



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 12:24 PM UTC

PDB ID : 9BN0 / pdb_00009bn0
EMDB ID : EMD-44717
Title : State-7 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.60 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

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<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

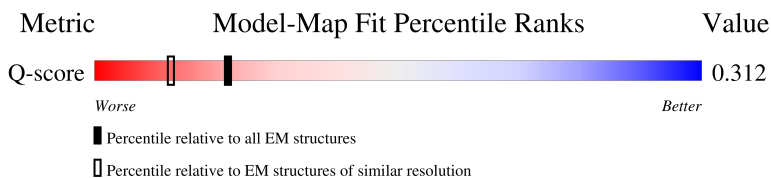
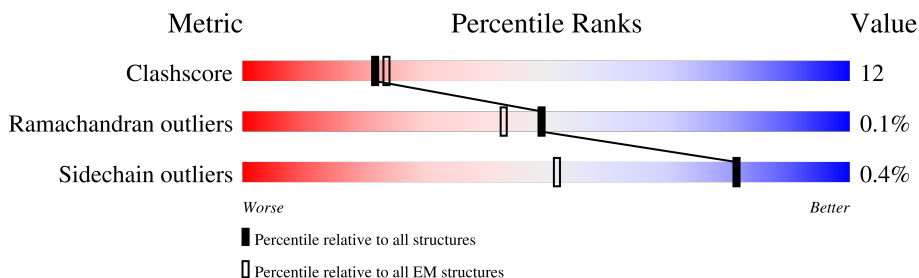
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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](#)

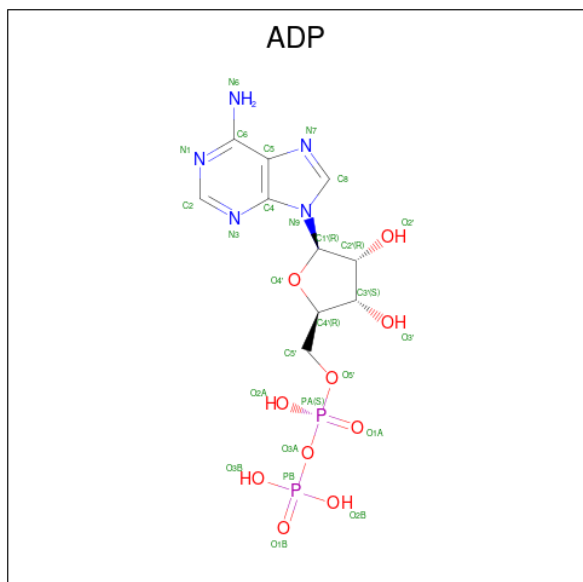
There are 4 unique types of molecules in this entry. The entry contains 23497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2909	Total	C	N	O	S	0	0
			23384	14885	4038	4344	117		

- 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	1	Total 1	Mg 1	0

L2097	M1961	L1792	E1639	F1568	M1502	LYS	ASN	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
R2107	E1964	L1797	I1641	F1570	S1503	GLU	GLU	TRP	ALA	GLU	PHE	PHE	LEU	LEU	LEU	LEU	PHE
G2119	E1965	L1797	I1641	S1570	Y1504	ALA	ALA	GLU	GLU	GLU	THR	THR	VAL	THR	GLN	GLN	GLN
A2121	R1966	Q1800	K1645	I1571	S1505	ILE	VAL	VAL	VAL	VAL	PRO	PRO	ILE	MET	ASN	GLY	LYS
V2122	M1967	R1804	K1649	S1572	M1506	LYS	LYS	GLN	ASP	THR	TRP	TRP	VAL	PRO	GLN	ILE	VAL
D2123	Q1979	E1814	K1652	T1573	K1508	ASP	VAL	ARG	LEU	THR	TRP	TRP	VAL	ASP	VAL	GLY	VAL
T2127	P1988	L1815	H1653	F1574	L1509	VAL	LEU	LEU	GLY	GLY	TYR	TYR	GLY	GLY	LEU	LEU	LEU
N1989	N1989	V1816	F1654	F1575	S1510	VAL	VAL	GLY	VAL	ARG	ASP	ASP	THR	ALA	ASN	GLY	ILE
Q2133	D1991	H1817	K1655	L1576	P1511	VAL	ALA	TYR	TRP	PRO	ASN	ASN	PHE	LEU	PRO	VAL	ILE
Q2134	Y1990	Q1818	F1658	L1577	Y1512	GLN	GLN	MET	SER	GLU	ILE	ILE	ASP	GLU	ARG	VAL	GLU
E2135	D1991	I1826	Y1661	M1579	Y1513	GLY	GLY	LYS	GLU	GLU	GLY	GLY	ASN	GLU	GLU	LEU	LYS
V2146	T1993	M1842	S1662	K1580	K1514	ILE	ILE	ILE	ALA	ALA	GLY	GLY	ASN	GLY	GLY	ALA	LYS
L2149	R1843	R1843	S1663	K1581	V1515	MET	ASN	MET	SER	LEU	GLY	GLY	GLY	TYR	GLY	ALA	ILE
V2150	S1994	F1844	I1664	V1582	F1516	ALA	ALA	LEU	VAL	ALA	GLY	GLY	VAL	VAL	ARG	LEU	LEU
A2151	A1995	Y1845	E1668	S1583	E1517	GLU	GLU	SER	TRP	LEU	ALA	ALA	VAL	VAL	ARG	LEU	GLY
E2152	N2012	L1857	D1669	K1584	D1518	ILE	ILE	ILE	GLU	THR	PHE	PHE	GLU	GLU	LYS	VAL	GLU
L2160	T2017	M1861	I1676	M1589	S1523	ALA	ALA	ALA	LYS	ASP	ARG	ARG	VAL	VAL	LYS	ALA	VAL
L2161	N2018	A1864	S1677	D1590	E1522	LEU	LEU	LEU	GLU	GLY	LYS	LYS	THR	THR	GLY	THR	ASP
V2164	P2020	Y1868	R1679	V1591	E1524	LYS	LYS	GLN	ILE	TYR	ASN	ASN	PHE	THR	THR	TRP	TRP
F2185	G2021	L1872	K1697	N1592	K1526	ASP	ASP	GLN	GLY	GLY	ILE	ILE	GLY	VAL	GLN	GLY	GLY
P2186	TYR	Y1873	I1698	M1593	D1525	GLY	SER	SER	GLY	LYS	ASP	ASP	VAL	VAL	GLY	GLY	GLY
F2187	ALA	L1874	N1699	I1594	K1527	GLU	GLU	GLU	TRP	LYS	ASP	ASP	VAL	VAL	LYS	ASP	LYS
G2188	GLY	L1875	E1700	I1594	L1527	ALA	ALA	GLY	TRP	GLN	ILE	ILE	GLY	GLY	GLY	GLY	GLY
R2172	ARG	G1874	W1701	D1590	M1528	LEU	LEU	GLN	SER	GLN	GLN	GLN	THR	THR	LEU	LEU	LEU
E2181	S2026	L1879	L1702	V1591	N1528	LEU	LEU	GLN	VAL	VAL	GLN	GLN	SER	VAL	LEU	LEU	LEU
L2182	N2031	V1880	T1703	Q1595	R1529	ARG	ARG	GLN	PRO	PRO	VAL	VAL	GLY	GLY	GLY	GLY	GLY
K2183	L2035	Q1881	L1704	F1596	I1530	MET	MET	LYS	ARG	CYS	ALA	ALA	ASN	ASN	PRO	ASP	ASP
K2184	M2041	T1882	V1705	V1597	M1531	LYS	LYS	LYS	LYS	ALA	ALA	ALA	GLN	GLN	ARG	MET	LEU
M2189	M2041	P1883	E1706	Q1598	A1532	ARG	ARG	GLY	LEU	LYS	LEU	LEU	CYS	CYS	GLN	ASP	ASP
Y2190	L2045	L1884	E1706	R1599	A1532	LEU	LEU	LEU	ARG	LYS	GLY	GLY	TRP	TRP	ILE	ASP	ASP
L2191	D2045	T1885	L1717	L1601	L1533	HIS	HIS	GLN	ASN	LYS	MET	MET	ASP	ASP	GLN	ALA	ALA
T2192	L2048	T1885	L1717	L1601	F1534	D1476	D1476	VAL	ASN	LYS	GLY	GLY	TRP	TRP	GLN	GLN	GLN
Y2193	L2049	M1892	V1721	D1602	D1535	L1477	L1477	VAL	ASN	LYS	PHE	PHE	ASP	ASP	ILE	ILE	ILE
V2207	V2052	E1897	V1724	R1603	D1535	V1478	V1478	GLU	ASP	ALA	GLY	GLY	TRP	TRP	GLN	GLN	GLN
T2213	M2053	G1902	F1727	A1605	V1536	M1479	M1479	GLU	ALA	VAL	VAL	VAL	GLY	GLY	VAL	VAL	VAL
T2214	L2065	T1910	F1727	L1604	Y1480	N1481	N1481	LEU	LEU	GLU	GLU	GLU	ASP	ASP	GLY	GLY	GLY
H2218	A2066	G1911	Y1738	A1605	W1537	Q1481	Q1481	THR	THR	ASP	ASP	ASP	VAL	VAL	GLY	GLY	GLY
G2219	L2069	K1912	L1607	D1606	I1538	K1483	K1483	GLY	GLY	THR	THR	THR	VAL	VAL	LEU	LEU	LEU
L2220	F2072	R1925	Q1746	L1607	V1545	L1486	L1486	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
M2221	L2075	F1928	L1749	L1608	E1548	I1487	I1487	LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY
M2222	L2090	V1927	L1750	G1609	E1548	R1488	R1488	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
S2231	L2093	L1948	G1771	K1610	E1548	G1489	G1489	LEU	LEU	SER	THR	THR	ASP	ASP	GLY	GLY	GLY
M2232	K2094	L1948	G1772	K1612	E1548	W1490	W1490	LEU	LEU	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY
A2233	L2093	L1948	G1772	K1612	E1548	D1491	D1491	LEU	LEU	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY
M2234	L2093	L1948	G1772	K1612	E1548	D1492	D1492	LEU	LEU	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY
K2235	L2093	L1948	G1772	K1612	E1548	L1493	L1493	LEU	LEU	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY
V2236	L2093	L1948	G1772	K1612	E1548	F1494	F1494	LEU	LEU	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY



