



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 08:40 PM UTC

PDB ID : 8X2I / pdb_00008x2i
EMDB ID : EMD-38011
Title : Cryo-EM structure of the TcsL at pH 5.0 in its open conformation
Authors : Zhan, X.; Tao, L.
Deposited on : 2023-11-09
Resolution : 2.50 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

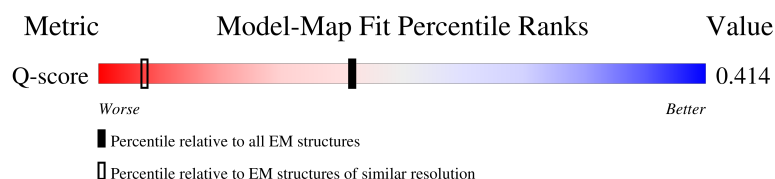
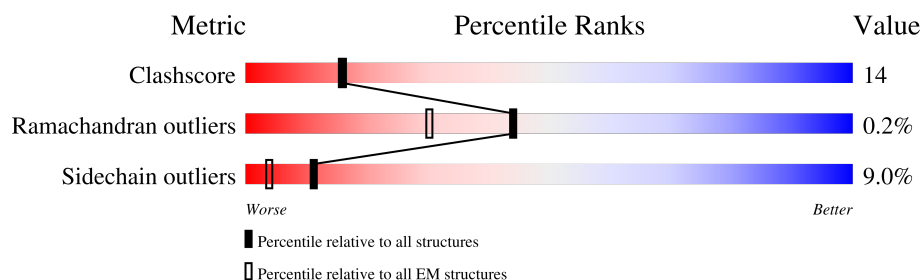
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	25% 64% 29% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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	2303	Total	C	N	O	S	0	0
			18644	11942	2959	3697	46		

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).

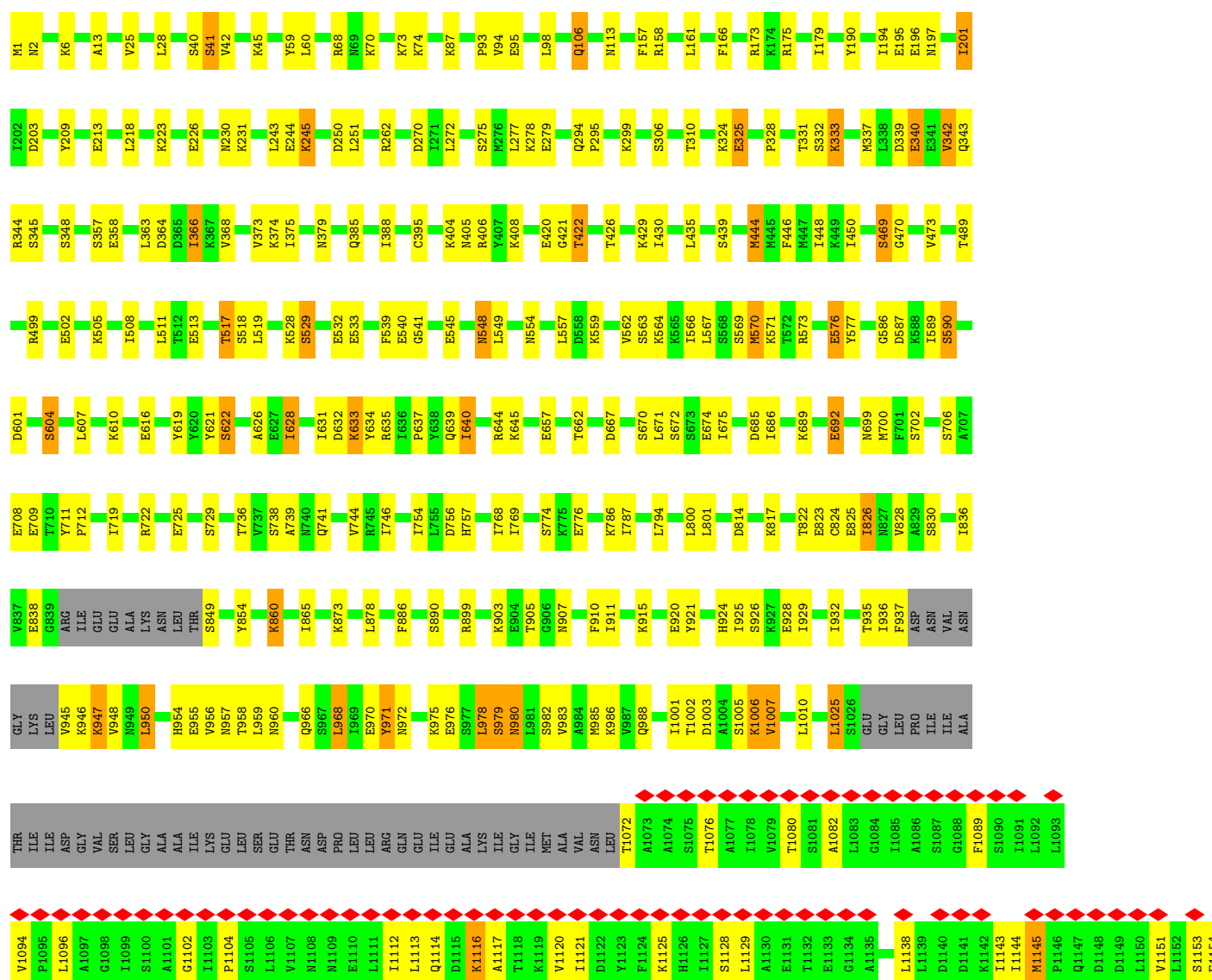
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

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

Chain A: 



