



wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 10:43 PM EDT

PDB ID : 9BN4 / pdb_00009bn4
EMDB ID : EMD-44721
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class2
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.90 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

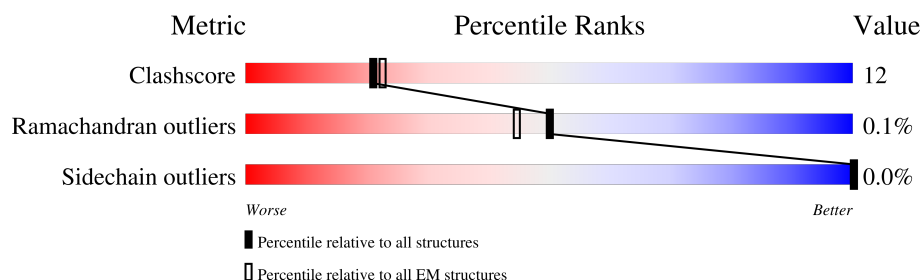
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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 3 unique types of molecules in this entry. The entry contains 23078 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.

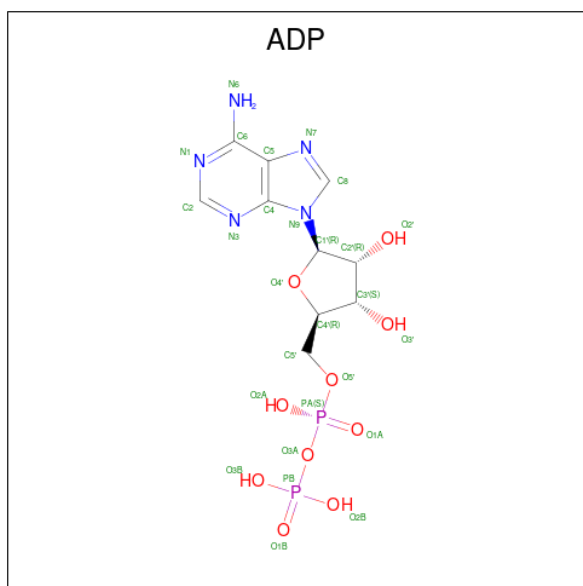
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2855	Total	C	N	O	S	0	0
			22962	14643	3963	4241	115		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

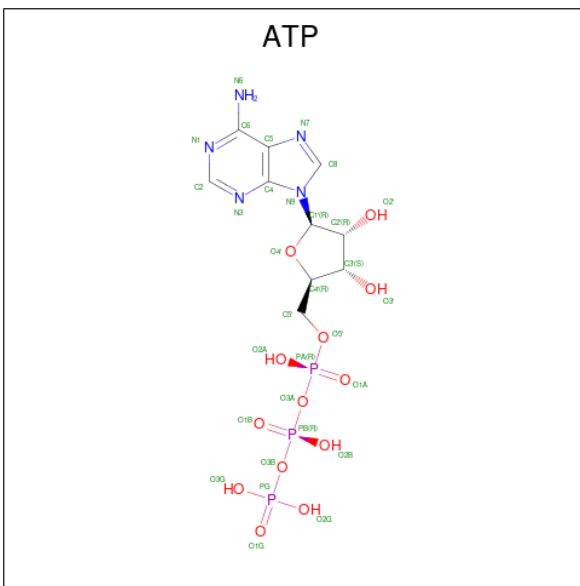
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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).

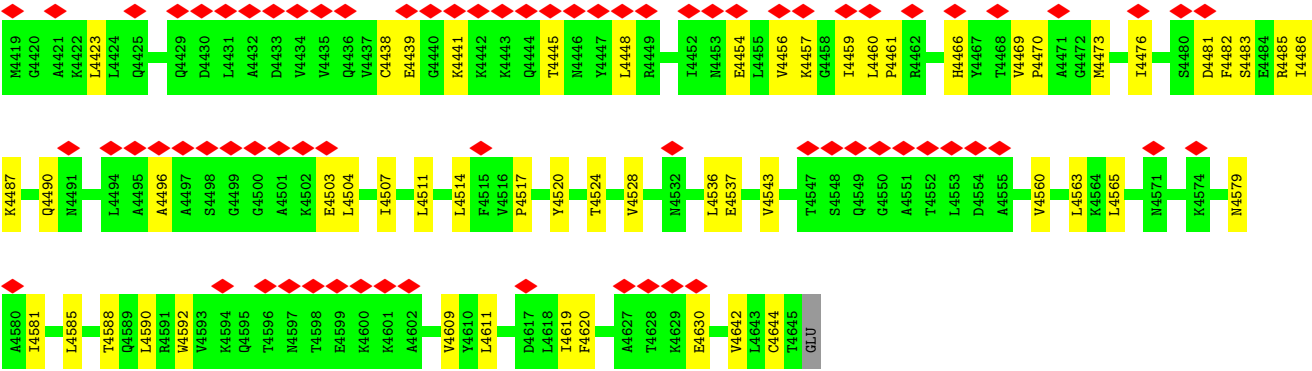


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

L1879	V1880	Q1881	T1882	P1883	L1884	R1887	M1892	L1900	G1901	G1902	S1903	P1907	E1914	L1923	G1924	R1925	D1933	E1934	D1937	F1938	Q1939	A1940	M1941	G1947	V1951	D1958	E1959	F1960	N1961	E1965	R1966	Q1976	C1977	I1978	Q1979	A1980	A1981	L1982	R1983	E1984	N1987	P1988	M1989	Y1990	D1991							
G1771	G1772	G1773	D1774	A1775	L1778	L1782	E1786	L1792	A1793	D1794	S1795	Q1800	R1804	R1805	R1806	K1807	L1808	E1809	H1810	I1811	I1812	R1823	S1824	L1825	K1827	D1831	N1832	F1836	E1837	W1838	L1839	R1843	K1849	V1853	L1854	Q1855	Q1856	L1857	N1867	Y1868	E1871	D1877	K1878									
L1575	L1576	A1577	K1580	K1581	V1582	K1584	S1585	P1586	L1587	V1588	M1589	D1590	V1591	L1592	N1593	I1594	Q1595	G1596	V1597	Q1598	R1599	S1600	L1601	E1602	R1603	L1604	A1605	D1606	L1607	L1608	I1611	Q1612	K1613	L1619	E1620	R1623	F1629	Y1630	F1631	V1632	G1633	D1634	E1635	D1636	L1637	L1638	E1639	I1640	K1646	A1648	K1649	
S1503	V1504	A1505	A1506	M1507	K1508	L1509	S1510	P1511	Y1512	Y1513	K1514	V1515	F1516	E1517	E1518	D1519	A1520	L1521	S1522	V1523	E1524	D1525	K1526	L1527	M1528	R1529	I1530	L1533	F1534	D1535	V1536	D1539	Q1541	Y1546	I1550	G1553	S1554	A1555	D1556	I1557	K1558	H1559	L1560	L1561	P1562	V1563	E1564	R1567	I1571	E1574		
LYS	ASN	GLU	ALA	ILE	VAL	LYS	ASP	VAL	GLN	GLY	GLU	ALA	GLU	PHE	L1463	K1464	Q1465	L1466	R1467	E1468	Y1469	W1470	N1471	T1472	Y1473	E1474	L1475	D1476	L1477	Y1478	N1479	Y1480	Q1481	N1482	K1483	C1484	R1485	L1486	I1487	D1491	L1492	L1493	F1494	N1495	K1496	V1497	K1498	E1499	H1500	I1501	M1502	
ALA	SER	TYR	GLU	PHE	VAL	GLN	ARG	GLY	TYR	MET	LYS	GLU	ILE	GLU	GLY	GLN	ILE	GLU	GLY	GLU	ASP	PRO	TRP	SER	GLN	GLU	ALA	LYS	ARG	GLN	ASN	TRP	ASP	VAL	VAL	GLU	GLY	ILE	TRP	LEU	GLN	ILE	TRP	ALA	ASP	VAL	ASP	GLN	GLN			
VAL	ALA	GLU	GLU	GLU	LEU	GLN	ASP	LEU	LYS	VAL	SER	GLU	TRP	SER	GLU	GLU	ALA	GLN	LEU	ILE	GLU	GLN	TRP	SER	VAL	VAL	GLN	GLU	ARG	GLN	ASN	GLU	ALA	LEU	LEU	VAL	VAL	SER	PHE	GLN	ILE	PRO	ALA	LEU	ARG	GLU	ARG	GLN	TYR			
TRP	GLU	LYS	THR	LYS	PRO	VAL	THR	THR	VAL	ARG	PRO	GLU	ILE	GLU	GLU	ALA	GLN	LEU	GLY	PHE	GLY	ARG	ASP	GLY	LYS	ASP	GLN	THR	ILE	LYS	GLN	LYS	ASP	GLU	ALA	LEU	LEU	THR	GLY	LEU	LEU	GLY	THR	ARG	GLY	THR	VAL	GLN				
ARG	PHE	GLN	PHE	PRO	PRO	SER	TRP	SER	TRP	ASN	ILE	GLU	GLY	THR	PHE	PHE	ASN	ASP	THR	THR	THR	ILE	ASP	GLY	THR	VAL	GLN	GLN	GLN	GLN	LYS	ASP	GLU	VAL	GLU	GLU	GLU	GLU	SER	ASN	GLY	THR	ARG	GLY	THR	THR	ASP					
GLU	LEU	ARG	ILE	THR	ASN	GLN	VAL	VAL	GLN	ASN	PRO	PRO	LEU	THR	LEU	VAL	ARG	GLY	THR	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL		
ASN	ALA	LEU	THR	MET	PRO	MET	ASP	GLY	THR	ALA	GLU	GLU	THR	LYS	VAL	MET	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
GLU	LEU	ARG	ILE	THR	ASN	GLN	VAL	VAL	GLN	ASN	PRO	PRO	LEU	THR	LEU	VAL	ARG	GLY	THR	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
ASN	LYS	LEU	ASP	MET	GLY	ILE	GLU	ILE	GLU	VAL	ARG	GLU	VAL	GLN	ALA	VAL	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
PHE	ASN	PHE	GLN	LYS	VAL	VAL	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP

