



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 07:45 AM EDT

PDB ID : 5TB2  
EMDB ID : EMD-8393  
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 2)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-11  
Resolution : 4.60 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.2

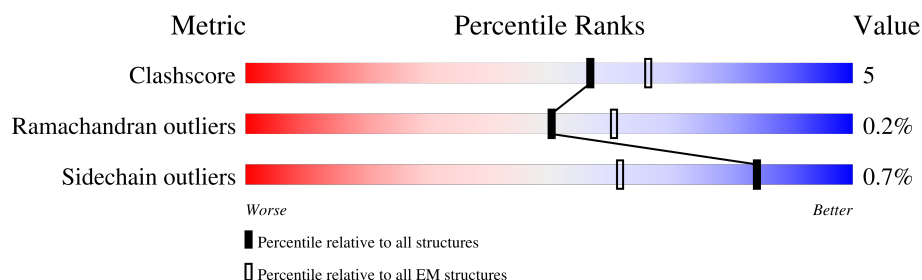
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 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	108	<div> <div>61%</div> <div>87%12%.</div> </div>
1	F	108	<div> <div>62%</div> <div>87%12%.</div> </div>
1	H	108	<div> <div>61%</div> <div>87%12%.</div> </div>
1	J	108	<div> <div>60%</div> <div>90%9%.</div> </div>
2	B	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	E	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	G	4416	<div> <div>51%</div> <div>84%11%5%</div> </div>
2	I	4416	<div> <div>52%</div> <div>84%11%5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

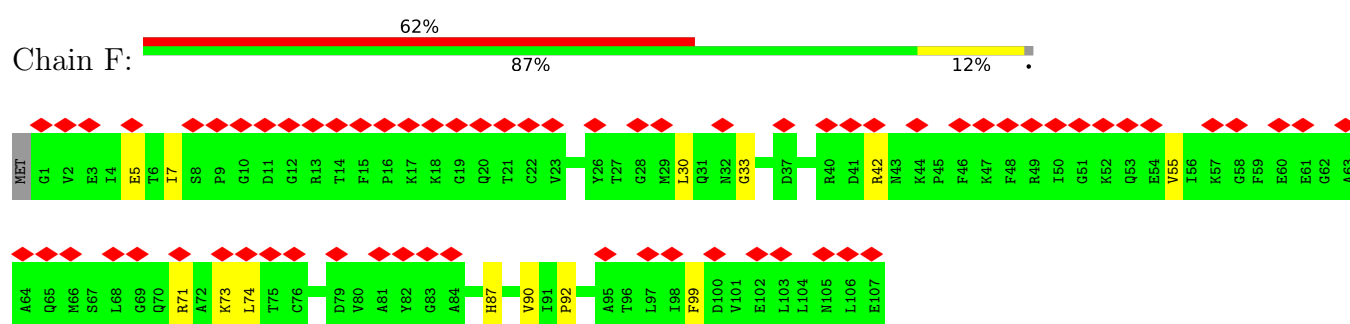
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

### 3 Residue-property plots [i](#)

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

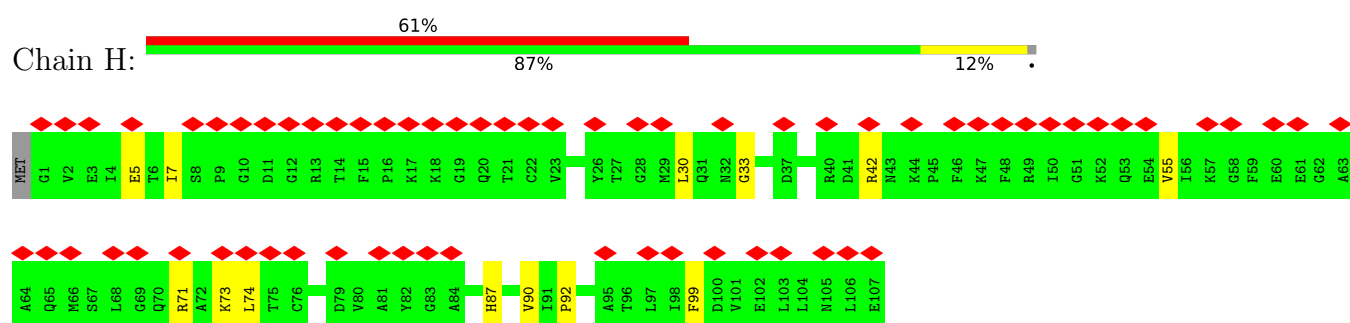
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



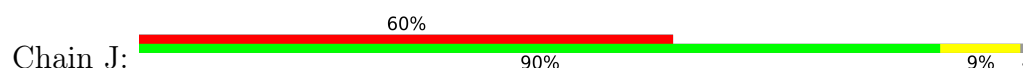
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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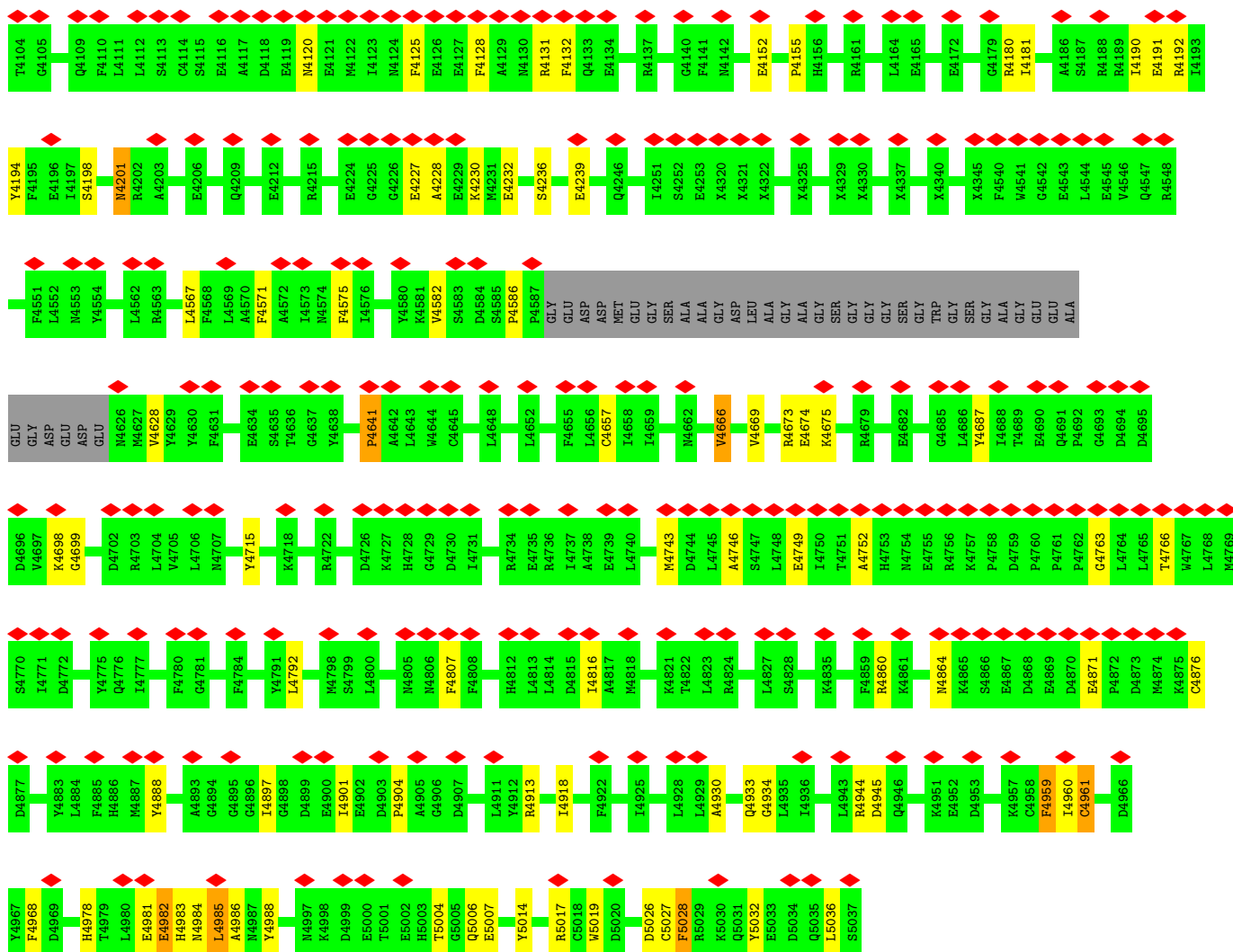




