



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 03:11 AM UTC

PDB ID : 9BLZ / pdb_00009blz
EMDB ID : EMD-44682
Title : State-1(phi motor) of full-length human dynein-1 in 5mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.20 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

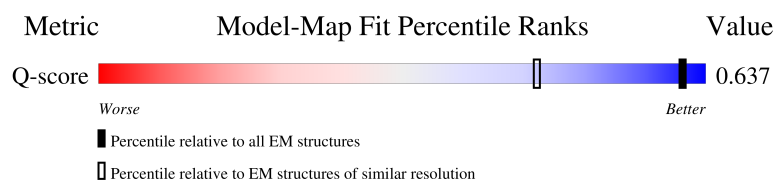
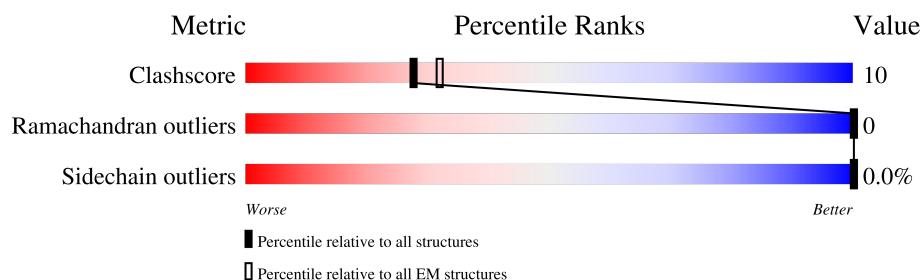
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	9% 48% 15% 38%

2 Entry composition [i](#)

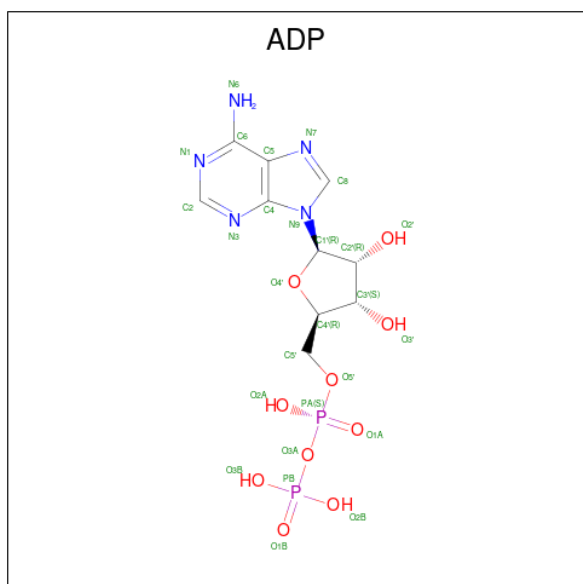
There are 5 unique types of molecules in this entry. The entry contains 25189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

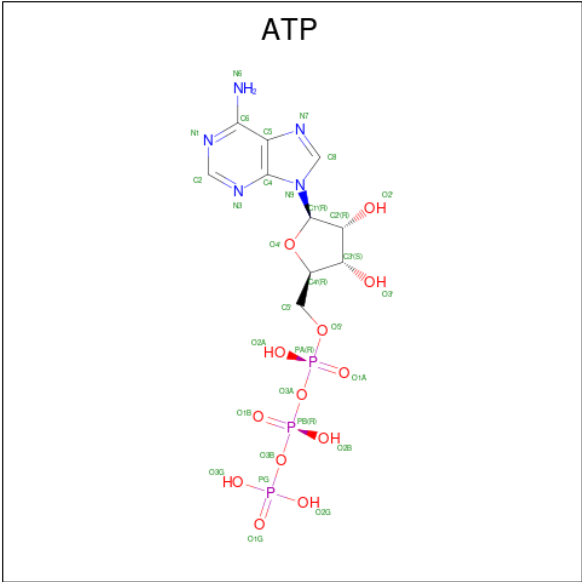
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2889	23218	14794	4002	4305	117	0	0

- 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).



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	0
			2	2	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	1857	Total	O	0
			1857	1857	





M4473	I4476	Q4477	W4478	S4480	D4481	R4485	L4489	Q4490	N4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	G4499	G4500	K4501	K4502	E4503	L4504	K4505	N4506	V4509	L4514	F4515	P4517	E4518	A4519	Y4520	R4525	Q4526	A4529	Q4530	N4531	S4532	S4533	W4534	S4535	L4536	E4537	F4538	E4538	L4541	E4542	V4543	T4546	T4547				
H4397	L4398	K4399	R4400	T4401	V4402	E4403	N4404	I4405	K4406	D4407	P4408	F4412	F4413	E4414	R4415	E4416	V4417	K4418	N4419	K4422	Q4425	D4426	Q4429	D4430	L4431	A4432	D4433	W4434	V4435	Q4436	W4437	C4438	E4439	G4440	K4441	K4442	K4443	Q4444	N4453	K4457	G4458	I4459	L4460	P4461	R4462	S4463	H4466	Y4467	T4468	A4471	G4472		
V4306	Q4307	W4308	F4318	N4325	N4326	K4342	N4346	Q4347	MET	LEU	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	LYS	THR	THR	ASP	GLY	ARG	P4374	A4375	W4376	N4377	N4378	T4379	L4380	H4381	T4382	S4385	N4386	W4387	L4388	H4389	L4390	Q4393	T4394	L4395	S4396					
I4190	A4197	W4201	Y4205	E4206	F4207	G4208	E4209	R4213	D4220	A4227	K4228	Q4231	N4232	I4233	S4234	D4235	D4236	S4250	I4251	Y4252	G4253	G4254	F4260	T4267	R4271	S4280	A4285	C4286	K4287	V4288	D4289	G4290	H4291	K4292	D4293	I4294	Q4295	P4296	P4297	D4298	R4301	K4302	E4303	F4304	F4305								
R3997	W4004	V4009	L4013	F4017	Q4023	P4024	P4037	N4038	T4039	G4048	D4057	E4061	Q4062	N4063	T4064	Q4065	I4071	A4087	V4088	R4092	L4096	V4099	L4116	Q4117	P4118	H4119	A4120	K4133	L4137	L4138	G4142	R4143	I4164	S4172	P4173	R4176																	
S3917	A3918	G3919	S3920	S3921	P3922	R3923	I3924	Q3925	G3926	V3929	E3930	Q3931	A3932	E3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	P3942	K3945	D3946	A3949	K3950	V3951	Q3952	D3954	E3955	Q3956	I3959	D3962	P3966	V3970	P3971	Y3972	L3973	W3974	S3975	E3976	E3977	L3978	P3979	A3980	Q3985	R3989	L3990				
V3794	E3795	T3796	V3797	Y3812	M3815	L3818	L3821	L3829	I3835	E3930	Y3836	H3837	N3838	V3839	E3842	N3843	K3847	G3848	V3849	T3850	D3851	Q3854	R3855	D3862	L3863	R3870	V3871	M3875	K3891	L3892	K3893	G3894	T3895	V3896	G3897	E3898	T3900	Y3901	R3910	G3911	N3912	E3913	I3914	V3915	L3916								
V3724	D3725	E3726	K3727	R3728	L3731	Q3735	L3740	R3741	L3742	R3743	Q3744	K3747	S3748	L3749	L3750	Q3751	E3755	V3756	K3757	G3758	R3759	I3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	L3768	T3769	L3770	E3771	N3772	R3775	E3776	A3777	E3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	I3789	V3790	M3791	Q3792	E3793
F3583	N3584	R3585	L3588	T3597	I3600	M3601	N3602	K3605	D3606	R3607	K3608	R3611	D3617	E3624	R3628	L3634	V3638	N3650	R3651	E3652	R3655	T3656	G3657	V3660	L3661	K3624	R3625	L3628	Q3667	D3668	I3669	T3681	D3691	L3692	C3693	S3694	R3695	R3705	V3716	P3721	P3722	D3723											
A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	E3489	E3490	K3491	T3492	S3493	E3494	T3495	F3496	K3497	R3498	Q3499	K3500	I3503	S3510	I3514	A3515	Y3516	A3517	F3520	K3524	R3525	L3528	H3534	H3535	Q3538	D3546	I3547	E3551	Y3552	L3553	D3557	E3558	R3559	L3580	K3581	R3582						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	872840	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)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.322	Depositor
Minimum map value	-0.575	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	183.04001, 183.04001, 183.04001	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.416, 0.416, 0.416	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/23717	0.37	0/32148

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	23218	0	23256	452	0
2	A	81	0	36	7	0
3	A	31	0	12	5	0
4	A	2	0	0	0	0
5	A	1857	0	0	38	0
All	All	25189	0	23304	452	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 10.

