



wwPDB EM Validation Summary Report ⓘ

May 13, 2025 – 09:31 PM EDT

PDB ID : 9DHA / pdb_00009dha
EMDB ID : EMD-46861
Title : State-7-Post-1 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg²⁺
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-09-03
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

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

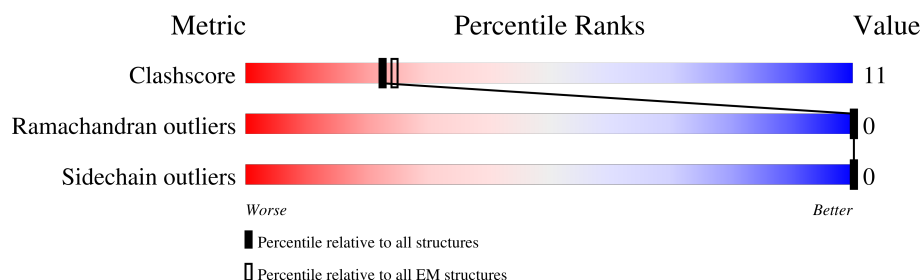
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24588 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.

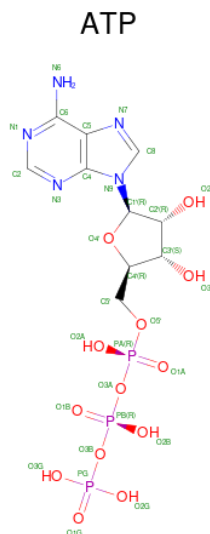
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3038	Total	C	N	O	S	0	0
			24471	15586	4225	4538	122		

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



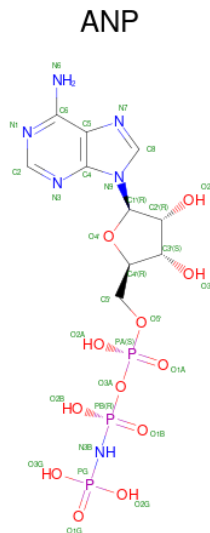
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- 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 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

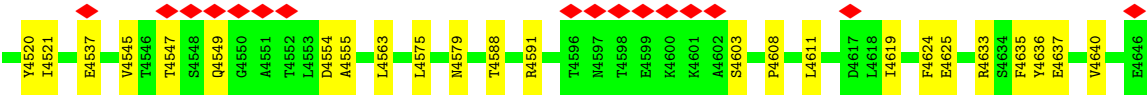
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

K1992	A1862	E1706	L1592	Y1513	K1441	A1381	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
T1993	L1879	R1710	N1593	K1514	N1442	S1382	ALA	GLU	PHE	PHE	LEU	LYS	LEU	LYS	ASN
S1994	V1880		I1594	Y1515	E1443	Y1383	GLU	THR	PHE	THR	VAL	THR	ILE	ASP	PHE
A1995	Q1881	V1721	Q1596	F1516	A1444	E1384	GLU	LYS	PRO	GLN	ILE	GLN	THR	MET	GLN
P1996	T1882	V1724	G1596	E1517	I1445	F1385	LEU	VAL	PRO	ILE	ARG	ASN	VAL	GLY	LYS
I1997	T1885		V1597	E1518	V1446	V1386		THR	TRP	SER	LYS	VAL	GLN	ILE	GLY
L2001		G1728	Q1598	A1520	K1447	Q1387	Q1327	THR	VAL	THR	Q1327	VAL	GLN	ILE	GLY
L2002	C1888	K1729	R1599	L1521	D1448	R1388	D1328	ASN	THR	GLY	L1328	GLY	VAL	GLU	ASP
N2003	P1889	T1730	E1602	W1522	V1449	L1389	L1329	ILE	TYR	GLN	K1330	VAL	VAL	LEU	ASP
V2006	M1892	T1731	R1603	E1524	L1450	L1390	G1331	PRO	ASN	GLU	G1331	THR	ALA	GLY	ILE
K2007	S1903	S1732	G1609	D1525	A1453	K1391	V1332	ILE	ILE	GLU	V1332	ASP	PHE	VAL	VAL
P2008	P1904	T1739	K1610	K1526	V1462	G1392	W1333	GLU	GLY	GLN	W1333	ASN	GLU	LEU	LYS
D2011	F1905	T1740	I1611	W1527	Q1454	Y1393	S1334	ALA	GLY	GLY	S1334	GLY	GLU	ALA	ILE
M2012	T1910	W1741	M1612	M1528	G1455	M1394	E1335	TRP	TRP	VAL	L1336	SER	CYS	GLY	ASP
G1911	G1911	V1750	K1613	I1530	E1456	K1395	L1336	GLY	GLY	ASP	S1337	ALA	ARG	LEU	LEU
E1914		E1763	P1627	M1531	L1459	I1396	S1337	ALA	ALA	THR	S1337	VAL	TYR	ARG	GLU
F1926		L1766	E1635	D1535	E1460	M1397	K1338	THR	PHE	VAL	V1339	ALA	LYS	ARG	VAL
N1931		M1769	D1636	D1539	E1461	L1398	W1340	GLY	ILE	SER	W1340	MET	LYS	ALA	VAL
C1932		G1770	E1639	V1540	L1463	Y1400	E1341	LYS	ASP	GLY	Q1342	THR	GLY	THR	THR
D1933		G1771	E1639	Q1541	K1464	I1401	I1343	PHE	ARG	ALA	I1343	VAL	VAL	LEU	THR
E1934		G1772	K1645	R1542	Q1465	E1402	I1344	THR	LYS	THR	D1344	ASP	GLY	ALA	TYR
T1935		G1773	N1646	R1543	I1466	L1403	Q1345	ILE	SER	ILE	Q1345	LYS	TYR	ALA	ALA
V1946		D1774	K1649	Y1546	E1468	K1404	M1346	LYS	ILE	THR	M1346	VAL	VAL	GLY	HIS
L1947			K1649	L1547	N1471	S1405	K1347	ASP	GLN	VAL	K1347	VAL	VAL	ASP	LYS
L1948		V1781	H1653	G1549	T1472	A1407	E1348	ARG	GLN	GLN	E1348	TRP	LEU	ALA	PHE
Q1950		M1784	F1654	I1550	L1475	L1408	Q1349	GLU	GLY	SER	Q1349	SER	GLY	LEU	LYS
V1951		V1785	K1655	F1551	L1476	K1409	P1350	CYS	VAL	VAL	P1350	VAL	GLN	VAL	GLU
G1952			K1656	T1552	L1477	D1410	W1351	ALA	ASN	ALA	W1351	TYR	ARG	ASP	ILE
D1958		T1788	A1659	G1553	L1477	R1411	V1352	LYS	LEU	ASN	V1352	GLN	ILE	ASP	ASN
N1961		L1792	G1660	S1554	V1478	H1412	S1353	LYS	MET	LYS	S1353	TRP	GLN	ASP	VAL
R1962		Q1800	V1661	A1555	Q1481	W1413	V1354	GLY	LYS	GLN	V1354	ASP	GLN	ALA	GLN
R1966		R1804	E1668	D1557	N1482	K1414	Q1355	ALA	ILE	PHE	Q1355	TRP	MET	ALA	LYS
S1969		L1811	S1671	K1558	N1482	Q1415	P1356	GLU	VAL	LYS	P1356	GLN	ARG	VAL	VAL
Q1973		I1812	I1676	E1564	R1485	L1416	R1357	GLU	GLY	GLN	R1357	VAL	GLN	VAL	VAL
T1978		K1829	R1679	E1574	L1486	M1417	K1357	THR	ASP	GLY	K1357	GLY	VAL	SER	ASP
E1984		I1830	M1685	F1575	L1487	K1418	L1359	THR	ARG	GLY	L1359	THR	ILE	HIS	LYS
H1985		D1831	M1685	L1576	G1489	R1419	R1360	GLY	VAL	VAL	R1360	ASN	TYR	PRO	ASN
S1986		N1832	S1691	A1577	W1490	H1421	Q1361	LEU	GLU	GLY	Q1361	ARG	GLY	GLY	HIS
N1987		A1833	L1692	M1579	D1491	V1422	L1363	THR	THR	THR	L1363	THR	GLY	PRO	GLY
P1988		W1838	T1693	K1580	F1494	W1424	D1364	SER	SER	SER	D1364	ASP	GLY	ILE	LYS
N1989		R1843	E1694	N1495	N1495	V1425	A1365	GLY	GLY	GLY	A1365	LEU	LEU	ASP	ASN
Y1990		F1844	K1697	V1582	K1496	V1426	L1366	ARG	LEU	LEU	L1366	ASN	GLY	LYS	PRO
D1991		M1861	I1698	K1584	V1497	S1427	L1367	VAL	THR	THR	L1367	TRP	VAL	ASN	ILE
S2082			W1701	S1583	A1506	E1428	Q1368	GLY	GLU	ASN	Q1368	GLY	GLY	ASN	VAL
Q2083			V1705	L1587	K1507	L1429	Q1369	THR	GLY	GLY	L1370	GLY	GLY	VAL	VAL
Y2086			D1590	V1591	M1508	T1430	K1371	ARG	GLY	GLY	K1371	GLY	GLY	ASN	GLY
			S1510	P1511	L1509	L1431	S1372	THR	THR	THR	S1372	ASP	GLY	LYS	PRO
						G1432	F1373	GLY	VAL	VAL	F1373	ASP	GLY	ASN	ILE
						Q1433	A1375	GLY	THR	THR	A1375	TRP	GLN	VAL	VAL
						I1434	R1376	GLY	THR	THR	R1376	GLN	GLY	THR	HIS
						D1436	L1377	GLY	THR	THR	L1377	GLY	GLY	GLY	GLY
						V1437	R1378	GLY	THR	THR	V1437	ASP	GLY	LEU	LEU
						D1438	Q1379	THR	THR	THR	D1438	LEU	GLY	LEU	LEU
						L1439	Y1380	ARG	THR	THR	L1439	ASN	GLY	LYS	PRO
						Q1440		GLN	ASP	ASP	Q1440	GLN	THR	THR	ARG



