



wwPDB EM Validation Summary Report ⓘ

May 12, 2025 – 06:55 PM EDT

PDB ID : 5W1R / pdb_00005w1r
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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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
MolProbity : 4-5-2 with Phenix2.0rc1
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

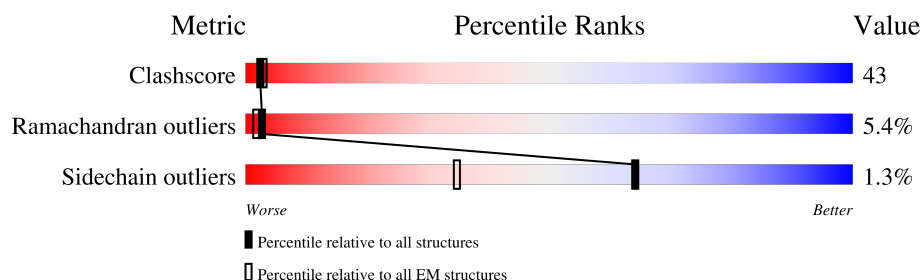
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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



L1419	L1420	E1421	L1422	I1423	T1424	N1350	T1351	Q1426	S1427	P1353	E1354	K1357	L1358	A1433	V1434	N1435	L1436	Y1437	G1438	P1439	D1440	A1441	R1442	L1443	A1449	V1452	S1453	L1463	L1464	H1465	L1466	L1467	P1469	S1470	Q1471	D1474	L1475	H1476	V1479	E1482	L1486	Y1487	K1489	G1490	D1495	E1496	K1497	C1499																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
R1340	I1341	M1342	E1343	F1344																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

T2355	T2356	G2276	L2277	K2200	L2201	T2202	T2203	G2204	V2205	D2208	L2216	N2217	F2218	L2219	N2220	K2221	L2222	V2223	F2224	H2225	P2226	K2227	L2228	A2229	V2230	F2231	H2232	K2233	N2234	L2238	L2239	L2241	C2244	D2247	C2248	L2249	G2324	L2325	L2326	L2327	R2328	Y2329	V2330	K2334	N2335	L2336	E2343	L2344	V2345	Q2348	L2349	K2350	Q2351	H2352	Q2353	N2354
G2363	L2364	N2365	V2366	T2367	T2368	K2369	S2370	F2371	P2372	A2375	D2376	F2377	N2378	N2379	N2380	A2381	V2382	F2383	F2384	L2385	L2386	P2387	P2388	PHE	HIS	GLY	V2392	L2393	L2394	T2395	L2396	C2397	L2398	E2399	V2400	L2402	C2403	R2404	V2405	G2407	E2410	L2411	T2412	F2413	Q2414	L2415										
N2135	F2136	V2137	V2138	P2139	L2140	N2141	T2142	K2143	F2144	L2145	A2146	K2147	K2148	L2149	V2150	L2151	N2152	T2153	E2154	E2155	V2156	P2159	K2162	H2163	W2164	L2165	S2166	T2167	L2168	L2169	Q2170	L2171	A2172	A2173	S2174	E2175	N2176	N2177	G2178	G2179	I2182	H2183	Y2184	M2185	V2186	L2187	E2188	L2189	V2190	I2193	L2194	S2195	G2198	L2199		
E2070	Q2071	H2077	D2078	D2079	V2080	L2081	L2083	L2084	N2085	D2086	E2087	L2088	N2089	R2090	H2091	E2092	C2093	N2094	A2095	P2096	L2097	T2098	A2099	L2100	V2101	K2102	H2103	M2104	H2105	R2106	S2107	L2108	G2109	PRO	GLN	GLY	GLU	GLU	ASP	S2117	V2118	P2119	R2120	D2121	L2122	P2123	S2124	W2125	M2126	F2127	L2128	H2130	G2131	G2134		
V1994	E1995	V1996	E1999	R2000	K2001	L1933	R1937	R1938	L1939	H1941	A1944	Y1945	I1949	S1950	V1951	I1952	C1953	C1954	V1955	E1958	L1959	K1960	F1961	Y1962	Q1963	G1964	F1965	L1966	F1967	S1968	V1889	H1890	A1891	K1892	F1900	H1901	C1904	I1905	T1906	E1907	G1908	N1909	E1910	L1911	R1986	L1987	Y1988	N1989	F1990	P1991	V1992	E1993				
ASP	VAL	LEU	LYS	ARG	PHE	THR	K1857	L1858	F1863	D1864	T1865	Q1866	T1868	K1869	M1870	G1872	Y1873	K1875	I1876	D1877	D1878	M1879	F1881	S1882	L1883	L1884	P1885	K1886	V1889	H1890	A1891	K1892	F1900	H1901	C1904	I1905	T1906	E1907	G1908	N1909	E1910	L1911	R1986	L1987	Y1988	N1989	F1990	P1991	V1992	E1993						
ARG	GLY	SER	CYS	VAL	THR	GLN	VAL	GLY	L1798	V1801	E1802	E1803	M1804	F1805	R1806	K1807	D1808	D1809	P1810	R1811	L1812	S1813	F1814	A1815	T1816	Q1817	S1818	PHE	VAL	ASP	ARG	SER	LEU	THR	LEU	LEU	TRP	HIS	CYS	SER	LEU	ASP	ALA	LEU	ARG	GLU	PHE	SER	THR	ILE	VAL	ASP	ALA	ILE		
F1722	M1723	Q1725	R1726	R1727	E1728	F1729	P1730	P1731	G1732	T1733	P1734	R1735	F1736	N1737	Y1738	V1740	M1743	K1744	K1745	F1746	L1747	D1748	A1749	L1750	E1751	L1752	L1759	E1760	T1763	GLU	VAL	LEU	CYS	ARG	GLU	GLN	HIS	VAL	MET	GLU	GLU	PHE	GLN	SER	PHE	ARG	ILE	ALA	ARG							
A1647	L1648	A1649	K1651	Q1654	S1658	VAL	SER	PHE	ASN	THR	SER	HIS	GLY	TYR	I1676	S1677	L1678	L1679	A1680	D1681	K1682	L1683	D1684	D1685	L1686	L1687	L1688	Q1691	T1694	L1695	L1696	P1697	F1698	S1706	L1707	E1708	E1709	L1710	R1711	R1712	L1713	V1714	Q1715	Q1716	L1717											
I1567	L1571	L1572	N1574	L1575	D1576	L1577	A1578	V1579	L1580	E1581	L1582	S1585	S1586	V1587	D1588	N1589	K1591	M1592	V1593	S1594	A1595	V1596	N1597	N1598	G1599	M1600	A1609	ASN	GLN	LYS	HIS	GLN	LEU	LEU	LEU	LEU	ALA	THR	THR	ILE	GLN	HIS	TRP	LYS	LYS	CYS	D1630	E1640	A1644	V1645	L1646					
L1500	F1501	S1502	L1503	D1504	L1505	S1506	C1507	K1508	Q1509	L1510	A1511	F1519	A1520	F1521	L1524	C1525	E1526	ARG	LEU	VAL	SER	LEU	SER	LEU	LEU	LEU	THR	THR	ALA	ALA	SER	SER	GLY	SER	GLN	G1548	S1549	V1550	I1551	H1552	F1553	S1554	H1555	G1556	E1557	Y1558	F1559	Y1560	S1561	L1562	F1563	E1564	T1566			



