



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:43 PM JST

PDB ID : 7CF9  
EMDB ID : EMD-30343  
Title : Structure of RyR1 (Ca<sup>2+</sup>/CHL)  
Authors : Ma, R.; Haji-Ghassemi, O.; Ma, D.; Lin, L.; Samurkas, A.; Van Petegem, F.; Yuchi, Z.  
Deposited on : 2020-06-24  
Resolution : 4.70 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](mailto: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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.31.3

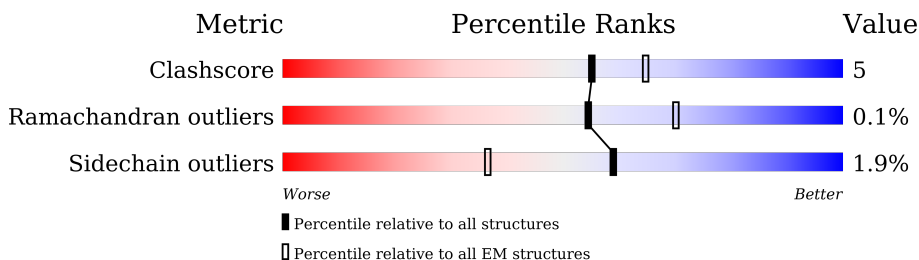
# 1 Overall quality at a glance

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  $\geq 3$ , 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	5037	
1	C	5037	
1	E	5037	
1	G	5037	
2	B	107	
2	D	107	
2	F	107	
2	H	107	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 116104 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 Ryanodine receptor 1,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	C	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	E	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	G	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	D	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

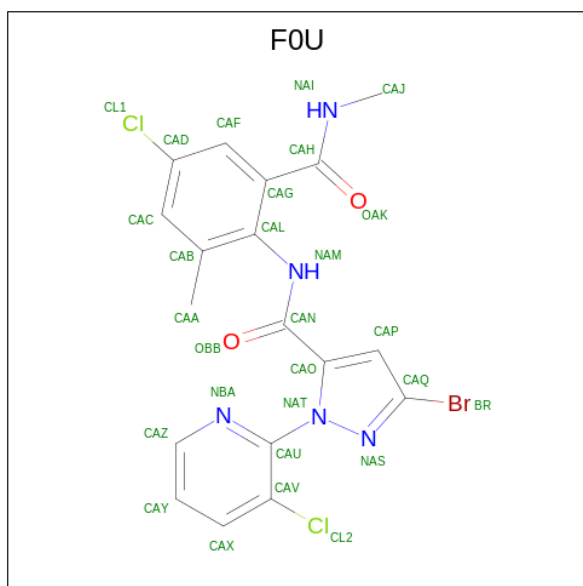
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	E	1	Total	Ca	0
			1	1	
3	G	1	Total	Ca	0
			1	1	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	

- Molecule 5 is 5-bromanyl-N-[4-chloranyl-2-methyl-6-(methylcarbamoyl)phenyl]-2-(3-chloranypyridin-2-yl)pyrazole-3-carboxamide (three-letter code: F0U) (formula: C<sub>18</sub>H<sub>14</sub>BrCl<sub>2</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

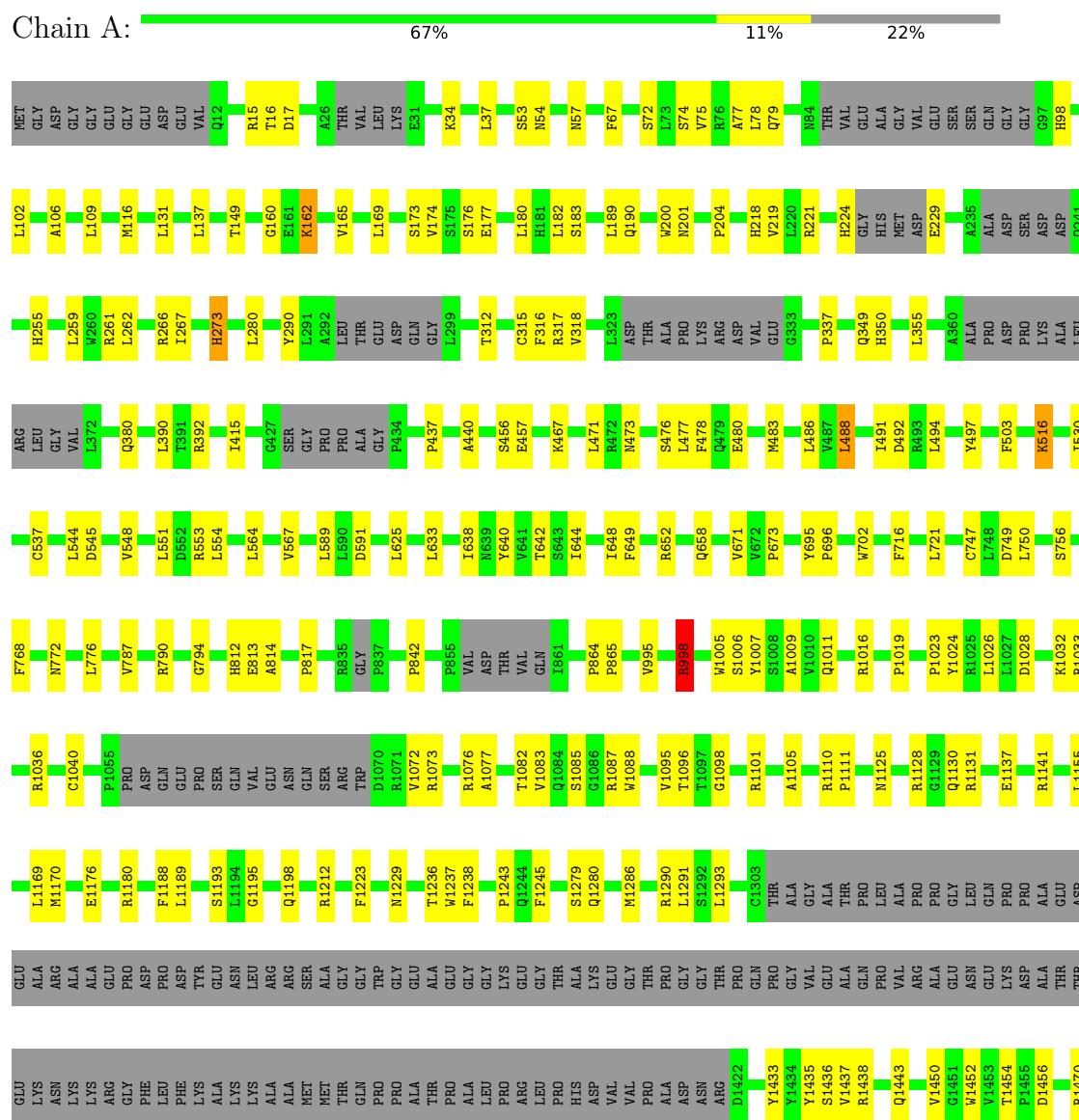


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	C	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	E	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	G	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	

