



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 04:49 PM UTC

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.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

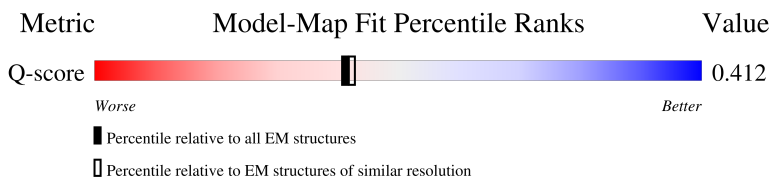
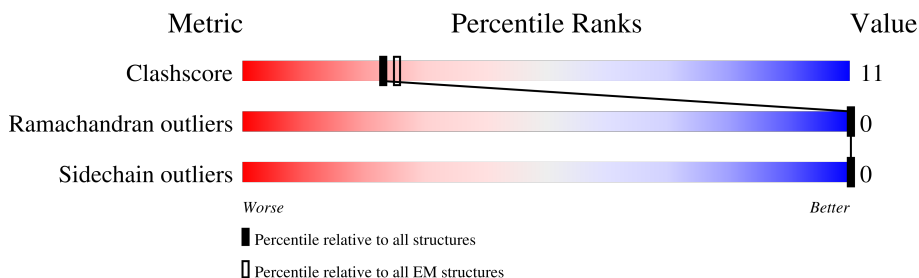
1 Overall quality at a glance

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 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.

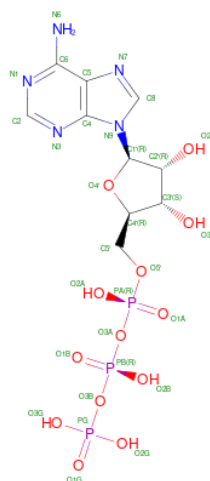
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3038	Total	C	N	O	S	0	0
			24471	15586	4225	4538	122		

- 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).



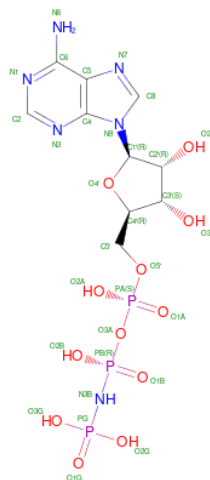
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- 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

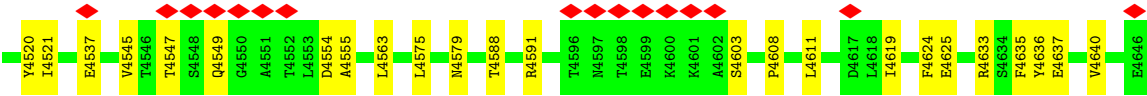
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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	I1594	Y1515	E1443	Y1383	GLU	GLU	THR	THR	VAL	THR	ILE	ASP	PHE
A1995	Q1881	V1721	Q1596	F1516	A1444	E1384	LEU	LEU	PRO	PRO	ILE	ARG	MET	GLY	LYS
P1996	T1882	V1724	G1596	E1518	I1445	F1385	Q1327	TRP	TRP	SER	ILE	VAL	GLN	ILE	GLY
I1997	T1885	V1724	V1597	E1519	V1446	V1386	D1328	THR	THR	VAL	VAL	VAL	GLN	ILE	VAL
L2001	G1728	G1728	Q1598	A1520	K1447	Q1387	L1329	THR	THR	GLY	ASP	PRO	ASN	GLY	VAL
L2002	C1888	K1729	R1599	S1522	D1448	R1388	K1330	ASN	TYR	LEU	ARG	PRO	TYR	ILE	ASP
N2003	C1889	T1730	E1602	W1523	V1449	L1389	G1331	ILE	ILE	GLN	THR	ALA	GLY	LEU	LEU
V2006	M1892	T1731	R1603	E1524	L1450	L1390	V1332	ASN	ASN	LEU	THR	PRO	VAL	ILE	ILE
K2007	S1903	S1732	G1609	K1526	A1453	K1391	W1333	GLU	ILE	GLU	ASP	GLU	ARG	GLU	GLU
P2008	P1904	T1739	K1610	L1527	V1462	G1392	M1334	ALA	GLY	GLN	ASN	ILE	LEU	LEU	LYS
V2008	F1905	T1740	I1611	M1528	Q1454	Y1393	E1335	LEU	GLY	SER	GLY	ALA	GLY	ILE	LYS
D2011	T1910	W1741	Q1612	R1529	G1455	M1394	L1336	TRP	TRP	VAL	THR	THR	CYS	ASP	ASP
M2012	G1911	V1750	K1613	I1530	E1456	K1395	S1337	GLY	GLY	ASP	LYS	VAL	ARG	LEU	LEU
M2018	E1914	E1763	P1627	M1531	L1459	I1396	K1338	LEU	PHE	THR	LYS	TYR	ARG	LEU	GLU
G2021	F1926	L1766	E1635	D1535	E1460	M1397	V1339	ILE	ILE	ALA	GLU	LYS	ALA	ALA	VAL
ALA	N1931	M1769	D1636	D1539	F1461	L1398	W1340	GLY	ILE	THR	MET	LYS	THR	GLY	THR
GLY	C1932	G1770	E1639	V1540	L1463	Y1400	E1341	LYS	ASP	THR	GLY	THR	GLN	THR	GLY
ARG	D1933	G1770	E1639	Q1541	K1464	I1401	Q1342	PHE	ARG	ALA	VAL	VAL	VAL	GLY	VAL
S2026	E1934	G1772	K1645	R1543	Q1465	E1402	I1343	LYS	LYS	THR	VAL	ILE	VAL	LEU	CYS
N2027	T1935	G1773	N1646	E1546	R1467	L1403	D1344	ARG	ASP	PHE	THR	GLN	GLN	TRP	ALA
D2030	V1946	D1774	K1649	L1547	E1468	K1404	Q1345	LYS	LYS	THR	THR	VAL	VAL	MET	GLY
K2033	L1947	V1781	H1653	G1549	N1471	S1405	K1347	ASP	ASP	VAL	GLN	VAL	VAL	VAL	LYS
S2038	C1949	M1784	F1654	I1550	T1472	A1407	E1348	ARG	GLN	GLN	GLN	LEU	LEU	ALA	PHE
P2044	Q1950	V1785	F1655	F1551	L1475	K1408	Q1349	GLU	GLY	VAL	LYS	SER	VAL	GLY	GLY
Q2047	V1951	G1792	K1655	T1552	D1476	K1409	P1350	CYS	LYS	VAL	ASN	TYR	GLN	ASP	ILE
I2049	G1952	T1788	K1656	G1553	L1477	D1410	W1351	ALA	ALA	ASN	LEU	ARG	PRO	MET	LEU
L2054	D1958	L1792	A1659	S1554	V1478	R1411	V1352	LYS	GLN	LEU	LYS	ILE	ILE	ASP	ASN
R2060	N1961	Q1800	G1660	A1555	Q1481	H1412	S1353	LYS	LYS	MET	LYS	THR	THR	ASP	THR
E2063	R1962	R1804	V1661	D1557	N1482	W1413	V1354	ALA	ILE	VAL	GLN	TRP	TRP	ALA	GLN
V2064	R1966	L1811	S1671	K1558	R1485	L1416	Q1355	GLU	VAL	GLU	ALA	GLN	VAL	VAL	VAL
L2065	S1969	I1812	I1676	E1564	L1486	M1417	P1356	GLU	GLU	GLU	GLY	GLY	SER	SER	ASP
A2066	Q1973	I1829	R1679	E1574	I1487	K1418	R1357	THR	ASP	VAL	VAL	ILE	GLY	HIS	GLY
I2069	T1978	I1830	M1685	F1575	G1489	R1419	L1359	THR	ARG	GLU	LEU	TYR	PRO	ASN	ASN
V2070	E1984	D1831	M1685	L1576	W1490	H1420	Q1361	GLY	GLU	ARG	GLY	GLY	GLY	GLY	GLY
F2073	H1985	N1832	S1691	A1577	D1491	H1421	N1362	SER	ARG	GLY	GLY	GLY	PRO	ILE	LYS
D2077	S1986	A1833	L1692	M1579	D1492	V1422	L1363	THR	THR	THR	THR	ASP	GLY	LEU	LEU
N1987	T1987	W1838	T1693	K1580	F1494	W1424	D1364	GLU	GLU	GLU	LEU	LEU	LEU	ASP	ASP
P1988	N1987	R1843	E1694	N1495	K1496	V1425	A1365	GLU	GLU	GLU	LEU	LEU	LEU	ASN	LYS
N1989	F1844	F1845	K1697	V1582	R1497	V1426	L1366	LEU	LEU	LEU	LEU	LEU	LEU	ASN	ASN
Y1990	Y1845	M1861	I1698	K1583	V1497	S1427	L1367	ARG	THR	THR	THR	LYS	LYS	VAL	VAL
Q2083	D1991		W1701	K1584	A1506	E1428	N1368	GLN	ASP	THR	THR	GLN	GLN	TRP	TRP
Y2086			V1705	L1587	M1507	L1429	Q1369	VAL	LYS	GLY	GLY	GLY	GLY	VAL	HIS

