



wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 06:18 am BST

PDB ID : 7POG
EMDB ID : EMD-13574
Title : High-resolution structure of native toxin A from Clostridioides difficile
Authors : Boesen, T.; Joergensen, R.; Aminzadeh, A.; Engelbrecht Larsen, C.
Deposited on : 2021-09-08
Resolution : 2.83 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

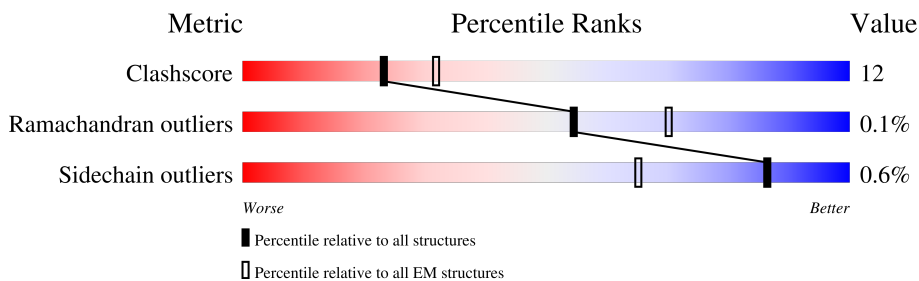
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2710	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19199 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 Toxin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2382	19198	12290	3103	3773	32	0	0

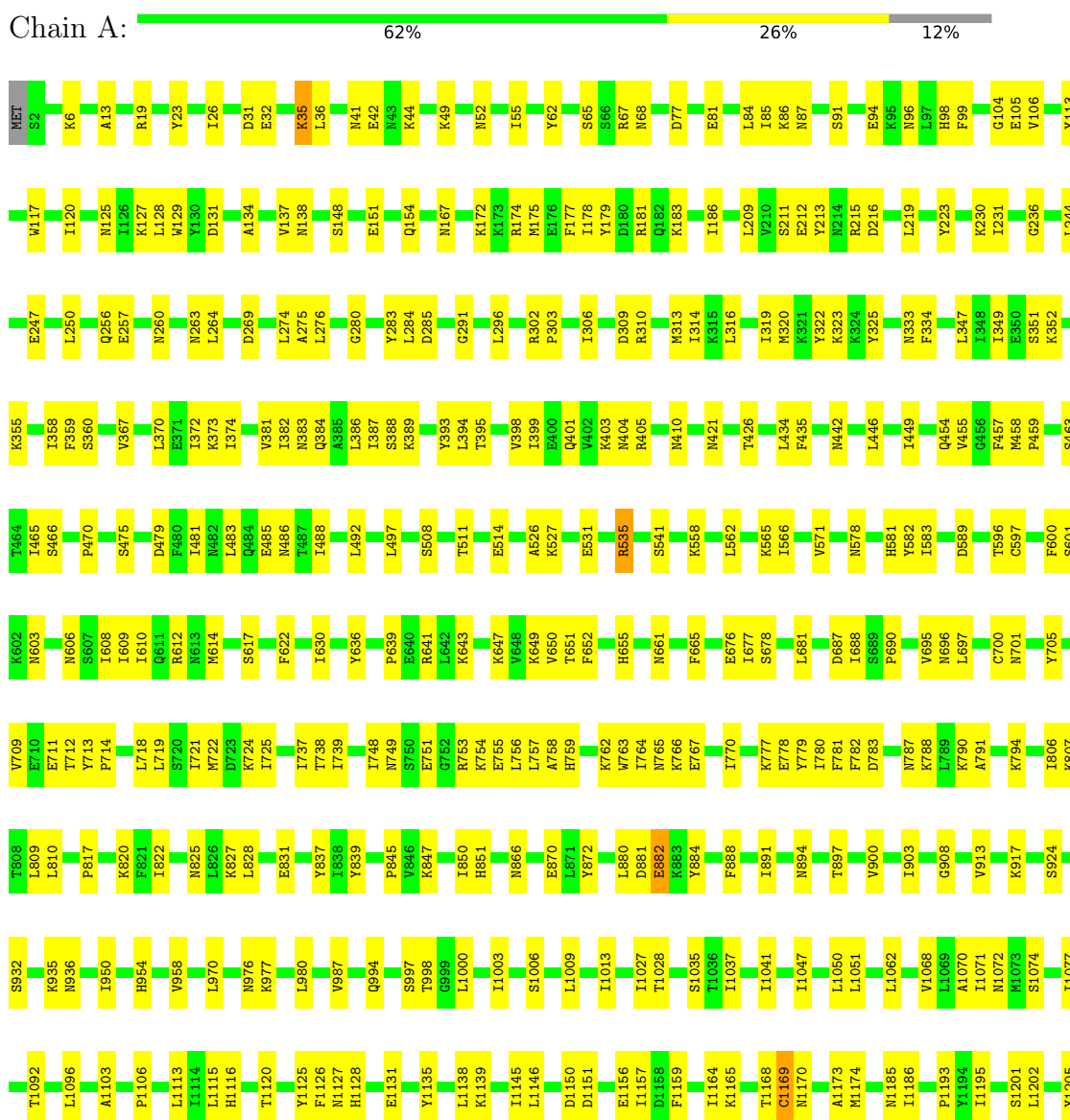
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots [i](#)

