



## wwPDB EM Validation Summary Report ⓘ

Dec 4, 2023 – 02:27 PM JST

PDB ID : 8X2I  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
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) : 2.36

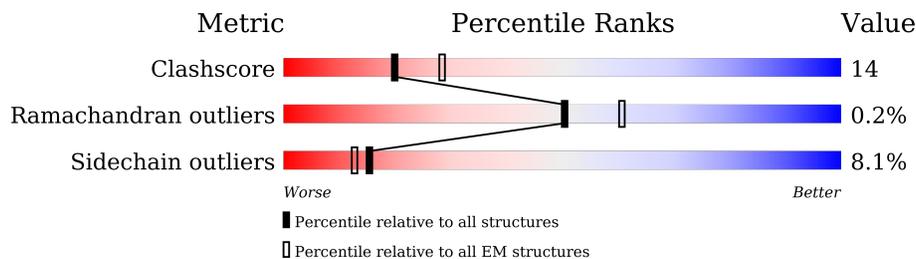
# 1 Overall quality at a glance i

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)
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  $\geq 3$ , 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 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
			Total	C	N	O	S		
1	A	2303	18644	11942	2959	3697	46	0	0

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

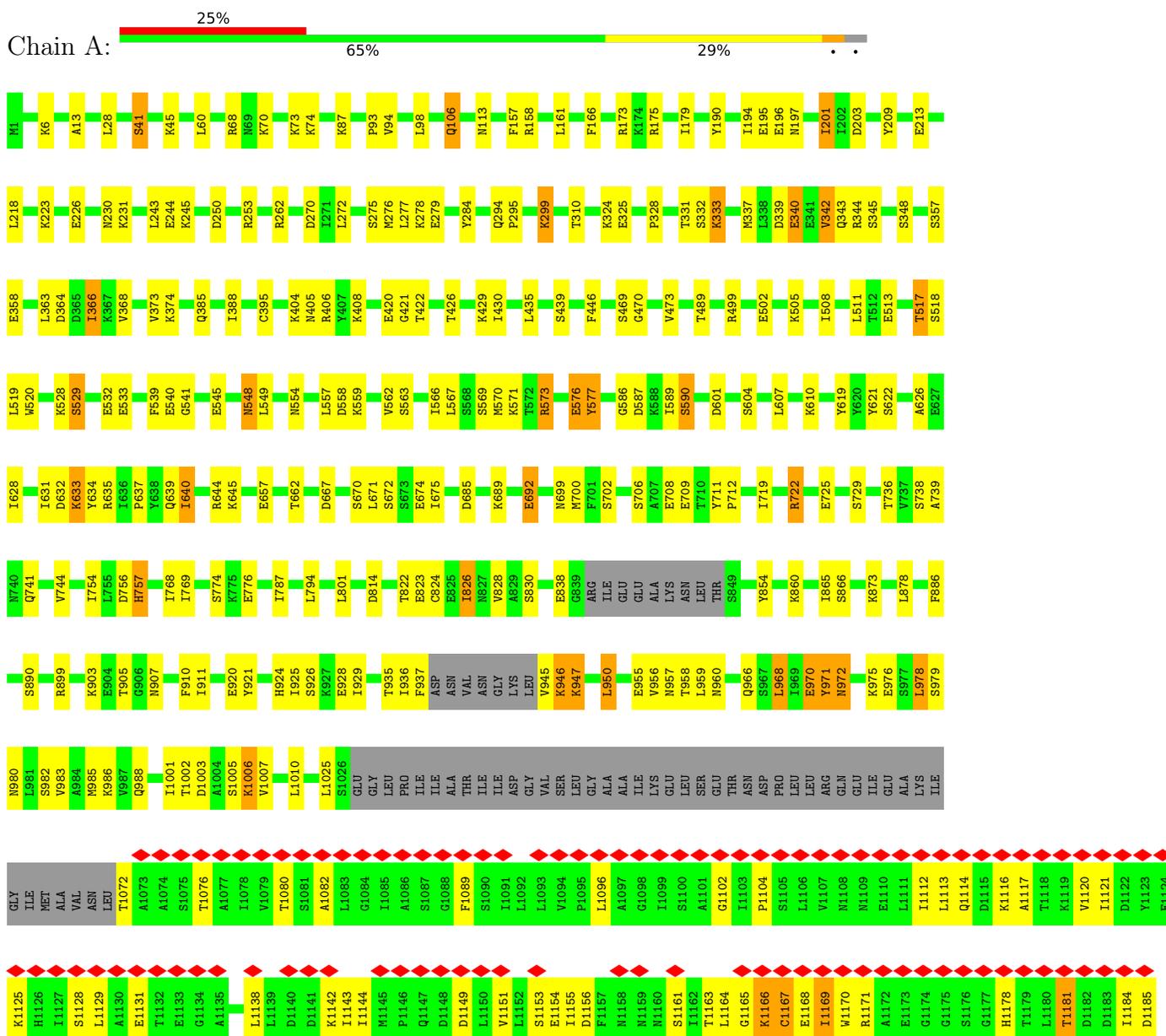
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