GLN	Q3198	D3096	R3007	E2914	R2831	L2744	F2635	Y2517	E2406	I2301	I2213	R2091	GLN
GLU	M3199	T3099	M3008	V2915	Q2834	I2747	D2636	I2518	E2407	V2302	T2214	A2092	GLU
ILE	H3201	A3100	L3012	H2918	D2835	I2752	R2642	T2522	A2408	D2306	H2218	L2093	ILE
GLU	N3202	A3101	A3013	V2919	R2836	N2752	R2643	P2527	A2409	E2310	G2219	L2097	GLU
LEU	V3203	N3014	N3014	T2922	E2839	M2755	M2646	T2528	M2412	W2311	K2220	K2104	LEU
HIS	G3204	G3019	G3019	R2923	D2840	L2766	Q2647	P2529	L2413	D2320	K2230	R2107	HIS
GLN	L3205	L3019	L3019	R2924	E2841	L2767	V2648	A2529	Q2416	D2321	K2231	T2111	GLN
GLN	R3206	F3021	F3021	T2925	E2842	R2758	V2649	P2530	Q2416	N2322	M2221	R2112	GLN
GLU	I3208	G3022	G3022	F2926	R2843	L2759	L2650	N2531	I2422	K2323	M2222	R2113	GLU
VAL	K3209	Q2928	Q2928	R2927	D2847	I2762	L2655	I2532	L2437	L2324	G2229	E2114	VAL
ILE	K3209	Q2928	Q2928	R2927	D2847	L2762	L2655	S2540	L2437	N2329	K2230	R2115	ILE
ASP	T3211	Q2929	Q2929	Q2930	L2855	P2768	Q2656	S2541	H2445	P2336	S2231	E2116	ASP
ASP	T3212	E3025	E3025	Q2930	K2856	L2769	K2657	S2542	H2446	N2338	M2232	R2117	ASP
GLN	D3213	Y3026	Y3026	L2933	H2857	T2770	W2658	G2543	I2446	R2340	W2234	E2118	GLN
GLN	Q3214	M3030	M3030	L2934	F2858	A2771	V2660	E2544	M2447	T2341	W2236	R2119	GLN
SER	Q3214	M3030	M3030	L2934	F2858	A2771	V2660	W2545	D2448	K2342	L2238	E2120	SER
VAL	V3215	D3124	D3124	K2943	I2861	M2773	D2664	A2563	T2449	M2345	K2239	R2121	VAL
VAL	E3216	V3125	V3125	T2944	R2862	M2773	E2665	D2566	T2450	P2337	E2248	E2122	VAL
GLU	E3217	V3128	V3128	T2945	R2863	E2774	E2665	D2569	R2451	N2339	G2249	E2123	GLU
ASP	L3218	Y3129	Y3129	L2946	E2864	E2775	W2667	T2571	L2452	R2340	K2257	E2124	ASP
LEU	R3219	Y3130	Y3130	V2950	K2865	T2778	L2668	V2570	L2455	T2341	Y2265	E2125	LEU
ASP	R3220	D3131	D3131	V2950	K2865	M2778	L2668	T2571	L2455	M2342	Y2266	E2126	ASP
LYS	D3221	K3132	K3132	K2962	R2869	F2784	T2676	D2572	Q2464	F2343	Y2267	E2127	LYS
LEU	LEU	F3136	F3136	H2963	P2870	D2787	F2682	D2573	R2467	E2344	G2266	E2128	LEU
PRO	ARG	S3137	S3137	V2964	L2871	D2787	L2683	D2574	R2467	Y2350	T2267	E2129	PRO
ALA	ALA	S3138	S3138	H2964	L2872	D2787	L2683	D2575	R2467	M2361	T2272	E2133	ALA
ILE	ILE	R3139	R3139	K2965	L2872	D2787	L2683	D2576	R2467	V2362	R2273	E2136	ILE
GLU	GLU	R3140	R3140	K2966	N2875	Y2792	W2685	R2577	M2481	W2363	E2274	E2137	GLU
GLN	GLN	N3145	N3145	Y2967	N2875	I2793	W2686	E2577	E2484	W2364	W2275	E2138	GLN
GLN	GLN	N3145	N3145	Y2967	N2875	I2793	W2686	E2577	E2484	S2365	T2276	E2139	GLN
ASN	ASN	V3148	V3148	E2970	K2879	P2796	E2687	E2578	Q2485	P2386	D2277	E2147	ASN
VAL	VAL	L3154	L3154	D2971	D2880	R2797	E2688	E2578	Q2485	D2387	T2281	K2148	VAL
LYS	LYS	L3154	L3154	D2972	D2880	R2797	E2688	E2578	Q2485	E2388	H2282	V2150	LYS
SER	SER	L3154	L3154	D2973	V2884	M2799	R2694	Y2582	Q2485	E2389	V2283	L2157	SER
ALA	ALA	L3050	L3050	E2974	D2885	M2799	R2694	Y2582	Q2485	G2390	L2284	L2161	ALA
ALA	ALA	Y3051	Y3051	L2976	Q2886	L2801	L2703	K2589	Y2489	E2391	K2286	E2172	ALA
ALA	ALA	Y3051	Y3051	L2976	Q2886	L2801	L2703	K2589	Y2489	E2392	K2286	E2173	ALA
ASN	ASN	R3167	R3167	E2975	L2889	V2802	E2705	P2590	Q2491	E2393	L2287	E2174	ASN
GLN	GLN	R3168	R3168	L2976	L2889	V2802	E2705	P2590	Q2491	A2394	D2289	E2175	GLN
GLN	GLN	R3169	R3169	L2976	L2889	V2802	E2705	P2590	Q2491	Q2395	D2289	E2175	GLN
HIS	HIS	T3172	T3172	C2985	K2894	F2807	C2712	C2594	Y2496	R2396	R2292	L2182	HIS
VAL	VAL	H3175	H3175	E2986	K2894	F2807	C2712	C2594	Y2496	E2397	R2292	L2182	VAL
VAL	VAL	Y3176	Y3176	E2986	K2894	F2807	C2712	C2594	Y2496	E2397	R2292	L2182	VAL
ARG	ARG	T3180	T3180	M2994	K2898	L2813	R2720	G2600	S2503	E2397	R2292	L2182	ARG
SER	SER	T3180	T3180	M2994	K2898	L2813	R2720	G2600	S2503	E2397	R2292	L2182	SER
MET	MET	A3184	A3184	E2995	F2900	T2815	L2728	L2606	Q2504	D2392	K2286	E2176	MET
ALA	ALA	A3184	A3184	E2995	F2900	T2815	L2728	L2606	Q2504	E2393	K2286	E2176	ALA
ASN	ASN	R3191	R3191	E2996	E2902	L2816	R2729	M2614	D2505	E2394	K2286	E2176	ASN
PRO	PRO	S3192	S3192	E2997	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	PRO
ALA	ALA	E3193	E3193	N2998	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	ALA
GLU	GLU	L3194	L3194	N2998	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	GLU
ALA	ALA	E3195	E3195	N2998	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	ALA
LYS	LYS	E3196	E3196	N2998	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	LYS
VAL	VAL	Q3197	Q3197	N2998	E2903	L2822	H2730	M2614	D2505	E2394	K2286	E2176	VAL
MET	MET	R3088	R3088	L3000	L2909	A2826	V2734	P2628	A2512	E2399	G2293	L2208	MET
SER	SER	N3092	N3092	D3001	V2910	H2827	V2736	E2629	E2513	E2402	L2294	E2209	SER
				G3003	L2911	E2828	V2736	E2629	E2513	E2403	L2294	E2209	
				F3004	F2912	L2830	P2739	K2633	E2516	E2404	Q2296	L2210	





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

5.1 Standard geometry

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

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	-	33,33,33	0.91	4 (12%)	45,52,52	0.61	0
2	ADP	A	4704	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
3	ATP	A	4702	5	32,33,33	0.34	0	48,52,52	0.30	0
2	ADP	A	4701	-	28,29,29	1.44	5 (17%)	43,45,45	1.80	7 (16%)

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	-	-	2/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.69	1.47	1.39
2	A	4701	ADP	C5-C4	4.67	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4701	ADP	C5-C6	2.66	1.48	1.41
4	A	4703	ANP	PG-O1G	2.45	1.49	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.86	118.64	126.72
2	A	4704	ADP	C5-C4-N3	-5.81	118.72	126.72
2	A	4701	ADP	N3-C4-N9	4.65	135.08	127.17
2	A	4704	ADP	N3-C4-N9	4.54	134.90	127.17
2	A	4704	ADP	C2-N3-C4	3.68	120.82	111.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

