



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 02:02 am GMT

PDB ID : 8AJB
EMDB ID : EMD-15476
Title : Cryo-EM structure of crescentin filaments (stutter mutant, C2 symmetry and large box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-28
Resolution : 4.30 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.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

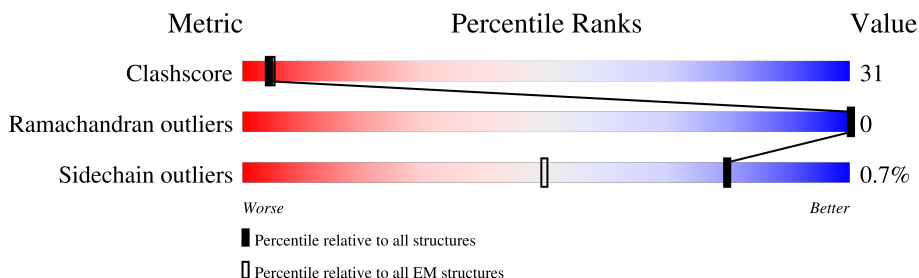
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






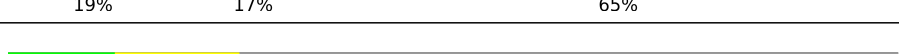


The reported resolution of this entry is 4.30 Å.

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	460	
1	B	460	
1	C	460	
1	D	460	
1	G	460	
1	H	460	
1	I	460	
1	J	460	

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Mol	Chain	Length	Quality of chain
1	M	460	
1	N	460	
1	O	460	
1	P	460	
1	S	460	
1	T	460	
1	U	460	
1	V	460	
2	E	907	
2	F	907	
2	K	907	
2	L	907	
2	Q	907	
2	R	907	
2	W	907	
2	X	907	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 30088 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 Crescentin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1876	1127	366	382	1		
1	B	238	Total	C	N	O	S	0	0
			1828	1099	358	370	1		
1	C	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	D	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	G	155	Total	C	N	O	S	0	0
			1203	727	234	241	1		
1	H	163	Total	C	N	O	S	0	0
			1264	764	244	255	1		
1	I	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	J	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	M	245	Total	C	N	O	S	0	0
			1876	1127	366	382	1		
1	N	238	Total	C	N	O	S	0	0
			1828	1099	358	370	1		
1	O	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	P	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	S	155	Total	C	N	O	S	0	0
			1203	727	234	241	1		
1	T	163	Total	C	N	O	S	0	0
			1264	764	244	255	1		
1	U	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	V	120	Total	C	N	O	S	0	0
			934	555	192	185	2		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP A0A8F8EC09
A	407	ALA	-	insertion	UNP A0A8F8EC09
A	408	THR	-	insertion	UNP A0A8F8EC09
B	406	SER	-	insertion	UNP A0A8F8EC09
B	407	ALA	-	insertion	UNP A0A8F8EC09
B	408	THR	-	insertion	UNP A0A8F8EC09
C	406	SER	-	insertion	UNP A0A8F8EC09
C	407	ALA	-	insertion	UNP A0A8F8EC09
C	408	THR	-	insertion	UNP A0A8F8EC09
D	406	SER	-	insertion	UNP A0A8F8EC09
D	407	ALA	-	insertion	UNP A0A8F8EC09
D	408	THR	-	insertion	UNP A0A8F8EC09
G	406	SER	-	insertion	UNP A0A8F8EC09
G	407	ALA	-	insertion	UNP A0A8F8EC09
G	408	THR	-	insertion	UNP A0A8F8EC09
H	406	SER	-	insertion	UNP A0A8F8EC09
H	407	ALA	-	insertion	UNP A0A8F8EC09
H	408	THR	-	insertion	UNP A0A8F8EC09
I	406	SER	-	insertion	UNP A0A8F8EC09
I	407	ALA	-	insertion	UNP A0A8F8EC09
I	408	THR	-	insertion	UNP A0A8F8EC09
J	406	SER	-	insertion	UNP A0A8F8EC09
J	407	ALA	-	insertion	UNP A0A8F8EC09
J	408	THR	-	insertion	UNP A0A8F8EC09
M	406	SER	-	insertion	UNP A0A8F8EC09
M	407	ALA	-	insertion	UNP A0A8F8EC09
M	408	THR	-	insertion	UNP A0A8F8EC09
N	406	SER	-	insertion	UNP A0A8F8EC09
N	407	ALA	-	insertion	UNP A0A8F8EC09
N	408	THR	-	insertion	UNP A0A8F8EC09
O	406	SER	-	insertion	UNP A0A8F8EC09
O	407	ALA	-	insertion	UNP A0A8F8EC09
O	408	THR	-	insertion	UNP A0A8F8EC09
P	406	SER	-	insertion	UNP A0A8F8EC09
P	407	ALA	-	insertion	UNP A0A8F8EC09
P	408	THR	-	insertion	UNP A0A8F8EC09
S	406	SER	-	insertion	UNP A0A8F8EC09
S	407	ALA	-	insertion	UNP A0A8F8EC09
S	408	THR	-	insertion	UNP A0A8F8EC09
T	406	SER	-	insertion	UNP A0A8F8EC09
T	407	ALA	-	insertion	UNP A0A8F8EC09
T	408	THR	-	insertion	UNP A0A8F8EC09
U	406	SER	-	insertion	UNP A0A8F8EC09

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Chain	Residue	Modelled	Actual	Comment	Reference
U	407	ALA	-	insertion	UNP A0A8F8EC09
U	408	THR	-	insertion	UNP A0A8F8EC09
V	406	SER	-	insertion	UNP A0A8F8EC09
V	407	ALA	-	insertion	UNP A0A8F8EC09
V	408	THR	-	insertion	UNP A0A8F8EC09

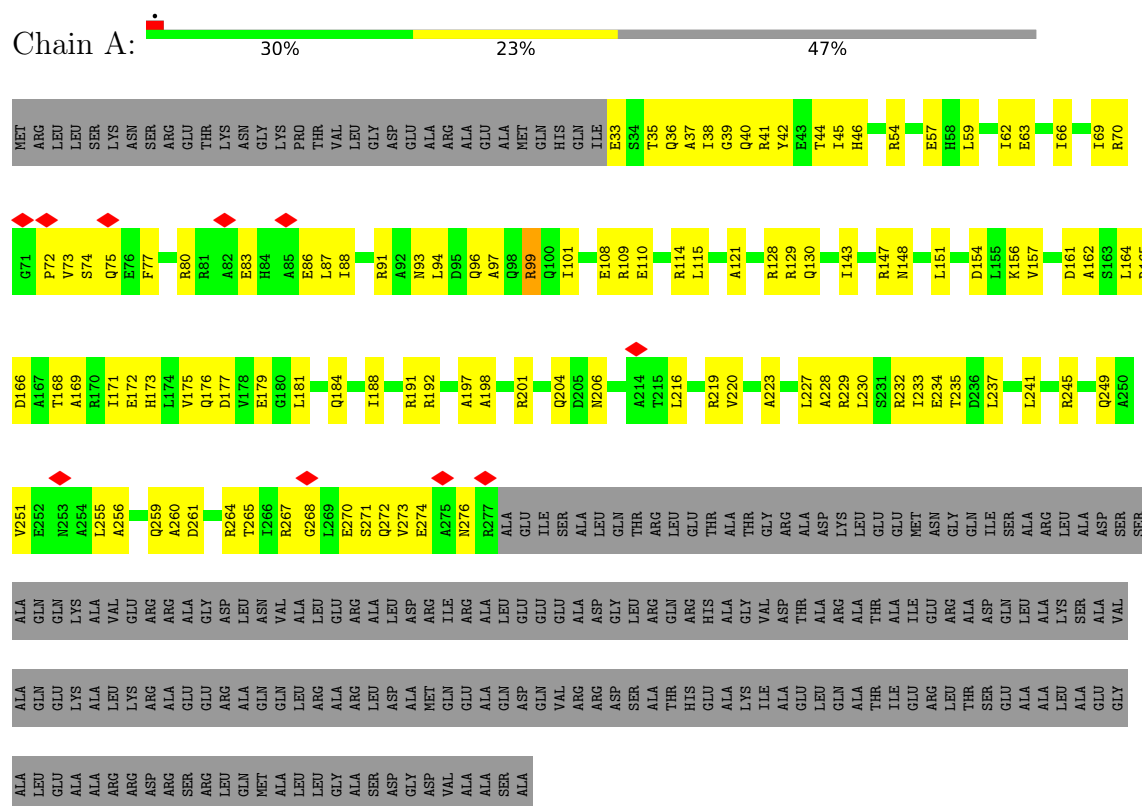
- Molecule 2 is a protein called Crescentin-specific megabody MB13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	F	111	Total	C	N	O	S	0	0
			861	535	154	167	5		
2	K	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	L	105	Total	C	N	O	S	0	0
			820	508	148	159	5		
2	Q	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	R	111	Total	C	N	O	S	0	0
			861	535	154	167	5		
2	W	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	X	105	Total	C	N	O	S	0	0
			820	508	148	159	5		

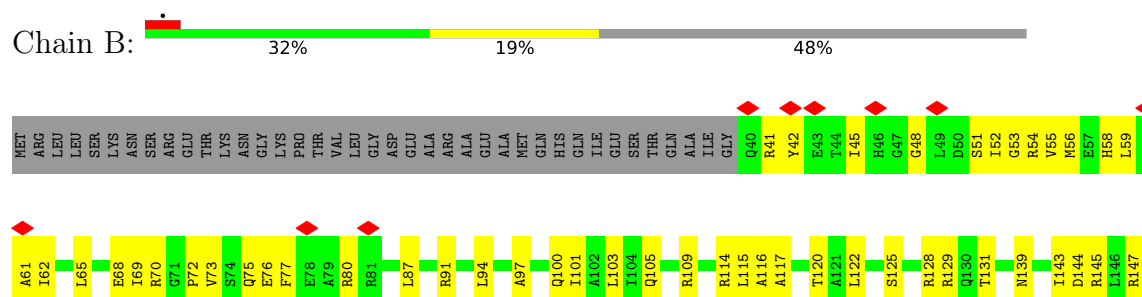
3 Residue-property plots

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.

