



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 02:51 AM EDT

PDB ID : 5T9V
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

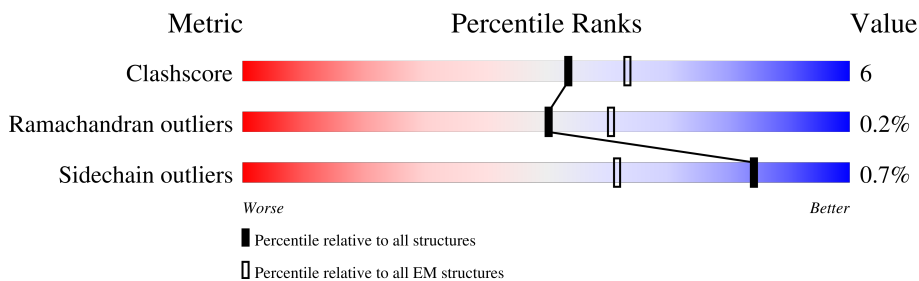
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition [i](#)

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.

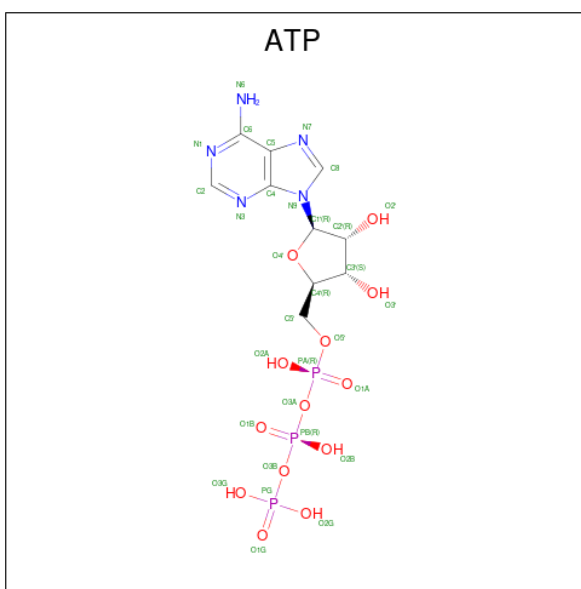
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

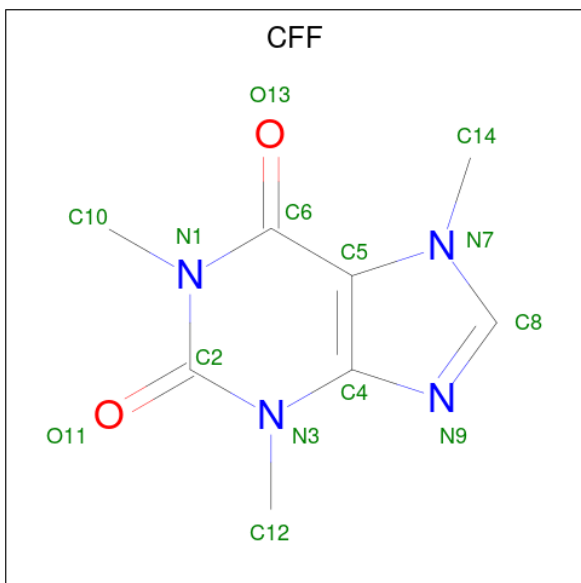
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0
2	I	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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 (three-letter code: 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 (three-letter code: 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	

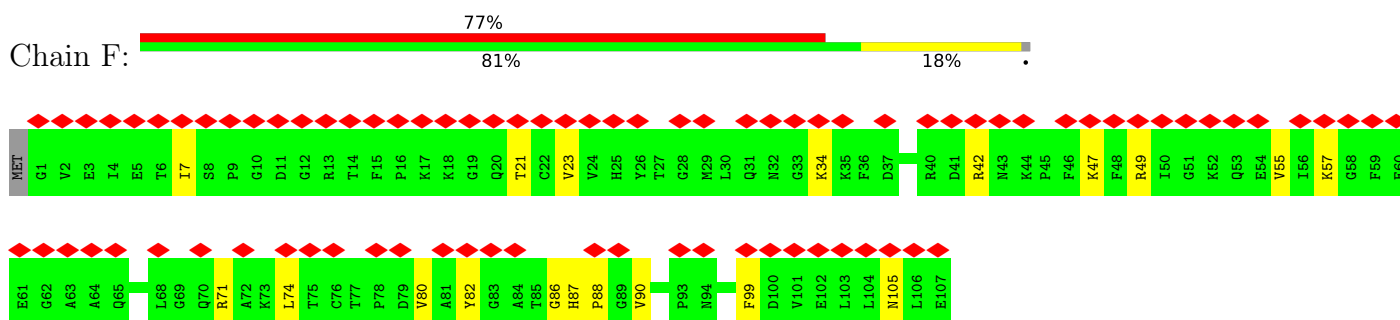
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	

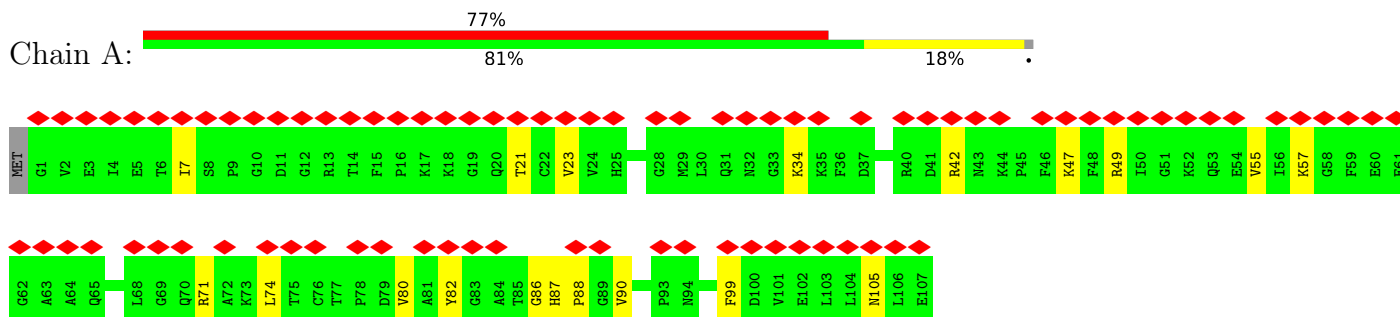
3 Residue-property plots [i](#)

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.

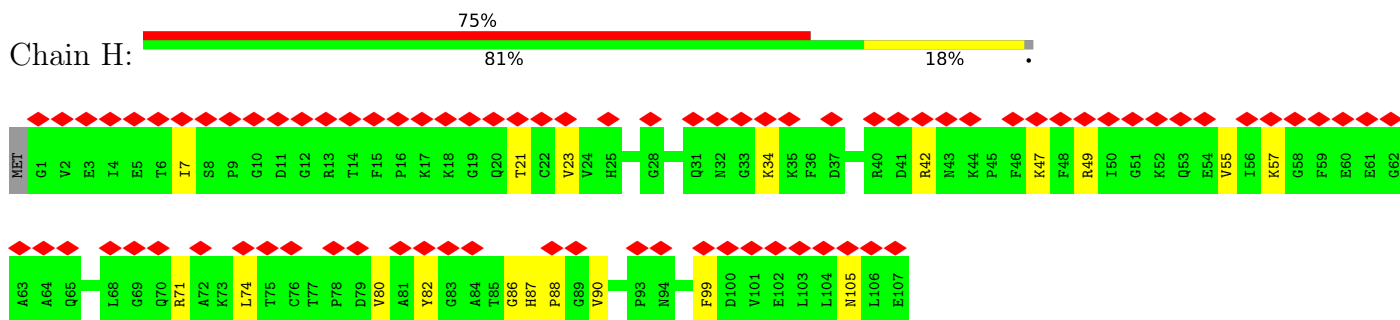
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