G4097	L4098	S4099	E4100	T4102	Q4103	V4104	L4107	M4108	D4109	Q4110	A4111	I4116	L4117	G4118	R4119	T4120	W4121	W4124	E4125	P4126	W4127	MET																																		
N4032	V4033	A4034	E4035	K4036	N4037	V4038	Y4039	P4040	R4041	Q4042	K4043	I4044	C4045	Y4046	A4047	K4048	R4049	K4050	L4051	A4052	G4053	N4054	N4055	P4056	A4057	V4058	L4059	T4060	G4061	D4062	L4065	L4066	K4070	A4071	P4072	A4073	F4074	R4075	D4076	W4077	V4078	A4079	V4080	A4081	A4082	G4083	S4084	K4085	D4086	H4087	N4088	I4089	A4090	A4091	E4095	S4096
R3965	Q3966	F3967	I3968	N3969	L3970	N3971	L3972	P3973	N3974	K3975	E3976	T3977	G3978	L3979	M3980	Y3981	S3982	T3983	M3984	A3987	K3991	S3992	S3993	D3994	P3995	G3996	L3997	L3998	T4001	M4002	V4006	K4007	E4008	P4009	S4010	F4011	D4012	W4013	K4014	M4015	Q4018	K4019	M4020	L4021	K4022	K4023	G4024	G4025	I4028	Q4029	E4030	I4031				
T3892	S3893	F3897	L3898	A3899	L3900	R3901	S3902	H3903	F3904	A3905	S3906	S3907	H3908	A3909	L3910	T3911	C3912	I3913	H3915	K3916	T3917	L3918	G3919	R3920	G3921	D3922	R3923	H3924	N3925	N3926	N3927	V3930	A3931	T3934	G3935	G3936	V3937	I3938	H3944	G3947	S3948	F3952	L3953	P3954	V3955	M3959	F3961	R3962	T3963	T3964						
R3733	R3734	P3735	K3736	R3737	I3738	L3739	R3740	R3741	G3742	H3743	D3744	E3745	P3749	F3750	L3758	D3761	Q3762	R3763	V3764	E3765	T3766	L3767	F3768	Q3769	V3770	M3771	N3772	G3773	I3774	L3775	A3776	Q3777	D3778	A3785	L3786	Q3787	L3788	R3789	Y3790	Y3791	S3792	P3795	K3796	T3797	S3798	R3799	E3804	W3805	L3806	E3807	N3808	T3809				
L3812	K3813	L3816	L3817	L3818	T3819	R3820	S3821	Q3822	G3823	E3824	K3825	A3826	A3827	Y3828	L3829	S3830	D3831	P3832	R3833	A3834	P3835	P3836	C3837	E3838	F3839	K3840	L3843	T3844	S3847	D3851	M3856	L3857	M3858	Y3859	K3860	R3864	E3875	S3876	K3877	V3878	P3879	A3880	D3881	L3882	L3883	K3884	R3885	A3886	F3887	M3890	S3891					
T3892	S3893	F3897	L3898	A3899	L3900	R3901	S3902	H3903	F3904	A3905	S3906	S3907	H3908	A3909	L3910	T3911	C3912	I3913	H3915	K3916	T3917	L3918	G3919	R3920	G3921	D3922	R3923	H3924	N3925	N3926	N3927	V3930	A3931	T3934	G3935	G3936	V3937	I3938	H3944	G3947	S3948	F3952	L3953	P3954	V3955	M3959	F3961	R3962	T3963	T3964						
R3965	Q3966	F3967	I3968	N3969	L3970	N3971	L3972	P3973	N3974	K3975	E3976	T3977	G3978	L3979	M3980	Y3981	S3982	T3983	M3984	A3987	K3991	S3992	S3993	D3994	P3995	G3996	L3997	L3998	T4001	M4002	V4006	K4007	E4008	P4009	S4010	F4011	D4012	W4013	K4014	M4015	Q4018	K4019	M4020	L4021	K4022	K4023	G4024	G4025	I4028	Q4029	E4030	I4031				
N4032	V4033	A4034	E4035	K4036	N4037	V4038	Y4039	P4040	R4041	Q4042	K4043	I4044	C4045	Y4046	A4047	K4048	R4049	K4050	L4051	A4052	G4053	N4054	N4055	P4056	A4057	V4058	L4059	T4060	G4061	D4062	L4065	L4066	K4070	A4071	P4072	A4073	F4074	R4075	D4076	W4077	V4078	A4079	V4080	A4081	A4082	G4083	S4084	K4085	D4086	H4087	N4088	I4089	A4090	A4091	E4095	S4096
SER	SER	SER	GLU	ASP	SER	GLU	LYS	V3373	I3374	A3375	G3376	L3377	Q3378	R3380	A3381	S3386	E3387	A3388	V3389	Q3390	A3391	A3392	E3393	E3394	E3395	A3396	Q3397	P3398	P3399	S3400	W3401	G3404	P3405	A3406	A3407	G3408	V3409	I3410	Y3413	M3414	T3415	L3416	A3417	C3420	Q3423	L3424	R3425	K3426	E3427	N3430	GLU	LEU	SER			