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: Toxin A



GLY	ALA	GLY	ASN	GLY	A2174	K2087	T1944	N1818	Y1684	F1516	C1407	T1296	I1208
LEU	ALA	LEU	ASN	SER	T2178	Y2089	R1947	A1819	I1685	M1517	E1408	R1297	G1209
PHE	GLY	THR	LYS	THR	Y2089	F2284	R1947	T1820	V1688	K1518	L1409	R1299	I1210
ILE	THR	THR	LYS	THR	N2182	K1953	K1953	E1825	L1689	M1522	I1413	F1299	K1211
ASP	THR	THR	LYS	THR	I2183	A2097	P1988	K1831	I1690	T1523	M1301	M1301	T1212
ASP	THR	THR	THR	THR	A2098	A2098	P1988	G1832	A1691	I1524	I1416	P1302	E1213
ASN	THR	THR	THR	THR	T2099	A1984	A1984	L1833	P1682	T1525	I1422	E1308	N1214
ASN	THR	THR	THR	THR	T2103	L2103	L1967	F1841	Y1706	Y1528	V1422	I1309	K1220
ILE	THR	THR	THR	THR	I2104	L2104	L1967	Y1842	Y1710	D1539	A1423	I1309	K1220
ASP	THR	THR	THR	THR	K2200	Q1968	Q1968	F1843	Y1710	D1539	K1424	I1221	I1221
ASP	THR	THR	THR	THR	Y2203	G2106	Y1976	F1843	I1715	F1540	S1426	Y1315	M1222
GLY	THR	THR	THR	THR	K2107	K2107	Y1976	L1850	I1745	S1541	L1426	S1316	M1223
THR	THR	THR	THR	THR	K2108	K2108	Y1976	L1850	I1745	I1542	L1429	F1317	L1224
THR	THR	THR	THR	THR	Y2109	Y2109	K1986	Q1855	P1719	S1543	L1429	D1318	A1227
THR	THR	THR	THR	THR	Y2110	Y2110	K1986	Q1855	P1719	S1543	L1429	D1318	A1227
THR	THR	THR	THR	THR	D2207	D2207	F1998	K1860	K1725	K1551	G1432	L1327	R1230
THR	THR	THR	THR	THR	A2210	A2210	F1998	K1860	K1725	K1551	D1433	L1328	R1230
THR	THR	THR	THR	THR	I2211	I2211	T2002	F1864	W1739	Y1556	G1432	L1327	R1230
THR	THR	THR	THR	THR	T2212	T2212	A2003	T1864	S1740	Y1556	D1433	L1327	R1230
THR	THR	THR	THR	THR	K2221	K2221	F2019	T1868	E1742	Y1562	K1434	L1328	V1231
THR	THR	THR	THR	THR	F2224	F2224	N2034	A1870	E1742	Y1562	L1437	L1328	F1232
THR	THR	THR	THR	THR	I2230	I2230	R2029	Y1875	I1747	Y1565	S1455	L1344	W1233
THR	THR	THR	THR	THR	L2235	L2235	F2039	L1893	K1757	F1581	E1466	L1344	W1233
THR	THR	THR	THR	THR	C2236	C2236	A2041	F1896	K1758	F1581	S1466	L1344	W1233
THR	THR	THR	THR	THR	Y2243	Y2243	P2041	F1896	K1762	L1586	E1466	L1344	W1233
THR	THR	THR	THR	THR	Y2244	Y2244	A2042	Y1904	R1764	L1589	Y1470	L1363	R1257
THR	THR	THR	THR	THR	Y2247	Y2247	R2043	F1905	I1765	L1594	Y1470	L1363	R1257
THR	THR	THR	THR	THR	L2251	L2251	T2044	A1906	K1777	L1603	A1473	L1368	K1263
THR	THR	THR	THR	THR	Q2252	Q2252	N2046	P1907	I1778	V1603	K1476	V1372	F1264
THR	THR	THR	THR	THR	N2253	N2253	N2048	A1908	S1779	I1604	L1373	L1373	Y1265
THR	THR	THR	THR	THR	I2258	I2258	N2048	Q1911	I1778	D1605	D1377	D1377	Y1265
THR	THR	THR	THR	THR	E2259	E2259	N2048	Q1911	S1779	T1609	I1378	I1378	R1267
THR	THR	THR	THR	THR	R2260	R2260	N2048	Q1911	S1779	T1609	K1487	M1379	A1270
THR	THR	THR	THR	THR	F2265	F2265	Q2057	L1920	I1788	L1622	K1487	M1379	A1270
THR	THR	THR	THR	THR	D2266	D2266	Q2057	L1920	I1788	L1622	K1487	M1379	A1270
THR	THR	THR	THR	THR	A2267	A2267	K2087	L1927	E1805	L1501	L1501	Q1388	L1279
THR	THR	THR	THR	THR	N2268	N2268	K2087	L1927	E1805	L1501	E1502	Q1388	L1279
THR	THR	THR	THR	THR	N2269	N2269	N2072	T1928	R1808	D1630	F1502	S1393	K1280
THR	THR	THR	THR	THR	E2270	E2270	N2072	L1929	R1808	D1630	F1502	S1393	K1280
THR	THR	THR	THR	THR	S2271	S2271	N2073	L1929	R1808	D1630	F1502	S1393	K1280
THR	THR	THR	THR	THR	K2272	K2272	S2074	D1937	D1809	I1631	N1504	K1399	Y1283
THR	THR	THR	THR	THR	M2273	M2273	S2074	D1937	D1809	I1631	N1504	K1399	Y1283
THR	THR	THR	THR	THR	Y2274	Y2274	V2077	D1937	H1810	M1652	A1510	D1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	V2077	D1937	H1810	M1652	A1510	D1401	K1289
THR	THR	THR	THR	THR	Y2275	Y2275	V2077	D1939	K1814	I1681	I1513	R1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	N2080	V1943	D1817	D1682	M1514	R1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	N2080	V1943	D1817	D1682	M1514	R1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	N2080	V1943	D1817	D1682	M1514	R1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	N2080	V1943	D1817	D1682	M1514	R1401	K1289
THR	THR	THR	THR	THR	T2275	T2275	N2080	V1943	D1817	D1682	M1514	R1401	K1289