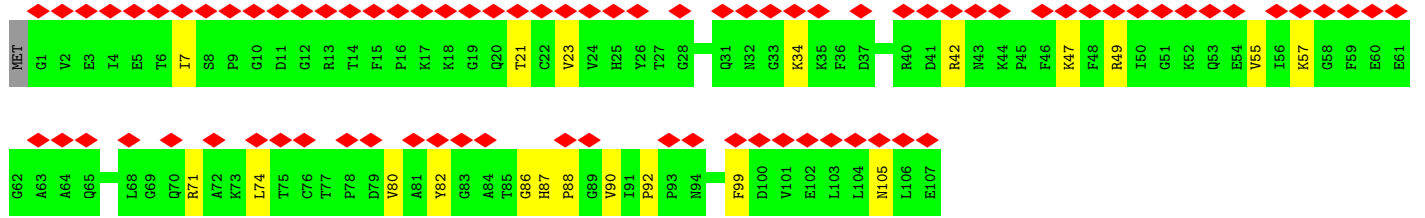


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

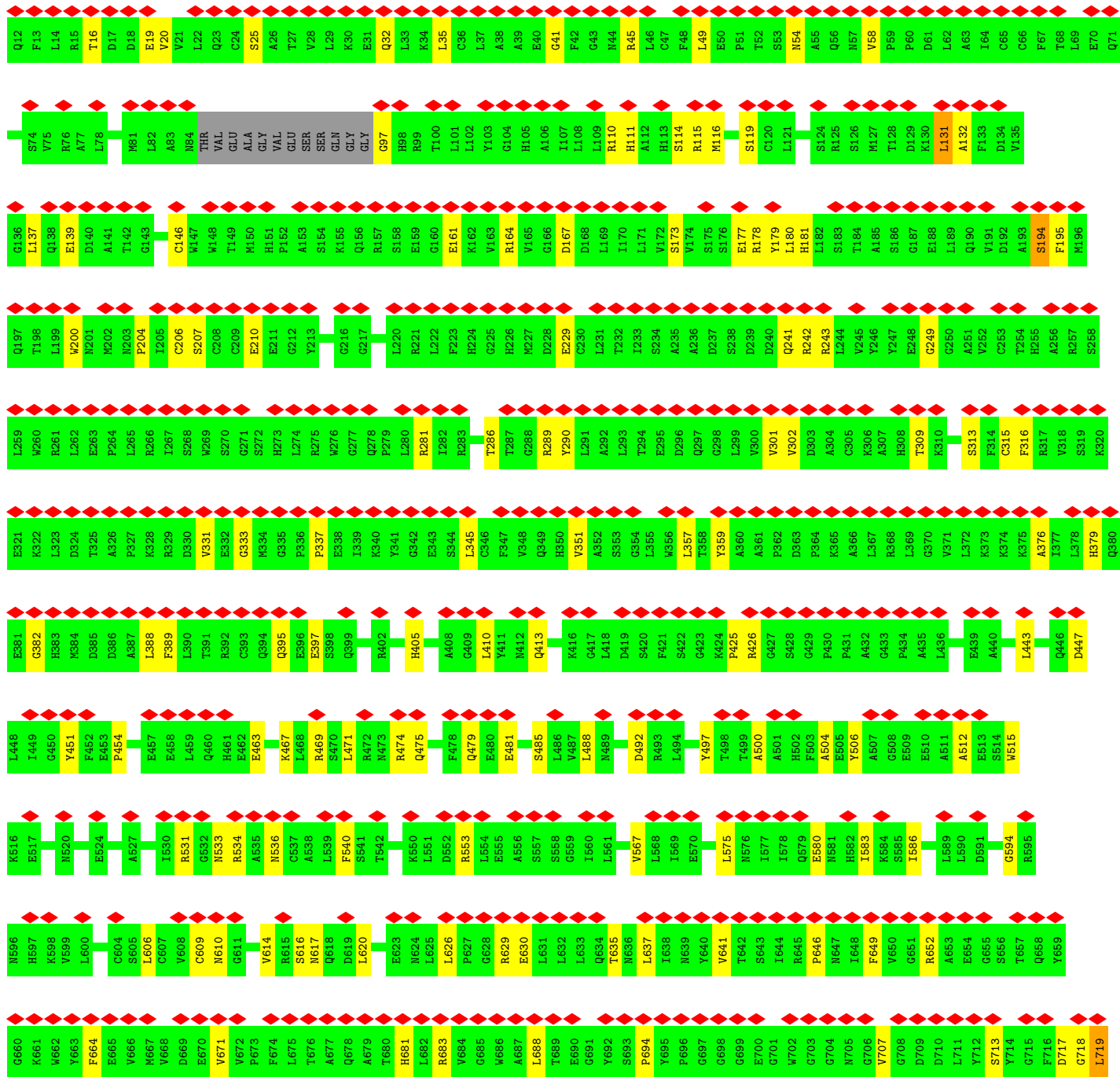
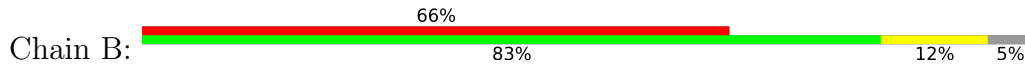


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

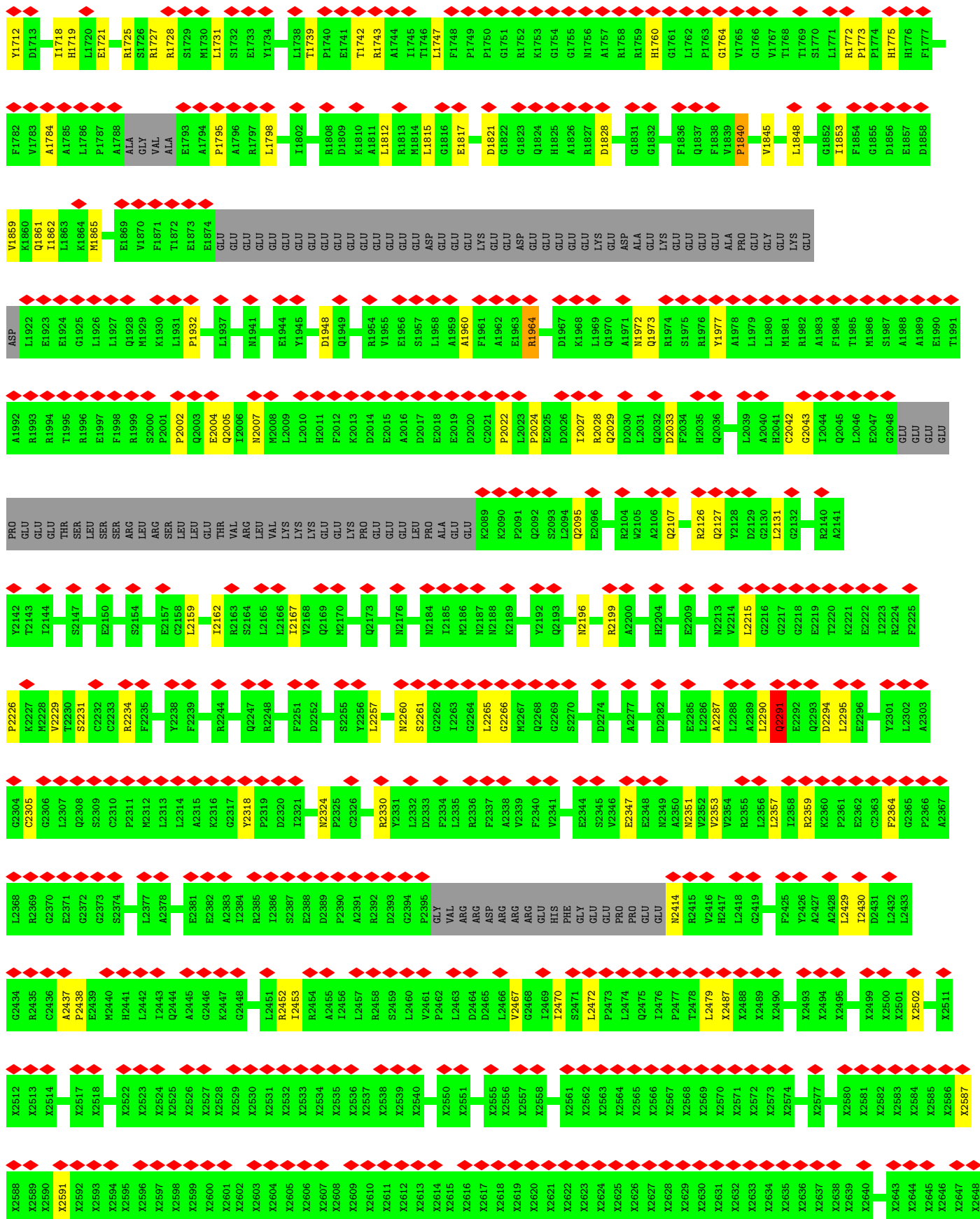




• Molecule 2: Ryanodine receptor 1

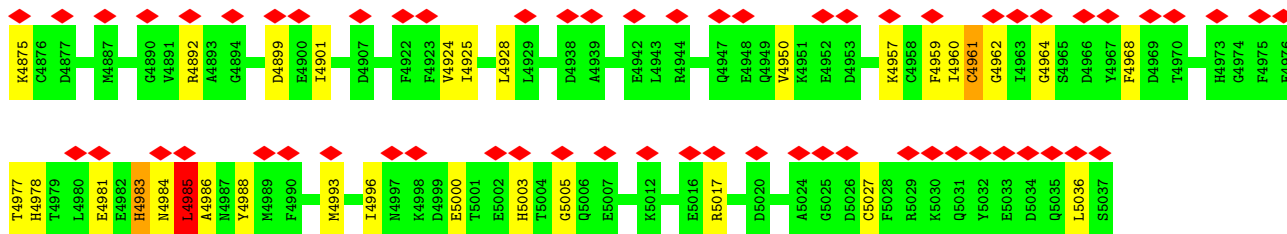


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X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1291	X1292	X1293	X1294	X1297	X1430	X1431	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444	X1445	X1446	X1447	X1448	X1449	X1450	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1468	X1469	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1484	X1485	X1486						
F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	C1222	F1223	I1228	M1229	M1230	Q1231	P1232	V1234	T1235	W1237	K1240	P1243	Q1244	F1245	E1246	P1247	P1250	E1251	H1254	Y1255	E1256	V1257	G1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	T1266	C1269	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281							
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Y1089	F1090	E1091	F1092	E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	M1104	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	L1134	G1135	S1136	E1137	P1138	F1139	G1140	R1141	M1142	W1143	Q1144	S1145	G1146	D1147	V1148	V1149
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P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964
S784	A785	G786	K787	R788	V789	R790	F791	L792	L793	G794	G795	R796	E799	F900	K901	F902	P904	P905	P906	G907	Y908	A909	P910	C911	H912	E913	A814	V815	L816	P917	R918	E919	R820	L821	R822	L823	E824	P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	H838	L839	V840	G841	P842	S843	R844		
H720	L721	W722	T723	G724	W726	A727	R728	P729	V730	T731	S732	F733	G734	W735	K736	L737	L738	A739	P740	E741	S745	C746	C747	L748	D749	L750	S751	V752	P753	S754	V755	S756	F757	R758	I759	N760	G761	C762	P763	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	P778	V780	V781	S782	F783			