The worst 5 of 452 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.56	0.86
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.08	0.85
1:A:4571:ASN:O	1:A:4574:LYS:HB2	1.82	0.80
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.64	0.79
1:A:3194:LEU:HD23	1:A:3500:MET:HE2	1.66	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	2881/4646 (62%)	2838 (98%)	43 (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	2567/4125 (62%)	2566 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	1973	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3198	GLN
1	A	4262	GLN
1	A	3202	ASN
1	A	3826	GLN
1	A	4429	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	4704	-	28,29,29	0.46	0	43,45,45	0.51	0
2	ADP	A	4701	4	28,29,29	0.46	0	43,45,45	0.52	0
2	ADP	A	4703	-	28,29,29	0.46	0	43,45,45	0.49	0
3	ATP	A	4702	4	32,33,33	0.55	0	48,52,52	0.58	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	4704	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

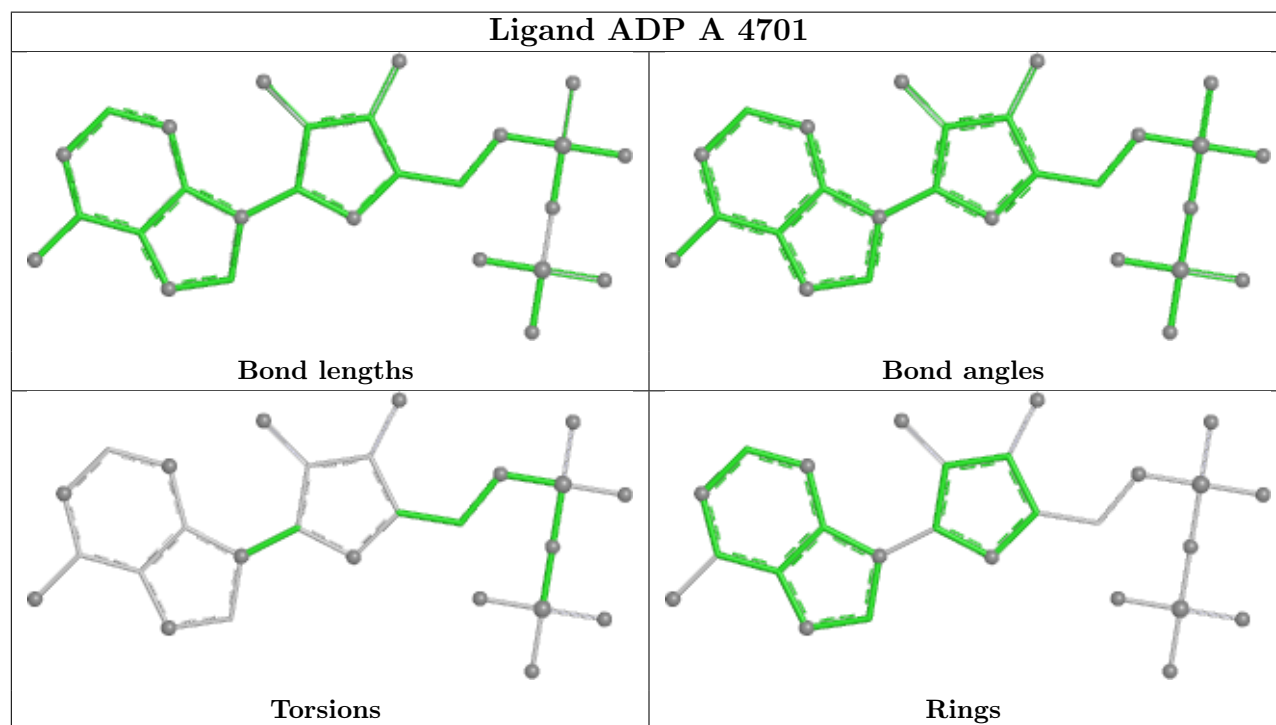
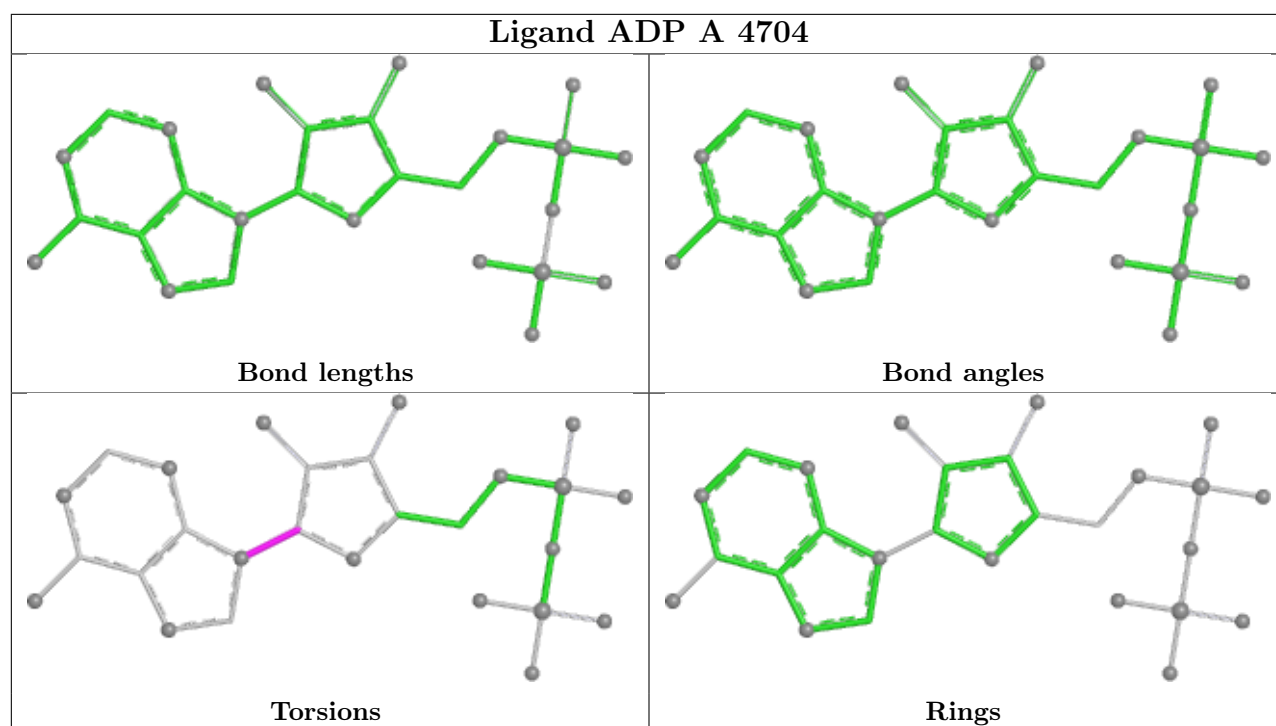
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C2'-C1'-N9-C8
2	A	4704	ADP	C2'-C1'-N9-C8

