



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 8JB5 / pdb_00008jb5
EMDB ID : EMD-36141
Title : The cryo-EM structure of Paeniclostridium sordellii lethal toxin (TcsL)
Authors : Zhan, X.; Tao, L.
Deposited on : 2023-05-08
Resolution : 2.90 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

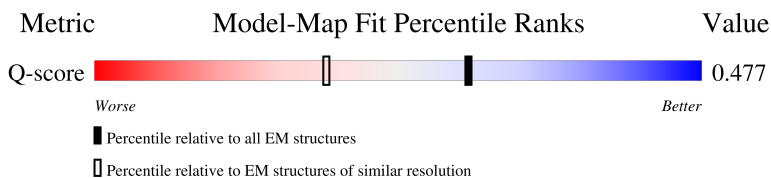
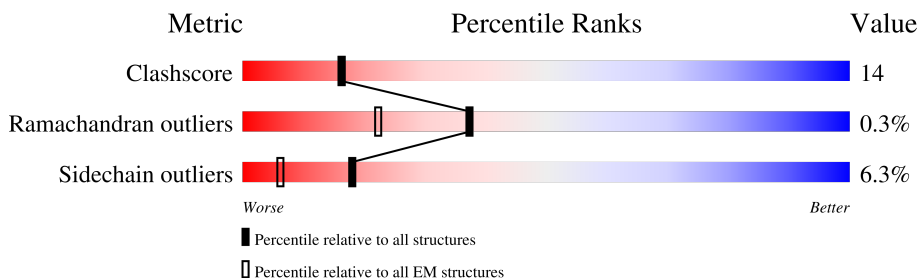
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	2372	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19027 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 Cytotoxin-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2355	Total	C	N	O	S	0	0
			19026	12183	3022	3774	47		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2365	HIS	-	expression tag	UNP T0D3N5
A	2366	HIS	-	expression tag	UNP T0D3N5
A	2367	HIS	-	expression tag	UNP T0D3N5
A	2368	HIS	-	expression tag	UNP T0D3N5
A	2369	HIS	-	expression tag	UNP T0D3N5
A	2370	HIS	-	expression tag	UNP T0D3N5
A	2371	HIS	-	expression tag	UNP T0D3N5
A	2372	HIS	-	expression tag	UNP T0D3N5

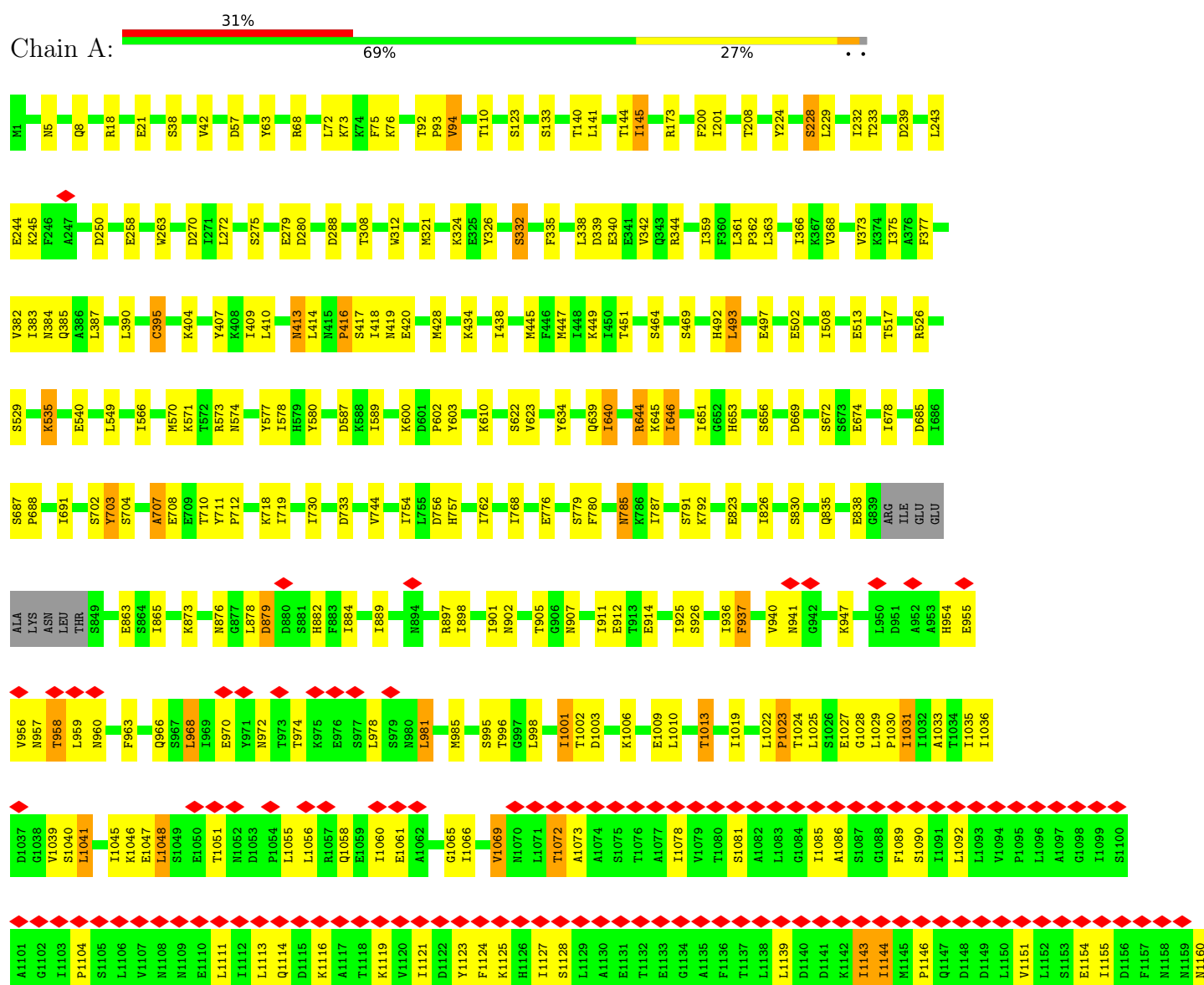
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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: Cytotoxin-L



