



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 10:18 AM EDT

PDB ID : 5W1R
EMDB ID : EMD-8751
Title : Cryo-EM structure of DNAPKcs
Authors : Sharif, H.; Li, Y.; Wu, H.
Deposited on : 2017-06-04
Resolution : 4.40 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.dev113
MolProbity : 4.02b-467
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) : 2.39

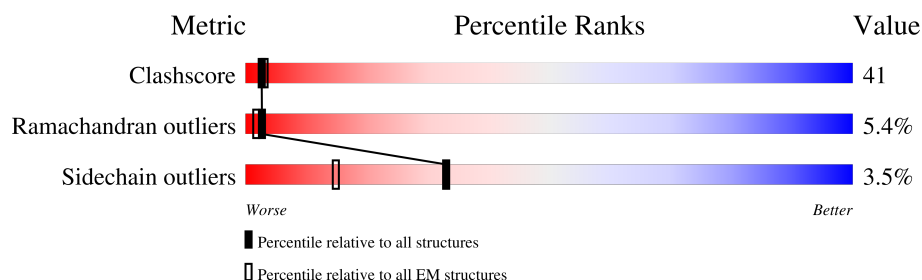
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	4128	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25559 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3563	Total	C	N	O	S	0	0
			25559	16187	4350	4889	133		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent protein kinase catalytic subunit



I1423	F1344	V1276	LEU	B1132	L1068	F1001	M937	L862	L800	C729	L670	MET
T1424	F1350	G1277	LEU	H1133	H1069	E1002	V938	G863	K801	L730	S871	ILE
A1425	N1350	A1278	PRO	L1134	P1070	S1003		G864	T802	T731	I872	PRO
Q1426	N1351	L1279	GLY	L1135	N1071	Q1004	M941	Q865	S803	F732	T873	T805
S1427	T1351	Q1280	ARG	I1138	A1072	D1005	L942	I866	S804	L733	T874	A610
I1428	S1352	V1281	ASN	E1139	F1073	V1006	G943	N867	L805	L734	V874	N611
E1429	P1353	L1282	SER	E1139	A1073	A1008	K944	K868	S806	S735	G875	L612
E1430	E1354	G1283	PRO	K1141	F1074	L1009	A945	N869	ASP	L736	N876	H613
L1431	E1354	L1283	ASN	K1141	R1075	L1009	T946	L870	GLU	L737	P877	P614
C1432	K1357	T1284	LEU	H1142	A1078	E1011	M948	L871	THR	H738	A677	A615
A1433	L1358	V1143	TRP	V1143	S1079	E1012	P949	T872	LYS	N739	K678	K616
A1433	L1358	E1285	LEU		S1079	A1013		V873	ASN	I740	K679	P617
V1434	K1361	A1286	LYS	K1147	L1080	I1013	E950	T874	ASN	V745	I680	K618
N1435	D1362	Q1287	ASP	A1148	A1081	L1014	G951	S875	TRP		K681	D619
L1436	L1363	S1288	VAL	K1149	F1082	D1015	G951	S876	GLU	V749	K682	F620
Y1437	G1364	L1289	LEU	K1150	N1083	G1016	Q953	D877	VAL	A751	P882	S821
G1436	N1365	K1213	K1213	R1151	N1084	I1017		E878	ALA	L752	GLY	A622
P1439	L1365	E1214	E1215	R1152	I1085	V1018	P956		LEU	L752	GLY	F623
D1440	L1368	G1290	G1291	L1153	Y1086	D1019	P957	K881	SER	L758	VAL	I624
A1441	M1369	A1292	V1217	P1154	E1088	P1020	M958	S882	ARG	G759	PRO	N625
	R1370	V1294	L1220	F1157	F1089	V1021	Y959	K882	ALA	L760	LYS	L626
R1447	V1371	A1295	L1221	P1158	E1090	S1023	Q960	Y883	ALA	S761	SER	V627
L1448	L1372	F1296	N1222	P1159	E1091	T1024			GLN	Y762	LEU	F629
	Q1374	F1297	L1223	S1160	S1094	L1025			LYS	T763	HIS	C630
V1452	T1375	E1299	F1224	A1161	L1086	R1026			GLY	L765	ASN	R631
L1463	L1376	G1228	G1228	L1163	V1096	D1027			PHE	A766	PRO	E632
L1464	P1379	Q1231	Q1231	L1165	E1097	G1030			VAL	E767	GLU	I633
H1465	G1383	L1236	L1236	L1166	F1098	R1031			VAL	G769	LEU	L634
N1466	F1384	A1237	A1237	D1167	F1099	C1032			VAL	E769	LYS	P635
I1467	N1385	Q1238	Q1238	L1168	V1100	I1033			VAL	G770	LEU	E636
L1468	L1386	Q1238	Q1238	V1169	F1101	E1035			VAL	N771	PHE	K637
P1469	I1387	P1239	P1239	K1170	E1102	R1034			LEU	A772	LYS	Q638
S1470	G1387	L1245	L1245	L1172	A1103	F1036			HIS	L773	LYS	A639
Q1471	D1388	CYS	CYS	L1173	V1105	L1037			THR	E774	THR	E840
		G1246	G1246	L1173	Y1107	K1038			LYS	E775	ASN	F641
D1474	V1391	P1247	P1247	C1176	S1110	S1040			LYS	S777	THR	F642
L1475	M1392	F1248	F1248	G1177	L1113	I1041			ASN	W776	LYS	E643
H1476	A1393	S1249	S1249	R1178	H1114	Q1042			LEU	S777	THR	E644
	H1394	L1250	L1250	P1179	H1115	Q1043			SER	W778	LYS	E645
V1479	L1395	ALA	ALA	Q1180	A1116	T1044			ASN	Y779	THR	V646
E1482	P1396	Q1251	Q1251	THR	A1116	I1044			GLU	L780	GLY	Y647
	D1397	T1253	T1253	GLU	A1116	T1045			ALA	D781	K712	S648
L1486	V1398	L1254	L1254	CYS	D1117	Q1048			I846	H783	E713	F649
V1487	N1401	L1257	L1257	ARG	E1118	Q1049			S847	V784	V714	S650
Y1488	K1404	D1258	D1258	LYS	K1119	E1050			L848	M785	A715	E852
K1489	Y1411	L1259	L1259	SER	S1120	K1051			E849	M785	V716	E853
G1490	K1404	L1260	L1260	ILE	L1121	S1052			E850	Q786	K717	I654
	Y1411	C1266	C1266	GLU	G1122	P1053			E851	Q787	M718	I655
	L1414	LYS	LYS	LEU	I1124	V1054			R852	Y788	K719	Q656
D1495	L1415	T1271	T1271	PHE	C1127	M1055			R853	Y789	Q720	S657
E1496	H1418	G1272	G1272	THR	C1128	V1056			R854	D791	T721	T658
R1497	L1419	VAL	VAL	LYR	D1129	A929			V855	I792	K723	R659
Q1498	E1273	PRO	PRO	VAL	PHE	A930			V856	L793	D724	L660
C1499	R1421	E1274	E1274		N977	C931			K959	L796	E725	P661
L1500	K1422	T1275	T1275		N988	E832			L859	Y799	L726	E662
P1501					K1000	L934					S728	S664
S1502												
L1503												
D1504												
L1505												