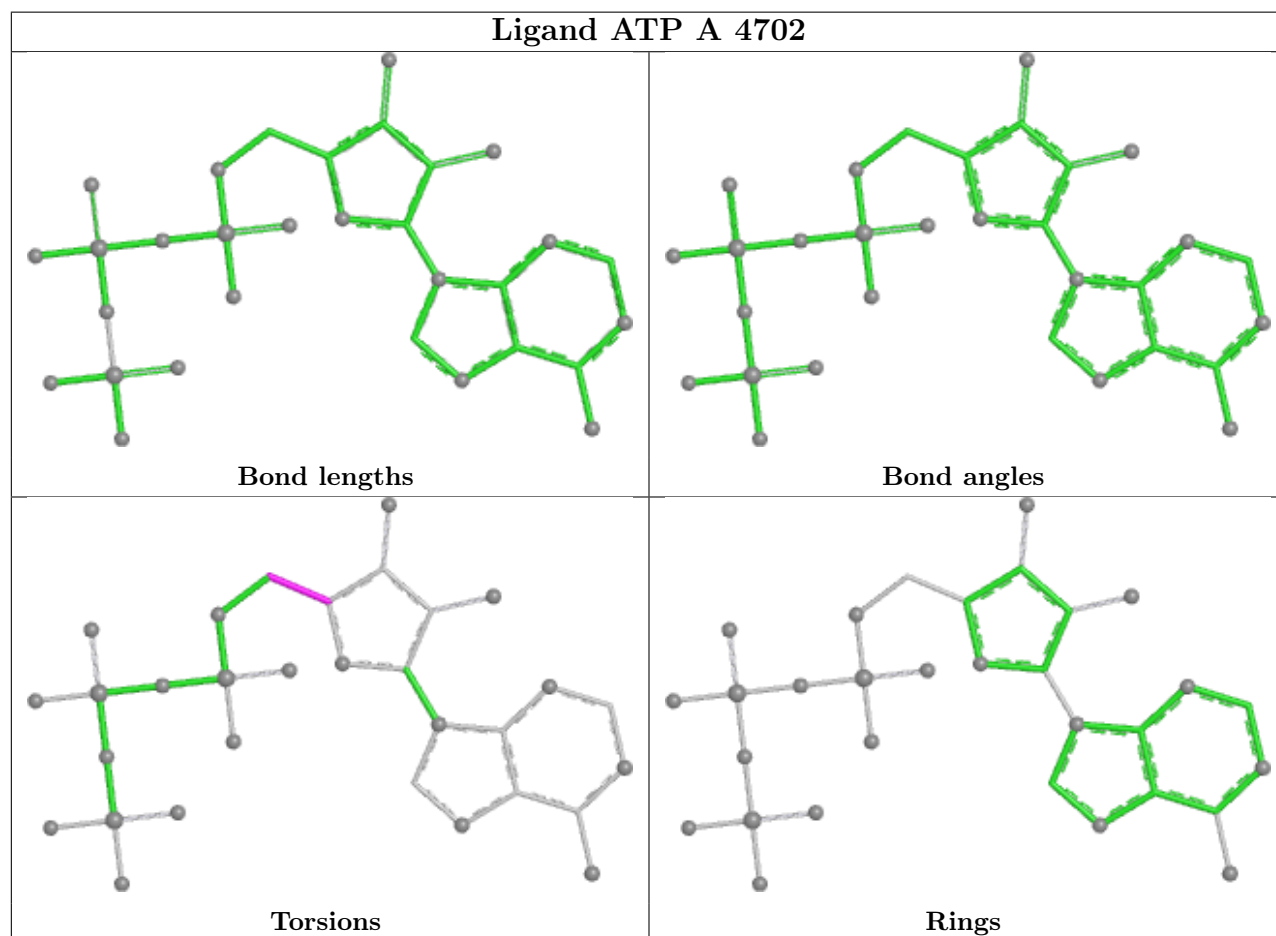
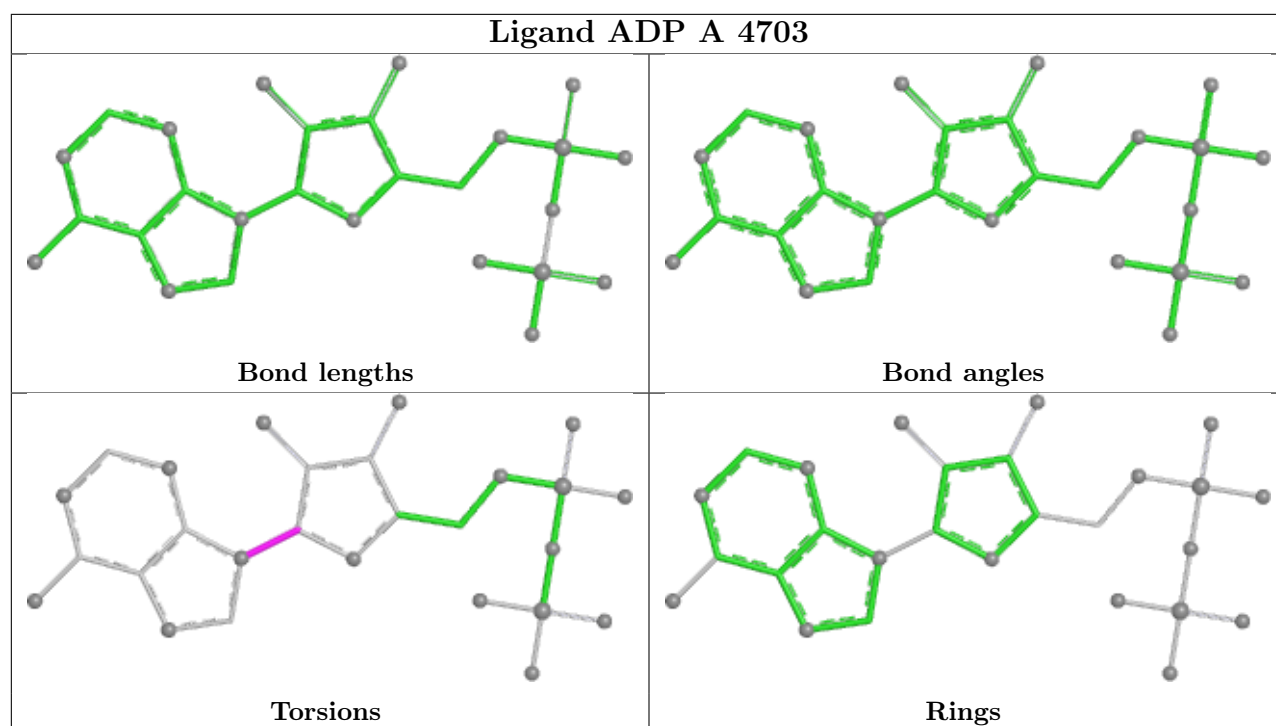
There are no ring outliers.

3 monomers are involved in 12 short contacts:

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

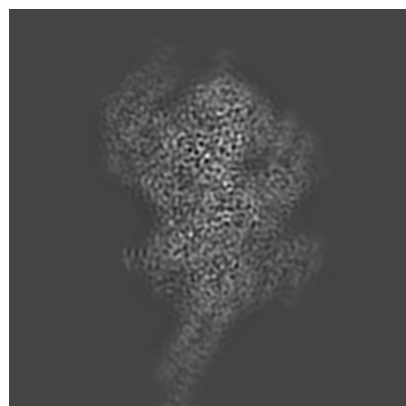
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44682. These allow visual inspection of the internal detail of the map and identification of artifacts.