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	900000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.239	Depositor
Minimum map value	-0.090	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0359	Depositor
Map size (\AA)	419.84, 419.84, 419.84	wwPDB
Map dimensions	656, 656, 656	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.64, 0.64, 0.64	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	0.27	0/19599	0.46	0/26540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19198	0	18832	468	0
2	A	1	0	0	0	0
All	All	19199	0	18832	468	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 12.

The worst 5 of 468 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:2266:ASP:O	1:A:2271:SER:HA	1.68	0.92
1:A:310:ARG:HH21	1:A:719:LEU:HD13	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:ILE:HD13	1:A:1515:VAL:HG13	1.68	0.75
1:A:1944:THR:HB	1:A:1958:PRO:HA	1.69	0.74
1:A:372:ILE:HG22	1:A:394:LEU:HD22	1.69	0.73

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	2380/2710 (88%)	2198 (92%)	180 (8%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	GLU
1	A	1498	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	2151/2412 (89%)	2138 (99%)	13 (1%)	86 93

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1434	LYS
1	A	1487	LYS
1	A	2376	LYS
1	A	2253	ASN
1	A	2260	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	HIS
1	A	824	ASN
1	A	1170	ASN
1	A	1892	GLN

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.

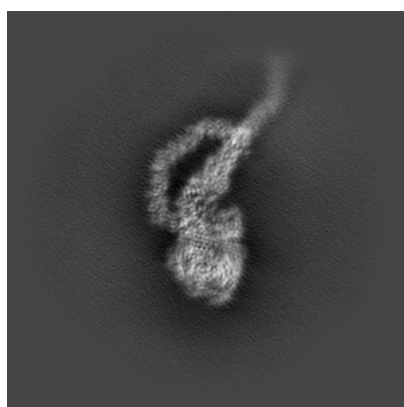
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13574. These allow visual inspection of the internal detail of the map and identification of artifacts.

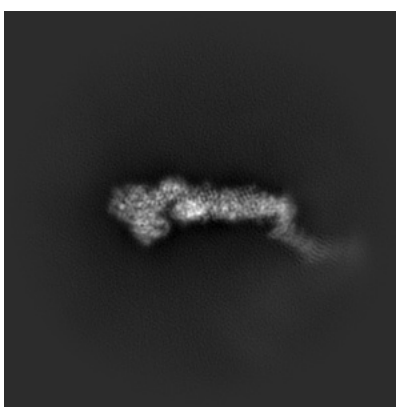
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

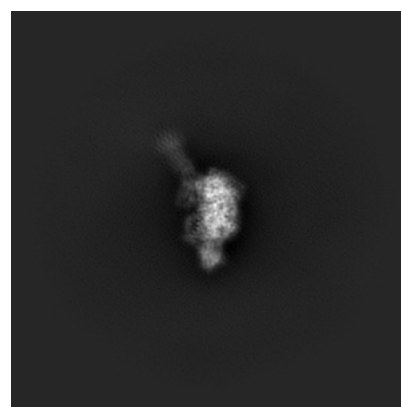
6.1.1 Primary map



X



Y

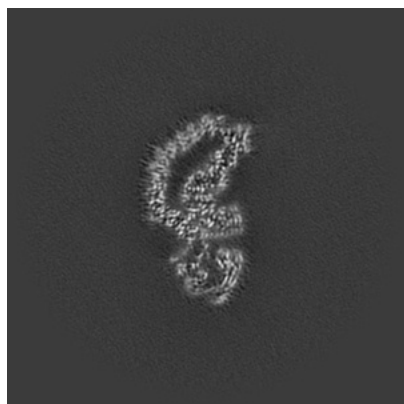


Z

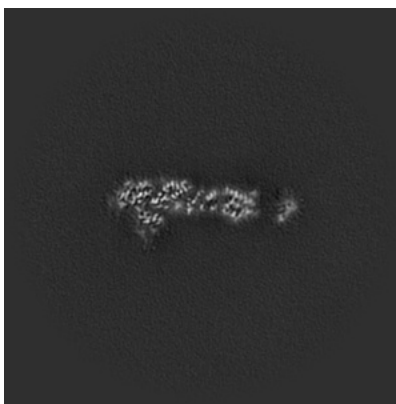
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 328



