



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 5NP1 / pdb_00005np1
EMDB ID : EMD-3672
Title : Open protomer of human ATM (Ataxia telangiectasia mutated)
Authors : Baretic, D.; Pollard, H.K.; Fisher, D.I.; Johnson, C.M.; Santhanam, B.; Truman, C.M.; Kouba, T.; Fersht, A.R.; Phillips, C.; Williams, R.L.
Deposited on : 2017-04-13
Resolution : 5.70 Å(reported)

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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
MolProbity : 4-5-2 with Phenix2.0
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

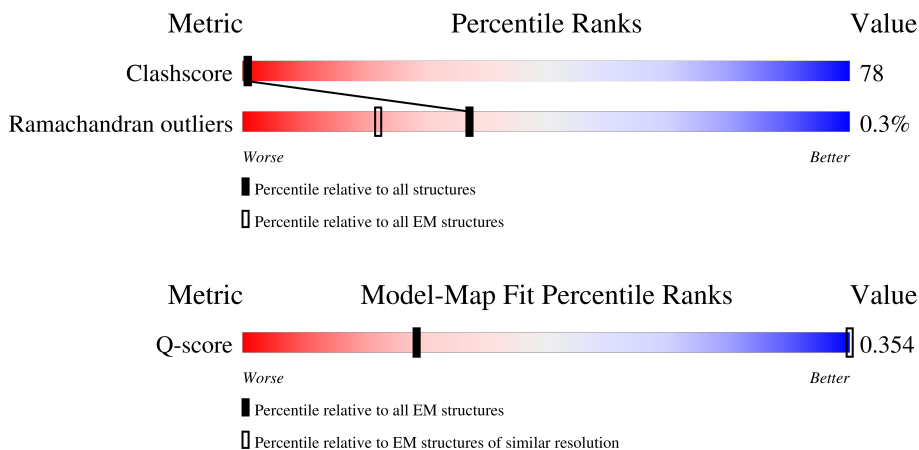
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	-
Q-score	-	25397	503 (5.20 - 6.20)

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	3066	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12201 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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2460	Total	C	N	O	0	0
			12201	7281	2460	2460		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q13315
A	-8	ASP	-	expression tag	UNP Q13315
A	-7	TYR	-	expression tag	UNP Q13315
A	-6	LYS	-	expression tag	UNP Q13315
A	-5	ASP	-	expression tag	UNP Q13315
A	-4	ASP	-	expression tag	UNP Q13315
A	-3	ASP	-	expression tag	UNP Q13315
A	-2	ASP	-	expression tag	UNP Q13315
A	-1	LYS	-	expression tag	UNP Q13315
A	0	HIS	-	expression tag	UNP Q13315