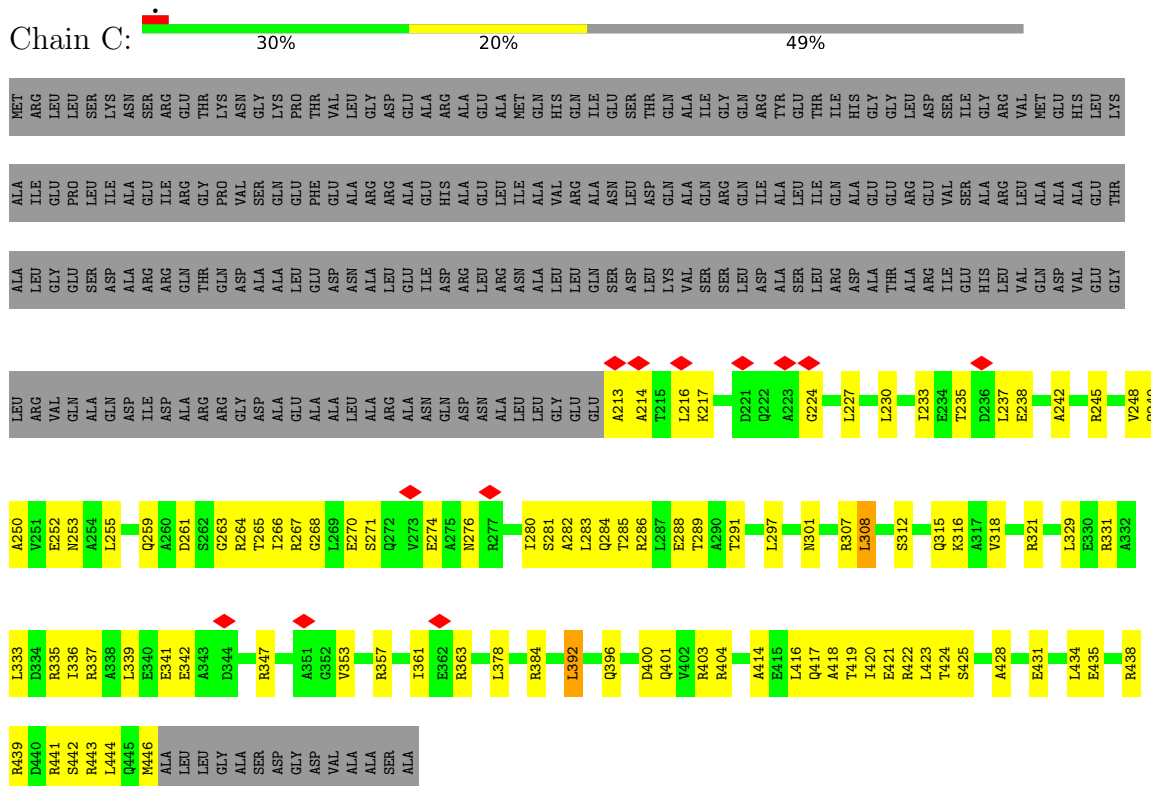
• Molecule 1: Crescentin



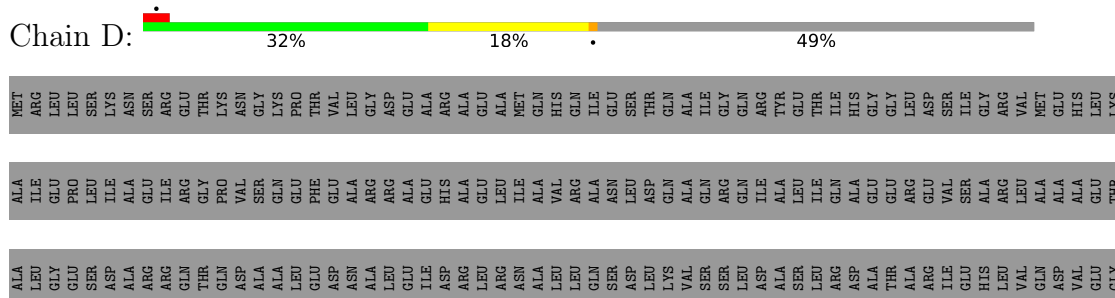
• Molecule 1: Crescentin



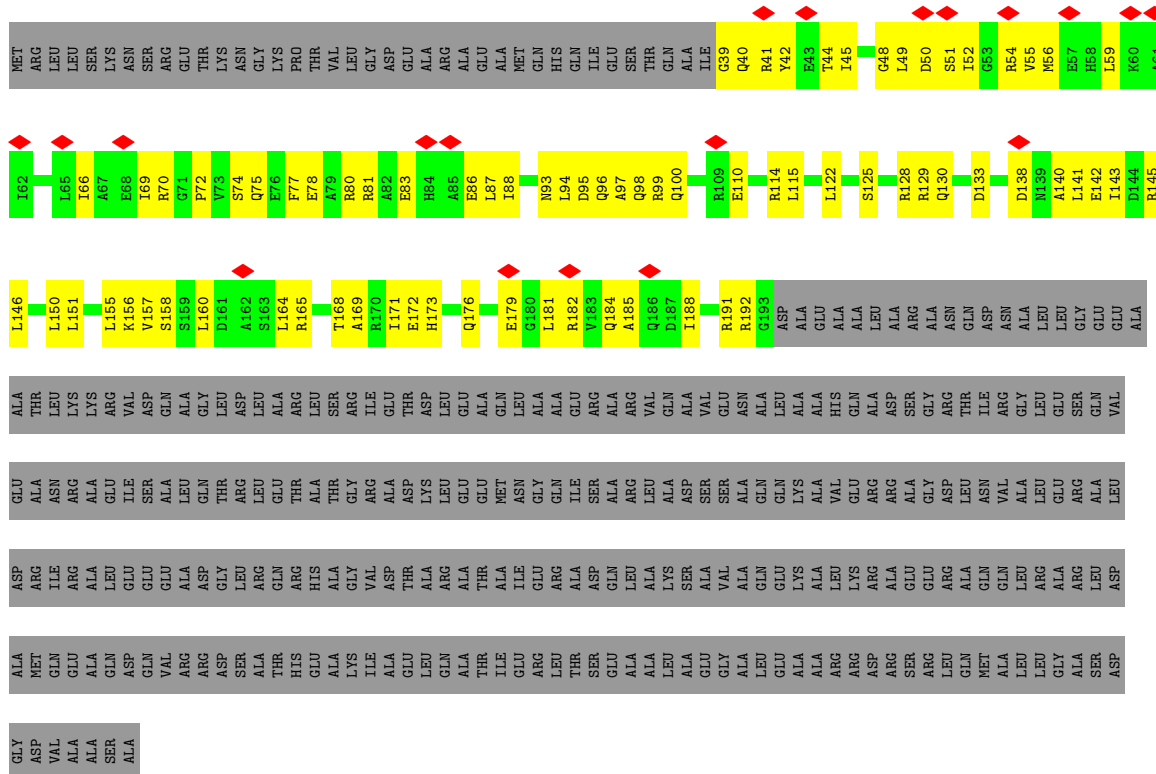
- Molecule 1: Crescentin



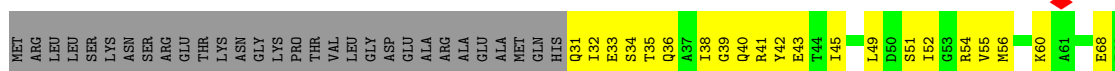
- Molecule 1: Crescentin

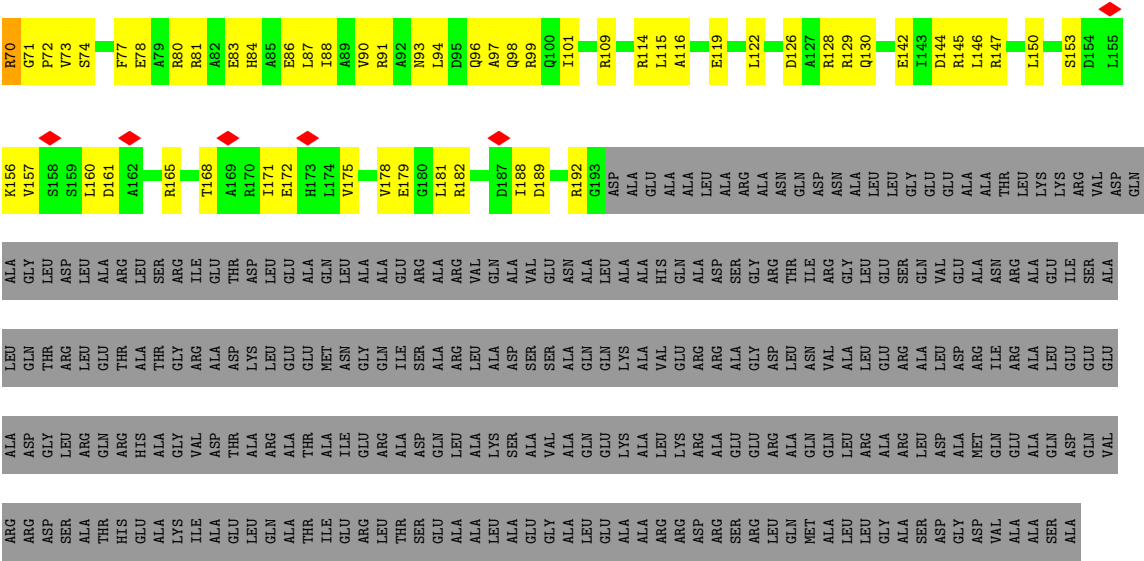


- Molecule 1: Crescentin

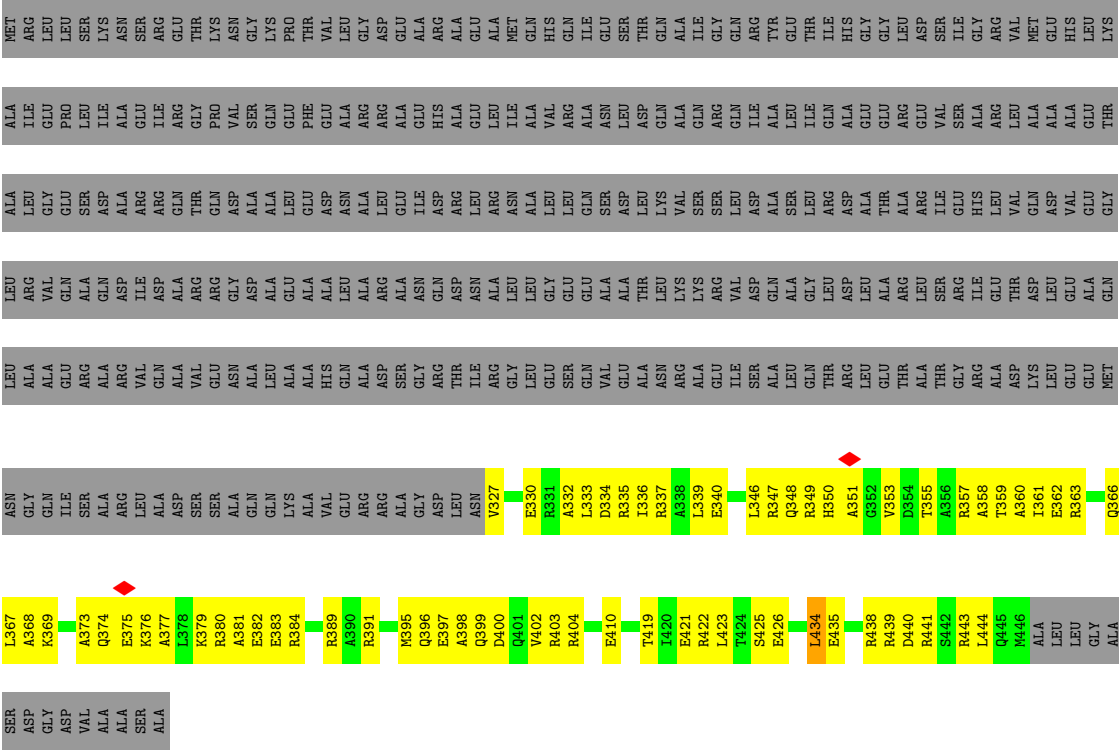


- Molecule 1: Crescentin

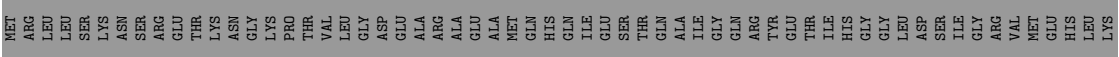




● Molecule 1: Crescentin

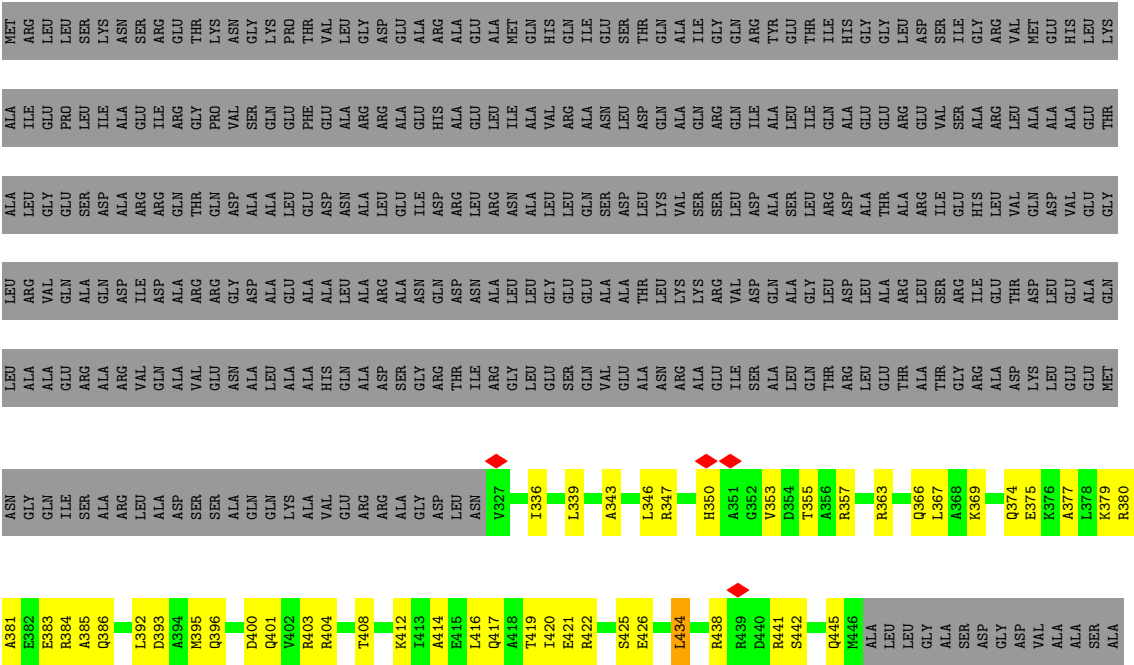


● Molecule 1: Crescentin









• Molecule 2: Crescentin-specific megabody MB13

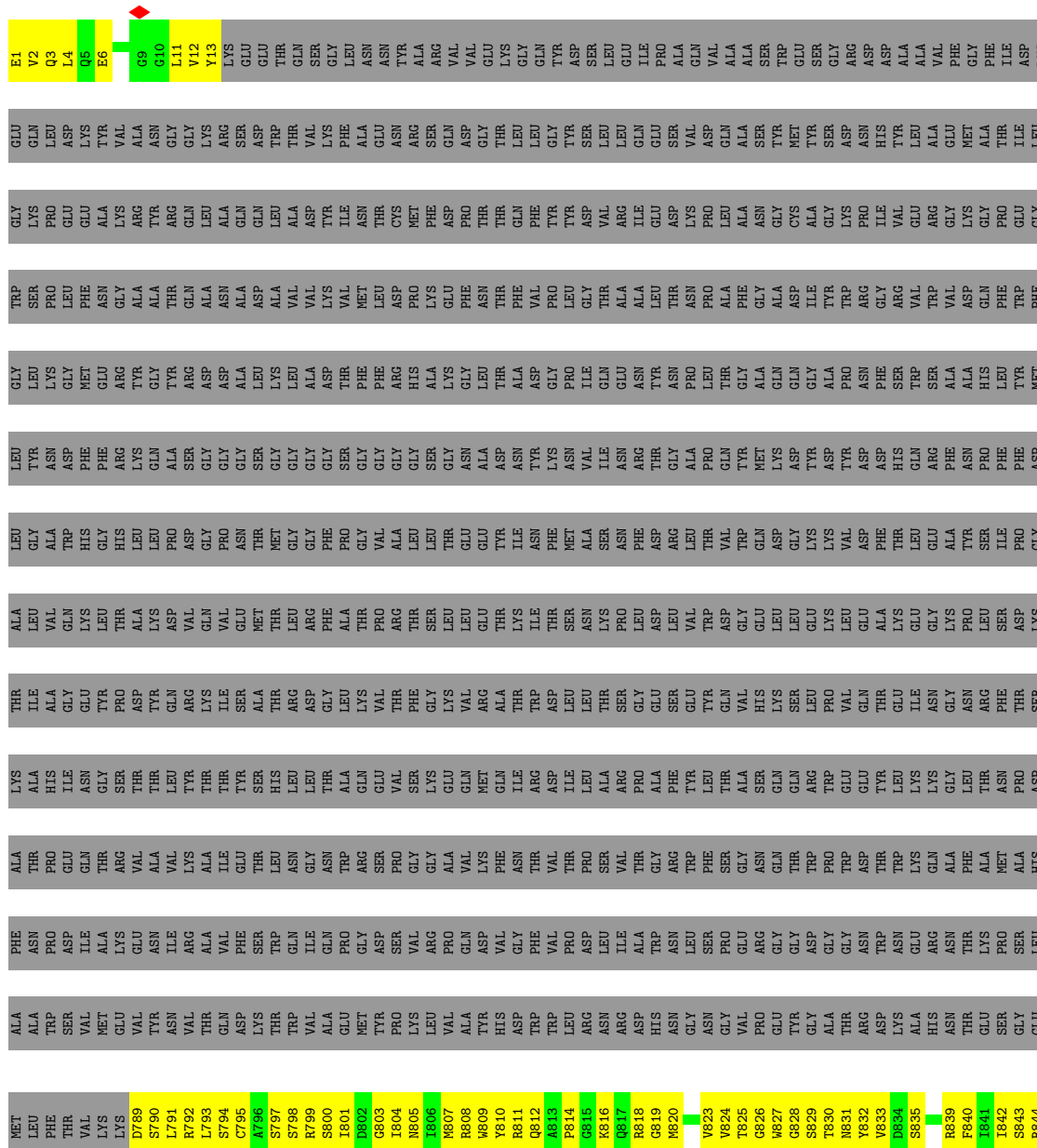






- Molecule 2: Crescentin-specific megabody MB13

Chain K: 8% 88%



Y851	Y852	Y853	Q854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	A870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000
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Chain R: 5% 7% 88%



