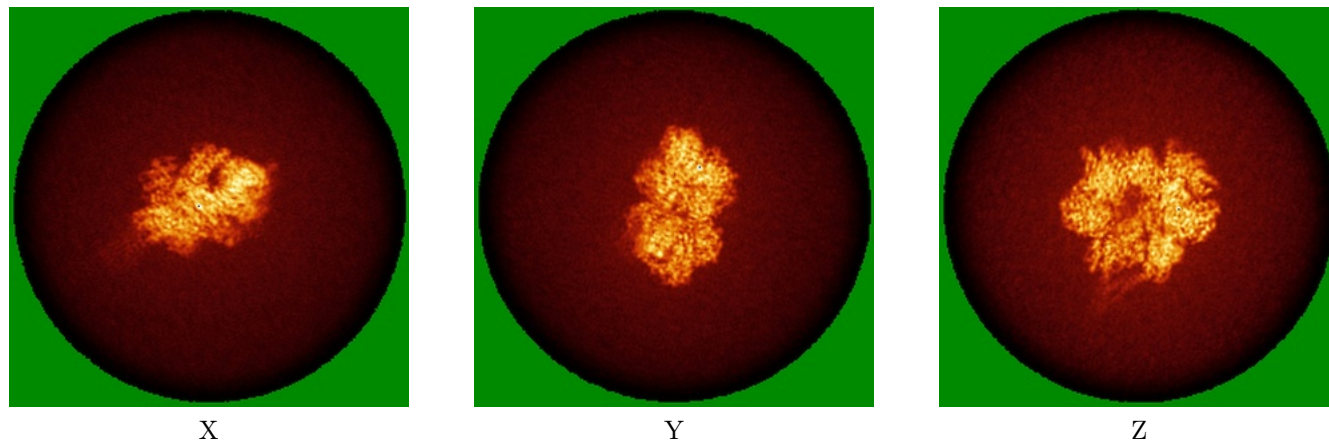


Z Index: 0

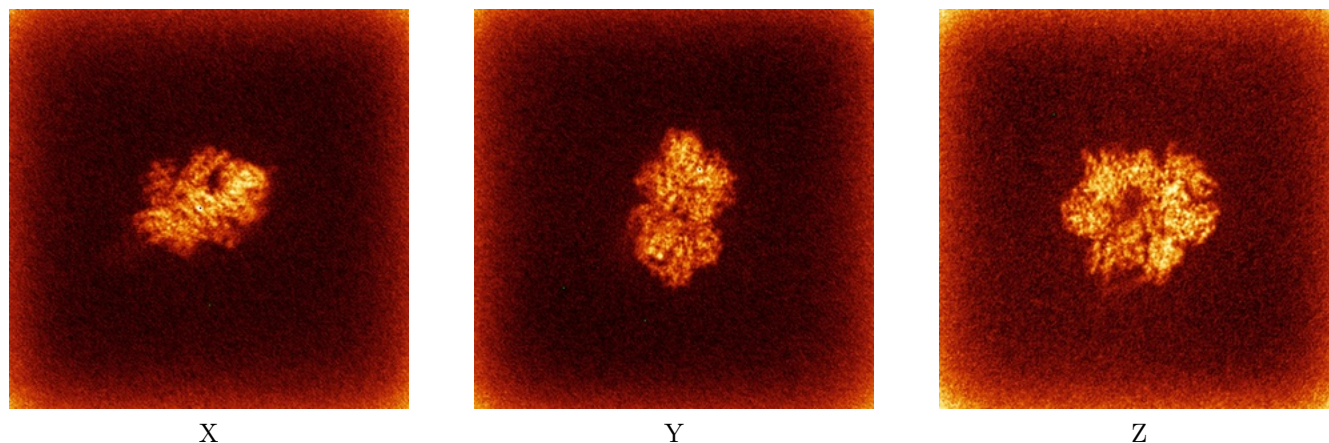
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

