



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 08:53 AM UTC

PDB ID : 8CPZ / pdb_00008cpz
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

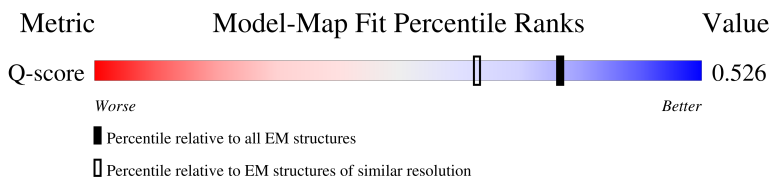
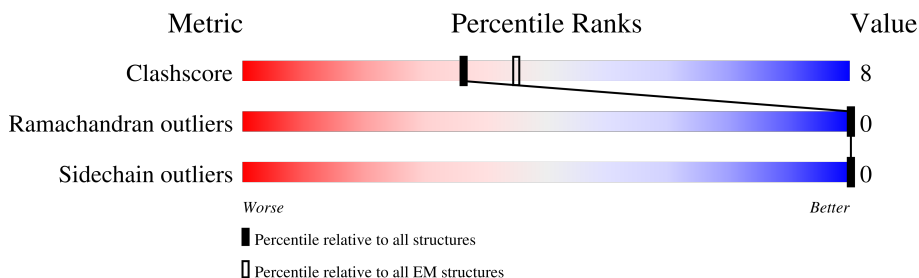
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	 67% 16% 16%
1	B	2535	 67% 16% 16%
1	C	2535	 68% 16% 16%
1	D	2535	 68% 16% 16%

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Mol	Chain	Length	Quality of chain
1	E	2535	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 67%, a yellow segment representing 16%, and a grey segment representing 16%. A small red dot is visible at the beginning of the green segment.

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
1	A	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	B	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	C	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	D	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	E	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		

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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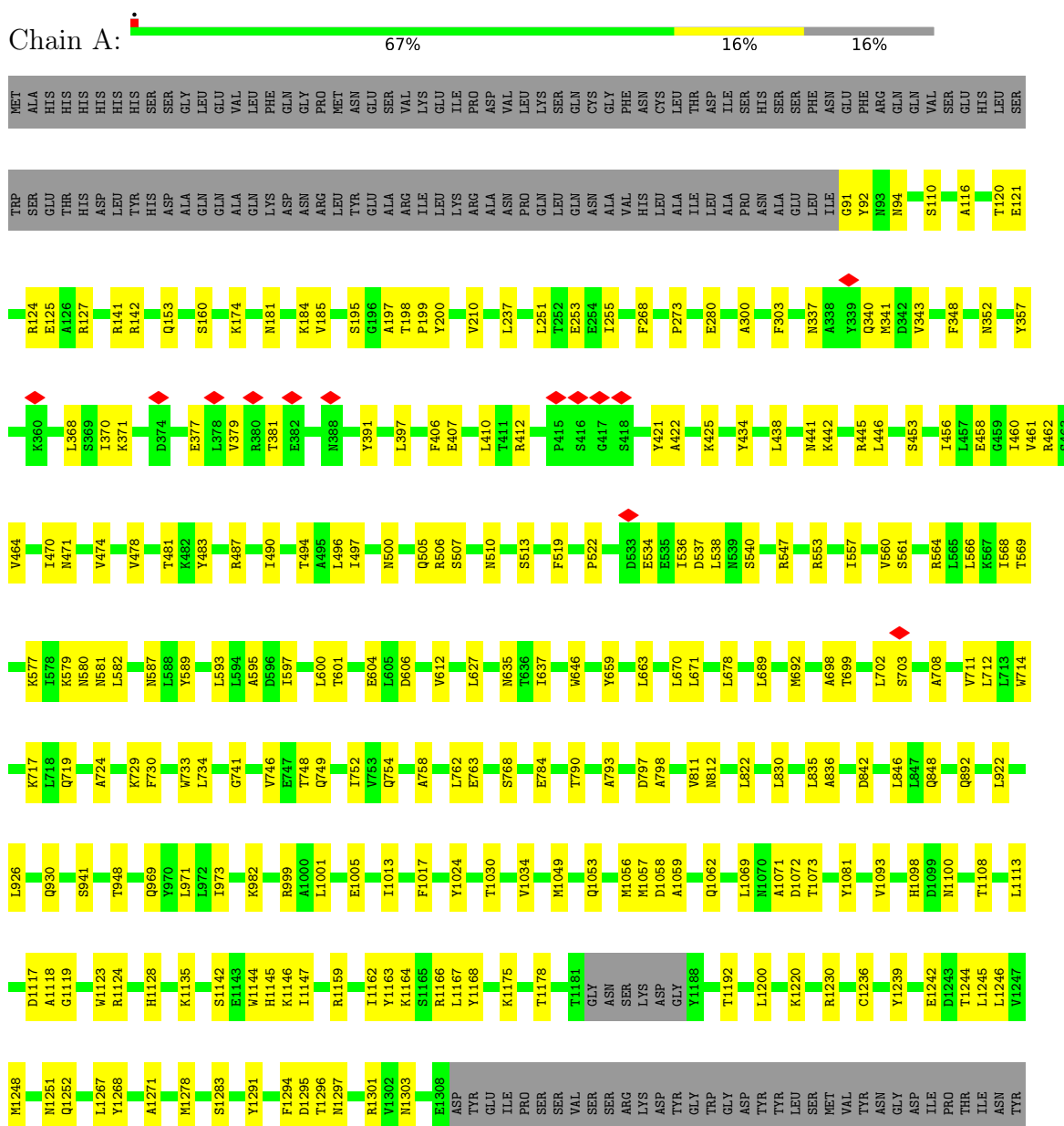
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	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

3 Residue-property plots

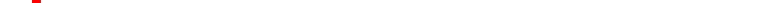
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

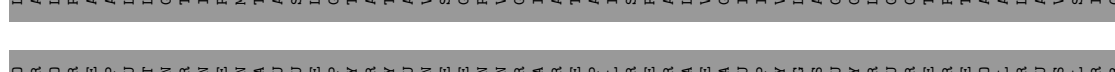
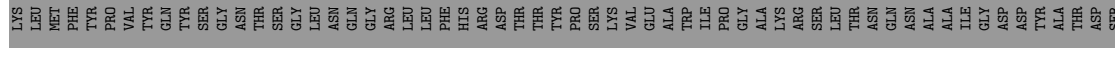
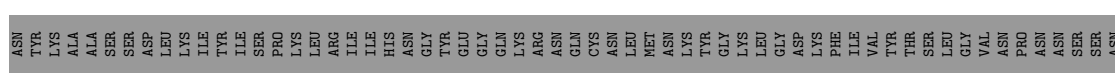
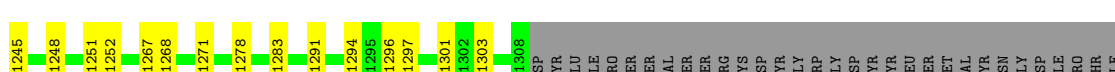
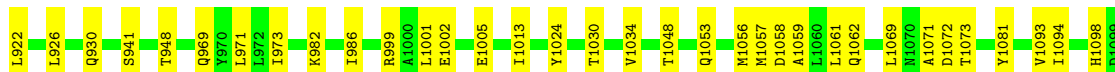
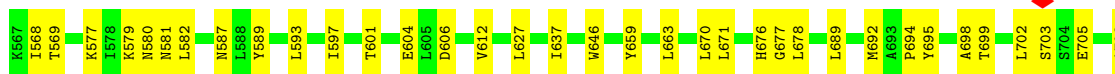
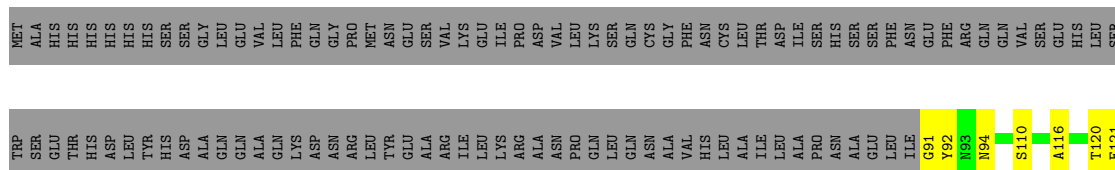
• Molecule 1: TcdA1



