



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:17 AM UTC

PDB ID : 5LKI / pdb_00005lki
EMDB ID : EMD-4068
Title : Cryo-EM structure of the Tc toxin TcdA1 in its pore state
Authors : Gatsogiannis, C.; Merino, F.; Prumbaum, D.; Roderer, D.; Leidreiter, F.;
Meusch, D.; Raunser, S.
Deposited on : 2016-07-22
Resolution : 3.46 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:

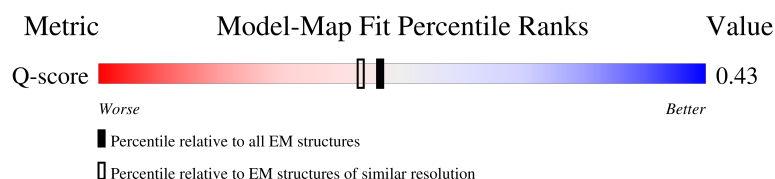
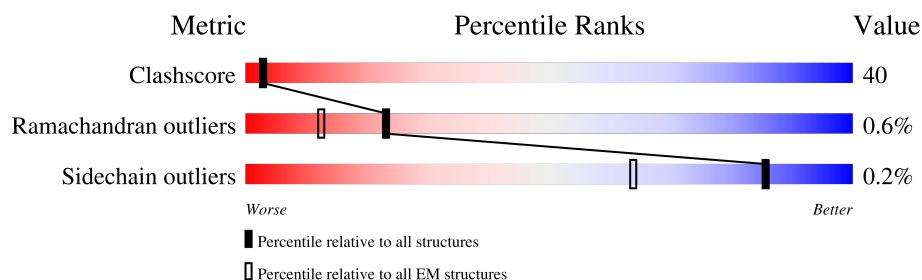
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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	2516	10% 29% 27% 43%
1	B	2516	10% 29% 28% 43%
1	C	2516	10% 29% 27% 43%
1	D	2516	10% 29% 27% 43%

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Mol	Chain	Length	Quality of chain
1	E	2516	

2 Entry composition

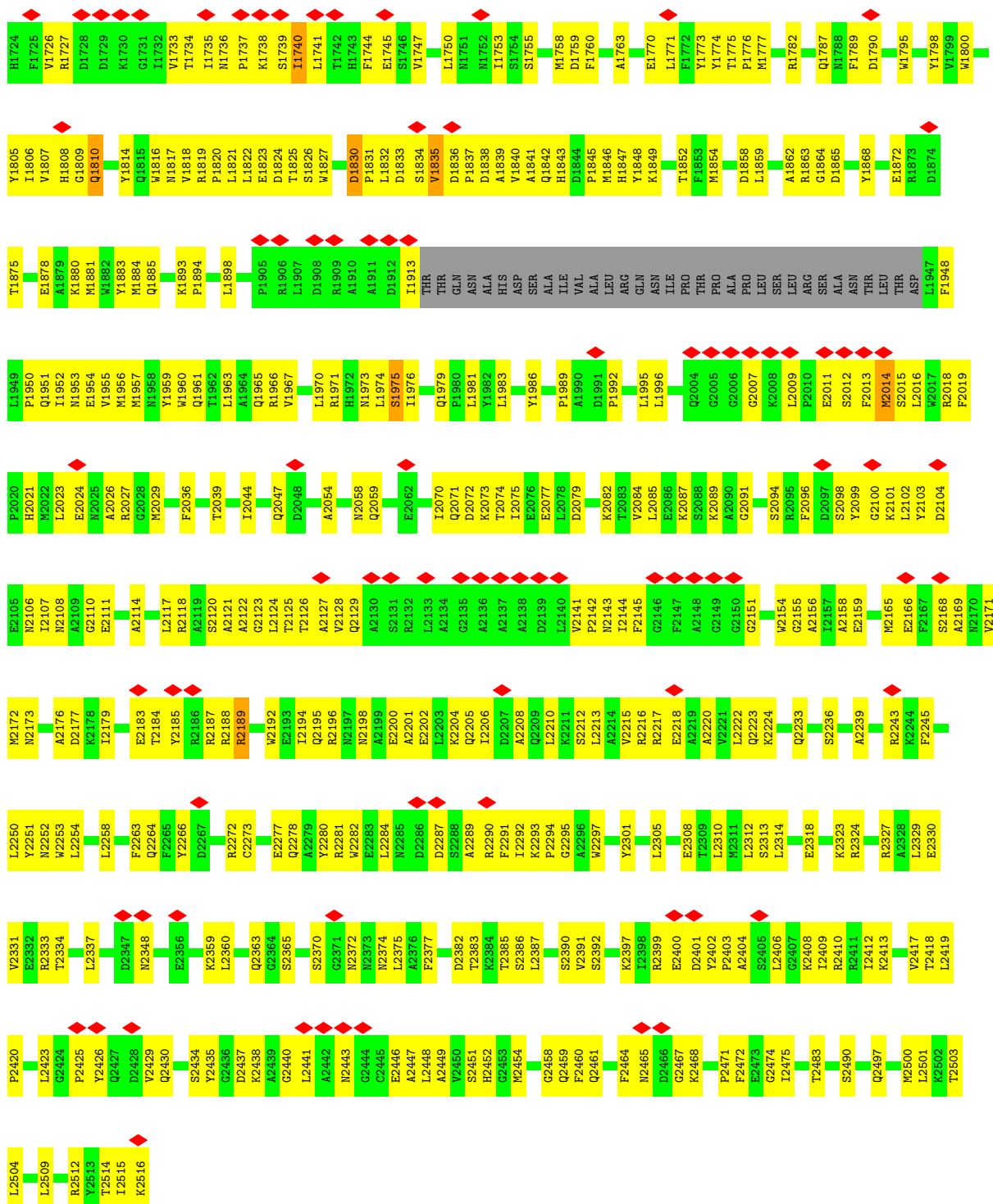
There is only 1 type of molecule in this entry. The entry contains 55415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

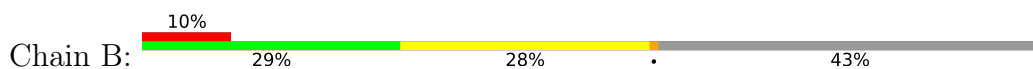
- Molecule 1 is a protein called TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	B	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	C	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	D	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0
1	E	1427	Total 11083	C 7001	N 1914	O 2130	S 38	0	0





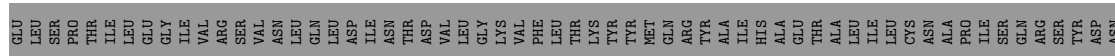
• Molecule 1: TcdA1



MET	ASN	GLU	SER	SER	VAL	LVS	GLU	ILE	PRO	ASP	VAL	LEU	LVS	SER	GLN	CYS	GLY	PHE	ASN	CYS	LEU	THR	ASP	ASP	ILE	SER	SER	SER	PHE	ASN	GLU	PHE	ARG	GLN	GLN	VAL	SER	SER	GLU	LEU	TRP	SER	GLU	THR	ASP	ASP	TTR	HIS	ASP	ASP	ALA	GLN	GLN	ALA	GLN	LVS	ASP	ASN	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

