wwPDB EM Validation Summary Report

Oct 28, 2023 – 12:35 PM EDT

PDB ID	:	8TXB
EMDB ID	:	EMD-41679
Title	:	Characterization of the Chlamydomonas Flagellar Mastigoneme Filament Structure at 3.9A
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*
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:

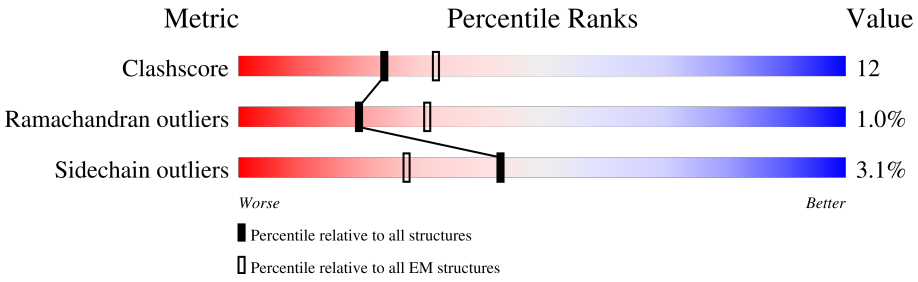
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	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 <=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	69% 25% • 5%
1	B	1987	69% 24% • 5%
1	C	1987	70% 24% • 5%
1	D	1987	70% 24% • 5%

2 Entry composition (i)

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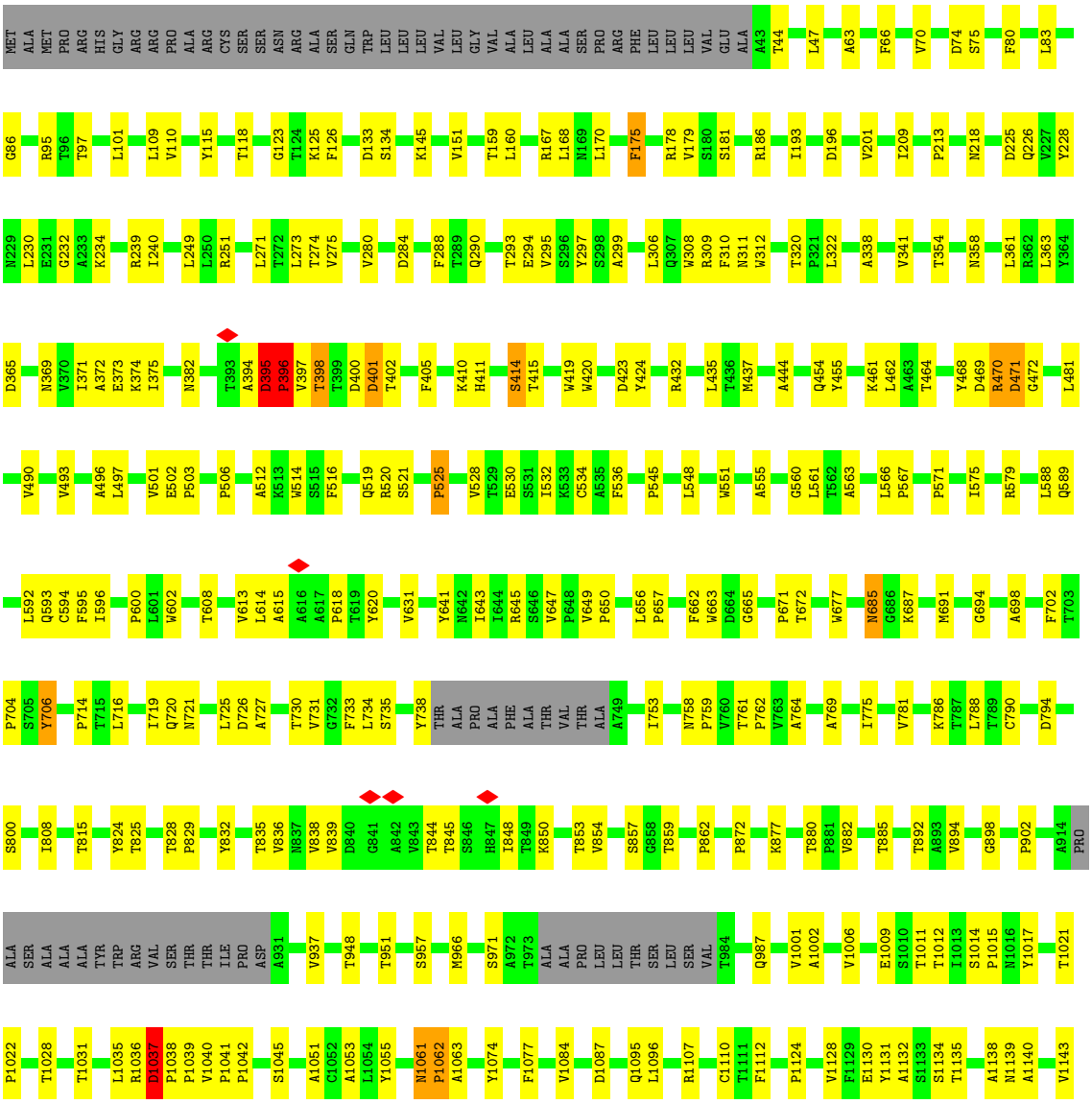
Chain	Residue	Modelled	Actual	Comment	Reference
D	1986	ASP	-	expression tag	UNP Q8LRM7
D	1987	GLU	-	expression tag	UNP Q8LRM7

