



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 07:58 PM UTC

PDB ID : 9MFW / pdb_00009mfw
EMDB ID : EMD-48240
Title : Motor domain with ADP AAA1 and ADP AAA3 from yeast full-length dynein-1 in 0.1 mM ATP condition
Authors : Geohring, I.C.; Chai, P.; Iyer, B.R.
Deposited on : 2024-12-10
Resolution : 4.10 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

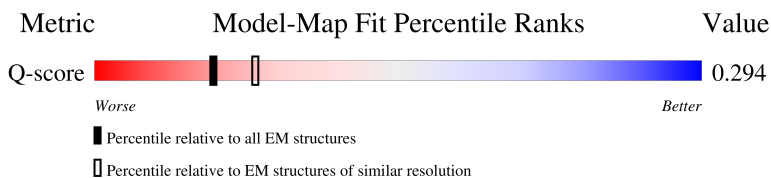
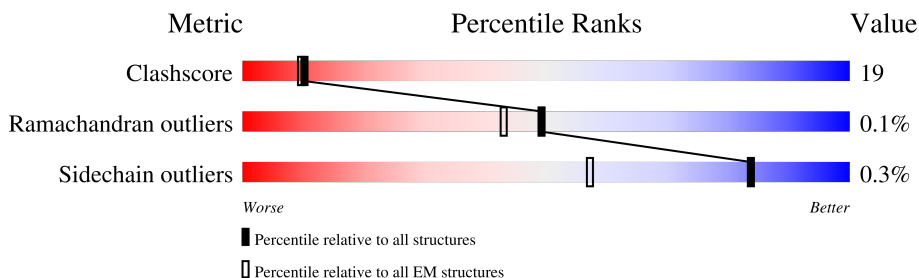
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	4092	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21037 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2583	20925	13431	3476	3920	98	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 31	C 10	N 5	O 13	P 3	0

L1310	Q1736	E1637	R1536	V1443	A1381	D1321	L1261	MET	LYS	ASN	ARG	VAL	GLN	ASP	THR
Q1811	K1737	E1637	F1537	H1444	Q1382	I1322	Q1262	HIS	HIS	ASN	ILE	ILE	LYS	ILE	ASN
R1815	N1738	V1640	Y1538	W1445	Y1383	G1323	S1263	VAL	ARG	ASN	ARG	VAL	GLU	ALA	VAL
V1816	D1739	V1640	Y1538	W1445	E1384	G1323	D1264	ALA	ARG	ASN	SER	PHE	PHE	LEU	ASP
V1817	T1740	Q1646	D1543	V1446	E1447	K1324	R1264	ALA	ARG	ASN	LYS	LEU	LEU	LEU	HIS
V1818	L1741	Q1646	D1544	V1448	I1386	R1325	A1266	ALA	HIS	ASN	MET	TRP	GLN	ASN	ILE
V1819	L1742	W1656	L1545	V1448	V1385	Q1326	A1266	ALA	HIS	ASN	LEU	LEU	GLN	LEU	SER
F1820	D1743	W1656	L1546	V1448	V1385	Q1326	A1266	ALA	HIS	ASN	LEU	LEU	GLN	LEU	SER
N1821	L1744	V1660	K1547	V1448	H1388	I1327	M1267	LYS	THR	THR	ASP	VAL	THR	VAL	THR
C1822	N1745	V1660	I1548	V1448	S1389	Q1328	F1268	LYS	THR	THR	ASP	VAL	THR	VAL	THR
D1823	S1746	C1663	I1549	V1448	S1390	K1329	F1269	GLU	GLU	GLU	ASP	VAL	THR	VAL	THR
D1824	V1747	L1664	D1464	V1465	G1391	N1330	R1270	ILE	ILE	ILE	ILE	ALA	ASN	ASN	ASN
S1825	S1748	N1667	I1465	V1465	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
F1826	S1750	N1667	F1468	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
D1827	L1755	S1670	H1554	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
Y1828	L1756	S1670	H1554	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
Q1829	L1756	W1672	H1554	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
V1830	Q1757	W1672	H1554	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
L1831	Y1758	K1674	H1554	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
S1832	K1759	E1675	K1563	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
R1833	F1760	E1675	K1563	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
L1834	Y1761	V1676	M1565	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
L1835	Y1762	M1678	F1566	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
I1838	I1765	K1679	F1566	V1469	L1392	L1331	R1271	PRO	PRO	PRO	PHE	PHE	ALA	ASN	ILE
A1843	P1766	I1680	I1569	T1467	A1404	K1340	Q1280	GLU	GLU	GLU	ASP	PHE	ALA	ASN	ILE
D1848	L1769	L1683	E1570	T1467	A1404	K1340	Q1280	GLU	GLU	GLU	ASP	PHE	ALA	ASN	ILE
E1849	I1770	L1683	E1570	T1467	A1404	K1340	Q1280	GLU	GLU	GLU	ASP	PHE	ALA	ASN	ILE
L1853	P1773	D1685	I1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
K1855	I1777	D1685	I1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
V1857	L1781	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
L1858	T1782	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
N1864	D1784	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
I1865	S1785	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
I1868	L1786	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
Q1869	H1787	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
K1789	Q1788	L1683	E1571	R1489	K1406	F1342	F1282	VAL	VAL	VAL	THR	THR	VAL	VAL	VAL
L1872	Y1790	L1701	L1592	L1504	N1419	L1354	M1293	ALA	ALA	ALA	ASP	ASP	ASP	ASP	ASP
Q1873	F1794	L1702	L1592	L1504	N1419	L1354	M1293	ALA	ALA	ALA	ASP	ASP	ASP	ASP	ASP
L1881	F1795	L1702	L1592	L1504	N1419	L1354	M1293	ALA	ALA	ALA	ASP	ASP	ASP	ASP	ASP
L1882	G1796	F1708	Q1603	L1509	L1423	I1358	S1297	ILE	ILE	ILE	PHE	PHE	ILE	ILE	ILE
E1883	G1796	F1708	Q1603	L1509	L1423	I1358	S1297	ILE	ILE	ILE	PHE	PHE	ILE	ILE	ILE
E1884	T1800	I1712	Q1605	L1516	E1425	E1359	M1299	THR	THR	THR	THR	THR	THR	THR	THR
E1885	G1713	I1712	Q1605	L1516	E1425	E1359	M1299	THR	THR	THR	THR	THR	THR	THR	THR
K1802	Q1714	I1712	Q1605	L1516	E1425	E1359	M1299	THR	THR	THR	THR	THR	THR	THR	THR
T1803	K1721	I1721	L1609	L1523	D1427	Q1362	V1303	THR	THR	THR	THR	THR	THR	THR	THR
E1804	L1611	L1727	L1611	L1529	L1429	E1364	E1304	THR	THR	THR	THR	THR	THR	THR	THR
V1805	L1611	L1727	L1611	L1529	L1429	E1364	E1304	THR	THR	THR	THR	THR	THR	THR	THR
K1807	L1611	L1727	L1611	L1529	L1429	E1364	E1304	THR	THR	THR	THR	THR	THR	THR	THR
V1894	E1614	F1734	E1614	Q1533	L1431	V1366	K1306	THR	THR	THR	THR	THR	THR	THR	THR
F1895	V1619	V1735	V1619	P1534	E1432	I1367	D1307	THR	THR	THR	THR	THR	THR	THR	THR