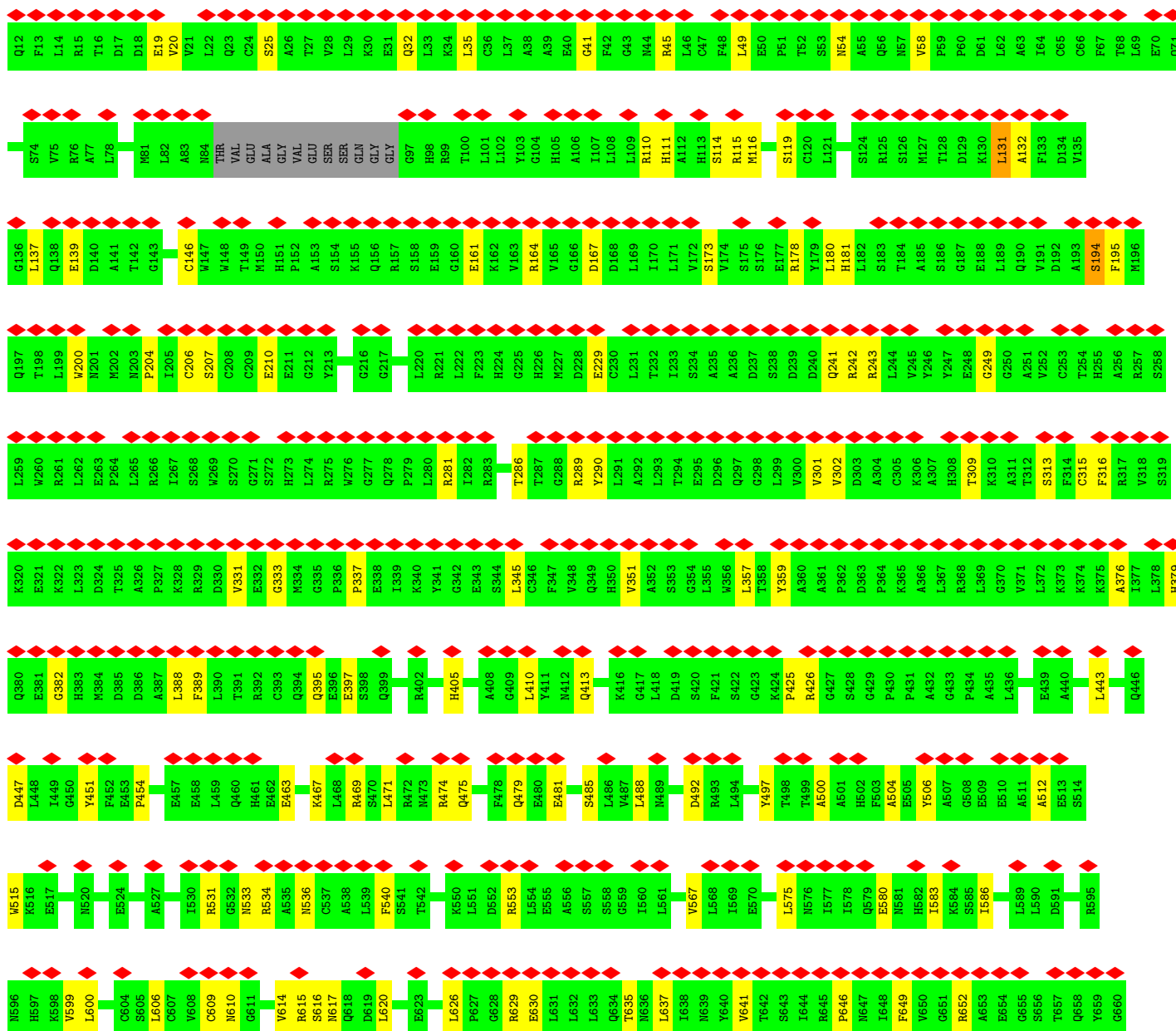
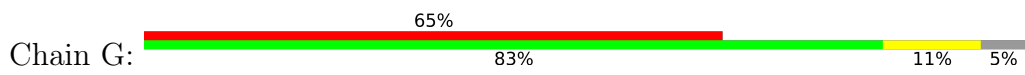


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X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058																																										
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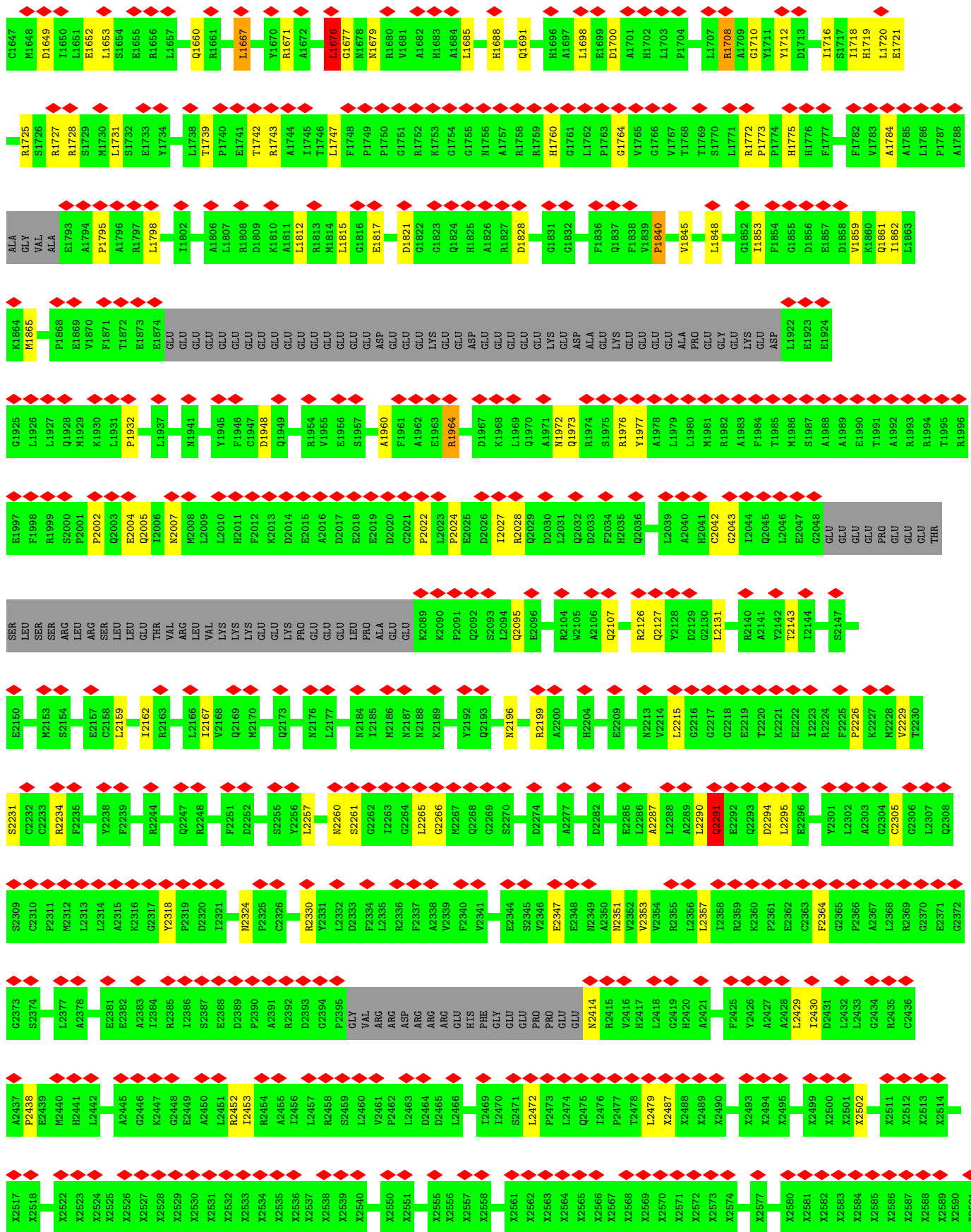
Table with 14 columns and approximately 85 rows of data, representing validation metrics for protein residues. Each cell contains a residue ID and a corresponding validation value. The values are color-coded: red for high values (e.g., 3.30), yellow for medium values (e.g., 1.00), green for low values (e.g., 0.00), and grey for missing values (e.g., 0.00). Small diamond symbols are placed above and below each cell, likely indicating specific validation flags or thresholds.