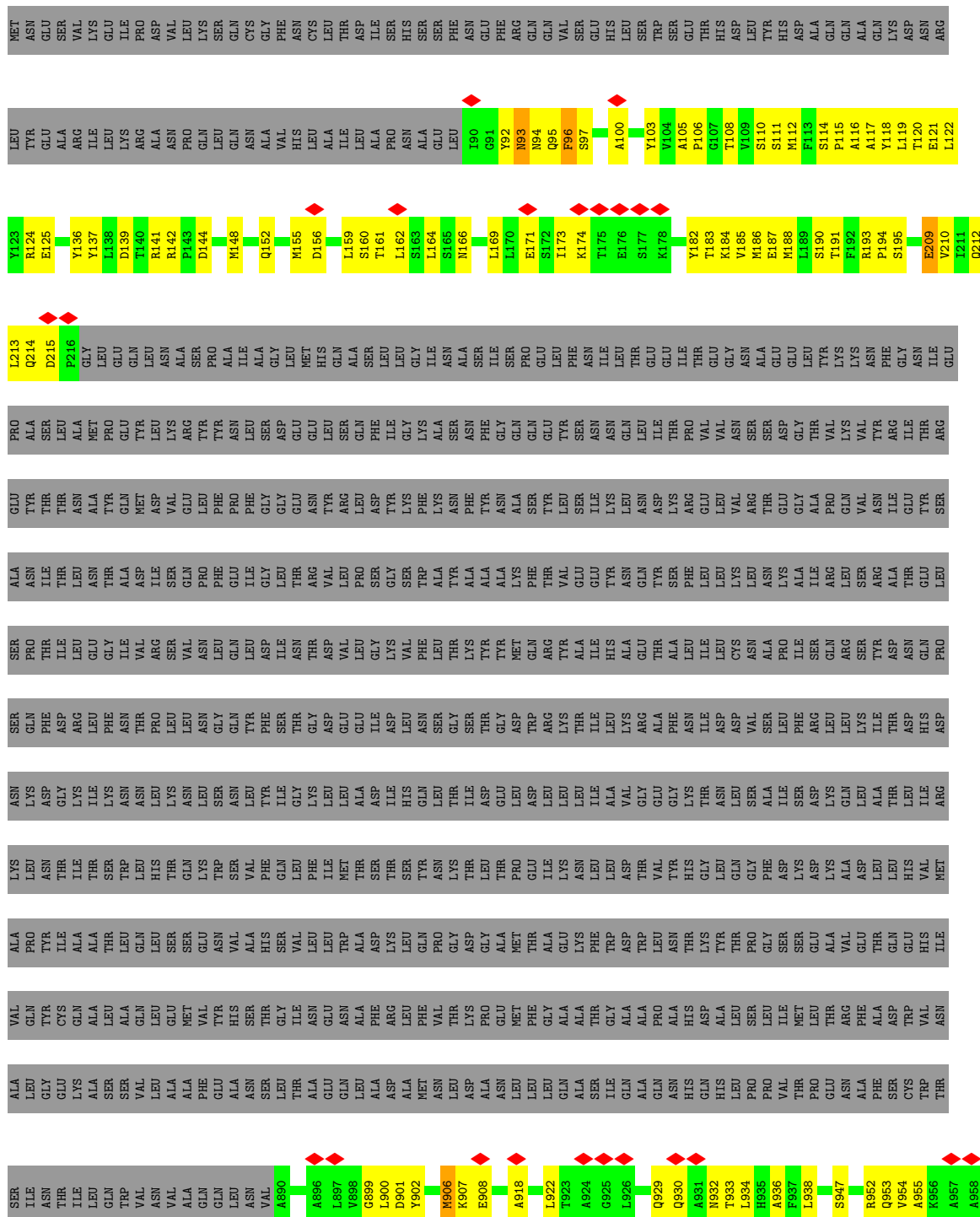




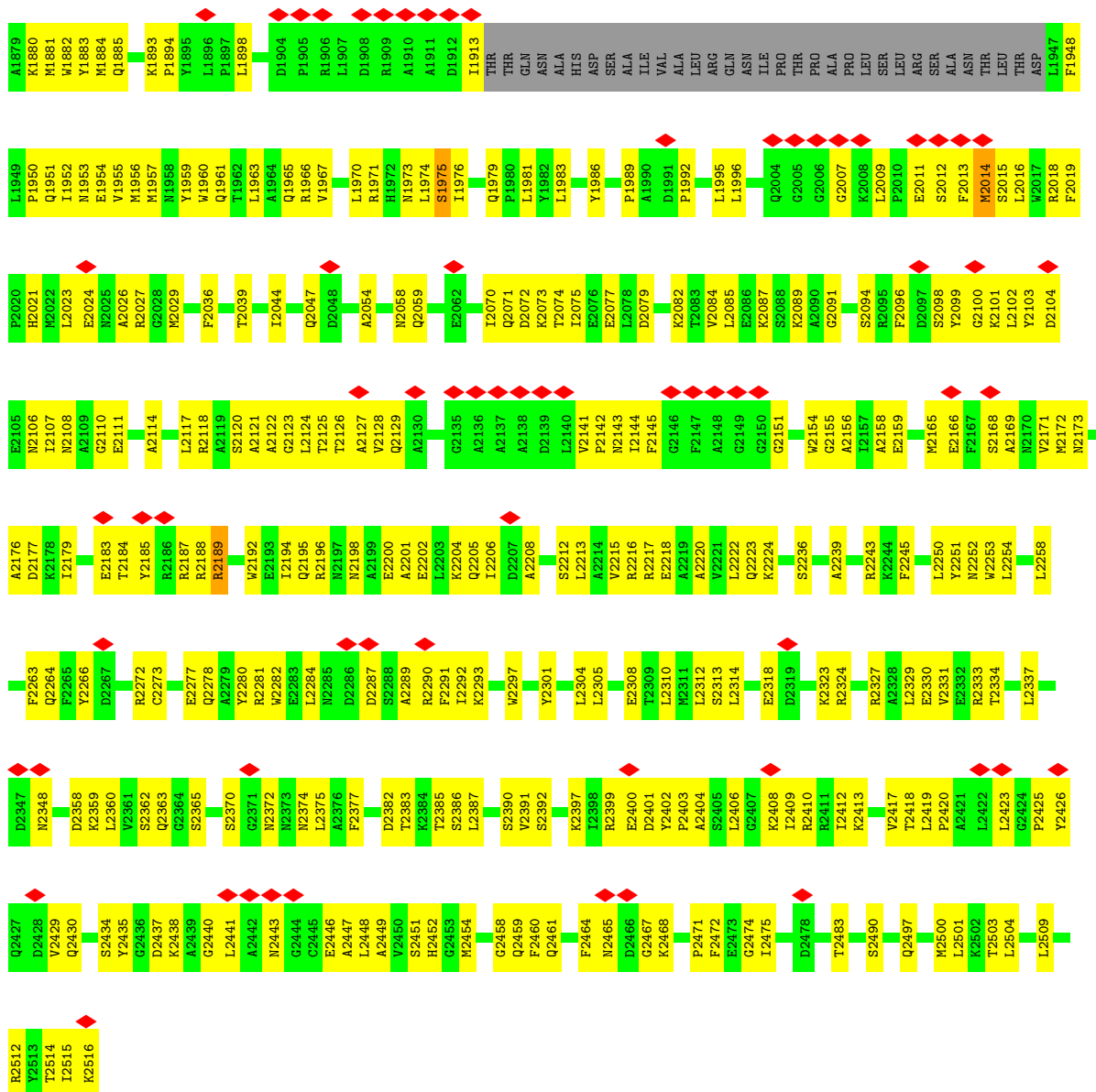




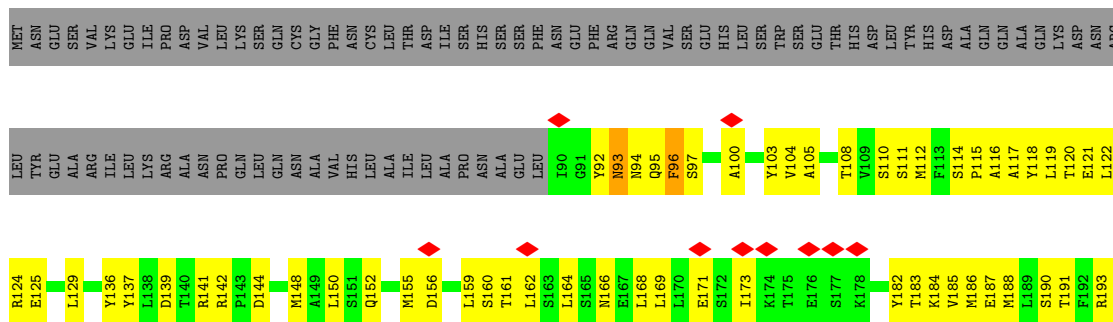
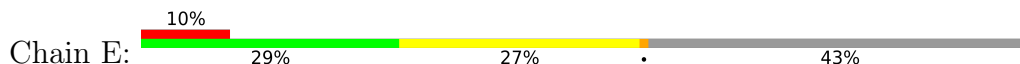
R2410	R2411	L2412	K2413	V2417	T2418	L2419	P2420	A2421	L2422	L2423	G2424	P2425	V2426	Q2427	D2428	V2429	Q2430	S2434	Y2435	G2436	D2437	K2438	A2439	G2440	L2441	A2442	N2443	G2444	E2445	E2446	A2447	L2448	A2449	V2450	S2451	H2452	G2453	N2454	G2458	Q2459	F2460	Q2461	F2464	N2465	G2466	G2467	K2468	P2471	F2472	E2473	G2474	I2475	T2483			
R2324	R2327	K2328	L2329	E2330	V2331	E2332	R2333	T2334	L2337	D2347	N2348	D2358	K2359	L2360	V2361	S2362	Q2363	G2364	S2365	S2370	G2371	N2372	N2373	N2374	L2375	A2376	F2377	D2382	T2383	K2384	S2385	G2386	L2387	S2390	V2391	S2392	D2395	L2396	K2397	I2398	R2399	E2400	D2401	Y2402	P2403	A2404	S2405	L2406	G2407	K2408	I2409					
A2239	R2243	K2244	F2245	L2250	Y2251	N2252	W2253	L2254	L2258	F2263	Q2264	F2265	Y2266	R2272	C2273	E2277	Q2278	A2279	Y2280	R2281	W2282	E2283	L2284	N2285	D2286	D2287	S2288	A2289	R2290	F2291	L2292	K2293	W2297	Y2301	L2304	L2305	E2308	T2309	L2310	M2311	L2312	S2313	L2314	E2318	D2319	K2323										
R2324	R2327	A2328	L2329	E2330	V2331	E2332	R2333	T2334	L2337	D2347	N2348	D2358	K2359	L2360	V2361	S2362	Q2363	G2364	S2365	S2370	G2371	N2372	N2373	N2374	L2375	A2376	F2377	D2382	T2383	K2384	S2385	G2386	L2387	S2390	V2391	S2392	D2395	L2396	K2397	I2398	R2399	E2400	D2401	Y2402	P2403	A2404	S2405	L2406	G2407	K2408	I2409					
R2410	R2411	L2412	K2413	V2417	T2418	L2419	P2420	A2421	L2422	L2423	G2424	P2425	V2426	Q2427	D2428	V2429	Q2430	S2434	Y2435	G2436	D2437	K2438	A2439	G2440	L2441	A2442	N2443	G2444	E2445	E2446	A2447	L2448	A2449	V2450	S2451	H2452	G2453	N2454	G2458	Q2459	F2460	Q2461	F2464	N2465	G2466	G2467	K2468	P2471	F2472	E2473	G2474	I2475	T2483			
S2094	R2095	F2096	D2097	S2098	Y2099	G2100	K2101	L2102	Y2103	D2104	E2105	P2106	L2107	N2108	A2109	G2110	E2111	A2114	L2117	R2118	A2119	S2120	A2121	A2122	G2123	L2124	T2125	A2126	T2127	V2128	Q2129	A2130	S2131	G2135	A2136	A2137	D2138	L2139	L2140	V2141	P2142	N2143	I2144	F2145	G2146	F2147	A2148	G2149	G2150	G2151	V2154	G2155	I2157	A2158		