E4537	A4375	L4223	K4082	K3945	H3837	K3747	L3661	N3576	L3478
T4547	H4381	D4224	I4084	K3946	N3838	S3748	I3662	A3577	L3479
Q4549	V4387	I4233	A4087	L3947	V3839	L3749	T3663	I3578	K3480
G4550	V4391	V4086	V4086	V3951	L3840	L3750	L3664	L3580	S3481
A4551	I4398	G4091	G4091	F3957	K3847	Q3751	G3665	K3581	L3482
D4554	L4398	R4092	R4092	F3966	I3859	A3752	D3666	R3585	S3483
F4558	N4404	L4096	L4096	E3967	L3863	L3753	Q3667	L3588	A3484
G4559	E4414	V4099	V4099	L3973	F3864	V3756	L3671	I3589	E3485
V4560	R4415	W4105	W4105	E3977	Q3865	K3757	S3672	I3590	R3486
K4564	E4416	L4106	L4106	E3977	V3866	G3758	P3673	D3591	E3487
K4574	K4422	M4107	M4107	T3983	F3869	R3759	T3681	A3596	K3489
L4575	L4423	L4113	L4113	L3992	R3870	I3760	D3682	T3597	E3490
S4576	R4428	L4116	L4116	F3996	V3871	L3761	D3683	T3600	K3491
L4577	Q4429	P4118	P4118	R4000	R3872	D3762	P3684	M3601	T3492
P4586	D4430	C4121	C4121	L4001	R3873	D3763	D3692	N3602	S3493
K4594	C4438	F4122	F4122	L4002	G3874	D3764	L3693	E3603	E3494
E4599	K4441	M4339	M4339	L4012	M3875	T3765	C3693	D3606	F3496
P4608	K4442	M4343	M4343	L4013	H3880	I3766	S3694	R3607	M3500
V4609	K4443	L4344	L4344	L4013	A3888	I3767	R3695	T3611	I3503
W4610	Q4444	K4345	K4345	M4021	R3889	T3768	V3696	T3612	S3510
L4611	T4445	M4346	M4346	M4021	R3892	T3769	T3697	L3615	F3513
I4619	W4446	Q4347	Q4347	L4025	L3892	L3770	V3699	D3616	D3617
F4624	Y4447	M4348	M4348	V4031	F3908	E3771	F3701	A3618	A3619
A4627	K4457	L4349	L4349	G4032	R3909	N3772	T3702	F3619	F3620
T4628	G4458	V4134	V4134	T4033	R3910	L3773	T3702	K3621	F3519
E4637	I4459	P4135	P4135	E4034	E3913	K3774	Q3709	N3622	F3520
R4638	L4460	M4137	M4137	E4034	I3914	E3776	V3716	L3623	K3524
V4642	P4461	R4140	R4140	P4037	V3915	A3777	V3724	L3627	H3535
E4646	R4462	ALA	ALA	M4038	L3916	A3778	D3725	R3628	L3536
	S4463	F4147	F4147	P4040	S3917	E3779	E3726	F3629	Q3537
	W4464	L4158	L4158	H4054	A3918	V3780	K3727	P3632	I3541
	H4466	GLU	GLU	L4058	S3920	T3781	R3728	Q3636	R3549
	V4475	R4176	R4176	L4068	T3921	R3782	S3729	V3638	E3551
	I4476	L4179	L4179	N4063	L3927	K3783	D3729	V3644	T3552
	A4501	Y4180	Y4180	T4064	T3928	V3784	D3730	V3653	L3553
	K4502	L4183	L4183	Q4065	V3929	E3785	L3731	R3654	S3554
	K4505	THR	THR	T4069	E3930	E3786	L3732	R3655	T3560
	L4511	R4193	R4193	A4070	A3934	T3787	K3733	T3656	W3562
	T4524	S4202	S4202	L4071	V3935	D3788	L3734	G3657	G3658
	W4534	Y4205	Y4205	F4077	V3936	I3789	Q3735	R3659	L3567
	S4535	A4215	A4215	Q4078	R3937	V3790	E3737	V3660	E3575
	L4536	ARG	ARG	Q4080	C3940	Q3792	F3738		
		D4220	D4220	D4081	L3941	E3795	Q3739		
					P3842	T3796	L3740		
						V3797	L3742		
							R3743		
							Q3744		
							L3745		
							L3824		
							S3828		
							L3833		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67545	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	1.172	Depositor
Minimum map value	-0.520	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.15	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, MG, 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	0.28	0/23881	0.42	1/32360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3129	VAL	N-CA-C	-5.20	107.76	113.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3695	ARG	Sidechain

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	23384	0	23414	546	0
2	A	81	0	36	9	0
3	A	31	0	12	2	0
4	A	1	0	0	0	0
All	All	23497	0	23462	546	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 546 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:3034:LYS:HA	1:A:3050:LEU:HD22	1.57	0.86
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.62	0.81
1:A:2581:LEU:HD22	1:A:2591:LEU:HD21	1.68	0.76
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	1.68	0.75
1:A:2320:ASP:OD2	1:A:2321:ASP:N	2.20	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	2901/4646 (62%)	2832 (98%)	66 (2%)	3 (0%)	48 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2987	ASN
1	A	2943	LYS
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	2583/4125 (63%)	2572 (100%)	11 (0%)	84 81

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3096	ASP
1	A	3125	TYR
1	A	4343	MET
1	A	3126	MET
1	A	2191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4062	GLN
1	A	4258	ASN
1	A	4506	ASN
1	A	2209	GLN
1	A	2171	HIS

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

Of 5 ligands modelled in this entry, 1 is 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	4701	-	28,29,29	0.45	0	43,45,45	0.49	0
2	ADP	A	4704	-	28,29,29	0.45	0	43,45,45	0.52	0
2	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.51	0
3	ATP	A	4702	-	32,33,33	0.51	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	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

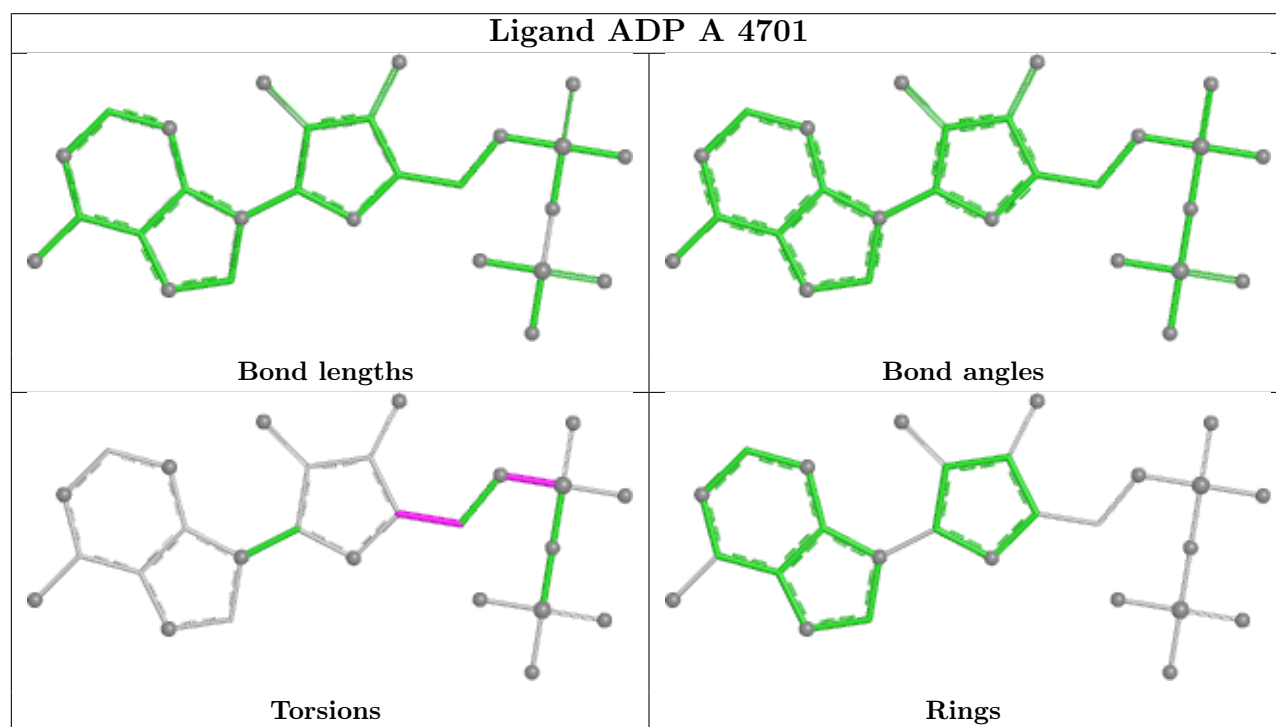
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C2'-C1'-N9-C8