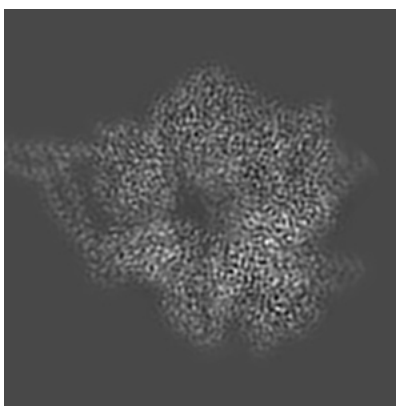
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

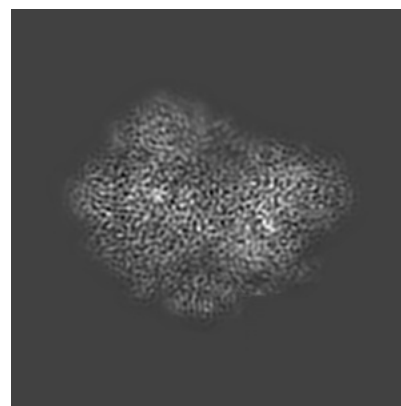
6.1.1 Primary map



X

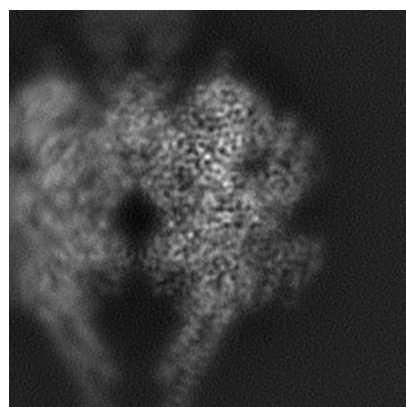


Y

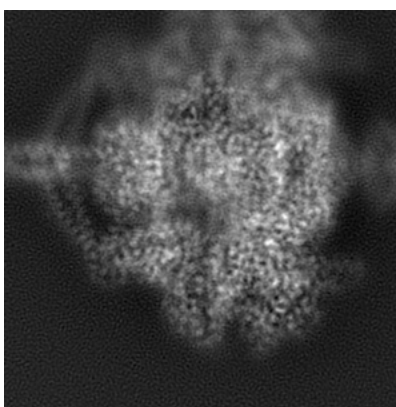


Z

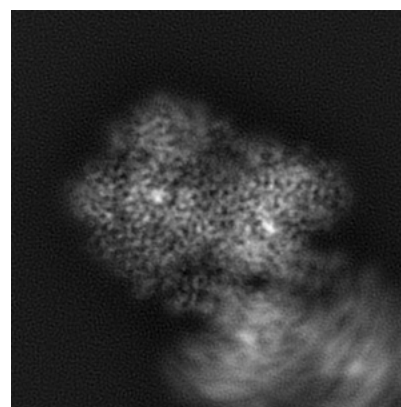
6.1.2 Raw map



X



Y

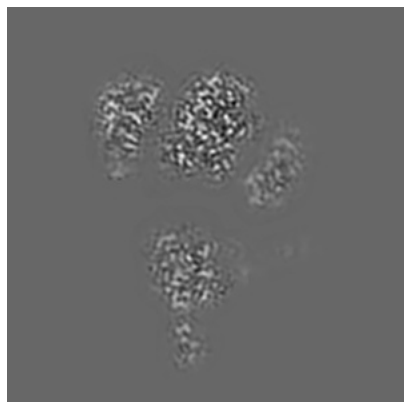


Z

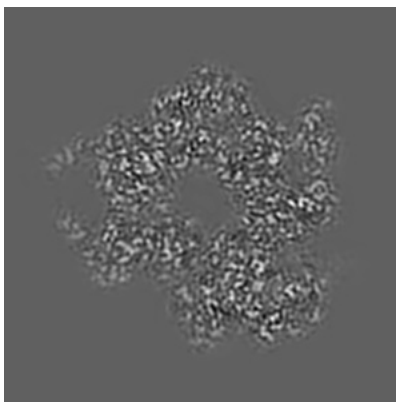
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

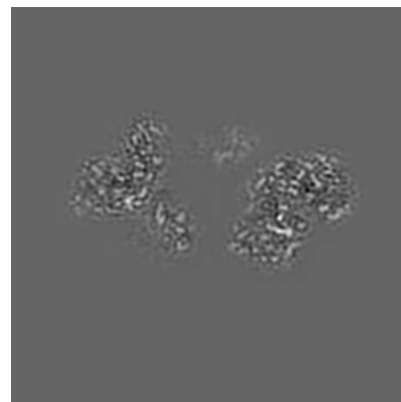
6.2.1 Primary map



X Index: 220

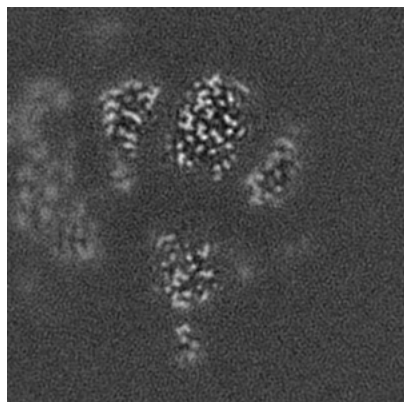


Y Index: 220

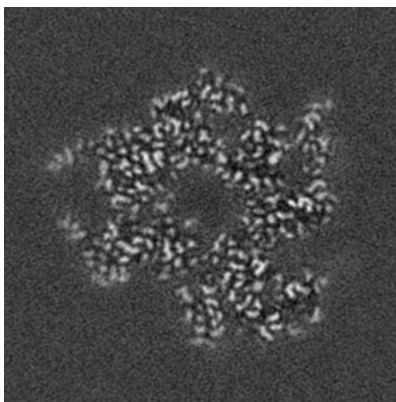


Z Index: 220

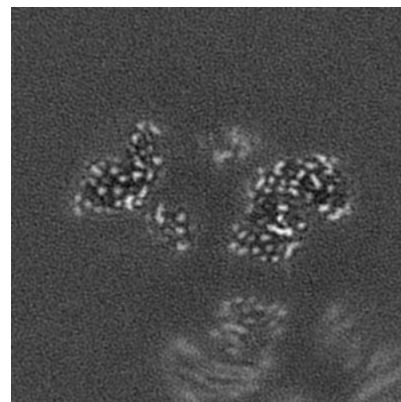
6.2.2 Raw map



X Index: 220



Y Index: 220

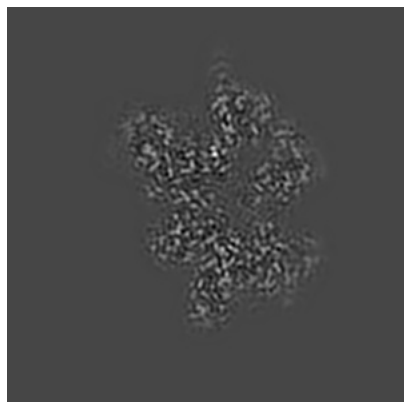


Z Index: 220

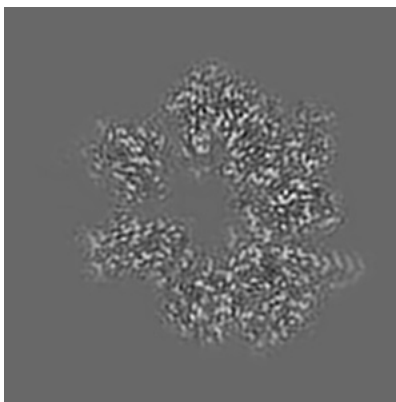
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