L2009	P2010	E2011	S2012	F2013	M2014	S2015	L2016	W2017	R2018	P2019	H2020	H2021	K2022	L2023	E2024	H2025	A2026	R2027	G2028	N2029	F2036	T2039	L2044	Q2047	D2048	A2054	N2058	Q2059	E2062	T2070	Q2071	D2072	K2073	T2074	L2075	E2076	E2077	L2078	D2079	K2082	T2083	V2084	L2085	E2086	K2087	S2088	K2089	A2090	G2091	V2154	G2155	I2157	A2158			
ARG	SER	ALA	ASN	THR	LEU	THR	ASP	L1947	F1948	L1949	P1950	Q1951	I1952	M1953	E1954	V1955	M1956	M1957	H1958	Y1959	W1960	Q1961	L1962	L1963	A1964	Q1965	R1966	V1967	L1970	R1971	H1972	M1973	L1974	S1975	I1976	D1977	G1978	Q1979	P1980	L1981	Y1982	L1983	Y1986	P1989	A1990	D1991	P1992	L1995	L1996	Q2004	G2005	G2006	G2007	K2008		
A1862	R1863	G1864	D1865	Y1868	E1872	R1873	D1874	T1875	E1878	A1879	K1880	M1881	V1882	Y1883	M1884	Q1885	K1893	P1894	L1898	P1905	R1906	L1907	D1908	R1909	A1910	A1911	D1912	I1913	THR	THR	GLN	ASN	ALA	HIS	ASP	SER	ALA	ILE	VAL	VAL	ALA	LEU	ARG	GLN	ASN	ILE	THR	PRO	ALA	PRO	LEU	SER	LEU			
D1790	W1795	Y1798	Y1799	W1800	S1803	G1804	Y1805	V1806	V1807	H1808	G1809	Q1810	Y1814	Q1815	W1816	V1817	V1818	R1819	P1820	L1821	L1822	E1823	D1824	T1825	S1826	W1827	D1830	L1832	D1833	S1834	V1835	D1836	P1837	D1838	A1839	V1840	A1841	Q1842	H1843	D1844	P1845	M1846	H1847	Y1848	K1849	T1852	M1853	D1858	L1859							
G1718	T1719	W1720	G1721	G1722	P1723	H1724	F1725	V1726	R1727	D1728	V1729	K1730	G1731	I1732	V1733	T1734	I1735	M1736	P1737	K1738	S1739	I1740	L1741	T1742	H1743	F1744	E1745	S1746	V1747	L1750	I1753	S1754	S1755	M1758	D1759	F1760	A1763	E1770	L1771	F1772	Y1773	Y1774	T1775	P1776	M1777	L1778	V1779	R1782	L1783	Q1787	N1788	F1789				
D1657	T1658	L1659	H1657	H1658	W1660	F1661	N1659	E1659	Q1594	Y1595	M1596	K1666	H1667	V1668	Q1669	K1730	Y1601	R1602	T1603	R1604	L1605	N1606	A1610	R1611	Y1614	A1615	R1616	D1622	T1623	L1624	L1625	S1626	T1629	Q1633	E1634	P1635	Q1636	L1637	G1638	K1639	G1640	F1641	Y1642	A1643	T1644	V1645	V1646	T1647	P1648	P1649	Y1650	N1651	L1652	S1653	T1654	H1655
SER	PHE	ASP	GLU	MET	ASN	TYR	GLN	PHE	GLN	ASN	ASN	ALA	LEU	GLU	ILE	ASP	GLY	SER	GLY	LEU	ASN	PHE	ILE	ASN	SER	ALA	THR	PHE	THR	ALA	PHE	ALA	GLU	ASP	GLY	ARG	LYS	LEU	LEU	GLY	TYR	GLU	SER	PRO	ILE	PRO	VAL	THR	LEU	LYS	VAL	SER	T1580	D1581	N1582	A1583