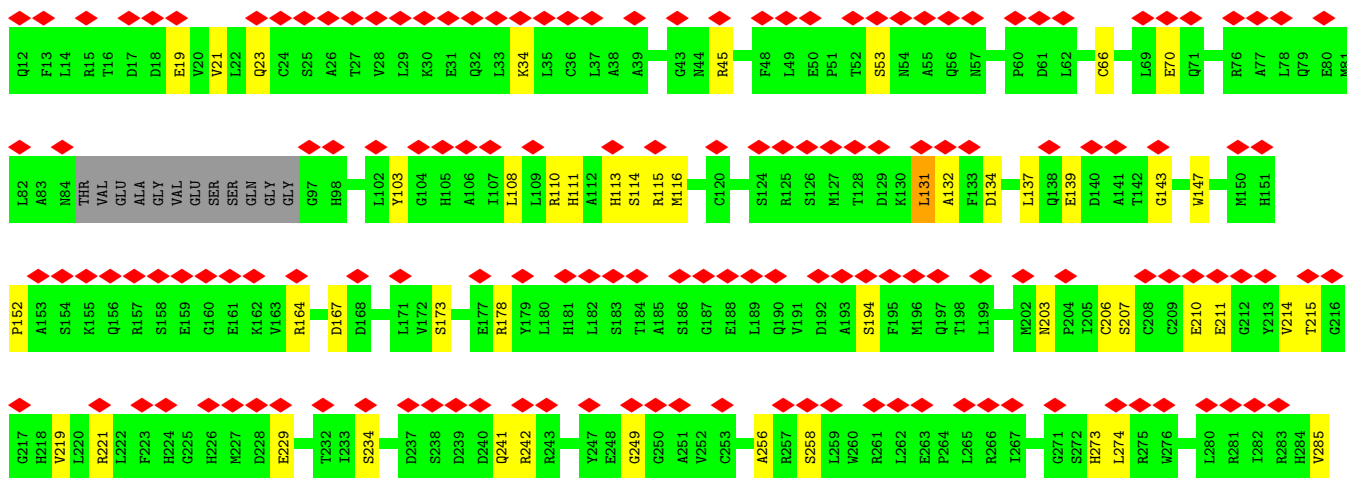
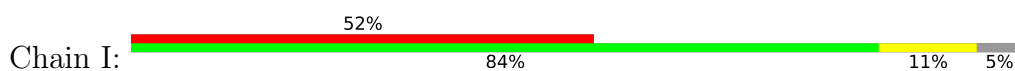
G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	R2928	F2929	L2930	Q2931	N2932	L2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952		X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
ARG	LYS	LYS	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	M2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	S2867	R2868	E2869	E2870	L2871	Q2872	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	E2882	H2883	N2884	T2885	W2886	R2887	G2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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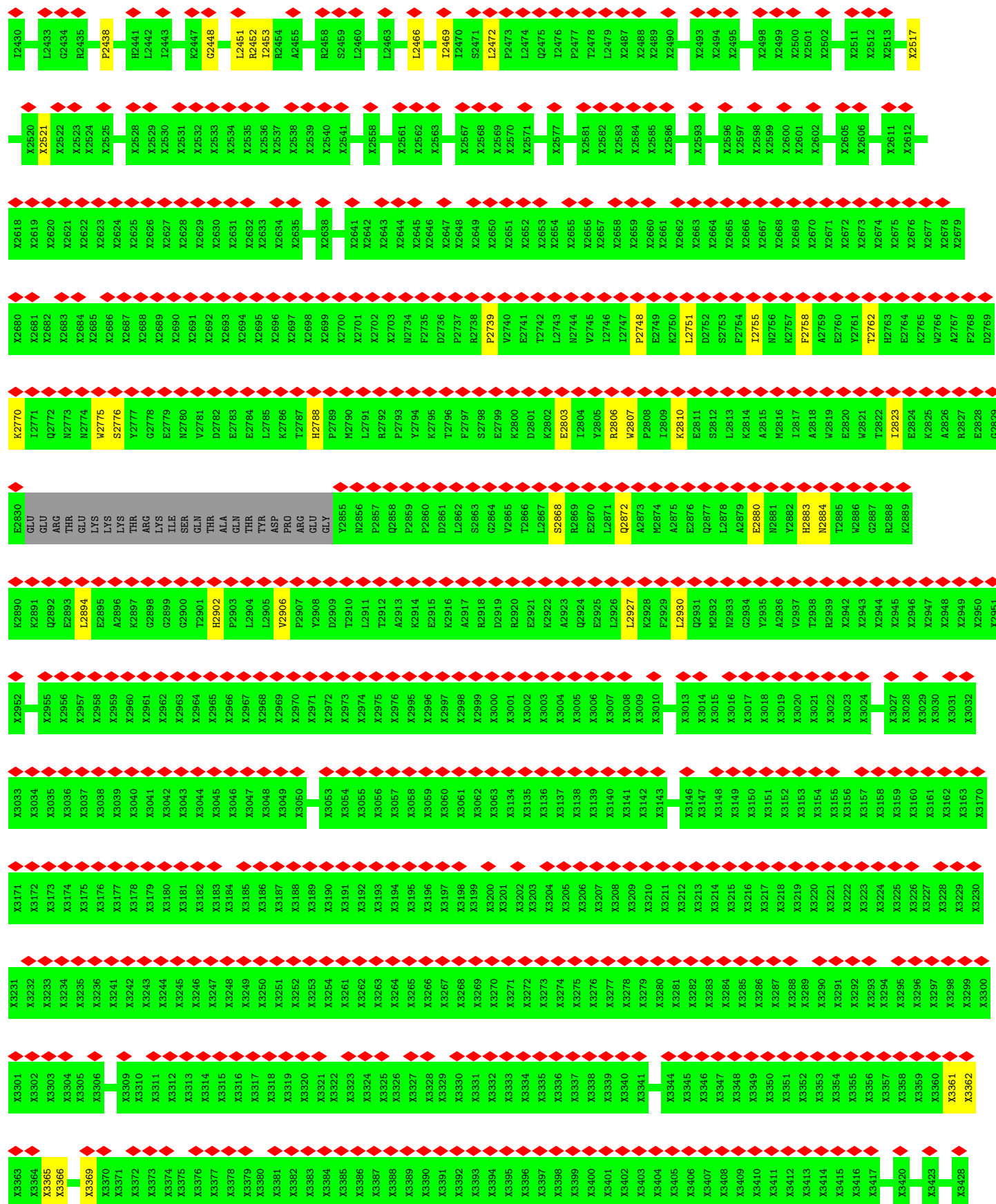