Q4444	T4445	M4446	Y4447	L4448	R4449	T4450	L4451	L4452	N4453	L4454	L4455	V4456	K4457	G4458	I4459	L4460	P4461	R4462	S4463	V4464	S4465	H4466	V4469	G4472	M4473	T4474	V4475	I4476	Q4477	V4478	V4479	F4482	R4485	I4486	Q4490	M4491	I4492	S4493	L4494	M4495	A4496	S4497	S4498	G4499	G4500	A4501	L4504	K4505	G4513	V4516	P4517																																												
THR	SER	ASP	GLY	ARG	PRG	A4376	V4376	M4377	R4378	T4379	T4382	T4383	A4384	S4385	N4386	V4387	L4388	H4389	T4394	L4395	K4399	E4403	N4404	I4405	K4406	F4410	R4411	F4412	F4413	E4414	R4415	E4416	L4423	L4424	Q4425	D4426	ASP	LEU	ALA	TTR	ALA	ALA	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443																																									
R4123	M4128	E4129	I4130	M4131	P4132	K4133	M4137	L4138	L4139	F4145	V4146	V4153	M4157	T4160	I4169	R4176	M4177	M4178	V4185	I4189	E4192	M4193	L4194	R4195	L4212	D4220	T4226	R4230	P4235	P4239	D4257	P4260	L4265	M4266	T4267	F4268	L4269	E4270	T4274	R4276	S4277	F4278	D4279	S4280	E4281	D4289	G4290	H4291	K4292	M4296	P4297	D4298	R4301	R4302	V4308	L4321	N4326	R4329	G4336	I4340	S4341	K4342	M4343	Q4347	M4348	L4349	E4350	D4351	E4352	D4353	ASP	LEU	ALA	TTR	ALA	ALA	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443							
L4042	D4050	V4055	E4056	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	S4068	I4071	G4072	S4073	A4074	E4075	G4076	F4077	A4080	D4081	K4082	A4083	I4084	N4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	M4095	L4096	K4097	N4098	V4099	H4100	M4105	L4106	M4107	Q4108	L4109	E4110	L4113	L4116	Q4117	P4118	Q3931	A3932	V3935	V3936	K3945	D3946	L3947	V3951	Q3952	A3953	D3954	E3955	Q3956	F3957	L3961	P3966	E3967	S3975	E3976	E3977	T3978	L3983	R3987	P3998	D3999	R4000	L4001	A4002	M4004	A4005	F4008	T4011	N4012	L4013	G4014	E4015	M4018	S4019	L4020	M4021	E4022	D4026	I4030	V4031	V4035	
L3824	F3832	I3835	V3836	V3839	L3846	D3851	R3855	L3863	R3870	V3871	A3872	R3873	G3874	M3875	L3876	D3879	L3886	R3889	I3890	K3893	G3897	E3898	D3902	A3903	E3904	L3909	N3912	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	Q3925	G3926	L3927	T3928	Q3931	A3932	V3935	V3936	K3945	D3946	L3947	V3951	Q3952	A3953	D3954	E3955	Q3956	F3957	L3961	P3966	E3967	S3975	E3976	E3977	T3978	L3983	R3987	P3998	D3999	R4000	L4001	A4002	M4004	A4005	F4008	T4011	N4012	L4013	G4014	E4015	M4018	S4019	L4020	M4021	E4022	D4026	I4030	V4031	V4035									
Q3735	G3736	R3743	Q3744	L3745	E3746	K3747	R3748	L3749	A3752	L3753	N3754	Q3755	E3756	K3757	G3758	R3759	L3760	L3761	D3762	D3763	T3764	T3765	I3766	I3767	T3768	T3769	R3770	E3771	N3772	L3773	K3774	R3775	E3776	E3779	R3782	K3783	V3784	E3785	E3786	T3787	D3788	V3797	C3808	S3809	F3813	E3816	S3817	Q3820	K3621	N3631	V3638	E3639	D3642	R3651	E3652	V3653	R3654	R3655	T3656	Q3657	G3658	R3659	V3660	L3661	L3664	G3665	D3666	Q3667	R3668	T3669	D3670	S3670	K3671	T3674	R3682	D3683	P3684	E3687	F3688	L3692	C3693	S3694	R3695	V3696	T3697	F3701	T3702	L3708	V3716	R3723	V3724	D3725	R3728	S3729	D3730
S3501	T3502	I3503	L3508	L3509	S3510	I3514	A3515	Y3516	D3521	L3536	F3543	R3544	T3545	I3546	L3553	S3554	N3555	E3558	R3561	S3566	L3567	D3570	D3570	K3471	V3472	N3473	R3474	S3475	T3476	A3477	Y3586	P3587	D3591	T3597	E3598	F3599	I3600	M3601	K3608	R3611	L3615	D3616	D3617	A3618	F3496	K3497	N3498	Q3499	K3500	ASP	LEU	ALA	VAL	ASP	GLY	ASN	GLN	GLN	LYS	LYS	LYS	ASN	ASN	THR	THR	THR	ASP	SER	ILE																										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40983	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	0.956	Depositor
Minimum map value	-0.343	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/24989	0.32	0/33856

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	24471	0	24527	545	0
2	A	54	0	24	10	0
3	A	31	0	12	6	0
4	A	31	0	13	5	0
5	A	1	0	0	0	0
All	All	24588	0	24576	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 11.

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:3211:THR:HG21	1:A:3753:LEU:HD21	1.51	0.93
1:A:3208:ILE:HD11	1:A:3482:LEU:HD22	1.55	0.88
1:A:3202:ASN:HB3	1:A:3206:ARG:HH12	1.37	0.86
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.11	0.81
1:A:2481:MET:HE3	1:A:2485:GLN:HG2	1.61	0.81

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	3028/4646 (65%)	2940 (97%)	88 (3%)	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	2703/4125 (66%)	2703 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4156	ASN
1	A	4532	ASN
1	A	4174	ASN
1	A	4347	GLN
1	A	4566	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 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	$\# Z > 2$
4	ANP	A	4703	-	29,33,33	1.12	4 (13%)	31,52,52	0.88	1 (3%)
3	ATP	A	4702	5	28,33,33	0.67	0	34,52,52	0.60	1 (2%)
2	ADP	A	4704	-	24,29,29	0.90	0	29,45,45	1.23	2 (6%)
2	ADP	A	4701	-	24,29,29	0.95	1 (4%)	29,45,45	1.18	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	4703	-	-	2/14/38/38	0/3/3/3
3	ATP	A	4702	5	-	3/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4703	ANP	PG-O1G	2.45	1.49	1.46
4	A	4703	ANP	PG-N3B	2.41	1.69	1.63
4	A	4703	ANP	PB-O1B	2.35	1.49	1.46
4	A	4703	ANP	PB-O3A	-2.32	1.56	1.59
2	A	4701	ADP	PA-O3A	2.27	1.61	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4701	ADP	N3-C2-N1	-3.60	123.79	128.67
2	A	4704	ADP	C4-C5-N7	-2.65	106.53	109.34
2	A	4701	ADP	C4-C5-N7	-2.46	106.74	109.34
4	A	4703	ANP	C5-C6-N6	2.33	123.86	120.31