Y1807	D1728	K1666	M1596	PHE	GLY	TYR	Q1292	R1232	L1170	M1103	S1029	A960
H1808	D1729	H1667	Q1597	ASN	ASN	ILE	Q1293	G1233	W1171	D1104	T1030	I961
G1809	K1730	V1668	W1598	THR	THR	SER	F1294	L1234	L1172	Q1105	W1031	K962
Q1810	G1731	V1669	S1600	GLU	GLU	PRO	D1295	Y1235	G1106	G1106	G1033	S963
Y1814	I1732	D1670	ILE	LYS	LEU	LEU	D1296	C1236	T1108	T1108	V1034	D965
Q1815	V1733	M1671	GLY	ASP	ASN	ARG	W1297	A1237	Y1109	Y1109	V1038	D966
W1816	T1734	N1672	GLY	THR	GLN	ILE	N1298	G1238	G1112	G1112	Y1039	L967
N1817	I1735	S1673	SER	ALA	GLN	ILE	N1299	L1239			Y1040	Y968
W1818	N1736	H1674	THR	THR	ARG	HIS	V1299	Q1240			P1041	Q969
R1819	N1737	L1675	LEU	LEU	ASN	GLY	R1300	G1241			N1042	Y970
P1820	K1738	I1676	VAL	VAL	LEU	TYR	R1301	E1242			N1043	
L1821	L1739	Y1677	GLY	SER	PHE	TYR	V1302	D1243			Y1044	Y973
L1822			GLY	GLY	HIS	GLU	N1303	T1244			Y1045	D974
E1823	A1740	Q1680	PRO	PRO	ARG	GLN	M1304	L1245			D1046	
T1825	L1741	L1681	VAL	VAL	THR	LYS	R1305	L1246				K976
S1826	T1742	T1682	ILE	ILE	ASN	ARG	TYR	W1247			M1049	Y977
W1827	H1743	D1683	THR	THR	PRO	GLN	ALA	M1248			R1050	S978
D1830	E1745	T1684	ALA	ALA	TRP	CYS	GLU	F1249			I1051	
P1831	S1746	M1685	THR	THR	GLY	ASN	ASP	Y1250			G1052	Y981
L1832	V1747	I1686	ILE	ILE	LEU	LEU	TYR	Y1251			Q1053	K982
D1833		M1687	SER	PRO	GLU	MET	ILE	K1251			D1127	T983
S1834	L1750	T1688	ALA	ALA	ALA	ASN	ILE	Q1252			Y1121	T984
V1835		I1689	LYS	LYS	THR	LYS	PRO	D1254			F1131	R985
D1836	I1753	F1691	VAL	VAL	GLN	TYR	SER	D1255			D1058	I986
P1837	S1754	I1692	ILE	ILE	PRO	GLY	VAL	T1255			L1059	
D1838	S1755	T1693	ILE	ILE	GLY	LEU	SER	L1256			D1132	A991
A1839	M1758	L1694	VAL	VAL	LYS	GLY	ARG	L1257			D1133	S992
V1840	D1759	D1695	ALA	ALA	ARG	ASP	LYS	S1258			G1134	I993
A1841	F1760	D1696	LYS	LYS	LEU	PHE	ASP	A1261			F1136	Q994
K1842		VAL	GLY	GLY	GLY	ILE	TYR	H1262			A1137	L996
H1843	A1763	PRO	GLY	GLY	GLN	VAL	TRP	I1263			N1139	N998
P1845	E1770	LEU	F1641	GLU	GLN	TYR	GLY	N1261			A1140	R999
M1846	L1771	ASN	A1642	THR	ASN	THR	ASP	A1262			W1141	
H1847	F1772	D1702	PHE	THR	ALA	SER	TYR	S1263			E1142	E1002
Y1848	Y1773	Y1703	THR	THR	ILE	GLY	TYR	D1264			E1143	N1003
K1849	I1774		PRO	PRO	ALA	VAL	LEU	Q1265			W1144	V1004
	T1775	K1706	VAL	VAL	ASP	ASN	SER	G1266			H1145	E1005
	P1776	V1707	THR	THR	ASP	PRO	MET	L1267			K1146	E1006
	L1777	Y1708	LEU	LEU	TYR	ASN	VAL	I1268			T1147	N1007
	M1778	M1709	VAL	VAL	ASN	ASN	GLY	F1269			D1148	A1008
	V1779	T1710	ILE	ILE	SER	SER	ASP	F1270			P1153	I1013
	R1782	F1711	GLN	GLN	ASN	ASN	ILE	A1271			Y1154	S1014
	L1783	K1712	PRO	PRO	LYS	LYS	PRO	D1272			K1155	R1015
	Q1787	K1713	SER	SER	ASN	LEU	THR	M1218			S1156	Q1016
	N1788	S1714	PRO	PRO	PRO	MET	ILE	K1219			T1157	F1017
	F1789	P1715	PHE	PHE	THR	TYR	ASN	K1220			P1160	F1018
	D1790	S1716	ASP	ASP	PRO	TYR	LYS	T1221			V1161	I1019
	W1795	D1717	GLY	GLY	VAL	VAL	ALA	S1222			I1162	D1020
	Y1796	G1718	MET	MET	TYR	TYR	ALA	E1223			Y1097	W1021
	Y1798	T1719	ASN	ASN	GLN	GLN	SER	L1224			Y1098	D1022
	W1799	W1720	TYR	TYR	TYR	TYR	ASP	K1225			D1099	M1025
	L1800	W1721	GLN	GLN	ILE	LEU	LYS	P1280			N1100	K1026
	Y1806	G1722	ILE	ILE	SER	LEU	ASP	E1281			L1166	R1027
	L1806	P1723	THR	THR	SER	ILE	ILE	Q1282			L1167	Y1028
		H1724						S1283			L1168	
		F1725						R1284			L1169	
		W1726						Y1285				
		R1727						R1286				
								D1288				
								N1289				
								S1290				
								I1291				



• Molecule 1: TcdA1







[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	13000	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 ($e^-/\text{\AA}^2$)	15.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	29.239	Depositor
Minimum map value	-15.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.75	Depositor
Map size (Å)	442.74002, 442.74002, 442.74002	wwPDB
Map dimensions	282, 282, 282	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	Depositor

5 Model quality

5.1 Standard geometry

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	0.60	1/11313 (0.0%)	0.75	19/15367 (0.1%)
1	B	0.60	1/11313 (0.0%)	0.75	19/15367 (0.1%)
1	C	0.60	1/11313 (0.0%)	0.75	19/15367 (0.1%)
1	D	0.60	1/11313 (0.0%)	0.75	19/15367 (0.1%)
1	E	0.60	1/11313 (0.0%)	0.75	19/15367 (0.1%)
All	All	0.60	5/56565 (0.0%)	0.75	95/76835 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1830	ASP	C-N	-9.53	1.01	1.34
1	D	1830	ASP	C-N	-9.52	1.01	1.34
1	C	1830	ASP	C-N	-9.51	1.02	1.34
1	B	1830	ASP	C-N	-9.50	1.02	1.34
1	A	1830	ASP	C-N	-9.49	1.02	1.34

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1789	PHE	N-CA-C	10.81	123.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1789	PHE	N-CA-C	10.80	123.06	111.28
1	A	1789	PHE	N-CA-C	10.80	123.05	111.28
1	E	1789	PHE	N-CA-C	10.79	123.04	111.28
1	B	1789	PHE	N-CA-C	10.79	123.04	111.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1005	GLU	Peptide
1	B	1005	GLU	Peptide
1	C	1005	GLU	Peptide
1	D	1005	GLU	Peptide
1	E	1005	GLU	Peptide

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	A	11083	0	10580	1116	0
1	B	11083	0	10579	1116	0
1	C	11083	0	10579	1131	0
1	D	11083	0	10580	1143	0
1	E	11083	0	10579	1121	0
All	All	55415	0	52897	4295	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 40.