F2163	D2164	T2165	P2166	D2167	G2168	Y2169	K2170	F2171	T2172	A2173	P2174	L2175	L2176	T2177	V2178	D2179	D2180	N2181	I2182	Y2183	G2184	Q2185	A2186	V2187	K2188	Y2189	S2190	G2191	L2192	V2193	R2194	V2195	N2196	E2197	D2198	V2199	Y2200	Y2201	F2202	G2203	E2204	T2205	Y2206	K2207	L2208	E2209	T2210	G2211	I2212	E2214	N2215	L2216	T2217	D2218	Y2219	Y2220	Y2221	F2222	
T2103	V2104	I2105	N2106	D2107	C2108	K2109	Y2110	Y2111	D2112	D2113	D2114	N2115	G2116	I2117	R2118	Q2119	L2120	G2121	F2122	I2123	T2124	I2125	N2126	D2127	L2128	I2129	F2130	Y2131	S2132	S2133	E2134	G2135	N2136	D2137	F2138	Y2139	K2140	Y2141	Y2142	Q2143	D2144	I2145	N2146	G2147	N2148	F2149	F2150	Y2151	D2152	N2153	N2154	S2155	G2156	L2157	V2158	I2159	G2160	V2161	L2162
K2043	D2044	D2045	D2046	L2047	G2048	T2049	E2050	E2051	E2052	E2053	L2054	T2055	L2056	Y2057	N2058	G2059	L2060	L2061	N2062	F2063	N2064	G2065	K2066	I2067	L2068	Y2069	F2070	D2071	I2072	S2073	N2074	T2075	A2076	V2077	V2078	G2079	V2080	G2081	T2082	L2083	D2084	D2085	G2086	S2087	T2088	Y2089	Y2090	Y2091	D2092	D2093	N2094	T2095	A2096	E2097	A2098	C2099	L2100	G2101	L2102
N1983	G1984	I1985	M1986	Q1987	T1988	G1989	F1990	I1991	T1992	I1993	N1994	D1995	K1996	V1997	F1998	Y1999	F2000	N2001	N2002	D2003	G2004	V2005	K2006	G2007	V2008	G2009	Y2010	I2011	E2012	N2013	G2015	K2016	Y2017	T1963	G1964	E1965	L1966	G1967	K1968	G1969	L1970	H1971	Q1972	I1973	G1974	I1975	N1976	K1977	Y1978	F1979	F1980	D1981	D1982						
L1737	S1738	V1742	N1745	I1751	S1756	Q1761	P1762	Q1763	R1767	V1771	F1772	D1775	T1776	D1779	P1634	Y1635	F1636	Y1649	G1650	G1651	L1652	R1653	L1656	Y1662	H1663	L1664	G1668	N1669	I1670	S1671	D1686	R1687	V1692	L1698	I1714	I1719	D1722	I1726	S1588	I1591																			
I1497	Y1498	M1499	D1501	S1502	N1503	N1504	L1505	F1506	I1507	D1512	L1513	L1514	L1515	I1516	K1521	G1522	D1523	K1533	D1534	F1535	S1539	L1540	S1541	F1542	T1543	D1546	T1547	N1548	T1549	I1550	K1551	L1552	N1553	Y1556	L1557	G1561	K1573	S1574	A1575	N1577	T1578	L1582	F1585	S1588	I1591														
S1407	I1408	L1409	E1410	D1411	I1412	N1413	I1414	I1415	I1416	E1417	I1418	D1419	L1420	V1421	S1424	Y1425	I1427	G1433	L1436	I1437	E1438	L1439	S1440	S1441	D1442	G1445	K1446	L1447	D1448	H1449	L1450	G1451	F1452	N1453	G1454	E1455	H1456	Q1457	K1458	Y1459	P1461	Y1462	S1463	Y1464	D1465	N1467	E1468	T1469	K1470	R1495	N1496								
W1344	V1345	V1348	D1349	M1350	V1351	V1352	K1353	N1354	I1355	T1356	I1357	I1358	S1359	E1361	S1360	D1360	E1361	S1297	F1298	I1299	V1302	I1303	T1304	T1305	E1306	Q1307	I1308	R1309	K1310	N1311	L1312	S1313	Y1314	R1315	F1316	Y1317	G1318	S1319	G1320	S1321	S1322	Y1323	S1324	L1325	S1326	L1327	S1328	P1329	Y1330	N1331	M1332	N1333	I1334	D1335	I1336	M1337	L1338	V1339	E1340
S1161	I1162	T1163	L1164	G1165	K1166	C1167	E1168	I1169	W1170	R1171	A1172	E1173	G1174	G1175	S1176	G1177	H1178	T1179	L1180	T1181	D1182	D1183	I1184	D1185	H1186	F1187	F1188	S1189	S1190	P1191	S1192	I1193	T1194	Y1195	R1196	K1197	P1198	W1199	L1200	S1201	I1202	Y1203	D1204	V1205	L1206	N1207	I1208	K1209	K1210	E1211	K1212	I1213	D1214	F1215	S1216	K1217	D1218	L1219	M1220
V1221	L1222	P1223	N1224	A1225	L1226	N1227	R1228	V1229	F1230	G1231	E1232	E1233	M1234	G1235	I1236	T1237	P1238	G1239	F1240	R1241	S1242	L1243	D1244	N1245	D1246	G1247	T1248	K1249	N1250	L1251	D1252	R1253	I1254	R1255	D1256	H1257	I1258	E1259	G1260	Q1261	I1262	Y1263	W1264	R1265	L1266	F1267	A1268	F1269	I1270	A1271	D1272	A1273	L1274	I1275	T1276	K1277	L1278	K1279	P1280

S2343	F2283	F2283	D2223
L2344	G2284	G2284	P2224
T2345	K2285	K2285	E2225
I2346	D2286	D2286	T2226
L2347	G2287	G2287	K2227
G2348	K2288	K2288	K2228
T2349	M2289	M2289	A2229
M2350	Q2290	Q2290	Y2230
Y2351	I2291	I2291	K2231
Y2352	G2292	G2292	G2232
F2353	V2293	V2293	L2233
D2354	T2294	T2294	N2234
P2355	N2295	N2295	V2235
D2356	T2296	T2296	Y2236
T2357	P2297	P2297	D2237
A2358	D2298	D2298	U2238
E2359	G2299	G2299	L2239
L2360	F2300	F2300	K2240
V2361	K2301	K2301	Y2241
V2362	Y2302	Y2302	Y2242
S2363	T2303	T2303	F2243
E2364	A2304	A2304	D2244
HIS	H2305	H2305	E2245
HIS	Q2306	Q2306	N2246
HIS	T2307	T2307	G2247
HIS	T2308	T2308	T2248
HIS	L2309	L2309	M2249
HIS	D2310	D2310	R2250
HIS	E2311	E2311	T2251
HIS	M2312	M2312	G2252
HIS	F2313	F2313	L2253
HIS	E2314	E2314	T2254
HIS	G2315	G2315	S2255
HIS	E2316	E2316	F2256
HIS	S2317	S2317	E2257
HIS	L2318	L2318	N2258
HIS	M2319	M2319	N2259
HIS	Y2320	Y2320	N2260
HIS	T2321	T2321	Y2261
HIS	G2322	G2322	Y2262
HIS	F2323	F2323	F2263
HIS	L2324	L2324	N2264
HIS	D2325	D2325	E2265
HIS	L2326	L2326	D2266
HIS	D2327	D2327	G2267
HIS	G2328	G2328	K2268
HIS	K2329	K2329	M2269
HIS	R2330	R2330	Q2270
HIS	T2331	T2331	F2271
HIS	Y2332	Y2332	G2272
HIS	F2333	F2333	Y2273
HIS	T2334	T2334	L2274
HIS	D2335	D2335	N2275
HIS	E2336	E2336	T2276
HIS	Y2337	Y2337	K2277
HIS	T2338	T2338	D2278
HIS	A2339	A2339	K2279
HIS	A2340	A2340	N2280
HIS	T2341	T2341	F2281
HIS	G2342	G2342	Y2282

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.099	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	321.752, 321.752, 321.752	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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:
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	0.43	1/19409 (0.0%)	0.61	4/26261 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	ILE	C-O	6.21	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	PRO	CA-N-CD	-13.11	93.65	112.00
1	A	1947	VAL	CA-C-N	5.88	132.77	121.54
1	A	1947	VAL	C-N-CA	5.88	132.77	121.54
1	A	1069	VAL	N-CA-C	-5.28	107.22	111.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	GLY	Peptide
1	A	1452	PHE	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	19026	0	18584	534	0
2	A	1	0	0	0	0
All	All	19027	0	18584	534	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 14.

