



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:11 PM UTC

PDB ID : 5T9V / pdb_00005t9v
EMDB ID : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

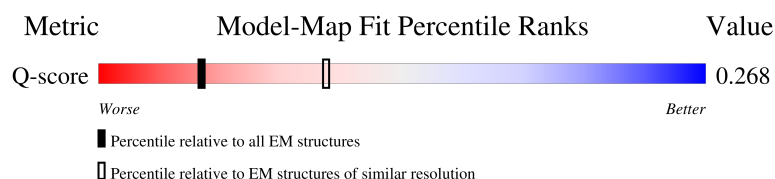
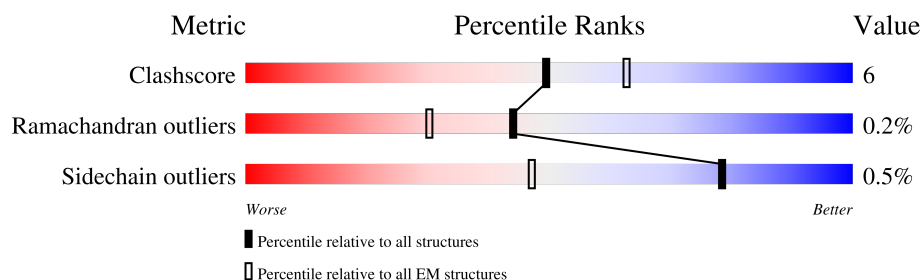
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	108	77% 80% 19% .
1	F	108	77% 80% 19% .
1	H	108	75% 80% 19% .
1	J	108	75% 79% 20% .

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

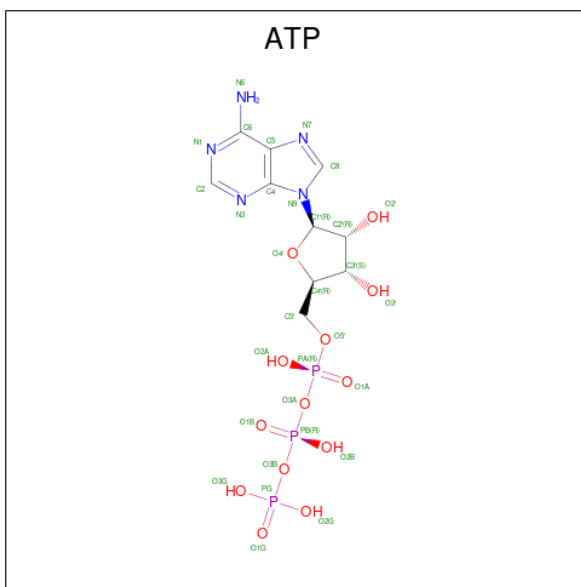
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

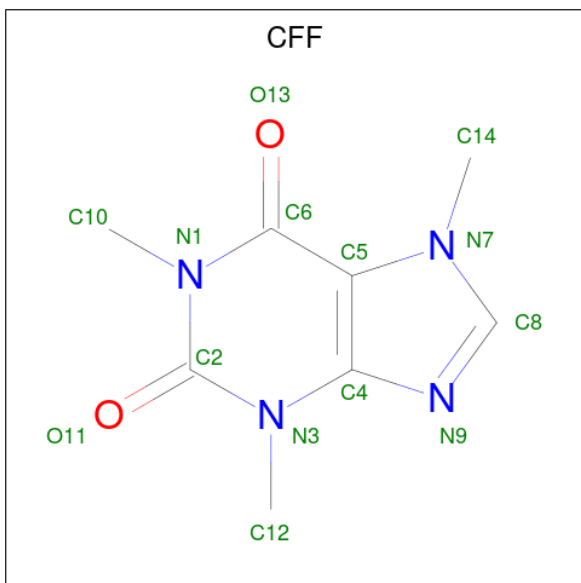
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

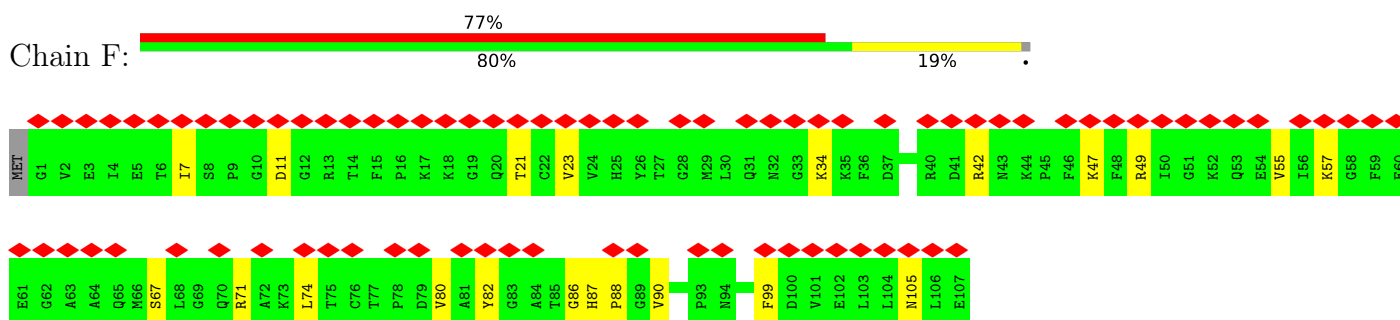
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

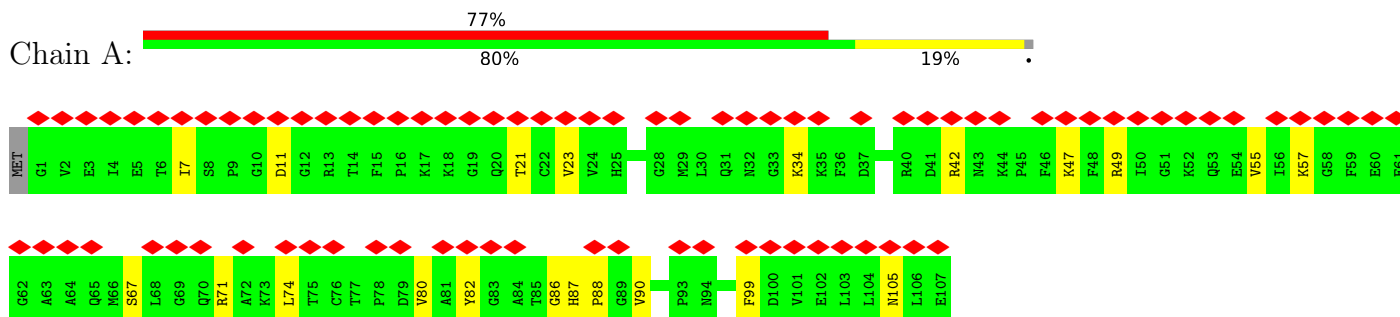
3 Residue-property plots [i](#)

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.

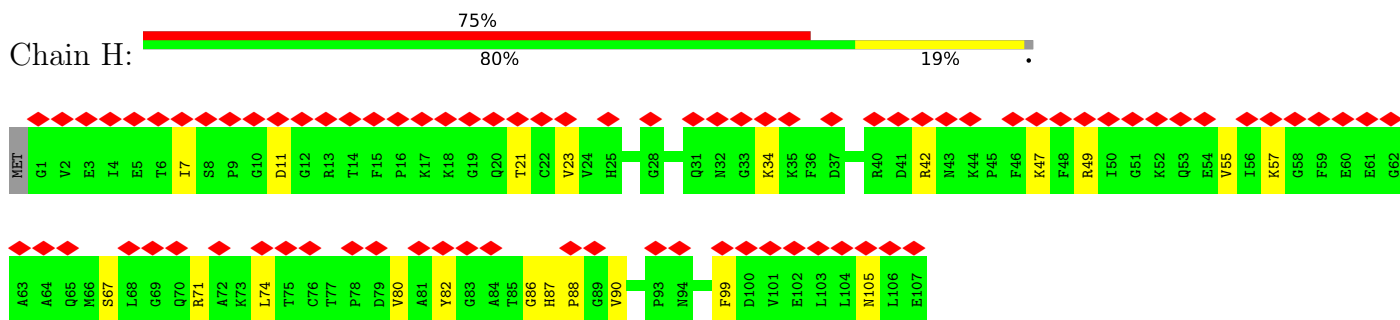
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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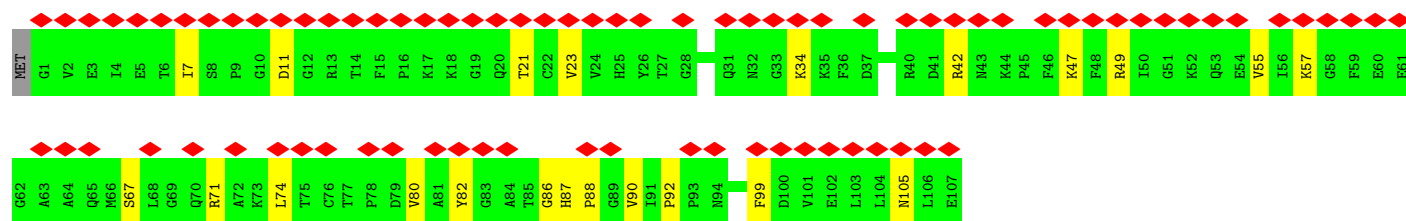


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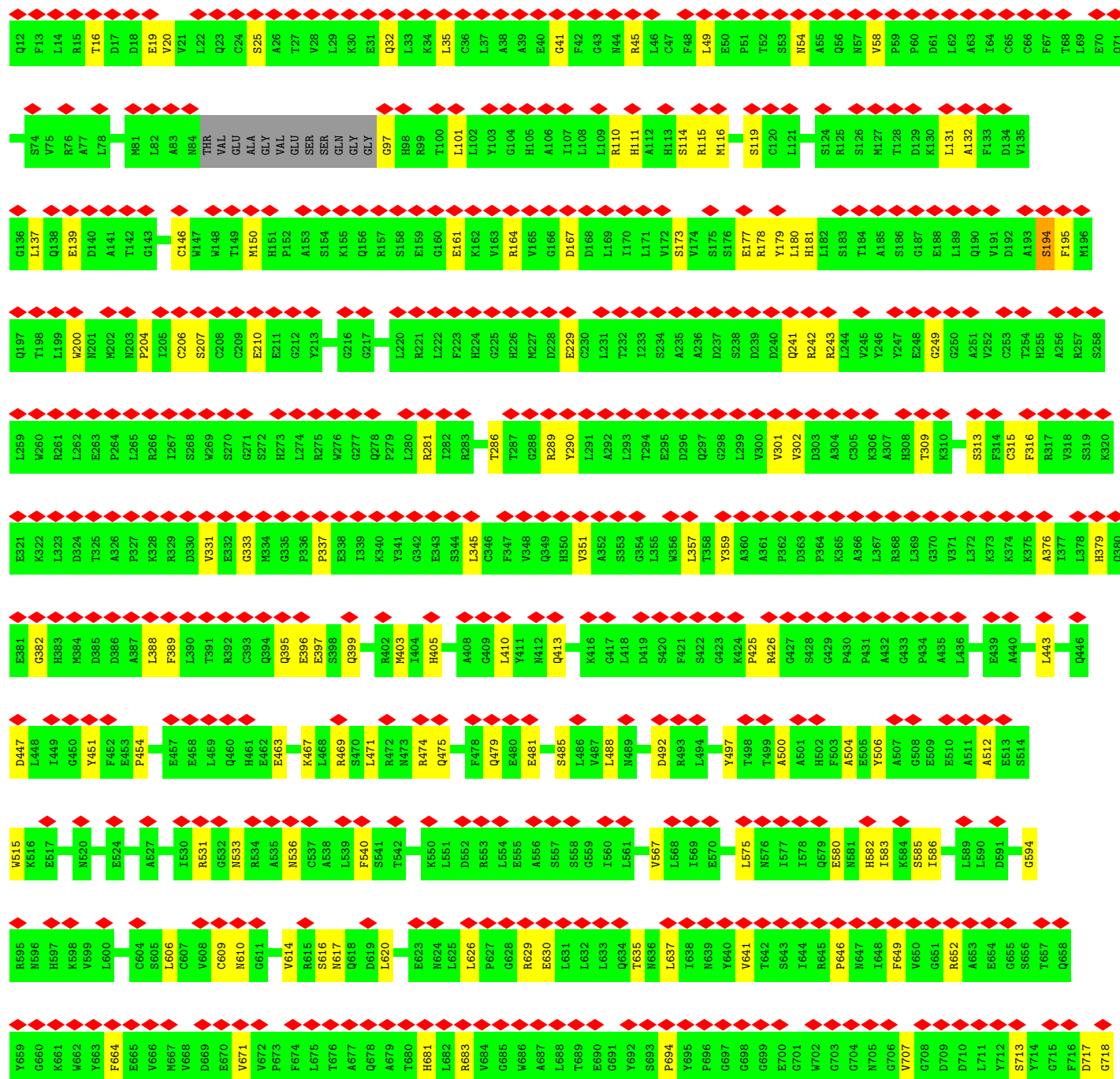
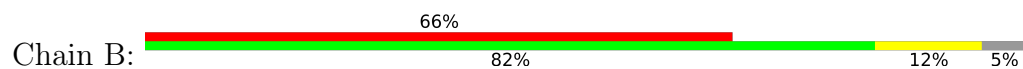