K1992	T1993	S1994	A1995	P1996	C1999	E2000	L2001	L2002	N2003	K2004	G2005	V2006	M2012	I2016	T2017	N2018	N2019	PRO	GLY	TYR	ALA	GLY	ARG	SER	ASN	L2028	P2029	I2030	N2031	L2035	F2036	R2037	S2038	L2039	A2040	M2041	T2042	L2048	I2049	V2052	N2053	F2059	R2060	E2063	V2064	L2065	A2066	N2067	V2068	L2069				
K2074	L2075	Q2079	A2092	L2093	K2094	S2099	L2100	A2100	G2101	N2102	K2004	R2105	E2106	R2107	R2113	E2114	LVS	GLU	GLU	ARG	GLY	ALA	GLU	VAL	ASP	GLU	GLY	I2127	A2128	E2129	E2135	S2140	M2145	L2149	L2157	L2160	Q2169	Y2170	H2171	R2172	Q2173	E2174	M2175	G2194	N2195	G2196	E2197							
E2198	W2203	V2204	K2206	V2207	L2208	Q2209	Y2211	Q2212	L2213	T2214	Q2215	T2216	L2220	M2221	G2227	K2230	S2231	W2234	L2237	L2241	K2257	S2260	D2262	R2263	L2264	Y2265	G2266	T2267	N2271	L2284	S2290	V2291	R2292	G2293	E2294	L2295	Q2296	K2297	Q2298	Q2299	W2300	V2307	D2308											
P2309	E2310	W2311	D2320	D2321	L2324	P2328	R2332	P2336	N2338	V2339	M2342	R2343	E2344	Q2346	D2347	K2349	Y2350	A2351	T2352	R2358	F2364	S2370	T2371	D2372	L2382	R2383	P2386	D2389	GLY	ASP	GLU	ALA	GLN	ARG	ARG	LVS	GLY	LVS	GLU	ASP	V2307	D2308												
GLU	GLU	ALA	S2410	L2413	Q2416	A2420	M2423	Q2424	P2425	T2426	S2429	G2431	H2439	Q2442	H2445	I2446	M2447	D2448	L2449	L2452	R2453	C2454	S2457	M2461	L2462	Y2472	D2478	F2479	P2480	M2481	E2484	R2488	R2492	V2495	L2498	L2499	W2500	S2501	L2502															
S2503	G2504	D2505	S2506	R2507	L2508	K2509	M2510	L2514	T2522	T2523	V2524	P2525	L2526	T2527	T2528	A2529	P2530	N2531	T2532	E2544	V2545	P2565	D2566	D2573	R2576	L2581	T2582	T2583	P2590	L2593	C2594	G2595	P2596	K2601	T2602	L2605	F2606	L2609	P2613	D2614	M2615	E2616	V2617											
N2621	F2622	S2623	T2626	T2627	P2628	E2629	H2637	Y2638	T2644	P2645	N2646	G2647	V2648	P2652	V2653	Q2654	K2657	W2658	L2659	F2662	C2663	D2664	E2665	L2666	P2667	L2668	P2669	D2670	F2682	M2686	T2689	V2701	R2705	V2709	C2712	N2713	P2714	R2720	K2721	R2729	H2730	V2731	P2732	V2733										
V2734	S2743	L2744	T2747	F2751	N2752	R2753	A2754	M2755	L2756	R2757	L2758	T2759	P2760	S2761	L2762	R2763	T2764	Y2765	A2766	E2767	P2768	L2769	A2772	M2773	V2774	E2775	E2782	R2783	F2784	T2785	Q2786	T2787	T2788	Q2789	P2790	H2791	T2792	T2793	Y2794	S2795	P2796	E2798	M2799	T2800	W2802	V2803	R2804	E2814	T2815	L2816	P2817			
V2818	E2819	G2820	L2821	T2822	R2823	D2840	R2844	L2855	K2856	H2857	P2858	P2859	N2860	T2861	D2862	R2863	E2864	K2865	A2866	M2867	S2868	R2869	T2870	L2871	L2872	S2874	N2875	W2876	L2877	S2878	K2879	P2883	V2884	D2885	Q2886	E2887	E2888	D2891	Y2892	R2896	L2897	K2898	V2899	E2902	E2903	D2906	L2909	L2911						
V2915	H2918	L2922	L2925	F2926	R2927	Q2928	P2929	Q2930	G2931	L2932	L2933	L2934	K2943	T2944	R2948	M2953	S2957	R2965	K2966	G2969	E2970	L2976	R2977	T2978	V2979	L2980	R2981	M2987	E2988	K2989	I2990	A2991	F2992	D2995	E2996	S2997	M2998	S3002	G3003	F3004	L3005	E3006	F3007	M3008										
L3011	L3012	E3022	G3023	D3024	E3025	Y3026	A3027	T3028	L3029	K3030	T3031	K3034	E3035	Q3038	K3039	E3040	G3041	L3042	K3043	L3044	D3045	S3046	H3047	E3048	E3049	T3055	T3059	R3060	L3061	A3062	K3064	P3070	SER	GLU	GLY	LEU	LVS	ASP	ARG	ALA	THR	S3082	N3087	R3088	L3091	F3094	W3097							
M3113	N3119	D3124	Y3125	V3128	V3129	Y3130	D3131	K3132	L3133	Q3134	Q3135	P3136	P3137	R3140	V3144	N3145	F3149	V3150	H3151	H3155	Q3156	A3157	N3158	A3159	R3160	L3161	A3162	K3163	G3166	R3167	T3168	M3169	P3173	R3174	H3175	Y3176	E3189	K3190	R3191	S3192	L3193	L3194	E3195	Q3198	M3199	H3200	L3201							
N3202	V3203	G3204	L3205	R3206	K3207	T3208	K3209	E3210	T3211	V3212	D3213	Q3214	V3215	E3216	E3217	L3218	R3219	R3220	ASP	LEU	ARG	ILE	LVS	SER	GLN	GLU	LEU	VAL	LVS	ASN	ALA	ALA	ALA	ASN	ASP	LVS	LEU	GLY	LYS	VAL	ASP	GLN	GLU	ALA	GLU	LYS	LYS	VAL	MET	SER	GLN	GLU	ILE	GLN





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91718	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-1.197	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1458, 1.1458, 1.1458	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	1/23454 (0.0%)	0.39	8/31791 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2328	PRO	CG-CD	-6.02	1.30	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2328	PRO	N-CD-CG	-11.60	85.79	103.20
1	A	2328	PRO	CA-N-CD	-10.21	97.70	112.00
1	A	2714	PRO	N-CD-CG	-8.44	90.54	103.20
1	A	2714	PRO	CA-CB-CG	-7.95	89.40	104.50
1	A	2714	PRO	CA-N-CD	-7.19	101.93	112.00

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	22962	0	23030	537	0
2	A	54	0	24	2	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	62	0	24	0	0
All	All	23078	0	23078	537	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 537 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:2925:ILE:HG13	1:A:2933:LEU:HD13	1.59	0.85
1:A:2929:PRO:HB3	1:A:3060:ARG:HA	1.56	0.85
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.10	0.85
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.61	0.82
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.59	0.82

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	2841/4646 (61%)	2765 (97%)	72 (2%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	1730	ALA
1	A	2871	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	2540/4125 (62%)	2539 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	2637	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4079	GLN
1	A	4262	GLN
1	A	4612	ASN
1	A	2689	HIS
1	A	2677	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](#)

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	4701	-	24,29,29	0.88	0	29,45,45	1.24	2 (6%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
3	ATP	A	4703	-	28,33,33	0.67	0	34,52,52	0.60	1 (2%)
3	ATP	A	4702	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	5/18/38/38	0/3/3/3
3	ATP	A	4702	-	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4704	ADP	N3-C2-N1	-3.58	123.81	128.67
2	A	4704	ADP	C4-C5-N7	-2.63	106.56	109.34
2	A	4701	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4702	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

5 of 18 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

Continued on next page...

Continued from previous page...