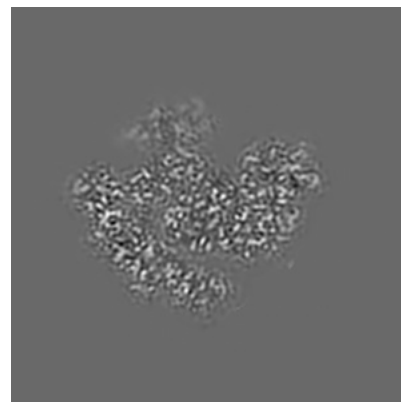
6.3.1 Primary map



X Index: 166

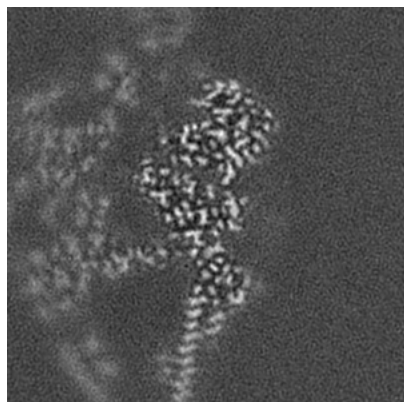


Y Index: 238

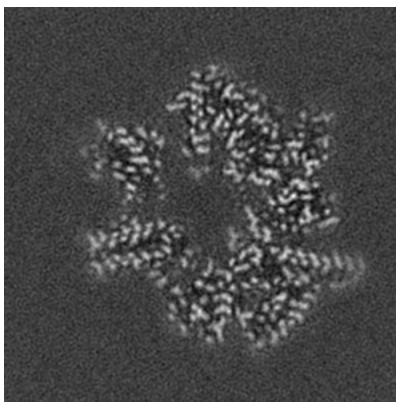


Z Index: 296

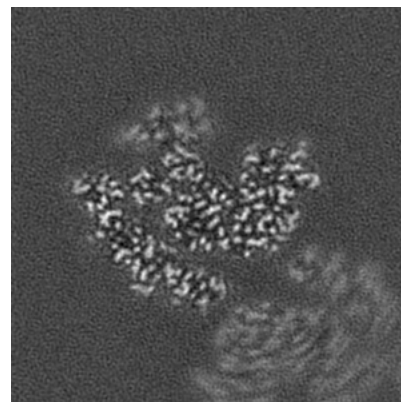
6.3.2 Raw map



X Index: 286



Y Index: 238

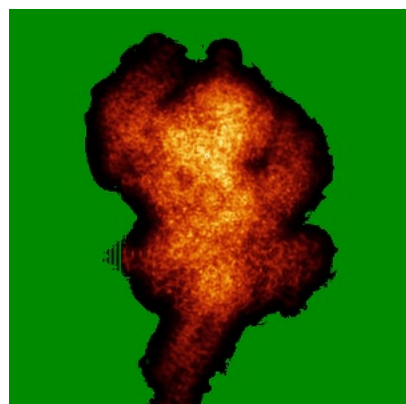


Z Index: 296

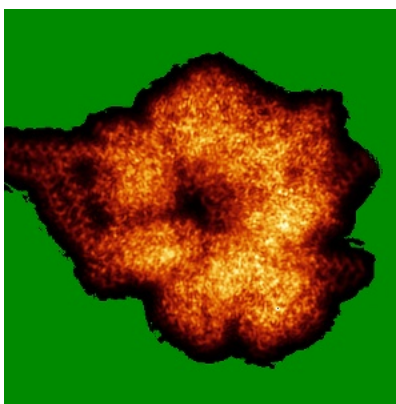
The images above show the largest variance slices of the map in three orthogonal directions.

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

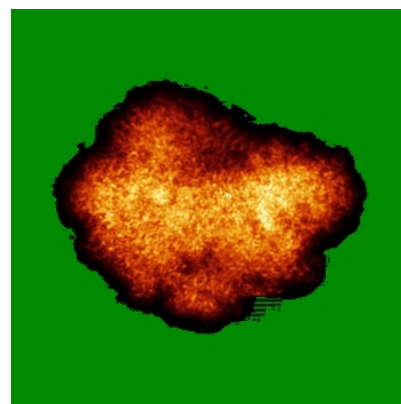
6.4.1 Primary map



X

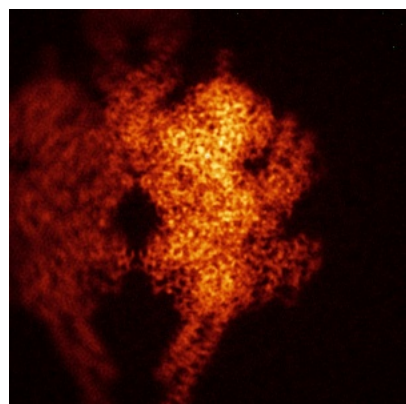


Y

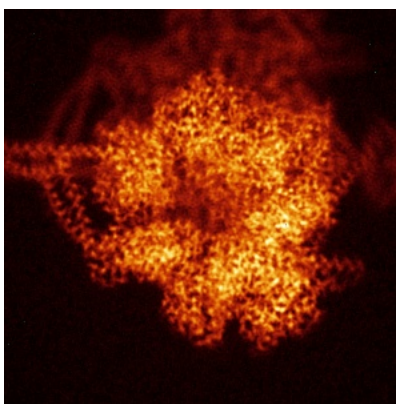


Z

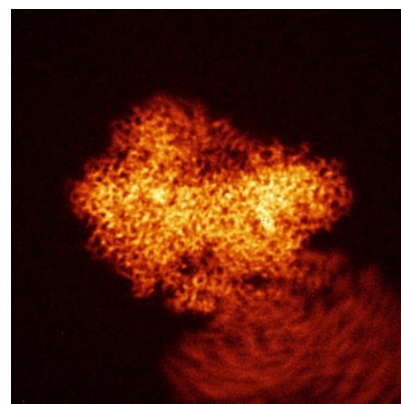
6.4.2 Raw map



X



Y

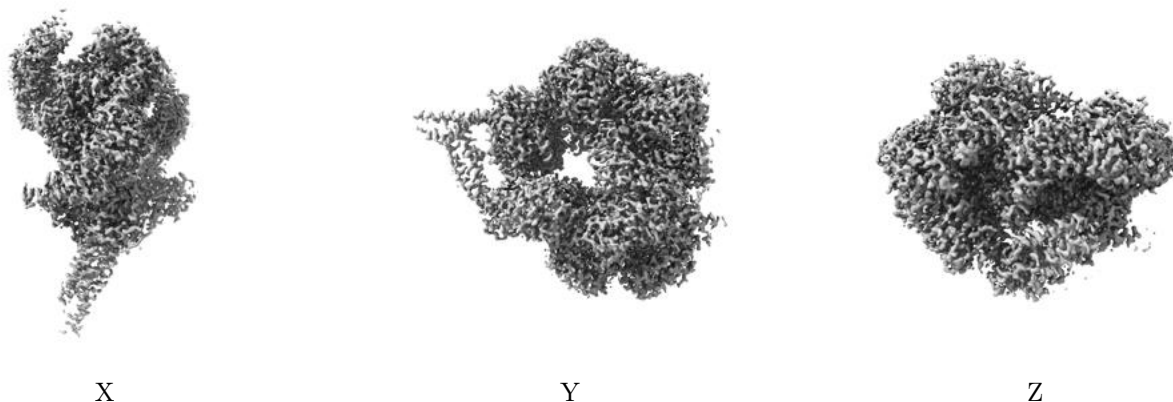


Z

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.

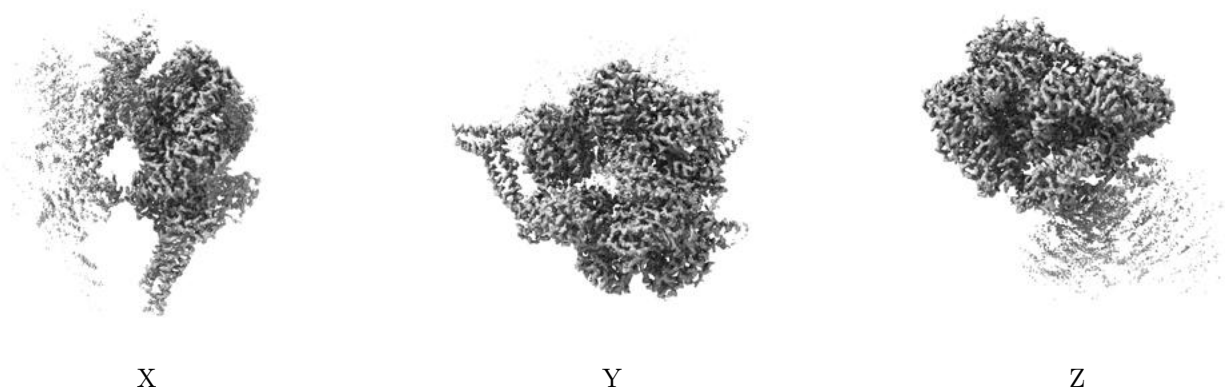
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

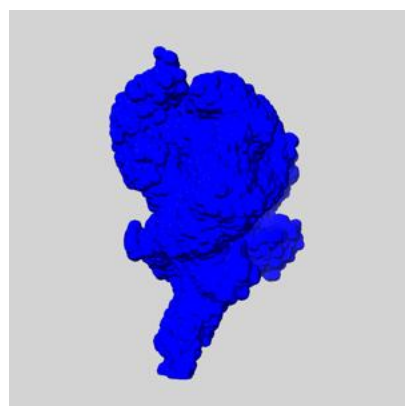
6.6 Mask visualisation [i](#)

