



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 02:46 PM JST

PDB ID : 7ELB
EMDB ID : EMD-31179
Title : Structure of Machupo virus L polymerase in complex with Z protein (dimeric form)
Authors : Peng, R.; Xu, X.; Peng, Q.; Shi, Y.
Deposited on : 2021-04-09
Resolution : 4.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

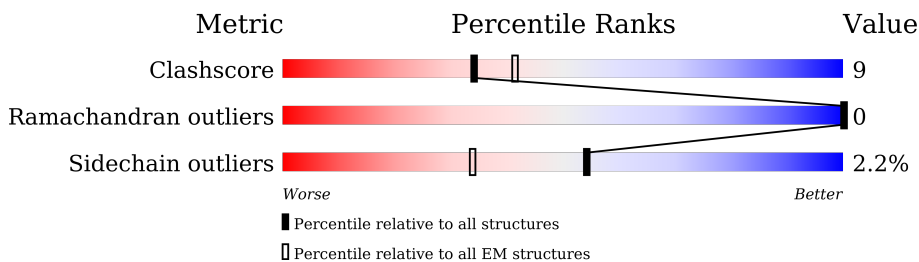
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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

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	2209	
1	C	2209	
2	B	94	
2	D	94	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 31012 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		
1	C	1937	Total	C	N	O	S	0	0
			15094	9621	2518	2861	94		

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	49	Total	C	N	O	S	0	0
			407	257	73	68	9		
2	D	49	Total	C	N	O	S	0	0
			407	257	73	68	9		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mn	0
			1	1	
3	C	1	Total	Mn	0
			1	1	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	
4	B	2	Total	Zn	0
			2	2	
4	C	2	Total	Zn	0
			2	2	

Continued on next page...

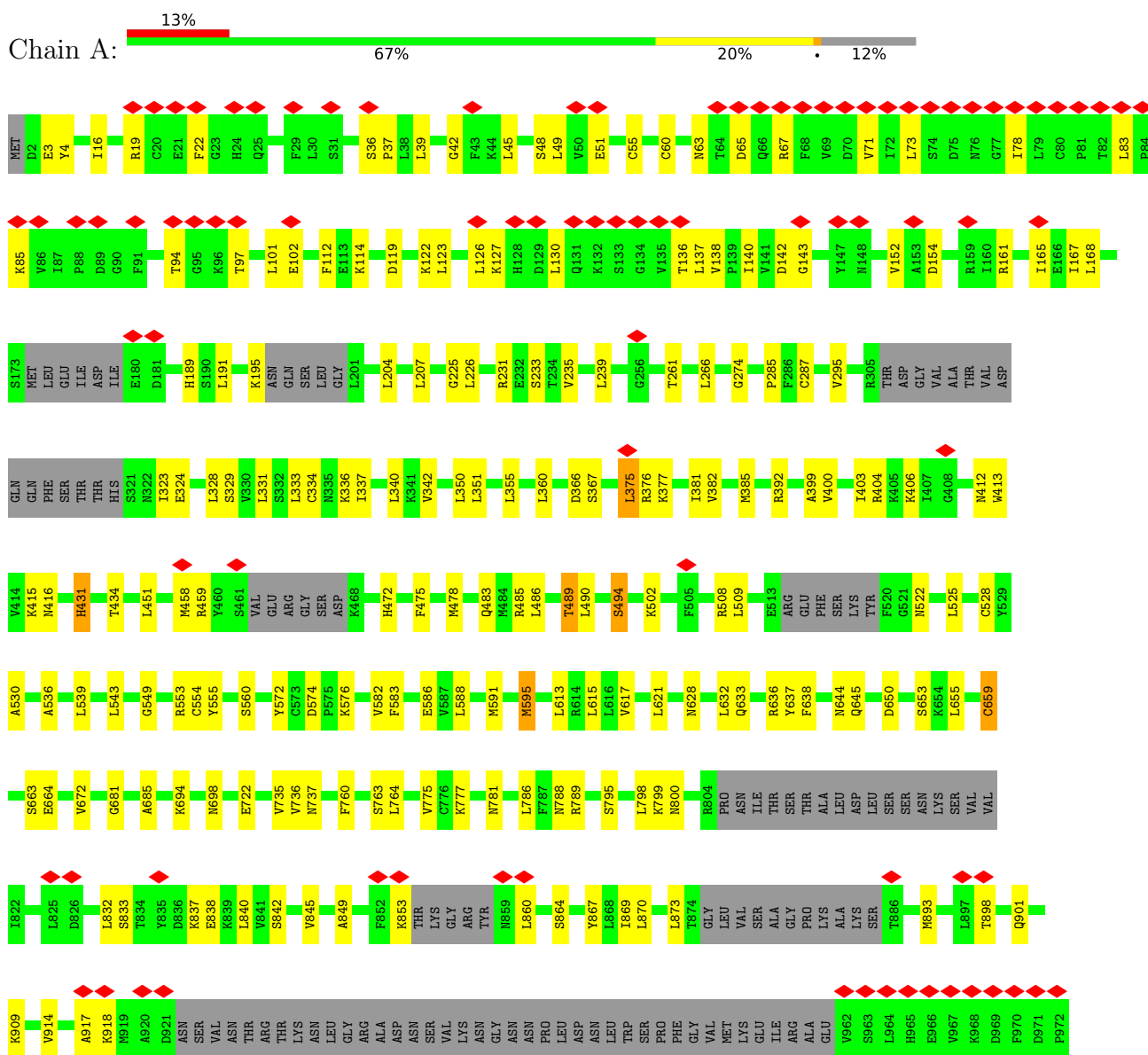
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	D	2	2	2	0

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: RNA-directed RNA polymerase L

