



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2023 – 06:55 AM EDT

PDB ID : 8U95
EMDB ID : EMD-42024
Title : The structure of myosin heavy chain from *Drosophila melanogaster* flight muscle thick filaments
Authors : Abbasi Yeganeh, F.; Rastegarpouyani, H.; Li, J.; Taylor, K.A.
Deposited on : 2023-09-18
Resolution : 4.70 Å(reported)

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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.dev50
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) : 2.35.1

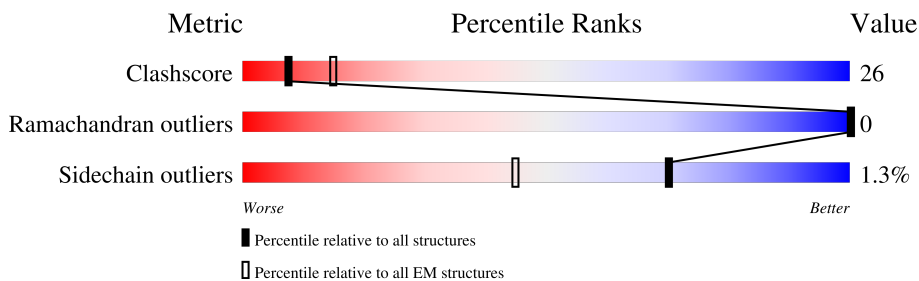
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1949	<p>52% (Poor fit), 26% (0 outliers), 25% (1 outlier), 48% (Not modelled)</p>
1	B	1949	<p>52% (Poor fit), 25% (0 outliers), 26% (1 outlier), 48% (Not modelled)</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16352 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 Myosin heavy chain, isoform U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1009	Total	C	N	O	S	0	0
			8176	4946	1527	1695	8		
1	B	1009	Total	C	N	O	S	0	0
			8176	4946	1527	1695	8		

VAL	SER	ARG	ILE	ASP	GLU	ILE	ALA	LEU	GLU	GLY	LYS	ALA	LEU	GLN	ASP	TYR																																																																																																							
Q1561	L1562	E1563	L1564	S1565	Q1566	V1567	R1568	E1569	E1570	I1571	D1572	R1573	R1574	I1575	Q1576	E1577	K1578	E1579	E1580	E1581	F1582	E1583	M1584	T1585	R1586	K1587	M1588	H1589	E1590	R1591	A1592	L1593	D1594	S1595	M1596	Q1597	S1598	S1599	L1600	E1601	A1602	E1603	A1604	K1605	G1606	K1607	A1608	E1609	A1610	L1611	R1612	M1613	K1614	R1615	K1616	L1617	E1618	A1619	D1620																																																												
A1441	E1442	K1443	K1444	Q1445	K1446	A1447	F1448	D1449	K1450	I1451	I1452	G1453	A1454	W1455	K1456	L1457	K1458	V1459	D1460	D1461	L1462	A1463	A1464	E1465	L1466	D1467	A1468	S1469	Q1470	K1471	E1472	C1473	R1474	M1475	Y1476	S1477	T1478	E1479	L1480	F1481	L1482	L1483	K1484	G1485	A1486	Y1487	E1488	E1489	Q1490	Q1491	Q1492	Q1493	L1494	E1495	A1496	V1497	R1498	R1499	E1500																																																												
M1501	K1502	M1503	L1504	A1505	D1506	V1507	V1508	K1509	D1510	L1511	L1512	D1513	Q1514	I1515	G1516	E1517	K1518	G1519	R1520	M1521	I1522	H1523	E1524	I1525	I1526	K1527	A1528	R1529	K1530	R1531	L1532	E1533	A1534	E1535	K1536	D1537	E1538	L1539	Q1540	A1541	A1542	L1543	E1544	E1545	A1546	E1547	A1548	A1549	L1550	E1551	Q1552	Q1553	E1554	E1555	M1556	K1557	V1558	L1559	R1560	E1561	E1562	E1563	E1564	E1565	E1566	E1567	E1568	E1569	E1570	E1571	E1572	E1573	E1574	E1575	E1576	E1577	E1578	E1579	E1580	E1581	E1582	E1583	E1584	E1585	E1586	E1587	E1588	E1589	E1590	E1591	E1592	E1593	E1594	E1595	E1596	E1597	E1598	E1599	E1600	E1601	E1602	E1603	E1604	E1605	E1606	E1607	E1608	E1609	E1610	E1611	E1612	E1613	E1614	E1615	E1616	E1617	E1618	E1619	E1620
R1381	S1382	E1383	E1384	L1385	E1386	E1387	A1388	K1389	R1390	K1391	L1392	Q1393	A1394	R1395	L1396	A1397	E1398	A1399	E1400	E1401	T1402	I1403	E1404	S1405	L1406	N1407	Q1408	K1409	C1410	I1411	G1412	L1413	E1414	K1415	T1416	K1417	R1418	L1419	L1420	S1421	T1422	E1423	V1424	A1425	D1426	L1427	Q1428	L1429	K1430	V1431	R1432	S1433	R1434	A1435	M1436	I1437	A1438	M1439	A1440																																																												
K1261	L1262	D1263	E1264	T1265	N1266	R1267	T1268	L1269	N1270	D1271	F1272	D1273	A1274	S1275	K1276	K1277	K1278	L1279	S1280	I1281	E1282	M1283	S1284	D1285	L1286	L1287	R1288	Q1289	L1290	E1291	A1292	A1293	E1294	S1295	Q1296	V1297	S1298	Q1299	L1300	S1301	K1302	L1303	K1304	L1305	L1306	L1307	T1308	T1309	Q1310	L1311	E1312	D1313	T1314	K1315	R1316	L1317	D1318	D1319	E1320																																																												
E1321	S1322	R1323	E1324	R1325	L1326	T1327	L1328	L1329	G1330	K1331	F1332	R1333	M1334	L1335	E1336	H1337	D1338	L1339	D1340	M1341	L1342	R1343	E1344	Q1345	V1346	E1347	E1348	E1349	A1350	E1351	G1352	L1353	A1354	D1355	L1356	Q1357	R1358	Q1359	L1360	S1361	K1362	A1363	M1364	A1365	E1366	A1367	Q1368	V1369	M1370	R1371	L1372	K1373	Y1374	E1375	S1376	D1377	E1378	V1379	A1380																																																												
E1201	M1202	A1203	E1204	Q1205	V1206	D1207	Q1208	L1209	M1210	K1211	L1212	K1213	A1214	L1215	A1216	E1217	K1218	E1219	K1220	E1221	Y1222	Y1223	Y1224	G1225	Q1226	L1227	M1228	D1229	L1230	S1231	K1232	L1233	G1234	V1235	D1236	H1237	T1238	M1239	E1240	K1241	A1242	A1243	Q1244	E1245	K1246	I1247	A1248	K1249	Q1250	M1251	Q1252	H1253	T1254	L1255	E1256	N1257	V1258	Q1259	S1260																																																												
R1081	K1082	D1083	K1084	E1085	L1086	S1087	S1088	L1089	T1090	A1091	K1092	L1093	E1094	D1095	E1096	Q1097	V1098	V1099	V1100	L1101	K1102	H1103	Q1104	R1105	L1106	T1107	K1108	E1109	L1110	Q1111	A1112	R1113	I1114	E1115	L1116	L1117	E1118	E1119	E1120	V1121	E1122	A1123	E1124	R1125	Q1126	A1127	R1128	A1129	K1130	A1131	E1132	K1133	Q1134	R1135	E1136	D1137	L1138	A1139	R1140																																																												
E1141	L1142	E1143	E1144	G1145	E1146	E1147	R1148	L1149	E1150	E1151	A1152	G1153	E1154	A1155	T1156	S1157	A1158	Q1159	I1160	E1161	L1162	M1163	K1164	K1165	R1166	E1167	A1168	E1169	L1170	S1171	K1172	L1173	R1174	E1175	D1176	L1177	E1178	E1179	A1180	M1181	I1182	Q1183	H1184	E1185	S1186	T1187	L1188	A1189	M1190	L1191	R1192	K1193	K1194	H1195	M1196	D1197	A1198	V1199	A1200																																																												
K1021	V1022	K1023	A1024	L1025	L1026	E1027	Q1028	T1029	L1030	D1031	E1032	L1033	A1034	D1035	S1036	L1037	E1038	R1039	E1040	K1041	K1042	V1043	R1044	G1045	D1046	V1047	E1048	K1049	S1050	K1051	R1052	K1053	V1054	E1055	G1056	D1057	L1058	K1059	L1060	T1061	Q1062	E1063	A1064	V1065	G1066	D1067	L1068	E1069	R1070	M1071	K1072	E1073	E1074	L1075	E1076	Q1077	T1078	I1079	Q1080																																																												
Q961	K962	A963	E964	Q965	D966	K967	A968	T969	K970	D971	H972	Q973	I974	R975	N976	L977	N978	D979	E980	I981	A982	H983	Q984	D985	E986	L987	I988	N989	R990	L991	N992	K993	E994	Q997	K998	M999	K940	R941	A942	D943	Q944	E945	Q1003	K1004	T1005	G1006	E1007	E1008	L1009	Q1010	A1011	A1012	E1013	D1014	K1015	I1016	M1017	H1018	L1019	N1020																																																											
GLN	GLU	ARG	ASN	ALA	LYS	LEU	GLU	GLY	ASN	D913	L914	E915	N916	Q917	L918	R919	D920	I921	Q922	E923	R924	L925	H926	Q927	E928	E929	E930	A931	R932	N933	Q934	L935	F936	Q937	K938	K939	K940	R941	A942	D943	Q944	E945	Q1003	K1004	T1005	G1006	E1007	E1008	L1009	Q1010	A1011	A1012	E1013	D1014	K1015	I1016	M1017	H1018	L1019	N1020																																																											