### • Molecule 2: Ryanodine receptor 1

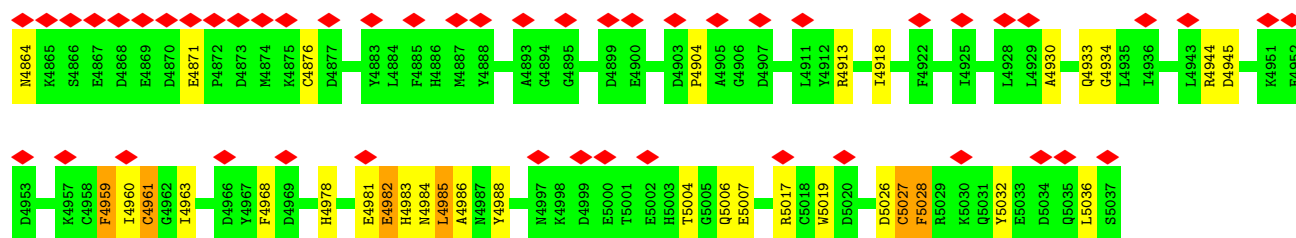


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Y1049	G1050	Y1051	M1052	I1053	G1054	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	R1072	R1073	I1074	F1075	R1076	A1077	E1078	S1080	Y1081	R1087	W1088	Y1089	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	G1103	W1104	A1105	H1106	P1107	E1108	L1109	R1110	P1111	D1112	G1174	S1175	E1176	T1177	A1178	F1179																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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Q981	T982	T983	L984	V985	D986	R987	L988	A989	G992	H993	N994	D999	R1000	V1001	Y1007	S1008	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	D1044	T1045	L1046	G1047	G1048																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1115	L1116	A1117	L1118	E1119	L1120	A1121	L1122	V1123	F1124	N1125	G1126	H1127	R1128	G1129	Q1130	R1131	W1132	H1133	L1134	G1135	S1136	E1137	G1140	R1141	S1145	G1146	D1147	V1148	V1149	G1150	G1151	M1152	I1153	D1154	L1155	T1156	E1157	I1160	L1161	T1163	L1164	E1167	V1168	L1169	M1170	S1171	D1172	P1173	G1174	S1175	E1176	T1177	A1178	F1179																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
F947	V948	Q949	H950	V951	A952	S953	G954	L955	W956	L957	T958	Y959	A960	A961	P962	D963	P964	K965	L966	A967	A968	E969	A970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041	E1042	E1043	E1044	E1045	E1046	E1047	E1048	E1049	E1050	E1051	E1052	E1053	E1054	E1055	E1056	E1057	E1058	E1059	E1060	E1061	E1062	E1063	E1064	E1065	E1066	E1067	E1068	E1069	E1070	E1071	E1072	E1073	E1074	E1075	E1076	E1077	E1078	E1079	E1080	E1081	E1082	E1083	E1084	E1085	E1086	E1087	E1088	E1089	E1090	E1091	E1092	E1093	E1094	E1095	E1096	E1097	E1098	E1099	E1100	E1101	E1102	E1103	E1104	E1105	E1106	E1107	E1108	E1109	E1110	E1111	E1112	E1113	E1114	E1115	E1116	E1117	E1118	E1119	E1120	E1121	E1122	E1123	E1124	E1125	E1126	E1127	E1128	E1129	E1130	E1131	E1132	E1133	E1134	E1135	E1136	E1137	E1138	E1139	E1140	E1141	E1142	E1143	E1144	E1145	E1146	E1147	E1148	E1149	E1150	E1151	E1152	E1153	E1154	E1155	E1156	E1157	E1158	E1159	E1160	E1161	E1162	E1163	E1164	E1165	E1166	E1167	E1168	E1169	E1170	E1171	E1172	E1173	E1174	E1175	E1176	E1177	E1178	E1179	E1180	E1181	E1182	E1183	E1184	E1185	E1186	E1187	E1188	E1189	E1190	E1191	E1192	E1193	E1194	E1195	E1196	E1197	E1198	E1199	E1200	E1201	E1202	E1203	E1204	E1205	E1206	E1207	E1208	E1209	E1210	E1211	E1212	E1213	E1214	E1215	E1216	E1217	E1218	E1219	E1220	E1221	E1222	E1223	E1224	E1225	E1226	E1227	E1228	E1229	E1230	E1231	E1232	E1233	E1234	E1235	E1236	E1237	E1238	E1239	E1240	E1241	E1242	E1243	E1244	E1245	E1246	E1247	E1248	E1249	E1250	E1251	E1252	E1253	E1254	E1255	E1256	E1257	E1258	E1259	E1260	E1261	E1262	E1263	E1264	E1265	E1266	E1267	E1268	E1269	E1270	E1271	E1272	E1273	E1274	E1275	E1276	E1277	E1278	E1279	E1280	E1281	E1282	E1283	E1284	E1285	E1286	E1287	E1288	E1289	E1290	E1291	E1292	E1293	E1294	E1295	E1296	E1297	E1298	E1299	E1300	E1301	E1302	E1303	E1304	E1305	E1306	E1307	E1308	E1309	E1310	E1311	E1312	E1313	E1314	E1315	E1316	E1317	E1318	E1319	E1320	E1321	E1322	E1323	E1324	E1325	E1326	E1327	E1328	E1329	E1330	E1331	E1332	E1333	E1334	E1335	E1336	E1337	E1338	E1339	E1340	E1341	E1342	E1343	E1344	E1345	E1346	E1347	E1348	E1349	E1350	E1351	E1352	E1353	E1354	E1355	E1356	E1357	E1358	E1359	E1360	E1361	E1362	E1363	E1364	E1365	E1366	E1367	E1368	E1369	E1370	E1371	E1372	E1373	E1374	E1375	E1376	E1377	E1378	E1379	E1380	E1381	E1382	E1383	E1384	E1385	E1386	E1387	E1388	E1389	E1390	E1391	E1392	E1393	E1394	E1395	E1396	E1397	E1398	E1399	E1400	E1401	E1402	E1403	E1404	E1405	E1406	E1407	E1408	E1409	E1410	E1411	E1412	E1413	E1414	E1415	E1416	E1417	E1418	E1419	E1420	E1421	E1422	E1423	E1424	E1425	E1426	E1427	E1428	E1429	E1430	E1431	E1432	E1433	E1434	E1435	E1436	E1437	E1438	E1439	E1440	E1441	E1442	E1443	E1444	E1445	E1446	E1447	E1448	E1449	E1450	E1451	E1452	E1453	E1454	E1455	E1456	E1457	E1458	E1459	E1460	E1461	E1462	E1463	E1464	E1465	E1466	E1467	E1468	E1469	E1470	E1471	E1472	E1473	E1474	E1475	E1476	E1477	E1478	E1479	E1480	E1481	E1482	E1483	E1484	E1485	E1486	E1487	E1488	E1489	E1490	E1491	E1492	E1493	E1494	E1495	E1496	E1497	E1498	E1499	E1500	E1501	E1502	E1503	E1504	E1505	E1506	E1507	E1508	E1509	E1510	E1511	E1512	E1513	E1514	E1515	E1516	E1517	E1518	E1519	E1520	E1521	E1522	E1523	E1524	E1525	E1526	E1527	E1528	E1529	E1530	E1531	E1532	E1533	E1534	E1535	E1536	E1537	E1538	E1539	E1540	E1541	E1542	E1543	E1544	E1545	E1546	E1547	E1548	E1549	E1550	E1551	E1552	E1553	E1554	E1555	E1556	E1557	E1558	E1559	E1560	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	E1621	E1622	E1623	E1624	E1625	E1626	E1627	E1628	E1629	E1630	E1631	E1632	E1633	E1634	E1635	E1636	E1637	E1638	E1639	E1640	E1641	E1642	E1643	E1644	E1645	E1646	E1647	E1648	E1649	E1650	E1651	E1652	E1653	E1654	E1655	E1656	E1657	E1658	E1659	E1660	E1661	E1662	E1663	E1664	E1665	E1666	E1667	E1668	E1669	E1670	E1671	E1672	E1673	E1674	E1675	E1676	E1677	E1678	E1679	E1680	E1681	E1682	E1683	E1684	E1685	E1686	E1687	E1688	E1689	E1690	E1691	E1692	E1693	E1694	E1695	E1696	E1697	E1698	E1699	E1700	E1701	E1702	E1703	E1704	E1705	E1706	E1707	E1708	E1709	E1710	E1711	E1712	E1713	E1714	E1715	E1716	E1717	E1718	E1719	E1720	E1721	E1722	E1723	E1724	E1725	E1726	E1727	E1728	E1729	E1730	E1731	E1732	E1733	E1734	E1735	E1736	E1737	E1738	E1739	E1740	E1741	E1742	E1743	E1744	E1745	E1746	E1747	E1748	E1749	E1750	E1751	E1752	E1753	E1754	E1755	E1756	E1757	E1758	E1759	E1760	E1761	E1762	E1763	E1764	E1765	E1766	E1767	E1768	E1769	E1770	E1771	E1772	E1773	E1774	E1775	E1776	E1777	E1778	E1779	E1780	E1781	E1782	E1783	E1784	E1785	E1786	E1787	E1788	E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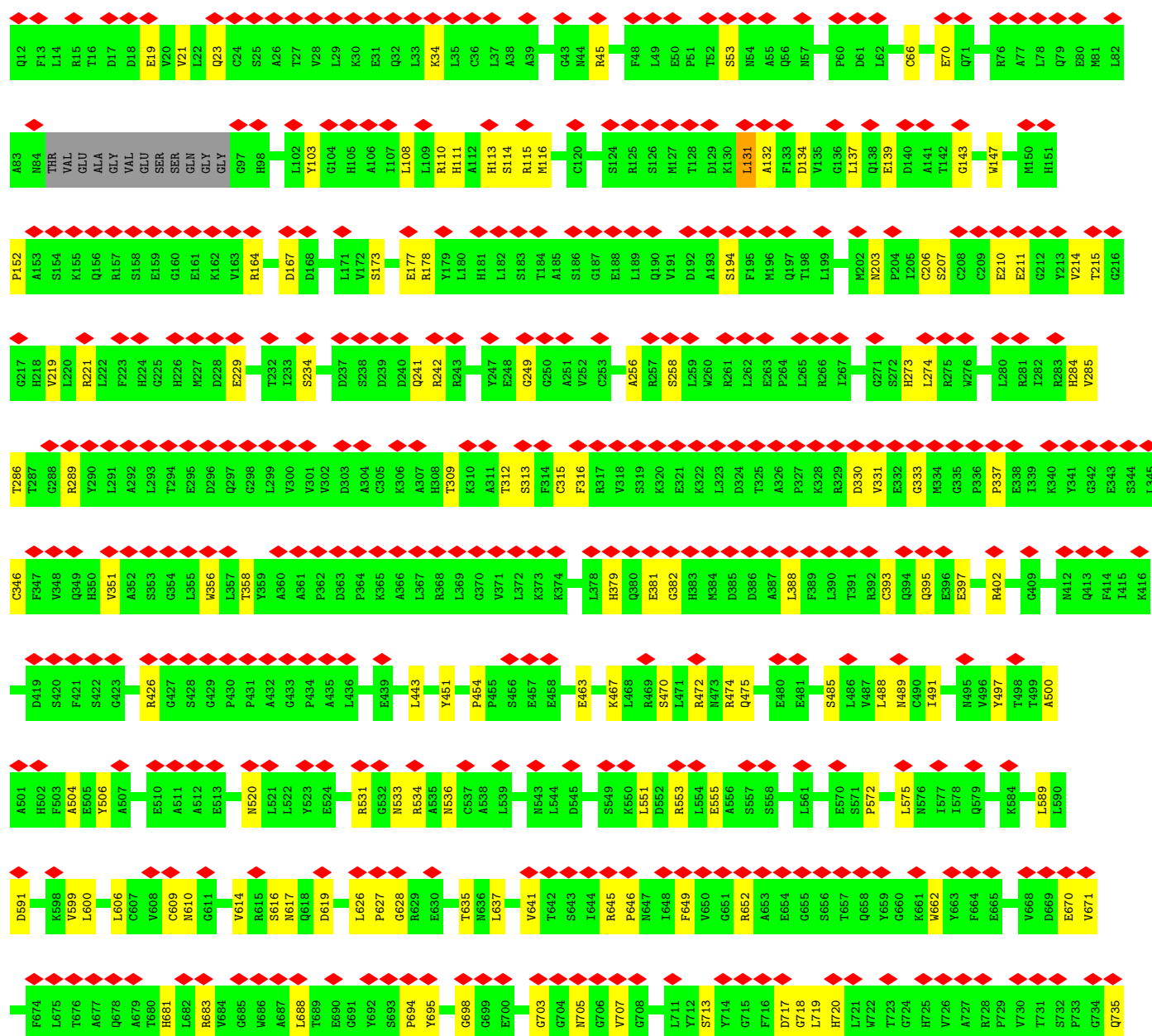


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• Molecule 2: Ryanodine receptor 1

Chain E:

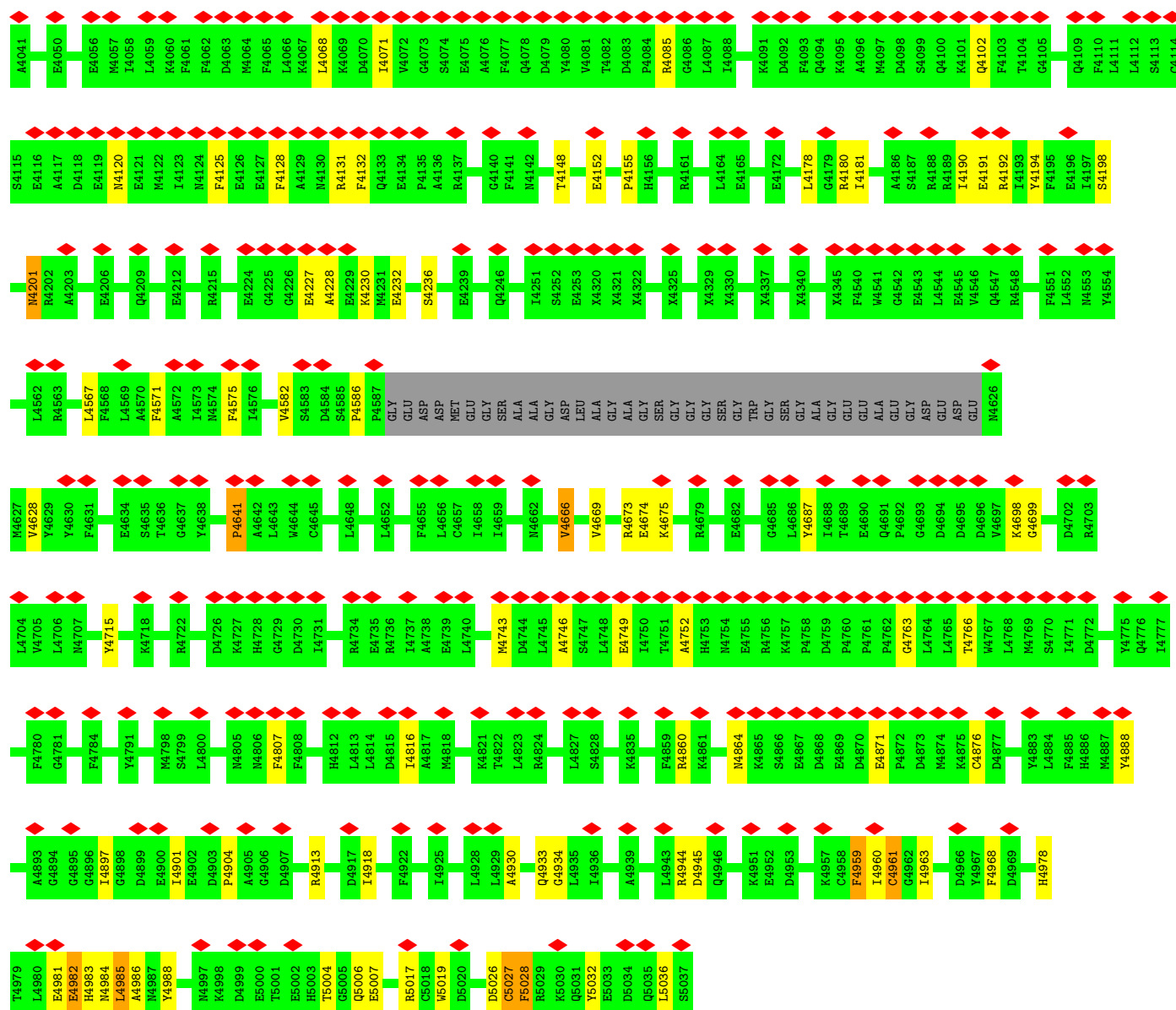




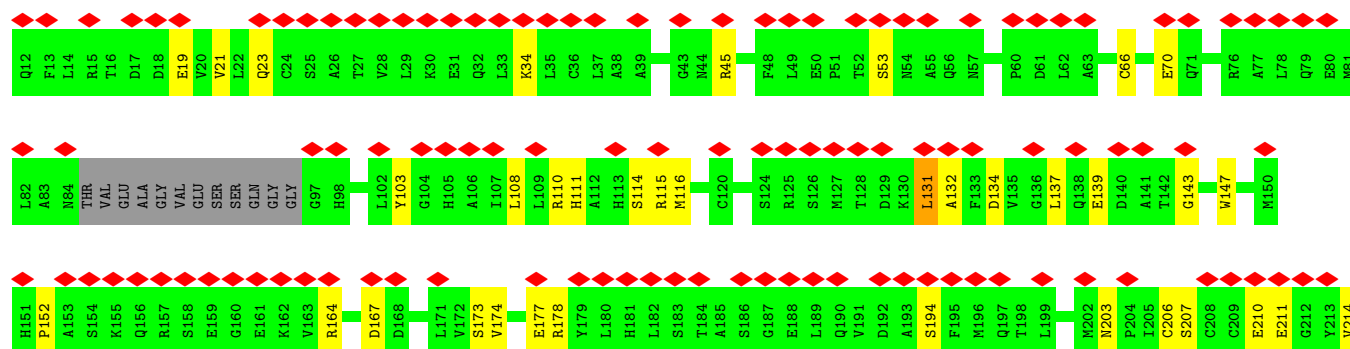
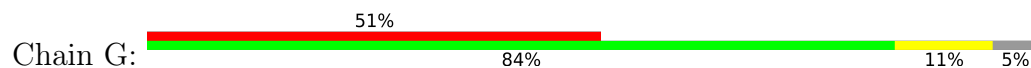




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• Molecule 2: Ryanodine receptor 1

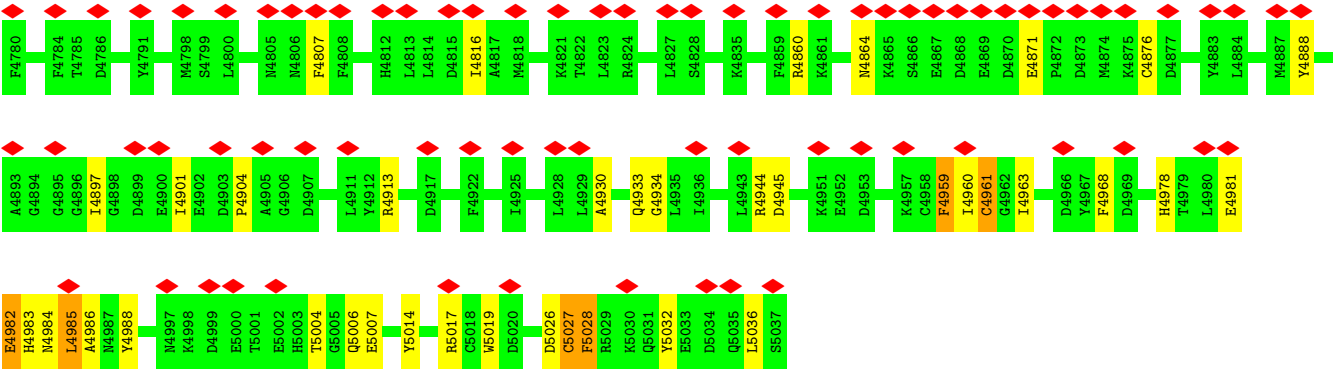


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GLN	L988	T928	E868	K801	H736	V671	D591	A501	D419	C346	T286	G217
PRO	A989	L929	R869	F802	L737	F674	K998	H502	S420	F347	G288	H218
SER	G992	K930	R870	P806	A739	L675	V599	A504	F421	V348	R289	V219
GLN	H993	T931	R871	G807	P740	L676	L600	E505	S422	H350	R290	L220
VAL	H994	L932	E872	Y808	E741	T677	L606	Y506	G423	V351	L222	R221
ASN	D999	L933	K873	A809	S745	Q678	C607	A507	G426	A352	L291	F223
GLN	Y1007	A934	L874	H812	C746	Q679	V608	E510	G427	L293	A292	F224
SER	A1009	L935	E876	E813	C747	A679	G609	A511	S353	G225	L294	H226
ARG	VAL	G936	E877	V815	L748	L682	N610	A512	G354	E295	D296	H227
TRP	Y1007	H938	L878	L816	D749	R683	G611	E513	S355	L357	Q297	D228
D1070	S1008	H939	L879	L817	L750	V684	V614	N520	A352	T358	G298	E229
R1071	ASP	G940	R879	L816	S751	G685	R615	L521	G427	Y359	L299	T232
V1072	GLN	E941	E880	L816	W752	G686	S616	L522	A432	A360	V300	I233
R1073	ASP	M941	L881	P817	W753	A687	N617	Y523	G433	A361	V301	S234
I1074	ILE	A942	W892	R820	S754	L688	Q618	E524	G434	P362	D303	D237
F1075	ALA	E943	A883	L821	W755	T689	D619	E524	A435	P363	A304	S238
R1076	ARG	E944	A883	L821	W756	E690	L626	R531	L436	P364	A307	D240
ARG	ARG	R822	L884	L823	S757	G691	P627	G532	E439	K365	A307	Q241
E1078	ASN	K945	T885	L823	R758	Y692	R629	N533	L443	K366	H308	R242
K1079	PRO	A946	R886	E824	W759	Y695	E630	R534	Y451	L367	T309	R243
Y1089	R1020	E947	L887	R827	W760	G699	T635	R535	P454	G370	K310	Y247
F1092	L1021	D948	E888	E828	G761	E700	N636	C537	S456	V371	T312	E248
E1093	V1022	N949	Q889	Y829	G762	G699	L637	L539	E457	L372	F314	G249
A1094	P1023	L950	C890	R830	W763	E700	L637	L539	E458	K373	C315	G250
V1095	Y1024	K951	W891	R831	G764	E700	T635	N536	E458	K374	F316	A256
T1096	L1026	K952	T892	E832	Q765	E700	N636	R536	E458	K374	F316	A256
T1097	L1027	T953	Y893	G833	Q766	E700	N636	R536	E458	K374	F316	A256
G1098	L1027	K954	G894	P834	W767	E700	N636	R536	E458	K374	F316	A256
E1099	E1029	L955	P895	R835	W768	E700	N636	R536	E458	K374	F316	A256
M1100	A1030	P956	V896	R836	W769	E700	N636	R536	E458	K374	F316	A256
G1103	T1031	K957	D897	P837	W770	E700	N636	R536	E458	K374	F316	A256
W1104	K1032	T958	D898	R838	W771	E700	N636	R536	E458	K374	F316	A256
A1105	R1033	Y959	N900	L839	W772	E700	N636	R536	E458	K374	F316	A256
P1107	S1034	M960	K901	S843	W773	E700	N636	R536	E458	K374	F316	A256
E1108	R1035	M961	K902	R844	W774	E700	N636	R536	E458	K374	F316	A256
L1109	R1036	S962	R902	R845	W775	E700	N636	R536	E458	K374	F316	A256
R1110	D1037	N963	L903	R846	W776	E700	N636	R536	E458	K374	F316	A256
P1111	S1038	G964	H904	L846	W777	E700	N636	R536	E458	K374	F316	A256
D1112	L1039	P965	P905	L846	W778	E700	N636	R536	E458	K374	F316	A256
V1113	C1040	K966	C906	L846	W779	E700	N636	R536	E458	K374	F316	A256
E1114	Q1041	P967	C907	L846	W780	E700	N636	R536	E458	K374	F316	A256
G1116	A1042	A968	V908	L846	W781	E700	N636	R536	E458	K374	F316	A256
A1117	R1043	P969	N909	L846	W782	E700	N636	R536	E458	K374	F316	A256
D1118	T1045	L970	F910	C854	W783	E700	N636	R536	E458	K374	F316	A256
E1119	T1046	D971	H911	P855	W784	E700	N636	R536	E458	K374	F316	A256
L1120	L1047	L972	S912	P856	W785	E700	N636	R536	E458	K374	F316	A256
A1121	G1048	S973	L913	D857	W786	E700	N636	R536	E458	K374	F316	A256
Y1122	H1049	H974	P914	THR	W787	E700	N636	R536	E458	K374	F316	A256
V1123	G1050	V975	E915	VAL	W788	E700	N636	R536	E458	K374	F316	A256
F1124	R976	S976	P916	GLN	W789	E700	N636	R536	E458	K374	F316	A256
M1125	Y1051	L977	E917	L861	W790	E700	N636	R536	E458	K374	F316	A256
	M1052	T978	R918	THR	W791	E700	N636	R536	E458	K374	F316	A256
	I1053	P979	N919	GLN	W792	E700	N636	R536	E458	K374	F316	A256
	E1054	A980	Y920	L863	W793	E700	N636	R536	E458	K374	F316	A256
	PRO	Q981	N921	P864	W794	E700	N636	R536	E458	K374	F316	A256
		T982	L922	P865	W795	E700	N636	R536	E458	K374	F316	A256
		T983	N924		W796	E700	N636	R536	E458	K374	F316	A256
		L984			W797	E700	N636	R536	E458	K374	F316	A256
		V985			W798	E700	N636	R536	E458	K374	F316	A256



X3317	X3318	X3319	X3320	X3321	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378																																																																		
X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316																																																																
X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127	X3128	X3129	X3130	X3131	X3132	X3133	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3146	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185
X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250																																																																	
X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047																																																
L2904	L2905	V2906	P2907	D2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2916	K2917	A2918	D2919	A2920	E2921	K2922	A2923	K2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966																																																																	
E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	P2792	P2793	V2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	V2805	K2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	V2819	E2820	V2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLN	THR	ALA	GLN	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	P2783																																																														
GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2864	K2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	E2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903																																																																	
X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693																																																																	
X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2558	X2561	X2562	X2563	X2567	X2568	X2569	X2570	X2571	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2593	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2605	X2606	X2611	X2612	X2613	X2614	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652																																																					
K2447	G2448	L2451	R2452	L2453	R2454	A2455	R2458	S2459	L2460	L2463	L2466	I2469	S2471	L2472	P2473	L2474	Q2475	I2476	P2477	P2478	L2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2498	X2499	X2500	X2511	X2512	X2513	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2528	X2529	X2532	X2533																																																																												
S2374	G2375	L2376	L2377	A2378	A2379	I2380	E2381	E2382	A2383	I2384	S2387	E2388	D2389	P2390	A2391	D2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	GLU	N2414	R2415	V2416	H2417	L2418	G2419	M2423	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	H2440	H2441																																																																							