D2153	D2154	S2155	G2156	L2157	V2158	L2159	L2160	G2161	V2162	F2163	D2164	L2165	P2166	D2167	G2168	Y2169	K2170	Y2171	F2172	A2173	D2174	L2175	N2176	T2177	N2178	N2179	D2180	N2181	G2182	Y2183	G2184	Q2185	A2186	Q2187	K2188	Y2189	S2190	G2191	L2192	V2193	R2194	V2195	N2196	E2197	D2198	V2199	Y2200	Y2201	F2202	G2203	E2204	T2205	Y2206	K2207	L2208	E2209	T2210	G2211	W2212
D2093	M2094	T2095	A2096	E2097	C2099	L2100	G2101	L2102	L2103	V2104	L2105	M2106	D2107	C2108	T2109	Y2110	Y2111	F2112	D2113	D2114	M2115	G2116	L2117	R2118	Q2119	L2120	G2121	N2122	F2123	L2124	L2125	M2126	D2127	N2128	L2129	F2130	Y2131	F2132	S2133	S2134	G2135	L2136	L2137	E2138	L2139	L2140	G2141	Q2142	L2143	M2144	L2145	G2146	G2147	N2148	E2209	T2210	G2211	W2212	
T2033	P2034	D2035	G2036	F2037	K2038	F2039	F2040	G2041	P2042	K2043	D2044	D2045	D2046	L2047	G2048	T2049	E2050	E2051	G2052	E2053	L2054	T2055	L2056	Y2057	M2058	G2059	L2060	L2061	N2062	F2063	N2064	G2065	K2066	L2067	Y2068	F2069	F2070	D2071	L2072	S2073	N2074	T2075	A2076	T2077	V2078	G2079	W2080	G2081	T2082	L2083	D2084	D2085	G2086	S2087	T2088	Y2089	Y2090	F2091	D2092
I1973	G1974	D1975	N1976	K1977	Y1978	F1980	D1981	F1982	N1983	G1984	I1985	M1986	Q1987	T1988	F1989	F1990	I1991	T1992	M1994	D1995	K1996	V1997	F1998	Y1999	M2001	N2002	D2003	G2004	V2005	M2006	Q2007	V2008	G2009	Y2010	I2011	E2012	V2013	N2014	G2015	K2016	Y2017	F2018	Y2019	A2020	G2021	K2022	N2023	G2024	E2025	R2026	Q2027	L2028	G2029	M2030	F2031	N2032			
I1641	K1642	E1643	L1644	S1645	Y1646	T1647	G1651	N1652	R1653	Q1654	N1655	S1661	Y1662	M1667	Q1679	L1682	Y1683	G1684	R1687	I1693	L1698	T1706	P1707	K1710	M1711	M1712	Y1713	I1714	P1716	D1722	I1726	K1729	L1737	Y1741	S1748	L1750	I1751	A1754	E1758																				
L1540	S1541	F1542	D1546	L1552	Y1556	E1559	Q1564	I1565	L1566	M1570	K1573	S1574	A1575	T1578	L1582	M1583	L1586	E1587	S1588	I1589	M1590	I1591	K1592	I1594	M1598	M1610	I1613	S1614	G1615	S1616	M1617	S1618	Q1621	L1624	K1628	D1629	P1634	M1638	F1639	K1640																			
I1449	I1450	F1452	M1453	G1454	E1455	H1456	Q1457	Y1458	I1460	I1463	Y1462	S1463	I1464	I1465	D1466	N1467	Y1471	Y1477	S1478	K1479	K1480	F1484	E1491	M1496	I1497	P1500	N1503	M1504	L1505	S1510	K1511	D1512	L1513	K1514	D1515	I1516	R1517	D1523	M1530	Y1531	F1532	K1533	D1534	D1535	M1536	S1539													
I1383	L1384	M1385	H1386	Y1387	T1388	I1389	F1391	D1394	I1395	M1396	E1397	M1398	N1399	R1400	F1406	I1407	S1403	L1404	T1405	L1406	S1407	I1408	L1409	M1413	I1414	I1415	I1416	L1420	V1421	S1422	K1423	S1424	Y1425	I1427	S1430	G1431	M1432	K1435	L1436	I1437	E1438	M1439	S1440	S1441	D1442	I1443	I1444	Q1445	Q1446	I1447	D1448								
G1247	T1248	K1249	L1250	L1251	D1252	R1253	I1254	R1255	D1256	H1257	Y1258	E1259	G1260	Q1261	F1262	Y1263	W1264	R1265	Y1266	F1267	A1268	F1269	I1270	A1271	D1272	I1273	L1274	I1275	K1277	L1278	K1279	P1280	R1281	Y1282	E1283	D1284	R1288	I1289	N1290	F1291	G1292	Y1293	E1293	M1294	R1296	I1299	V1300	I1303	T1304	T1305	E1306	Q1307	I1308	R1309	K1310				
M1311	L1312	S1313	F1316	Y1317	G1318	S1319	S1322	Y1323	S1324	I1325	S1326	L1327	M1332	M1333	I1334	D1335	L1336	M1337	L1338	V1339	E1340	M1341	V1345	I1346	D1347	V1348	V1351	V1352	K1353	L1354	I1355	T1356	E1357	I1358	D1360	E1361	I1362	Q1363	E1366	I1367	I1368	E1369	N1370	I1371	G1372	S1373	K1374	L1375	M1376	D1379	M1380								
H1186	F1187	F1188	S1189	S1190	F1191	I1193	T1194	Y1195	R1196	K1197	F1198	W1199	L1200	S1201	Y1202	I1203	D1204	V1205	L1206	N1207	I1208	K1209	K1210	E1211	K1212	I1213	D1214	F1215	K1217	L1218	L1219	M1220	V1221	M1224	A1225	P1226	M1227	R1228	V1229	F1230	G1231	Y1232	E1233	M1234	G1235	W1236	T1237	P1238	G1239	F1240	R1241	S1242	L1243	D1244	N1245	D1246			



## 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	0.45	2/19023 (0.0%)	0.56	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	TYR	CD1-CE1	-5.46	1.31	1.39
1	A	284	TYR	CD2-CE2	-5.22	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1505	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	1982	ASP	CB-CG-OD2	5.10	122.89	118.30

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	508	0
2	A	1	0	0	0	0
All	All	18645	0	18175	508	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 508 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%)	47 68

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%)	1919 (92%)	169 (8%)	<b>11</b> <b>23</b>

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1465	ILE
1	A	1722	ASP
1	A	1517	ARG
1	A	1628	LYS
1	A	1841	ASP

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

Mol	Chain	Res	Type
1	A	1290	ASN
1	A	2058	ASN
1	A	1449	HIS
1	A	2260	ASN
1	A	1724	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 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.

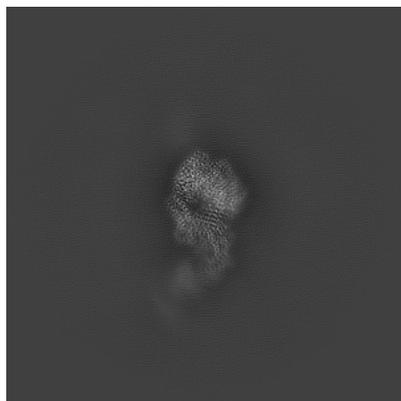
## 6 Map visualisation [i](#)

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

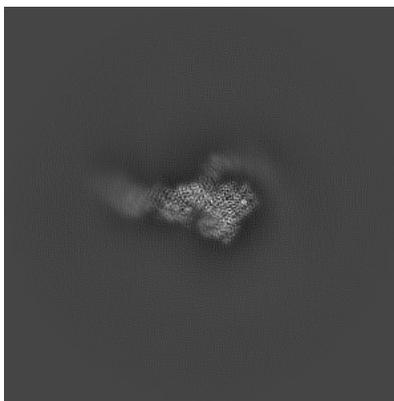
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