The worst 5 of 4295 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:2176:ALA:CB	1:D:2117:LEU:HD22	1.13	1.59
1:D:2176:ALA:CB	1:E:2117:LEU:HD22	1.13	1.59
1:D:2169:ALA:CB	1:E:2124:LEU:HD22	1.29	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2169:ALA:HB2	1:B:2124:LEU:CD2	1.14	1.58
1:A:2117:LEU:HD22	1:E:2176:ALA:CB	1.16	1.58

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	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	21	53
1	B	1415/2516 (56%)	1297 (92%)	110 (8%)	8 (1%)	21	53
1	C	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	21	53
1	D	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	21	53
1	E	1415/2516 (56%)	1298 (92%)	109 (8%)	8 (1%)	21	53
All	All	7075/12580 (56%)	6489 (92%)	546 (8%)	40 (1%)	23	53

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PHE
1	A	954	VAL
1	A	1810	GLN
1	A	2144	ILE
1	B	96	PHE

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	1135/2157 (53%)	1133 (100%)	2 (0%)	87	84
1	B	1135/2157 (53%)	1133 (100%)	2 (0%)	87	84
1	C	1135/2157 (53%)	1133 (100%)	2 (0%)	87	84
1	D	1135/2157 (53%)	1133 (100%)	2 (0%)	87	84
1	E	1135/2157 (53%)	1133 (100%)	2 (0%)	87	84
All	All	5675/10785 (53%)	5665 (100%)	10 (0%)	85	84

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2189	ARG
1	E	1213	ILE
1	E	2189	ARG
1	B	2189	ARG
1	C	1213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1053	GLN
1	E	1298	ASN
1	E	2071	GLN
1	B	2321	HIS
1	B	2198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1830:ASP	C	1831:PRO	N	1.02
1	B	1830:ASP	C	1831:PRO	N	1.02
1	C	1830:ASP	C	1831:PRO	N	1.02
1	D	1830:ASP	C	1831:PRO	N	1.02
1	E	1830:ASP	C	1831:PRO	N	1.02

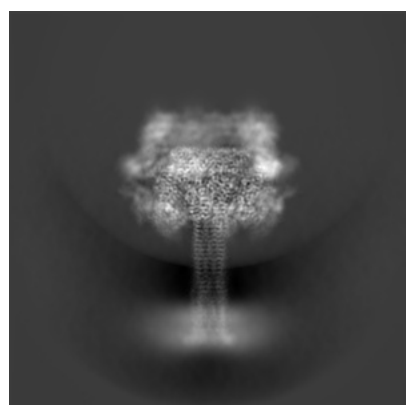
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4068. These allow visual inspection of the internal detail of the map and identification of artifacts.

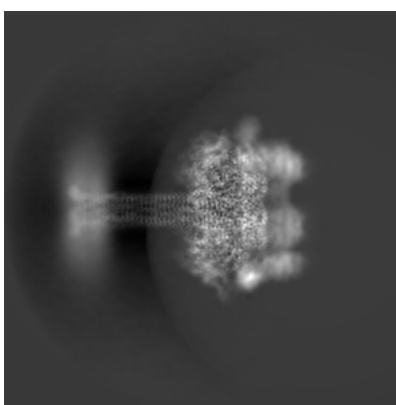
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

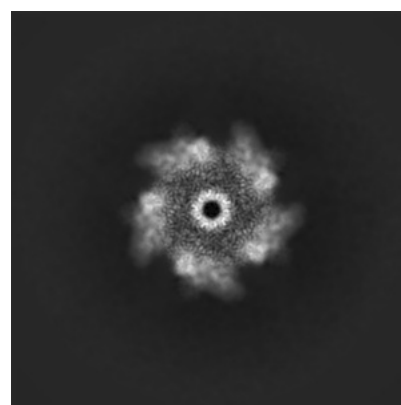
6.1.1 Primary map



X



Y



Z

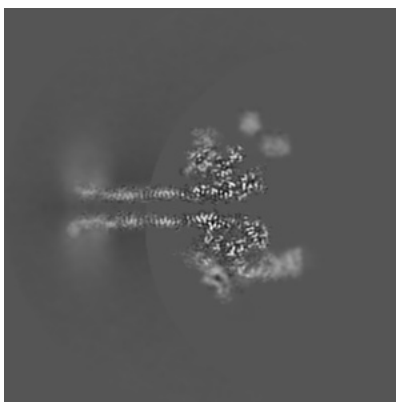
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

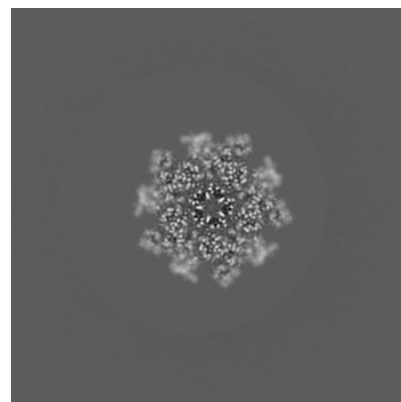
6.2.1 Primary map



X Index: 141



Y Index: 141

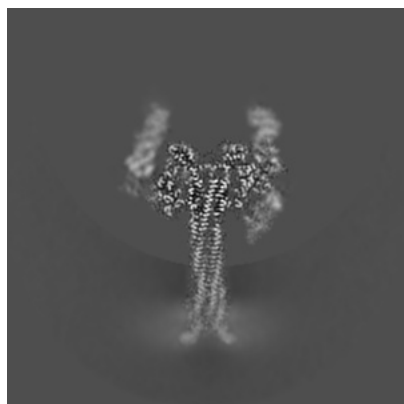


Z Index: 141

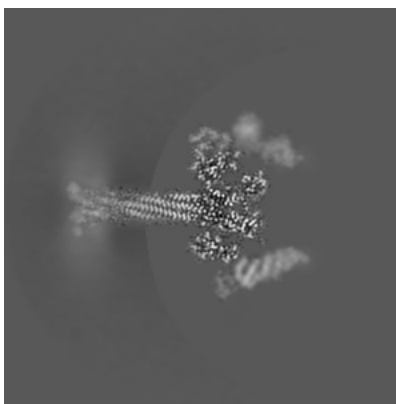
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

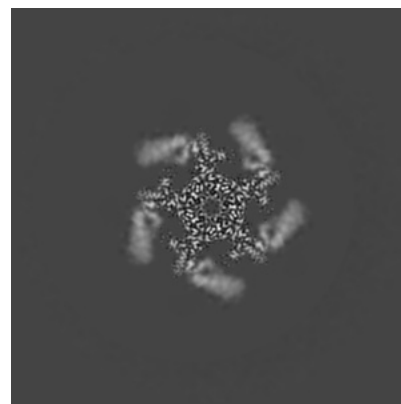
6.3.1 Primary map



X Index: 134



Y Index: 132

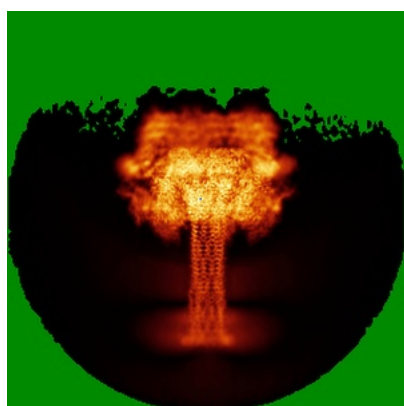


Z Index: 169

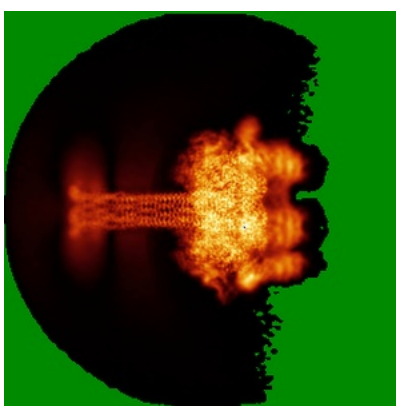
The images above show the largest variance slices of the map in three orthogonal directions.