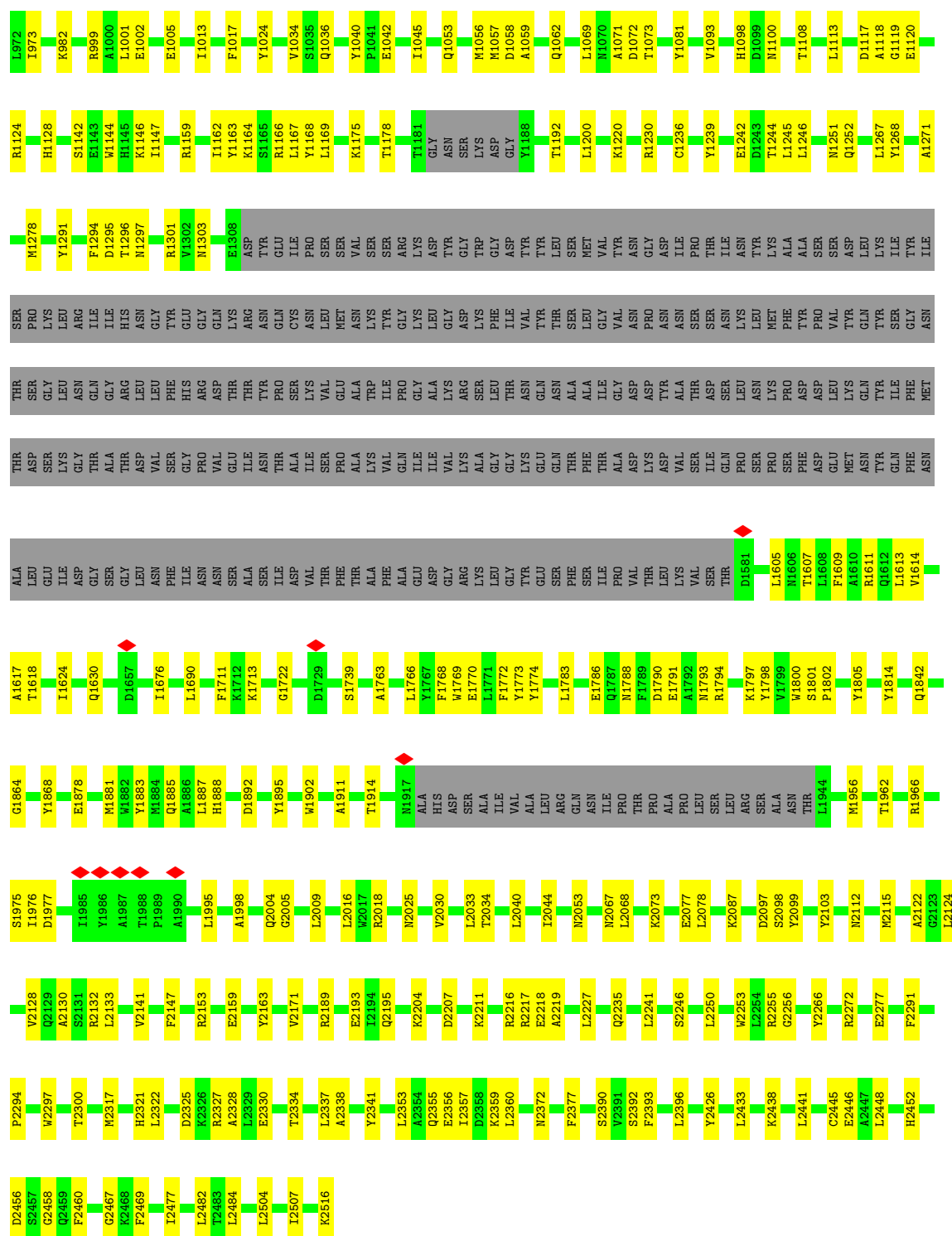


- Molecule 1: TcdA1

Chain C:  68% 16% 16%





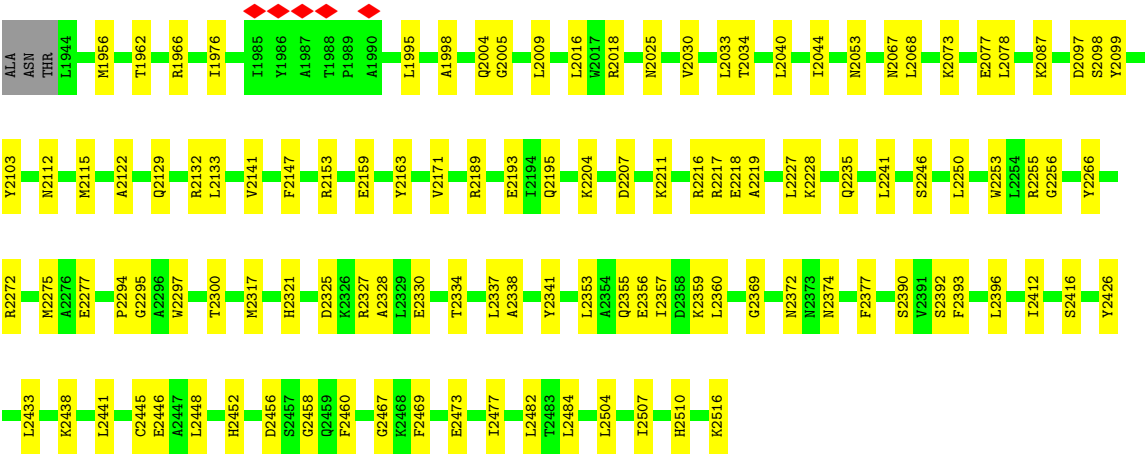


• Molecule 1: TcdA1

Chain E: 67% 16% 16%

MET	ALA	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	GLU	VAL	VAL	PHE	GLN	GLY	PRO	MET	ASN	GLU	ILE	ASP	ASP	VAL	LEU	LYS	SER	GLN	CYS	PHE	ASN	CYS	LEU	THR	ASP	ILE	SER	HIS	SER	SER	SER	PHE	ASN	GLU	PHE	ARG	GLN	VAL	SER	GLU	HIS	LEU	SER
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TRP	Y1798	D1581	PRO	LEU	LYS	ASN	L1245	L1113	E705	I568	V464	Y357	R124	TRP
SER	Y1799	L1605	SER	ASN	LEU	TYR	M1248	D1117	A708	I569	I470	N364	R127	SER
GLU	Y1800	L1606	PRO	LYS	PHE	ALA	N1251	A1118	V711	K577	M471	R129	R130	GLU
THR	S1801	T1607	PHE	PRO	THR	ALA	Q1252	G1119	L712	K578	N474	L368	R141	HIS
ASP	P1802	L1608	ASP	VAL	VAL	SER	Q1253	E1120	L713	N579	V478	S369	R142	ASP
LEU	Y1805	F1609	LEU	THR	THR	ASP	L1267	W1123	W714	N580	V478	N371	Q153	LEU
LEU	Q1842	A1610	ASN	GLN	GLN	LEU	Y1268	R1124	Q719	N581	T481	D374	Q154	HIS
GLN	Q1864	Q1612	GLN	THR	THR	ILE	A1271	H1128	A724	K482	Y483	E377	S160	ASP
ASP	D1865	V1614	PHE	PHE	GLY	ASN	H1278	K1135	F730	N587	Y483	L379	K174	GLN
ASN	Y1868	A1617	ASN	THR	THR	ILE	S1283	K1136	L734	L588	R487	V379	N181	ALA
GLN	E1878	T1618	LEU	THR	THR	SER	Y1291	S1142	L735	L589	Y487	L379	K174	GLN
GLN	E1878	T1618	SER	THR	THR	PRO	Y1292	S1143	L736	L590	R487	V379	N181	GLN
GLN	E1878	T1618	LYS	THR	THR	LYS	Y1293	S1144	L737	L591	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	Y1294	S1145	L738	L592	R487	V379	N181	GLN
GLN	E1878	T1618	ILE	THR	THR	ILE	F1294	H1146	L739	L593	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	D1295	H1147	L740	L594	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	N1297	K1148	L741	L595	R487	V379	N181	GLN
GLN	E1878	T1618	ASP	THR	THR	ASP	Y1301	K1149	L742	L596	R487	V379	N181	GLN
GLN	E1878	T1618	VAL	THR	THR	VAL	R1302	K1150	L743	L597	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	Y1303	K1151	L744	L598	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	E1308	K1152	L745	L599	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	ASP	K1153	L746	L600	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1154	L747	L601	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1155	L748	L602	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1156	L749	L603	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	TYR	K1157	L750	L604	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	GLY	K1158	L751	L605	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	ASN	K1159	L752	L606	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	LEU	K1160	L753	L607	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	THR	K1161	L754	L608	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	ASP	K1162	L755	L609	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1163	L756	L610	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1164	L757	L611	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1165	L758	L612	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	TYR	K1166	L759	L613	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1167	L760	L614	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1168	L761	L615	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	LEU	K1169	L762	L616	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	THR	K1170	L763	L617	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	ASN	K1171	L764	L618	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1172	L765	L619	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1173	L766	L620	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1174	L767	L621	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1175	L768	L622	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1176	L769	L623	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1177	L770	L624	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1178	L771	L625	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1179	L772	L626	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1180	L773	L627	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1181	L774	L628	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1182	L775	L629	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1183	L776	L630	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1184	L777	L631	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1185	L778	L632	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1186	L779	L633	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1187	L780	L634	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1188	L781	L635	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1189	L782	L636	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1190	L783	L637	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1191	