V3433	I3434	D3435	S3436	A3437	E3438	L3439	Q3440	P3443	A3444	L3445	V3446	V3447	E3448	K3449	M3450	L3451	N3457	S3458	N3459	E3460	A3461	R3462	L3463	K3464	F3465	P3466	I3471	I3472	P3476	E3477	E3478	T3479	L3480	S3481	L3482	E3486	I3487	S3488	SER	VAL	C3492	W3493	F3495	I3496	S3497	W3498	L3499	S3500	H3501	M3502	V3503	A3504				
L3505	L3506	D3509	Q3510	A3511	V3512	A3513	V3514	Q3515	H3516	S3517	V3518	E3519	E3520	I3521	T3522	D3523	N3524	Y3525	P3526	V3530	Y3531	P3532	F3533	T3534	L3535	S3536	S3537	E3538	S3539	V3540	S3541	N3551	K3552	E3553	R3557	I3558	K3559	S3560	K3561	L3562	D3563	Q3564	G3565	G3566	W3567	F3568	Q3569	A3574	L3575	D3576	S3579	K3580	P3581			
E3682	F3685	K3686	W3687	W3688	R3689	A3694	K3698	T3699	K3603	K3604	N3605	L3606	E3607	Y3610	Y3614	L3617	G3618	D3619	P3620	K3621	A3622	P3623	G3626	A3627	F3628	R3629	R3630	K3631	F3632	I3633	Q3634	F3635	F3636	G3637	F3640	D3641	F3644	G3645	K3646	S3649	L3655	L3656	S3657	L3658	V3659	A3674	L3675	D3676	S3679	K3680	P3681					
N3660	D3661	T3662	T3663	K3664	K3665	K3670	N3671	K3672	K3675	P3676	P3677	L3680	K3681	E3682	C3683	S3684	P3685	W3686	K3687	S3688	D3689	V3692	E3693	F3694	L3695	K3696	N3697	GLU	LEU	GLU	ILE	P3702	G3703	Q3704	Y3705	D3706	G3707	K3710	P3711	L3712	Y3715	R3718	L3719	A3720	E3724	R3725	K3730	S3731	L3732							
R3733	R3734	P3735	K3736	R3737	I3738	L3739	R3740	R3741	G3742	H3743	D3744	E3745	P3749	F3750	L3758	D3761	Q3762	R3763	V3764	E3765	T3766	L3767	F3768	Q3769	V3770	M3771	N3772	G3773	I3774	L3775	A3776	Q3777	D3778	A3785	L3786	Q3787	L3788	R3789	Y3790	Y3791	S3792	P3795	K3796	T3797	S3798	R3799	E3804	W3805	L3806	E3807	N3808	T3809				
L3812	K3813	L3816	L3817	L3818	T3819	R3820	S3821	Q3822	G3823	E3824	K3825	A3826	A3827	Y3828	L3829	S3830	D3831	P3832	R3833	A3834	P3835	P3836	C3837	E3838	F3839	K3840	L3843	T3844	S3847	D3851	M3856	L3857	M3858	Y3859	K3860	R3864	E3875	S3876	K3877	V3878	P3879	A3880	D3881	L3882	L3883	K3884	R3885	A3886	F3887	M3890	S3891					
T3892	S3893	F3897	L3898	A3899	L3900	R3901	S3902	H3903	F3904	A3905	S3906	S3907	H3908	A3909	L3910	T3911	C3912	I3913	H3915	K3916	T3917	L3918	G3919	R3920	G3921	D3922	R3923	H3924	N3925	N3926	N3927	V3930	A3931	T3934	G3935	G3936	V3937	I3938	H3944	G3947	S3948	F3952	L3953	P3954	V3955	M3959	F3961	R3962	T3963	T3964						
R3965	Q3966	F3967	I3968	N3969	L3970	N3971	L3972	P3973	N3974	K3975	E3976	T3977	G3978	L3979	M3980	Y3981	S3982	T3983	M3984	A3987	K3991	S3992	S3993	D3994	P3995	G3996	L3997	L3998	T4001	M4002	V4006	K4007	E4008	P4009	S4010	F4011	D4012	W4013	K4014	M4015	Q4018	K4019	M4020	L4021	K4022	K4023	G4024	G4025	I4028	Q4029	E4030	I4031				
N4032	V4033	A4034	E4035	K4036	N4037	V4038	Y4039	P4040	R4041	Q4042	K4043	I4044	C4045	Y4046	A4047	K4048	R4049	K4050	L4051	A4052	G4053	N4054	N4055	P4056	A4057	V4058	L4059	T4060	G4061	D4062	L4065	L4066	K4070	A4071	P4072	A4073	F4074	R4075	D4076	W4077	V4078	A4079	V4080	A4081	A4082	G4083	S4084	K4085	D4086	H4087	N4088	I4089	A4090	A4091	E4095	S4096