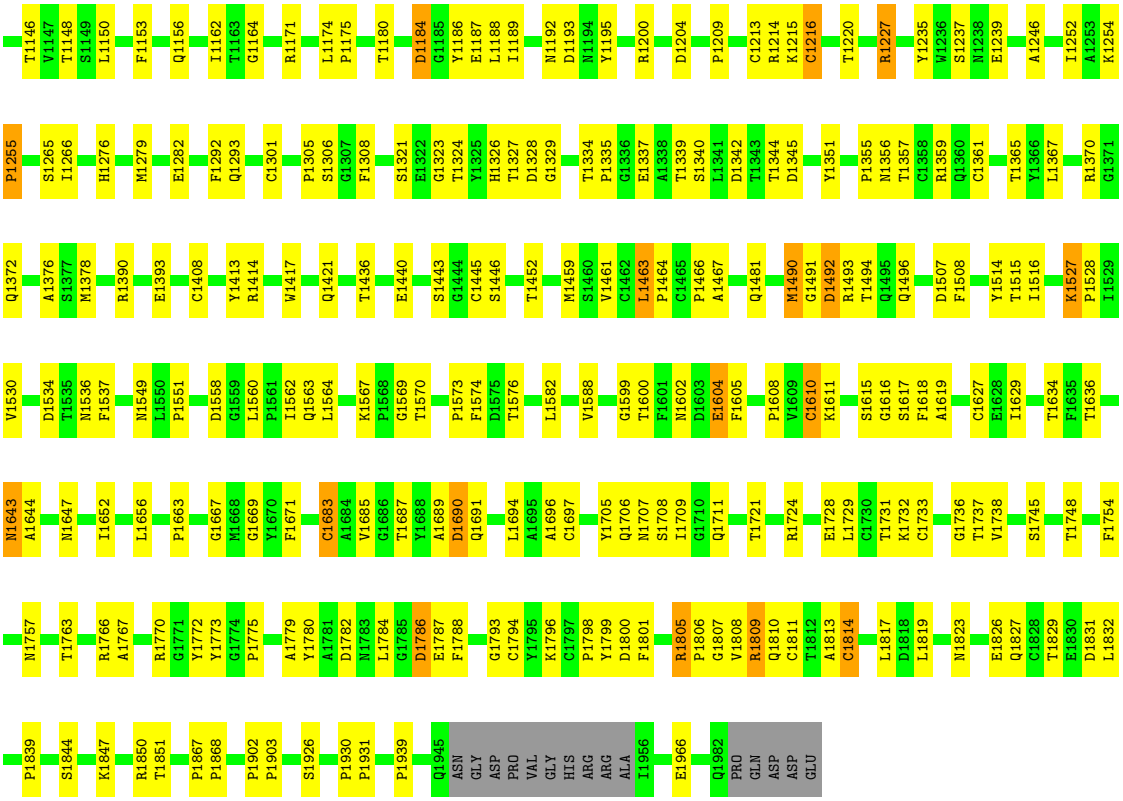
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mastigoneme-like protein

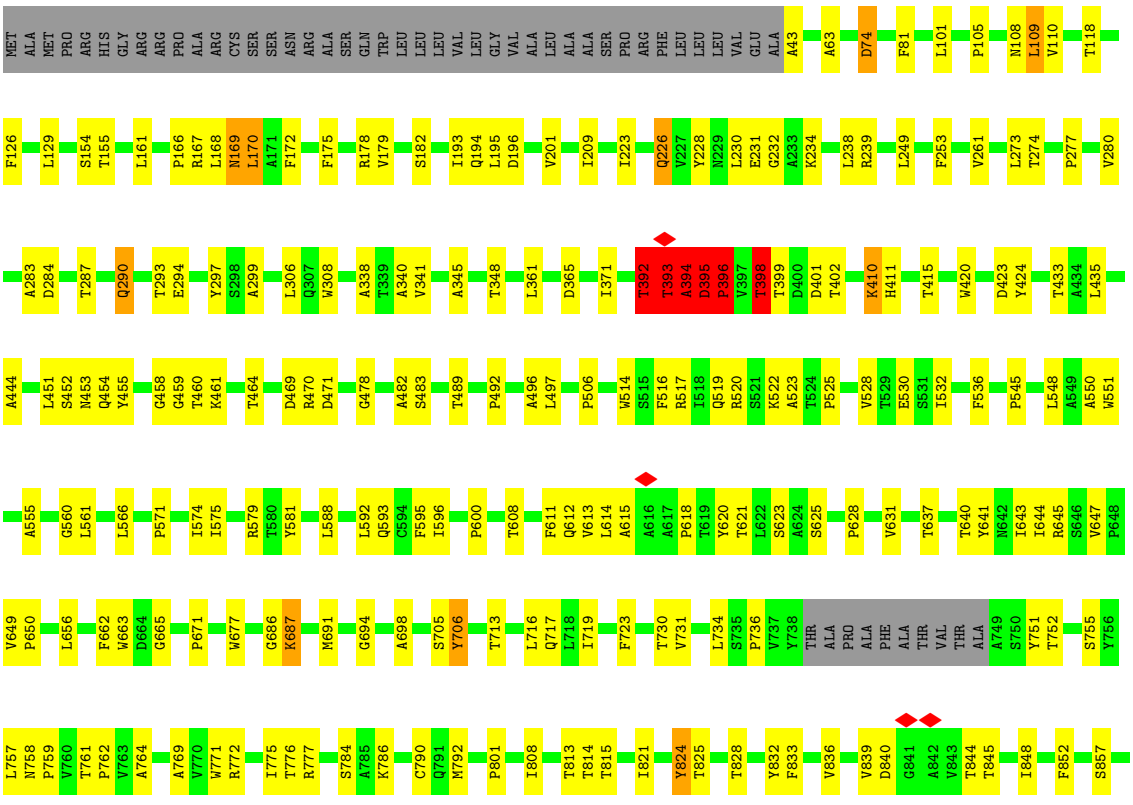
Chain A:

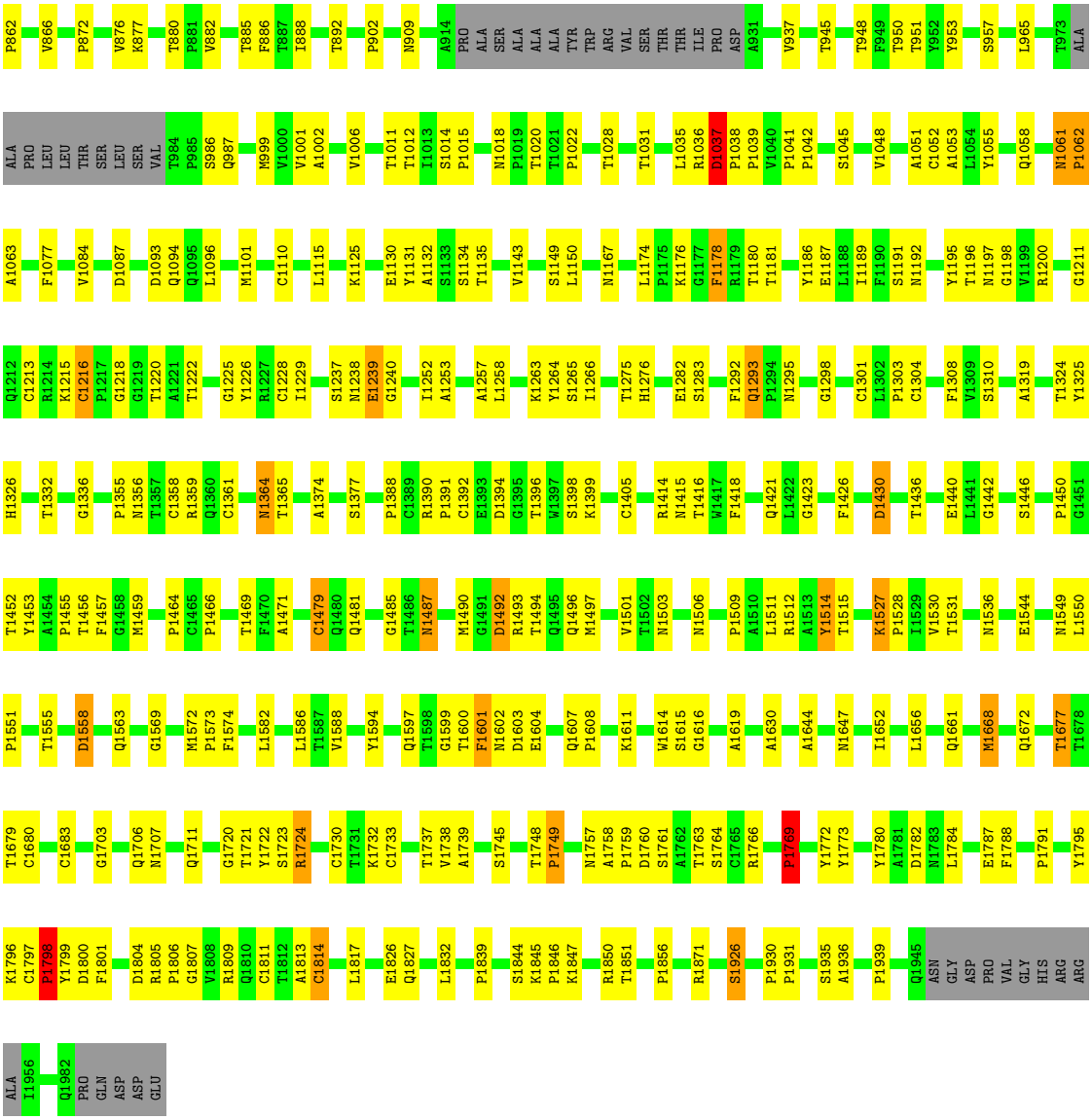




• Molecule 1: Mastigoneme-like protein

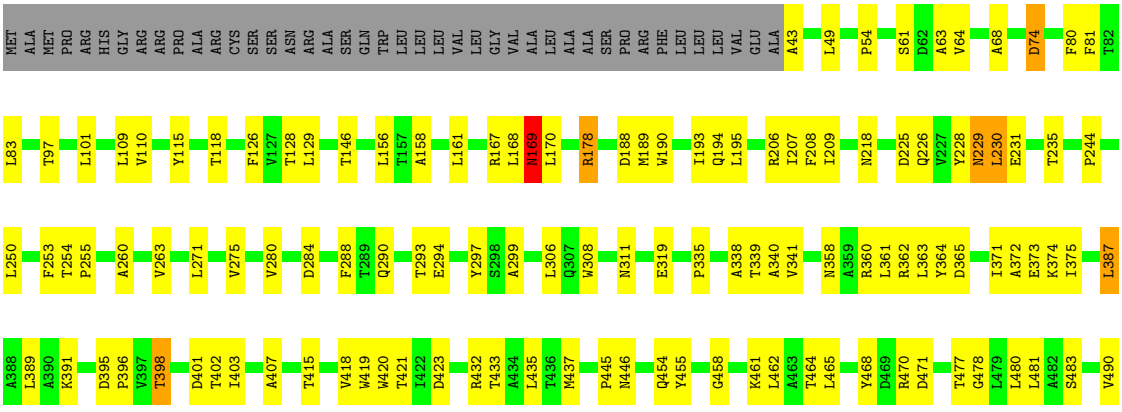
Chain B:

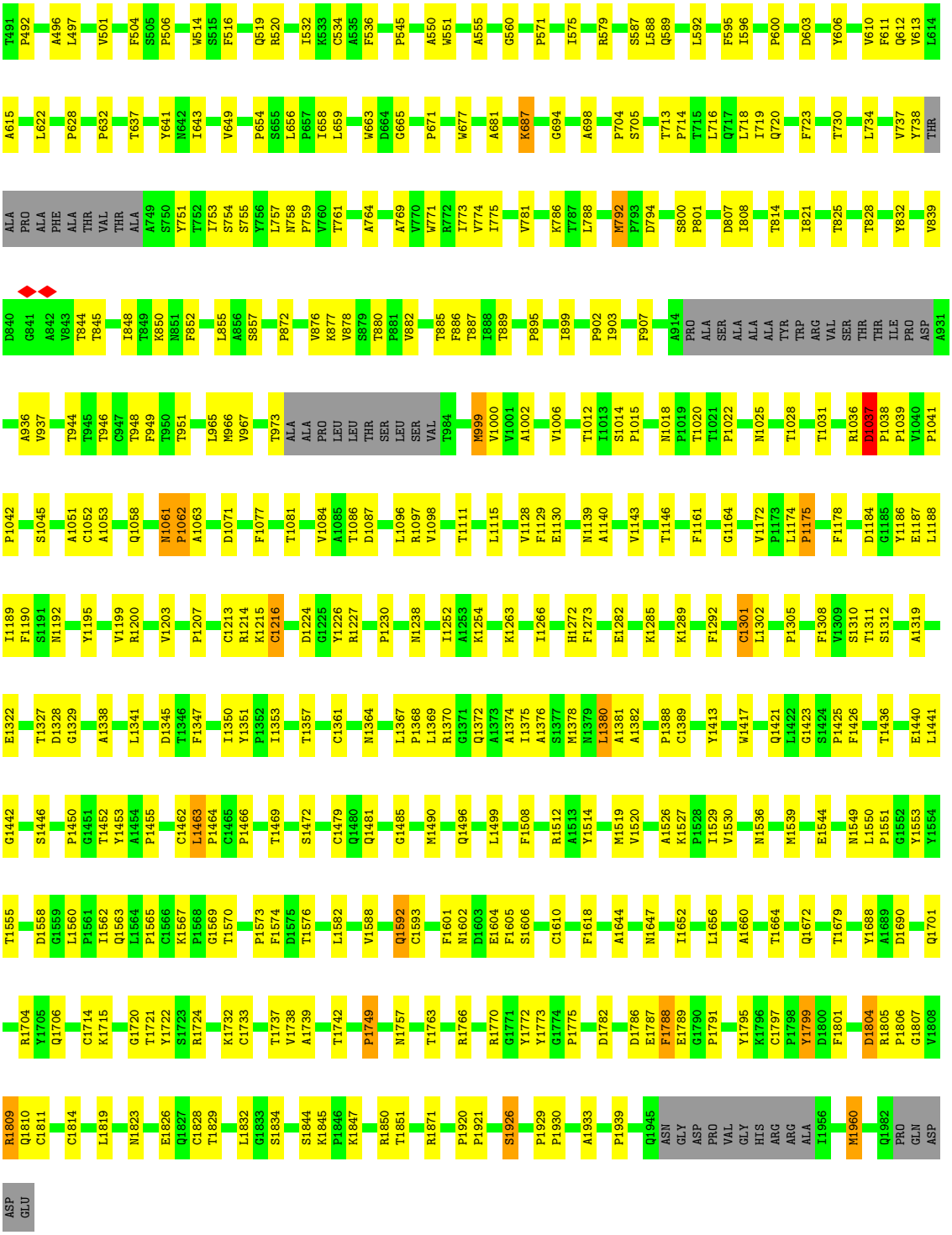




• Molecule 1: Mastigoneme-like protein

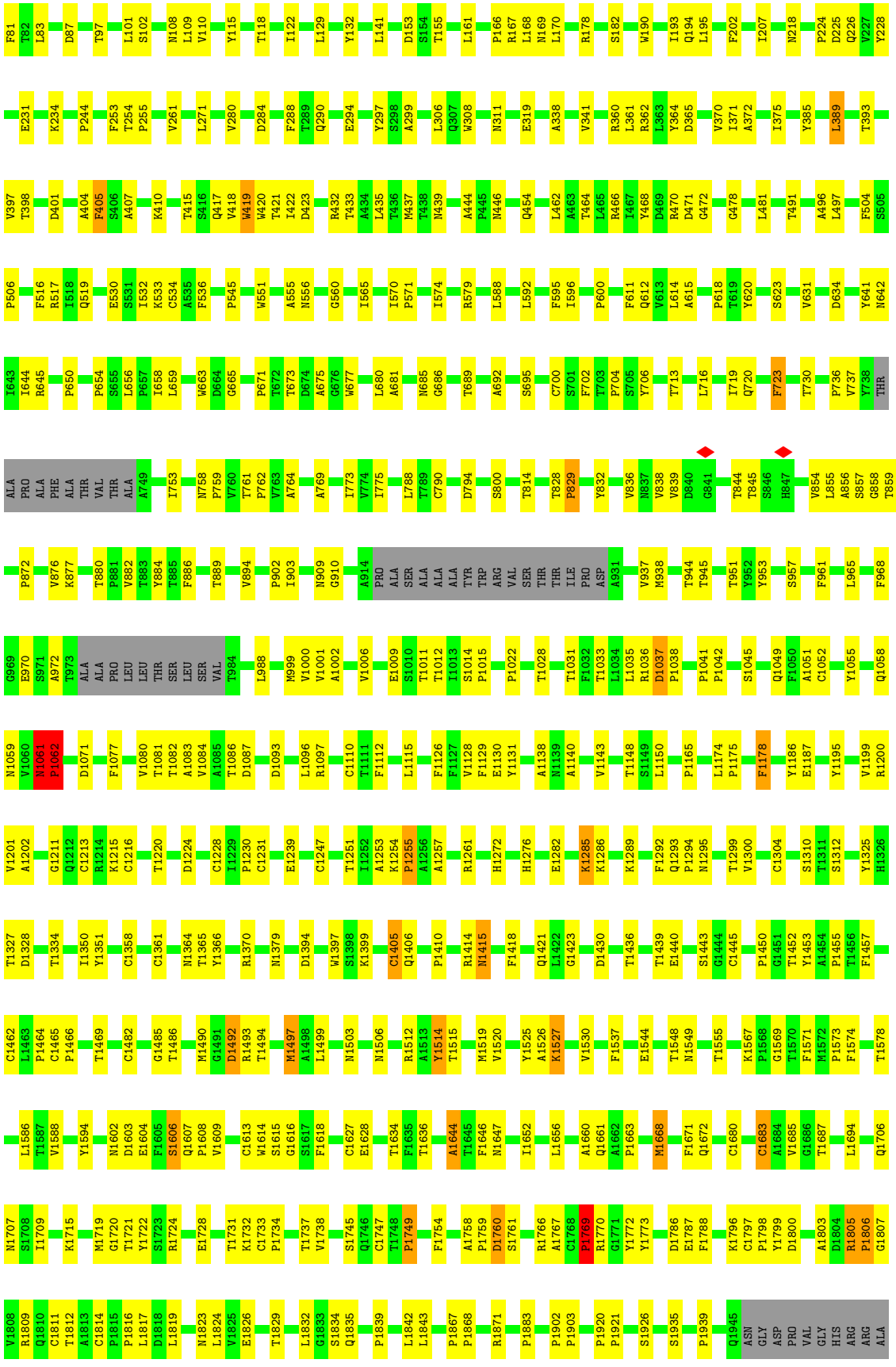
Chain C:





• Molecule 1: Mastigoneme-like protein

Chain D: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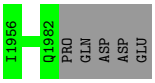
E231 K234 P244 F253 T254 P255 V261 L271 V280 D284 F288 T289 Q290 E294 Y297 S298 A299 L306 Q307 W308 N311 E319 A338 V341 R360 L361 R362 L363 Y364 D365 V370 I371 A372 I375 Y385 L389 T393
V397 T398 D401 A404 F405 S406 A407 K410 T415 S416 Q417 V418 W419 W420 T421 I422 D423 R432 T433 A434 L435 T436 M437 T438 N439 A444 P445 N446 Q454 L462 A463 T464 L465 R466 I467 Y468 D469 R470 D471 G472 G478 L481 T491 A496 L497 F504 S505
P506 F516 R517 I518 Q519 E530 S531 I532 K533 C534 A535 F536 P545 W551 A555 N556 G560 I565 L570 P571 I574 R579 L588 L592 F595 I596 P600 F611 Q612 V613 L614 A615 P618 T619 Y620 S623 V631 D634 P636 V737 Y738 THR
I643 I644 R645 P650 P654 S655 L656 P657 I658 L659 W663 D664 G665 P671 T672 T673 D674 A675 G676 W677 L680 A681 N685 G686 T689 A692 S695 C700 S701 F702 T703 P704 S705 Y706 T713 L716 I719 Q720 F723 T730 P736 V737 Y738 THR
ALA PRO ALA PHE ALA THR VAL THR ALA A749 I753 N758 P759 V760 T761 P762 V763 A764 A769 I773 V774 I775 L788 T789 C790 D794 S800 T814 T828 P829 Y832 V836 N837 V838 V839 D840 G841 T844 T845 S846 H847 V854 L855 A856 S857 G858 T859
P872 V876 K877 T880 P881 V882 T883 Y884 T885 F886 T889 V894 P902 I903 N909 G910 A914 PRO ALA SER ALA ALA ALA TYR TRP ARG VAL SER THR THR ILE PRO ASP A931 V937 M938 T944 T945 T951 Y952 Y953 S957 F961 L965 F968
G969 E970 S971 A972 T973 ALA ALA PRO LEU LEU THR SER LEU SER VAL T984 L988 M999 V1000 V1001 A1002 V1006 E1009 S1010 T1011 T1012 I1013 S1014 P1015 P1022 T1028 T1031 F1032 T1033 L1034 L1035 R1036 D1037 P1038 P1041 P1042 S1045 Q1049 F1050 A1051 C1052 Y1055 Q1058
N1059 V1060 N1061 P1062 D1071 F1077 V1080 T1081 T1082 A1083 V1084 A1085 T1086 D1087 D1093 L1096 R1097 C1110 T1111 F1112 L1115 F1126 F1127 V1128 F1129 E1130 Y1131 A1138 N1139 A1140 V1143 T1148 S1149 L1150 P1165 L1174 P1175 F1178 Y1186 E1187 Y1195 V1199 R1200
V1201 A1202 G1211 Q1212 C1213 R1214 K1215 C1216 T1220 D1224 C1228 I1229 P1230 C1231 E1239 C1247 T1251 I1252 A1253 K1254 P1255 A1256 A1257 R1261 H1272 H1276 E1282 K1285 K1286 K1289 F1292 Q1293 P1294 N1295 T1299 V1300 C1304 S1310 T1311 S1312 Y1325 H1326
T1327 D1328 T1334 I1350 Y1351 C1358 C1361 N1364 T1365 Y1366 R1370 N1379 D1394 W1397 S1398 K1399 C1405 Q1406 P1410 R1414 N1415 F1418 Q1421 L1422 G1423 D1430 T1436 T1439 E1440 S1443 G1444 C1445 P1450 G1451 T1452 Y1453 A1454 P1455 T1456 F1457
C1462 L1463 P1464 C1465 P1466 T1469 C1482 G1485 T1486 M1490 G1491 D1492 R1493 T1494 M1497 A1498 L1499 N1503 N1506 R1512 A1513 Y1514 T1515 M1519 V1520 Y1525 A1526 K1527 V1530 F1537 E1544 T1548 N1549 T1555 K1567 P1568 G1569 T1570 F1571 M1572 P1573 F1574 T1578
L1586 T1587 V1588 Y1594 N1602 D1603 E1604 F1605 S1606 Q1607 P1608 V1609 C1613 W1614 S1615 G1616 S1617 F1618 C1627 E1628 T1634 F1635 T1636 A1644 T1645 F1646 N1647 I1652 L1656 A1660 Q1661 A1662 P1663 M1668 F1671 Q1672 C1680 C1683 A1684 V1685 G1686 T1687 Q1706
N1707 S1708 I1709 K1715 M1719 G1720 T1721 Y1722 S1723 R1724 E1728 T1731 K1732 C1733 P1734 T1737 V1738 S1745 Q1746 C1747 T1748 P1749 F1754 A1758 P1759 D1760 S1761 R1766 A1767 C1768 P1769 R1770 G1771 Y1772 Y1773 D1786 E1787 F1788 K1796 C1797 P1798 Y1799 D1800 A1803 D1804 R1805 P1806 G1807
V1808 R1809 Q1810 C1811 T1812 A1813 C1814 P1815 P1816 L1817 D1818 L1819 N1823 L1824 V1825 E1826 T1829 L1832 G1833 S1834 Q1835 P1839 L1842 L1843 P1867 P1868 R1871 P1883 P1902 P1903 P1920 P1921 S1926 S1935 P1939 Q1945 ASN GLY ASP PRO VAL GLY HIS ARG ARG ALA


I1956
Q1962
PRO
GLN
ASP
ASP
GLU

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	229.8, 229.8, 919.2	wwPDB
Map dimensions	200, 200, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.149, 1.149, 1.149	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	0.38	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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	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 (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	1884/1987 (95%)	1738 (92%)	132 (7%)	14 (1%)	22	60
1	B	1884/1987 (95%)	1725 (92%)	133 (7%)	26 (1%)	11	46
1	C	1884/1987 (95%)	1727 (92%)	139 (7%)	18 (1%)	15	52
1	D	1884/1987 (95%)	1726 (92%)	137 (7%)	21 (1%)	14	51
All	All	7536/7948 (95%)	6916 (92%)	541 (7%)	79 (1%)	20	52

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 (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	1488/1571 (95%)	1445 (97%)	43 (3%)	42	65
1	B	1488/1571 (95%)	1437 (97%)	51 (3%)	37	62
1	C	1488/1571 (95%)	1443 (97%)	45 (3%)	41	64
1	D	1488/1571 (95%)	1441 (97%)	47 (3%)	39	63
All	All	5952/6284 (95%)	5766 (97%)	186 (3%)	43	64

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 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.