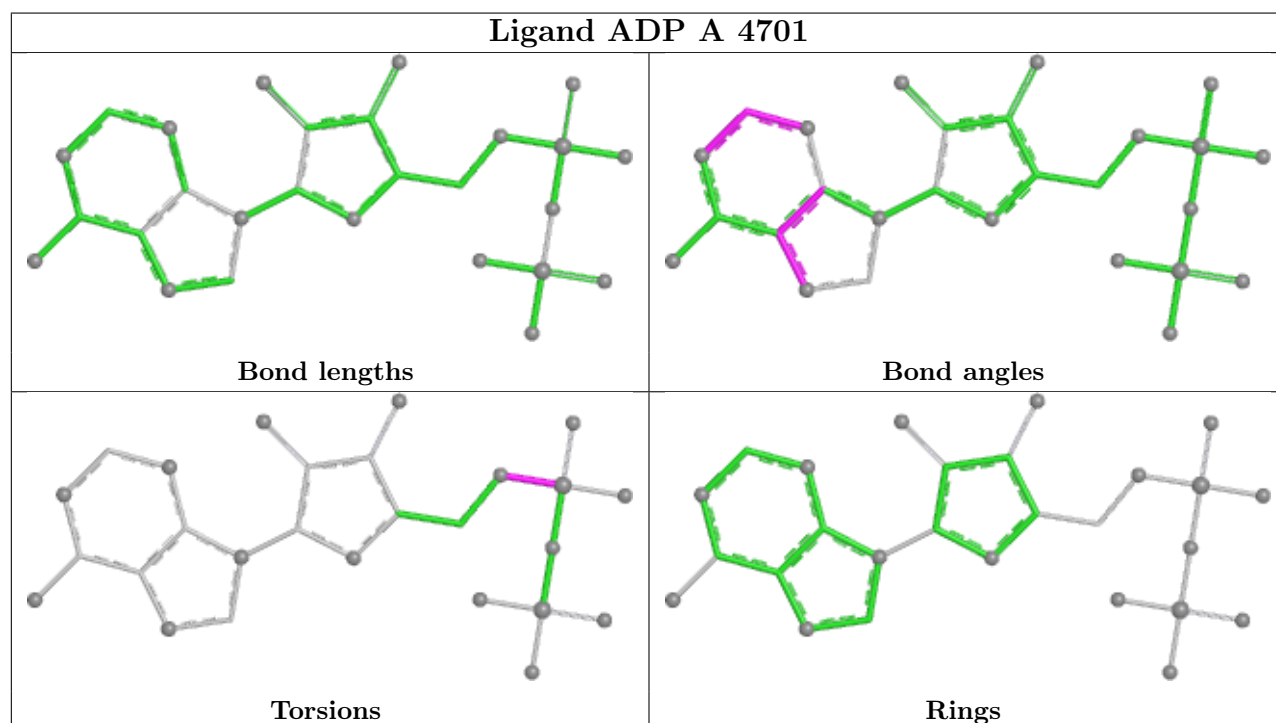
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'

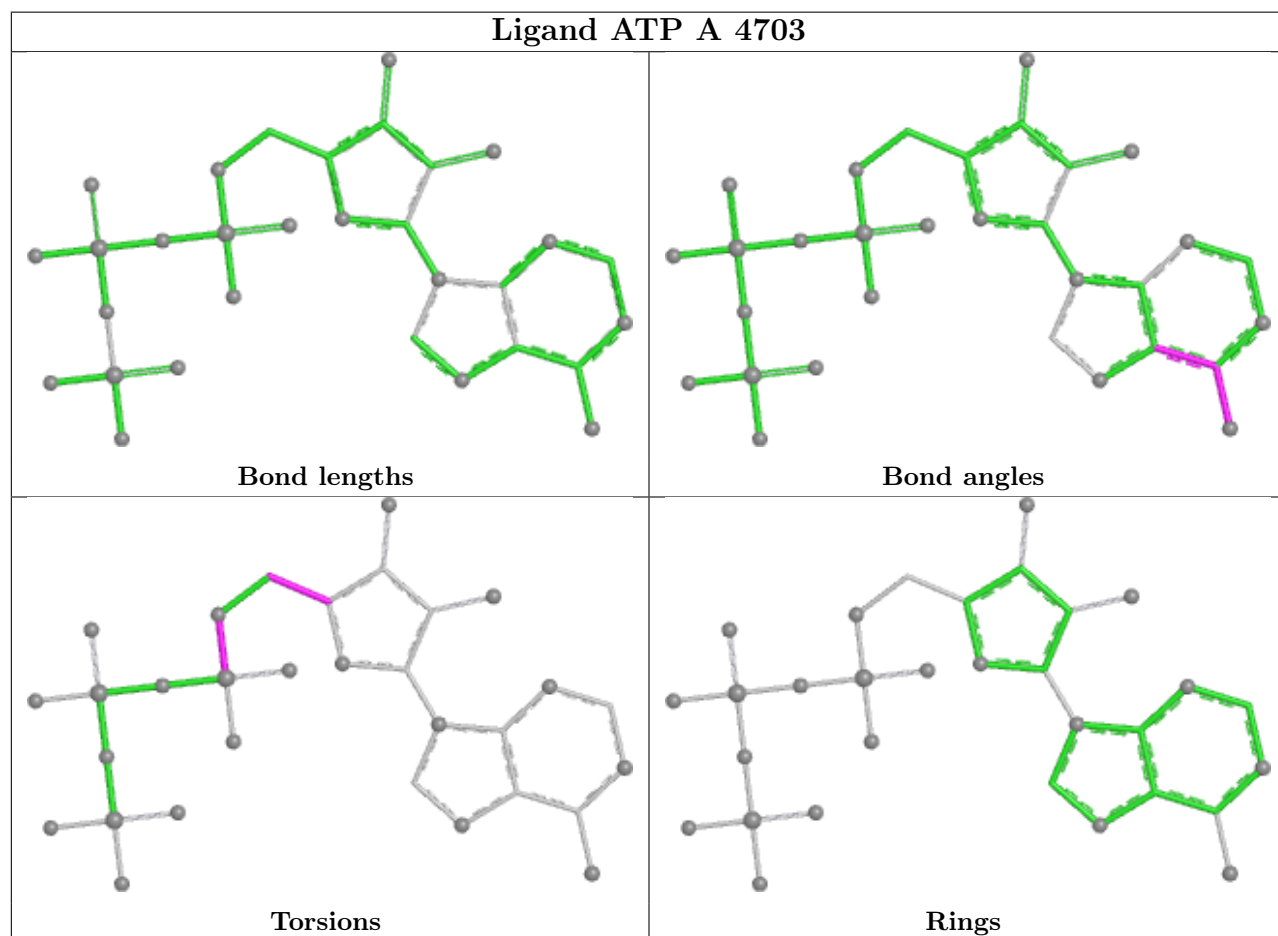
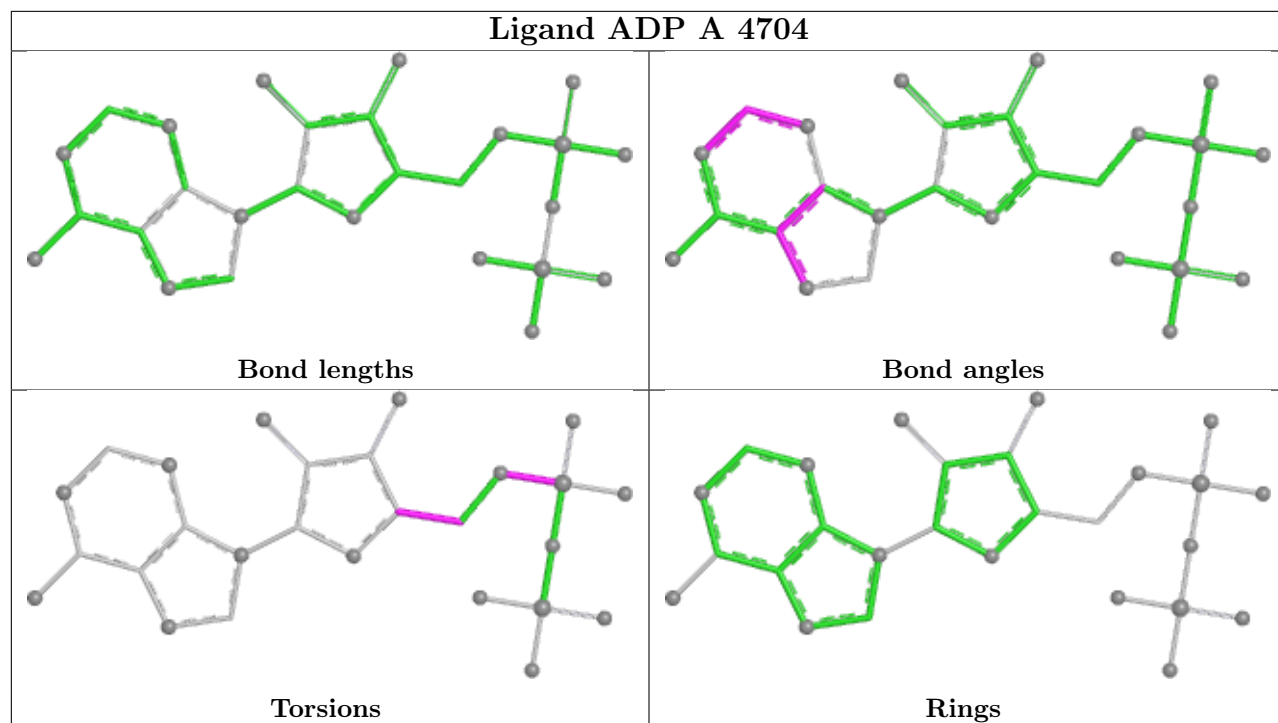
There are no ring outliers.