L2361	L2362	C2363	L2364	N2365	N2366	V2367	T2368	P2371	P2372	A2375	D2376	R2377	F2378	N2379	N2380	A2381	V2382	F2383	F2384	L2385	K2388	PHE	HIS	GLY	V2392	L2393	K2394	T2395	L2396	L2397	L2398	E2399	V2400	V2401	L2402	C2403	R2404	V2405	E2406	G2407	E2410	L2411	L2412	F2413	Q2414	L2415	V2418	Q2422	R2425	H2426	E2427	L2428								
N2283	D2284	L2285	P2286	P2287	Y2288	D2289	P2290	Q2291	S2297	E2298	Y2299	A2302	L2303	N2306	Y2312	K2313	E2314	V2315	V2316	A2317	A2318	A2319	A2320	E2321	V2322	L2323	G2324	C2397	L2325	L2326	L2327	R2328	Y2329	V2330	K2334	N2335	L2336	E2343	L2344	V2345	Q2348	L2349	K2350	Q2351	H2352	Q2353	N2354	T2355	L2356	E2357	V2358	D2359	K2360	A2282						
V2205	D2208	L2216	N2217	F2218	L2219	N2220	K2221	L2222	V2223	F2224	H2225	P2226	K2227	R2228	A2229	F2231	R2232	H2233	N2234	L2238	L2241	C2244	C2248	L2249	L2250	L2251	P2252	Y2253	G2254	L2255	E2258	K2259	F2260	S2261	G2262	P2265	N2266	S2267	K2268	S2271	V2272	L2276	G2277	L2278	L2279	N2280	N2281	F2202	T2203	G2204										
L2140	N2141	L2142	R2143	L2144	F2145	L2146	A2147	K2148	L2149	V2150	L2151	N2152	T2153	E2154	E2155	V2156	P2159	K2162	H2163	W2164	L2165	S2166	L2168	L2169	Q2170	L2171	A2172	A2173	S2174	E2175	N2176	N2177	G2178	G2179	L2182	H2183	Y2184	M2185	V2186	V2187	E2188	L2189	V2190	L2193	L2194	S2195	G2198	L2199	A2200	T2201	P2202	T2203	G2204							
V2079	V2080	L2081	E2082	L2083	E2084	M2085	E2086	D2087	L2088	N2089	H2090	C2093	M2094	A2095	P2096	L2097	T2098	A2099	L2100	V2101	K2102	H2103	N2104	H2105	R2106	S2107	L2108	G2109	PRO	GLN	GLY	GLU	ASP	S2117	V2118	P2119	R2120	D2121	L2122	P2123	S2124	W2125	M2126	K2127	F2128	L2129	H2130	G2131	N2134	N2135	P2136	T2137	V2138	P2139						
R2000	K2001	K2002	K2003	Y2004	K2009	E2010	A2011	D2018	G2021	P2022	S2023	Y2024	M2025	S2026	S2027	L2028	L2031	A2032	D2033	S2034	S2037	E2038	S2041	Q2042	F2043	D2044	F2045	S2046	T2047	G2048	V2049	Q2050	S2051	S2055	S2056	Q2057	D2058	P2059	R2060	P2061	A2062	T2063	F2066	R2067	R2068	R2069	E2070	Q2071	H2077	D2078										
L1933	R1937	R1938	L1939	Y1940	H1941	A1944	Y1945	I1949	S1950	V1951	I1952	C1953	C1954	V1955	E1958	L1959	K1960	F1961	Y1962	G1964	L1966	F1967	S1968	E1969	E1972	K1973	N1974	L1975	L1976	I1977	F1978	E1979	N1980	L1981	I1982	D1983	L1984	K1985	L1986	R1987	Y1988	N1989	F1990	P1991	V1992	L1918	C1919	Y1920	F1923	E1999										
ARG	PHE	THR	L1858	F1863	D1864	T1865	Q1866	T1867	L1868	K1869	K1870	M1871	G1872	Y1873	Y1874	K1875	L1876	L1877	D1878	V1879	M1880	Y1881	S1882	R1883	L1884	P1885	K1886	V1889	H1890	A1891	K1892	F1900	H1901	C1904	I1905	T1906	E1907	N1909	E1910	L1911	T1912	K1913	T1914	L1915	I1916	K1917	L1918	C1919	Y1920	F1923	E1930									
THR	GLN	VAL	GLY	LEU	L1798	V1801	Y1802	E1803	F1804	M1805	R1806	K1807	D1808	D1809	P1810	R1811	L1812	S1813	F1814	L1815	R1816	Q1817	S1818	PHE	VAL	ASP	ARG	LEU	LEU	LEU	THR	LEU	LEU	TRP	HIS	CYS	VAL	GLU	ASP	ALA	LEU	LEU	GLU	PHE	GLN	SER	PHE	SER	THR	ILE	VAL	VAL	ASP	ALA	ILE	ASP	VAL	LEU	LYS	SER
S1726	R1727	E1728	F1729	P1730	P1731	G1732	T1733	P1734	R1735	F1736	M1737	N1738	Y1739	V1740	M1743	Y1744	K1745	F1746	L1747	D1748	A1749	L1750	E1751	L1752	L1759	E1760	T1763	GLU	VAL	LEU	CYS	ARG	GLU	GLN	GLN	HIS	VAL	MET	GLU	GLU	ALA	LEU	PHE	ARG	THR	ARG	ILE	ALA	ALA	ARG	ARG	GLY	CYS	VAL						
Q1854	S1857	VAL	SER	PHE	ASN	THR	SER	HIS	GLY	SER	L1524	C1525	F1526	ARG	LEU	VAL	SER	LEU	LEU	LEU	ASN	PRO	ALA	VAL	LEU	SER	THR	ALA	ALA	LEU	GLY	SER	SER	GLN	ALA	G1548	S1549	V1550	T1551	H1552	F1553	S1554	H1555	G1556	E1557	Y1558	F1559	Y1560	S1561	L1562	F1563	S1564	E1565	T1566	I1567	L1571	L1572	K1573		
L1575	D1576	L1577	A1578	V1579	L1580	E1581	L1582	S1585	S1586	V1587	D1588	M1589	T1590	K1591	M1592	V1593	S1594	A1595	V1596	L1597	M1600	A1609	ASN	GLN	LYS	HIS	GLN	GLY	LEU	LYS	ALA	THR	THR	ILE	LEU	GLN	HIS	TRP	LYS	LYS	CYS	D1630	S1637	E1640	A1644	V1645	L1646	L1648	L1649	A1650	K1651									