L784	L638	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1192	L785	L639	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1193	L786	L640	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1194	L787	L641	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1195	L788	L642	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1196	L789	L643	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1197	L790	L644	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1198	L791	L645	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1199	L792	L646	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1200	L793	L647	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1201	L794	L648	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1202	L795	L649	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1203	L796	L650	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1204	L797	L651	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1205	L798	L652	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1206	L799	L653	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1207	L800	L654	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1208	L801	L655	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1209	L802	L656	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1210	L803	L657	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1211	L804	L658	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1212	L805	L659	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1213	L806	L660	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1214	L807	L661	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1215	L808	L662	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1216	L809	L663	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1217	L810	L664	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1218	L811	L665	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1219	L812	L666	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1220	L813	L667	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1221	L814	L668	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1222	L815	L669	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1223	L816	L670	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1224	L817	L671	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1225	L818	L672	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1226	L819	L673	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1227	L820	L674	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1228	L821	L675	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1229	L822	L676	R487	V379	N181	GLN
GLN	E1878	T1618	PRO	THR	THR	PRO	ASN	K1230	L823	L677	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1231	L824	L678	R487	V379	N181	GLN
GLN	E1878	T1618	GLY	THR	THR	GLY	TYR	K1232	L825	L679	R487	V379	N181	GLN
GLN	E1878	T1618	LEU	THR	THR	LEU	ASN	K1233	L826	L680	R487	V379	N181	GLN
GLN	E1878	T1618	ASN	THR	THR	ASN	GLY	K1234	L827	L681	R487	V379	N181	GLN
GLN	E1878	T1618	THR	THR	THR	THR	ASN	K1235	L828	L682	R487	V379		



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	0.15	0/17247	0.42	0/23428
1	B	0.15	0/17247	0.42	0/23428
1	C	0.15	0/17247	0.42	0/23428
1	D	0.15	0/17247	0.42	0/23428
1	E	0.15	0/17247	0.42	0/23428
All	All	0.15	0/86235	0.42	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	289	0
1	B	16884	0	16507	291	0
1	C	16884	0	16507	281	0
1	D	16884	0	16507	284	0
1	E	16884	0	16507	290	0
All	All	84420	0	82535	1282	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 8.

The worst 5 of 1282 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:341:MET:HE1	1:B:410:LEU:HD22	1.49	0.95
1:C:341:MET:HE1	1:C:410:LEU:HD22	1.49	0.93
1:A:341:MET:HE1	1:A:410:LEU:HD22	1.50	0.93
1:D:341:MET:HE1	1:D:410:LEU:HD22	1.50	0.91
1:E:341:MET:HE1	1:E:410:LEU:HD22	1.49	0.91

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	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

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%)	1816 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1816/2173 (84%)	1816 (100%)	0	100	100
1	C	1816/2173 (84%)	1816 (100%)	0	100	100
1	D	1816/2173 (84%)	1816 (100%)	0	100	100
1	E	1816/2173 (84%)	1816 (100%)	0	100	100
All	All	9080/10865 (84%)	9080 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1100	ASN
1	E	1842	GLN
1	D	93	ASN
1	E	1812	GLN
1	E	914	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

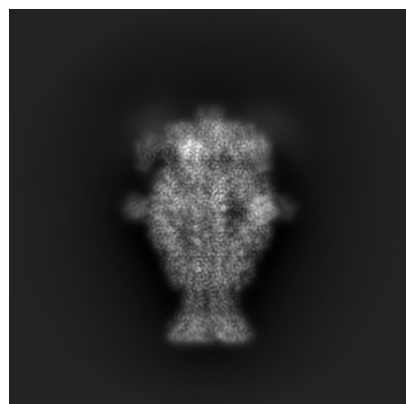
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16791. These allow visual inspection of the internal detail of the map and identification of artifacts.

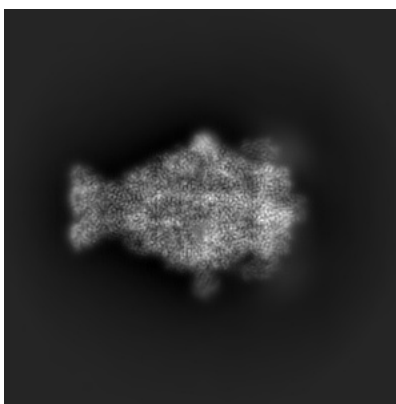
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