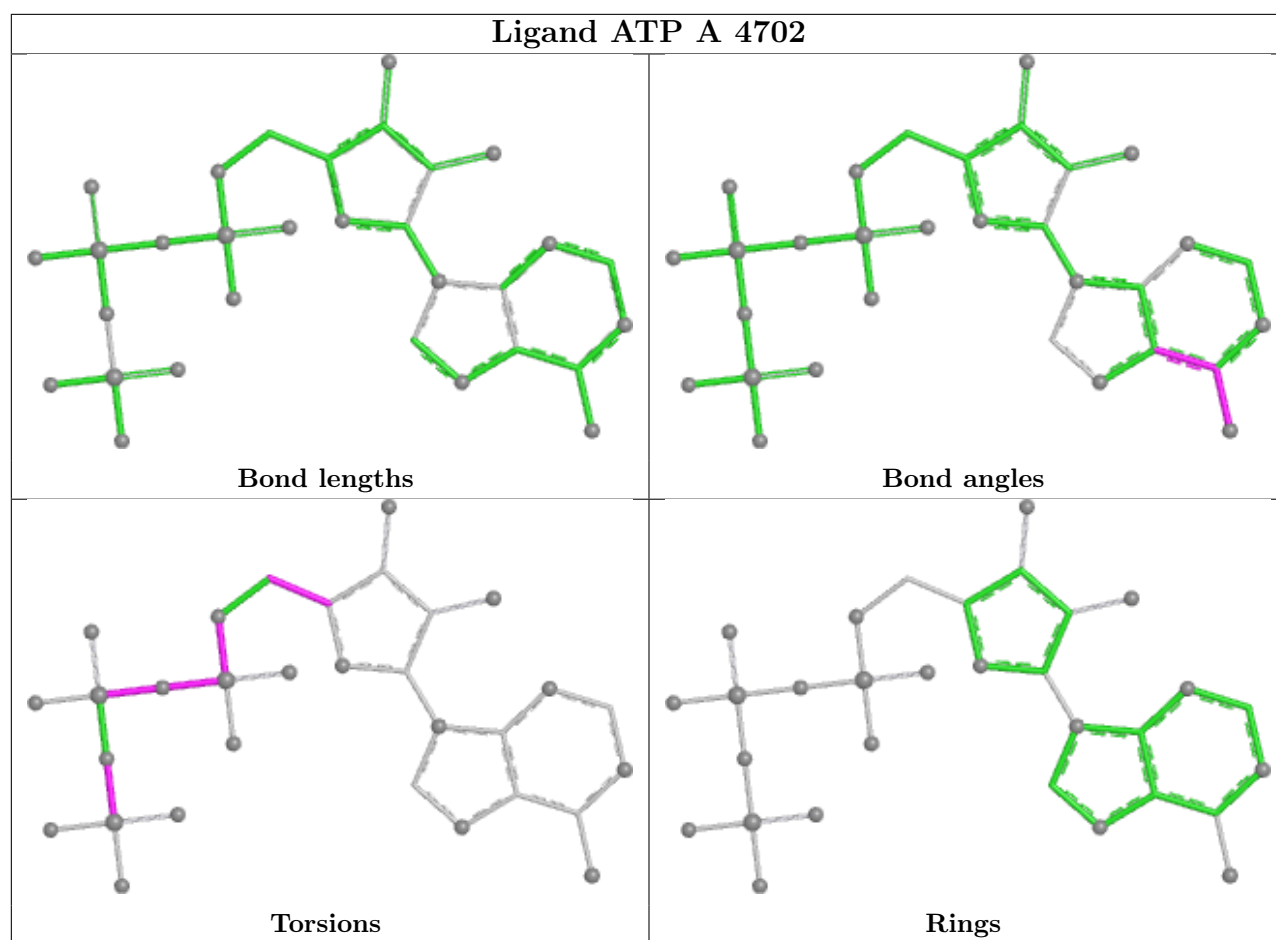
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
2	A	4704	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

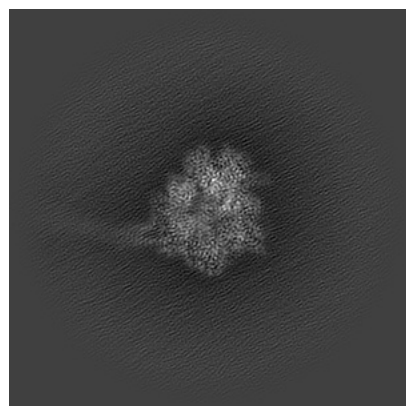
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44721. These allow visual inspection of the internal detail of the map and identification of artifacts.

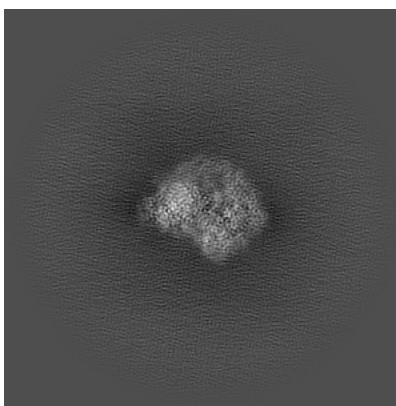
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

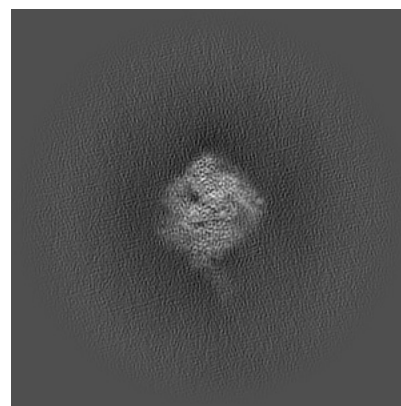
6.1.1 Primary map



X

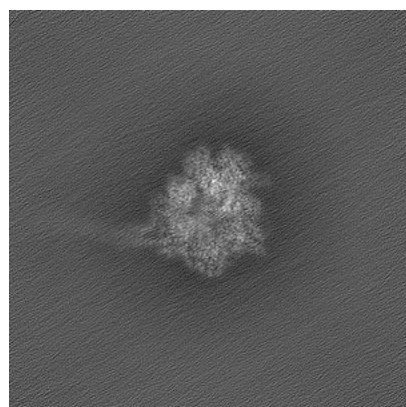


Y

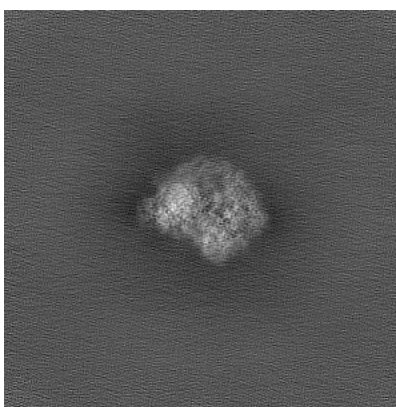


Z

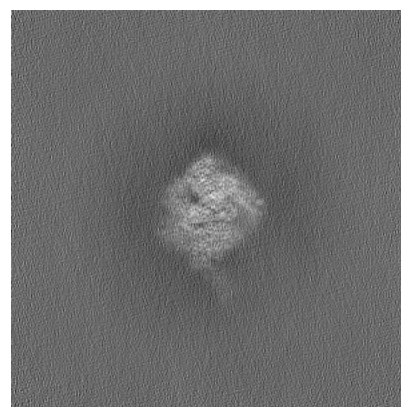
6.1.2 Raw map



X



Y

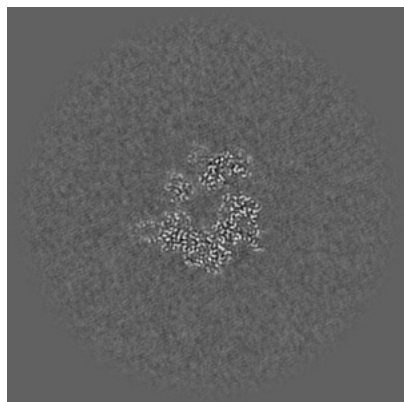


Z

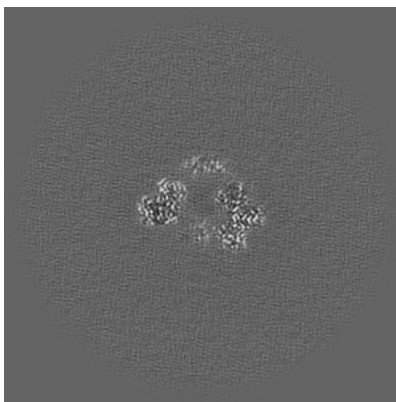
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