LEU	LYS	GLY	TYR	ASN	ASP	PHE	GLY	THR	LEU	PHE	LEU	Y852	Y853	L853	Y854	Q854	Y855	M855	Y856	G856	N857	L858	K859	P860	E861	D862	T863	A864	Y865	Y866	Y867	Y868	Y869	Y870	A871	L871	Y872	Y873	G874	E875	S876	Y877	Y878	T882	Q883	Y884	T885	Y886	S887	Y888	Y889	Y890	Y891	L791	R792	L793	T794	C795	A796	Y797	Y798	D802	G803	I804	R805	M806	M807	L808	Y809	Y810	R811	Q812	A813	Y814	K816	Q817	R818	G819	M820	Y823	T824	T825	G826	Y827	S828	S829	T830	N831	Y832	Y833	D834	Y835	S836	Y837	G838	R839	F840	I841	T842	S843	R844	Y845	D849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000	Y1001	Y1002	Y1003	Y1004	Y1005	Y1006	Y1007	Y1008	Y1009	Y1010	Y1011	Y1012	Y1013	Y1014	Y1015	Y1016	Y1017	Y1018	Y1019	Y1020	Y1021	Y1022	Y1023	Y1024	Y1025	Y1026	Y1027	Y1028	Y1029	Y1030	Y1031	Y1032	Y1033	Y1034	Y1035	Y1036	Y1037	Y1038	Y1039	Y1040	Y1041	Y1042	Y1043	Y1044	Y1045	Y1046	Y1047	Y1048	Y1049	Y1050	Y1051	Y1052	Y1053	Y1054	Y1055	Y1056	Y1057	Y1058	Y1059	Y1060	Y1061	Y1062	Y1063	Y1064	Y1065	Y1066	Y1067	Y1068	Y1069	Y1070	Y1071	Y1072	Y1073	Y1074	Y1075	Y1076	Y1077	Y1078	Y1079	Y1080	Y1081	Y1082	Y1083	Y1084	Y1085	Y1086	Y1087	Y1088	Y1089	Y1090	Y1091	Y1092	Y1093	Y1094	Y1095	Y1096	Y1097	Y1098	Y1099	Y1100	Y1101	Y1102	Y1103	Y1104	Y1105	Y1106	Y1107	Y1108	Y1109	Y1110	Y1111	Y1112	Y1113	Y1114	Y1115	Y1116	Y1117	Y1118	Y1119	Y1120	Y1121	Y1122	Y1123	Y1124	Y1125	Y1126	Y1127	Y1128	Y1129	Y1130	Y1131	Y1132	Y1133	Y1134	Y1135	Y1136	Y1137	Y1138	Y1139	Y1140	Y1141	Y1142	Y1143	Y1144	Y1145	Y1146	Y1147	Y1148	Y1149	Y1150	Y1151	Y1152	Y1153	Y1154	Y1155	Y1156	Y1157	Y1158	Y1159	Y1160	Y1161	Y1162	Y1163	Y1164	Y1165	Y1166	Y1167	Y1168	Y1169	Y1170	Y1171	Y1172	Y1173	Y1174	Y1175	Y1176	Y1177	Y1178	Y1179	Y1180	Y1181	Y1182	Y1183	Y1184	Y1185	Y1186	Y1187	Y1188	Y1189	Y1190	Y1191	Y1192	Y1193	Y1194	Y1195	Y1196	Y1197	Y1198	Y1199	Y1200	Y1201	Y1202	Y1203	Y1204	Y1205	Y1206	Y1207	Y1208	Y1209	Y1210	Y1211	Y1212	Y1213	Y1214	Y1215	Y1216	Y1217	Y1218	Y1219	Y1220	Y1221	Y1222	Y1223	Y1224	Y1225	Y1226	Y1227	Y1228	Y1229	Y1230	Y1231	Y1232	Y1233	Y1234	Y1235	Y1236	Y1237	Y1238	Y1239	Y1240	Y1241	Y1242	Y1243	Y1244	Y1245	Y1246	Y1247	Y1248	Y1249	Y1250	Y1251	Y1252	Y1253	Y1254	Y1255	Y1256	Y1257	Y1258	Y1259	Y1260	Y1261	Y1262	Y1263	Y1264	Y1265	Y1266	Y1267	Y1268	Y1269	Y1270	Y1271	Y1272	Y1273	Y1274	Y1275	Y1276	Y1277	Y1278	Y1279	Y1280	Y1281	Y1282	Y1283	Y1284	Y1285	Y1286	Y1287	Y1288	Y1289	Y1290	Y1291	Y1292	Y1293	Y1294	Y1295	Y1296	Y1297	Y1298	Y1299	Y1300	Y1301	Y1302	Y1303	Y1304	Y1305	Y1306	Y1307	Y1308	Y1309	Y1310	Y1311	Y1312	Y1313	Y1314	Y1315	Y1316	Y1317	Y1318	Y1319	Y1320	Y1321	Y1322	Y1323	Y1324	Y1325	Y1326	Y1327	Y1328	Y1329	Y1330	Y1331	Y1332	Y1333	Y1334	Y1335	Y1336	Y1337	Y1338	Y1339	Y1340	Y1341	Y1342	Y1343	Y1344	Y1345	Y1346	Y1347	Y1348	Y1349	Y1350	Y1351	Y1352	Y1353	Y1354	Y1355	Y1356	Y1357	Y1358	Y1359	Y1360	Y1361	Y1362	Y1363	Y1364	Y1365	Y1366	Y1367	Y1368	Y1369	Y1370	Y1371	Y1372	Y1373	Y1374	Y1375	Y1376	Y1377	Y1378	Y1379	Y1380	Y1381	Y1382	Y1383	Y1384	Y1385	Y1386	Y1387	Y1388	Y1389	Y1390	Y1391	Y1392	Y1393	Y1394	Y1395	Y1396	Y1397	Y1398	Y1399	Y1400	Y1401	Y1402	Y1403	Y1404	Y1405	Y1406	Y1407	Y1408	Y1409	Y1410	Y1411	Y1412	Y1413	Y1414	Y1415	Y1416	Y1417	Y1418	Y1419	Y1420	Y1421	Y1422	Y1423	Y1424	Y1425	Y1426	Y1427	Y1428	Y1429	Y1430	Y1431	Y1432	Y1433	Y1434	Y1435	Y1436	Y1437	Y1438	Y1439	Y1440	Y1441	Y1442	Y1443	Y1444	Y1445	Y1446	Y1447	Y1448	Y1449	Y1450	Y1451	Y1452	Y1453	Y1454	Y1455	Y1456	Y1457	Y1458	Y1459	Y1460	Y1461	Y1462	Y1463	Y1464	Y1465	Y1466	Y1467	Y1468	Y1469	Y1470	Y1471	Y1472	Y1473	Y1474	Y1475	Y1476	Y1477	Y1478	Y1479	Y1480	Y1481	Y1482	Y1483	Y1484	Y1485	Y1486	Y1487	Y1488	Y1489	Y1490	Y1491	Y1492	Y1493	Y1494	Y1495	Y1496	Y1497	Y1498	Y1499	Y1500	Y1501	Y1502	Y1503	Y1504	Y1505	Y1506	Y1507	Y1508	Y1509	Y1510	Y1511	Y1512	Y1513	Y1514	Y1515	Y1516	Y1517	Y1518	Y1519	Y1520	Y1521	Y1522	Y1523	Y1524	Y1525	Y1526	Y1527	Y1528	Y1529	Y1530	Y1531	Y1532	Y1533	Y1534	Y1535	Y1536	Y1537	Y1538	Y1539	Y1540	Y1541	Y1542	Y1543	Y1544	Y1545	Y1546	Y1547	Y1548	Y1549	Y1550	Y1551	Y1552	Y1553	Y1554	Y1555	Y1556	Y1557	Y1558	Y1559	Y1560	Y1561	Y1562	Y1563	Y1564	Y1565	Y1566	Y1567	Y1568	Y1569	Y1570	Y1571	Y1572	Y1573	Y1574	Y1575	Y1576	Y1577	Y1578	Y1579	Y1580	Y1581	Y1582	Y1583	Y1584	Y1585	Y1586	Y1587	Y1588	Y1589	Y1590	Y1591	Y1592	Y1593	Y1594	Y1595	Y1596	Y1597	Y1598	Y1599	Y1600	Y1601	Y1602	Y1603	Y1604	Y1605	Y1606	Y1607	Y1608	Y1609	Y1610	Y1611	Y1612	Y1613	Y1614	Y1615	Y1616	Y1617	Y1618	Y1619	Y1620	Y1621	Y1622	Y1623	Y1624	Y1625	Y1626	Y1627	Y1628	Y1629	Y1630	Y1631	Y1632	Y1633	Y1634	Y1635	Y1636	Y1637	Y1638	Y1639	Y1640	Y1641	Y1642	Y1643	Y1644	Y1645	Y1646	Y1647	Y1648	Y1649	Y1650	Y1651	Y1652	Y1653	Y1654	Y1655	Y1656	Y1657	Y1658	Y1659	Y1660	Y1661	Y1662	Y1663	Y1664	Y1665	Y1666	Y1667	Y1668	Y1669	Y1670	Y1671	Y1672	Y1673	Y1674	Y1675	Y1676	Y1677	Y1678	Y1679	Y1680	Y1681	Y1682	Y1683	Y1684	Y1685	Y1686	Y1687	Y1688	Y1689	Y1690	Y1691	Y1692	Y1693	Y1694	Y1695	Y1696	Y1697	Y1698	Y1699	Y1700	Y1701	Y1702	Y1703	Y1704	Y1705	Y1706	Y1707	Y1708	Y1709	Y1710	Y1711	Y1712	Y1713	Y1714	Y1715	Y1716	Y1717	Y1718	Y1719	Y1720	Y1721	Y1722	Y1723	Y1724	Y1725	Y1726	Y1727	Y1728	Y1729	Y1730	Y1731	Y1732	Y1733	Y1734	Y1735	Y1736	Y1737	Y1738	Y1739	Y1740	Y1741	Y1742	Y1743	Y1744	Y1745	Y1746	Y1747	Y1748	