



wwPDB EM Validation Summary Report ⓘ

May 19, 2024 – 06:49 am BST

PDB ID : 6Z6G
EMDB ID : EMD-11093
Title : Cryo-EM structure of La Crosse virus polymerase at pre-initiation stage
Authors : Arragain, B.; Effantin, G.; Gerlach, P.; Reguera, J.; Schoehn, G.; Cusack, S.; Malet, H.
Deposited on : 2020-05-28
Resolution : 3.06 Å(reported)
Based on initial model : 5AMQ

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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

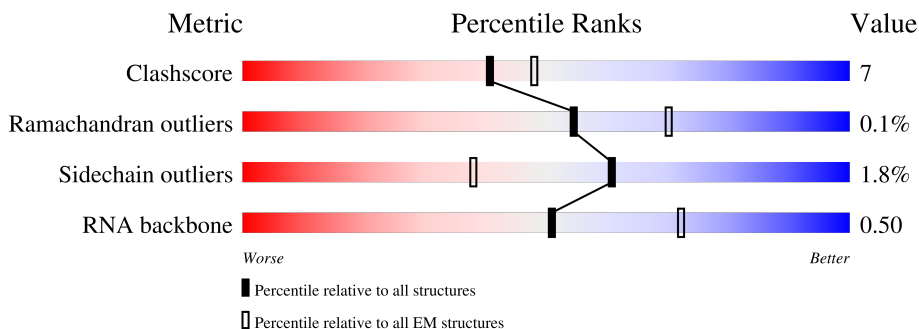
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	U	10	
2	X	8	
3	H	16	
4	A	2285	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18068 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 RNA chain called 5'vRNA 1-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	10	Total	C	N	O	P	0	0
			216	96	39	71	10		

- Molecule 2 is a RNA chain called 5'vRNA 9-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	5	Total	C	N	O	P	0	0
			101	47	18	32	4		

- Molecule 3 is a RNA chain called 3'vRNA 1-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	13	Total	C	N	O	P	0	0
			274	123	47	91	13		

- Molecule 4 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2142	Total	C	N	O	S	0	0
			17475	11184	2924	3256	111		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A5HC98
A	-20	GLY	-	expression tag	UNP A5HC98
A	-19	HIS	-	expression tag	UNP A5HC98
A	-18	HIS	-	expression tag	UNP A5HC98
A	-17	HIS	-	expression tag	UNP A5HC98
A	-16	HIS	-	expression tag	UNP A5HC98
A	-15	HIS	-	expression tag	UNP A5HC98
A	-14	HIS	-	expression tag	UNP A5HC98
A	-13	ASP	-	expression tag	UNP A5HC98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	TYR	-	expression tag	UNP A5HC98
A	-11	ASP	-	expression tag	UNP A5HC98
A	-10	ILE	-	expression tag	UNP A5HC98
A	-9	PRO	-	expression tag	UNP A5HC98
A	-8	THR	-	expression tag	UNP A5HC98
A	-7	THR	-	expression tag	UNP A5HC98
A	-6	GLU	-	expression tag	UNP A5HC98
A	-5	ASN	-	expression tag	UNP A5HC98
A	-4	LEU	-	expression tag	UNP A5HC98
A	-3	TYR	-	expression tag	UNP A5HC98
A	-2	PHE	-	expression tag	UNP A5HC98
A	-1	GLN	-	expression tag	UNP A5HC98
A	0	GLY	-	expression tag	UNP A5HC98

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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.

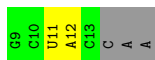
- Molecule 1: 5'vRNA 1-10

Chain U: 



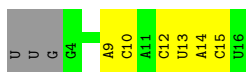
- Molecule 2: 5'vRNA 9-16

Chain X: 




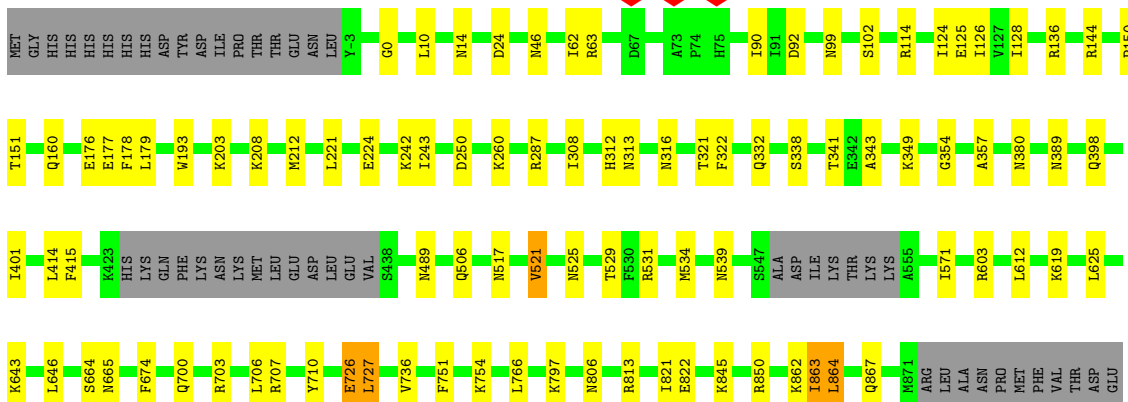
- Molecule 3: 3'vRNA 1-16

Chain H: 



- Molecule 4: RNA-directed RNA polymerase L

Chain A: 