### 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: Ryanodine receptor 1, RyR1







L2038	L2047	L2058	L2069	L2080	L2091	L2102	L2113	L2124	L2135	L2146	L2157	L2168	L2179	L2190	L2201	L2212	L2223	L2234	L2245	L2256	L2267	L2278	L2289	L2300	L2311	L2322	L2333	L2344	L2355	L2366	L2377	L2388	L2399	L2410	L2421	L2432	L2443	L2454	L2465	L2476	L2487	L2498	L2509	L2520	L2531	L2542	L2553	L2564	L2575	L2586	L2597	L2608	L2619	L2630	L2641	L2652	L2663	L2674	L2685	L2696	L2707	L2718	L2729	L2740	L2751	L2762	L2773	L2784	L2795	L2806	L2817	L2828	L2839	L2850	L2861	L2872	L2883	L2894	L2905	L2916	L2927	L2938	L2949	L2960	L2971	L2982	L2993	L3004	L3015	L3026	L3037	L3048	L3059	L3070	L3081	L3092	L3103	L3114	L3125	L3136	L3147	L3158	L3169	L3180	L3191	L3202	L3213	L3224	L3235	L3246	L3257	L3268	L3279	L3290	L3301	L3312	L3323	L3334	L3345	L3356	L3367	L3378	L3389	L3400	L3411	L3422	L3433	L3444	L3455	L3466	L3477	L3488	L3499	L3510	L3521	L3532	L3543	L3554	L3565	L3576	L3587	L3598	L3609	L3620	L3631	L3642	L3653	L3664	L3675	L3686	L3697	L3708	L3719	L3730	L3741	L3752	L3763	L3774	L3785	L3796	L3807	L3818	L3829	L3840	L3851	L3862	L3873	L3884	L3895	L3906	L3917	L3928	L3939	L3950	L3961	L3972	L3983	L3994	L4005	L4016	L4027	L4038	L4049	L4060	L4071	L4082	L4093	L4104	L4115	L4126	L4137	L4148	L4159	L4170	L4181	L4192	L4203	L4214	L4225	L4236	L4247	L4258	L4269	L4280	L4291	L4302	L4313	L4324	L4335	L4346	L4357	L4368	L4379	L4390	L4401	L4412	L4423	L4434	L4445	L4456	L4467	L4478	L4489	L4500	L4511	L4522	L4533	L4544	L4555	L4566	L4577	L4588	L4599	L4610	L4621	L4632	L4643	L4654	L4665	L4676	L4687	L4698	L4709	L4720	L4731	L4742	L4753	L4764	L4775	L4786	L4797	L4808	L4819	L4830	L4841	L4852	L4863	L4874	L4885	L4896	L4907	L4918	L4929	L4940	L4951	L4962	L4973	L4984	L4995	L5006	L5017	L5028	L5039	L5050	L5061	L5072	L5083	L5094	L5105	L5116	L5127	L5138	L5149	L5160	L5171	L5182	L5193	L5204	L5215	L5226	L5237	L5248	L5259	L5270	L5281	L5292	L5303	L5314	L5325	L5336	L5347	L5358	L5369	L5380	L5391	L5402	L5413	L5424	L5435	L5446	L5457	L5468	L5479	L5490	L5501	L5512	L5523	L5534	L5545	L5556	L5567	L5578	L5589	L5600	L5611	L5622	L5633	L5644	L5655	L5666	L5677	L5688	L5699	L5710	L5721	L5732	L5743	L5754	L5765	L5776	L5787	L5798	L5809	L5820	L5831	L5842	L5853	L5864	L5875	L5886	L5897	L5908	L5919	L5930	L5941	L5952	L5963	L5974	L5985	L5996	L6007	L6018	L6029	L6040	L6051	L6062	L6073	L6084	L6095	L6106	L6117	L6128	L6139	L6150	L6161	L6172	L6183	L6194	L6205	L6216	L6227	L6238	L6249	L6260	L6271	L6282	L6293	L6304	L6315	L6326	L6337	L6348	L6359	L6370	L6381	L6392	L6403	L6414	L6425	L6436	L6447	L6458	L6469	L6480	L6491	L6502	L6513	L6524	L6535	L6546	L6557	L6568	L6579	L6590	L6601	L6612	L6623	L6634	L6645	L6656	L6667	L6678	L6689	L6700	L6711	L6722	L6733	L6744	L6755	L6766	L6777	L6788	L6799	L6810	L6821	L6832	L6843	L6854	L6865	L6876	L6887	L6898	L6909	L6920	L6931	L6942	L6953	L6964	L6975	L6986	L6997	L7008	L7019	L7030	L7041	L7052	L7063	L7074	L7085	L7096	L7107	L7118	L7129	L7140	L7151	L7162	L7173	L7184	L7195	L7206	L7217	L7228	L7239	L7250	L7261	L7272	L7283	L7294	L7305	L7316	L7327	L7338	L7349	L7360	L7371	L7382	L7393	L7404	L7415	L7426	L7437	L7448	L7459	L7470	L7481	L7492	L7503	L7514	L7525	L7536	L7547	L7558	L7569	L7580	L7591	L7602	L7613	L7624	L7635	L7646	L7657	L7668	L7679	L7690	L7701	L7712	L7723	L7734	L7745	L7756	L7767	L7778	L7789	L7800	L7811	L7822	L7833	L7844	L7855	L7866	L7877	L7888	L7899	L7910	L7921	L7932	L7943	L7954	L7965	L7976	L7987	L7998	L8009	L8020	L8031	L8042	L8053	L8064	L8075	L8086	L8097	L8108	L8119	L8130	L8141	L8152	L8163	L8174	L8185	L8196	L8207	L8218	L8229	L8240	L8251	L8262	L8273	L8284	L8295	L8306	L8317	L8328	L8339	L8350	L8361	L8372	L8383	L8394	L8405	L8416	L8427	L8438	L8449	L8460	L8471	L8482	L8493	L8504	L8515	L8526	L8537	L8548	L8559	L8570	L8581	L8592	L8603	L8614	L8625	L8636	L8647	L8658	L8669	L8680	L8691	L8702	L8713	L8724	L8735	L8746	L8757	L8768	L8779	L8790	L8801	L8812	L8823	L8834	L8845	L8856	L8867	L8878	L8889	L8900	L8911	L8922	L8933	L8944	L8955	L8966	L8977	L8988	L8999	L9010	L9021	L9032	L9043	L9054	L9065	L9076	L9087	L9098	L9109	L9120	L9131	L9142	L9153	L9164	L9175	L9186	L9197	L9208	L9219	L9230	L9241	L9252	L9263	L9274	L9285	L9296	L9307	L9318	L9329	L9340	L9351	L9362	L9373	L9384	L9395	L9406	L9417	L9428	L9439	L9450	L9461	L9472	L9483	L9494	L9505	L9516	L9527	L9538	L9549	L9560	L9571	L9582	L9593	L9604	L9615	L9626	L9637	L9648	L9659	L9670	L9681	L9692	L9703	L9714	L9725	L9736	L9747	L9758	L9769	L9780	L9791	L9802	L9813	L9824	L9835	L9846	L9857	L9868	L9879	L9890	L9901	L9912	L9923	L9934	L9945	L9956	L9967	L9978	L9989	L9990	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

















Chain F: 

72%

26%

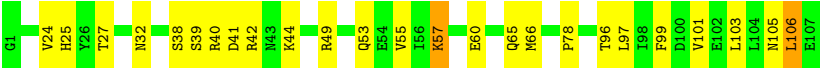


● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 

77%

21%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.001	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, FOU

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	0.32	0/26486	0.72	40/36018 (0.1%)
1	C	0.32	0/26486	0.72	40/36018 (0.1%)
1	E	0.32	0/26486	0.72	40/36018 (0.1%)
1	G	0.32	0/26486	0.72	40/36018 (0.1%)
2	B	0.33	0/820	0.76	0/1105
2	D	0.34	0/820	0.76	0/1105
2	F	0.34	0/820	0.76	0/1105
2	H	0.34	0/820	0.76	0/1105
All	All	0.32	0/109224	0.72	160/148492 (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	2
1	C	0	2
1	E	0	2
1	G	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	998	ARG	CA-CB-CG	8.63	132.39	113.40
1	E	998	ARG	CA-CB-CG	8.61	132.35	113.40
1	A	998	ARG	CA-CB-CG	8.61	132.34	113.40
1	G	998	ARG	CA-CB-CG	8.61	132.34	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4211	LYS	CD-CE-NZ	8.17	130.49	111.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4018	ASP	Peptide
1	A	749	ASP	Peptide
1	C	4018	ASP	Peptide
1	C	749	ASP	Peptide
1	E	749	ASP	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28192	0	24933	290	0
1	C	28192	0	24933	285	0
1	E	28192	0	24933	291	0
1	G	28192	0	24933	291	0
2	B	804	0	812	8	0
2	D	804	0	812	9	0
2	F	804	0	812	11	0
2	H	804	0	812	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	28	0	0	0	0
5	C	28	0	0	0	0
5	E	28	0	0	0	0
5	G	28	0	0	0	0
All	All	116104	0	102980	1155	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 5.

The worst 5 of 1155 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:C:652:ARG:HD3	1:C:750:LEU:HB3	1.69	0.74
1:E:652:ARG:HD3	1:E:750:LEU:HB3	1.69	0.73
1:E:2304:GLY:O	1:E:2308:GLN:HB2	1.88	0.73
1:A:2304:GLY:O	1:A:2308:GLN:HB2	1.88	0.73
1:G:652:ARG:HD3	1:G:750:LEU:HB3	1.69	0.73

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	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	C	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	E	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	G	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
2	B	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	D	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	14128/20576 (69%)	13240 (94%)	880 (6%)	8 (0%)	54	85

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	673	PRO
1	C	318	VAL
1	C	673	PRO
1	E	318	VAL

### 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	2495/3416 (73%)	2460 (99%)	35 (1%)	67	81
1	C	2495/3416 (73%)	2461 (99%)	34 (1%)	67	81
1	E	2495/3416 (73%)	2460 (99%)	35 (1%)	67	81
1	G	2495/3416 (73%)	2461 (99%)	34 (1%)	67	81
2	B	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	D	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	F	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	H	84/88 (96%)	70 (83%)	14 (17%)	2	14
All	All	10316/14016 (74%)	10122 (98%)	194 (2%)	59	75

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3677	LEU
2	F	101	VAL
1	E	4211	LYS
1	E	5002	GLU
1	G	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2551	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	44	ASN
1	E	3767	GLN
1	E	4124	ASN
1	G	1229	ASN

### 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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	F0U	E	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	C	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	A	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	G	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.44	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F0U	E	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	C	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	A	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	G	5203	-	-	0/11/18/18	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5203	F0U	CAU-NAT	-6.50	1.33	1.44
5	G	5203	F0U	CAU-NAT	-6.50	1.33	1.44
5	C	5203	F0U	CAU-NAT	-6.46	1.33	1.44
5	E	5203	F0U	CAU-NAT	-6.46	1.33	1.44
5	E	5203	F0U	CAG-CAH	-5.20	1.39	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5203	F0U	CAJ-NAI-CAH	-4.31	117.00	121.89
5	C	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	A	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	E	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	A	5203	F0U	CAZ-NBA-CAU	4.11	120.63	115.98