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D3097	R3098	A3099	K3100	Y3101	Y3102	I3103	Q3104	N3105	G3106	I3107	Q3108	S3109	F3110	M3111	Q3112	N3113	Y3114	I3117	D3118	V3119	L3120	L3121	R3125	L3126	T3127	K3128	L3129	Q3130	A3134	L3135	T3136	E3137	I3138	Q3139	F3140	H3070	G3071	E3072	L3073	A3076	I3077	L3078	E3079	L3080	H3081	Y3082	E3085	L3088	L3091	L3092	Q3093	D3094					
L2801	F2802	K2806	Q2807	L2808	F2809	L2812	F2813	S2814	G2815	I2816	M2820	D2821	F2823	L2826	T2833	L2836	F2840	M2841	R2842	F2843	L2844	N2845	T2846	S2849	F2850	F2851	P2852	F2853	V2855	L2858	Q2859	D2860	I2861	H2865	A2866	A2867	L2868	L2869	S2870	D2871	F2873	A2874	A2875	V2876	S2877	A2878											
G2879	C2880	L2884	P2887	T2890	R2891	L2892	L2897	L2898	R2899	L2900	LEU	PRO	ALA	GLU	LEU	PRO	V2910	R2911	G2912	K2913	A2914	R2915	L2916	P2917	P2918	V2919	D2920	L2921	R2922	W2923	V2924	E2925	L2926	ALA	L2929	Y2930	R2931	S2932	I2933	G2934	D2937	V2938	L2939	R2940	G2941	T2942	F2943	T2944	S2945	E2946							
L2947	G2948	T2949	K2950	Q2951	L2952	T2953	Q2954	S2955	L2958	A2959	E2960	E2967	Q2971	E2974	A2975	L2976	N2977	Q2978	Q2979	D2980	D2983	P2986	T2987	E2988	A2989	E2990	K2991	D2992	F2993	W2994	E2995	S2998	L2999	D3000	C3001	Y3002	N3003	H3004	L3005	A3006	E3007	L3011	E3012	Y3013	I3019	D3020	S3021	P3024									
D3026	L3027	I3030	E3033	P3034	F3035	Y3036	Q3037	E3038	T3039	P3042	T3045	R3046	S3047	K3048	L3049	K3050	L3052	Q3054	G3055	E3056	A3057	S3060	L3061	L3062	T3063	I3065	D3066	K3067	A3068	W3069	H3070	G3071	E3072	L3073	A3076	I3077	L3078	E3079	L3080	H3081	Y3082	E3085	L3088	L3091	L3092	Q3093	D3094										
D3097	R3098	A3099	K3100	Y3101	Y3102	I3103	Q3104	N3105	G3106	I3107	Q3108	S3109	F3110	M3111	Q3112	N3113	Y3114	I3117	D3118	V3119	L3120	L3121	R3125	L3126	T3127	K3128	L3129	Q3130	A3134	L3135	T3136	E3137	I3138	Q3139	F3140	H3070	G3071	E3072	L3073	A3076	I3077	L3078	E3079	L3080	H3081	Y3082	E3085	L3088	L3091	L3092	Q3093	D3094					
L2429	E2430	R2431	Q2432	K2433	V2434	C2435	L2436	D2437	L2438	L2439	Y2440	K2441	H2442	R2443	K2445	P2448	L2451	R2452	F2453	L2454	P2457	V2458	V2459	E2460	F2461	V2462	S2463	H2464	F2465	S2466	C2469	R2470	E2471	L2536	Q2472	R2473	V2474	N2475	L2476	L2477	N2478	V2479	I2480	H2481	D2482	N2483	V2484	R2485	D2486	F2487	E2488	S2489	L2490	T2491	D2492		
N2493	D2494	S2495	Q2496	F2499	K2500	K2503	D2504	L2505	V2506	L2507	L2510	I2511	D2512	E2513	N2514	L2517	Q2518	L2519	I2520	L2521	R2522	N2523	F2524	W2525	S2526	H2527	E2528	L2529	R2530	S2533	N2534	T2535	L2536	D2537	R2538	L2539	L2542	N2543	S2544	L2545	Y2546	S2547	K2549	V2552	H2553	F2554	L2555	S2556	L2557	A2558	T2559						
N2560	F2561	L2562	E2564	M2565	T2566	M2568	S2569	P2570	D2571	Y2572	P2573	N2574	PRO	MET	PHE	GLU	HIS	PRO	LEU	SER	GLU	CYS	GLU	PHE	GLN	GLY	THR	ASP	ASP	ASP	TRP	ARG	PHE	LEU	ARG	SER	THR	VAL	LEU	PRO	MET	PHE	VAL	GLU	THR	GLN	ALA	SER	PRO	GLN	SER	GLY	THR	LEU	GLN	THR	ARG
THR	GLN	GLY	GLY	SER	LEU	SER	ALA	ARG	TRP	PRO	VAL	ALA	PRO	VAL	PRO	ASP	PHE	GLY	LYS	LYS	ASP	PHE	LEU	GLY	GLN	ASP	VAL	GLY	ASN	LYS	VAL	LYS	GLY	ALA	ALA	THR	GLY	ARG	THR	ASP	LEU	ARG	ARG	ARG	PHE	MET	THR	ARG	ASP	GLN	GLY	LYS	LEU	LEU			
SER	LEU	MET	TRP	ARG	ALA	LYS	VAL	ALA	GLU	GLN	LYS	ARG	GLU	LYS	ILE	GLU	GLY	VAL	PRO	ASP	PHE	GLY	GLN	HIS	LYS	LYS	MET	LYS	GLN	ASP	VAL	LYS	VAL	LYS	GLY	THR	THR	ASP	LEU	ARG	ARG	ARG	ARG	PHE	MET	THR	ARG	ASP	GLN	GLY	LYS	LEU	LEU				
L2776	H2777	G2778	D2779	L2780	P2781	D2782	I2783	K2786	H2787	S2788	S2789	L2790	I2791	T2792	P2793	L2794	Q2795	A2796	V2797	A2798	S2799	R2800																																			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (\AA)	241.6, 241.6, 241.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.51, 1.51, 1.51	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	0.33	0/25994	0.59	18/35463 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	GLU	C-N-CD	8.55	146.35	128.40
1	A	1070	PRO	CA-N-CD	-7.38	101.16	111.50
1	A	560	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	644	PRO	CA-N-CD	-6.82	101.95	111.50
1	A	1812	LEU	CA-CB-CG	6.69	130.68	115.30