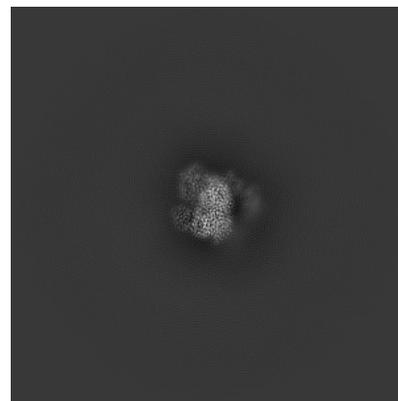
#### 6.1.1 Primary map



X

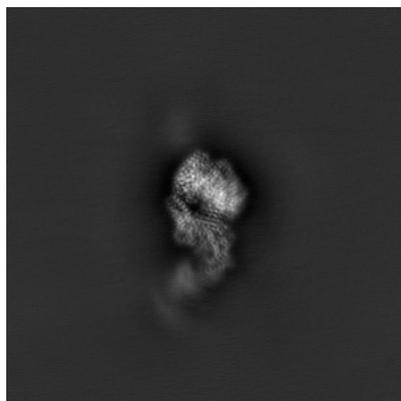


Y

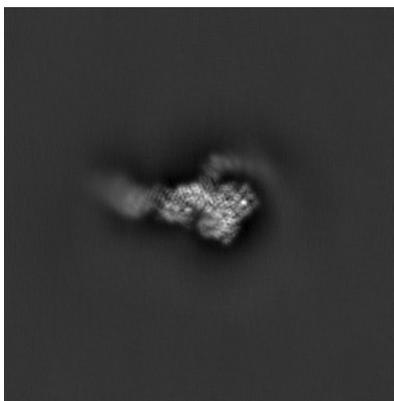


Z

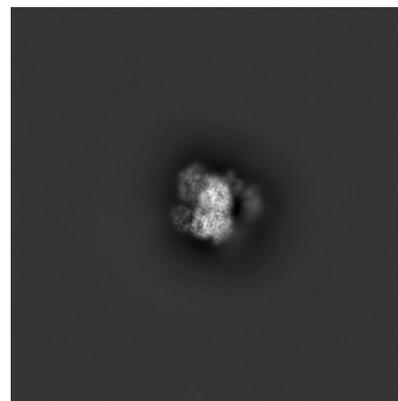
#### 6.1.2 Raw map



X



Y

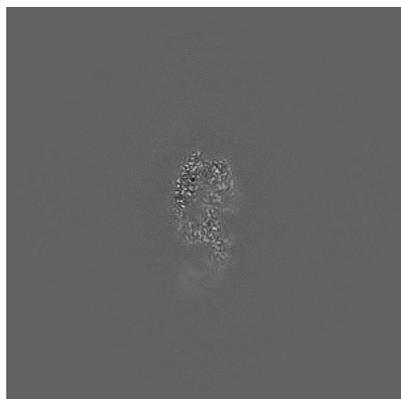


Z

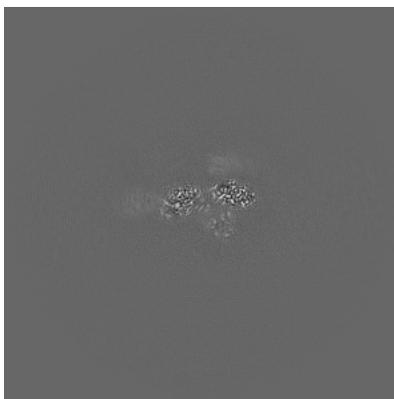
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

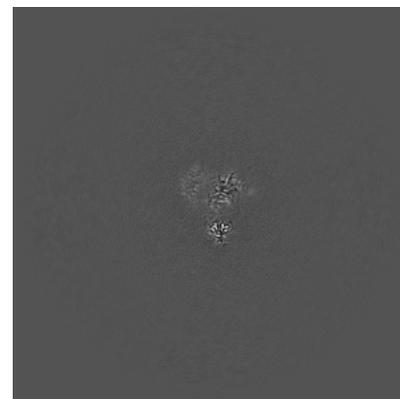
### 6.2.1 Primary map



X Index: 200

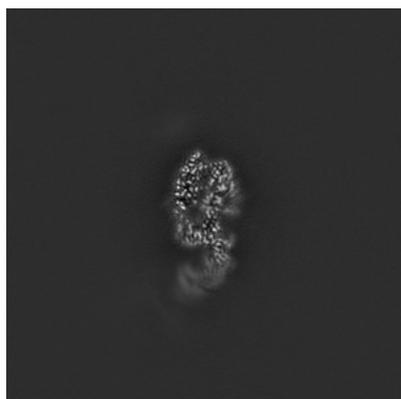


Y Index: 200

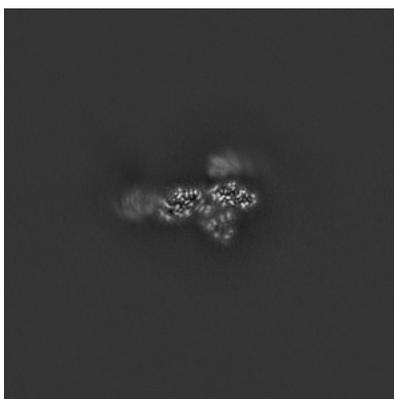


Z Index: 200

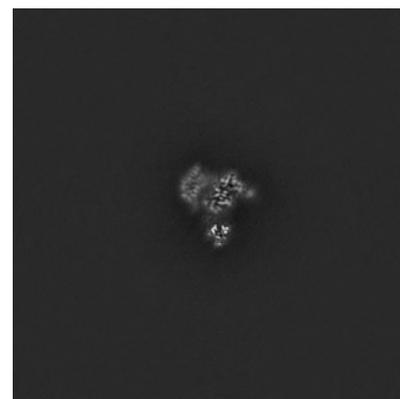
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

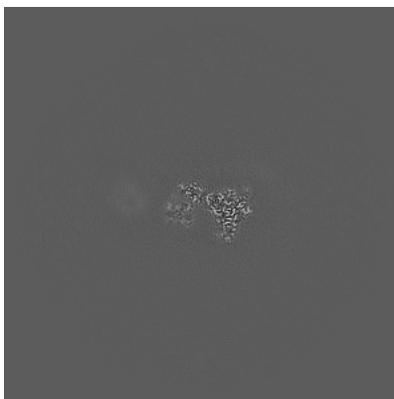
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

