



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2024 – 04:41 pm GMT

PDB ID : 8CPZ
EMDB ID : EMD-16791
Title : Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K1179W mutant
Authors : Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.
Deposited on : 2023-03-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
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) : 2.36

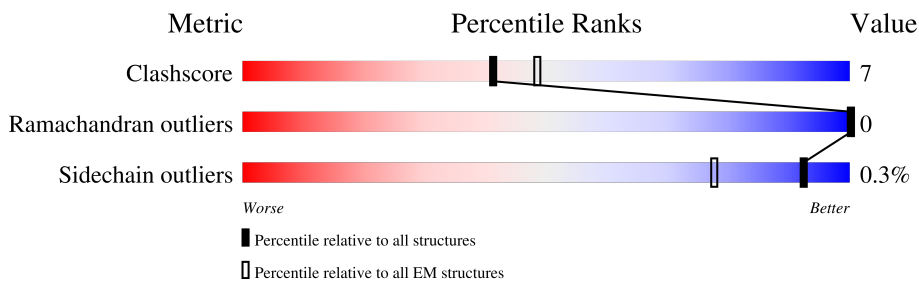
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2535	
1	B	2535	
1	C	2535	
1	D	2535	
1	E	2535	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 84420 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
			Total	C	N	O	S		
1	A	2122	16884	10699	2868	3262	55	0	0
1	B	2122	16884	10699	2868	3262	55	0	0
1	C	2122	16884	10699	2868	3262	55	0	0
1	D	2122	16884	10699	2868	3262	55	0	0
1	E	2122	16884	10699	2868	3262	55	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	1179	TRP	LYS	engineered mutation	UNP Q9RN43

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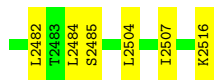
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	1179	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	1179	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
D	-8	GLY	-	expression tag	UNP Q9RN43
D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	1179	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	1179	TRP	LYS	engineered mutation	UNP Q9RN43

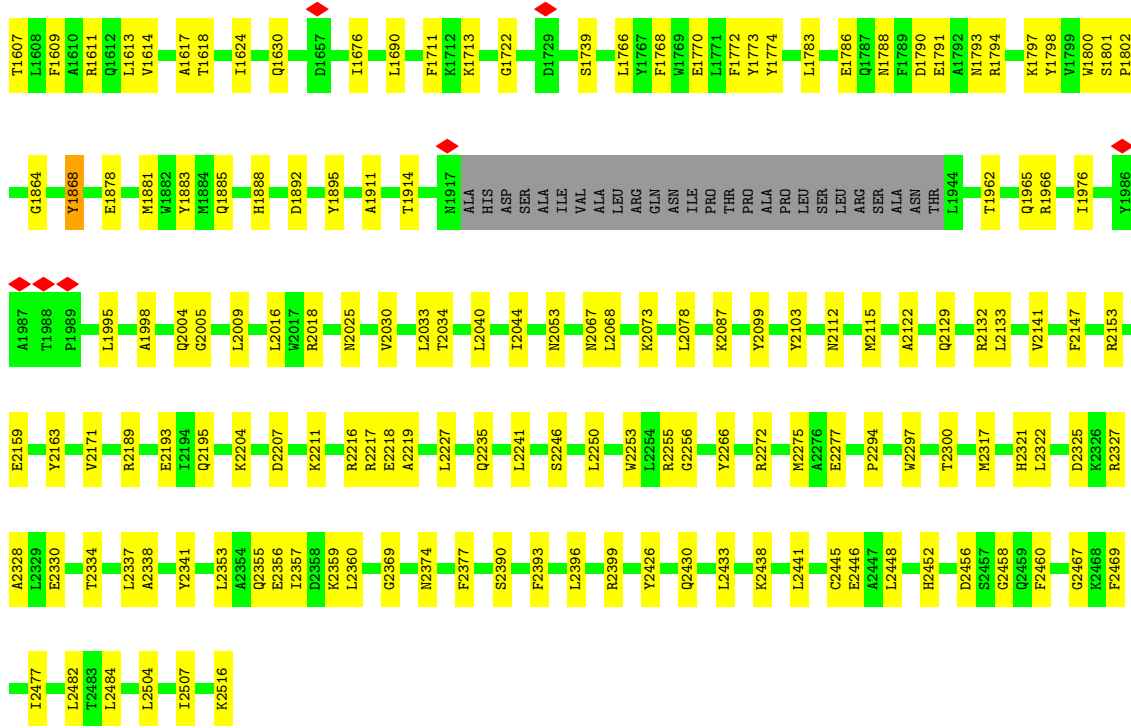
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Y2163	S2188	V2171	R2189	E2193	Q2195	K2204	D2207	K2211	R2218	A2219	L2227	Q2235	L2241	S2246	L2250	W2253	L2254	R2255	G2256	Y2266	R2272	N2275	A2276	E2277	F2294	G2295	A2296	W2297	T2300	N2317	H2321	L2322	D2325	K2326	F2329	R2327												
Q2004	G2005	L2009	L2016	W2017	R2018	N2025	V2030	L2033	T2034	L2040	L2044	N2053	T2066	N2067	L2068	K2073	L2078	K2087	D2097	S2098	Y2099	Y2103	N2112	M2115	A2122	G2123	L2124	V2128	Q2129	R2132	L2133	V2141	F2147	R2153	E2159													
W1882	Y1883	W1884	Q1885	H1888	D1892	Y1895	A1911	N1917	ALA	HIS	ASP	SER	ALA	VAL	ALA	LEU	ARG	GLN	ASN	PRO	THR	PRO	PRO	ALA	L1944	T1962	Q1965	R1966	I1976	I1985	Y1986	A1987	T1988	P1989	A1990	L1995	A1998											
A1617	T1618	I1624	Q1630	D1657	I1676	L1690	F1711	K1712	K1713	G1722	D1729	S1739	L1766	F1767	W1769	E1770	F1772	Y1773	Y1774	R1782	L1783	E1786	Q1787	N1788	F1789	D1790	E1791	A1792	N1793	R1794	K1797	Y1798	Y1799	W1800	S1801	P1802	G1864	Y1868	E1878	M1881								
ALA	LEU	GLU	ILE	ASP	GLY	SER	GLY	LEU	ASN	PHE	ILE	ASN	ASN	THR	PHE	ALA	ALA	GLU	ASP	GLY	ARG	LYS	LEU	GLY	TYR	PHE	SER	ILE	PRO	VAL	THR	D1581	L1605	N1606	T1607	L1608	F1609	A610	R1611	Q1612	L1614	V1614						
THR	ASP	SER	LYS	GLY	THR	ALA	VAL	THR	PRO	ALA	LYS	VAL	GLN	ILE	ILE	VAL	VAL	GLY	GLY	LYS	GLU	GLN	THR	PHE	THR	ALA	ALA	LYS	ASP	VAL	THR	ALA	THR	PRO	PRO	PHE	ASP	GLU	ASP	MET	ASN	TYR	GLN	TYR	PHE	ASN		
THR	SER	GLY	LEU	ASN	ARG	HIS	ASP	ASN	LEU	GLY	THR	ASP	GLY	VAL	THR	GLY	GLY	VAL	THR	LEU	THR	THR	THR	PHE	ILE	VAL	VAL	ASP	ASP	THR	THR	ASN	GLN	LEU	MET	PHE	TYR	ALA	ALA	SER	VAL	VAL	TYR	GLN	TYR	ILE	THR	
SER	PRO	LYS	LEU	ARG	HIS	ASN	ASN	LYS	THR	ASP	THR	THR	GLN	THR	VAL	THR	GLY	GLY	VAL	THR	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
A1118	G1119	E1120	R1124	H1128	S1142	E1143	W1144	H1145	K1146	I1147	I1162	Y1163	K1164	S1165	R1166	L1167	Y1168	L1169	K1175	T1178	T1181	GLY	ASN	SER	GLY	ASP	GLY	TYR	THR	LEU	GLY	VAL	L1200	K1220	R1230	C1236	Y1239	E1242	D1243	T1244	L1245	L1246	N1251	Q1252	L1267	Y1268		
S941	T948	Q969	Y970	L971	L972	L973	K982	R989	A1000	L1001	T1005	E1005	T1013	Y1024	T1030	Y1034	T1048	M1049	R1050	Q1053	M1056	Y1057	D1058	A1059	L1060	L1061	Q1062	L1069	N1070	A1071	D1072	T1073	Y1081	Y1093	H1098	D1099	N1100	T1108	L1113	D1117								
W714	Q719	A724	F730	W733	L734	G741	V746	E747	T748	Q749	E750	H751	I752	W753	Q754	A758	L762	E763	S768	E784	T790	D797	A798	V811	N812	L822	L830	L835	A836	D842	L846	Q848	L922	L926	Q930	L938												
S463	V464	I470	N471	V474	V478	Y483	R487	I490	E493	T494	A495	L496	L497	Q505	R506	S507	N510	S513	R517	I518	F519	P522	D533	E534	E535	I536	D537	L538	N539	S540	R547	R553	I557	V560	S561	R564	L566	R567	I568	T569								
K577	I578	K579	N580	N581	L582	N587	Y589	L593	I597	T601	E604	D605	D606	V612	M635	T636	I637	W646	Y659	K661	L663	L670	L671	L678	L689	M692	A693	P694	A698	T699	L702	S703	S704	E705	A708	V711	L712	L713										



