



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 12:45 AM EDT

PDB ID : 8TXB
EMDB ID : EMD-41679
Title : Characterization of the Chlamydomonas Flagellar Mastigoneme Filament Structure at 3.9Å
Authors : Yue, W.; Kai, Z.
Deposited on : 2023-08-23
Resolution : 3.90 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

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<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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

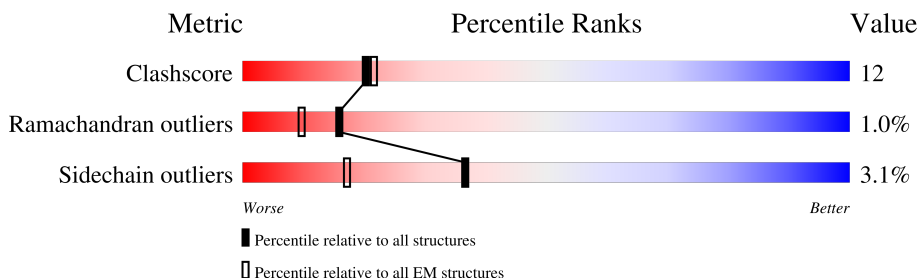
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1987	
1	B	1987	
1	C	1987	
1	D	1987	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54748 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 Mastigoneme-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	B	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	C	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	D	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	VAL	conflict	UNP Q8LRM7
A	142	LEU	THR	conflict	UNP Q8LRM7
A	143	ALA	GLY	conflict	UNP Q8LRM7
A	144	SER	LEU	conflict	UNP Q8LRM7
A	145	LYS	GLU	conflict	UNP Q8LRM7
A	146	THR	ASP	conflict	UNP Q8LRM7
A	147	VAL	GLY	conflict	UNP Q8LRM7
A	149	ILE	HIS	conflict	UNP Q8LRM7
A	150	TYR	LEU	conflict	UNP Q8LRM7
A	151	VAL	CYS	conflict	UNP Q8LRM7
A	517	ARG	LYS	conflict	UNP Q8LRM7
A	530	GLU	GLY	conflict	UNP Q8LRM7
A	619	THR	ALA	conflict	UNP Q8LRM7
A	800	SER	THR	conflict	UNP Q8LRM7
A	820	SER	PHE	conflict	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	THR	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	TYR	deletion	UNP Q8LRM7
A	?	-	PHE	deletion	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q8LRM7
A	1399	LYS	ARG	conflict	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLU	deletion	UNP Q8LRM7
A	1868	PRO	ALA	conflict	UNP Q8LRM7
A	1897	PRO	GLN	conflict	UNP Q8LRM7
A	1914	PRO	ARG	conflict	UNP Q8LRM7
A	1915	PRO	ARG	conflict	UNP Q8LRM7
A	1917	PRO	HIS	conflict	UNP Q8LRM7
A	1919	SER	ALA	conflict	UNP Q8LRM7
A	1920	PRO	ARG	conflict	UNP Q8LRM7
A	1921	PRO	ARG	conflict	UNP Q8LRM7
A	1924	ASN	THR	conflict	UNP Q8LRM7
A	1925	ARG	ALA	conflict	UNP Q8LRM7
A	1926	SER	LEU	conflict	UNP Q8LRM7
A	1935	SER	PRO	conflict	UNP Q8LRM7
A	1978	ASP	-	expression tag	UNP Q8LRM7
A	1979	ALA	-	expression tag	UNP Q8LRM7
A	1980	GLU	-	expression tag	UNP Q8LRM7
A	1981	MET	-	expression tag	UNP Q8LRM7
A	1982	GLN	-	expression tag	UNP Q8LRM7
A	1983	PRO	-	expression tag	UNP Q8LRM7
A	1984	GLN	-	expression tag	UNP Q8LRM7
A	1985	ASP	-	expression tag	UNP Q8LRM7
A	1986	ASP	-	expression tag	UNP Q8LRM7
A	1987	GLU	-	expression tag	UNP Q8LRM7
B	141	LEU	VAL	conflict	UNP Q8LRM7
B	142	LEU	THR	conflict	UNP Q8LRM7
B	143	ALA	GLY	conflict	UNP Q8LRM7
B	144	SER	LEU	conflict	UNP Q8LRM7
B	145	LYS	GLU	conflict	UNP Q8LRM7
B	146	THR	ASP	conflict	UNP Q8LRM7
B	147	VAL	GLY	conflict	UNP Q8LRM7
B	149	ILE	HIS	conflict	UNP Q8LRM7
B	150	TYR	LEU	conflict	UNP Q8LRM7
B	151	VAL	CYS	conflict	UNP Q8LRM7
B	517	ARG	LYS	conflict	UNP Q8LRM7
B	530	GLU	GLY	conflict	UNP Q8LRM7
B	619	THR	ALA	conflict	UNP Q8LRM7
B	800	SER	THR	conflict	UNP Q8LRM7
B	820	SER	PHE	conflict	UNP Q8LRM7
B	?	-	GLY	deletion	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	GLY	deletion	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	TYR	deletion	UNP Q8LRM7
B	?	-	PHE	deletion	UNP Q8LRM7
B	?	-	LEU	deletion	UNP Q8LRM7
B	1399	LYS	ARG	conflict	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	GLU	deletion	UNP Q8LRM7
B	1868	PRO	ALA	conflict	UNP Q8LRM7
B	1897	PRO	GLN	conflict	UNP Q8LRM7
B	1914	PRO	ARG	conflict	UNP Q8LRM7
B	1915	PRO	ARG	conflict	UNP Q8LRM7
B	1917	PRO	HIS	conflict	UNP Q8LRM7
B	1919	SER	ALA	conflict	UNP Q8LRM7
B	1920	PRO	ARG	conflict	UNP Q8LRM7
B	1921	PRO	ARG	conflict	UNP Q8LRM7
B	1924	ASN	THR	conflict	UNP Q8LRM7
B	1925	ARG	ALA	conflict	UNP Q8LRM7
B	1926	SER	LEU	conflict	UNP Q8LRM7
B	1935	SER	PRO	conflict	UNP Q8LRM7
B	1978	ASP	-	expression tag	UNP Q8LRM7
B	1979	ALA	-	expression tag	UNP Q8LRM7
B	1980	GLU	-	expression tag	UNP Q8LRM7
B	1981	MET	-	expression tag	UNP Q8LRM7
B	1982	GLN	-	expression tag	UNP Q8LRM7
B	1983	PRO	-	expression tag	UNP Q8LRM7
B	1984	GLN	-	expression tag	UNP Q8LRM7
B	1985	ASP	-	expression tag	UNP Q8LRM7
B	1986	ASP	-	expression tag	UNP Q8LRM7
B	1987	GLU	-	expression tag	UNP Q8LRM7
C	141	LEU	VAL	conflict	UNP Q8LRM7
C	142	LEU	THR	conflict	UNP Q8LRM7
C	143	ALA	GLY	conflict	UNP Q8LRM7
C	144	SER	LEU	conflict	UNP Q8LRM7
C	145	LYS	GLU	conflict	UNP Q8LRM7
C	146	THR	ASP	conflict	UNP Q8LRM7
C	147	VAL	GLY	conflict	UNP Q8LRM7
C	149	ILE	HIS	conflict	UNP Q8LRM7
C	150	TYR	LEU	conflict	UNP Q8LRM7
C	151	VAL	CYS	conflict	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	517	ARG	LYS	conflict	UNP Q8LRM7
C	530	GLU	GLY	conflict	UNP Q8LRM7
C	619	THR	ALA	conflict	UNP Q8LRM7
C	800	SER	THR	conflict	UNP Q8LRM7
C	820	SER	PHE	conflict	UNP Q8LRM7
C	?	-	GLY	deletion	UNP Q8LRM7
C	?	-	THR	deletion	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	GLY	deletion	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	TYR	deletion	UNP Q8LRM7
C	?	-	PHE	deletion	UNP Q8LRM7
C	?	-	LEU	deletion	UNP Q8LRM7
C	1399	LYS	ARG	conflict	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	GLU	deletion	UNP Q8LRM7
C	1868	PRO	ALA	conflict	UNP Q8LRM7
C	1897	PRO	GLN	conflict	UNP Q8LRM7
C	1914	PRO	ARG	conflict	UNP Q8LRM7
C	1915	PRO	ARG	conflict	UNP Q8LRM7
C	1917	PRO	HIS	conflict	UNP Q8LRM7
C	1919	SER	ALA	conflict	UNP Q8LRM7
C	1920	PRO	ARG	conflict	UNP Q8LRM7
C	1921	PRO	ARG	conflict	UNP Q8LRM7
C	1924	ASN	THR	conflict	UNP Q8LRM7
C	1925	ARG	ALA	conflict	UNP Q8LRM7
C	1926	SER	LEU	conflict	UNP Q8LRM7
C	1935	SER	PRO	conflict	UNP Q8LRM7
C	1978	ASP	-	expression tag	UNP Q8LRM7
C	1979	ALA	-	expression tag	UNP Q8LRM7
C	1980	GLU	-	expression tag	UNP Q8LRM7
C	1981	MET	-	expression tag	UNP Q8LRM7
C	1982	GLN	-	expression tag	UNP Q8LRM7
C	1983	PRO	-	expression tag	UNP Q8LRM7
C	1984	GLN	-	expression tag	UNP Q8LRM7
C	1985	ASP	-	expression tag	UNP Q8LRM7
C	1986	ASP	-	expression tag	UNP Q8LRM7
C	1987	GLU	-	expression tag	UNP Q8LRM7
D	141	LEU	VAL	conflict	UNP Q8LRM7
D	142	LEU	THR	conflict	UNP Q8LRM7
D	143	ALA	GLY	conflict	UNP Q8LRM7
D	144	SER	LEU	conflict	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	145	LYS	GLU	conflict	UNP Q8LRM7
D	146	THR	ASP	conflict	UNP Q8LRM7
D	147	VAL	GLY	conflict	UNP Q8LRM7
D	149	ILE	HIS	conflict	UNP Q8LRM7
D	150	TYR	LEU	conflict	UNP Q8LRM7
D	151	VAL	CYS	conflict	UNP Q8LRM7
D	517	ARG	LYS	conflict	UNP Q8LRM7
D	530	GLU	GLY	conflict	UNP Q8LRM7
D	619	THR	ALA	conflict	UNP Q8LRM7
D	800	SER	THR	conflict	UNP Q8LRM7
D	820	SER	PHE	conflict	UNP Q8LRM7
D	?	-	GLY	deletion	UNP Q8LRM7
D	?	-	THR	deletion	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	GLY	deletion	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	TYR	deletion	UNP Q8LRM7
D	?	-	PHE	deletion	UNP Q8LRM7
D	?	-	LEU	deletion	UNP Q8LRM7
D	1399	LYS	ARG	conflict	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	GLU	deletion	UNP Q8LRM7
D	1868	PRO	ALA	conflict	UNP Q8LRM7
D	1897	PRO	GLN	conflict	UNP Q8LRM7
D	1914	PRO	ARG	conflict	UNP Q8LRM7
D	1915	PRO	ARG	conflict	UNP Q8LRM7
D	1917	PRO	HIS	conflict	UNP Q8LRM7
D	1919	SER	ALA	conflict	UNP Q8LRM7
D	1920	PRO	ARG	conflict	UNP Q8LRM7
D	1921	PRO	ARG	conflict	UNP Q8LRM7
D	1924	ASN	THR	conflict	UNP Q8LRM7
D	1925	ARG	ALA	conflict	UNP Q8LRM7
D	1926	SER	LEU	conflict	UNP Q8LRM7
D	1935	SER	PRO	conflict	UNP Q8LRM7
D	1978	ASP	-	expression tag	UNP Q8LRM7
D	1979	ALA	-	expression tag	UNP Q8LRM7
D	1980	GLU	-	expression tag	UNP Q8LRM7
D	1981	MET	-	expression tag	UNP Q8LRM7
D	1982	GLN	-	expression tag	UNP Q8LRM7
D	1983	PRO	-	expression tag	UNP Q8LRM7
D	1984	GLN	-	expression tag	UNP Q8LRM7
D	1985	ASP	-	expression tag	UNP Q8LRM7