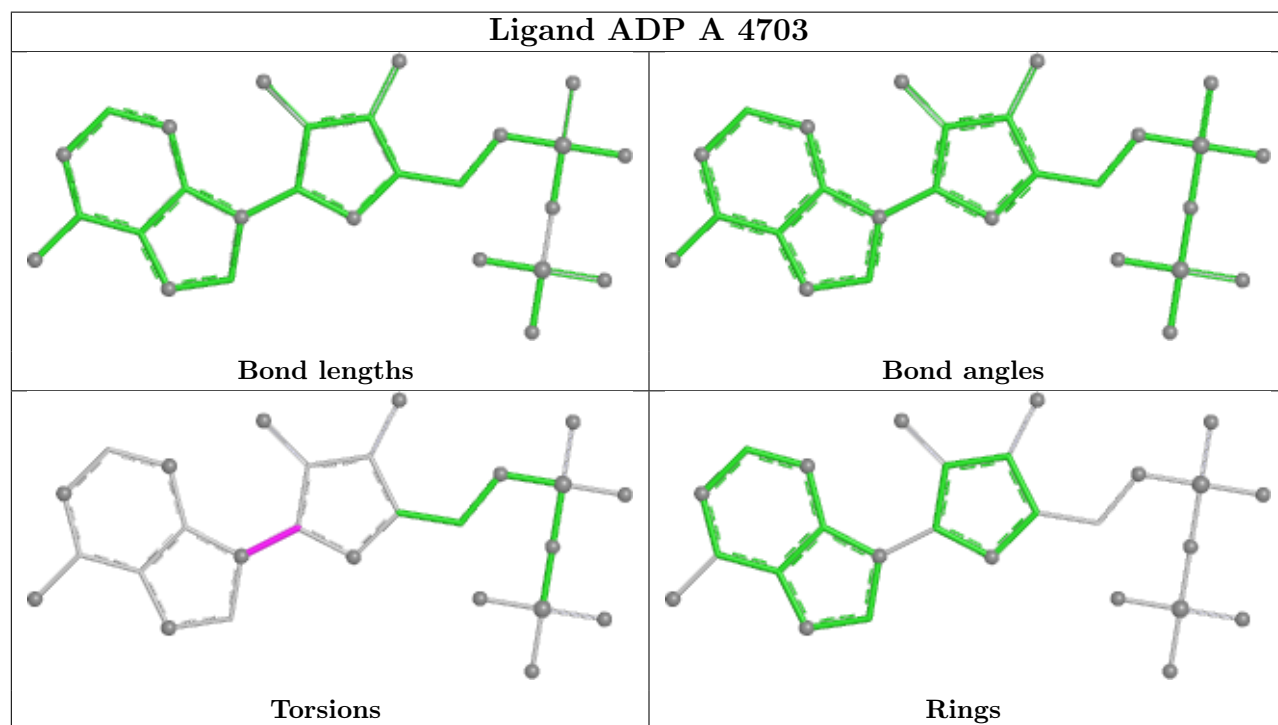
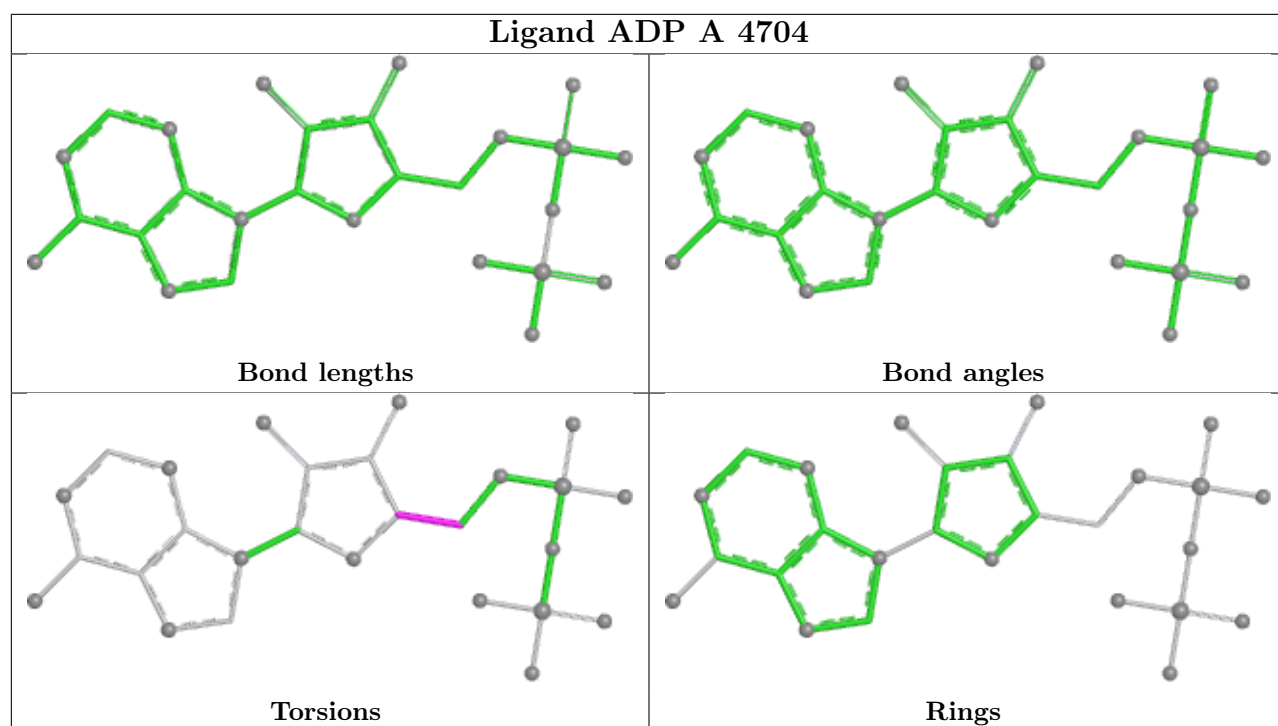
There are no ring outliers.