L2250	L2251	L2159	N2160	S2161	S2067	T1959	I1998	Y1836	THR	ALA	E1380	A1031	GLN	VAL	CYS	GLY	TYR	GLU	VAL	GLY	HIS	CYS
M2251	M2252	N2161	N2162	N2163	N2071	I1961	R1901	A1838	HIS	LEU	N1383	THR	THR	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
M2253	M2254	N2164	N2165	N2166	N2072	Y1962	L1902	A1839	I1710	GLU	D1391	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
M2255	M2256	N2167	N2168	N2169	N2073	N1963	L1903	A1840	S1715	PRO	N1392	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M2257	M2258	N2170	N2171	N2172	N2074	N1964	L1904	A1841	L1724	ILE	L1400	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
M2259	M2260	N2173	N2174	N2175	N2075	N1965	G1905	A1842	L1729	LEU	R1401	I1042	I1043	I1044	I1045	I1046	I1047	I1048	I1049	I1050	I1051	I1052
M2261	M2262	N2176	N2177	N2178	N2076	N1966	R1906	A1843	Y1736	G1545	V1404	K1054	K1055	K1056	K1057	K1058	K1059	K1060	K1061	K1062	K1063	K1064
M2263	M2264	N2179	N2180	N2181	N2077	N1967	R1907	A1844	Q1743	N1580	PRO	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077
M2265	M2266	N2182	N2183	N2184	N2078	N1968	H1908	A1845	L1744	T1590	ASP	K1072	K1073	K1074	K1075	K1076	K1077	K1078	K1079	K1080	K1081	K1082
M2267	M2268	N2185	N2186	N2187	N2079	N1969	G1909	A1846	S1746	S1594	THR	D1080	D1081	D1082	D1083	D1084	D1085	D1086	D1087	D1088	D1089	D1090
M2269	M2270	N2188	N2189	N2190	N2080	N1970	L1910	A1847	G1747	P1599	GLY	N1112	N1113	N1114	N1115	N1116	N1117	N1118	N1119	N1120	N1121	N1122
M2271	M2272	N2191	N2192	N2193	N2081	N1971	K1911	A1848	A1751	M1603	THR	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168
M2273	M2274	N2194	N2195	N2196	N2082	N1972	F1912	A1849	Q1764	N1615	ASP	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154
M2275	M2276	N2197	N2198	N2199	N2083	N1973	E1913	A1850	A1752	LEU	MET	V1155	V1156	V1157	V1158	V1159	V1160	V1161	V1162	V1163	V1164	V1165
M2277	M2278	N2200	N2201	N2202	N2084	N1974	L1914	A1851	Q1765	GLY	THR	R1424	R1425	R1426	R1427	R1428	R1429	R1430	R1431	R1432	R1433	R1434
M2279	M2280	N2203	N2204	N2205	N2085	N1975	M1915	A1852	A1753	HIS	ASP	K1431	K1432	K1433	K1434	K1435	K1436	K1437	K1438	K1439	K1440	K1441
M2281	M2282	N2206	N2207	N2208	N2086	N1976	S1916	A1853	Q1766	THR	ASP	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2283	M2284	N2209	N2210	N2211	N2087	N1977	K1917	A1854	A1754	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2285	M2286	N2212	N2213	N2214	N2088	N1978	I1918	A1855	A1755	LEU	ASP	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2287	M2288	N2215	N2216	N2217	N2089	N1979	Q1919	A1856	Q1767	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2289	M2290	N2218	N2219	N2220	N2090	N1980	THR	A1857	A1756	HIS	ASP	K1431	K1432	K1433	K1434	K1435	K1436	K1437	K1438	K1439	K1440	K1441
M2291	M2292	N2221	N2222	N2223	N2091	N1981	TYR	A1858	A1757	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2293	M2294	N2224	N2225	N2226	N2092	N1982	PRO	A1859	A1758	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2295	M2296	N2227	N2228	N2229	N2093	N1983	GLY	A1860	A1759	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2297	M2298	N2230	N2231	N2232	N2094	N1984	THR	A1861	A1760	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2299	M2300	N2233	N2234	N2235	N2095	N1985	PRO	A1862	A1761	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2301	M2302	N2236	N2237	N2238	N2096	N1986	GLY	A1863	A1762	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2303	M2304	N2239	N2240	N2241	N2097	N1987	THR	A1864	A1763	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2305	M2306	N2242	N2243	N2244	N2098	N1988	TYR	A1865	A1764	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2307	M2308	N2245	N2246	N2247	N2099	N1989	GLY	A1866	A1765	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2309	M2310	N2248	N2249	N2250	N2100	N1990	THR	A1867	A1766	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2311	M2312	N2251	N2252	N2253	N2101	N1991	PRO	A1868	A1767	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2313	M2314	N2254	N2255	N2256	N2102	N1992	GLY	A1869	A1768	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2315	M2316	N2257	N2258	N2259	N2103	N1993	THR	A1870	A1769	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2317	M2318	N2260	N2261	N2262	N2104	N1994	TYR	A1871	A1770	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2319	M2320	N2263	N2264	N2265	N2105	N1995	PRO	A1872	A1771	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2321	M2322	N2266	N2267	N2268	N2106	N1996	GLY	A1873	A1772	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2323	M2324	N2269	N2270	N2271	N2107	N1997	THR	A1874	A1773	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2325	M2326	N2272	N2273	N2274	N2108	N1998	TYR	A1875	A1774	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2327	M2328	N2275	N2276	N2277	N2109	N1999	PRO	A1876	A1775	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2329	M2330	N2278	N2279	N2280	N2110	N2000	GLY	A1877	A1776	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2331	M2332	N2281	N2282	N2283	N2111	N2001	THR	A1878	A1777	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2333	M2334	N2284	N2285	N2286	N2112	N2002	TYR	A1879	A1778	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2335	M2336	N2287	N2288	N2289	N2113	N2003	PRO	A1880	A1779	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2337	M2338	N2290	N2291	N2292	N2114	N2004	GLY	A1881	A1780	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2339	M2340	N2293	N2294	N2295	N2115	N2005	THR	A1882	A1781	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2341	M2342	N2296	N2297	N2298	N2116	N2006	TYR	A1883	A1782	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2343	M2344	N2299	N2300	N2301	N2117	N2007	PRO	A1884	A1783	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2345	M2346	N2302	N2303	N2304	N2118	N2008	GLY	A1885	A1784	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2347	M2348	N2305	N2306	N2307	N2119	N2009	THR	A1886	A1785	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2349	M2350	N2308	N2309	N2310	N2120	N2010	TYR	A1887	A1786	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2351	M2352	N2311	N2312	N2313	N2121	N2011	PRO	A1888	A1787	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2353	M2354	N2314	N2315	N2316	N2122	N2012	GLY	A1889	A1788	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2355	M2356	N2317	N2318	N2319	N2123	N2013	THR	A1890	A1789	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2357	M2358	N2320	N2321	N2322	N2124	N2014	TYR	A1891	A1790	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2359	M2360	N2323	N2324	N2325	N2125	N2015	PRO	A1892	A1791	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2361	M2362	N2326	N2327	N2328	N2126	N2016	GLY	A1893	A1792	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447
M2363	M2364	N2329	N2330	N2331	N2127	N2017	THR	A1894	A1793	GLY	THR	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447
M2365	M2366	N2332	N2333	N2334	N2128	N2018	TYR	A1895	A1794	GLY	THR	R1450	R1451	R1452	R1453	R1454	R1455	R1456	R1457	R1458	R1459	R1460
M2367	M2368	N2335	N2336	N2337	N2129	N2019	PRO	A1896	A1795	GLY	THR	S1437	S1438	S1439	S1440	S1441	S1442	S1443				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57660	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)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	247.79999, 247.79999, 247.79999	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