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

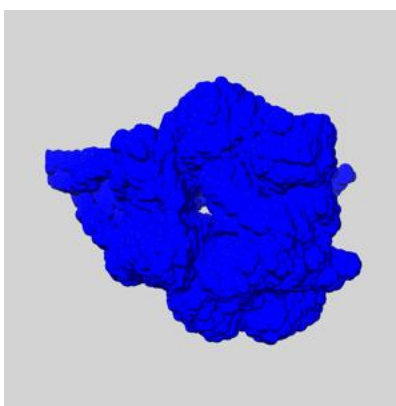
A mask typically either:

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

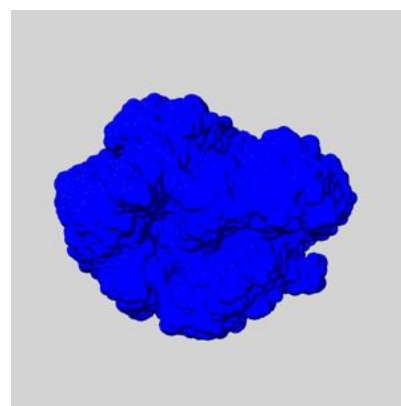
6.6.1 emd_44682_msk_1.map [i](#)



X



Y

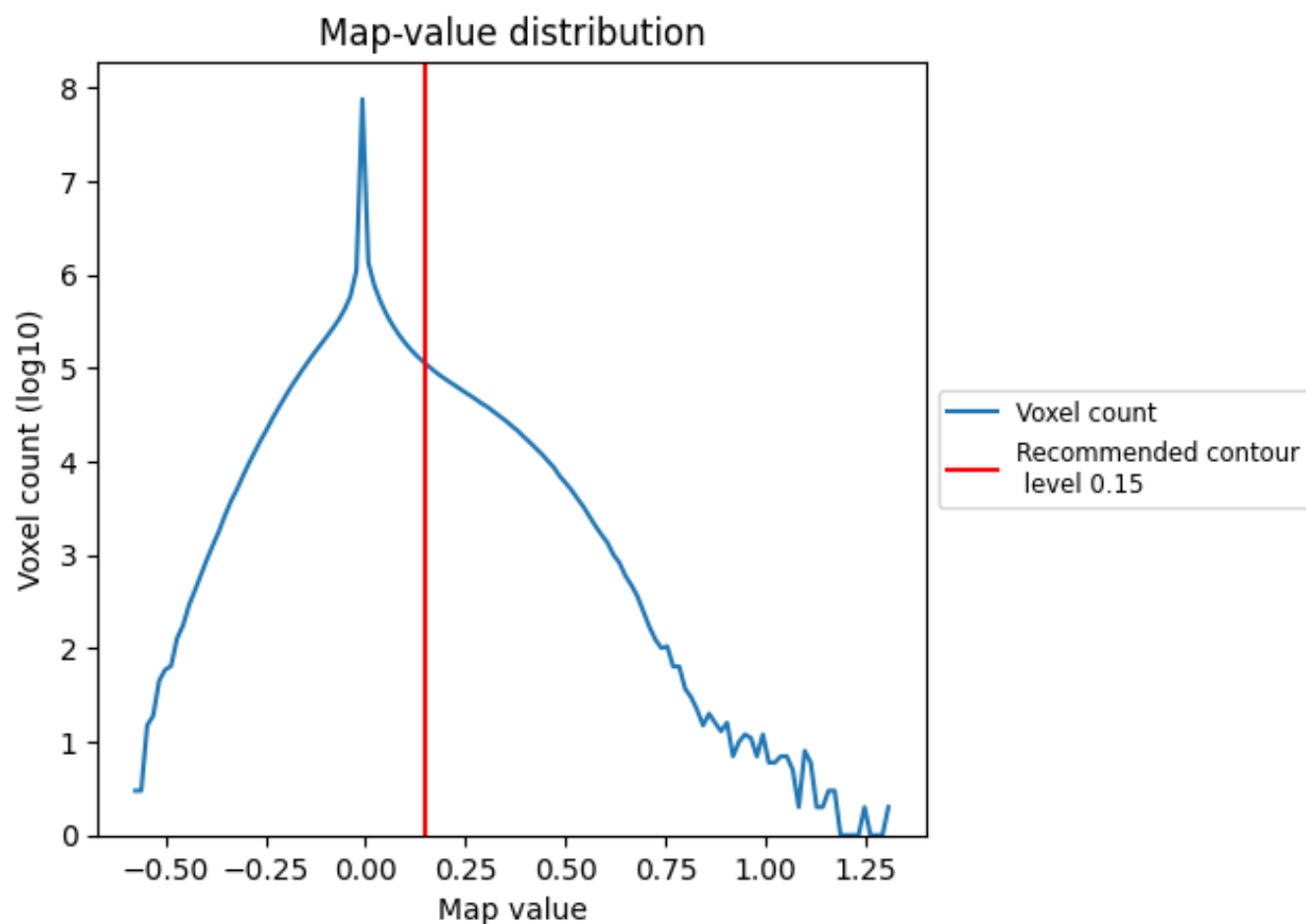


Z

7 Map analysis [i](#)

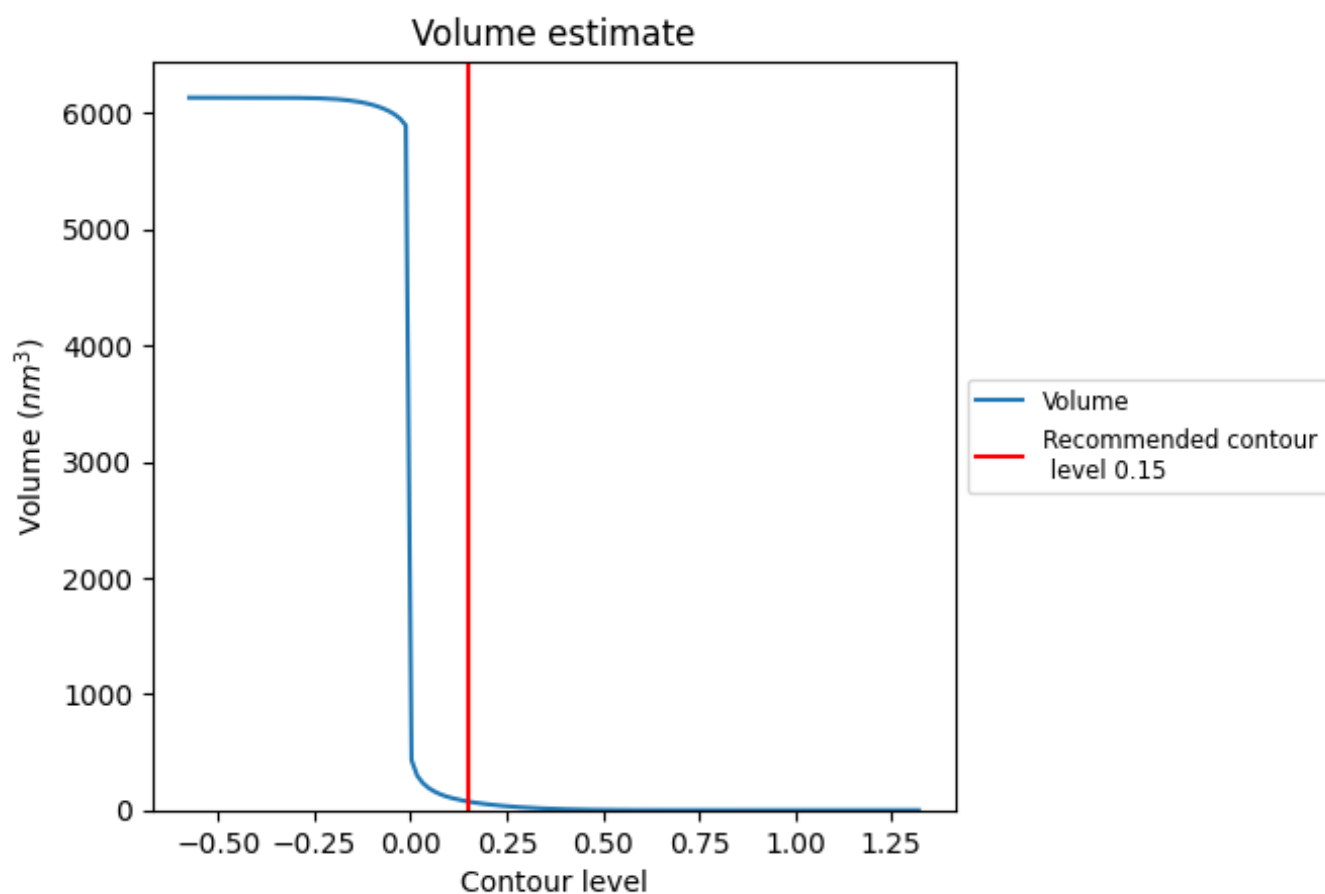
This section contains the results of statistical analysis of the map.