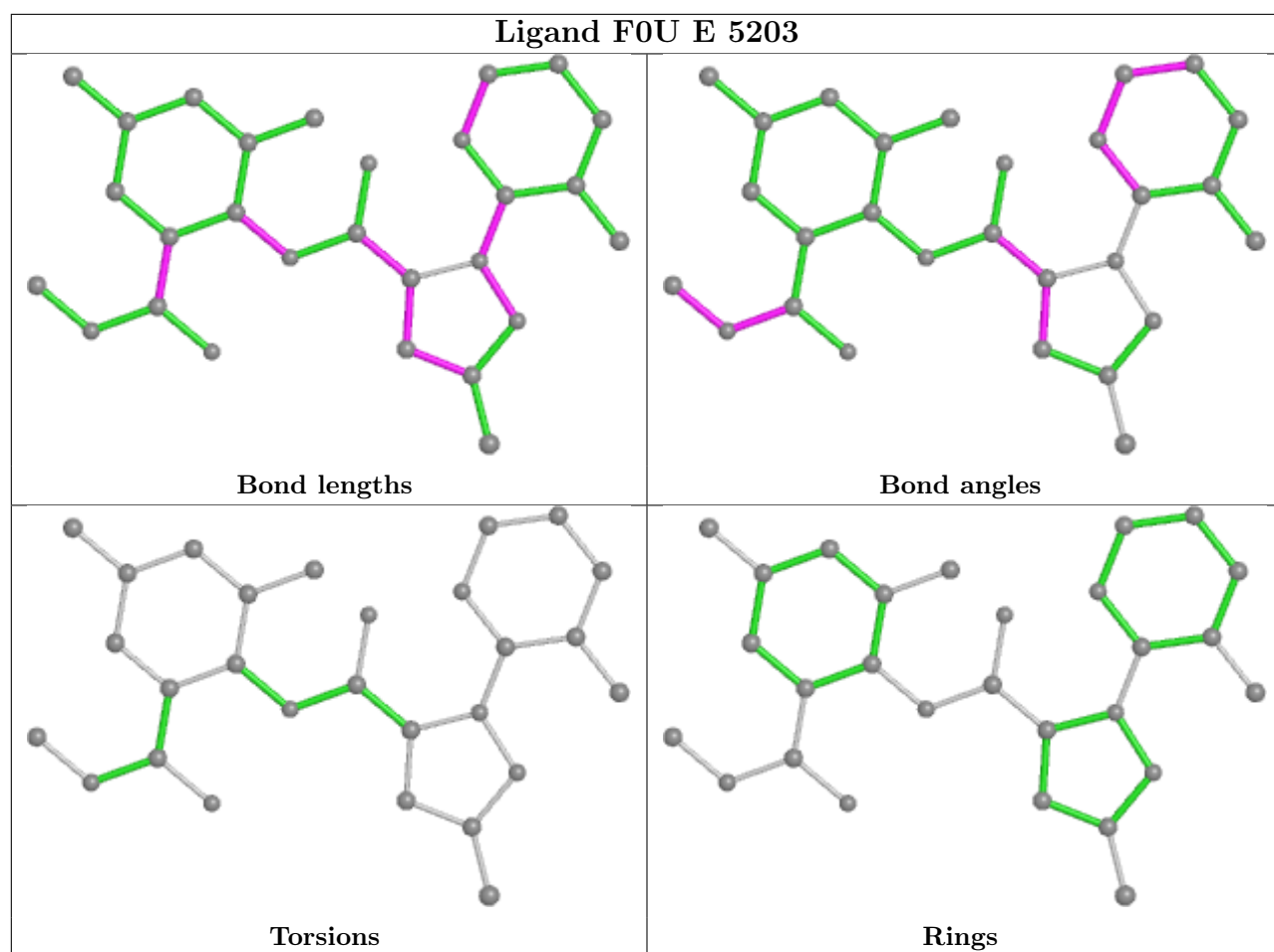
There are no chirality outliers.

There are no torsion outliers.

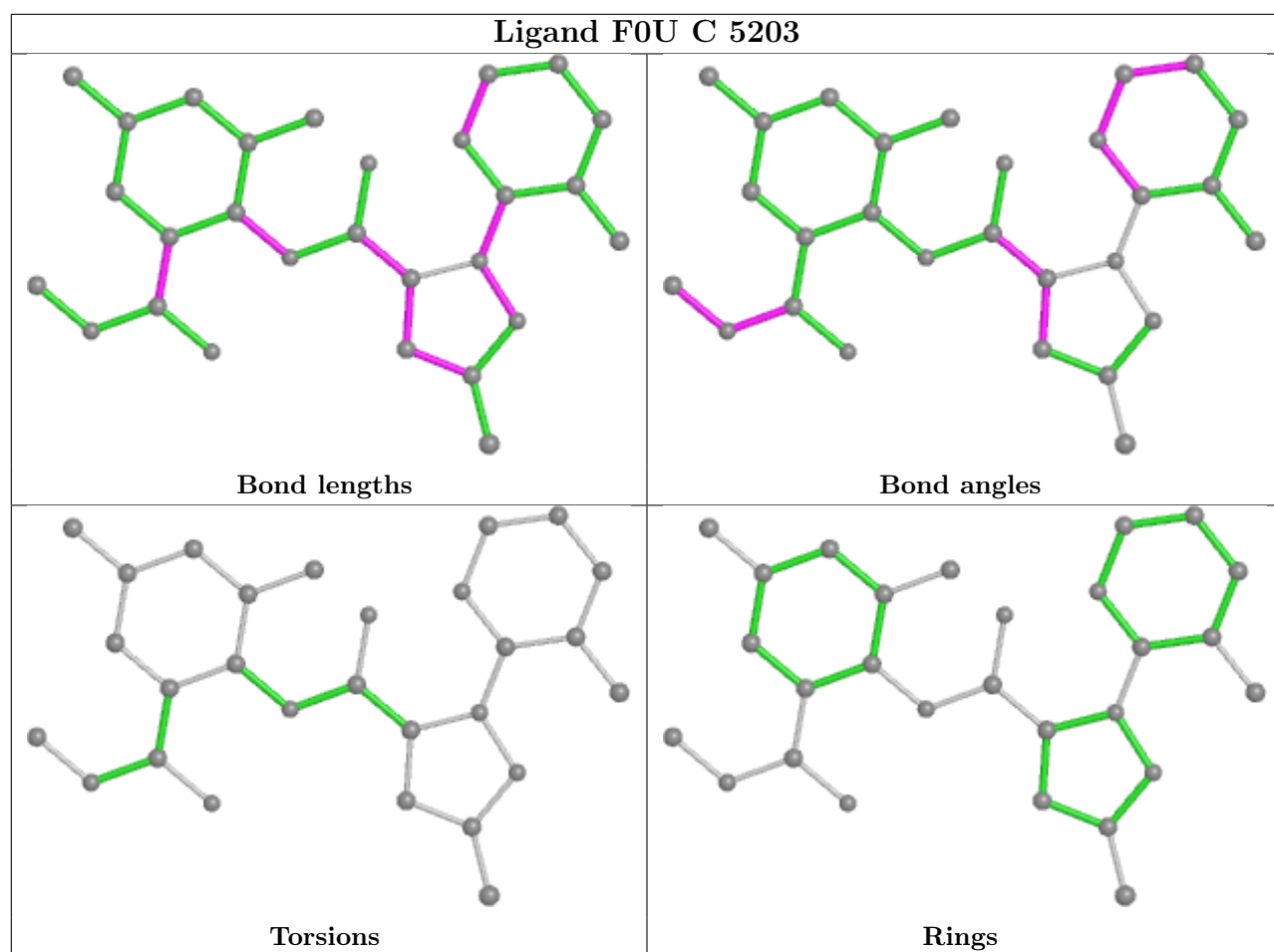
There are no ring outliers.