The worst 5 of 534 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:1023:PRO:HG3	1:A:1649:TYR:CZ	1.49	1.48
1:A:1956:THR:HG23	1:A:1986:MET:N	1.21	1.45
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1023:PRO:CG	1:A:1649:TYR:CZ	2.18	1.26
1:A:1180:LEU:HD21	1:A:1185:ASP:OD1	1.34	1.22

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	2351/2372 (99%)	2210 (94%)	135 (6%)	6 (0%)	36 65

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	ALA
1	A	1948	GLU
1	A	1029	LEU
1	A	1762	PRO
1	A	2342	GLY

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	2130/2146 (99%)	1995 (94%)	135 (6%)	16 45

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1870	THR
1	A	1927	ILE
1	A	2181	ASN
1	A	897	ARG
1	A	884	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1520	ASN
1	A	1763	GLN
1	A	1553	ASN
1	A	1731	ASN
1	A	2058	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

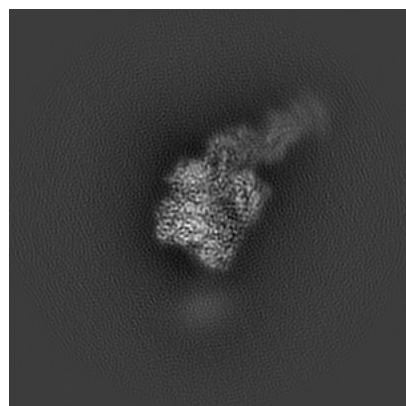
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36141. These allow visual inspection of the internal detail of the map and identification of artifacts.

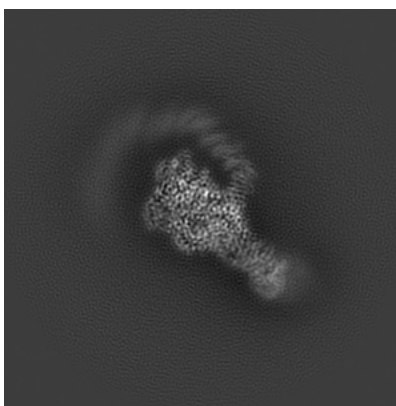
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

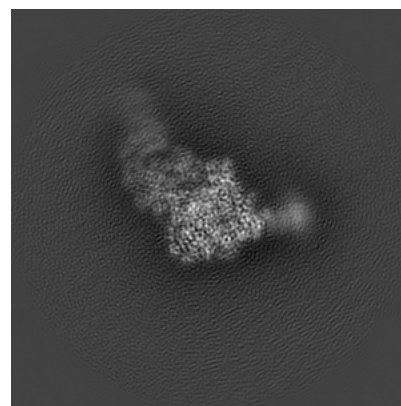
6.1.1 Primary map



X

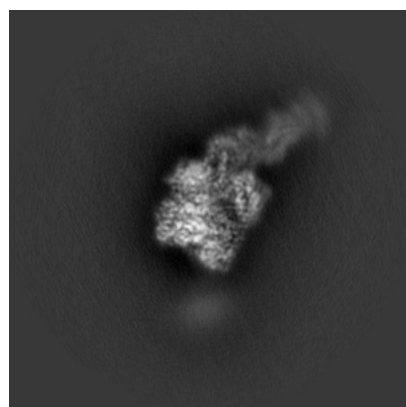


Y

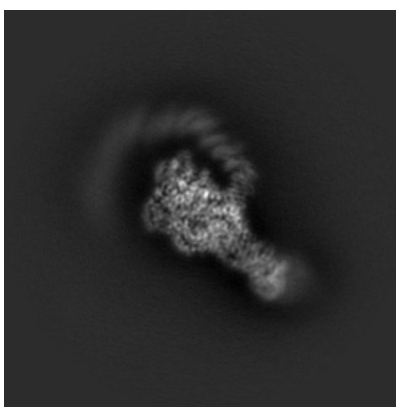


Z

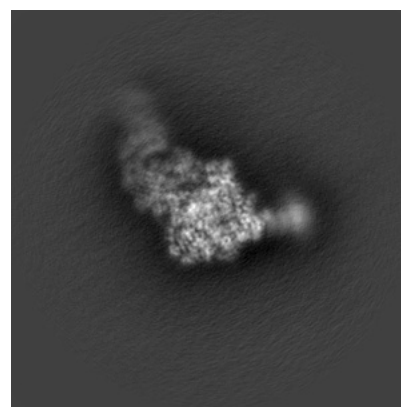
6.1.2 Raw map



X



Y

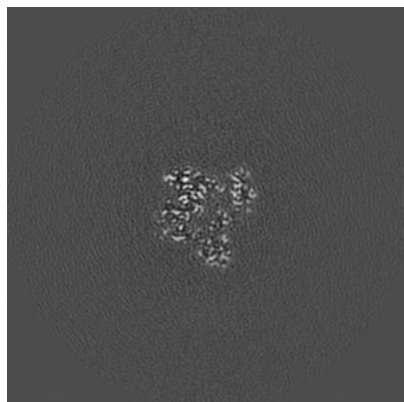


Z

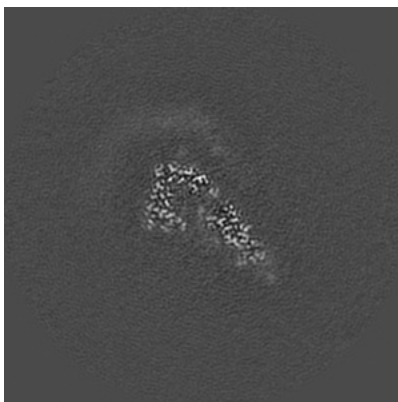
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