L3938	L3939	T3940	A3941	B3944	B3945	M3946	W3950	V3951	L3955	V3959	E3960	E3961	T3962	K3963	A3964	L3968	N3975	S3976	T3977	N3978	N3979	I3980	K3981	L3984	R3989	T3989	F3989	L4009	L4010	C4011	A4012	D4019	Q4022	V4024	V4027	R4028	I4029	P4030	L4033	L4034	Q4035	Q4036																
I3839	L3840	L3841	Q3842	N3843	I3844	Q3845	M3846	W3850	V3851	L3855	V3859	E3860	E3861	T3862	K3863	A3864	A3865	E3866	E3867	F3871	N3870	Y3875	F3876	T3877	M3878	A3879	S3879	E3881	L3884	R3891	T3891	F3895	V3896	E3898	D3899	I3900	I3903		F3915	F3916		K3919		W3924	W3934	F3935	H3936	A3937										
V3733	P3734	K3735	L3736	T3737	V3738	D3739	T3740	N3741	N3742	D3743	L3744	R3745	Y3746	L3747	L3760	N3761	W3762	F3767	F3768	V3769	D3770		N3780	Y3785	F3786	T3787	M3788	A3789	S3790	E3791	K3799	L3800	L3801	E3802	L3803	A3804	K3805	E3809	S3810	L3811	K3812	L3813	L3814	P3815	L3819	S3820	N3821	L3822	N3823	Q3826	W3838							
R3655	V3656	K3659	K3660	S3661	K3662	E3663	T3664	R3665	A3666	A3667	R3668	T3669	R3670	V3671	D3672	E3673	L3674	W3675	W3676	L3677	L3678	Y3679	V3682	F3686	S3687	T3688	A3689	L3690	K3693	F3694	K3695	K3696	L3697	M3698	A3699	M3700	T3701	M3702	K3707	F3708	D3709	L3710	E3711	S3712	E3713	Y3714	Y3715	K3716	E3728	S3729	S3730	D3731	G3732					
T3586	L3587	N3588	N3589	L3590	K3591	K3592	E3593	A3594	M3595	N3596	I3597	E3598	K3599	K3600	L3601	S3602	E3603	S3604	E3605	E3606	F3607	F3608	P3609	Q3610	F3611	D3612	N3613	L3614	V3615	E3616	E3617	T3620	I3621	G3622	K3623	F3629	S3630	M3631	L3632	E3633	K3634	F3635	Q3636	Q3637	F3638	H3639	W3640	F3641	L3644	I3645	I3646	S3651	C3652	F3653	K3654			
K3522	E3523	S3524	I3525	E3526	T3527	R3528	I3529	F3530	D3531	L3532	T3533	E3534	E3540	M3541	Q3542	R3543	K3544	R3545	F3546	D3547	L3548	L3549	K3550	L3551	N3552	T3553	F3554	Y3555	K3556	L3557	K3558	L3559	K3560	N3561	L3562	E3563	K3564	R3565	L3566	L3567	E3568	E3569	F3570	N3571	N3572	S3573	Q3574	G3575	N3576	S3577	L3578	E3579	N3580	D3581	E3582	L3583	M3584	Y3585
Q3453	D3454	F3457	P3460	I3461	S3462	R3463	L3464	L3465	L3466	R3468	E3469	F3470	A3473	G3474	N3475	R3476	V3479	E3480	I3481	G3482	D3483	H3484	E3485	V3486	D3487	V3488	S3489	G3490	D3491	F3492	K3493	L3494	F3495	P3501	S3502	G3503	D3504	I3505	P3506	L3507	F3508	L3509	R3510	S3511	R3512	V3513	R3514	L3515	V3516	H3517	T3520	N3521						
I3367	D3368	Y3369	L3370	L3373	D3374	E3375	K3376	K3377	L3380	E3381	L3384	D3385	K3386	N3387	D3388	F3389	L3391	N3394	S3395	L3396	V3397	N3398	N3399	S3400	Q3401	D3402	F3406	L3407	L3408	D3409	M3414	N3424	K3425	T3426	V3427	L3428	L3429	S3430	F3431	L3432	E3433	E3434	R3439	G3447	S3448	V3449	V3450	I3451	I3452									
K3297	S3298	L3299	T3300	F3301	E3302	K3303	E3304	R3306	W3306	L3307	N3308	T3309	T3310	K3311	Q3312	F3313	S3314	K3315	T3316	S3317	Q3318	E3319	L3320	N3323	C3324	I3325	I3329	Y3330	Y3333	F3334	G3335	H3336	L3337	N3338	E3339	R3340	L3346	L3349	K3350	R3351	L3352	L3353	G3354	K3355	K3359	Y3360	D3361	Y3364	R3365	F3366								
THR	LEU	ASP	LYS	GLN	MET	LEU	MET	GLU	GLN	ASN	ASN	SER	SER	GLU	ARG	GLU	VAL	ASN	GLY	ALA	THR	GLU	GLU	ILE	LEU	VAL	ASN	ARG	LYS	LYS	LEU	GLN	TRP	ARG	ASP	ILE	ASP	GLN	GLN	LYS	THR	ILE	GLU	ALA	VAL	GLY	THR	ASP	LYS	ASN								
ILE	LYS	LYS	GLN	GLN	MET	LEU	THR	GLU	THR	ILE	LYS	MET	GLU	ALA	ASN	VAL	PHE	THR	GLN	THR	THR	GLN	ASP	LEU	GLU	THR	ALA	ASN	TYR	GLN	TRP	TRP	ARG	ASP	ILE	ASP	GLN	GLN	LYS	THR	ILE	GLU	ALA	VAL	GLY	THR	ASP	LYS	ASN									
HIS	MET	PRO	PRO	GLN	ILE	ARG	LYS	LYS	TYR	LYS	MET	GLU	ALA	ASN	GLU	PHE	LEU	LEU	ALA	ASP	PRO	GLY	VAL	ASN	THR	GLN	THR	ASN	GLY	TYR	GLN	TRP	TRP	ARG	ASP	ILE	ASP	ALA	ALA	GLN	LYS	THR	ILE	GLU	ASP	GLN	GLY	VAL	THR	LYS	ASN							
ARG	ILE	GLU	PHE	GLU	SER	SER	LYS	THR	THR	THR	ALA	ALA	LEU	LEU	LEU	PHE	LEU	LEU	ALA	ASP	GLU	GLU	MET	THR	THR	GLN	ASP	LEU	ALA	ALA	GLY	TYR	GLN	TRP	ARG	ASP	ILE	ASP	GLU	VAL	VAL	ASN	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					

S4.037	E4.038	E4.039	R4.044	L4.049	S4.050	M4.051	T4.052	S4.058	M4.062	L4.063	Q4.064	L4.065	Y4.073	E4.074	R4.075	K4.079	E4.080	Y4.081	A4.082	S4.083	S4.084	T4.085	E4.086	L4.089	Q4.090	E4.091	M4.092

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53499	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)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.881	Depositor
Minimum map value	-0.306	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.18	0/21346	0.37	0/28844

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1373	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	20925	0	21047	810	0
2	A	81	0	36	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	5	0
All	All	21037	0	21095	810	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 19.

The worst 5 of 810 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:1364:GLU:CG	1:A:1420:TYR:CD2	1.83	1.62
1:A:1364:GLU:CD	1:A:1420:TYR:C	1.84	1.46
1:A:1364:GLU:HG3	1:A:1420:TYR:CD2	1.41	1.42
1:A:1364:GLU:CD	1:A:1420:TYR:O	1.66	1.39
1:A:1364:GLU:CG	1:A:1420:TYR:O	1.69	1.38

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	2579/4092 (63%)	2453 (95%)	124 (5%)	2 (0%)	48 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2499	SER
1	A	3525	ILE

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	2358/3759 (63%)	2352 (100%)	6 (0%)	86 85

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

Mol	Chain	Res	Type
1	A	1376	LYS
1	A	1379	LYS
1	A	1380	GLU
1	A	1374	ILE
1	A	1372	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2513	GLN
1	A	2741	HIS
1	A	3984	GLN
1	A	2671	GLN
1	A	2832	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4101	-	28,29,29	1.38	4 (14%)	43,45,45	1.82	10 (23%)
3	ATP	A	4102	-	32,33,33	0.44	0	48,52,52	0.30	0
2	ADP	A	4104	-	28,29,29	1.42	4 (14%)	43,45,45	1.89	9 (20%)
2	ADP	A	4103	-	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4101	-	-	7/16/32/32	0/3/3/3
3	ATP	A	4102	-	-	9/22/38/38	0/3/3/3
2	ADP	A	4104	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4103	-	-	7/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4104	ADP	C5-C4	4.75	1.47	1.39
2	A	4103	ADP	C5-C4	4.63	1.47	1.39
2	A	4101	ADP	C5-C4	4.59	1.47	1.39
2	A	4104	ADP	C5-C6	2.75	1.48	1.41
2	A	4103	ADP	C5-C6	2.63	1.48	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4104	ADP	C5-C4-N3	-6.17	118.22	126.72
2	A	4103	ADP	C5-C4-N3	-5.90	118.59	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4101	ADP	C5-C4-N3	-5.66	118.92	126.72
2	A	4104	ADP	N3-C4-N9	4.79	135.32	127.17
2	A	4103	ADP	N3-C4-N9	4.66	135.10	127.17