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

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	U	0.95	0/241	1.26	5/374 (1.3%)
2	X	0.50	0/112	1.11	0/173
3	H	0.93	0/305	1.00	2/472 (0.4%)
4	A	0.47	0/17824	0.57	1/24023 (0.0%)
All	All	0.49	0/18482	0.60	8/25042 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	8	U	N3-C2-O2	-8.67	116.13	122.20
1	U	8	U	N1-C2-O2	8.36	128.65	122.80
1	U	8	U	C6-N1-C2	-6.24	117.25	121.00
3	H	12	C	N1-C2-O2	6.04	122.53	118.90
1	U	8	U	C5-C6-N1	5.96	125.68	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	216	0	108	0	0
2	X	101	0	53	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	274	0	140	1	0
4	A	17475	0	17524	266	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	18068	0	17825	268	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 7.

The worst 5 of 268 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)
4:A:2151:LEU:HD13	4:A:2204:PHE:CE2	1.35	1.57
4:A:1838:ALA:HA	4:A:1868:TYR:CE1	1.47	1.50
4:A:2151:LEU:HD13	4:A:2204:PHE:CZ	1.50	1.46
4:A:2151:LEU:CD1	4:A:2204:PHE:CE2	1.99	1.44
4:A:1838:ALA:HA	4:A:1868:TYR:CZ	1.60	1.33

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
4	A	2116/2285 (93%)	1974 (93%)	139 (7%)	3 (0%)	51 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	2153	LYS
4	A	1186	SER
4	A	1969	CYS

5.3.2 Protein sidechains ⓘ

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
4	A	1968/2107 (93%)	1932 (98%)	36 (2%)	59 80

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1985	ARG
4	A	2209	ASN
4	A	2011	LYS
4	A	2103	ARG
4	A	1133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	1133	ASN
4	A	1954	HIS
4	A	1392	ASN
4	A	2141	ASN
4	A	1842	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	9/10 (90%)	4 (44%)	0
2	X	4/8 (50%)	0	0
3	H	12/16 (75%)	3 (25%)	0
All	All	25/34 (73%)	7 (28%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	6	U
1	U	7	G

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Mol	Chain	Res	Type
1	U	8	U
1	U	9	G
3	H	9	A

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

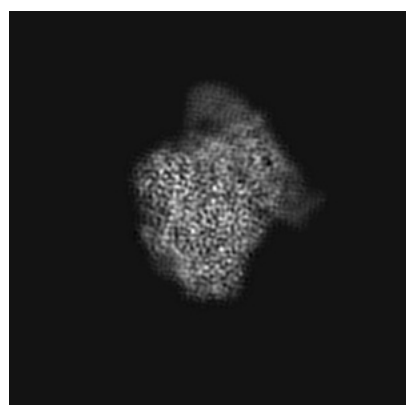
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11093. These allow visual inspection of the internal detail of the map and identification of artifacts.

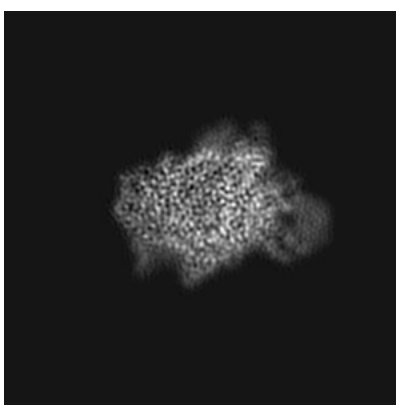
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

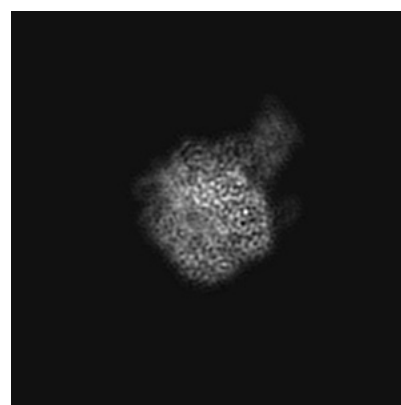
6.1.1 Primary map



X



Y

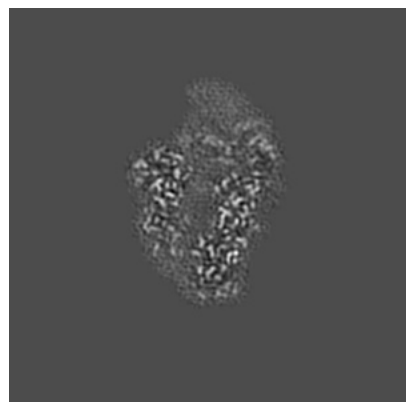


Z

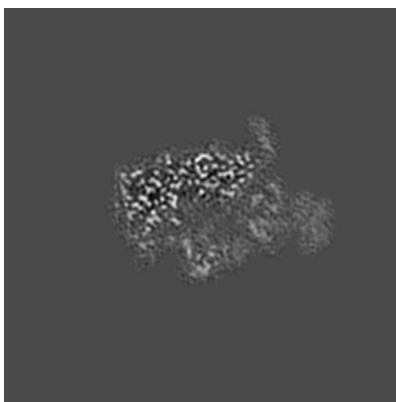
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