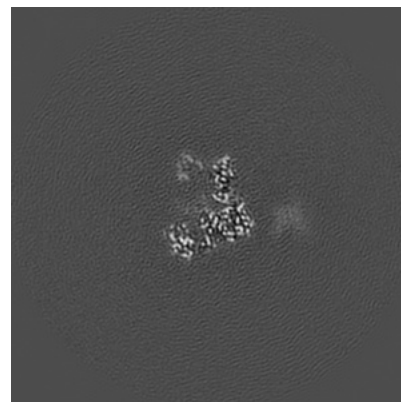
6.2.1 Primary map



X Index: 148

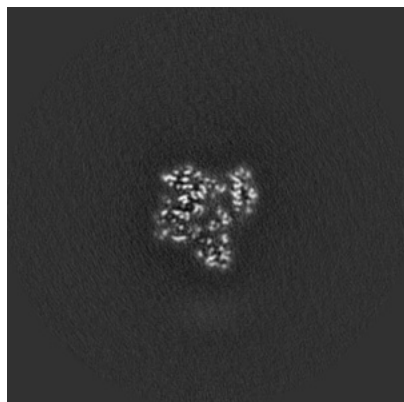


Y Index: 148

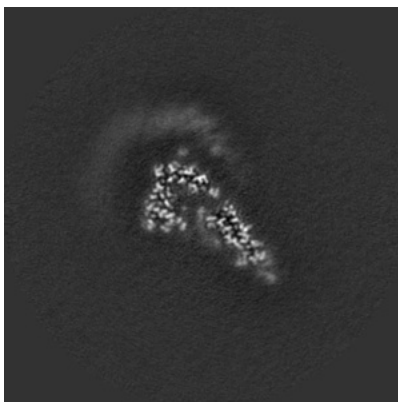


Z Index: 148

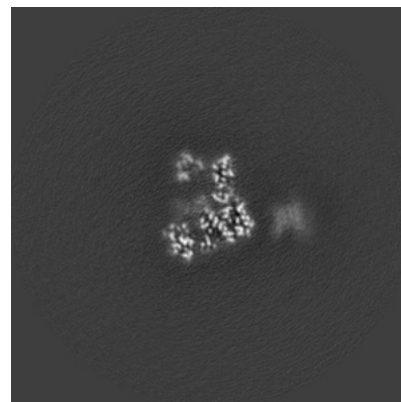
6.2.2 Raw map



X Index: 148



Y Index: 148

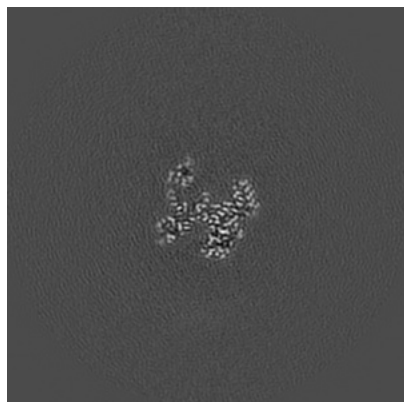


Z Index: 148

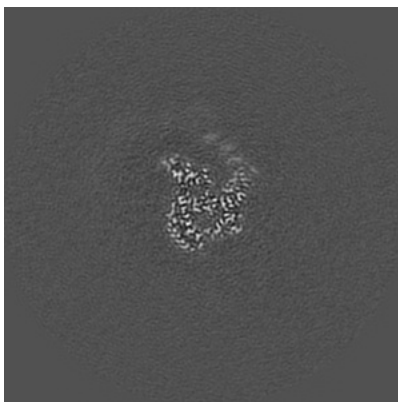
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