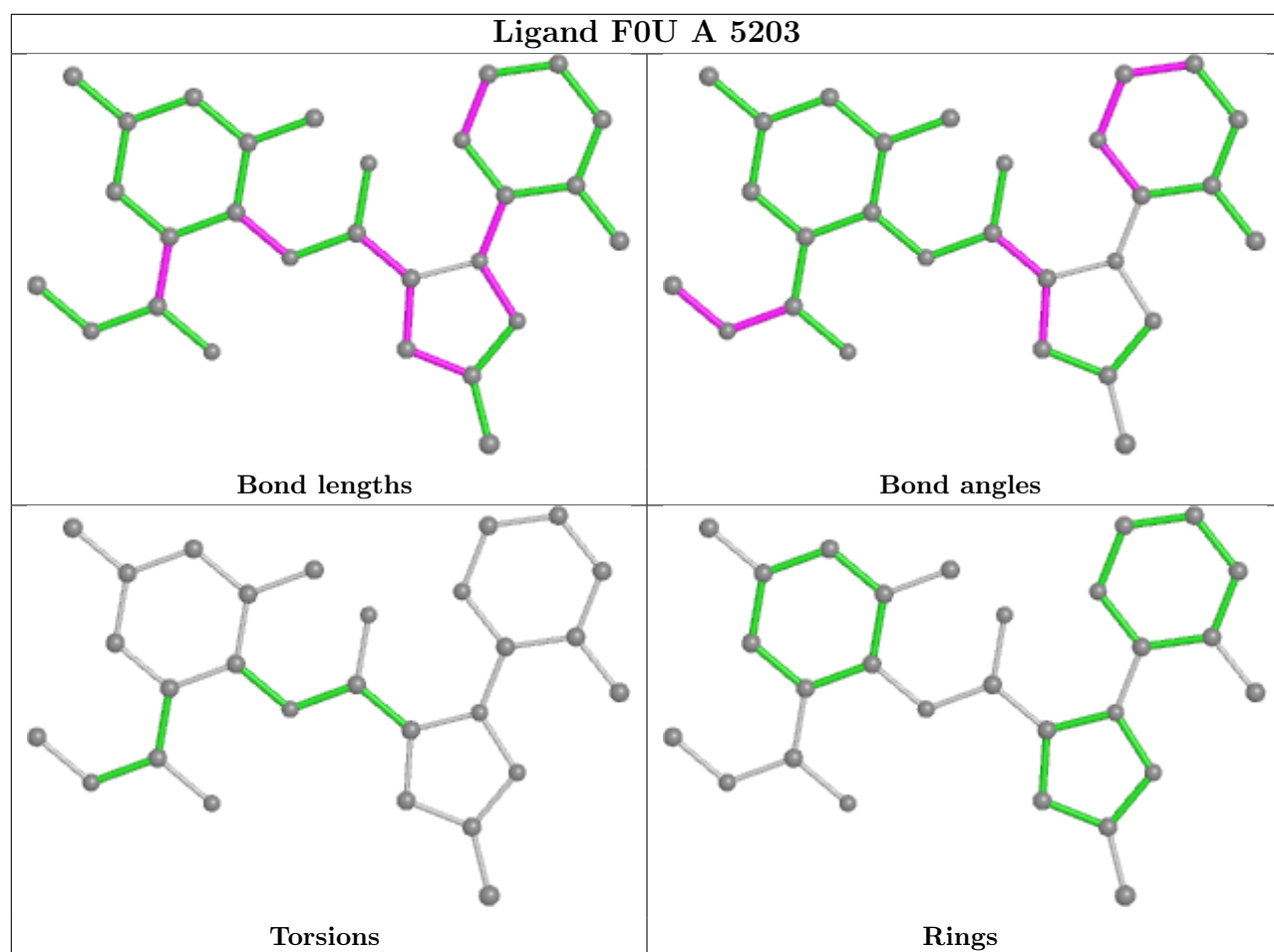
No monomer is involved in short contacts.

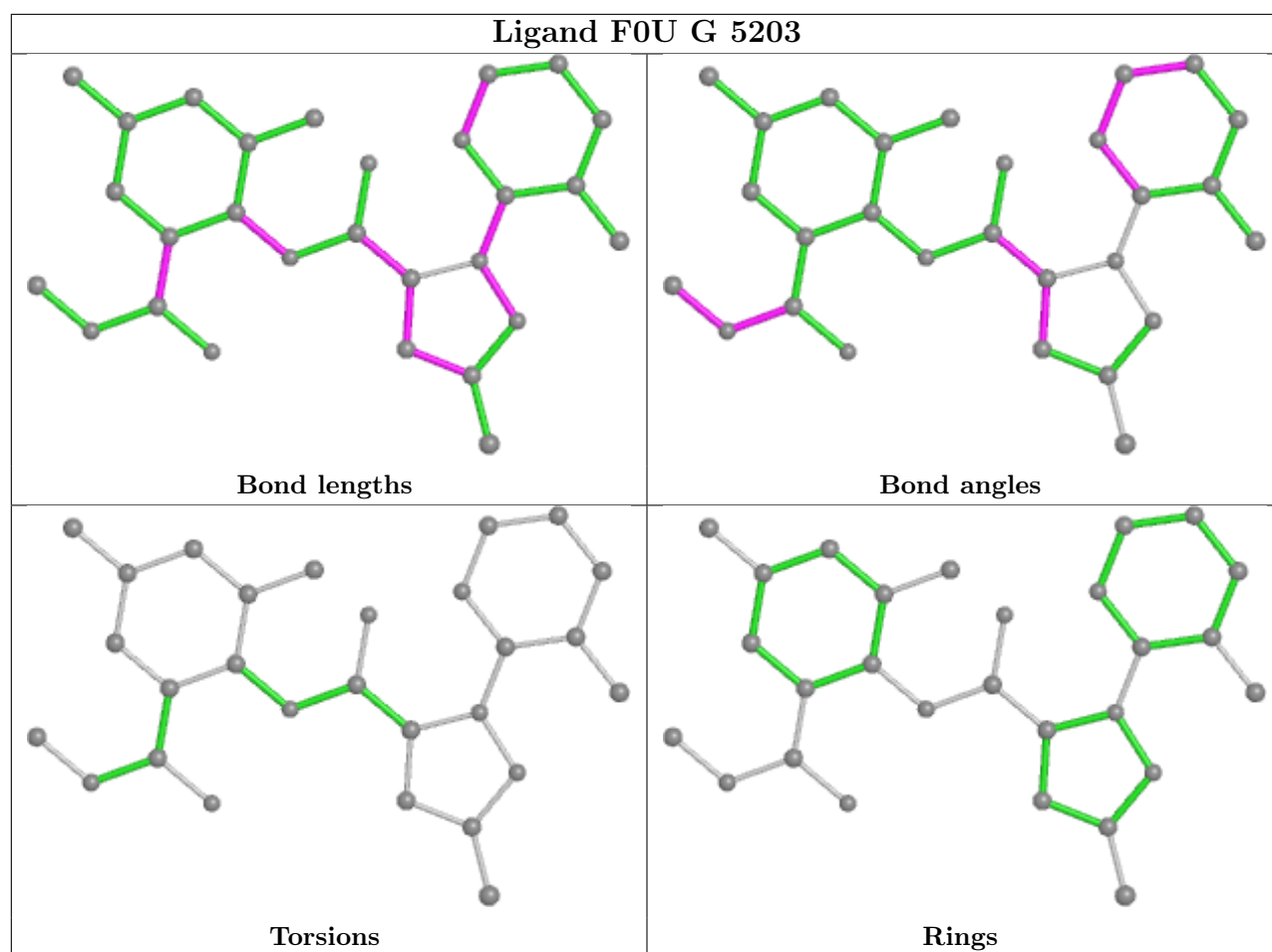
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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.

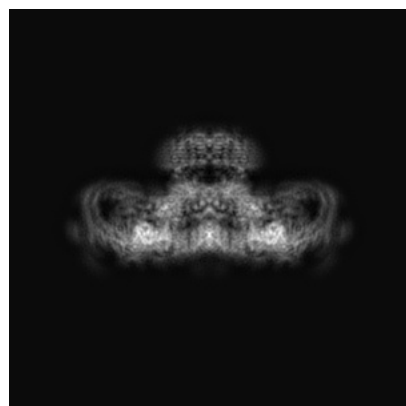
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30343. These allow visual inspection of the internal detail of the map and identification of artifacts.

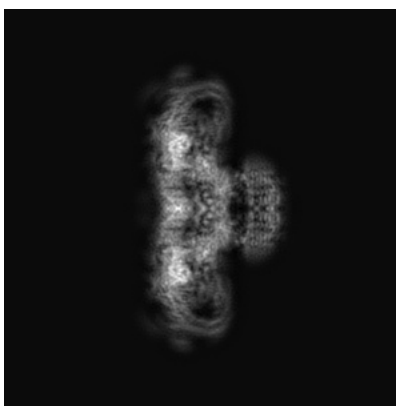
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