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	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	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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

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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	33/142628 (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
2	B	0	17
2	E	0	17
2	G	0	16
2	I	0	16
All	All	0	66

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	G	131	LEU	CA-CB-CG	8.35	134.51	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.48	115.30
2	E	131	LEU	CA-CB-CG	8.33	134.46	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1676	LEU	CA-CB-CG	6.33	129.86	115.30

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	818	0	824	8	0
1	F	818	0	824	8	0
1	H	818	0	824	8	0
1	J	818	0	824	5	0
2	B	29499	0	24751	284	0
2	E	29499	0	24751	290	0
2	G	29499	0	24751	288	0
2	I	29499	0	24751	286	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102300	1147	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 1147 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:I:4190:ILE:CD1	2:I:5026:ASP:OD2	1.76	1.33
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	1.77	1.33
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	1.77	1.32
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	1.76	1.31
2:B:4190:ILE:HD11	2:B:5026:ASP:OD2	1.31	1.26

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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	335 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	G	3235/4416 (73%)	2893 (89%)	334 (10%)	8 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	336 (10%)	8 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1387 (10%)	32 (0%)	50	81

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	I	5028	PHE
2	E	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

### 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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84	90

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	131	LEU
2	G	4120	ASN
2	G	553	ARG
2	G	3762	ARG
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4120	ASN
2	G	3781	GLN
2	E	520	ASN
2	G	3766	GLN
2	G	4553	ASN

### 5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	I	14
2	E	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.35
1	I	4345:UNK	C	4540:PHE	N	73.35
1	E	4345:UNK	C	4540:PHE	N	73.35
1	G	4345:UNK	C	4540:PHE	N	73.35

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	45.90

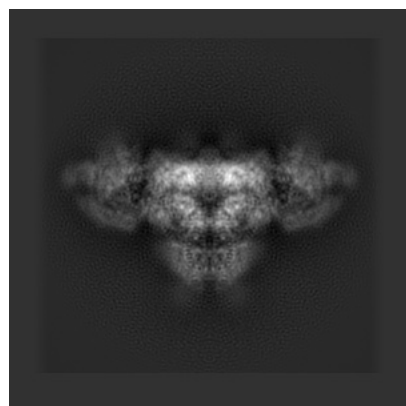
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8393. These allow visual inspection of the internal detail of the map and identification of artifacts.

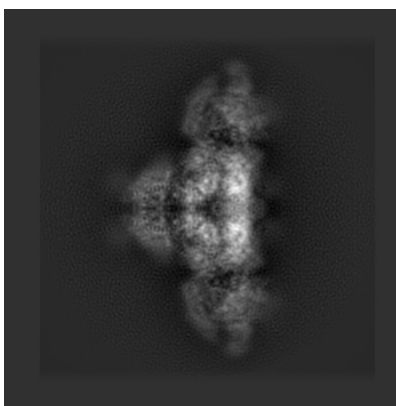
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

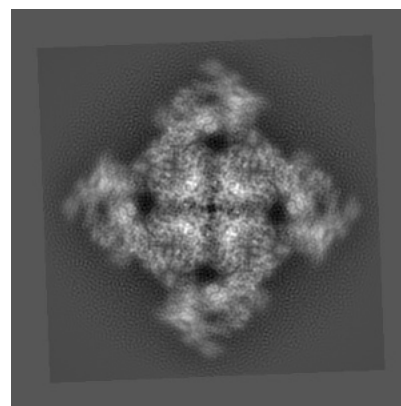
#### 6.1.1 Primary map



X

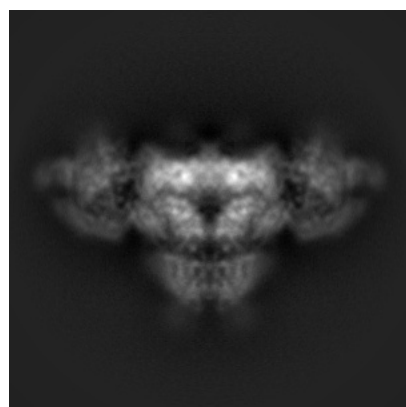


Y

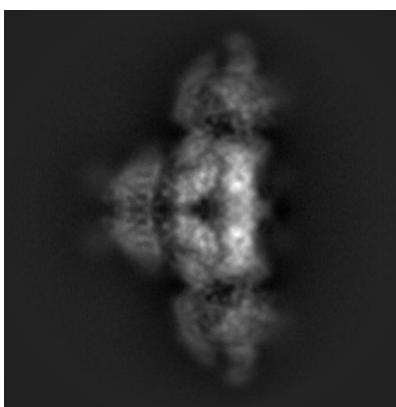


Z

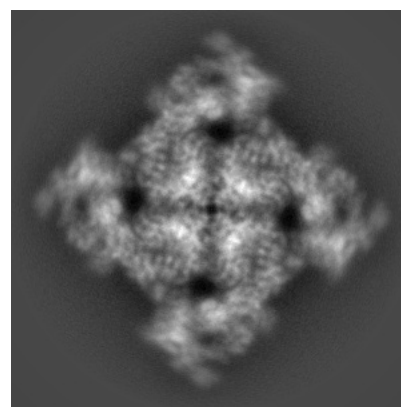
#### 6.1.2 Raw map



X



Y

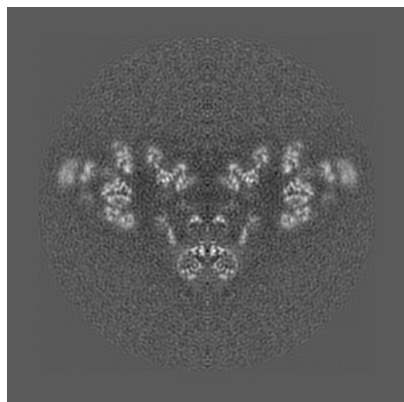


Z

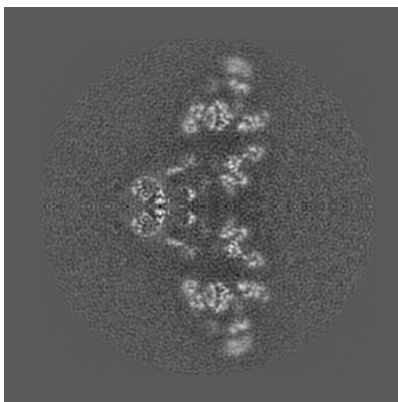
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