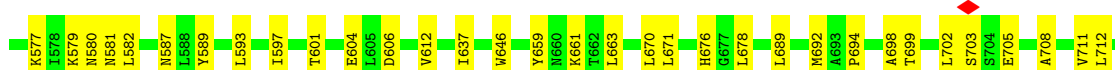
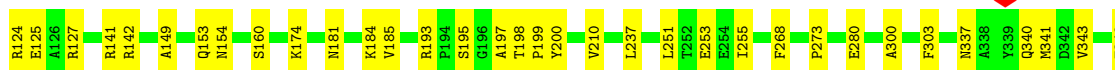
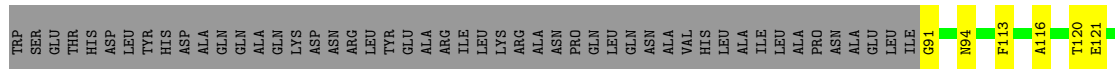
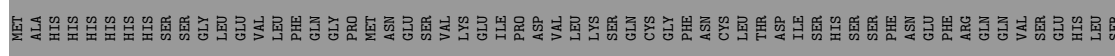
● Molecule 1: TcdA1

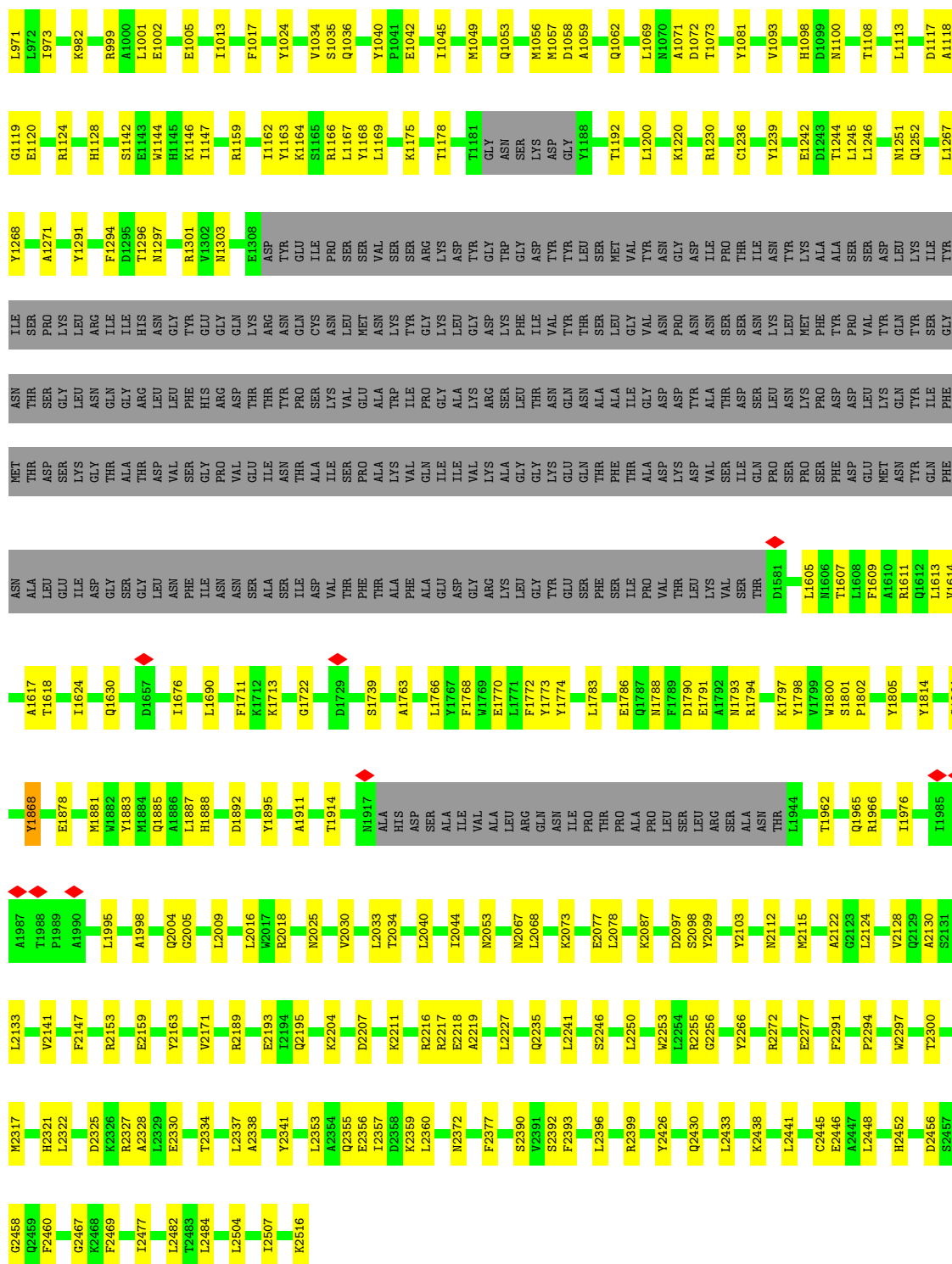


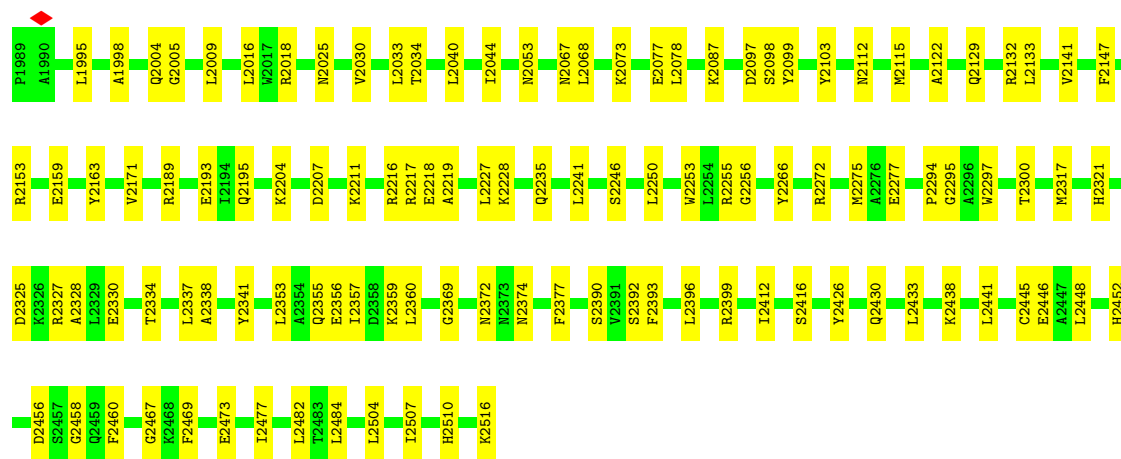
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TRP	SER	GLU	THR	HIS	HIS	ASP	LEU	TYR	HIS	THR	ALA	GLN	ALA	ALA	GLN	LYS	ASN	ASN	ARG	LEU	TYR	GLU	GLU	ALA	ILE	LEU	LEU	ARG	ARG	LEU	ASN	ASN	LEU	ALA	ILE	ILE	LEU	ALA	PRO	ALA	ILE	LEU	LEU	GLN	ASP	ARG	GLN	VAL	VAL	GLN	GLU	GLU	LEU	LEU	LEU	SER
R124	R127	R357	R358	F359	R141	R142	Q153	M154	S160	K174	M181	K184	V185	S195	G196	A197	T198	P199	Y200	V210	L237	L251	T252	E253	L255	T256	E257	F288	P273	E280	K283	L293	A300	F303	N337	F113	A338	Y339	Q340	M341	F348															
N352	Y357	F359	N364	L368	S369	L370	K371	D374	E377	L378	V379	R380	T381	E382	N388	Y391	L397	F406	E407	L410	T411	R412	P415	S416	G417	S418	Y421	K425	Y431	Y434	L438	M441	K442	R445	L446	S453	L456																			
E458	G459	V461	V464	T470	M471	V474	V478	T481	K482	Y483	T490	T494	A495	L496	I497	N500	Q505	R506	S507	N510	S513	F519	P522	D533	E534	E535	L536	D537	N539	S540	R547	R553	I557	S561	R564	L566																				
V567	L568	T569	K577	K578	N580	N581	L582	N587	N588	V589	L593	I597	T601	E604	L605	D606	V612	L627	I637	W646	Y659	L663	L670	L671	H676	G677	L678	L689	M692	A693	P694	Y695	A698	T699	L702	S703	S704	E705	A708																	
V711	L712	L713	W714	Q719	A724	K729	F730	W733	L734	G741	W746	E747	I748	Q749	L1001	E1002	E1005	I1013	Y1024	E763	S768	I790	D797	A798	V811	N812	L822	L830	A693	L835	A836	D842	L845	L846	L847	Q848	V881																			
L922	L926	Q930	S941	T948	Q969	F730	L971	L972	I973	K982	L986	R999	L1001	E1002	E1005	I1013	Y1024	E763	S768	I790	D797	A798	V811	N812	L822	L830	A693	L835	A836	D842	L845	L846	L847	Q848	V881																					
H1098	D1099	M1100	T1108	L1113	D1117	A1118	G1119	E1120	R1124	H1128	K1135	S1142	E1143	W1144	H1145	K1146	I1147	R1159	I1162	Y1163	K1164	S1165	R1166	L1167	Y1168	L1169	K1175	T1178	W1179	Q1180	T1181	GLY	ASN	SER	LYS	ASP	GLY	ASN	ASN	GLY	T1192	L1200	L1200	K1220	R1250	C1236										
T1244	L1245	M1251	Q1252	L1267	Y1268	A1271	Y1291	F1294	D1295	T1296	M1297	R1301	V1302	M1303	E1308	ASP	TYR	GLU	ILE	PRO	ILE	PRO	LEU	LYS	TRP	TRP	GLY	ASP	TRP	GLY	ASP	TYR	VAL	VAL	VAL	VAL	TYR	LEU	SER	MET	LYS	ASP	ASP	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP				
ALA	SER	ASP	LEU	ASP	ASN	GLN	LEU	ILE	TYR	ASN	ILE	GLN	GLY	ILE	ARG	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN		
TYR	PRO	VAL	TYR	GLN	GLN	GLY	TYR	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN			