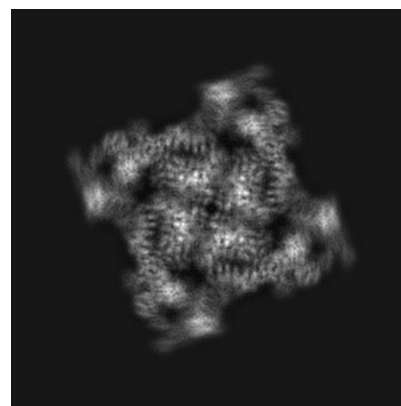
#### 6.1.1 Primary map



X

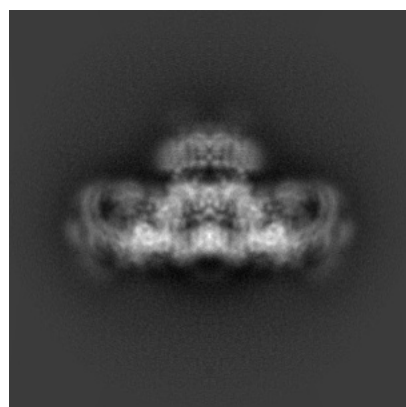


Y

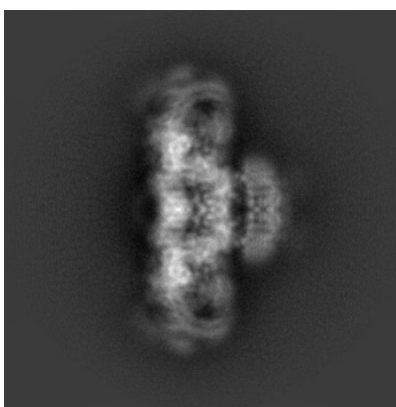


Z

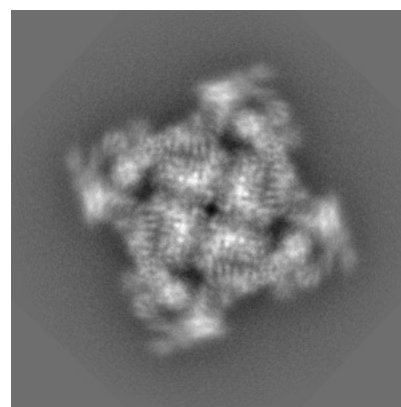
#### 6.1.2 Raw map



X



Y

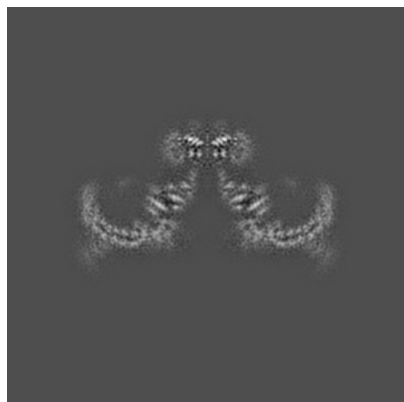


Z

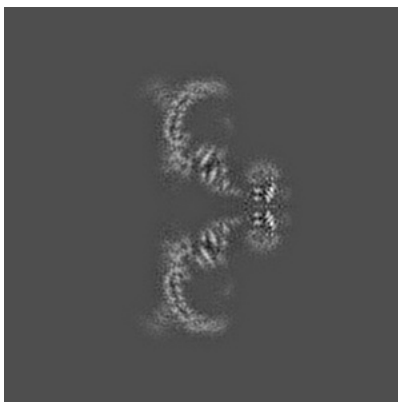
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

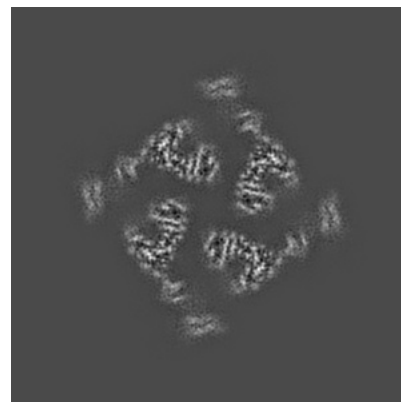
### 6.2.1 Primary map



X Index: 224

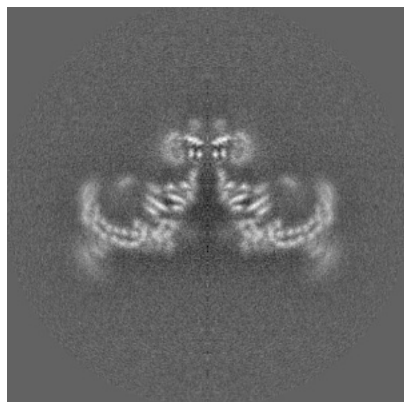


Y Index: 224

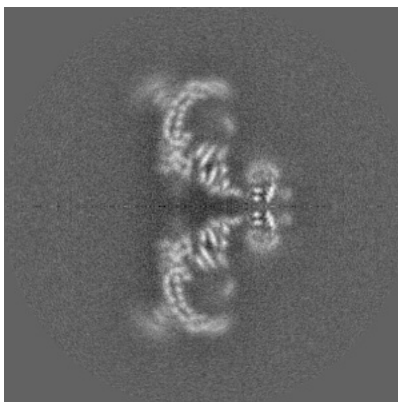


Z Index: 224

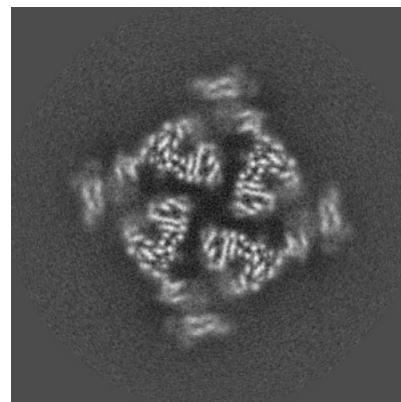
### 6.2.2 Raw map



X Index: 224



Y Index: 224

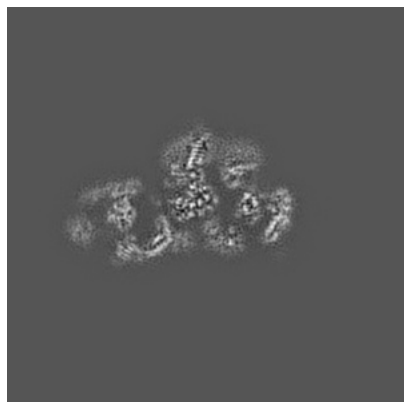


Z Index: 224

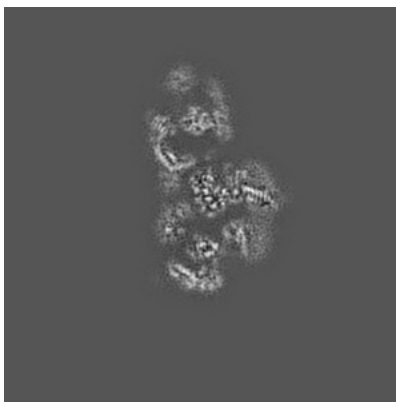
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