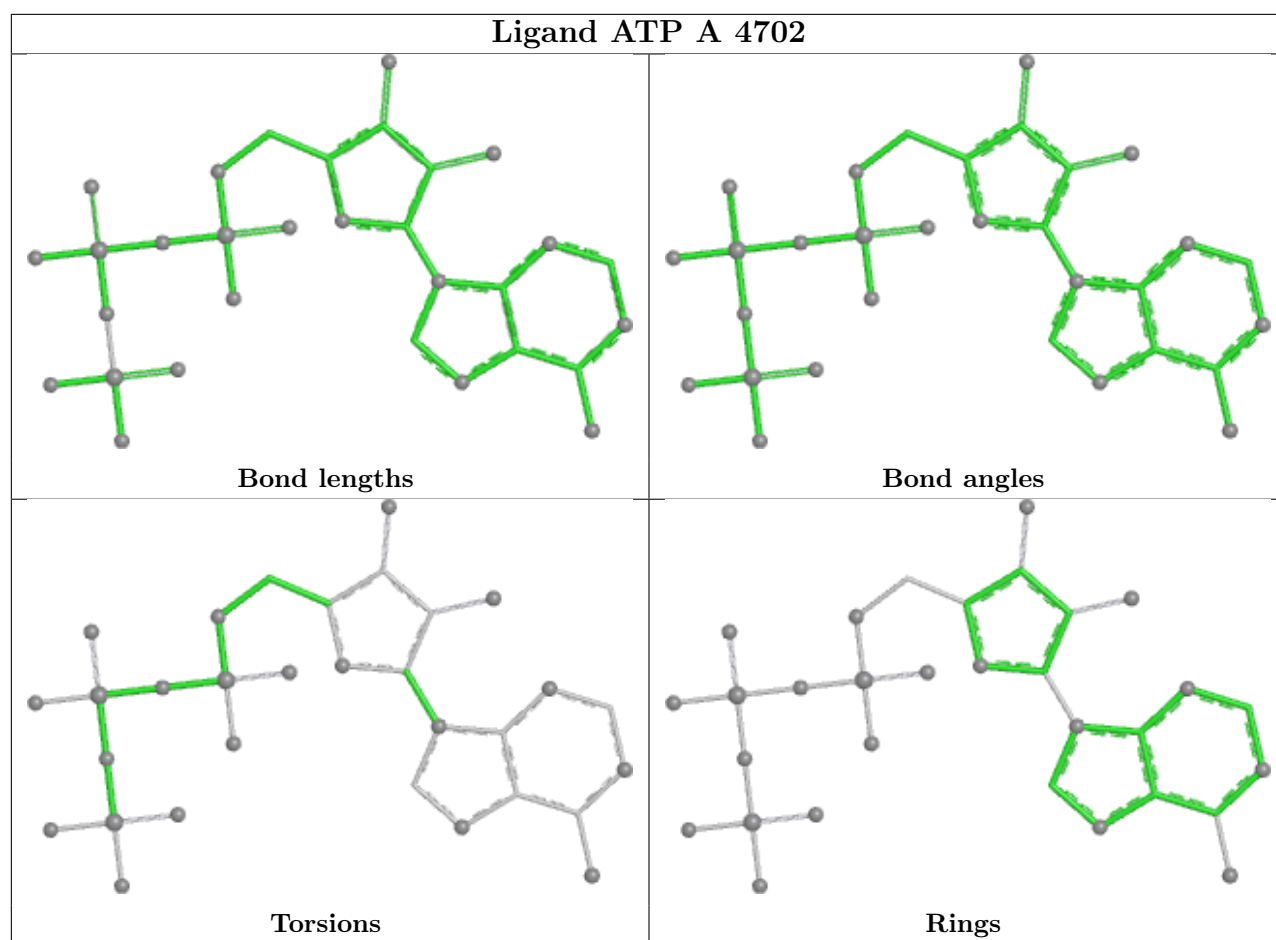
4 monomers are involved in 11 short contacts:

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

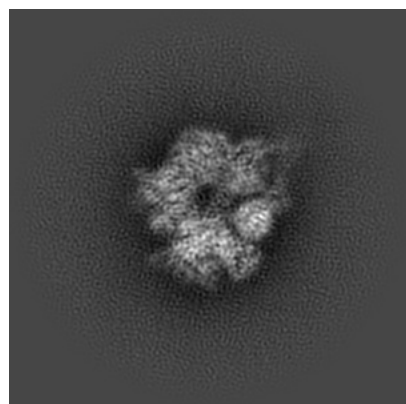
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44717. These allow visual inspection of the internal detail of the map and identification of artifacts.

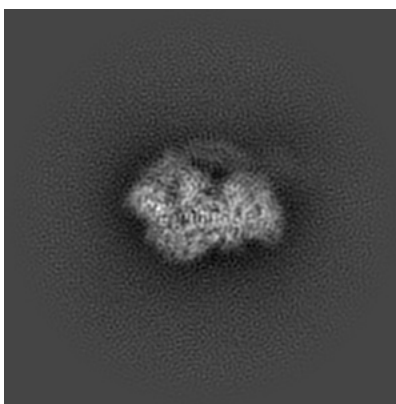
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

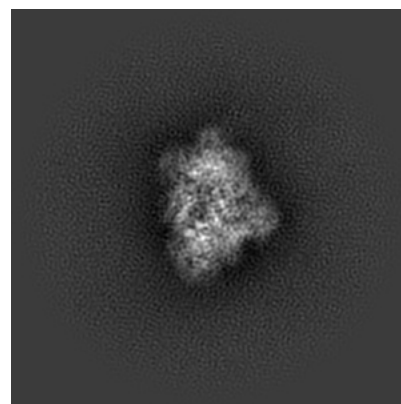
6.1.1 Primary map



X

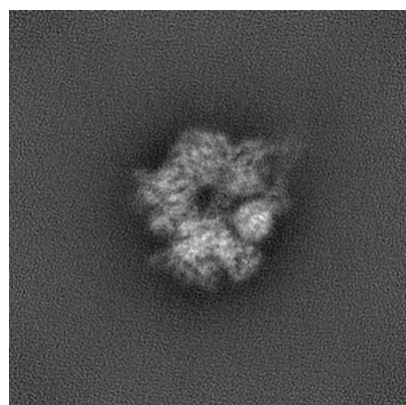


Y

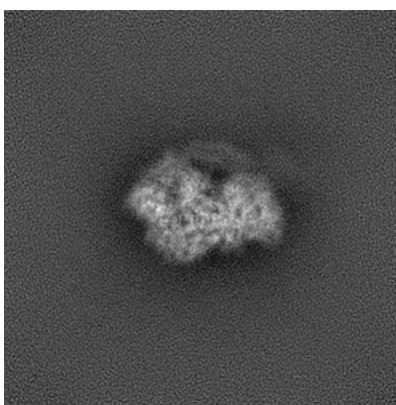


Z

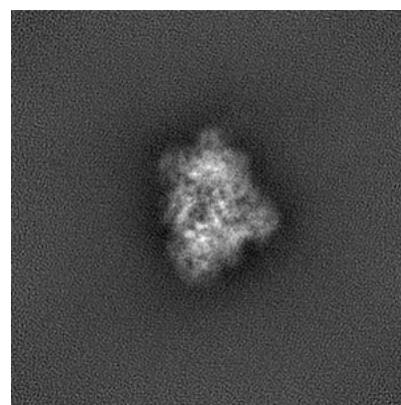
6.1.2 Raw map



X



Y

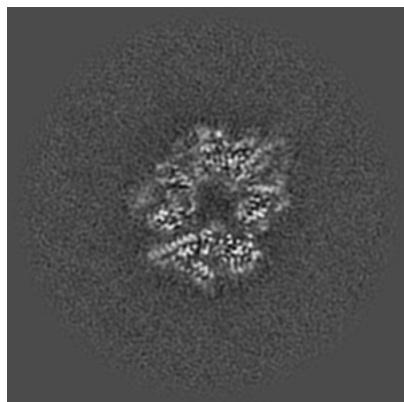


Z

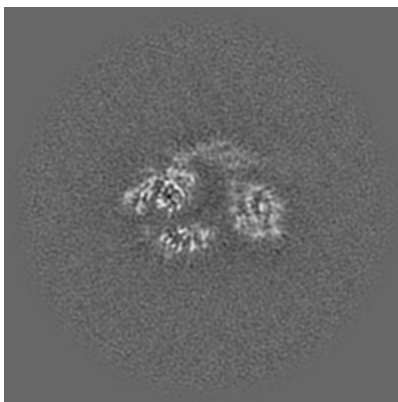
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