Y Index: 328

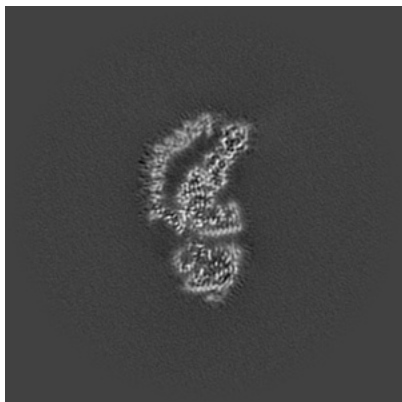


Z Index: 328

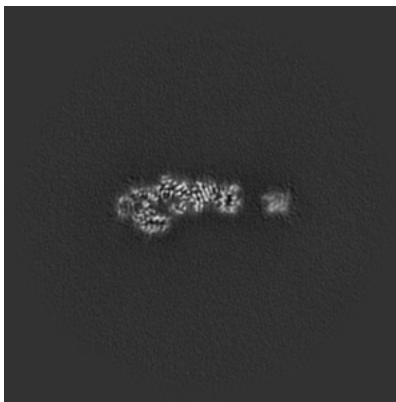
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

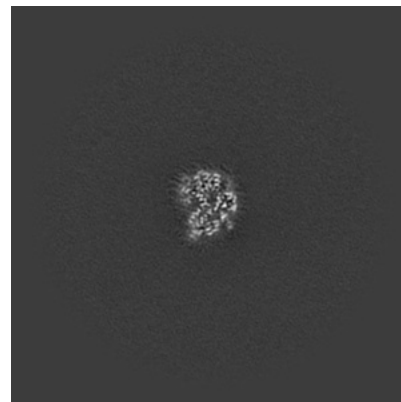
6.3.1 Primary map



X Index: 334



Y Index: 306



Z Index: 223

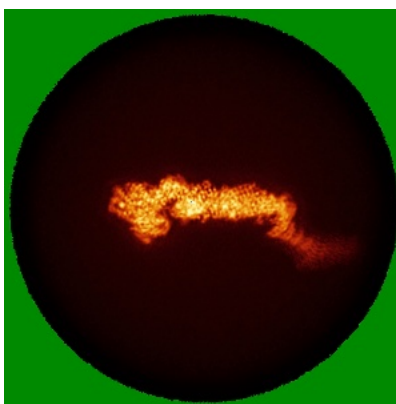
The images above show the largest variance slices of the map in three orthogonal directions.