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.

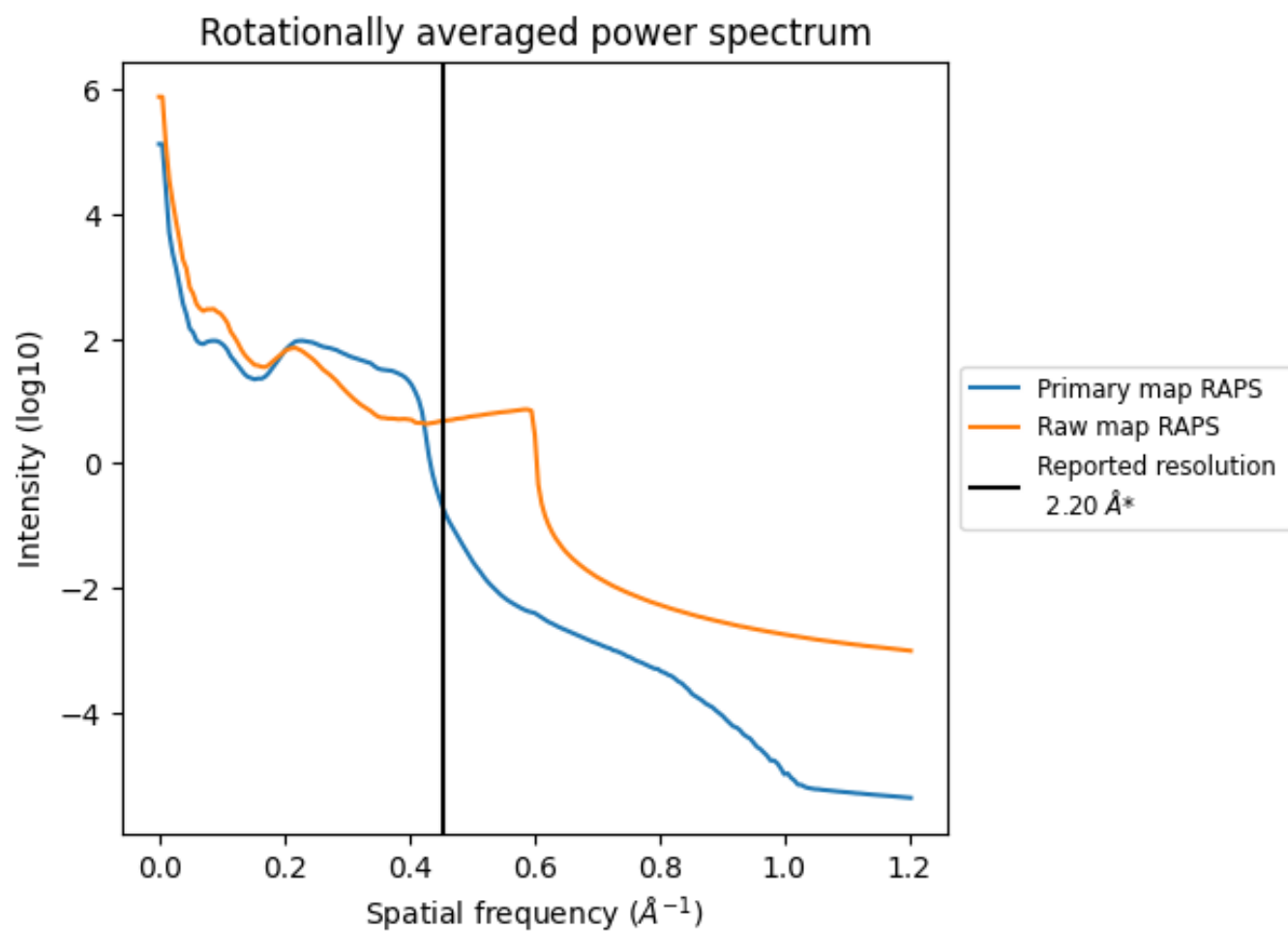
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 ⓘ