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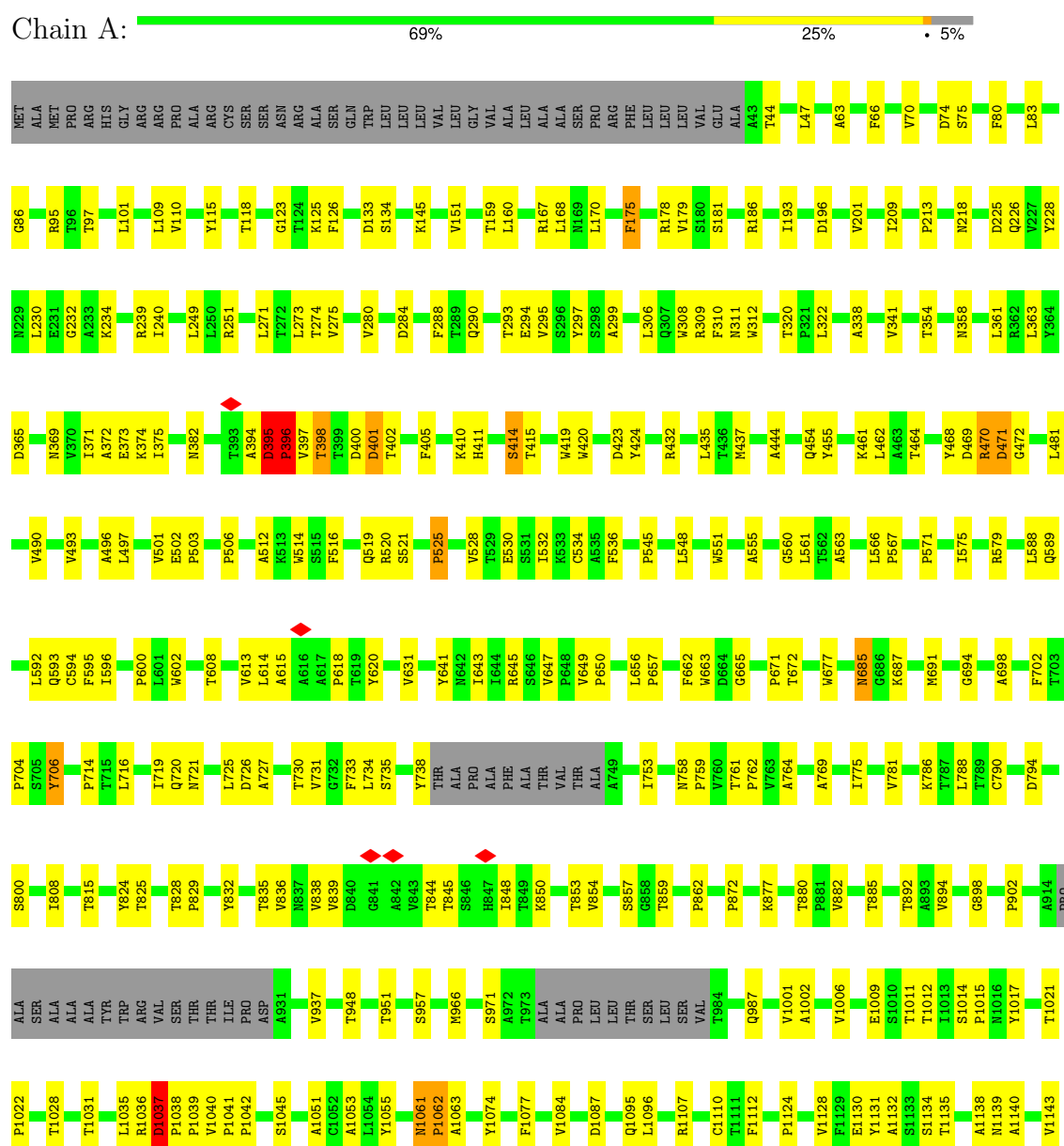
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1986	ASP	-	expression tag	UNP Q8LRM7
D	1987	GLU	-	expression tag	UNP Q8LRM7