Q2119	G2059	Y1999	L1930	Y1838	P1711	M1593	P1500	S1422	K1353	L1278	K1217	T1155
L2120	I2060	F2000	M1931	D1841	M1712	I1594	M1503	K1423	M1354	K1279	D1218	D1156
G2121	L2061	N2001	I1932	S1842	I1713	M1598	N1504	S1424	I1355	P1280	L1219	F1157
F2122	N2062	N2002	I1936	L1843	C1715	M1610	L1505	Y1425	T1356	R1281	M1220	N1158
T2123	F2063	D2003	Y1937	K1847	P1716	E1717	S1510	I1427	I1357	Y1282	V1221	M1159
L2124	G2064	D2004	Y1938		E1717				E1358	E1283	N1224	N1160
L2125	G2065	V2005	Y1947	N1851	D1722	I1613	D1512	S1430	S1359	D1284	A1225	S1161
N2126	K2066	Q2007	I1948	I1854	I1726	G1615	L1513	G1431	D1360	T1288	P1226	T1162
D2127	I2067	Q2007	K1949		I1726	S1616	K1514	N1432	E1361	I1289	N1227	T1163
N2128	G2068	V2008	K1950	F1857	K1729	M1617	D1515	C1433	I1362	N1290	R1228	G1165
F2069	F2069	G2009	L1951	T1858	K1729	S1618	L1516	M1434	I1362	N1291	G1166	C1167
L2129	L1952	T2010	L1952		L1737	Q1621	R1517	L1436	Q1363	L1291	F1230	C1167
F2130	D2071	G2010	D1953	K1864	E1737			I1437	E1366	G1293	G1231	E1168
Y2131	I2072	E2012	D1954	F1867	Y1741	L1624	G1522	I1437	L1367	D1293	E1225	T1169
F2132	S2073	V2013	E1955		Y1741		D1523	E1438	I1368	N1294	Y1232	I1169
S2133	N2074	N2014	T1956	S1872	S1748	K1628	V1524	N1439	E1369	T1295	E1233	W1170
E2134	T2075	G2015	Y1957	I1872	D1749			S1440	M1370	R1296	M1234	R1171
S2135	T2075	K2016	F1959	S1876	I1751	P1634	Y1531	D1441	L1371	I1299	G1235	A1172
G2136	A2076	K2017	M1960	I1877	I1751		F1532	D1442	L1372	V1300	W1236	E1173
K2137	V2077	F2017	P1961	I1880	A1754	K1638	K1533	I1443	S1373		T1237	G1174
T2138	G2078	F2018	K1638		E1758	F1638	D1534	Q1445	L1375	I1303	P1238	G1175
E2139	G2079	Y2019	K1640	I1641		K1640	D1536	K1446	M1376	T1304	G1239	S1176
L2140	W2080	F2020	I1641	K1642	M1770	K1642	D1536	I1447		T1305	F1240	G1177
G2141	G2081	G2021	E1643	E1643	F1771	T1644	L1540	D1448		E1306	R1241	H1178
G2142	T2082	K2022	Y1888	Y1646	F1772	S1645	S1541	I1449	D1379	Q1307	S1242	T1179
Y2143	L2083	N2023	I1646	T1647	D1779		F1542	I1450	G1451	I1308	S1242	T1179
Q2144	D2084	G2024	G1651		S1782	G1651	T1547	F1452	L1383	I1309	L1243	L1180
N2145	D2085	E2025	L1895		I1970	M1652		N1453	L1384	K1309	D1244	T1181
N2146	G2086	R2026	I1900		V1791	R1653	L1552	G1454	M1385	K1310	D1245	D1182
G2147	S2087	Q2027	N1901		K1795	Q1654	Y1556	I1455	N1386	N1311	N1246	D1183
T2088	Y2089	G2029	D1975		I1796	M1655		H1456	H1387	L1312	G1247	I1184
Y2149	Q2090	F2031	N1976		I1797		E1559	K1458	T1389	S1313	T1248	I1185
F2150	E2091	N2032	K1907		Y1662	S1661	L1566	I1459	N1390	F1316	K1249	H1186
T2151	D2092	N2033	Y1908		Q1679	Y1662	L1566	I1460	F1318	Y1317	K1250	F1187
D2153	G2093	T2033	F1911		S1801		N1570	P1461	I1395	G1319	D1251	F1188
E2154	N2094	P2034	S1912		S1806	L1682	K1573	S1463	N1396	S1322	D1252	S1189
T2155	G2095	D2035	G1913		D1807	Y1683	S1574	I1464	E1397	Y1323	R1253	P1191
G2156	A2096	G2036	T1914		G1808	G1684	A1575	I1465	S1398	S1324	R1255	S1192
L2157	E2097	F2037	I1984		Y1812		T1578	N1467	R1400	S1326	D1256	I1193
N2158	G2098	K2038	I1985		S1818	R1687		Y1471	S1403	L1327	H1257	T1194
L2159	C2099	F2039	M1986		S1818	K1691	L1582	Y1477	L1404	T1334	Y1258	Y1195
T2160	I2100	F2040	G1921		Y1823	V1692	M1583	S1478	T1405	D1335	E1259	R1196
G2161	G2101	G2041	S1923		N1827	I1693	L1586	K1479	F1406	L1336	G1260	K1197
V2162	L2102	P2042	N1924				L1587	S1479	S1407	N1337	Q1261	P1198
F2163	T2103	K2043	N1925				S1588	K1480	I1408	L1338	F1262	W1199
D2164	Y2104	D2044	F1926		N1831	T1706	I1589	F1484	L1409	E1340	Y1263	L1200
T2165	I2105	D2045	I1927			P1707	N1590	E1491	M1413	W1264	W1264	S1201
P2166	N2106	D2046	G1928		L1836		I1591	E1414	I1414	T1202	R1265	I1202
D2167	D2107	L2047	P1928		I1837		I1591	I1415	I1415	D1347	Y1266	Y1203
G2168	K2109	G2048	K1929				I1591	N1496	I1416	V1348	F1267	D1204
Y2169	Y2110	E2050					I1591	I1497		V1351	A1268	V1205
K2170	Y2111	E2051					I1591			V1352	F1269	L1206
F2171	F2112	G2052					I1591				I1270	N1207
A2173	D2113	E2053					I1591				A1271	I1208
P2174	D2114	L2054					I1591				D1272	K1212
L2175	N2115	T2055					I1591				A1273	I1213
N2176	G2116	L2056					I1591				I1275	F1215
T2177	I2117	Y2057					I1591				T1276	S1216
V2178	R2118	N2058					I1591				K1277	

E2359	L2360	V2361	V2362	S2363	E2364	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	E2299	L2239	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298
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															D2311	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															E2312	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															F2313	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															E2314	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															G2315	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															E2316	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															S2317	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G2252	L2253	I2254	S2255	F2256	E2257	N2258	N2259	N2260	V2261	F2262	F2263	N2264	E2265	D2266	G2267	K2268	N2269	Q2270	F2271	G2272	V2273	L2274	N2275	I2276	K2277	D2278	K2279	N2280	F2281	V2282	F2283	G2284	K2285	D2286	G2287	K2288	N2289	Q2290	I2291	G2292	V2293	F2294	N2295	T2296	P2297	N2298	
															I2318	K2240	V2241	F2242	F2243	D2244	E2245	N2246	Q2247	I2248	N2249	R2250	T2251	G22																																															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1045888	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	12.371	Depositor
Minimum map value	-8.281	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	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	0.39	0/19023	0.57	2/25734 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1947	VAL	CA-C-N	5.87	132.75	121.54
1	A	1947	VAL	C-N-CA	5.87	132.75	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1511	LYS	Peptide
1	A	364	ASP	Peptide

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	18644	0	18175	530	0
2	A	1	0	0	0	0
All	All	18645	0	18175	530	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 530 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:1956:THR:HG23	1:A:1986:MET:N	1.21	1.51
1:A:1956:THR:CG2	1:A:1986:MET:N	1.86	1.38
1:A:1956:THR:HG21	1:A:1986:MET:CA	1.71	1.19
1:A:1956:THR:HG21	1:A:1986:MET:CB	1.74	1.18
1:A:1956:THR:CG2	1:A:1986:MET:CB	2.34	1.05

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	2295/2372 (97%)	2163 (94%)	128 (6%)	4 (0%)	43 63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1948	GLU
1	A	633	LYS
1	A	2342	GLY
1	A	422	THR

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	2088/2146 (97%)	1901 (91%)	187 (9%)	9 19

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1270	ILE
1	A	1591	ILE
1	A	1345	VAL
1	A	1462	TYR
1	A	1647	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1520	ASN
1	A	1676	ASN
1	A	1530	ASN
1	A	1654	GLN
1	A	1727	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

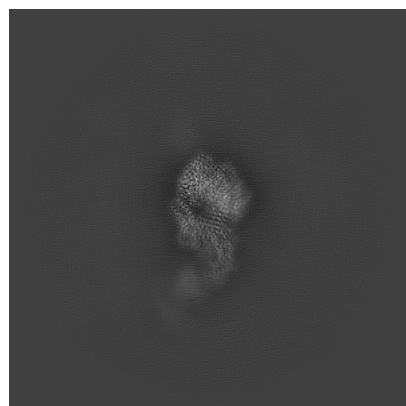
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38011. These allow visual inspection of the internal detail of the map and identification of artifacts.