R1381	E1321	K1261	E1201	E1141	R1081	K1021	Q961	GLN	VAL	GLY	MET	THR	LEU	LYS
S1382	S1322	L1262	M1202	L1142	K1082	V1022	K962	GLU	SER	ILE	ARG	THR	ASN	ALA
E1383	R1323	D1263	A1203	E1143	D1083	K1023	A963	ARG	ILE	MET	THR	LEU	ASP	THR
E1384	E1324	E1264	E1204	E1144	K1084	A1024	E964	ALA	GLN	SER	VAL	THR	VAL	GLN
L1385	R1325	T1265	Q1205	L1145	E1085	K1025	Q965	LEU	ASP	TRP	THR	GLN	ASP	PHE
E1386	A1326	R1266	Q1206	G1146	L1086	L1026	D966	THR	GLU	MET	GLN	PRO	GLN	SER
E1387	T1327	R1267	D1207	E1147	S1087	E1027	K967	ALA	ALA	TRP	HIS	HIS	PHE	LYS
A1388	L1328	T1268	Q1208	R1148	S1088	Q1028	A968	GLN	ARG	GLY	VAL	VAL	LYS	LYS
L1389	L1329	L1269	L1209	L1149	T1089	T1029	T969	LEU	LEU	ARG	VAL	VAL	LYS	LYS
R1390	G1330	M1270	M1210	E1150	T1090	T1030	K970	ASN	GLU	GLY	CYS	CYS	GLN	ASN
K1391	K1331	D1271	K1211	E1151	A1091	D1031	D971	L914	LYS	TYR	ILE	ILE	ASN	THR
L1392	F1332	F1272	L1212	A1152	K1092	E1032	H972	E915	ALA	LEU	ILE	ILE	LYS	HIS
Q1393	R1333	A1273	K1213	G1153	L1093	L1033	Q973	N916	LYS	ARG	PRO	PRO	LEU	LEU
A1394	M1334	D1274	A1214	G1154	E1094	L1034	I974	A917	ALA	LYS	GLU	GLU	ILE	LYS
R1395	L1335	S1275	K1215	A1155	D1095	D1035	R975	L918	GLU	PHE	MET	MET	GLU	SER
E1396	E1336	K1276	A1216	T1156	E1096	S1036	N976	R919	GLU	LYS	LYS	LYS	ILE	ALA
H1397	H1337	K1277	E1217	S1157	Q1097	L1037	R977	D920	LEU	THR	THR	GLN	PHE	PRO
E1398	D1338	K1278	K1218	A1158	V1098	E1038	N978	I921	ALA	VAL	VAL	VAL	ALA	LYS
A1399	L1339	L1279	E1219	Q1159	V1099	R1039	D979	Q922	VAL	ARG	ALA	ASP	GLN	PRO
E1400	D1340	S1280	K1220	I1160	L1100	E1040	E980	E923	LYS	THR	THR	HIS	SER	PRO
E1401	M1341	I1281	M1221	E1161	L1101	K1041	I981	R924	VAL	VAL	VAL	HIS	SER	PRO
T1402	L1342	E1282	E1222	L1162	K1102	K1042	A982	T926	ARG	ALA	VAL	GLY	GLY	LYS
T1403	R1343	M1283	Y1223	M1163	H1103	V1043	H983	T926	LYS	LEU	VAL	VAL	GLY	PRO
E1404	E1344	S1284	Y1224	K1164	Q1104	R1044	Q984	Q927	GLU	LEU	MET	MET	GLY	GLY
S1405	Q1345	D1285	G1225	K1165	R1105	R1045	D985	E928	LEU	VAL	HIS	HIS	GLU	GLN
L1406	L1346	L1286	L1226	R1166	Q1106	D1046	E986	E929	GLU	VAL	ASP	ASP	GLY	GLN
N1407	E1347	L1287	L1227	E1167	I1107	V1047	L987	E930	ALA	GLN	TYR	TYR	ALA	ALA
Q1408	E1348	R1288	N1228	A1168	K1108	E1048	I988	A931	ASN	ASN	ASN	CYS	GLY	ASN
R1409	E1349	Q1289	D1229	E1169	E1109	K1049	N989	R932	ALA	LEU	LEU	LEU	ARG	ALA
C1410	A1350	L1290	L1230	L1170	L1110	S1050	K990	N933	LYS	LEU	VAL	VAL	GLY	ALA
T1411	E1351	E1291	R1231	S1171	Q1111	K1051	L991	O934	LEU	TYR	THR	THR	ILE	ALA
G1412	G1352	E1292	A1232	K1172	A1112	R1052	N992	L936	ALA	LEU	GLY	GLY	LYS	HIS
L1413	R1353	A1293	G1233	L1173	R1113	K1053	K993	F936	GLY	GLM	VAL	VAL	GLY	TYR
E1414	A1354	E1294	V1234	R1174	I1114	V1054	E994	Q937	THR	LEU	ILE	ILE	GLY	ALA
K1415	D1355	S1295	D1235	R1175	E1115	E1055	K995	Q937	ALA	THR	ARG	ARG	PHE	CYS
T1416	L1356	Q1296	H1236	D1176	E1116	G1056	K996	O938	VAL	TRP	ALA	ALA	VAL	VAL
K1417	Q1357	V1297	L1237	L1177	L1117	D1057	M997	R940	LEU	PRO	GLY	THR	SER	SER
Q1418	R1358	S1298	T1238	E1178	E1118	L1058	Q998	F940	VAL	TRP	VAL	VAL	VAL	TYR
R1419	Q1359	Q1299	N1239	E1179	E1119	K1059	G999	R941	ASP	TYR	TYR	GLY	SER	ASN
L1420	L1360	L1300	E1240	A1180	E1120	L1060	E1000	A942	LEU	LEU	GLN	ALA	THR	ALA
S1421	S1361	S1301	K1241	M1181	V1121	T1061	D943	O944	SER	TRP	MET	TYR	ASN	TYR
T1422	K1362	K1302	A1242	I1182	E1122	Q1062	N1002	E945	TRP	GLM	GLU	GLU	LYS	LYS
E1423	A1363	I1303	A1243	Q1183	A1123	E1063	Q1003	I946	VAL	LYS	VAL	VAL	GLU	GLY
V1424	M1364	K1304	Q1244	H1184	E1124	A1064	K1004	S947	ALA	ALA	ARG	ARG	LEU	LEU
E1425	A1365	E1305	E1245	E1185	R1125	V1065	T1005	O948	ASP	ASP	VAL	VAL	ASN	ASN
D1426	E1366	S1306	K1246	E1186	Q1126	A1066	G1006	L949	TRP	TRP	TRP	TRP	LEU	LEU
L1427	A1367	L1307	T1247	T1187	A1127	D1067	E1007	R950	LEU	SER	GLY	GLY	LEU	LEU
Q1428	Q1368	T1308	L1248	L1188	R1128	L1068	E1008	K951	ALA	ALA	ALA	ALA	VAL	VAL
L1429	V1369	T1309	K1249	A1189	A1129	E1069	L1009	D952	LEU	LEU	GLY	GLY	GLU	GLU
E1430	W1370	Q1310	Q1250	N1190	K1130	R1070	Q1010	D953	ASP	ASP	VAL	VAL	GLU	GLY
V1431	R1371	L1311	L1251	L1191	A1131	M1071	A1011	E954	TRP	TRP	TRP	TRP	LEU	LEU
D1432	S1372	E1312	Q1252	R1192	A1132	K1072	A1012	D955	LYS	LYS	LYS	LYS	ASN	ASN
R1433	K1373	D1313	H1253	K1193	K1133	R1073	E1013	L956	ALA	ALA	ALA	ALA	SER	SER
A1434	Y1374	T1314	L1254	K1194	Q1134	E1074	D1014	L957	GLY	GLY	GLY	GLY	LEU	LEU
N1435	E1375	K1315	L1255	H1195	R1135	L1075	K1015	R959	VAL	VAL	VAL	VAL	ASN	ASN
A1436	S1376	R1316	M1256	E1196	A1136	E1076	I1016	N960	TRP	TRP	TRP	TRP	ASP	ASP
I1437	D1377	L1317	E1257	D1197	D1137	Q1077	N1017		PRO	PRO	PRO	PRO	ARG	ARG
A1438	G1378	A1318	V1258	A1198	L1138	T1078	H1018		GLN	GLN	GLN	GLN	LEU	LEU
N1439	V1379	D1319	Q1259	V1199	A1139	F1079	L1019		ASP	ASP	ASP	ASP	LEU	LEU
A1440	A1380	E1320	S1260	A1200	R1140	Q1080	N1020		TYR	TYR	TYR	TYR	ASP	PRO