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G2709	C2624	R2486	K2363	A2301	P2222	V2155	CYS	E1971	S1905	T1835	D1758
K2710	D2625	L2487	A2364	K2302	T2223	E2156	PRO	K1972	Q1906	D1836	P1759
R2711	A2626	V2365	E2368	E2304	M2224	E2157	E2094	R1973	R1907	V1841	A1762
R2712	Y2627	E2366	E2366	E2304	A2225	E2158	L2095	S1974	T1908	L1842	Y1763
K2713	L2628	V2367	V2367	Q2306	L2226	K2159	E2096	L1975	M1909	P1843	L1764
K2714	L2629	W2491	A2368	S2306	R2227	K2160	E2097	A1976	L1910	Y1844	Q1765
	L2630	L2492	G2369	L2307	T2228		L2098	PHE	A1911	L1845	
D2720	A2631	E2493	G2370	A2308	V2229	V2166	H2099	GLU	Y1912	L1846	R1768
D2721		M2494	TYR	L2309	L2230	V2167	L2230	GLU	V1913	L1847	T1769
R2723	D2634	M2494	ASP	S2310	L2231	S2168	Q2101	ALA	L1914	H1847	S1770
K2724	GLN	GLY	GLY	L2311	E2232	L2169	A2102	SER	Y1915	L1848	
D2725	THR	ASN	GLU	L2312	L2233	V2170	A2103	TRP	M1916	L1849	ARG
D2726	THR	ASN	SER	L2313		P2171	GLY	GLN	R1917	L1850	LYS
A2726	TRP	TYR	S2376	Q2314	E2236	T2172	R2105	THR		L1851	LYS
M2728	LYS	THR		M2315		L2173	M2106	ALA	K1920	Q1852	PHE
G2729	VAL	L2379	L2379	I2316	R2244	S2174	M2107	ALA			LEU
Q2730	LYS	R2380	R2380	K2317	E2245	R2175	Q2108	VAL	S1924	E1856	GLU
V2731	VAL	N2381	N2381	L2319	C2246	L2176		THR	G1925	S1857	GLU
V2732	GLN	G2382	G2382	L2319	L2247	Q2177	H2111	TRP	T1926	W1858	PRO
F2732	ARG	K2383	K2383	D2320	K2248	A2178	C2112	SER	T1927	R1859	ARG
Q2733	ARG	L2384	L2384	A2321	D2249	I2179		GLU	F1928	M1860	PHE
M2734	LEU	K2385	K2385	S2322	L2250	G2180	L2116	LYS	M1929	L1861	ASP
C2735	GLU	A2386	A2386	C2323	L2251	E2181	LYS	SER	D1930	L1862	ASP
A2649	GLU	F2387	F2387	A2324	T2252	L2182	GLU	LYS	A1931	S1863	GLU
N2736	LEU	L2388	L2388	ALA	T2252	L2183	VAL	ALA	F1932	T1864	ASN
T2737	ASP	S2389	S2389	ASN	H2254	E2183	GLU	PRO		H1865	PRO
L2738	E2449	L2390	L2390	ASN	H2254	S2184	GLU	E1996	W1933	H1866	PHE
L2739	L2450	L2391	L2391	P2328	L2255	I2185	GLY	R1998	L1934	Q1867	GLU
Q2740	L2451	R2392	R2392	P2328	V2256	G2186	THR	GLY	Y1938	G1868	GLY
	L2452	F2393	F2393		E2257	E2187		SER	L1939	F1869	LEU
T2743	L2453	R2394	R2394	K2331	L2258	S2190	Y2124	THR	A1940	F1870	ASP
E2744	A2454	S2394	S2394	L2332	S2259	R2191	H2125	GLN	E1941	T1871	ASP
T2745	L2455	D2395	D2395	T2333	L2260	SER	E2126	ALA	V1941	S1872	ILE
R2746	L2456	T2396	T2396	Y2334	L2261	VAL	S2127	ALA	A1942	C1873	ASN
K2747	E2457	Q2397	Q2397	T2336	A2262	L2128	Y2129	ILE	K1943	L1874	LEU
R2748	L2458	Q2399	Q2399	E2336	R2263	T2194	N2130	GLN	A1944	R1875	TRP
	LEU	R2400	R2400	C2337	T2264	H2195	A2131	ALA	A1945	H1876	ILE
T2682	R2459	K2460	K2460	L2338	F2265	Q2196	L2132	E2007	Q1946	P1877	
Q2684	R2461	F2462	F2462	R2339	K2266	Q2197	L2132	L2008		S1878	
S2685	F2462	E2462	E2462	V2340		L2198	Q2133	Y2009	A1949	Q1879	A1812
F2686	L2463	M2403	M2403	C2341	R2273	S2199	S2134	R2010	A1950	T1880	F1813
K2687	C2464	Y2404	Y2404	G2342	A2274	E2200	L2135	S2011	H1951	S1881	L1814
L2688	K2465	M2405	M2405	N2343	L2275	V2201	R2136	I2012	F1952	R1882	D1815
E2689	A2466	K2406	K2406	W2344	T2276	L2202	D2137	E2014	T1953	S1883	
	F2537	S2407	S2407	L2345	Q2277	I2203	ARG	E2014	A1954	G1817	G1818
	H2538	E2407	E2407	A2346	L2278	K2204	GLU	P2015	L1955	T1884	
	E2539	S2408	S2408	E2347	K2279	W2205	PHE	D2016	L1956	T1885	
	V2540	E2409	E2409	E2347	Q2280	Q2206	S2141	S2017	Y1957	P1886	
	L2541	F2410	F2410	T2348	Y2281	K2207	T2142	L2018	A1958	A1887	
	N2542	E2411	E2411	C2349	H2208	S2209	F2143	Y2019	E1959	M1888	
	N2543	N2412	N2412		N2282	Q2209	Y2144	G2020	T1960	L1889	
	C2473			N2352	V2284	Q2210	E2145	C2021	Y1961	D1890	
	L2474	GLN	GLN	P2353		L2211	S2146	G2022	A1962	S1891	
	L2475	ALA	ALA	A2354	L2293	L2212	L2147	G2023	D1963	L1827	
	S2476	LEU	LEU	V2355	E2294	K2213	K2148	GLY	K1964	S1893	
		LEU	LEU	L2356	E2295	E2216	Y2149	MET	P1895	E1894	
	H2480	LYS	LYS	Q2357	A2296	F2217	A2150	GLU	S1966	M1830	
	D2481	ARG	ARG	Q2358	Q2297		R2151	LEU	M1967	C1831	
	M2482	ALA	ALA	T2359	V2298		V2152	GLN	D1968	V1832	
	W2483	LYS	LYS	S2360	V2299		K2152	PRO	P1969	K1903	
	F2485	GLU	GLU	L2361	T2299		E2154	ILE	Q1970	K1834	
		GLU	GLU	E2362	W2300	E2221					
L2557	R2486	L2487	A2364	K2302	T2223	E2156					
F2558	L2487	V2365	E2368	E2304	M2224	E2157					
T2559	S2488	S2489	E2560	E2560	A2225	E2158					
L2561	L2490	W2491	A2562	S2306	L2226	K2159					
L2563	L2492	L2492	L2563	L2307	T2228						
A2564	E2493	E2493	A2564	A2308	V2229	V2166					
N2565	M2494	M2494	N2565	L2309	L2230	V2167					
A2566	S2495	S2495	A2566	S2310	L2231	S2168					
F2571	S2498	S2498	F2571	L2311	E2232	L2169					
LEU	E2499	E2499	LEU	L2312	L2233	V2170					
THR	V2500	V2500	THR	L2313		P2171					
LEU	M2501	M2501	LEU	Q2314	E2236	T2172					
THR	G2502	G2502	THR	M2315		L2173					
PRO	M2503	M2503	PRO	I2316	R2244	S2174					
VAL	M2504	M2504	VAL	K2317	E2245	R2175					
ALA	K2505	K2505	ALA	L2319	C2246	L2176					
ARG	R2506	R2506	ARG	D2320	K2248	A2178					
ARG	D2507	D2507	ARG	A2321	D2249	I2179					
SER	G2508	G2508	SER	S2322	L2250	G2180					
ILE	P2512	P2512	ILE	C2323	L2251	E2181					
THR	T2513	T2513	THR	A2324	T2252	L2182					
LYS	F2516	F2516	LYS	ALA	T2252	L2183					
ASN	L2517	L2517	ASN	ASN	H2254	S2184					
VAL	L2517	L2517	VAL	ASN	L2255	I2185					
PRO	L2452	L2452	PRO	P2328	V2256	G2186					
LYS	R2453	R2453	LYS		E2257	E2187					
GLN	A2454	A2454	GLN	K2331	L2258	S2190					
SER	L2455	L2455	SER	L2332	S2259	R2191					
GLN	A2456	A2456	GLN	T2333	L2260	SER					
LEU	E2457	E2457	LEU	Y2334	L2261	VAL					
D2595	R2458	R2458	D2595	E2336	R2263	T2194					
T2599	K2459	K2459	T2599	THR	Q2399	Q2196					
E2600	R2460	R2460	E2600	MET	R2400	Q2197					
A2602	F2462	F2462	A2602	MET	K2460	Q2197					
S2764	L2463	L2463	S2764	G2533	E2462	L2198					
G2765	C2464	C2464	G2765	G2534	M2403	S2199					
E2689	K2465	K2465	E2689	L2535	Y2404	E2200					
L2767	F2537	F2537	L2767	G2536	M2405	V2201					
E2768	H2538	H2538	E2768	E2537	K2406	L2202					
	E2539	E2539		E2539	S2407	I2203					
V2774	V2540	V2540	V2774	V2540	E2407	K2204					
T2775	L2541	L2541	T2775	L2541	S2408	W2205					
I2776	N2542	N2542	I2776	N2542	E2409	Q2206					
G2777	N2543	N2543	G2777	N2543	F2410	K2207					
E2778	L2544	L2544	E2778	L2544	E2411	S2209					
F2779	S2545	S2545	F2779	S2545	N2412	Q2210					
L2780	R2546	R2546	L2780	R2546	GLN	L2211					
V2781	L2547	L2547	V2781	L2547	ALA	L2212					
N2782	L2548	L2548	N2782	L2548	LEU	K2213					
C2783	S2549	S2549	C2783	S2549	LEU	E2216					
E2784	M2550	M2550	E2784	M2550	LYS	F2217					
V2705			V2705		ARG						
D2785	P2553	P2553	D2785	P2553	ALA						
G2786	E2622	E2622	G2786	E2622	LYS						
A2787	L2623	L2623	A2787	L2623	GLU						