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	25559	0	23509	2005	0
All	All	25559	0	23509	2005	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 41.

The worst 5 of 2005 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:2546:TYR:CD1	1:A:2554:PHE:CE1	1.81	1.66
1:A:995:PHE:CZ	1:A:1003:SER:N	1.69	1.57
1:A:660:LEU:HD11	1:A:733:LEU:CD2	1.34	1.54
1:A:488:ILE:HG23	1:A:616:LYS:CE	1.36	1.53
1:A:708:VAL:HG22	1:A:712:LYS:CE	1.33	1.52

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	3511/4128 (85%)	2776 (79%)	547 (16%)	188 (5%)	1 15

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	THR
1	A	565	TYR
1	A	623	PHE
1	A	624	ILE
1	A	638	GLN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2460/3671 (67%)	2374 (96%)	86 (4%)	31 52

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2554	PHE
1	A	3411	ASP
1	A	2566	THR
1	A	3114	TYR
1	A	3493	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3278	GLN
1	A	3291	GLN
1	A	3927	ASN
1	A	3515	GLN
1	A	993	HIS

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](#)

There are no chain breaks in this entry.

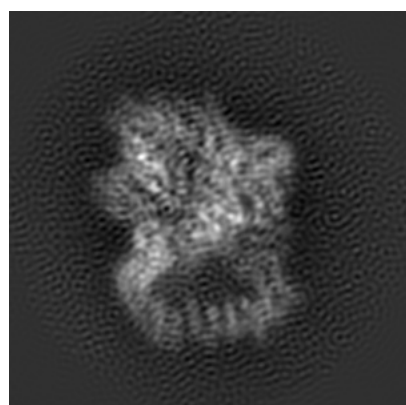
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8751. These allow visual inspection of the internal detail of the map and identification of artifacts.

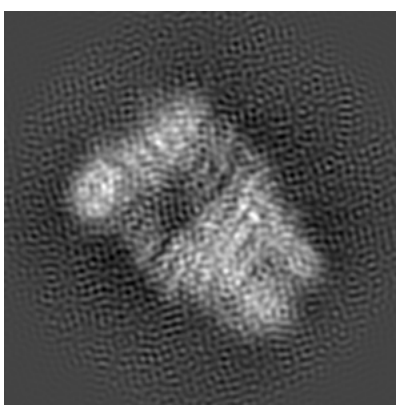
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

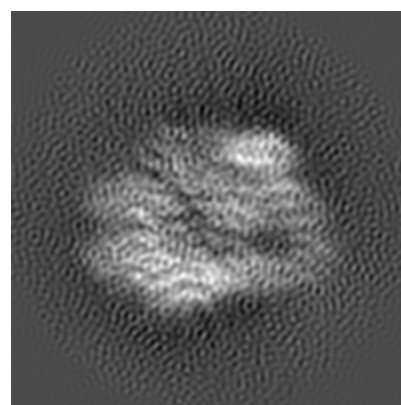
6.1.1 Primary map



X



Y

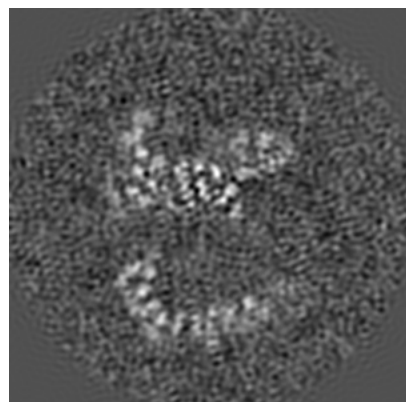


Z

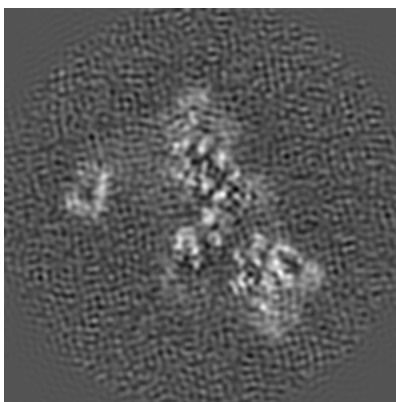
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

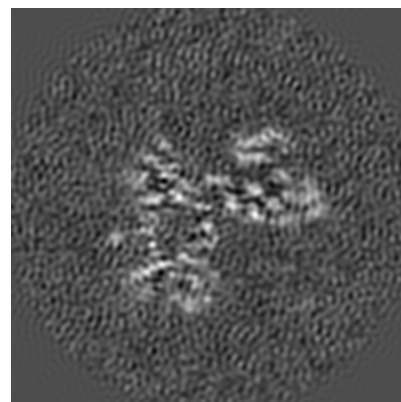
6.2.1 Primary map



X Index: 80



Y Index: 80

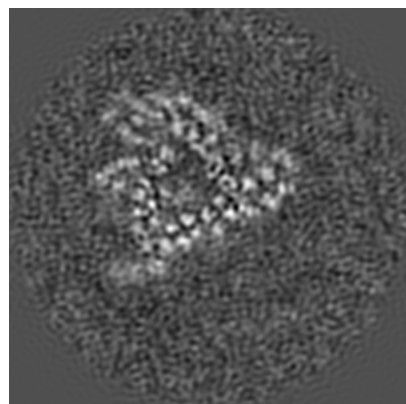


Z Index: 80

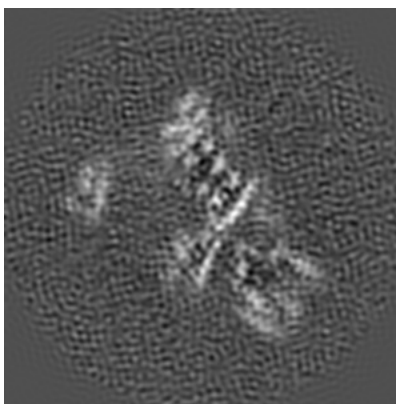
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