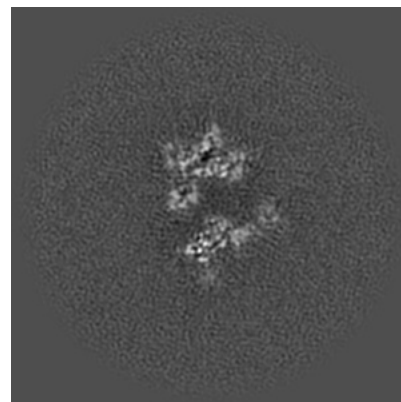
6.2.1 Primary map



X Index: 128

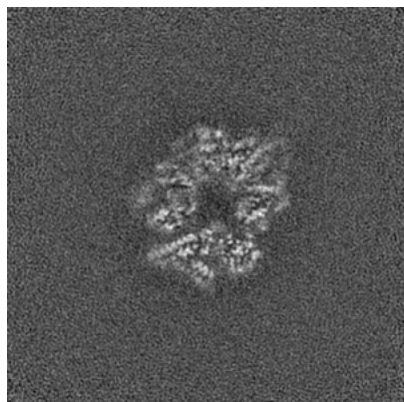


Y Index: 128

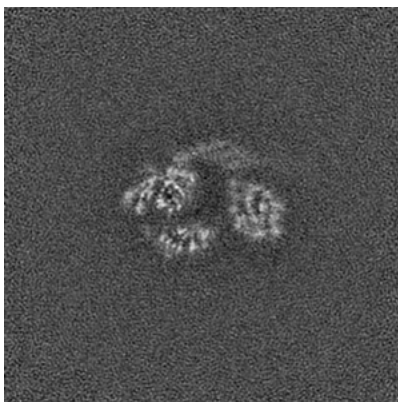


Z Index: 128

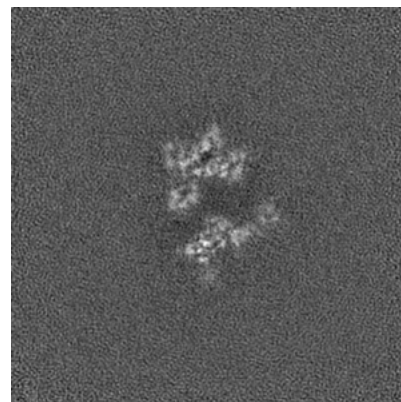
6.2.2 Raw map



X Index: 128



Y Index: 128

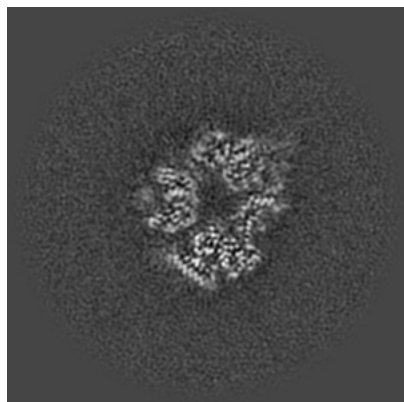


Z Index: 128

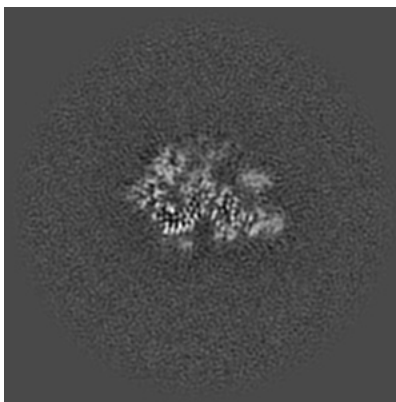
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

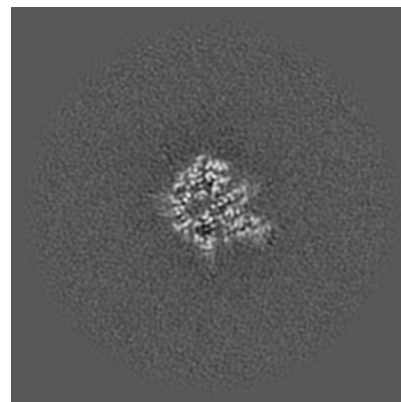
6.3.1 Primary map



X Index: 131

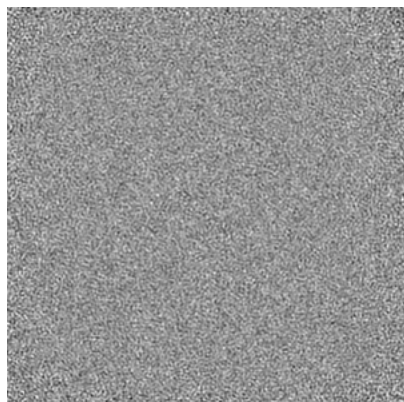


Y Index: 112

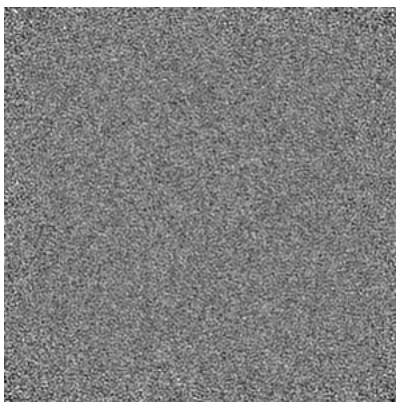


Z Index: 102

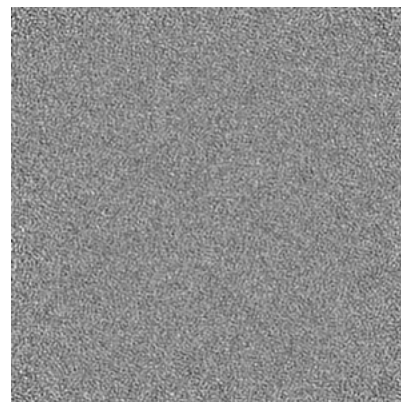
6.3.2 Raw map



X Index: 0



Y Index: 0

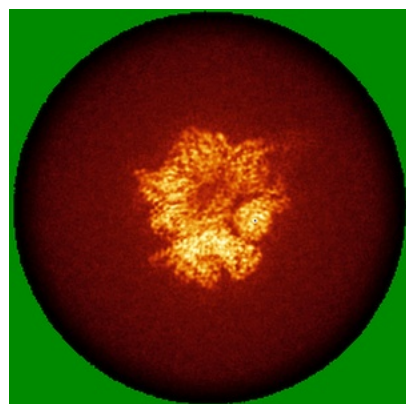


Z Index: 0

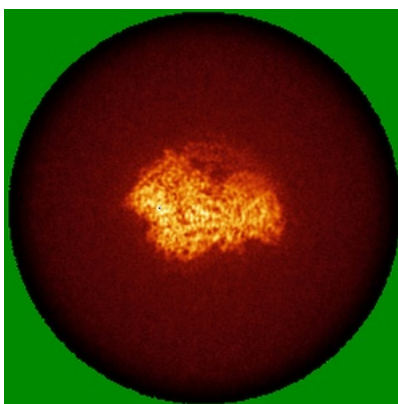
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

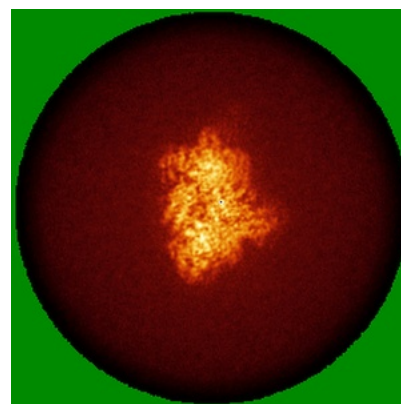
6.4.1 Primary map



X

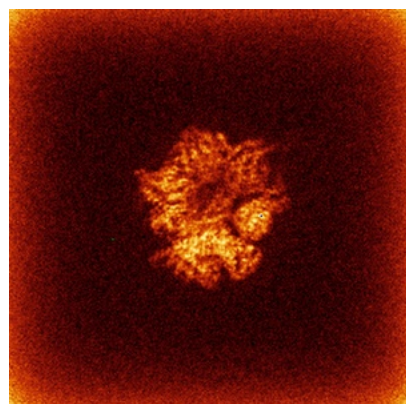


Y

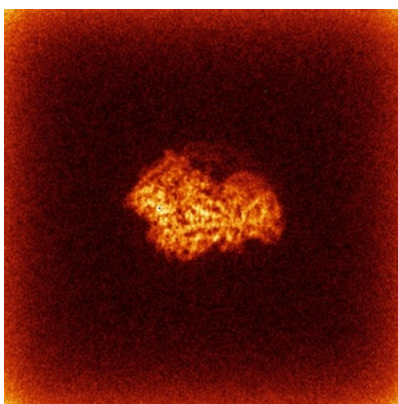


Z

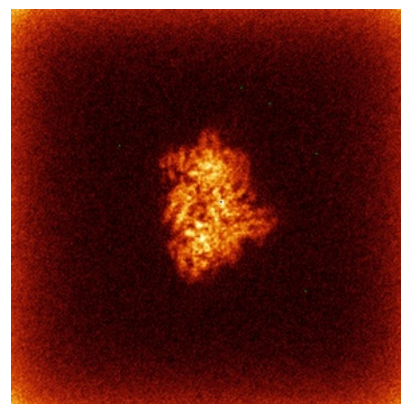
6.4.2 Raw map



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.

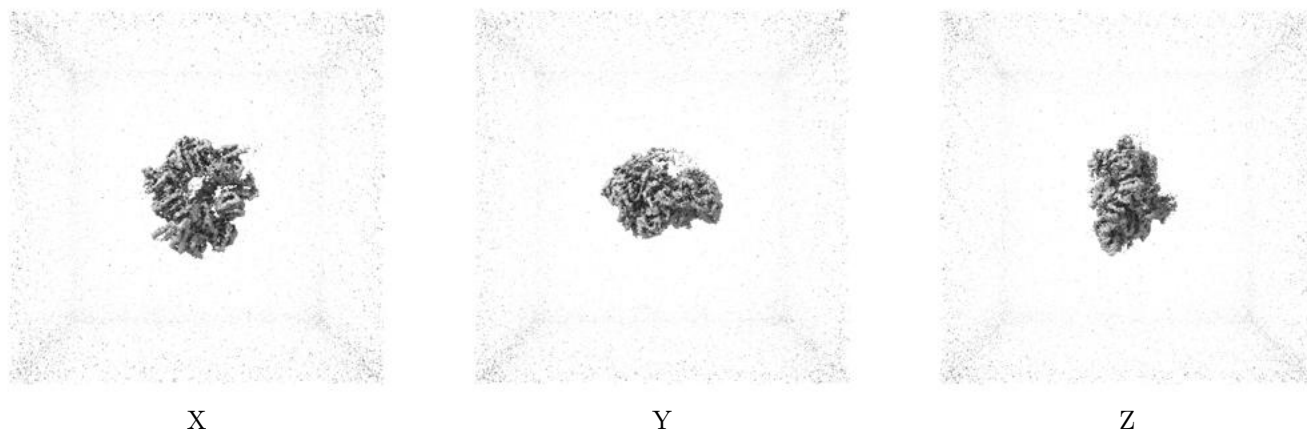
6.5 Orthogonal surface views [i](#)

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.