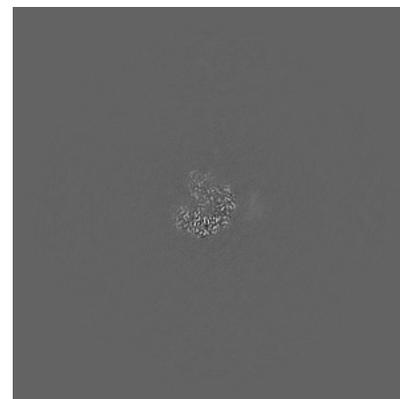
### 6.3.1 Primary map



X Index: 204

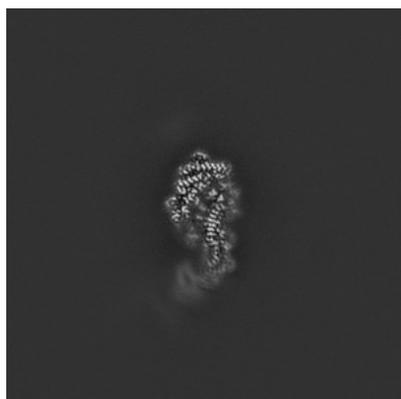


Y Index: 182

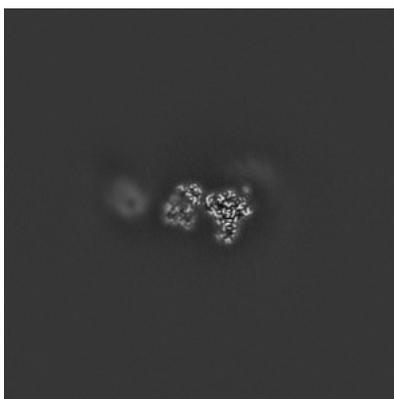


Z Index: 226

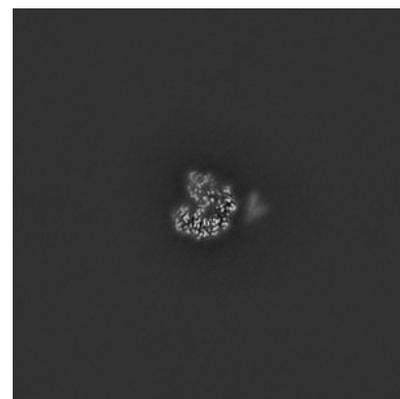
### 6.3.2 Raw map



X Index: 204



Y Index: 182

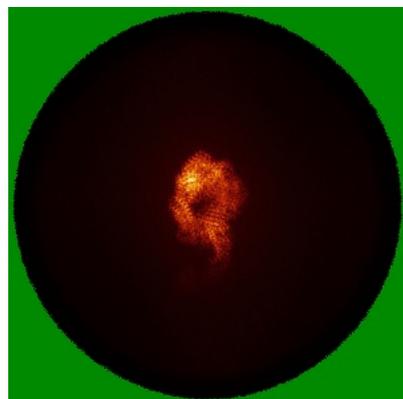


Z Index: 226

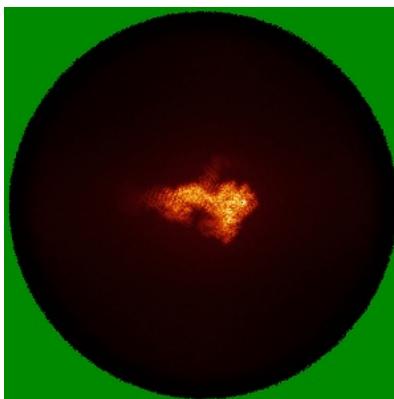
The images above show the largest variance slices of the map in three orthogonal directions.