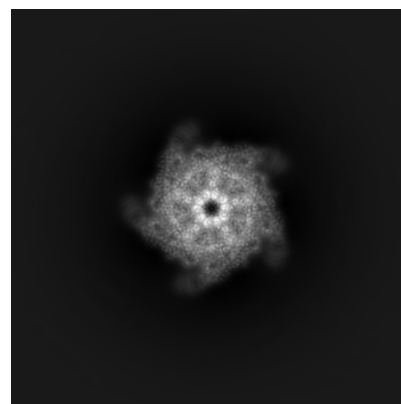
6.1.1 Primary map



X

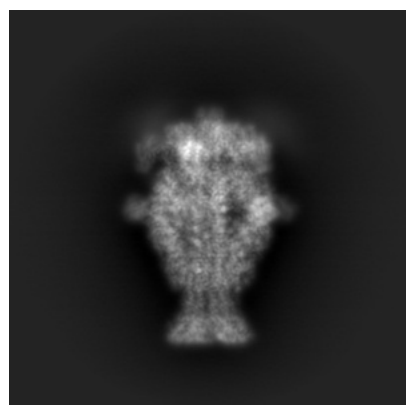


Y

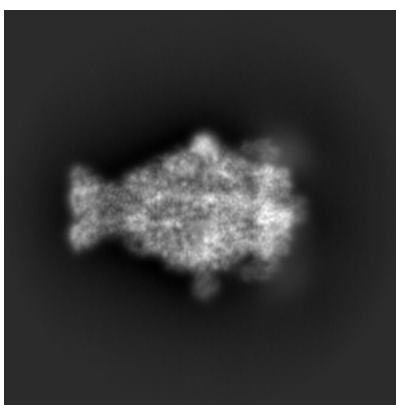


Z

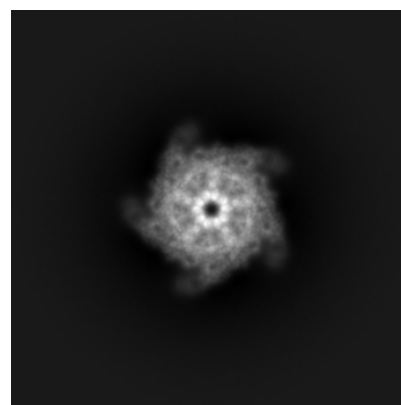
6.1.2 Raw map



X



Y



Z

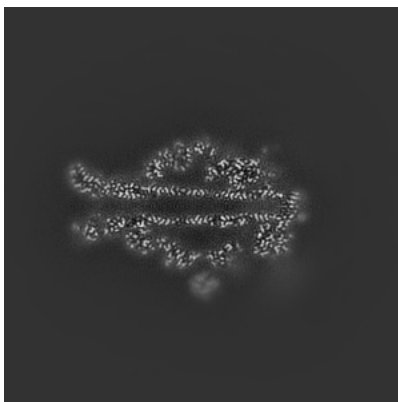
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

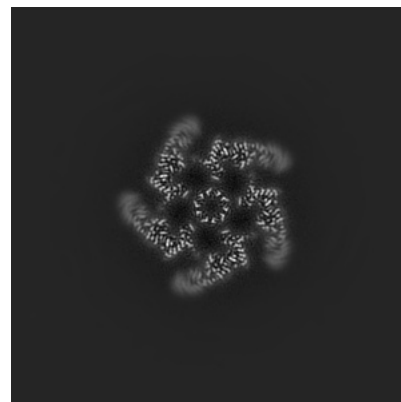
6.2.1 Primary map



X Index: 176

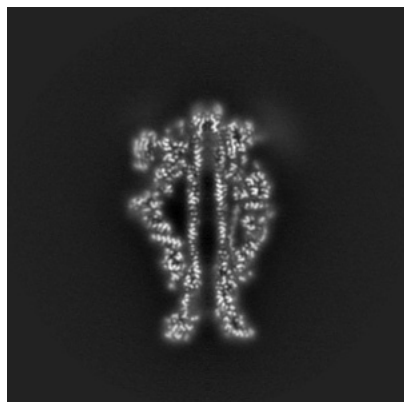


Y Index: 176

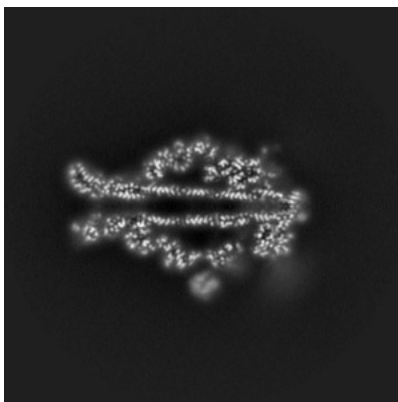


Z Index: 176

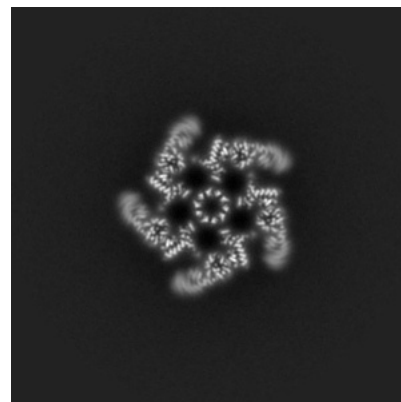
6.2.2 Raw map



X Index: 176



Y Index: 176

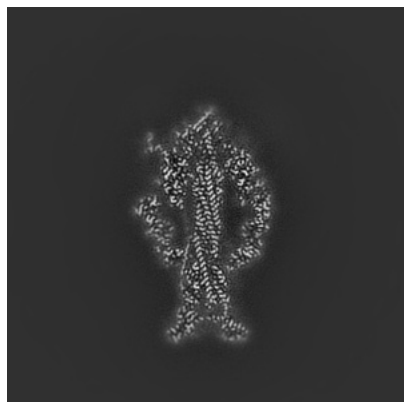


Z Index: 176

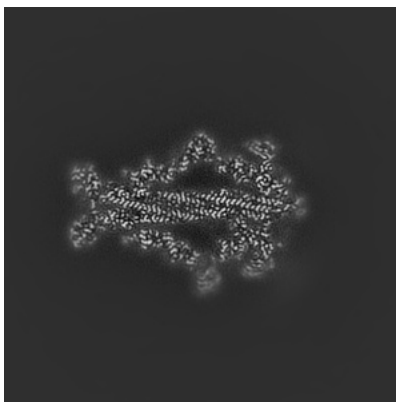
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

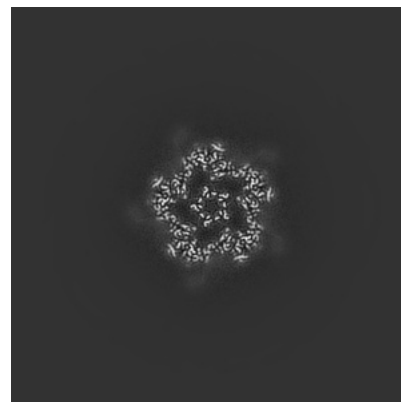
6.3.1 Primary map



X Index: 187

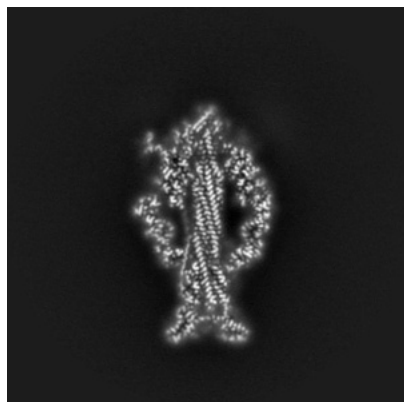


Y Index: 166

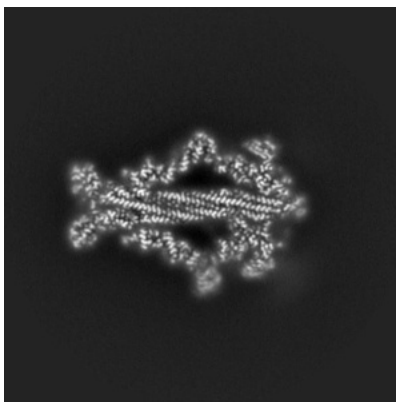


Z Index: 192

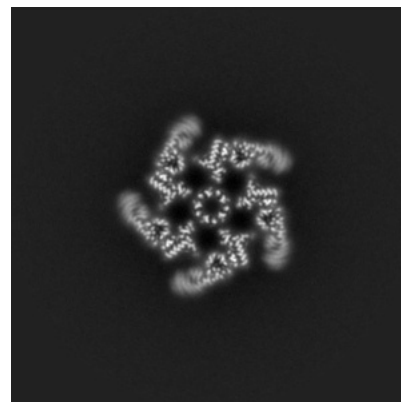
6.3.2 Raw map



X Index: 187



Y Index: 166

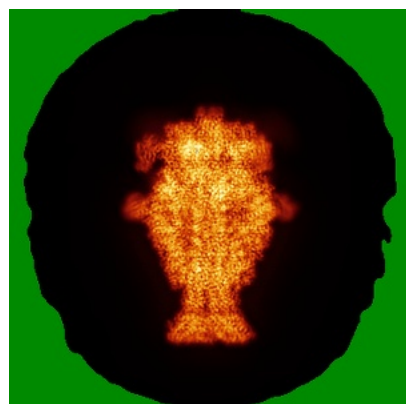


Z Index: 177

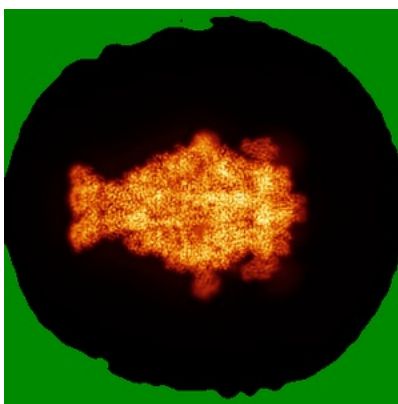
The images above show the largest variance slices of the map in three orthogonal directions.