A1441	A1442	A1443	K1444	K1445	K1446	K1447	F1448	D1449	K1450	I1451	I1452	G1453	E1454	M1455	K1456	L1457	K1458	V1459	D1460	D1461	L1462	A1463	A1464	A1465	L1466	D1467	A1468	S1469	Q1470	K1471	E1472	C1473	R1474	M1475	Y1476	S1477	T1478	E1479	L1480	F1481	R1482	L1483	K1484	G1485	A1486	Y1487	E1488	E1489	G1490	Q1491	E1492	Q1493	L1494	E1495	A1496	V1497	R1498	R1499	E1500	
M1501	K1502	N1503	L1504	A1505	D1506	E1507	V1508	K1509	D1510	L1511	L1512	D1513	Q1514	I1515	G1516	E1517	G1518	G1519	R1520	N1521	I1522	H1523	E1524	I1525	L1526	K1527	A1528	R1529	K1530	R1531	L1532	L1533	A1534	E1535	M1536	D1537	E1538	L1539	Q1540	A1541	A1542	L1543	E1544	E1545	A1546	E1547	A1548	A1549	L1550	E1551	Q1552	E1553	L1554	M1555	K1556	V1557	L1558	R1559	A1560	
Q1561	L1562	E1563	L1564	Q1565	V1567	R1568	Q1569	E1570	I1571	D1572	R1573	R1574	I1575	Q1576	E1577	K1578	E1579	E1580	E1581	F1582	E1583	M1584	T1585	R1586	K1587	M1588	H1589	R1590	R1591	A1592	L1593	D1594	S1595	M1596	Q1597	A1598	L1599	L1600	E1601	A1602	E1603	A1604	K1605	Q1606	K1607	A1608	E1609	A1610	L1611	Q1612	M1613	K1614	K1615	K1616	L1617	E1618	A1619	D1620		
I1621	M1622	E1623	L1624	E1625	I1626	A1627	L1628	D1629	H1630	A1631	M1632	K1633	A1634	M1635	A1636	E1637	A1638	Q1639	K1640	M1641	E1642	K1643	R1644	Y1645	R1646	Q1647	Q1648	L1649	K1650	D1651	A1652	Q1653	T1654	A1655	L1656	E1657	E1658	E1659	Q1660	R1661	A1662	R1663	D1664	D1665	A1666	R1667	E1668	Q1669	A1670	G1671	I1672	S1673	E1674	R1675	R1676	A1677	M1678	A1679	L1680	
Q1681	M1682	E1683	L1684	E1685	E1686	S1687	R1688	T1689	L1690	L1691	E1692	Q1693	A1694	D1695	R1696	G1697	R1698	R1699	Q1700	A1701	E1702	Q1703	E1704	L1705	A1706	D1707	A1708	H1709	E1710	Q1711	L1712	Q1713	E1714	V1715	S1716	A1717	Q1718	M1719	A1720	S1721	I1722	S1723	A1724	A1725	K1726	R1727	K1728	L1729	E1730	S1731	L1732	L1733	Q1734	T1735	L1736	H1737	S1738	D1739	L1740	
D1741	E1742	L1743	L1744	M1745	E1746	A1747	K1748	M1749	S1750	E1751	E1752	K1753	A1754	K1755	K1756	A1757	M1758	V1759	D1760	A1761	A1762	R1763	L1764	A1765	D1766	E1767	L1768	R1769	A1770	E1771	Q1772	D1773	H1774	A1775	Q1776	T1777	Q1778	E1779	L1780	L1781	R1782	K1783	A1784	L1785	E1786	Q1787	Q1788	I1789	E1790	E1791	L1792	Q1793	Q1794	V1795	R1796	L1796	D1797	K1798	M1799	E1800
A1801	M1802	A1803	L1804	K1805	G1806	G1807	K1808	K1809	A1810	I1811	Q1812	K1813	L1814	E1815	Q1816	R1817	V1818	R1819	E1820	L1821	E1822	M1823	E1824	L1825	E1826	G1827	E1828	Q1829	R1830	R1831	H1832	A1833	D1834	A1835	Q1836	K1837	M1838	L1839	R1840	K1841	S1842	E1843	R1844	R1845	E1846	V1846	K1847	E1848	L1849	D1850	F1851	Q1852	S1853	E1854	E1855	D1856	R1857	K1858	M1859	H1860
E1861	R1862	M1863	Q1864	D1865	L1866	V1867	D1868	K1869	L1870	Q1871	Q1872	K1873	I1874	K1875	T1876	Y1877	K1878	R1879	Q1880	I1881	E1882	E1883	A1884	E1885	E1886	I1887	A1888	A1889	L1890	M1891	L1892	A1893	K1894	F1895	R1896	K1897	A1898	Q1899	Q1900	E1901	L1902	E1903	E1904	A1905	A1906	V1846	E1907	R1908	A1909	D1910	L1911	A1912	E1913	Q1914	A1915	I1916	S1917	K1918	F1919	R1920
A1921	LYS	GLY	ARG	ALA	GLY	SER	VAL	GLY	ARG	GLY	ALA	PRO	THR	ALA	SER	GLY	ARG	LYS	SER	ALA	LEU	LEU	GLU	GLN																																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	19.048	Depositor
Minimum map value	-4.384	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.633	Depositor
Recommended contour level	2.79	Depositor
Map size (\AA)	1021.44006, 1021.44006, 1021.44006	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.33, 1.33, 1.33	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	0.29	0/8212	0.62	0/10958
1	B	0.31	0/8212	0.67	2/10958 (0.0%)
All	All	0.30	0/16424	0.65	2/21916 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1227	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	1729	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1331	LYS	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	8176	0	8192	457	0
1	B	8176	0	8192	487	0
All	All	16352	0	16384	844	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 26.

The worst 5 of 844 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:1224:TYR:HA	1:B:1227:LEU:HD12	1.50	0.93
1:A:1015:LYS:HZ1	1:B:1016:ILE:HG12	1.34	0.89
1:A:1223:TYR:OH	1:B:1226:GLN:NE2	2.09	0.85
1:A:1582:PHE:HB3	1:A:1586:ARG:HH12	1.45	0.82
1:B:1730:GLU:HB3	1:B:1734:GLN:HE22	1.46	0.80

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	1007/1949 (52%)	999 (99%)	8 (1%)	0	100	100
1	B	1007/1949 (52%)	989 (98%)	18 (2%)	0	100	100
All	All	2014/3898 (52%)	1988 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	866/1669 (52%)	856 (99%)	10 (1%)	71	84
1	B	866/1669 (52%)	854 (99%)	12 (1%)	67	81
All	All	1732/3338 (52%)	1710 (99%)	22 (1%)	70	82

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1218	LYS
1	B	1514	GLN
1	B	1482	ARG
1	B	1586	ARG
1	A	1409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1184	HIS
1	B	1734	GLN
1	B	1900	GLN
1	B	1899	GLN
1	A	1589	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

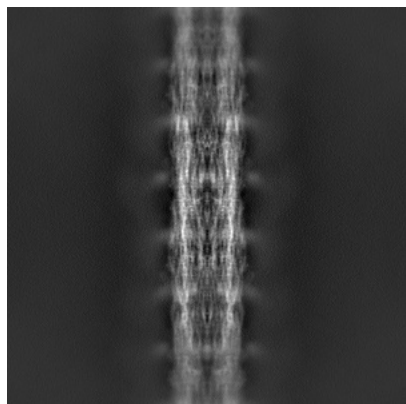
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42024. These allow visual inspection of the internal detail of the map and identification of artifacts.