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

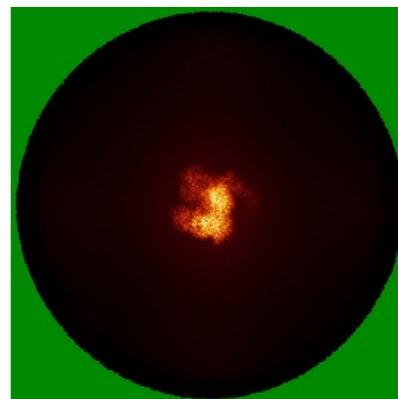
### 6.4.1 Primary map



X

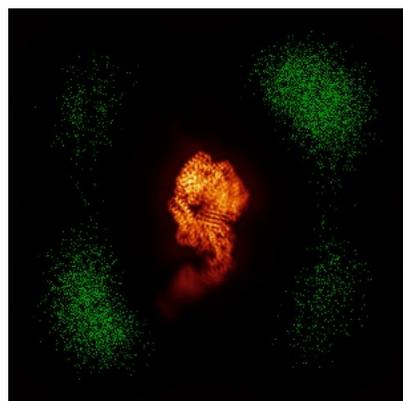


Y

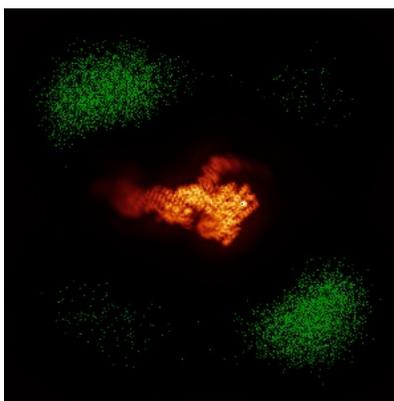


Z

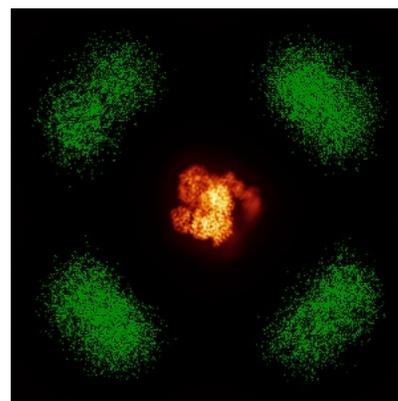
### 6.4.2 Raw map



X



Y

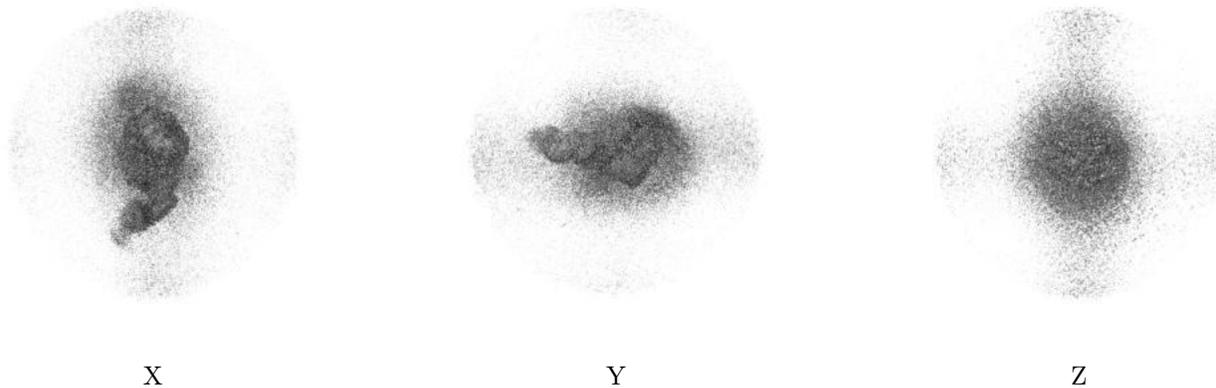


Z

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.

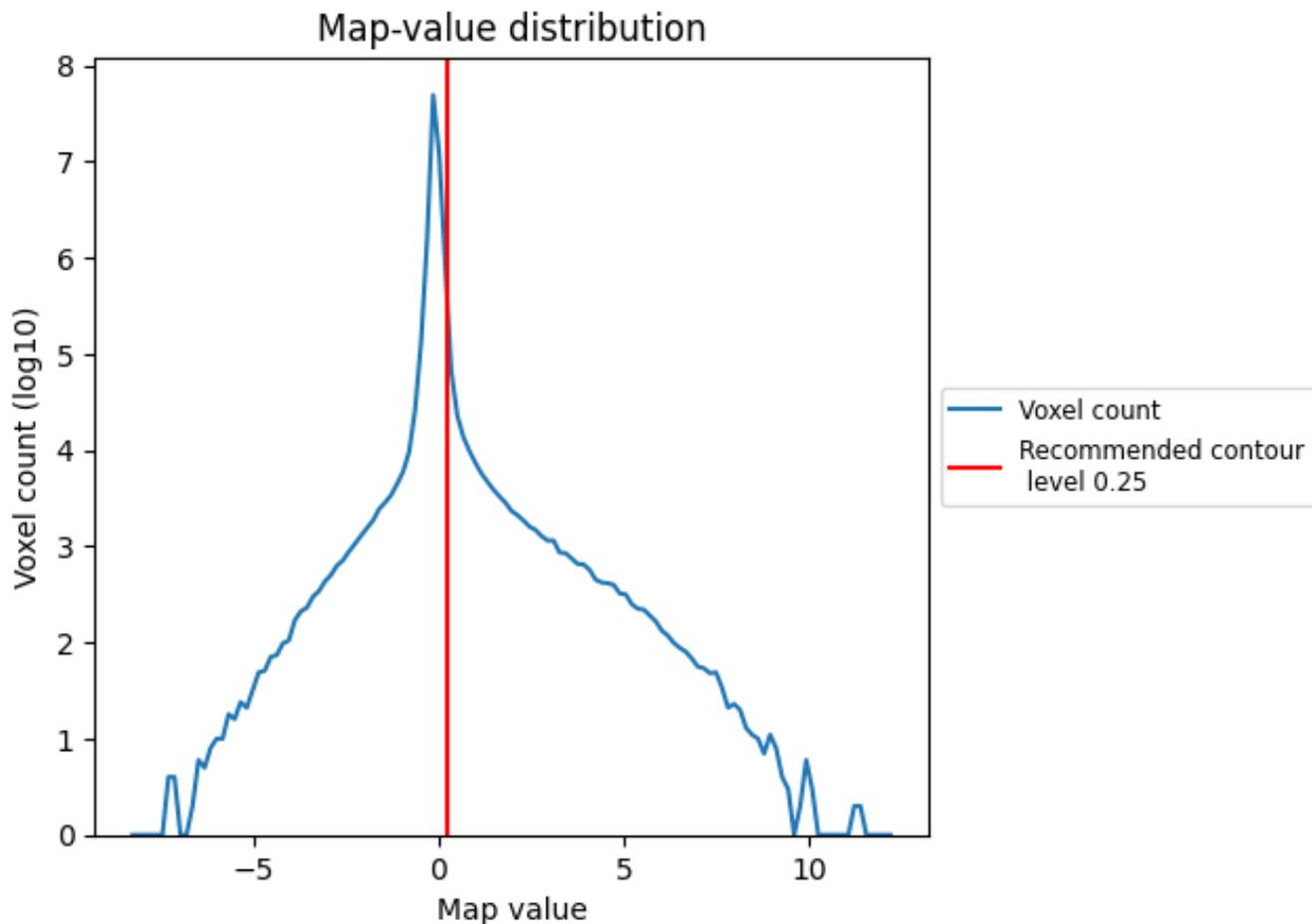
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