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

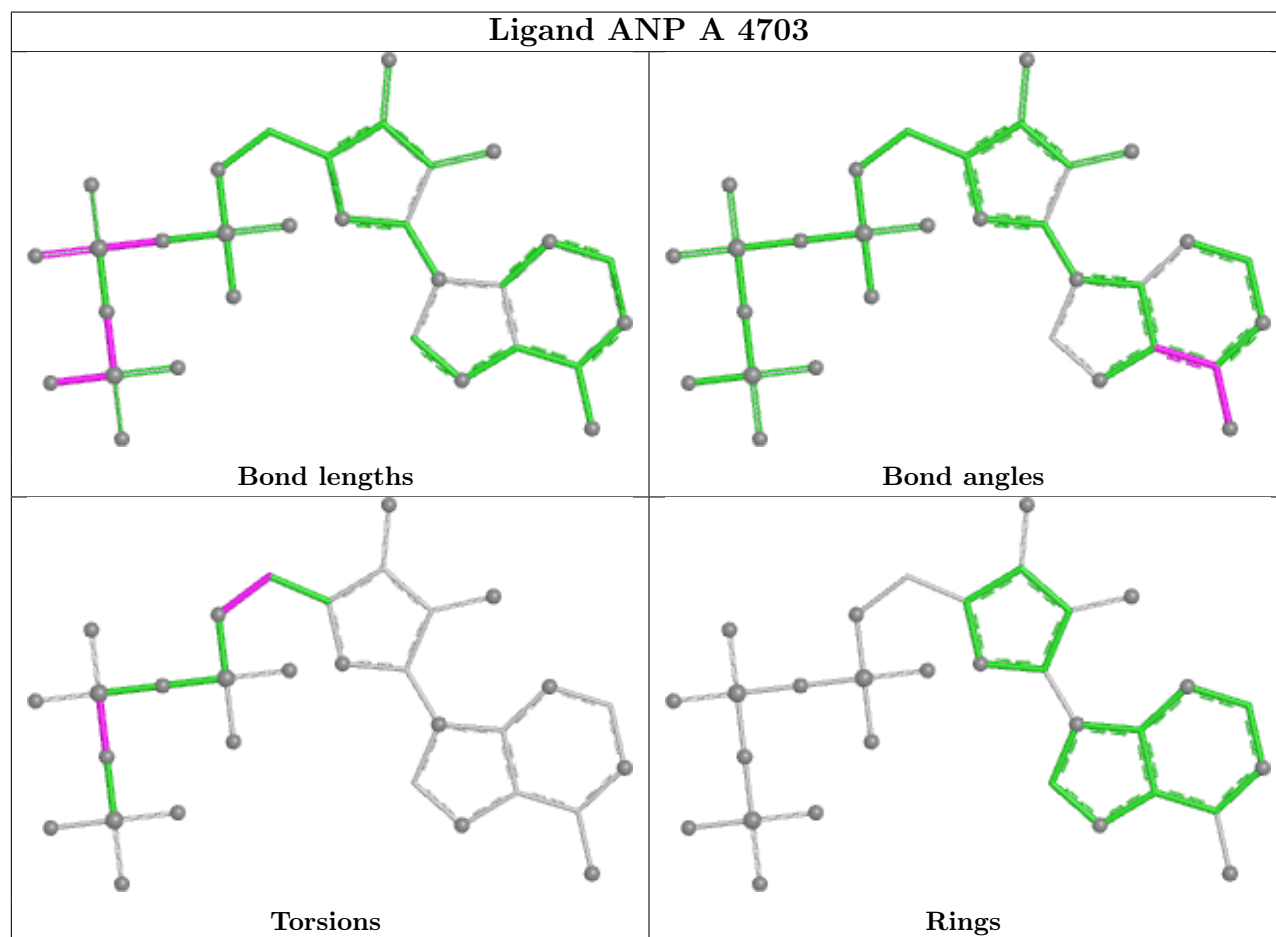
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	C5'-O5'-PA-O3A

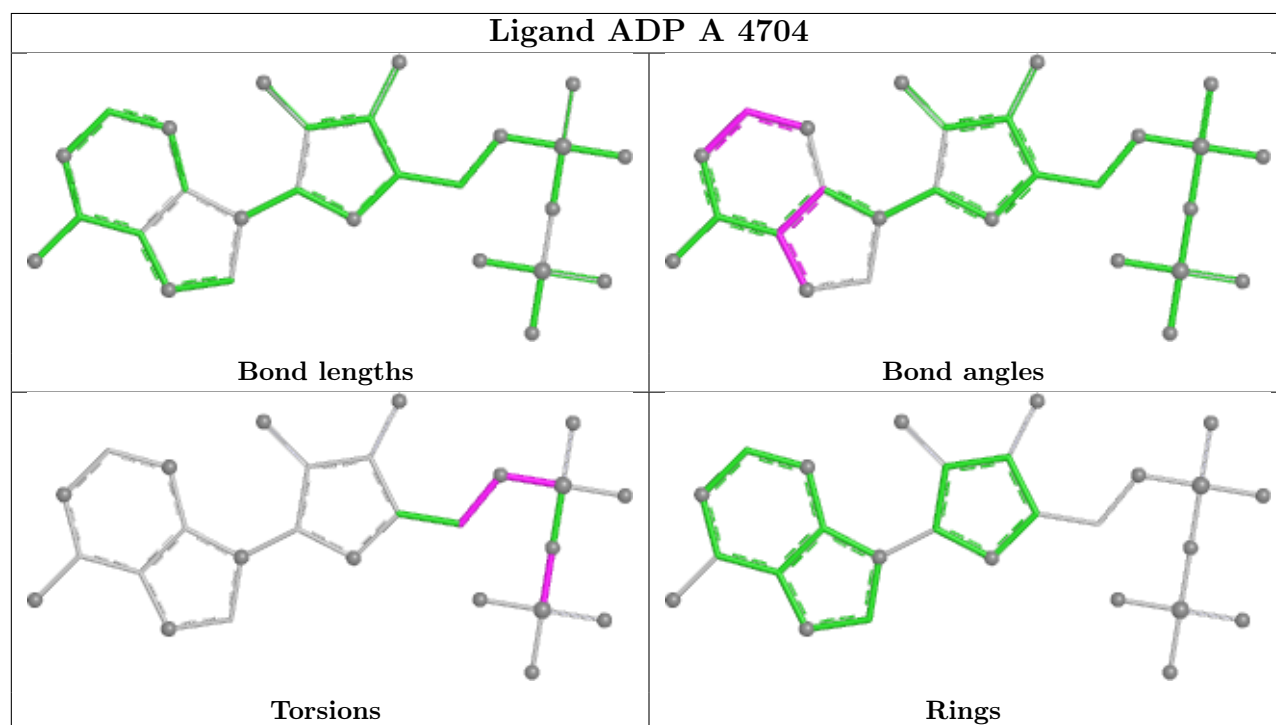
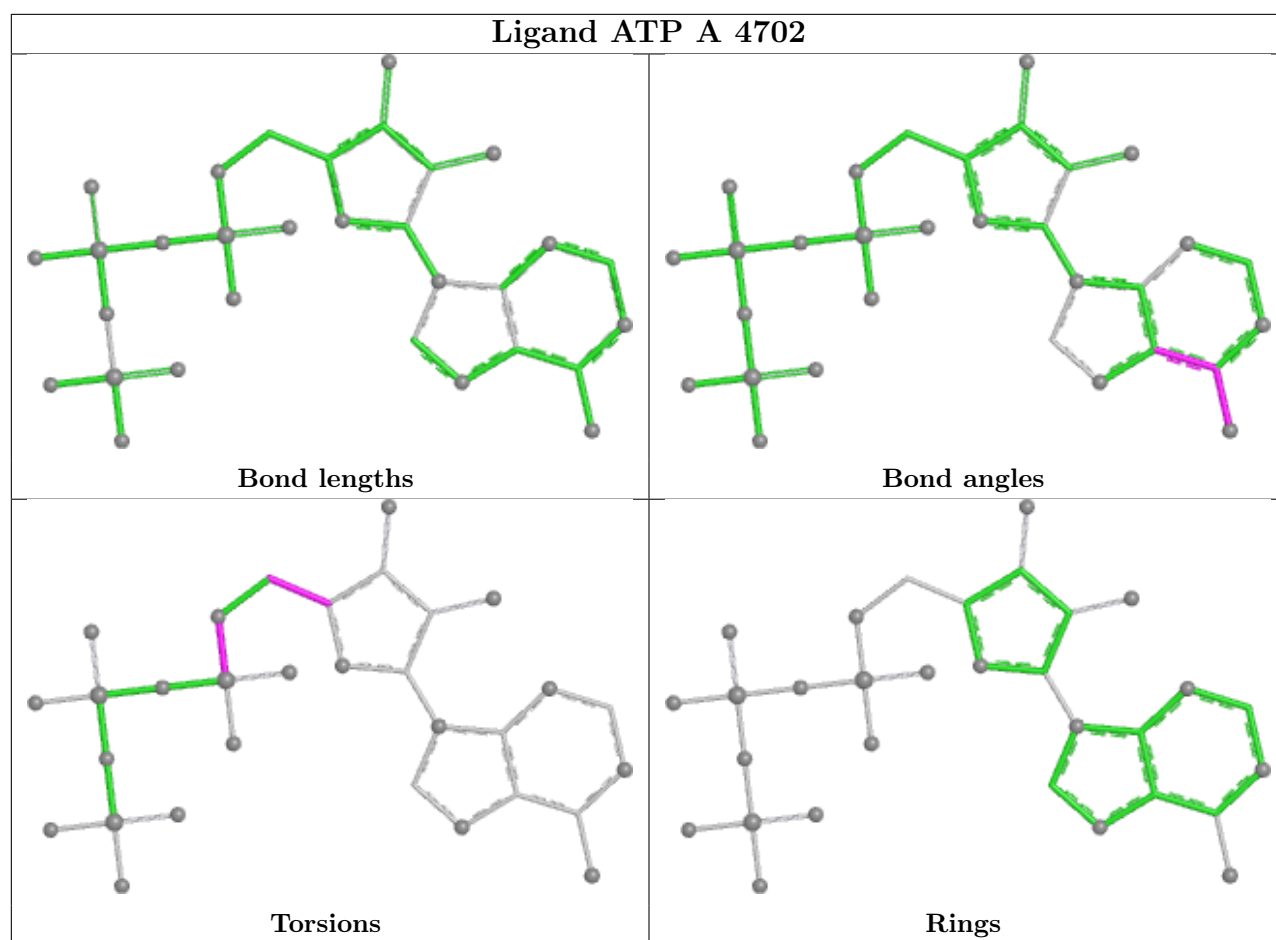
There are no ring outliers.