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

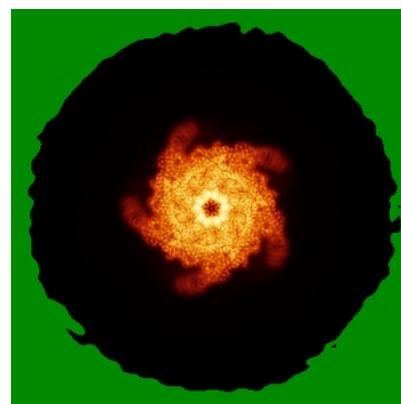
6.4.1 Primary map



X



Y

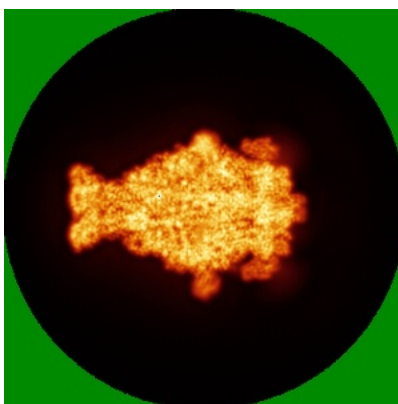


Z

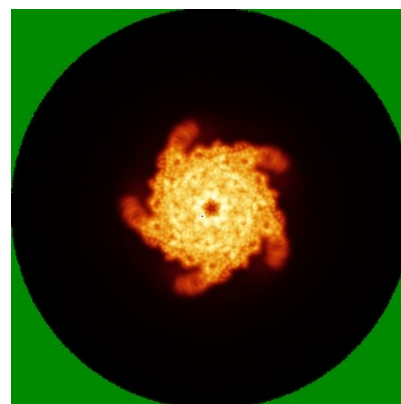
6.4.2 Raw map



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.

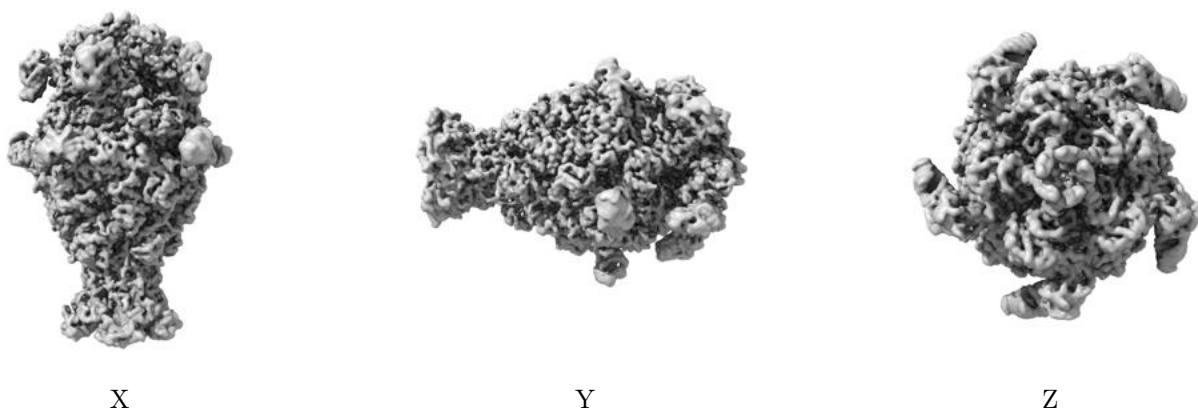
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

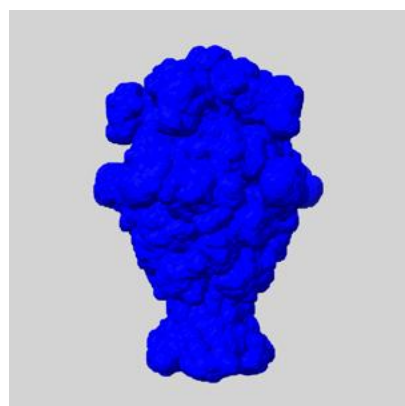
6.6 Mask visualisation [i](#)

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

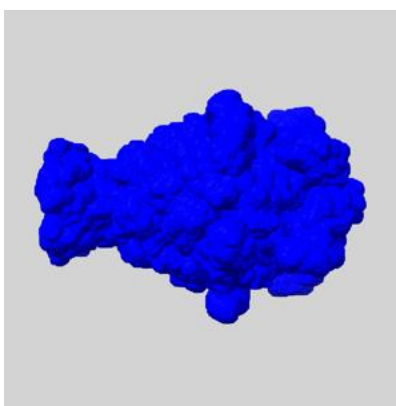
A mask typically either:

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

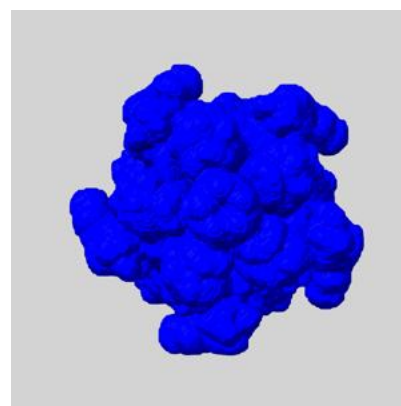
6.6.1 emd_16791_msk_1.map [i](#)