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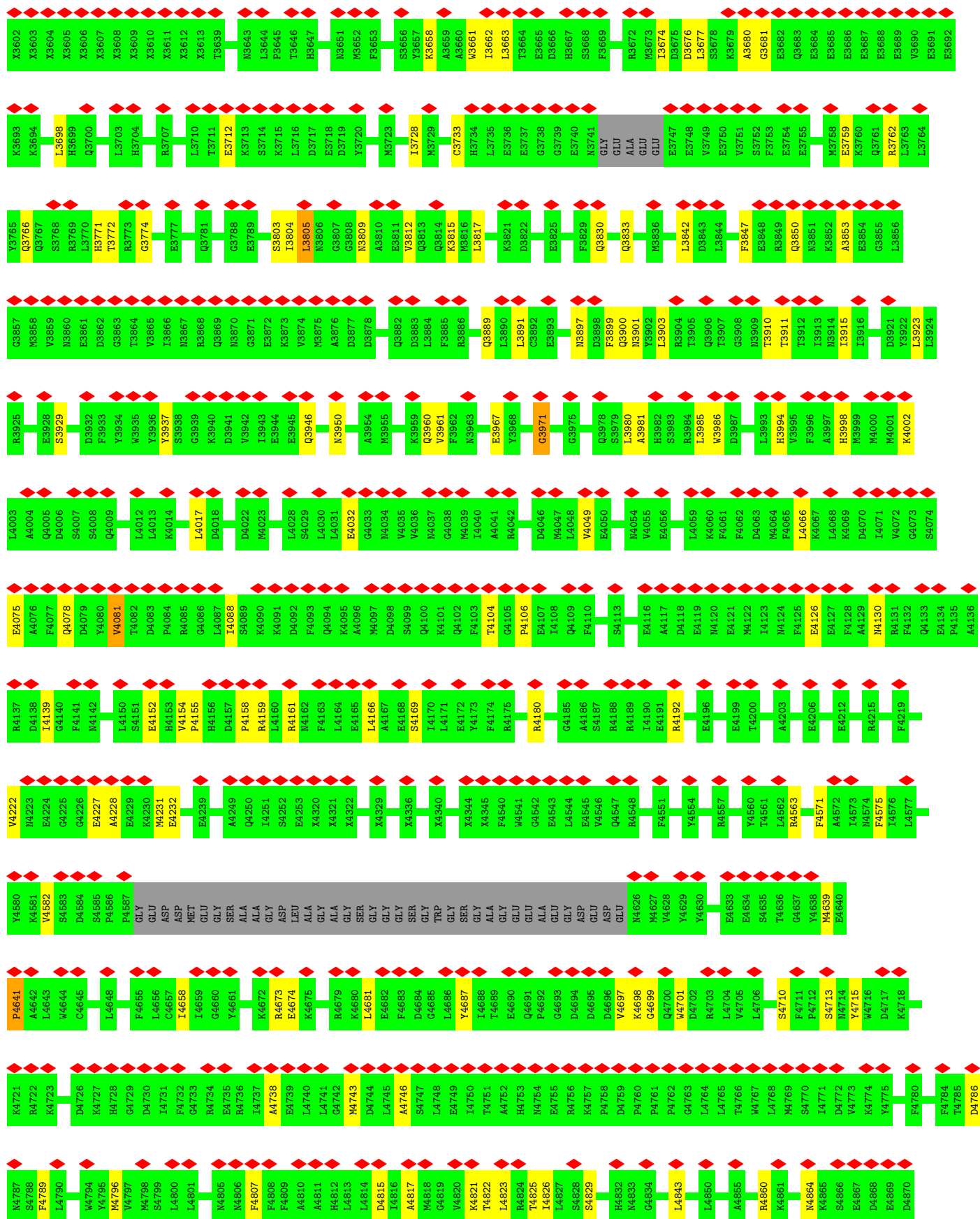
• Molecule 2: Ryanodine receptor 1

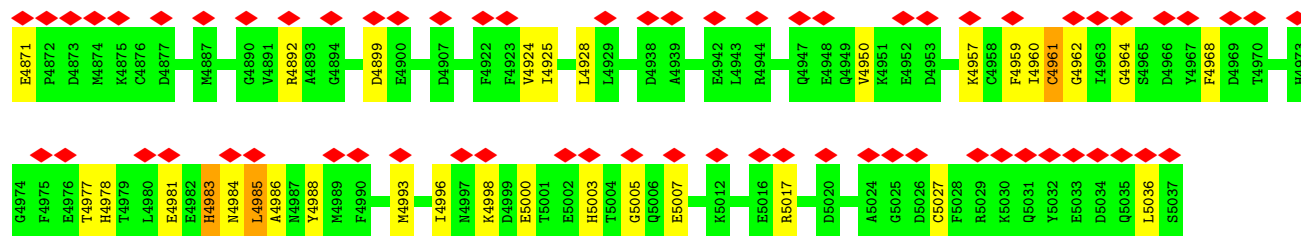


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X1557	X1558	M1573		P1574	L1575	S1576	A1577	L1578	M1579	F1580	L1581	S1582	E1583	R1584	K1585	N1586	P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	Q1598	M1599	L1600	S1604	W1605	R1606	R1607	M1608	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	H1702	L1703	P1704	Q1631	D1632	P1633	L1634	T1635				
X1486	X1487	X1488	X1492		X1493	X1494	X1495	X1496	X1497	X1503	X1504	X1505	X1506	X1507	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1536	X1537	X1541		X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556						
X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1291		X1292	X1293	X1294	X1297		X1430	X1431	X1435		X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1453		X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462		X1468	X1469	X1473		X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1484	X1485			
F1213	F1214	A1215	L1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	I1228		M1229	M1230	Q1231	R1232	P1233	T1234	T1235	T1236	W1237	K1240		P1243		Q1244	F1245	E1246	P1247	P1250		E1251	H1254		L1255	E1256	V1257	A1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266		C1269		L1270	R1271	L1272	A1273	H1274	R1275	L1276	X1277	X1278	X1279	X1280	
V1149	G1150	C1151	M1152	T1153	D1154	L1155	T1156	E1157	N1158	T1159	T1160	I1161	F1162	T1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	T1182	L1183	T1184	G1185	D1186	G1187	F1188	C1192		S1193	L1194	Q1198		V1199	H1201	L1202	N1203	L1204	G1205	Q1206	D1207	V1208	S1209	L1210	L1211	R1212			
W1088	Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	W1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	W1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	V1122	V1123	F1124	N1125	G1126	H1127	R1128	R1131		W1132	H1133	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148		
L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	T1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	L1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	THR	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	R1087			
G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	N991	G992	A997		R998	D999	R1000	V1001	A1002	Q1003	G1004	W1005	S1006	Y1007	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026			
R844	C945	C906	S947	H848	T949	D850	F951	V852	L853	C854	P855	V856	D857	THR	VAL	GLN	S861	V862	L863	P864	P865	H866	L867	R868	R869	L870	R871	H872	L873	K873	L874	A875	S876	N877	L878	H879	E880	L881	W882	A883	L884	P885	L886	K887	L888	Y829	R830	R831	L890	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	R842	S843
L719	H720	L721	H722	L723	G724	H725	V726	L727	R728	P729	V730	L731	S732	P733	Q734	H735	L736	L737	L738	P804	P805	P806	G807	Y808	A809	C747	L748	D749	L750	S751	V752	P753	S754	L755	S756	F757	R758	L759	N760	G761	C762	P763	V767		F768	E769	A770	F771	L772	N773	D774	G775	L776	F777	P778	P779	V780	L781	S782		

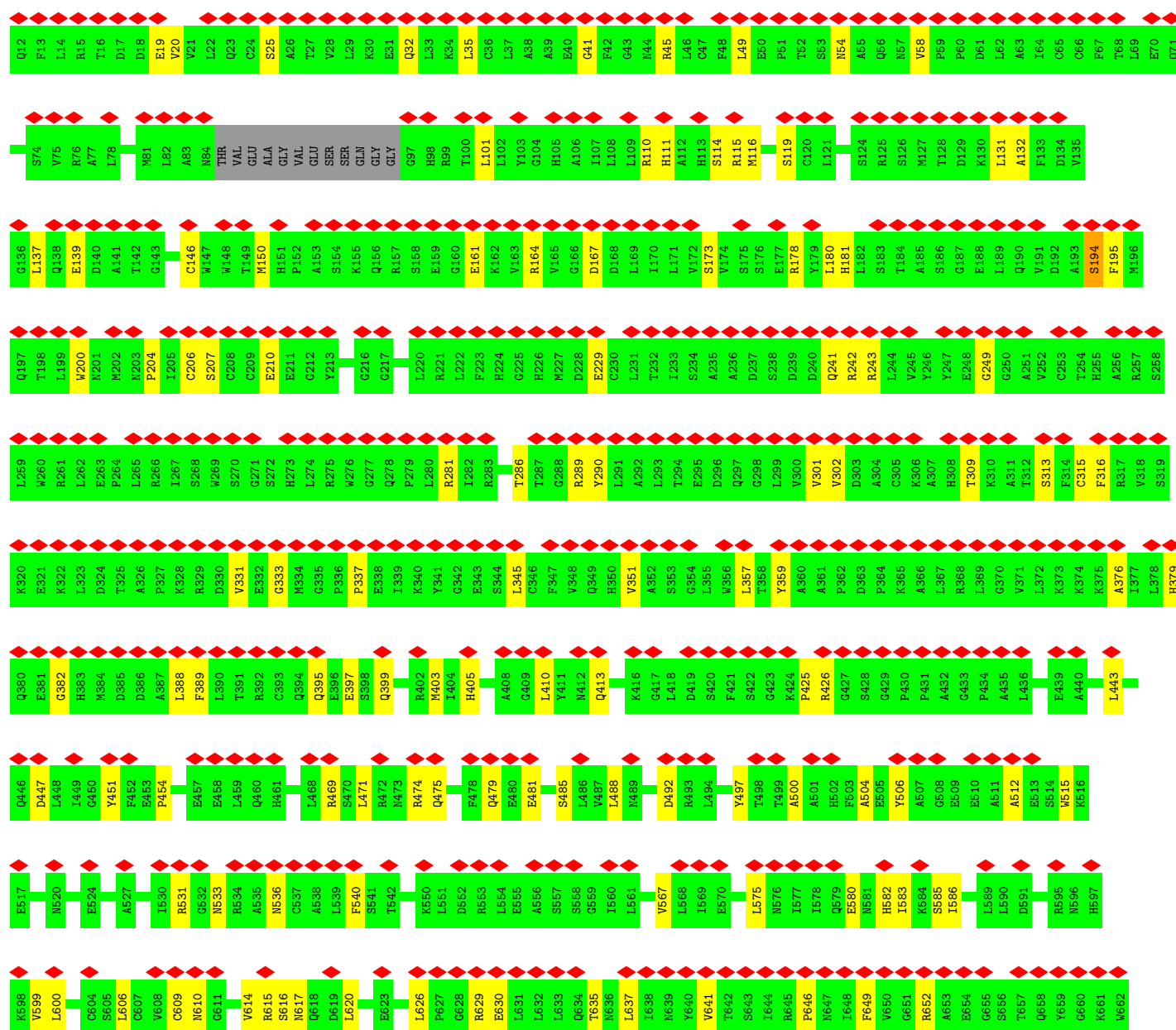
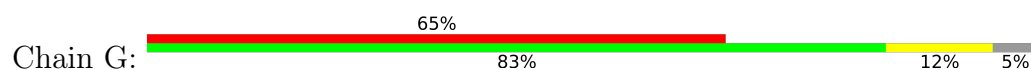