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

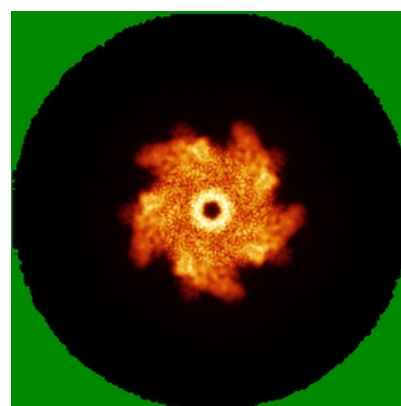
6.4.1 Primary map



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

This section was not generated.

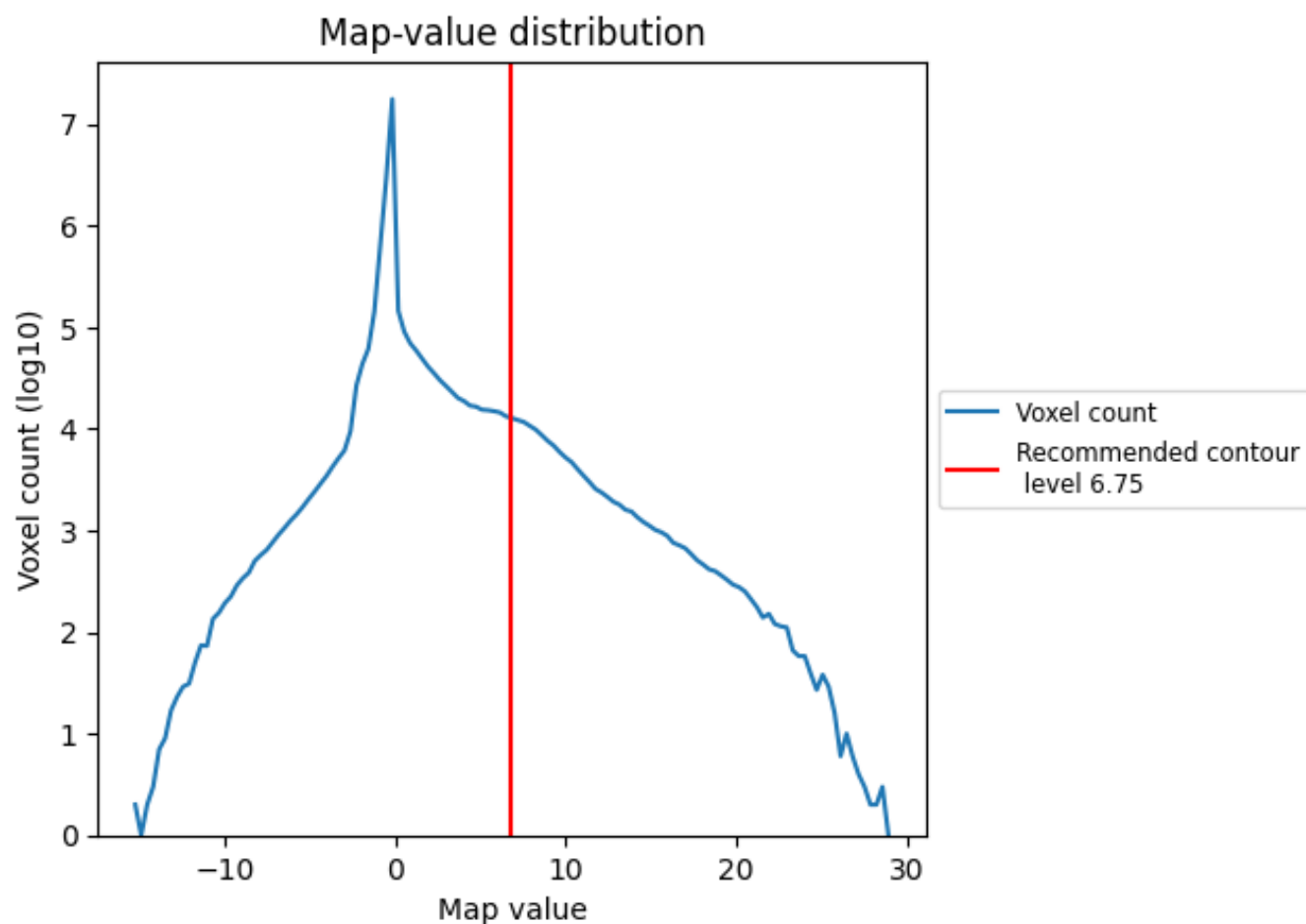
6.6 Mask visualisation

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

7 Map analysis [i](#)

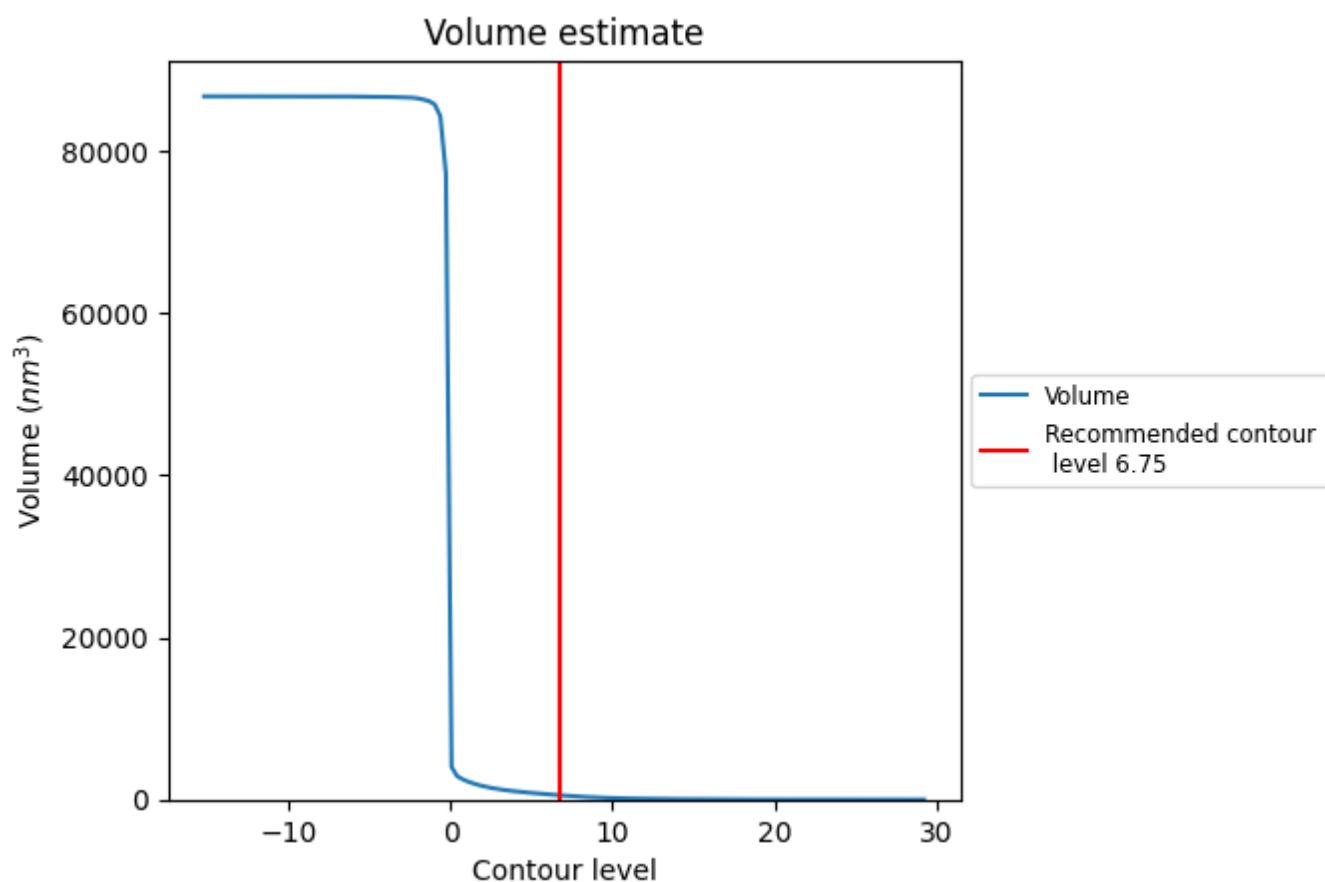
This section contains the results of statistical analysis of the map.