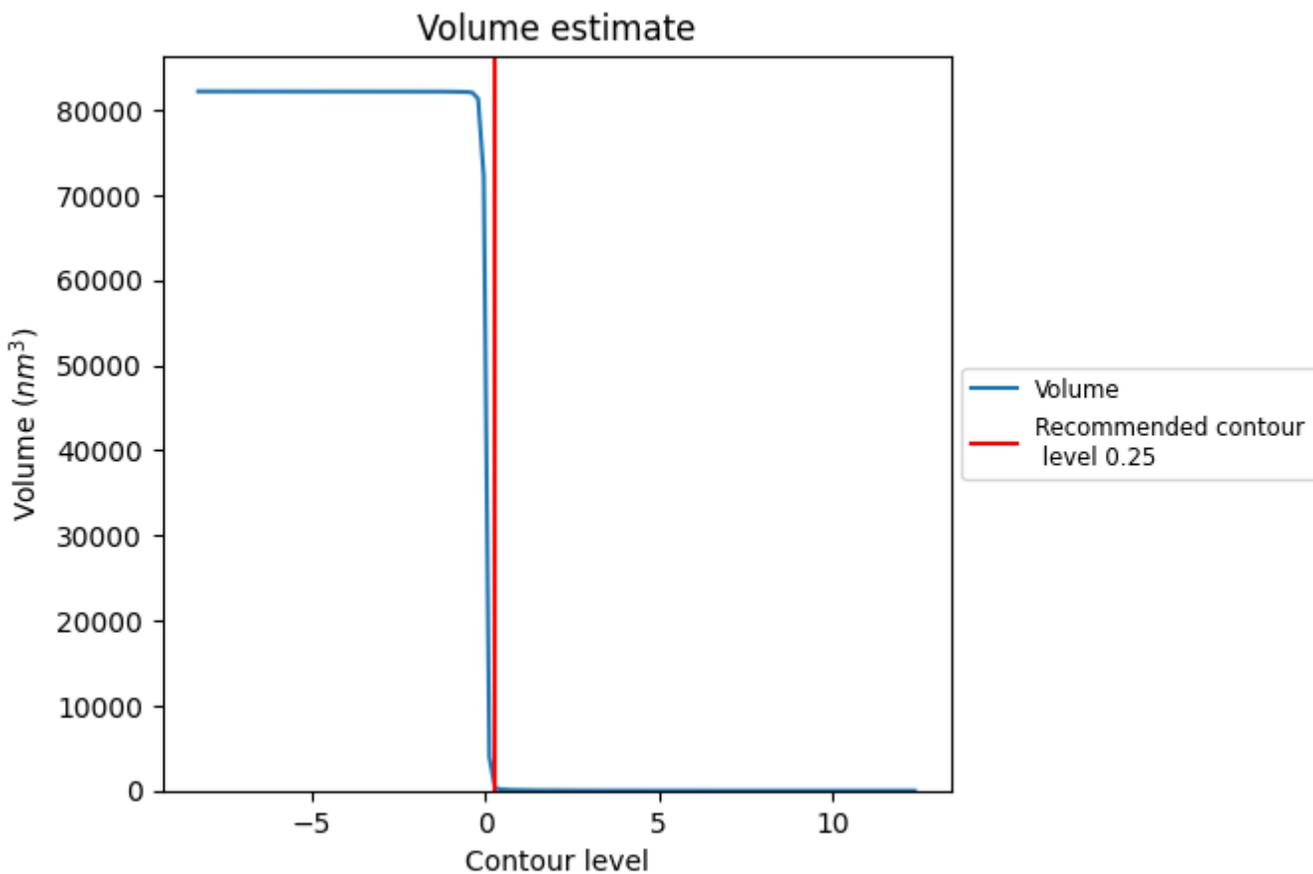
This section contains the results of statistical analysis of the map.

### 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.

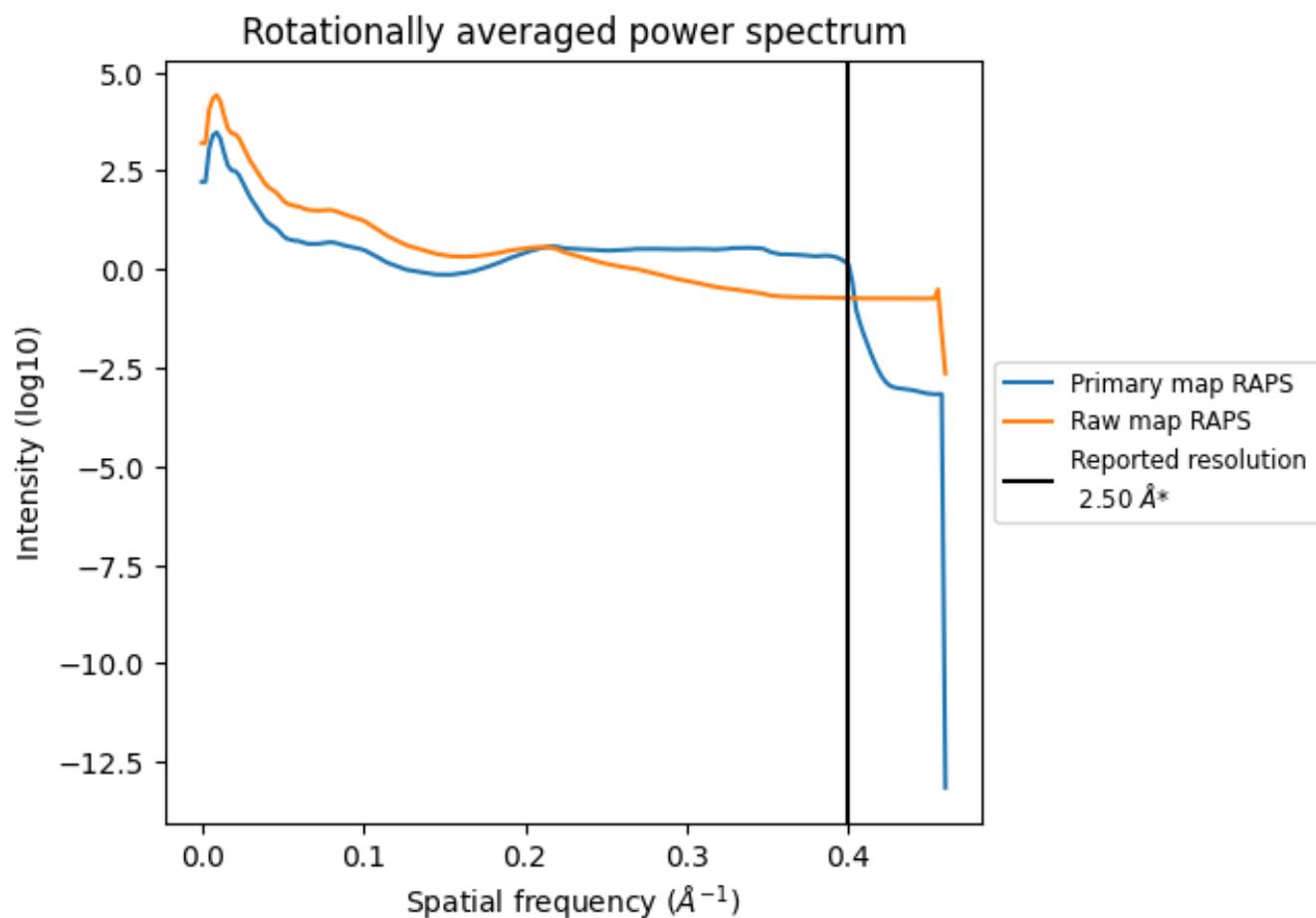
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm<sup>3</sup>; 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 [i](#)

