



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 6L7E / pdb_00006l7e
EMDB ID : EMD-0843
Title : Toxin Complex TcdA1-TcdB1-TccC2
Authors : Yan, Z.F.; Yang, G.W.
Deposited on : 2019-11-01
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

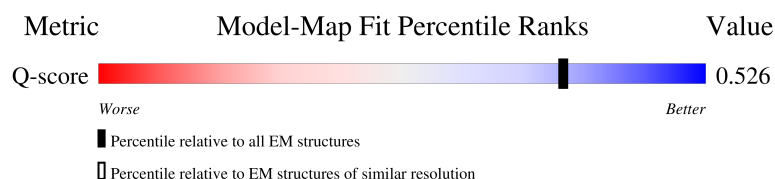
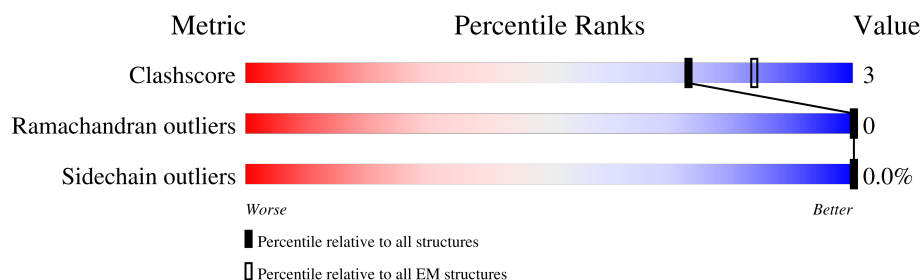
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	2516	 88% 10% .
1	B	2516	 88% 10% .
1	C	2516	 88% 9% .
1	D	2516	 87% 10% .

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	E	2516	 88% 10% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 97400 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

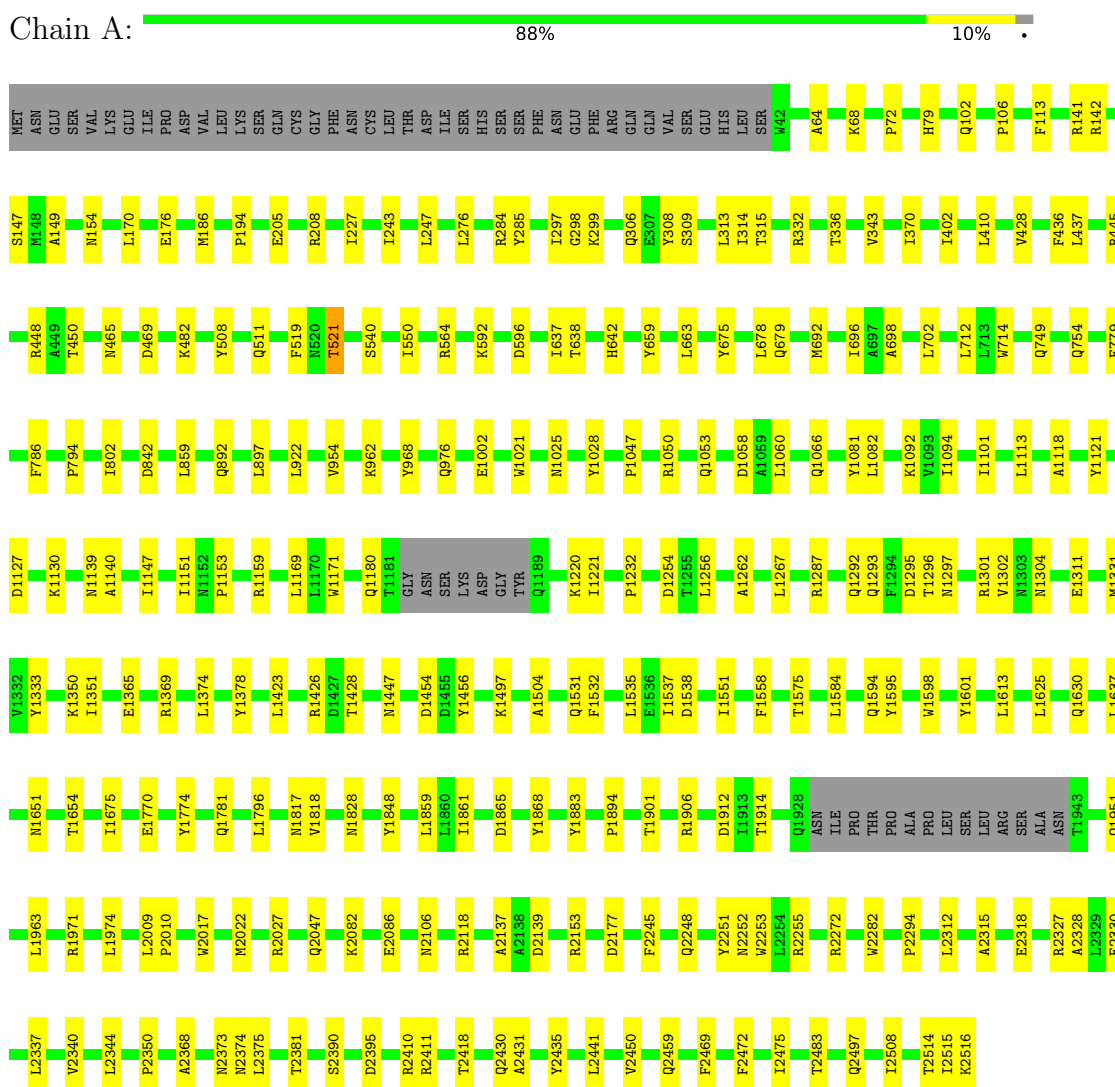
- Molecule 1 is a protein called TcdA1.