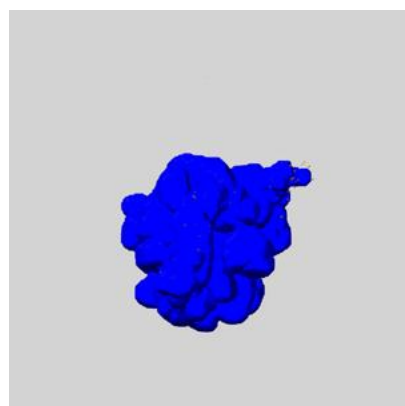
6.6 Mask visualisation [i](#)

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

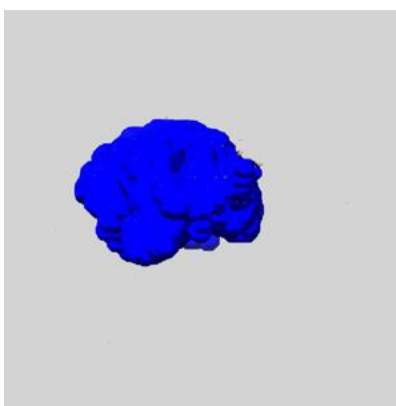
A mask typically either:

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

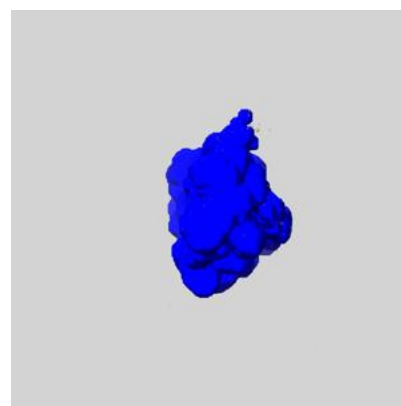
6.6.1 emd_44717_msk_1.map [i](#)



X



Y

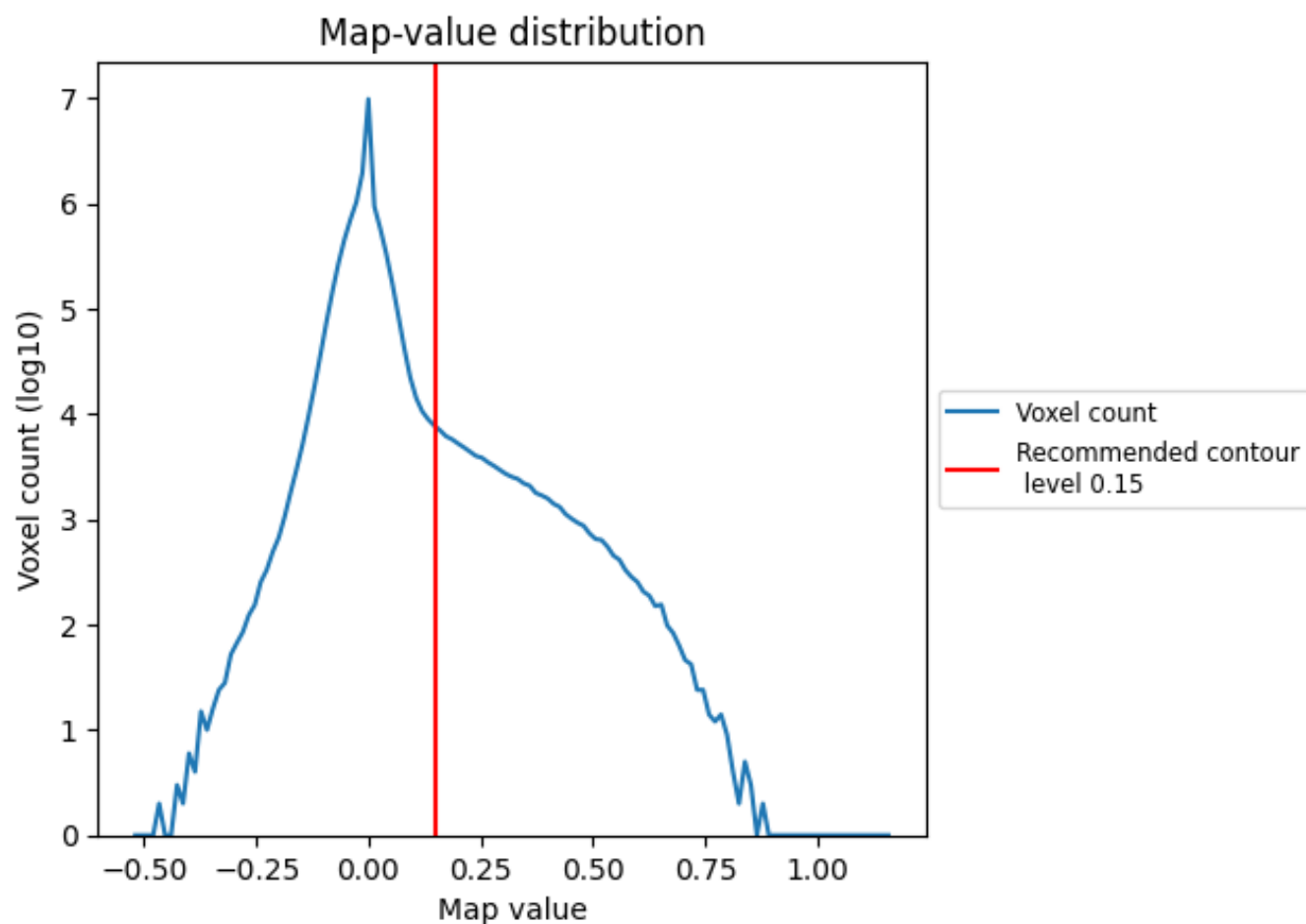


Z

7 Map analysis ⓘ

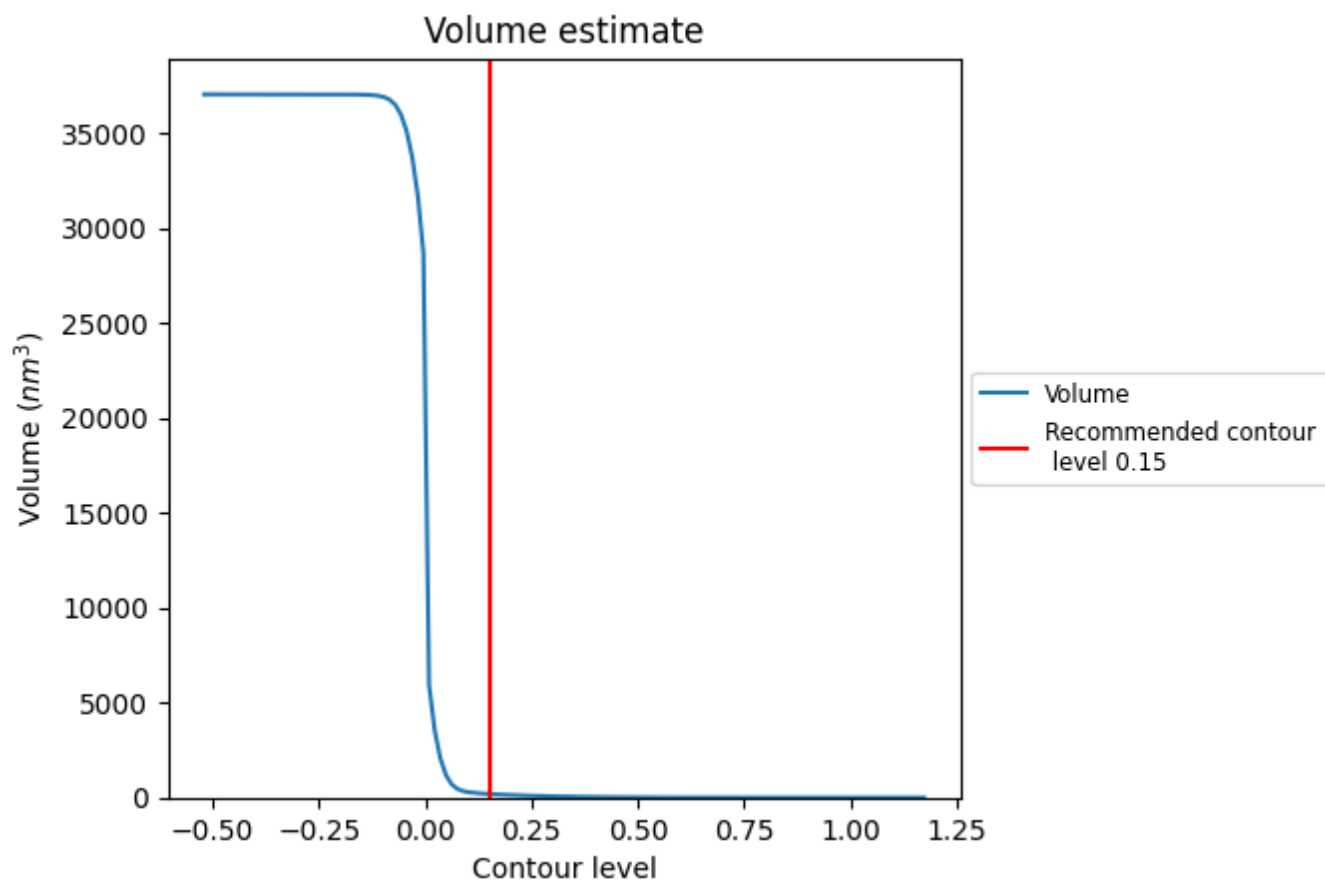
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