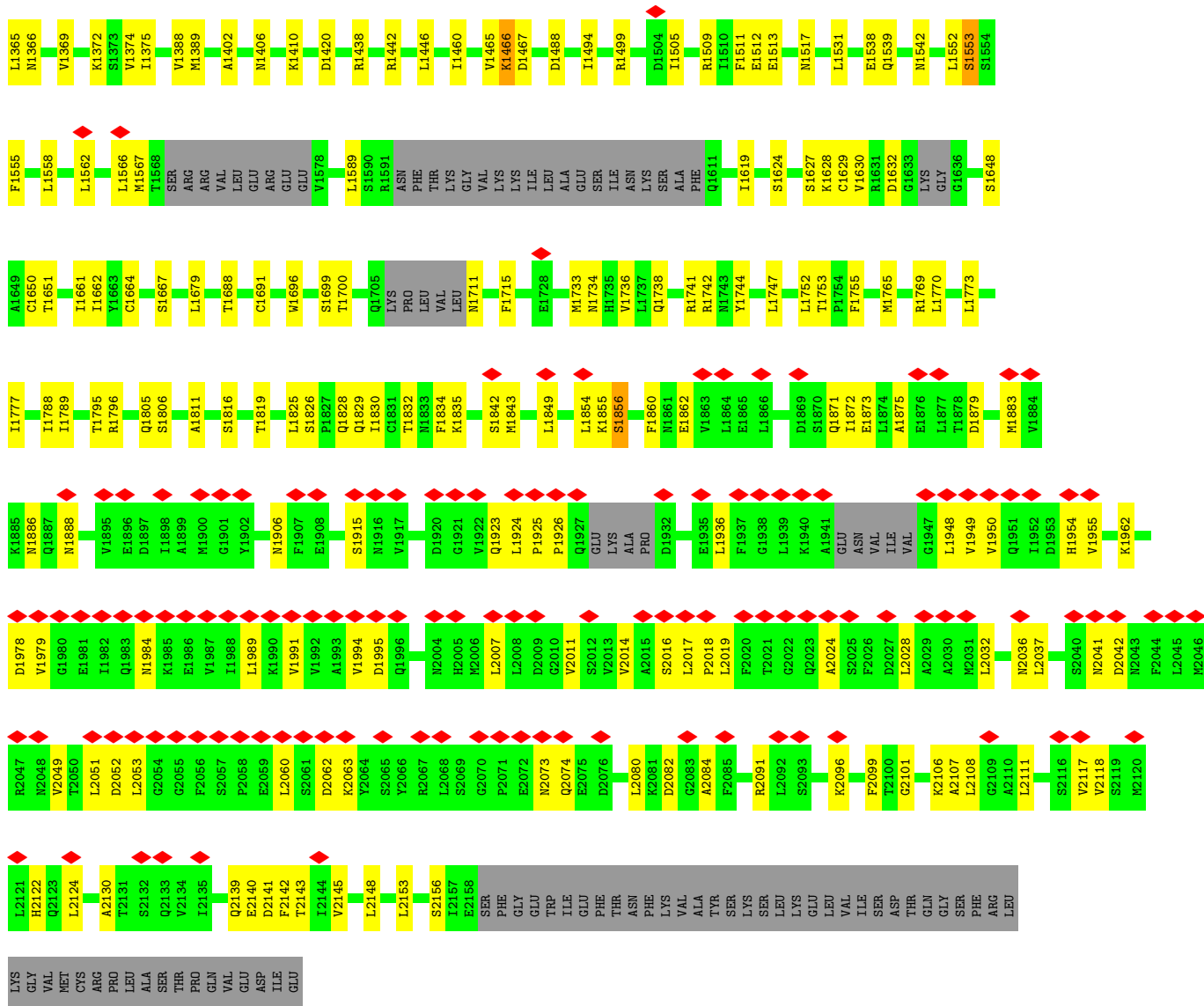


D973	D974	L974	P976	P977	E978	P979	P980	X981	E982	L983	C984	D985	A986	P987	P988	X989	S990	S991	E992	X993	C994	X995	F996	F997	L998	E999	G1000	V1001	L1002	D1003	V1004	C1005	F1006	L1007	G1008	L1009	L1010	L1011	K1012	N1013	L1014	T1015	T1016	S1017	S1018	Y1019	Y1024	F1025	M1026	C1027	F1028	K1029	Y1030	L1031	L1032	I1033	Q1034	G1035																																																																																																																																																																																																																																																																																																																																														
H1036	F1037	D1038	Q1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095																																																																																																																																																																																																																																																																																																																																													
S1109	G1113	G1113	M1137	M1141	T1142	R1143	E1146	D1147	E1150	A1151	V1152	S1155	T1159	L1183	S1184	C1185	H1189	S1190	L1200	A1203	L1204	E1209	L1210	R1211	T1212	D1215	R1216	D1220	L1221	D1222	S1223	I1227	E1237	V1238	G1249	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	Y1302	G1303	L1304	L1305	T1306	L1310	C1311	Y1312	T1326	S1327	S1328	Q1331	T1335	S1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	E1353	M1354	L1355	C1356	L1361	L1365	N1366																																																																																																																																																																																																																																																																																			
V1369	K1372	S1373	V1374	I1375	V1388	M1389	A1402	M1406	D1420	R1438	R1442	L1446	I1460	V1465	K1466	D1467	D1488	I1494	R1499	D1504	I1505	R1509	I1510	F1511	E1512	E1513	L1531	E1538	Q1539	M1542	L1552	S1553	S1554	F1555	L1558	L1562	R1563	T1564	K1565	L1566	M1567	T1568	S1569	ARG	ARG	VAL	LEU	GLU	ARG	GLU	V1578	K1588	L1589	S1590	R1591	ASN	PHE	THR	LYS	GLY	VAL	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	R1631	D1632	G1633	LYS	GLY	G1636	S1648	A1649	C1650	T1651	L1652	R1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	S1667	L1679	L1687	T1688	C1691	W1696	S1699	T1700	Q1705	PRO	LEU	VAL	LEU	M1711	F1715	E1728	M1733	H1734	H1735	L1736	L1737	Q1738	R1741	N1742	N1743	Y1744	L1747	L1752	T1753	P1754	F1755	Q1760	T1764	M1765	R1769	L1777	A1778	A1779	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	A1811	S1816	T1819	L1823	G1824	L1825	S1826	P1827	Q1828	Q1829	C1830	L1831	L1832	M1833	F1834	K1835	L1836	Q1837	S1842	M1843	L1849	L1854	K1855	S1856	W1859	F1860	M1861	E1862	V1863	L1866	D1869	Q1871	S1870	L1872	E1873	L1874	A1875	E1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	V1901	V1902	M1906	F1907	E1908	L1909	S1915	N1916	L1917	M1918	L1919	D1920	G1921	Q1923	L1924	P1925	P1926	Q1927	GLU	LYS	ALA	PRO	D1932	E1935	L1936	F1937	G1938	L1939	K1940	A1941	GLU	ASN	VAL	I1942	VAL	G1947	L1948	L1949	V1950	Q1951	L1952	L1953	L1954	L1955	K1962	D1978	V1979	G1980	E1981	I1982	Q1983	M1984	K1985	E1986	V1987	I1988	L1989	K1990	V1991	V1992	A1993	V1994	D1995	Q1996	N2004	H2005	M2006	L2007	L2008	D2009	G2010	V2011	S2012	V2013	V2014	A2015	S2016	L2017	P2018	L2019	F2020	T2021	G2022	Q2023	A2024	S2025	L2028	A2029	A2030	M2031	L2032	N2036	L2037	S2040	M2041	D2042	M2043	F2044	L2045	M2046	R2047	M2048	V2049	T2050	L2051	D2052	L2053	G2054	G2055	F2056	S2057	P2058	E2059	L2060	S2061	D2062	K2063	Y2064	S2065	Y2066	R2067	L2068	F2071	E2072	M2073	Q2074	E2075	D2076	L2080	R2081	D2082	G2083	A2084	F2085	R2091	L2092	S2093	K2096	F2099	T2100	G2101	L2108	L2111	S2116	V2117	V2118
H2122	Q2123	L2124	A2130	T2131	S2132	Q2133	V2134	I2135	E2140	D2141	F2142	T2143	V2144	L2145	L2148	L2153	S2156	T2157	E2158	SER	PHE	GLY	GLU	TRP	I1E	GLU	PHE	THR	ASN	PHE	LYS	VAL	ALA	TYR	SER	LYS	SER	LEU	LYS	GLU	GLU	VAL	ILE	SER	ASP	THR	GLN	GLY	SER	PHE	ARG	LEU	LYS	GLY	VAL	MET	CYS	ARG	PRO	ARG	PRO	ARG	PRO	GLN	VAL	GLU	ASP	ILE	GLU																																																																																																																																																																																																																																																																																																																																			