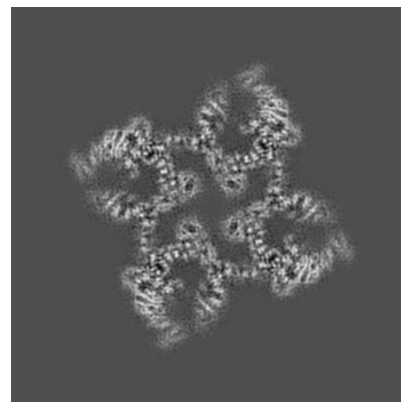
### 6.3.1 Primary map



X Index: 186

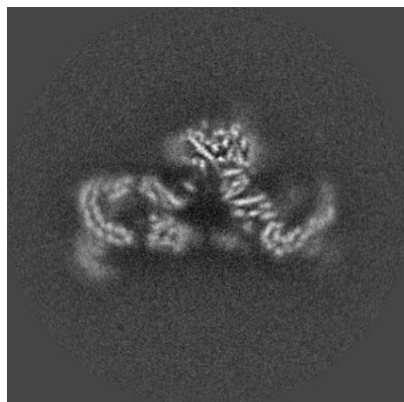


Y Index: 186

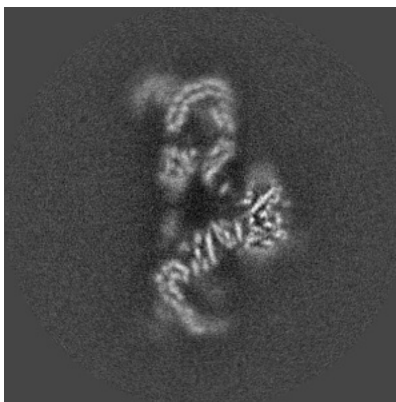


Z Index: 190

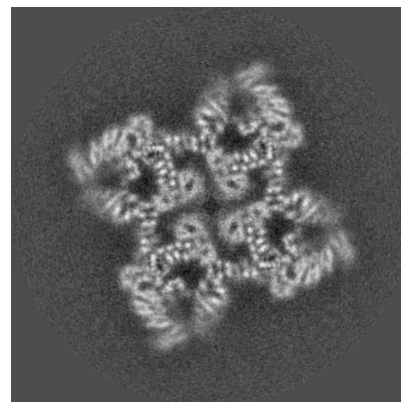
### 6.3.2 Raw map



X Index: 215



Y Index: 215

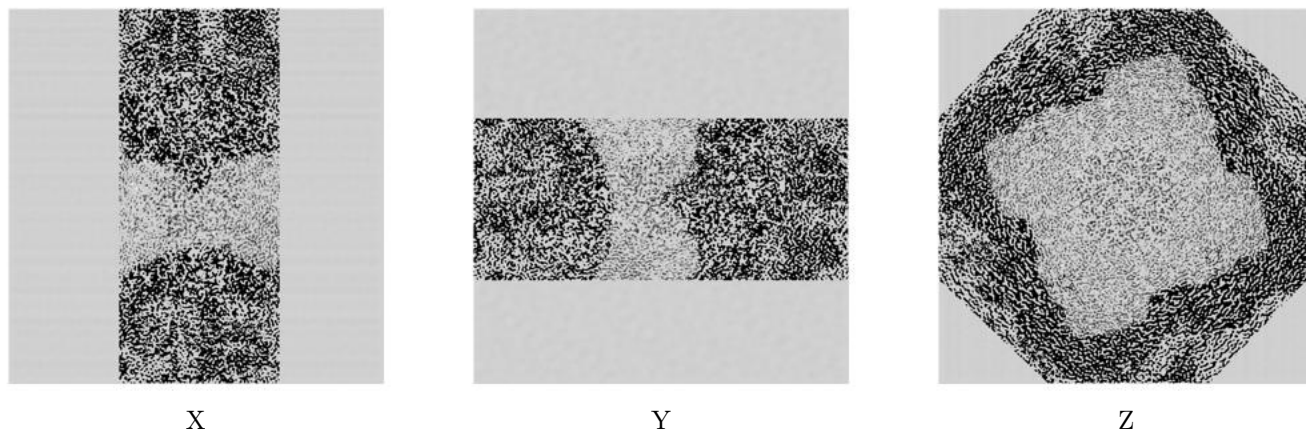


Z Index: 189

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

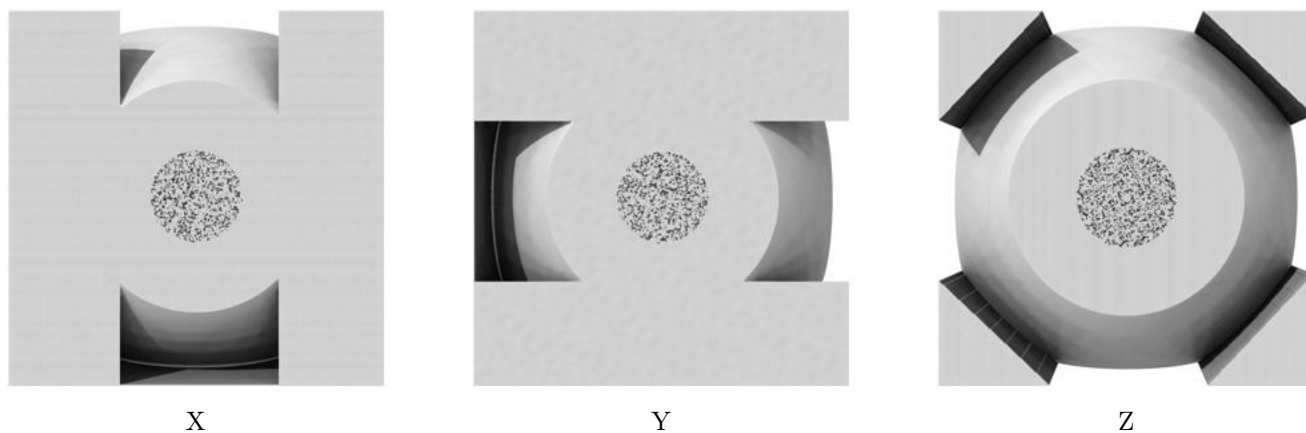
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

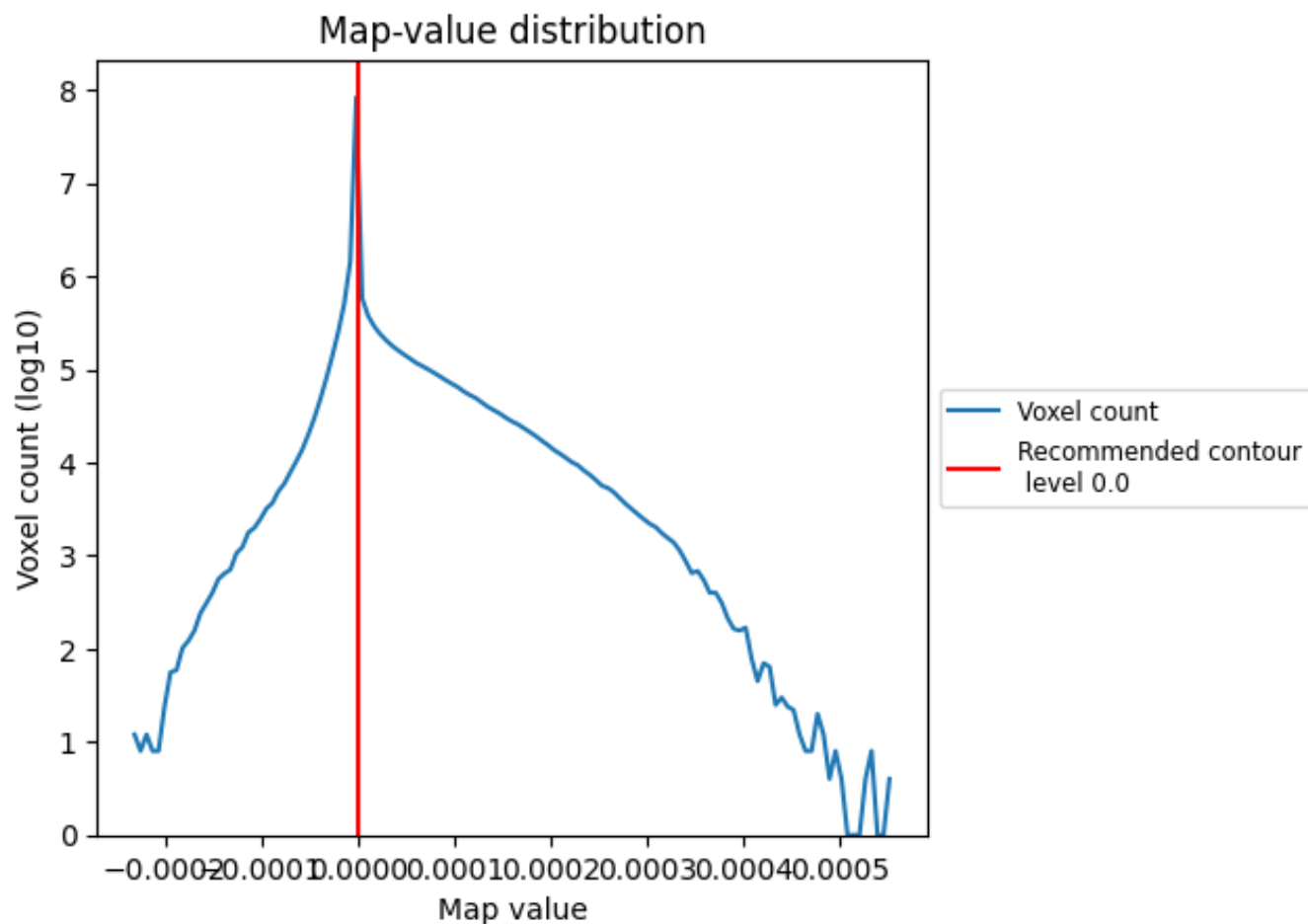
## 6.5 Mask visualisation [i](#)

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.

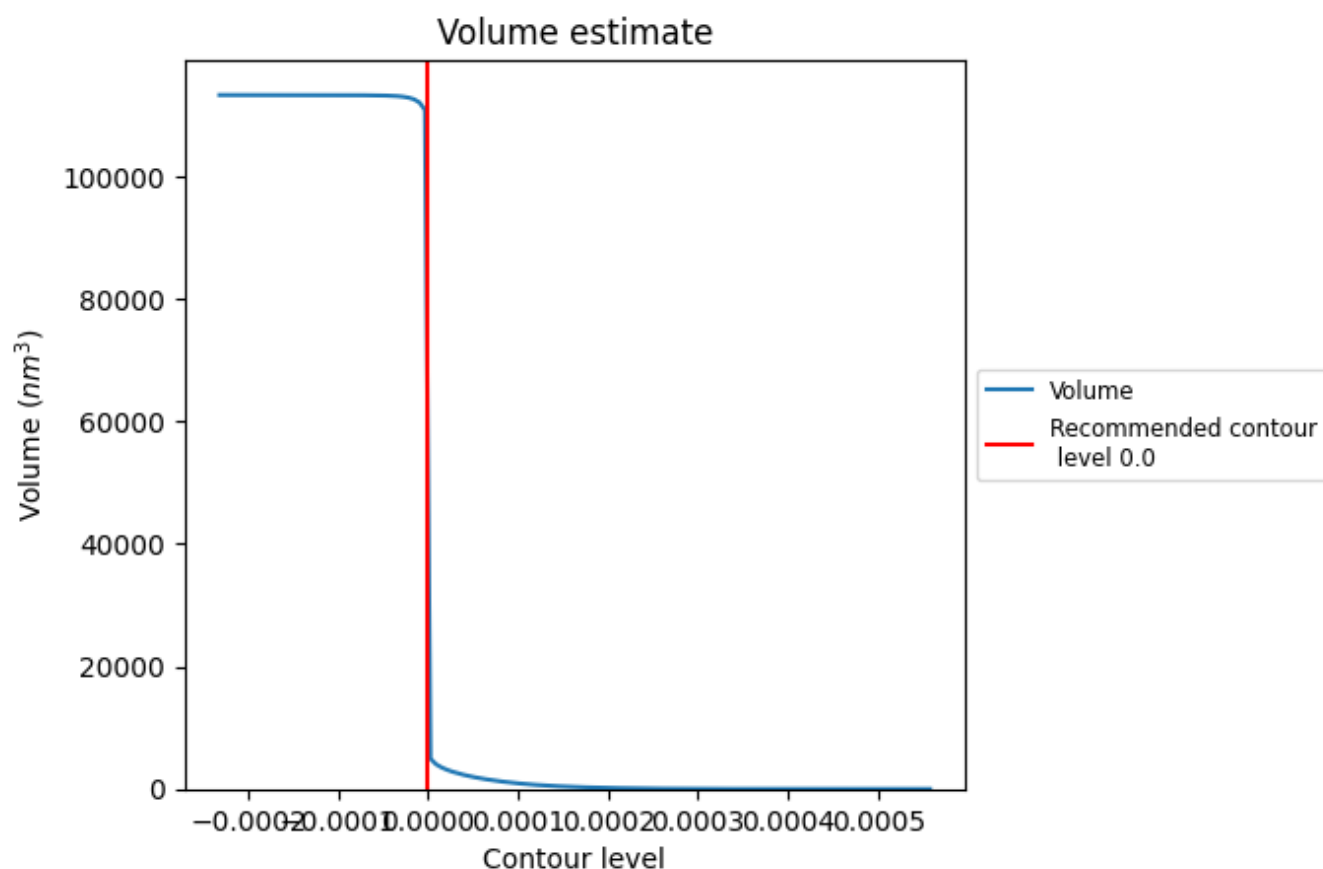
### 7.1 Map-value distribution [i](#)



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.