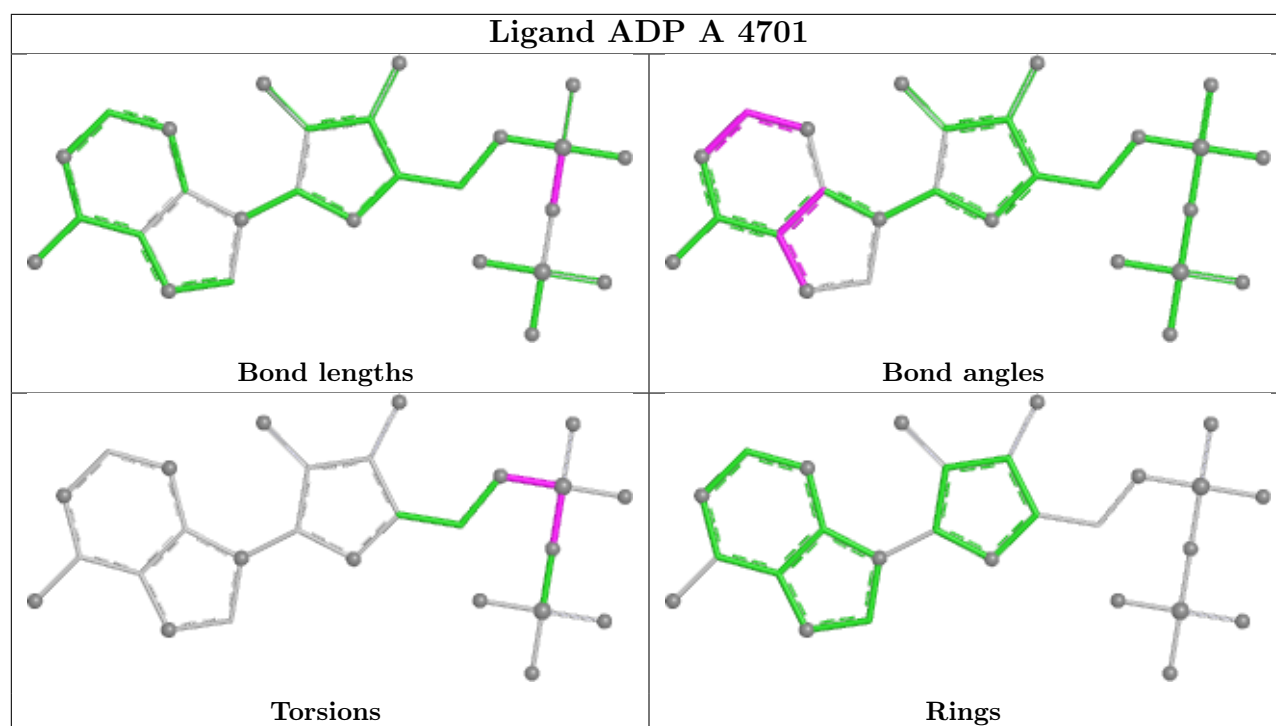
4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	5	0
3	A	4702	ATP	6	0
2	A	4704	ADP	2	0
2	A	4701	ADP	8	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.

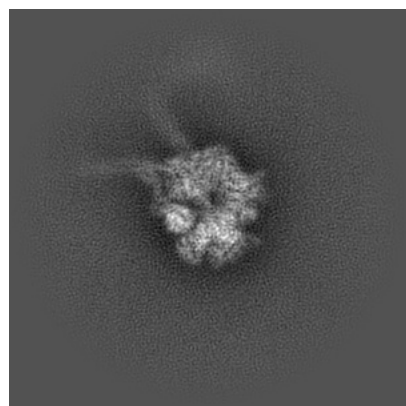
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46861. These allow visual inspection of the internal detail of the map and identification of artifacts.

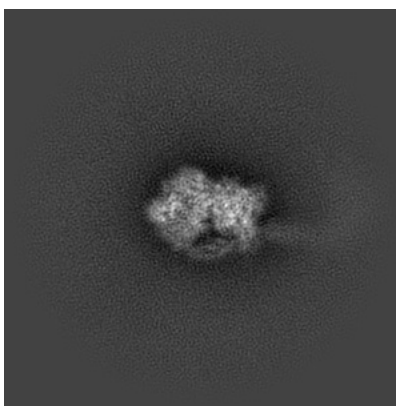
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

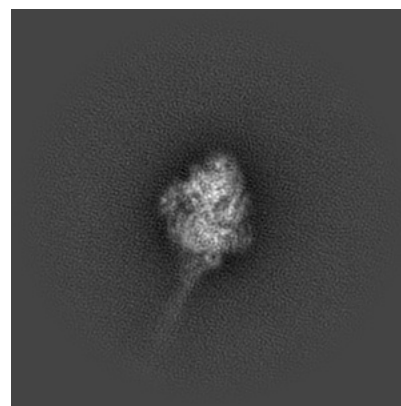
6.1.1 Primary map



X

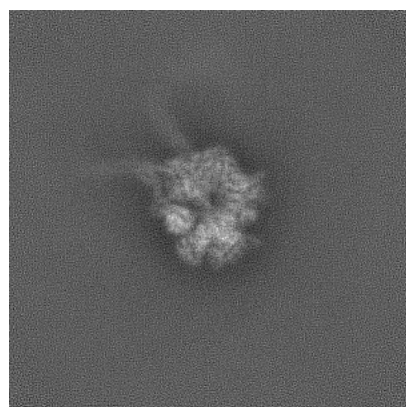


Y

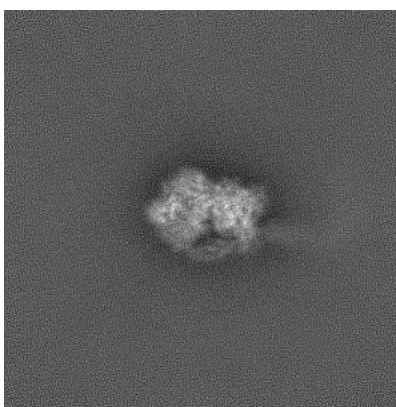


Z

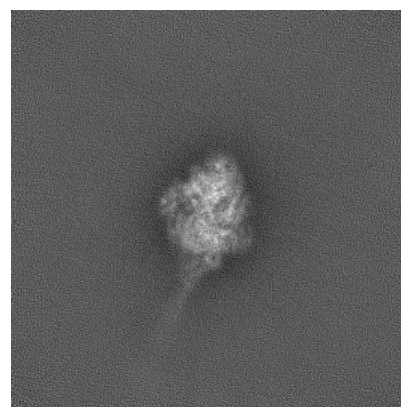
6.1.2 Raw map



X



Y

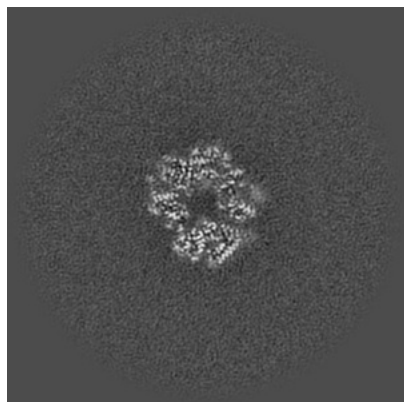


Z

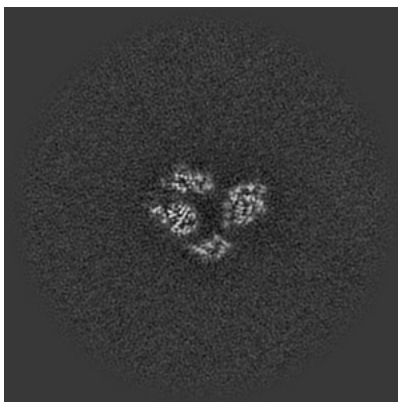
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