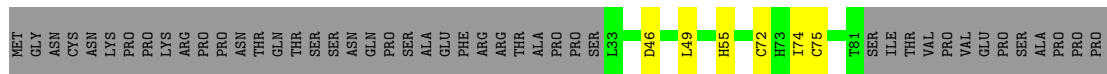
• Molecule 1: RNA-directed RNA polymerase L



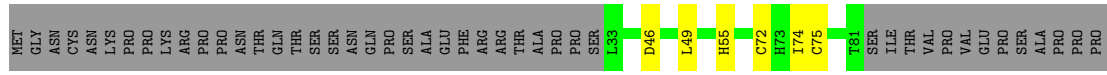
MET	D2	E3	Y4	R19	C20	E21	F22	G23	H24	I25	F29	L30	S31	S36	E113	P37	L38	L39	T40	E41	G42	F43	K44	L45	S48	L49	V50	E51	C55	O60	G61	A62	M63	T64	D65	Q66	R67	F68	D70	V71	I72	L73	S74	D75	M76	G77	I78	L79	C80	P81	T82	L83	P84					
K85	V86	I87	P88	D89	G90	F91	T94	G95	K96	T97	L101	E102	F112	E113	K114	D119	K122	L123	L124	N125	L126	K127	H128	D129	L130	Q131	K132	S133	G134	V135	T136	L137	V138	F139	I140	V141	D142	G143	Y147	M148	V152	A153	D154	R159	I160	R161	I165	E166	I167	L168								
S173	MET	LEU	GLU	ILE	ASP	ILE	E180	D181	H189	S190	L191	K195	ASN	GLN	SER	LEU	GLY	L201	L204	L207	G225	L226	R231	E232	S233	T234	V235	L239	G256	L266	G274	P285	F286	C287	V295	R305	THR	ASP	GLY	VAL	ALA	THR	VAL	ASP	GLN													
GLN	PHE	SER	THR	HIS	S321	N322	E324	L328	S329	V330	L331	S332	L333	C334	N335	K336	I337	L340	V341	V342	L350	L351	L355	L360	D366	S367	L375	R376	K377	I381	V382	M385	R392	V400	R404	K405	K406	I407	G408	N412	W413	W414	K415	N416														
H431	T434	L451	M458	R459	Y460	S461	VAL	GLU	ARG	GLY	SER	ASP	K468	H472	F475	M478	Q483	M484	R485	L486	T489	L490	S494	K502	R508	L509	E513	ARG	GLU	PHE	SER	LYS	TYR	F520	G521	M522	L525	C528	Y529	A530	F533	A536																
L539	V540	F541	F542	L543	G549	R553	K554	C554	Y555	S560	Y572	C573	D574	P575	K576	V582	F583	S584	E585	E586	V587	L588	M591	M595	L613	R614	L615	L616	V617	L621	N628	L632	Q633	R636	Y637	F638	M644	D650	S653	K654	L655	C659																
S663	E664	V672	G681	D684	A685	K694	M698	E722	V735	V736	N737	F760	V775	C776	K777	W781	L786	F787	N788	R789	S795	L798	K799	N800	R804	PRO	ASN	PRO	ILE	THR	SER	THR	ALA	LEU	ASP	LEU	SER	SER	ASN	LYS	VAL	VAL	I822	L825														
D826	E827	L832	S833	T834	Y835	D836	K837	E838	A920	K839	L840	V841	S842	V845	A849	F852	K853	THR	GLY	ARG	TYR	N859	L860	S864	Y867	L869	L870	L873	T874	LEU	VAL	SER	ALA	PRO	LYS	ALA	LEU	ARG	SER	T886	S891	L892	M893	L897	T898	E899	E900	Q901										
V902	K909	V914	A917	K918	M919	A920	D921	ASN	SER	VAL	ASN	THR	ARG	THR	LYS	ASN	GLY	ARG	ALA	ASN	VAL	LYS	ASN	GLY	ASN	PRO	PHE	GLY	VAL	MET	LYS	GLU	ILE	ARG	ALA	V962	S963	L964	K965	E966	V967	K968	D969	F970														
D971	P972	D973	V974	L975	P976	P977	E978	V979	V980	K981	E982	L983	C984	D985	A986	Y987	Y988	K989	S990	S991	E992	K993	C994	N995	F996	F997	L998	E999	G1000	G1000	V1001	L1002	D1003	V1004	G1005	P1006	L1007	G1008	L1009	L1010	L1011	K1012	M1013	L1014	T1015	T1016	S1017	S1018	Y1019	E1023	Y1024	F1028	K1029	Y1030	L1031	L1032	I1033	Q1034
G1035	H1036	F1037	D1038	Q1039	LYS	LEU	GLY	SER	TYR	HIS	L1146	D1147	E1150	A1151	V1152	S1155	T1159	L1183	S1184	C1185	H1189	S1190	L1200	A1203	L1204	E1209	L1210	R1211	T1212	D1215	R1216	L1221	D1222	S1223	I1227	E1237	V1238	G1249	LYS	LEU	LYS	M1093	Y1097															
S1109	G1113	D1135	L1136	M1137	T1138	K1139	M1140	M1141	T1142	R1143	E1146	D1147	E1150	A1151	V1152	S1155	T1159	L1183	S1184	C1185	H1189	S1190	L1200	A1203	L1204	E1209	L1210	R1211	T1212	D1215	R1216	L1221	D1222	S1223	I1227	E1237	V1238	G1249	LYS	LEU	LYS	M1093	Y1097															
LEU	GLY	MET	GLY	CYS	GLY	S1262	S1266	S1282	M1285	L1288	G1291	I1294	D1300	L1301	Y1302	G1303	L1304	T1305	T1306	L1310	C1311	Y1312	T1326	S1327	S1328	Q1331	T1335	S1339	LEU	ASP	ILE	GLU	GLY	GLY	SER	D1347	M1351	L1352	M1353	M1354	L1355	C1356	L1361															



• Molecule 2: RING finger protein Z



• Molecule 2: RING finger protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36056	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 ($e^-/\text{\AA}^2$)	60	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	0.042	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	A	0.25	0/15349	0.44	0/20744
1	C	0.24	0/15349	0.44	0/20744
2	B	0.22	0/419	0.45	0/569
2	D	0.22	0/419	0.46	0/569
All	All	0.25	0/31536	0.44	0/42626

There are no bond length outliers.