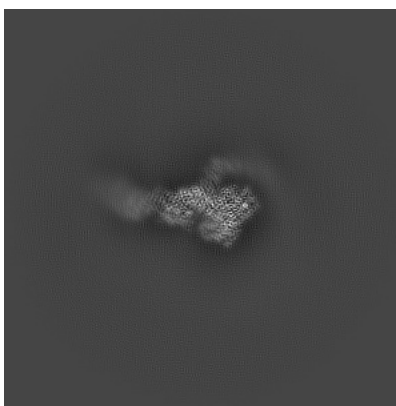
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

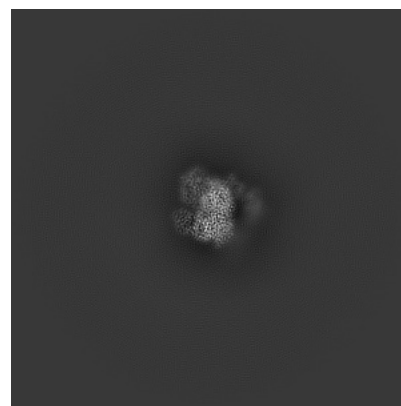
6.1.1 Primary map



X

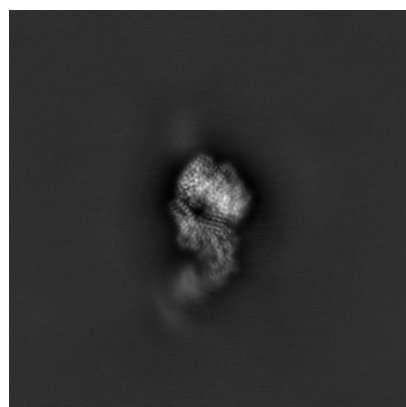


Y

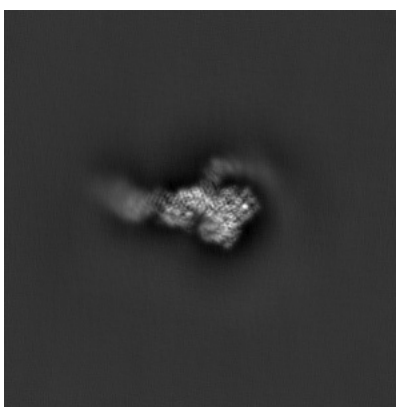


Z

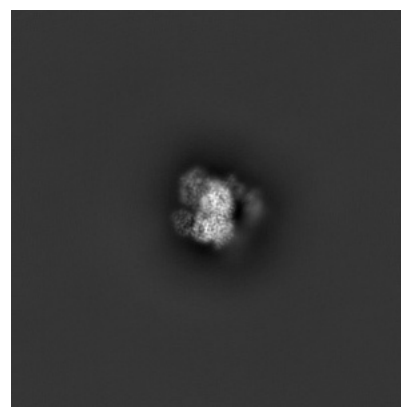
6.1.2 Raw map



X



Y

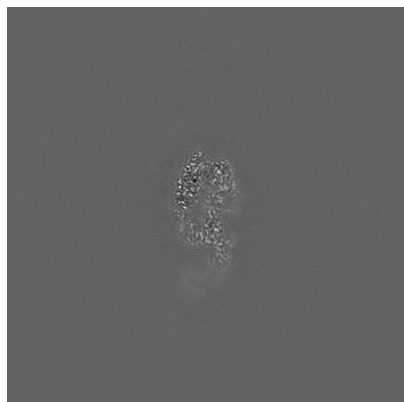


Z

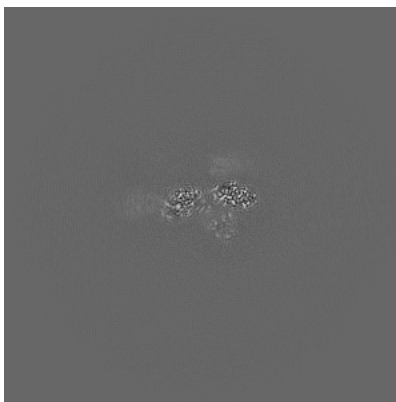
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