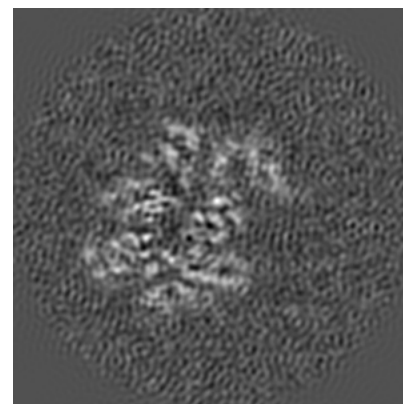
6.3.1 Primary map



X Index: 61



Y Index: 82

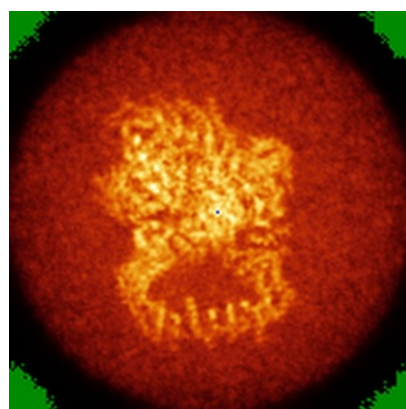


Z Index: 95

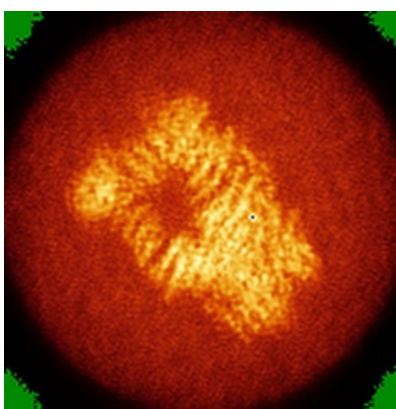
The images above show the largest variance slices of the map in three orthogonal directions.