ASP	ASP	LEU	GLN	TYR	ILE	PHE	ASP	MET	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP		
PHE	ASP	GLU	MET	TYR	GLN	PHE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
D1561	L1605	N1606																																																						



• Molecule 1: TcdA1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	230785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	425.92, 425.92, 425.92	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	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	0.27	0/17247	0.51	0/23428
1	B	0.27	0/17247	0.51	0/23428
1	C	0.27	0/17247	0.51	0/23428
1	D	0.27	0/17247	0.51	0/23428
1	E	0.26	0/17247	0.51	0/23428
All	All	0.27	0/86235	0.51	0/117140

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	16884	0	16507	277	0
1	B	16884	0	16507	280	0
1	C	16884	0	16507	275	0
1	D	16884	0	16507	277	0
1	E	16884	0	16507	280	0
All	All	84420	0	82535	1241	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 7.

The worst 5 of 1241 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:B:689:LEU:HD11	1:B:712:LEU:HB3	1.62	0.82
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.46	0.81
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.61	0.81
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.62	0.81
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.45	0.81

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	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	B	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	C	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	D	2114/2535 (83%)	2065 (98%)	49 (2%)	0	100	100
1	E	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
All	All	10570/12675 (83%)	10329 (98%)	241 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1816/2173 (84%)	1811 (100%)	5 (0%)	92	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1816/2173 (84%)	1811 (100%)	5 (0%)	92	98
1	C	1816/2173 (84%)	1811 (100%)	5 (0%)	92	98
1	D	1816/2173 (84%)	1811 (100%)	5 (0%)	92	98
1	E	1816/2173 (84%)	1811 (100%)	5 (0%)	92	98
All	All	9080/10865 (84%)	9055 (100%)	25 (0%)	92	98

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2430	GLN
1	D	1965	GLN
1	E	2430	GLN
1	D	1868	TYR
1	D	2399	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	892	GLN
1	E	852	GLN
1	C	969	GLN
1	D	969	GLN
1	C	892	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](#)

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-16791. These allow visual inspection of the internal detail of the map and identification of artifacts.

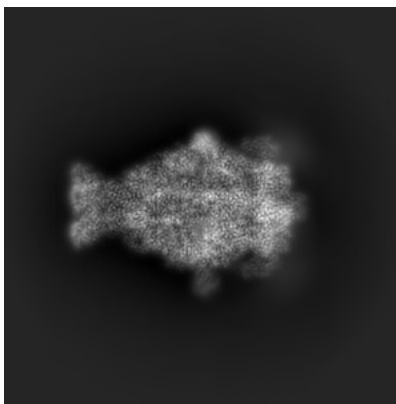
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