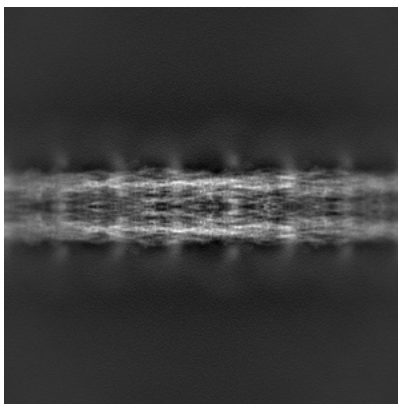
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

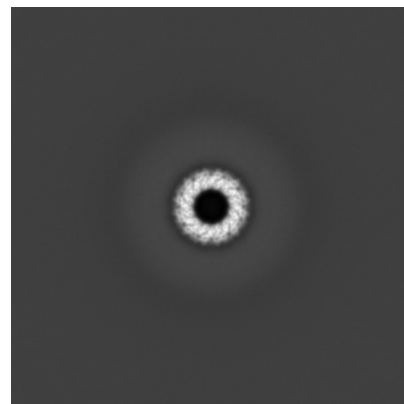
6.1.1 Primary map



X

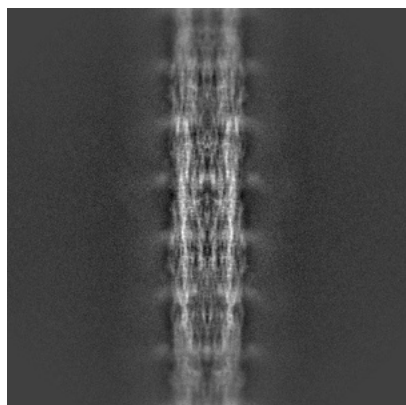


Y

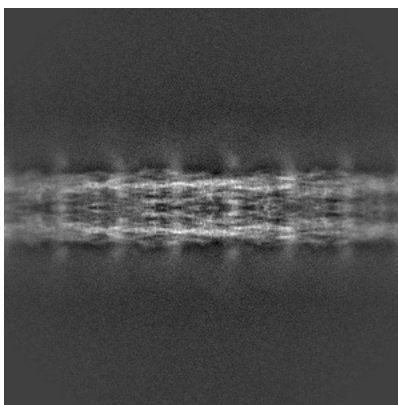


Z

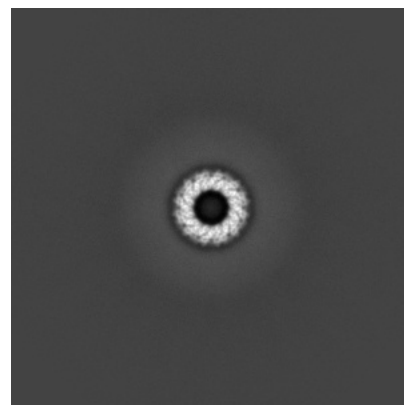
6.1.2 Raw map



X



Y

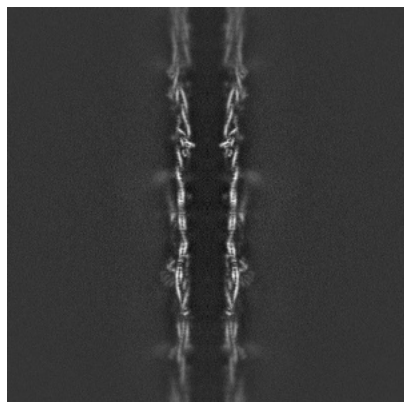


Z

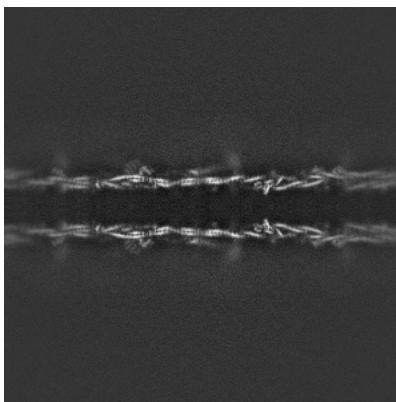
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

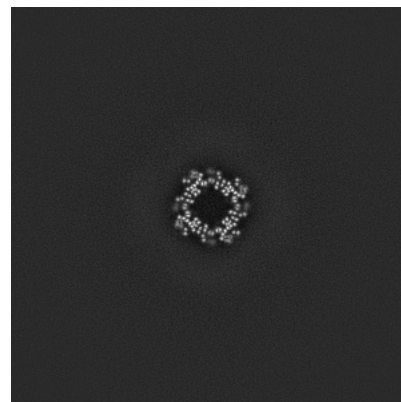
6.2.1 Primary map



X Index: 384

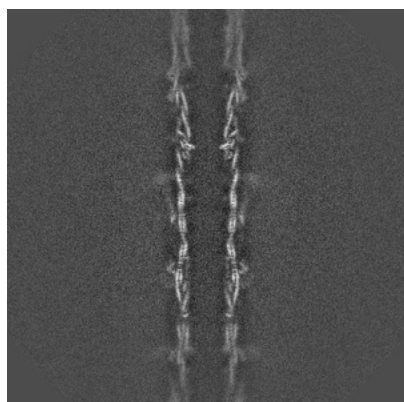


Y Index: 384

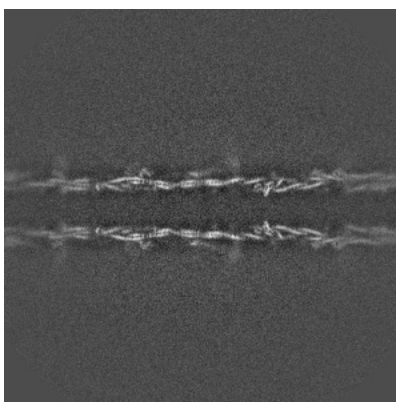


Z Index: 384

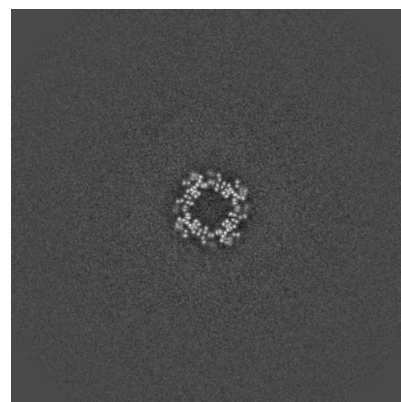
6.2.2 Raw map



X Index: 384



Y Index: 384

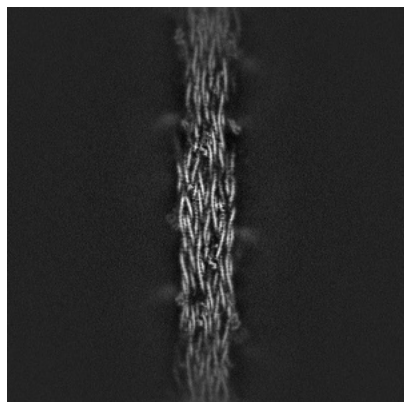


Z Index: 384

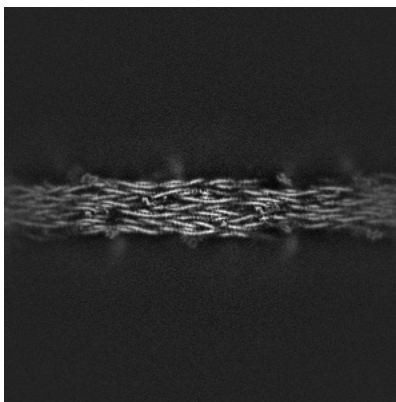
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