V3005	Q2942	S2859	H2788
	E2943	S2860	
	T2944	I2861	D2796
	L2945	V2862	F2796
	T2947	C2863	S2797
	T2948		A2798
	T2949	I2866	F2799
	T2949	C2867	Q2800
	L3013	E2950	C2801
	Q3014	V2951	Q2802
E3015	T2952	K2803	
K3016	T2953		
L3017		M2806	
K3018	T2956	GLU	
G3019	T2957	VAL	
V3020	F2958	GLN	
	D2959	LYS	
	V2960	LYS	
T3024	T2961	SER	
V3025	T2962	F2813	
L3026	N2962	E2815	
S3027	N2963	E2815	
Q3028		K2816	
G3029	A2967	V2817	
G3030	L2968	E2818	
Q3031	V2969	V2819	
V3032	L2970	F2820	
N3033	GLN	M2821	
L3034	GLN	D2822	
L3035	ARG	V2823	
I3036	PRO	Q2824	
Q3037	GLU	Q2825	
Q3038	ASP	F2827	
A3039	GLU		
I3040	THR	R2912	
I3041	GLU	D2913	
F3042	LEU	T2914	
K3043	HIS	T2915	
PR0	PR0	D2916	
THR	THR	D2917	
LEU	LEU	G2917	
ASN	ASN		
ALA	ALA	T2921	
ASP	ASP	C2922	
ASP	ASP	V2923	
GLN	GLN	E2924	
GLU	GLU	G2925	
CYS	CYS	V2926	
LYS	LYS	F2927	
ARG	ARG	R2928	
ASN	ASN	T2929	
LEU	LEU	C2930	
SER	SER	C2931	
ASP	ASP	E2932	
		K2933	
	T2984		
	T2986		
	D2999		
	Q3000		
	E2936		
	S3001		
	F3002		
	N3003		
	T3004		
		N2940	
		S2941	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.1	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.137	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.026	Depositor
Map size ($\text{\AA}$)	428.99997, 428.99997, 428.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.43, 1.43, 1.43	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.80	5/12155 (0.0%)	1.12	48/16884 (0.3%)

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	78

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLN	CA-C	-10.23	1.38	1.52
1	A	647	GLU	CA-C	-9.65	1.38	1.52
1	A	947	TYR	CA-C	-7.04	1.42	1.52
1	A	2961	THR	CA-C	-6.56	1.43	1.52
1	A	1111	LEU	C-N	-6.35	1.25	1.34

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1375	ALA	CA-C-N	21.70	141.08	119.82
1	A	1375	ALA	C-N-CA	21.70	141.08	119.82
1	A	1410	LYS	CA-C-N	-12.14	109.29	122.89
1	A	1410	LYS	C-N-CA	-12.14	109.29	122.89
1	A	1053	ASP	CA-C-N	-11.10	107.84	119.83

There are no chirality outliers.

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Peptide
1	A	111	ARG	Peptide
1	A	181	ASP	Peptide
1	A	248	ARG	Peptide
1	A	66	LYS	Peptide

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	12201	0	5285	1362	0
All	All	12201	0	5285	1362	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 78.

The worst 5 of 1362 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:1480:PRO:HA	1:A:1484:MET:H	1.16	1.10
1:A:1606:LEU:O	1:A:1608:LEU:N	1.88	1.07
1:A:2714:GLN:HA	1:A:2768:GLU:HA	1.40	1.01
1:A:2388:LEU:O	1:A:2392:ARG:N	1.94	1.00
1:A:1712:PHE:O	1:A:1715:LEU:N	1.96	0.99

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	2368/3066 (77%)	2142 (90%)	218 (9%)	8 (0%)	36 72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2776	ILE
1	A	1607	PRO
1	A	2645	ILE
1	A	1367	ASP
1	A	1688	ILE

5.3.2 Protein sidechains [i](#)

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

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	128:VAL	C	129:LYS	N	3.85
1	A	1200:THR	C	1201:PHE	N	3.19
1	A	163:GLN	C	164:TRP	N	3.09
1	A	1394:SER	C	1395:ASN	N	3.08

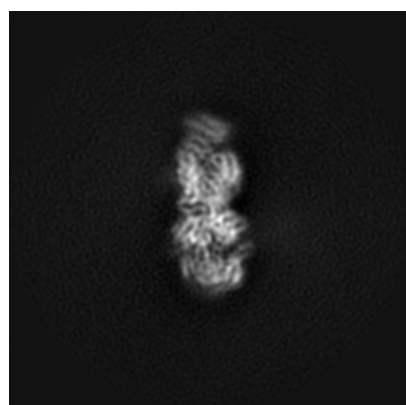
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3672. These allow visual inspection of the internal detail of the map and identification of artifacts.