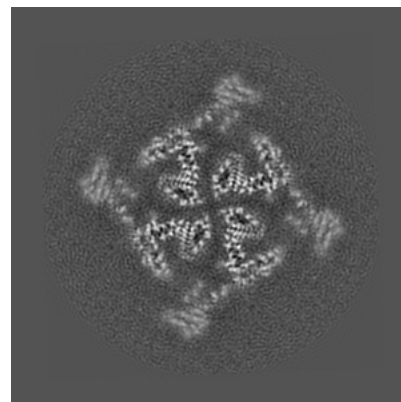
### 6.2.1 Primary map



X Index: 200

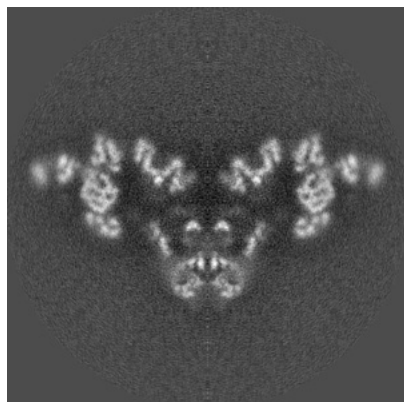


Y Index: 200

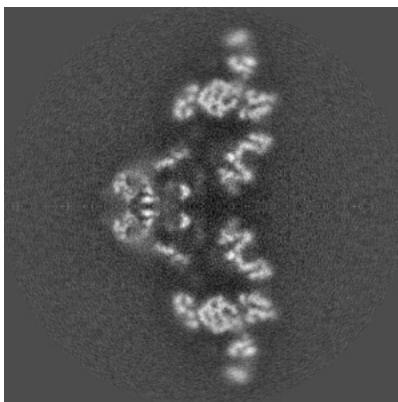


Z Index: 200

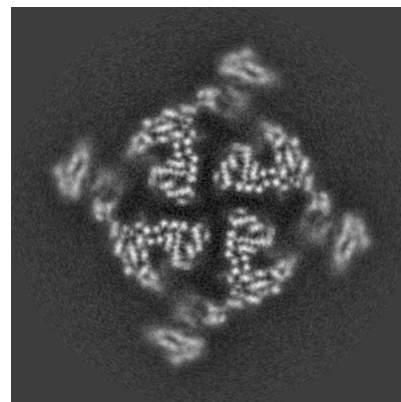
### 6.2.2 Raw map



X Index: 168



Y Index: 168



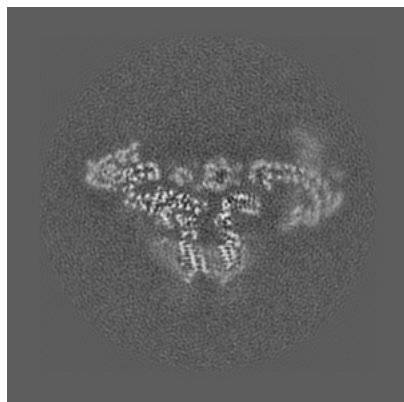
Z Index: 168

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

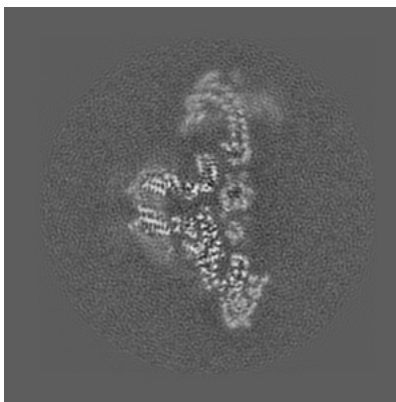


## 6.3 Largest variance slices [i](#)

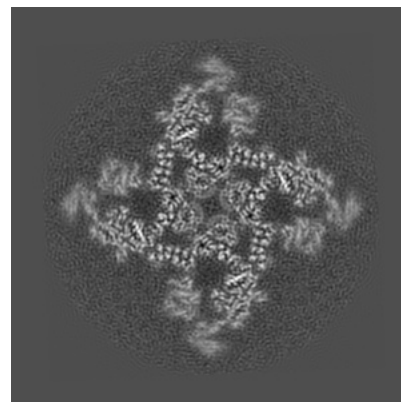
### 6.3.1 Primary map



X Index: 224

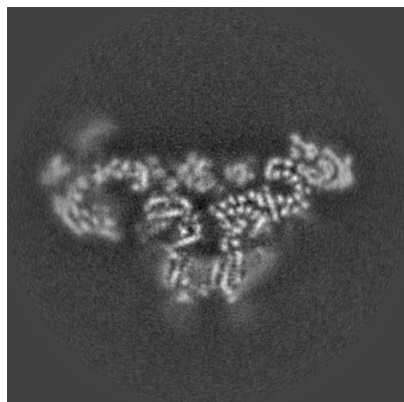


Y Index: 176

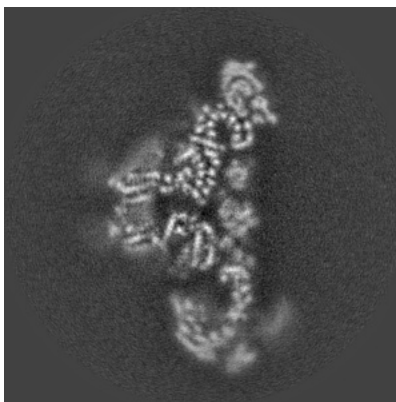


Z Index: 228

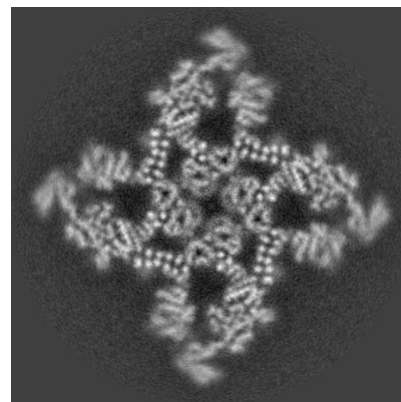
### 6.3.2 Raw map



X Index: 146



Y Index: 190

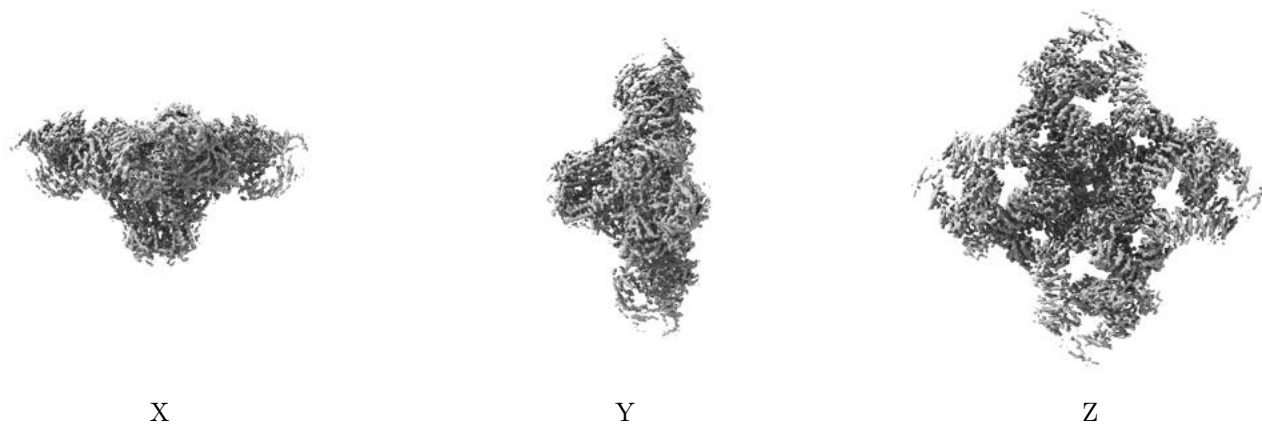


Z Index: 193

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

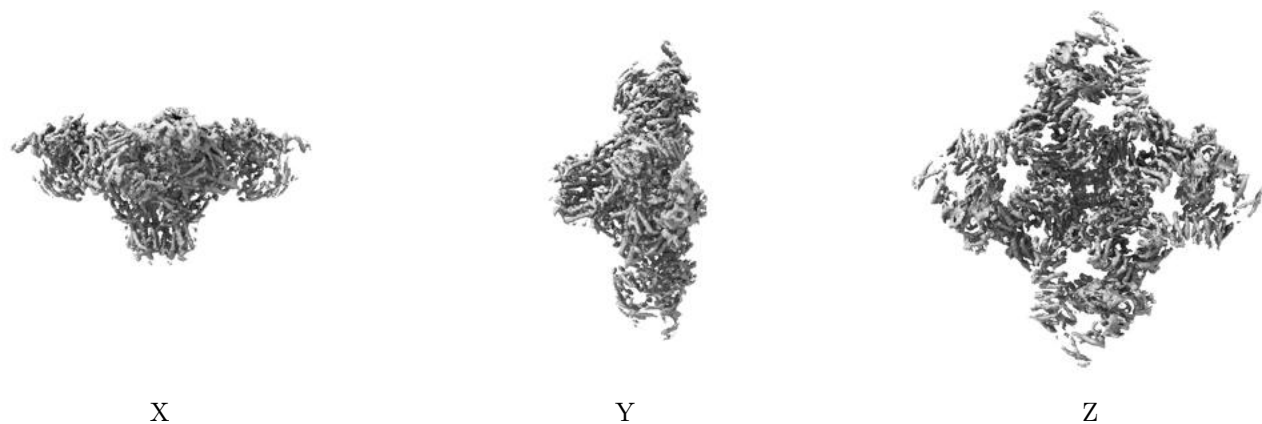
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

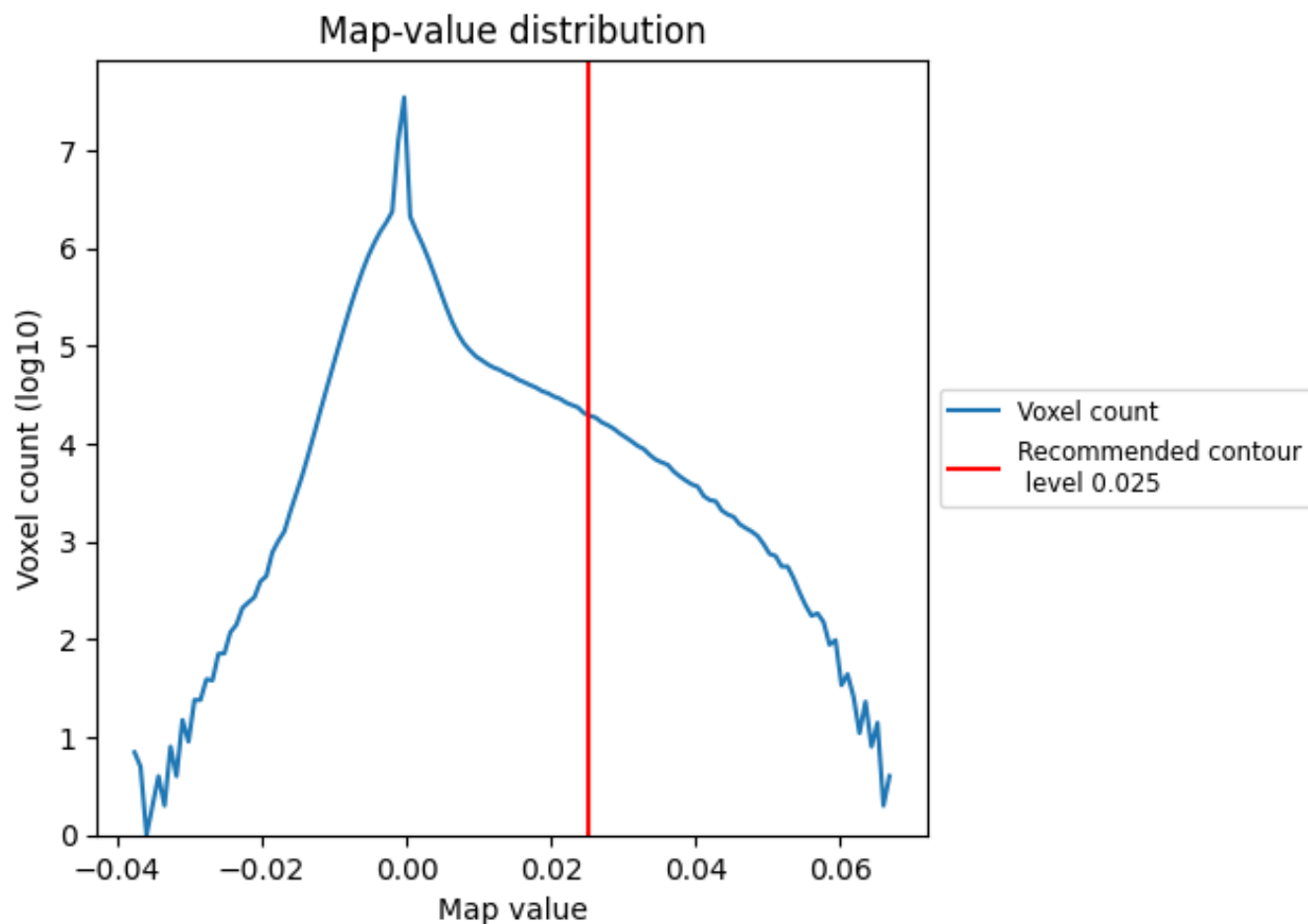
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