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

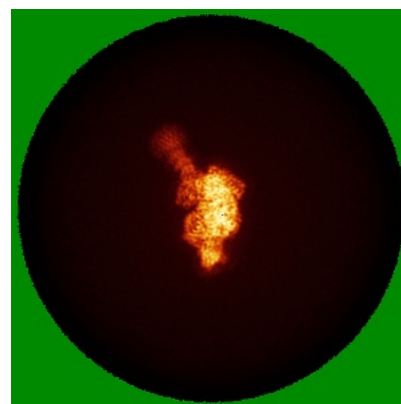
6.4.1 Primary map



X



Y

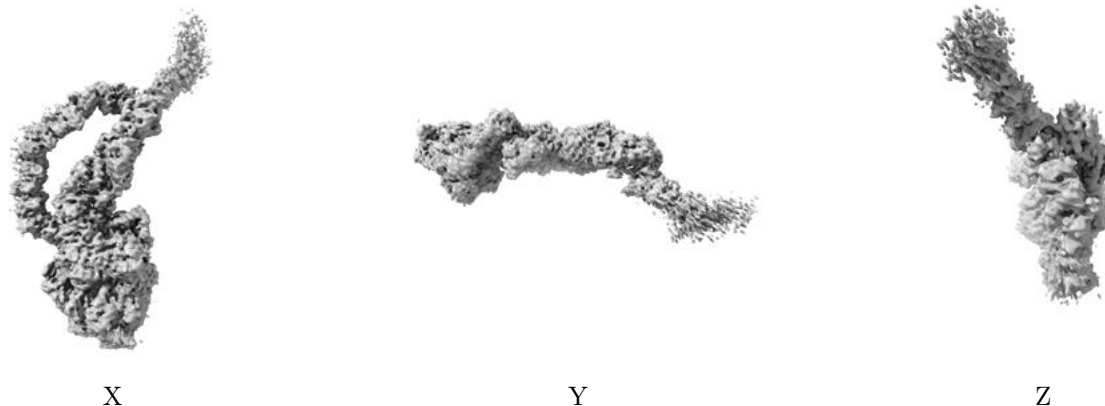


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

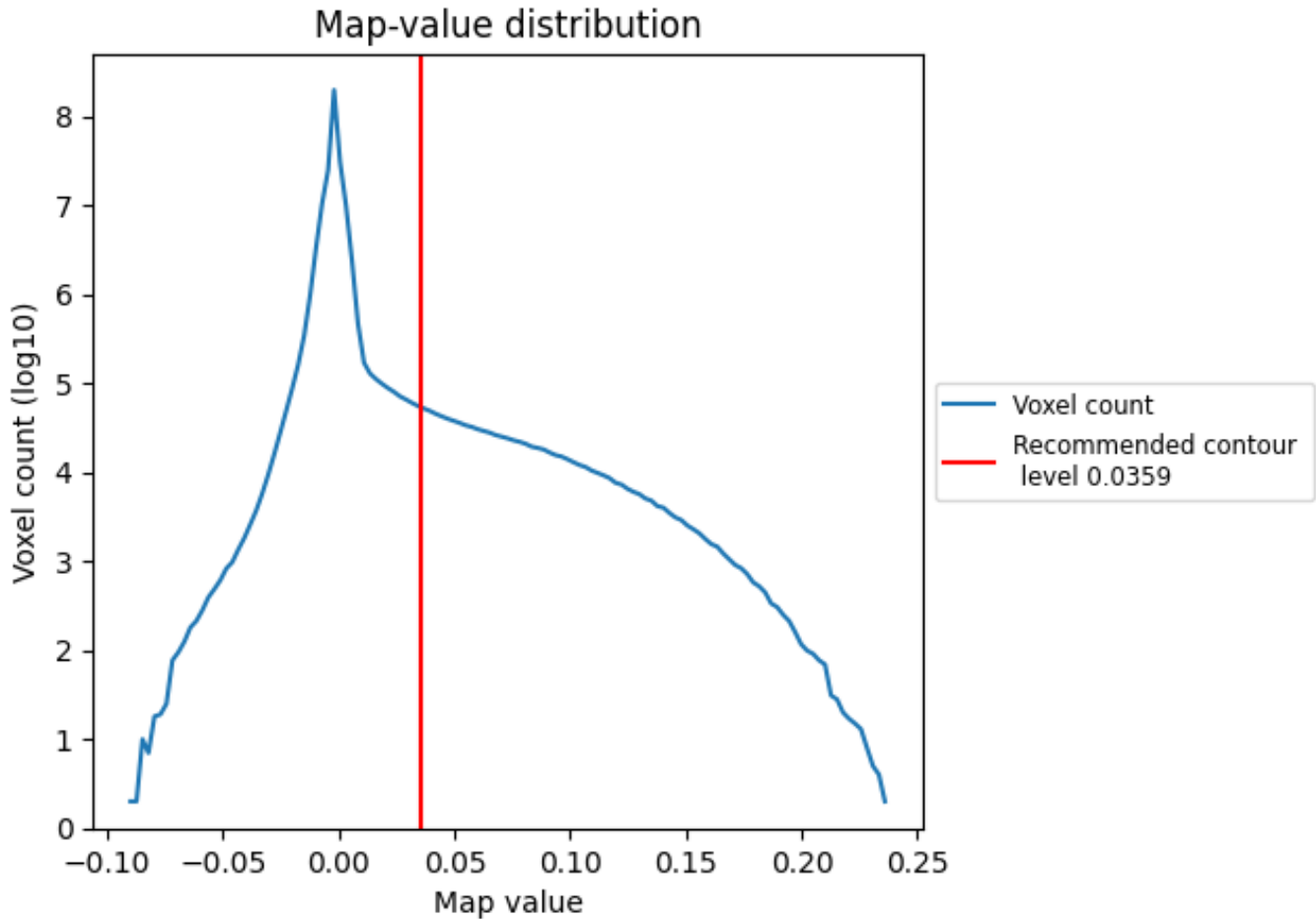
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