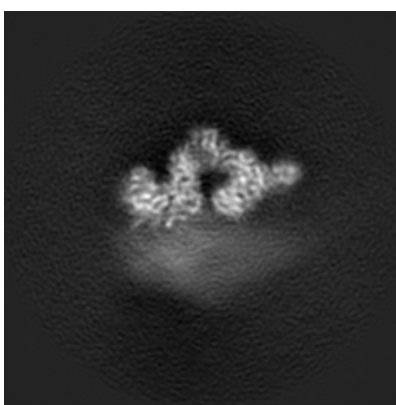
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

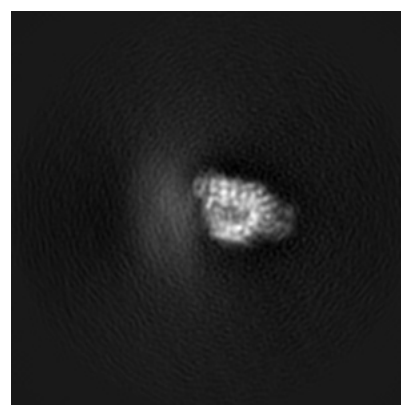
6.1.1 Primary map



X



Y

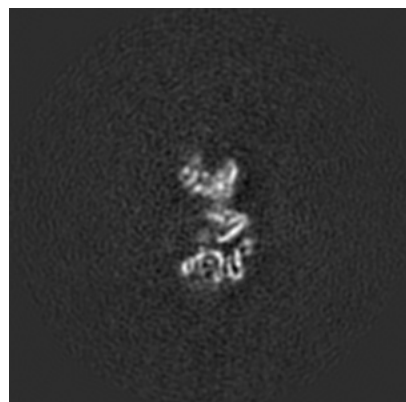


Z

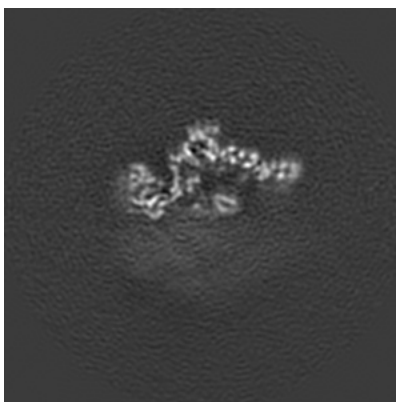
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

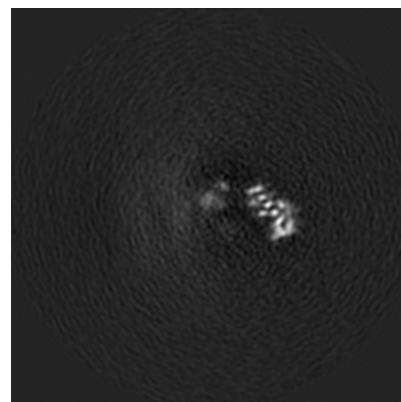
6.2.1 Primary map



X Index: 150



Y Index: 150

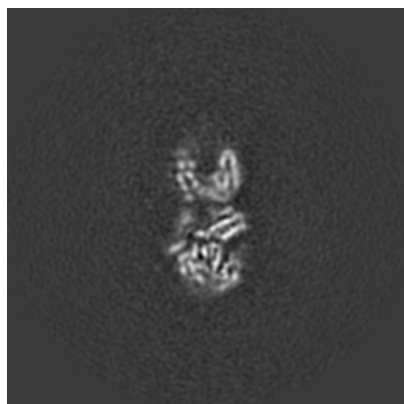


Z Index: 150

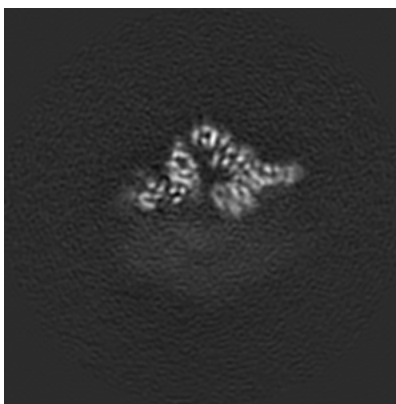
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

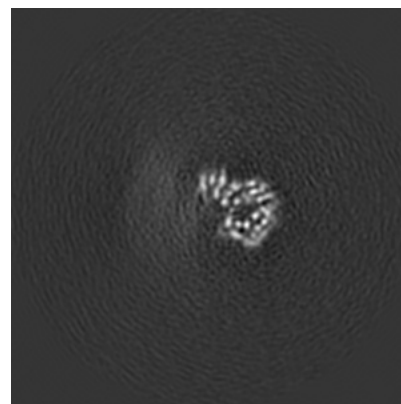
6.3.1 Primary map



X Index: 159



Y Index: 138

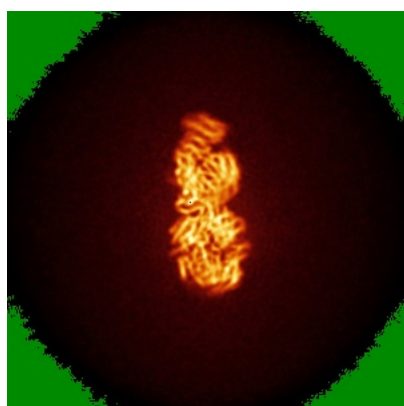


Z Index: 134

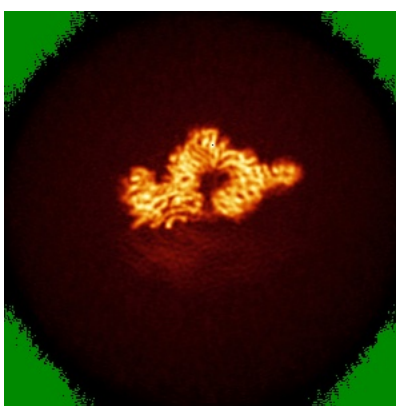
The images above show the largest variance slices of the map in three orthogonal directions.