• Molecule 2: Ryanodine receptor 1

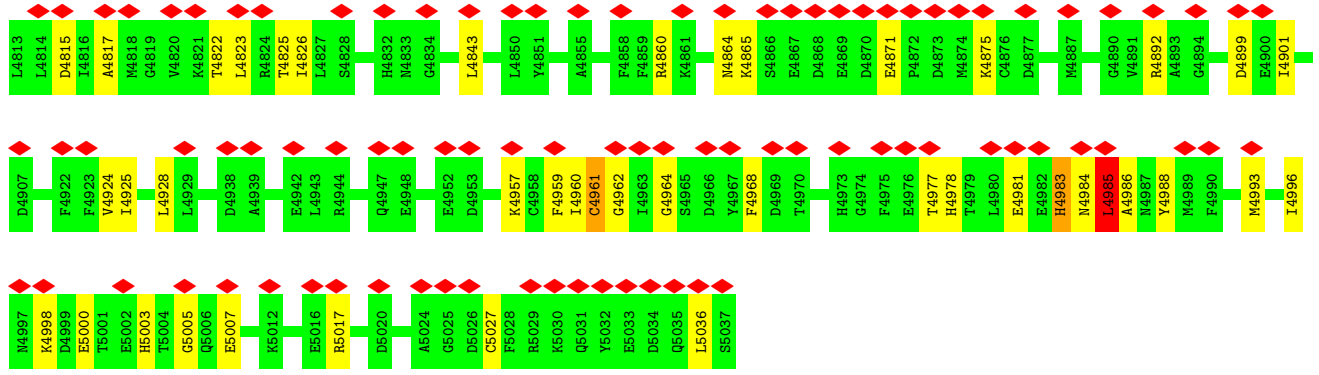


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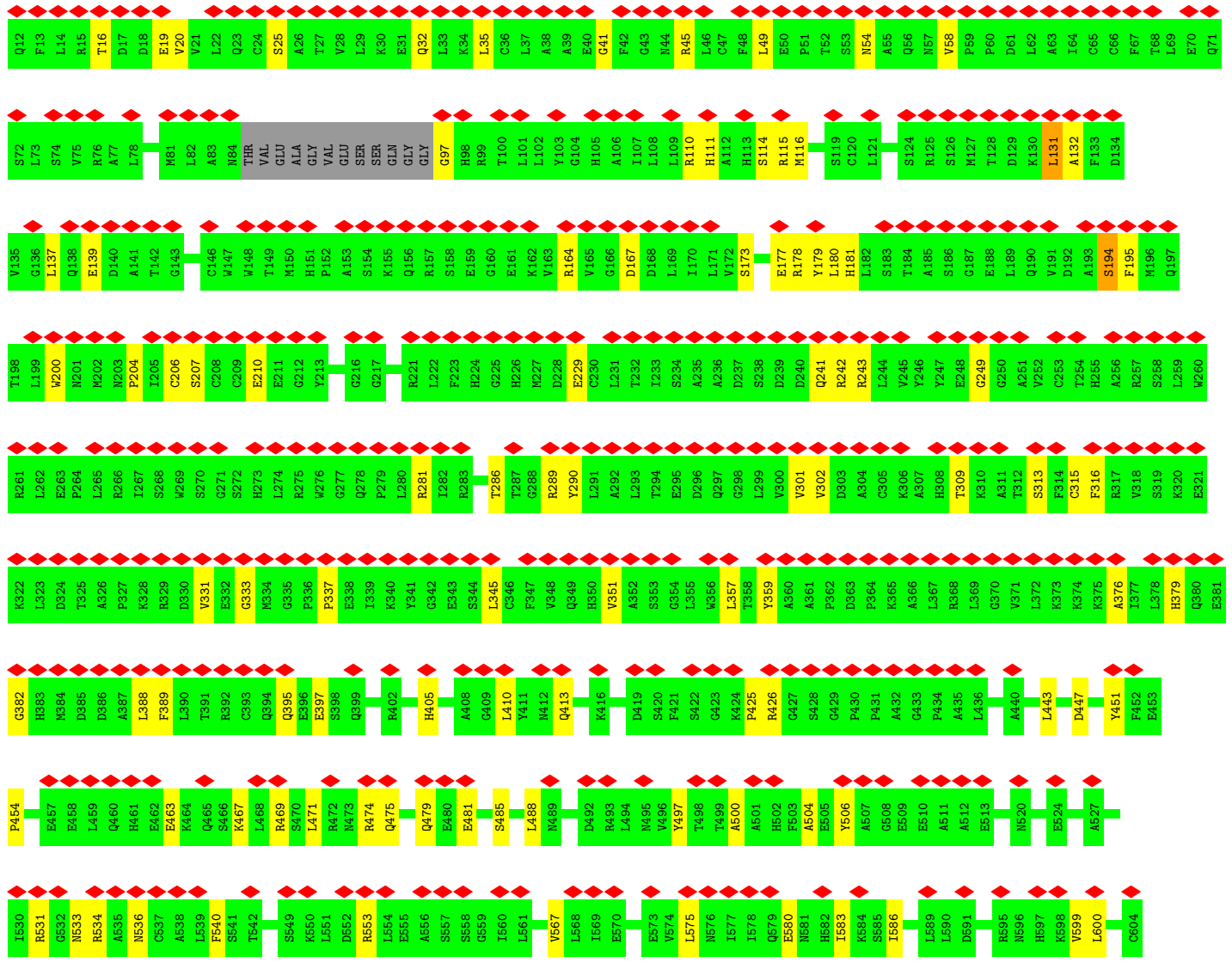
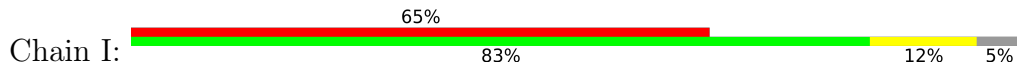


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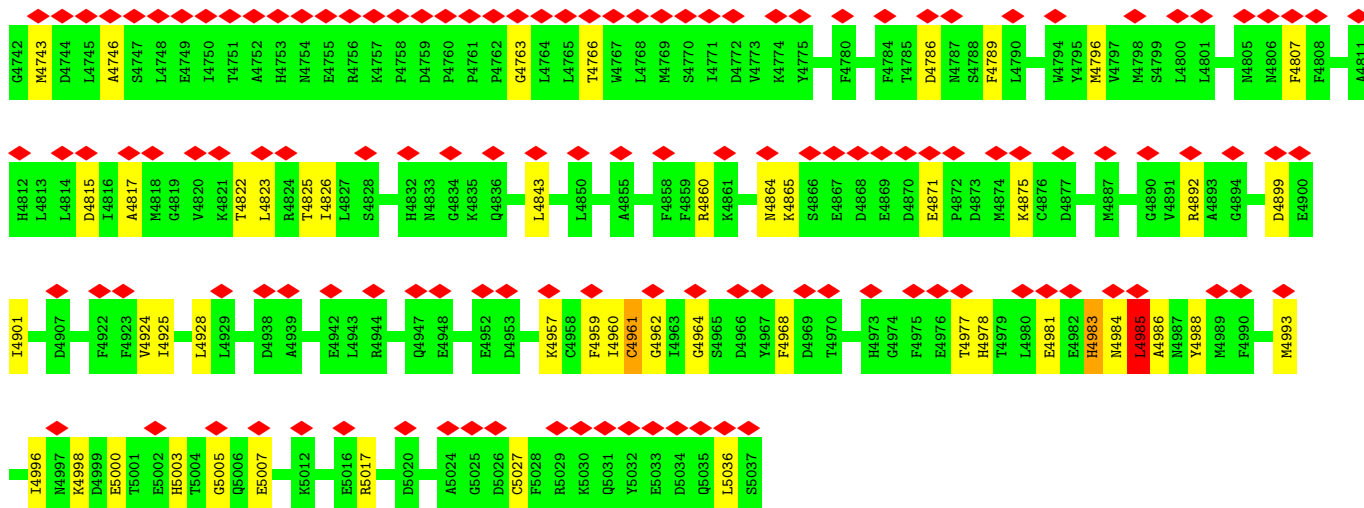
● Molecule 2: Ryanodine receptor 1



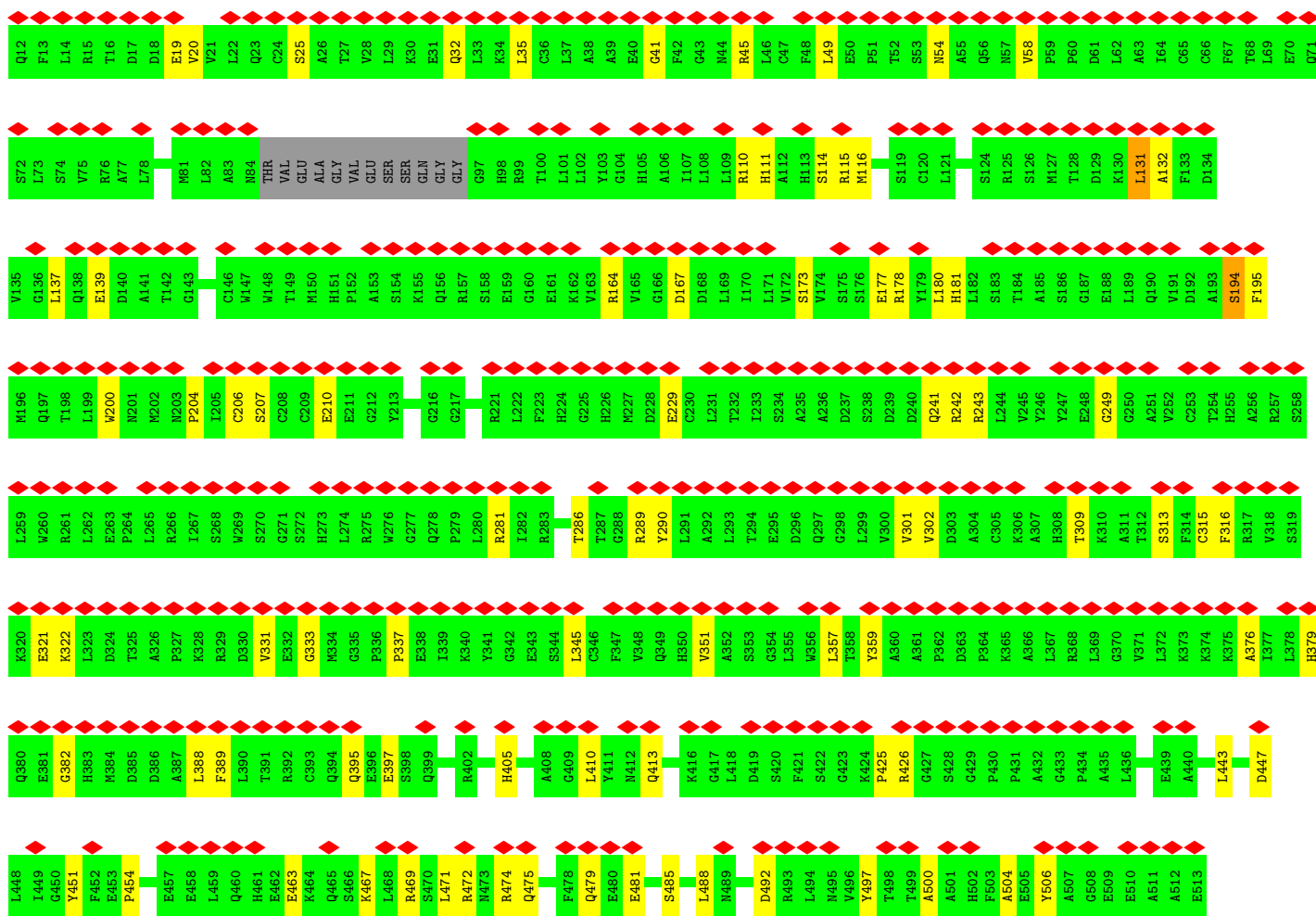
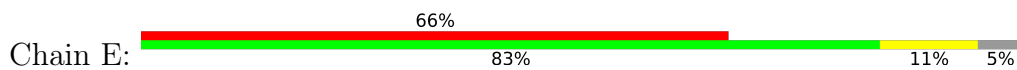
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X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2549	X2550	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2591	X2592	X2593	X2594	X2595												
X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656									
X2657	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	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	M2734	F2735	D2736	P2737	R2738	V2739	W2740	E2741	T2742	L2743	L2744	Y2745	I2746							