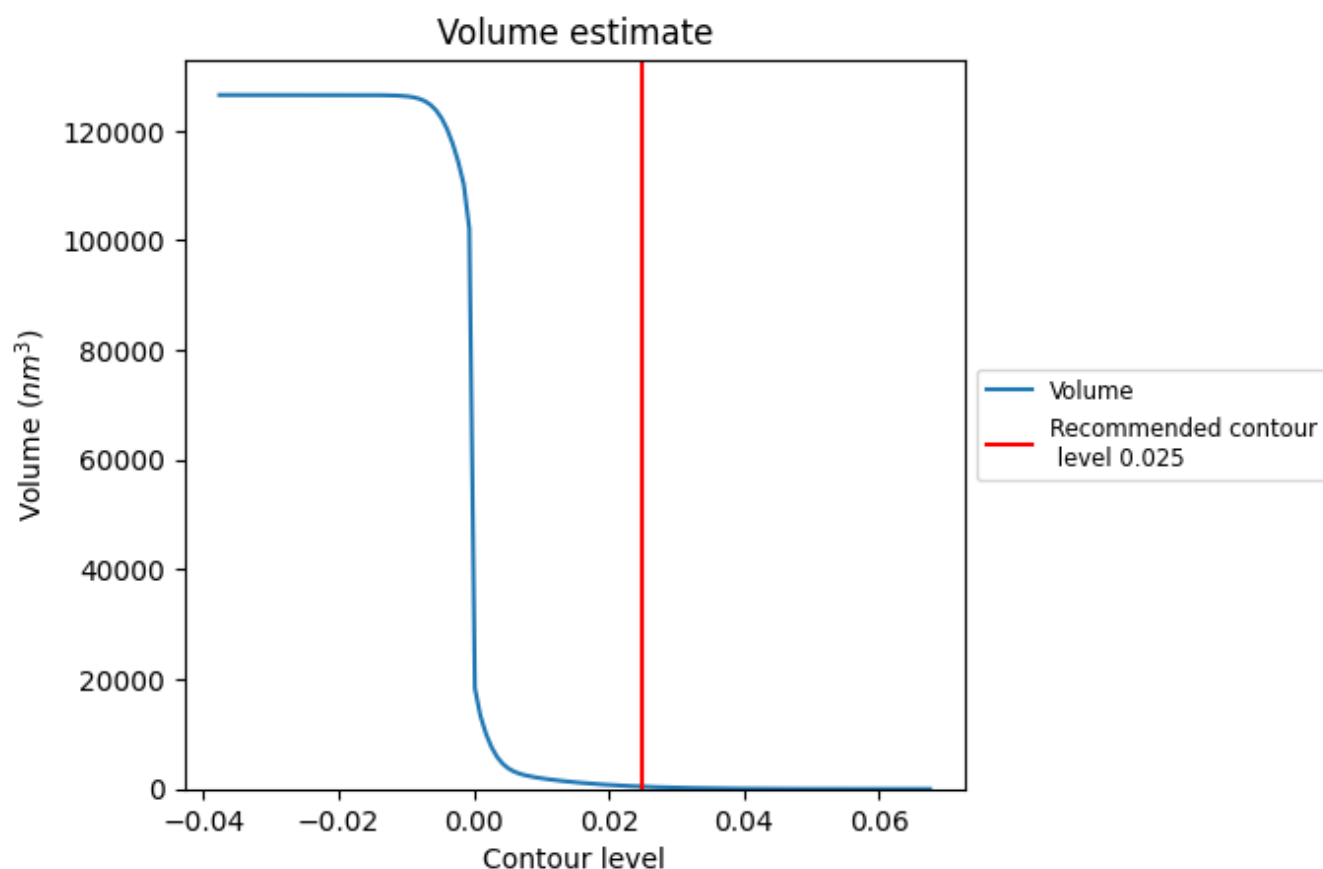
This section contains the results of statistical analysis of the map.

### 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.

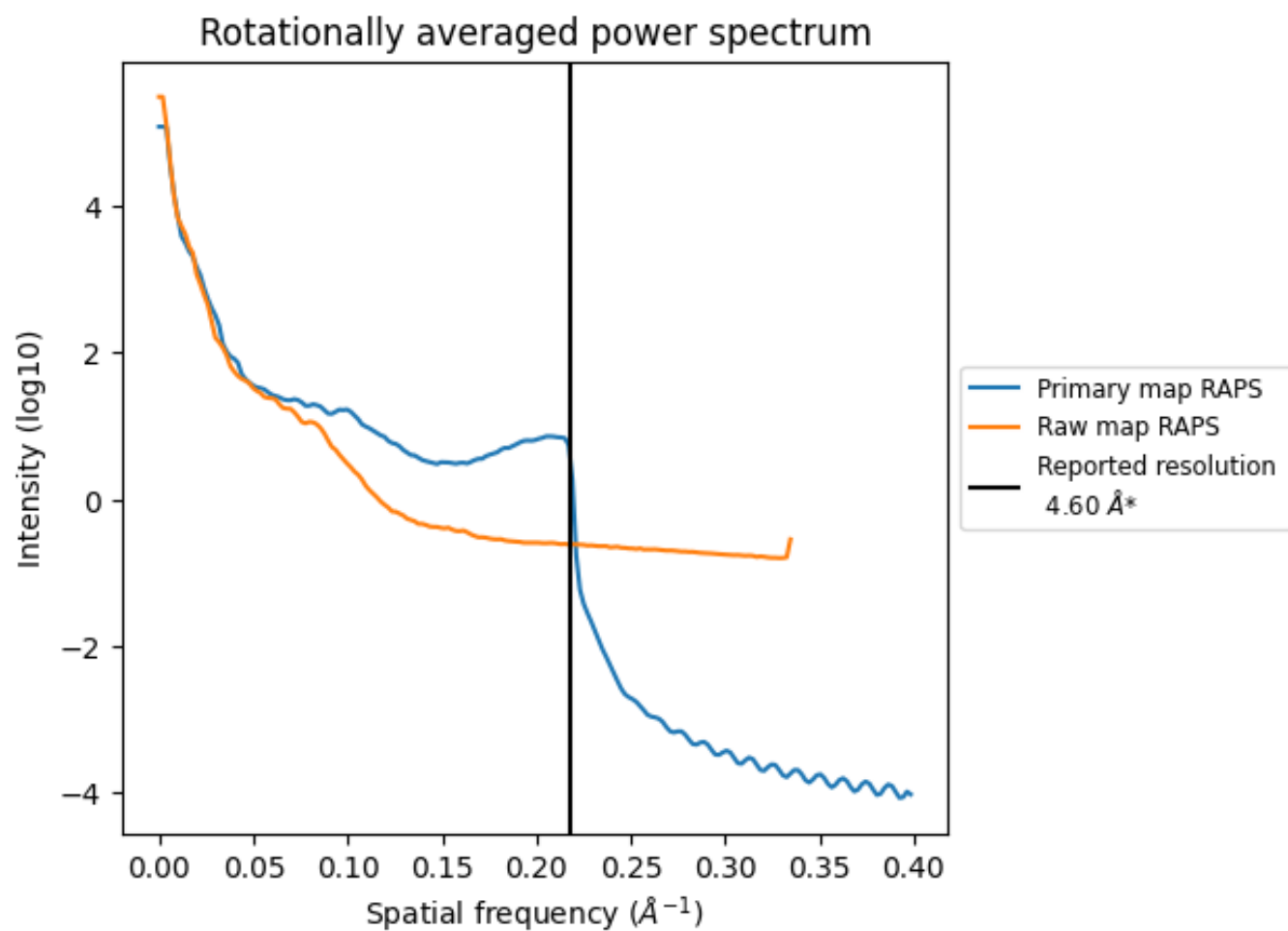
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm<sup>3</sup>; this corresponds to an approximate mass of 390 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](#)

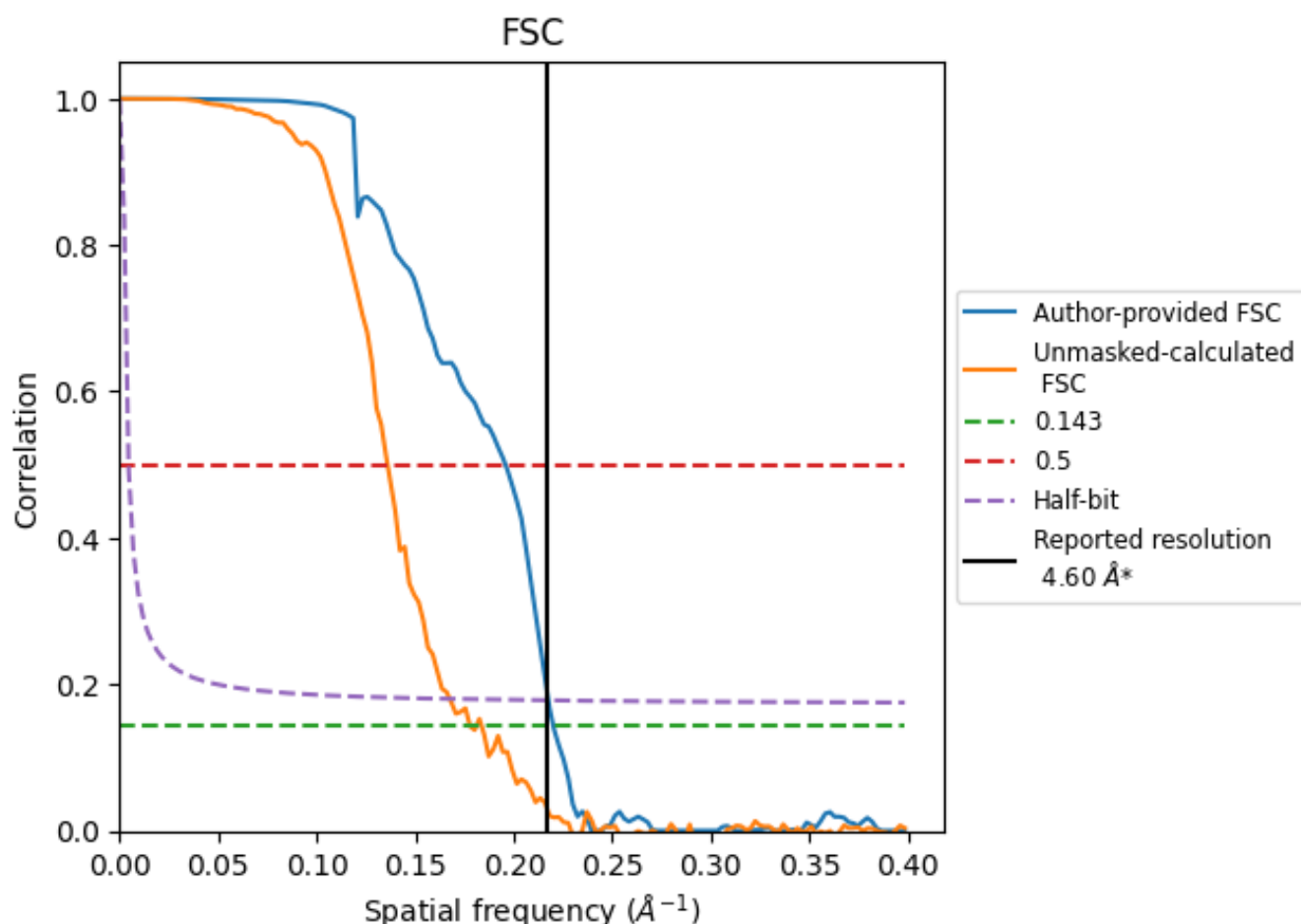


\*Reported resolution corresponds to spatial frequency of 0.217 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