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

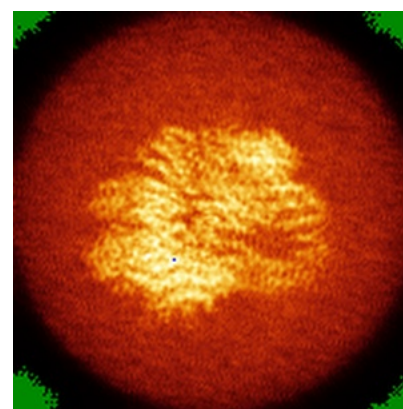
6.4.1 Primary map



X



Y

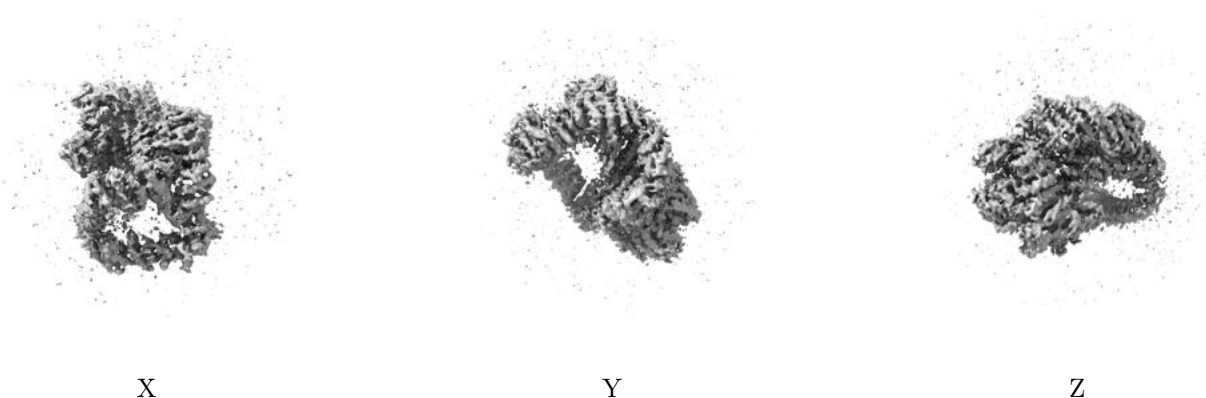


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

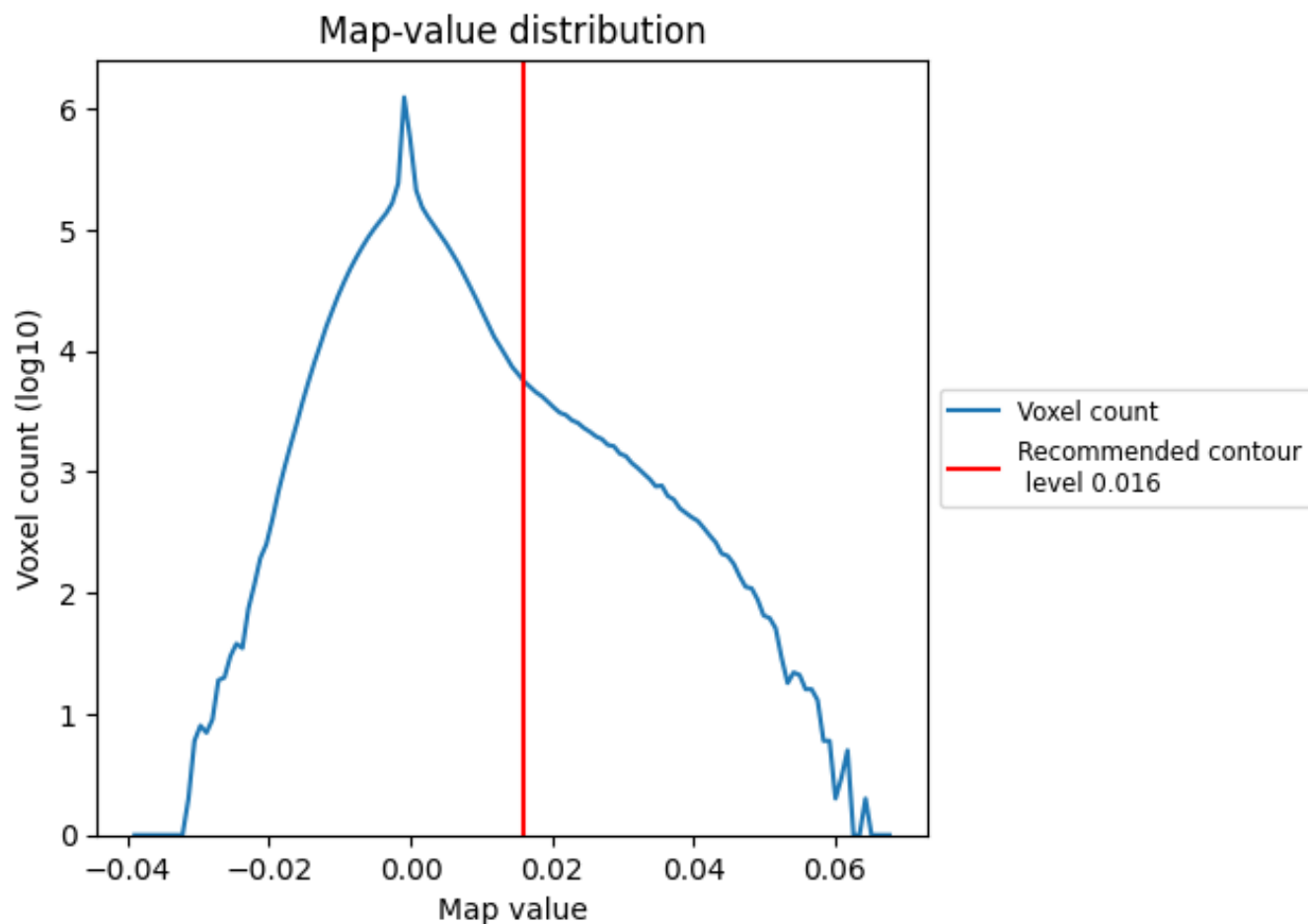
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

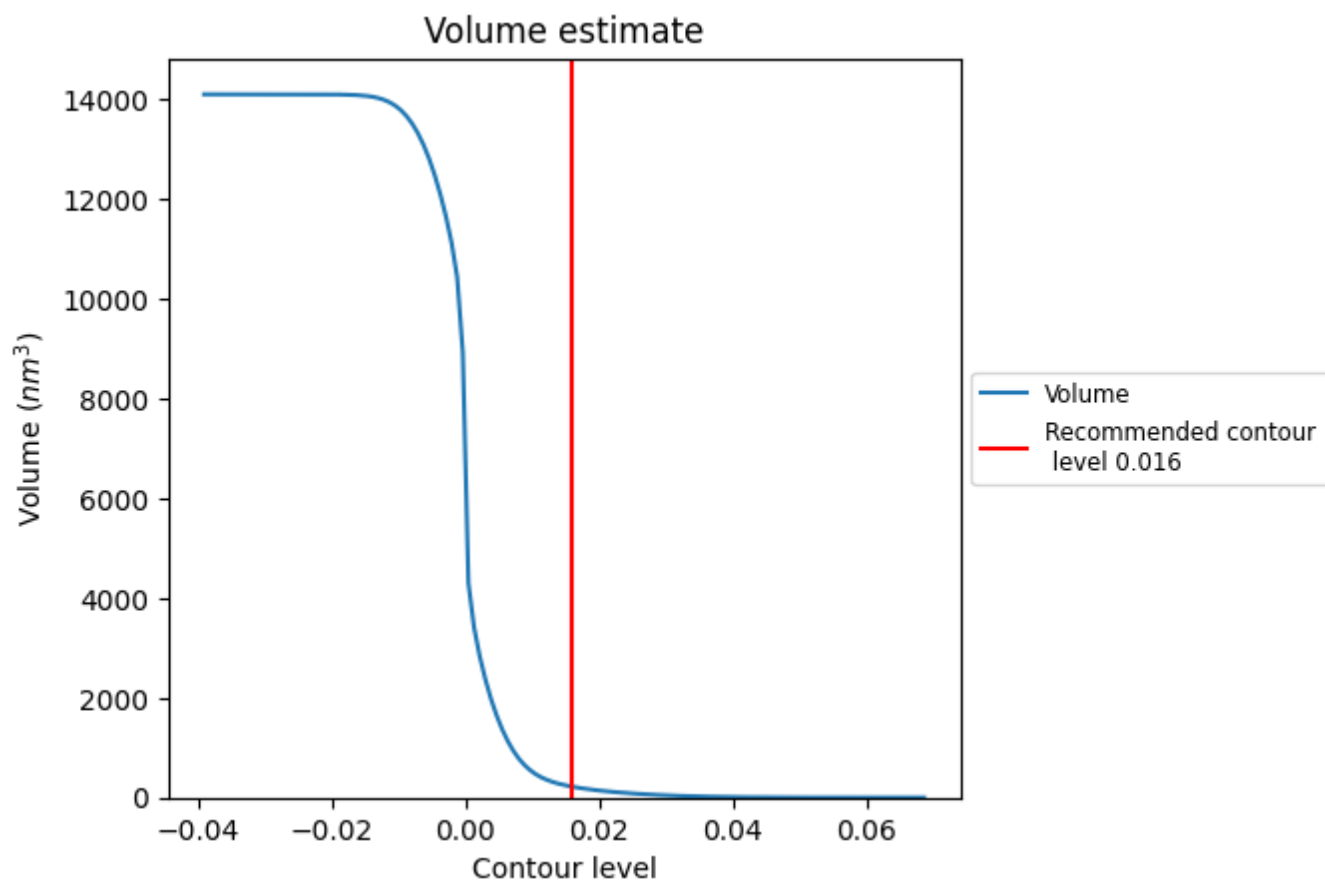
This section contains the results of statistical analysis of the map.

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.