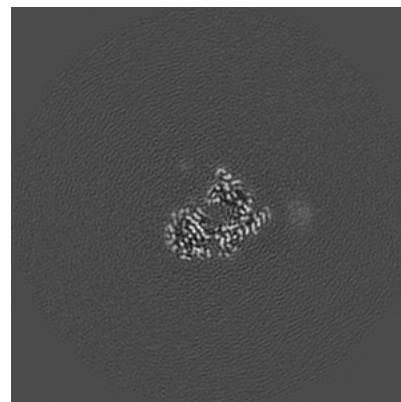
6.3.1 Primary map



X Index: 159

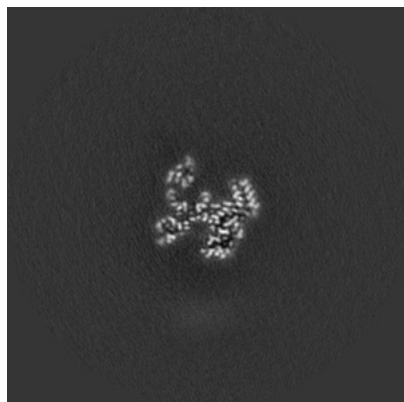


Y Index: 130

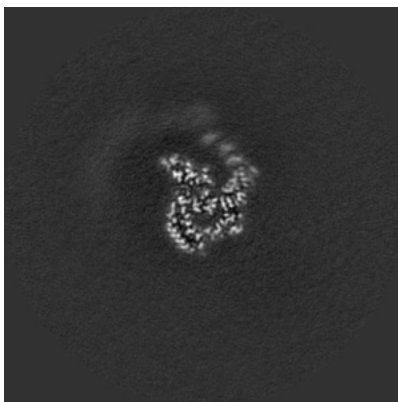


Z Index: 135

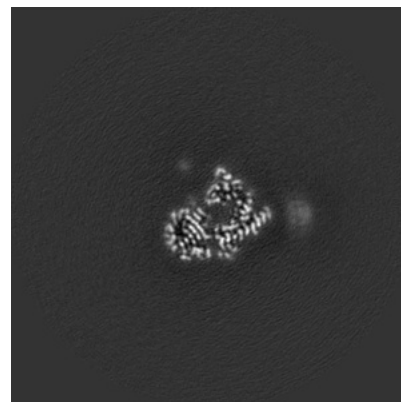
6.3.2 Raw map



X Index: 159



Y Index: 130

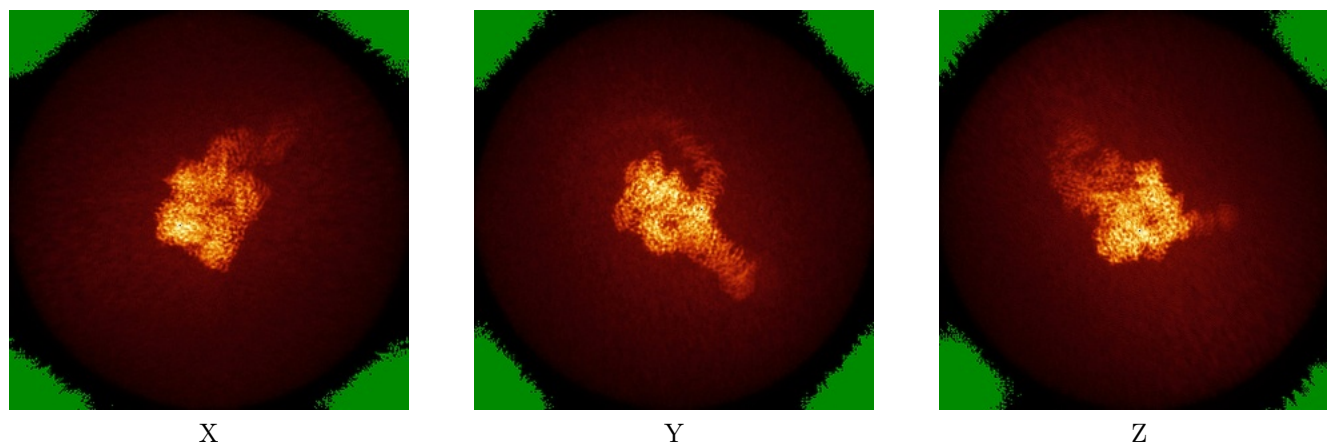


Z Index: 135

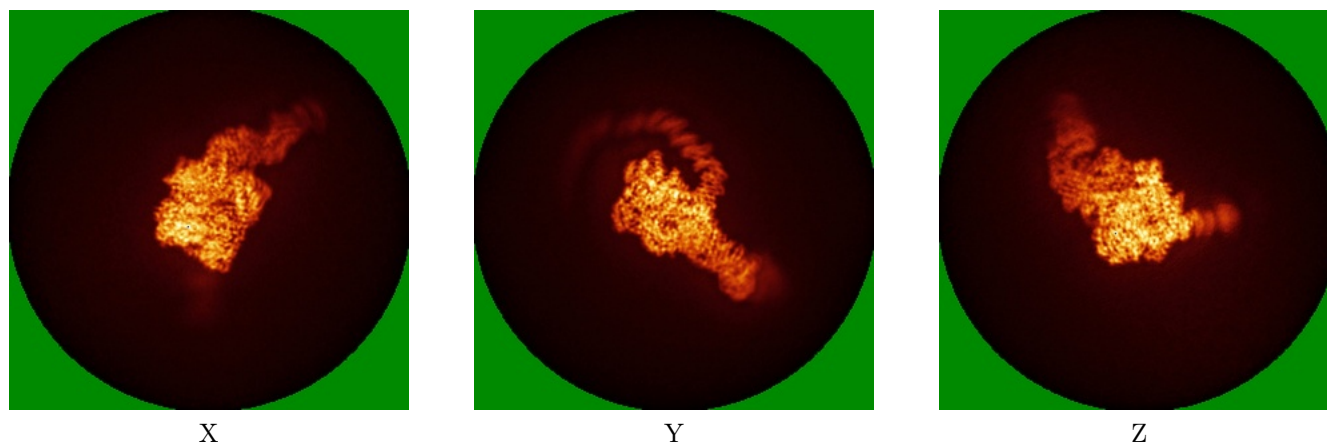
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

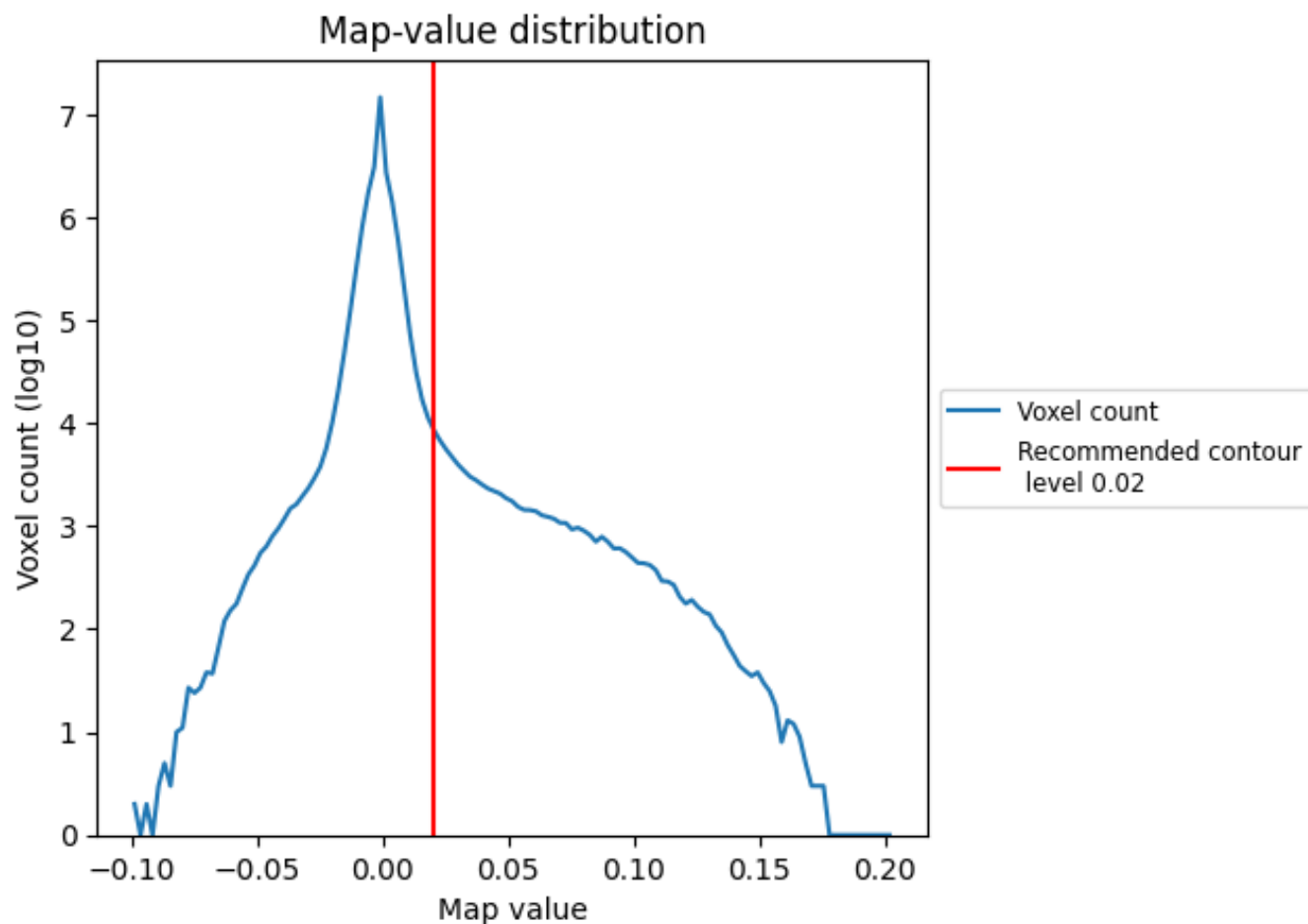
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