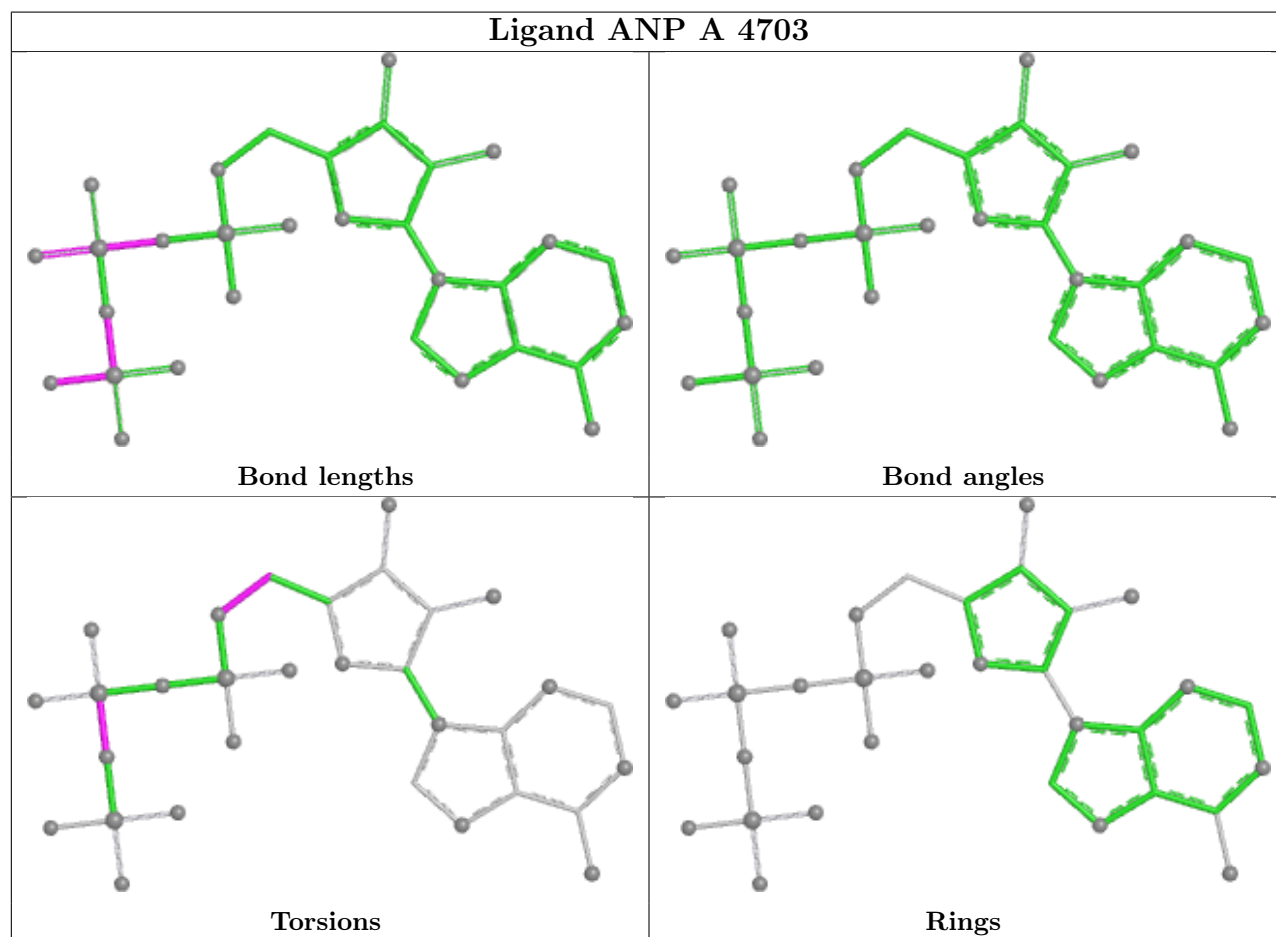
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	C5'-O5'-PA-O3A

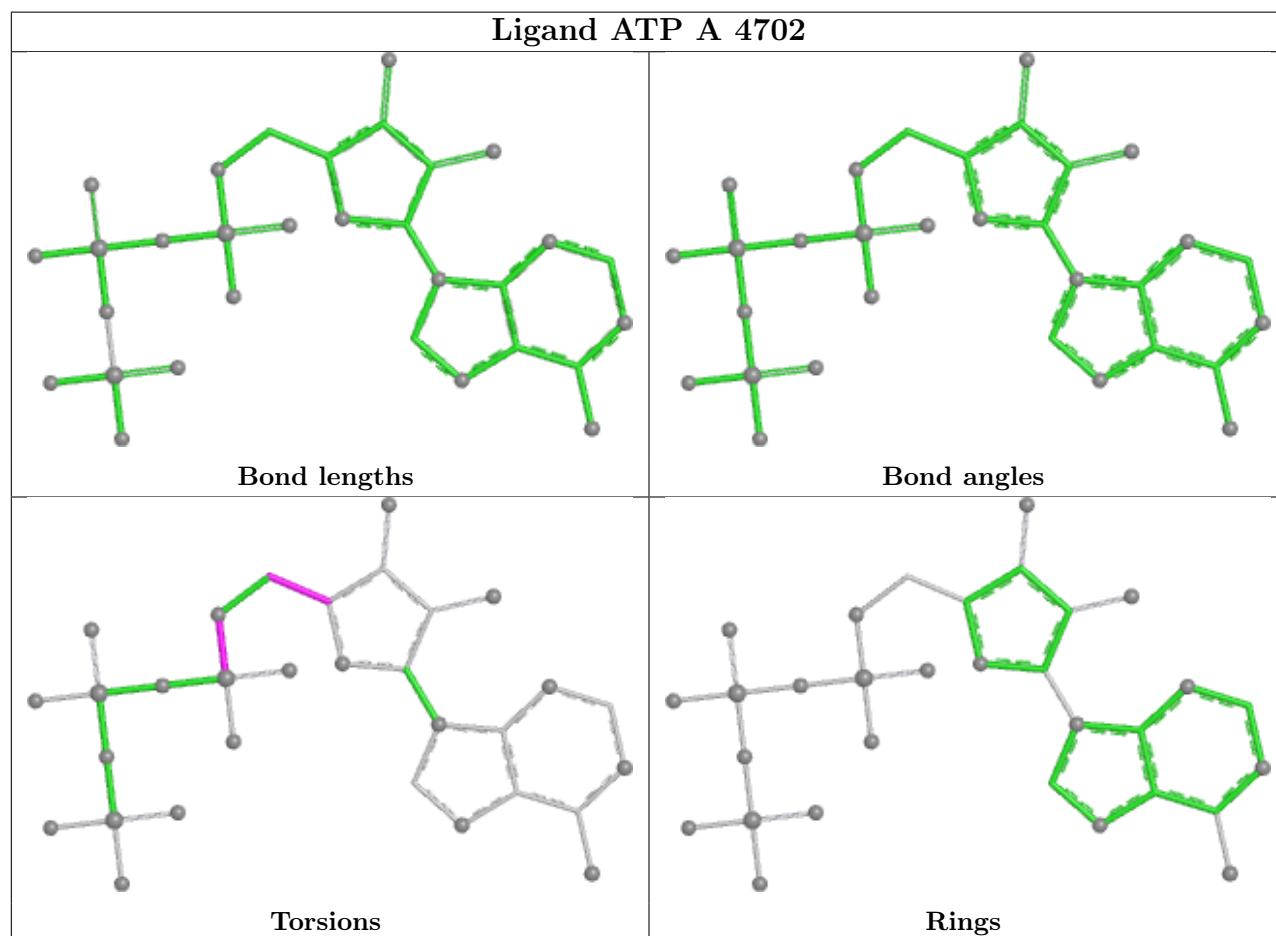
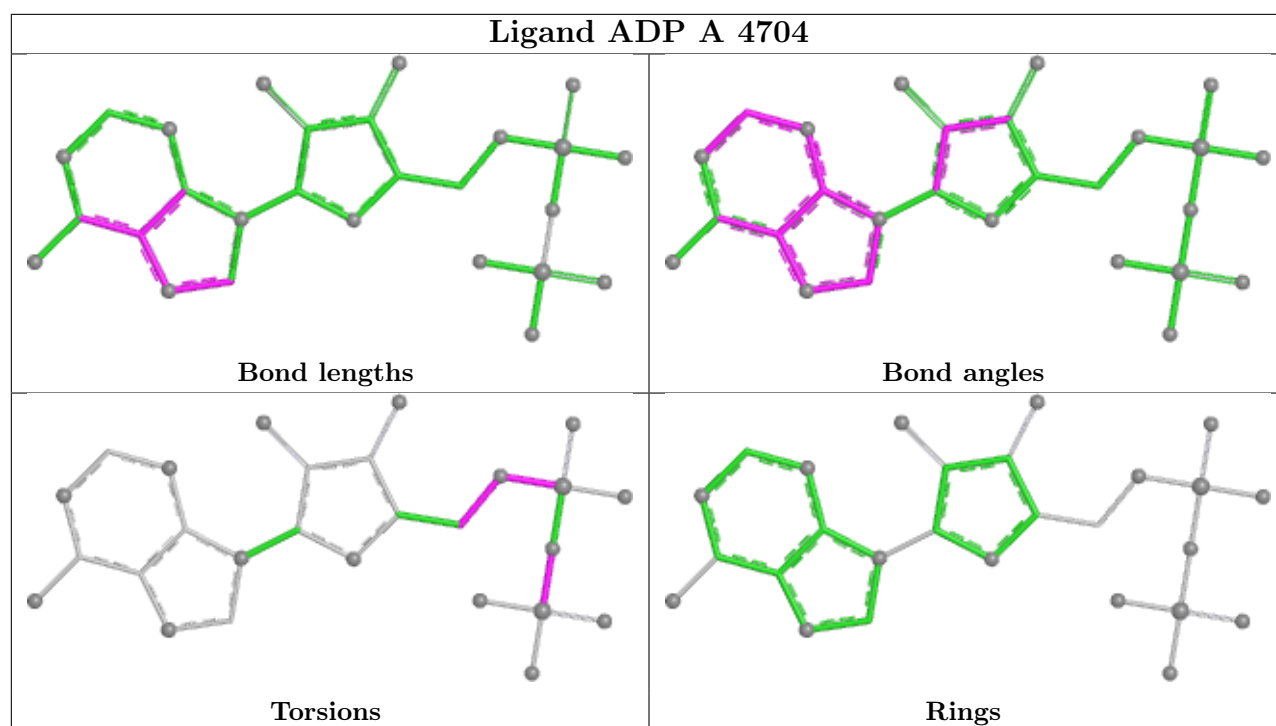
There are no ring outliers.