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

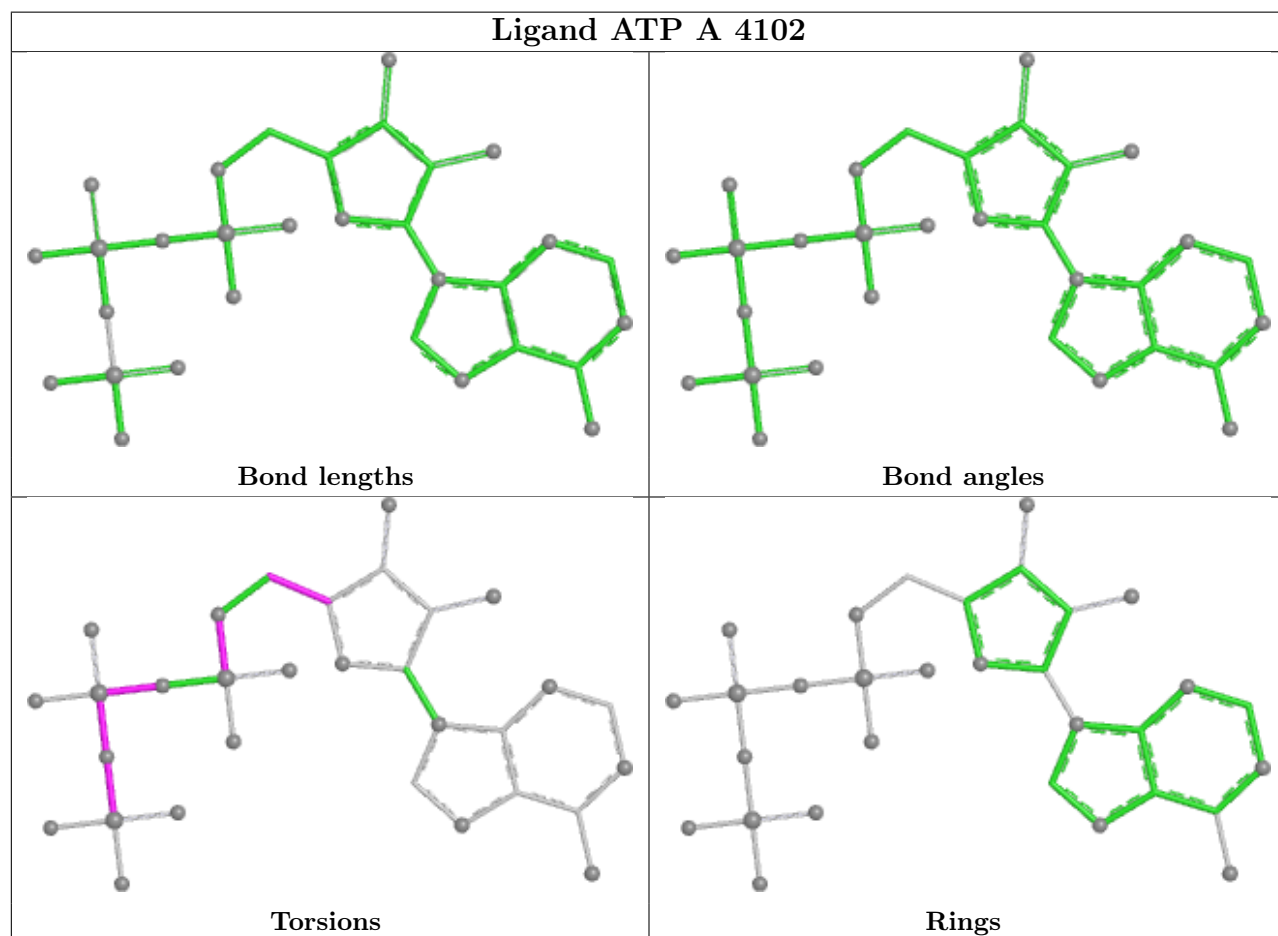
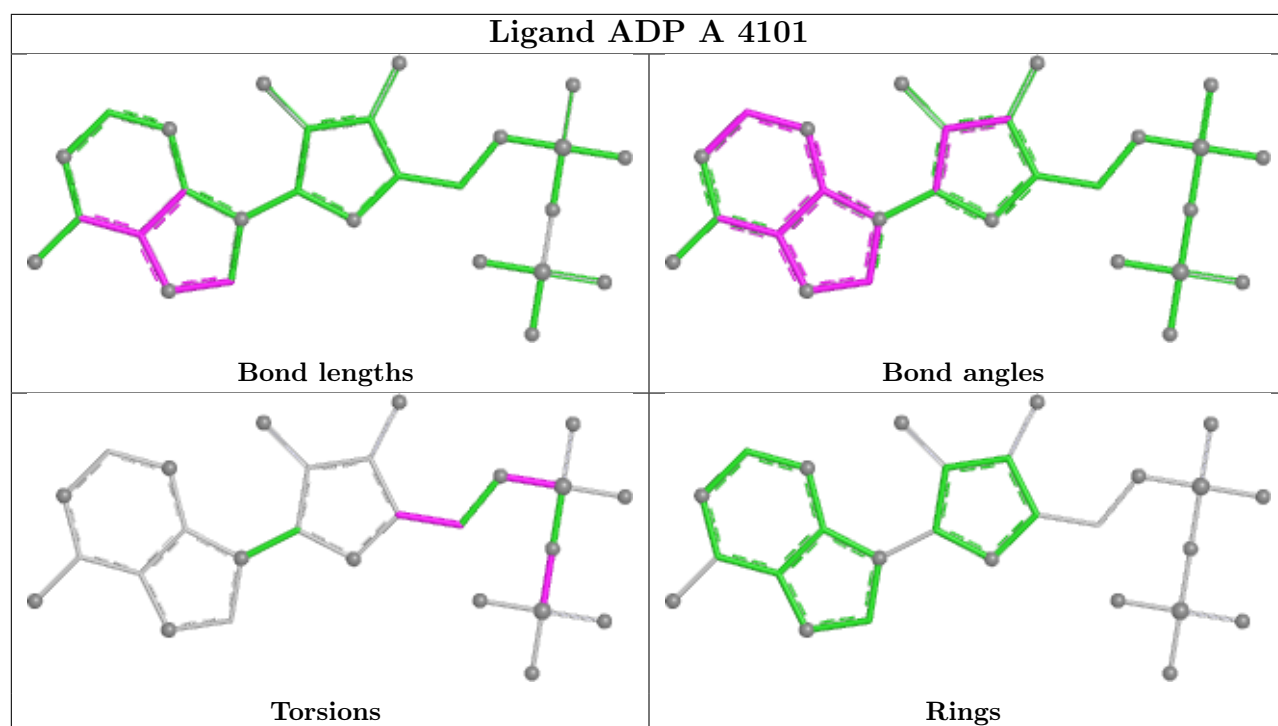
Mol	Chain	Res	Type	Atoms
2	A	4101	ADP	PA-O3A-PB-O2B
2	A	4101	ADP	PA-O3A-PB-O3B
2	A	4101	ADP	C5'-O5'-PA-O1A
2	A	4101	ADP	C5'-O5'-PA-O3A
2	A	4103	ADP	PA-O3A-PB-O2B

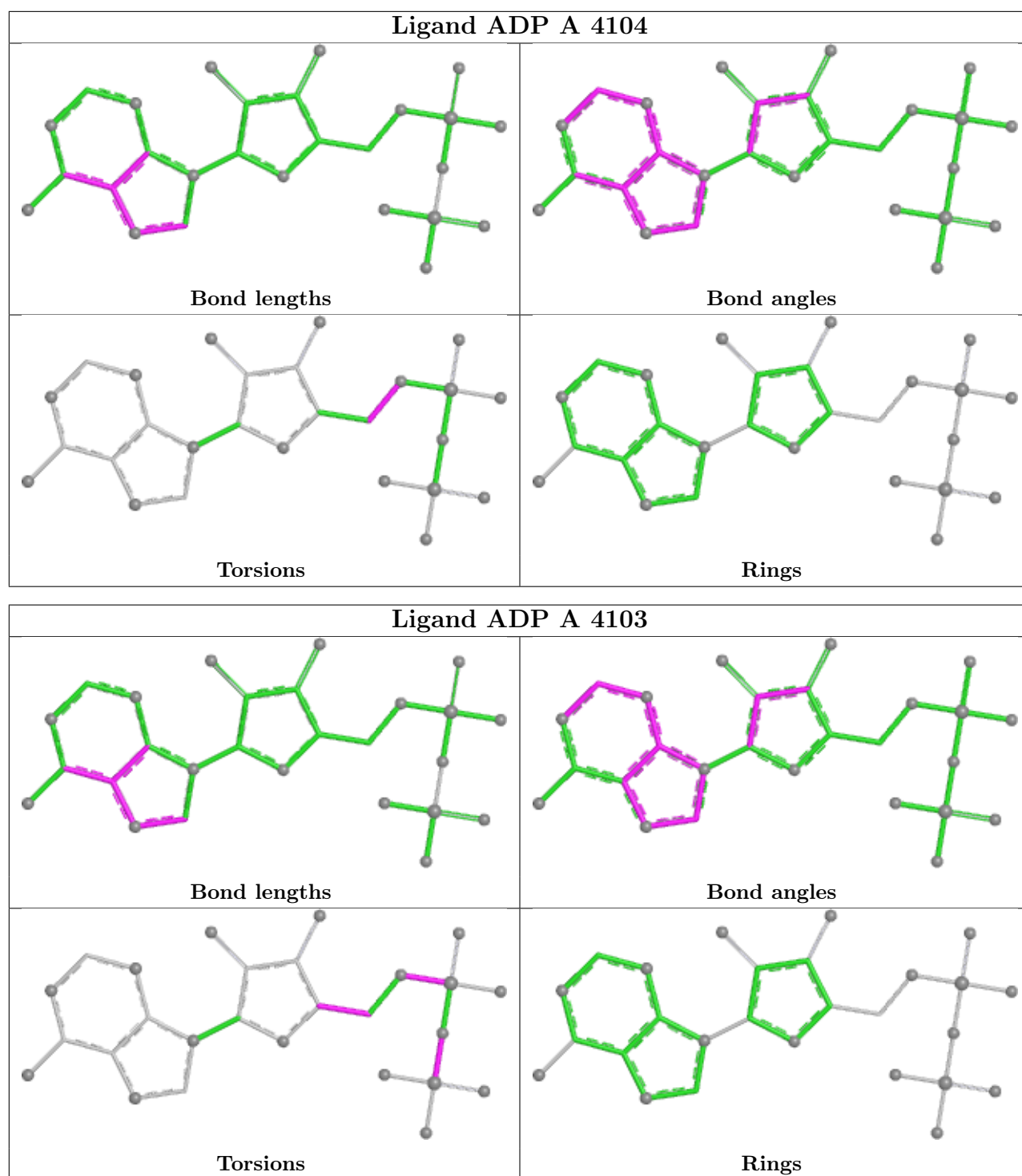
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4101	ADP	4	0
3	A	4102	ATP	5	0
2	A	4104	ADP	4	0
2	A	4103	ADP	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