• Molecule 2: Ryanodine receptor 1

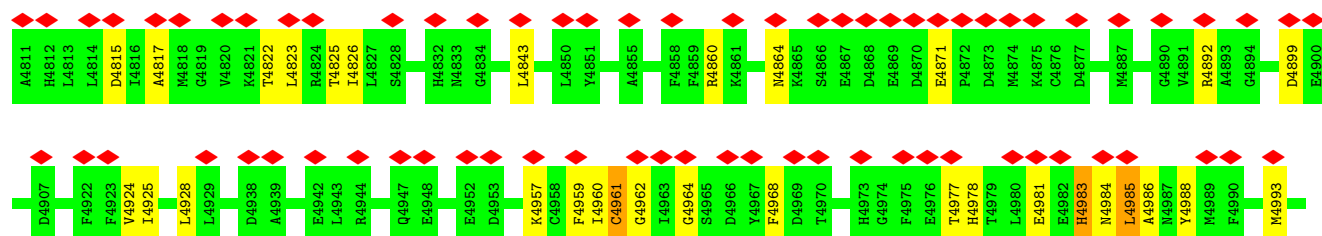


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L1581	S1582	E1583	R1584	K1585	P1587	X1497	X1503	X1291	Q1220	T1156	A1094	R1033	P969	N909	T849	K788	G724	F664
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R1584	K1585	P1587	X1497	X1291	X1430	X1431	X1505	X1297	F1223	T1159	T1096	N1035	L972	H911	F851	R790	V726	M667
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P1587	X1497	X1430	X1431	X1435	X1436	X1437	X1507	X1438	N1229	F1162	E1099	S1038	H974	P914	C854	G794	P729	E670
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X1430	X1431	X1435	X1436	X1437	X1438	X1439	X1511	X1440	Q1231	L1164	V1102	C1040	R976	P916	R856	G795	T731	V672
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X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1513	X1442	P1233	G1166	E1103	A1042	T978	R918	THR	E799	G734	F674
X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1514	X1443	V1234	E1167	A1105	V1043	P979	N919	VAL	E799	G734	F674
X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1515	X1444	T1235	E1168	A1106	R1044	A980	Y920	T861	F800	Q735	L675
X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1516	X1445	W1236	V1169	R1106	R1044	A980	Y920	T861	F800	Q735	L675
X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1519	X1446	W1237	L1169	E1106	T1045	Q981	N921	H736	K801	Q735	L675
X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1519	X1447	K1240	M1170	E1108	L1046	T982	N921	H736	K801	Q735	L675
X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1519	X1448	P1243	S1171	L1109	L1047	T983	Q923	L738	F802	Q735	L675
X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1520	X1449	Q1244	D1172	R1110	G1048	L984	M924	L738	F802	Q735	L675
X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1521	X1450	F1245	S1173	P1111	Y1049	V985	S925	L738	F802	Q735	L675
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X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1523	X1452	P1247	S1175	E1113	Y1051	R987	G926	L738	F802	Q735	L675
X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1524	X1453	E1247	E1114	V1113	I1053	R987	G926	L738	F802	Q735	L675
X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1525	X1454	P1247	E1116	E1114	I1053	R987	G926	L738	F802	Q735	L675
X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1526	X1455	P1247	T1177	L1115	I1053	R987	G926	L738	F802	Q735	L675
X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1527	X1456	P1250	A1178	G1116	E1054	R987	G926	L738	F802	Q735	L675
X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1528	X1457	E1251	F1179	A1117	PRD	G992	G926	L738	F802	Q735	L675
X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1529	X1458	E1251	R1180	E1119	GLN	A997	G926	L738	F802	Q735	L675
X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1530	X1459	H1254	E1181	E1119	GLU	A997	G926	L738	F802	Q735	L675
X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1531	X1460	Y1255	I1182	E1119	GLU	A997	G926	L738	F802	Q735	L675
X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1532	X1461	E1256	I1183	A1121	PRD	R998	G926	L738	F802	Q735	L675
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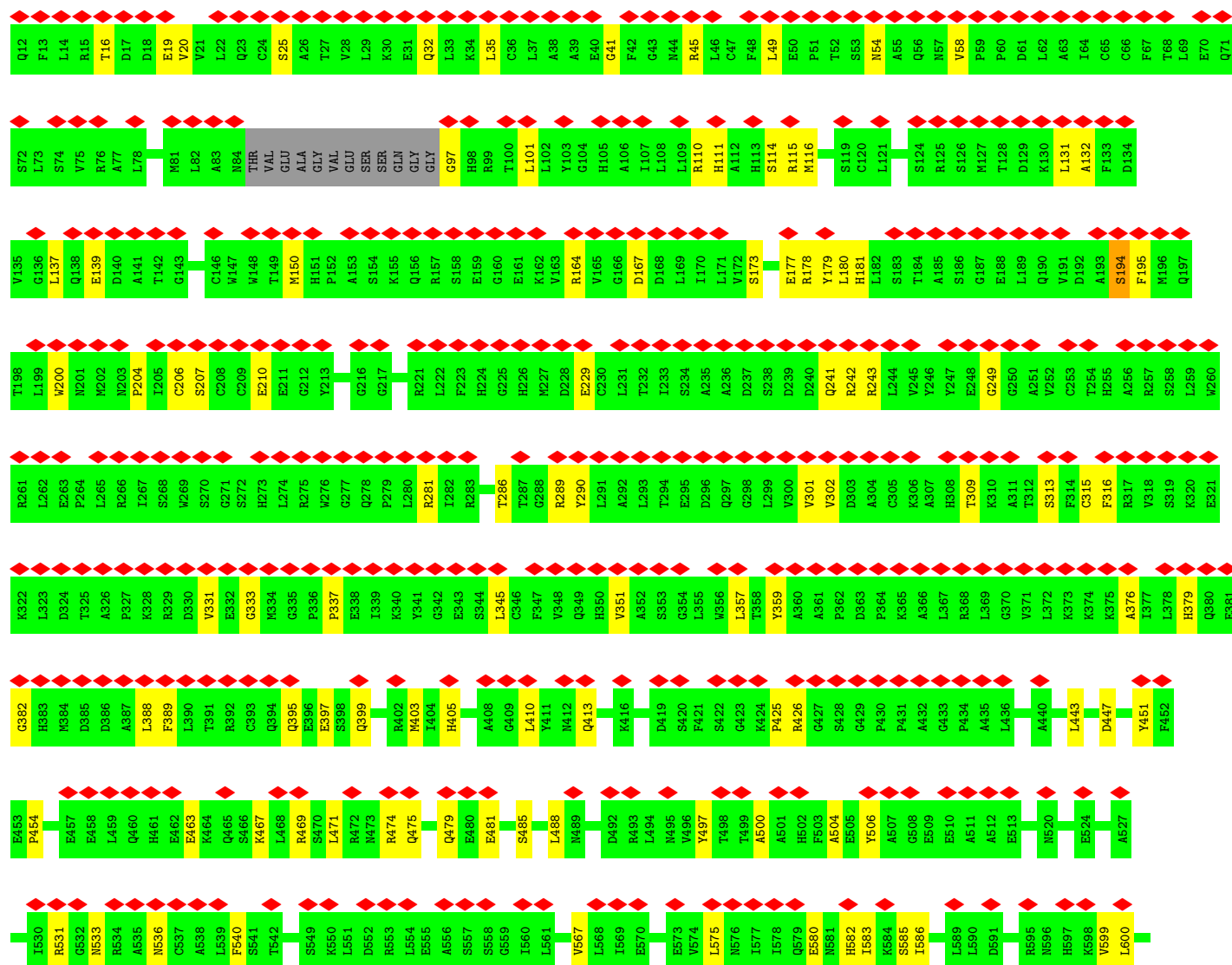
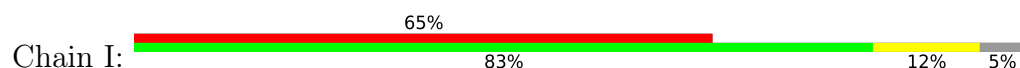


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● Molecule 2: Ryanodine receptor 1



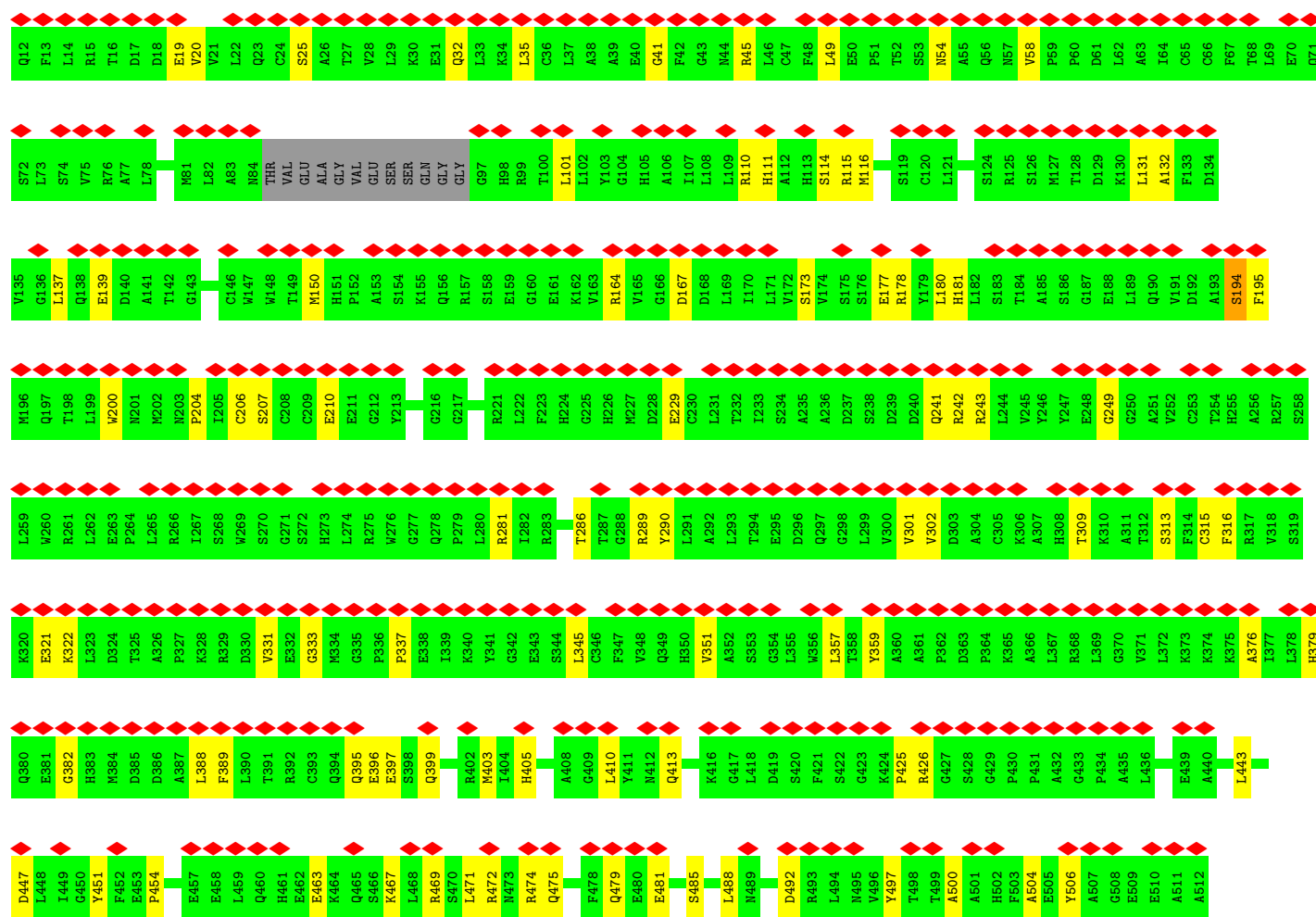
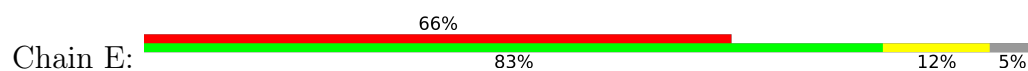
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- Molecule 2: Ryanodine receptor 1

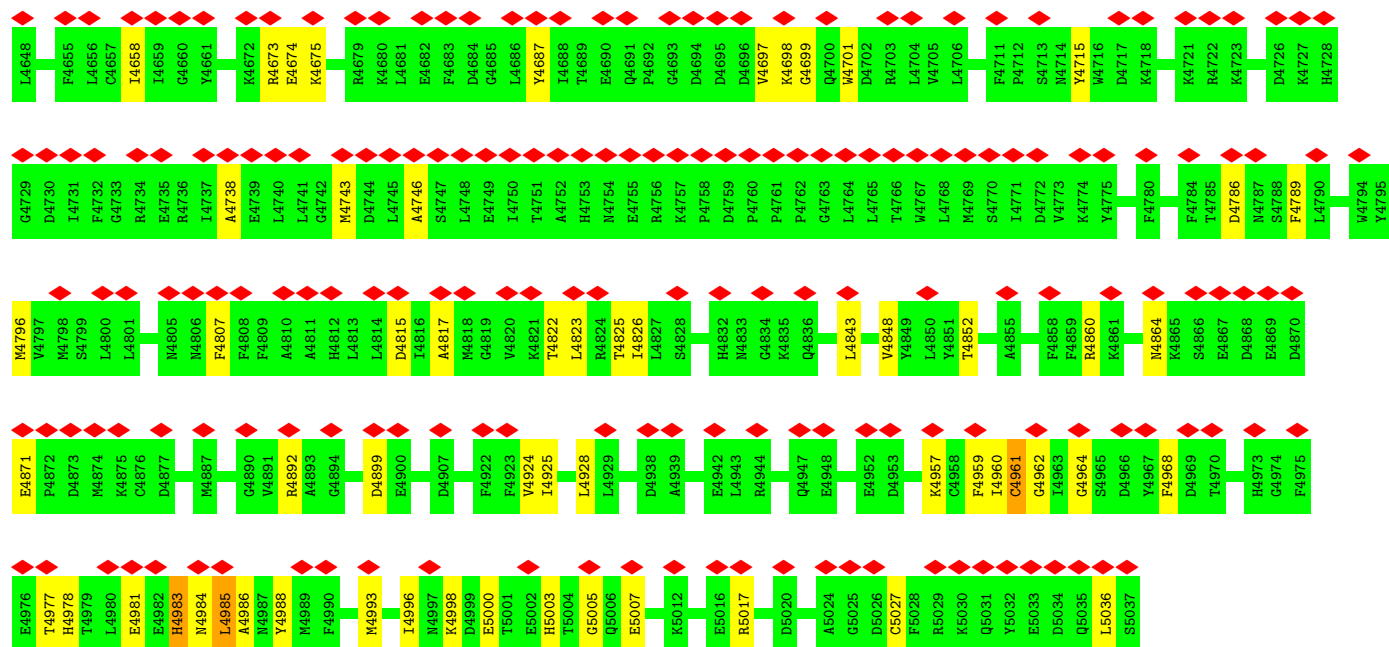


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F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	M1125	G1126	H1127	R1128	R1131	W1132	H1133	G1135	S1136	E1137	P1138	F1139	G1140	R1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	V1149	G1150	C1151	M1152					
I1153	D1154	L1155	T1156	E1157	T1159	I1160	T1161	F1162	T1163	L1164	M1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	C1192	S1193	L1194	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216						
T1031	K1032	R1033	S1034	M1035	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	A1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	M1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	GLN	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	S1085	G1086	R1087	W1088	Y1089	F1090	E1091					
P967	A968	P969	L970	D971	S972	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	Q923	M924	S925	Q926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	Q940	M941	A942	D943	E944	K945	A946	ASP	ILE	PRO	ALA	ARG	ASN	PRO	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966
S847	H848	T849	D850	F851	V852	C854	P853	C854	P855	V856	D857	THR	VAL	GLN	I861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	V882	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906		
G786	V787	K788	V789	F791	R792	L793	G794	G795	R796	E799	F900	K901	F902	L903	P904	P905	P906	G907	Y908	A909	P910	C911	H912	W913	A914	V915	L916	P917	S918	E919	R920	L921	R922	L923	E924	P925	I926	K927	E928	Y929	R930	R931	E932	G933	P934	R935	G936	P937	H938	L939	V940	G941	P942	S943	R944	C945	L946					
W722	T723	G724	H725	V726	A727	R728	P729	V730	T731	S732	P733	Q734	Q735	H736	L737	L738	A739	P740	E741	S745	C746	G747	L748	D749	L750	S751	V752	P753	S754	I755	S756	F757	R758	I759	N760	G761	C762	P763	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	W781	S782	F783	S784	A785					
K661	V662	Y663	F664	E665	V666	M667	V668	D669	E670	V671	P672	P673	F674	L675	T676	A677	Q678	A679	D680	H681	L682	R683	V684	G685	W686	A687	L688	T689	E690	L691	Y692	S693	P694	Y695	G696	G697	G698	G699	E700	S643	I644	R645	P646	N647	I648	E580	N581	F649	V650	G651	R652	A653	E654	G655	Q656	T657	Y659	W659	G660			
E513	E517	N520	E524	A527	I530	R531	N533	R534	A535	N536	C537	A538	F540	S541	T542	K550	L551	D552	R553	L554	E555	A556	S557	S558	G559	I560	L561	V567	L568	I569	E570	L575	N576	I577	I578	Q579	E580	N581	H582	I583	K584	S585	I586	L589	L590	D591	R595															