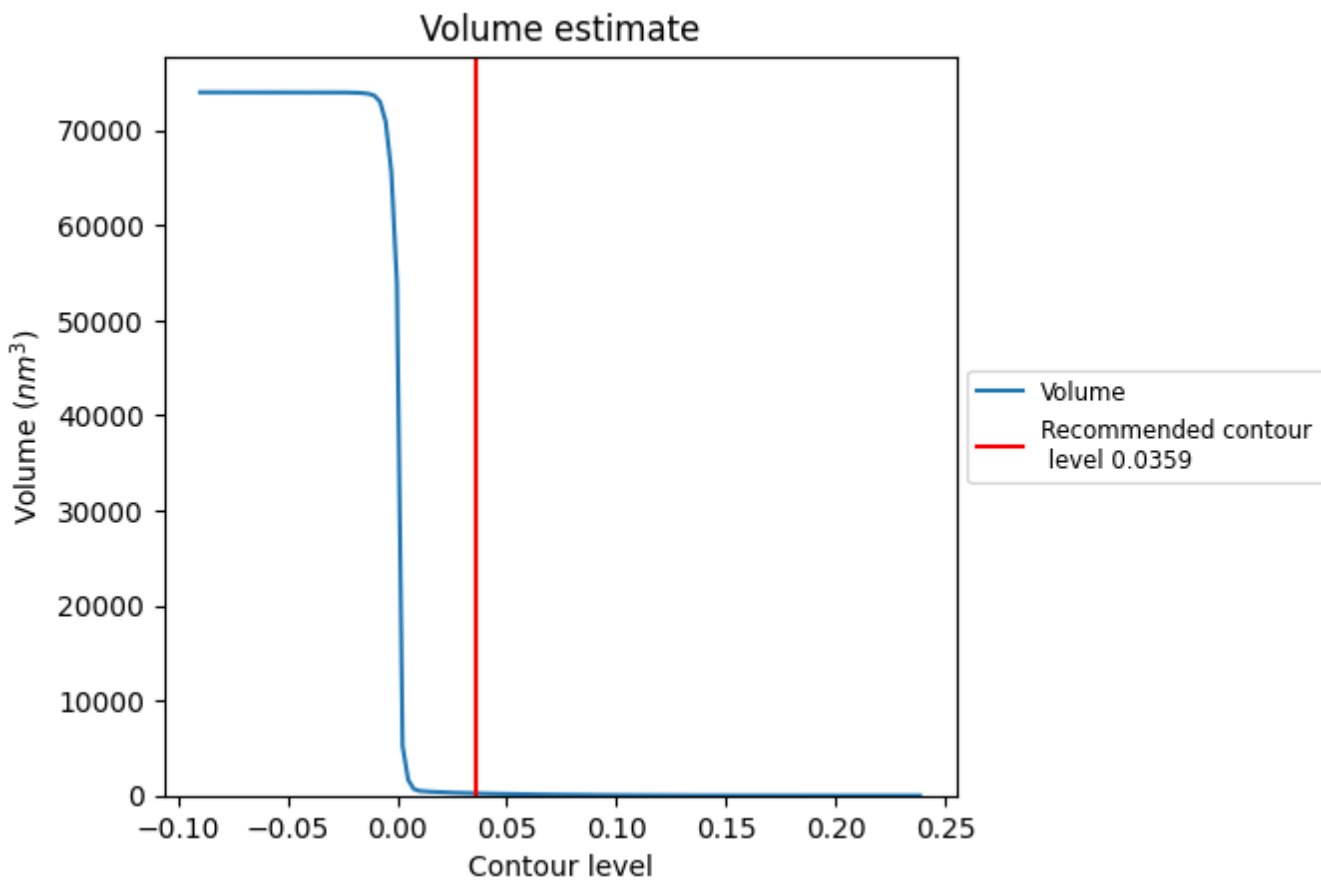
This section contains the results of statistical analysis of the map.

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.

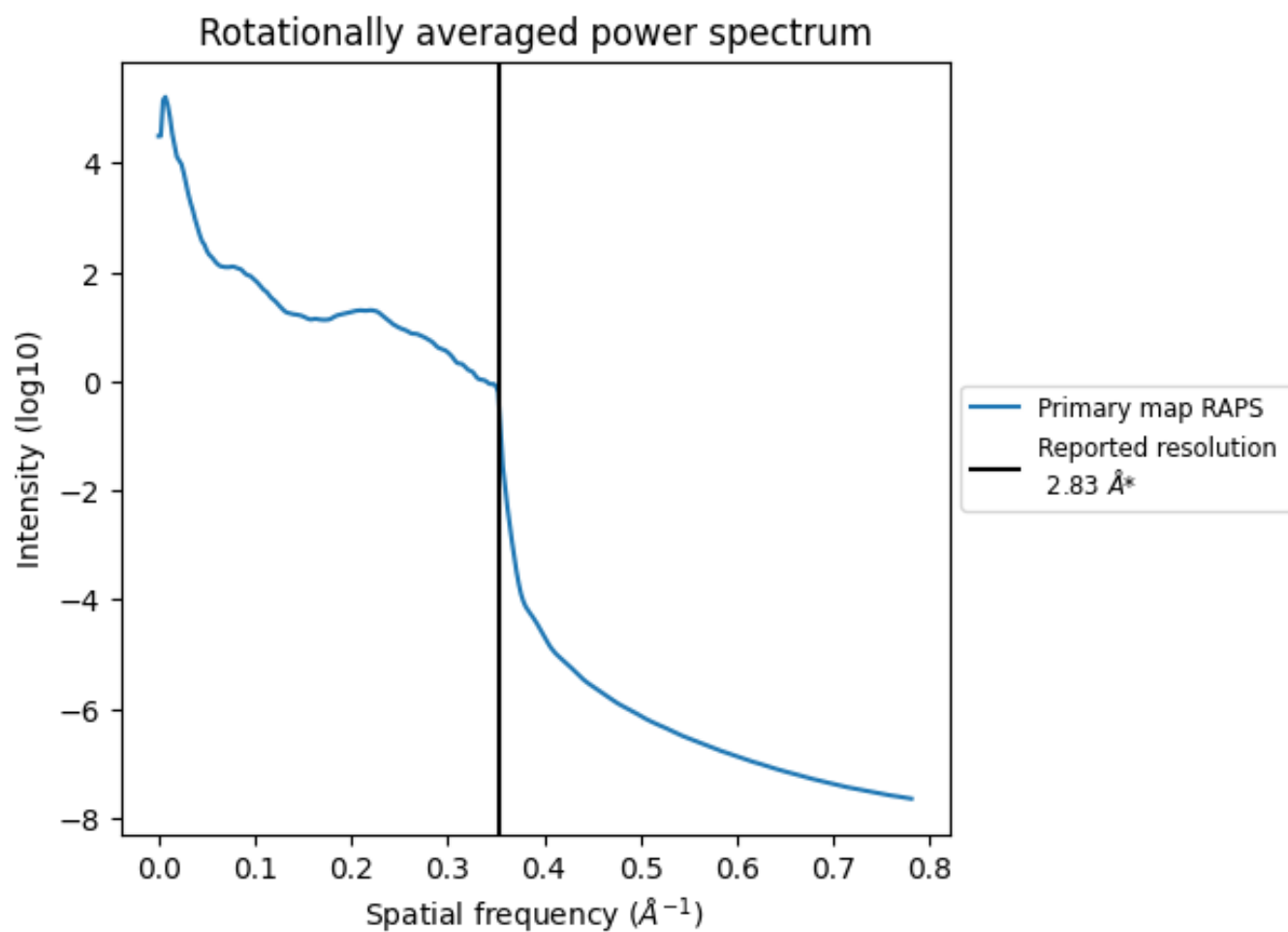
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 232 nm³; this corresponds to an approximate mass of 210 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 0.353\AA^{-1}