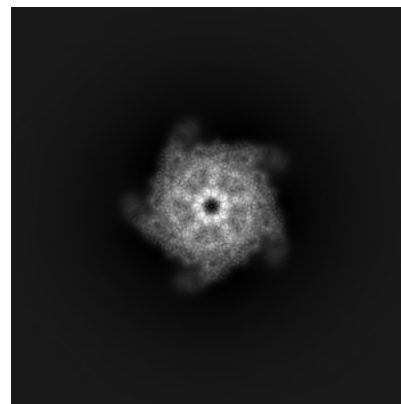
6.1.1 Primary map



X

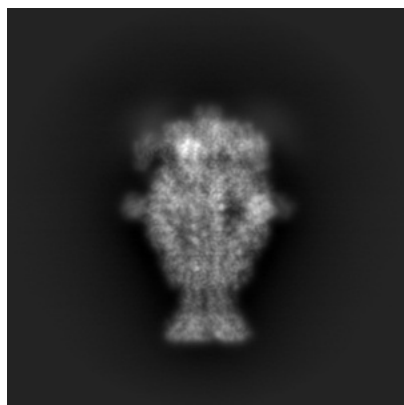


Y

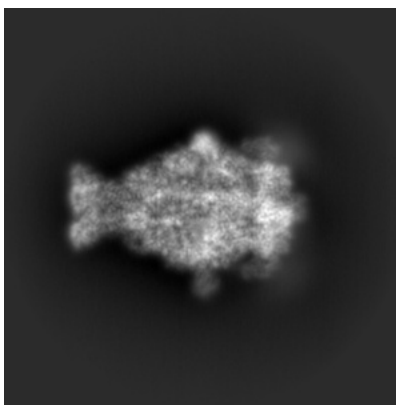


Z

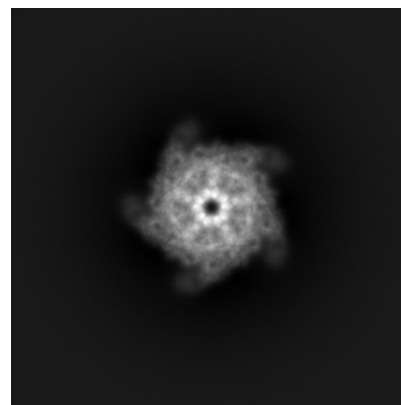
6.1.2 Raw map



X



Y



Z

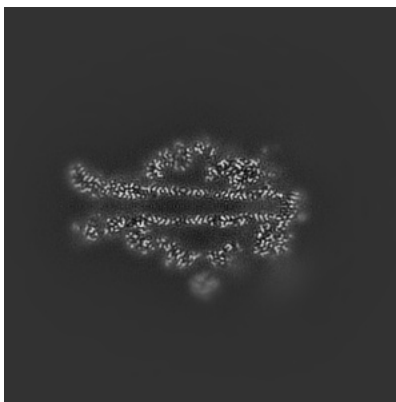
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

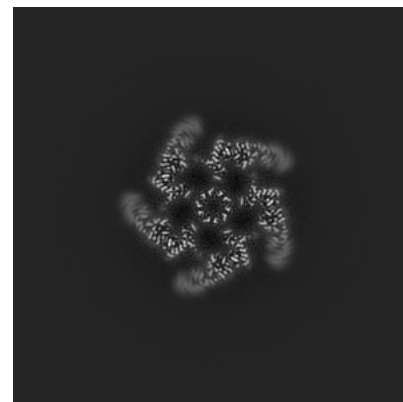
6.2.1 Primary map



X Index: 176

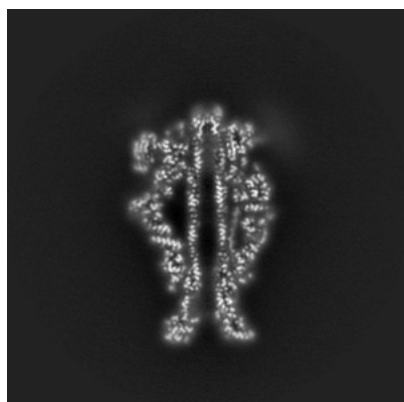


Y Index: 176

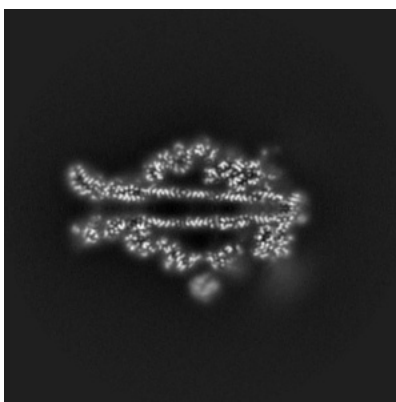


Z Index: 176

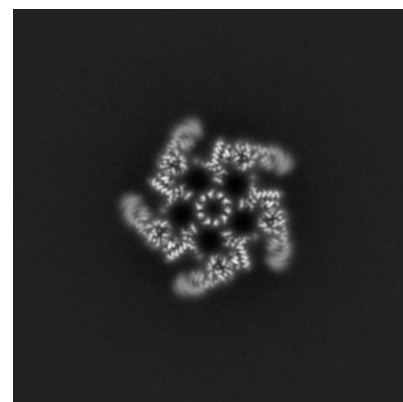
6.2.2 Raw map



X Index: 176



Y Index: 176

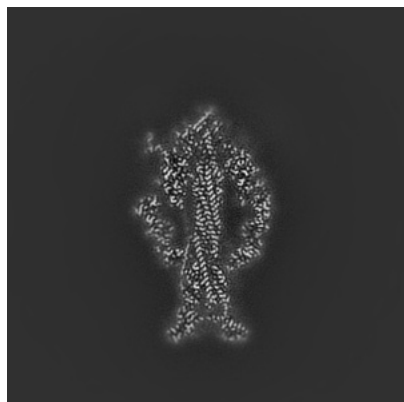


Z Index: 176

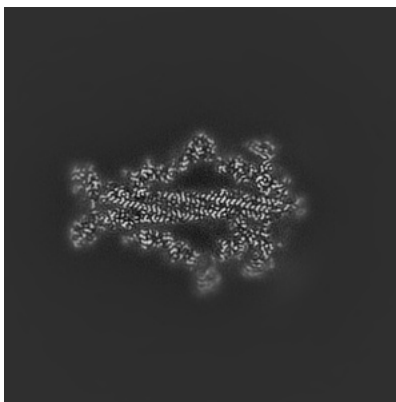
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