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X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3603	X3604	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	T3639	N3643	L3644	
P3645	T3646	H3647	R3648	A3649	C3650	N3651	N3652	F3653	S3656	Y3657	K3658	A3659	A3660	W3661	I3662	L3663	L3664	E3665	D3666	H3667	S3668	F3669	R3672	K3673	L3674	D3675	L3676	S3677	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3689	R3762	E3691	E3692	K3693	K3694	L3698	H3699	Q3700	H3704	R3772	R3773	G3774	L3710	T3711	E3712				
K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	H3723	L3728	K3731	S3732	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLY	R3742	ALA	GLU	D3743	E3744	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	M3758	E3759	K3760	Q3761	R3762	L3763	L3764	Y3765	Q3766	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	G3774	Q3781	S3784					
K3787	G3788	E3789	S3803	I3804	L3805	N3809	A3810	E3811	V3812	Q3813	Q3814	K3815	M3816	L3817	K3821	D3822	E3825	Q3830	Q3833	K3836	L3842	D3843	F3847	E3848	R3849	Q3850	N3851	K3852	A3853	E3854	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	I3866	R3867	R3868	Q3869	N3870	G3871	E3872	K3873									
V3874	K3875	A3876	D3877	D3878	Q3882	D3883	L3884	F3885	R3886	Q3889	L3890	L3891	C3892	E3893	N3896	A3898	S3898	F3899	Q3900	N3901	L3903	R3904	T3905	Q3906	T3907	G3908	N3909	T3910	T3911	T3912	L3913	N3914	L3915	D3921	R3925	E3928	S3929	D3932	F3933	Y3934	M3935	Y3936	Y3937	Q3939	Q3940	D3941	V3942	L3943	E3944									
E3946	Q3946	N3950	A3954	K3959	Q3960	N3963	E3967	Y3968	G3971	Q3978	L3980	A3981	H3982	S3983	R3984	L3985	W3986	D3987	L3989	L3993	L3994	L3995	H3994	V3995	F3996	A3997	H3998	N3999	M4000	M4001	M4002	L4003	A4004	Q4005	D4006	S4007	S4008	Q4009	L4012	L4013	K4014	L4017	D4018	D4022	M4023	L4028	S4029	L4030	L4031	K4091	D4092	F4093	Q4094	K4095	A4096			
E4032	G4033	M4034	V4035	V4036	M4037	G4038	M4039	M4040	A4041	R4042	D4046	M4047	L4048	V4049	E4050	S4053	M4054	V4055	E4056	L4059	K4060	F4061	F4062	D4063	M4064	F4065	L4066	K4067	L4068	K4069	D4070	L4071	V4072	G4073	S4074	E4075	A4076	F4077	Q4078	D4079	Y4080	V4081	T4082	D4083	P4084	R4085	G4086	L4088	K4091	D4092	F4093	Q4094	K4095	A4096				
M4097	D4098	S4099	Q4100	K4101	Q4102	F4103	T4104	G4105	P4106	Q4109	F4110	L4111	L4112	S4113	E4116	A4117	D4118	E4119	M4120	E4121	M4122	I4123	M4124	F4125	E4126	E4127	F4128	A4129	M4130	R4131	F4132	Q4133	E4134	A4135	R4137	D4138	I4139	G4140	F4141	M4142	L4150	S4151	E4152	H4153	W4154	P4155	H4156	D4157	P4158	R4159	S4160	R4161	M4162	F4163	L4164			
E4166	L4166	A4167	E4168	S4169	I4170	L4171	F4172	Y4173	F4174	R4180	Q4185	A4186	S4187	R4188	A4189	I4190	E4191	L4192	E4196	E4199	T4200	A4203	E4206	Q4209	L4212	E4215	E4216	R4215	F4219	M4223	E4224	Q4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	E4239	M4245	A4249	Q4250	I4251	S4252	F4253	X4320											
X4321	X4322	X4329	X4330	X4334	X4335	X4336	X4340	X4344	X4345	F4340	W4341	G4342	E4343	L4344	E4345	E4346	Q4347	R4348	E4351	Y4354	R4357	L4362	R4363	F4371	A4372	I4373	A4374	F4375	I4376	Y4380	K4381	V4382	S4383	D4384	S4385	P4386	P4387	GLY	GLU	ASP	ASP	ASP	GLY	GLU	MET	GLY	E4735	E4736	E4737	A4738	E4739	L4740	L4741					
ASP	LEU	ALA	GLY	ALA	GLY	SER	GLY	GLY	GLY	TRP	GLY	SER	GLY	ALA	GLY	GLY	ASP	GLU	ALA	GLY	GLY	ASP	GLU	M4626	M4627	Y4628	Y4629	Y4630	E4634	S4635	T4636	G4637	Y4638	M4639	E4640	P4641	A4642	L4643	W4644	C4645	L4646	F4655	L4656	C4657	I4658	I4659	G4660	Y4661	M4662	K4672	R4673	E4674						
X4675	R4679	K4680	L4681	E4682	F4683	D4684	G4685	L4686	Y4687	L4688	T4689	E4690	Q4691	P4692	G4693	D4694	D4695	D4696	V4697	K4698	C4699	Q4700	M4701	D4702	R4703	L4704	V4705	L4706	F4711	F4712	S4713	M4714	Y4715	Y4716	D4717	K4718	K4721	R4722	K4723	D4726	K4727	H4728	Q4729	D4730	I4731	G4732	G4733	R4734	R4736	L4737	A4738	E4739	L4740	L4741				



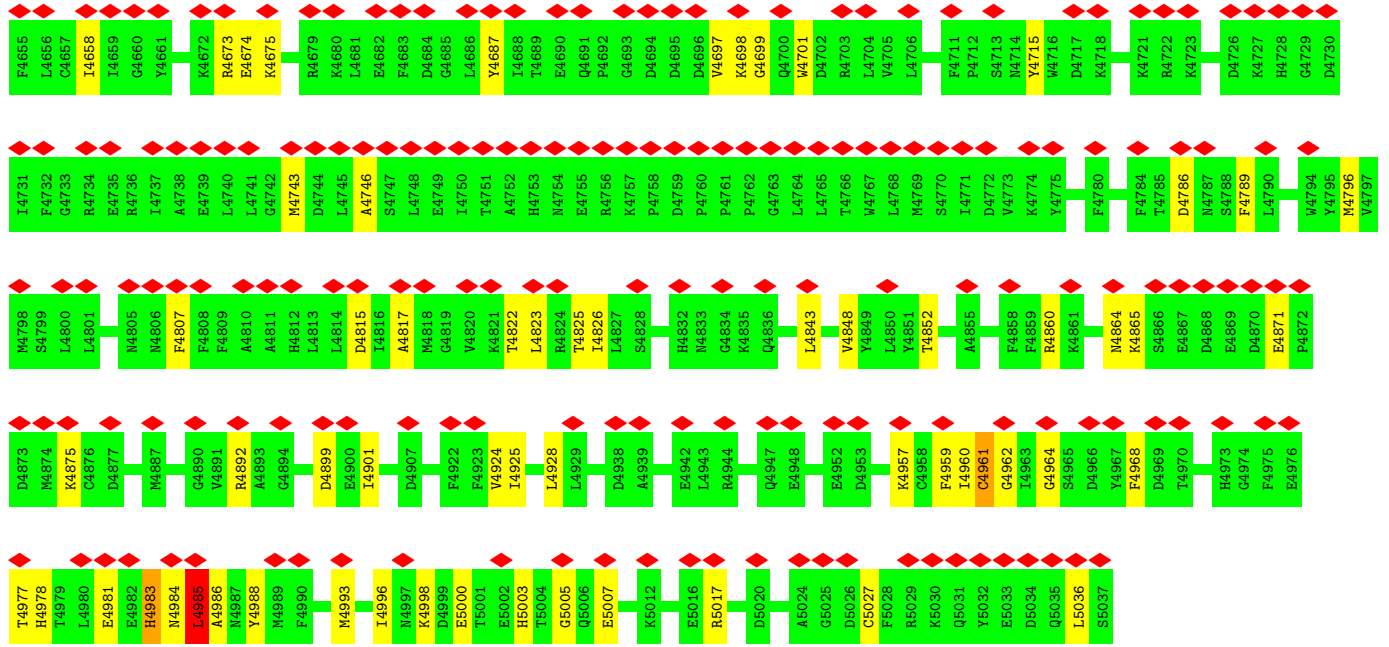
● Molecule 2: Ryanodine receptor 1



X1287	X1288	X1291	X1292	X1297	X1430	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	X1466	X1469	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1484	X1485	X1486	X1487	X1488	X1492	X1493	X1494	X1495	X1496								
G1218	L1219	Q1220	E1221	F1222	F1223	I1228	M1229	M1230	Q1231	R1232	R1233	V1234	T1235	T1236	W1237	K1240	P1243	Q1244	F1245	E1246	P1247	P1250	E1251	H1254	Y1255	E1256	V1257	M1258	R1259	M1260	D1261	G1262	T1263	V1264	D1265	C1269	L1270	R1271	L1272	A1273	H1274	R1275	X1276	X1277	X1278	X1279	X1280	X1281	X1282	X1285	X1286								
D1154	L1155	T1156	E1157	T1159	I1160	I1161	F1162	T1163	L1164	M1165	G1166	A1167	R1168	V1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	M1186	G1187	F1188	C1192	S1193	L1194	Q1198	V1199	G1200	H1201	L1202	M1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	G1217			
E1093	A1094	V1095	T1096	T1097	G1098	E1099	M1100	R1101	V1102	G1103	A1104	V1104	R1044	T1045	L1046	L1047	M1048	G1050	Y1051	M1052	I1053	E1054	PRO	ASP	GLN	GLU	PRO	SER	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	F1092		
A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	A989	E990	R991	G992	A997	R998	D999	R1000	N997	V1001	A1002	Q1003	G1004	V1005	S1008	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	R1020	G993	G994	G995	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	
Y908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	G926	E927	T928	R929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	N961	S962	N963	G964	Y965	K966	P967
H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	GLN	L861	V862	L863	P864	P865	H866	L867	E868	R869	L870	R871	E872	K873	L874	A875	E876	N877	R878	H879	E880	L881	W882	A883	L884	T885	R886	L887	E888	Q889	G890	M891	T892	V893	G894	R895	G896	P897	H898	D899	N900	K901	R902	L903	H904	P905	C906	L907
V867	K868	V869	L870	V871	V872	P873	G874	Q735	H736	L737	L738	Q739	P740	E741	S745	C746	L747	L748	D749	L750	S751	V752	P753	L633	G634	T835	M836	L637	I638	N639	Y640	V641	T642	S643	I644	R645	P646	N647	I648	F649	V650	G651	R652	A654	G655	S656	T657	Q658	Y659	G660	K661								
E517	H520	E524	A527	I530	R531	G532	M533	R534	A535	M536	C537	A538	L539	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	M581	I583	K584	S585	I586	L589	L590	D591	R595	N596											