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	0.31	8/25994 (0.0%)	0.74	69/35463 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3568	ILE	CA-C	6.95	1.61	1.52
1	A	3580	ASN	N-CA	6.42	1.55	1.45
1	A	1342	MET	SD-CE	6.37	1.95	1.79
1	A	3576	ASP	C-O	5.67	1.30	1.24
1	A	643	GLU	C-N	5.64	1.41	1.34

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	PHE	N-CA-C	10.57	122.80	111.28
1	A	3316	LEU	N-CA-C	-9.85	100.62	111.36
1	A	3580	ASN	N-CA-C	9.80	125.09	110.10
1	A	3348	LEU	N-CA-C	9.36	121.25	111.14
1	A	654	ILE	N-CA-C	9.00	119.81	110.72

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	2101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25559	0	23509	2101	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 43.

The worst 5 of 2101 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2460/3671 (67%)	2429 (99%)	31 (1%)	65 77

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1959	LEU
1	A	3568	ILE
1	A	2312	TYR
1	A	3953	LEU
1	A	3416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1466	ASN
1	A	2527	HIS
1	A	3927	ASN
1	A	1941	HIS
1	A	3278	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](#)

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.

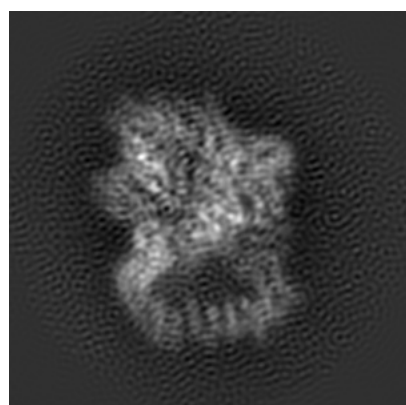
6 Map visualisation [i](#)

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.

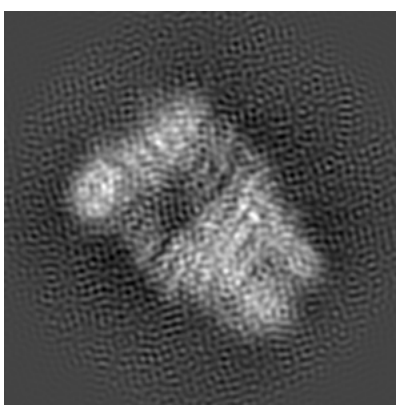
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

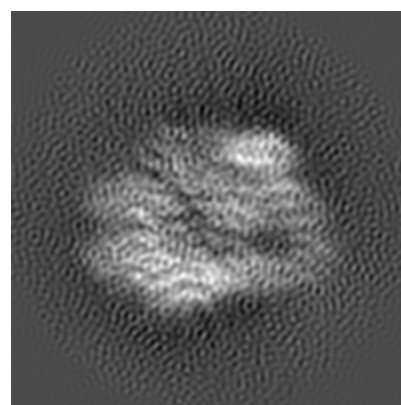
6.1.1 Primary map



X



Y

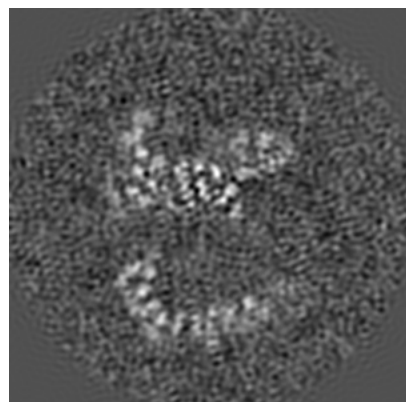


Z

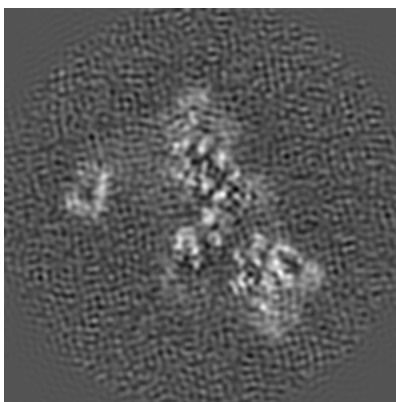
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

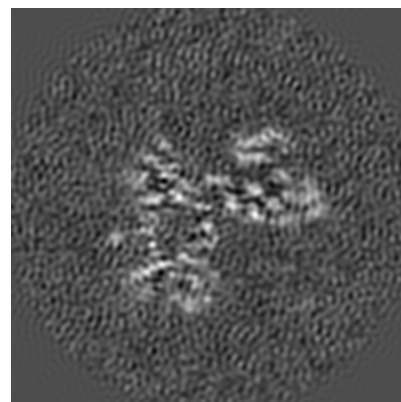
6.2.1 Primary map



X Index: 80



Y Index: 80

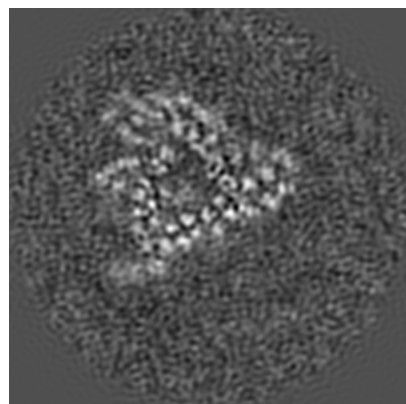


Z Index: 80

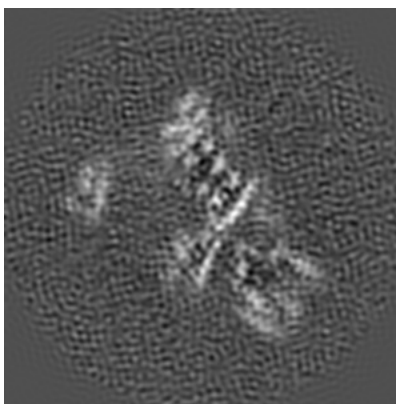
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

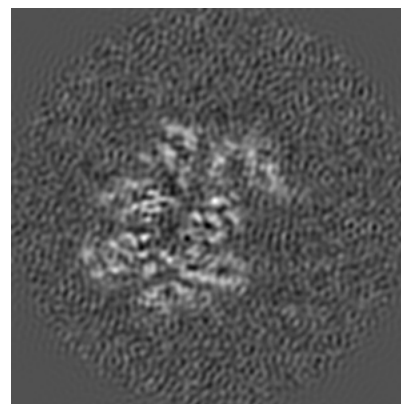
6.3.1 Primary map



X Index: 61



Y Index: 82

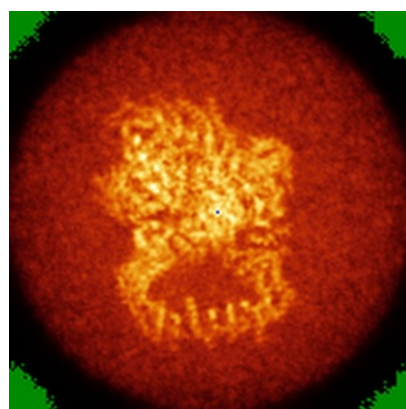


Z Index: 95

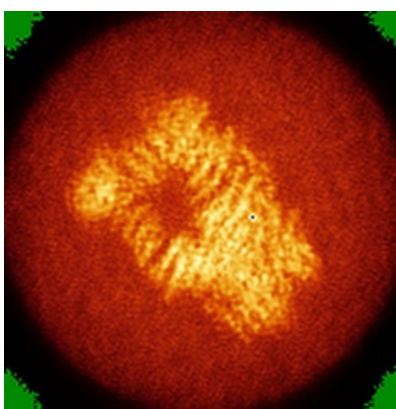
The images above show the largest variance slices of the map in three orthogonal directions.