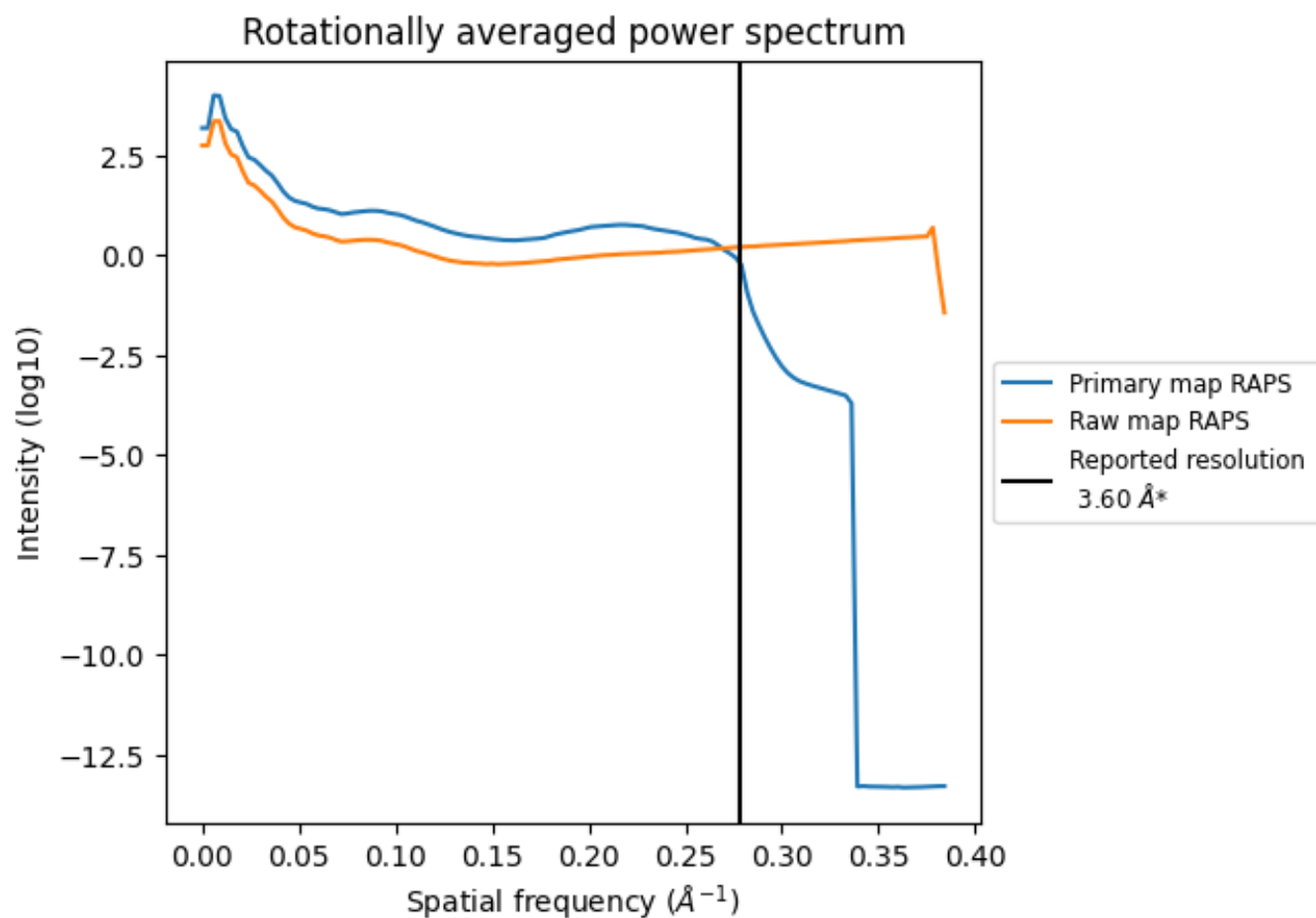
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm³; this corresponds to an approximate mass of 170 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 ⓘ