Y1749	Y1750	Y1751	Y1752	Y1753	Y1754	Y1755	Y1756	Y1757	Y1758	Y1759	Y1760	Y1761	Y1762	Y1763	Y1764	Y1765	Y1766	Y1767	Y1768	Y1769	Y1770	Y1771	Y1772	Y1773	Y1774	Y1775	Y1776	Y1777	Y1778	Y1779	Y1780	Y1781	Y1782	Y1783	Y1784	Y1785	Y1786	Y1787	Y1788	Y1789	Y1790	Y1791	Y1792	Y1793	Y1794	Y1795	Y1796	Y1797	Y1798	Y1799	Y1800	Y1801	Y1802	Y1803	Y1804	Y1805	Y1806	Y1807	Y1808	Y1809	Y1810	Y1811	Y1812	Y1813	Y1814	Y1815	Y1816	Y1817	Y1818	Y1819	Y1820	Y1821	Y1822	Y1823	Y1824	Y1825	Y1826	Y1827	Y1828	Y1829	Y1830	Y1831	Y1832	Y1833	Y1834	Y1835	Y1836	Y1837	Y1838	Y1839	Y1840	Y1841	Y1842	Y1843	Y1844	Y1845	Y1846	Y1847	Y1848	Y1849	Y1850	Y1851	Y1852	Y1853	Y1854	Y1855	Y1856	Y1857	Y1858	Y1859	Y1860	Y1861	Y1862	Y1863	Y1864	Y1865	Y1866	Y1867	Y1868	Y1869	Y1870	Y1871	Y1872	Y1873	Y1874	Y1875	Y1876	Y1877	Y1878	Y1879	Y1880	Y1881	Y1882	Y1883	Y1884	Y1885	Y1886	Y1887	Y1888	Y1889	Y1890	Y1891	Y1892	Y1893	Y1894	Y1895	Y1896	Y1897	Y1898	Y1899	Y1900	Y1901	Y1902	Y1903	Y1904	Y1905	Y1906	Y1907	Y1908	Y1909	Y1910	Y1911	Y1912	Y1913	Y1914	Y1915	Y1916	Y1917	Y1918	Y1919	Y1920	Y1921	Y1922	Y1923	Y1924	Y1925	Y1926	Y1927	Y1928	Y1929	Y1930	Y1931	Y1932	Y1933	Y1934	Y1935	Y1936	Y1937	Y1938	Y1939	Y1940	Y1941	Y1942	Y1943	Y1944	Y1945	Y1946	Y1947	Y1948	Y1949	Y1950	Y1951	Y1952	Y1953	Y1954	Y1955	Y1956	Y1957	Y1958	Y1959	Y1960	Y1961	Y1962	Y1963	Y1964	Y1965	Y1966	Y1967	Y1968	Y1969	Y1970	Y1971	Y1972	Y1973	Y1974	Y1975	Y1976	Y1977	Y1978	Y1979	Y1980	Y1981	Y1982	Y1983	Y1984	Y1985	Y1986	Y1987	Y1988	Y1989	Y1990	Y1991	Y1992	Y1993	Y1994	Y1995	Y1996	Y1997	Y1998	Y1999	Y2000	Y2001	Y2002	Y2003	Y2004	Y2005	Y2006	Y2007	Y2008</
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GLU	ASP	LEU	HIS	ASP	ALA
MET	ALA	ALA	PHE	ALA	THR
LEU	THR	ALA	ASN	THR	THR
PHE	TRP	ALA	PRO	ASP	GLU
THR	SER	VAL	ILE	GLN	GLN
VAL	VAL	VAL	ILE	THR	THR
LYS	MET	LYS	ALA	ARG	ARG
LYS	GLU	GLU	LYS	VAL	VAL
ASP	ASP	VAL	ASN	ASN	ALA
SER	SER	TYR	ASN	ILE	ALA
L791	L791	VAL	ASN	VAL	VAL
R792	R792	THR	ARG	LYS	LYS
L793	L793	THR	ALA	ALA	ALA
S794	S794	GLN	VAL	ILE	ILE
C795	C795	ASP	PHE	GLU	GLU
A796	A796	LYS	SER	THR	THR
S797	S797	THR	TRP	LEU	LEU
S798	S798	TRP	GLN	ASN	ASN
R799	R799	VAL	ILE	GLY	GLY
S800	S800	ALA	GLN	ASN	ASN
I801	I801	GLU	PRO	TRP	TRP
I804	I804	MET	GLY	ARG	ARG
N805	N805	TYR	ASP	GLY	GLY
I806	I806	PRO	SER	THR	THR
M807	M807	LYS	VAL	VAL	VAL
Q812	Q812	LEU	VAL	THR	THR
Q812	Q812	VAL	PRO	PRO	PRO
K816	K816	ALA	ASN	LEU	SER
Q817	Q817	TYR	LEU	ILE	VAL
R818	R818	HIS	ASP	ALA	THR
R818	R818	ASP	GLY	GLY	GLY
A822	A822	TRP	PHE	THR	THR
V823	V823	LEU	VAL	VAL	VAL
V824	V824	ARG	THR	THR	THR
T825	T825	ASN	PRO	ASP	ASP
G826	G826	ASN	ASN	LEU	SER
W827	W827	ASP	GLY	THR	THR
G828	G828	HIS	TRP	ALA	ALA
S829	S829	ASN	ALA	THR	THR
T830	T830	GLY	GLY	GLY	GLY
N831	N831	ASN	VAL	ASN	ASN
Y832	Y832	VAL	PRO	ARG	ARG
V833	V833	PRO	GLU	GLN	GLN
D834	D834	GLU	TYR	GLY	GLY
S835	S835	TYR	GLY	ASP	TRP
V836	V836	GLY	ALA	GLY	PRO
K837	K837	ALA	THR	TRP	TRP
G838	G838	THR	ARG	ASP	ASP
R839	R839	ARG	ASP	TRP	THR
F840	F840	ASP	LYS	ASN	TRP
I841	I841	LYS	ALA	GLU	LYS
I842	I842	ALA	HIS	ARG	GLN
S843	S843	HIS	ASN	THR	ALA
R844	R844	ASN	THR	PHE	ALA
D845	D845	THR	GLU	LYS	ALA
K848	K848	SER	PRO	MET	MET
D849	D849	GLY	SER	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	585252	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.736	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	954.0, 954.0, 954.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.59, 1.59, 1.59	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	0.35	0/1884	0.57	0/2540
1	B	0.34	0/1836	0.61	1/2475 (0.0%)
1	C	0.31	0/1795	0.60	2/2407 (0.1%)
1	D	0.31	0/1795	0.57	1/2407 (0.0%)
1	G	0.34	0/1210	0.60	0/1630
1	H	0.36	0/1271	0.61	0/1713
1	I	0.33	0/935	0.57	1/1251 (0.1%)
1	J	0.32	0/935	0.56	1/1251 (0.1%)
1	M	0.35	0/1884	0.57	0/2540
1	N	0.34	0/1836	0.61	1/2475 (0.0%)
1	O	0.31	0/1795	0.60	2/2407 (0.1%)
1	P	0.31	0/1795	0.57	1/2407 (0.0%)
1	S	0.34	0/1210	0.60	0/1630
1	T	0.35	0/1271	0.61	0/1713
1	U	0.33	0/935	0.57	1/1251 (0.1%)
1	V	0.32	0/935	0.56	1/1251 (0.1%)
2	E	0.52	0/883	0.64	0/1192
2	F	0.47	0/875	0.68	0/1181
2	K	0.44	0/883	0.58	0/1192
2	L	0.43	0/833	0.61	0/1124
2	Q	0.52	0/883	0.64	0/1192
2	R	0.46	0/875	0.68	0/1181
2	W	0.44	0/883	0.58	0/1192
2	X	0.43	0/833	0.61	0/1124
All	All	0.37	0/30270	0.60	12/40726 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	434	LEU	CA-CB-CG	-6.42	100.54	115.30
1	J	434	LEU	CA-CB-CG	-6.41	100.56	115.30
1	O	308	LEU	CA-CB-CG	-6.15	101.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	LEU	CA-CB-CG	-6.14	101.17	115.30
1	N	208	LEU	CA-CB-CG	5.83	128.71	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1876	0	1869	136	0
1	B	1828	0	1824	128	0
1	C	1793	0	1815	111	0
1	D	1793	0	1813	99	0
1	G	1203	0	1200	103	0
1	H	1264	0	1261	104	0
1	I	934	0	946	84	0
1	J	934	0	946	72	0
1	M	1876	0	1869	138	0
1	N	1828	0	1824	124	0
1	O	1793	0	1815	110	0
1	P	1793	0	1813	102	0
1	S	1203	0	1200	102	0
1	T	1264	0	1261	103	0
1	U	934	0	946	82	0
1	V	934	0	946	72	0
2	E	869	0	846	83	0
2	F	861	0	842	71	0
2	K	869	0	846	119	0
2	L	820	0	802	77	0
2	Q	869	0	846	81	0
2	R	861	0	842	72	0
2	W	869	0	846	117	0
2	X	820	0	802	76	0
All	All	30088	0	30020	1875	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 31.