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

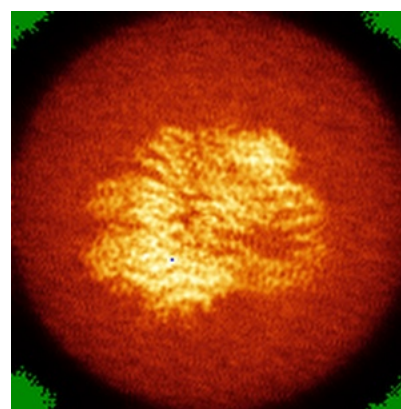
6.4.1 Primary map



X



Y

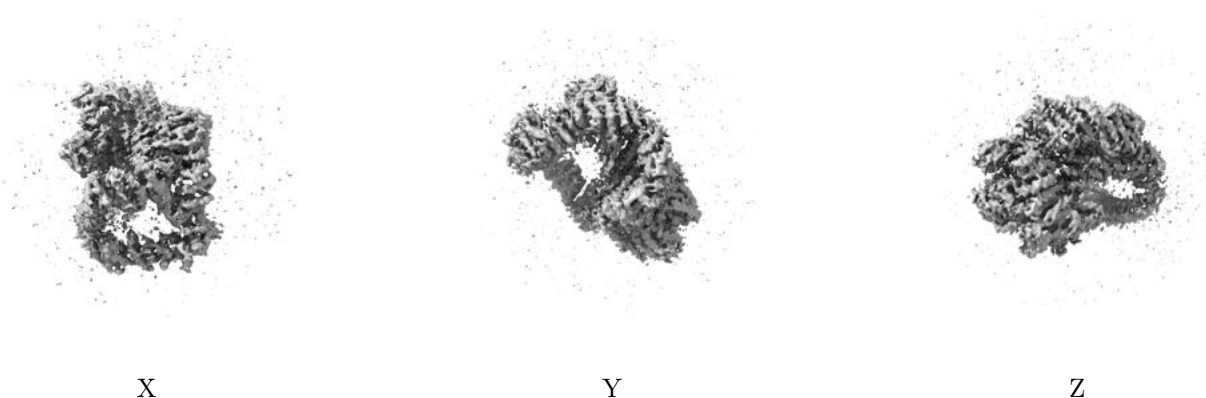


Z

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.

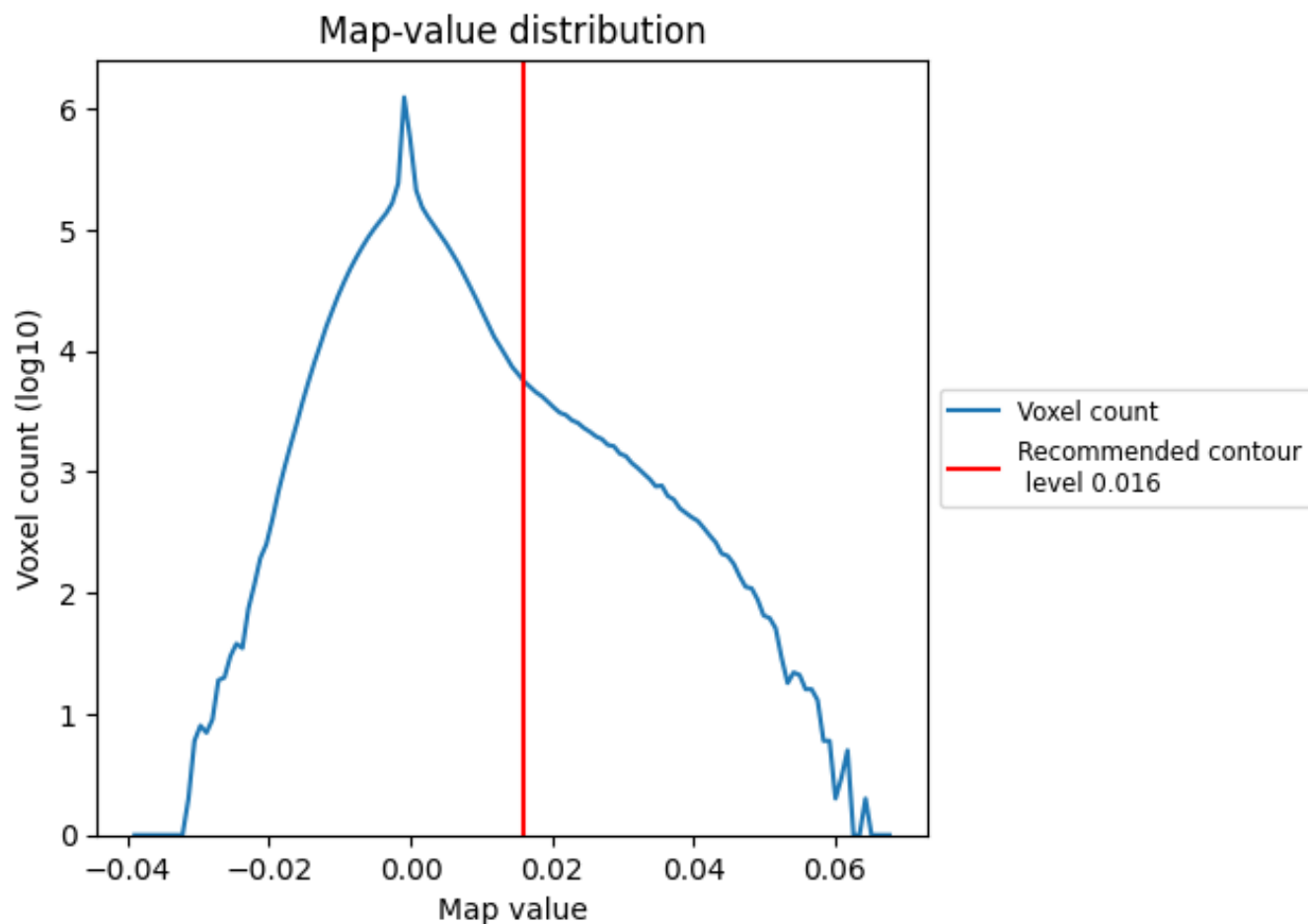
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