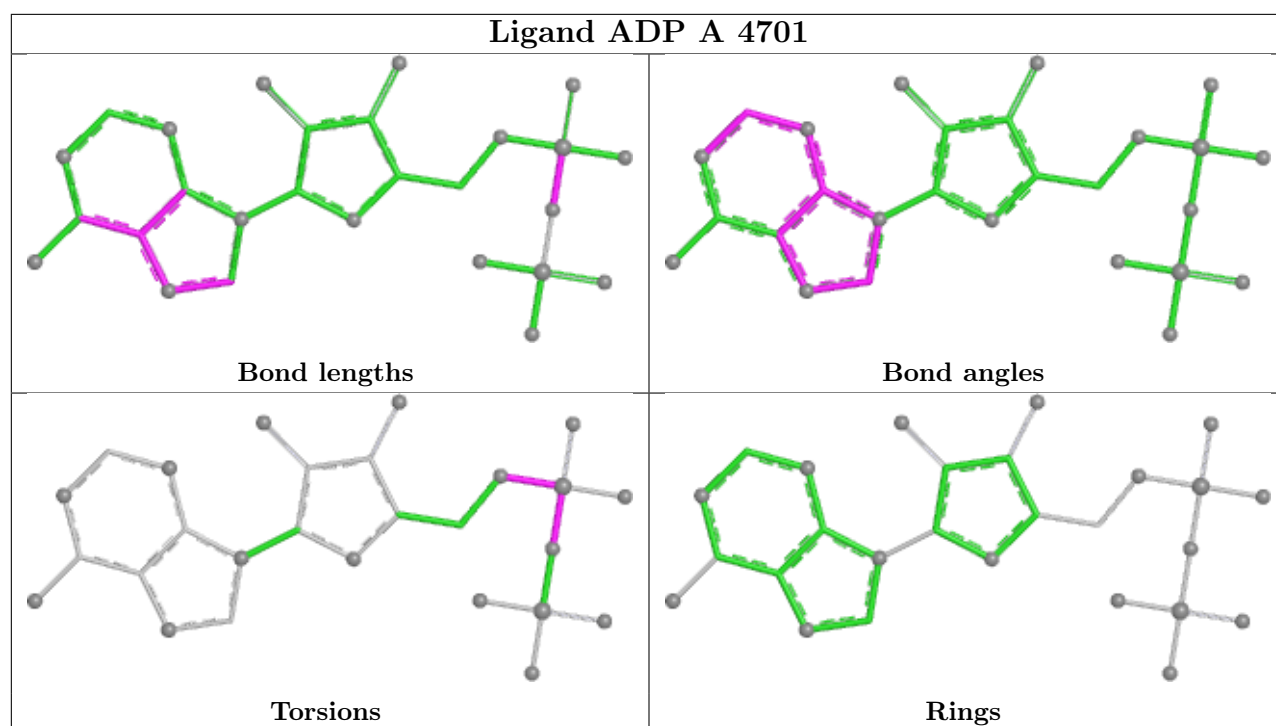
4 monomers are involved in 21 short contacts:

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

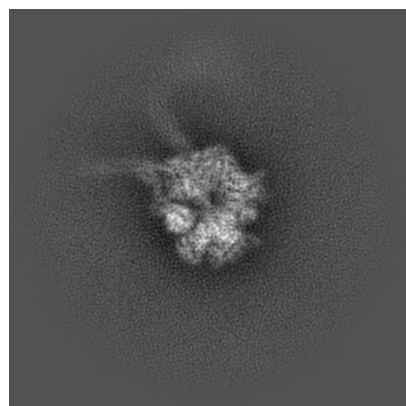
6 Map visualisation [i](#)

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.

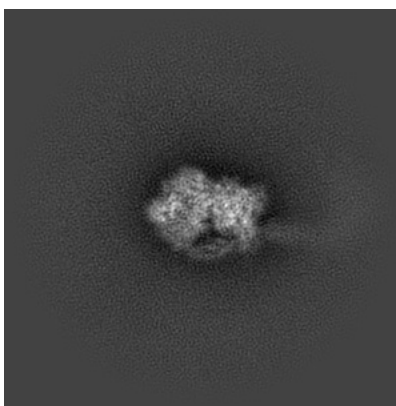
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

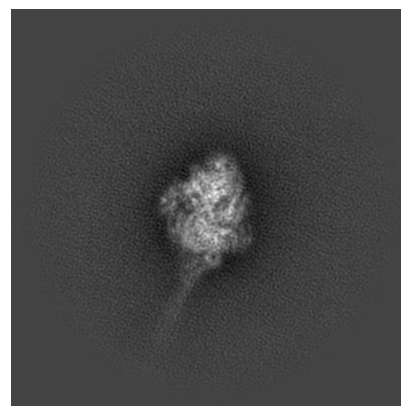
6.1.1 Primary map



X

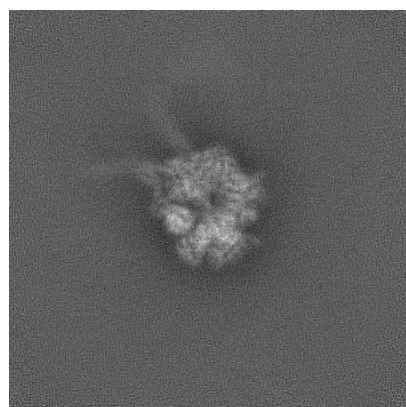


Y

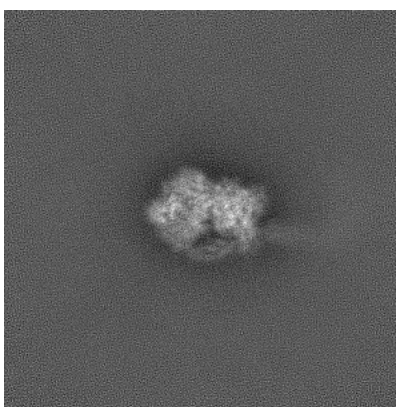


Z

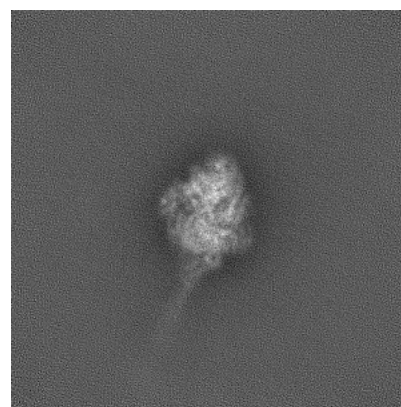
6.1.2 Raw map



X



Y

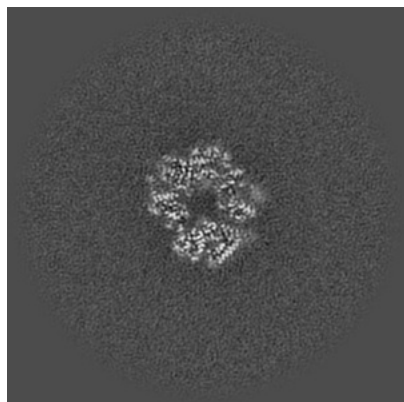


Z

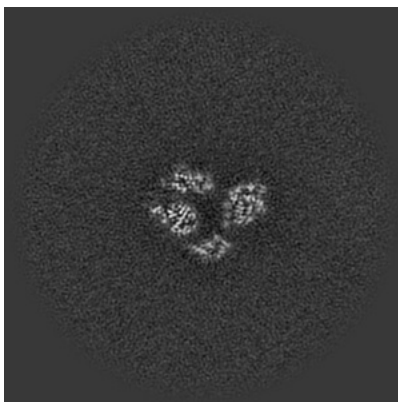
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