The worst 5 of 1875 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)
2:K:804:ILE:HB	2:K:872:TYR:CZ	1.30	1.66
2:K:804:ILE:HD13	2:K:872:TYR:CD2	1.28	1.64
2:W:804:ILE:HD13	2:W:872:TYR:CD2	1.28	1.63
2:W:804:ILE:HB	2:W:872:TYR:CZ	1.29	1.62
2:W:804:ILE:CB	2:W:872:TYR:CE1	1.85	1.60

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	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	B	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	C	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	D	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	G	153/460 (33%)	152 (99%)	1 (1%)	0	100	100
1	H	161/460 (35%)	159 (99%)	2 (1%)	0	100	100
1	I	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	J	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
1	M	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	N	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	O	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	P	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	S	153/460 (33%)	152 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	161/460 (35%)	159 (99%)	2 (1%)	0	100	100
1	U	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	V	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
2	E	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	F	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	K	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	L	101/907 (11%)	89 (88%)	12 (12%)	0	100	100
2	Q	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	R	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	W	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	X	101/907 (11%)	90 (89%)	11 (11%)	0	100	100
All	All	3834/14616 (26%)	3651 (95%)	183 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/347 (54%)	186 (100%)	1 (0%)	86	90
1	B	182/347 (52%)	182 (100%)	0	100	100
1	C	174/347 (50%)	174 (100%)	0	100	100
1	D	174/347 (50%)	170 (98%)	4 (2%)	45	65
1	G	122/347 (35%)	121 (99%)	1 (1%)	79	85
1	H	129/347 (37%)	127 (98%)	2 (2%)	58	74
1	I	89/347 (26%)	89 (100%)	0	100	100
1	J	89/347 (26%)	89 (100%)	0	100	100
1	M	187/347 (54%)	186 (100%)	1 (0%)	86	90
1	N	182/347 (52%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	174/347 (50%)	174 (100%)	0	100	100
1	P	174/347 (50%)	170 (98%)	4 (2%)	45	65
1	S	122/347 (35%)	121 (99%)	1 (1%)	79	85
1	T	129/347 (37%)	127 (98%)	2 (2%)	58	74
1	U	89/347 (26%)	89 (100%)	0	100	100
1	V	89/347 (26%)	89 (100%)	0	100	100
2	E	94/749 (13%)	94 (100%)	0	100	100
2	F	93/749 (12%)	93 (100%)	0	100	100
2	K	94/749 (13%)	94 (100%)	0	100	100
2	L	89/749 (12%)	87 (98%)	2 (2%)	47	66
2	Q	94/749 (13%)	94 (100%)	0	100	100
2	R	93/749 (12%)	93 (100%)	0	100	100
2	W	94/749 (13%)	94 (100%)	0	100	100
2	X	89/749 (12%)	87 (98%)	2 (2%)	47	66
All	All	3032/11544 (26%)	3012 (99%)	20 (1%)	80	87

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	438	ARG
1	T	93	ASN
2	X	799	ARG
2	X	792	ARG
1	H	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	249	GLN
1	O	301	ASN
1	V	374	GLN
1	M	276	ASN
1	N	259	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 [i](#)

There are no chain breaks in this entry.

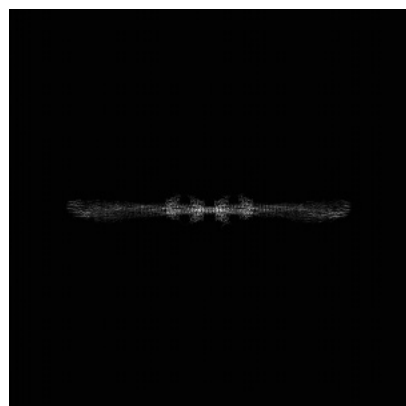
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15476. These allow visual inspection of the internal detail of the map and identification of artifacts.

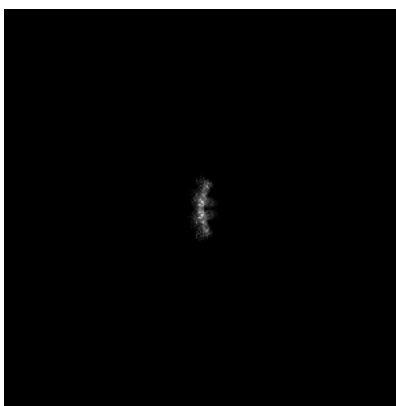
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

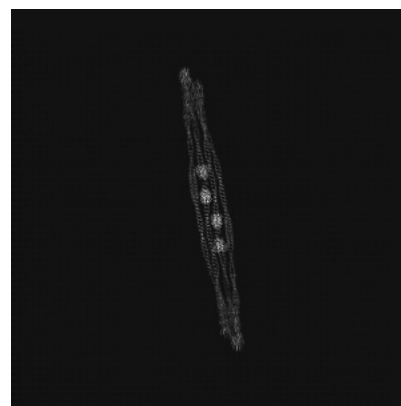
6.1.1 Primary map



X

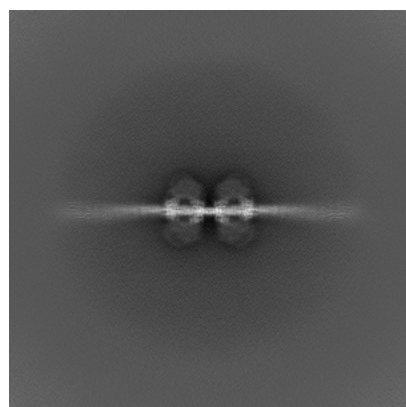


Y

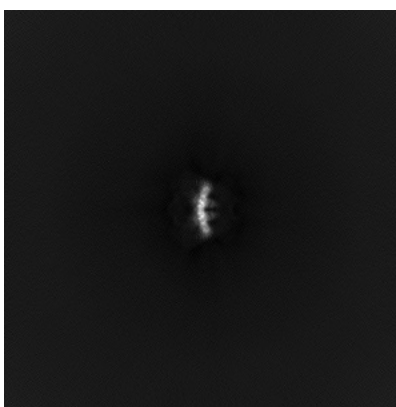


Z

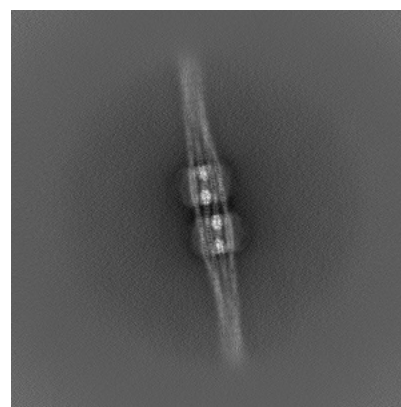
6.1.2 Raw map



X



Y

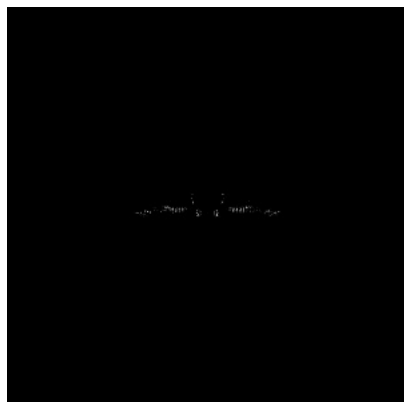


Z

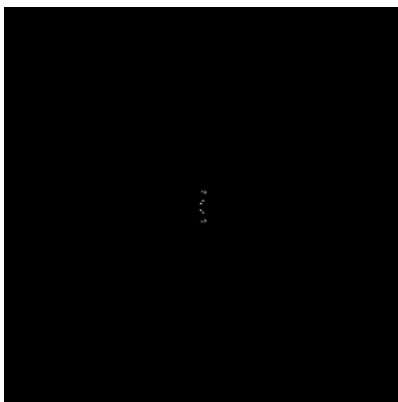
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