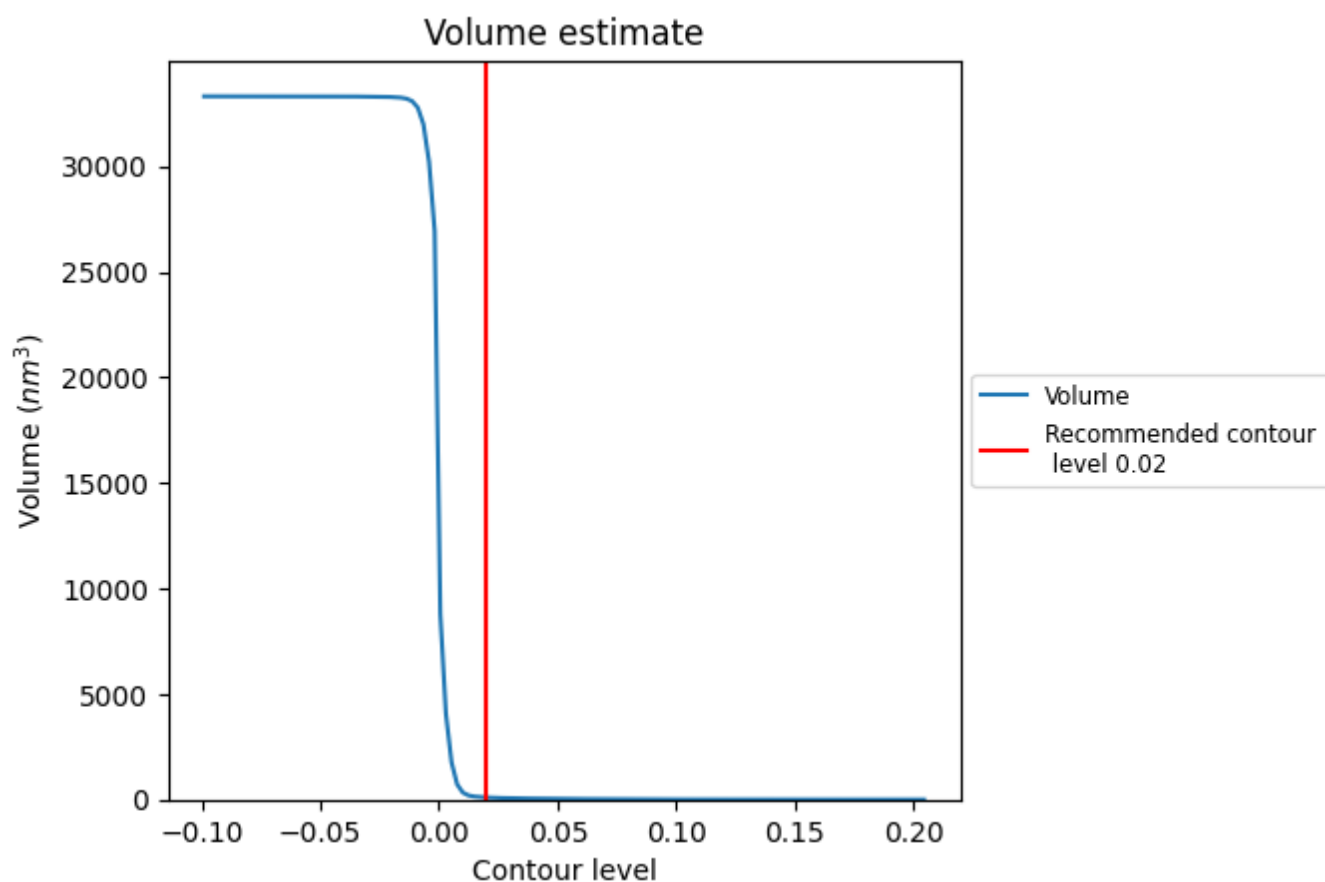
This section contains the results of statistical analysis of the map.

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.

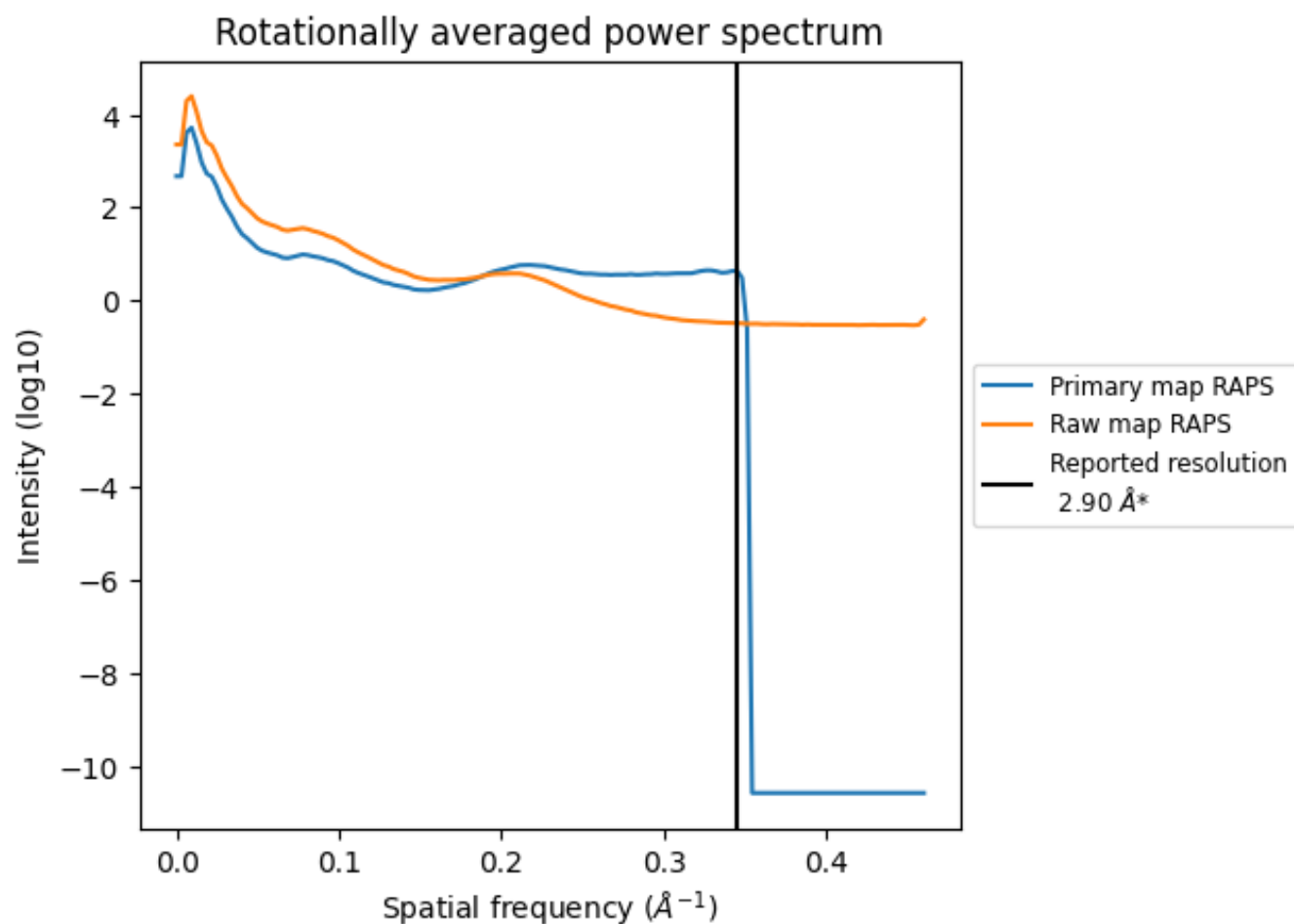
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm^3 ; this corresponds to an approximate mass of 90 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 ⓘ