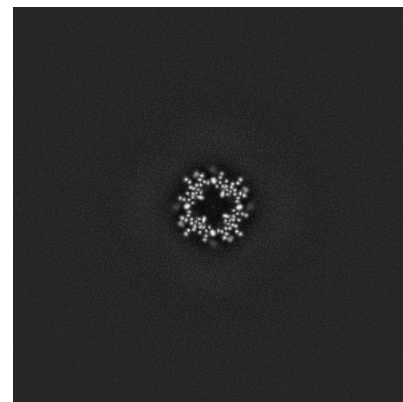
6.3.1 Primary map



X Index: 429

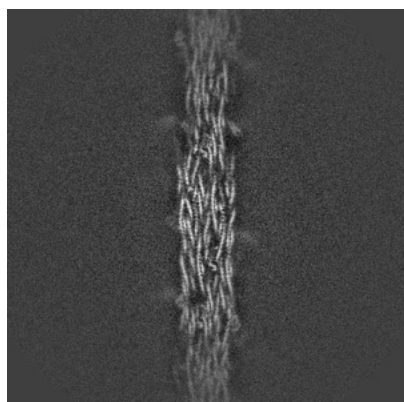


Y Index: 339

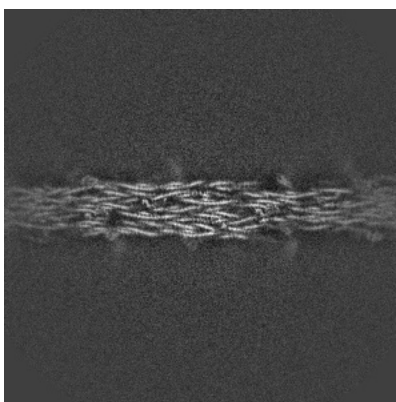


Z Index: 395

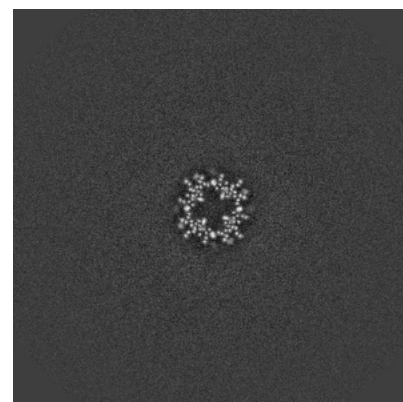
6.3.2 Raw map



X Index: 429



Y Index: 339

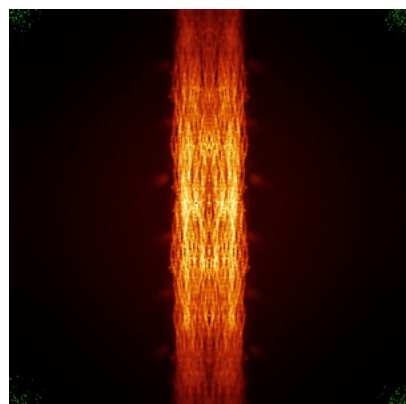


Z Index: 395

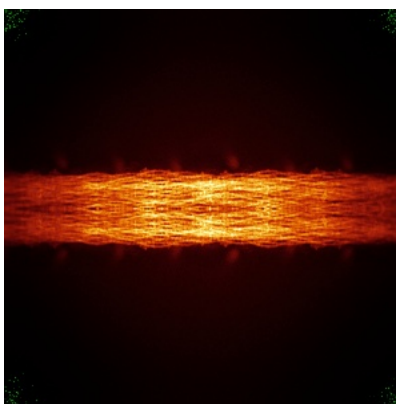
The images above show the largest variance slices of the map in three orthogonal directions.

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

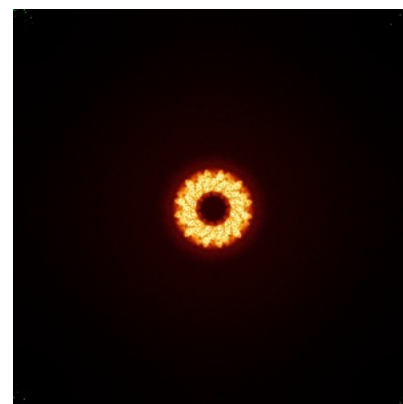
6.4.1 Primary map



X

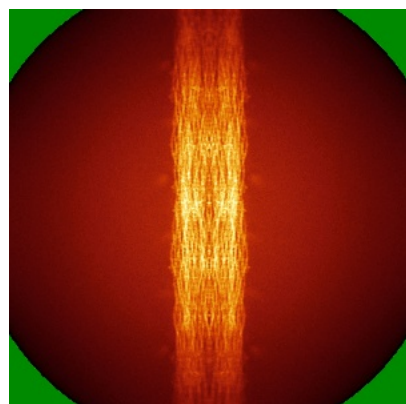


Y

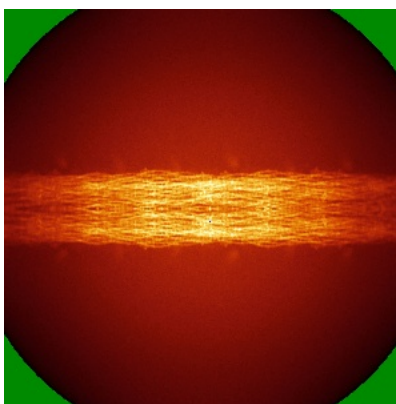


Z

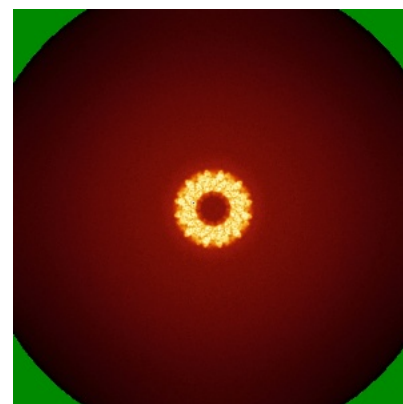
6.4.2 Raw map



X



Y

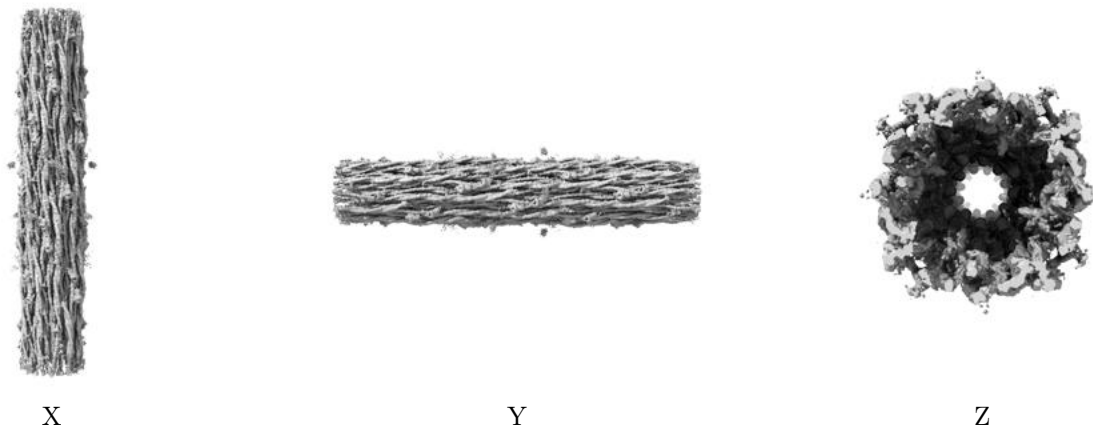


Z

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.

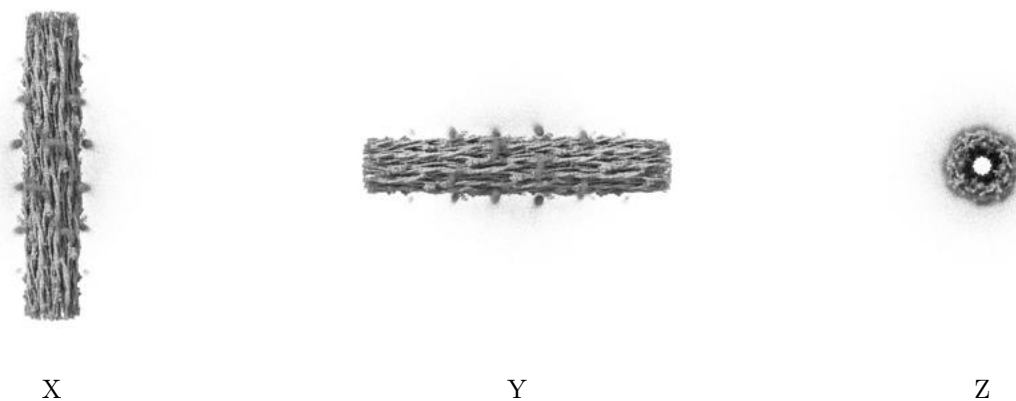
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.79. 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.