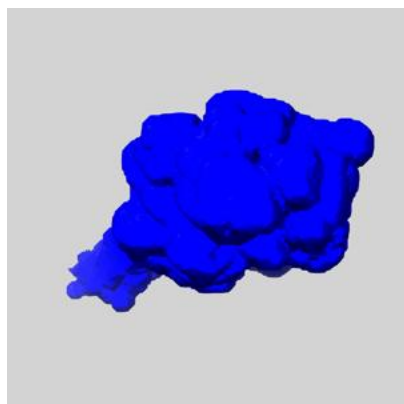
6.6 Mask visualisation [i](#)

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

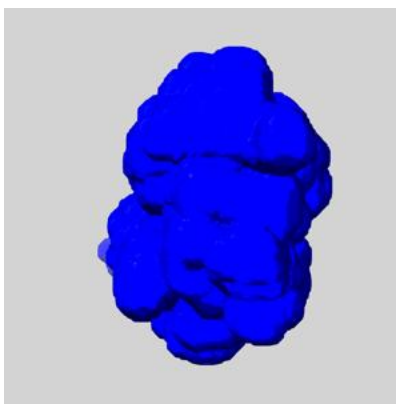
A mask typically either:

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

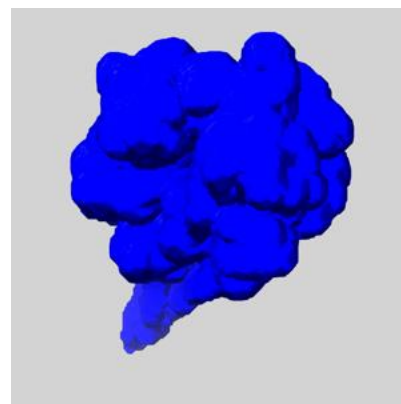
6.6.1 emd_44704_msk_1.map [i](#)