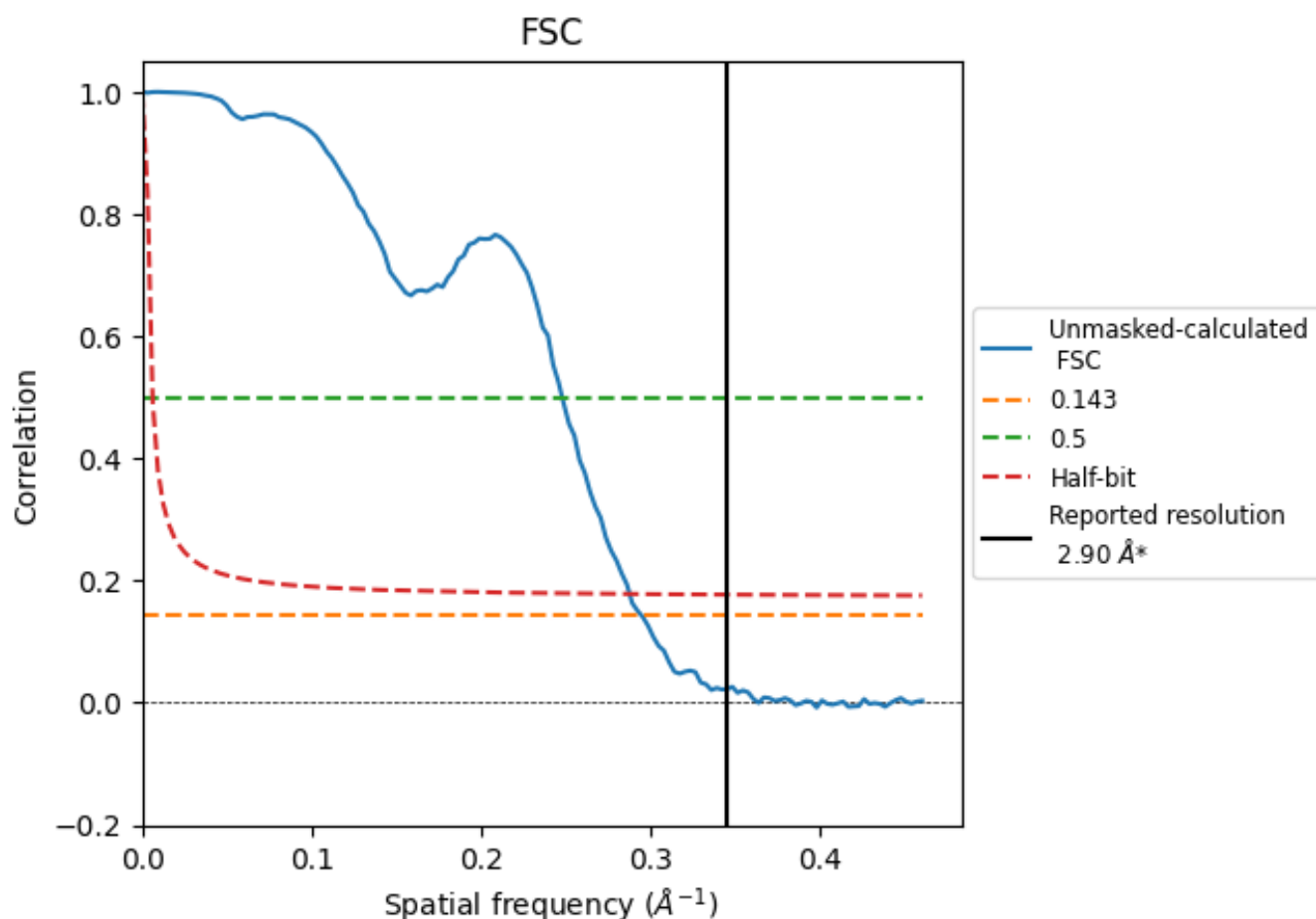


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

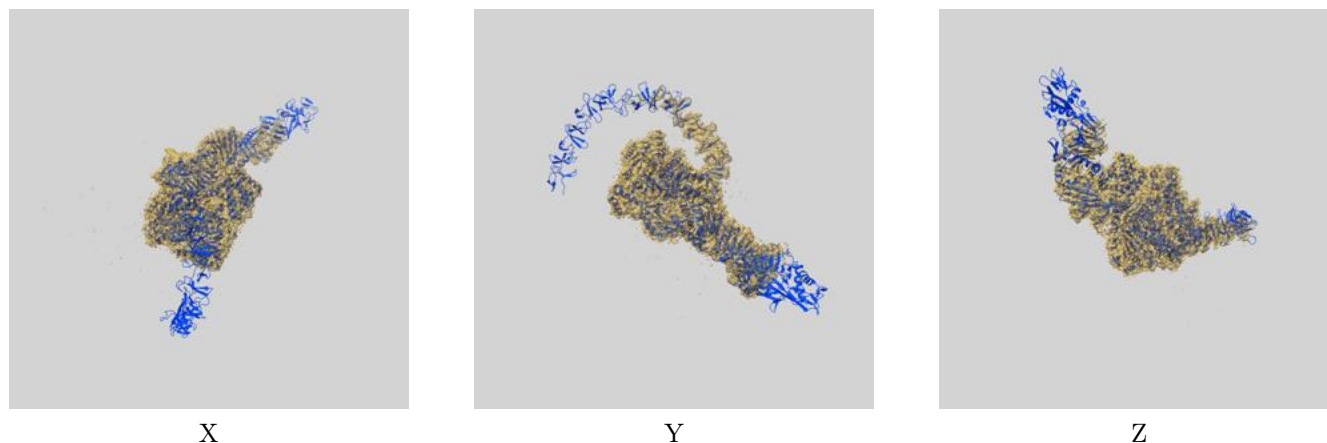
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.04	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