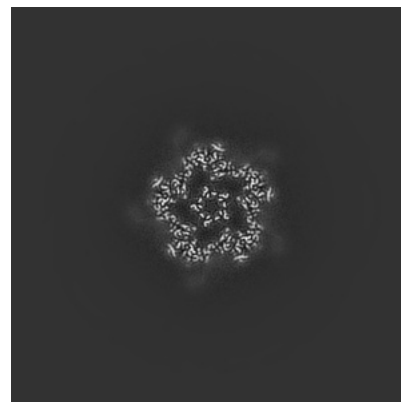
6.3.1 Primary map



X Index: 187

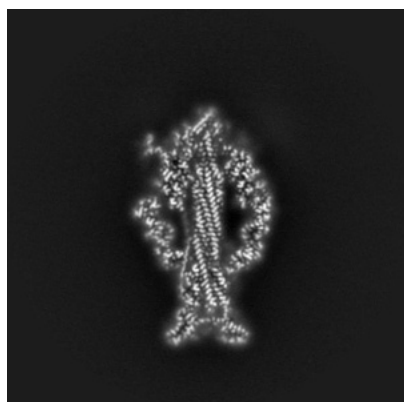


Y Index: 166

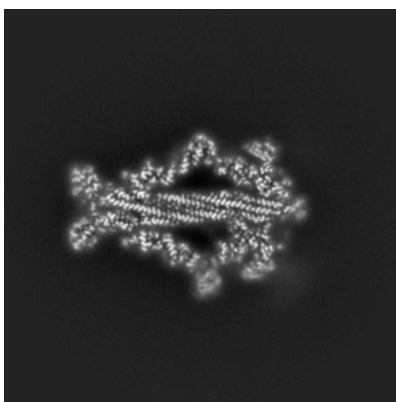


Z Index: 192

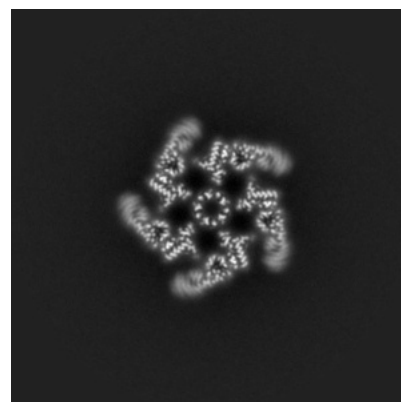
6.3.2 Raw map



X Index: 187



Y Index: 166

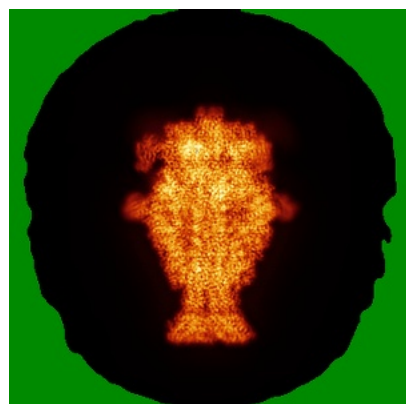


Z Index: 177

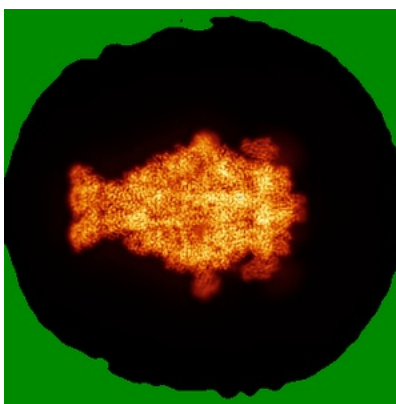
The images above show the largest variance slices of the map in three orthogonal directions.

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

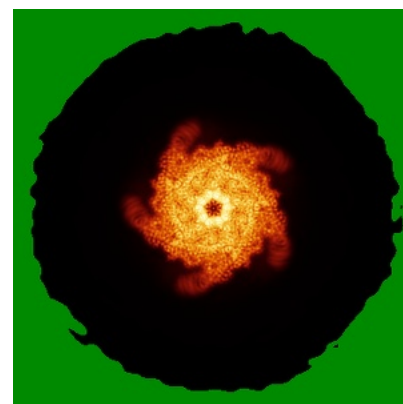
6.4.1 Primary map



X



Y

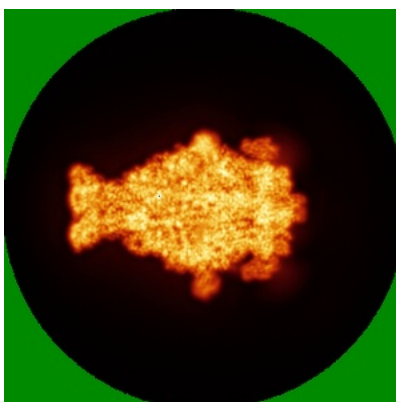


Z

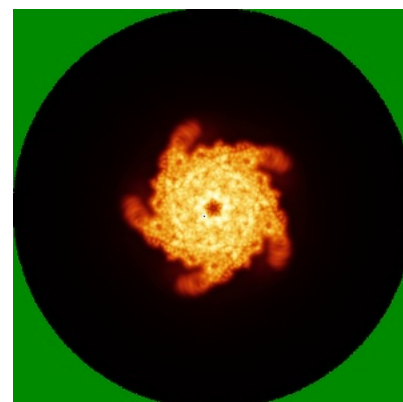
6.4.2 Raw map



X



Y

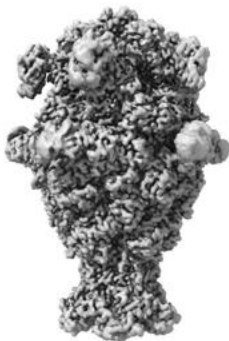


Z

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](#)

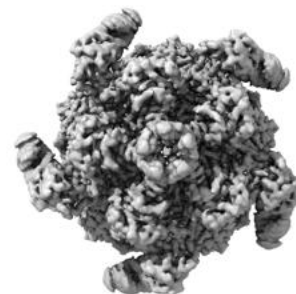
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

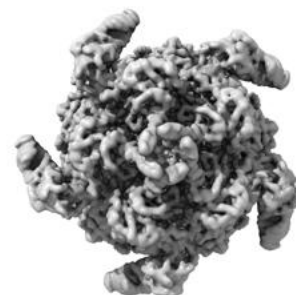
6.5.2 Raw map



X



Y



Z

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.

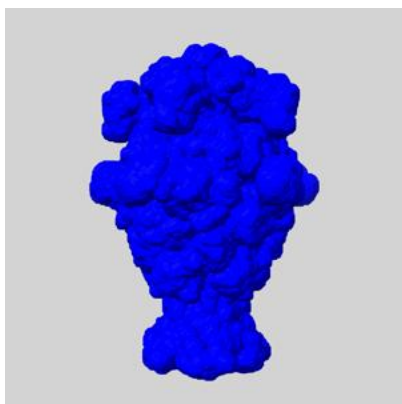
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

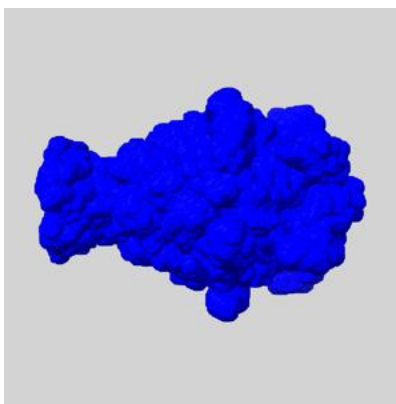
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

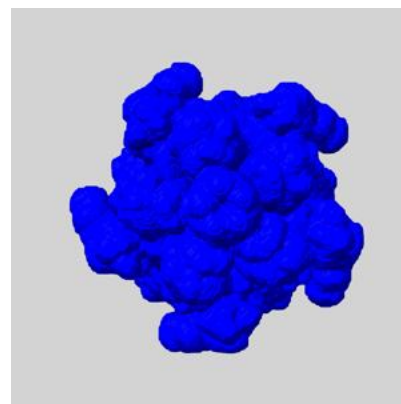
6.6.1 emd_16791_msk_1.map [i](#)