There are no bond angle outliers.

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	15094	0	14961	274	0
1	C	15094	0	14961	271	0
2	B	407	0	383	5	0
2	D	407	0	383	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
All	All	31012	0	30688	550	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 9.

The worst 5 of 550 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:C:1011:LEU:HD12	1:C:1034:GLN:HG2	1.60	0.83
1:A:1011:LEU:HD12	1:A:1034:GLN:HG2	1.60	0.81
1:A:1835:LYS:HD3	1:A:1872:ILE:HD12	1.67	0.76
1:C:287:CYS:HB3	1:C:472:HIS:HE1	1.51	0.75
1:A:287:CYS:HB3	1:A:472:HIS:HE1	1.51	0.74

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	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
1	C	1899/2209 (86%)	1744 (92%)	155 (8%)	0	100	100
2	B	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
2	D	47/94 (50%)	34 (72%)	13 (28%)	0	100	100
All	All	3892/4606 (84%)	3556 (91%)	336 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	1690/2007 (84%)	1651 (98%)	39 (2%)	50	70
1	C	1690/2007 (84%)	1651 (98%)	39 (2%)	50	70
2	B	47/88 (53%)	47 (100%)	0	100	100
2	D	47/88 (53%)	47 (100%)	0	100	100
All	All	3474/4190 (83%)	3396 (98%)	78 (2%)	54	71

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1031	LEU
1	C	1736	VAL
1	C	1036	HIS
1	C	1369	VAL
1	C	2052	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	522	ASN
1	C	901	GLN
1	C	1916	ASN
1	C	568	GLN
1	C	737	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

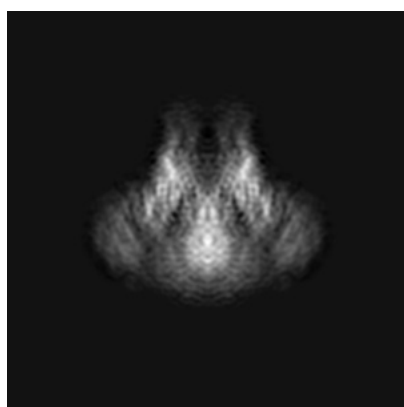
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31179. These allow visual inspection of the internal detail of the map and identification of artifacts.

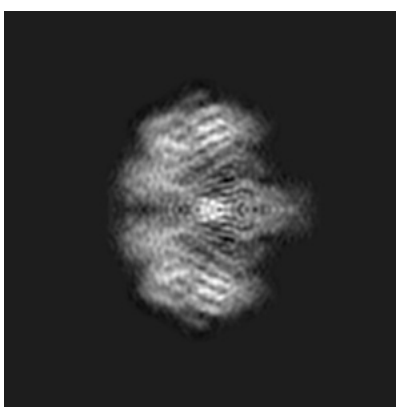
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

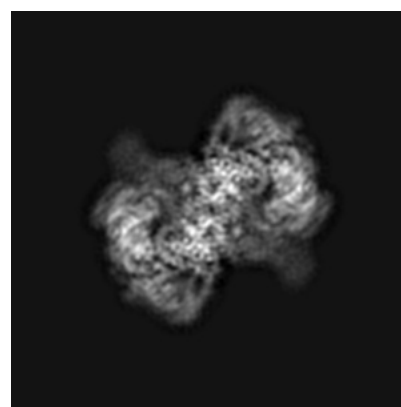
6.1.1 Primary map



X



Y



Z

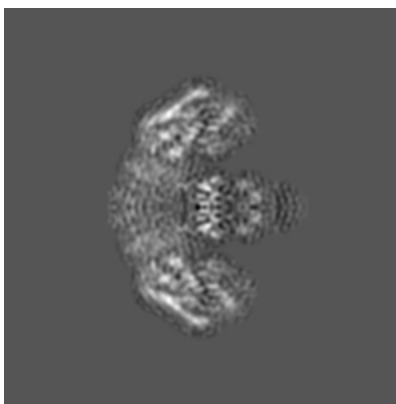
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

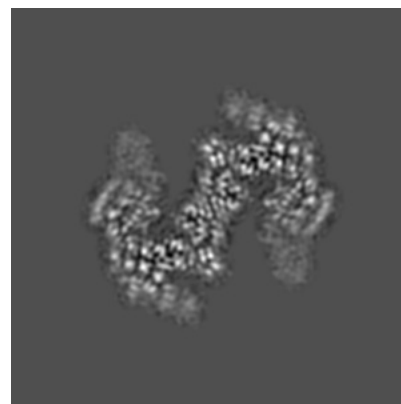
6.2.1 Primary map



X Index: 128



Y Index: 128

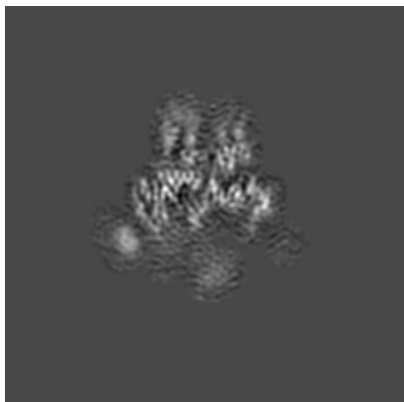


Z Index: 128

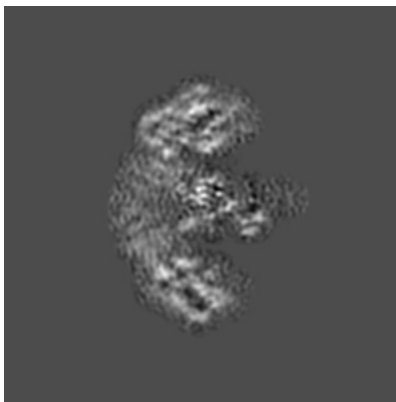
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