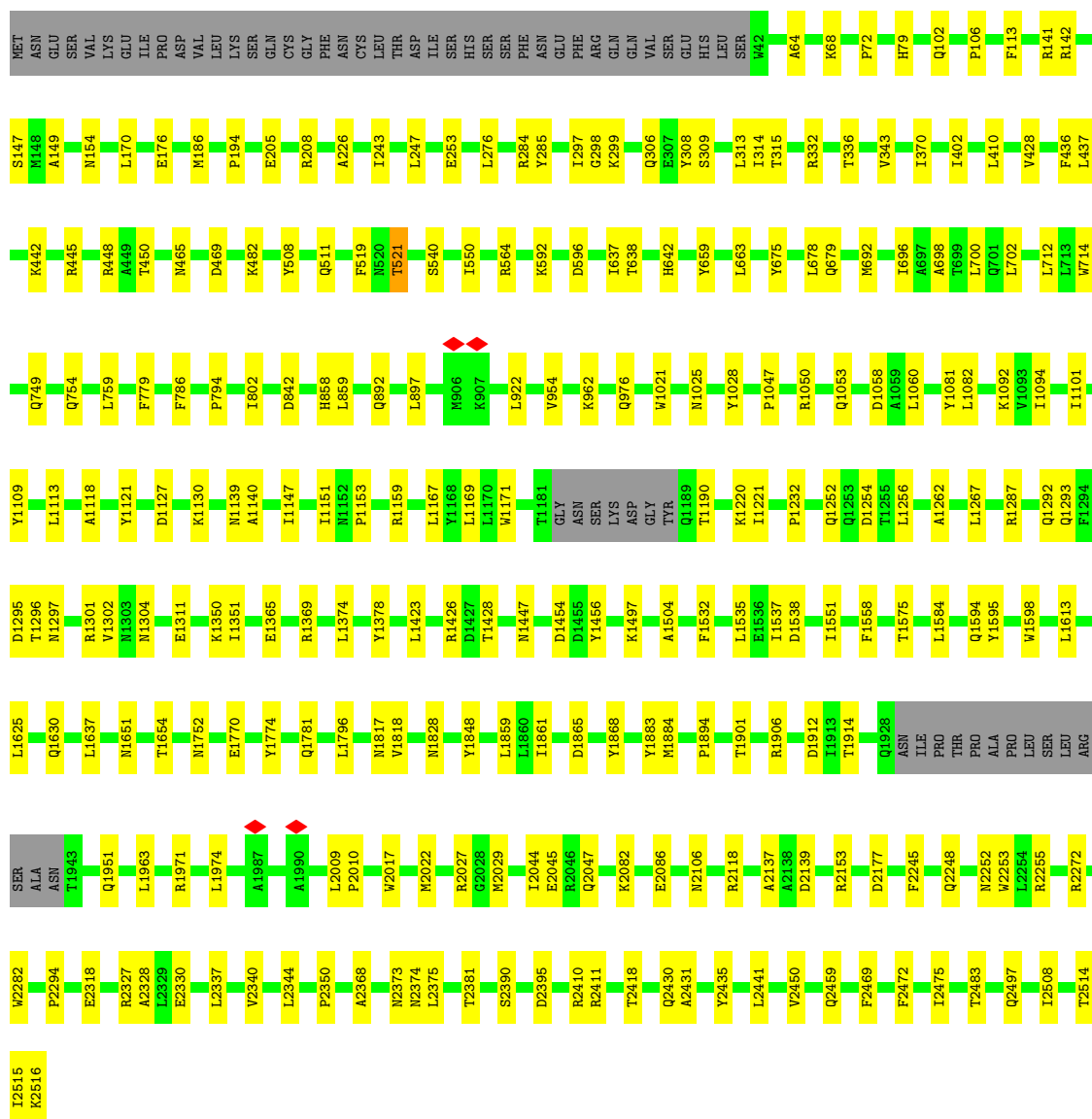
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2454	Total 19480	C 12333	N 3311	O 3775	S 61	0	0
1	B	2454	Total 19480	C 12333	N 3311	O 3775	S 61	0	0
1	C	2454	Total 19480	C 12333	N 3311	O 3775	S 61	0	0
1	D	2454	Total 19480	C 12333	N 3311	O 3775	S 61	0	0
1	E	2454	Total 19480	C 12333	N 3311	O 3775	S 61	0	0

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.