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: Mastigoneme-like protein





K1796	T1679	P1551	T1452	H1326	Q1212	A1063	ALA	P862
C1797	C1680	T1555	A1453	T1332	C1213	F1077	PRO	V866
P1799	C1683	T1555	A1454	T1332	R1214	F1077	LEU	V866
D1800	C1683	D1558	P1455	G1336	K1215	V1084	LEU	P872
F1801	G1703	D1558	T1456	G1336	C1216	V1084	THR	P872
	G1703	D1558	F1457	G1336	P1217	V1084	SER	V876
D1804	Q1706	Q1563	G1458	P1355	G1218	D1087	LEU	K977
R1805	N1707	G1569	M1459	N1356	G1219	D1087	SER	K977
P1806	N1707	G1569	G1459	P1356	T1220	D1093	VAL	V876
G1807	Q1711	P1572	P1464	C1358	T1221	Q1094		T880
V1808	Q1711	P1573	C1465	R1359	T1222	Q1095	P985	P881
R1809	G1720	F1574	P1466	Q1360	T1222	L1096	S986	V882
Q1810	T1721	P1574		C1361	G1225	L1096	Q987	V882
C1811	Y1722	L1582	T1469		Y1226	M1101		T885
T1812	S1723	L1582	F1470	N1364	R1227	M1101	M999	F886
A1813	S1723	L1582	A1471	T1365	C1228	C1110	V1000	T887
C1814	R1724	L1586		A1374	I1229	L1115	V1001	I888
		T1587	C1479	A1374			A1002	I888
L1817	C1730	V1588	Q1480		S1237			T892
	T1731	V1588	Q1481		N1238		V1006	T892
E1826	K1732	Y1594		S1377	E1239	K1125		P902
Q1827	C1733	Y1594		S1377	G1240	K1125		P902
		Q1597	G1485	P1388	G1240	E1130	T1011	N909
L1832	T1737	T1598	T1486	C1389		Y1131	T1012	N909
P1839	V1738	G1599	M1487	P1390	I1252	A1132	T1013	N909
	A1739	T1600		C1392	A1253	S1134	S1014	A914
		F1601	G1490	E1393		T1135	P1015	A914
S1844	S1745	D1602	G1491	E1393	A1257	V1143	N1018	ALA
K1845	T1748	D1603	R1492	G1395	L1258	V1143	P1019	SER
P1846	P1749	E1604	T1494	T1396	K1263	S1149	T1020	ALA
K1847		Q1607	Q1495	W1397	Y1264	S1149	T1021	ALA
		P1608	Q1496	S1398	S1265	L1150	P1022	ALA
R1850	N1757		M1497	K1399	I1266	L1150	TRP	TYR
T1851	P1759	K1611				N1167	ARG	ARG
P1856	D1760		V1501	C1405	T1275	N1167	VAL	VAL
R1871	S1761	W1614	T1502		H1276	L1174	SER	VAL
	A1762	S1615	N1503	R1414		P1175	THR	THR
	T1763	G1616	N1506	T1416	S1283	K1176	L1035	THR
S1926	S1764	S1765		W1417	S1283	G1177	R1036	ILE
	R1766	A1619	P1509	F1418	F1292	R1179	D1037	PRO
P1930		A1510	A1510		Q1293	T1180	P1038	ASP
P1931	P1769	A1530	L1511	Q1421	P1294	T1180	P1039	A931
S1935	Y1772	A1644	R1512	L1422	T1294	T1181	V1040	V937
A1936	Y1773	N1647	A1513	G1423	N1295	T1181	P1041	V937
			T1515	F1426	G1298	Y1186	P1042	T945
P1939	Y1780	T1552				E1187	S1045	T945
Q1945	A1781		K1527	D1430	C1301	L1188		T948
ASN	D1782	L1656	P1528	T1436	L1302	F1190	V1048	F949
GLY	N1783	L1656	T1529	T1436	P1303	S1191		T950
ASP	L1784	Q1661	V1530		C1304	N1192	A1051	T951
PRO		Q1661	T1531	E1440	F1308	Y1195	C1052	Y952
VAL	E1787	M1668	L1441	L1441	V1309	T1196	A1053	Y953
GLY	F1788	M1668	G1442	G1442	S1310	T1197	L1054	Y953
HIS		Q1672	M1536			G1198	Y1055	S957
ARG	P1791	Q1672	E1544	S1446	A1319	V1199	Q1058	L965
ARG	Y1705	T1677	N1549	P1450	A1319	R1200		L965
ARG	Y1705	T1677	L1550	C1454	T1324	C1311	M1061	T973
					P1325		P1062	ALA