X



Y

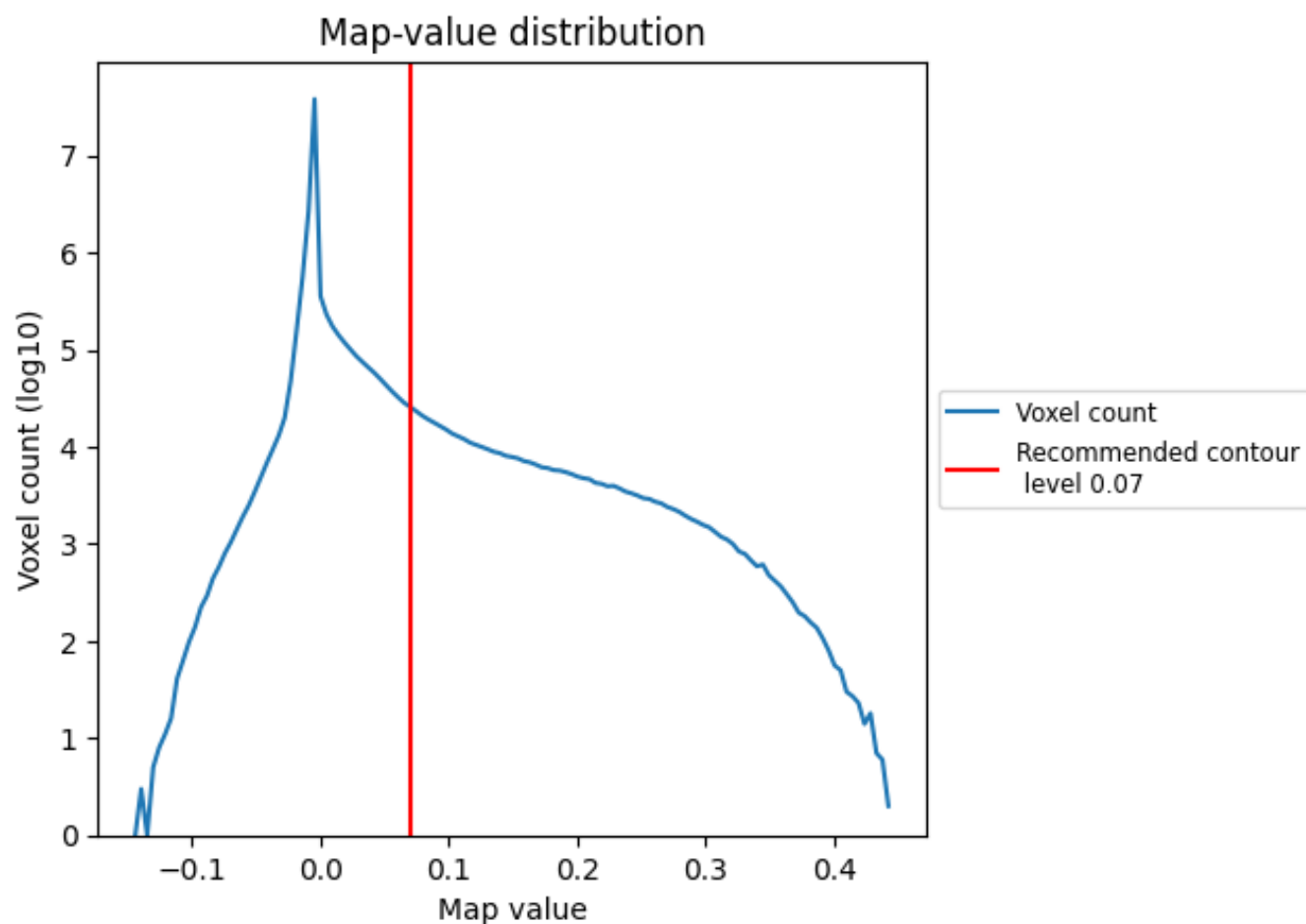


Z

7 Map analysis [i](#)

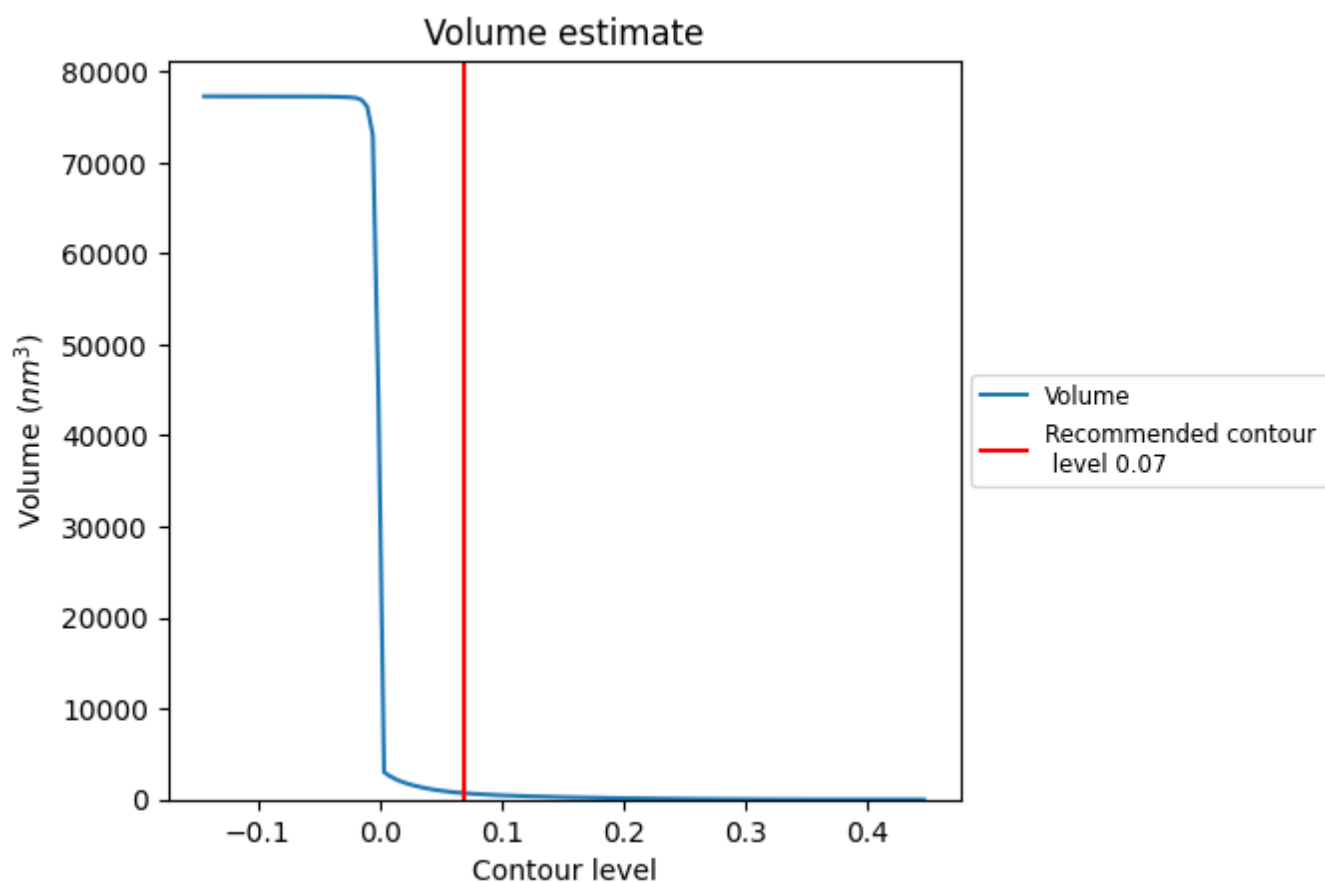
This section contains the results of statistical analysis of the map.

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.