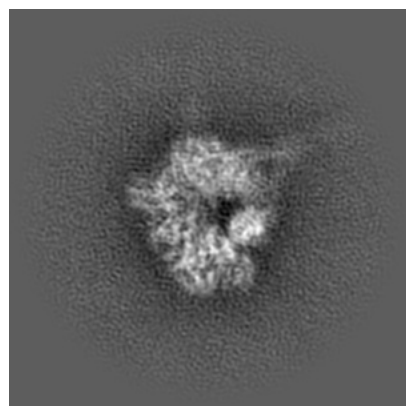
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48240. These allow visual inspection of the internal detail of the map and identification of artifacts.

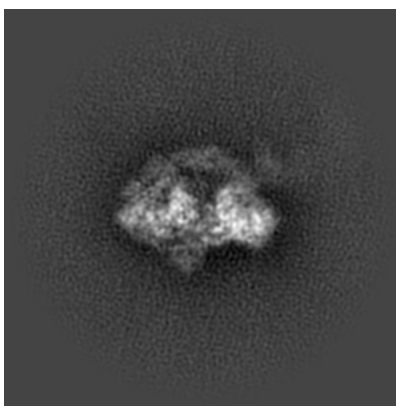
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

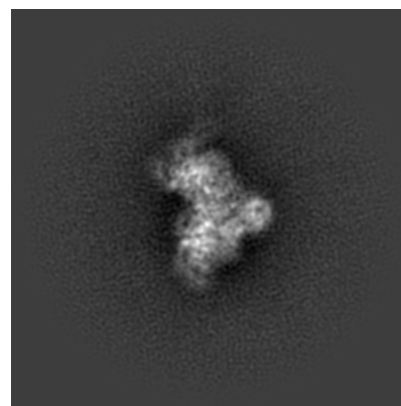
6.1.1 Primary map



X

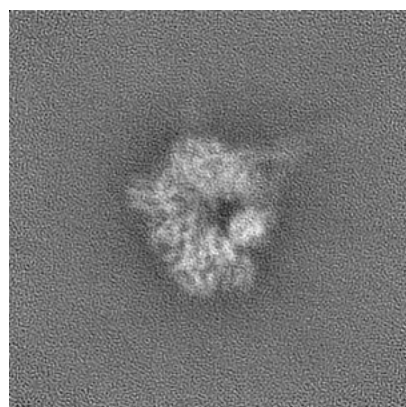


Y

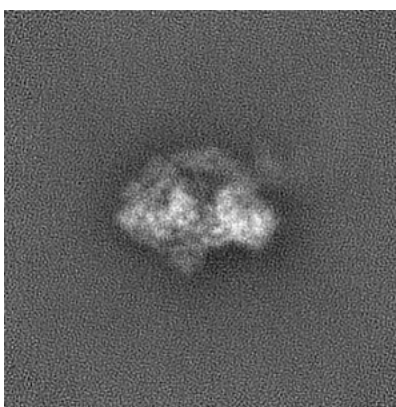


Z

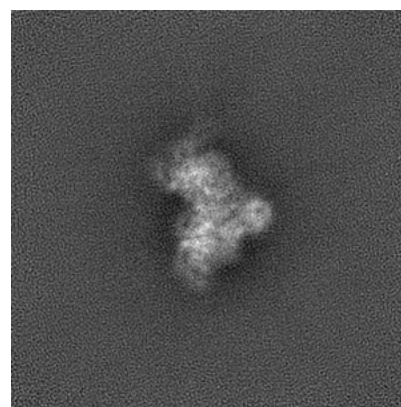
6.1.2 Raw map



X



Y

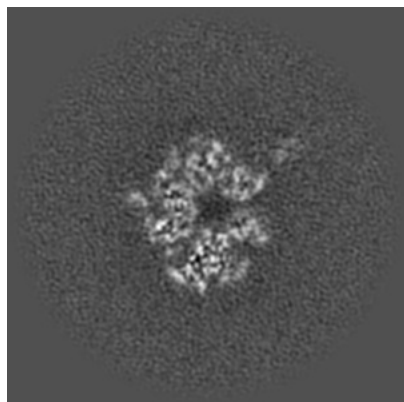


Z

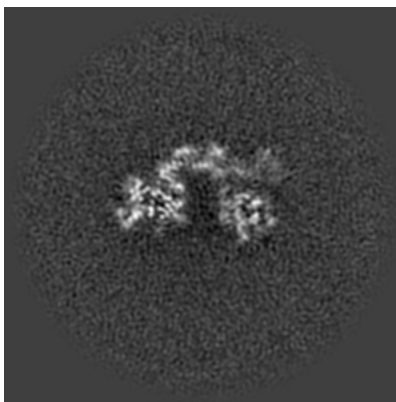
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

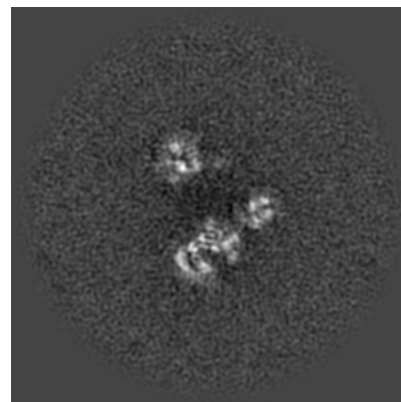
6.2.1 Primary map



X Index: 128

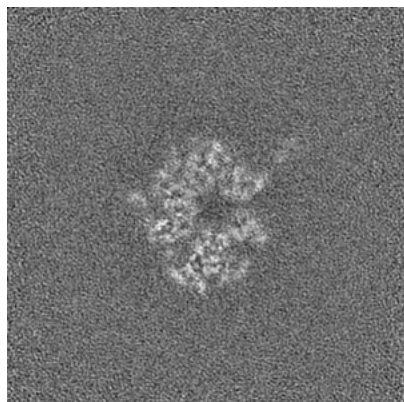


Y Index: 128

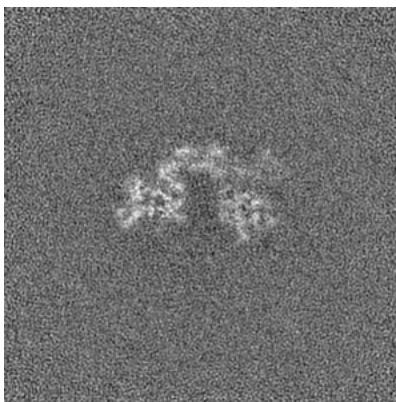


Z Index: 128

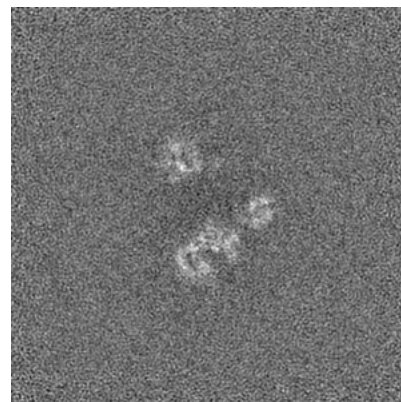
6.2.2 Raw map



X Index: 128



Y Index: 128

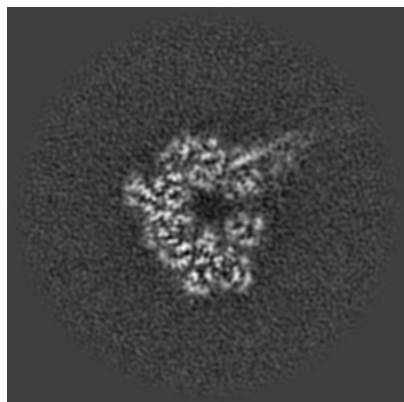


Z Index: 128

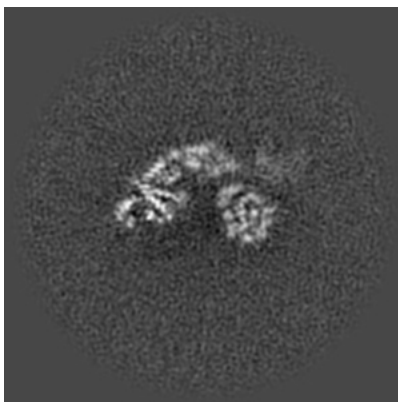
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