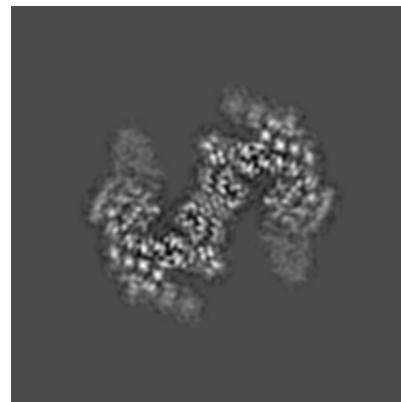
6.3.1 Primary map



X Index: 125



Y Index: 131



Z Index: 129

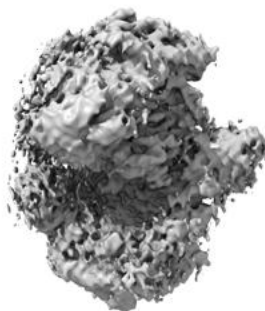
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

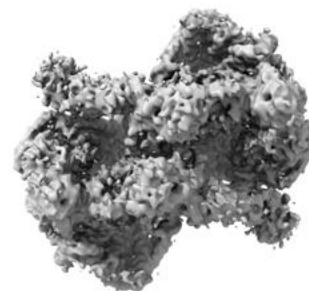
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