X



Y

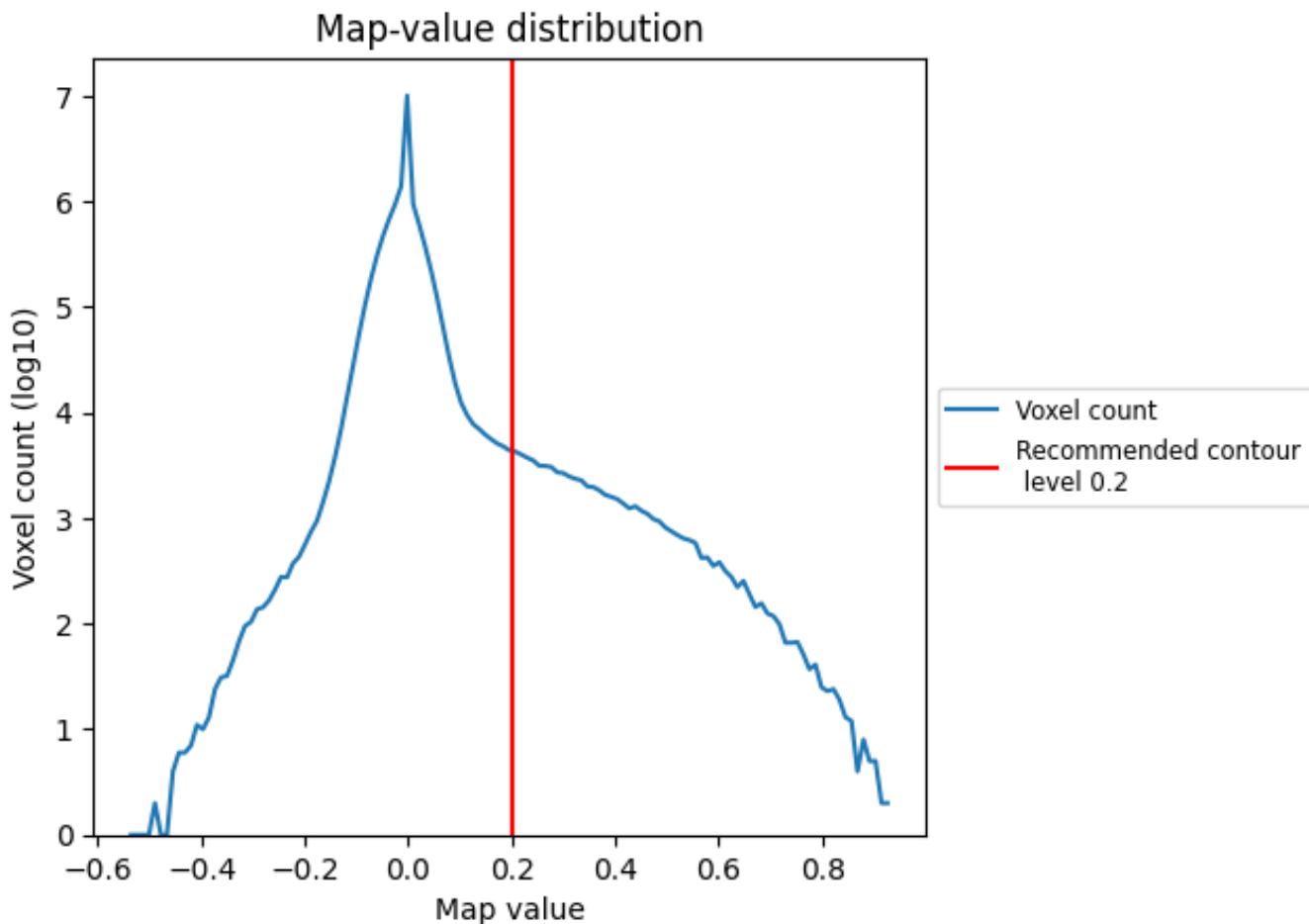


Z

7 Map analysis [i](#)

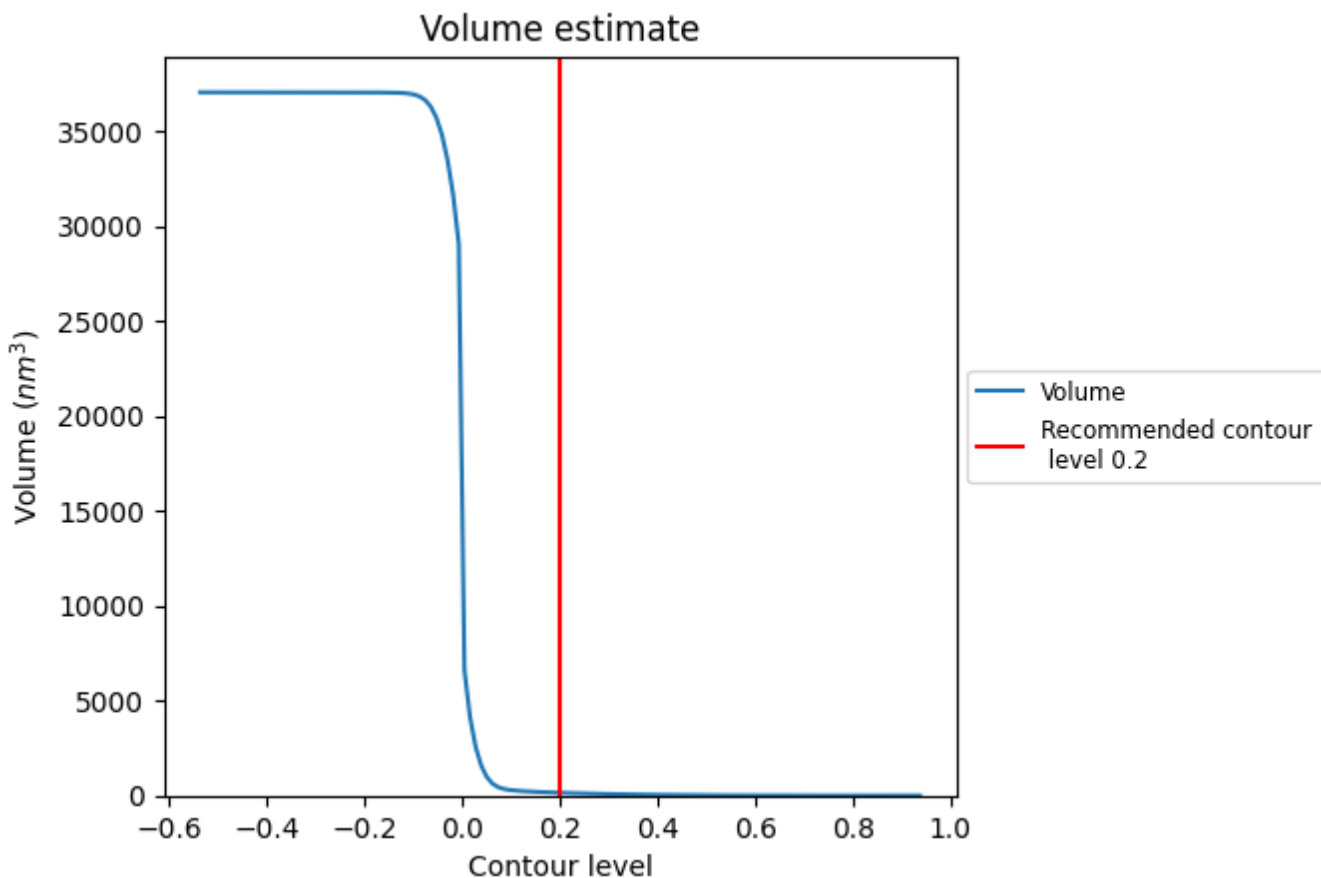
This section contains the results of statistical analysis of the map.

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.