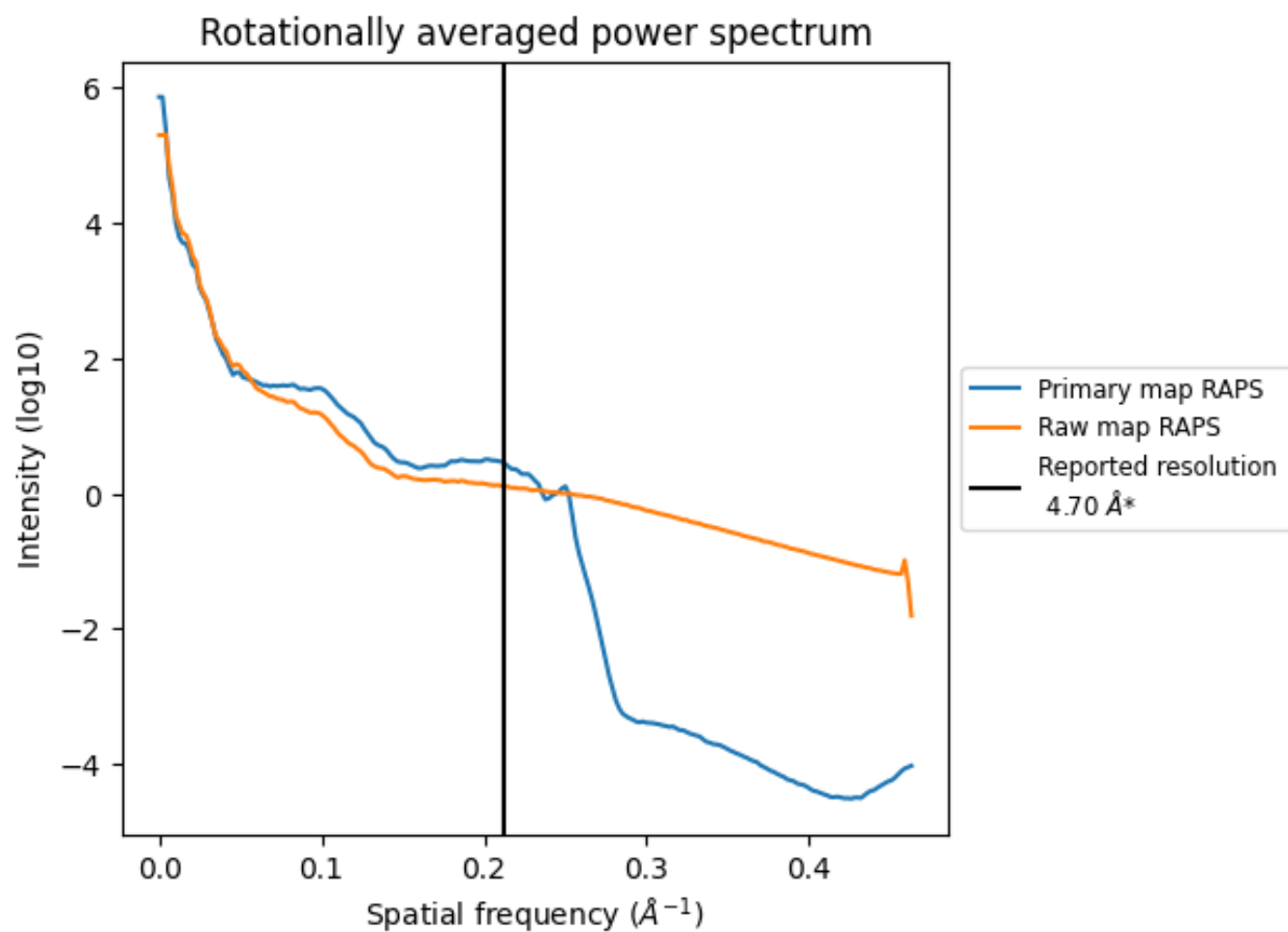
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51623  $\text{nm}^3$ ; this corresponds to an approximate mass of 46633 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 ⓘ

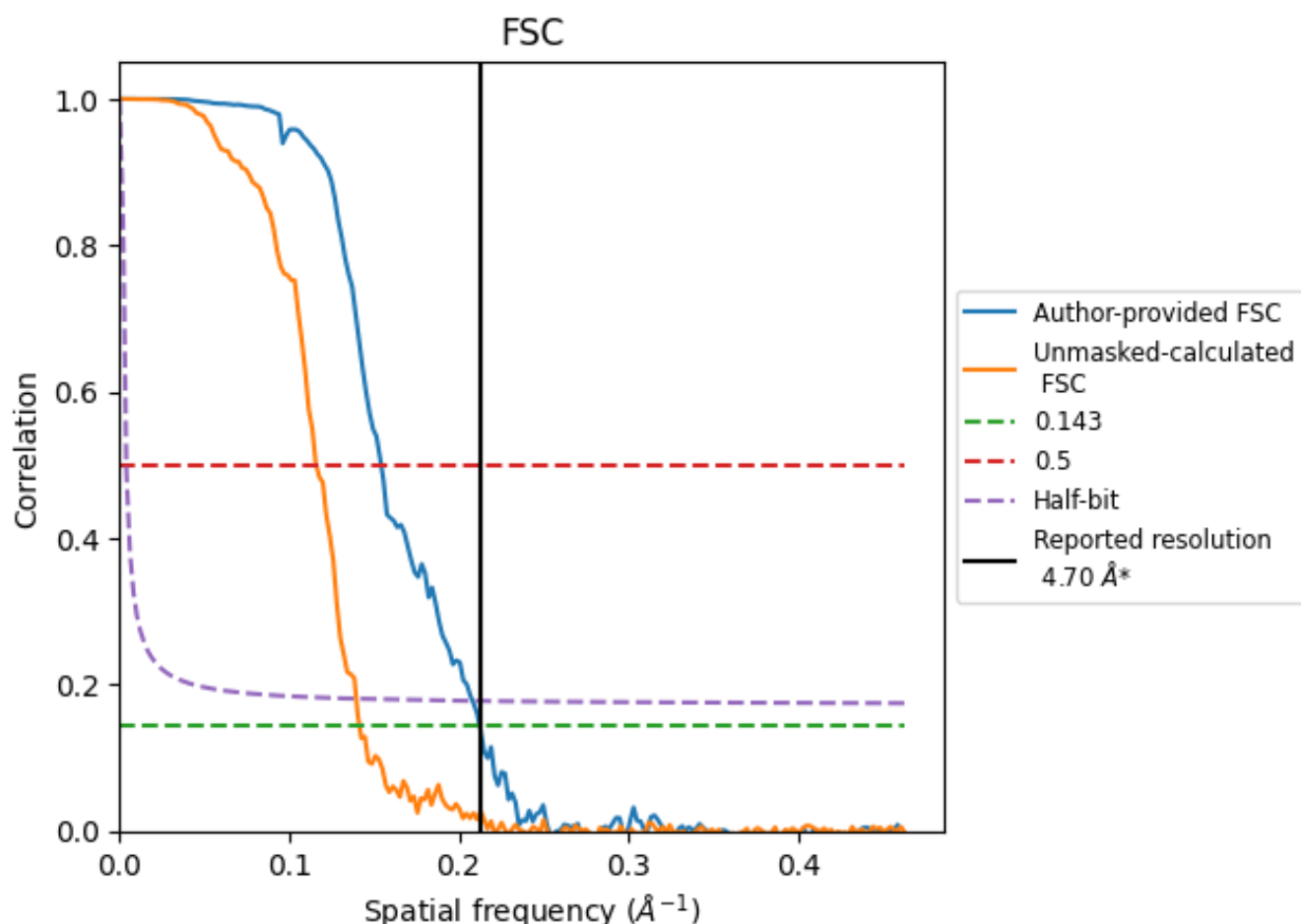


\*Reported resolution corresponds to spatial frequency of  $0.213 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