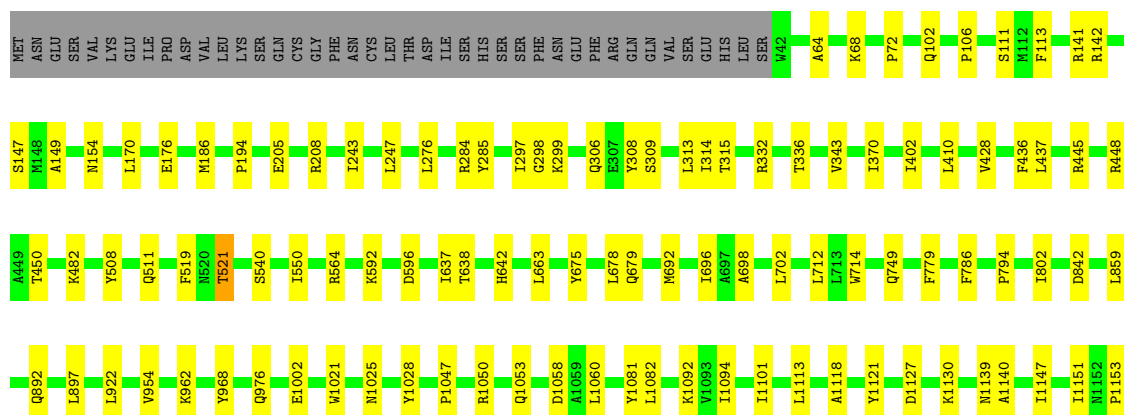
- Molecule 1: TcdA1

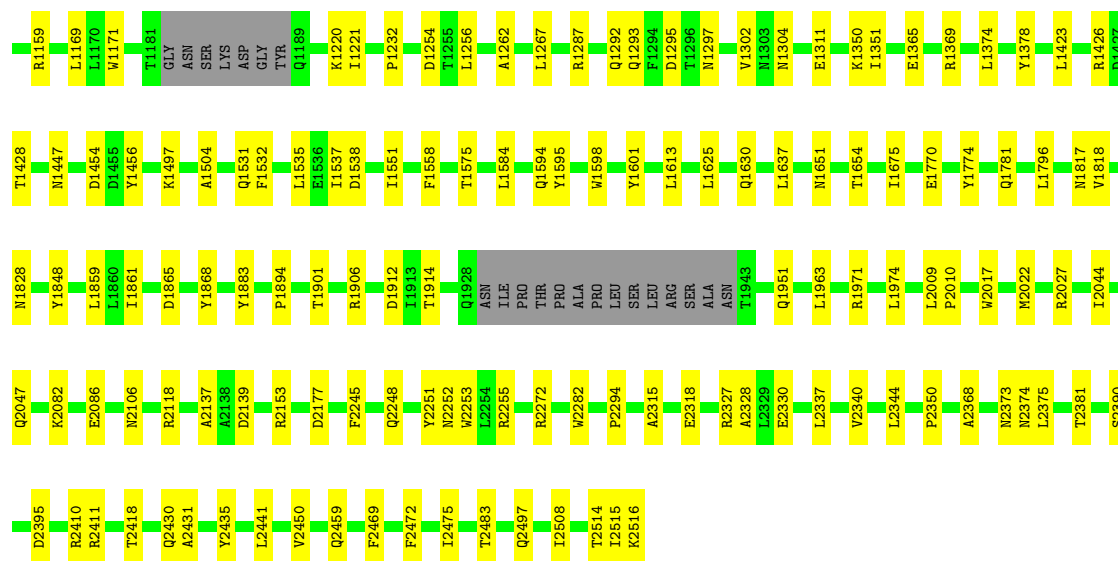




• Molecule 1: TcdA1

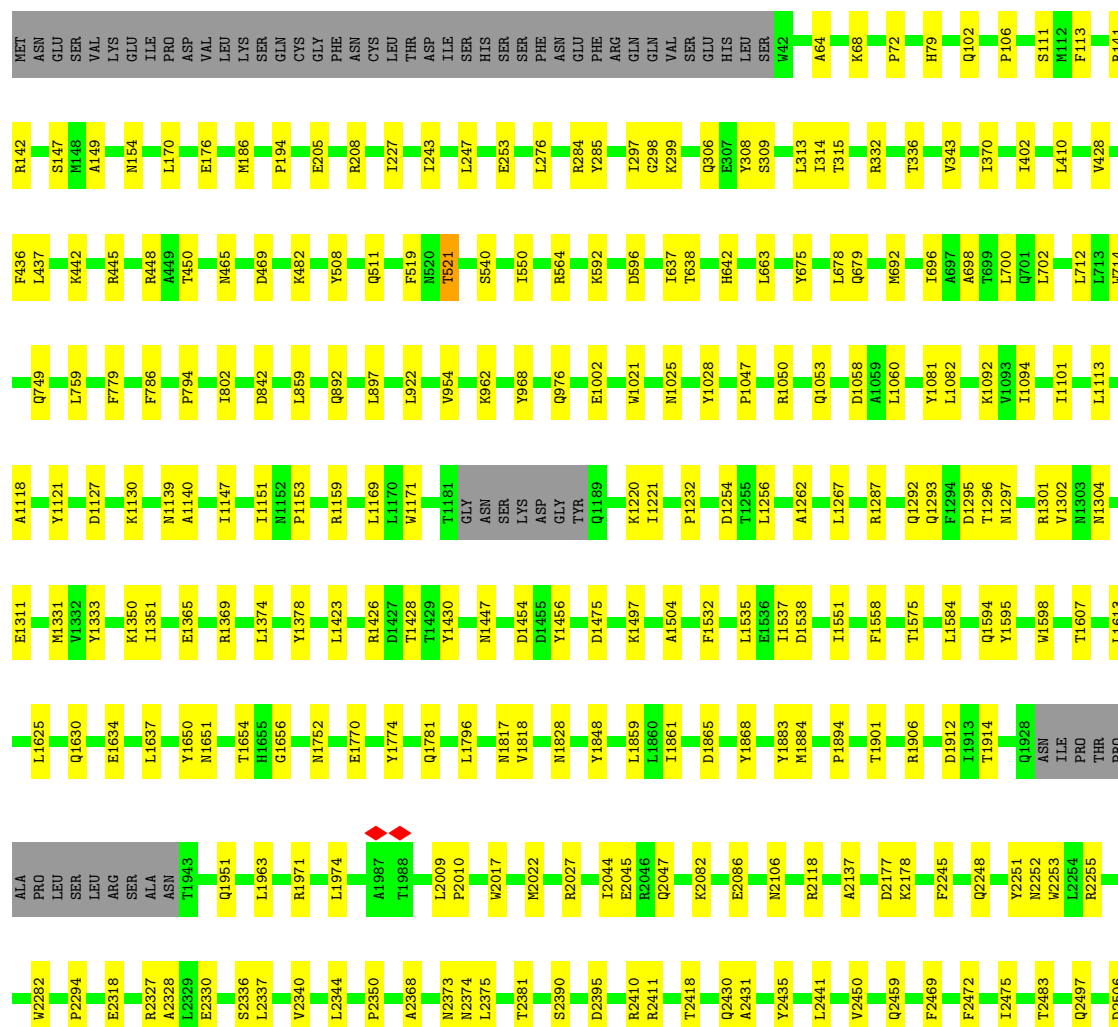
Chain C: 88% 9% •





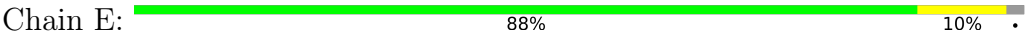
• Molecule 1: TcdA1

Chain D: 87% 10% .