• Molecule 1: Mastigoneme-like protein

Chain C:  70% 24% 5%

MET	ALA	MET	PRO	ARG	HIS	GLY	ARG	ARG	PRO	ALA	ARG	CYS	SER	SER	ASN	ALA	ALA	SER	PRO	ARG	PHE	LEU	LEU	LEU	VAL	LEU	GLY	VAL	ALA	LEU	ALA	ALA	SER	PRO	PRO	ARG	PHE	LEU	LEU	LEU	VAL	GLU	ALA	A43	L49	P54	S61	D62	A63	V64	A68	D74	F80	F81	T82
L83		T97	L101	L109	V110	Y115		T118	F126	V127	T128	L129		T146		L156	T157	A158		L161		R167	L168	A169	L170		R178	D188	M189	W190		I193	Q194	L195	R206	I207	F208	I209		N218		D225	Q226	V227	Y228	N229	L230	E231	T235	P244					
L250	F253	T254	P255	A260	V263	L271	V275	V280	D284	F288	T289	Q290	T293	E294	Y297	S298	A299	L306	Q307	W308	N311	E319	P335	A338	T339	A340	V341	N358	A359	L360	R361	Q362	L363	V364	D365		I371	L480	A372	E373	K374	I375		L387											
A388	L389	A390	K391	D395	P396	Y397	T398	D401	T402	I403	A407	T415	V418	W419	W420	T421	I422	D423	R432	T433	A434	L435	T436	M437	P445	N446	Q454	Y455	G458	K461	L462	A463	T464	L465	Y468	D469	R470	D471	T477	G478	L479	L480	L481	A482	S483	V490									



Y1808	N1707	C1462	T1327	V1201	N1059	G969	P872	ALA	I643	P506	V397	F81
R1809	S1708	L1463	D1328	A1202	Y1060	E970	P872	PRO	I644	F516	T398	T82
Q1810	I1709	P1464	T1334	A1202	X1061	S971	V876	ALA	R645	F517	D401	L83
T1812	K1715	C1465	T1334	Q1211	P1062	A972	K877	PHE	P650	K234	D87	D87
A1813	Y1594	P1466	I1350	Q1212	D1071	T973	T880	THR	P654	Q519	P244	T87
C1814	M1719	T1469	Y1351	C1213	F1077	ALA	P881	VAL	S685	F405	F253	L101
P1815	G1720	C1482	C1368	K1215	F1080	PRO	P882	THR	L686	S406	T254	S102
P1816	T1721	C1482	C1368	C1216	V1081	LEU	T883	THR	P657	A407	P255	
L1817	Y1722	G1485	C1361	T1220	T1081	THR	T884	THR	I658	K410	V261	N108
D1818	S1723	T1486	C1361	T1220	T1082	THR	T885	THR	L659	T415	L109	V110
L1819	R1724	T1486	C1361	D1224	A1083	LEU	P886	THR	S686	A535	L271	
N1823	E1728	M1490	T1365	D1224	V1084	SER	T889	THR	W683	F536	L271	
V1824	T1731	G1491	Y1366	C1229	A1085	VAL	T889	THR	D684	Q417	V280	Y115
V1825	K1732	D1492	T1229	I1229	T1086	T984	V894	THR	G685	V418	V280	
E1826	C1733	R1493	R1370	P1230	D1087	L988	P902	THR	W419	W419	D284	T118
T1829	P1734	T1494	M1379	C1231	D1093	L988	I903	THR	T421	W420	D284	T118
L1832	T1737	M1497	D1394	E1239	L1096	M999	P902	THR	T673	W551	D284	T118
G1833	V1738	A1498	D1394	C1247	R1097	V1000	I903	THR	T673	P671	D284	T118
S1834	F1618	L1499	W1397	C1247	R1097	V1000	I903	THR	D674	W551	D284	T118
Q1835	G1616	T1494	S1398	E1239	C1110	A1002	G910	THR	T673	A555	F288	I122
P1839	C1627	N1503	K1399	T1251	T1111	V1006	A914	THR	G676	N556	T289	L129
L1842	T1634	N1506	C1405	A1253	F1112	E1009	PRO	THR	W677	G560	Q290	L129
L1843	F1635	R1512	Q1406	P1255	L1115	S1010	ALA	THR	A434	I565	E294	Y132
P1867	T1636	A1513	P1410	A1256	F1126	T1011	ALA	THR	L435	I570	Y297	L141
P1868	A1644	T1515	P1410	A1257	F1127	T1012	ALA	THR	M436	P571	A299	D153
R1871	T1645	M1519	R1414	R1261	V1128	S1014	TYR	THR	T438	I574	L306	S154
P1883	F1646	V1520	M1415	H1272	F1129	P1015	TRP	THR	N439	R579	Q367	T155
P1902	M1647	Y1526	F1418	H1276	E1130	P1022	VAL	THR	A444	L588	W308	L161
P1903	I1652	A1526	Q1421	H1276	Y1131	P1022	VAL	THR	P445	L592	E319	
P1920	A1660	K1527	L1422	E1282	A1138	T1028	THR	THR	N446	L592	A338	
P1921	Q1661	V1530	G1423	K1285	H1139	T1031	THR	THR	L462	F595	A338	
S1926	A1662	F1537	D1430	K1286	A1140	F1032	ILE	THR	T464	I596	V341	R178
S1935	P1663	E1544	T1436	K1289	V1143	L1034	ASP	THR	R466	P600	R360	S182
S1939	M1668	T1548	T1439	F1282	T1148	L1035	V837	THR	I467	F611	L361	W190
G1945	F1671	N1549	E1440	Q1293	S1149	R1036	M938	THR	Y468	Q612	R362	
ASN	Q1672	T1555	S1443	P1294	L1150	D1037	M938	THR	D469	V613	L363	
GLY	C1680	T1555	G1444	N1295	P1165	P1038	T944	THR	D840	L614	Y364	I193
ASP	C1683	K1567	C1445	T1299	P1175	P1041	T945	THR	G472	A615	D471	Q194
ASP	C1683	P1569	P1450	V1300	F1178	P1042	T951	THR	G478	P618	V370	L195
PRO	V1685	T1570	G1451	C1304	Y1186	Q1049	Y952	THR	L481	T619	I371	F202
VAL	G1686	F1571	T1452	C1304	E1187	Y1050	Y953	THR	I375	Y620	A372	
GLY	T1687	M1572	A1454	S1310	Y1195	C1052	S957	THR	T491	S623	I375	
HIS	D1894	P1573	P1455	T1311	Y1195	C1052	F961	THR	A496	V631	Y365	N218
ARG	R1805	F1574	T1456	T1312	V1199	Y1055	L965	THR	L497	D634	L389	P224
ARG	P1806	T1578	F1457	Y1326	V1199	Y1055	L965	THR	F504	Y641	T393	D225
ALA	G1807	Q1706	H1326	H1326	R1200	Q1058	F968	THR	Y227	N642	Y228	Y228