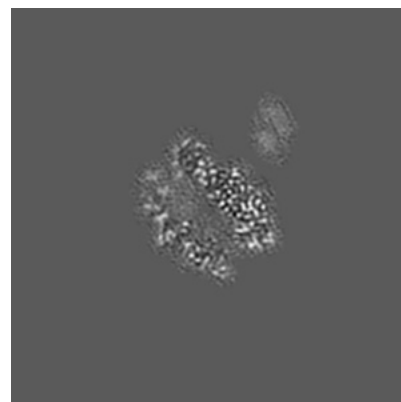
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

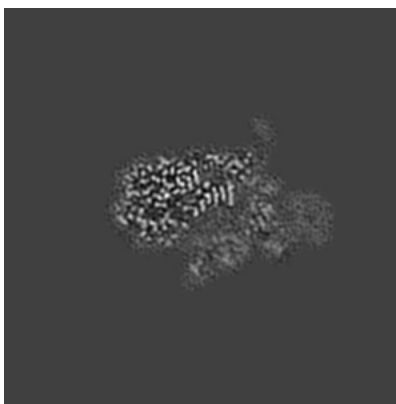
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

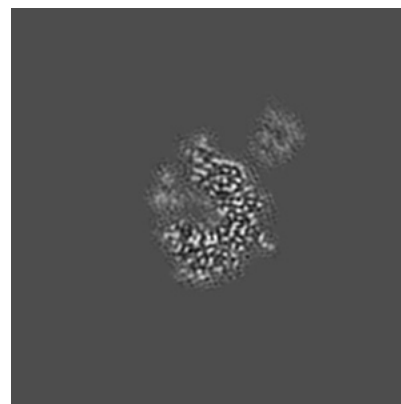
6.3.1 Primary map



X Index: 170



Y Index: 158

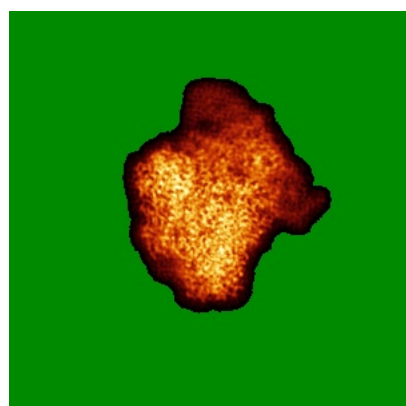


Z Index: 167

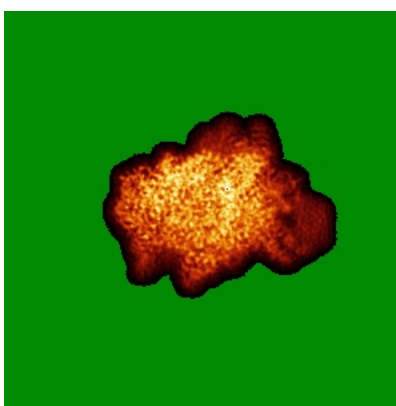
The images above show the largest variance slices of the map in three orthogonal directions.