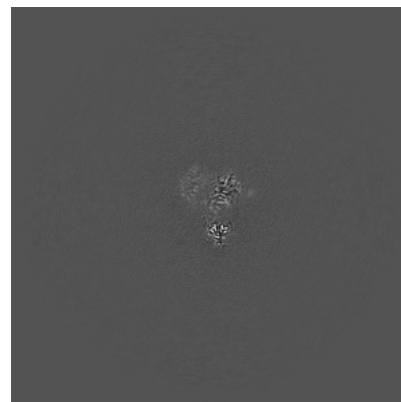
6.2.1 Primary map



X Index: 200

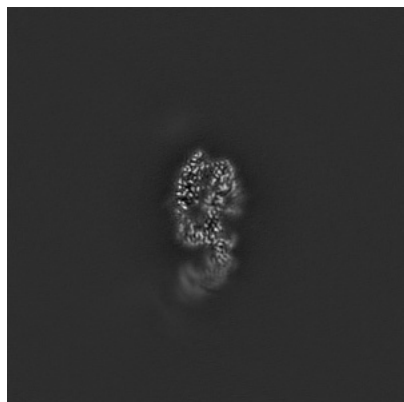


Y Index: 200

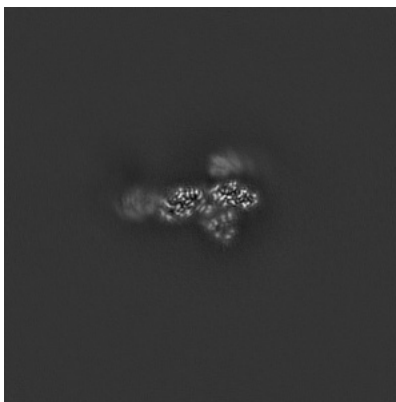


Z Index: 200

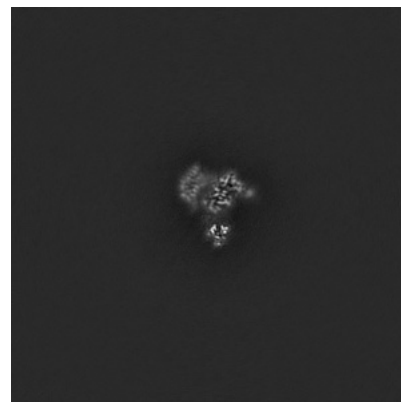
6.2.2 Raw map



X Index: 200



Y Index: 200

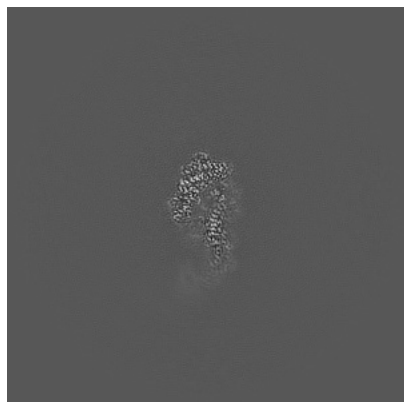


Z Index: 200

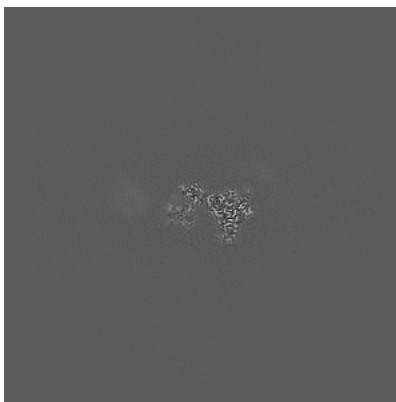
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

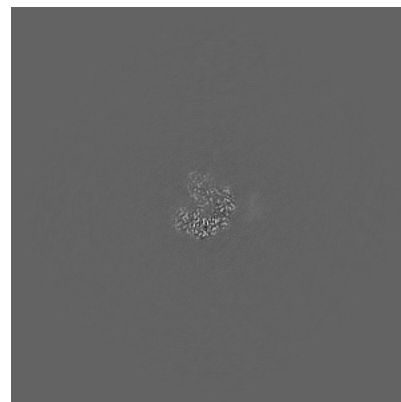
6.3.1 Primary map



X Index: 204

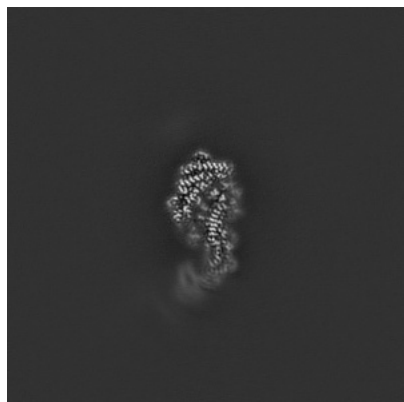


Y Index: 182

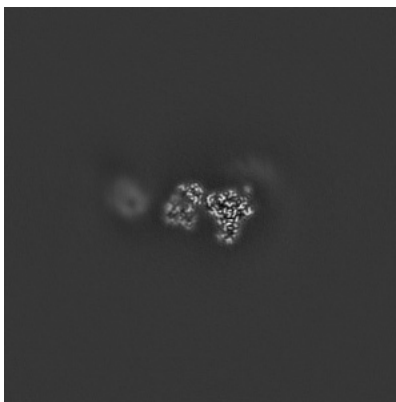


Z Index: 226

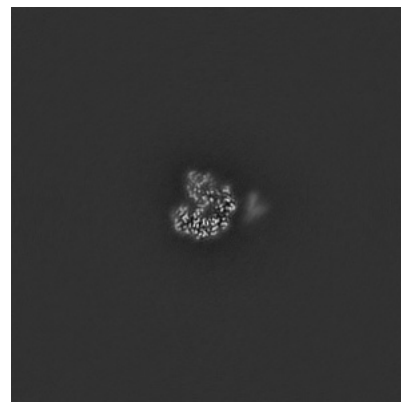
6.3.2 Raw map



X Index: 204



Y Index: 182

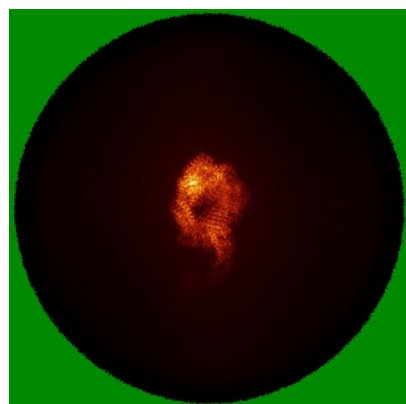


Z Index: 226

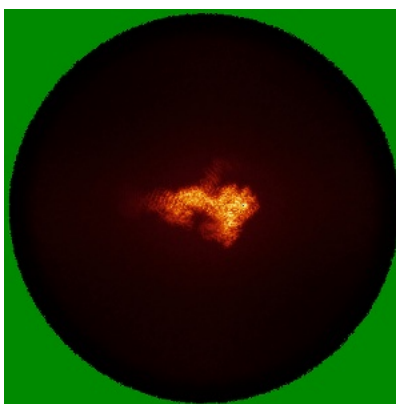
The images above show the largest variance slices of the map in three orthogonal directions.