11956	H	Q1982
		PRO
		GLN
		ASP
		ASP
		GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.733	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.0728	Depositor
Map size (\AA)	229.8, 229.8, 919.2	wwPDB
Map dimensions	200, 200, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.149, 1.149, 1.149	Depositor

5 Model quality

5.1 Standard geometry

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	0.38	6/14067 (0.0%)	0.63	15/19393 (0.1%)
1	B	0.49	7/14067 (0.0%)	0.70	26/19393 (0.1%)
1	C	0.41	5/14067 (0.0%)	0.60	16/19393 (0.1%)
1	D	0.41	5/14067 (0.0%)	0.65	18/19393 (0.1%)
All	All	0.42	23/56268 (0.0%)	0.65	75/77572 (0.1%)

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	4
1	B	0	10
1	C	0	1
1	D	0	2
All	All	0	17

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	396	PRO	CG-CD	-29.39	0.53	1.50
1	C	396	PRO	CG-CD	-27.30	0.60	1.50
1	D	1769	PRO	CG-CD	-21.49	0.79	1.50
1	B	1769	PRO	CG-CD	-20.80	0.82	1.50
1	A	396	PRO	CB-CG	19.42	2.47	1.50

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	PRO	CB-CG-CD	-27.30	0.04	106.50
1	D	1769	PRO	N-CD-CG	-26.92	62.81	103.20
1	D	1769	PRO	CA-CB-CG	-20.53	64.99	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1769	PRO	N-CD-CG	-19.02	74.66	103.20
1	B	1769	PRO	CA-CB-CG	-18.34	69.16	104.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1527	LYS	Peptide
1	A	395	ASP	Peptide
1	A	397	VAL	Peptide
1	A	398	THR	Peptide
1	B	392	THR	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	13687	0	13241	358	0
1	B	13687	0	13240	327	0
1	C	13687	0	13241	341	0
1	D	13687	0	13241	307	0
All	All	54748	0	52963	1295	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 1295 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:532:ILE:HD11	1:A:594:CYS:HB3	1.47	0.97
1:A:1515:THR:HG21	1:C:1192:ASN:HD22	1.40	0.85
1:C:659:LEU:HB2	1:C:719:ILE:O	1.76	0.85
1:C:401:ASP:OD1	1:C:402:THR:N	2.10	0.85
1:A:358:ASN:HB3	1:A:375:ILE:HD11	1.58	0.84

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	1884/1987 (95%)	1738 (92%)	132 (7%)	14 (1%)	19	54
1	B	1884/1987 (95%)	1725 (92%)	133 (7%)	26 (1%)	9	39
1	C	1884/1987 (95%)	1727 (92%)	139 (7%)	18 (1%)	13	46
1	D	1884/1987 (95%)	1726 (92%)	137 (7%)	21 (1%)	12	45
All	All	7536/7948 (95%)	6916 (92%)	541 (7%)	79 (1%)	16	46

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	THR
1	A	1062	PRO
1	A	1143	VAL
1	B	169	ASN
1	B	393	THR

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	1488/1571 (95%)	1445 (97%)	43 (3%)	37	59
1	B	1488/1571 (95%)	1437 (97%)	51 (3%)	32	55
1	C	1488/1571 (95%)	1443 (97%)	45 (3%)	36	58
1	D	1488/1571 (95%)	1441 (97%)	47 (3%)	34	56
All	All	5952/6284 (95%)	5766 (97%)	186 (3%)	37	56

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1238	ASN
1	D	389	LEU
1	C	1380	LEU
1	C	1601	PHE
1	D	723	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	446	ASN
1	C	1672	GLN
1	C	1272	HIS
1	D	218	ASN
1	A	1810	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 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 ⓘ

There are no chain breaks in this entry.

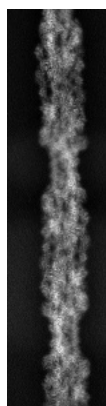
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41679. These allow visual inspection of the internal detail of the map and identification of artifacts.