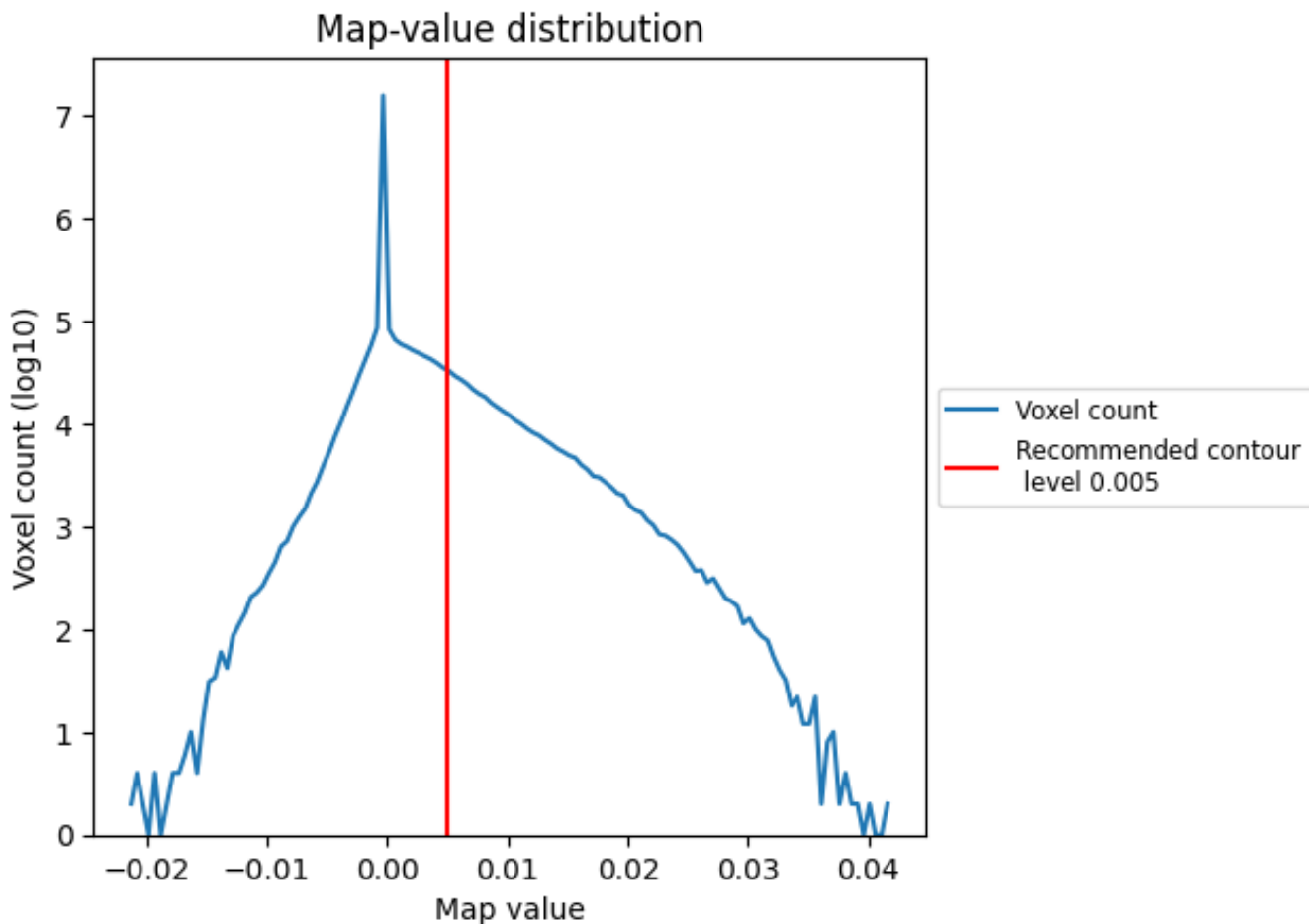
6.5 Mask visualisation

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

7 Map analysis [i](#)

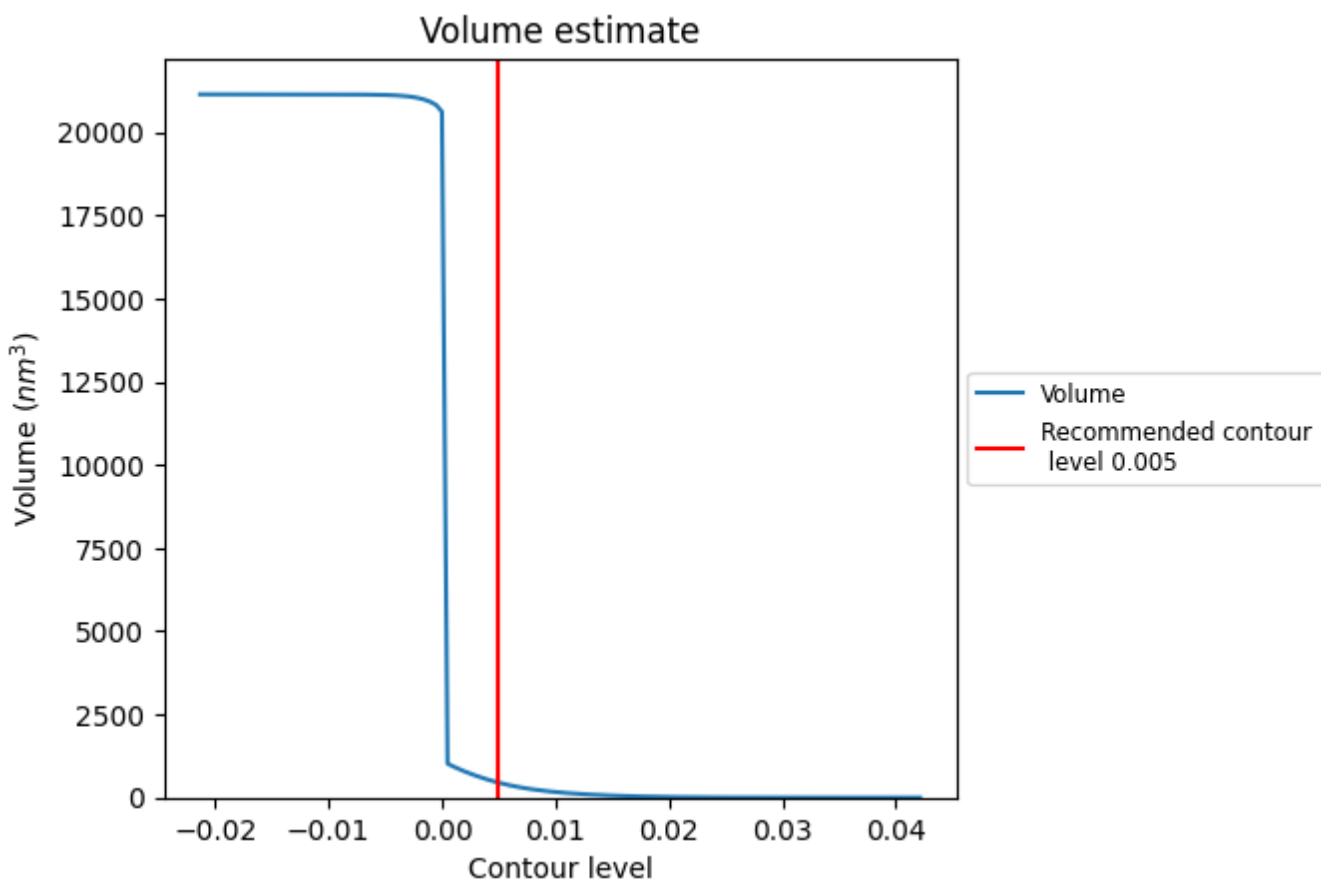
This section contains the results of statistical analysis of the map.

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.

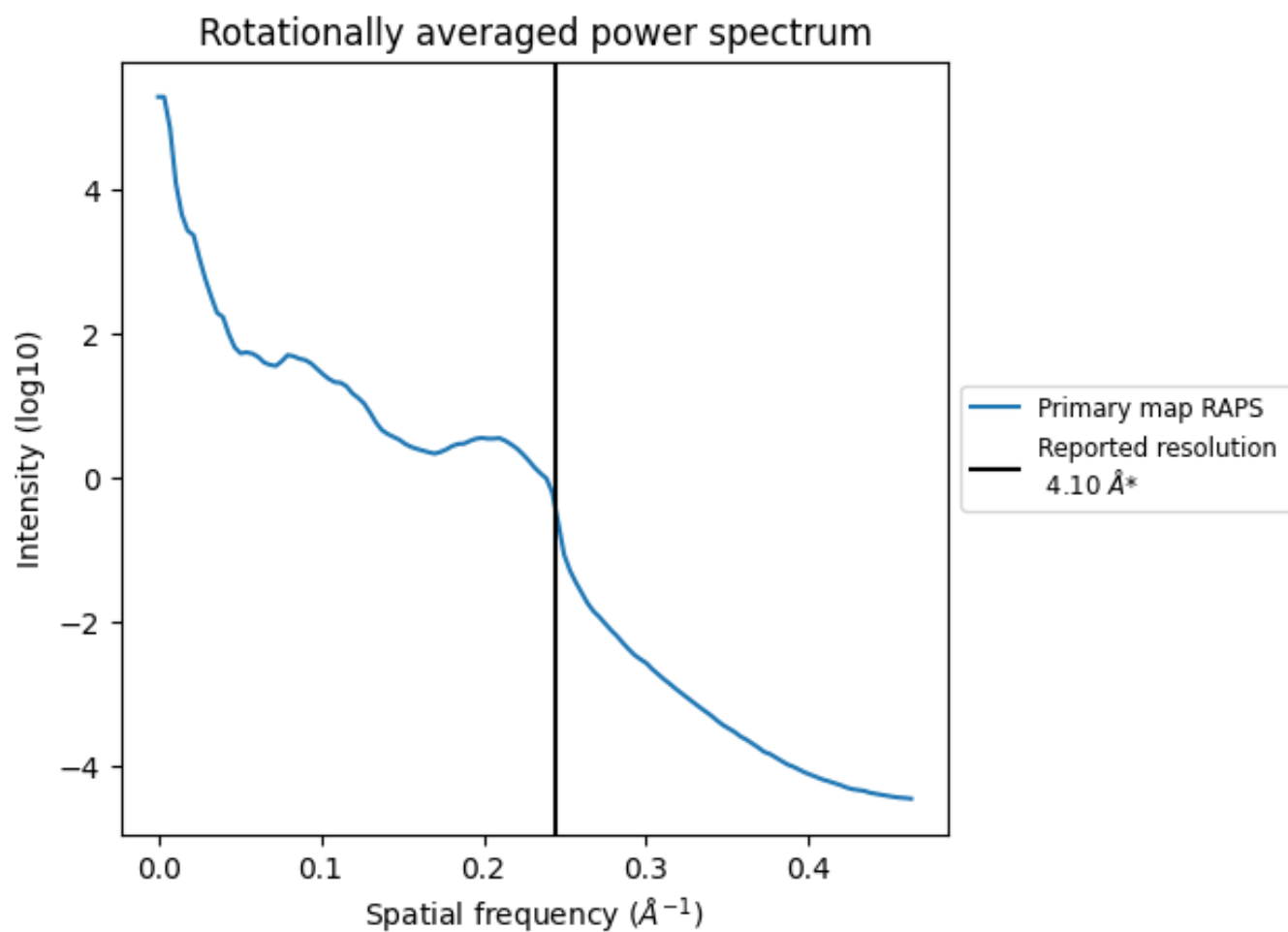
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 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 [i](#)