K2507
K2508
T2514
K2515
K2516

● Molecule 1: TcdA1



RET	ASN	GLU	SER	VAL	LYS	GLU	ILE	PRO	ASP	VAL	LEU	LYS	SER	GLN	CYS	GLY	PHE	ASN	CYS	LEU	THR	ASP	ILE	SER	HIS	SER	SER	PHE	ASN	GLU	PHE	ARG	GLN	GLN	VAL	SER	GLU	HIS	LEU	SER	W42	A64	K68	P72	H79	Q102	P106	S111	W112	F113	R141
R142	S147	N148	A149	M154	L170	E176	M186	P194	E205	R208	I243	L247	E253	L276	K283	K284	Y285	S289	T297	G298	K299	Q306	E307	Y308	S309	L313	I314	T315	R332	T336	V343	I370	L402	L410	V428																
F436	L437	K442	R445	R448	A449	T450	K477	K482	C499	Y508	Q511	F519	N520	T521	S540	T550	R564	K592	D596	I637	T638	H642	L663	Y675	L678	Q679	M692	T696	A697	A698	L702	L712	L713	W714																	
Q749	F779	F786	P794	I802	D842	L859	Q892	L897	L922	V954	K962	Q976	E1002	W1021	N1025	Y1028	P1047	R1050	Q1063	D1068	L1060	L1061	S1065	Y1081	L1082	K1092	V1093	I1094	I1101	L1113	A1118																				
Y1121	D1127	K1130	N1139	A1140	I1147	I1151	N1152	P1153	R1159	I1162	L1169	L1170	W1171	T1181	GLY	ASN	SER	LYS	ASP	GLY	TYR	Q1189	D1254	T1255	L1256	A1262	L1267	R1287	Q1292	Q1293	F1294	D1295	T1296	N1297	R1301	V1302	N1303	N1304													
E1311	I1351	E1365	R1369	L1374	Y1378	L1423	R1426	D1427	T1428	N1447	D1454	D1455	Y1456	K1497	A1504	F1532	L1535	E1536	I1537	I1551	F1558	T1575	L1584	Q1594	Y1595	W1598	Y1601	L1613	D1622	L1625	Q1630	E1634	P1635	Q1636																	
L1637	N1651	T1654	I1675	E1770	Y1774	Q1781	L1796	K1797	Y1798	N1817	V1818	M1828	Y1848	L1859	I1860	I1861	D1865	Y1868	Y1883	M1884	P1894	T1901	R1906	D1912	I1913	T1914	Q1928	ASN	ILE	PRO	THR	PRO	ALA	LEU	LEU	ARG	SER	ALA													
ASN	T1943	Q1951	L1963	R1971	L1974	L2009	P2010	W2017	M2022	R2027	G2028	M2029	I2044	E2045	R2046	Q2047	K2082	E2086	N2106	R2118	A2137	A2138	D2139	R2153	D2177	Q2248	N2252	W2253	L2254	R2255	T2261	R2272	W2282	P2294	E2318																
R2327	A2328	L2329	E2330	L2337	V2340	L2344	P2350	A2368	N2373	N2374	L2375	T2381	S2390	D2395	R2410	R2411	T2418	Q2430	A2431	Y2435	L2441	V2450	Q2469	F2469	F2472	T2475	T2483	R2255	T2261	R2272	W2282	P2294	E2318																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.218	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	508.44003, 508.44003, 508.44003	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.18	0/19899	0.46	3/27028 (0.0%)
1	B	0.18	0/19899	0.46	2/27028 (0.0%)
1	C	0.18	0/19899	0.46	2/27028 (0.0%)
1	D	0.18	0/19899	0.46	3/27028 (0.0%)
1	E	0.18	0/19899	0.46	2/27028 (0.0%)
All	All	0.18	0/99495	0.46	12/135140 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
All	All	0	25

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2381	THR	CA-C-N	5.16	131.39	121.54
1	A	2381	THR	C-N-CA	5.16	131.39	121.54
1	C	2381	THR	CA-C-N	5.16	131.39	121.54
1	C	2381	THR	C-N-CA	5.16	131.39	121.54
1	B	2381	THR	CA-C-N	5.13	131.34	121.54

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1598	TRP	Peptide
1	A	2106	ASN	Peptide
1	A	336	THR	Peptide
1	A	521	THR	Peptide
1	A	859	LEU	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	19480	0	19047	142	0
1	B	19480	0	19047	142	0
1	C	19480	0	19047	136	0
1	D	19480	0	19047	146	0
1	E	19480	0	19047	143	0
All	All	97400	0	95235	638	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 3.

The worst 5 of 638 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:714:TRP:HE1	1:A:794:PRO:HB2	1.62	0.65
1:B:714:TRP:HE1	1:B:794:PRO:HB2	1.62	0.64
1:D:714:TRP:HE1	1:D:794:PRO:HB2	1.62	0.63
1:E:714:TRP:HE1	1:E:794:PRO:HB2	1.62	0.63
1:C:714:TRP:HE1	1:C:794:PRO:HB2	1.62	0.63

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	2448/2516 (97%)	2368 (97%)	80 (3%)	0	100	100
1	B	2448/2516 (97%)	2368 (97%)	80 (3%)	0	100	100
1	C	2448/2516 (97%)	2366 (97%)	82 (3%)	0	100	100
1	D	2448/2516 (97%)	2367 (97%)	81 (3%)	0	100	100
1	E	2448/2516 (97%)	2365 (97%)	83 (3%)	0	100	100
All	All	12240/12580 (97%)	11834 (97%)	406 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	2100/2157 (97%)	2099 (100%)	1 (0%)	100	100
1	B	2100/2157 (97%)	2099 (100%)	1 (0%)	100	100
1	C	2100/2157 (97%)	2099 (100%)	1 (0%)	100	100
1	D	2100/2157 (97%)	2099 (100%)	1 (0%)	100	100
1	E	2100/2157 (97%)	2099 (100%)	1 (0%)	100	100
All	All	10500/10785 (97%)	10495 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	THR
1	B	521	THR
1	C	521	THR
1	D	521	THR
1	E	521	THR

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

Mol	Chain	Res	Type
1	E	511	GLN
1	E	852	GLN
1	E	1672	ASN
1	B	2042	ASN
1	B	1700	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

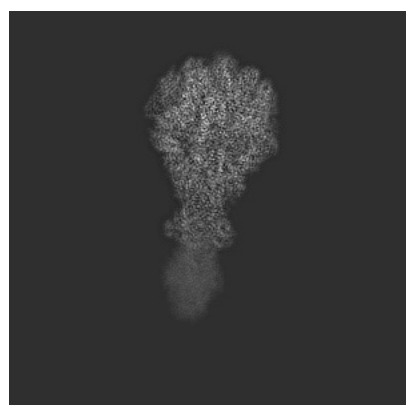
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0843. These allow visual inspection of the internal detail of the map and identification of artifacts.