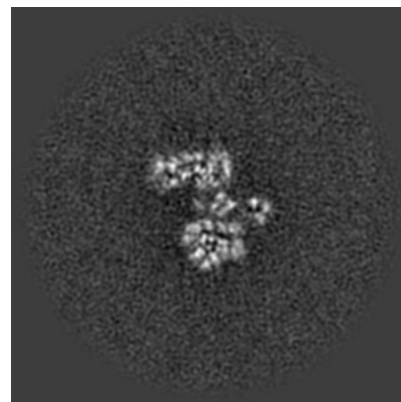
6.3.1 Primary map



X Index: 122

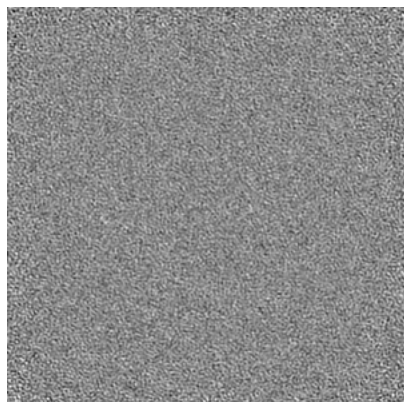


Y Index: 124

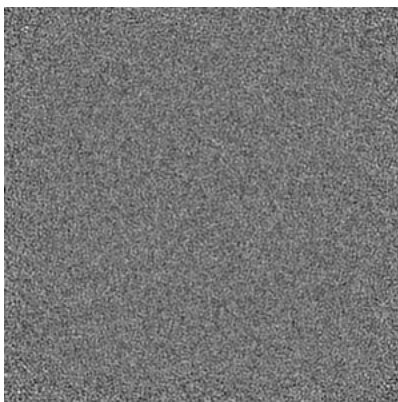


Z Index: 113

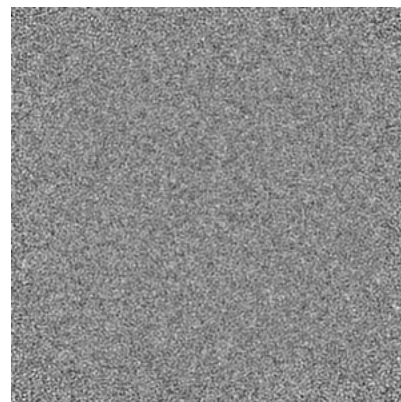
6.3.2 Raw map



X Index: 0



Y Index: 0

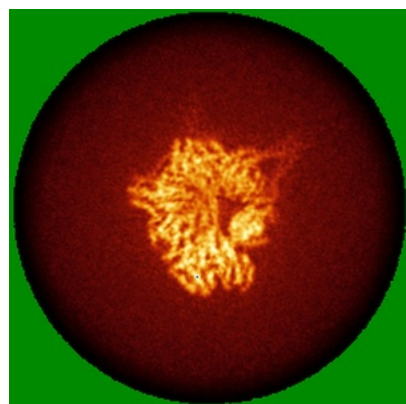


Z Index: 0

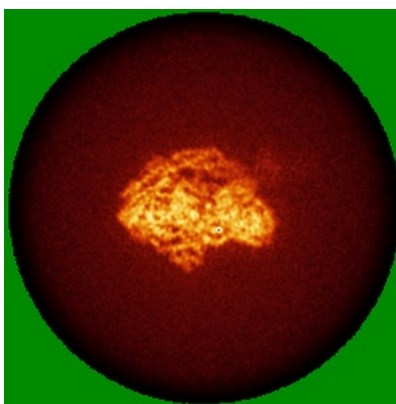
The images above show the largest variance slices of the map in three orthogonal directions.

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

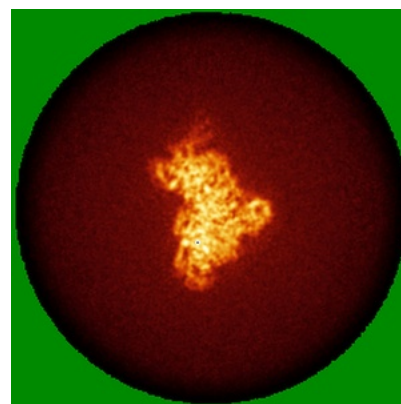
6.4.1 Primary map



X

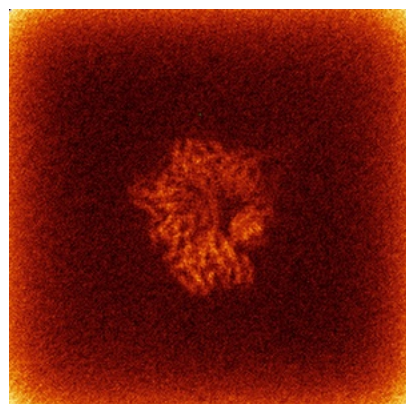


Y

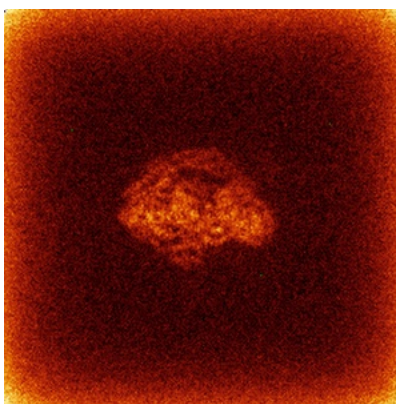


Z

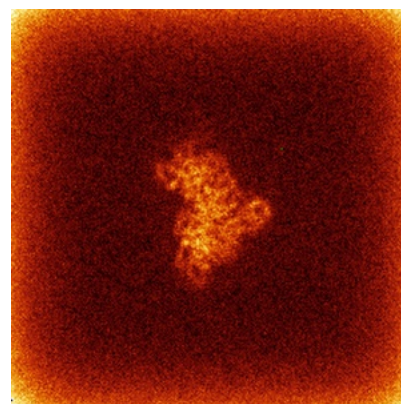
6.4.2 Raw map



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.

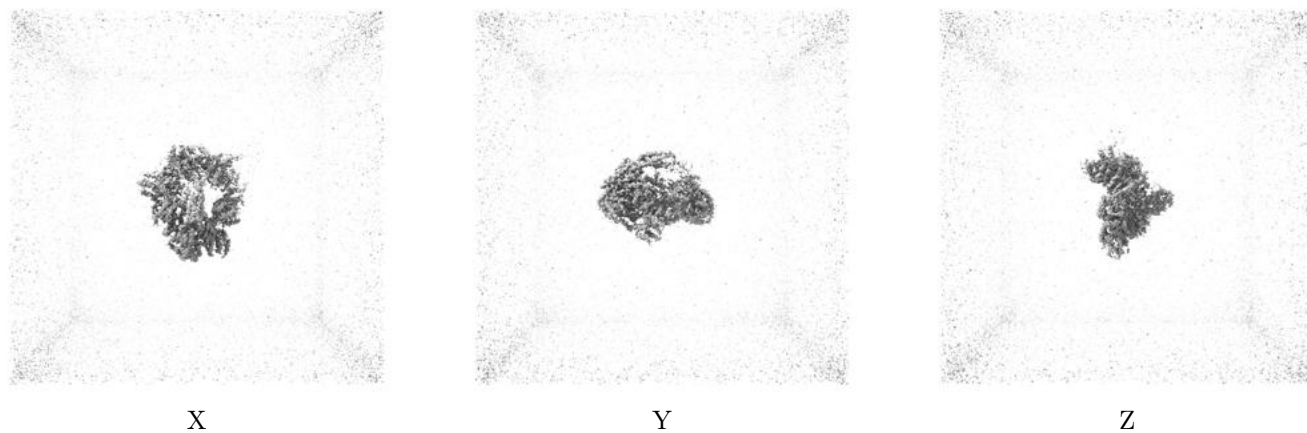
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