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

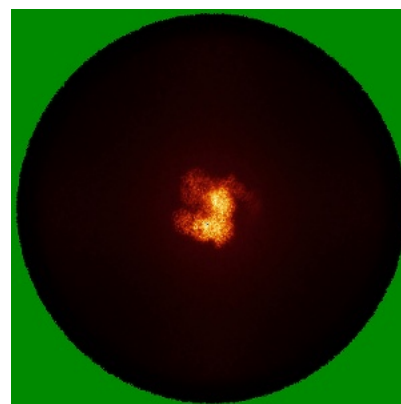
6.4.1 Primary map



X

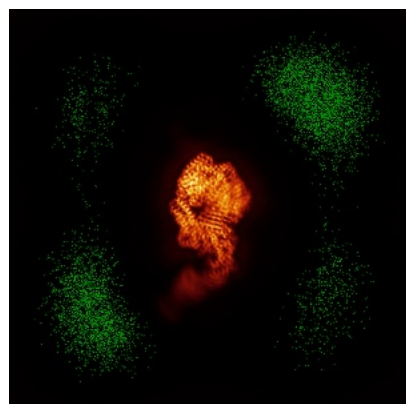


Y

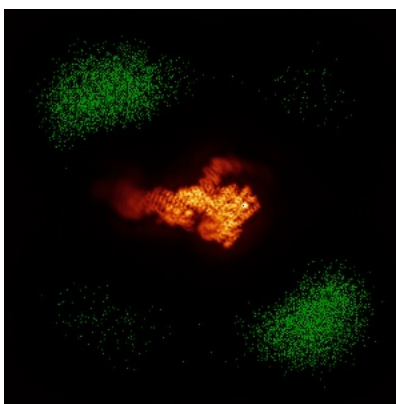


Z

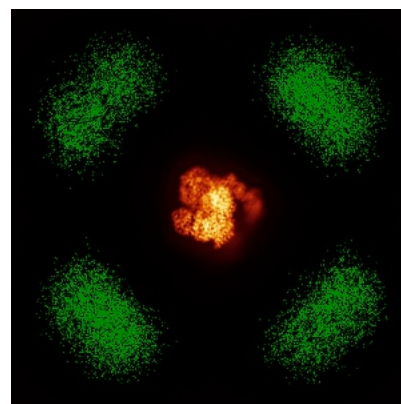
6.4.2 Raw map



X



Y

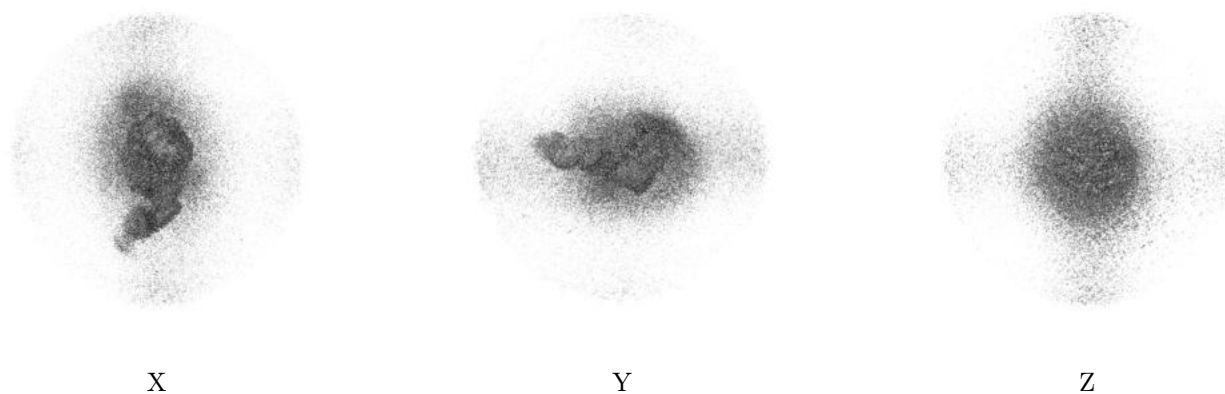


Z

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.

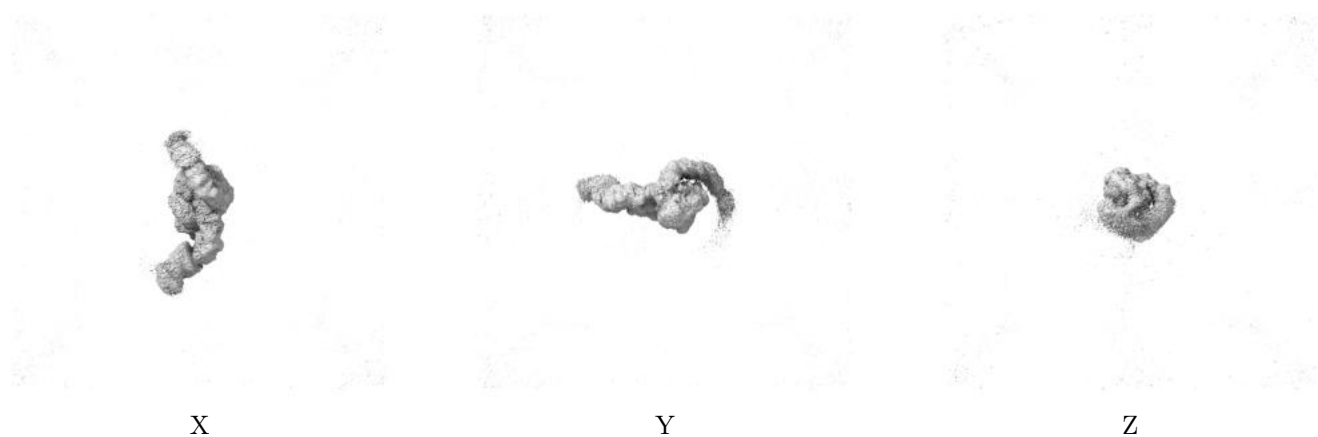
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

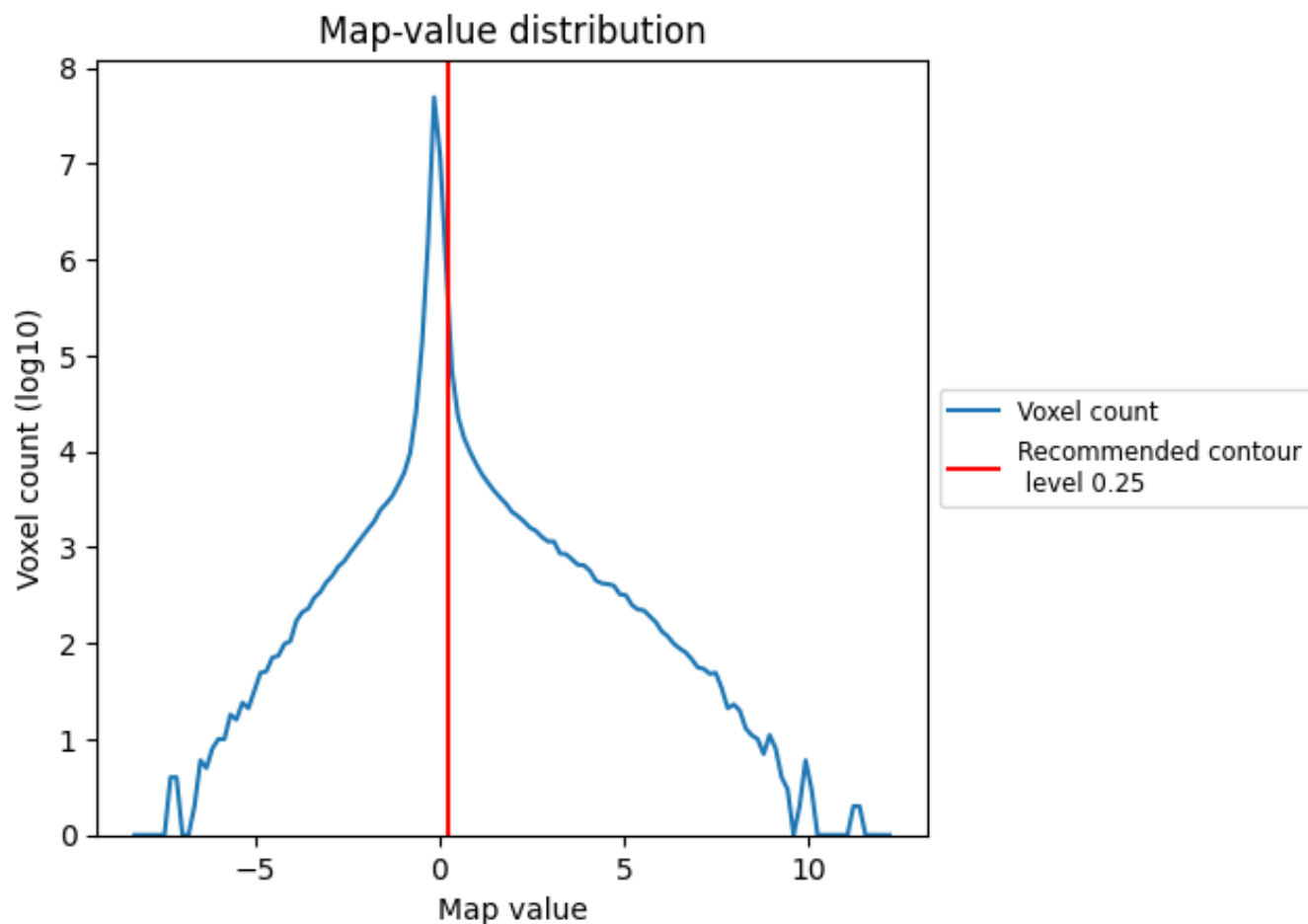
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