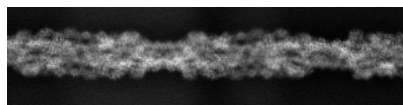
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

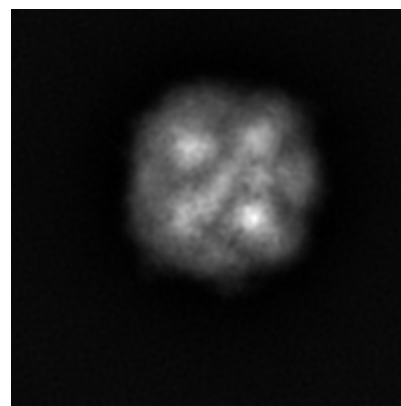
6.1.1 Primary map



X



Y

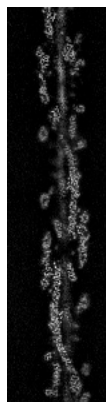


Z

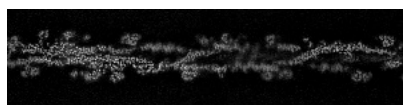
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

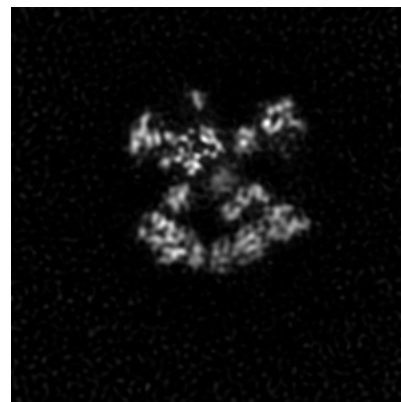
6.2.1 Primary map



X Index:
100



Y Index: 100

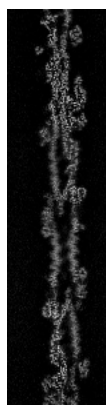


Z Index: 400

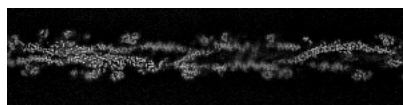
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

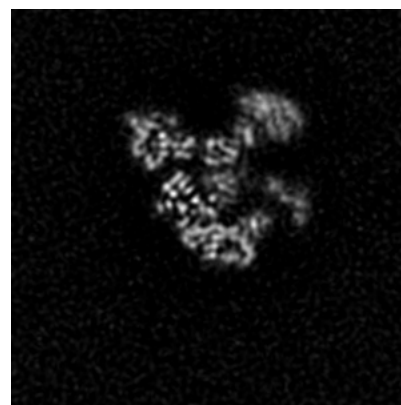
6.3.1 Primary map



X Index:
122



Y Index: 99

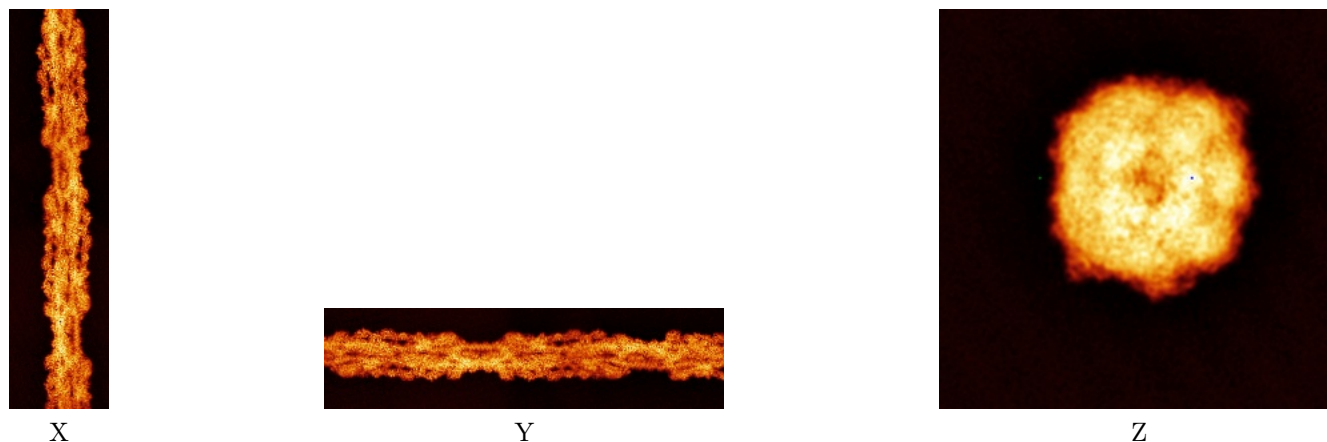


Z Index: 264

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

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

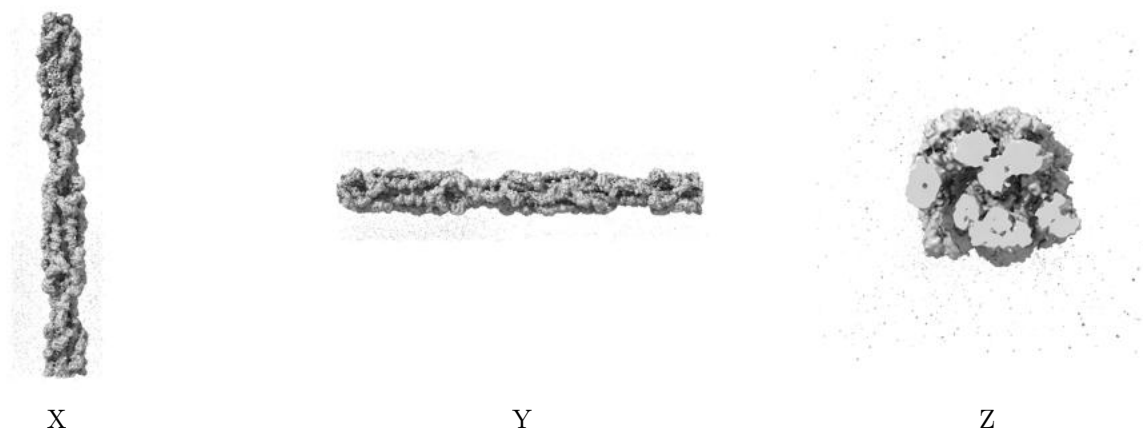
6.4.1 Primary map



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 0.0728. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