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

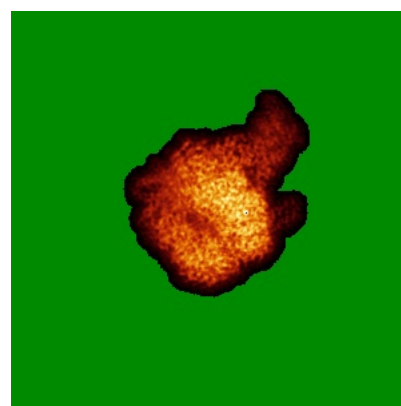
6.4.1 Primary map



X



Y

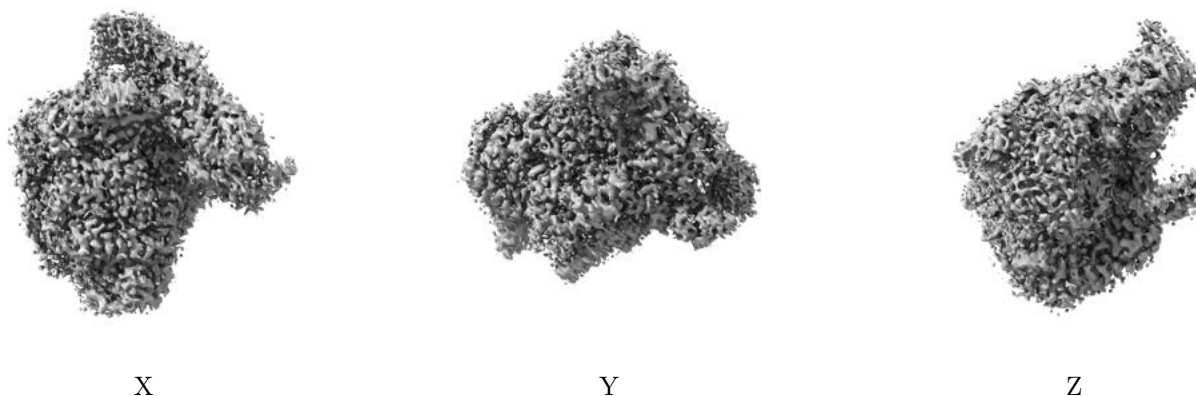


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

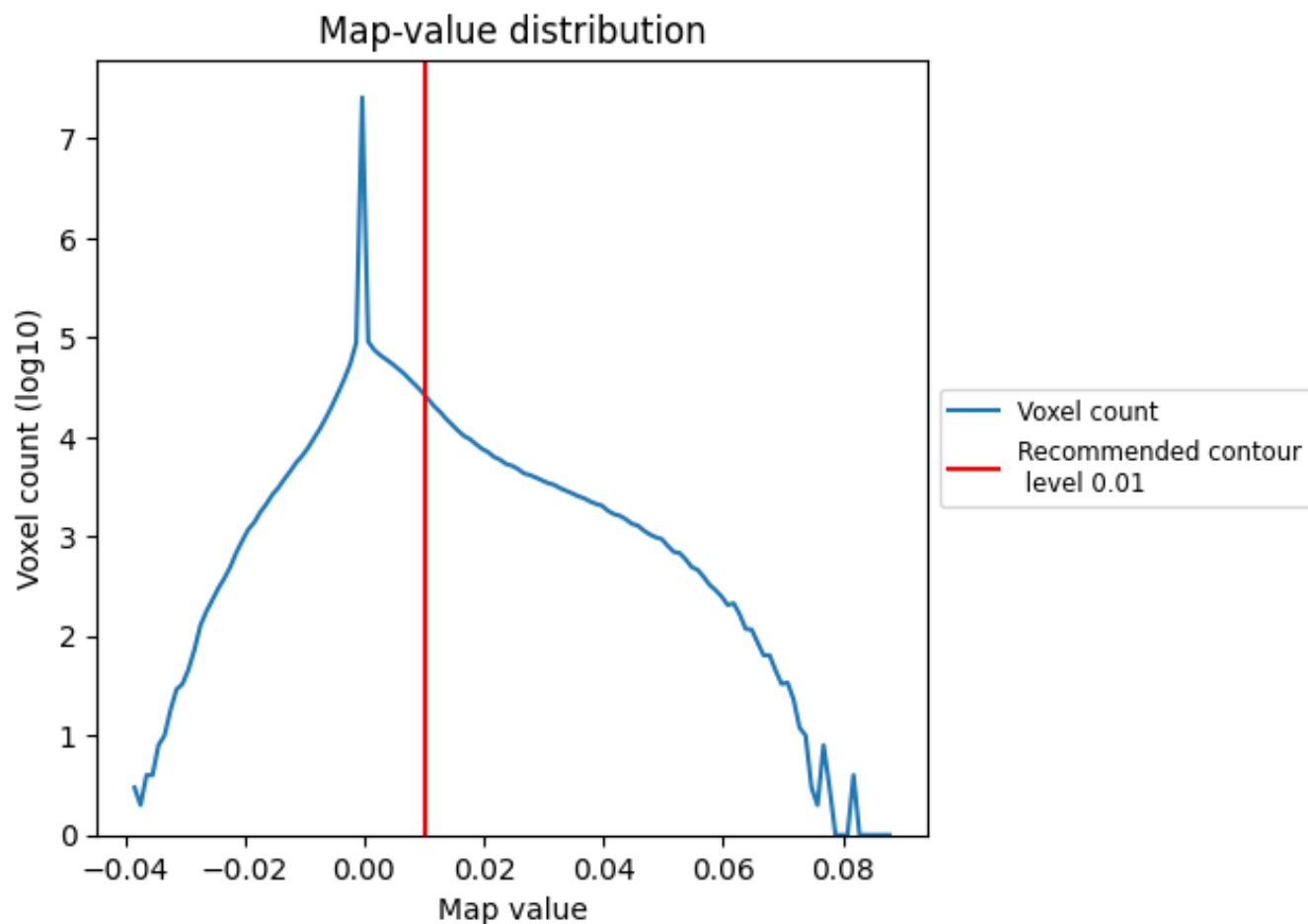
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

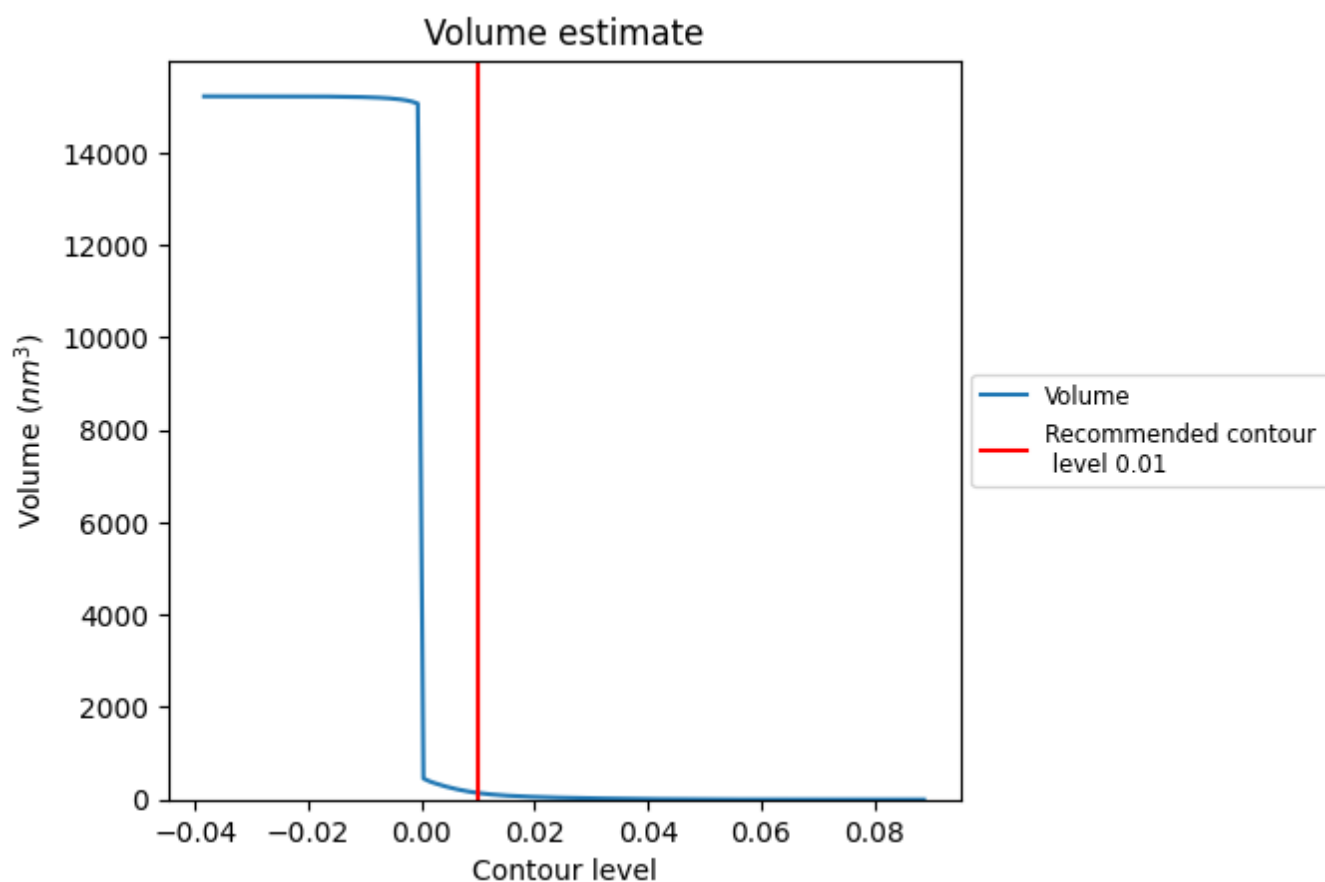
This section contains the results of statistical analysis of the map.