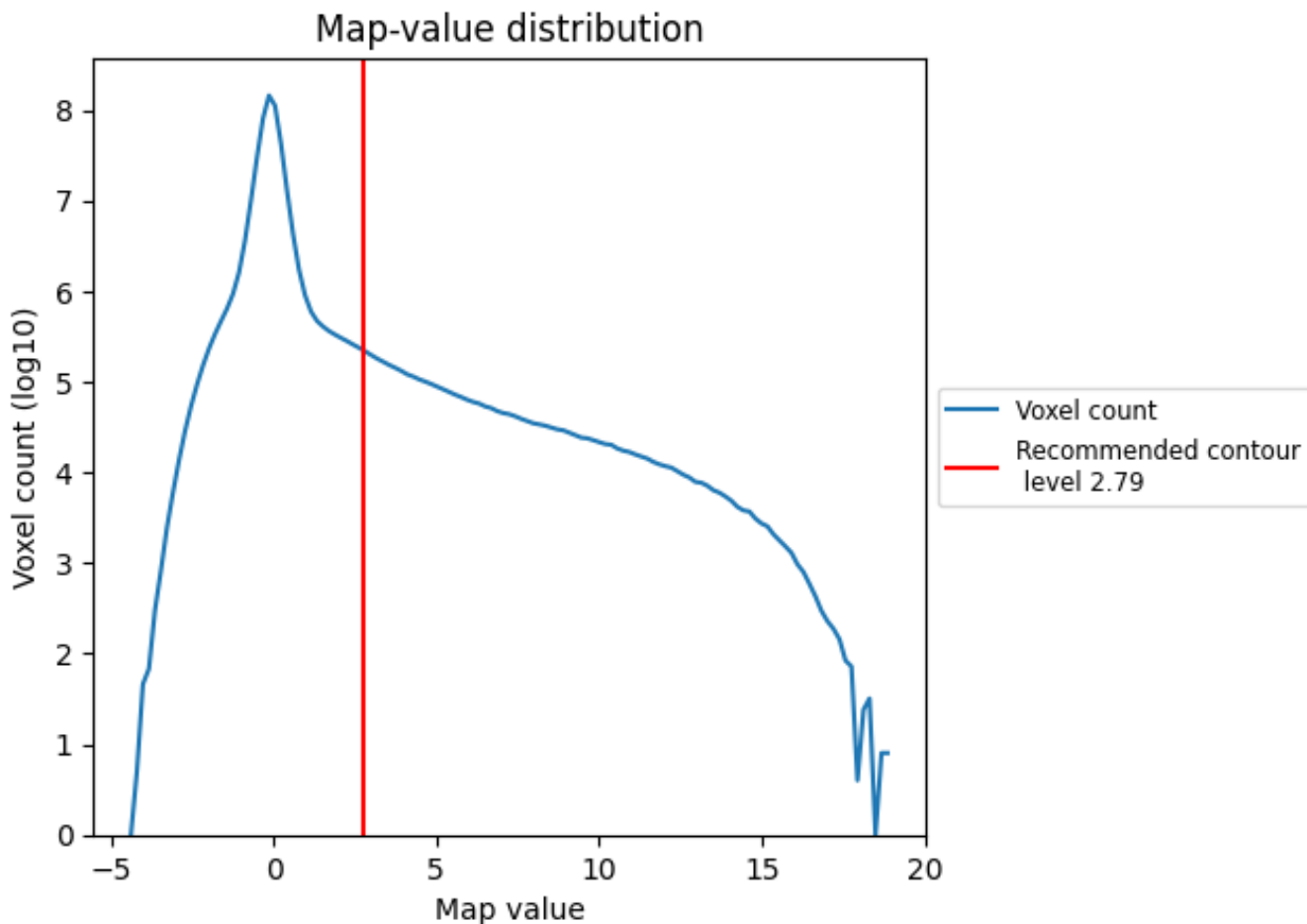
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

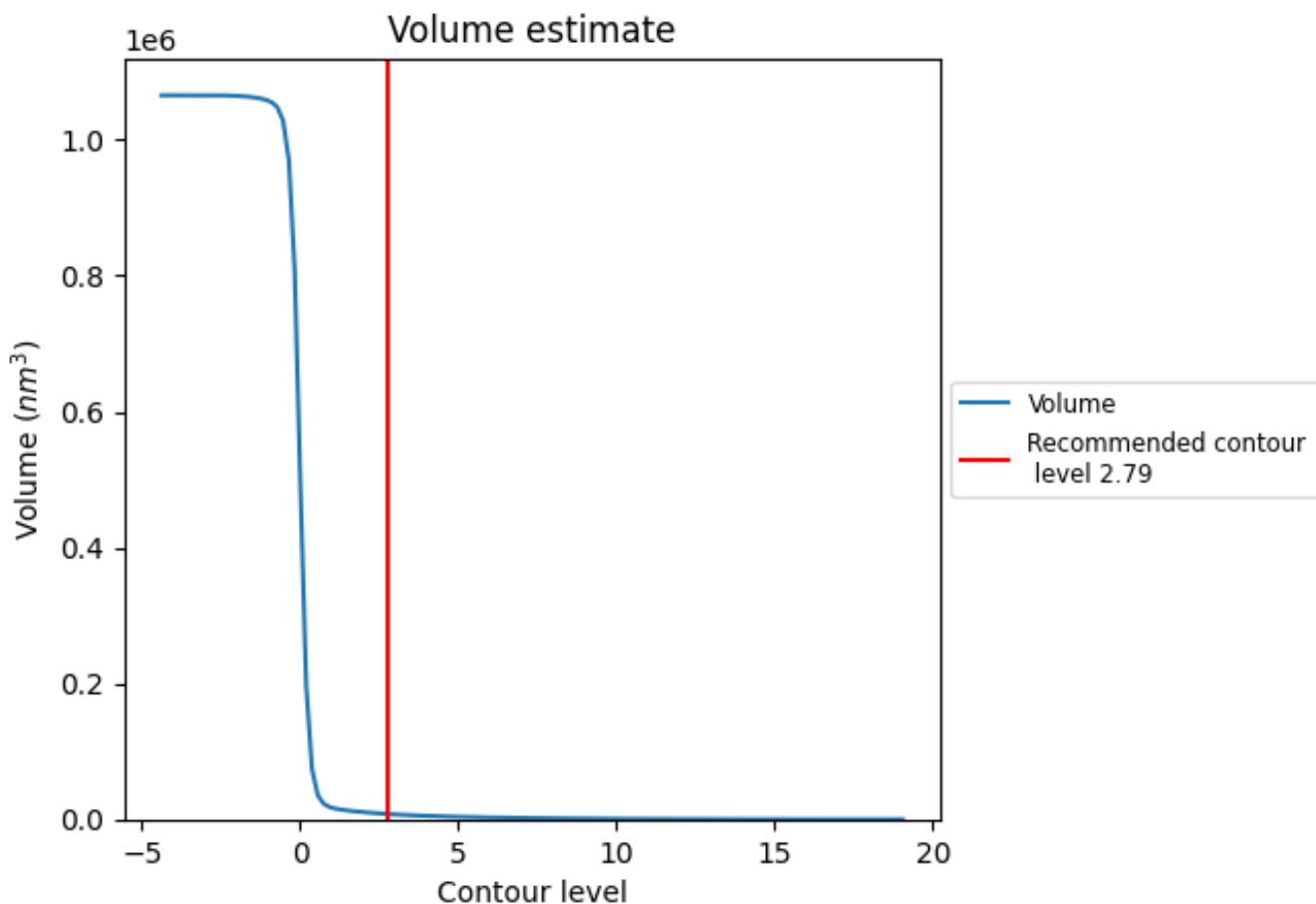
This section contains the results of statistical analysis of the map.

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.