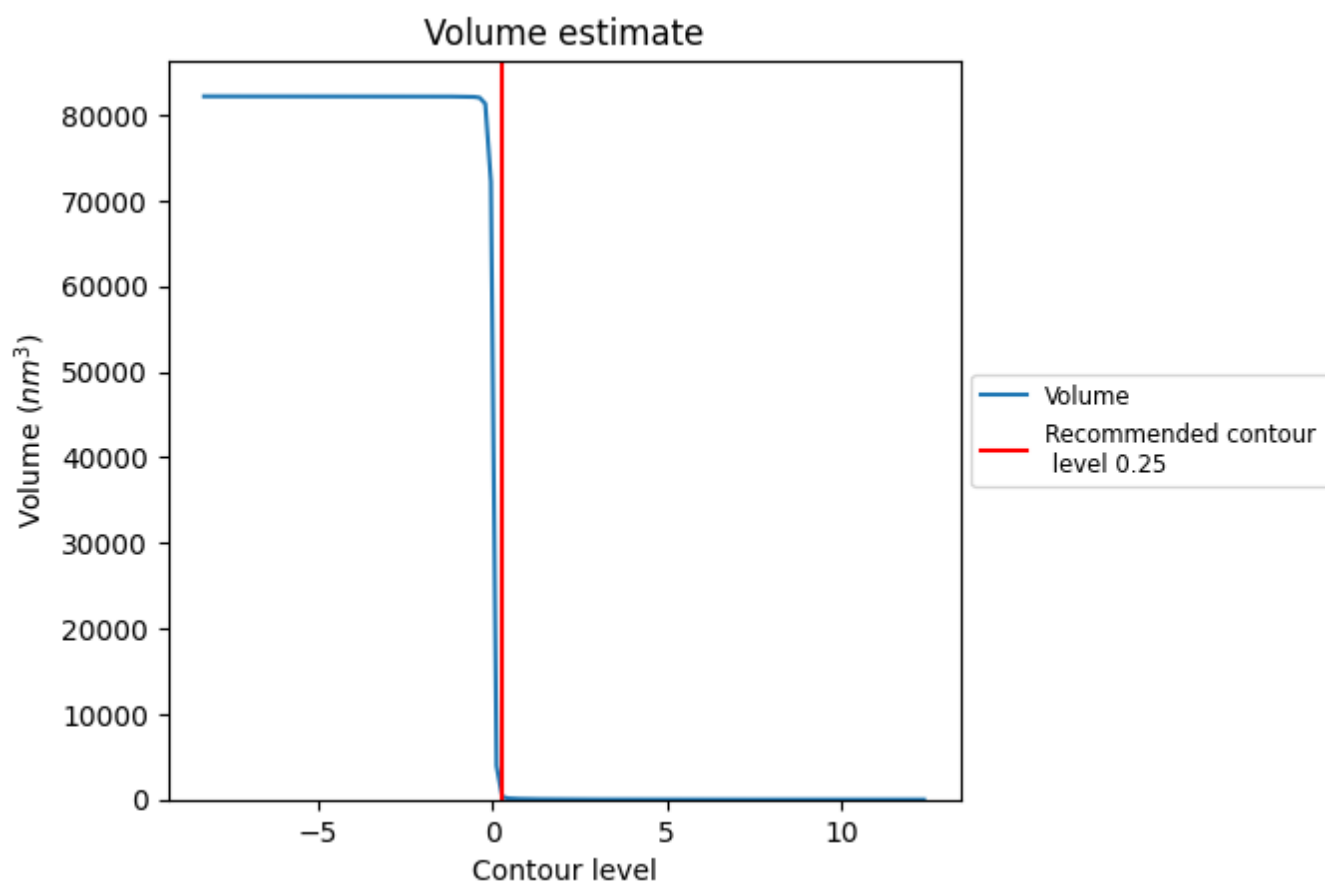
This section contains the results of statistical analysis of the map.

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.

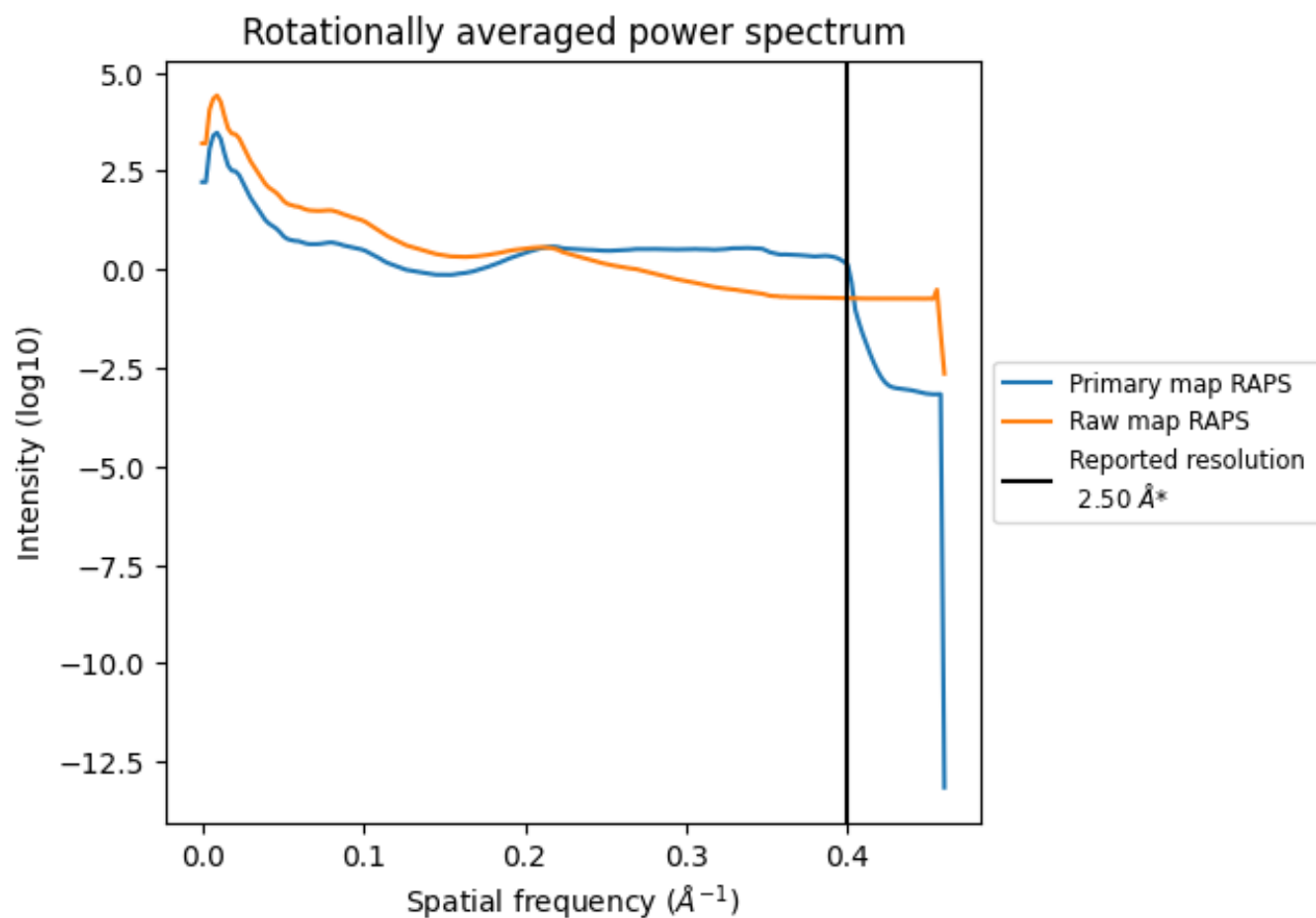
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 724 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 ⓘ