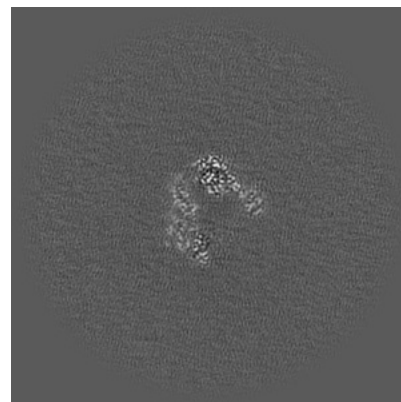
6.2.1 Primary map



X Index: 180

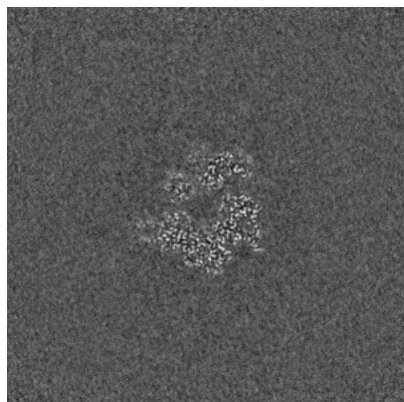


Y Index: 180

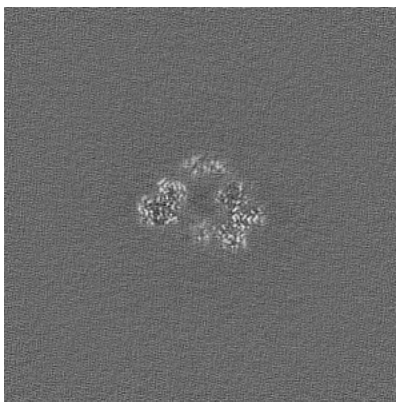


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

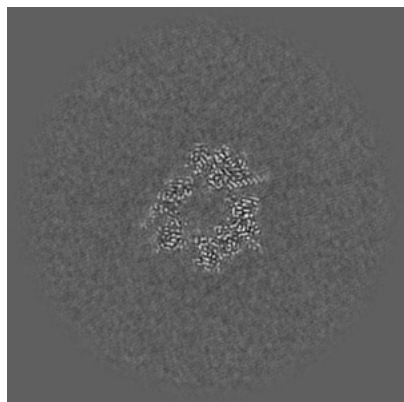


Z Index: 180

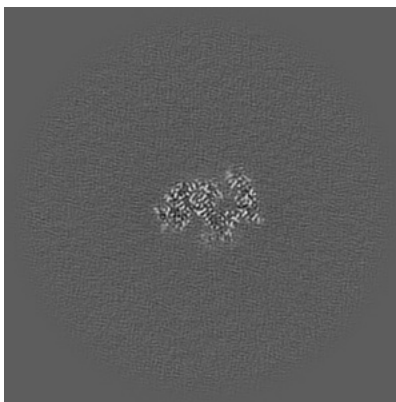
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

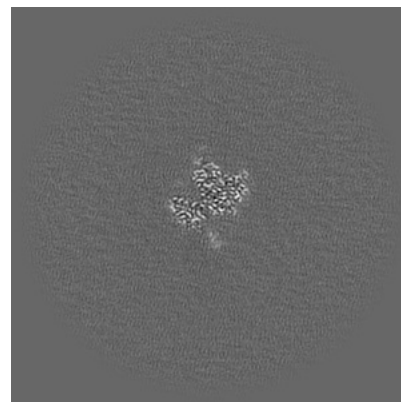
6.3.1 Primary map



X Index: 175

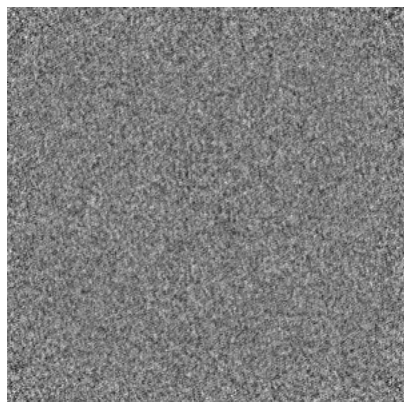


Y Index: 203

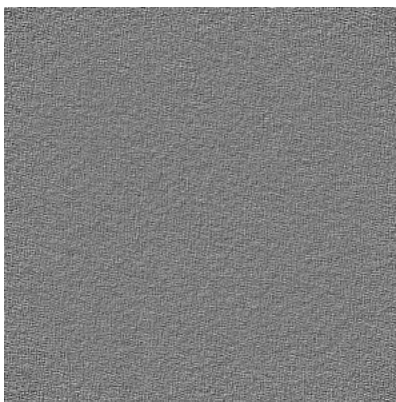


Z Index: 209

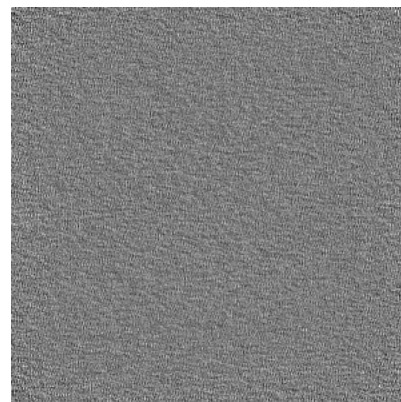
6.3.2 Raw map



X Index: 0



Y Index: 0

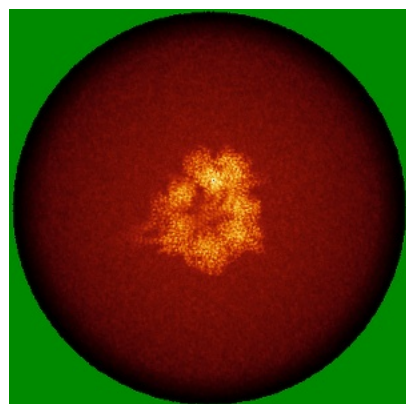


Z Index: 0

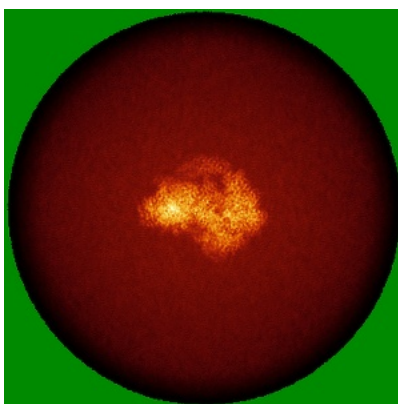
The images above show the largest variance slices of the map in three orthogonal directions.

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

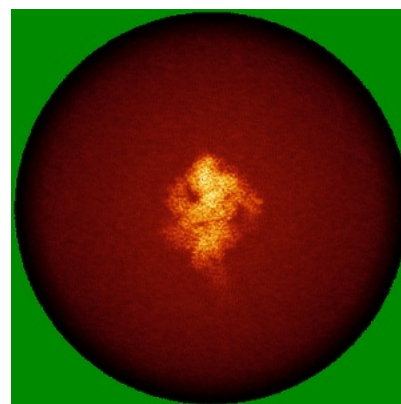
6.4.1 Primary map



X

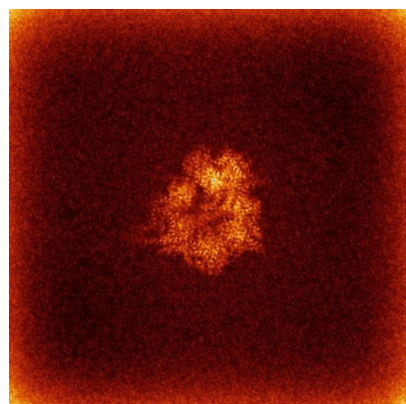


Y

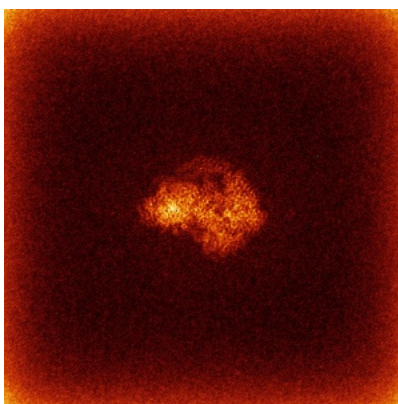


Z

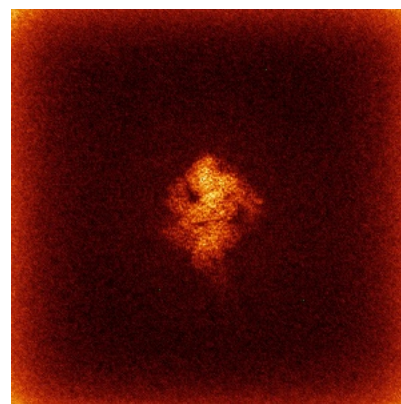
6.4.2 Raw map



X



Y

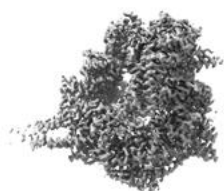


Z

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



X



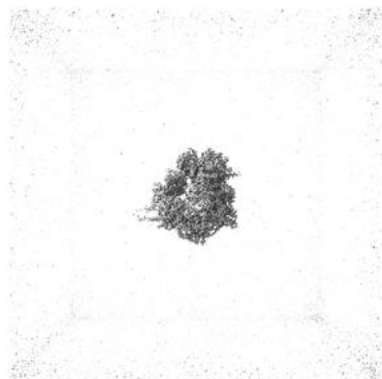
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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



X



Y



Z

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.