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

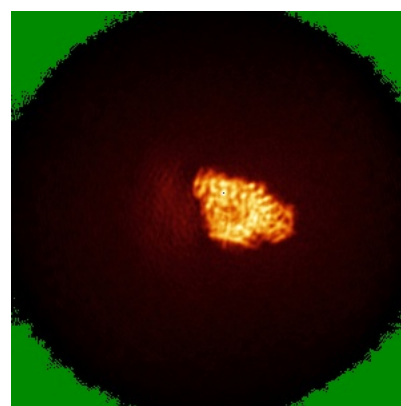
6.4.1 Primary map



X



Y



Z

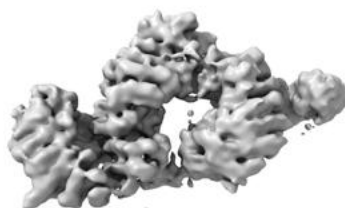
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

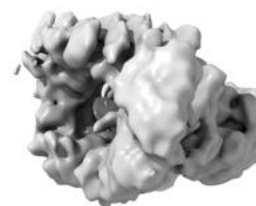
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

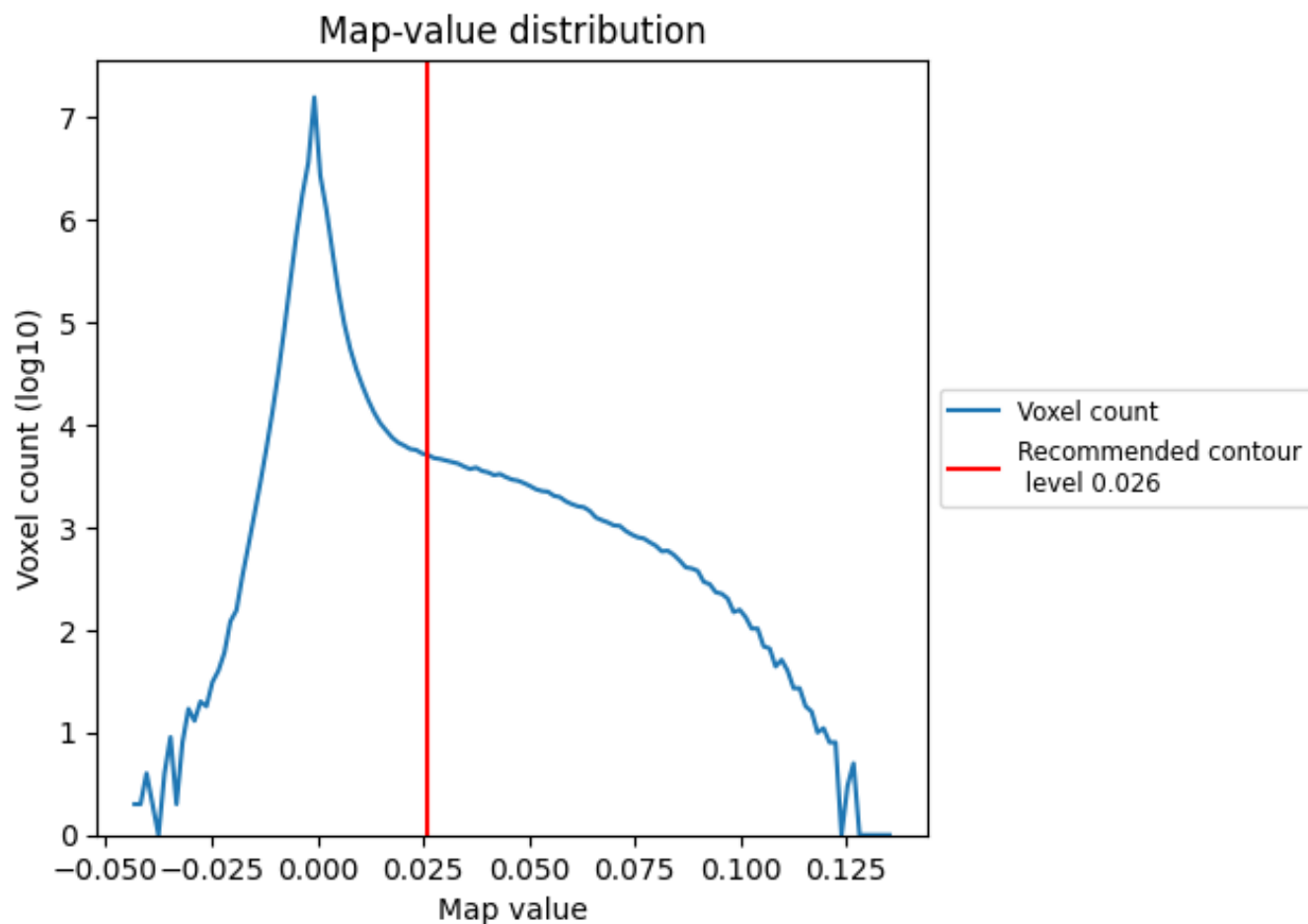
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