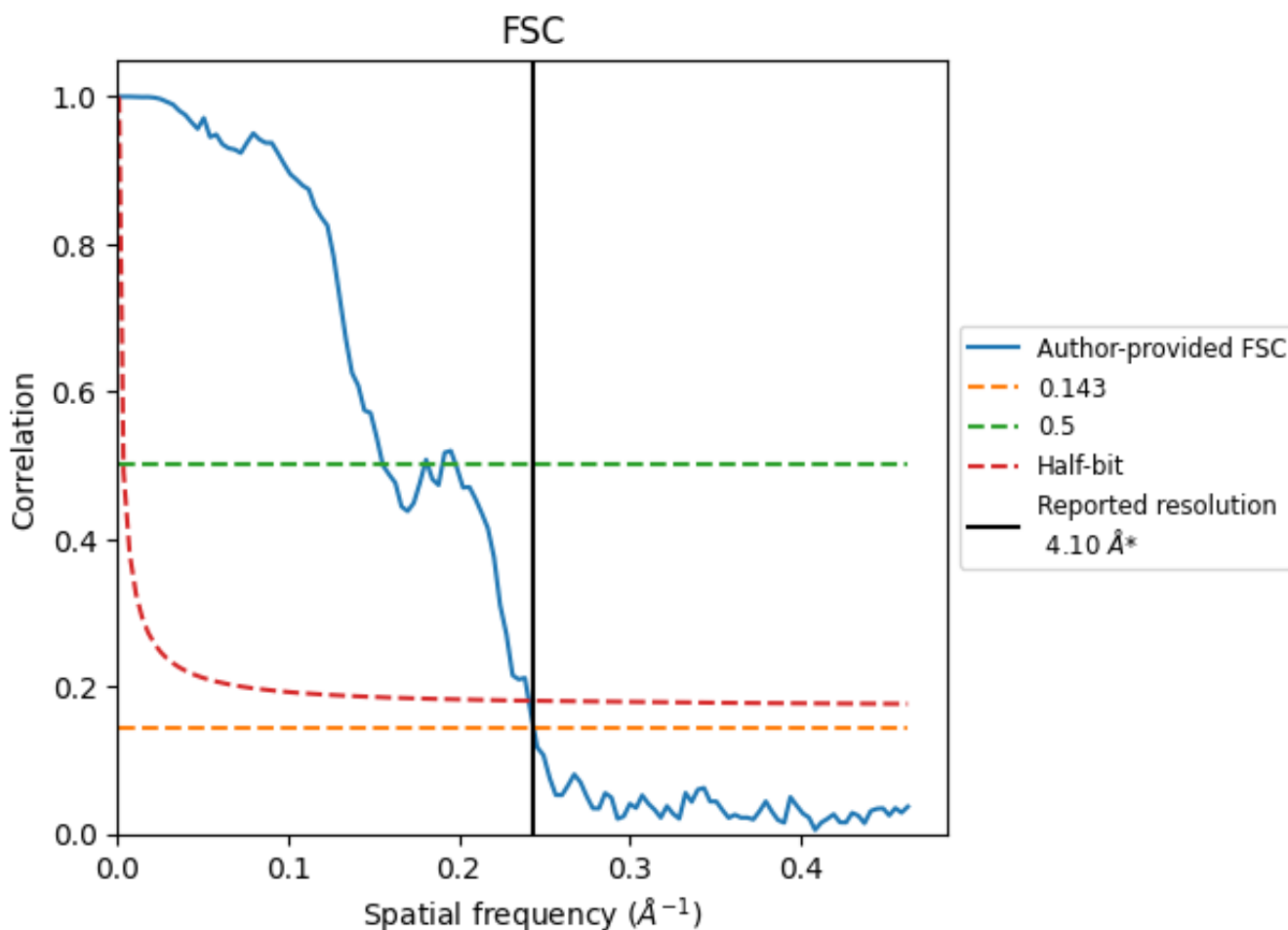


*Reported resolution corresponds to spatial frequency of 0.244\AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

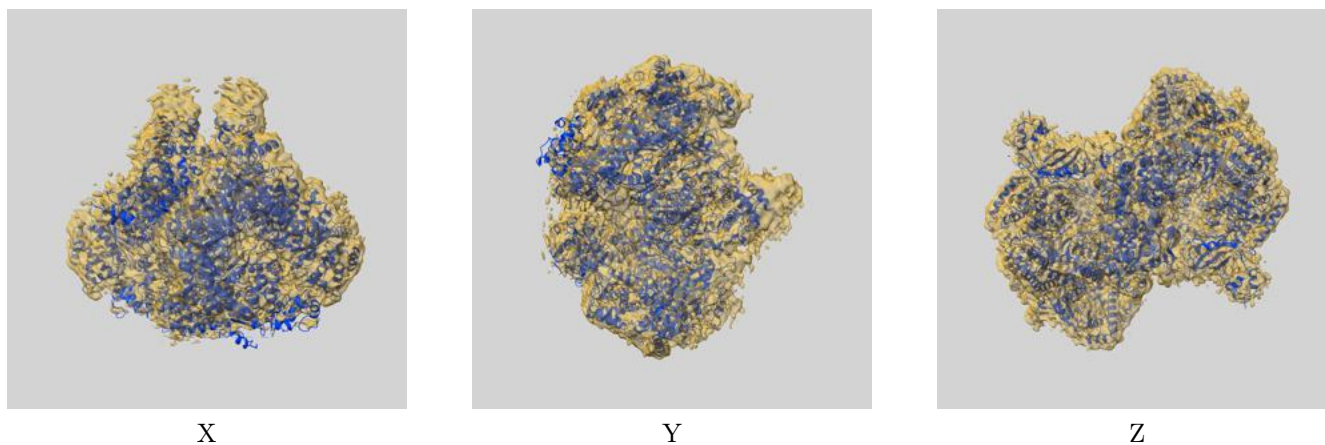
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	6.43	4.15
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

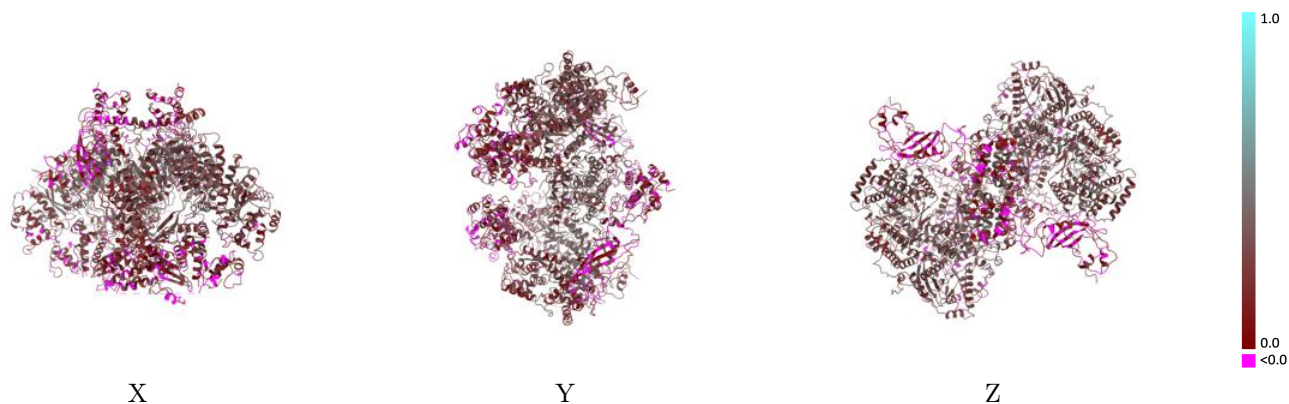
This section contains information regarding the fit between EMDB map EMD-31179 and PDB model 7ELB. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