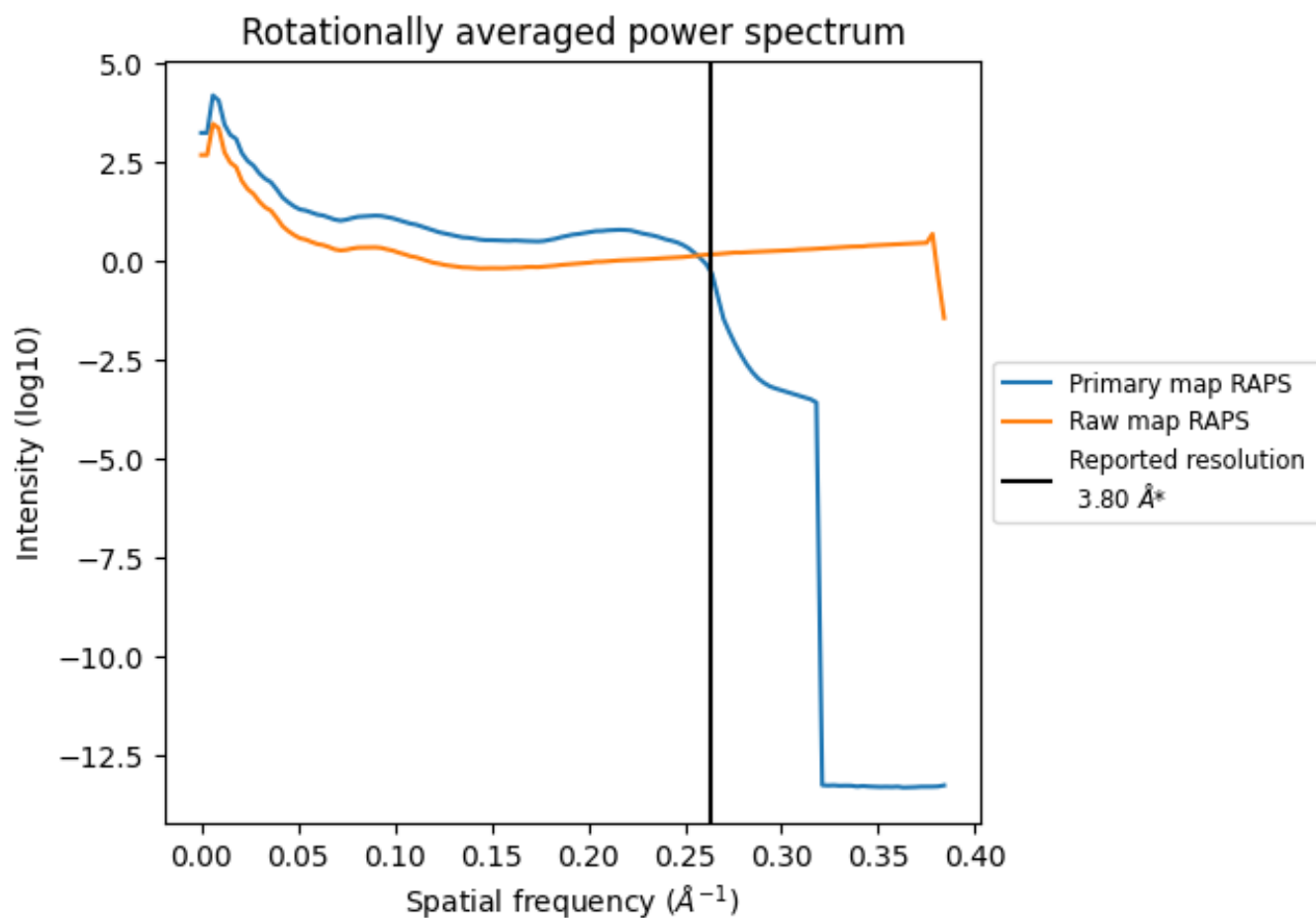
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm^3 ; this corresponds to an approximate mass of 133 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 [i](#)