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.

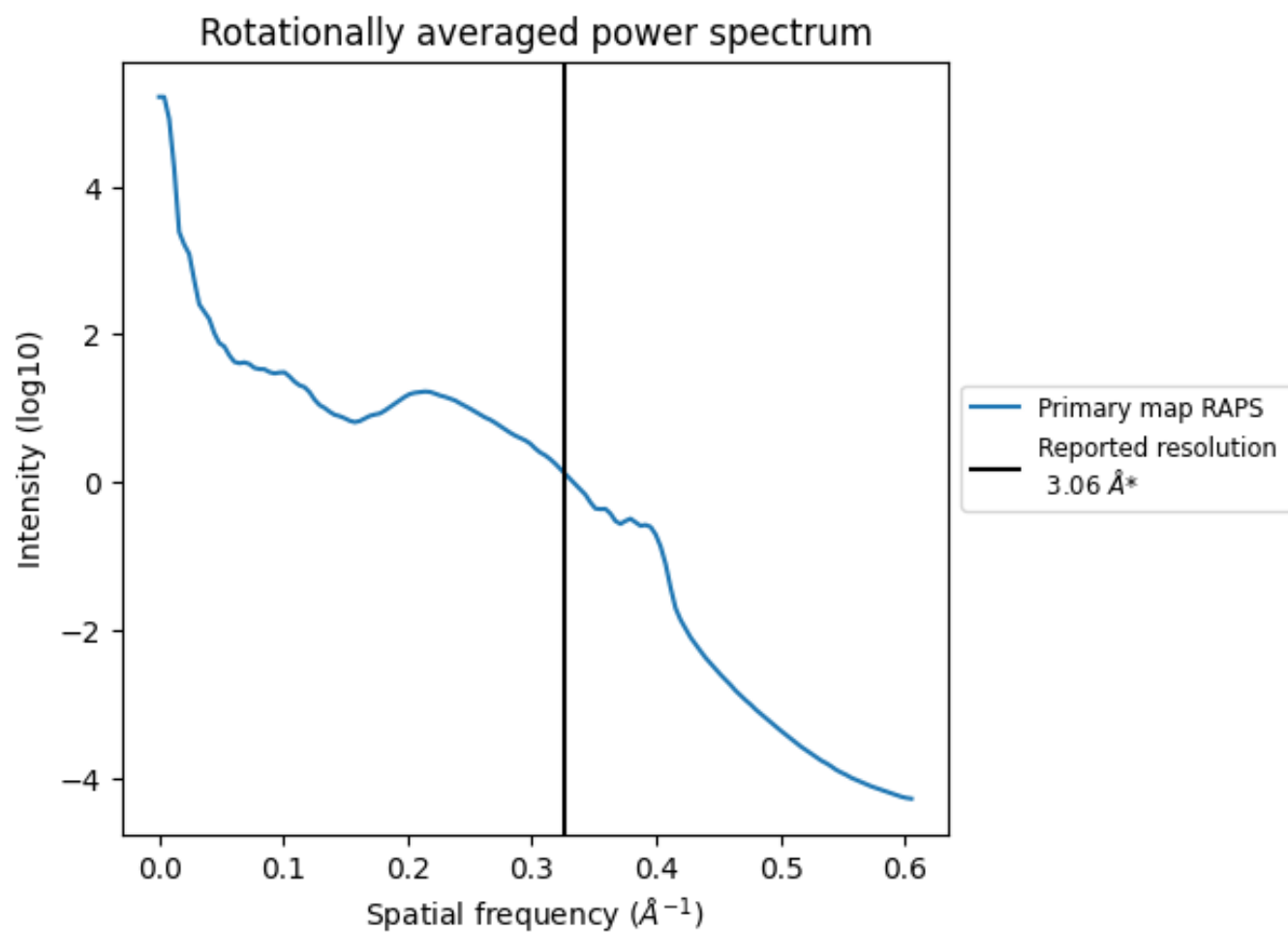
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