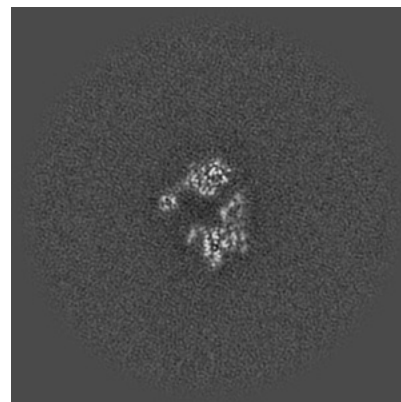
6.2.1 Primary map



X Index: 192

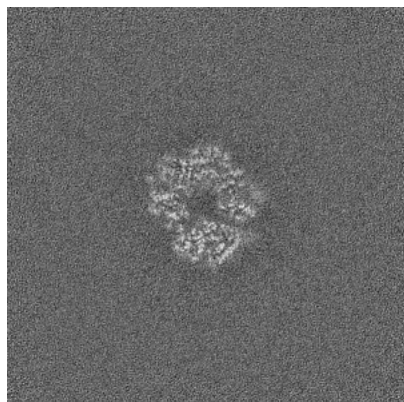


Y Index: 192

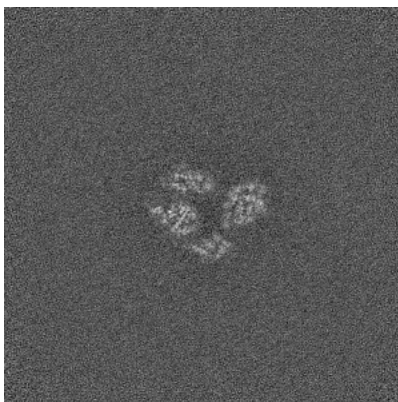


Z Index: 192

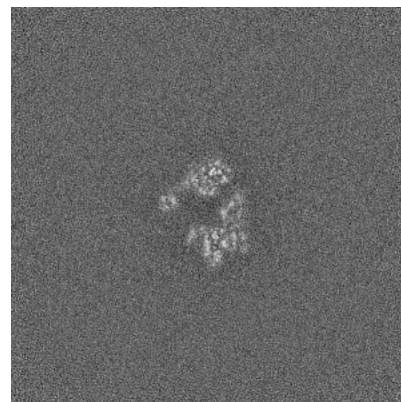
6.2.2 Raw map



X Index: 192



Y Index: 192

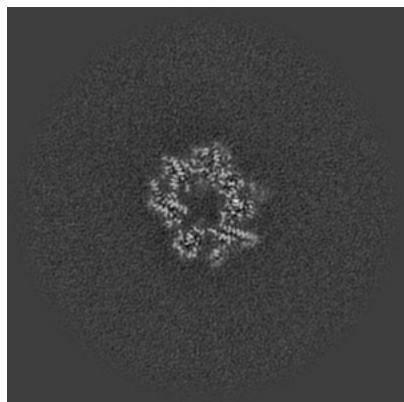


Z Index: 192

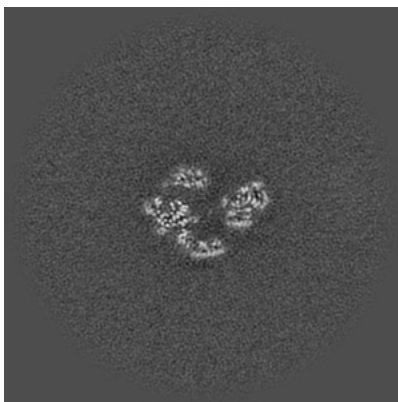
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

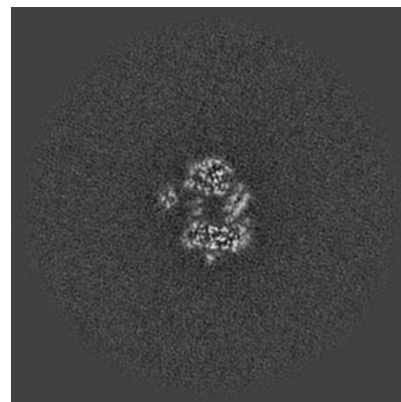
6.3.1 Primary map



X Index: 196

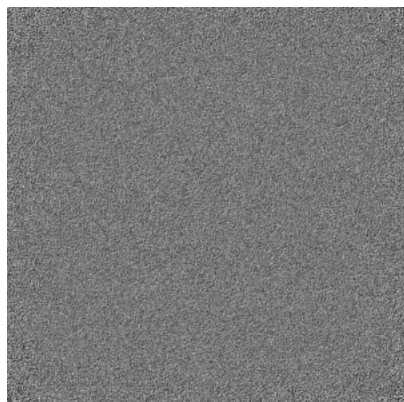


Y Index: 199

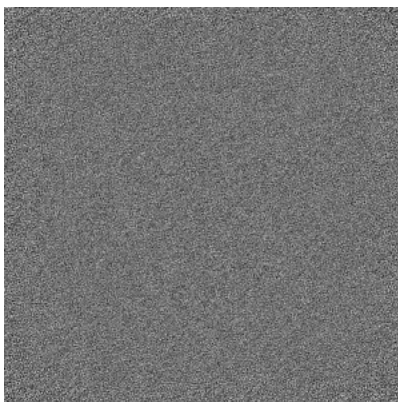


Z Index: 186

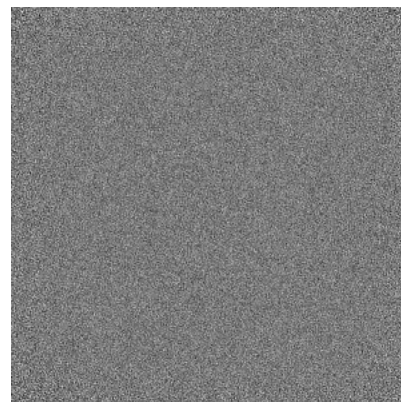
6.3.2 Raw map



X Index: 0



Y Index: 0

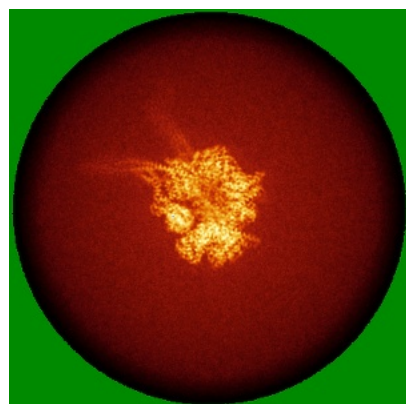


Z Index: 0

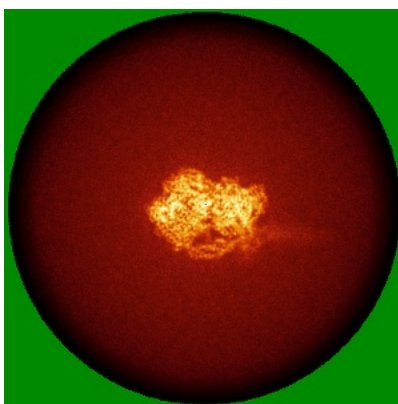
The images above show the largest variance slices of the map in three orthogonal directions.

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

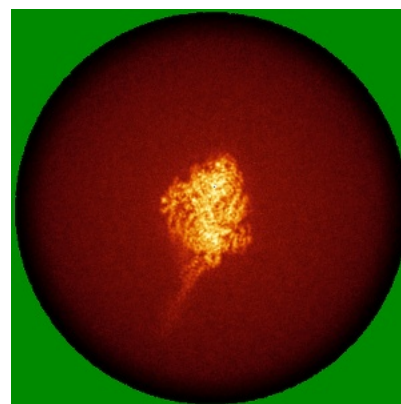
6.4.1 Primary map



X

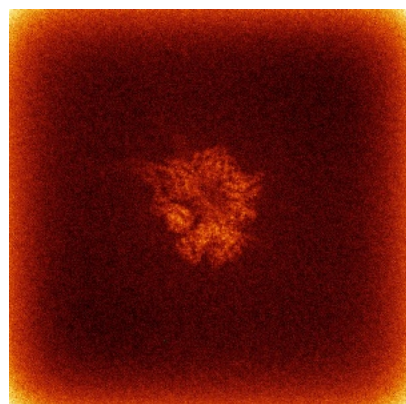


Y

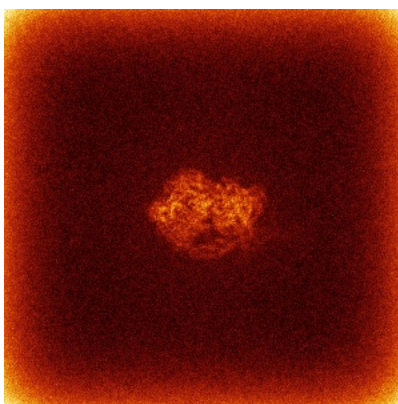


Z

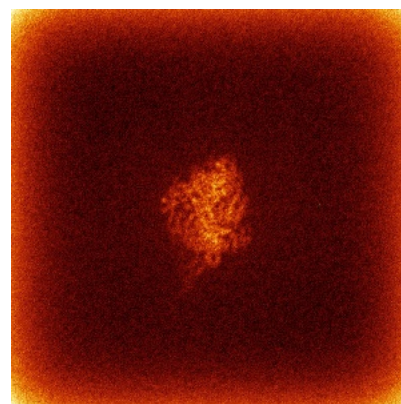
6.4.2 Raw map



X



Y

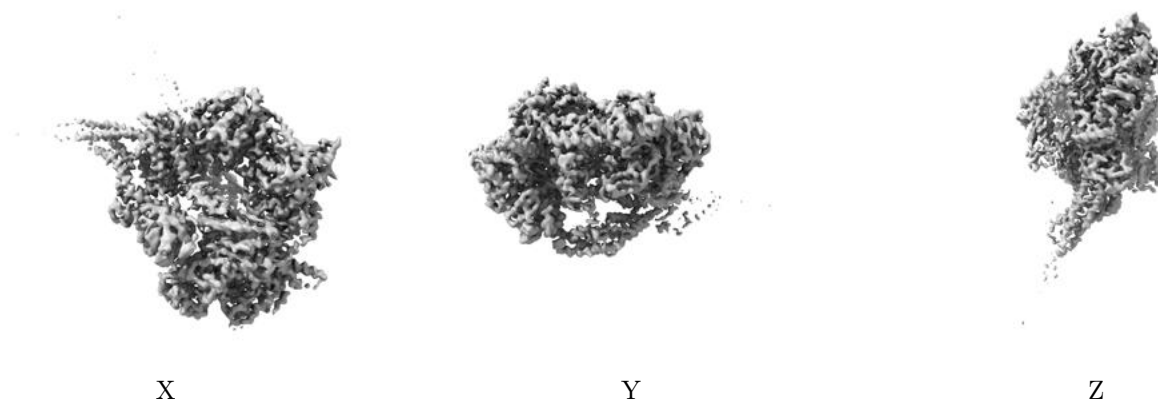


Z

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.