X3324	X3264	X3194	X3058	X2998	R2918	Q2858	S2798	R2738	X2648	X2587	G2434
X3325	X3265	X3195	X3059	X2999	D2919	P2859	E2799	P2739	X2649	X2588	R2435
X3326	X3266	X3196	X3060	X2999	R2920	P2860	K2800	P2740	X2650	X2589	C2436
X3327	X3267	X3197	X3061	X3001	R2921	D2861	D2801	E2741	X2651	X2590	A2437
X3328	X3268	X3198	X3062	X3002	R2922	L2862	E2802	T2742	X2652	X2591	P2438
X3329	X3269	X3199	X3063	X3003	A2923	S2863	E2803	L2743	X2653	X2592	E2439
X3330	X3270	X3200	X3064	X3004	Q2924	Q2864	L2804	N2744	X2654	X2593	N2440
X3331	X3271	X3201	X3065	X3005	E2925	V2865	R2805	V2745	X2655	X2594	H2441
X3332	X3272	X3202	X3136	X3006	R2926	T2866	R2806	L2746	X2656	X2595	L2442
X3333	X3273	X3203	X3137	X3007	L2927	L2867	W2807	L2747	X2657	X2596	
X3334	X3274	X3204	X3138	X3008	R2928	S2868	P2808	P2748	X2658	X2597	A2445
X3335	X3275	X3205	X3139	X3009	F2929	R2869	L2809	E2749	X2659	X2598	G2446
X3336	X3276	X3206	X3140	X3010	L2930	E2870	K2810	K2750	X2660	X2599	R2447
X3337	X3277	X3207	X3141	X3011	Q2931	L2871	E2811	L2751	X2661	X2600	E2448
X3338	X3278	X3208	X3142	X3012	M2932	Q2872	S2812	D2752	X2662	X2601	
X3339	X3279	X3209	X3143	X3013	N2933	A2873	L2813	S2753	X2663	X2602	
X3340	X3280	X3210	X3144	X3014	Q2934	M2874	K2814	F2754	X2664	X2603	A2450
X3341	X3281	X3211	X3145	X3015	V2935	A2875	A2815	L2755	X2665	X2604	L2451
X3342	X3282	X3212	X3146	X3016	A2936	E2876	M2816	N2756	X2666	X2605	R2454
X3343	X3283	X3213	X3147	X3017	V2937	Q2877	L2817	K2757	X2667	X2606	A2455
X3344	X3284	X3214	X3148	X3018	T2938	L2878	A2818	P2758	X2668	X2607	L2456
X3345	X3285	X3215	X3149	X3019	R2939	A2879	E2819	A2759	X2669	X2608	L2457
X3346	X3286	X3216	X3150	X3020	R2940	E2880	E2820	R2760	X2670	X2609	S2458
X3347	X3287	X3217	X3151	X3021	X2943	M2881	W2821	V2761	X2671	X2610	S2459
X3348	X3288	X3218	X3152	X3022	X2944	W2882	T2822	T2762	X2672	X2611	L2460
X3349	X3289	X3219	X3153	X3023	X2945	H2883	T2823	H2763	X2673	X2612	V2461
X3350	X3290	X3220	X3154	X3024	X2946	M2884	E2824	E2674	X2674	X2613	P2462
X3351	X3291	X3221	X3155	X3025	X2947	T2885	K2825	K2765	X2675	X2614	L2463
X3352	X3292	X3222	X3156	X3026	X2948	W2886	A2826	W2766	X2676	X2615	D2464
X3353	X3293	X3223	X3157	X3027	X2949	Q2887	R2827	A2767	X2677	X2616	D2465
X3354	X3294	X3224	X3158	X3028	X2950	R2888	E2828	F2768	X2678	X2617	L2466
X3355	X3295	X3225	X3159	X3029	X2951	K2889	G2829	D2769	X2679	X2618	V2467
X3356	X3296	X3226	X3160	X3030	X2952	K2890	E2830	K2770	X2680	X2619	G2468
X3357	X3297	X3227	X3161	X3031	X2953	K2891	GLU	L2771	X2681	X2620	L2469
X3358	X3298	X3228	X3162	X3032	X2954	Q2892	GLU	Q2772	X2682	X2621	S2471
X3359	X3299	X3229	X3163	X3033	X2955	E2893	ARG	N2773	X2683	X2622	L2472
X3360	X3300	X3230	X3170	X3034	X2956	L2894	THR	N2774	X2684	X2623	P2473
X3361	X3301	X3231	X3171	X3035	X2957	E2895	GLU	N2775	X2685	X2624	L2474
X3362	X3302	X3232	X3172	X3036	X2958	A2896	LYS	W2775	X2686	X2625	Q2475
X3363	X3303	X3233	X3173	X3037	X2959	K2897	LYS	S2776	X2687	X2626	L2476
X3364	X3304	X3234	X3174	X3038	X2960	G2898	THR	V2777	X2688	X2627	P2477
X3365	X3305	X3235	X3175	X3039	X2961	G2899	ARG	E2778	X2689	X2628	T2478
X3366	X3306	X3236	X3176	X3040	X2962	G2900	LYS	E2779	X2690	X2629	L2479
X3367	X3307	X3241	X3177	X3041	X2963	G2901	ILE	N2780	X2691	X2630	K2487
X3368	X3308	X3242	X3178	X3042	X2964	T2901	GLN	V2781	X2692	X2631	X2488
X3369	X3309	X3243	X3179	X3043	X2965	H2902	THR	D2782	X2693	X2632	X2489
X3370	X3310	X3244	X3180	X3044	X2966	P2903	ALA	E2783	X2694	X2633	X2490
X3371	X3311	X3245	X3181	X3045	X2967	L2904	THR	E2784	X2695	X2634	
X3372	X3312	X3246	X3182	X3046	X2968	L2905	TYR	L2785	X2696	X2635	X2493
X3373	X3313	X3247	X3183	X3047	X2969	V2906	ASP	T2786	X2697	X2636	X2494
X3374	X3314	X3248	X3184	X3048	X2969	P2907	PRO	K2786	X2698	X2637	X2495
X3375	X3315	X3249	X3185	X3049	X2970	V2908	ARG	T2787	X2699	X2638	X2496
X3376	X3316	X3250	X3186	X3050	X2971	D2909	GLU	H2788	X2700	X2639	X2497
X3377	X3317	X3251	X3187	X3051	X2972	T2910	GLY	P2789	X2701	X2640	X2498
X3378	X3318	X3252	X3188	X3052	X2973	L2911	V2855	M2790	X2702	X2643	X2499
X3379	X3319	X3253	X3189	X3053	X2974	T2912	N2856	L2791	X2703	X2644	X2500
X3380	X3320	X3254	X3190	X3054	X2975	A2913	P2857	R2792	X2704	X2645	X2501
X3381	X3321	X3255	X3191	X3055	X2976	E2914		P2793	N2734	X2646	X2502
X3382	X3322	X3256	X3192	X3056	X2977	E2915		K2795	F2735	X2647	
X3383	X3323	X3257	X3193	X3057	X2978	K2916		P2797	D2736		
					X2997	A2917			P2737		





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	0.060	Depositor
Minimum map value	-0.032	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, CFF, ATP, CA

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	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.21	0/25428	0.52	2/34534 (0.0%)
2	E	0.21	0/25428	0.53	2/34534 (0.0%)
2	G	0.21	0/25428	0.53	4/34534 (0.0%)
2	I	0.21	0/25428	0.53	4/34534 (0.0%)
All	All	0.21	0/105048	0.52	12/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4639	MET	CA-C-N	5.24	134.57	121.80
2	B	4639	MET	C-N-CA	5.24	134.57	121.80
2	I	4639	MET	CA-C-N	5.24	134.57	121.80
2	I	4639	MET	C-N-CA	5.24	134.57	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4639	MET	CA-C-N	5.23	134.57	121.80

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	194	SER	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	14	0
1	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	16	0
2	B	29499	0	24748	320	0
2	E	29499	0	24748	308	0
2	G	29499	0	24748	310	0
2	I	29499	0	24748	314	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102376	1276	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 6.

The worst 5 of 1276 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:4231:MET:HE1	2:I:4960:ILE:HA	1.43	1.01
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.43	1.00
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.43	1.00
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.43	0.99
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	43	77
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	43	77
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	43	77
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	44	77

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU

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%)	2479 (99%)	14 (1%)	78	80
2	E	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	G	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
2	I	2493/3022 (82%)	2479 (99%)	14 (1%)	78	80
All	All	10324/12444 (83%)	10268 (100%)	56 (0%)	78	81

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	131	LEU
2	E	4983	HIS
2	I	3663	LEU
2	E	4961	CYS

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Mol	Chain	Res	Type
2	E	3663	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	413	GLN
2	I	3900	GLN
2	E	4109	GLN
2	I	765	GLN
2	I	1775	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	CFF	I	5102	-	15,15,15	1.93	7 (46%)	23,23,23	2.72	10 (43%)
3	ATP	B	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.77	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.77	10 (20%)
4	CFF	B	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.73	10 (43%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.77	10 (20%)
4	CFF	G	5102	-	15,15,15	1.94	7 (46%)	23,23,23	2.73	10 (43%)
4	CFF	E	5102	-	15,15,15	1.93	8 (53%)	23,23,23	2.72	9 (39%)
3	ATP	G	5101	-	32,33,33	1.35	5 (15%)	48,52,52	1.76	10 (20%)

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
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	4/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	4/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	4/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	4/22/38/38	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.54	1.47	1.39
3	B	5101	ATP	C5-C4	4.53	1.47	1.39
3	E	5101	ATP	C5-C4	4.53	1.47	1.39
3	G	5101	ATP	C5-C4	4.51	1.47	1.39
4	G	5102	CFF	C6-N1	-3.96	1.32	1.40

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C14-N7-C8	-7.66	111.94	126.28
4	B	5102	CFF	C14-N7-C8	-7.65	111.96	126.28
4	G	5102	CFF	C14-N7-C8	-7.64	111.98	126.28
4	I	5102	CFF	C14-N7-C8	-7.64	111.99	126.28
3	I	5101	ATP	C5-C4-N3	-5.82	118.71	126.72