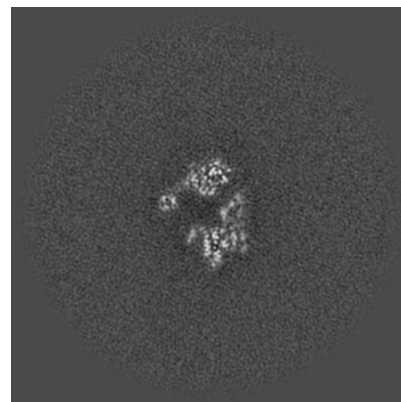
6.2.1 Primary map



X Index: 192

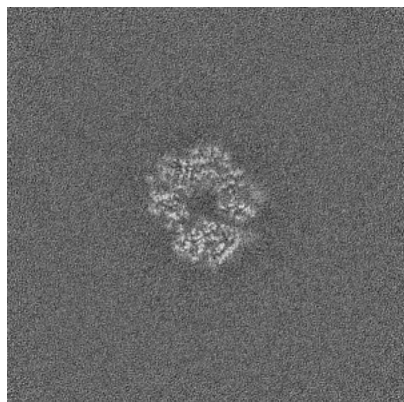


Y Index: 192

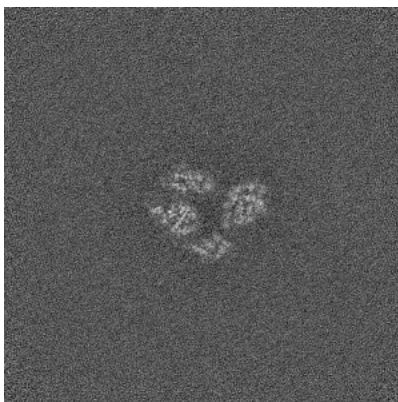


Z Index: 192

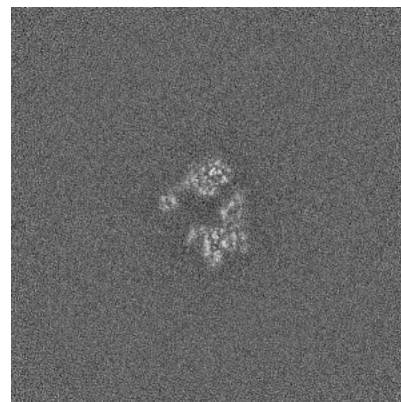
6.2.2 Raw map



X Index: 192



Y Index: 192

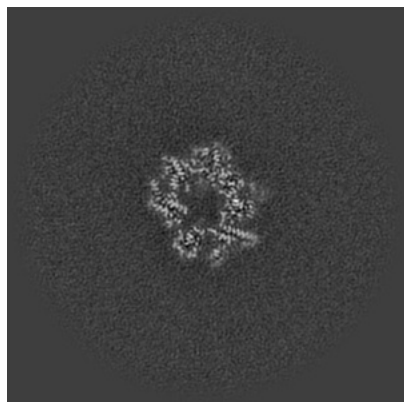


Z Index: 192

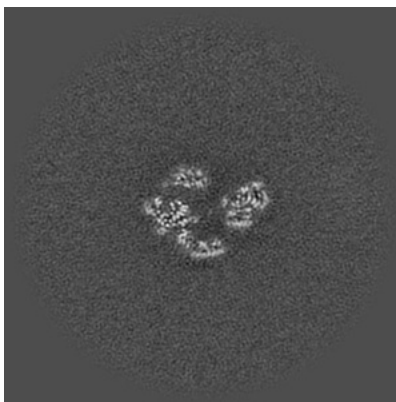
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

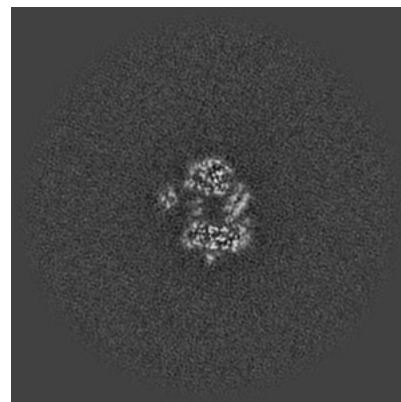
6.3.1 Primary map



X Index: 196

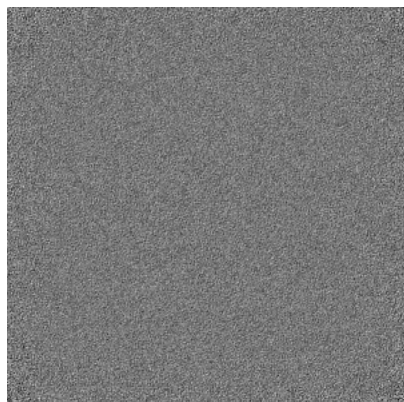


Y Index: 199

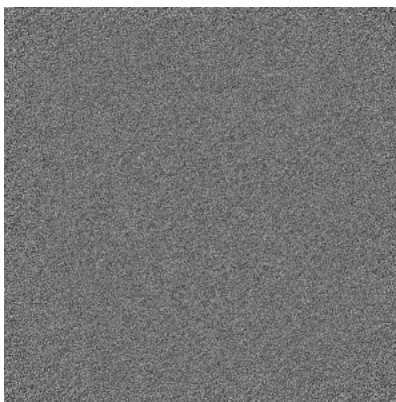


Z Index: 186

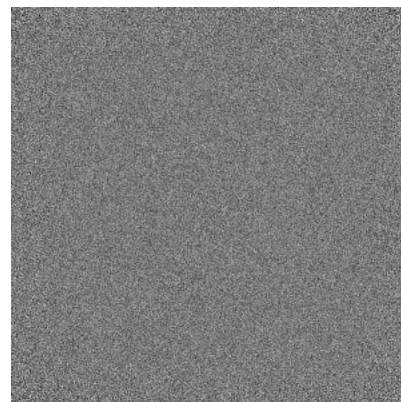
6.3.2 Raw map



X Index: 0



Y Index: 0

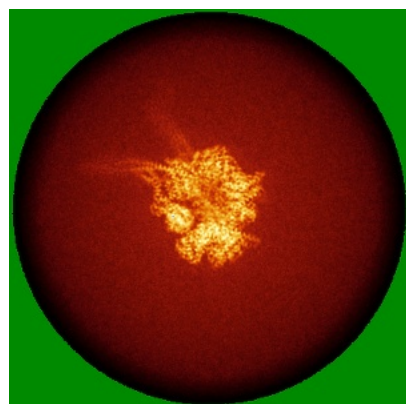


Z Index: 0

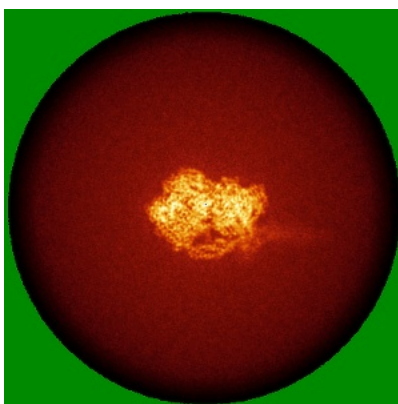
The images above show the largest variance slices of the map in three orthogonal directions.

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

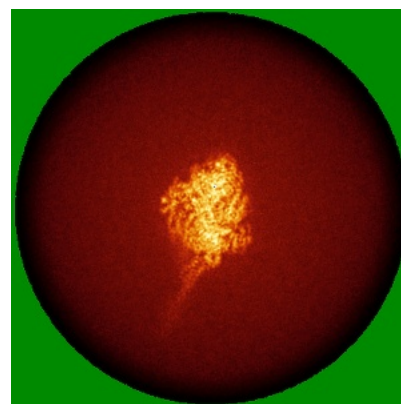
6.4.1 Primary map



X

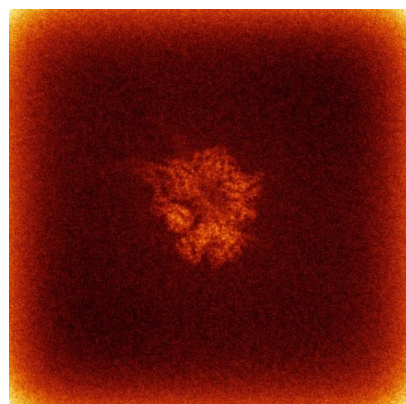


Y

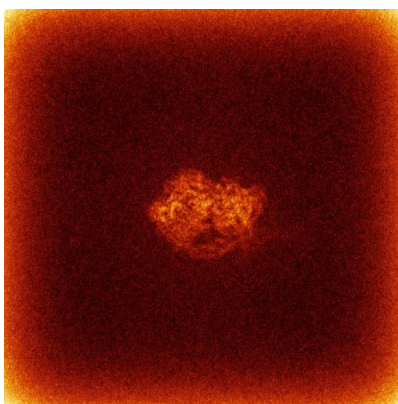


Z

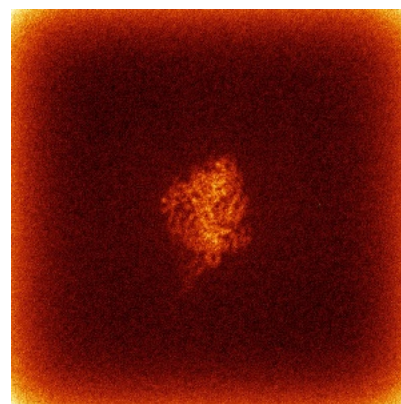
6.4.2 Raw map



X



Y

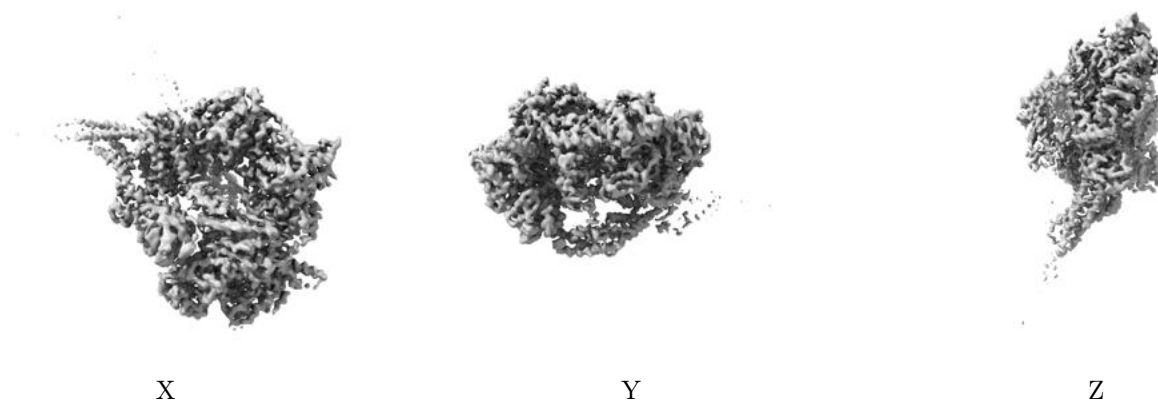


Z

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.