L2377	A2378	E2381	E2382	A2383	L2384	R2385	L2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415	V2416	H2417	L2418	G2419	H2420	A2421	L2422	N2423	S2424	F2425	Y2426	A2427	A2428	L2429	I2430	D2431	L2432	L2433	G2434	R2435	G2436	E2437	A1577	A1578	M1579
L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	I2321	N2324	R2325	C2326	E2329	R2330	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	Q2338	V2339	F2340	V2341	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	V2352	V2353	V2354	R2355	L2356	L2357	I2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374							
F2239	L2242	S2243	R2244	Q2247	R2248	F2251	D2252	Y2256	L2257	N2260	S2261	G2262	L2263	G2264	L2265	G2266	N2267	Q2268	G2269	S2270	D2274	A2277	D2282	E2285	L2286	A2287	L2288	A2289	L2290	Q2291	Q2293	D2294	L2295	E2296	V2299	S2300	Y2301	L2302	A2303	G2304	C2305	G2306	L2307	R2308	S2309	C2310	N2312															
C2158	L2159	I2162	R2163	L2166	I2167	Q2169	M2170	Q2173	M2176	L2177	N2184	N2187	N2188	K2189	Y2192	Q2193	N2196	R2199	A2200	H2204	E2209	N2213	V2214	L2215	G2216	G2217	G2218	T2220	K2221	E2222	L2223	R2224	F2225	P2226	K2227	M2228	V2229	T2230	S2231	C2232	C2233	R2234	F2235	Y2238																		
SER	LEU	LEU	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	LYS	GLU	LYS	PRO	GLU	GLU	LEU	LEU	PRO	ALA	GLU	K2089	K2090	P2091	Q2092	S2093	L2094	Q2095	E2096	R2104	Q2107	R2126	Q2127	Y2128	D2129	G2130	L2131	A2137	R2140	A2141	Y2142	T2143	I2144	S2147	E2150	M2153	S2154	E2157														
G2005	I2006	N2007	M2008	L2010	H2011	F2012	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	P2022	L2023	E2025	D2026	L2027	R2028	Q2029	D2030	L2031	Q2032	D2033	F2034	H2035	Q2036	D2037	L2038	L2039	A2040	H2041	C2042	G2043	I2044	Q2045	L2046	E2047	G2048	GLU	GLU	GLU	PRO	PRO	GLU	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG					
L1937	L1942	Y1945	F1946	C1947	D1948	Q1949	H1953	R1954	V1955	E1956	S1957	A1960	F1961	A1962	E1963	R1964	D1967	K1968	L1969	Q1970	A1971	N1972	Q1973	R1974	S1975	F1976	Y1977	A1978	L1979	M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	R1993	R1994	T1995	R1996	E1997	F1998	R1999	P2001	P2002	Q2003	E2004										
E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	LYS	GLU	ASP	GLU	GLU	GLU	GLU	ALA	ALA	LYS	GLU	GLU	GLU	GLU	ALA	PRO	GLU	GLY	LYS	L1922	E1923	E1924	G1925	L1926	L1927	Q1928	L1862	M1929	K1930	L1931	P1932	P1868	E1869	V1870	F1871	T1872	E1873										
R1797	L1798	A1806	L1807	R1808	D1809	K1810	A1811	L1812	H1813	M1814	L1815	G1816	E1817	D1821	G1822	G1823	Q1824	H1825	A1826	R1827	D1828	G1831	G1832	F1836	Q1837	F1838	V1839	P1840	V1841	V1845	L1848	G1852	F1854	G1855	D1856	E1857	D1858	K1860	Q1861	L1862	L1863	K1864	M1865	P1868	E1869	V1870	F1871	T1872	E1873													
L1731	S1732	E1733	Y1734	L1738	T1739	P1740	E1741	T1742	R1743	A1744	I1745	T1746	L1747	F1748	P1749	P1750	G1751	R1752	K1753	G1754	G1755	G1756	A1757	R1758	L1759	H1760	G1761	L1762	P1763	G1764	V1765	R1766	V1767	T1768	T1769	R1772	P1773	P1774	H1775	Y1776	F1777	F1782	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1794	P1795	A1796						
D1649	I1650	L1651	E1652	S1653	S1654	R1655	T1656	E1657	Q1660	R1661	L1667	Y1670	R1671	A1672	L1676	M1679	R1680	V1681	H1682	A1682	L1683	L1685	H1688	Q1691	L1698	E1699	D1700	A1701	H1702	L1703	P1704	L1707	R1708	A1709	G1710	Y1711	Y1712	D1713	I1718	H1719	L1720	E1721	R1725	S1726	R1727	R1728	S1729	M1730														
F1580	L1581	S1582	E1583	R1584	K1585	P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	Q1598	M1599	L1600	S1604	W1605	M1608	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	Q1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	L1639	H1640	E1644	N1645	R1646	C1647	M1648									
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	X1538	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1573	A1577	A1578	M1579										

X2438	X2439	X2440	X2441	X2442	X2445	X2446	X2447	X2448	X2449	X2450	X2451	X2452	X2453	X2454	X2455	X2456	X2457	X2458	X2459	X2460	X2461	X2462	X2463	X2464	X2465	X2466	X2467	X2468	X2469	X2470	X2471	X2472	X2473	X2474	X2475	X2476	X2477	X2478	X2479	X2487	X2488	X2489	X2490	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2502	X2511	X2512	X2513																																	
X2514	X2517	X2518	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2549	X2550	X2555	X2556	X2557	X2558	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590																																					
X2591	X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631	X2632	X2633	X2634	X2635	X2636	X2637	X2638	X2639	X2640	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651																															
X2652	X2653	X2654	X2655	X2656	X2657	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	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739	X2740	X2741
T2742	L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	E2759	E2760	I2761	T2762	H2763	E2764	K2765	T2766	F2767	F2768	D2769	K2770	I2771	Q2772	N2773	L2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	P2794	M2795	K2796	T2797	F2798	E2799	K2800	D2801																														
K2802	E2803	L2804	Y2805	K2806	P2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	E2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	K2858	P2859	P2860	D2861																																	
L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	L2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	V2907	P2908	D2909	T2910	L2911	T2912	P2913	P2914	K2915	K2916	A2917	R2918	D2919	R2920	E2921																														
K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	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	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061																														
X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3144	X3145	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	X3205	X3206	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	X3251	X3252	X3253	X3254	X3255	X3256	X3257	X3258	X3259	X3260	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	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327																														
X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	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	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387																														



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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (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 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	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	1234	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 1234 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:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78

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%)	47	81
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	47	81
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	47	81
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	50	81

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	E	131	LEU
2	E	4085	ARG
2	E	553	ARG
2	E	1964	ARG

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Mol	Chain	Res	Type
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1775	HIS
2	E	3896	ASN
2	E	4983	HIS
2	G	838	HIS
2	G	725	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	B	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.30	1 (12%)
4	CFF	G	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.62	5 (16%)
4	CFF	I	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.30	1 (12%)
4	CFF	E	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.29	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C5-C4	-4.39	1.33	1.39
4	E	5102	CFF	C5-C4	-4.39	1.33	1.39
4	B	5102	CFF	C5-C4	-4.35	1.33	1.39
4	G	5102	CFF	C5-C4	-4.34	1.33	1.39
4	G	5102	CFF	C6-N1	-4.21	1.32	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	PA-O3A-PB	-3.69	120.15	132.83
3	G	5101	ATP	PA-O3A-PB	-3.69	120.18	132.83
3	E	5101	ATP	PA-O3A-PB	-3.68	120.18	132.83
3	I	5101	ATP	PA-O3A-PB	-3.67	120.22	132.83
3	I	5101	ATP	C3'-C2'-C1'	3.55	106.33	100.98

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

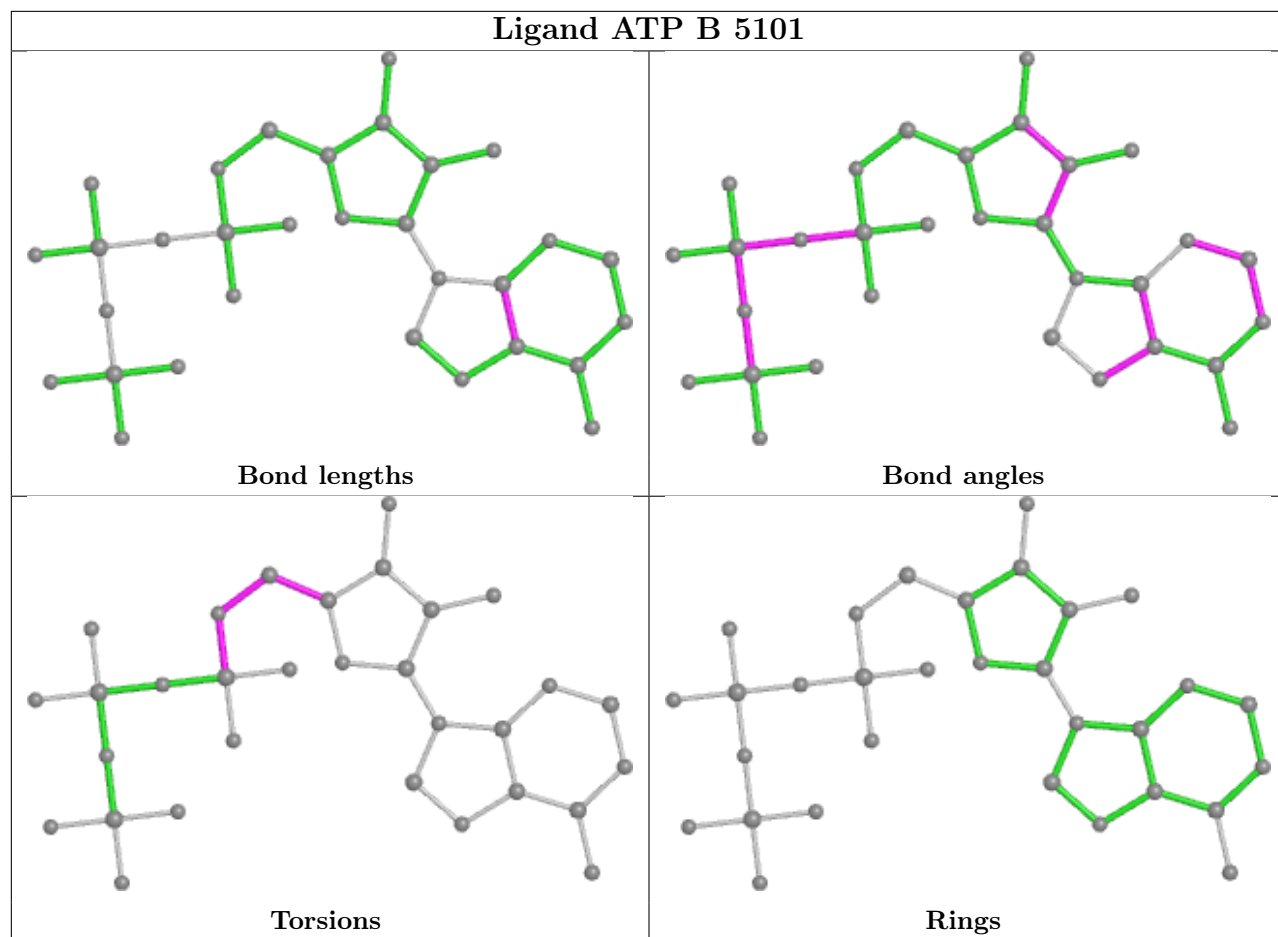
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C4'-C5'-O5'-PA