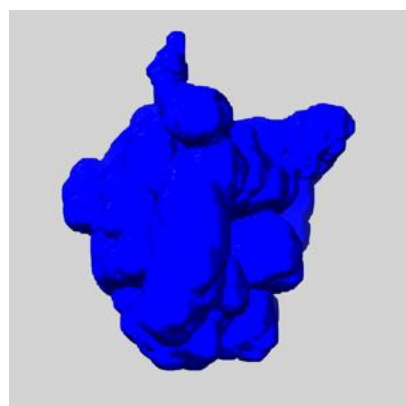
6.6 Mask visualisation [i](#)

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

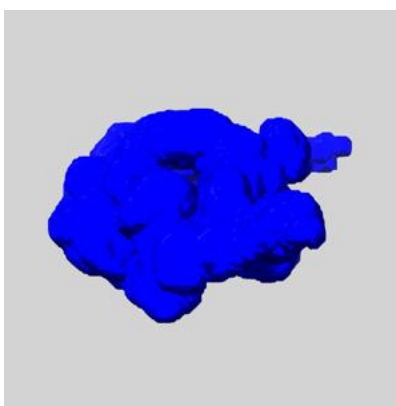
A mask typically either:

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

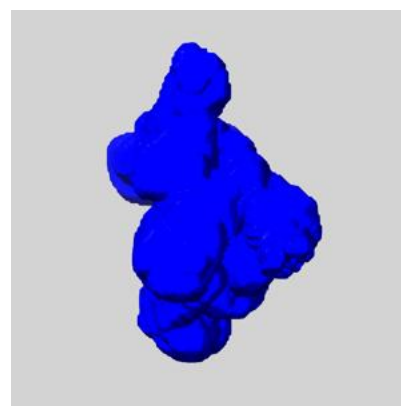
6.6.1 emd_48240_msk_1.map [i](#)



X



Y

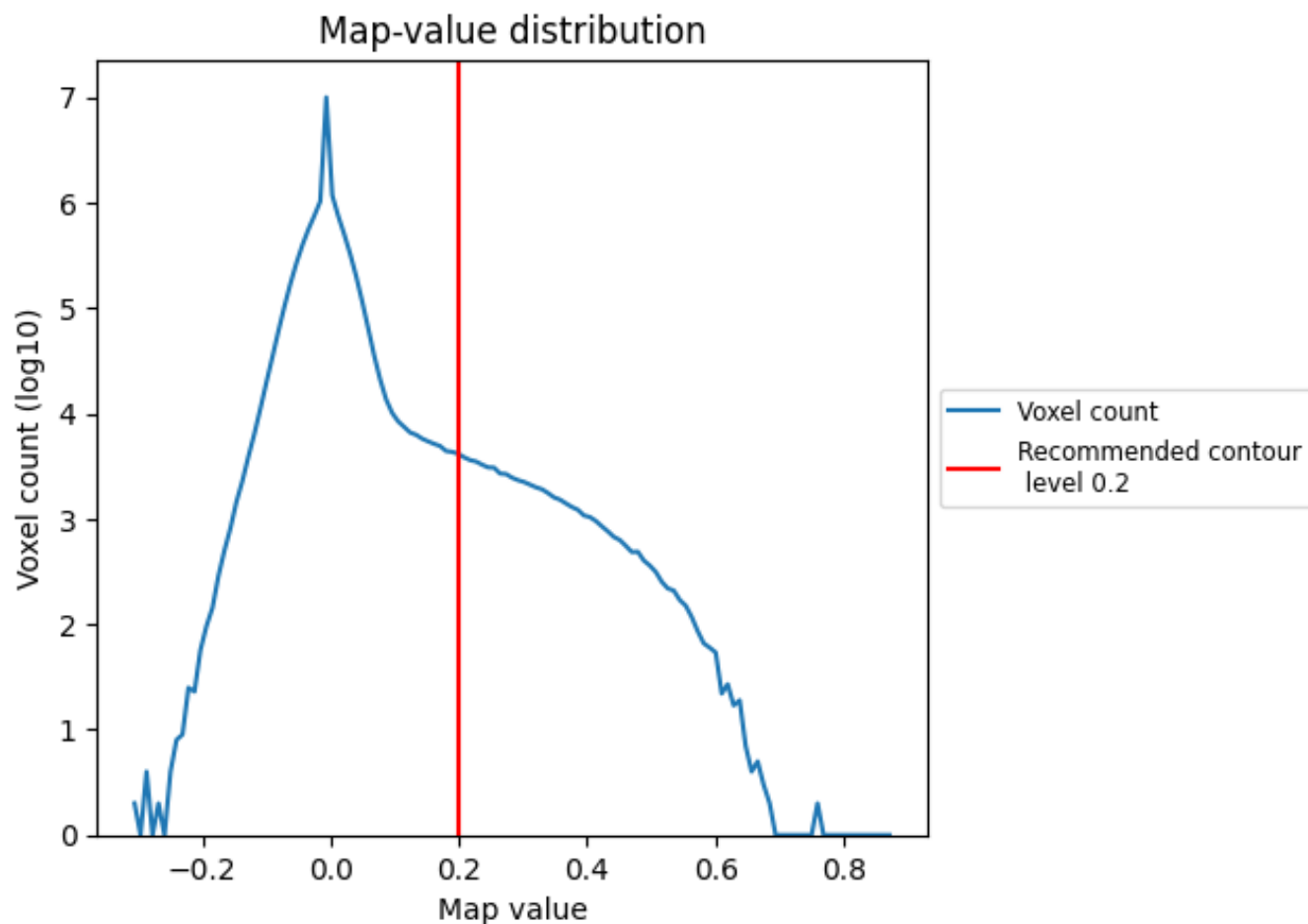


Z

7 Map analysis [i](#)

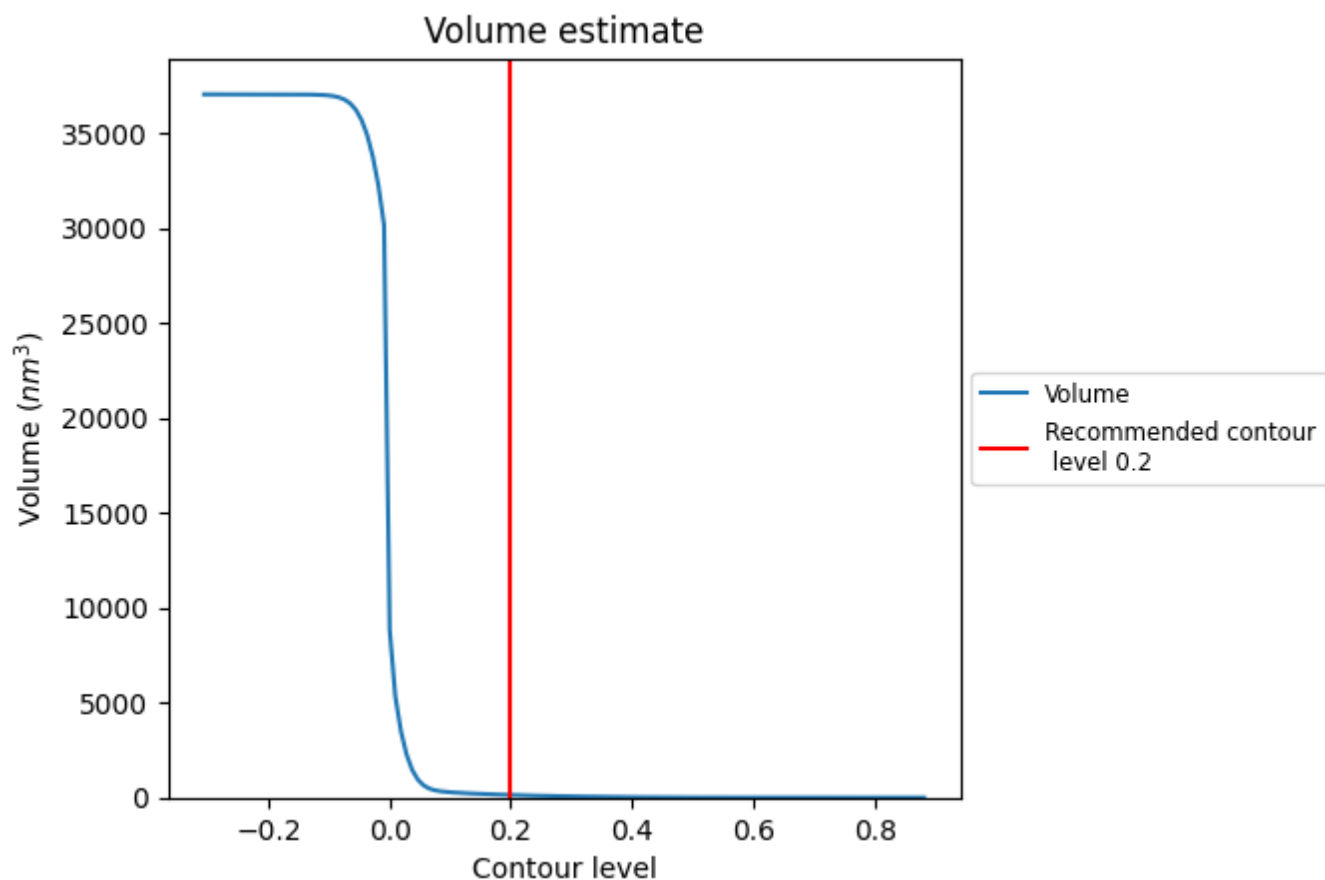
This section contains the results of statistical analysis of the map.