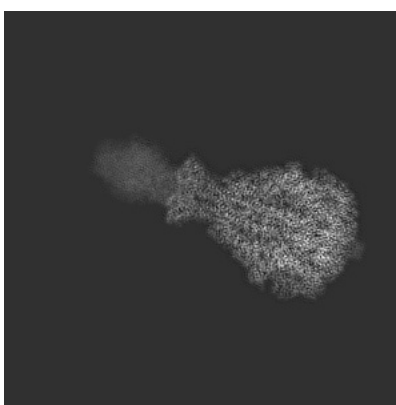
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

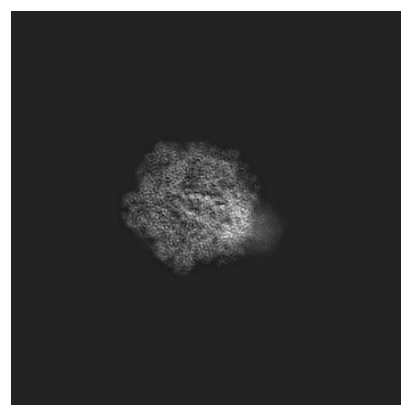
6.1.1 Primary map



X



Y



Z

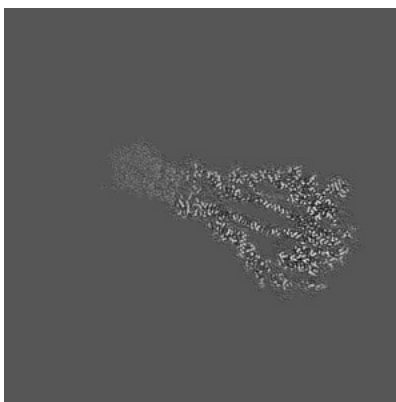
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

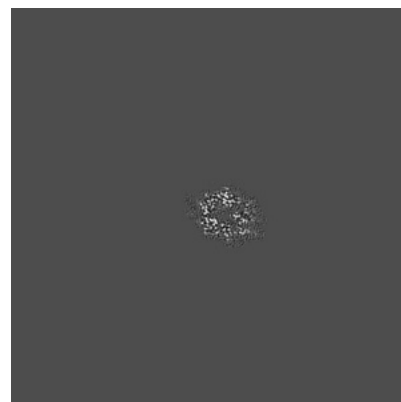
6.2.1 Primary map



X Index: 190



Y Index: 190



Z Index: 190

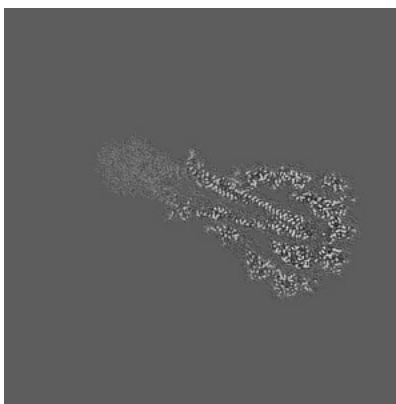
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

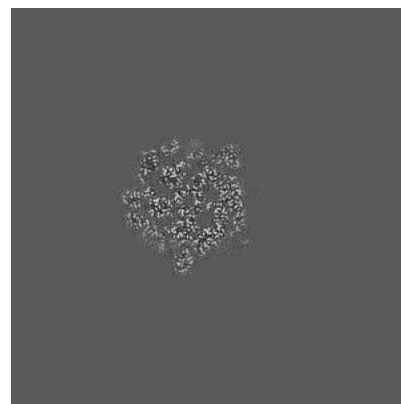
6.3.1 Primary map



X Index: 187



Y Index: 184

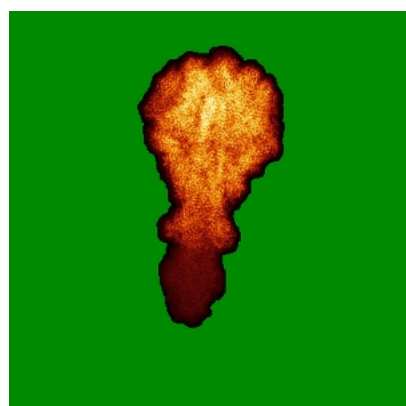


Z Index: 288

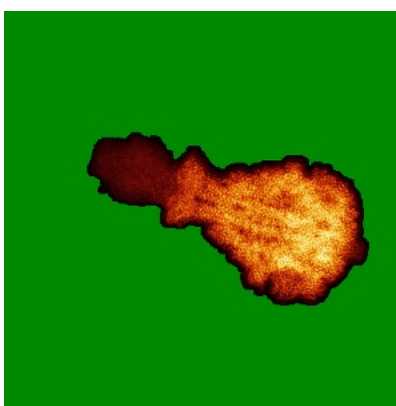
The images above show the largest variance slices of the map in three orthogonal directions.