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

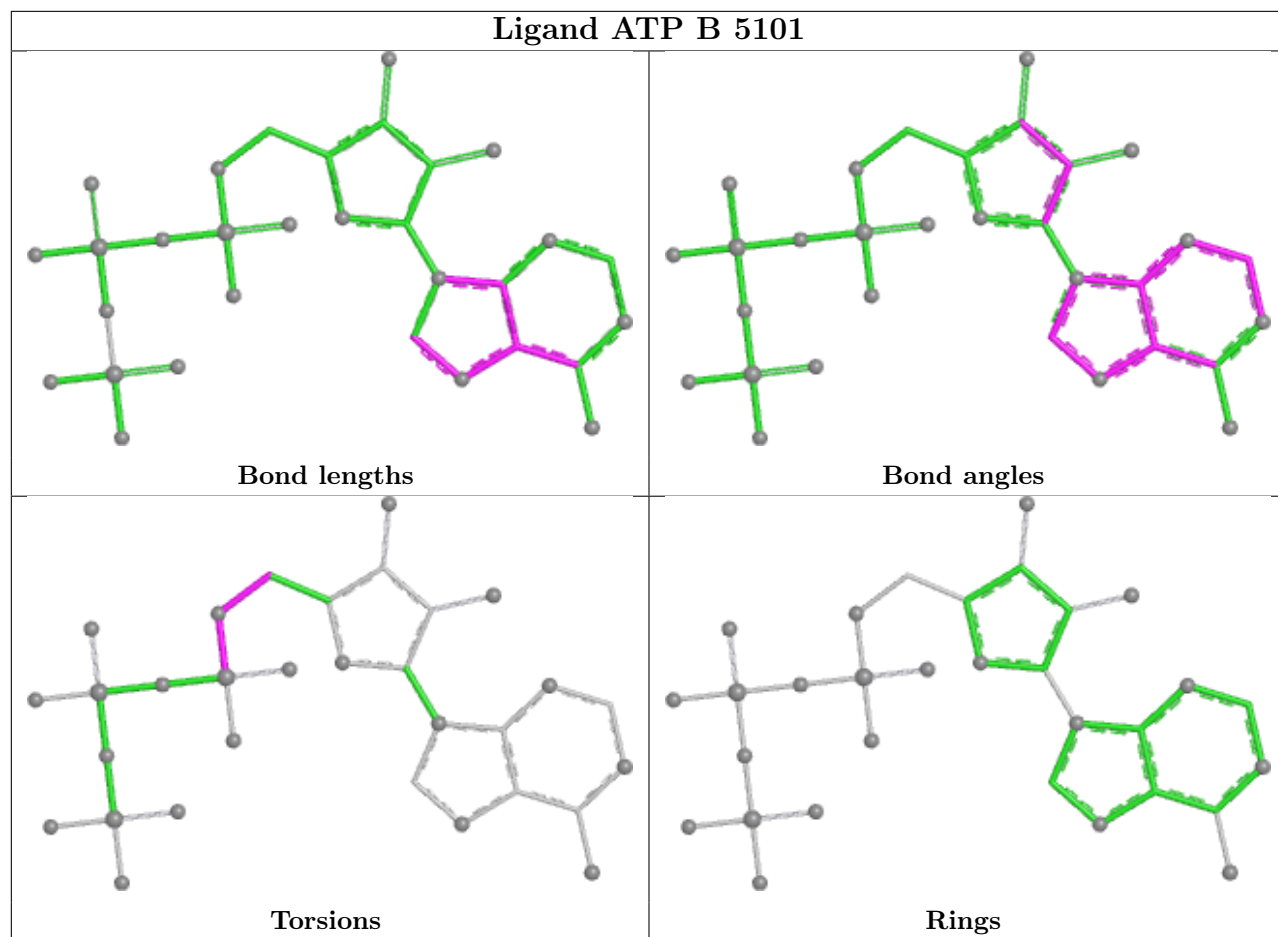
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C4'-C5'-O5'-PA

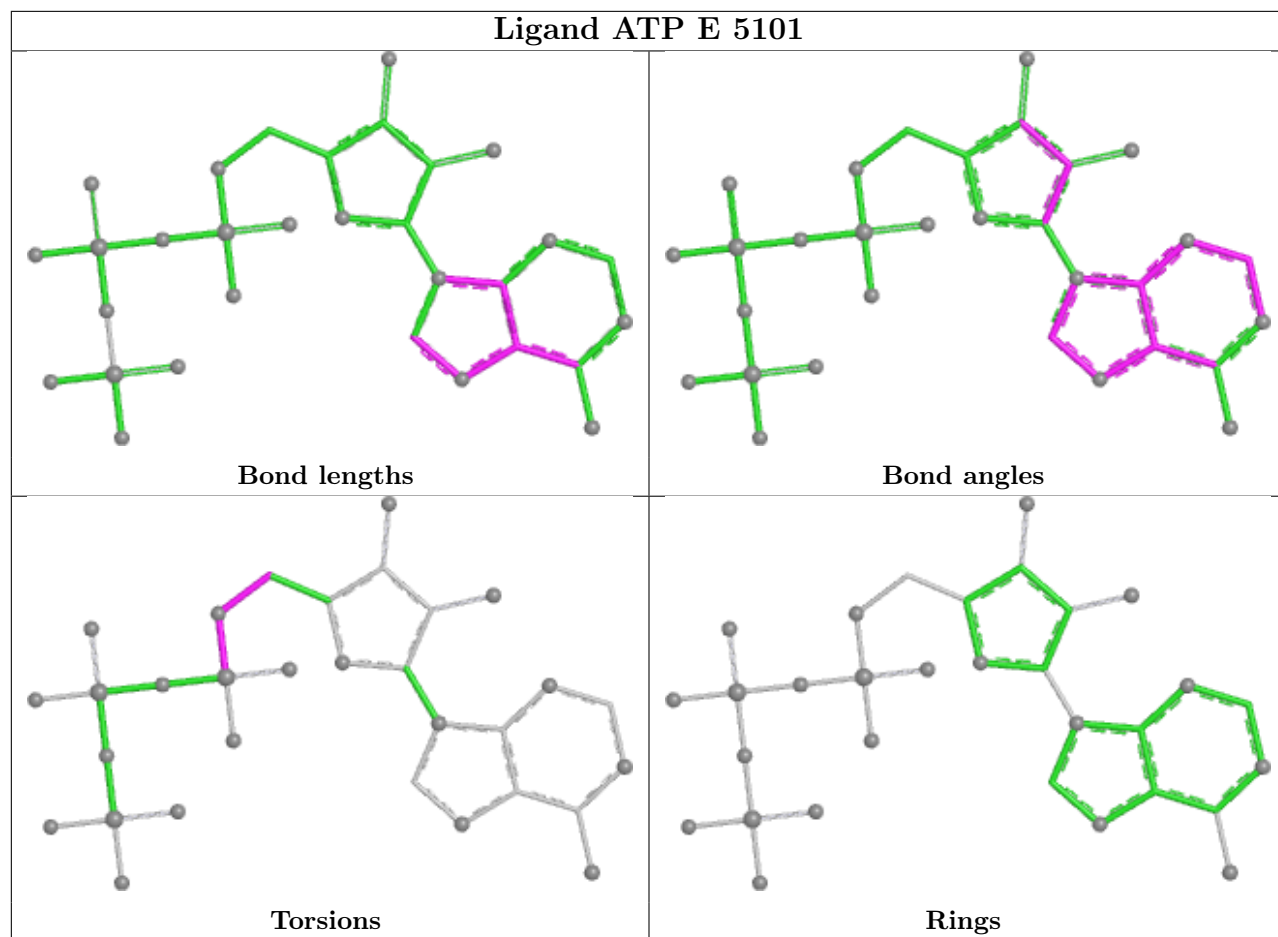
There are no ring outliers.

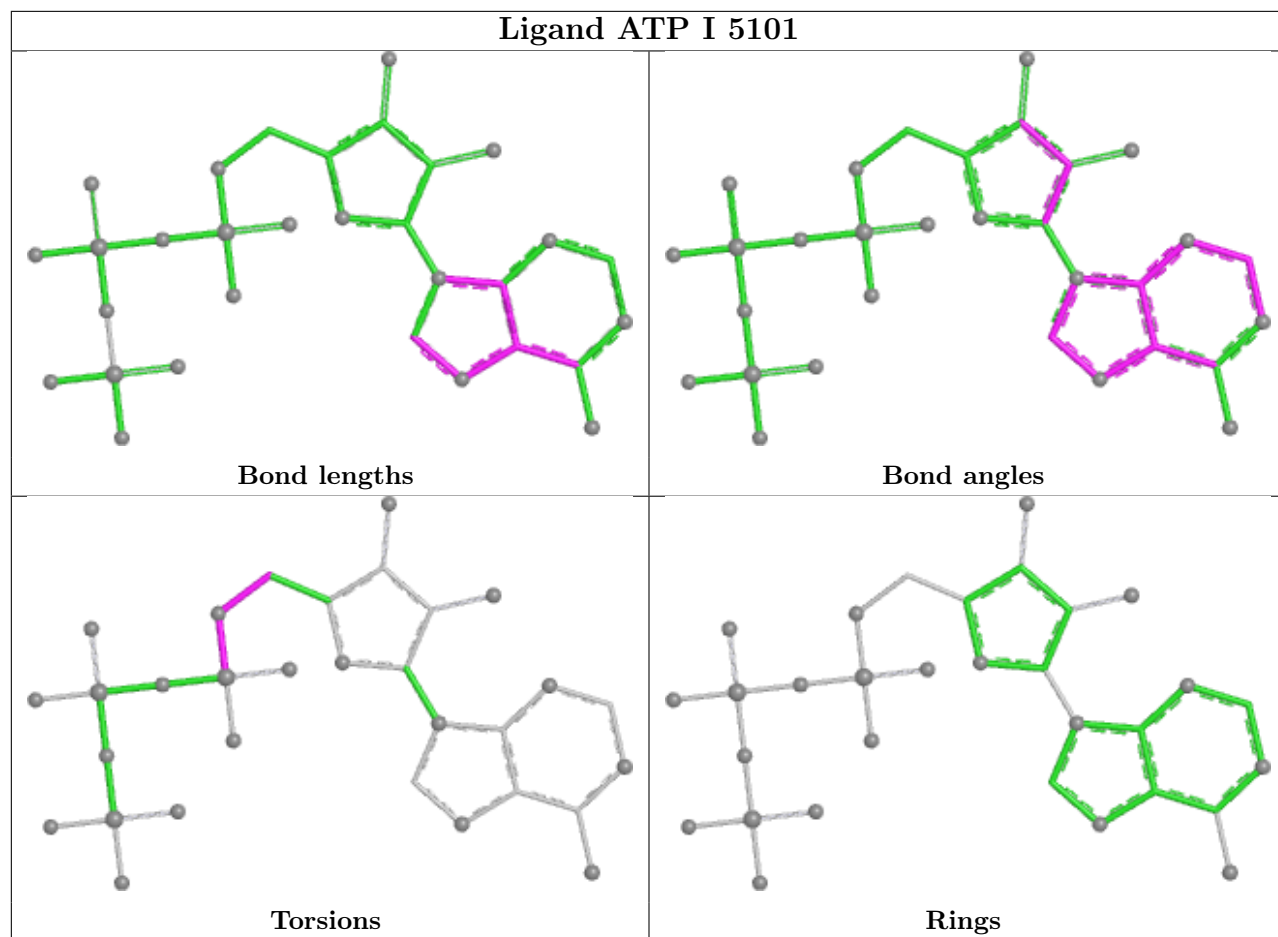
4 monomers are involved in 4 short contacts:

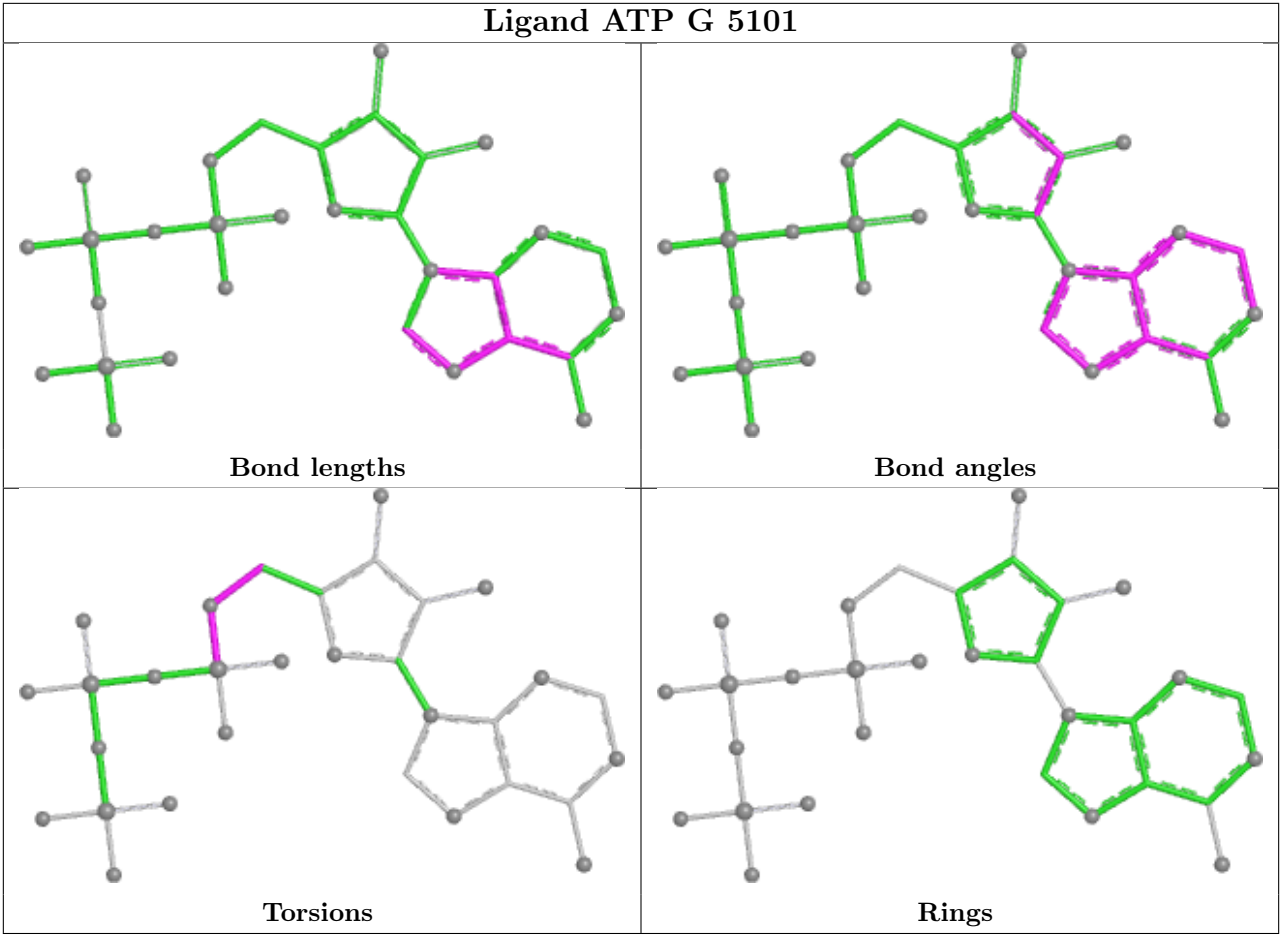
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	I	5101	ATP	1	0
3	G	5101	ATP	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	I	14
2	E	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	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62

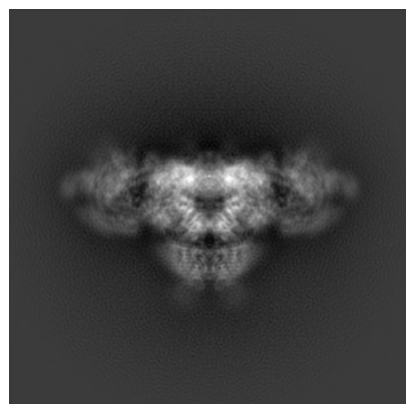
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8376. These allow visual inspection of the internal detail of the map and identification of artifacts.