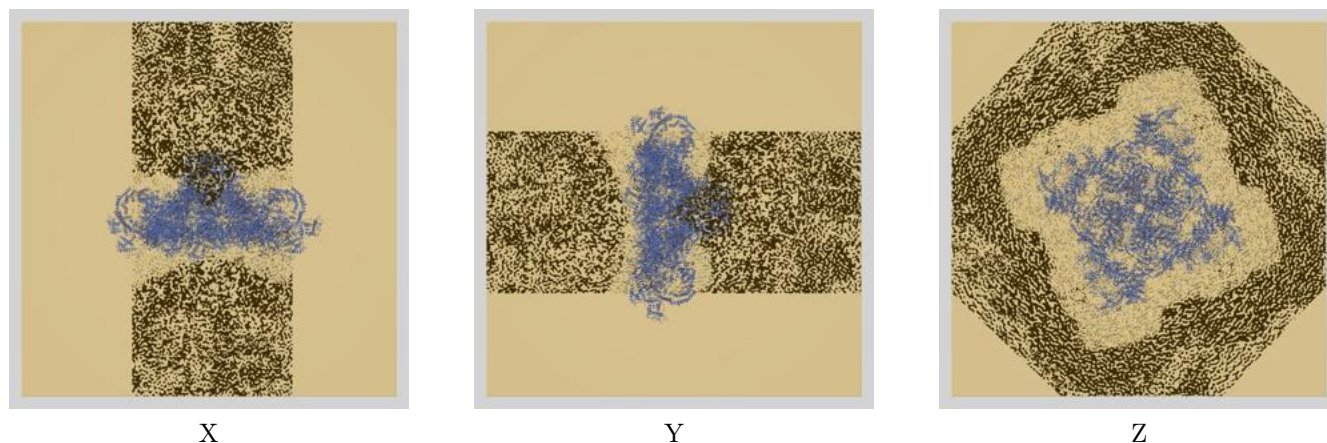
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	6.48	4.80
Unmasked-calculated*	7.07	8.62	7.16

\*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 7.07 differs from the reported value 4.7 by more than 10 %

## 9 Map-model fit [i](#)

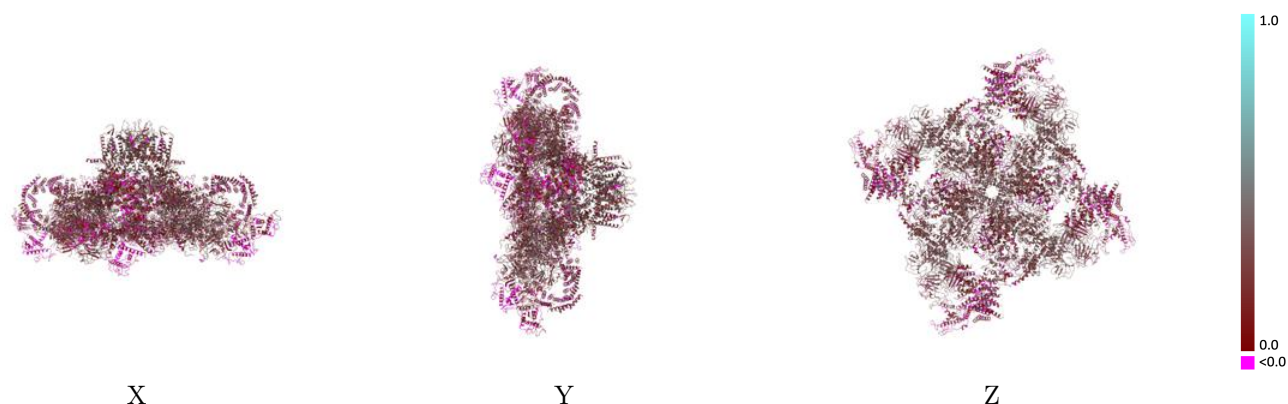
This section contains information regarding the fit between EMDB map EMD-30343 and PDB model 7CF9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



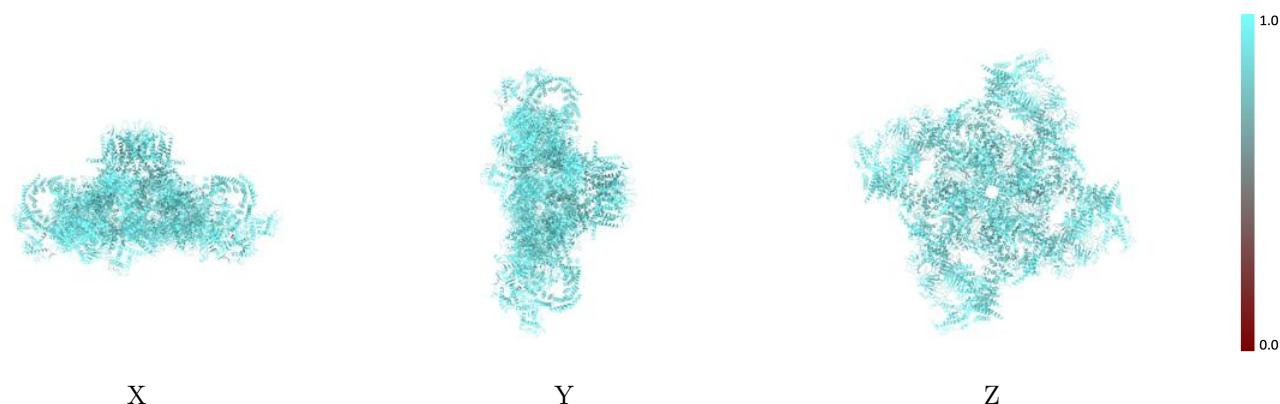
The images above show the 3D surface view of the map at the recommended contour level 0.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



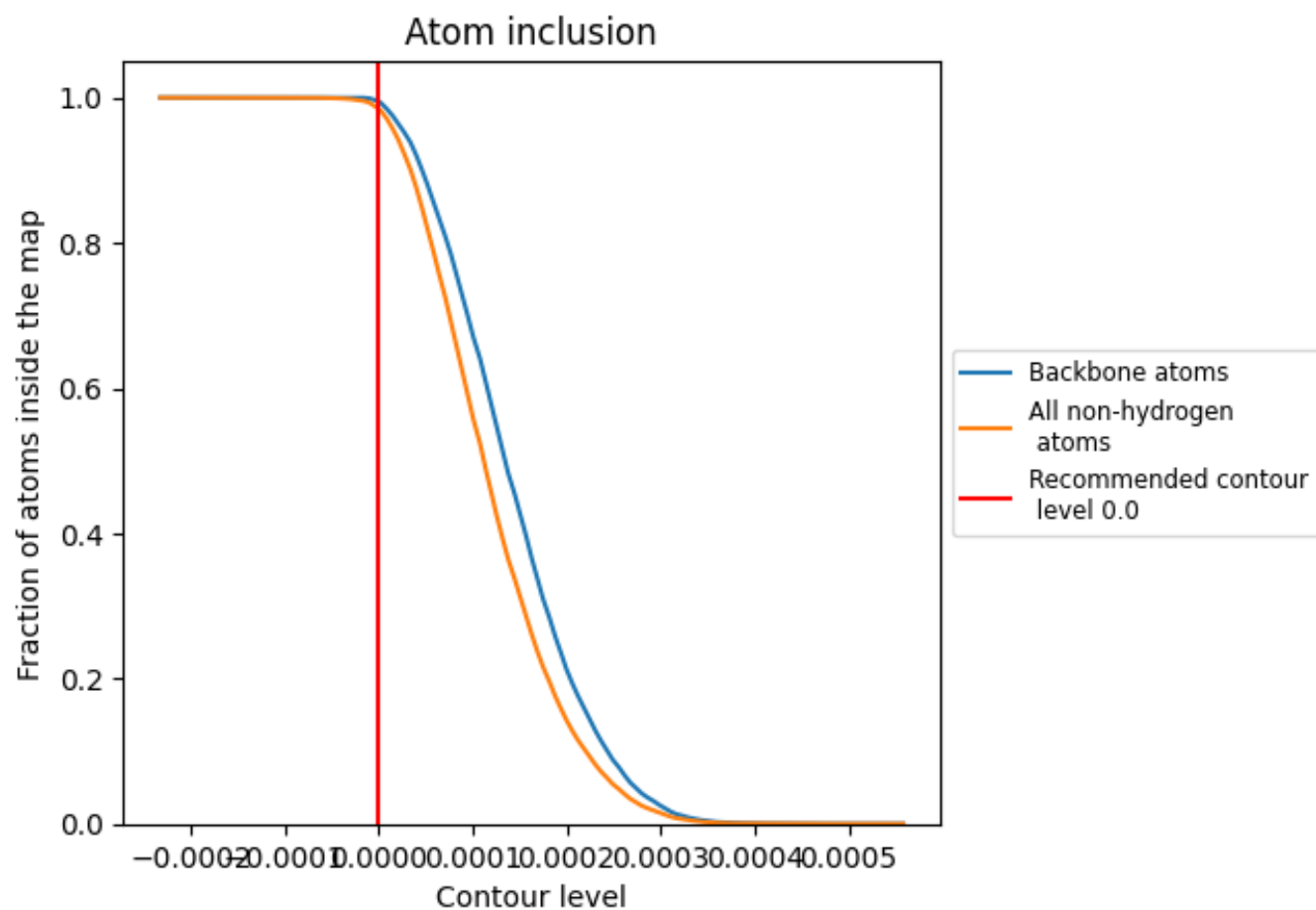
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9849	<div></div> 0.2320
A	<div></div> 0.9846	<div></div> 0.2300
B	<div></div> 0.9975	<div></div> 0.2860
C	<div></div> 0.9846	<div></div> 0.2300
D	<div></div> 0.9962	<div></div> 0.2840
E	<div></div> 0.9845	<div></div> 0.2300
F	<div></div> 0.9962	<div></div> 0.2840
G	<div></div> 0.9845	<div></div> 0.2300
H	<div></div> 0.9975	<div></div> 0.2860