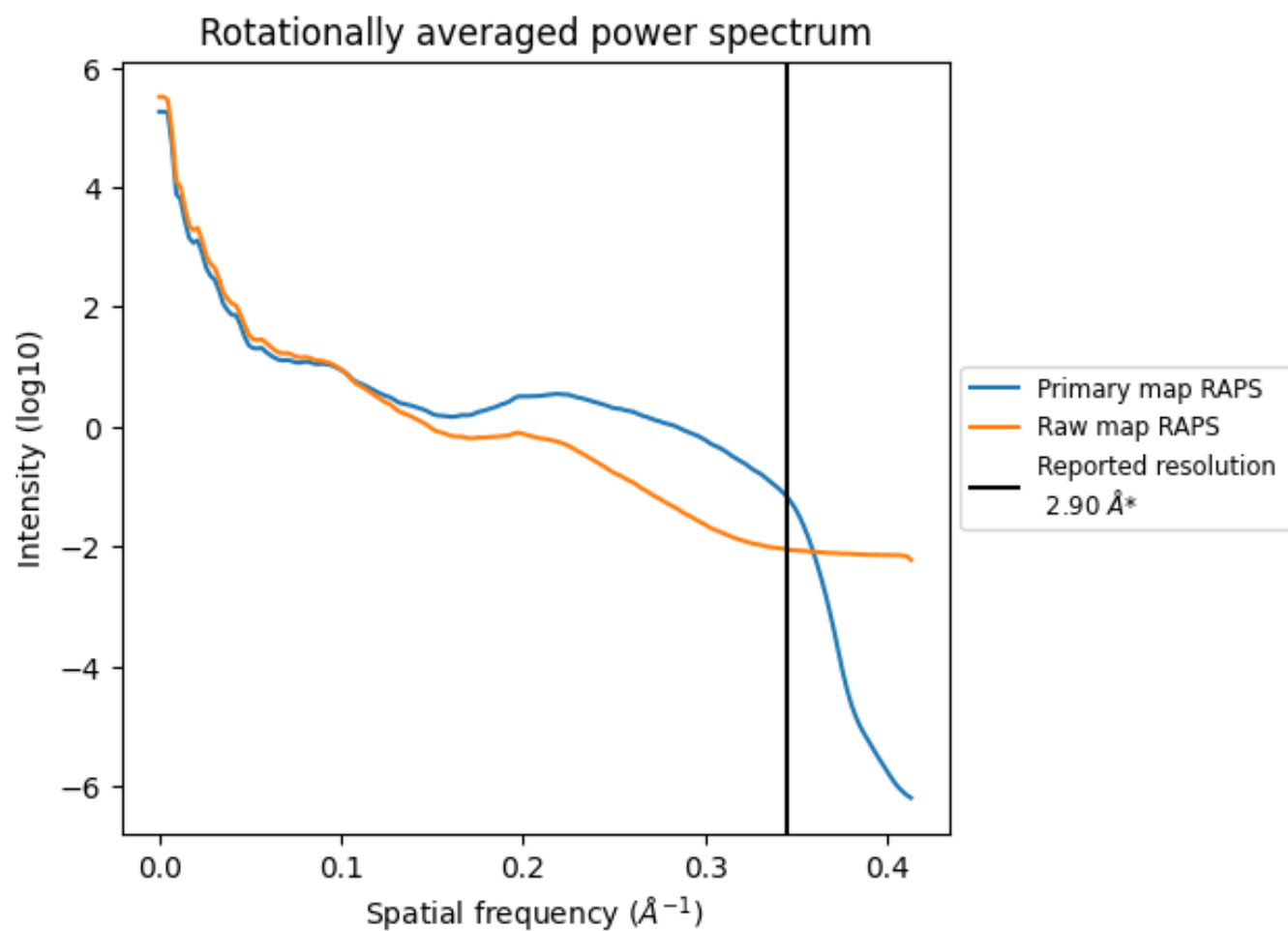
7.2 Volume estimate [i](#)



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 ⓘ

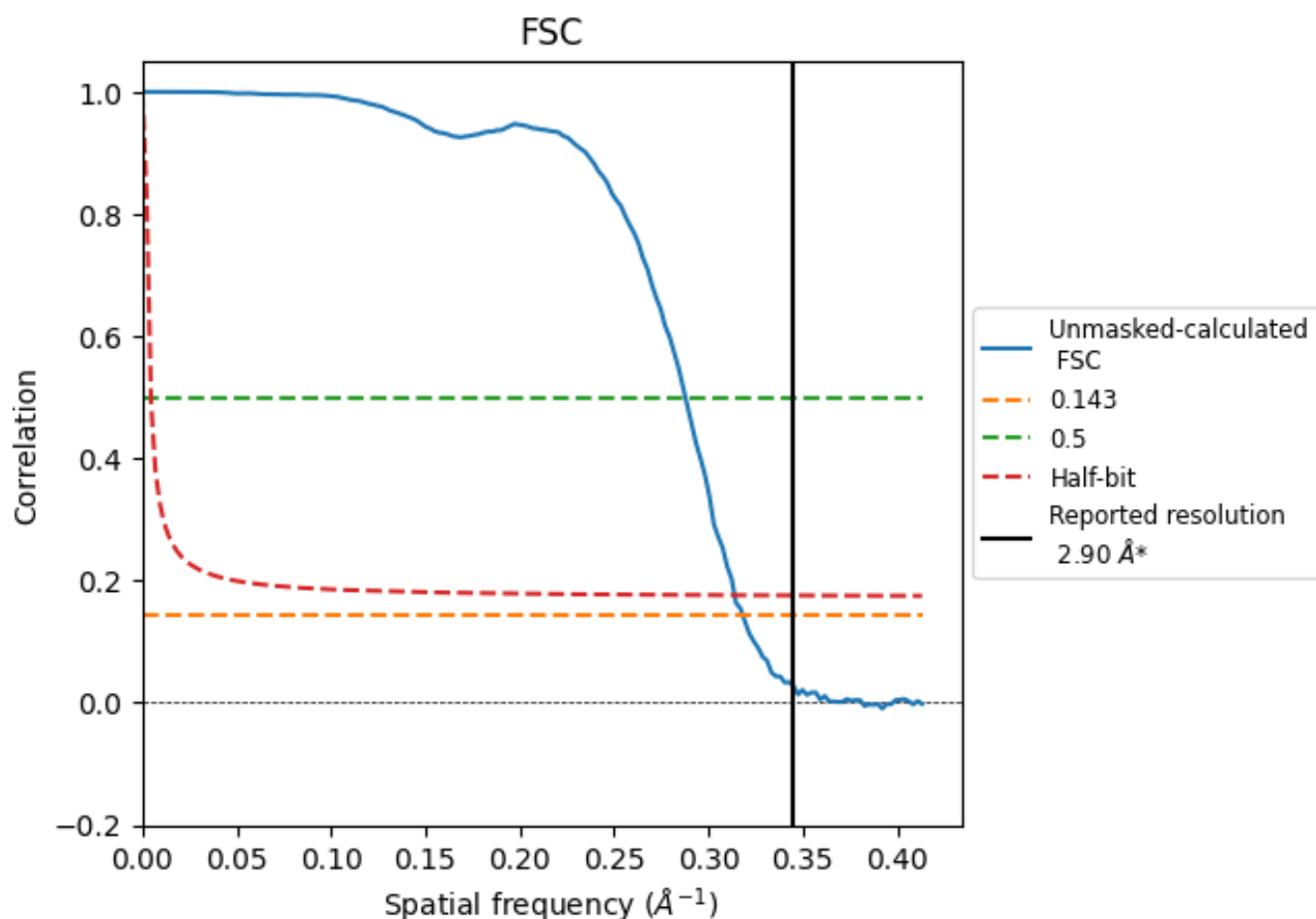


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

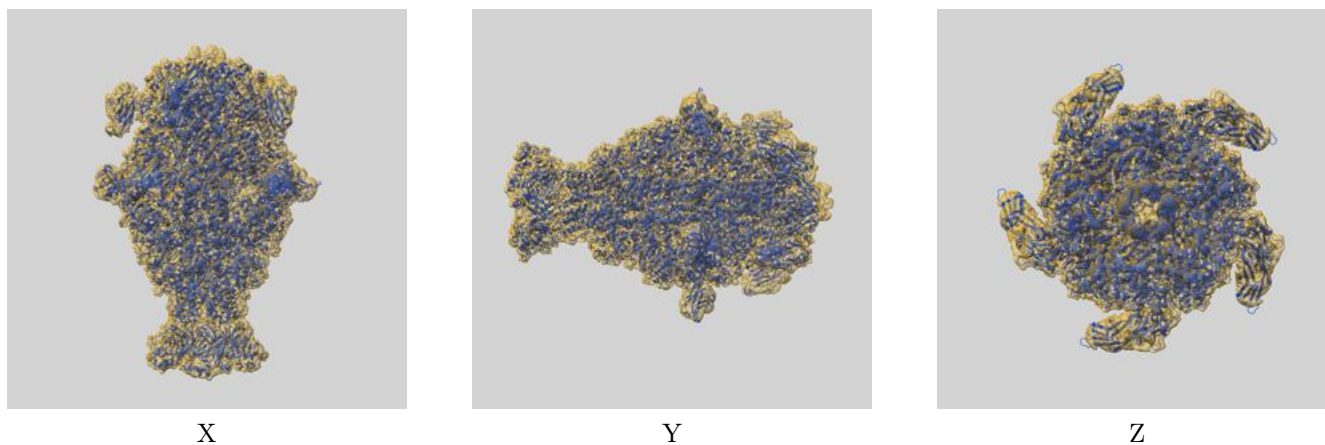
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.47	3.19