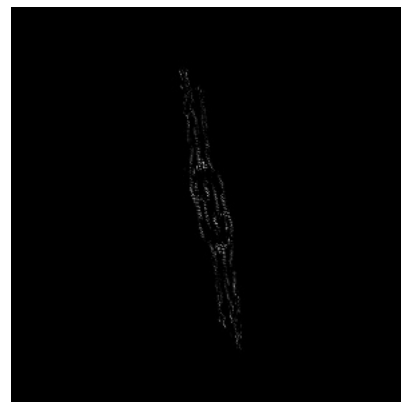
6.2.1 Primary map



X Index: 300

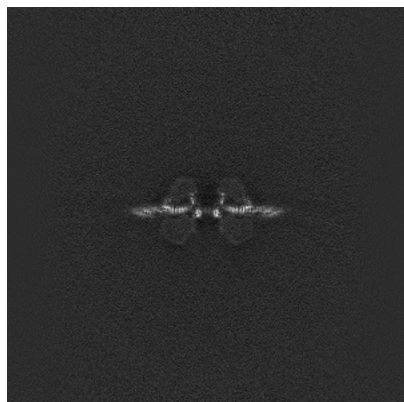


Y Index: 300

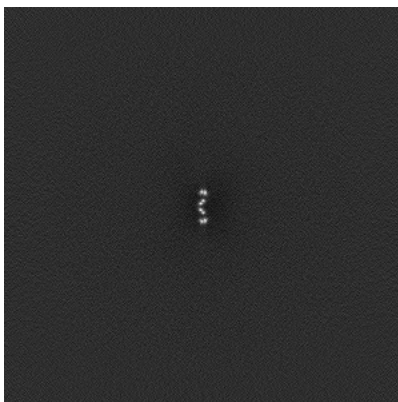


Z Index: 300

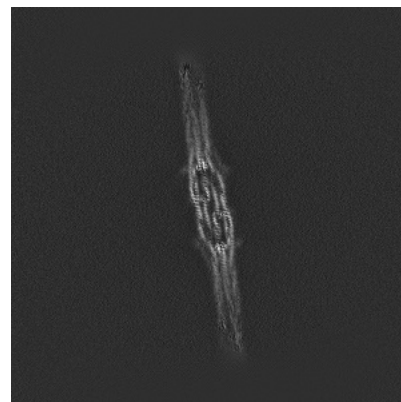
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

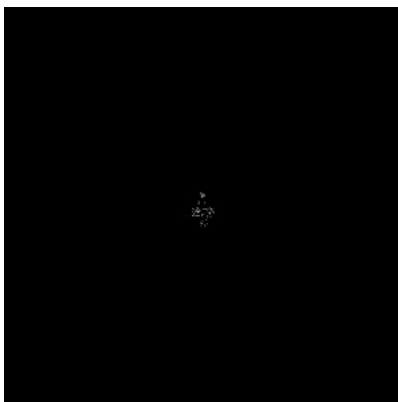
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 310

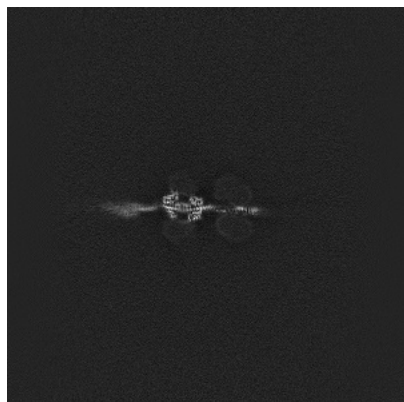


Y Index: 318

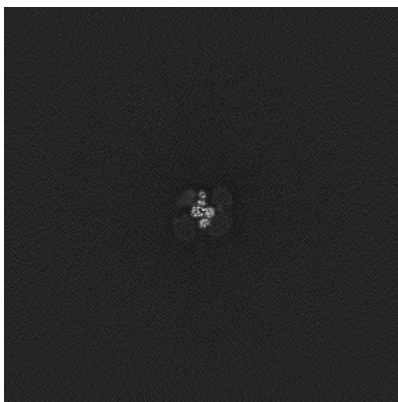


Z Index: 299

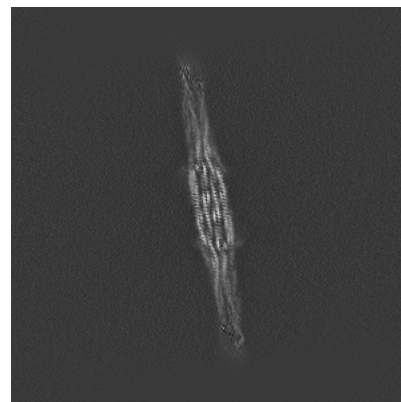
6.3.2 Raw map



X Index: 310



Y Index: 317

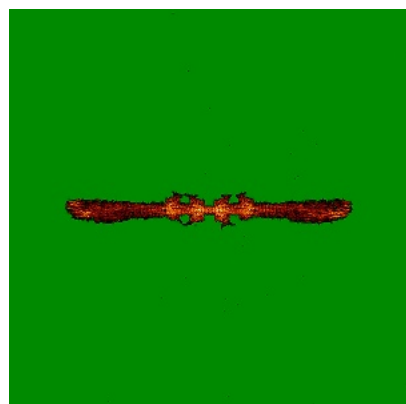


Z Index: 298

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X

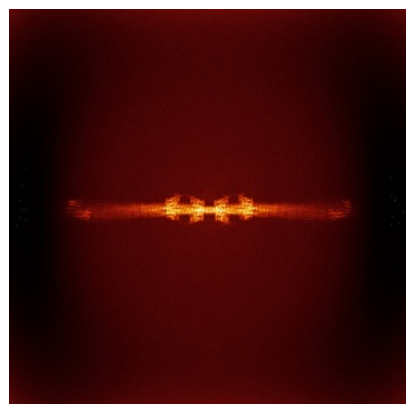


Y

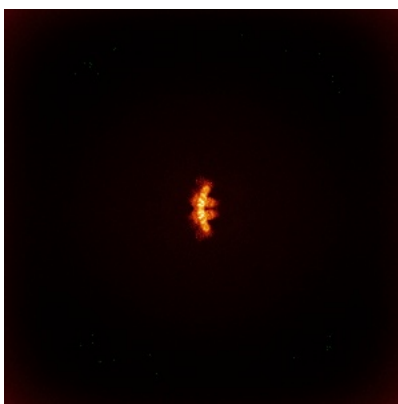


Z

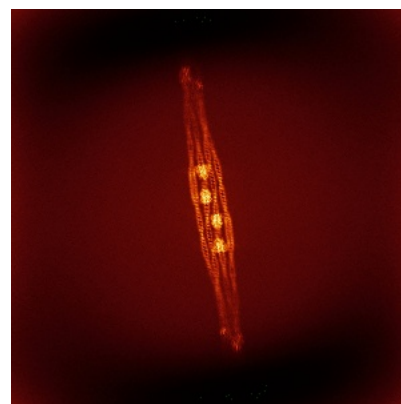
6.4.2 Raw map



X



Y

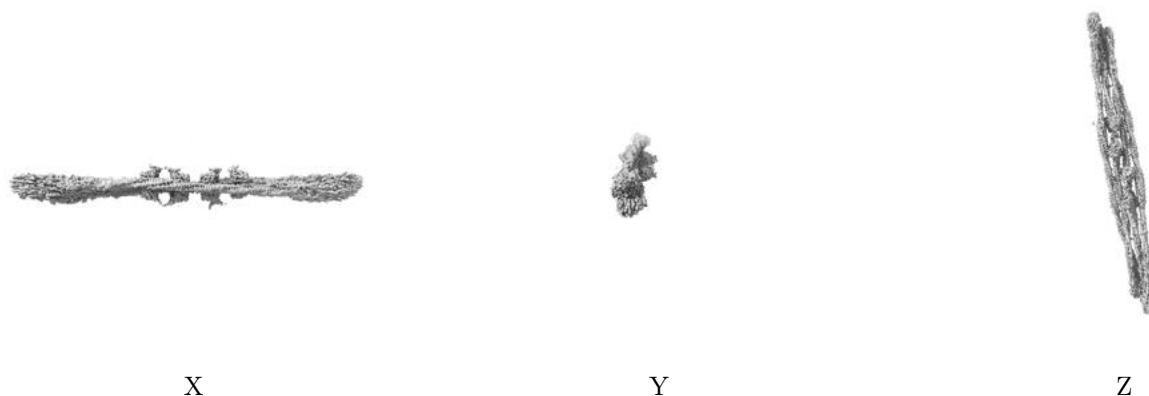


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

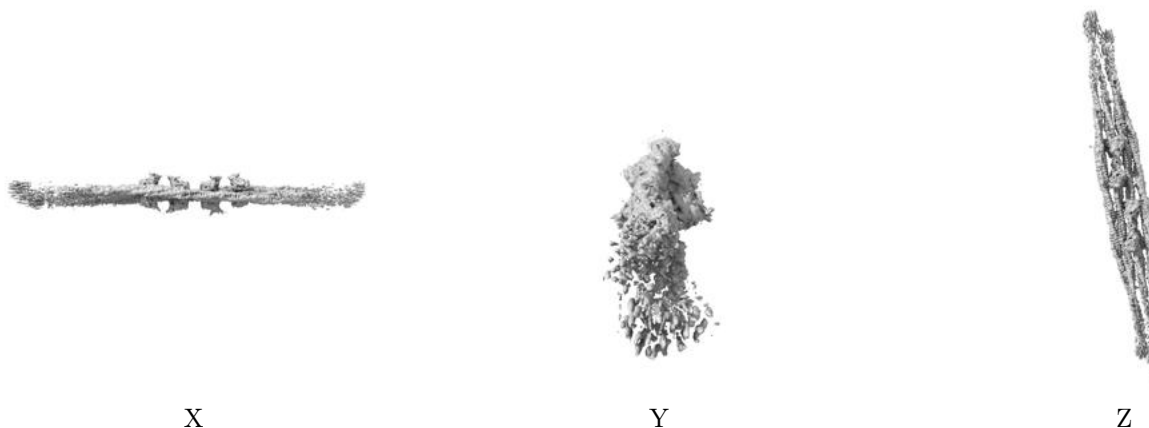
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

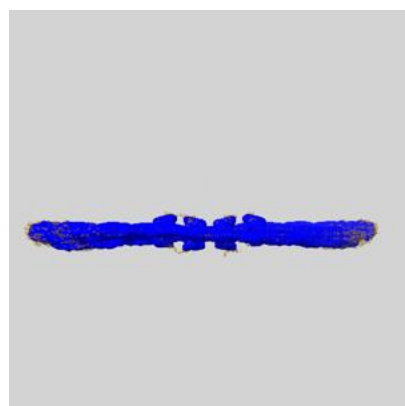
6.6 Mask visualisation [i](#)

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

A mask typically either:

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

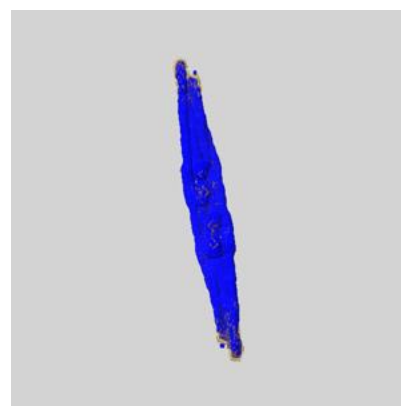
6.6.1 emd_15476_msk_1.map [i](#)