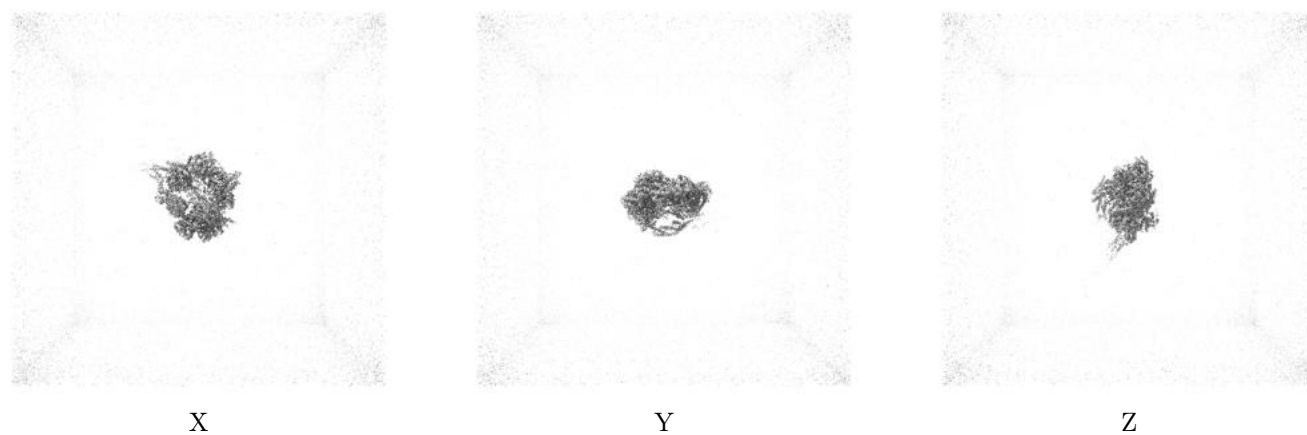
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

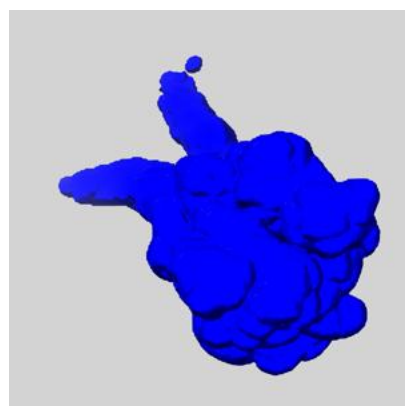
6.6 Mask visualisation [i](#)

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

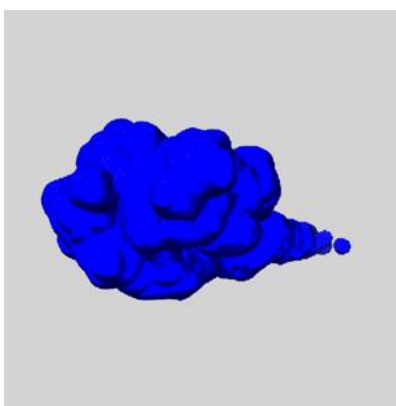
A mask typically either:

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

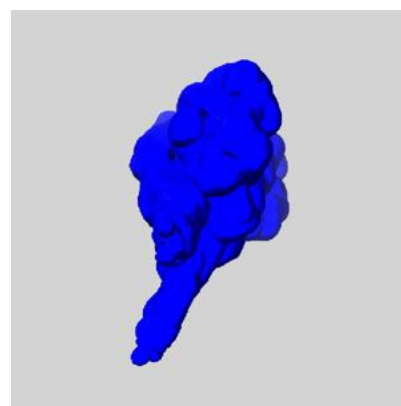
6.6.1 emd_46861_msk_1.map [i](#)



X



Y

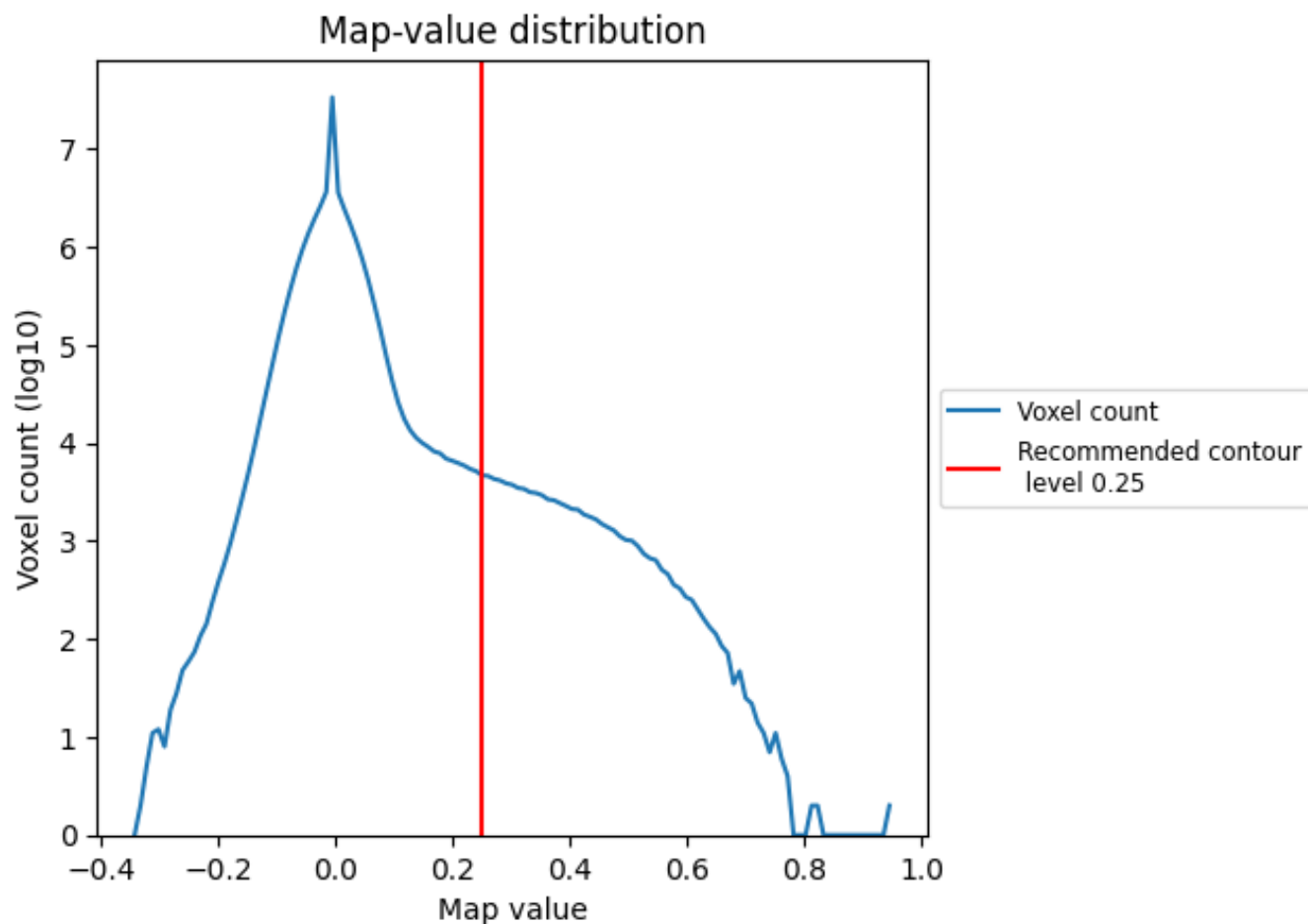


Z

7 Map analysis [i](#)

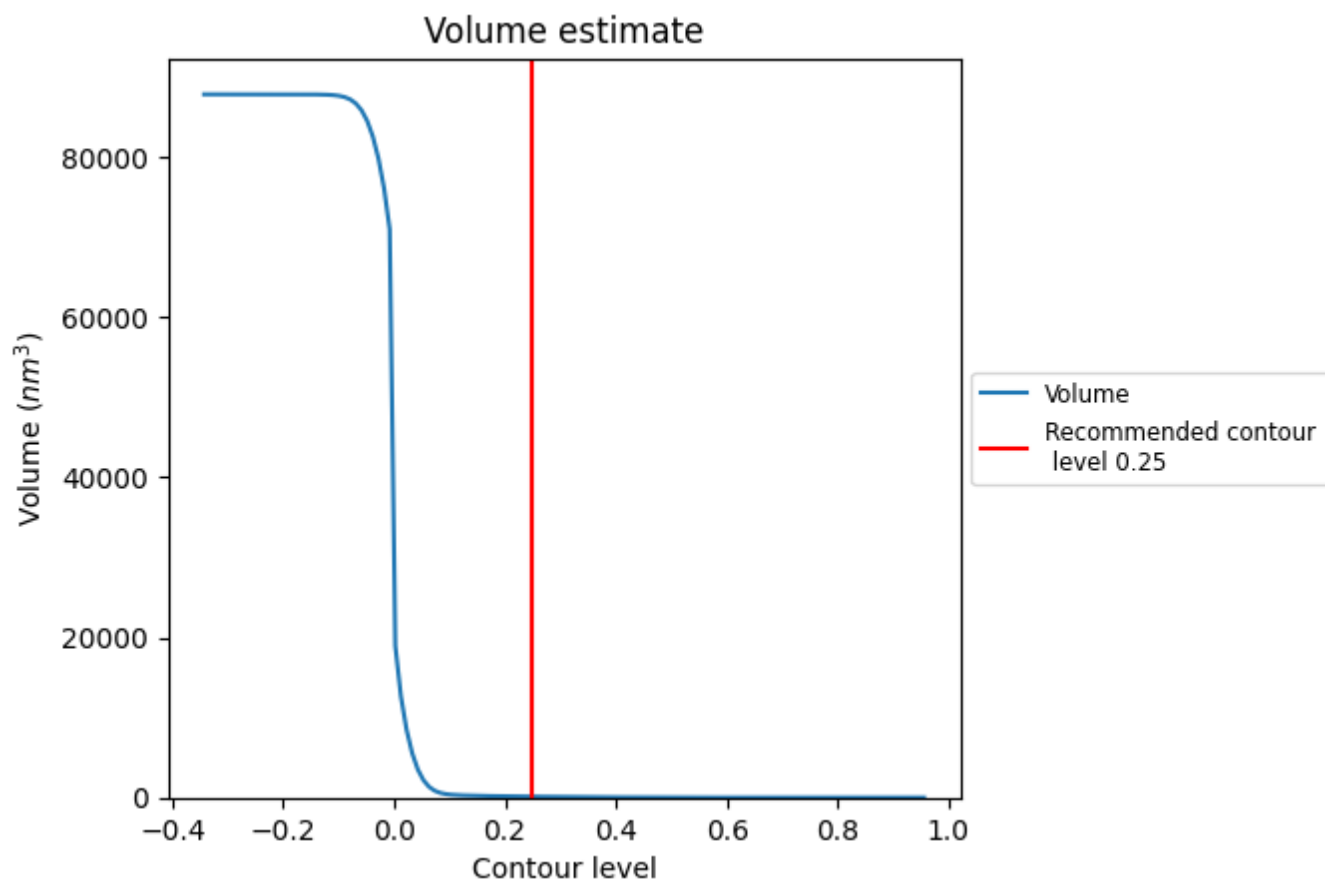
This section contains the results of statistical analysis of the map.