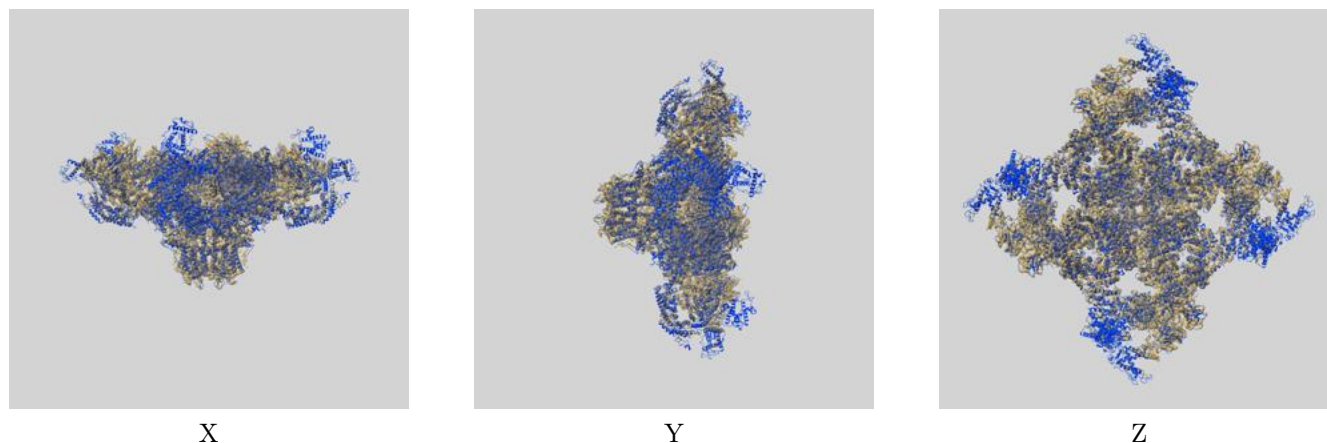
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.54	5.11	4.60
Unmasked-calculated*	5.62	7.35	5.97

\*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 5.62 differs from the reported value 4.6 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-8393 and PDB model 5TB2. Per-residue inclusion information can be found in section [3](#) on page [4](#).

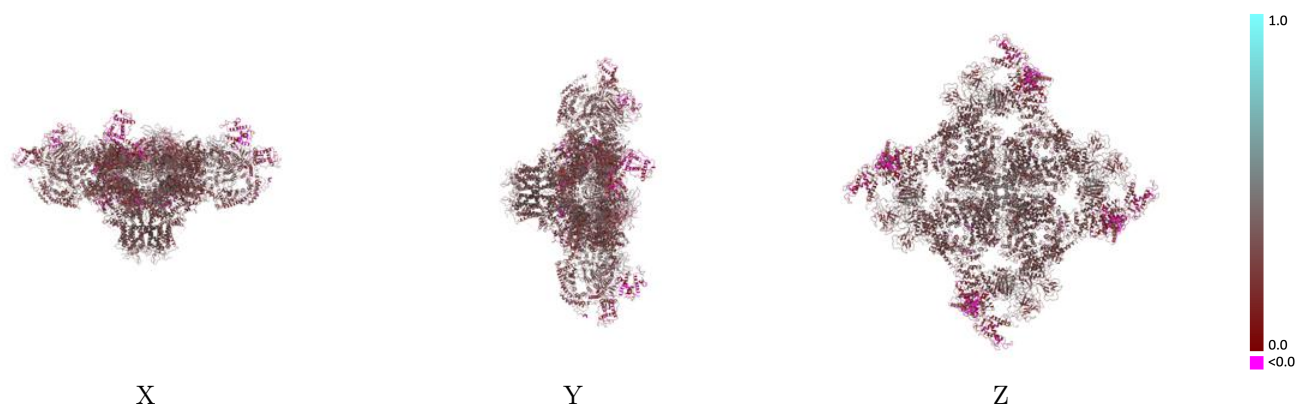
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

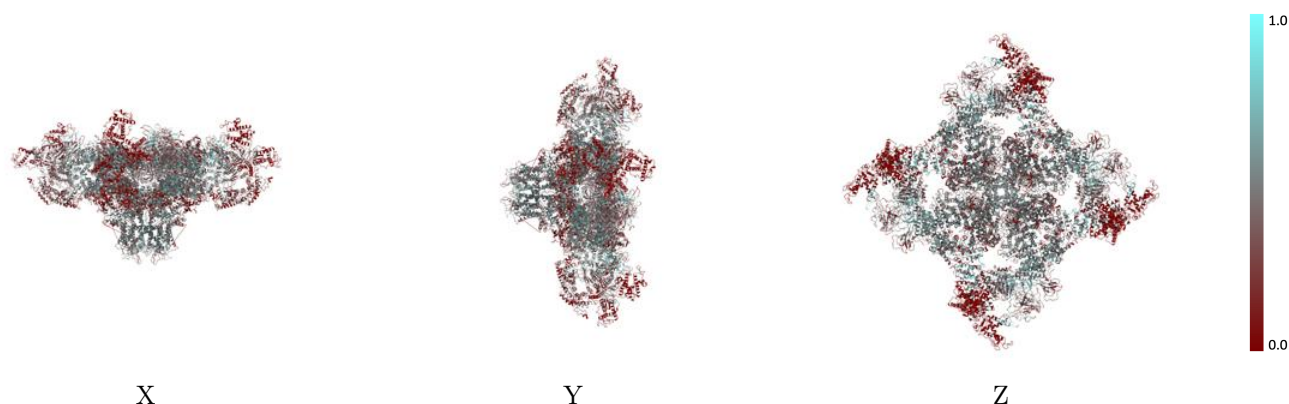


## 9.2 Q-score mapped to coordinate model [i](#)



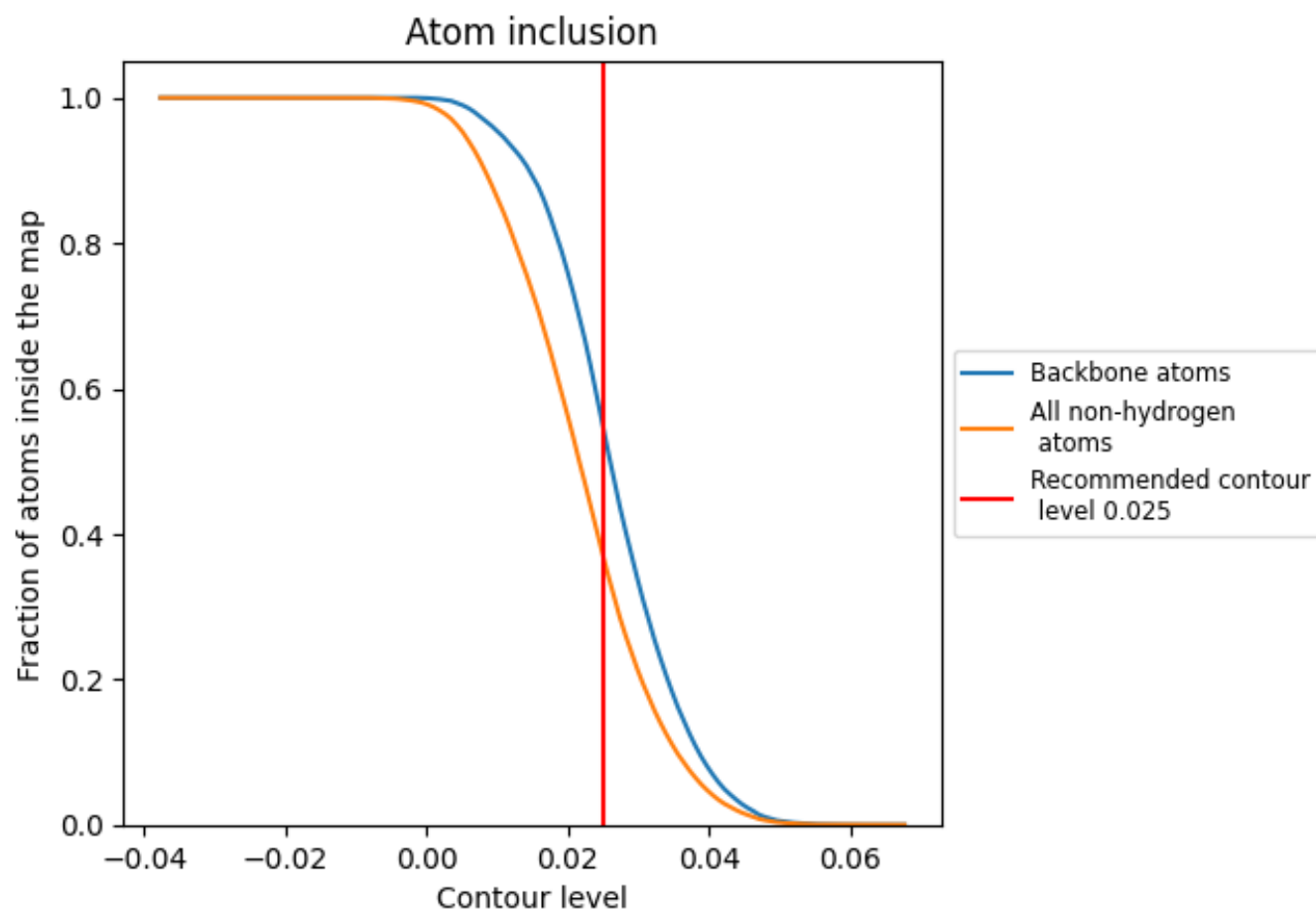
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 37% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3694	<div></div> 0.2880
A	<div></div> 0.3499	<div></div> 0.3000
B	<div></div> 0.3696	<div></div> 0.2880
E	<div></div> 0.3695	<div></div> 0.2880
F	<div></div> 0.3437	<div></div> 0.3030
G	<div></div> 0.3705	<div></div> 0.2880
H	<div></div> 0.3486	<div></div> 0.3040
I	<div></div> 0.3705	<div></div> 0.2870
J	<div></div> 0.3499	<div></div> 0.3030

1.0

0.0

<0.0