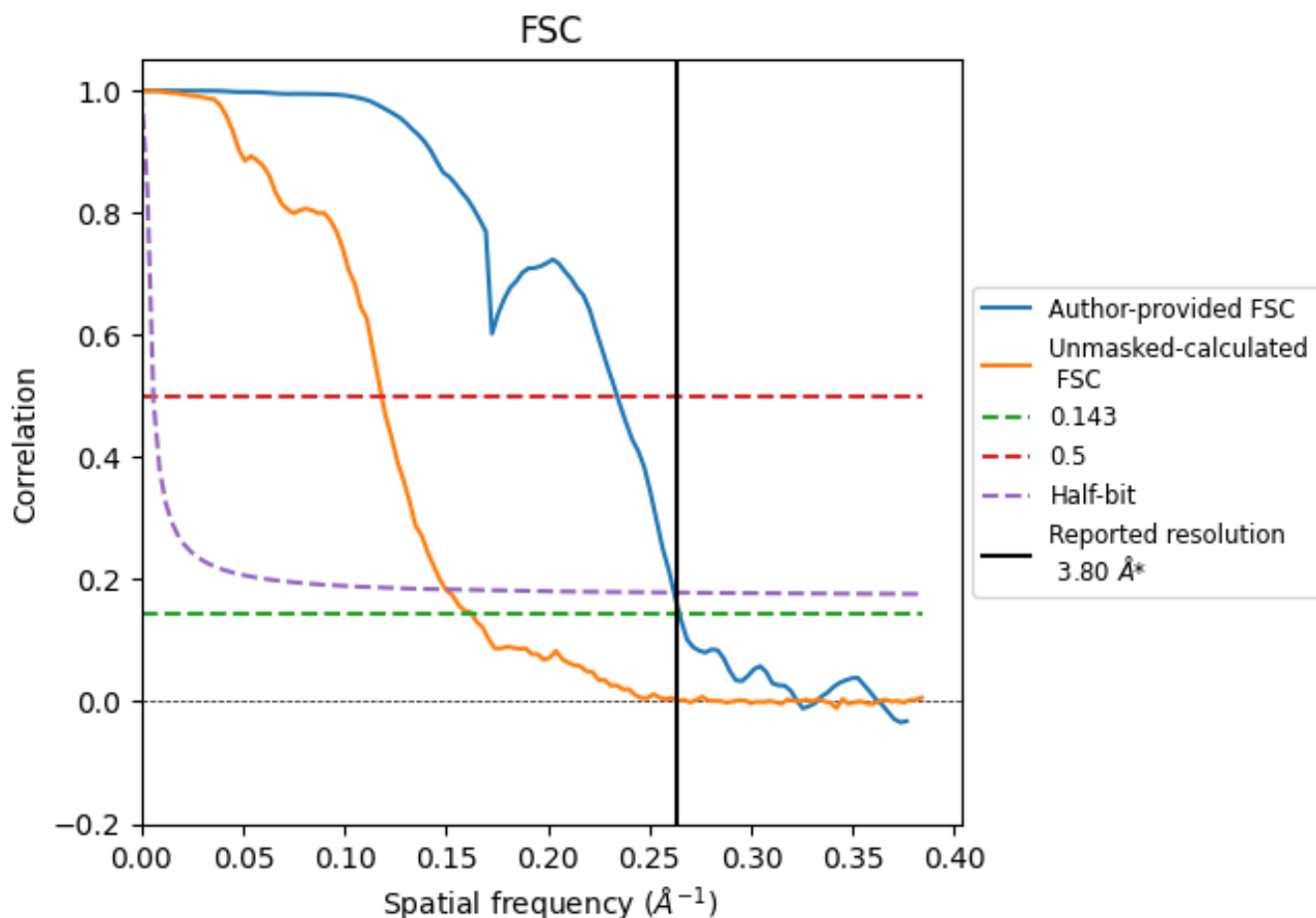


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

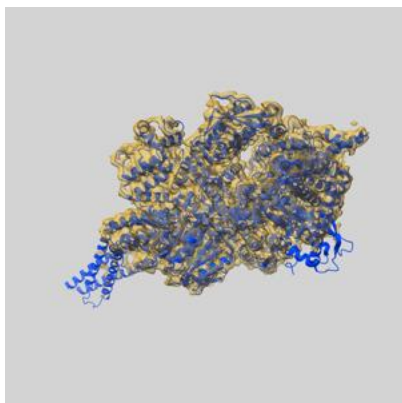
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.27	3.82
Unmasked-calculated*	6.15	8.45	6.67

*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 6.15 differs from the reported value 3.8 by more than 10 %

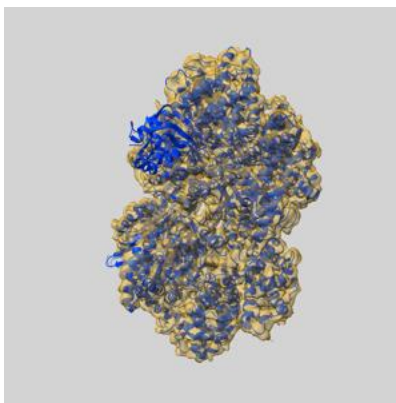
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44704 and PDB model 9BMN. Per-residue inclusion information can be found in section [3](#) on page [5](#).