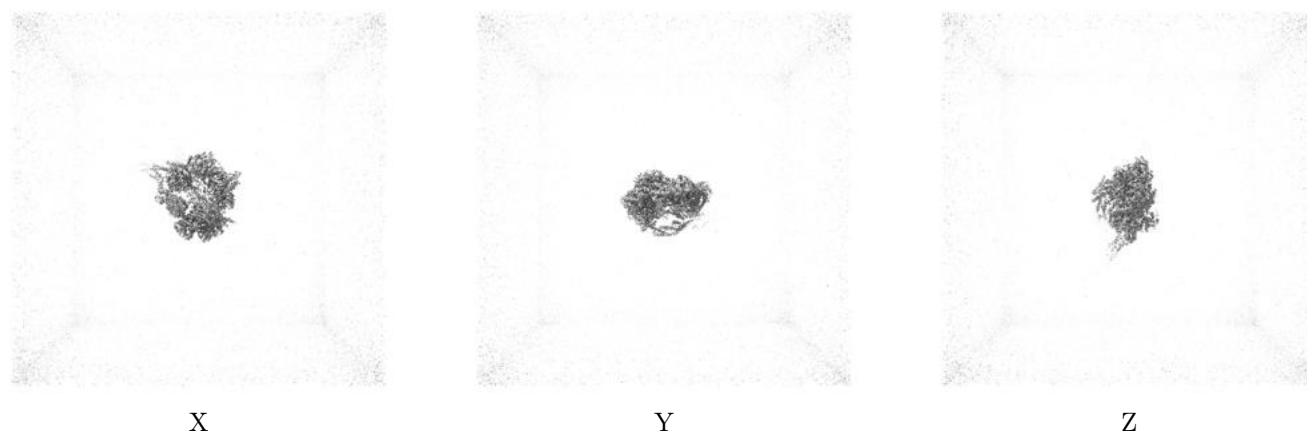
6.5 Orthogonal surface views [i](#)

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.

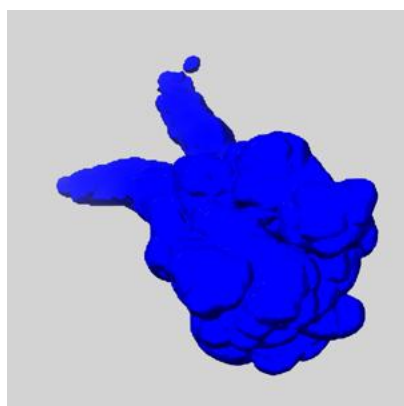
6.6 Mask visualisation [i](#)

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

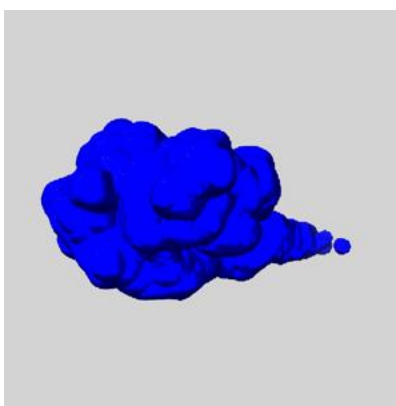
A mask typically either:

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

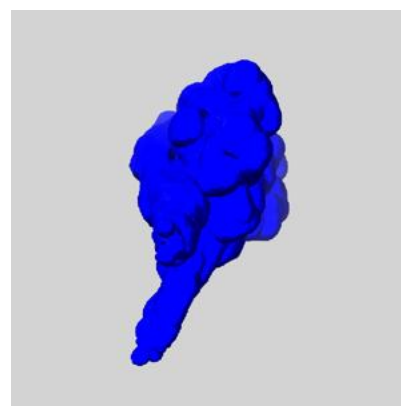
6.6.1 emd_46861_msk_1.map [i](#)



X



Y

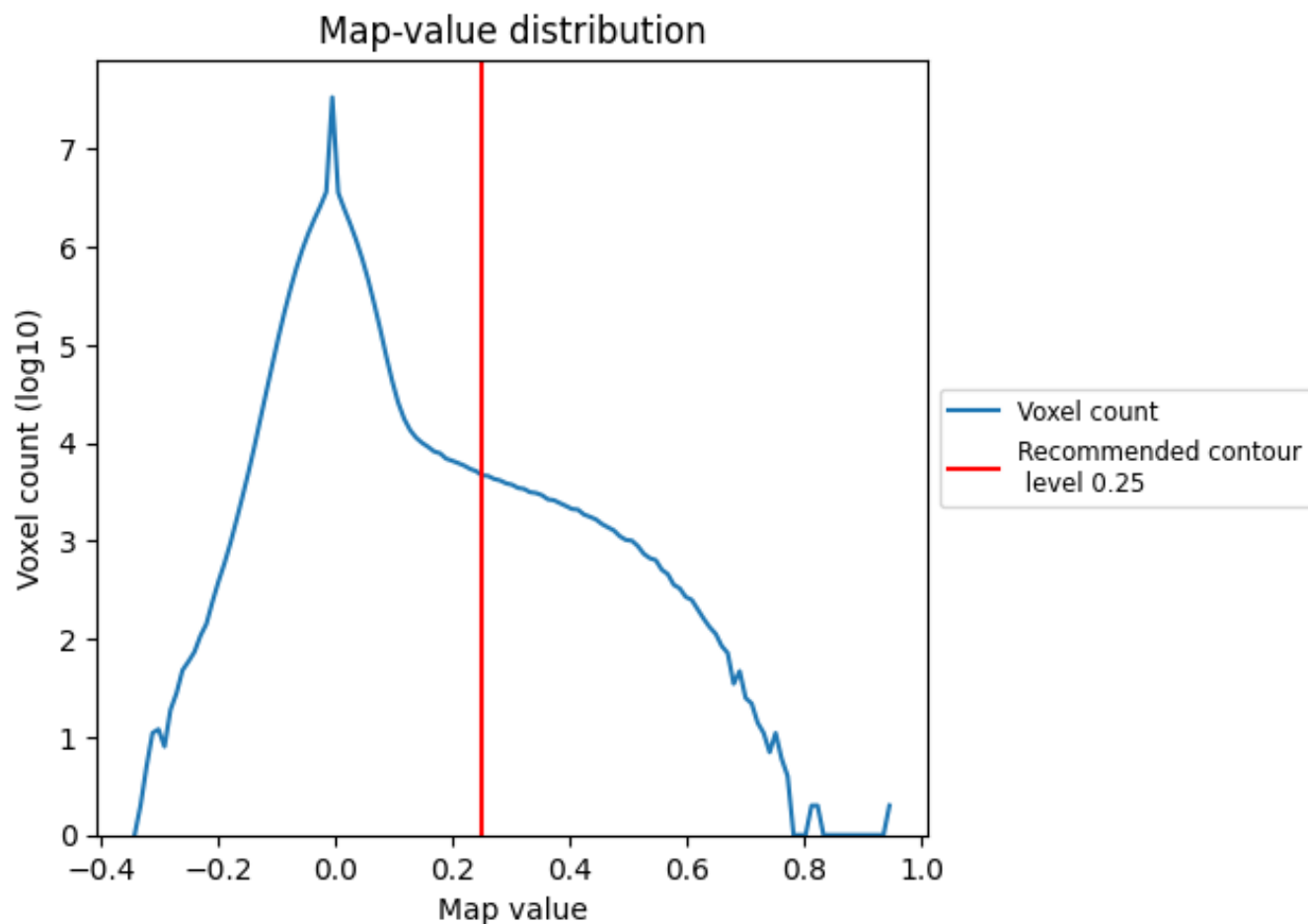


Z

7 Map analysis [i](#)

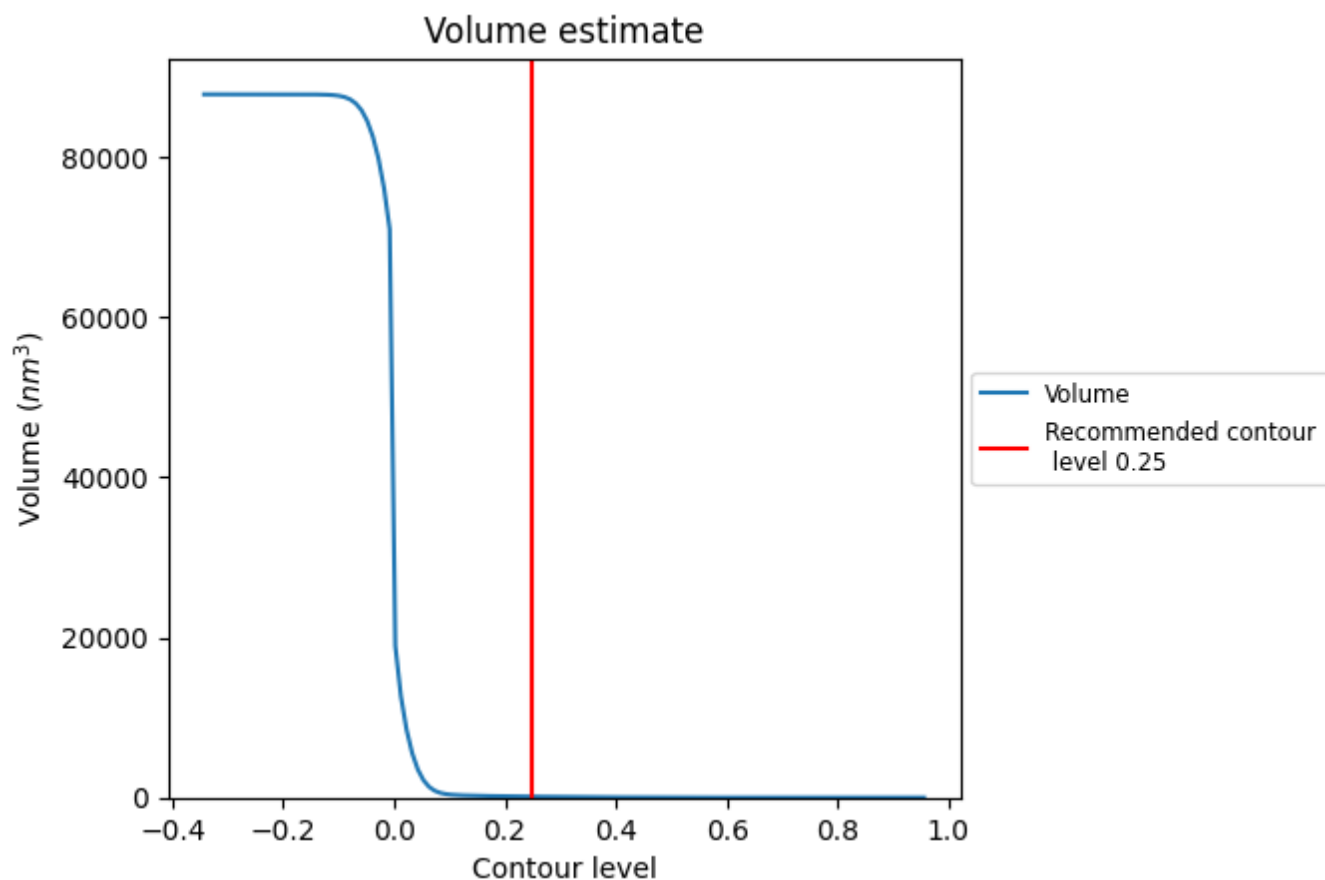
This section contains the results of statistical analysis of the map.