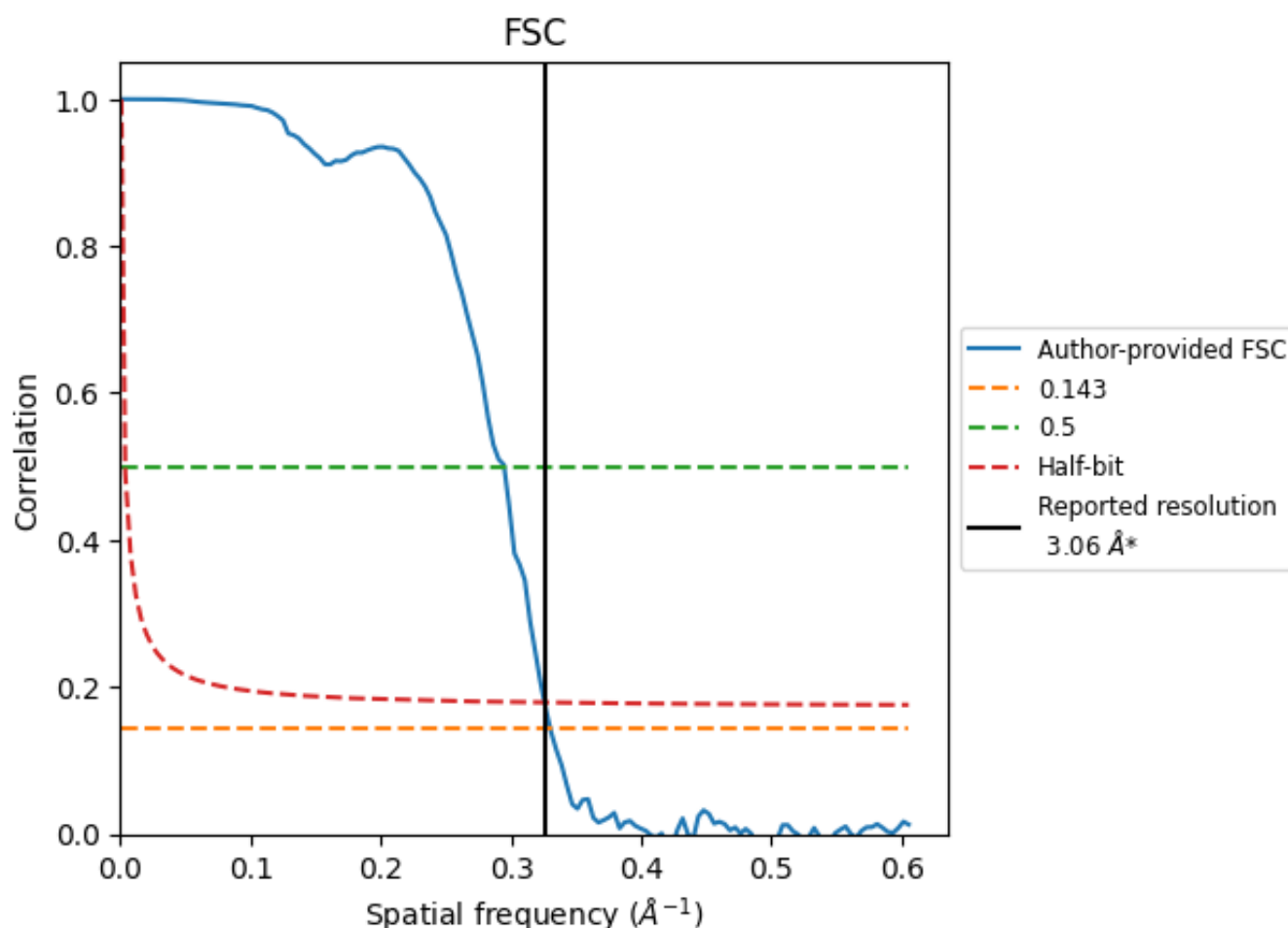


*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

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 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

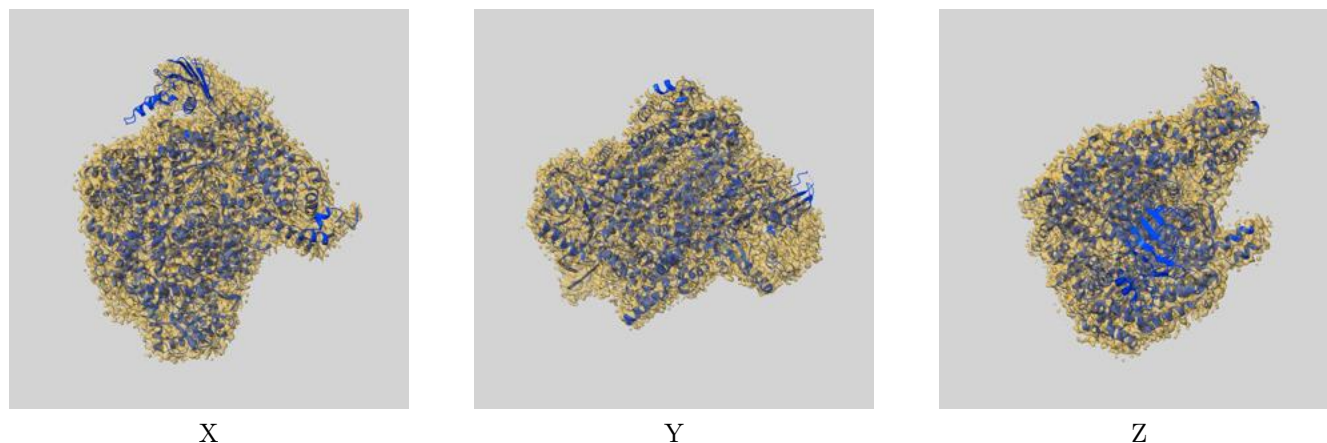
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.03	3.39	3.07
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

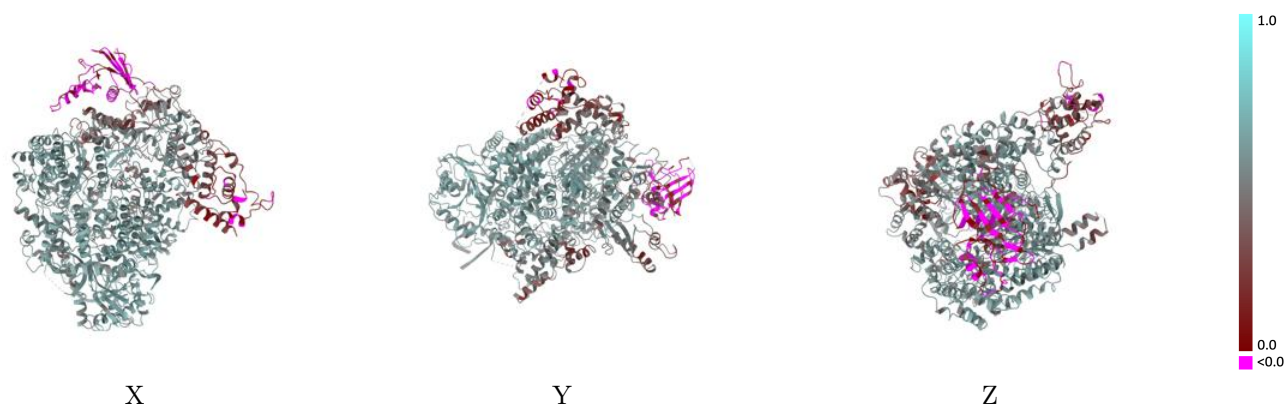
This section contains information regarding the fit between EMDB map EMD-11093 and PDB model 6Z6G. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