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

9 Map-model fit [i](#)

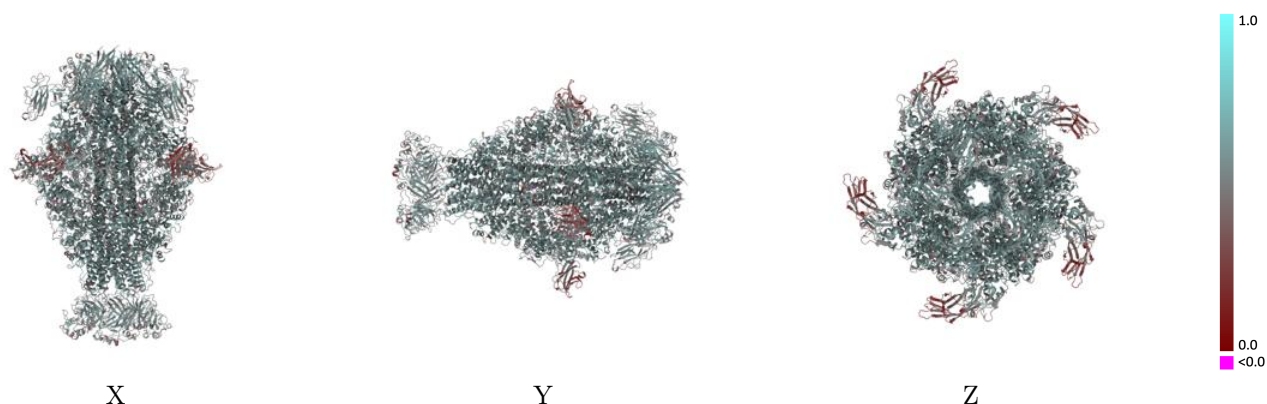
This section contains information regarding the fit between EMDB map EMD-16791 and PDB model 8CPZ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



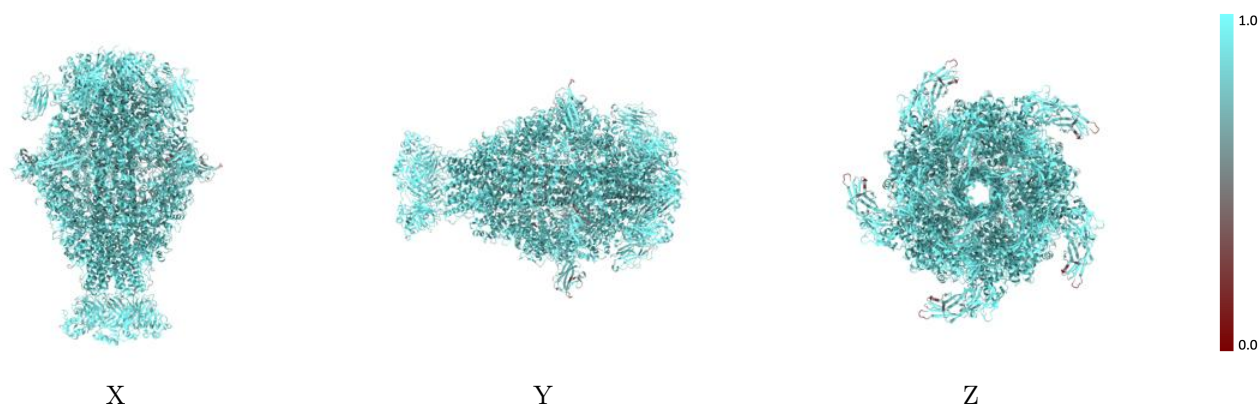
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



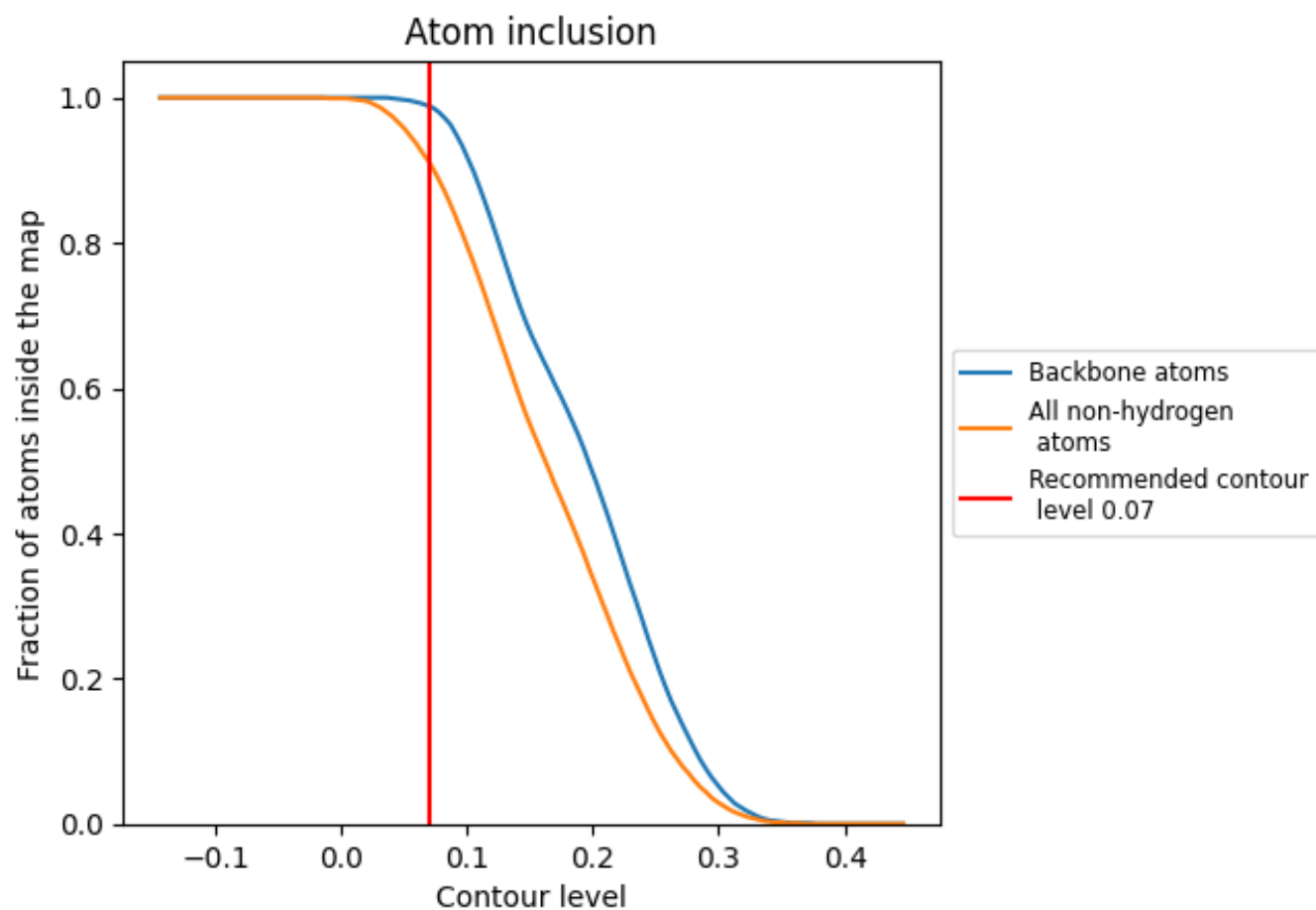
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