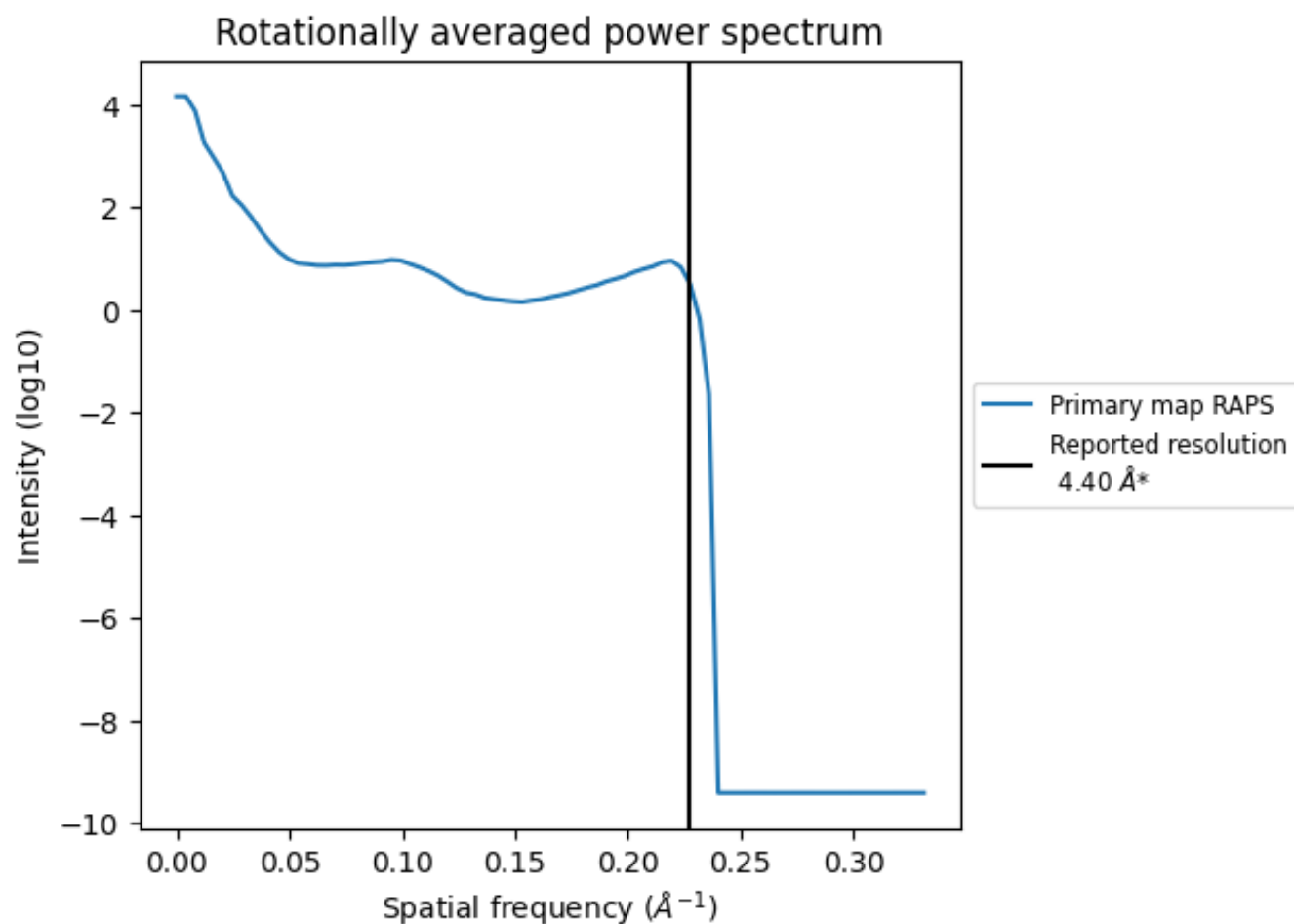
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 197 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 0.227 Å⁻¹

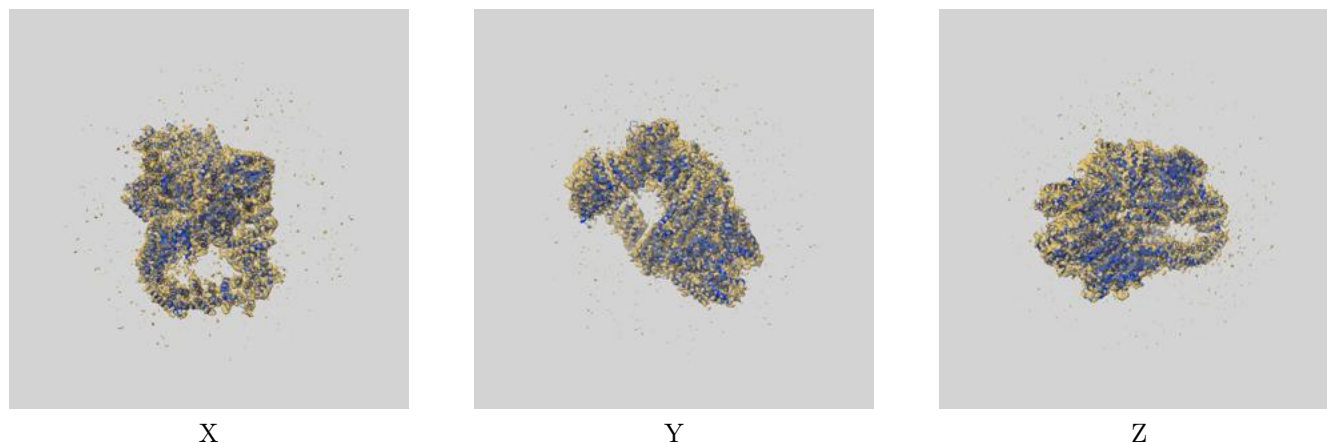
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

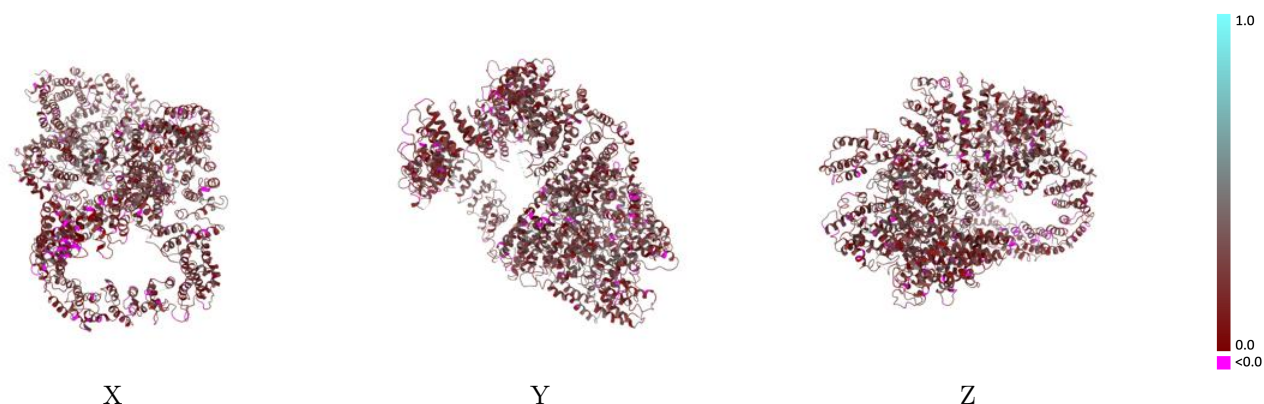
This section contains information regarding the fit between EMDB map EMD-8751 and PDB model 5W1R. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