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.

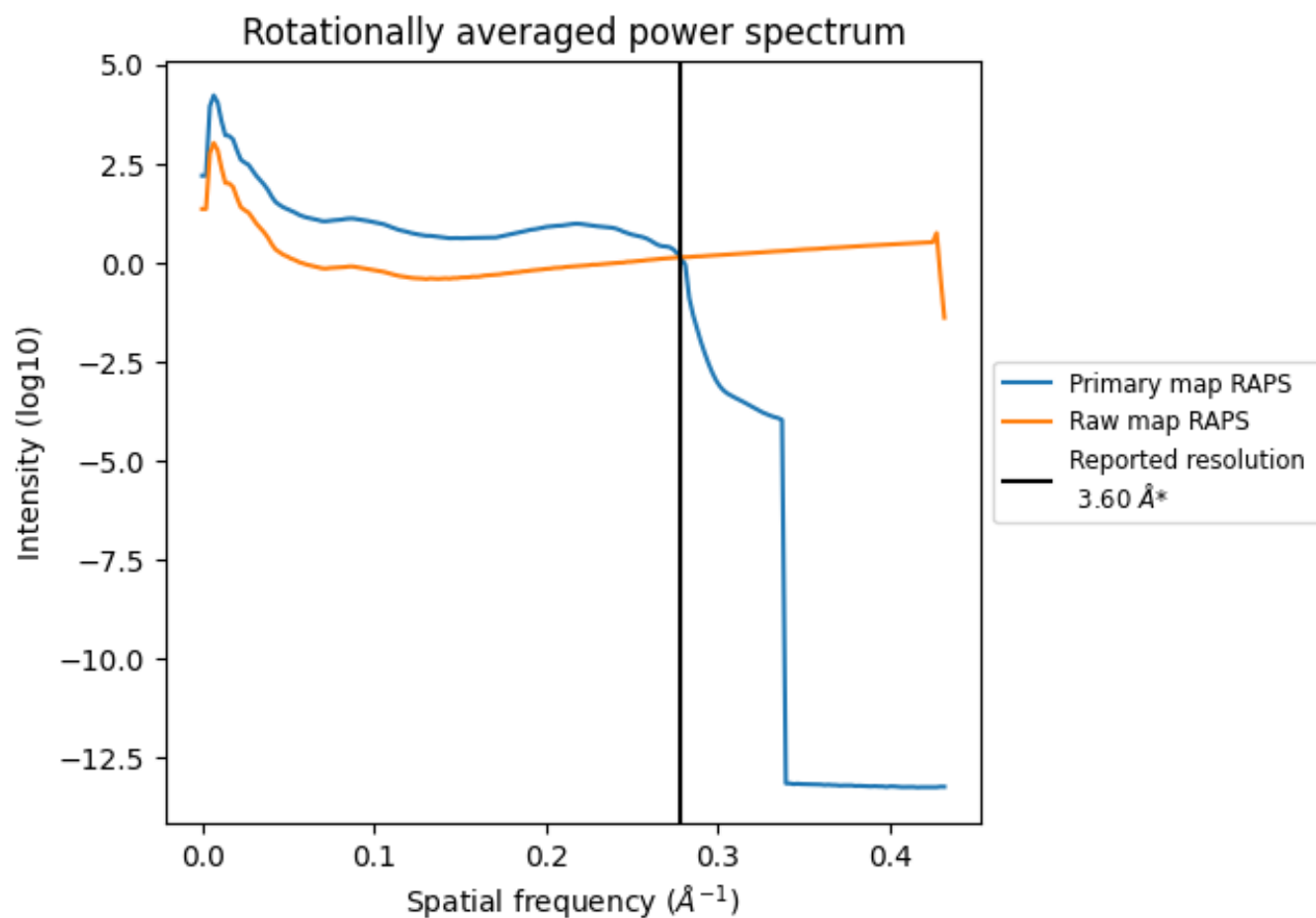
7.2 Volume estimate [i](#)



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 ⓘ

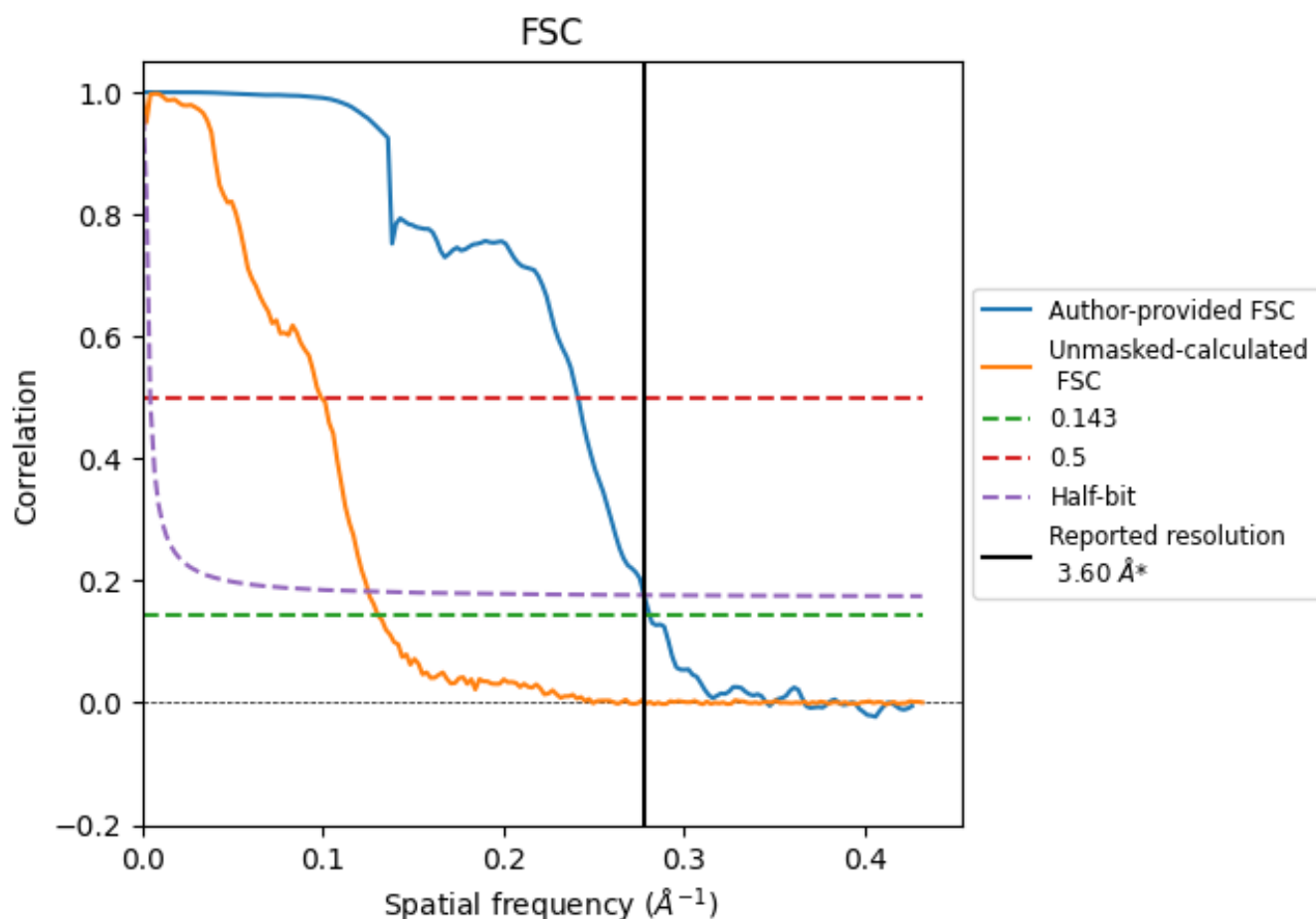


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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](#)