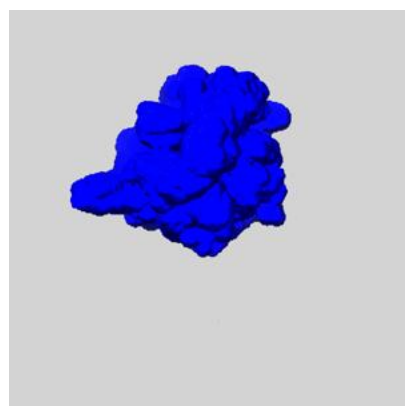
6.6 Mask visualisation [i](#)

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

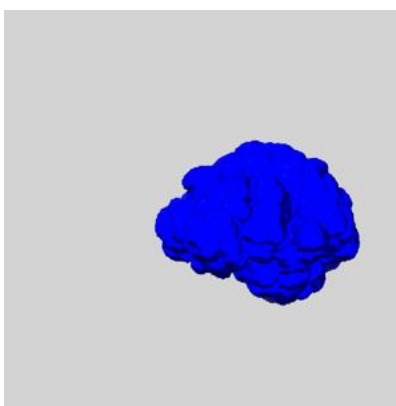
A mask typically either:

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

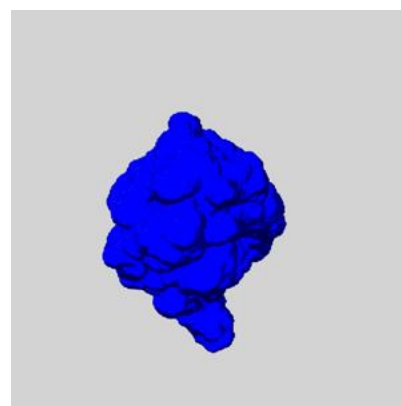
6.6.1 emd_44721_msk_1.map [i](#)



X



Y

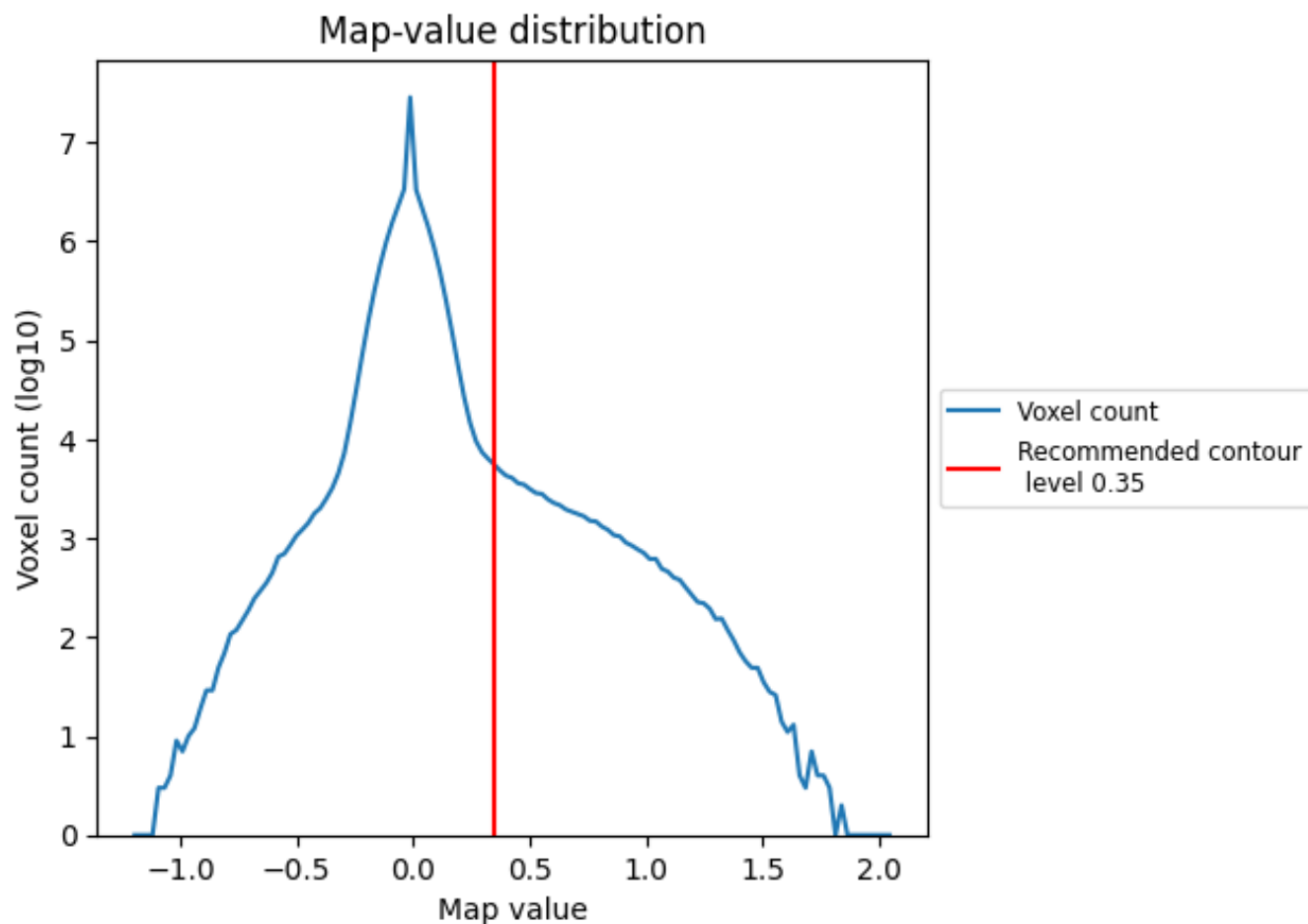


Z

7 Map analysis [i](#)

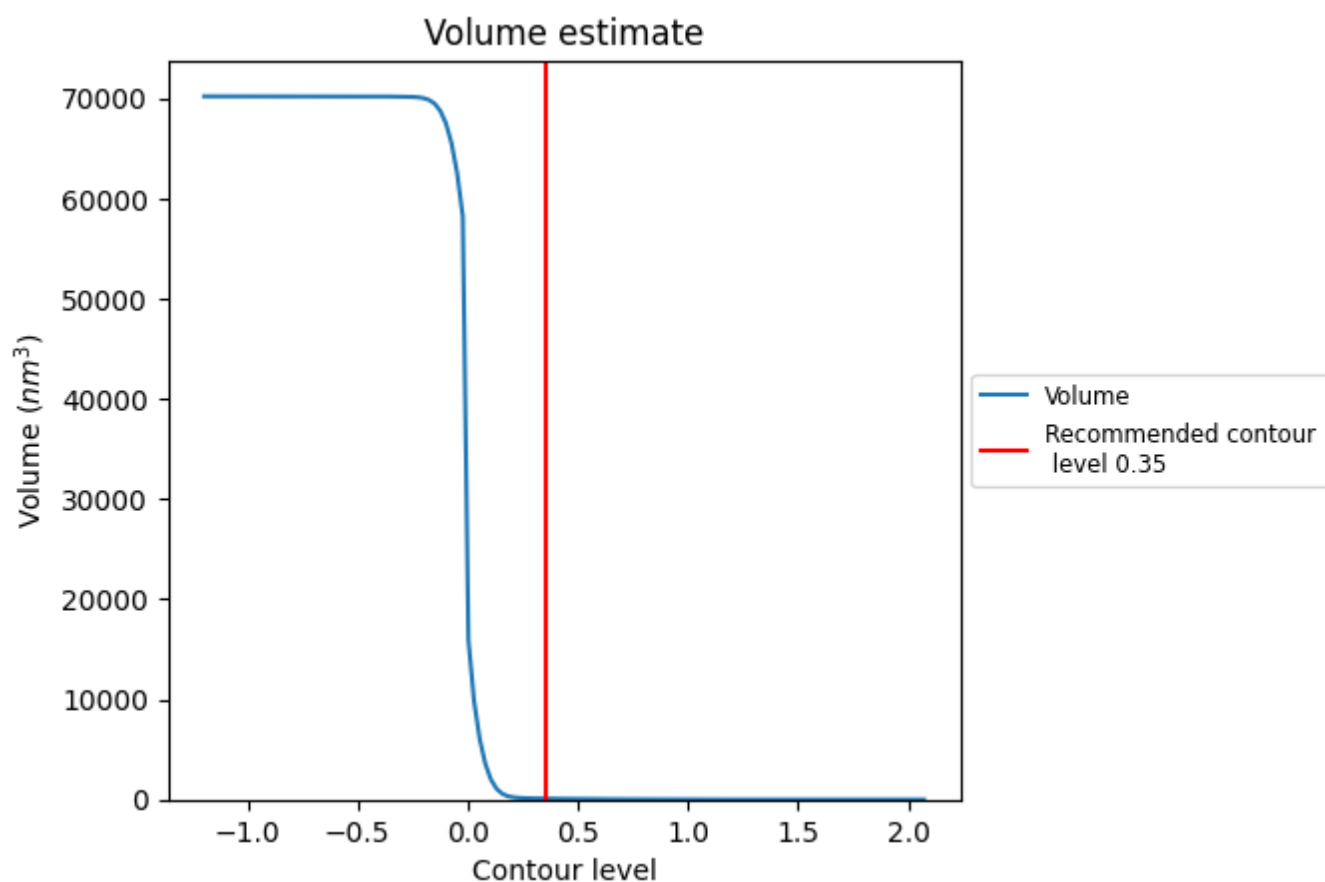
This section contains the results of statistical analysis of the map.