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.

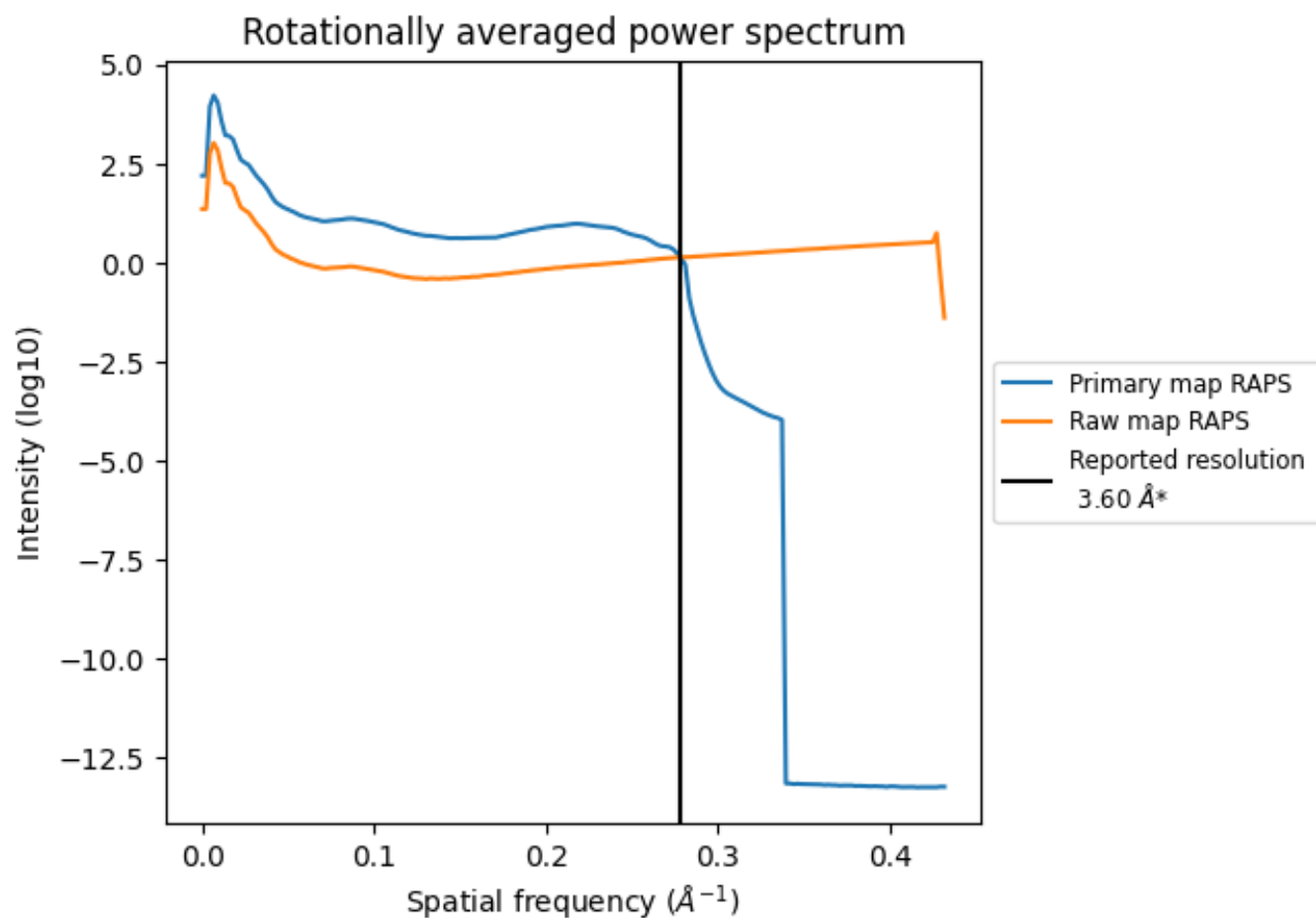
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 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 ⓘ

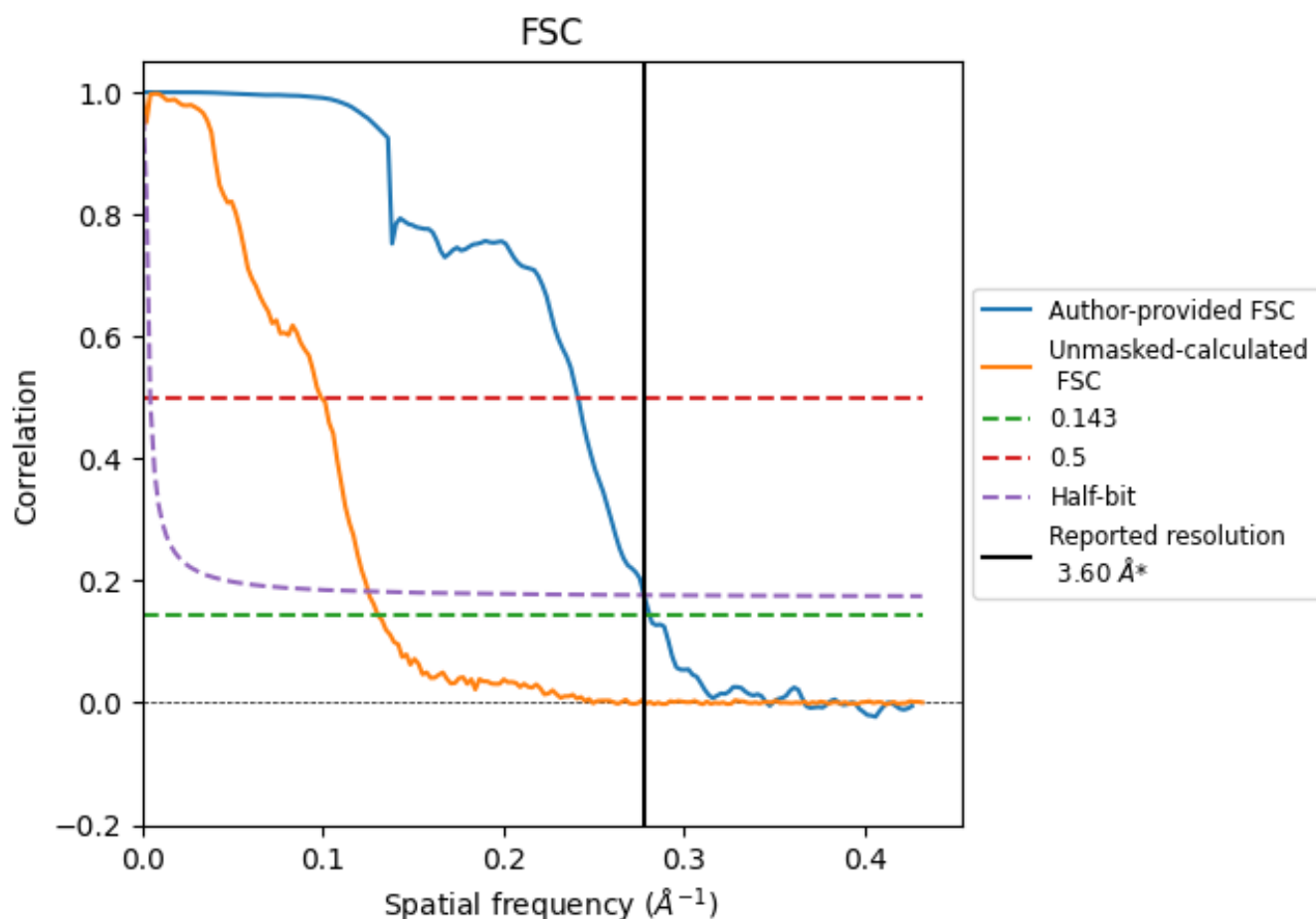


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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](#)