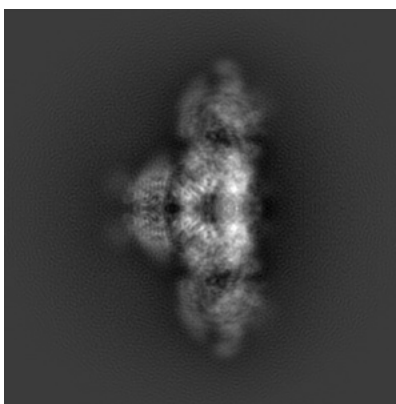
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

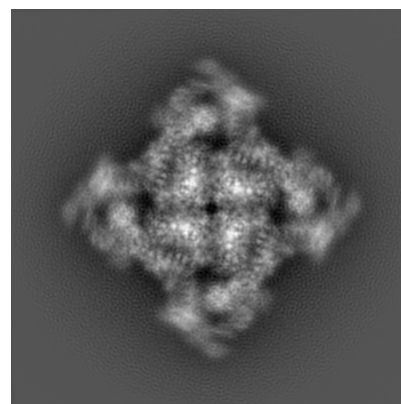
6.1.1 Primary map



X

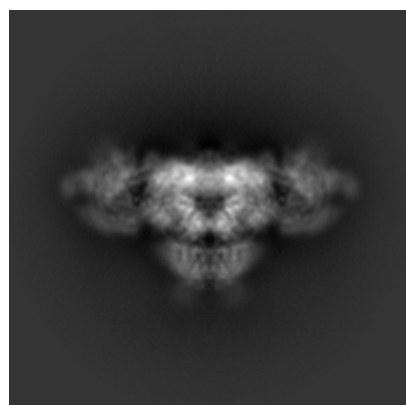


Y

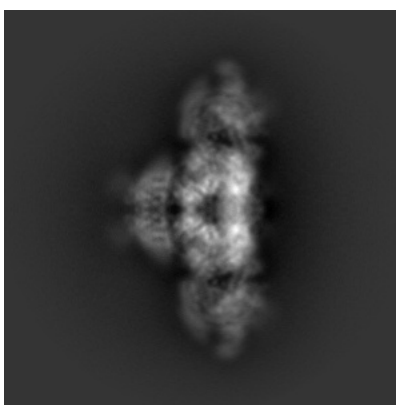


Z

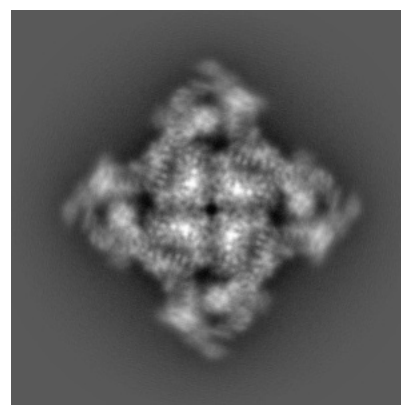
6.1.2 Raw map



X



Y

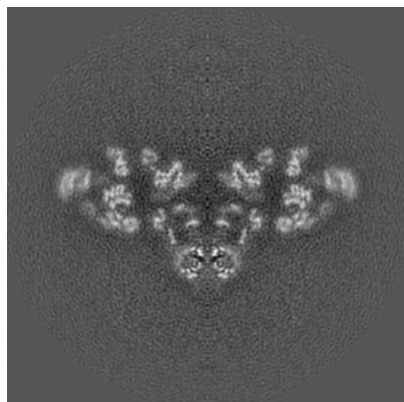


Z

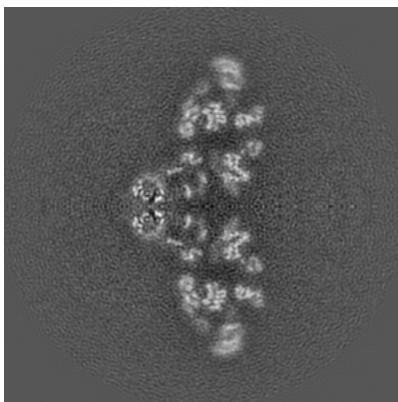
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

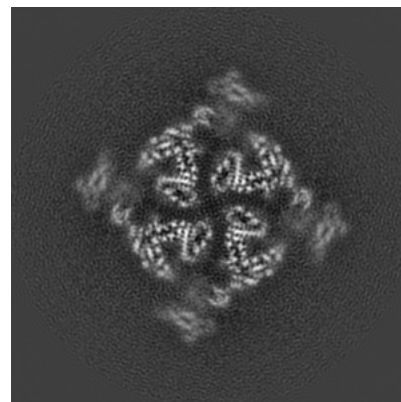
6.2.1 Primary map



X Index: 200

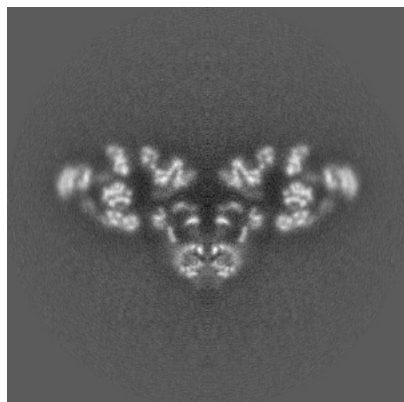


Y Index: 200

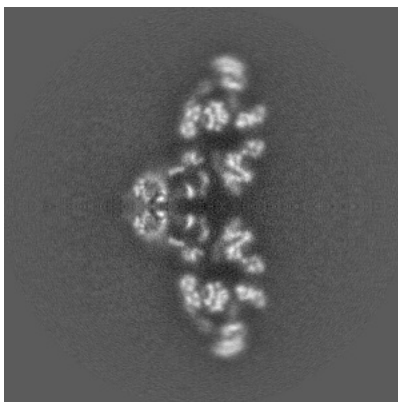


Z Index: 200

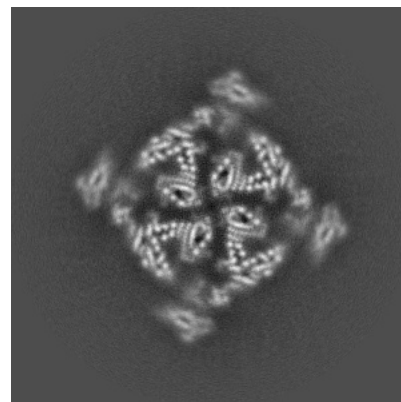
6.2.2 Raw map



X Index: 200



Y Index: 200

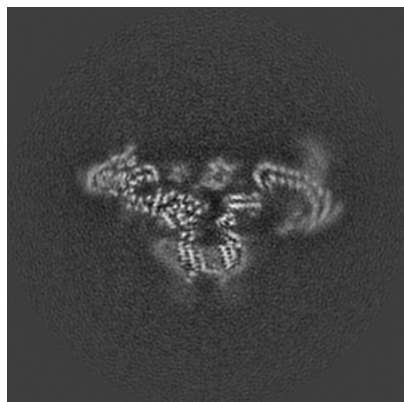


Z Index: 200

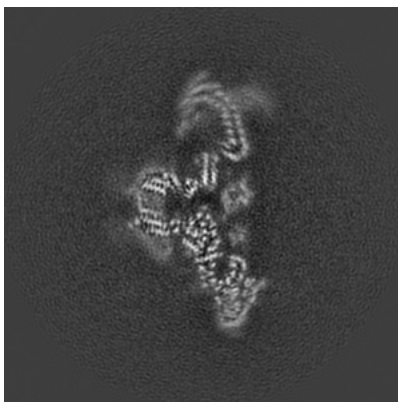
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

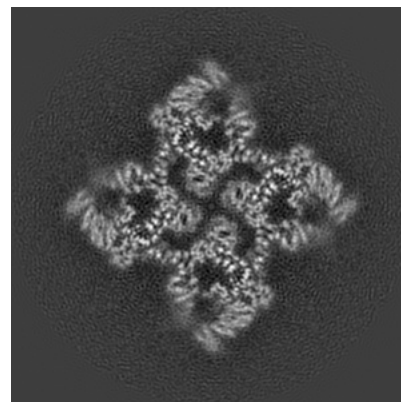
6.3.1 Primary map



X Index: 225

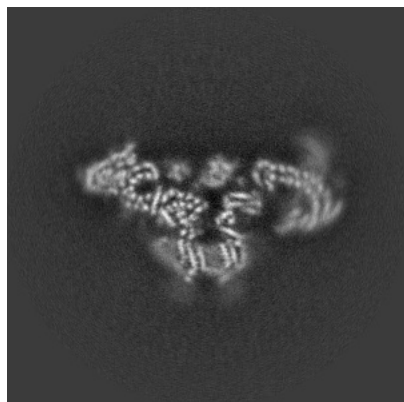


Y Index: 175

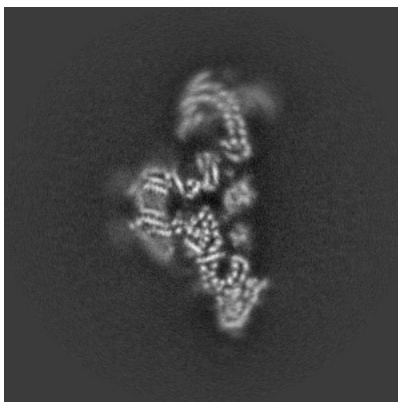


Z Index: 232

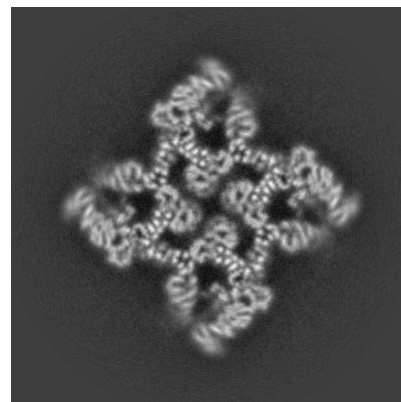
6.3.2 Raw map



X Index: 224



Y Index: 176

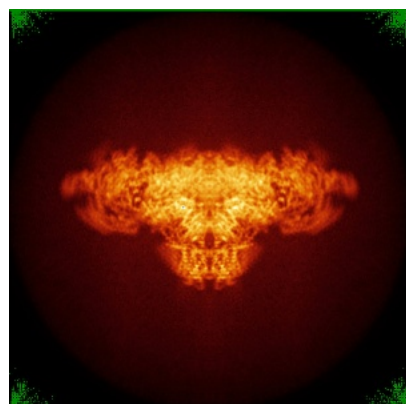


Z Index: 232

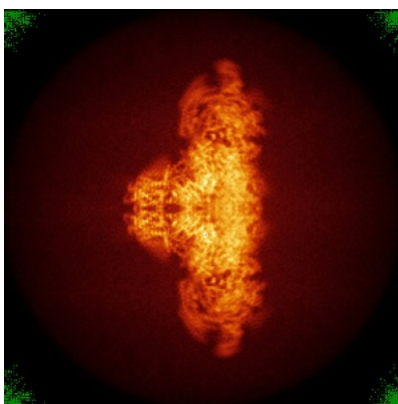
The images above show the largest variance slices of the map in three orthogonal directions.