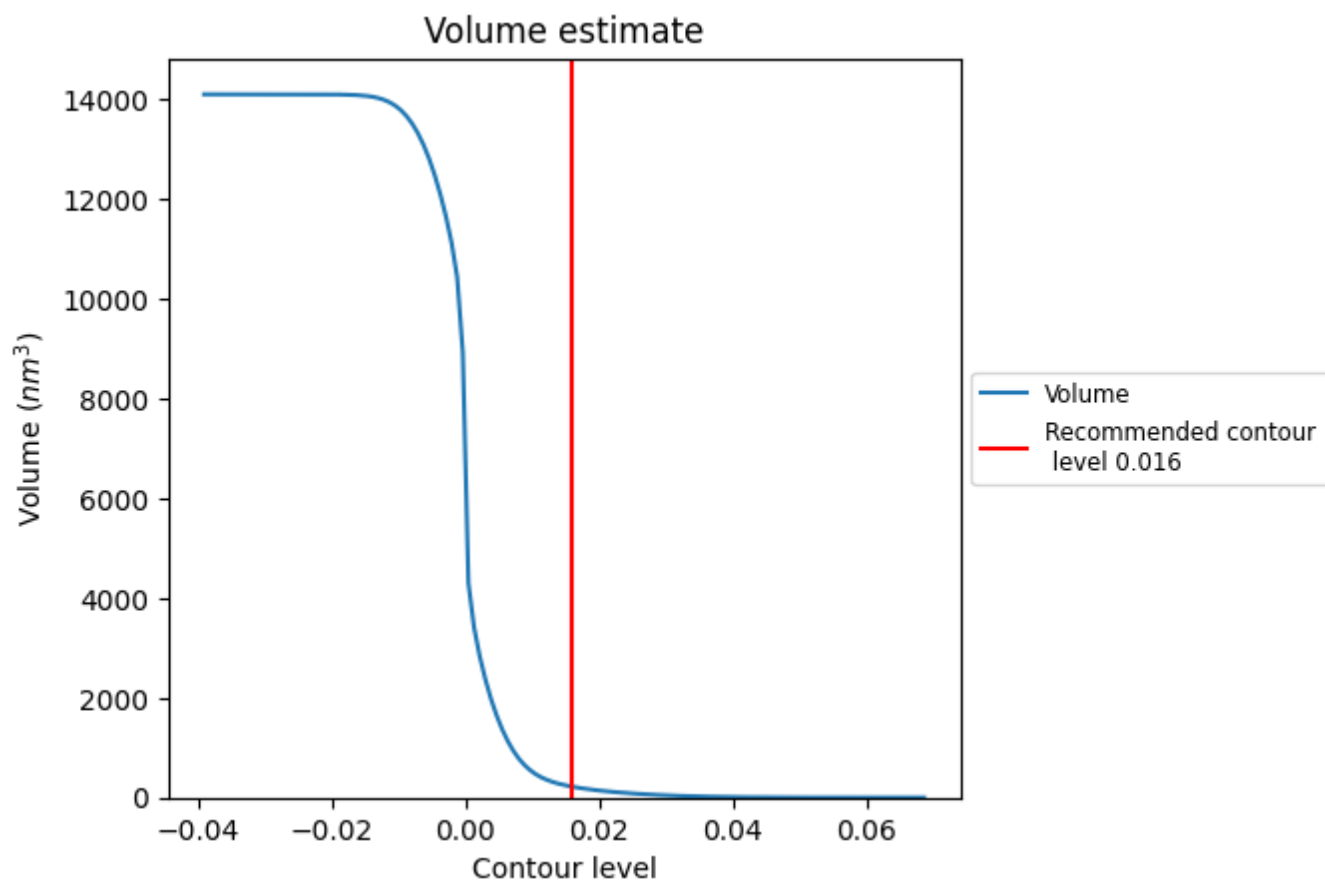
This section contains the results of statistical analysis of the map.

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.