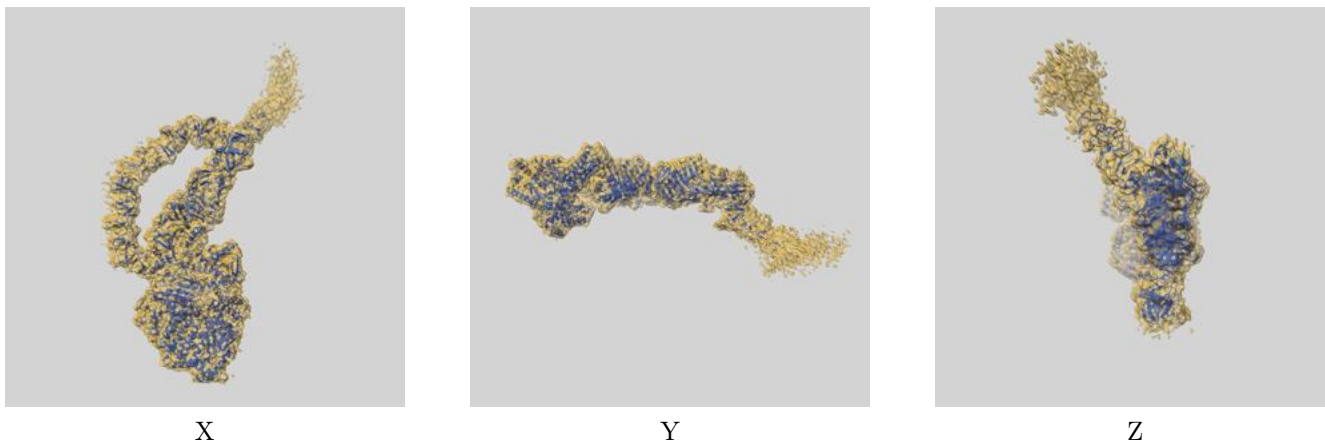
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

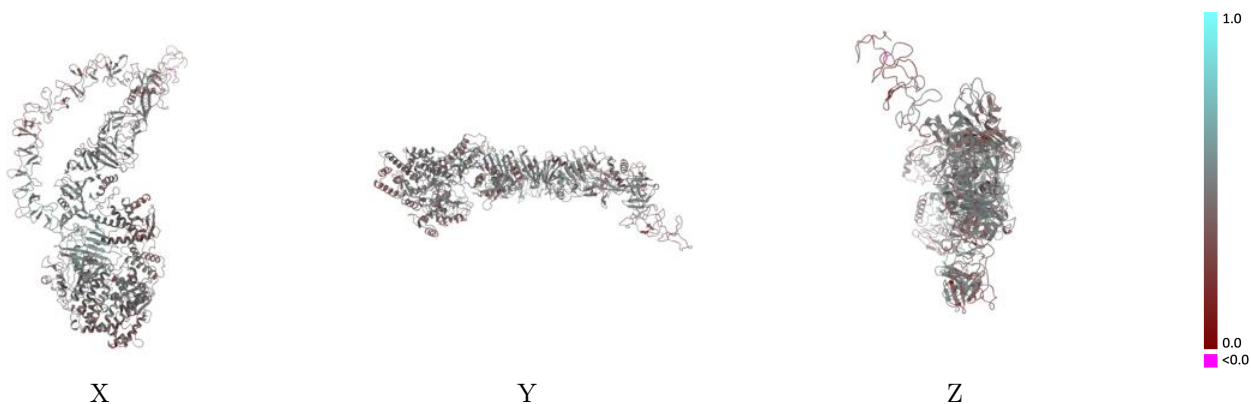
This section contains information regarding the fit between EMDB map EMD-13574 and PDB model 7POG. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