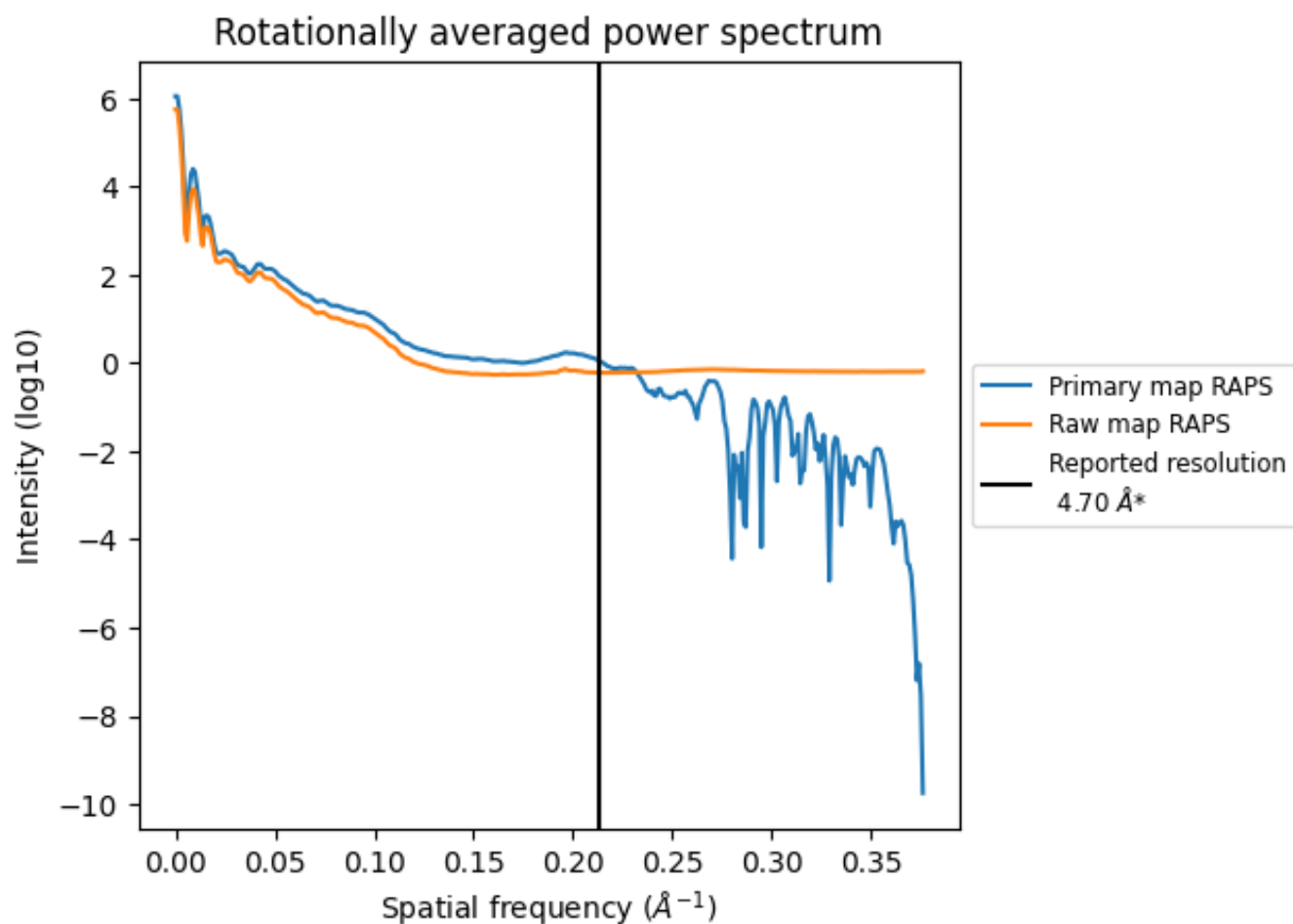
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7791 nm^3 ; this corresponds to an approximate mass of 7038 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

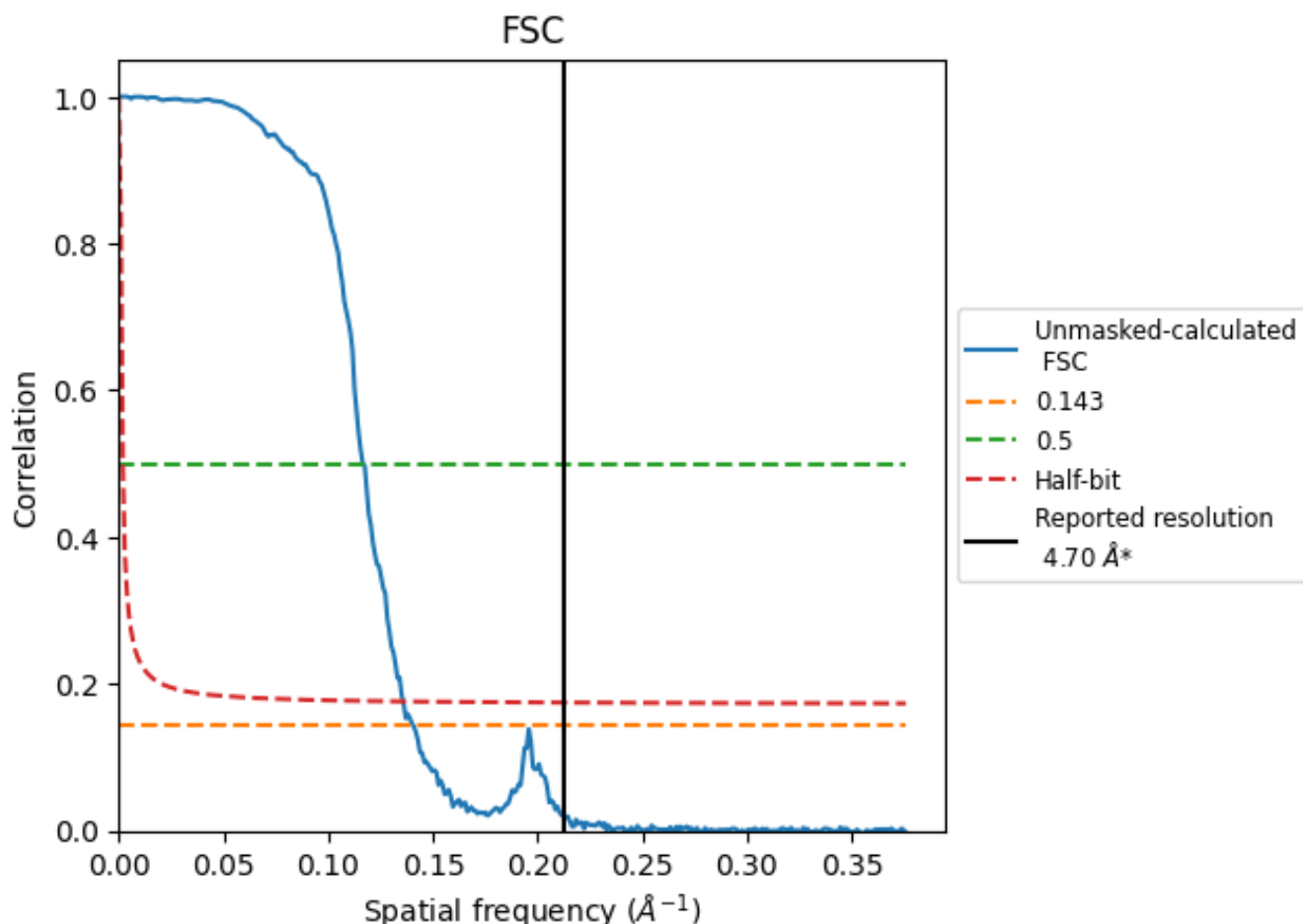


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

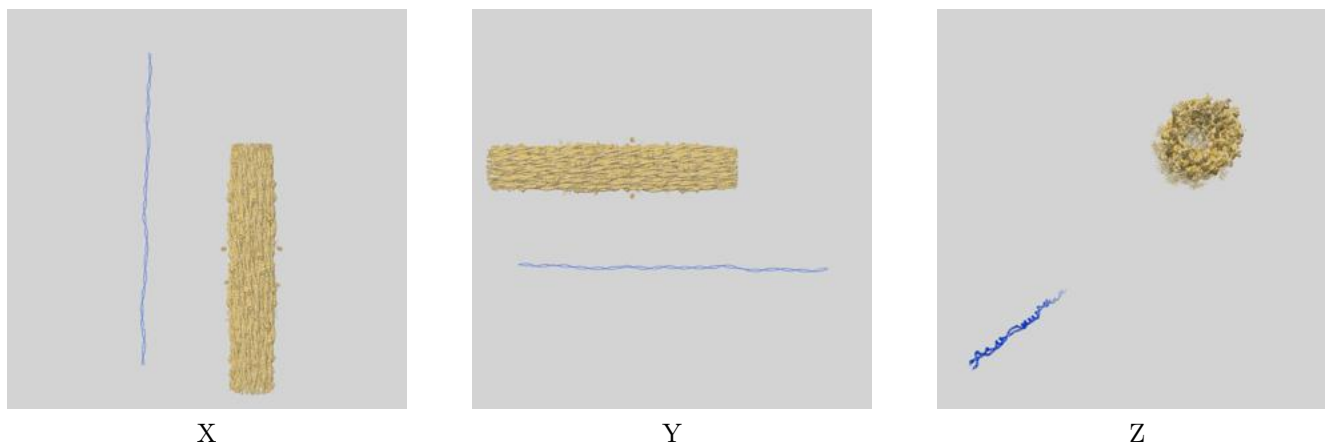
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	4.70
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	7.11	8.57	7.36	-