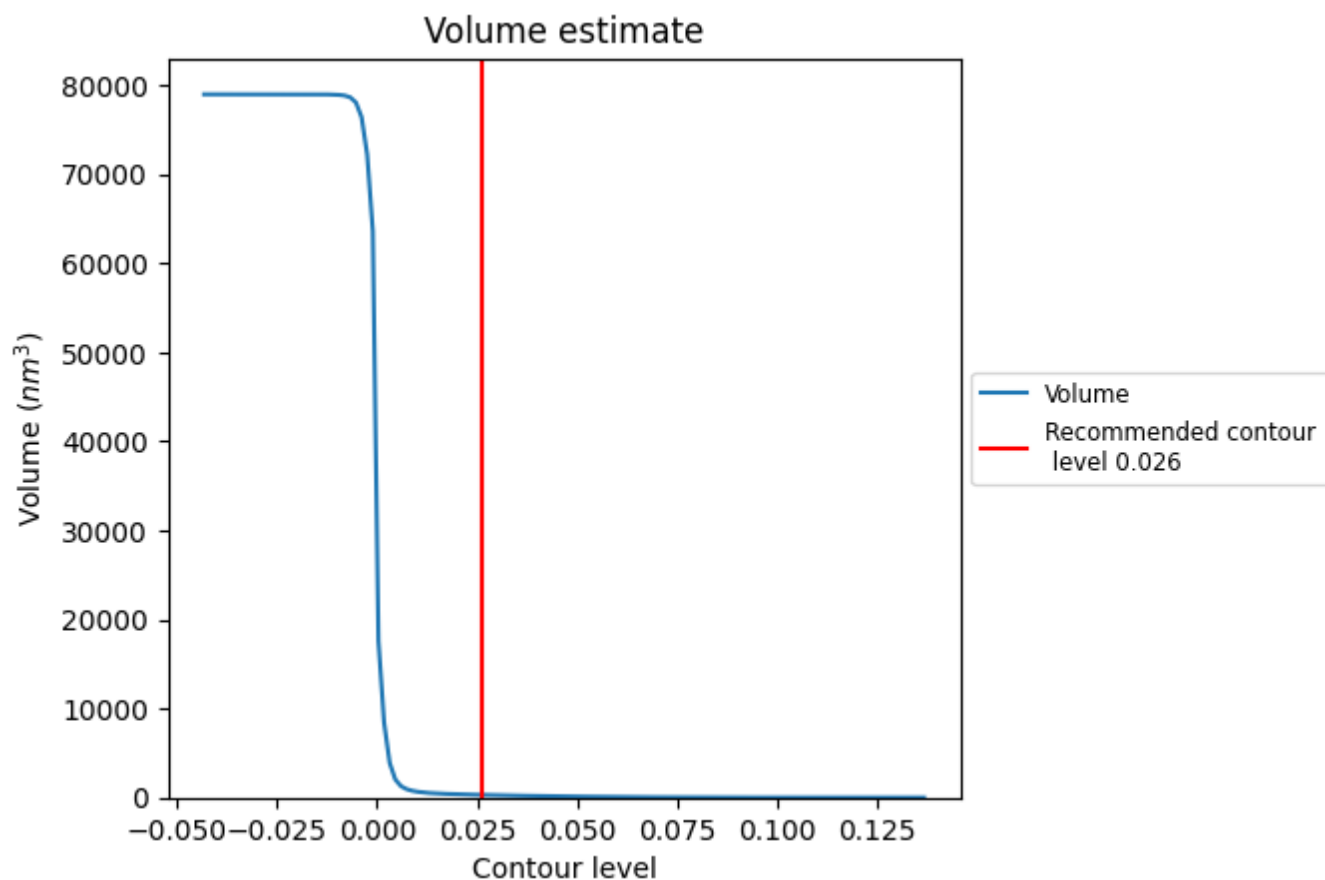
This section contains the results of statistical analysis of the map.

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.

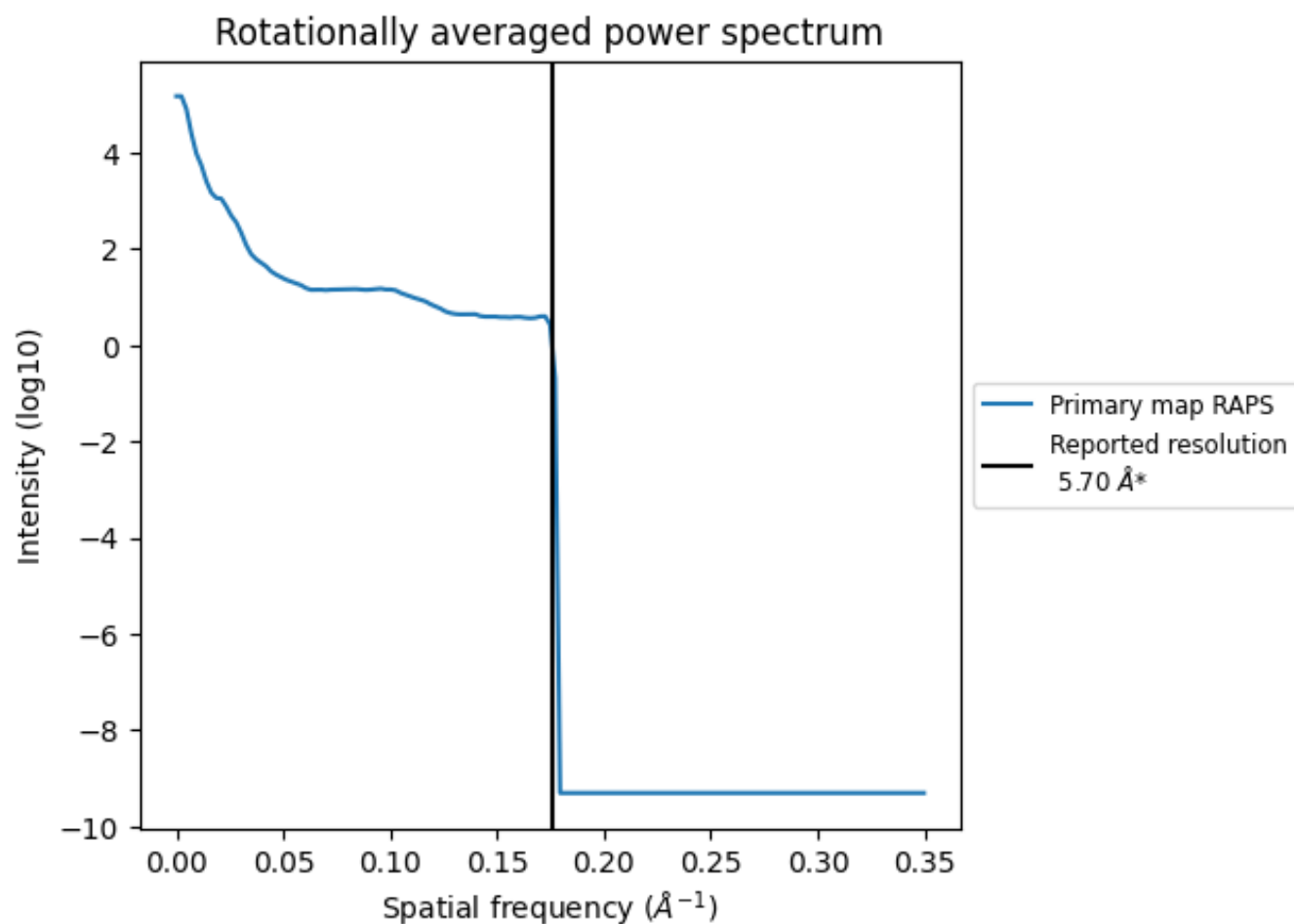
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm³; this corresponds to an approximate mass of 269 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 ⓘ