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.

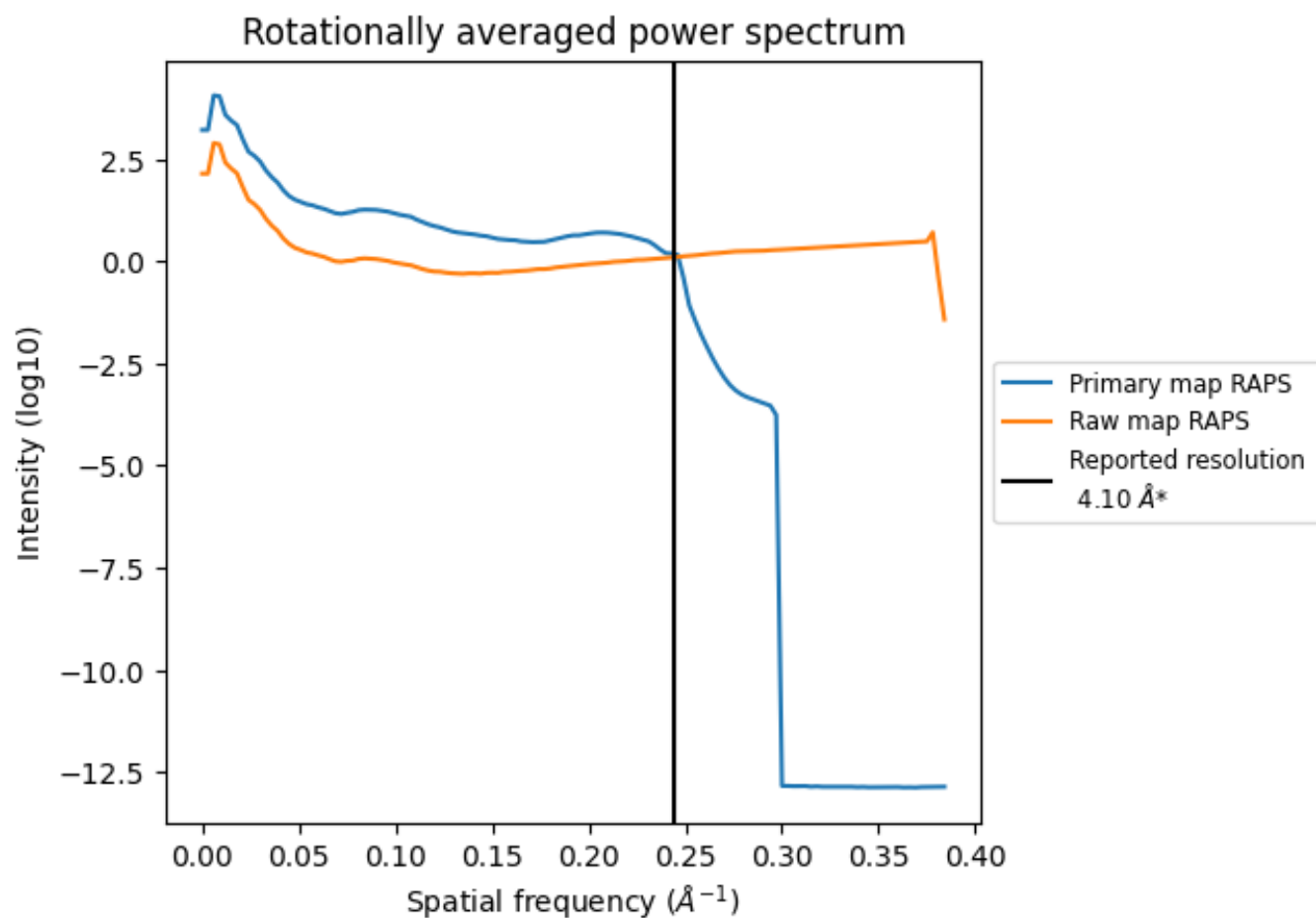
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

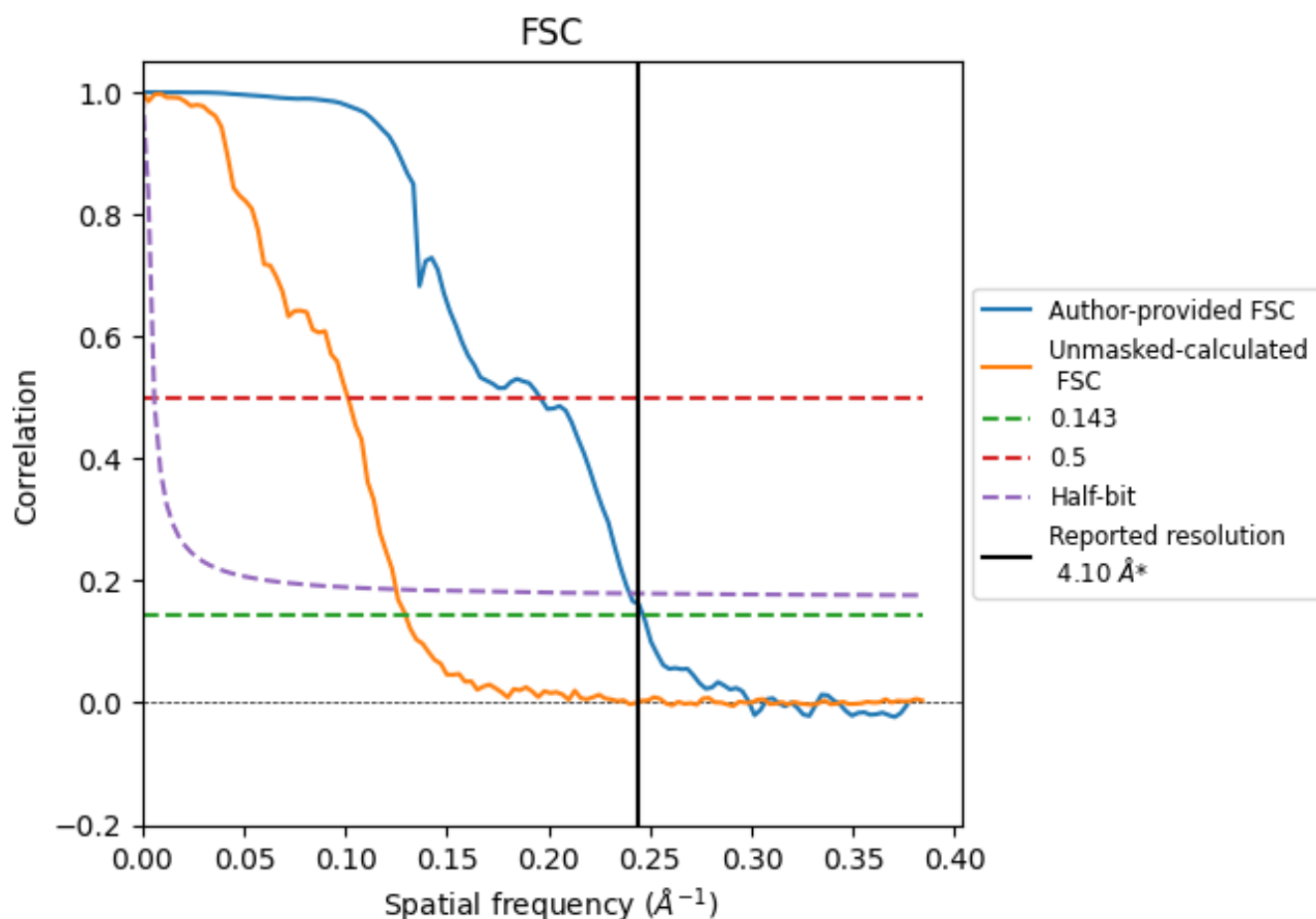


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

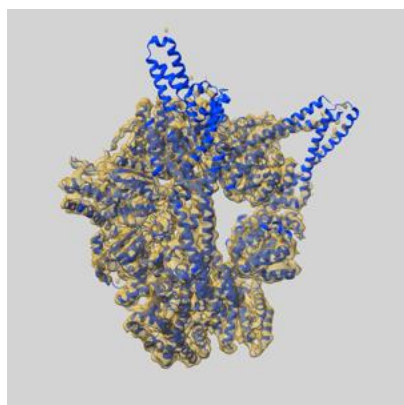
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.06	5.11	4.17
Unmasked-calculated*	7.71	9.88	8.00

*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 7.71 differs from the reported value 4.1 by more than 10 %

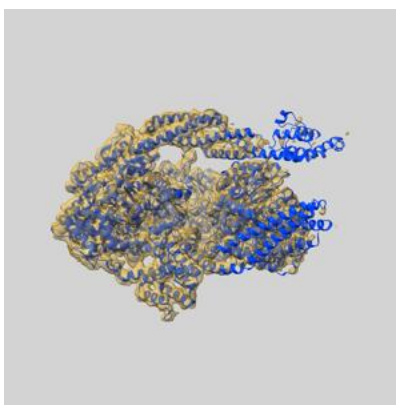
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48240 and PDB model 9MFW. Per-residue inclusion information can be found in section 3 on page 5.