X



Y

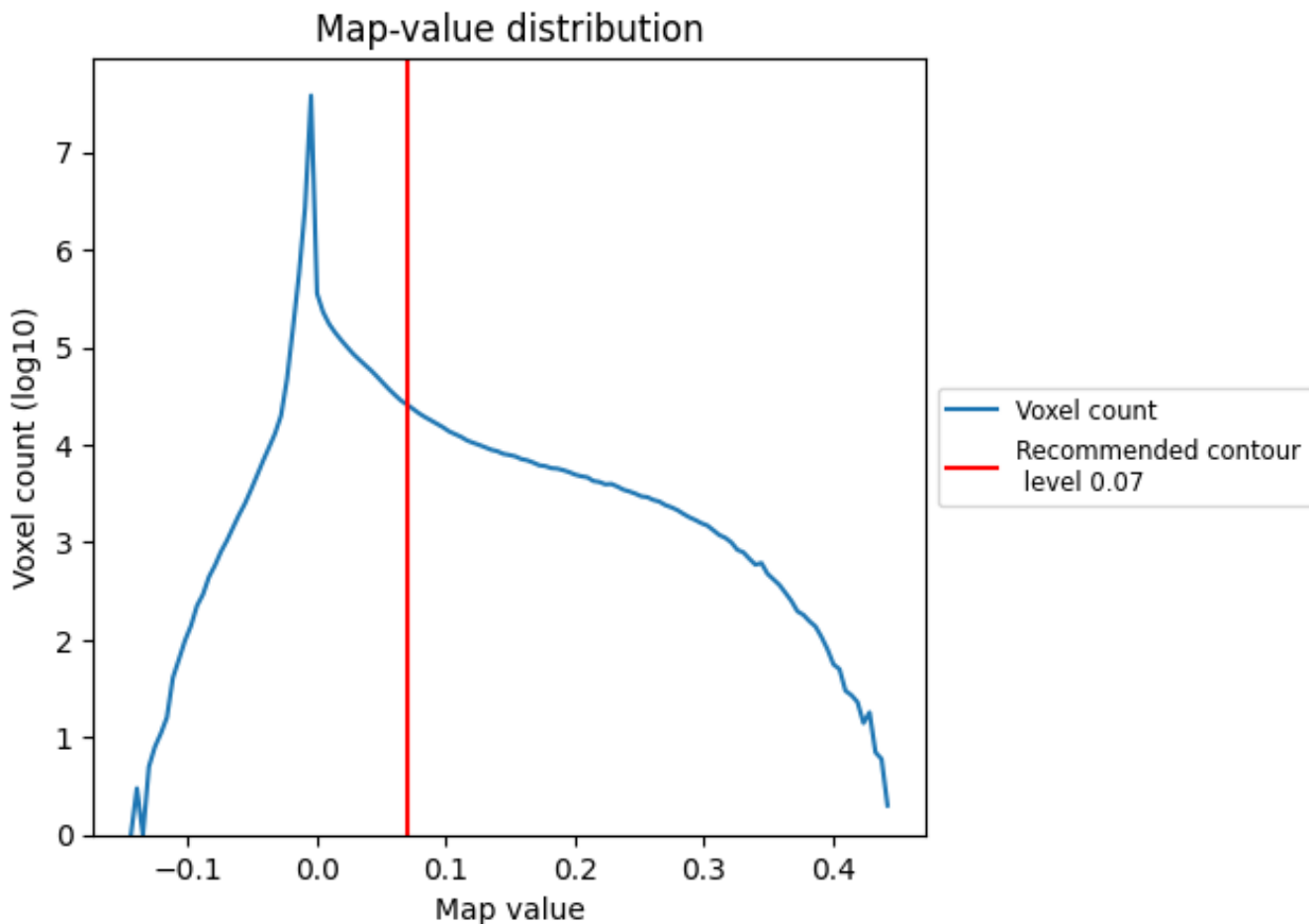


Z

7 Map analysis [i](#)

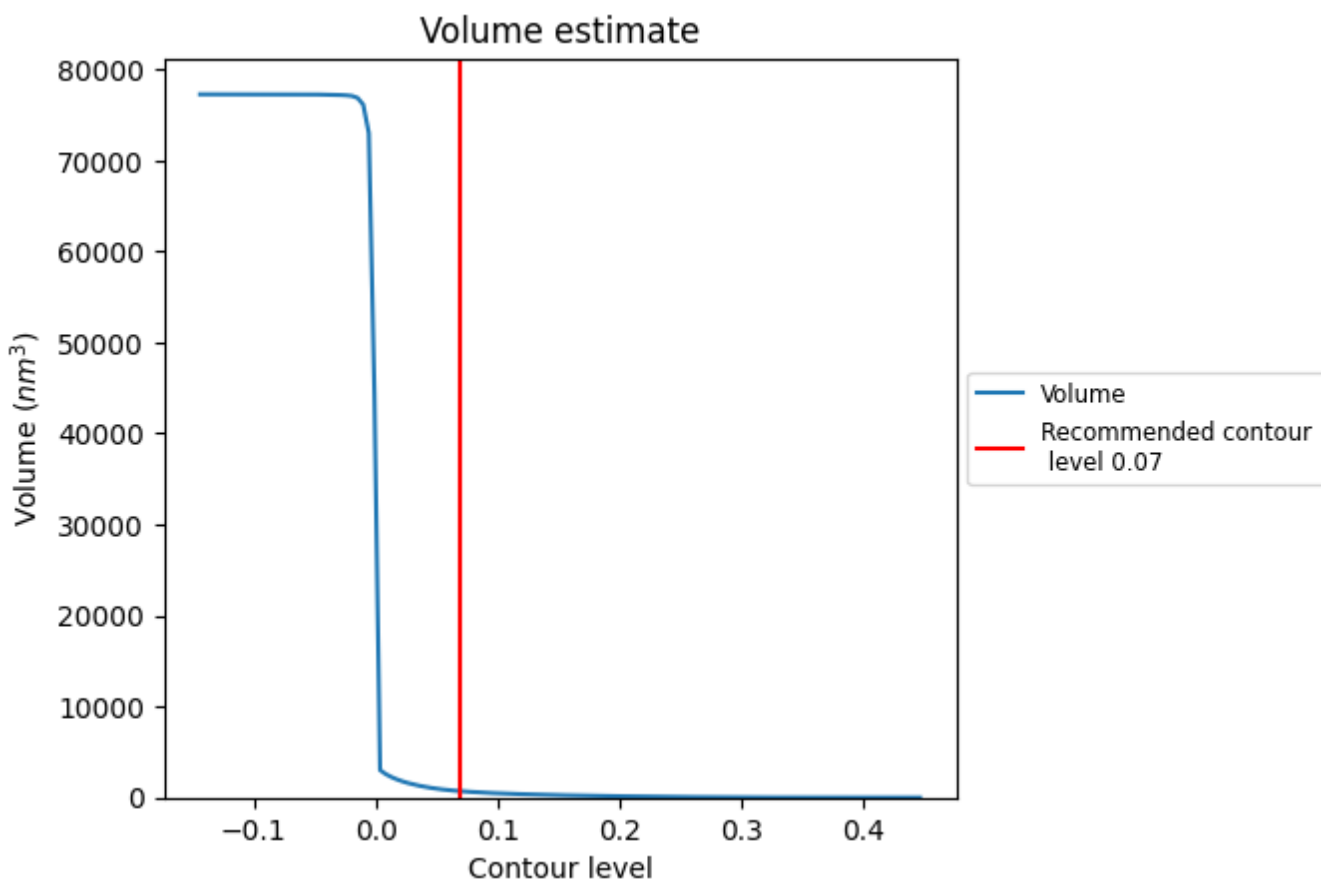
This section contains the results of statistical analysis of the map.

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.