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

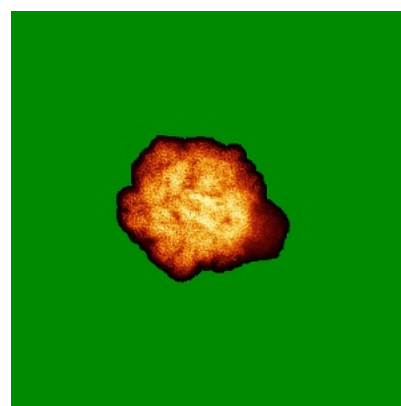
6.4.1 Primary map



X



Y

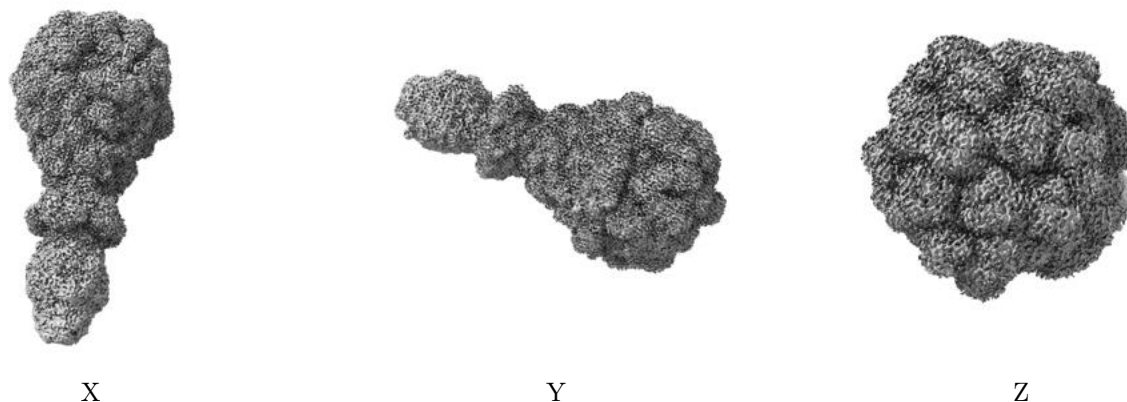


Z

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

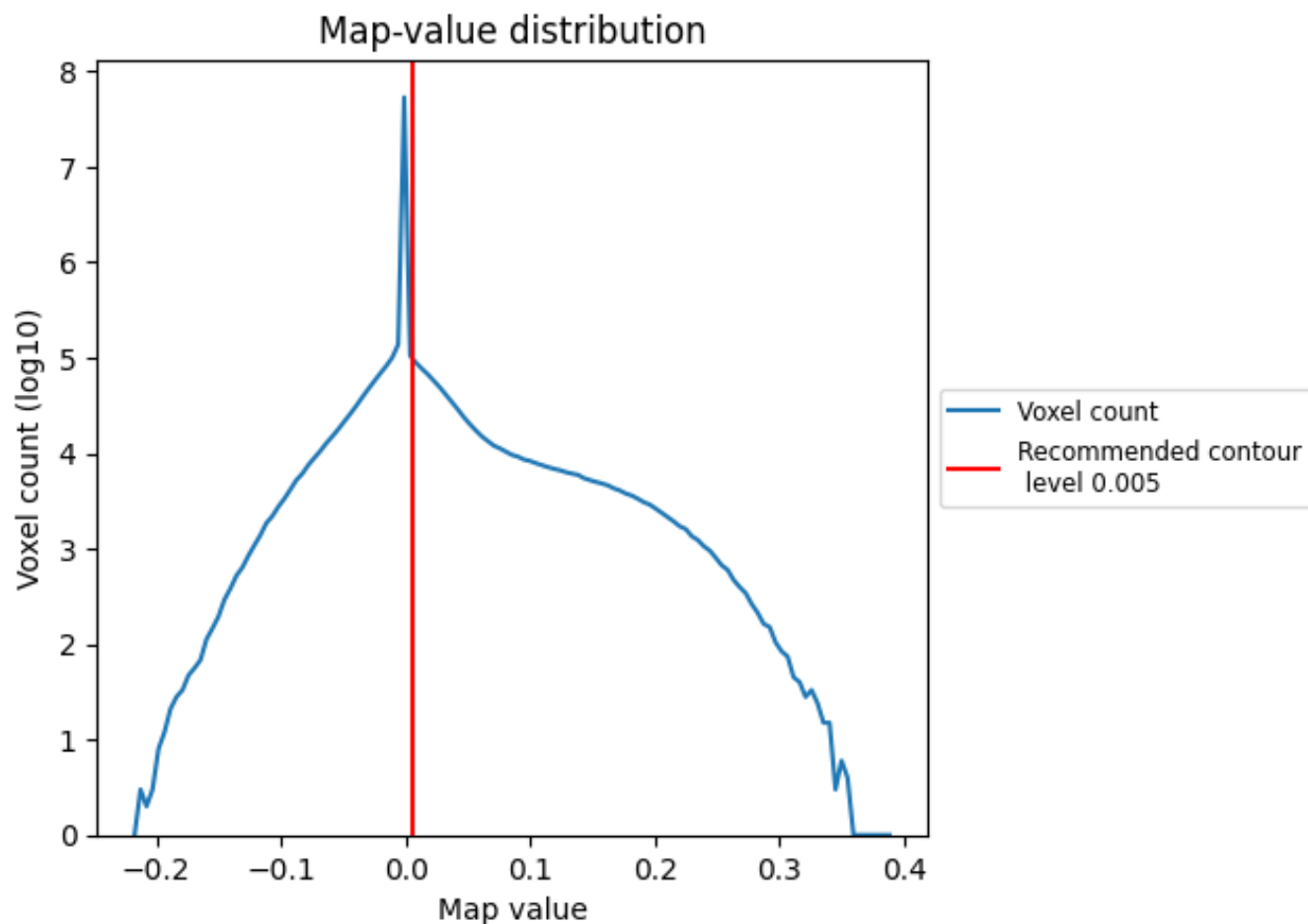
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

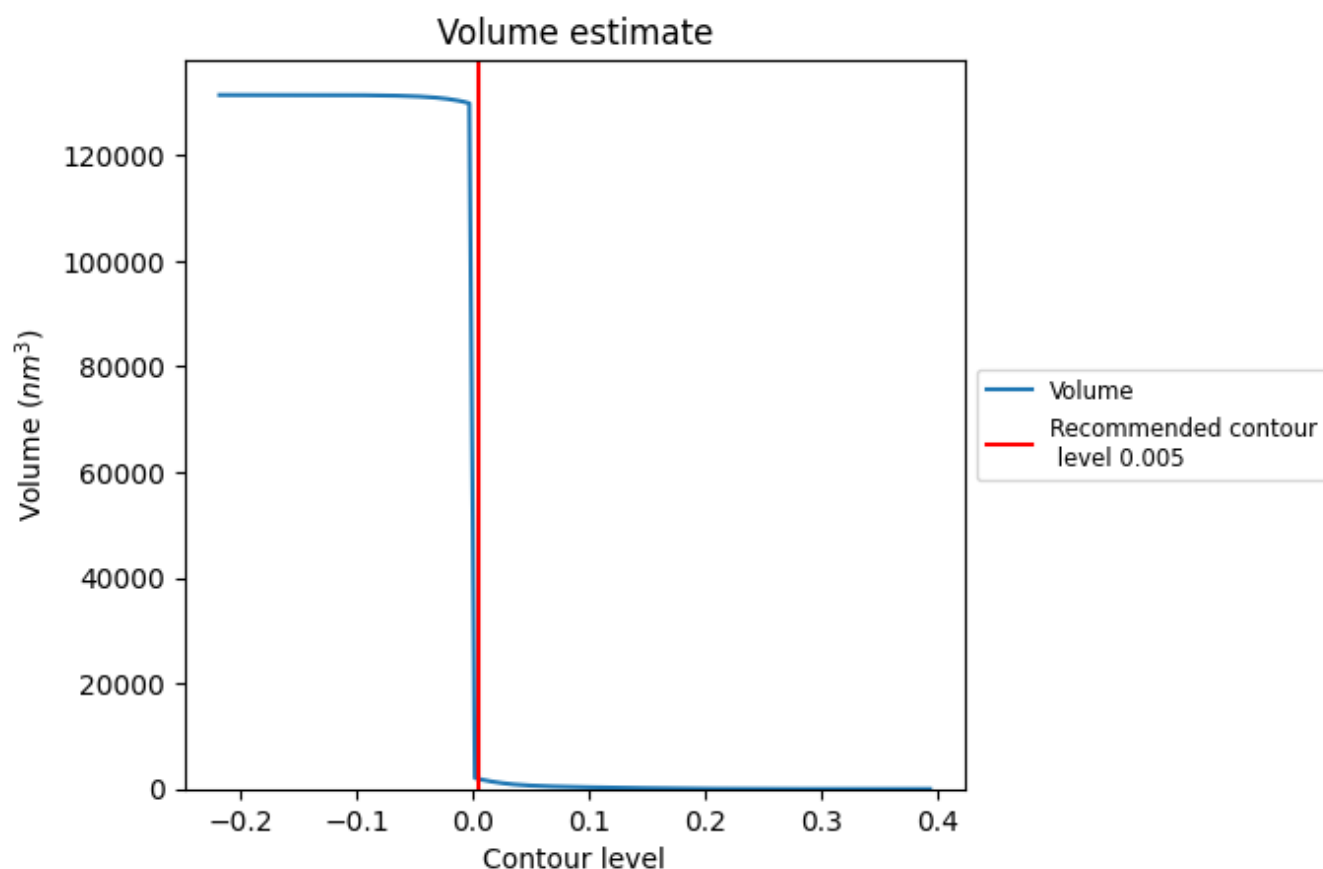
This section contains the results of statistical analysis of the map.