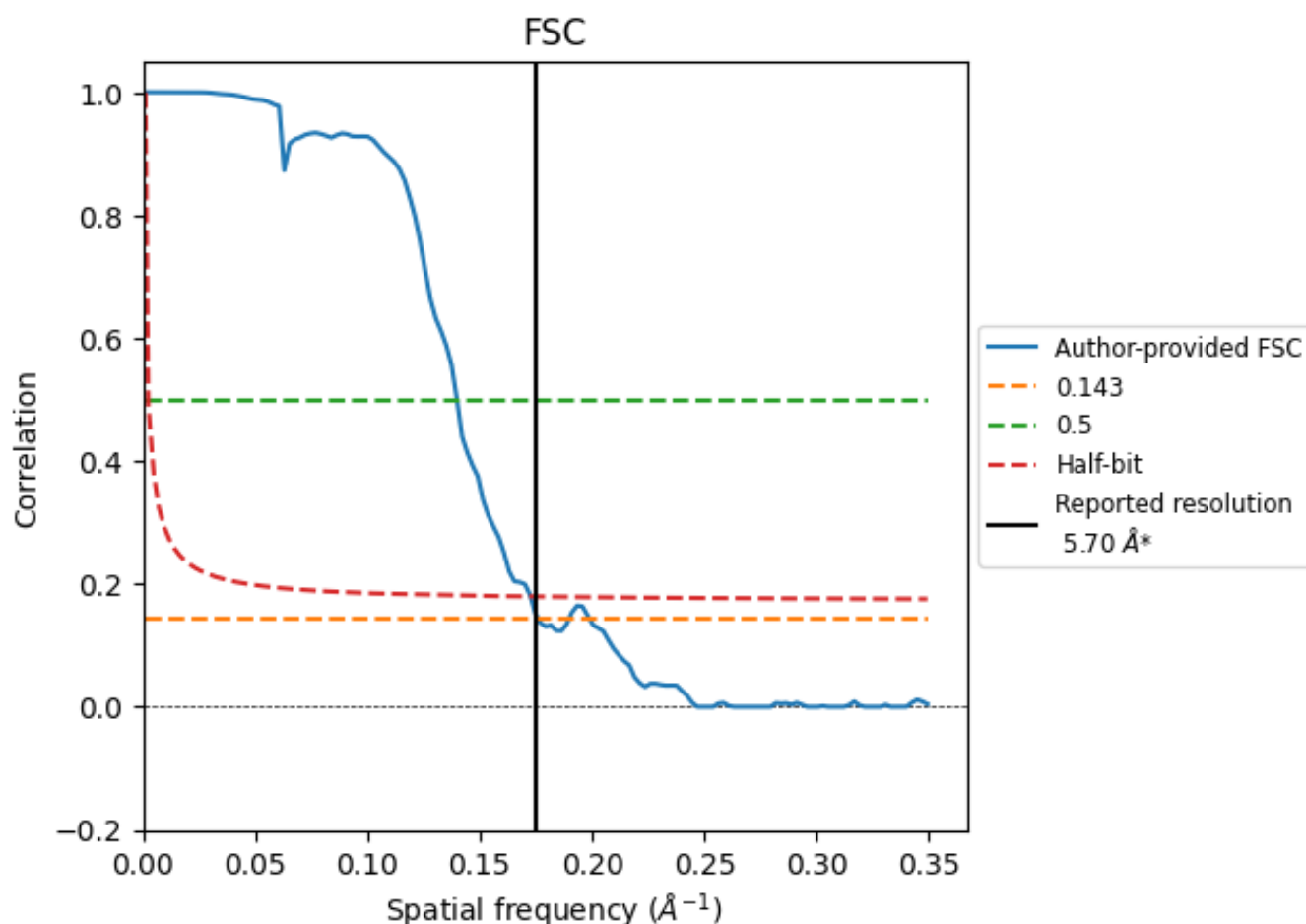


*Reported resolution corresponds to spatial frequency of 0.175 $\text{\AA}^{-1}$

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 0.175 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

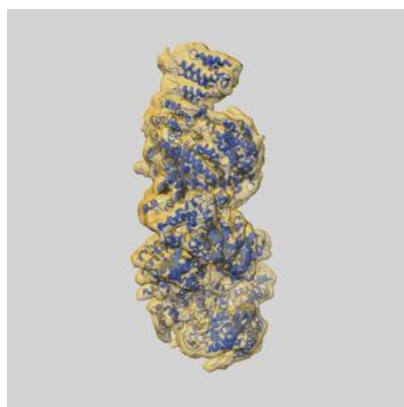
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.68	7.15	5.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

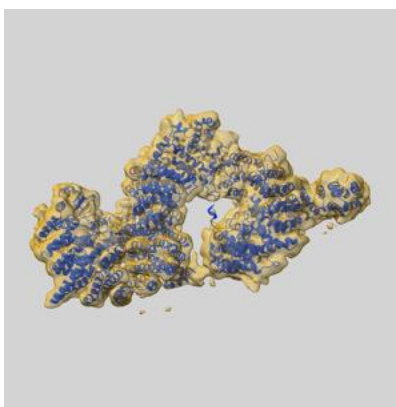
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3672 and PDB model 5NP1. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