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

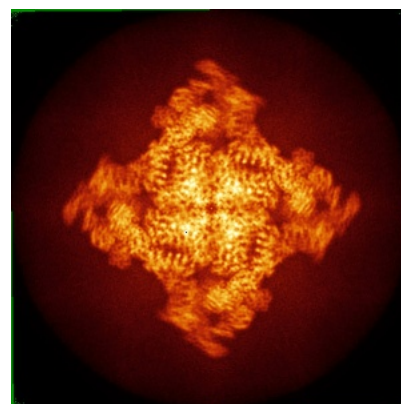
6.4.1 Primary map



X

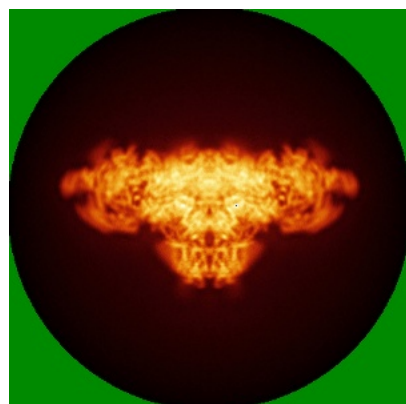


Y

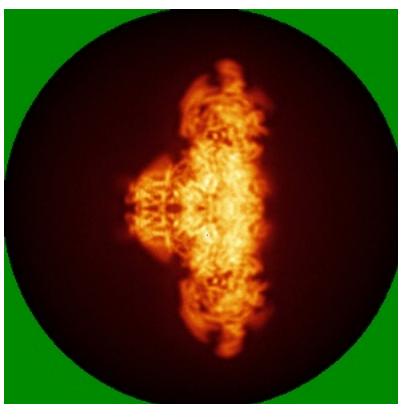


Z

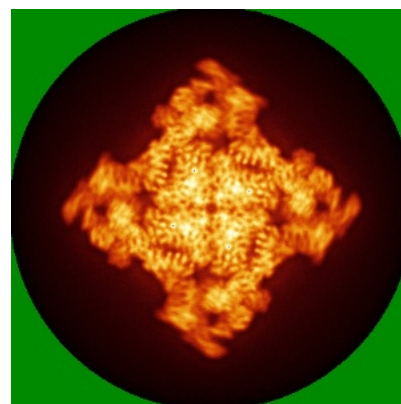
6.4.2 Raw map



X



Y

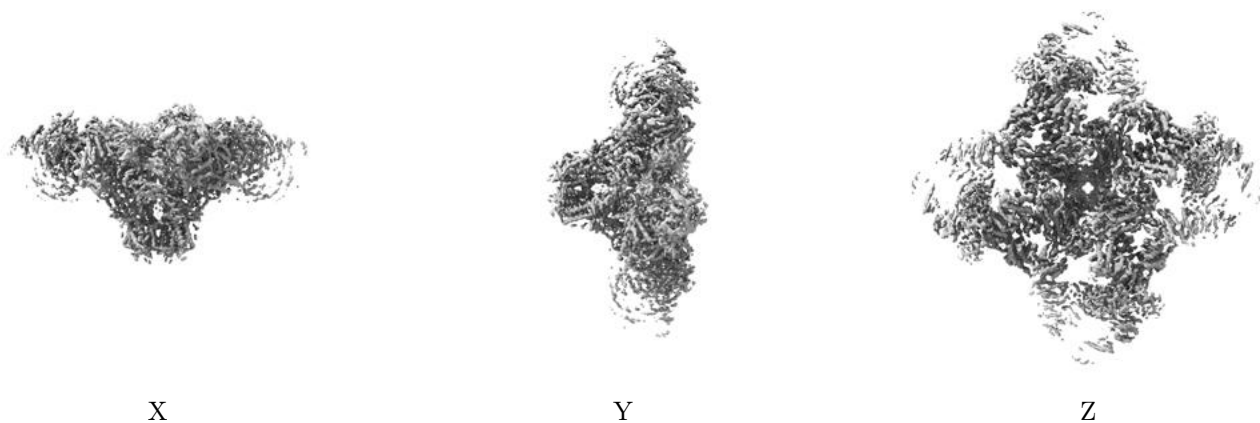


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

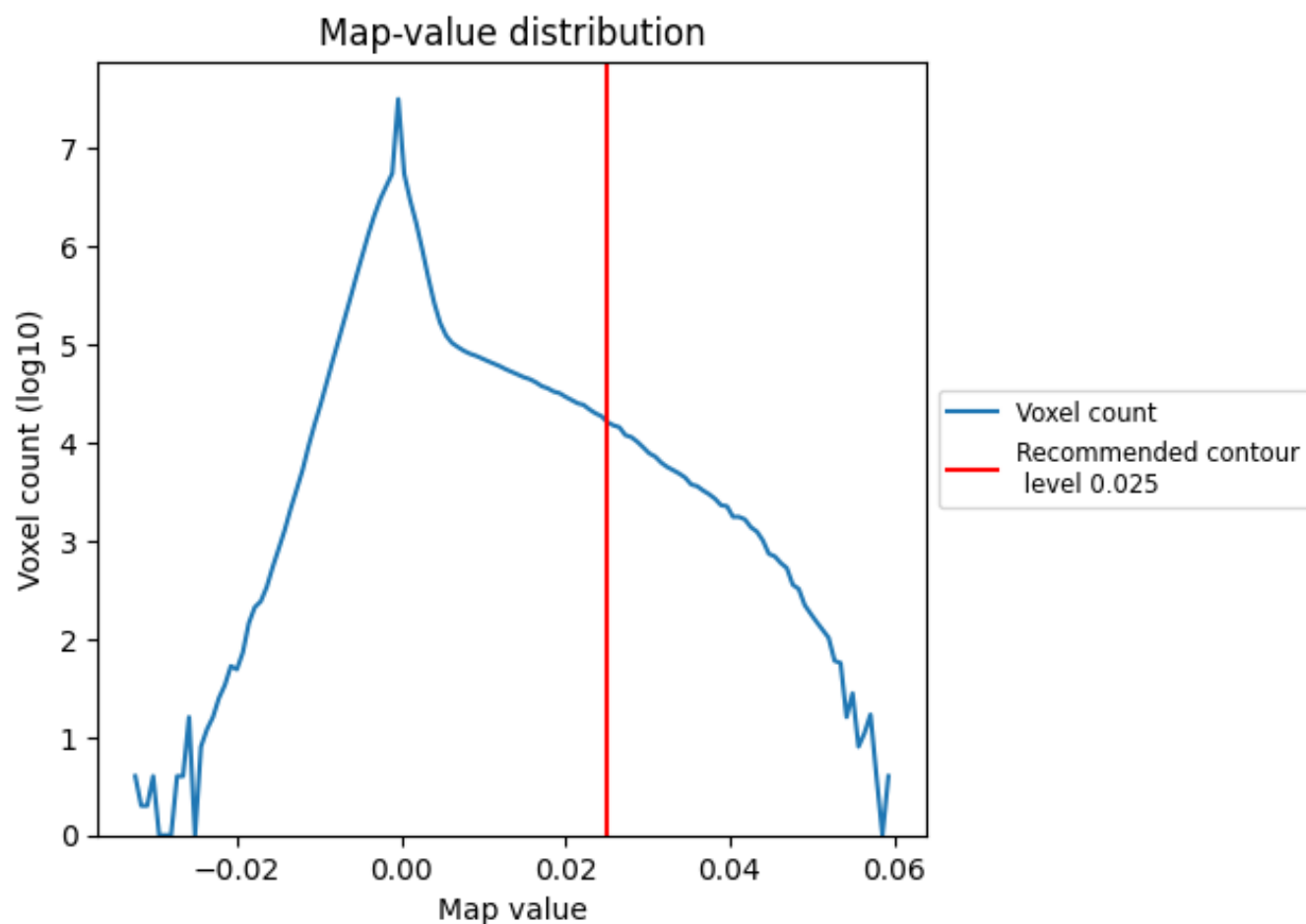
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

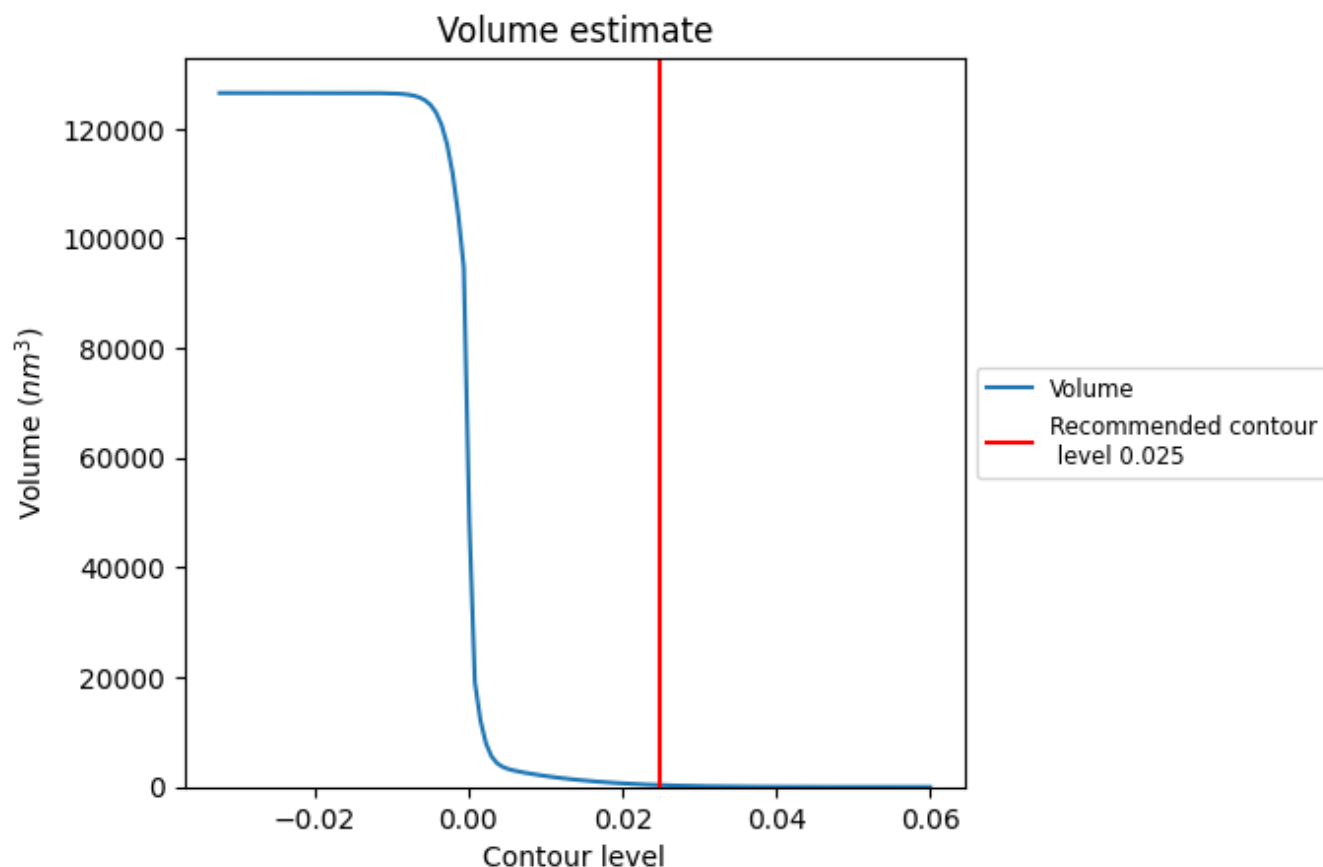
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

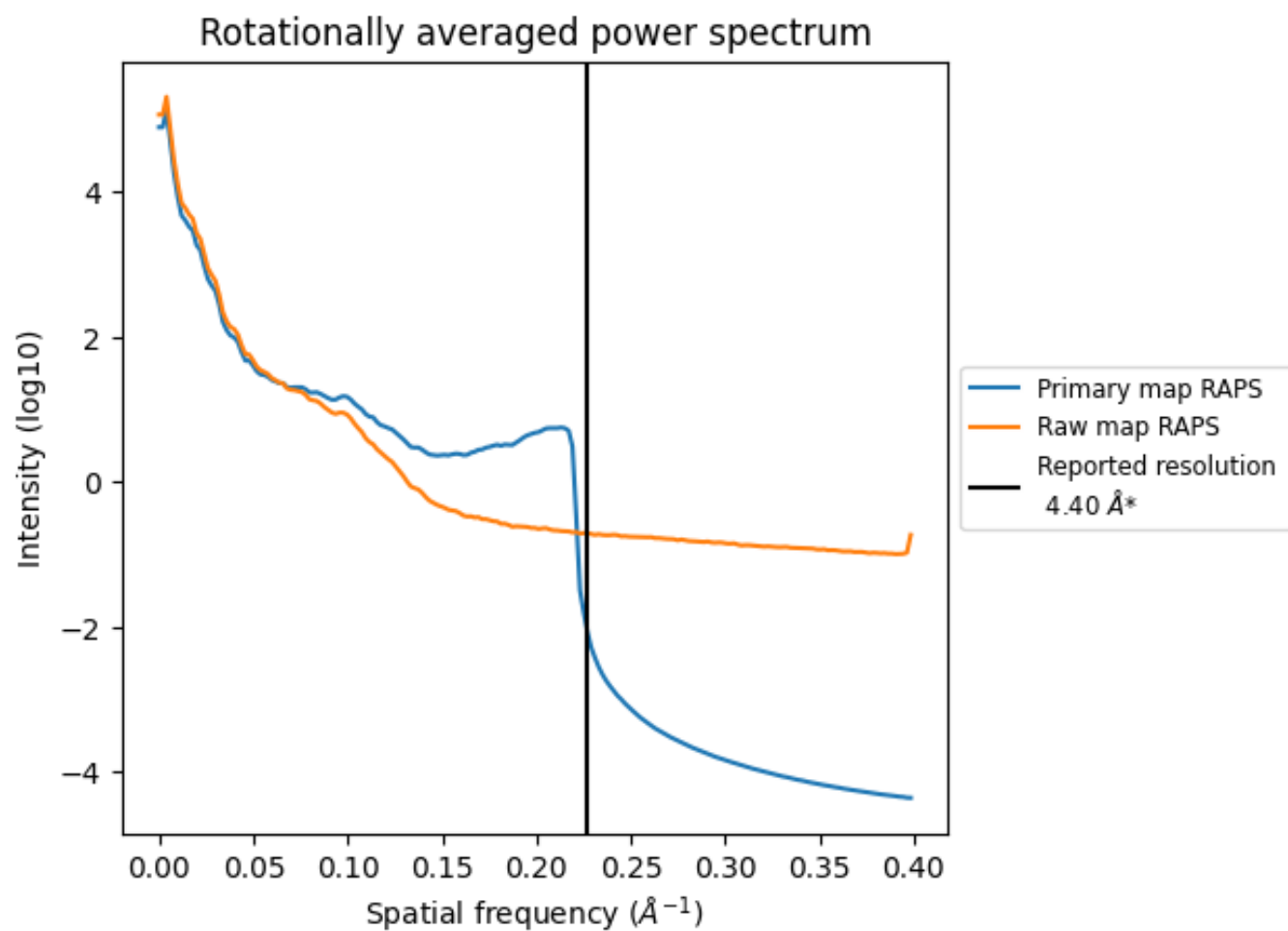
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm^3 ; this corresponds to an approximate mass of 299 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 ⓘ