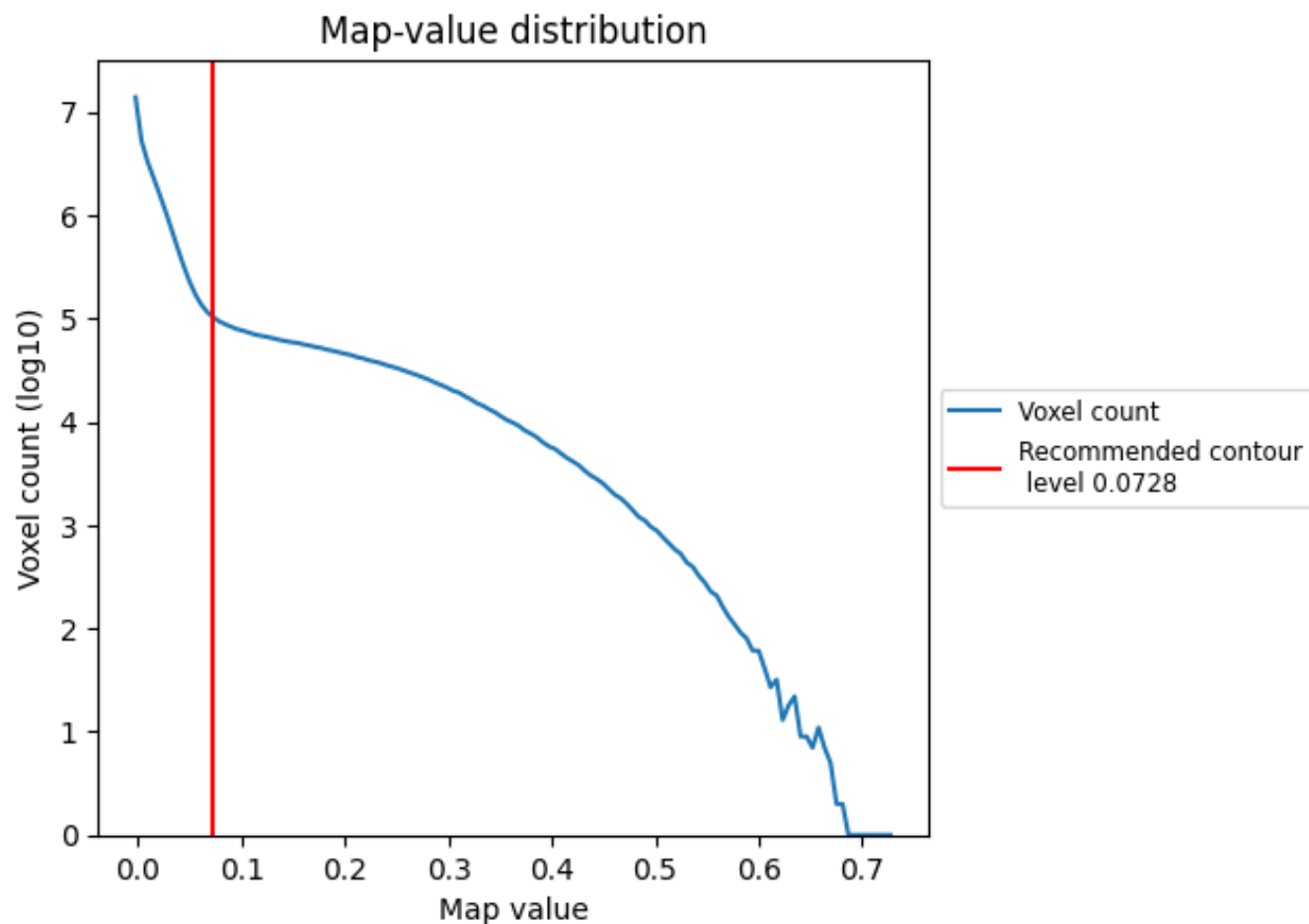
6.6 Mask visualisation

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

7 Map analysis [i](#)

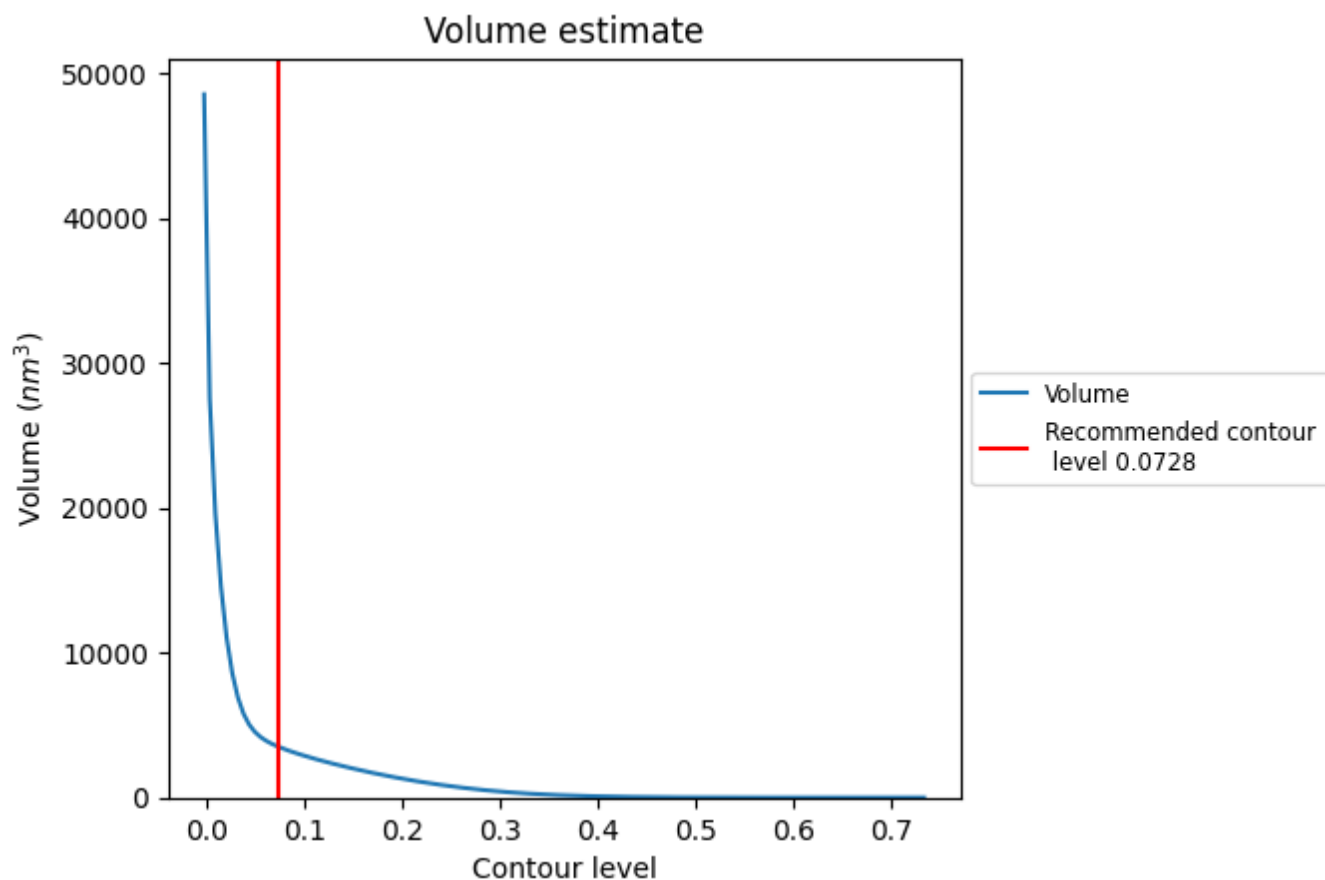
This section contains the results of statistical analysis of the map.