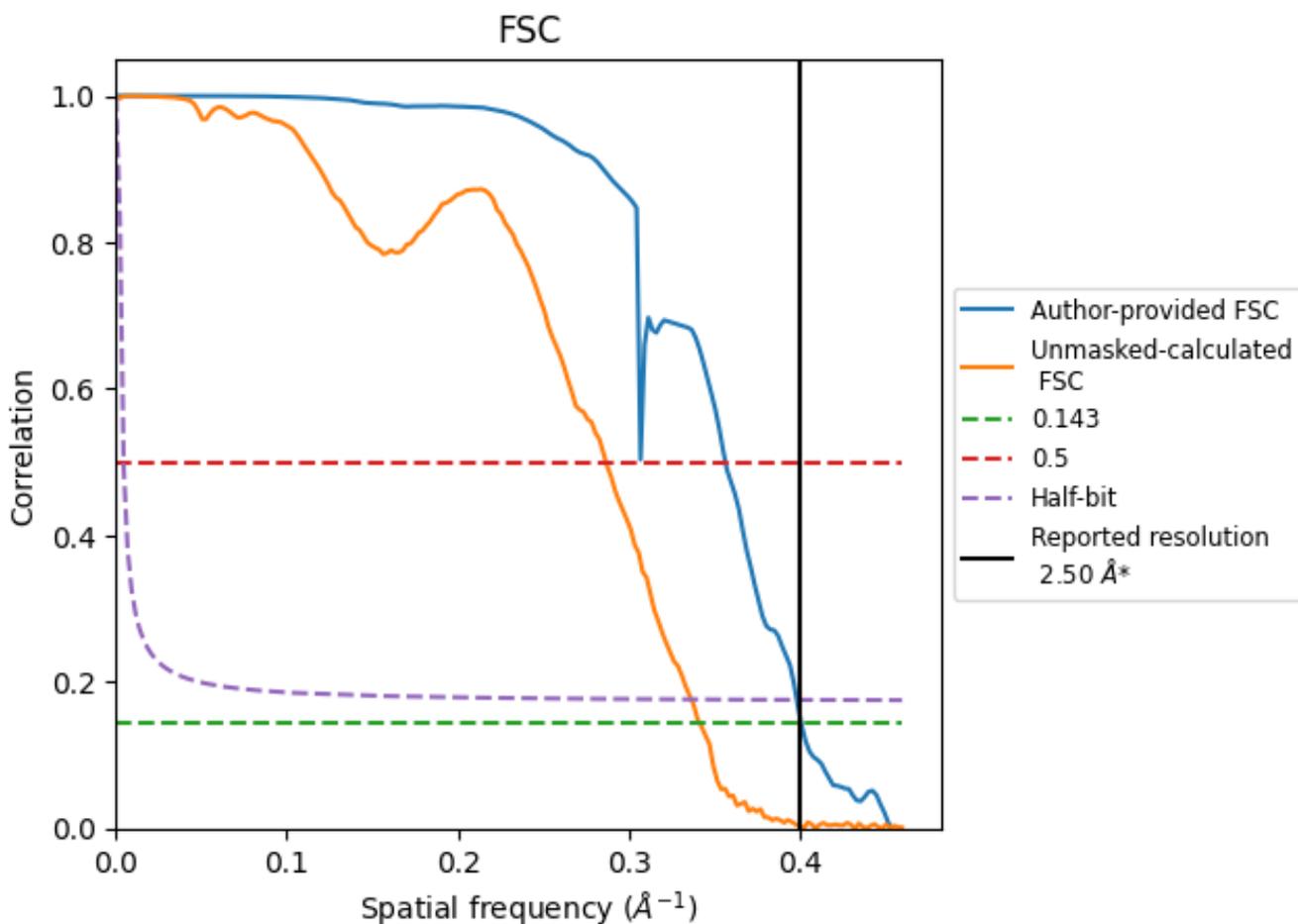


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

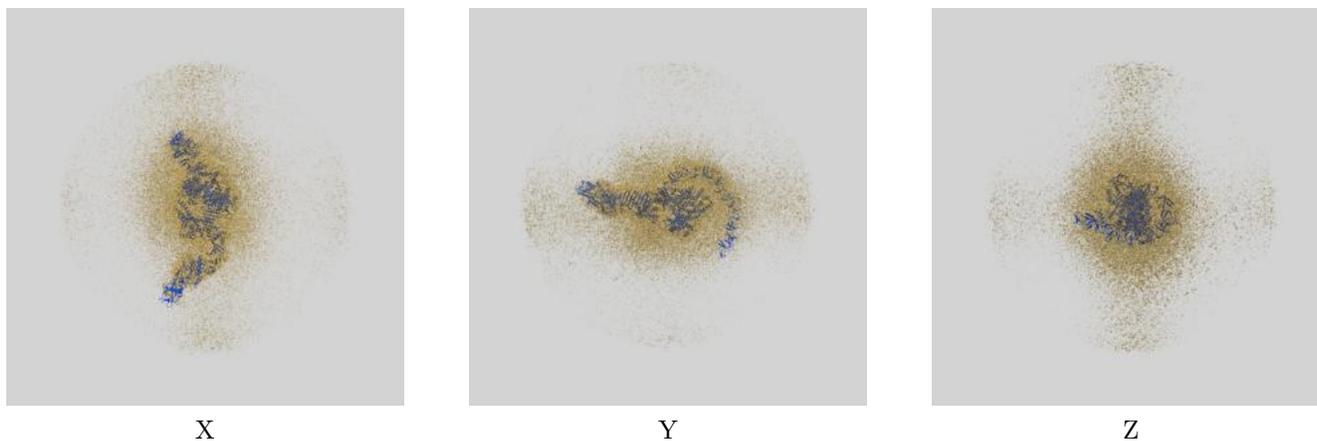
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.80	2.51
Unmasked-calculated*	2.93	3.49	2.97

\*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](#)