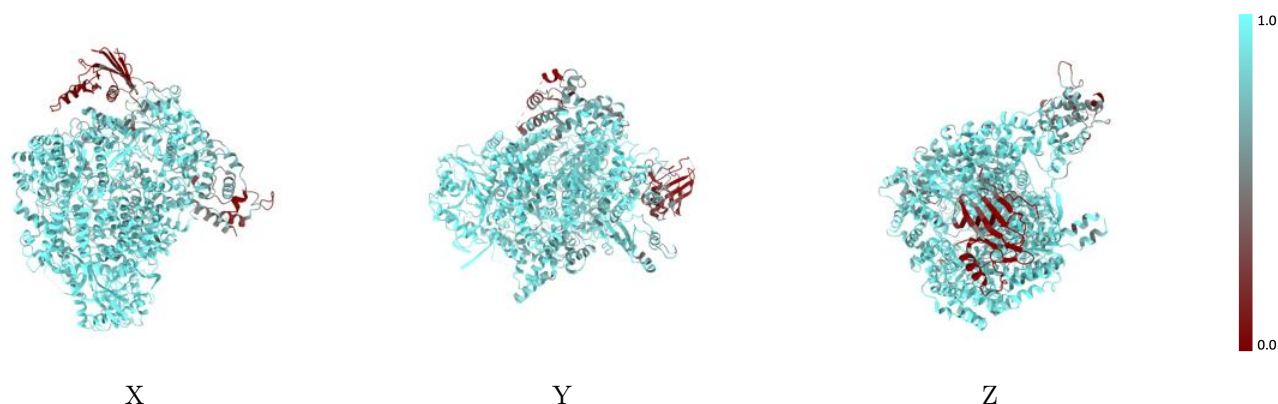
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



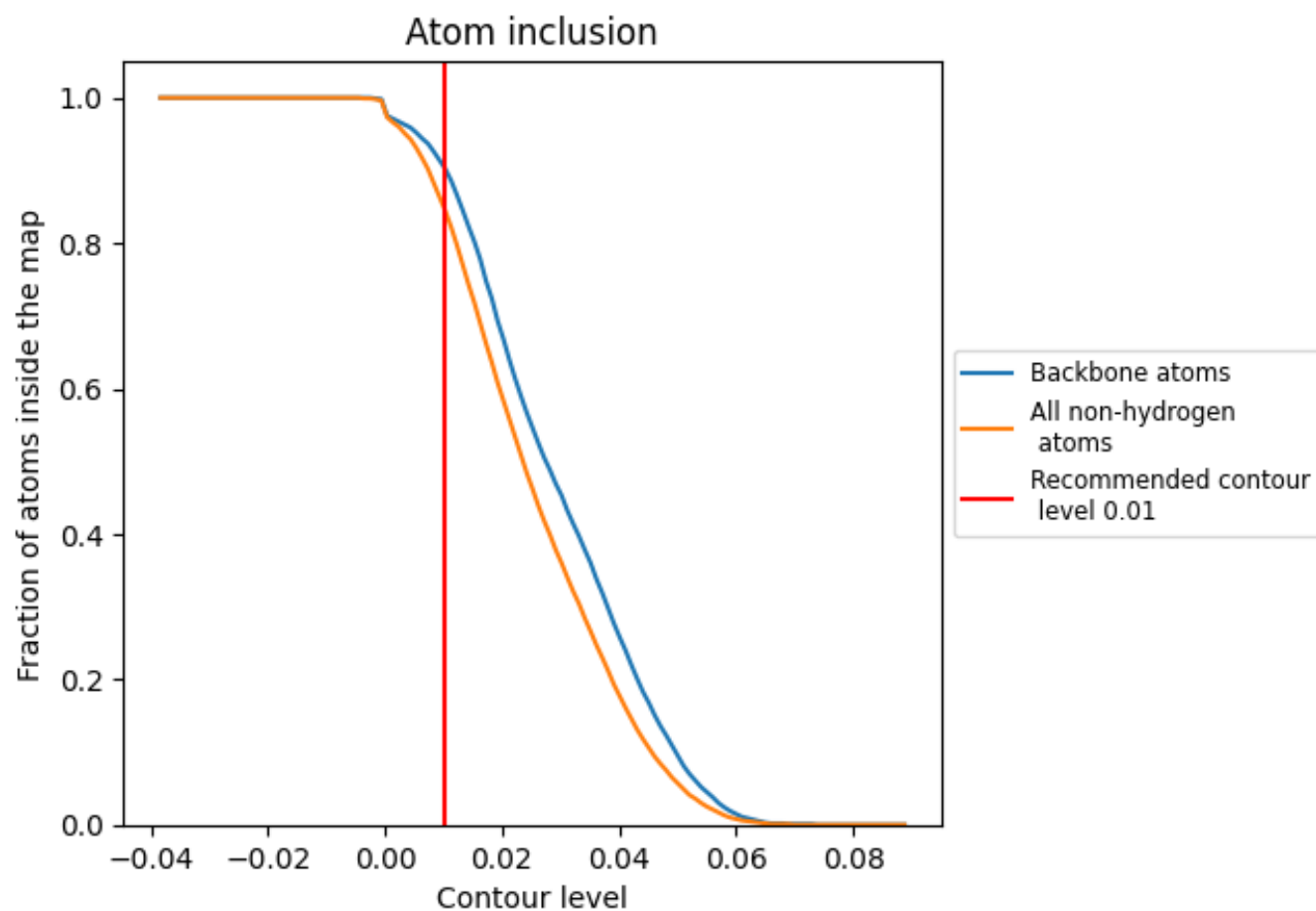
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8500	<div></div> 0.4990
A	<div></div> 0.8460	<div></div> 0.4970
H	<div></div> 0.9820	<div></div> 0.5870
U	<div></div> 0.9860	<div></div> 0.5910
X	<div></div> 0.9800	<div></div> 0.5130