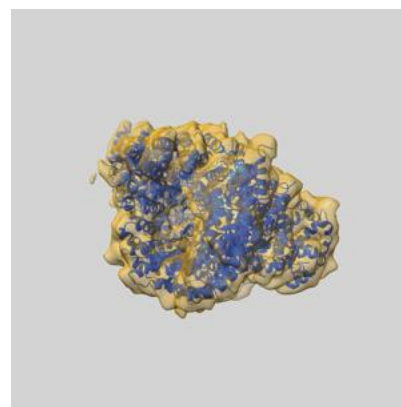
9.1 Map-model overlay [i](#)



X



Y



Z

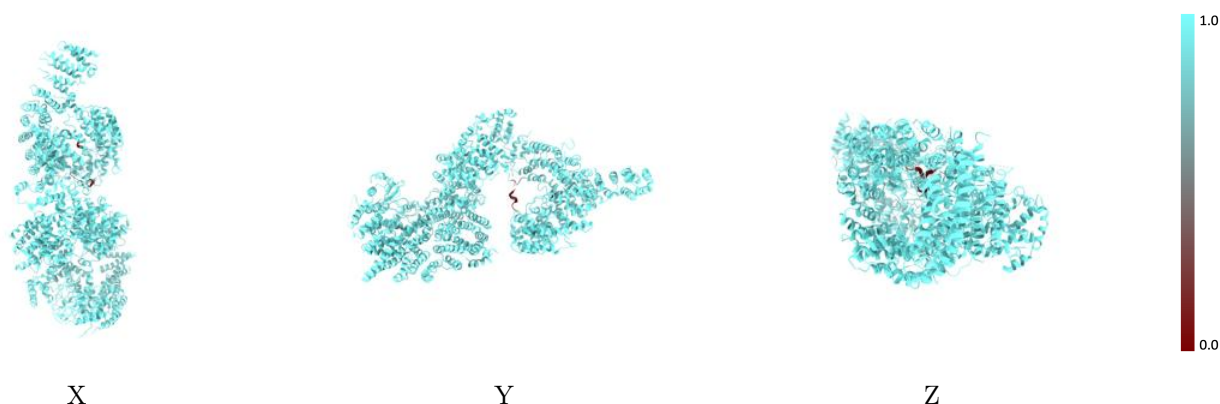
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



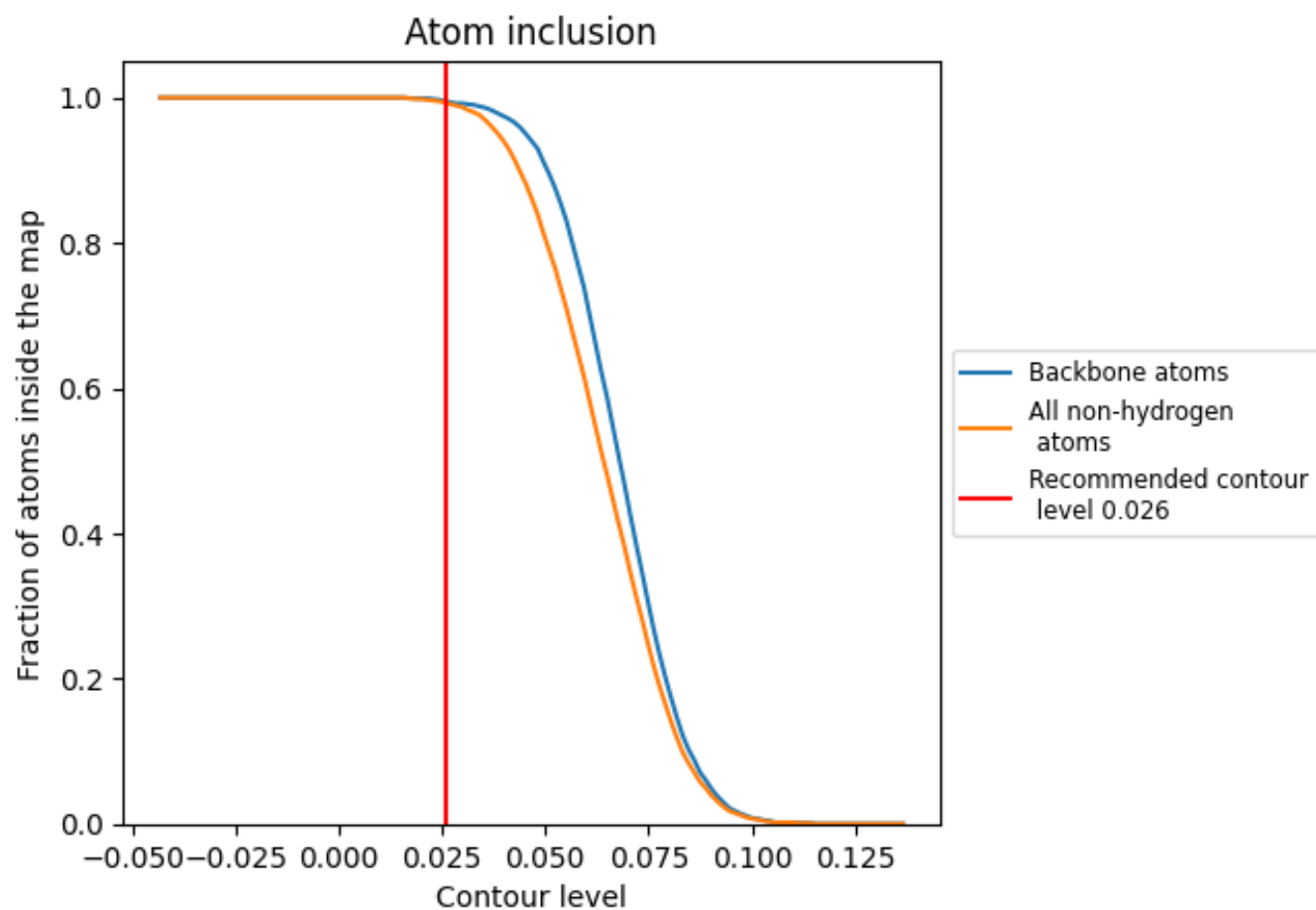
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.3540
A	0.9930	0.3540