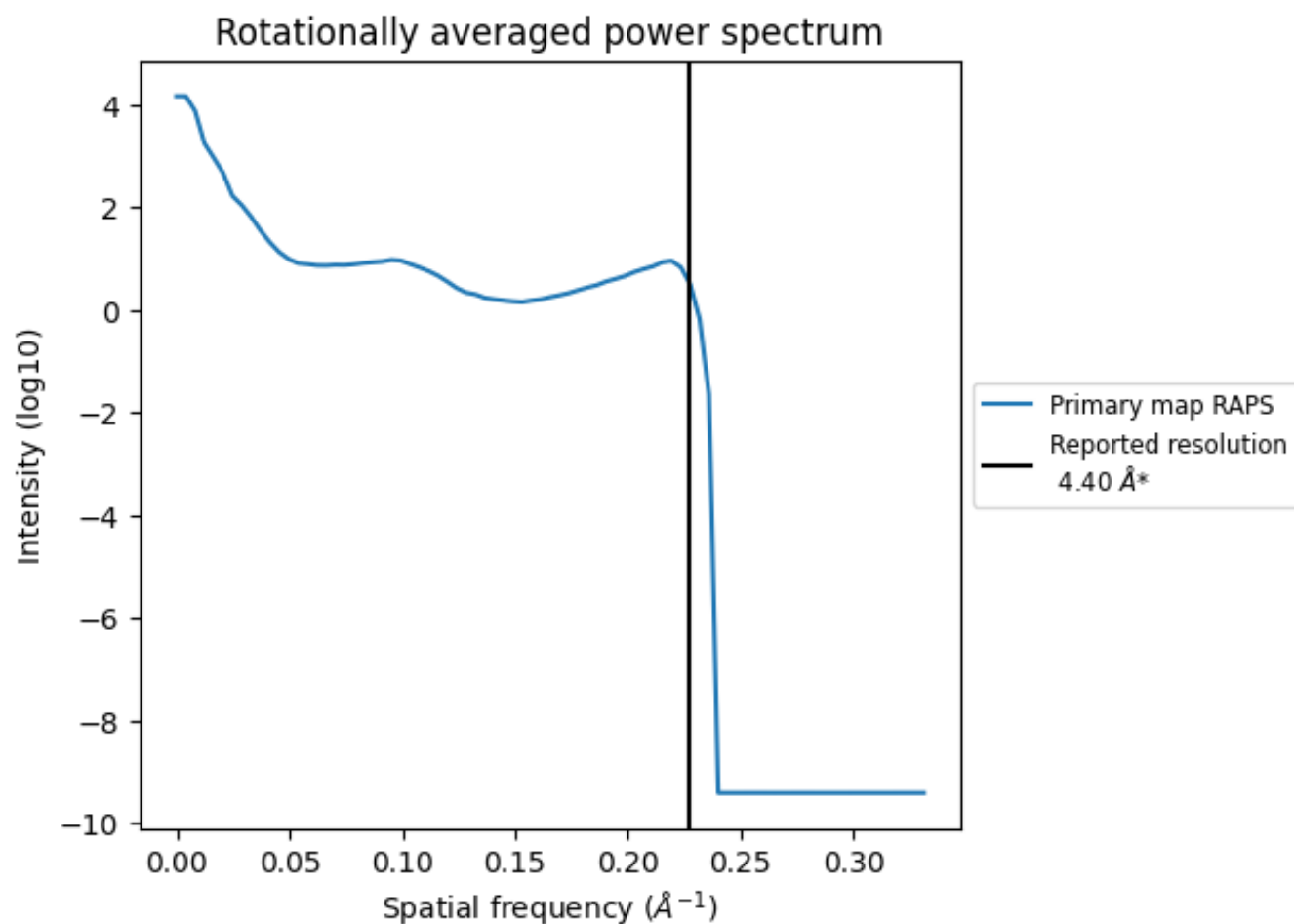
7.2 Volume estimate [i](#)



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 \AA^{-1}

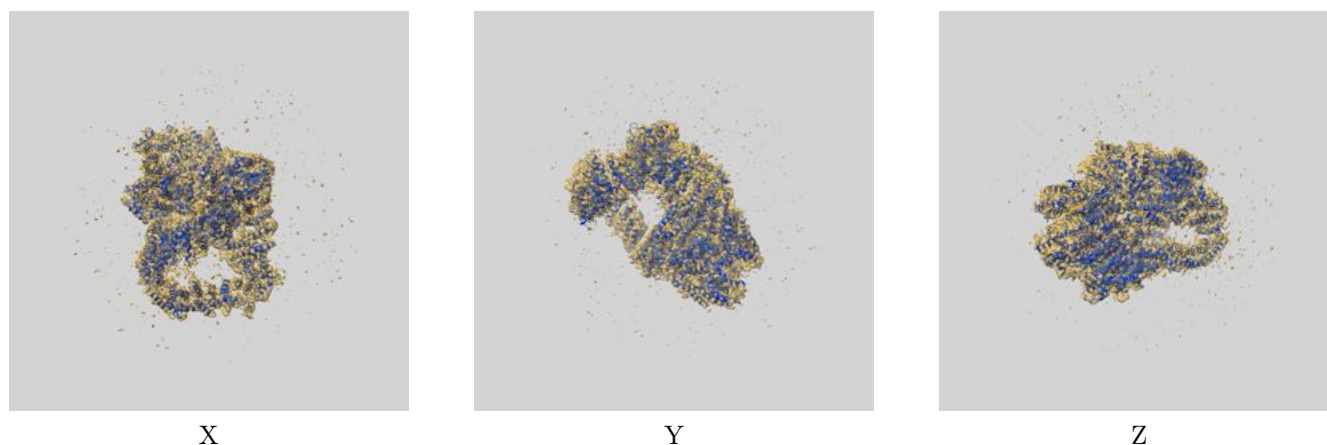
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

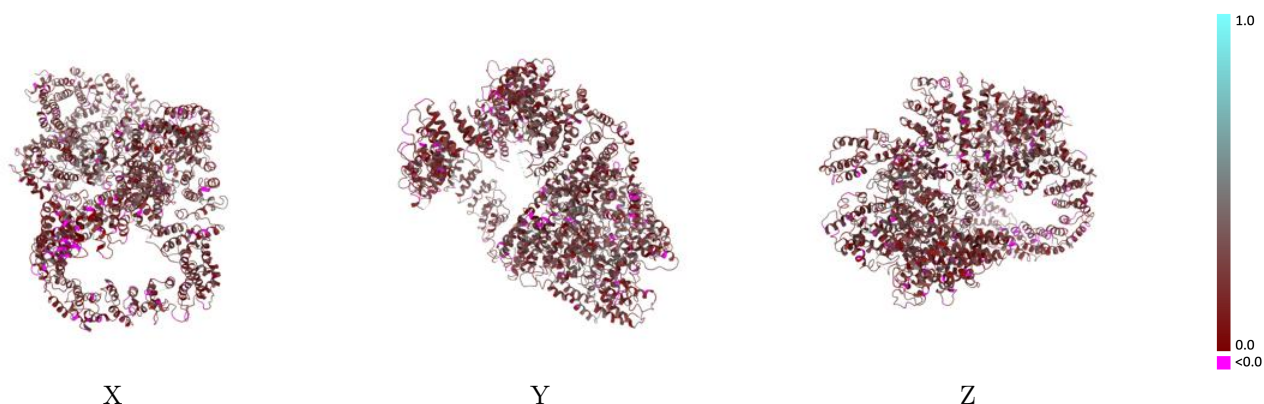
This section contains information regarding the fit between EMDB map EMD-8751 and PDB model 5W1R. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