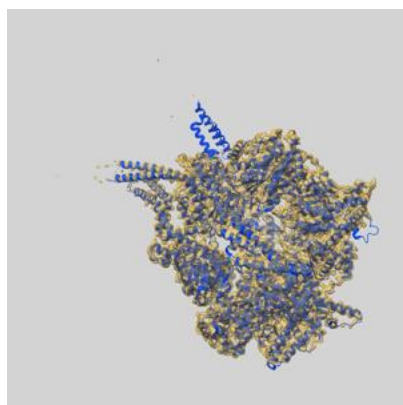
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	4.14	3.60
Unmasked-calculated*	7.65	10.09	7.99

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

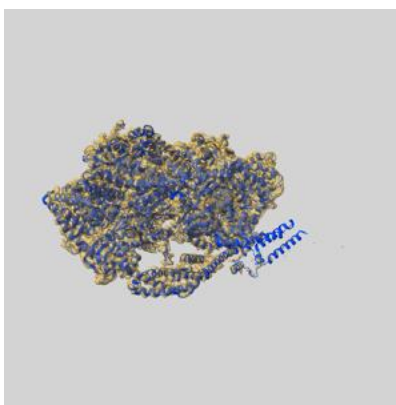
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46861 and PDB model 9DHA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

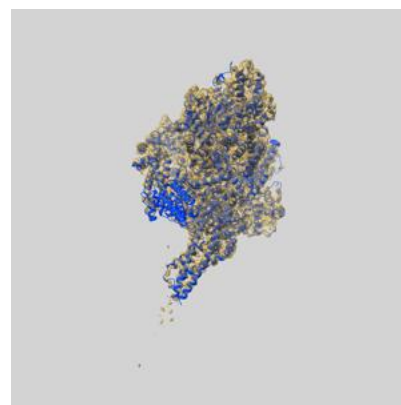
9.1 Map-model overlay [i](#)



X



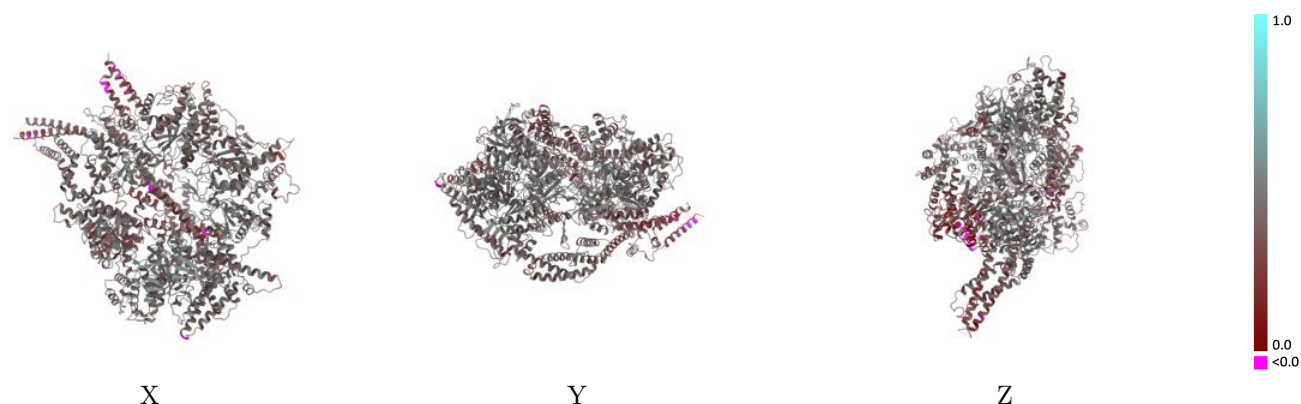
Y



Z

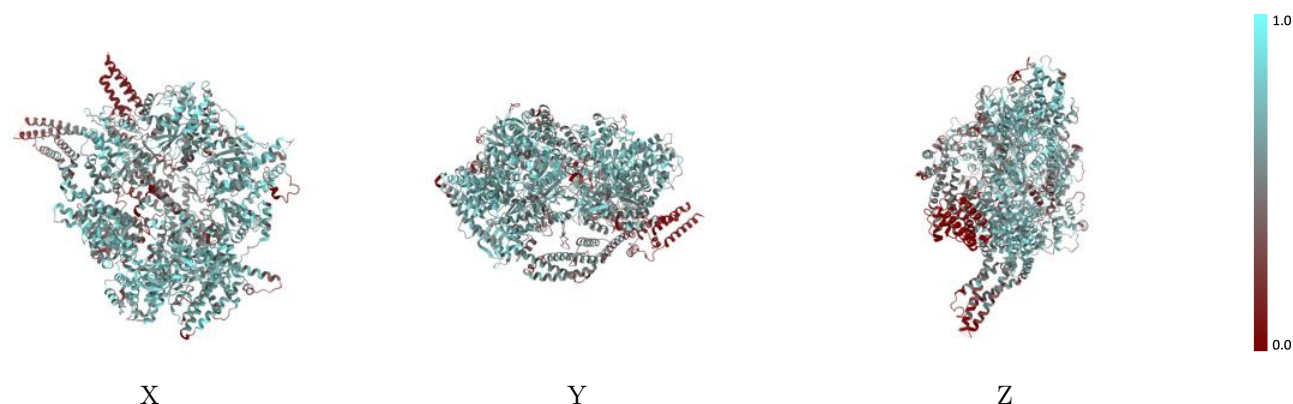
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



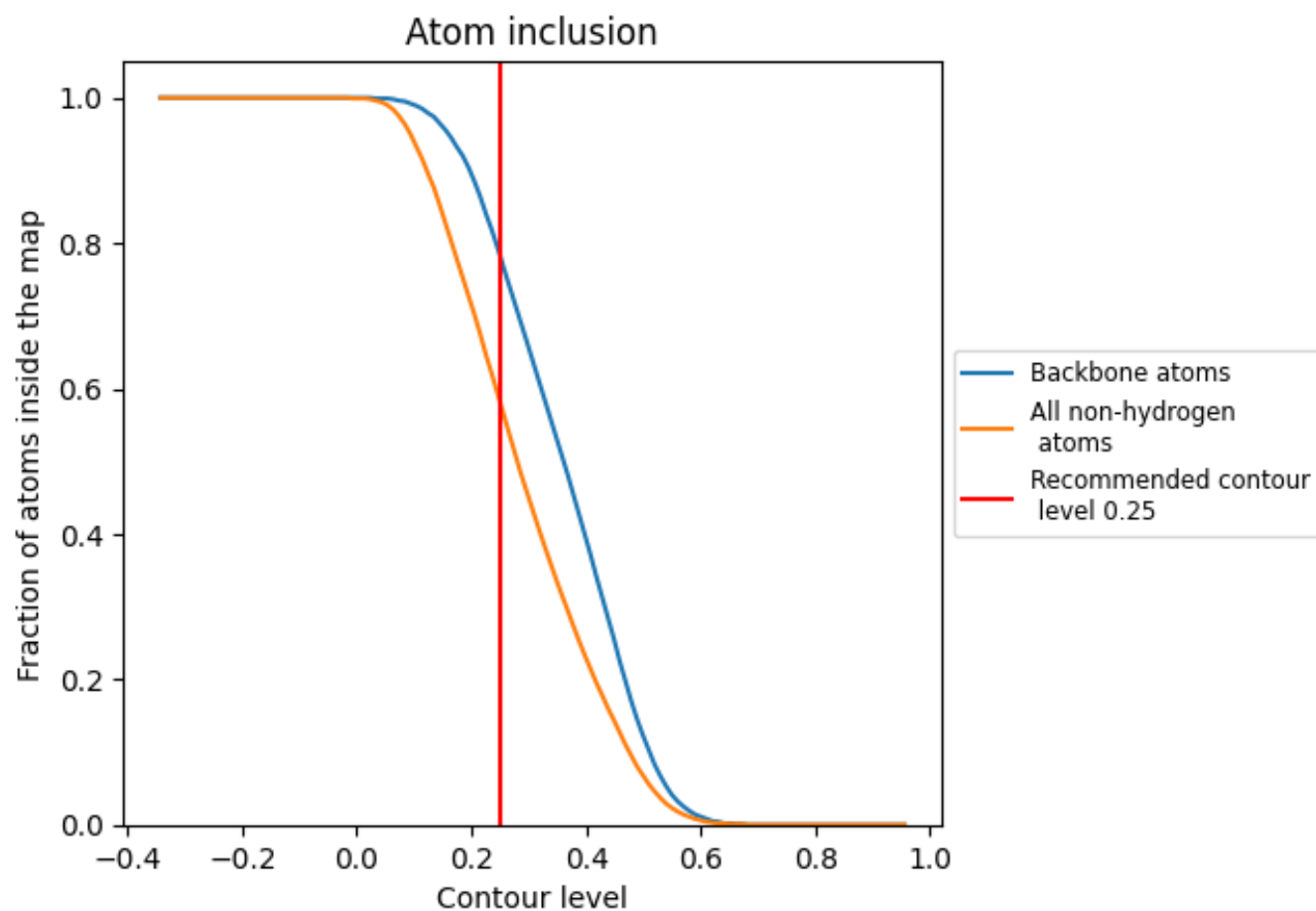
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 58% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5810	<div></div> 0.4120
A	<div></div> 0.5810	<div></div> 0.4120