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.

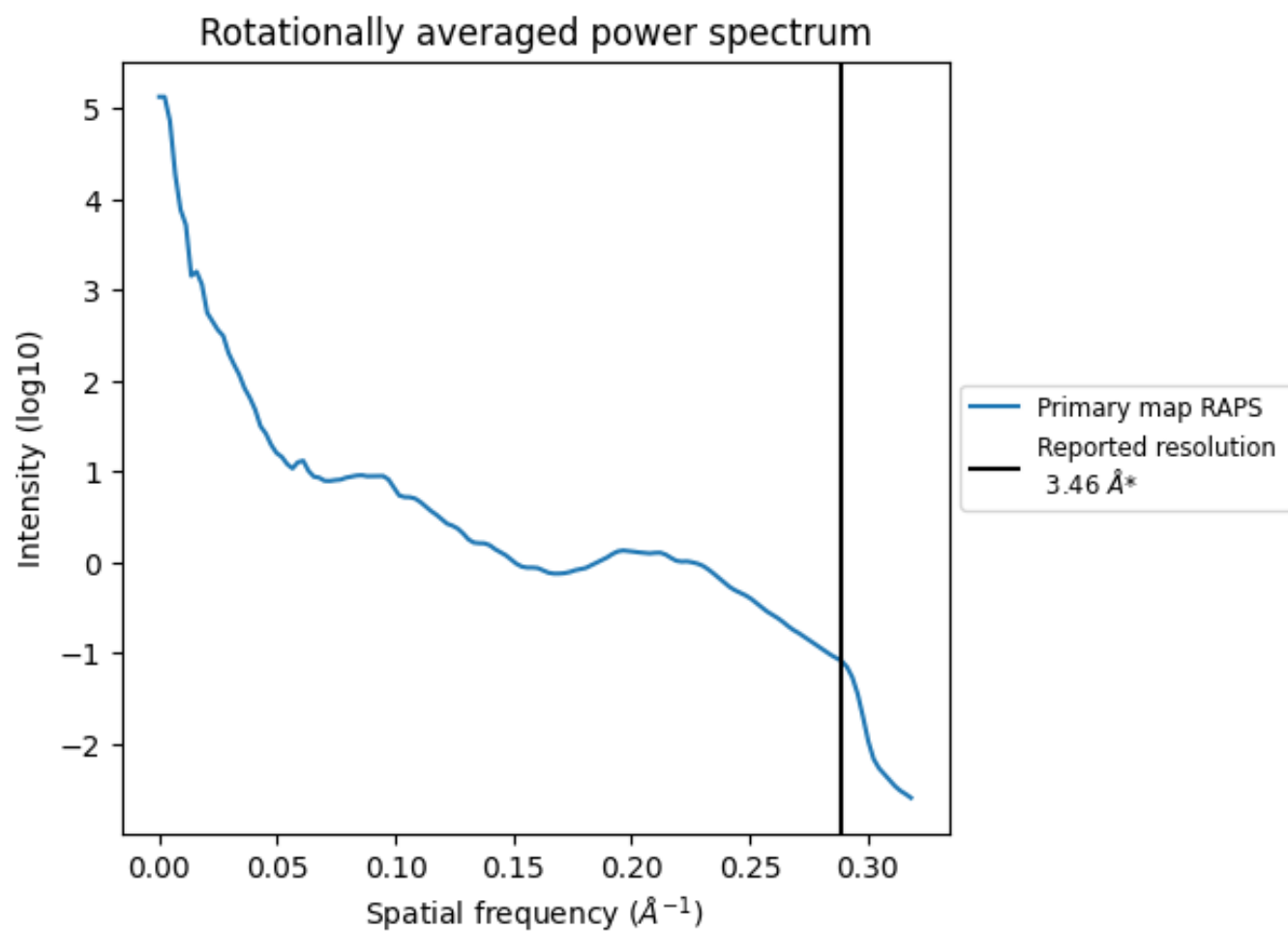
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 535 nm³; this corresponds to an approximate mass of 483 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 0.289 $\text{\AA}^{-1}$

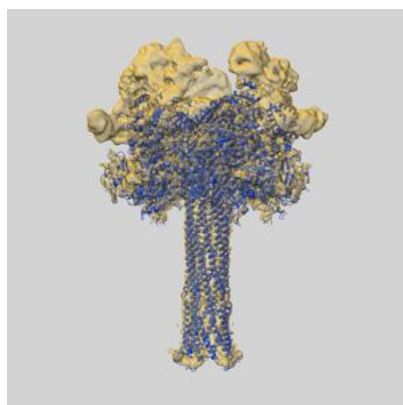
8 Fourier-Shell correlation

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

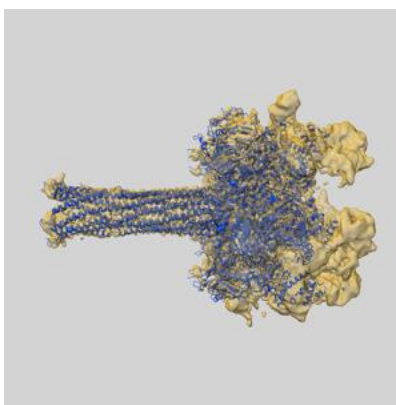
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4068 and PDB model 5LKI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

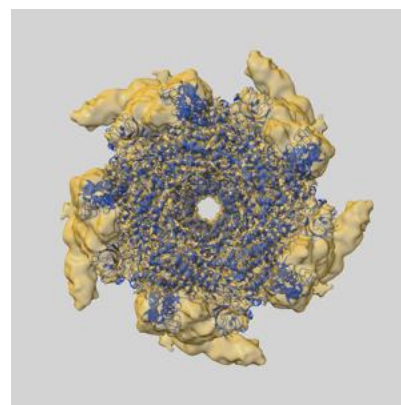
9.1 Map-model overlay [i](#)