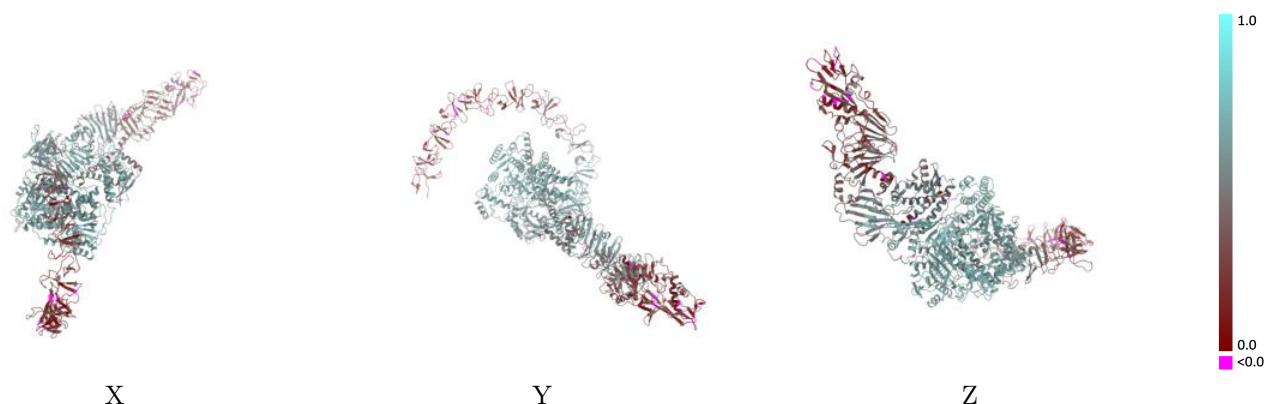
This section contains information regarding the fit between EMDB map EMD-36141 and PDB model 8JB5. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



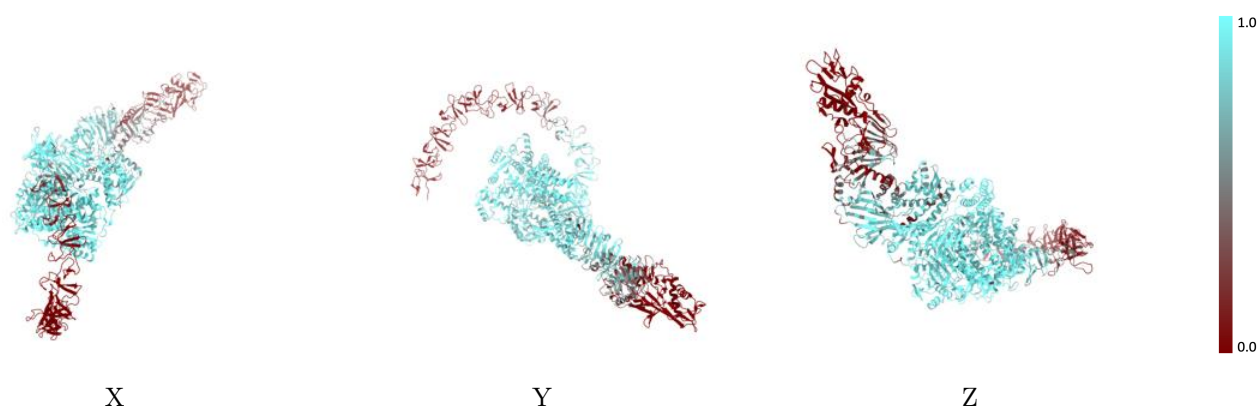
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



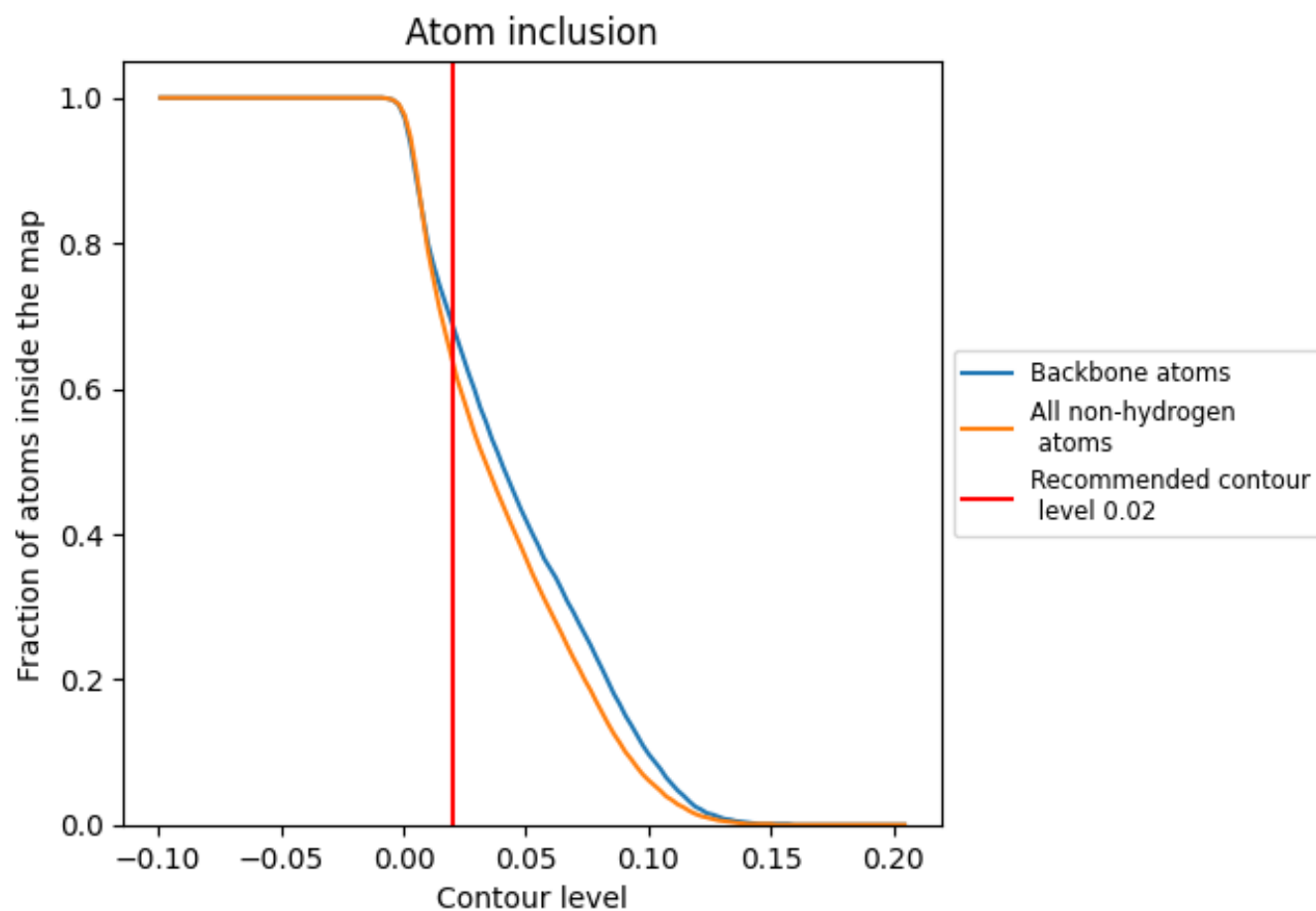
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 64% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.4770
A	0.6390	0.4770