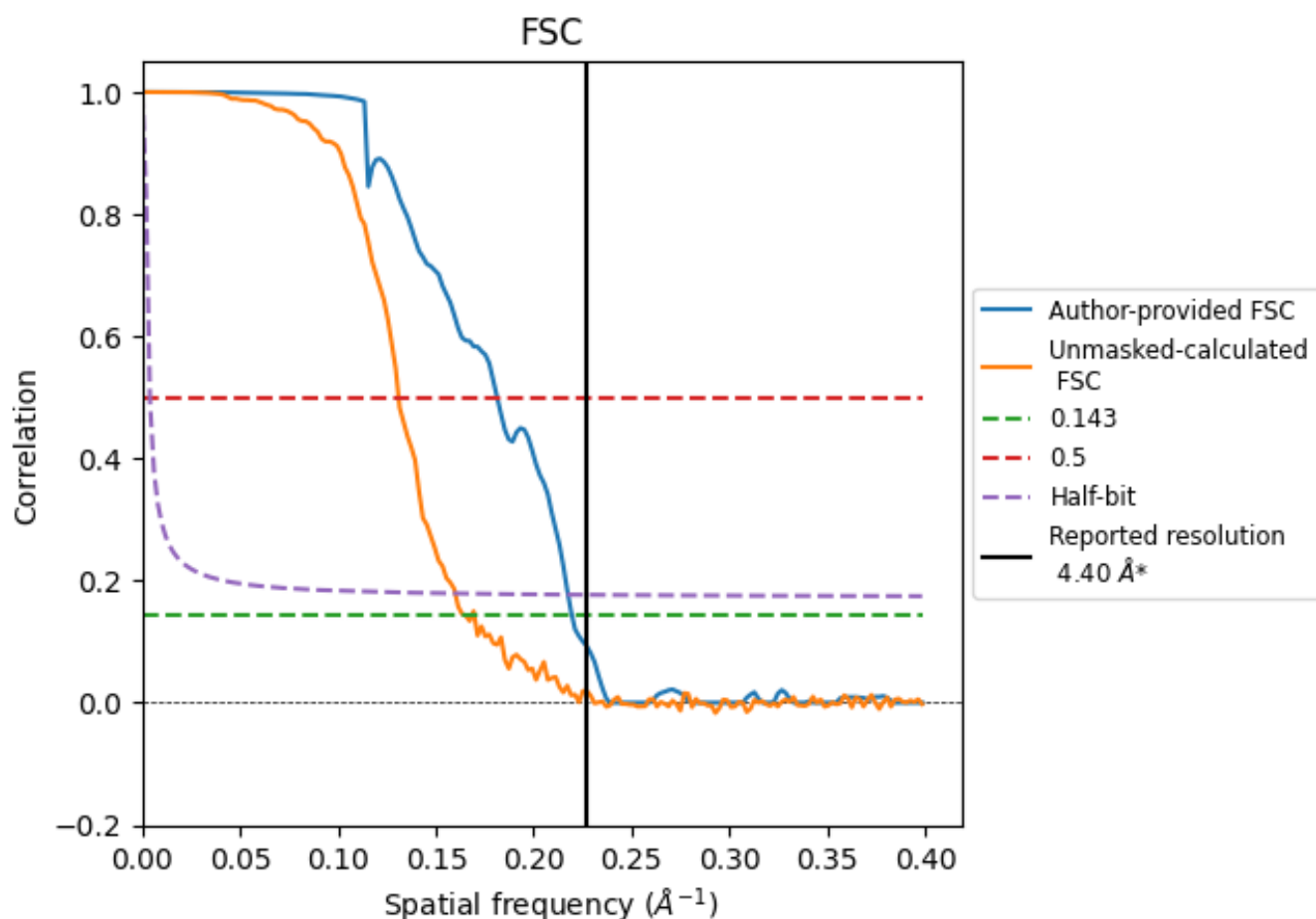


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 $0.227 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

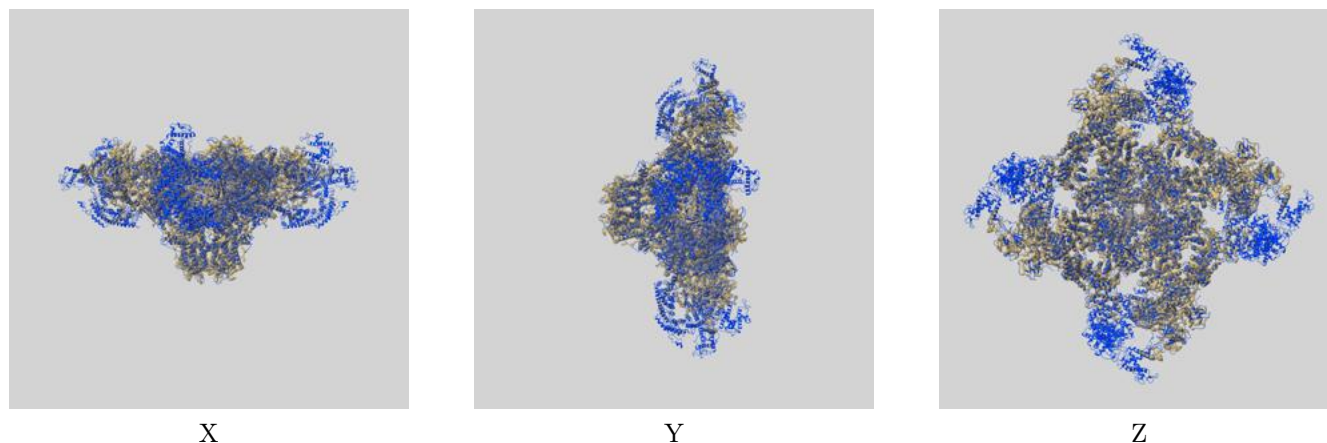
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.56	5.52	4.60
Unmasked-calculated*	6.06	7.64	6.25

*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 6.06 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

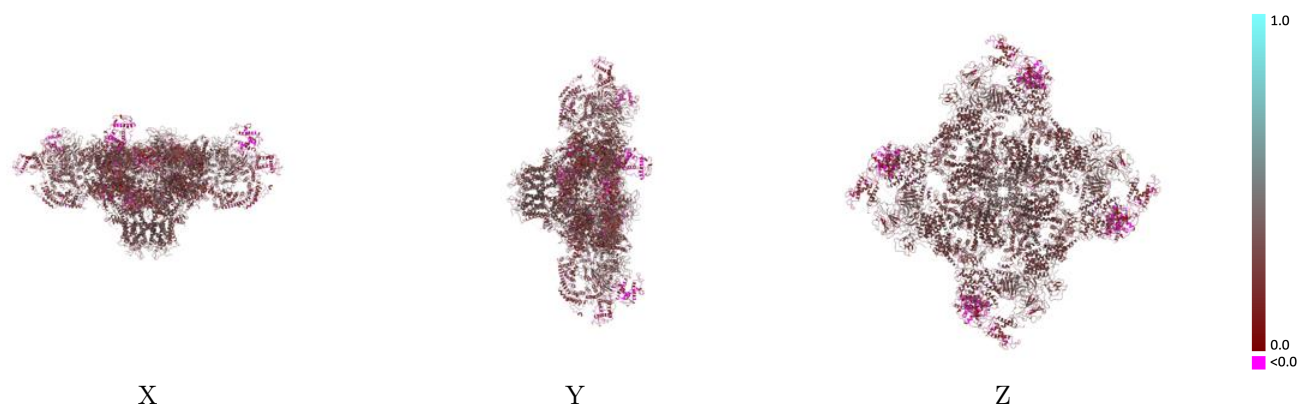
This section contains information regarding the fit between EMDB map EMD-8376 and PDB model 5T9V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



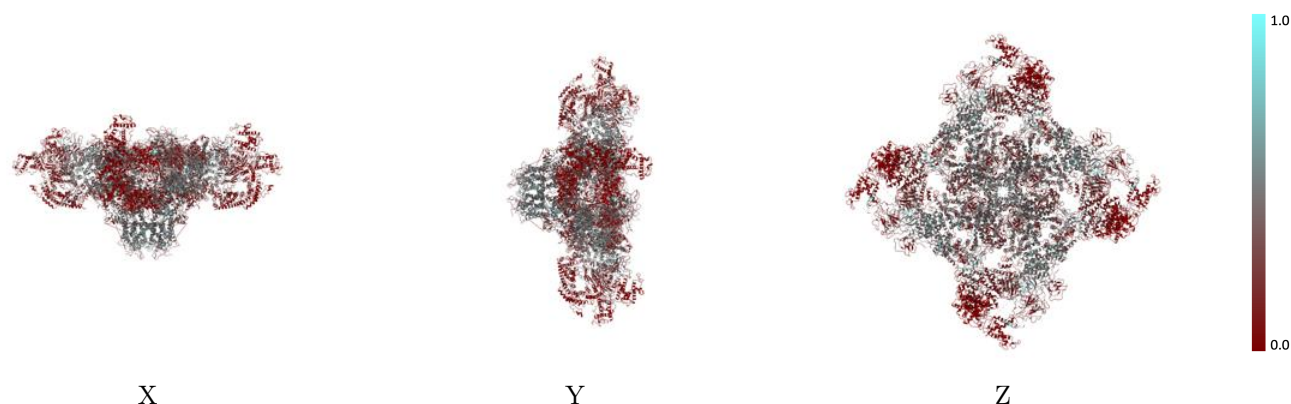
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



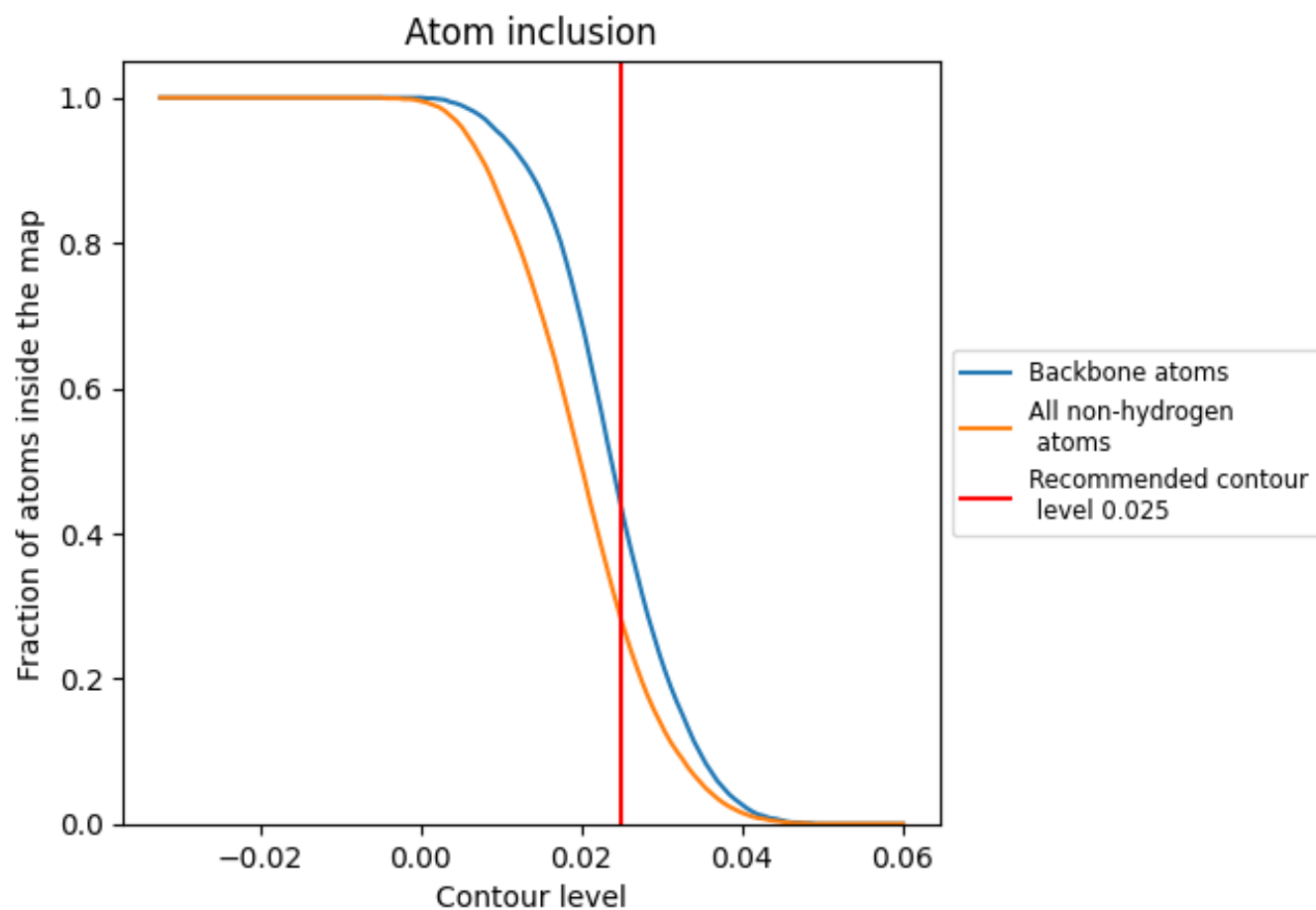
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 44% of all backbone atoms, 28% 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	0.2800	0.2680
A	0.2690	0.3040
B	0.2810	0.2690
E	0.2800	0.2650
F	0.2680	0.3070
G	0.2800	0.2680
H	0.2710	0.3040
I	0.2800	0.2660
J	0.2720	0.3050

1.0

0.0

<0.0