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.

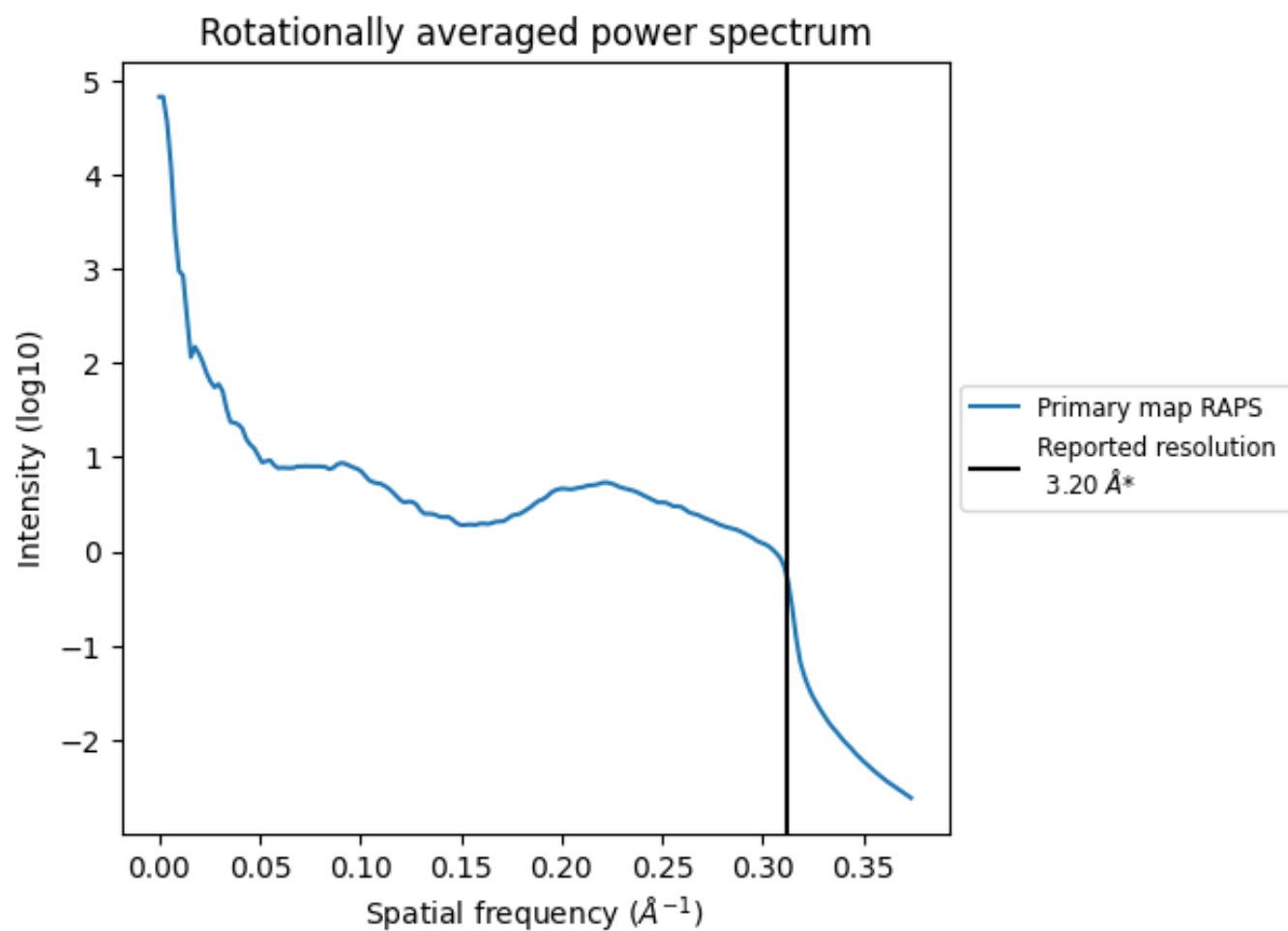
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1916 nm^3 ; this corresponds to an approximate mass of 1731 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 0.312 Å⁻¹

8 Fourier-Shell correlation

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

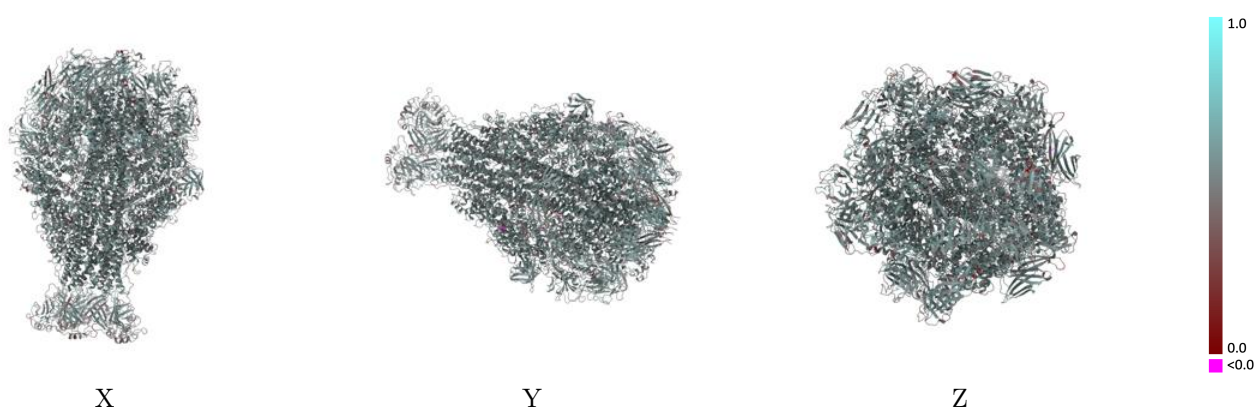
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0843 and PDB model 6L7E. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