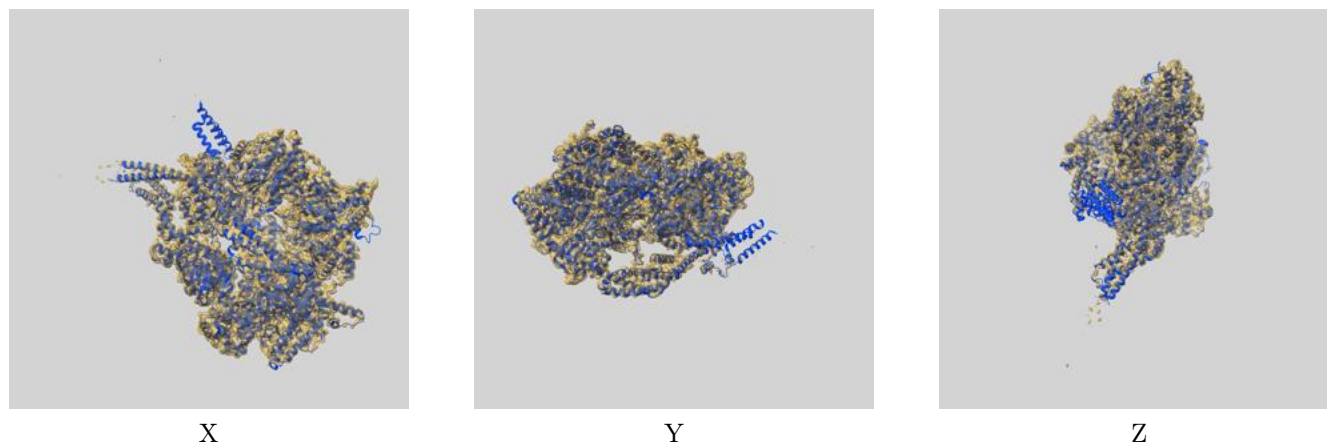
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	4.14	3.60
Unmasked-calculated*	7.65	10.09	7.99

*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](#)

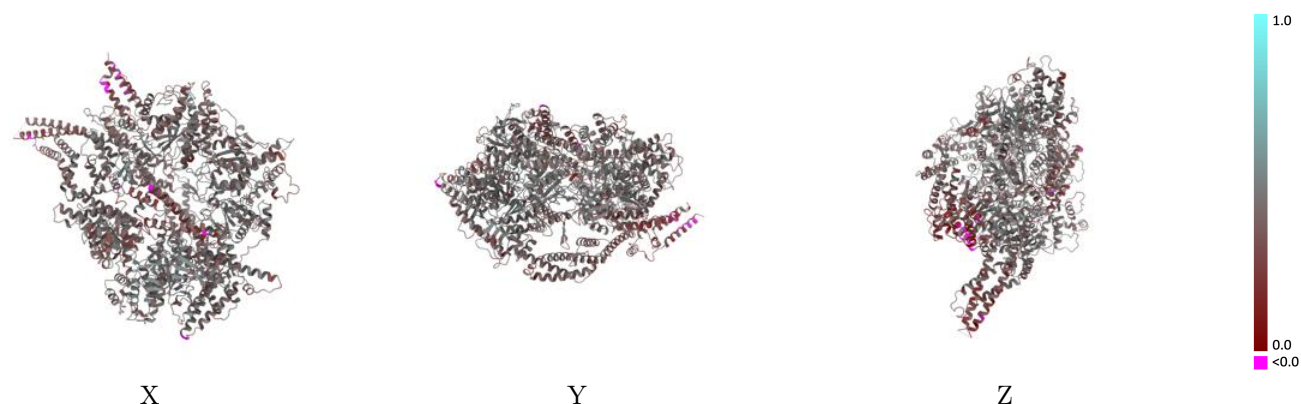
This section contains information regarding the fit between EMDB map EMD-46861 and PDB model 9DHA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



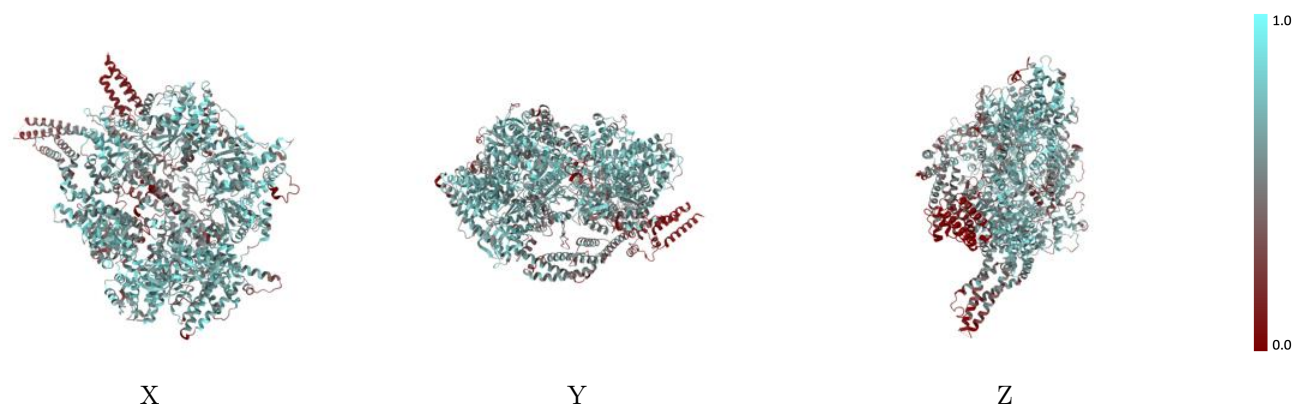
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



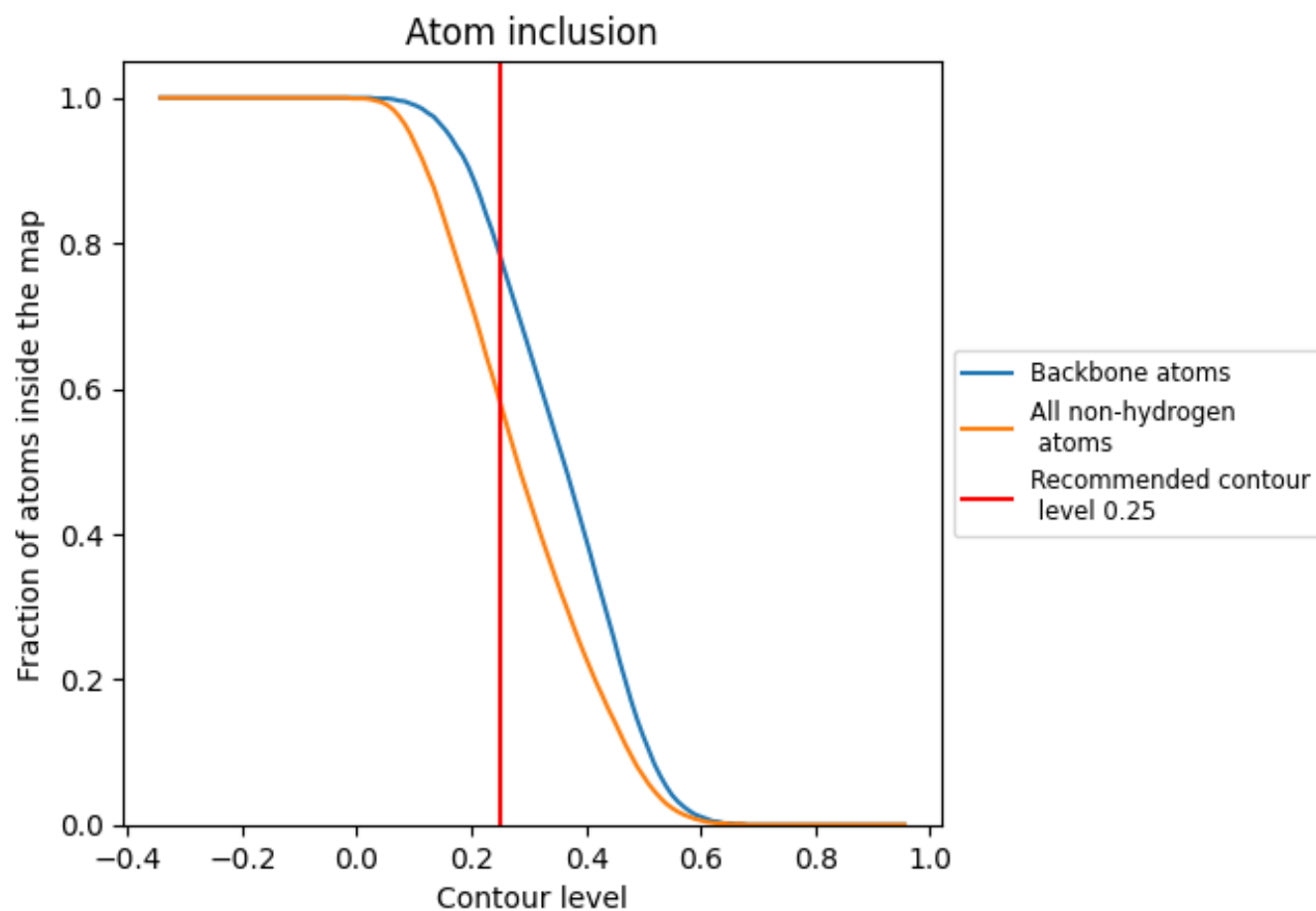
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.5810	0.4120
A	0.5810	0.4120