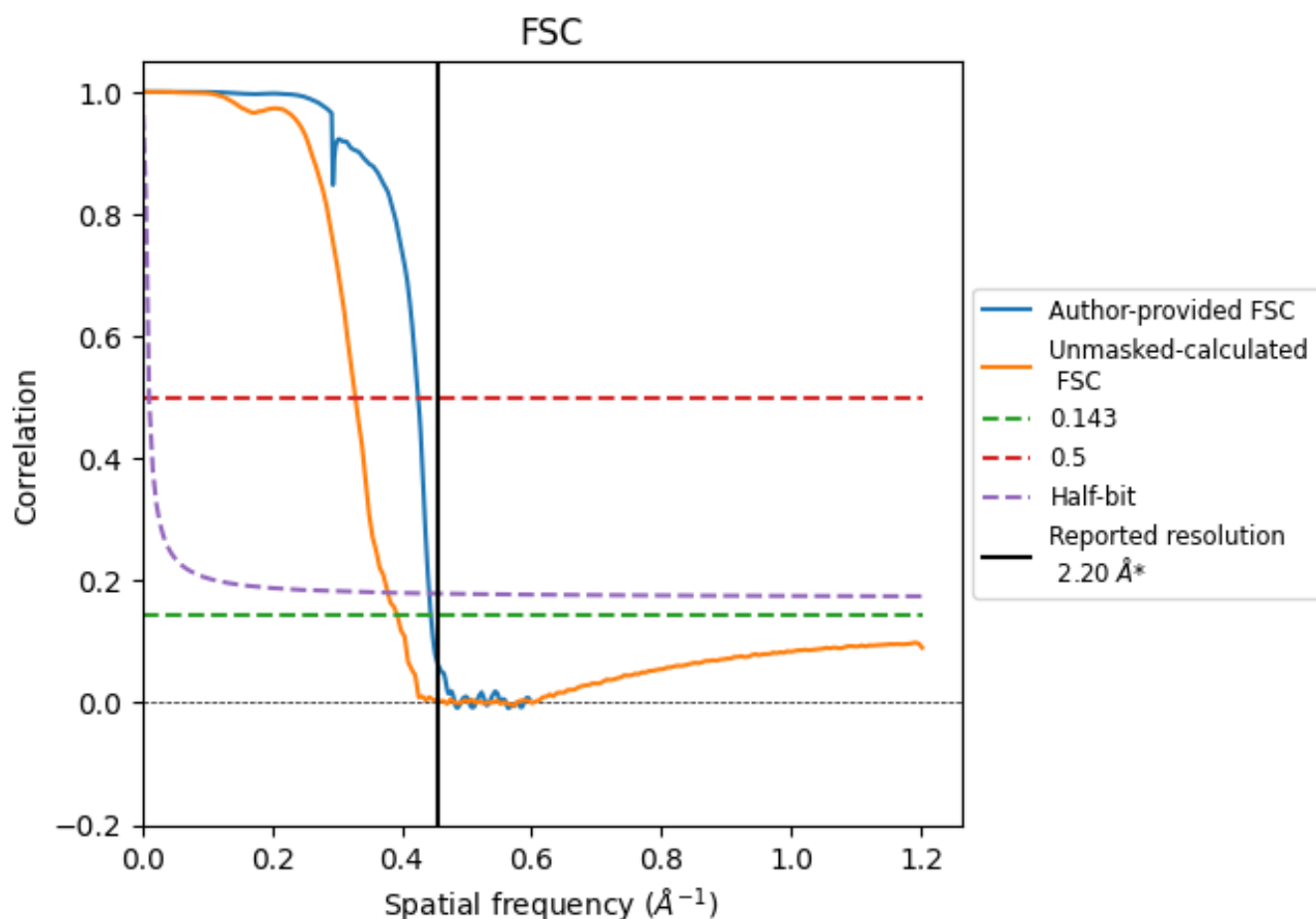


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

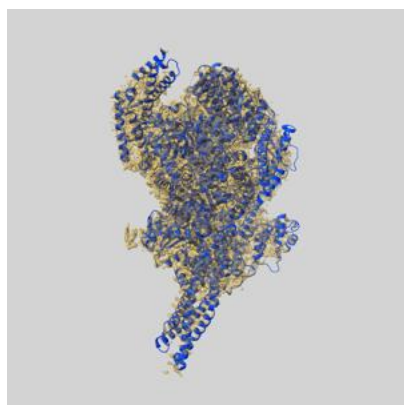
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.25	2.35	2.26
Unmasked-calculated*	2.54	3.05	2.64

*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 2.54 differs from the reported value 2.2 by more than 10 %

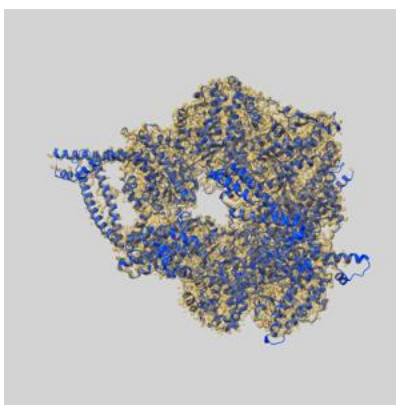
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44682 and PDB model 9BLZ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

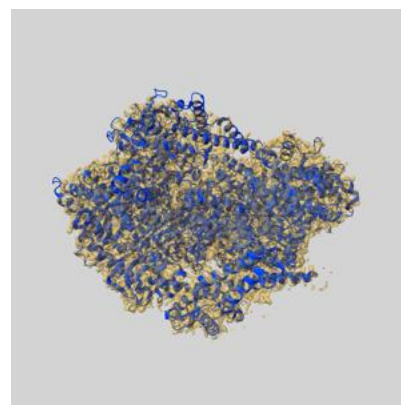
9.1 Map-model overlay [i](#)



X



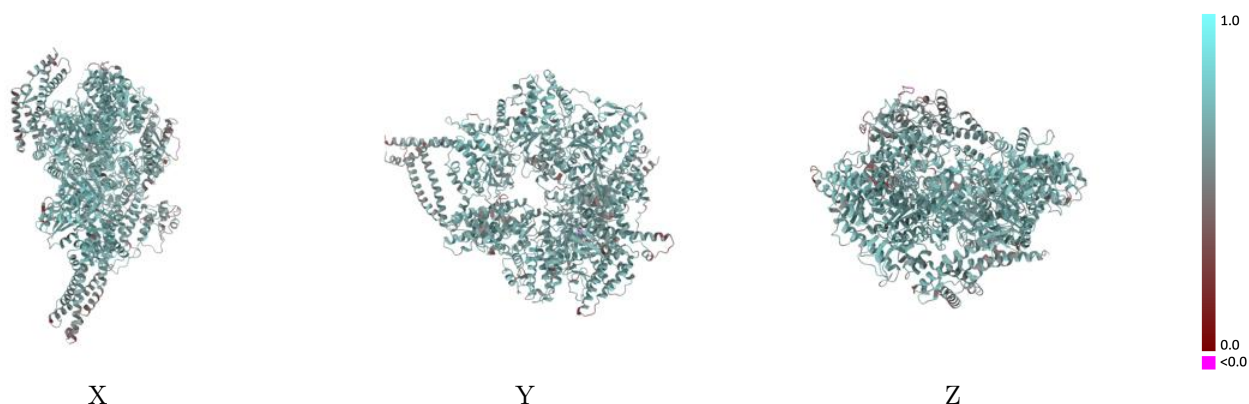
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)

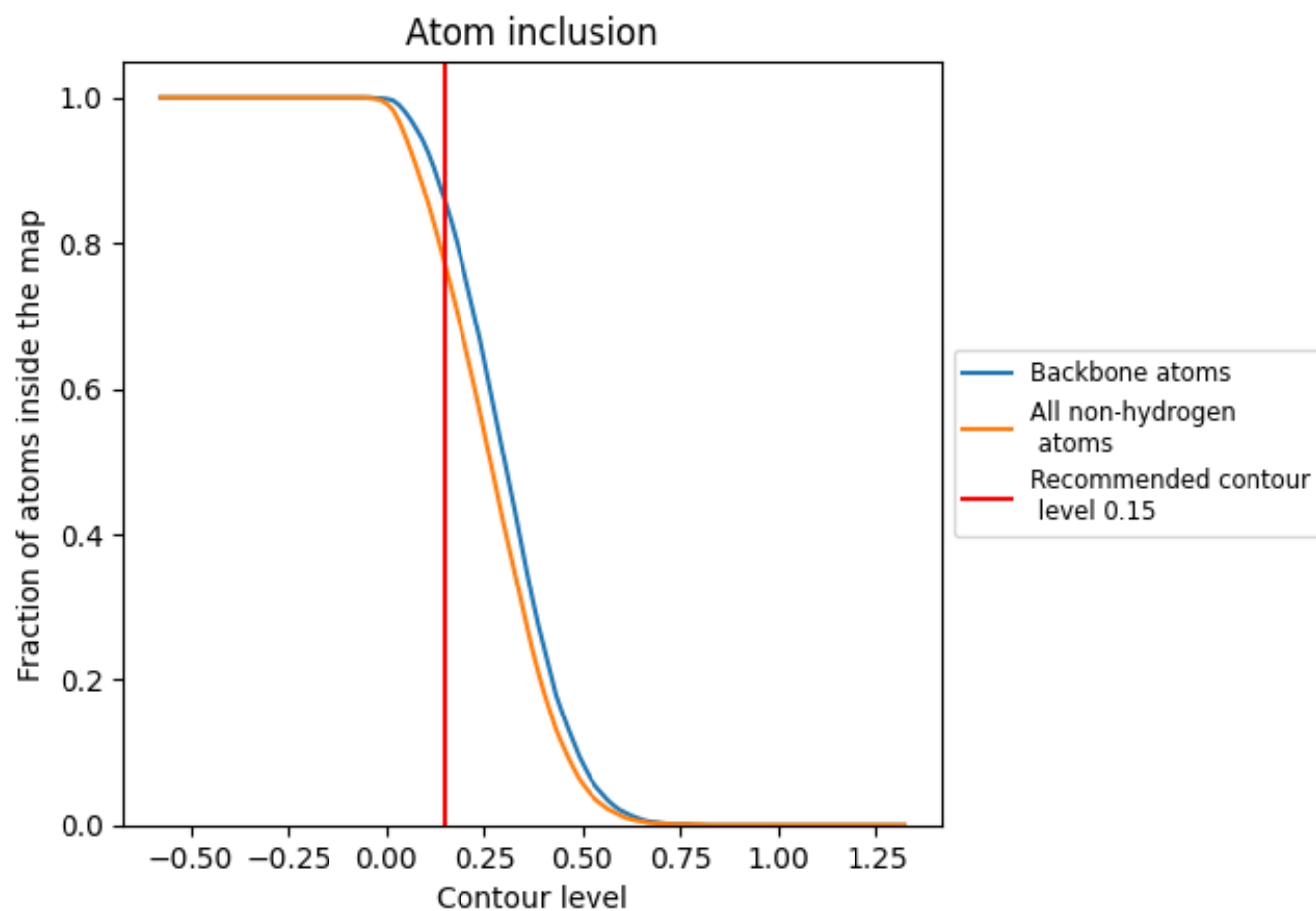


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.6370
A	0.7690	0.6370