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.

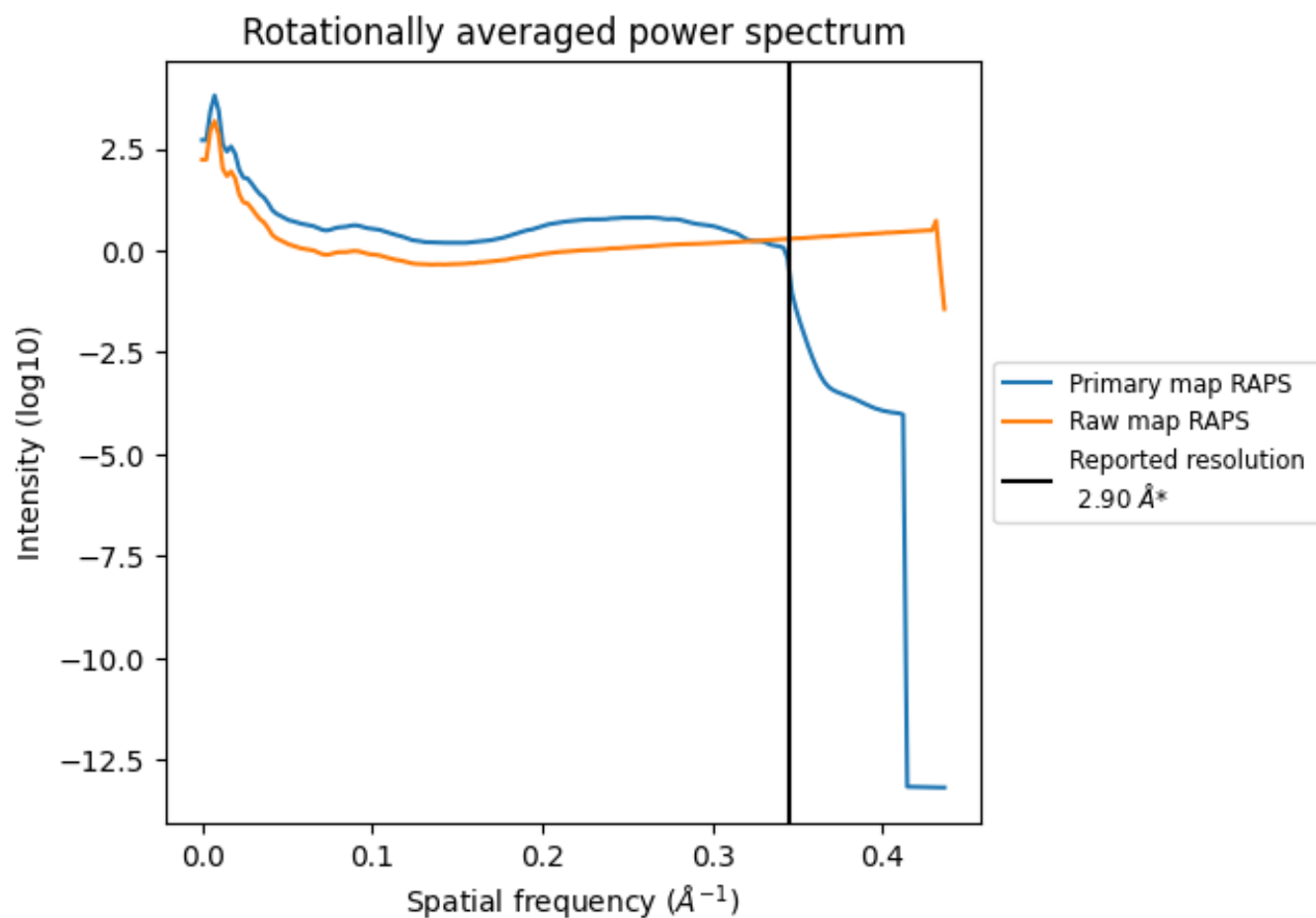
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 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 ⓘ