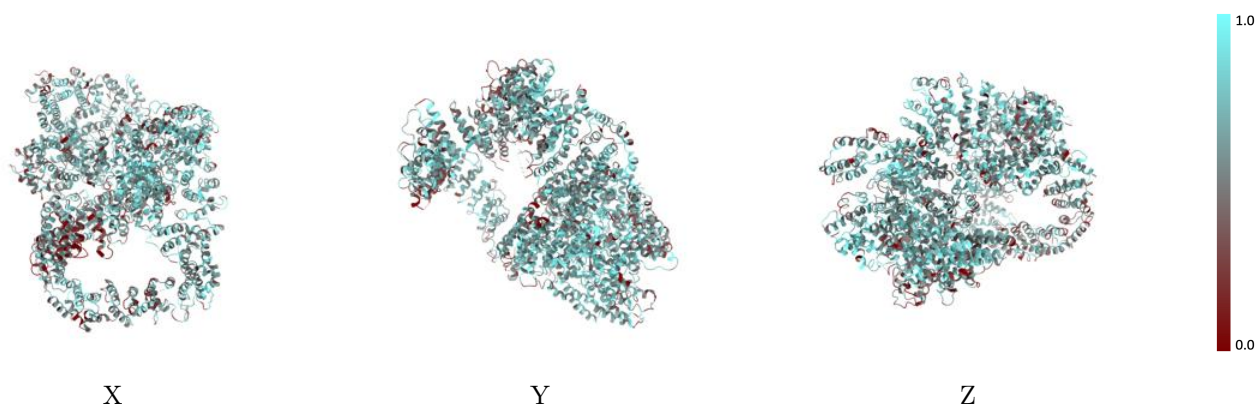
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



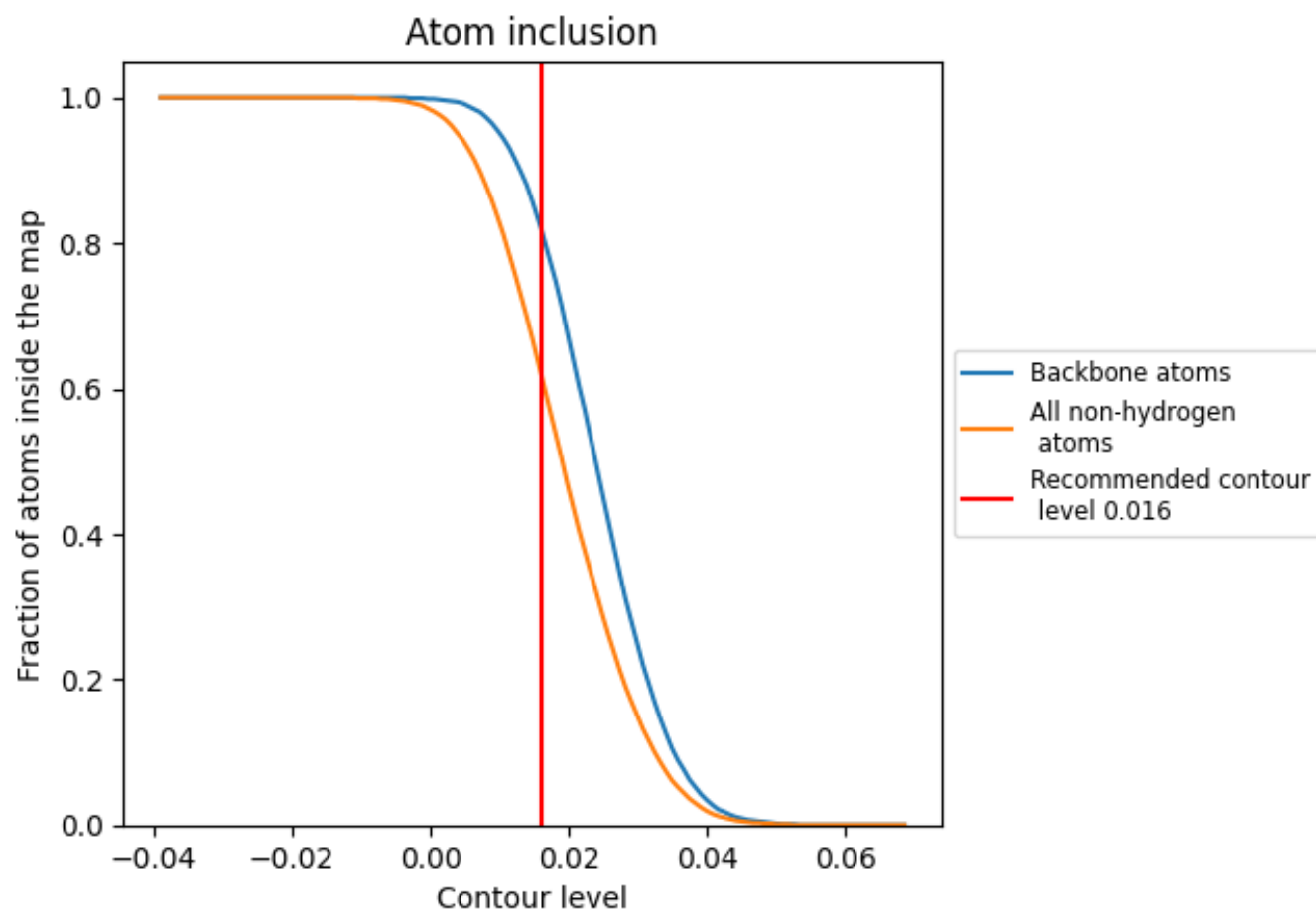
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6210	<div></div> 0.2350
A	<div></div> 0.6210	<div></div> 0.2350