X



Y

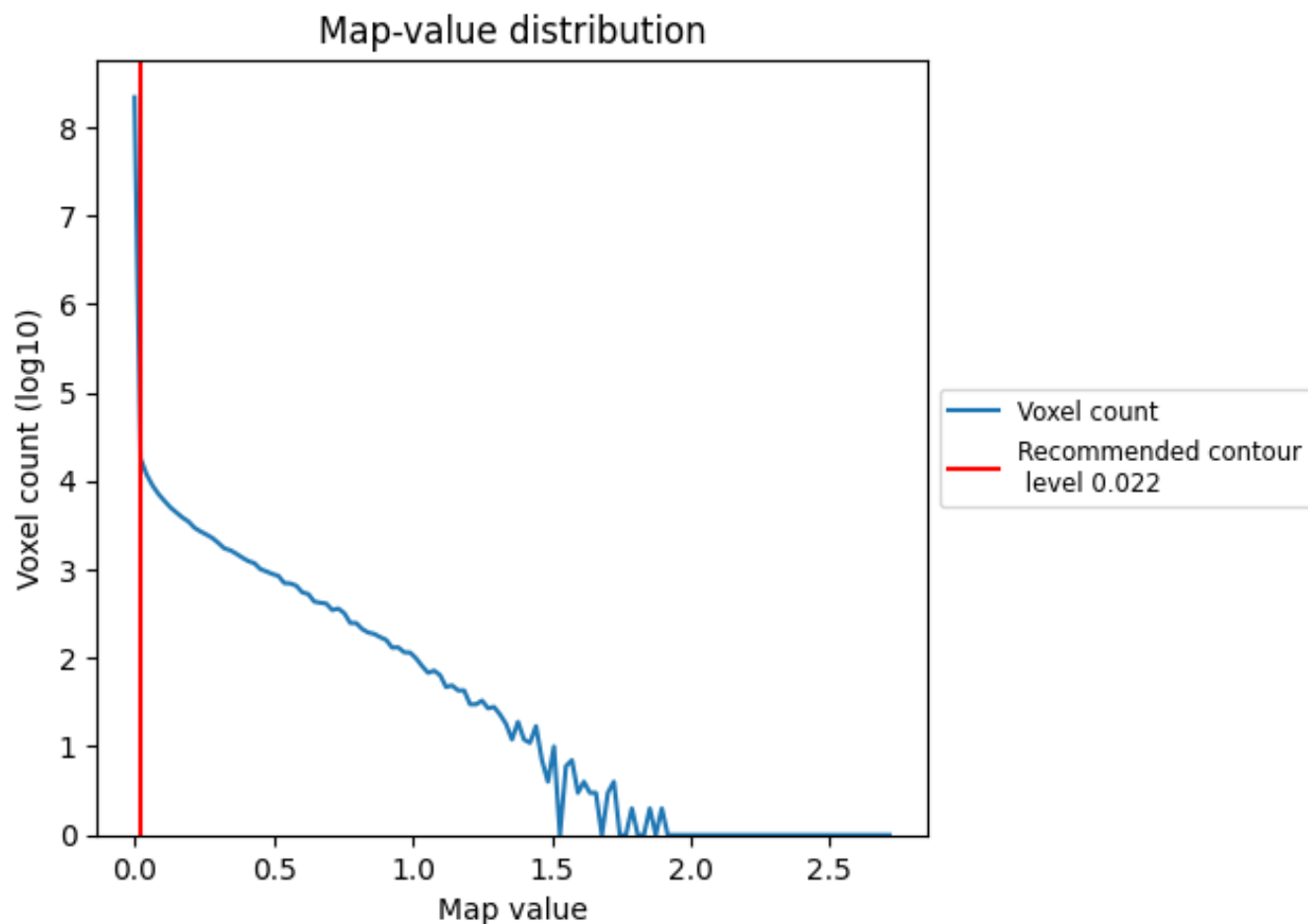


Z

7 Map analysis [i](#)

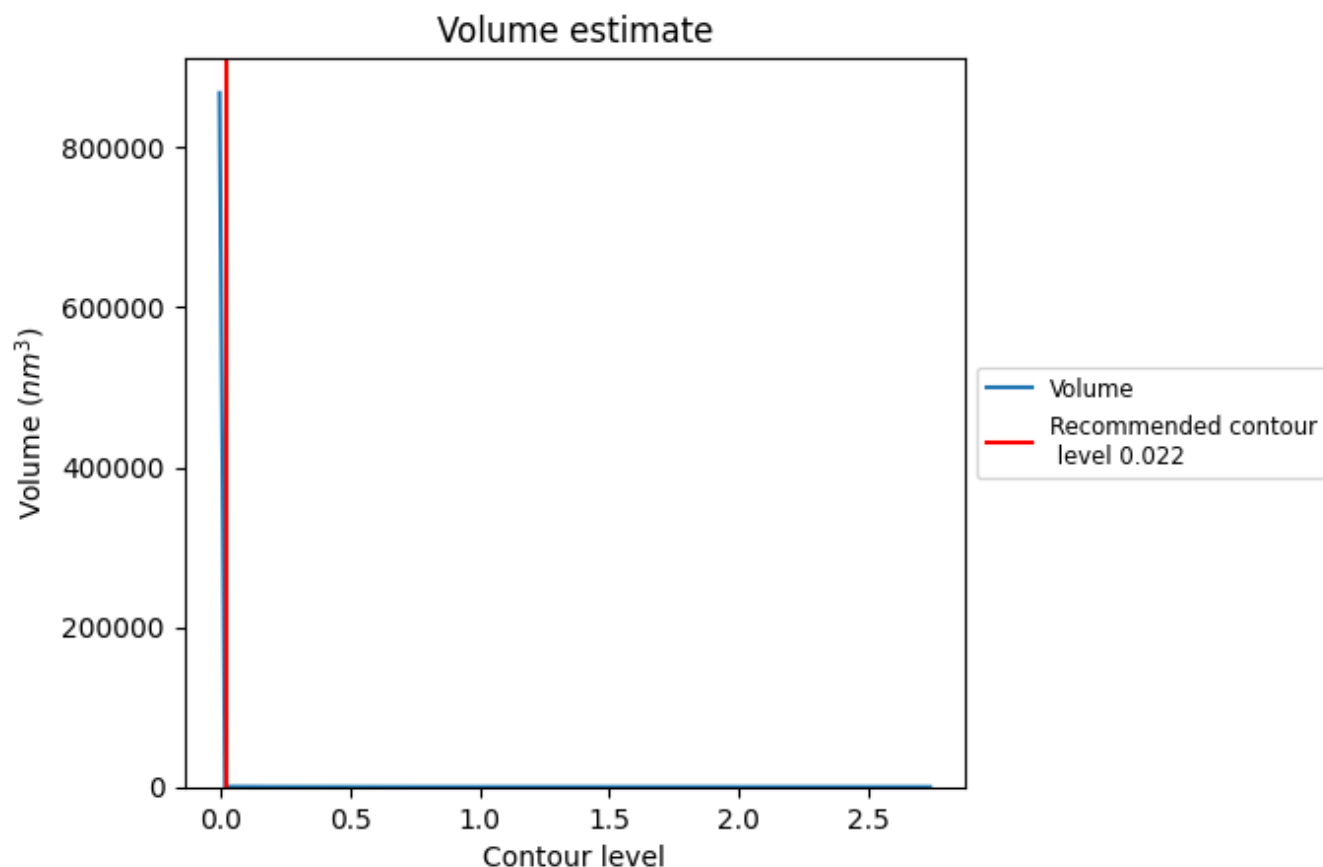
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

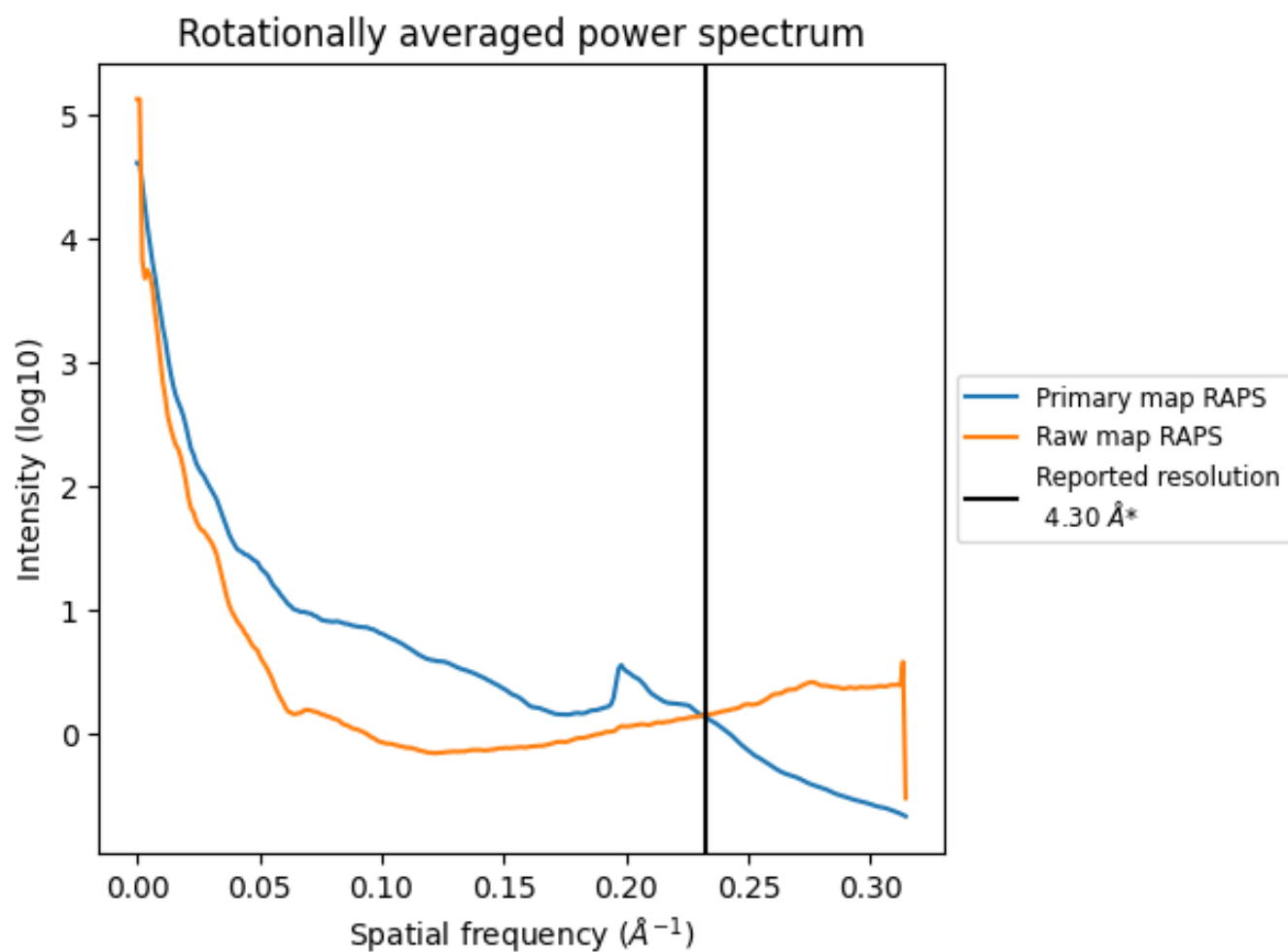
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