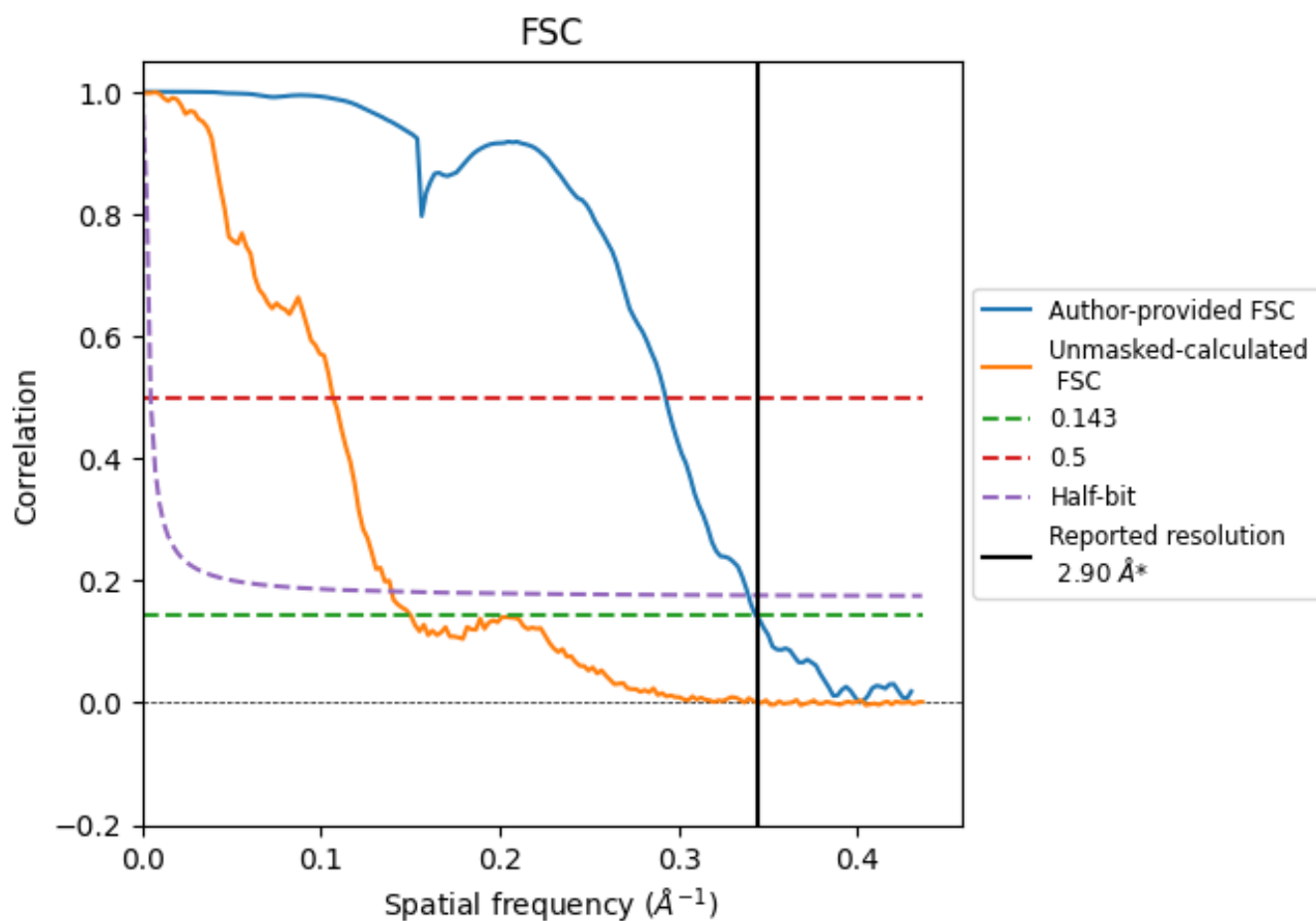


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

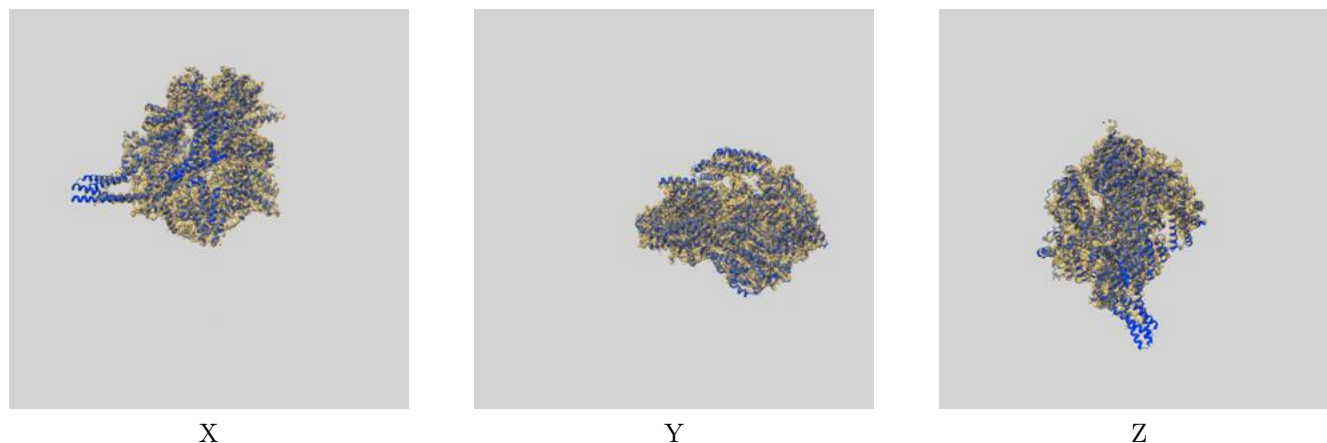
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.42	2.95
Unmasked-calculated*	6.66	9.37	7.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.66 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

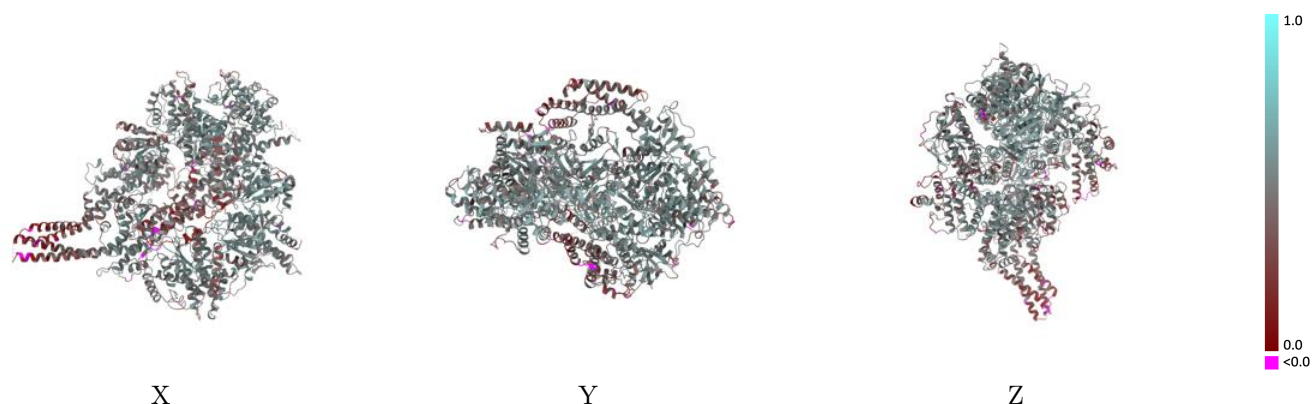
This section contains information regarding the fit between EMDB map EMD-44721 and PDB model 9BN4. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



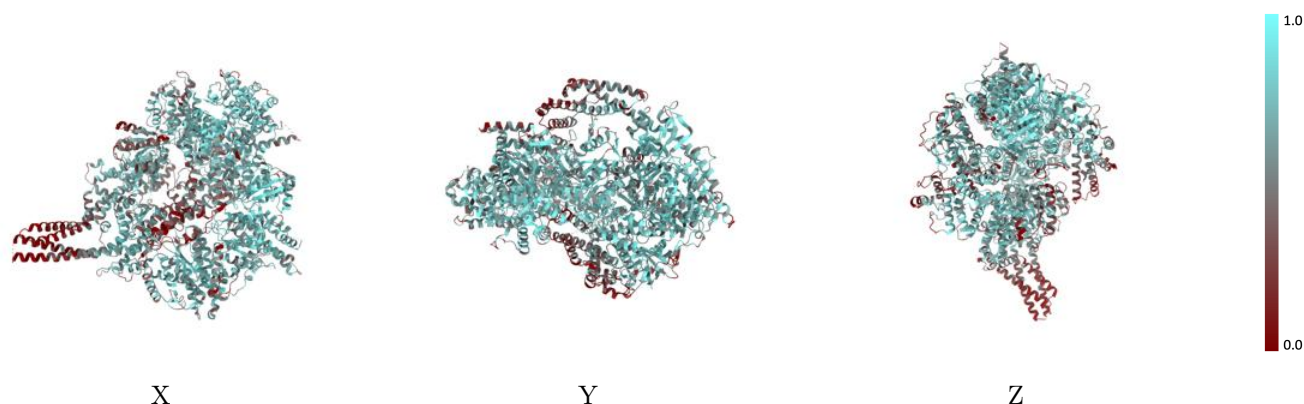
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



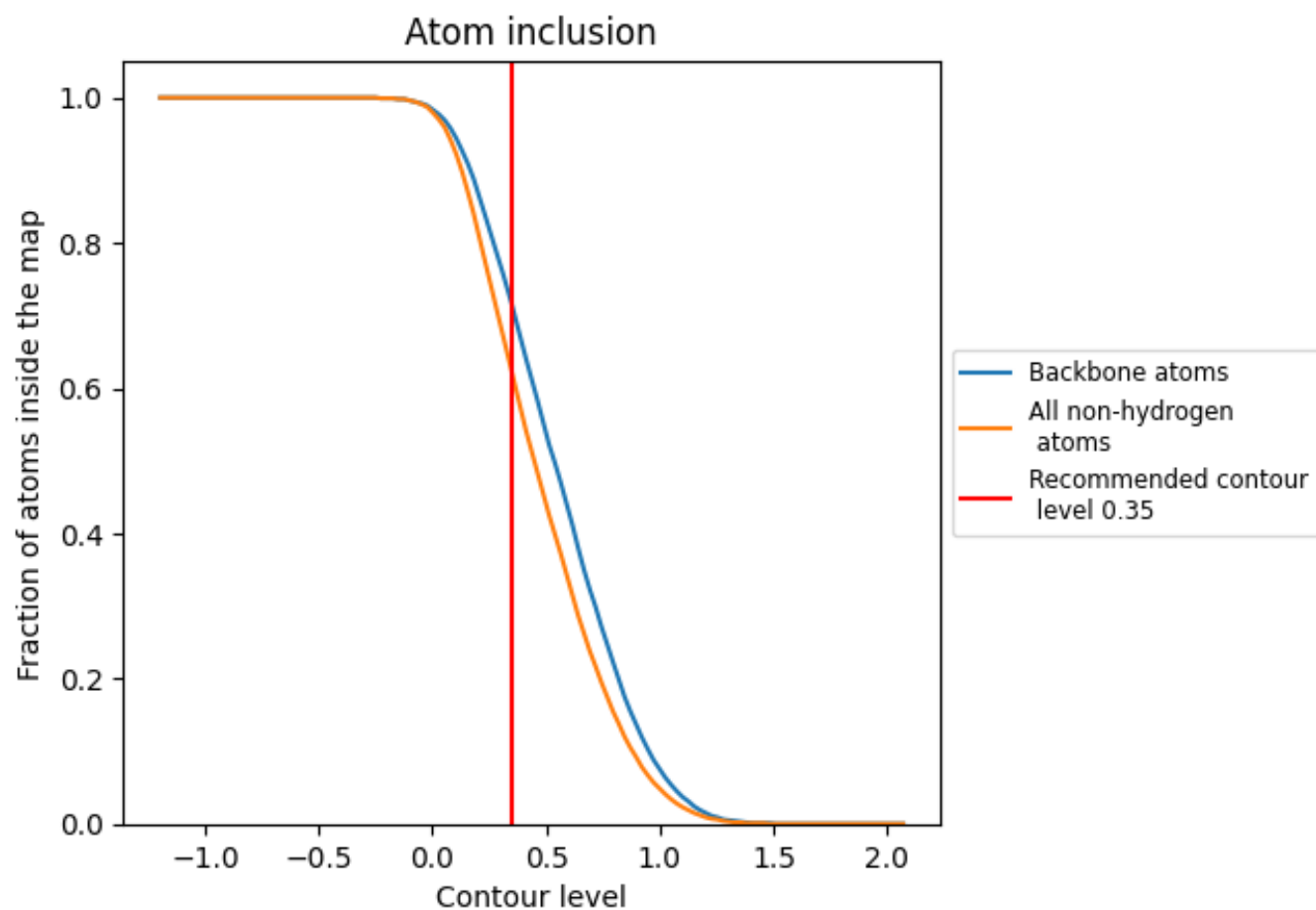
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6220	<div></div> 0.4680
A	<div></div> 0.6220	<div></div> 0.4680