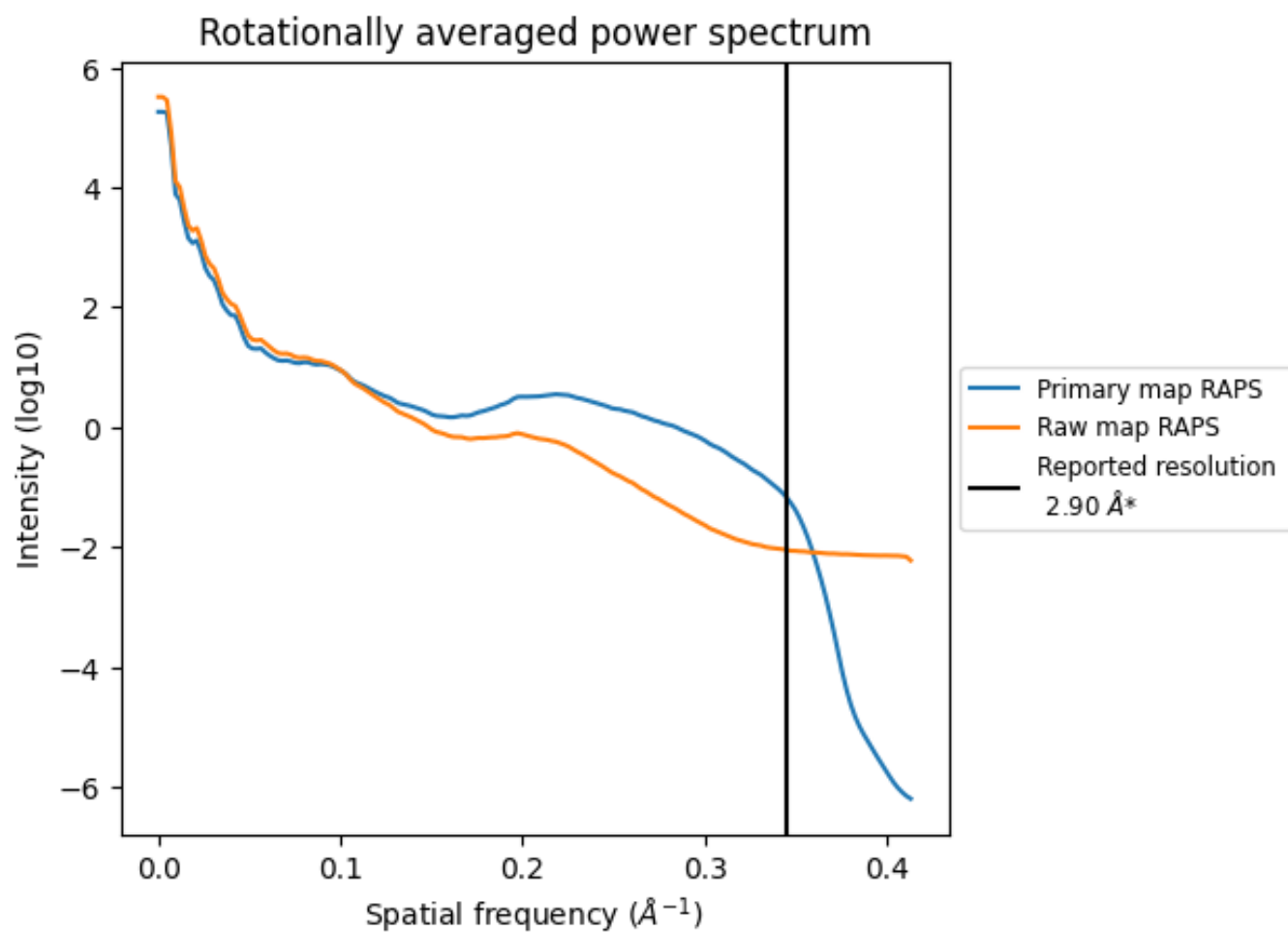
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 702 nm³; this corresponds to an approximate mass of 634 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

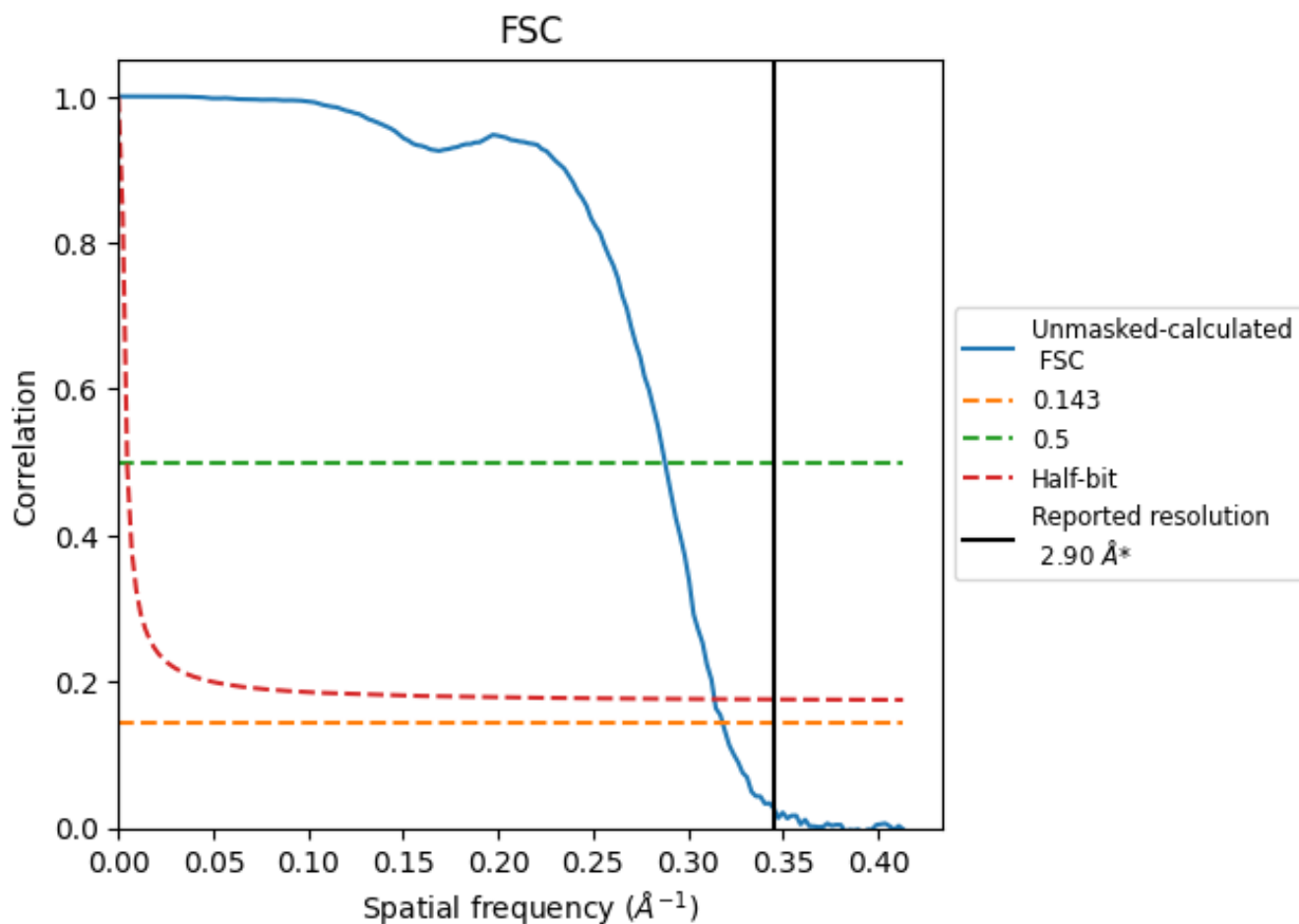


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345\AA^{-1}

8.2 Resolution estimates [i](#)

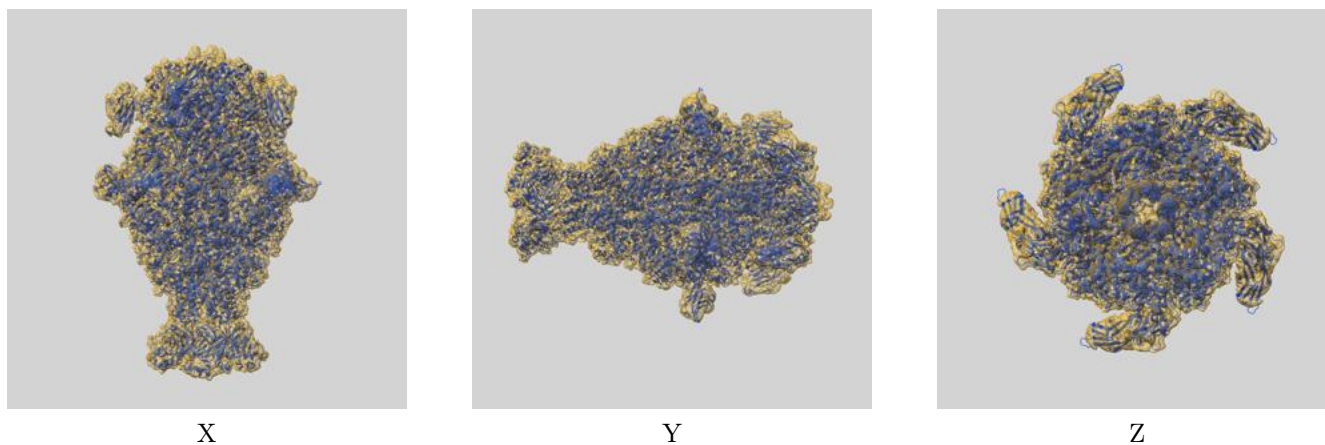
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.47	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