X



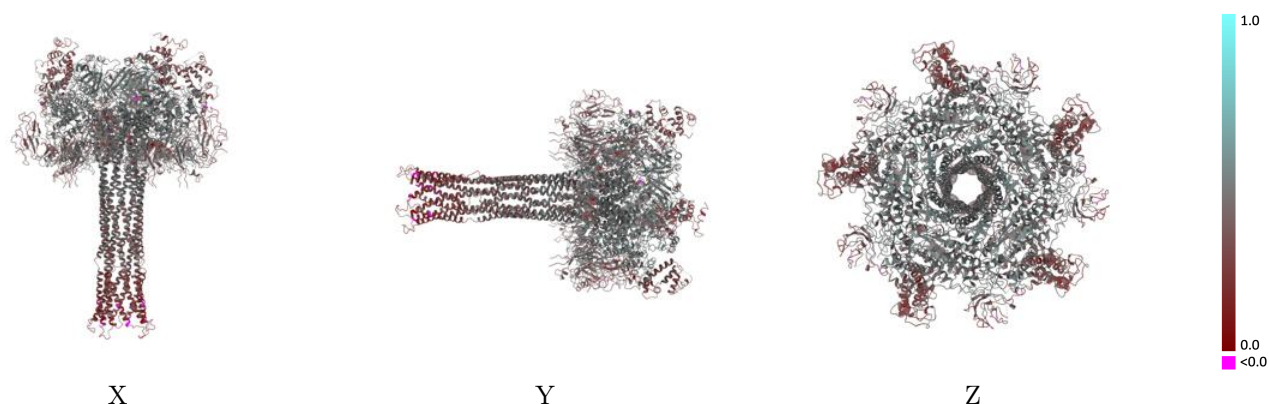
Y



Z

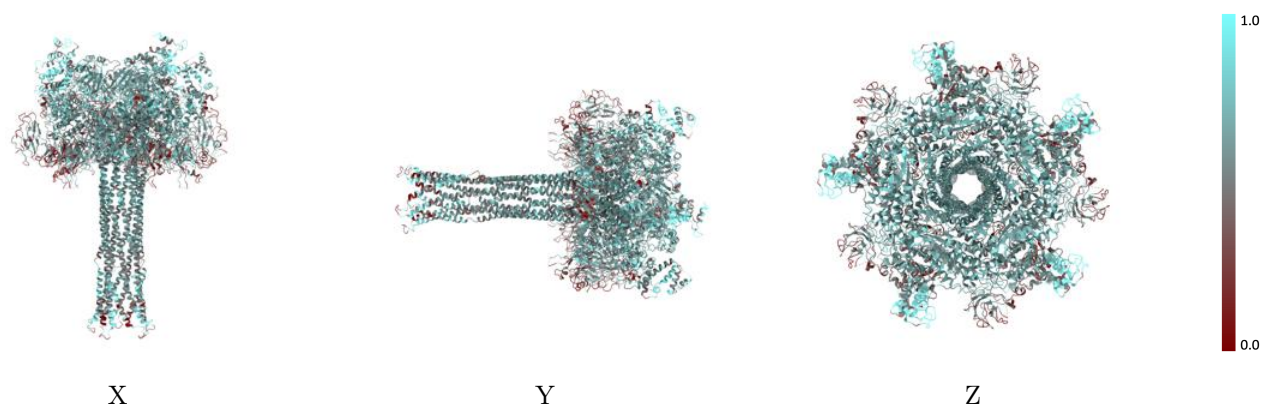
The images above show the 3D surface view of the map at the recommended contour level 6.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



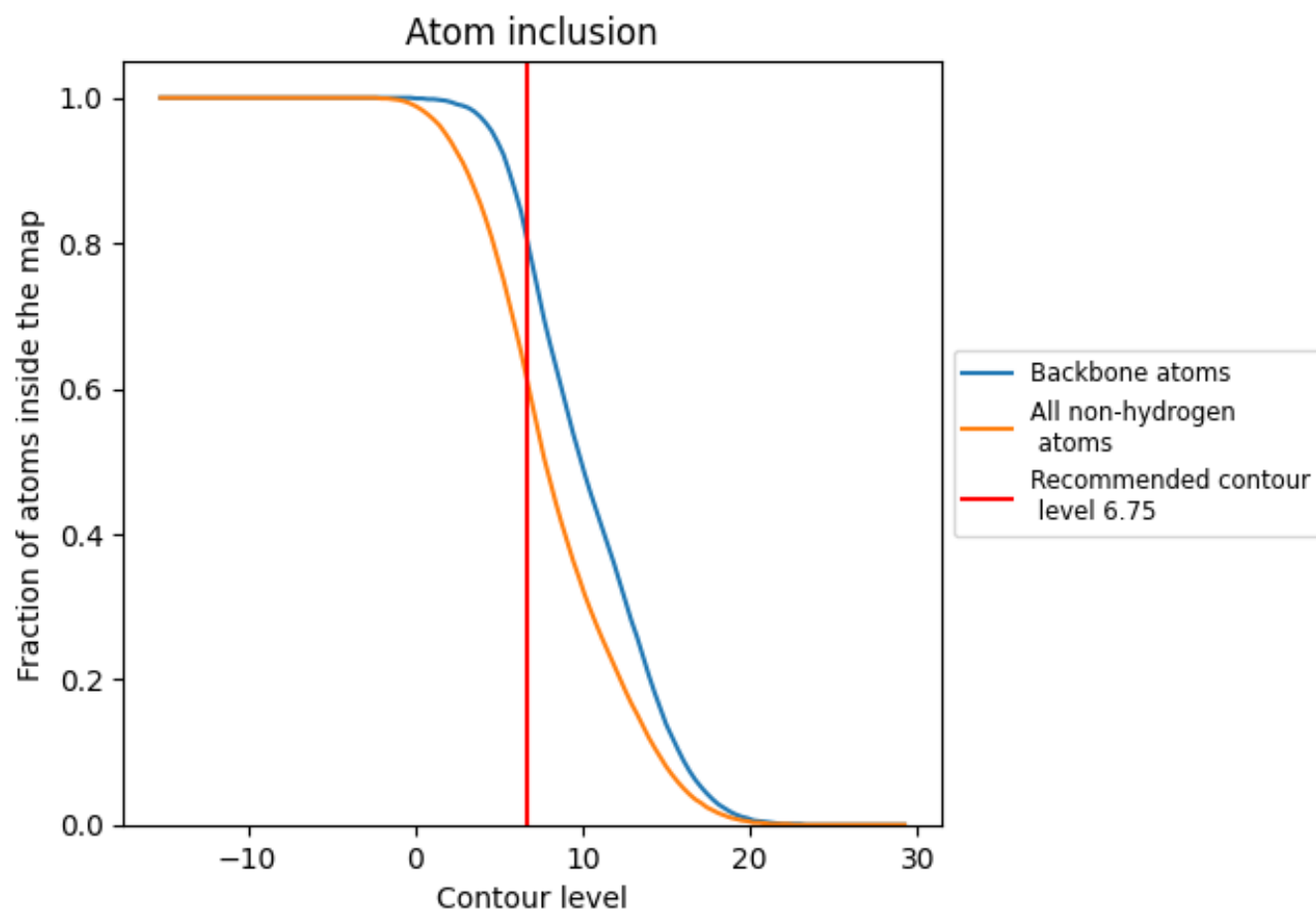
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 60% 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 (6.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6050	0.4300
A	0.6120	0.4380
B	0.6020	0.4270
C	0.6020	0.4270
D	0.6050	0.4280
E	0.6060	0.4300