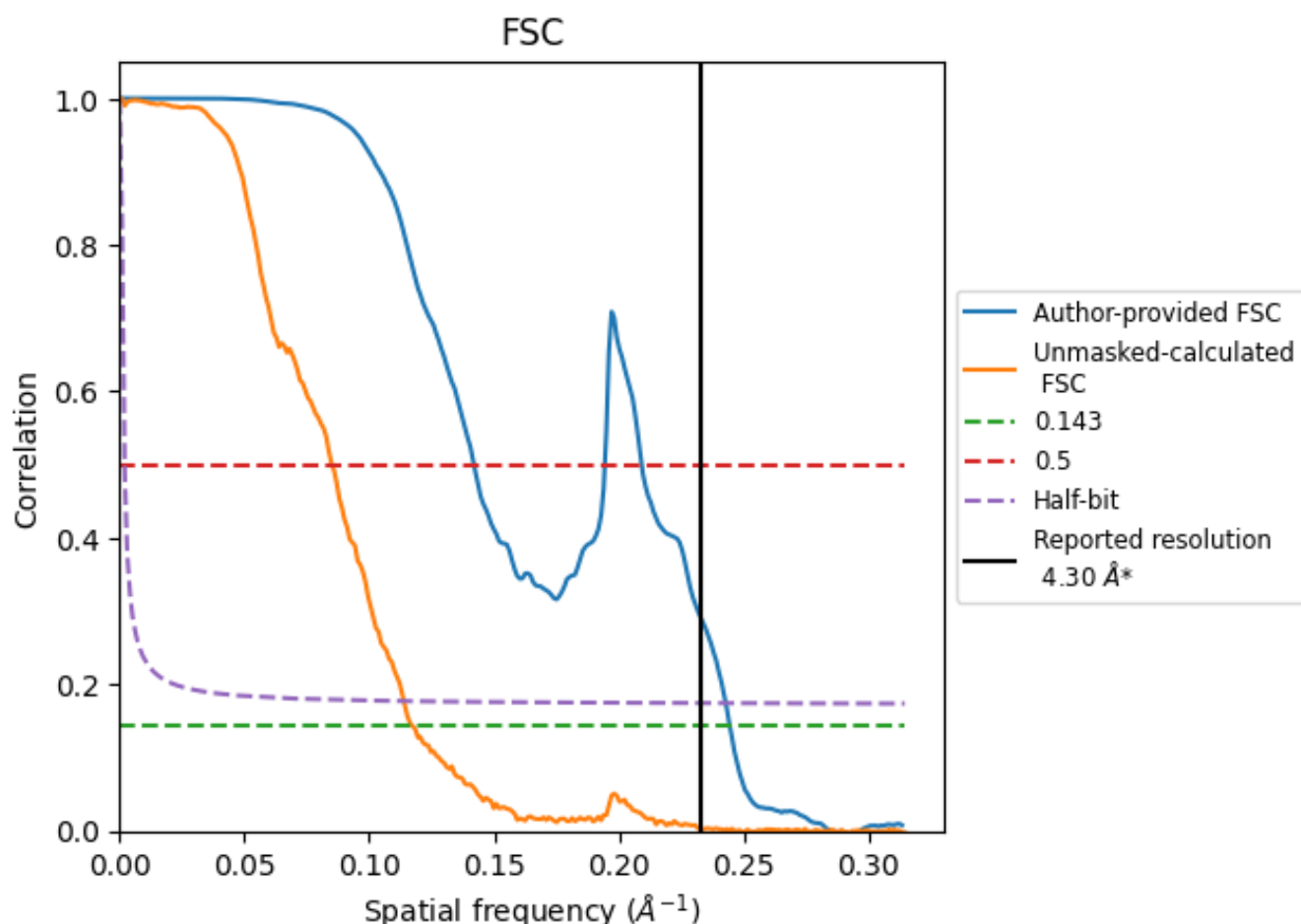


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 \AA^{-1}

8.2 Resolution estimates [i](#)

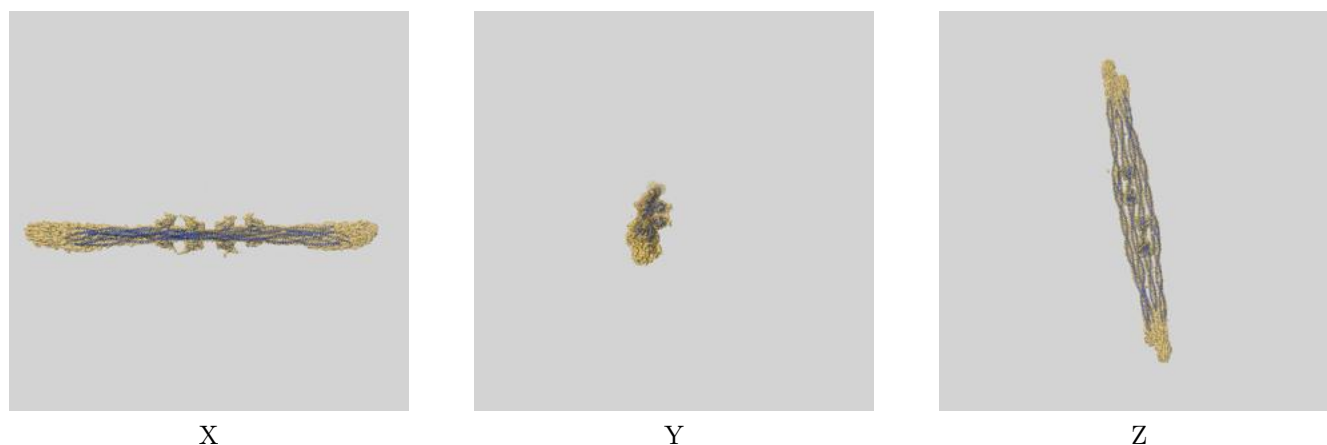
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.09	7.05	4.12
Unmasked-calculated*	8.53	11.75	8.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.53 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15476 and PDB model 8AJB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



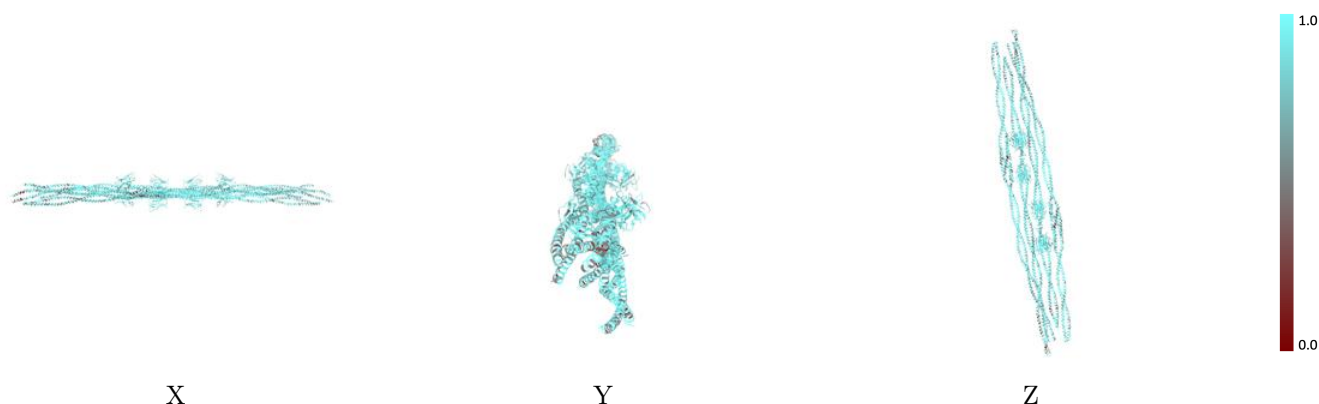
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



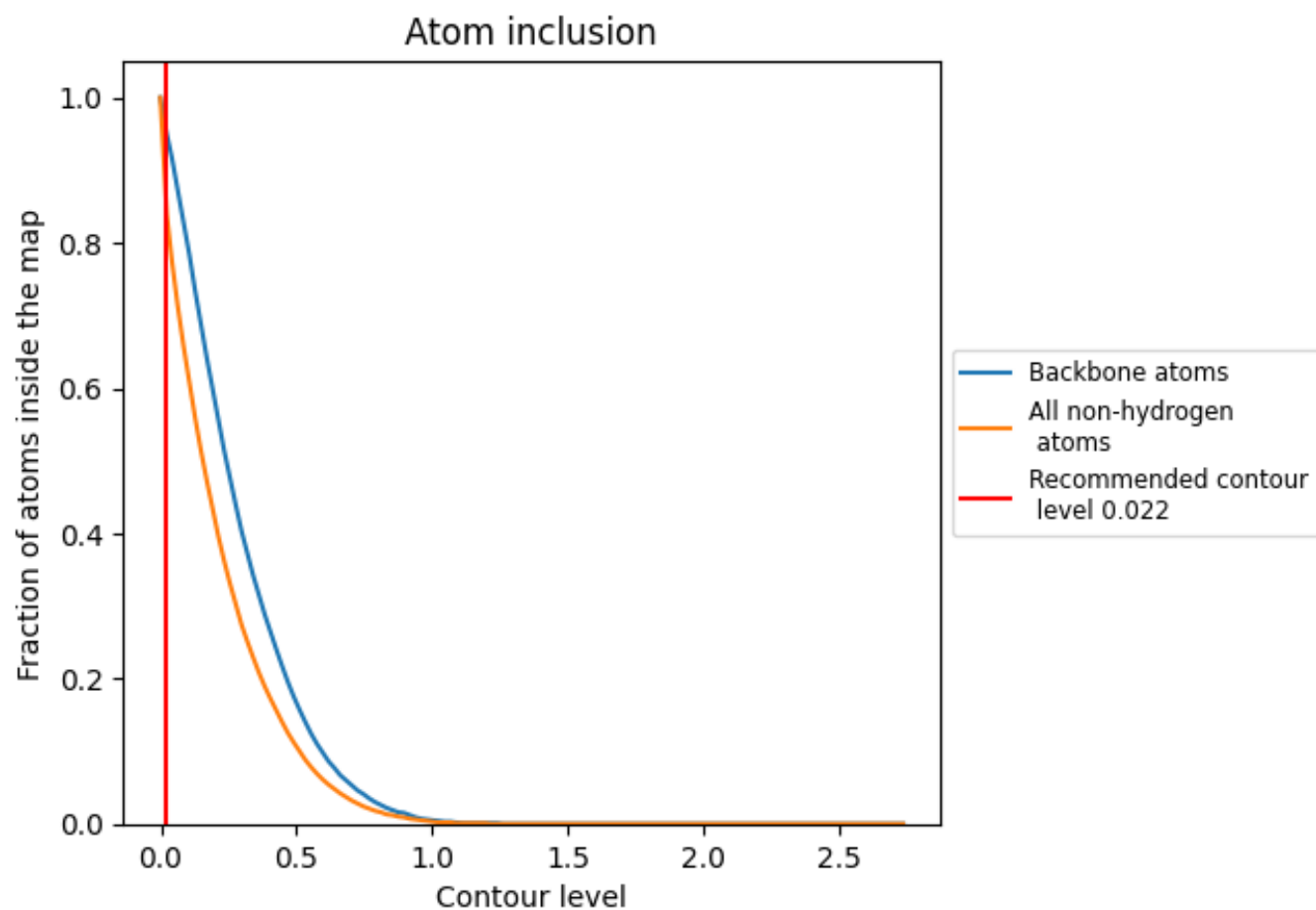
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).



















































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.1860
A	 0.8330	 0.1630
B	 0.8260	 0.1630
C	 0.8050	 0.1570
D	 0.8420	 0.1700
E	 0.9230	 0.3140
F	 0.9030	 0.2830
G	 0.7630	 0.0640
H	 0.8310	 0.0980
I	 0.8450	 0.1850
J	 0.8430	 0.1680
K	 0.9000	 0.2960
L	 0.8880	 0.3160
M	 0.8200	 0.1590
N	 0.8150	 0.1620
O	 0.8080	 0.1660
P	 0.8600	 0.1950
Q	 0.9050	 0.2970
R	 0.8990	 0.2710
S	 0.7620	 0.0650
T	 0.8280	 0.1230
U	 0.8440	 0.1940
V	 0.8330	 0.1830
W	 0.8920	 0.2850
X	 0.8960	 0.3280