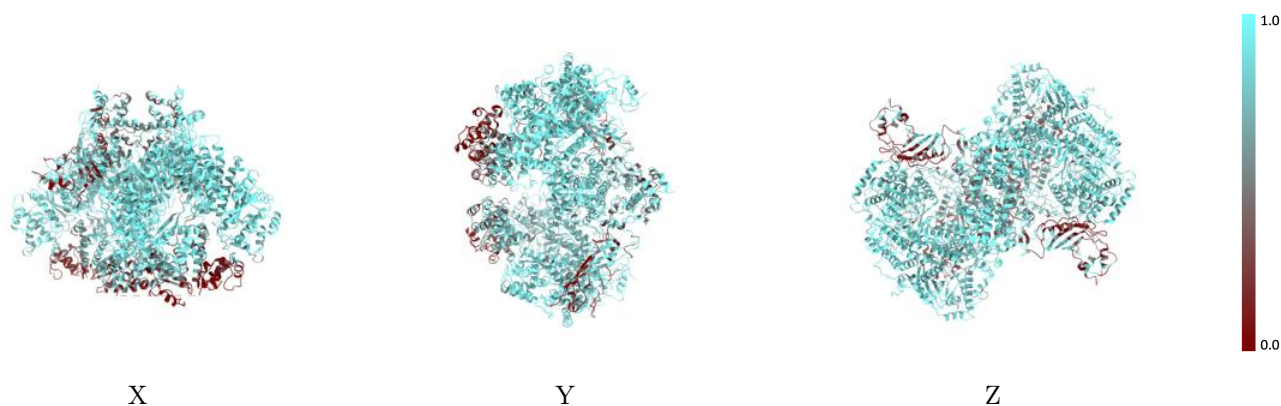
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



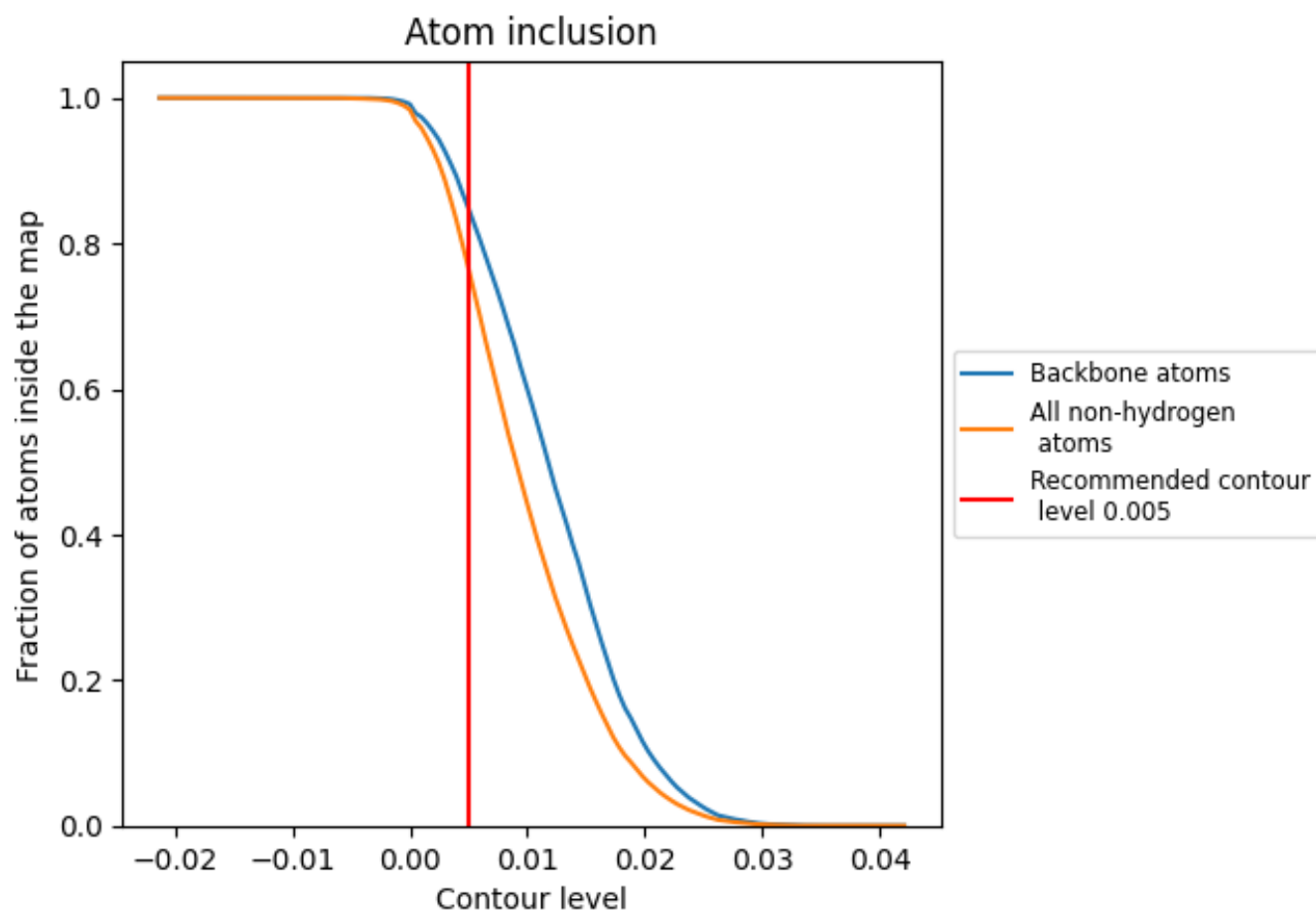
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).



9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7655	 0.2290
A	 0.7625	 0.2290
B	 0.9196	 0.2180
C	 0.7602	 0.2300
D	 0.9221	 0.2270