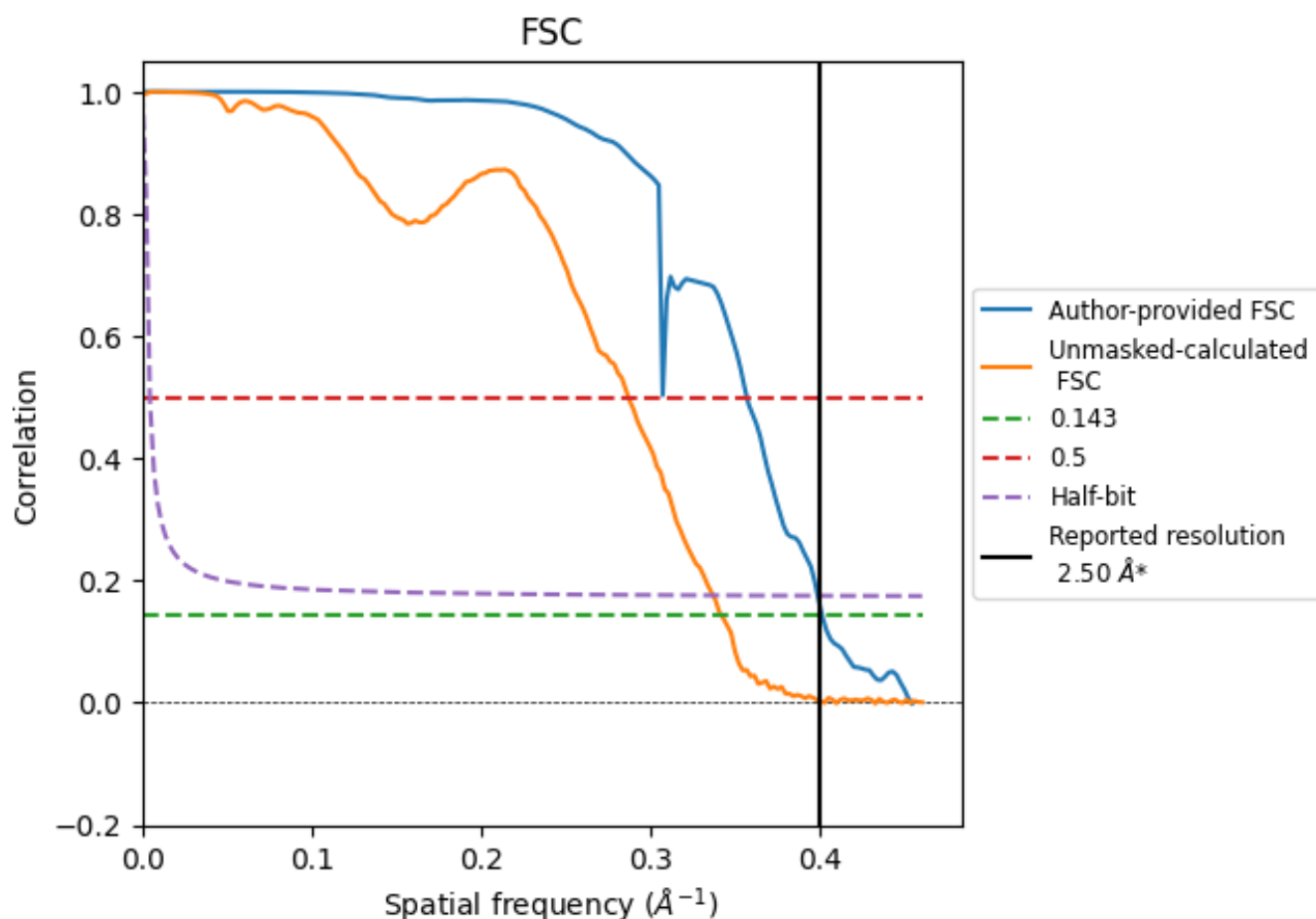


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

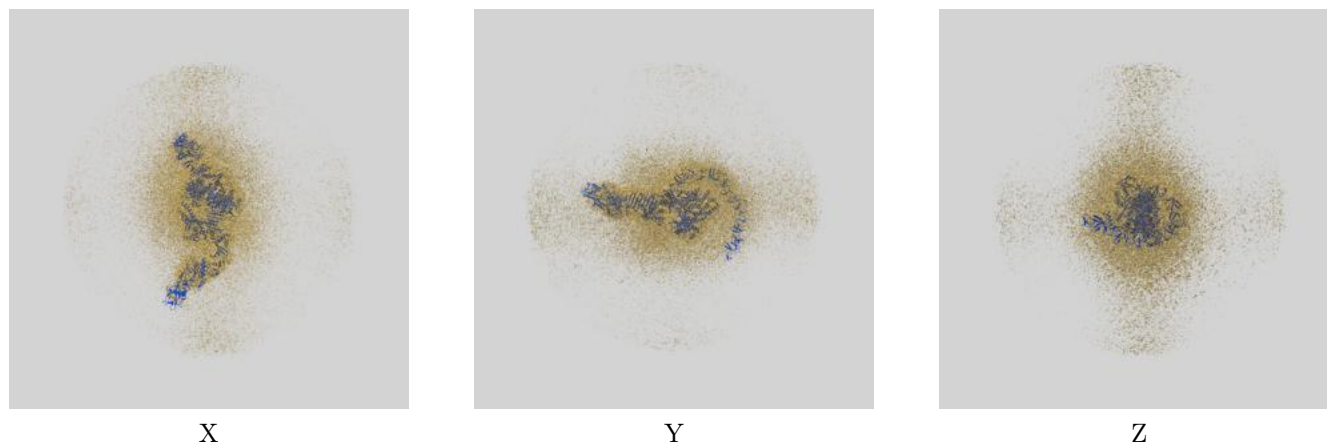
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.80	2.51
Unmasked-calculated*	2.93	3.49	2.97

*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 2.93 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