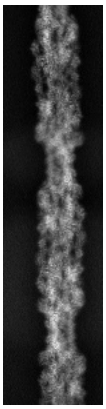
6 Map visualisation

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.

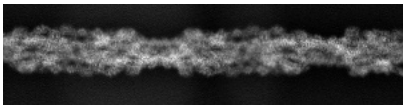
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

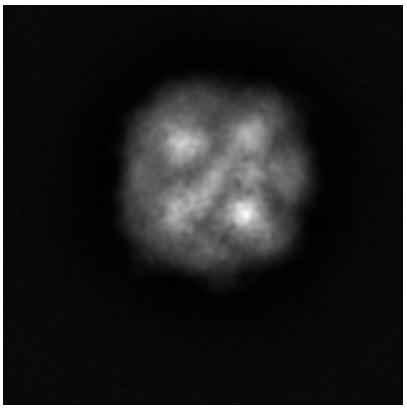
6.1.1 Primary map



X



Y

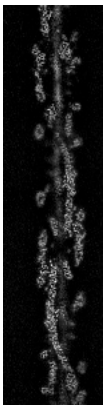


Z

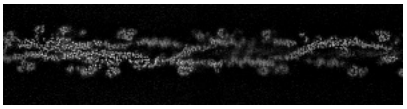
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

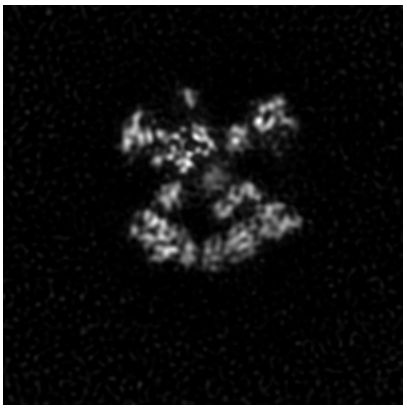
6.2.1 Primary map



X Index: 100



Y Index: 100

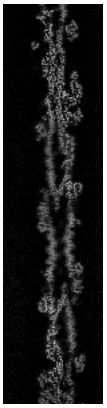


Z Index: 400

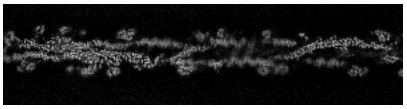
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

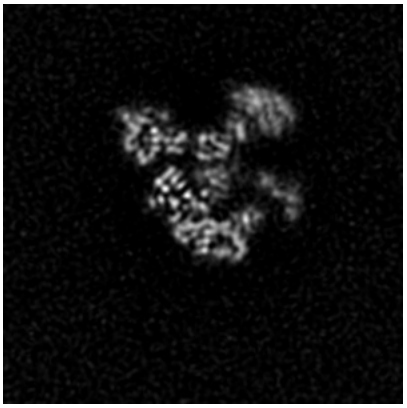
6.3.1 Primary map



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)