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 3533 nm³; this corresponds to an approximate mass of 3192 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

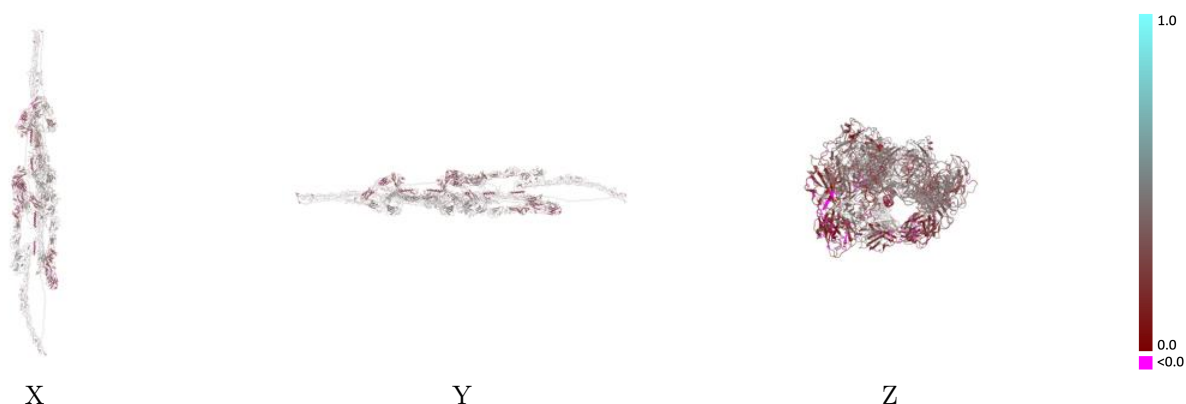
This section contains information regarding the fit between EMDB map EMD-41679 and PDB model 8TXB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0728 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](#)



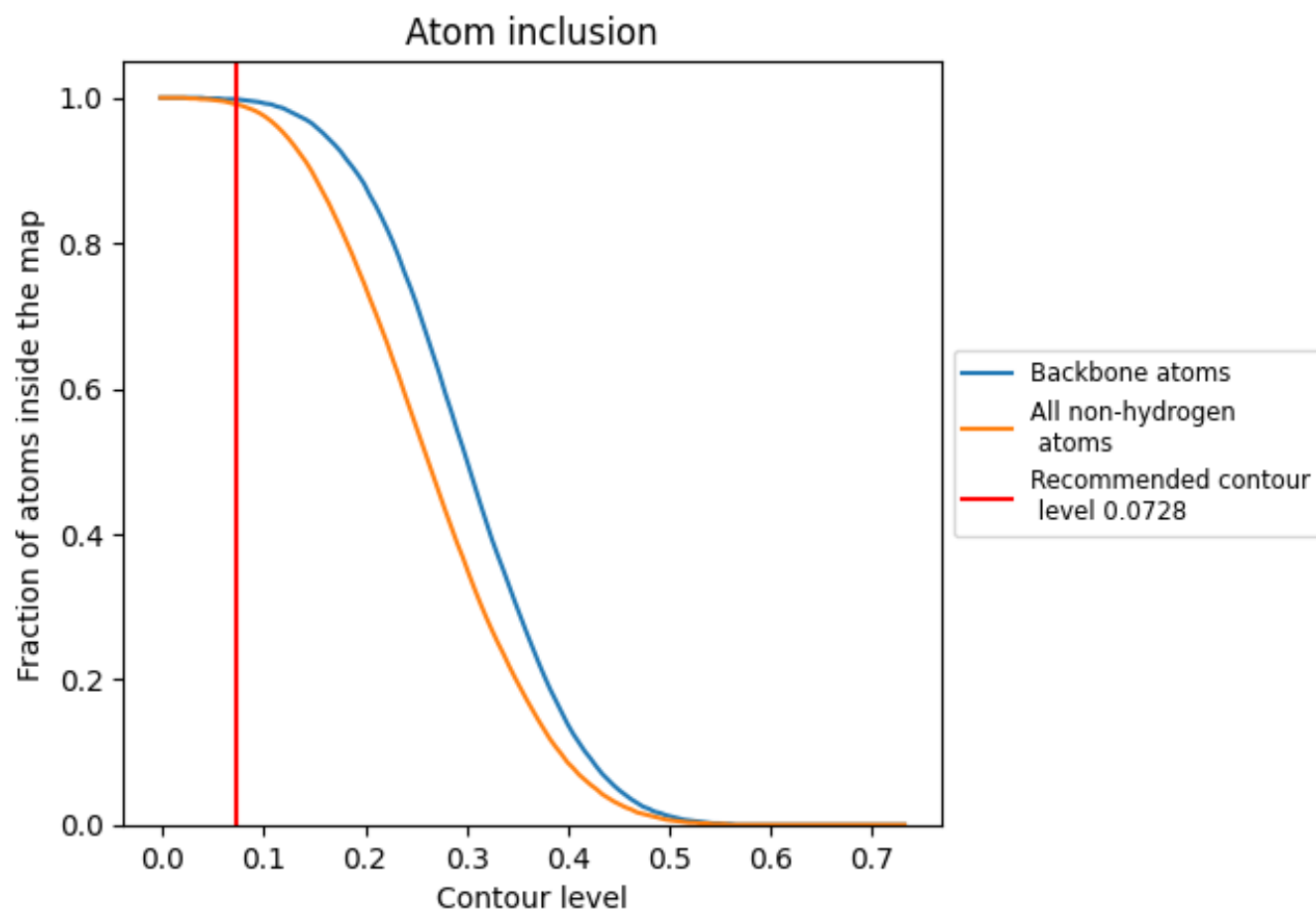
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0728).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0728) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9910	<div></div> 0.3500
A	<div></div> 0.9910	<div></div> 0.3490
B	<div></div> 0.9930	<div></div> 0.3620
C	<div></div> 0.9930	<div></div> 0.3500
D	<div></div> 0.9880	<div></div> 0.3360