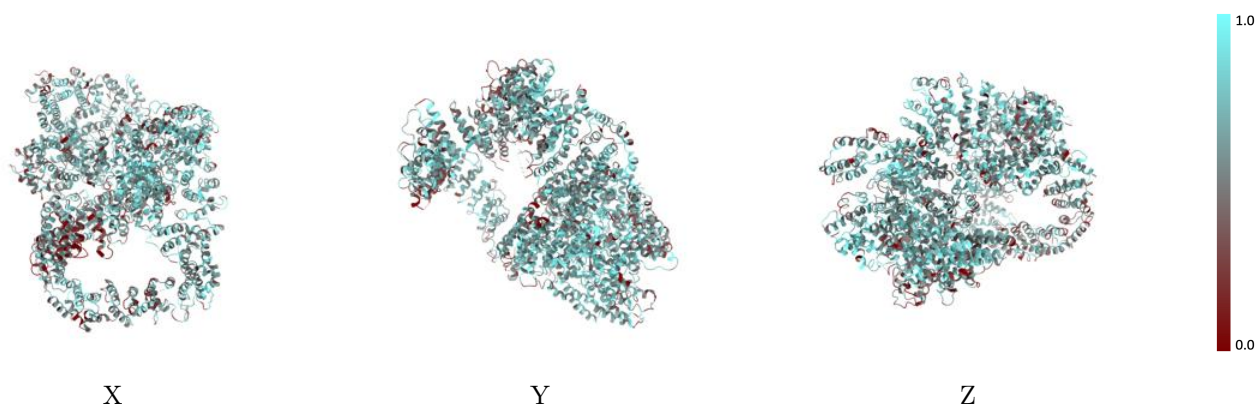
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



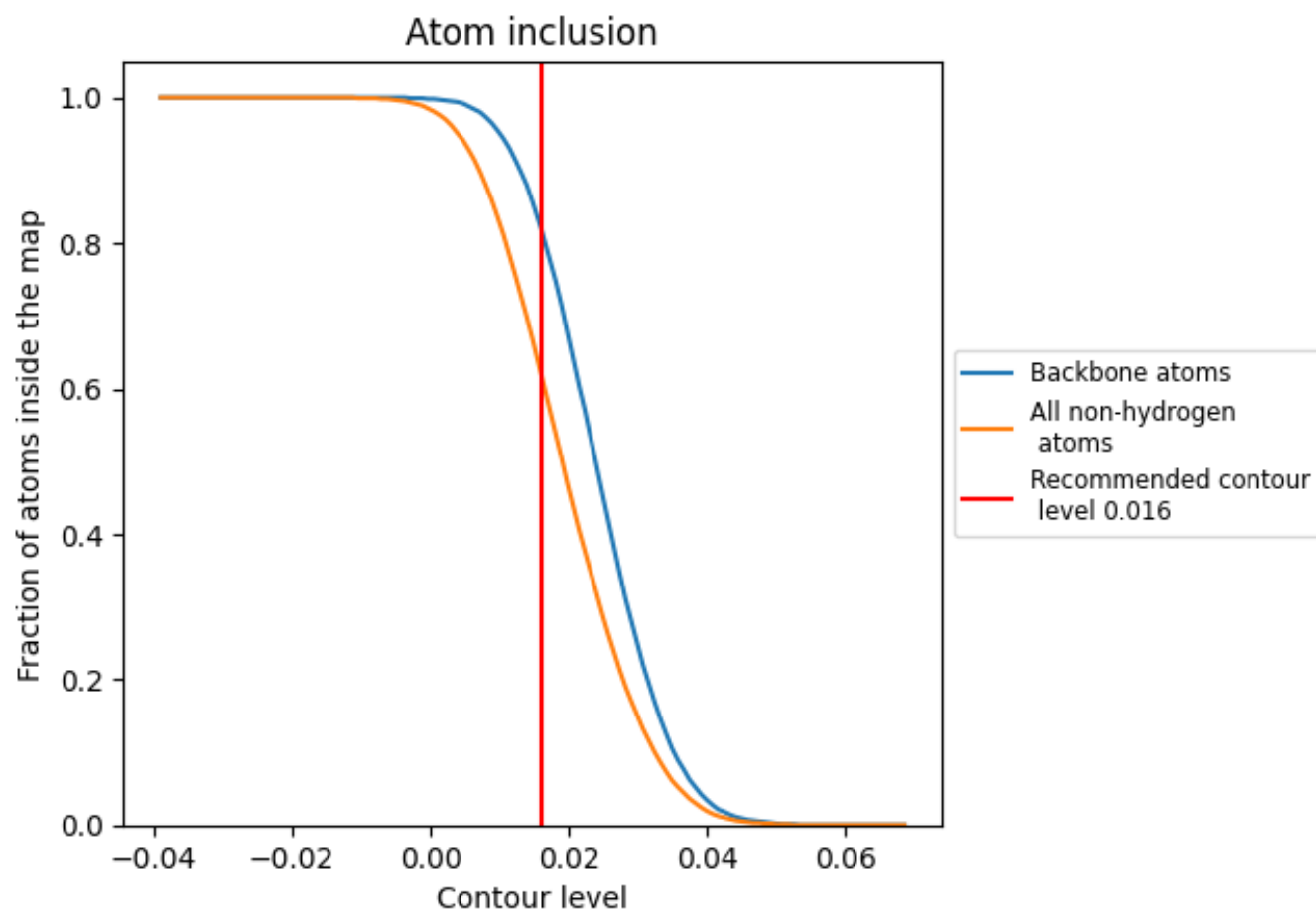
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