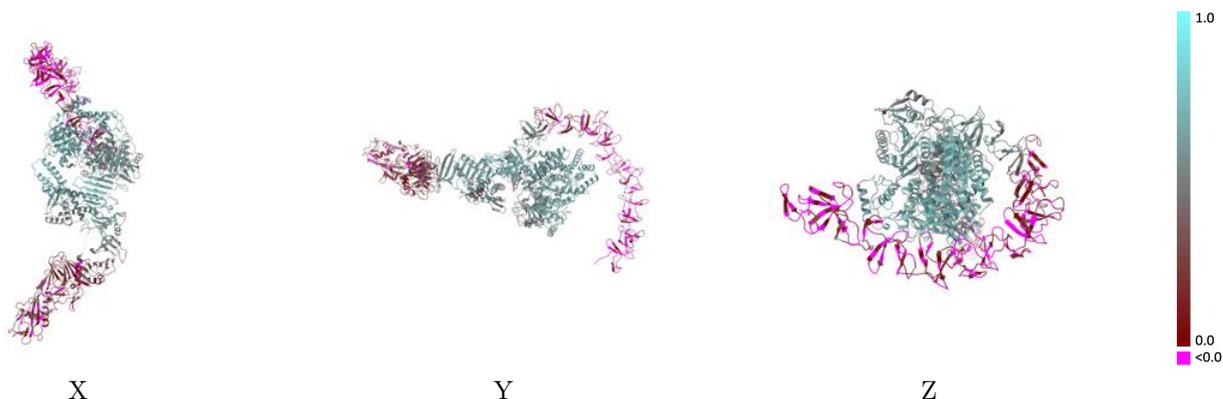
This section contains information regarding the fit between EMDB map EMD-38011 and PDB model 8X2I. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



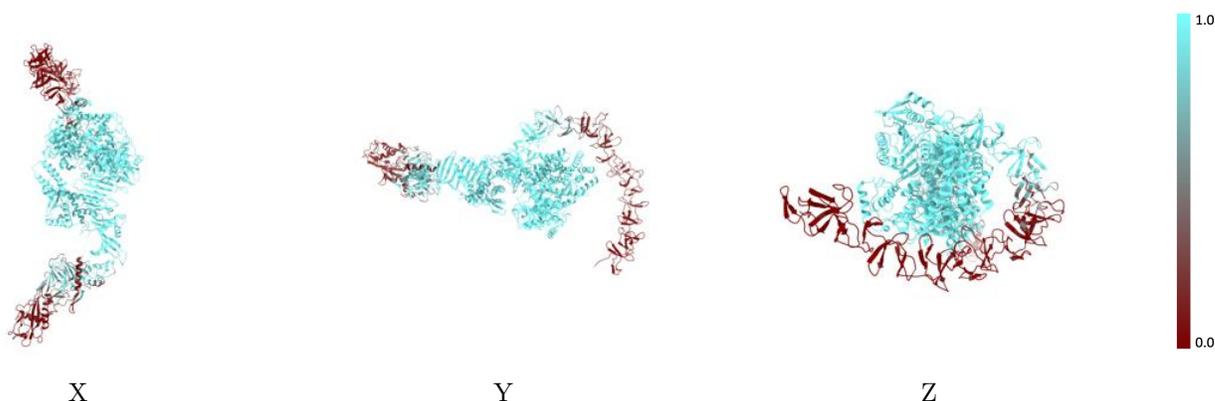
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



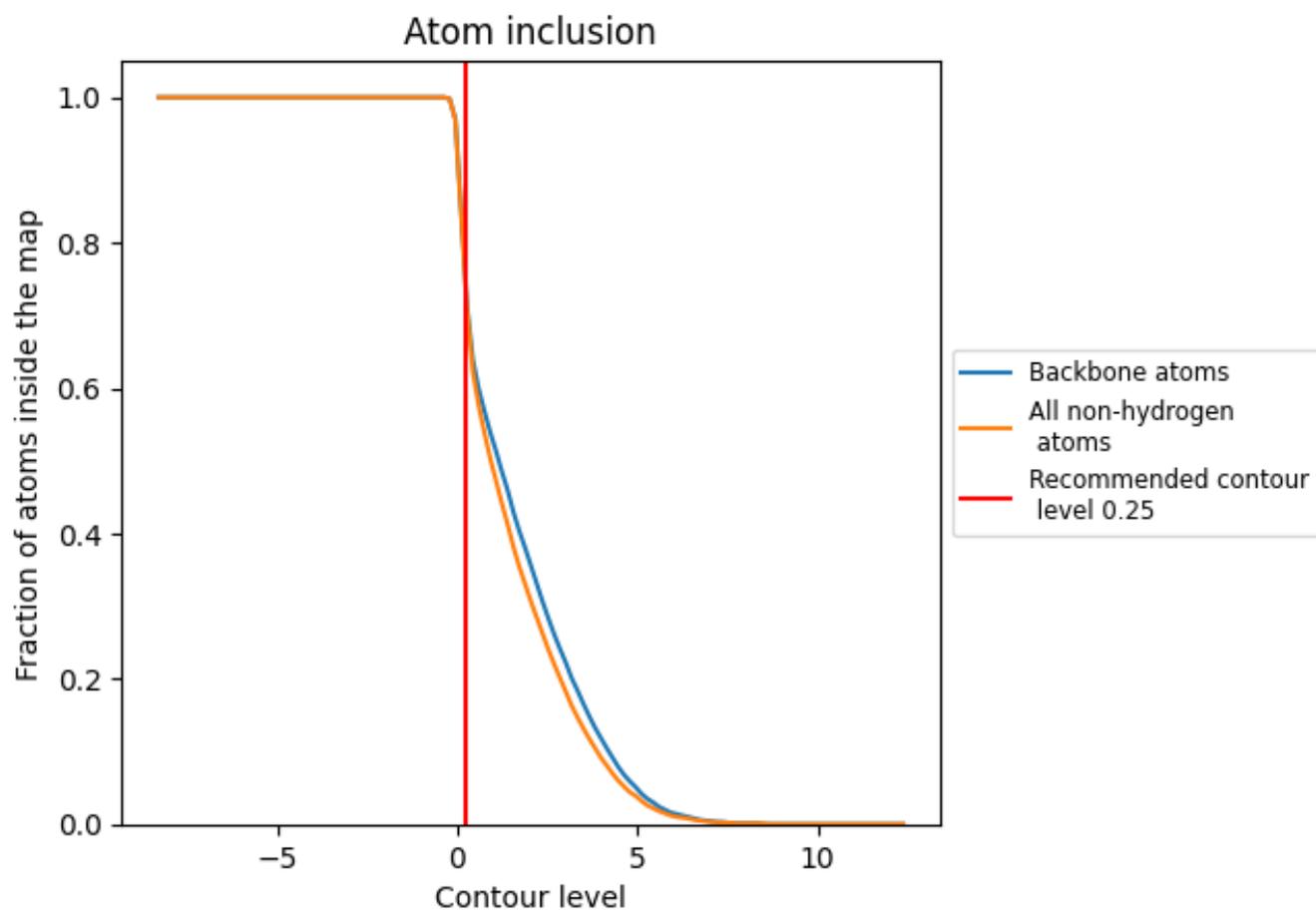
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