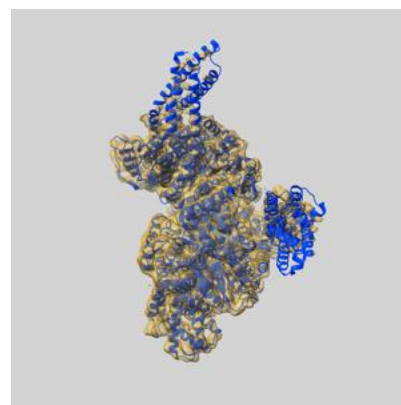
9.1 Map-model overlay [i](#)



X



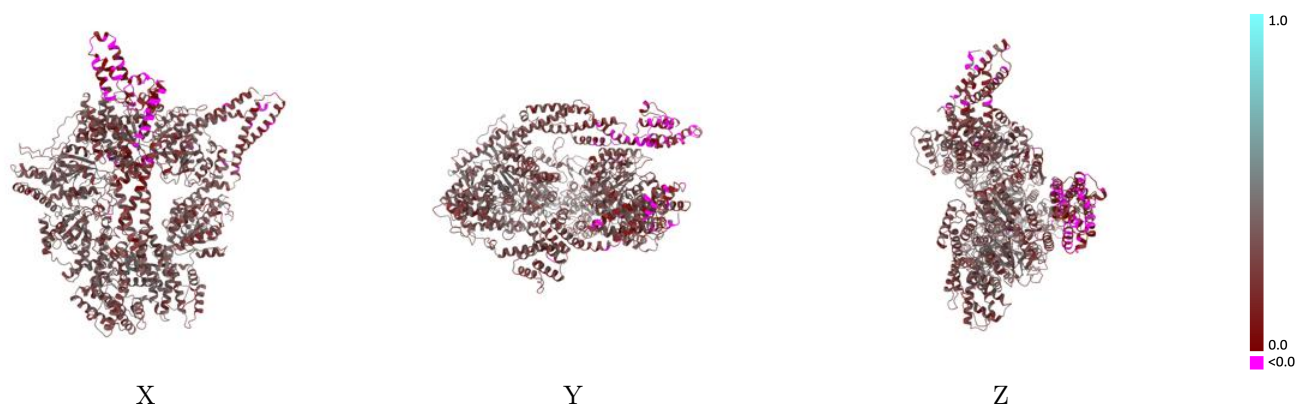
Y



Z

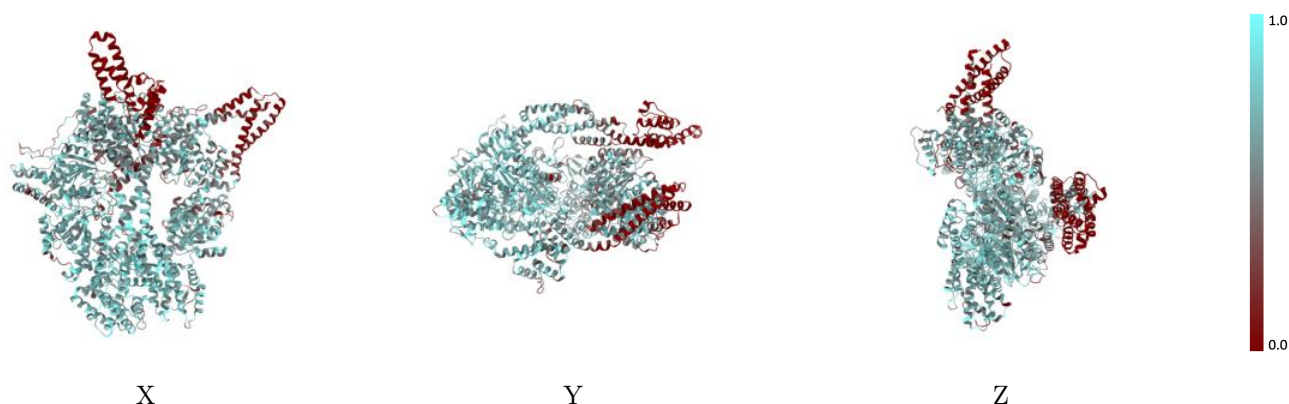
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



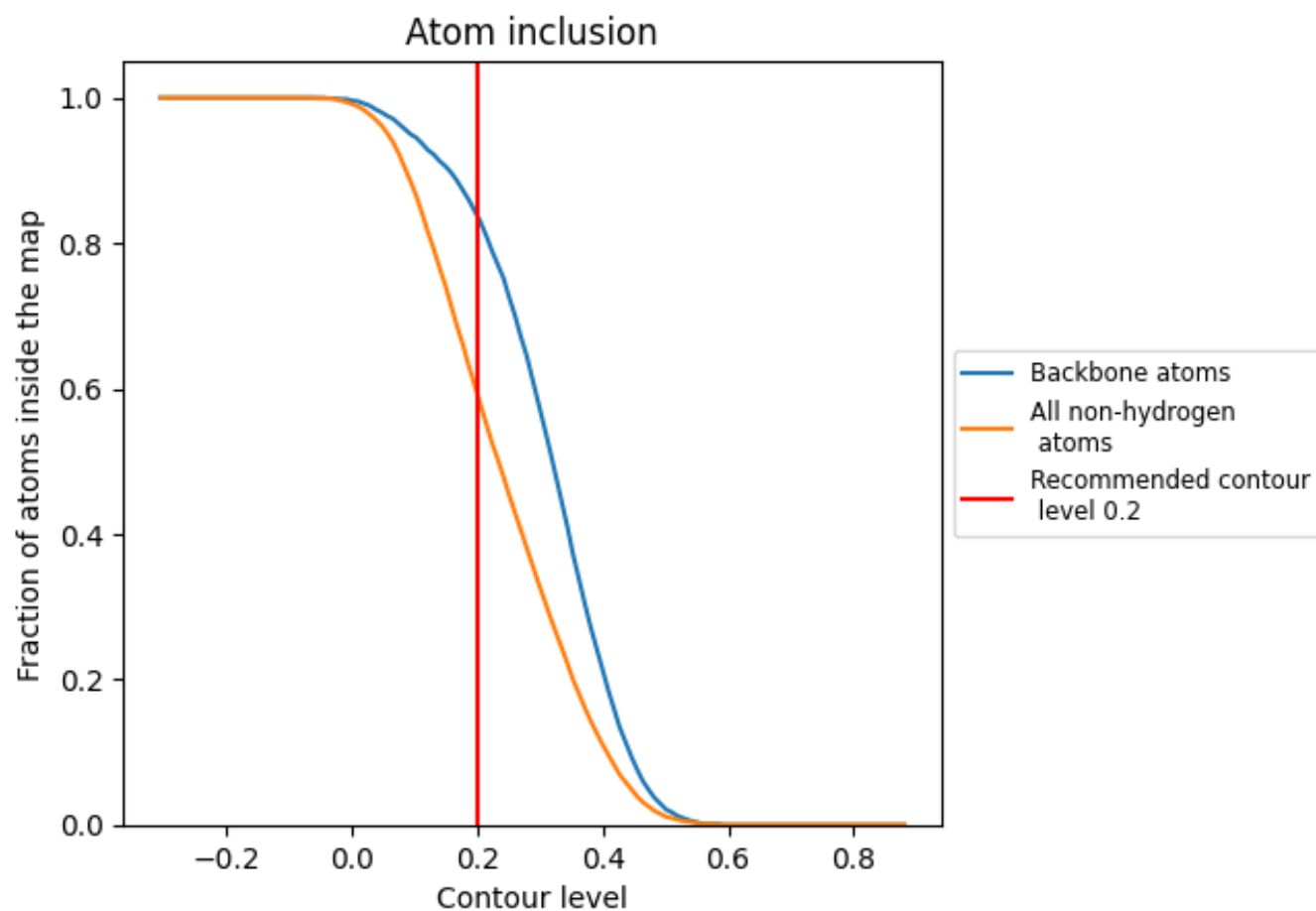
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 59% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.2940
A	0.5920	0.2940