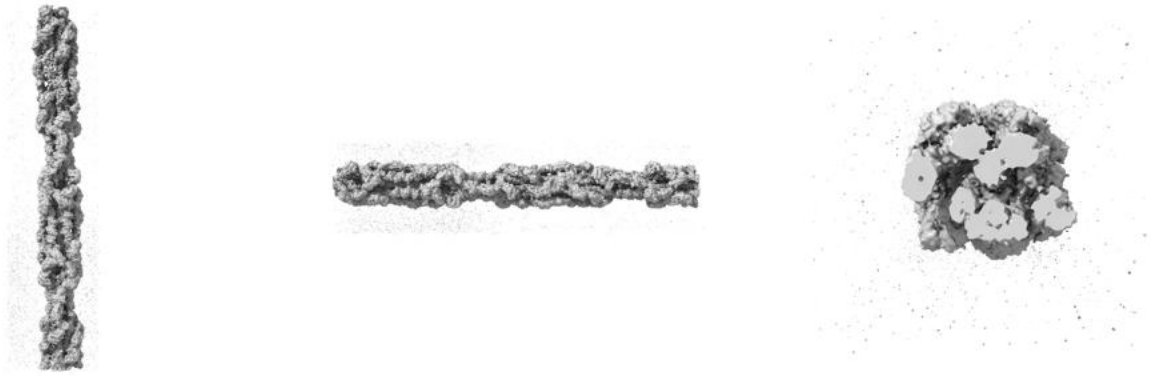
6.4.1 Primary map

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

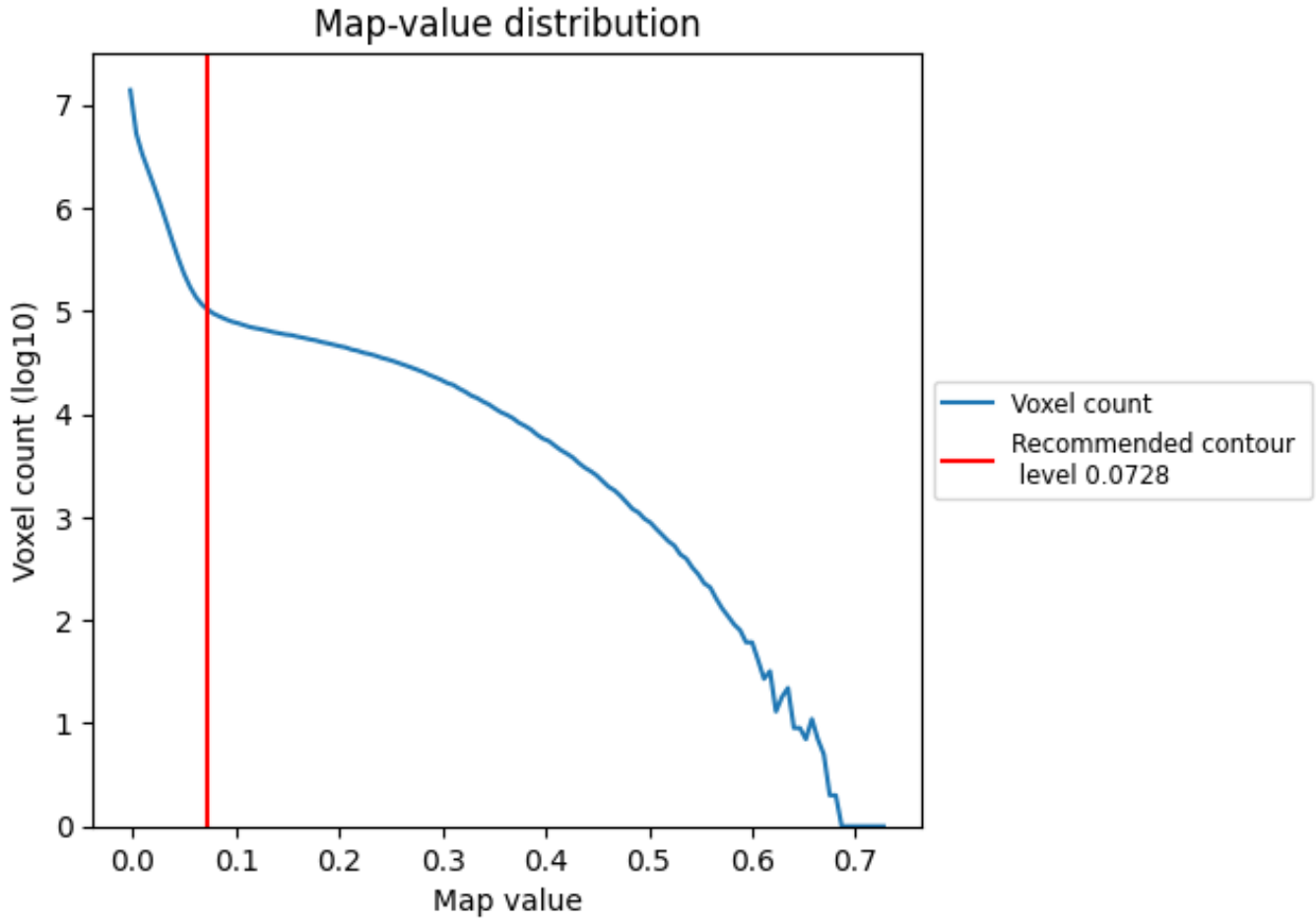
6.6 Mask visualisation (i)

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

7 Map analysis

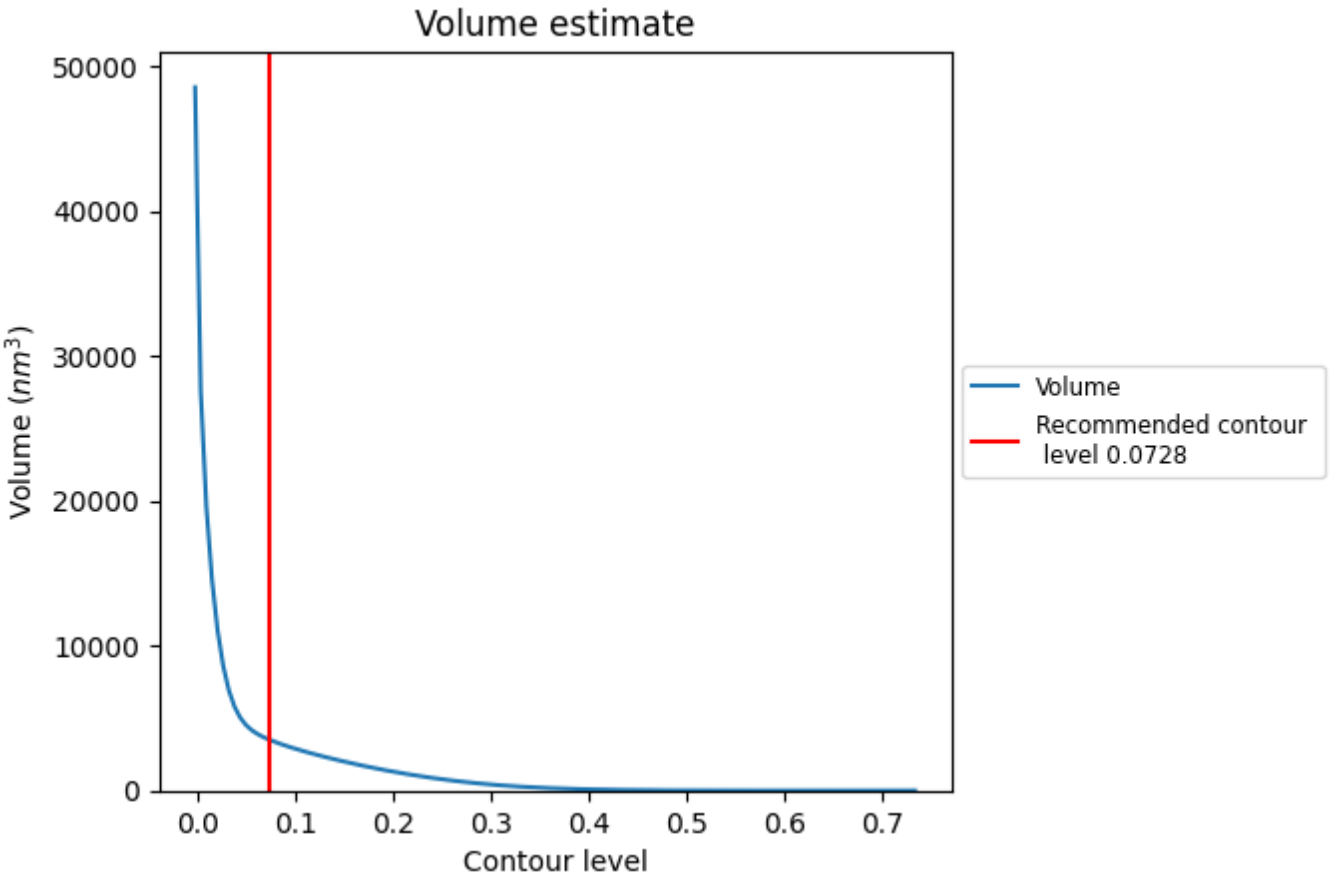
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 nm^3; 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 (i)

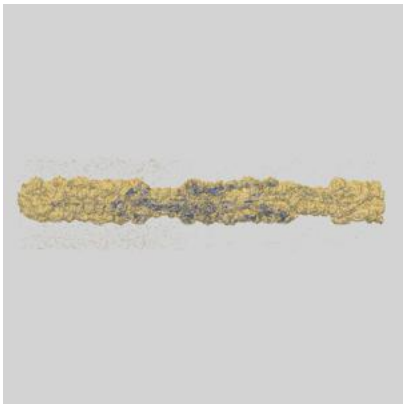
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