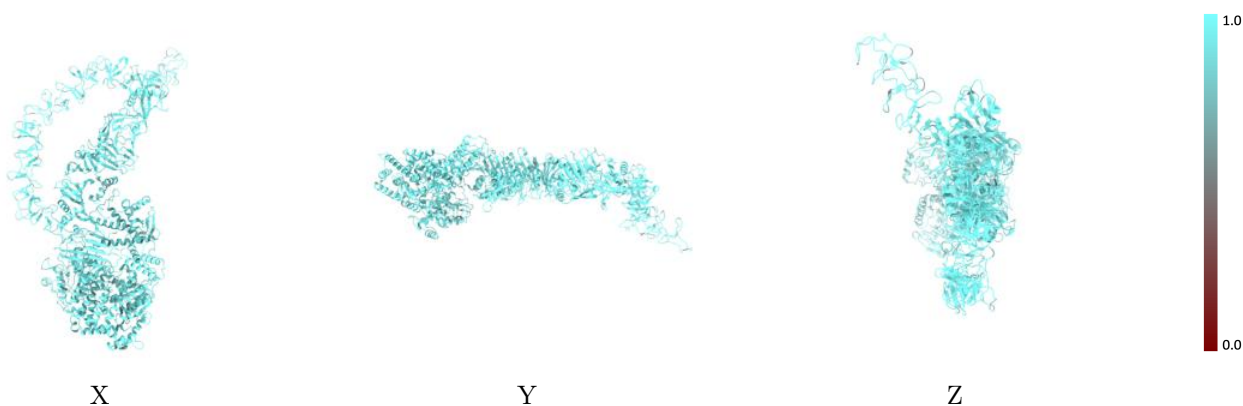
The images above show the 3D surface view of the map at the recommended contour level 0.0359 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



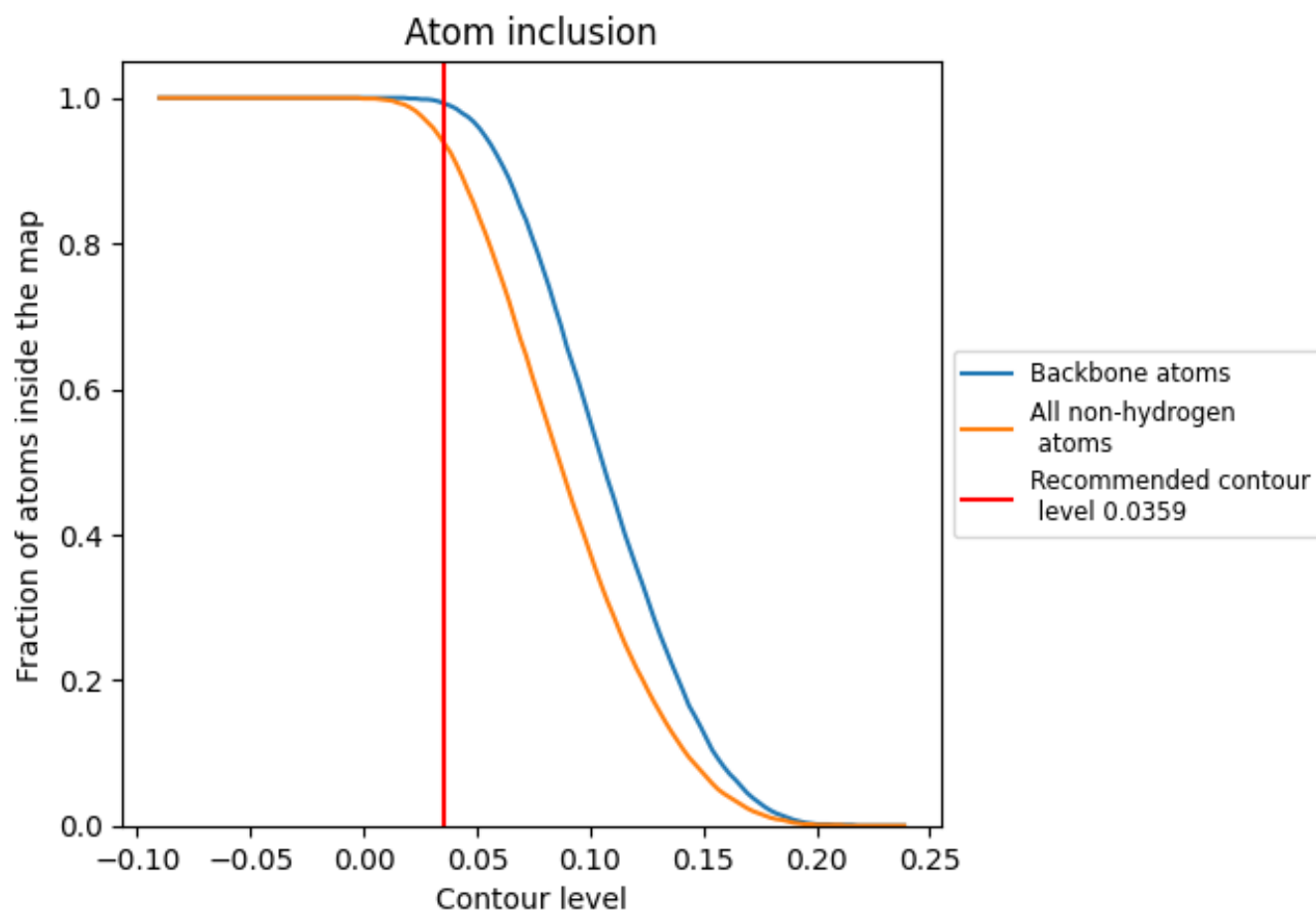
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0359).





9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.4550
A	 0.9360	 0.4550