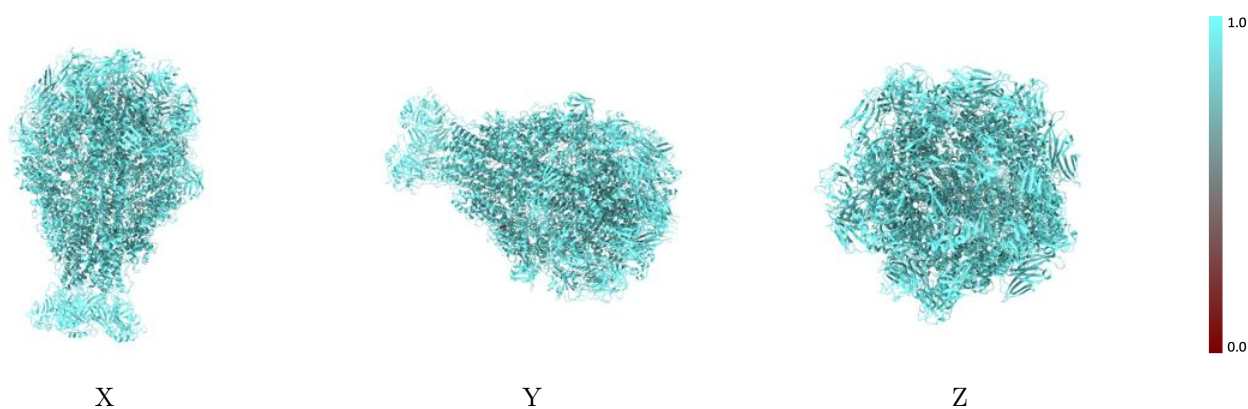
This section was not generated.

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



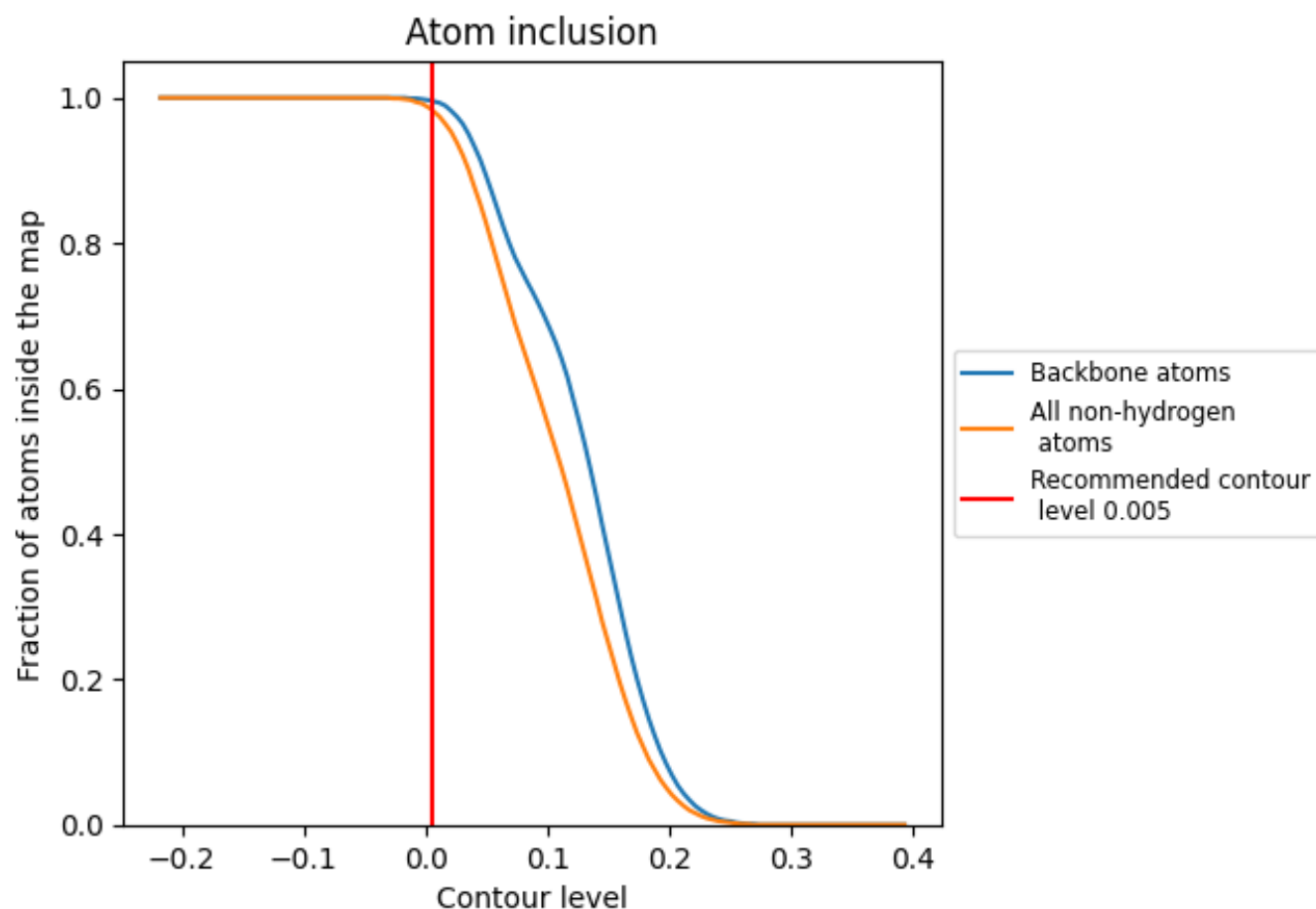
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9840	0.5260
A	0.9870	0.5320
B	0.9810	0.5210
C	0.9850	0.5250
D	0.9830	0.5260
E	0.9830	0.5270