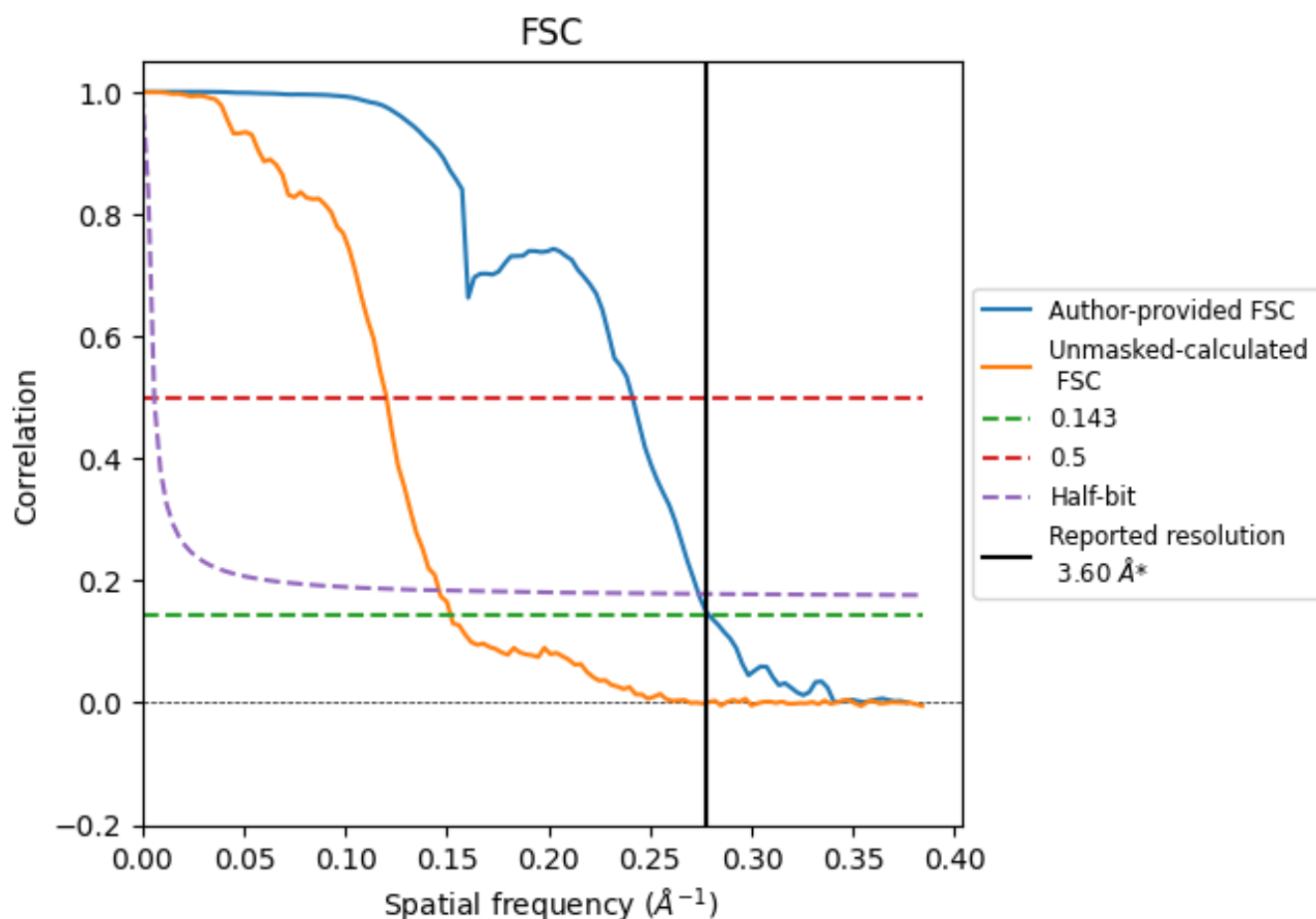


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

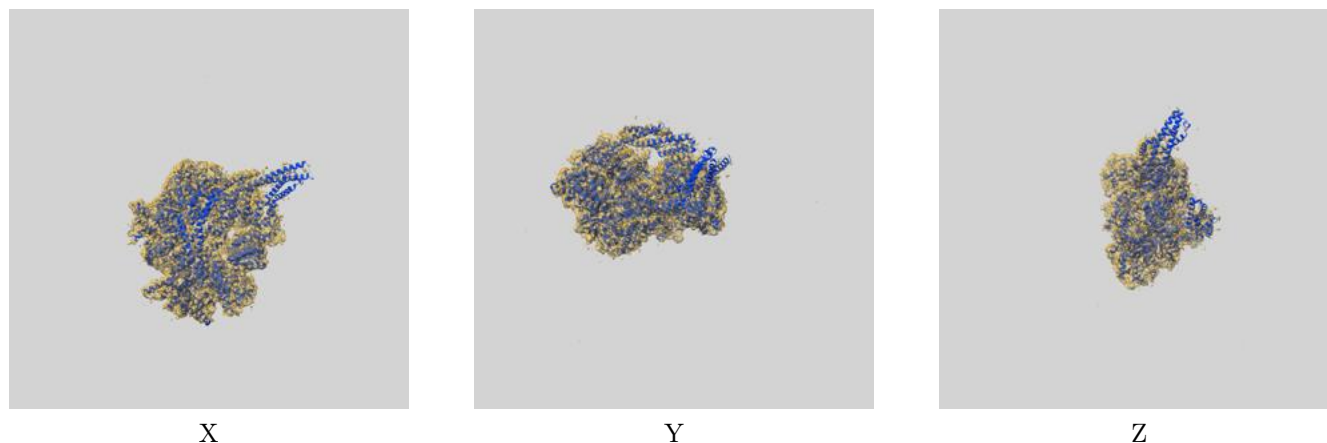
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.14	3.65
Unmasked-calculated*	6.58	8.32	6.84

*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 6.58 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

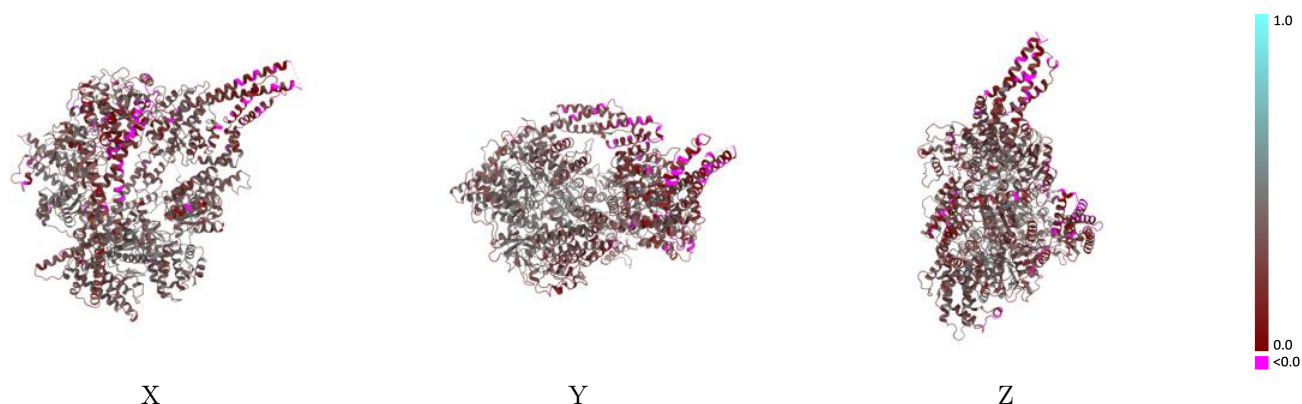
This section contains information regarding the fit between EMDB map EMD-44717 and PDB model 9BN0. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



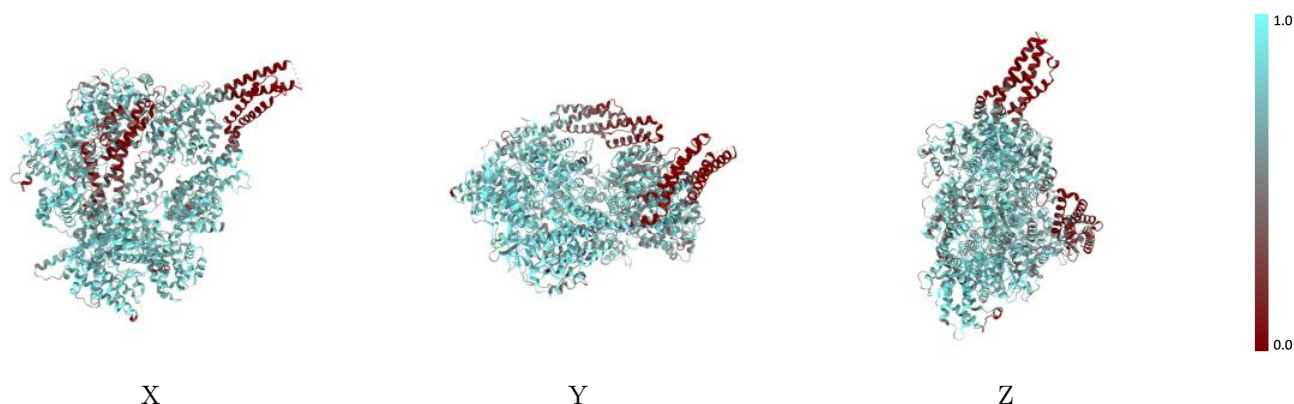
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



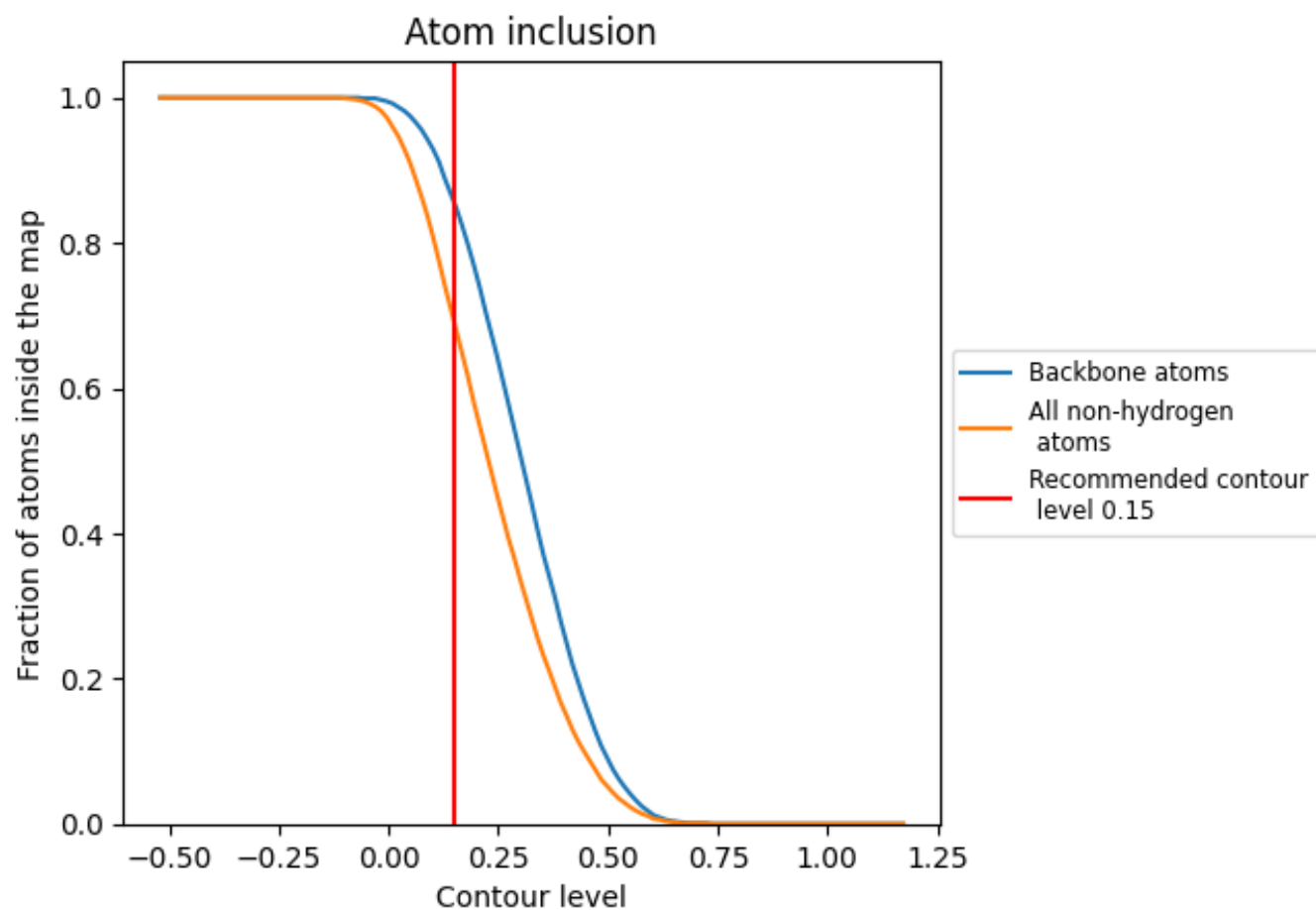
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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	0.6900	0.3120
A	0.6900	0.3120