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

9 Map-model fit [i](#)

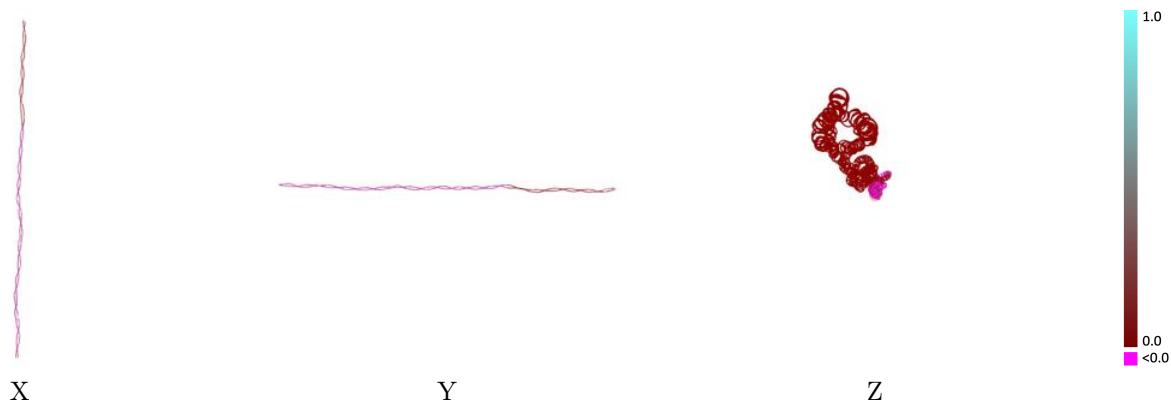
This section contains information regarding the fit between EMDB map EMD-42024 and PDB model 8U95. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



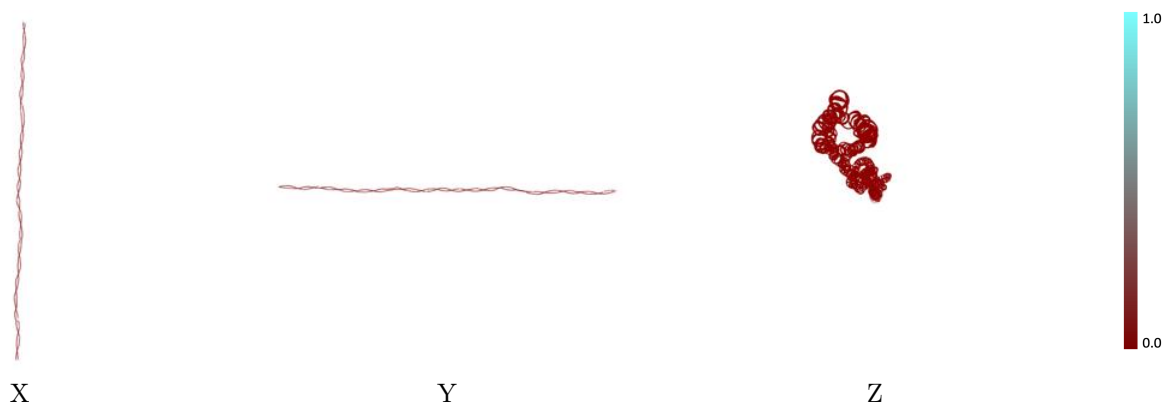
The images above show the 3D surface view of the map at the recommended contour level 2.79 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



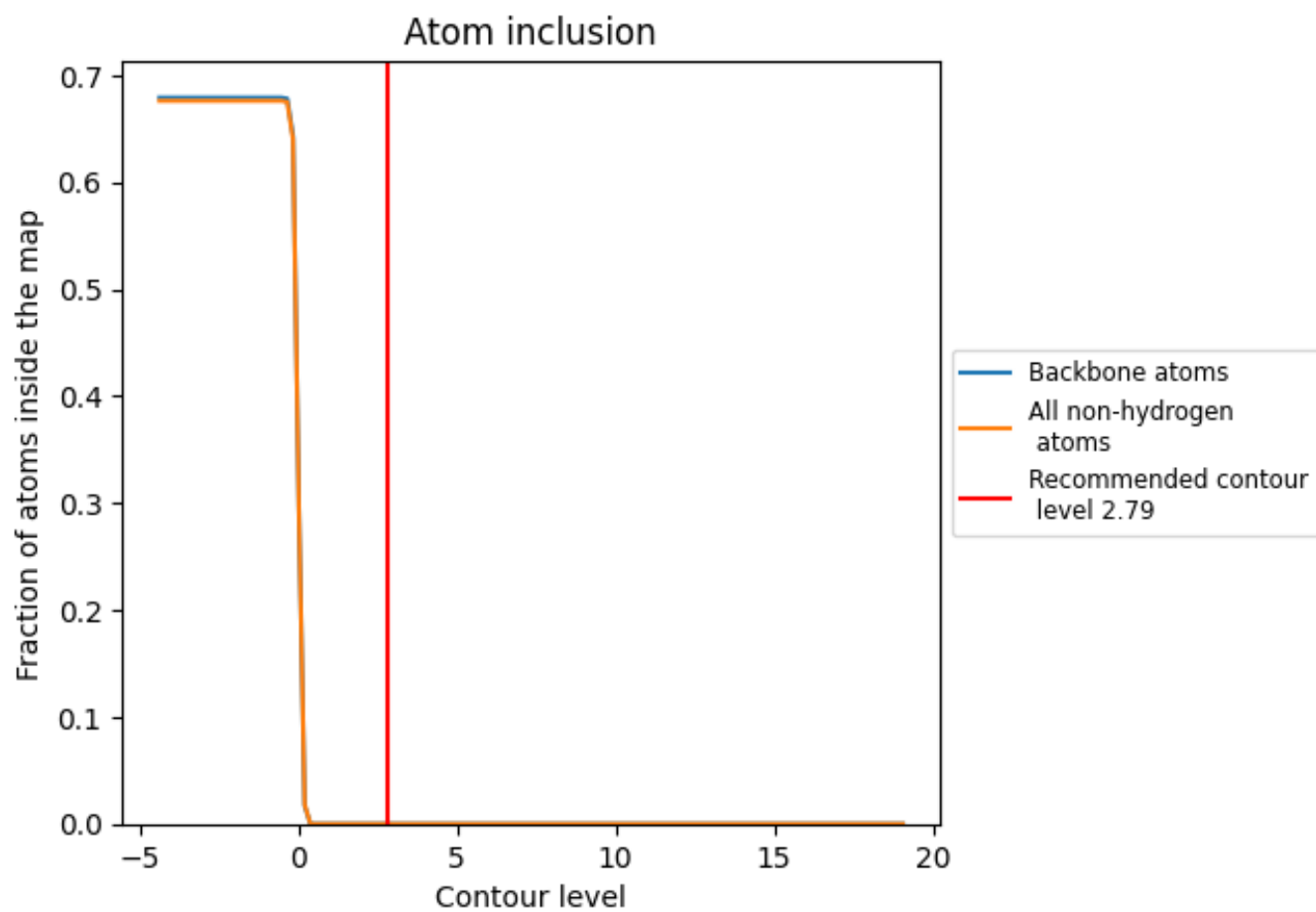
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.79).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (2.79) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 0.0010
A	 0.0000	 0.0030
B	 0.0000	 -0.0010