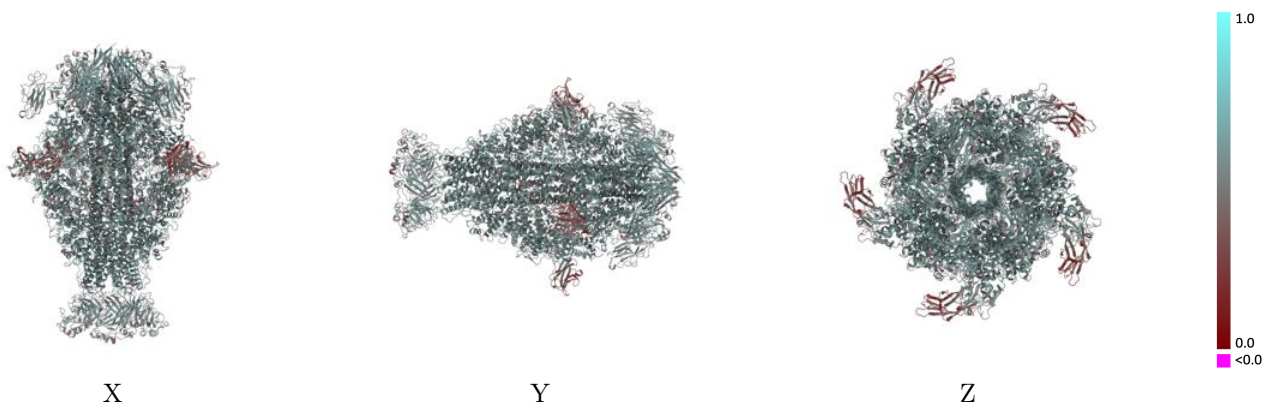
This section contains information regarding the fit between EMDB map EMD-16791 and PDB model 8CPZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



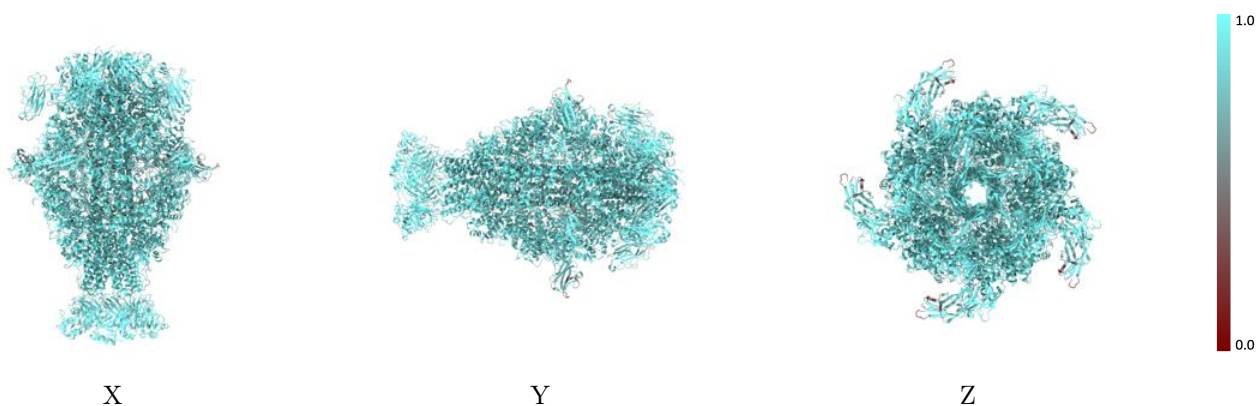
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



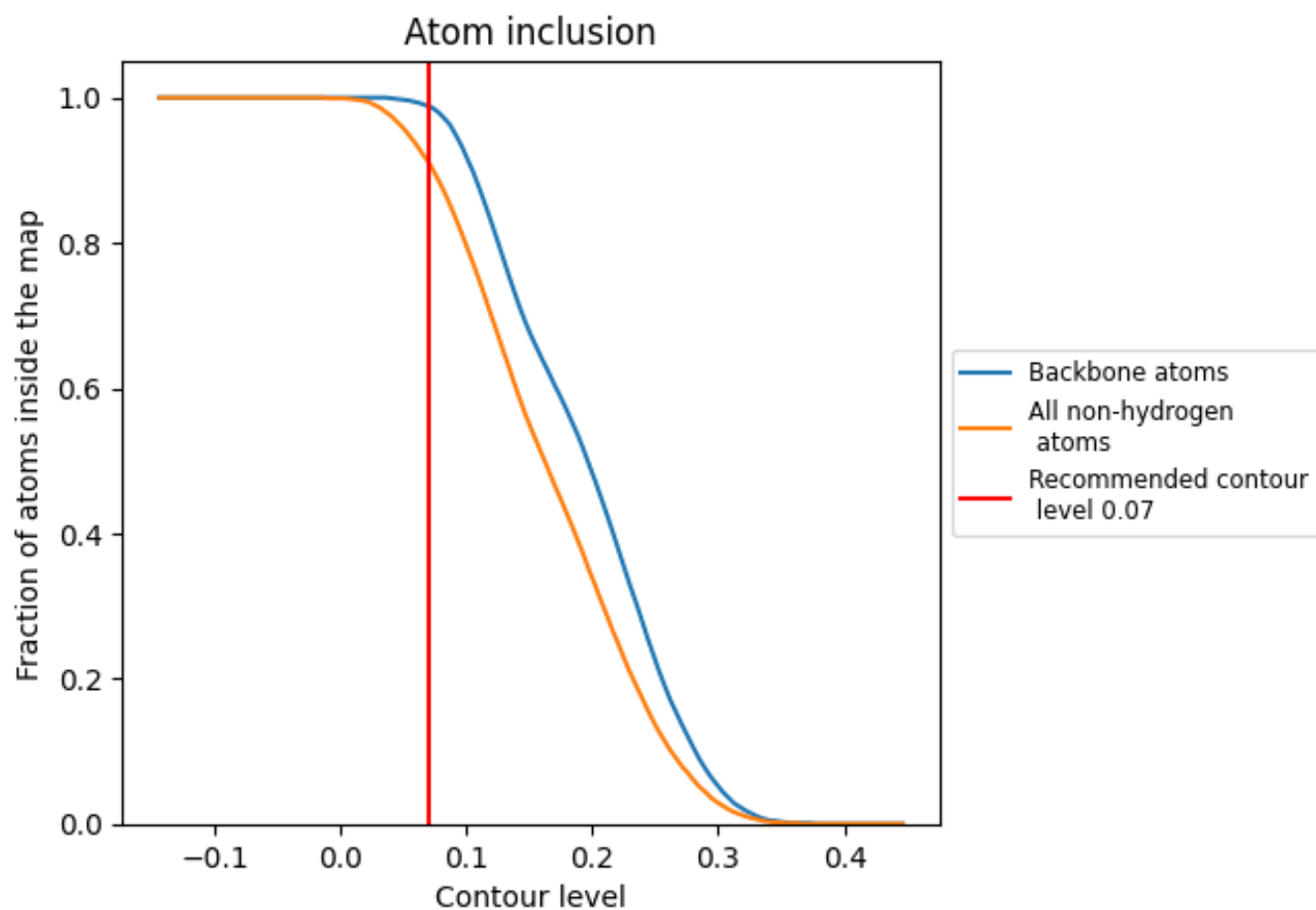
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).













9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5260
A	 0.9100	 0.5260
B	 0.9110	 0.5270
C	 0.9100	 0.5270
D	 0.9110	 0.5260
E	 0.9110	 0.5260