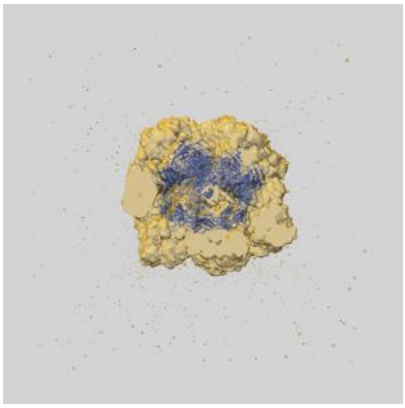
This section contains information regarding the fit between EMDB map EMD-41679 and PDB model 8TXB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay

X



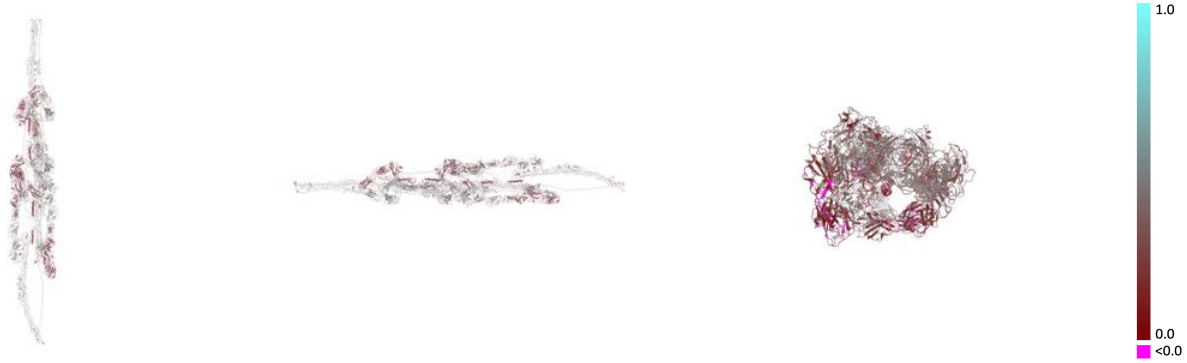
Y



Z

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



X Y Z

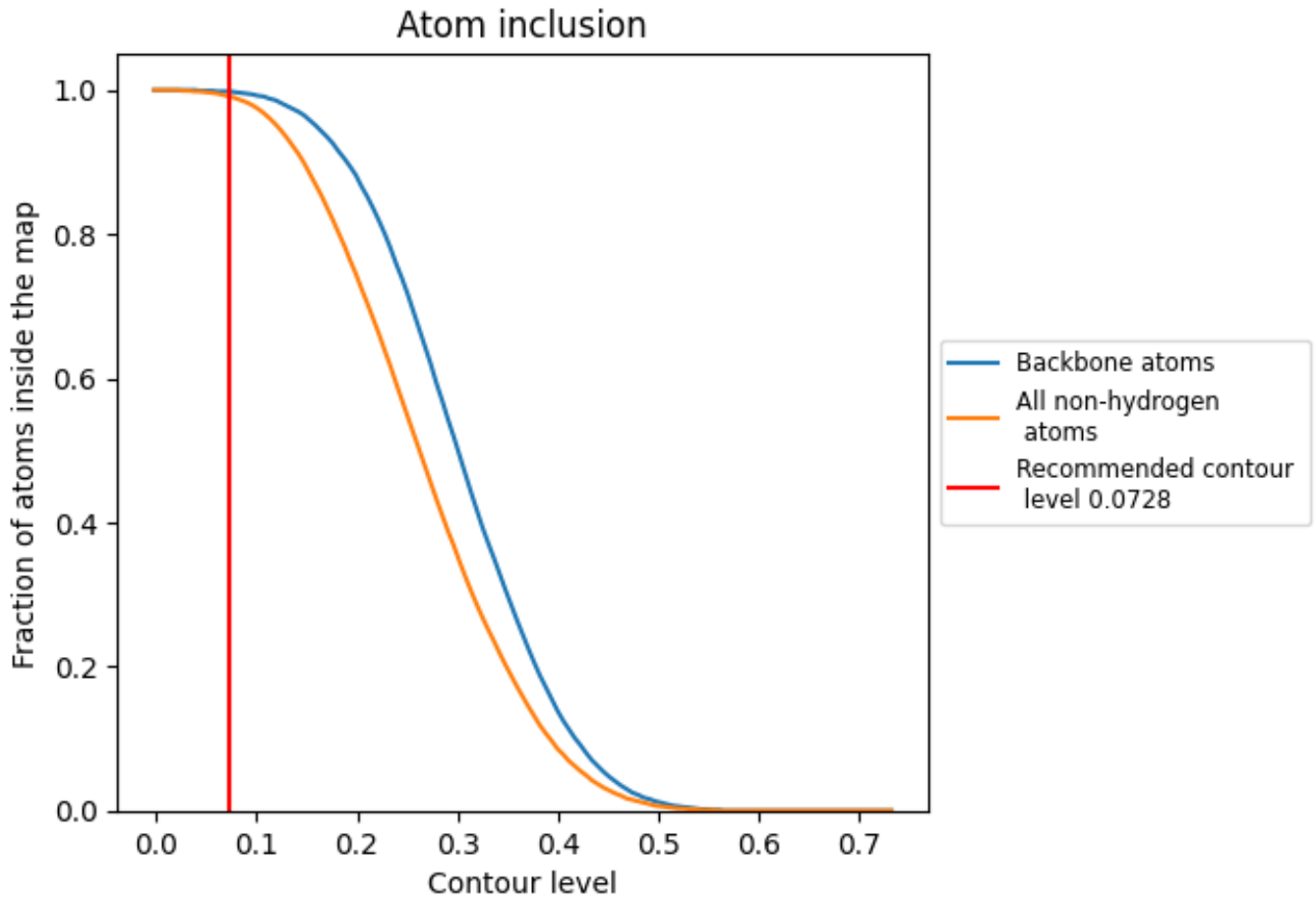
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (i)



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	0.9910	0.3500
A	0.9910	0.3490
B	0.9930	0.3620
C	0.9930	0.3500
D	0.9880	0.3360