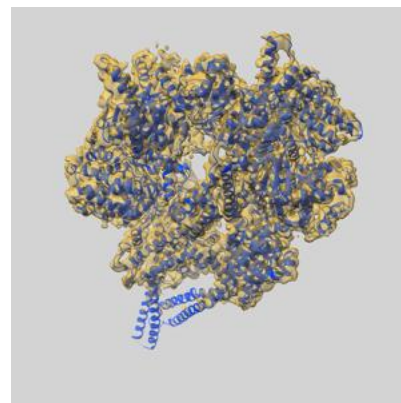
9.1 Map-model overlay [i](#)



X



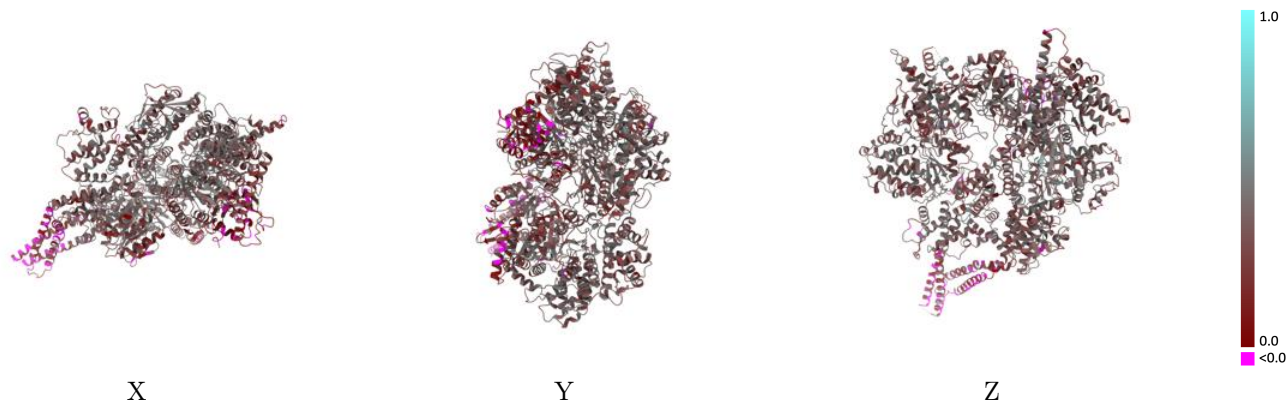
Y



Z

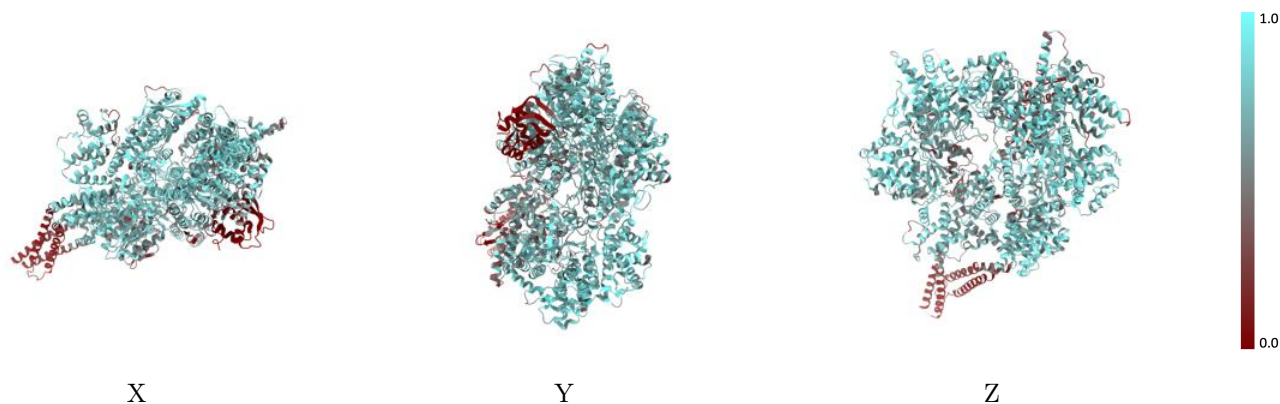
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