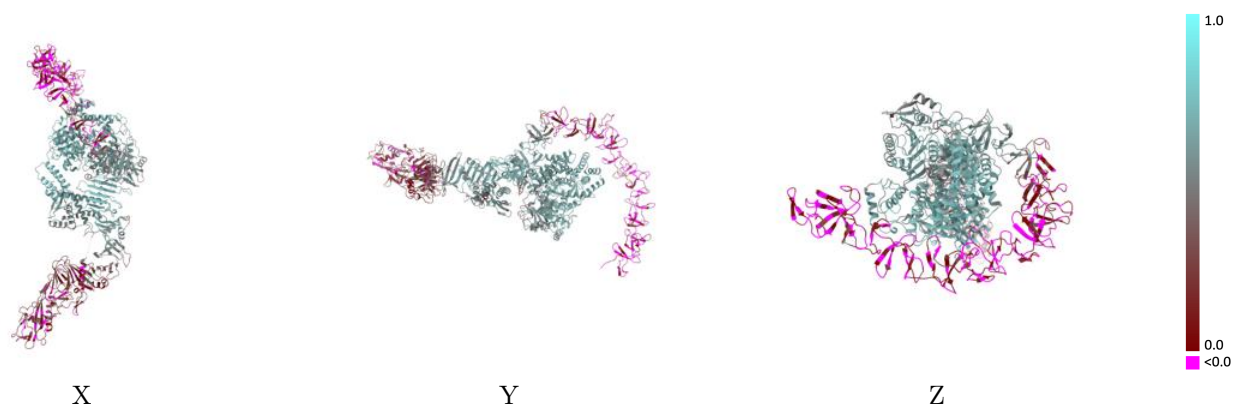
This section contains information regarding the fit between EMDB map EMD-38011 and PDB model 8X2I. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



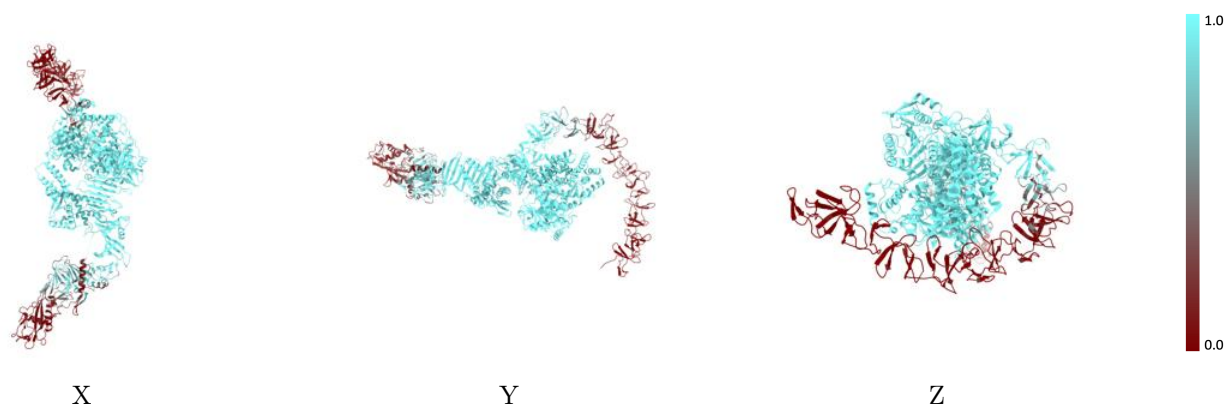
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



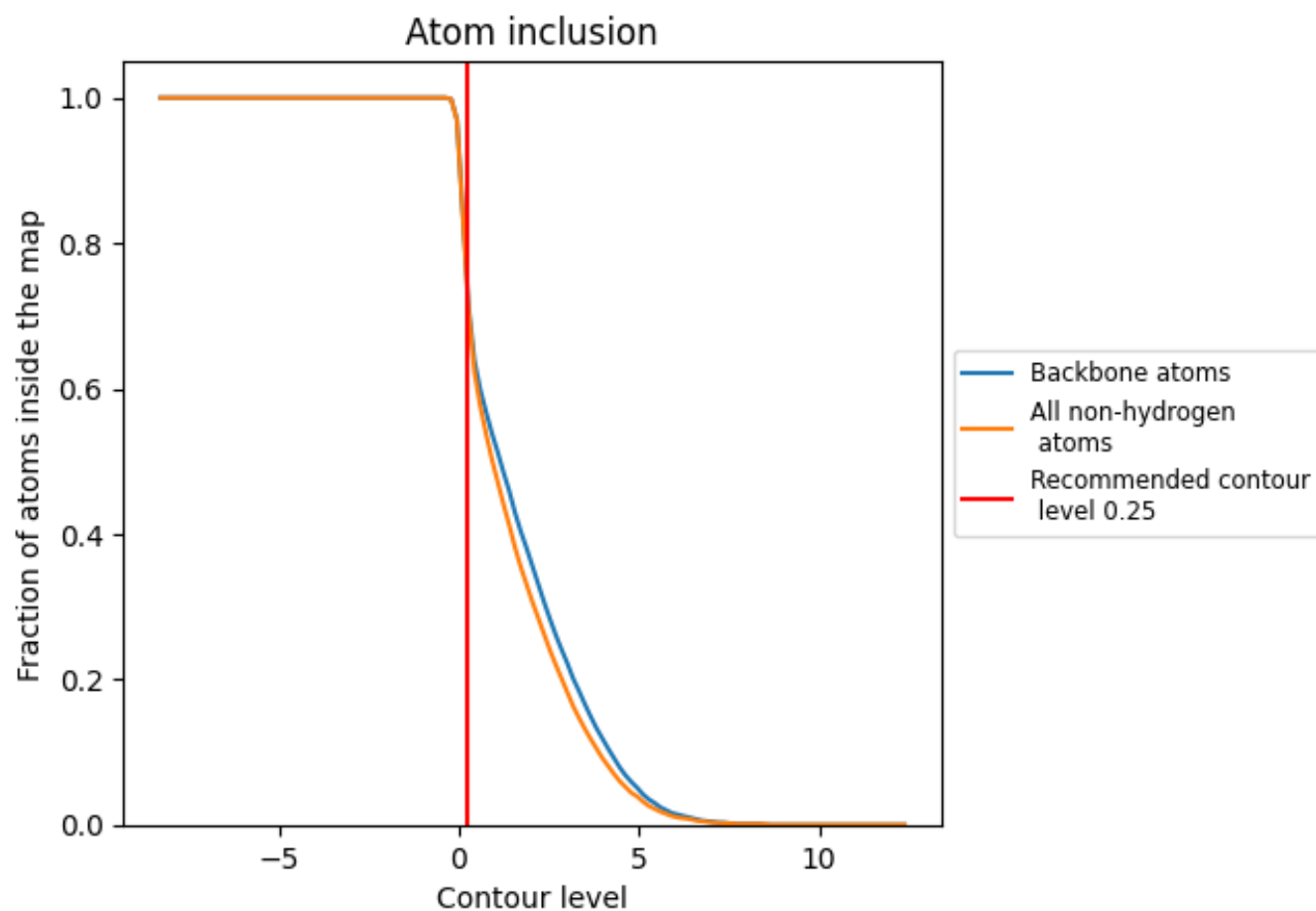
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4140
A	0.7210	0.4140