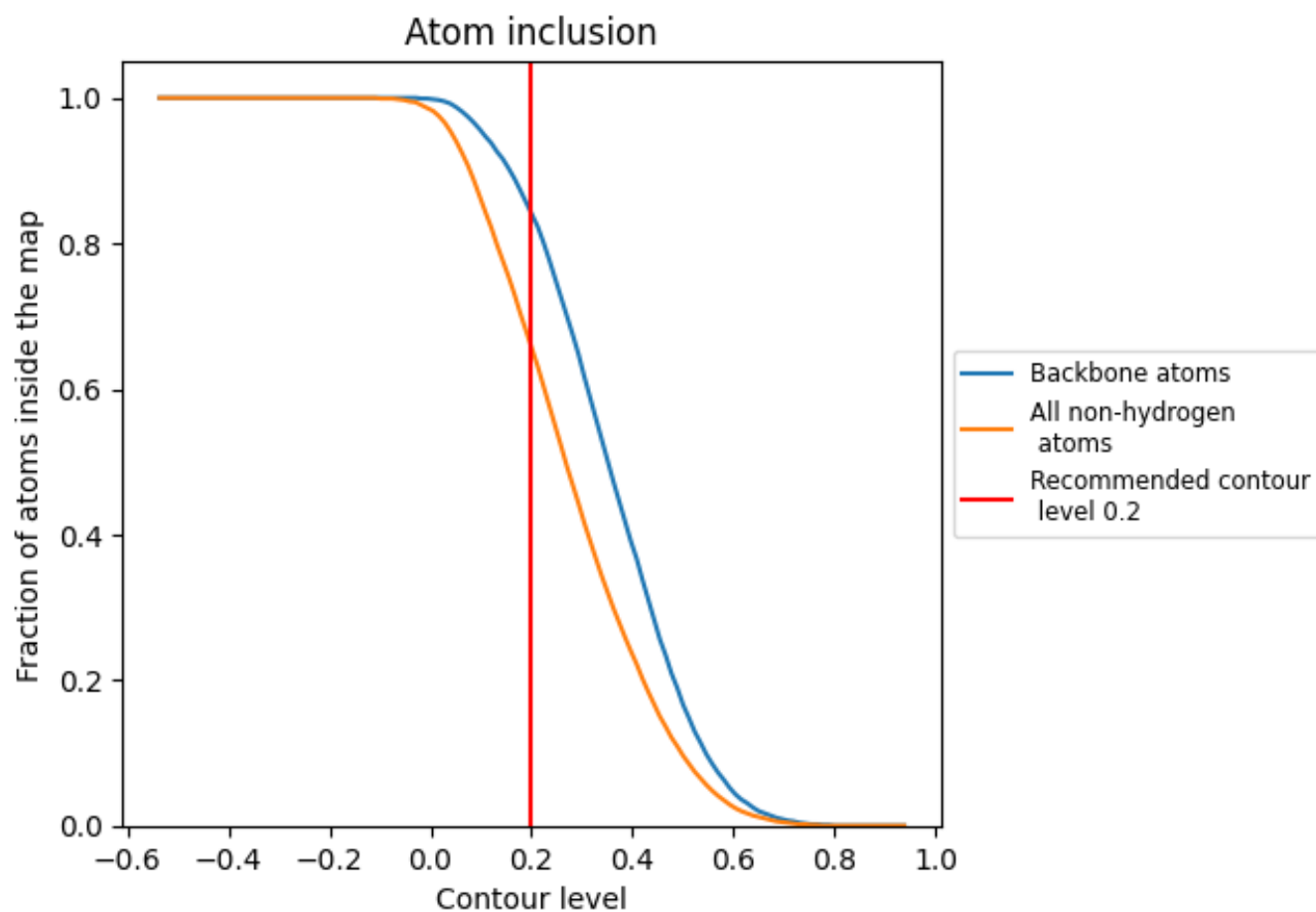
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

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	 0.6570	 0.3320
A	 0.6570	 0.3320