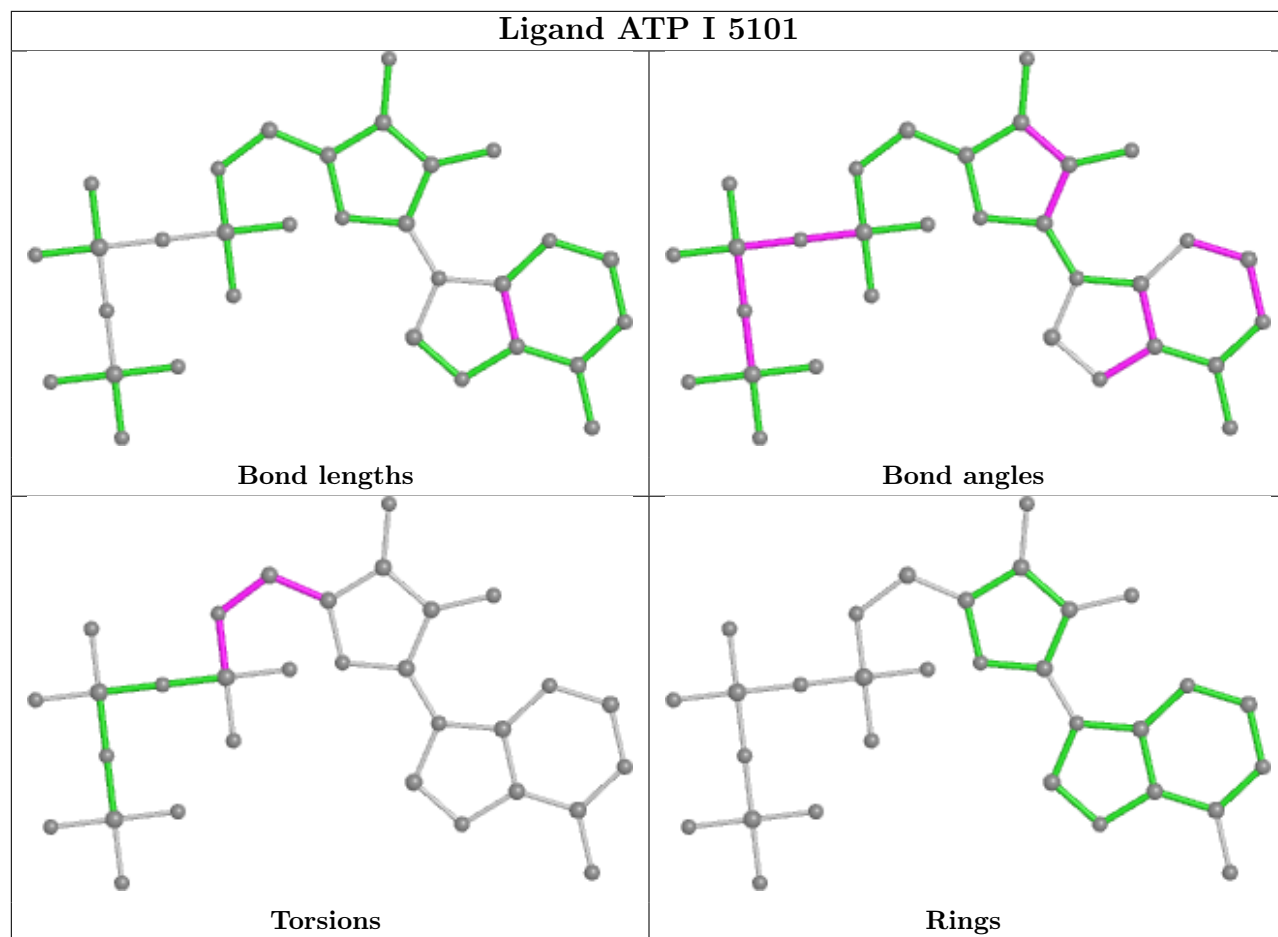
There are no ring outliers.

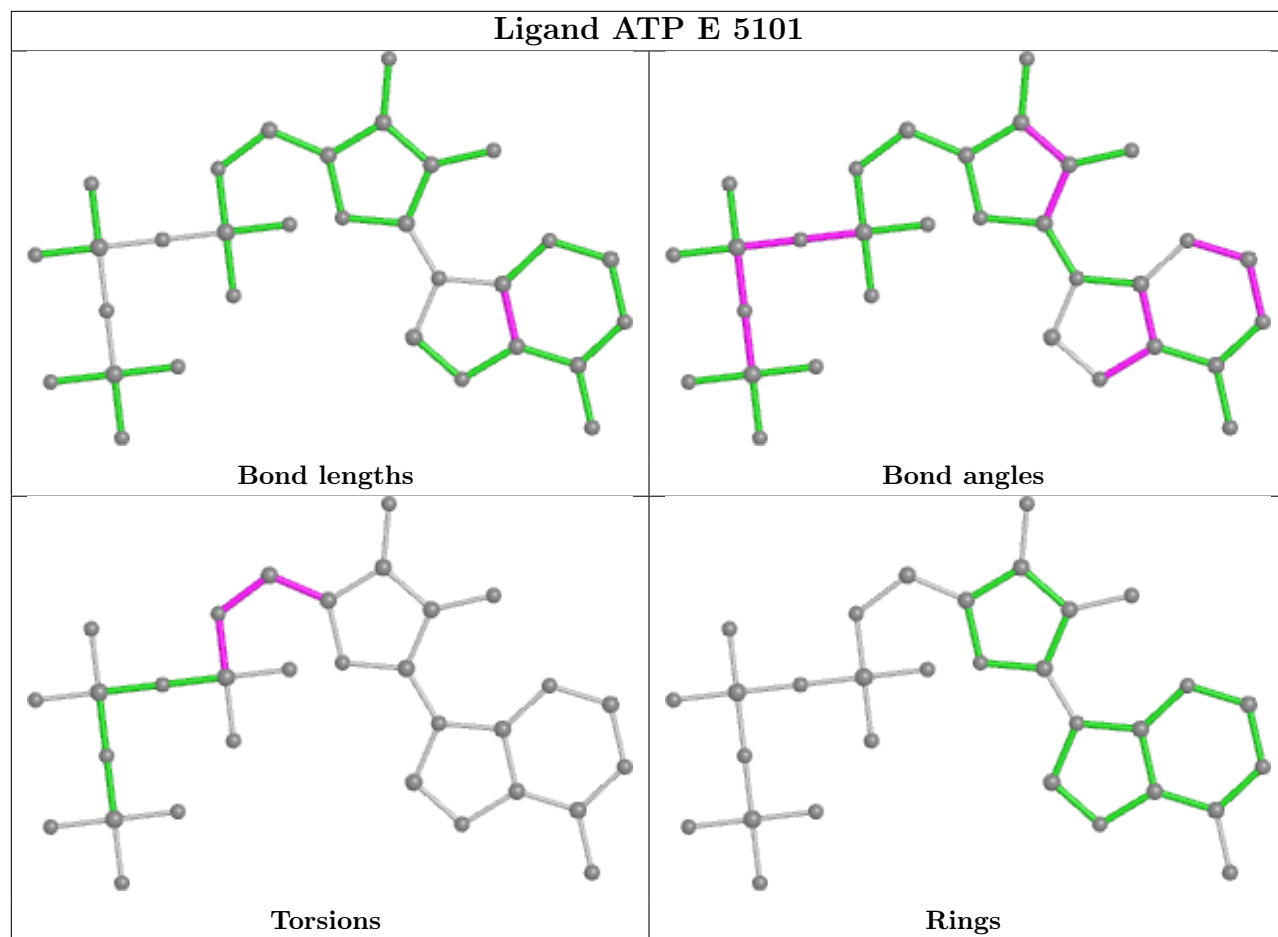
4 monomers are involved in 4 short contacts:

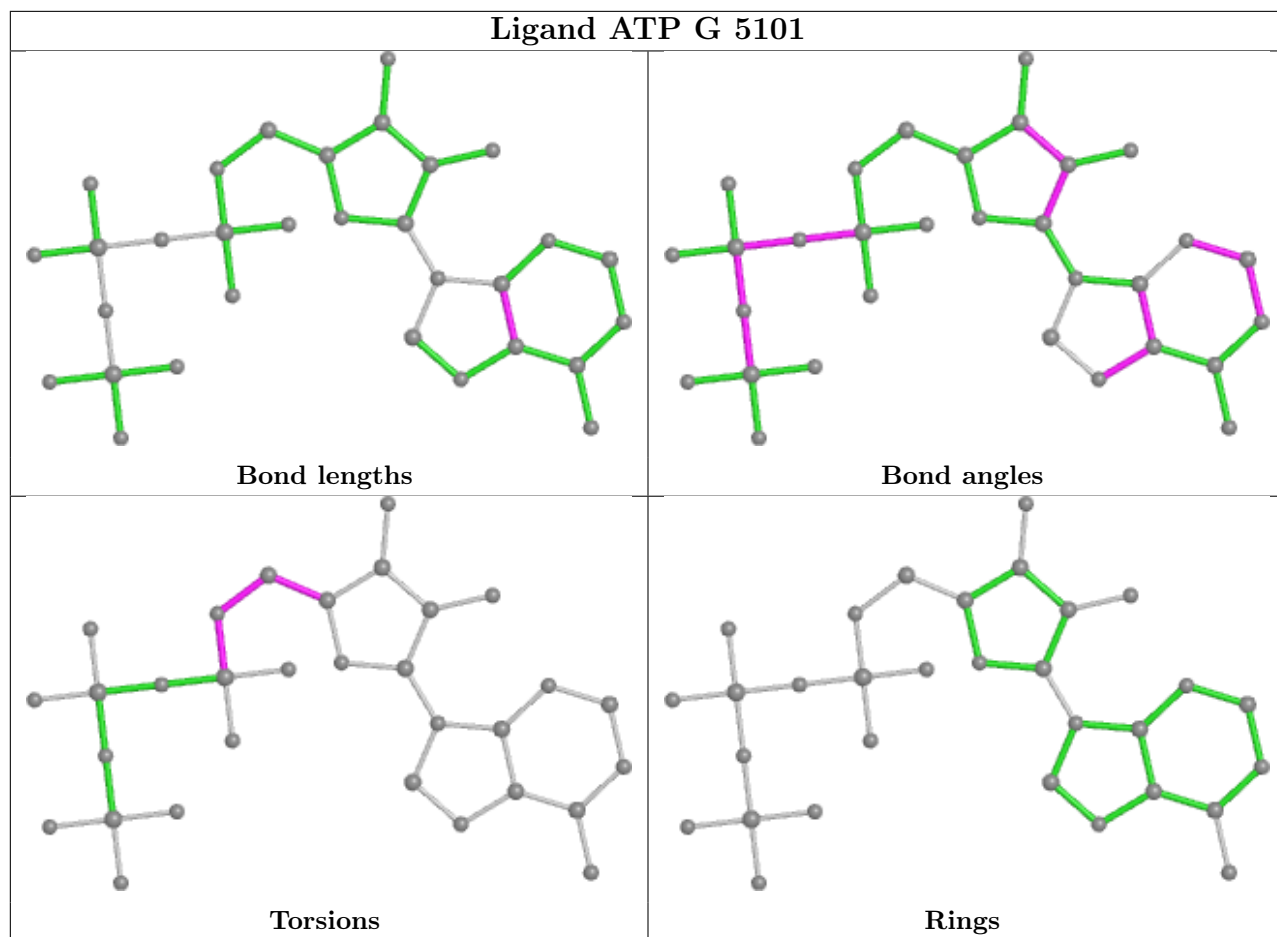
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0

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 [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	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

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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

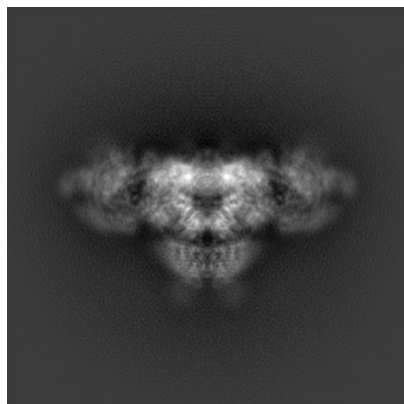
6 Map visualisation [i](#)

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.

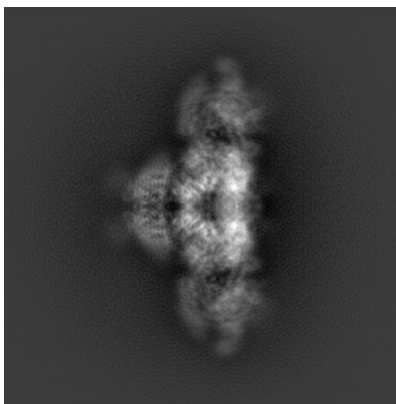
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

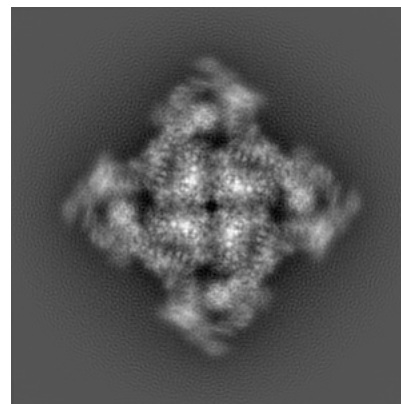
6.1.1 Primary map



X

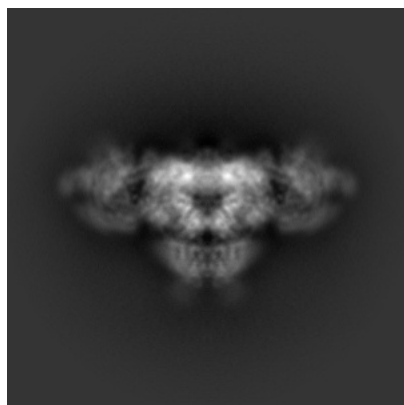


Y

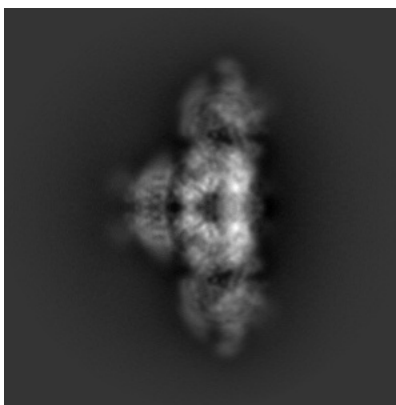


Z

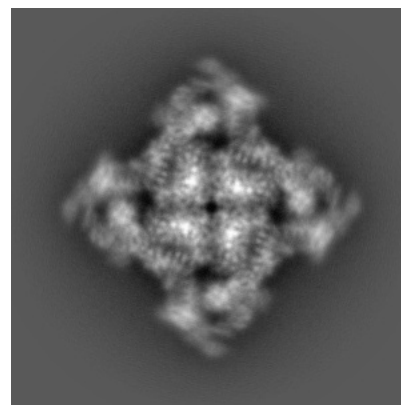
6.1.2 Raw map



X



Y

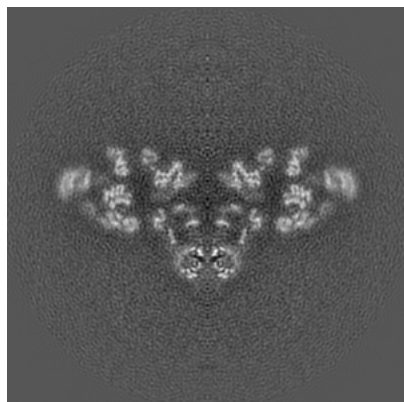


Z

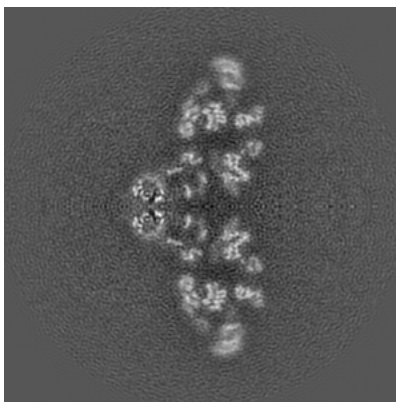
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

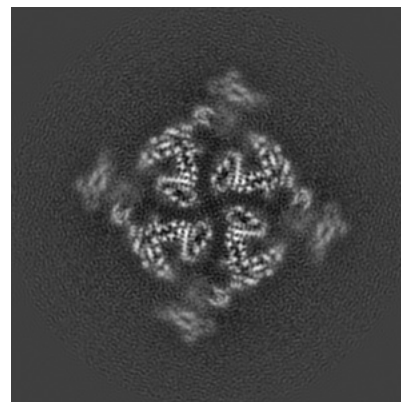
6.2.1 Primary map



X Index: 200

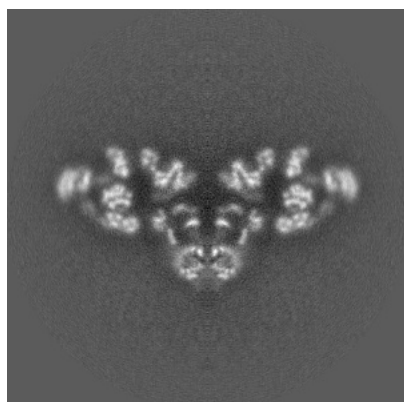


Y Index: 200

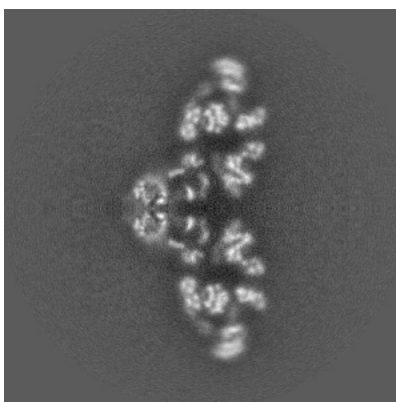


Z Index: 200

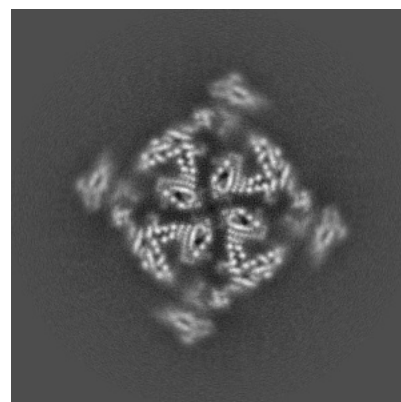
6.2.2 Raw map



X Index: 200



Y Index: 200

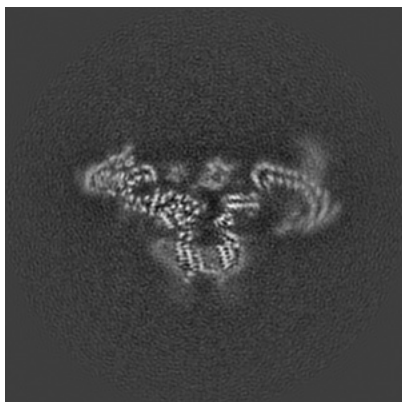


Z Index: 200

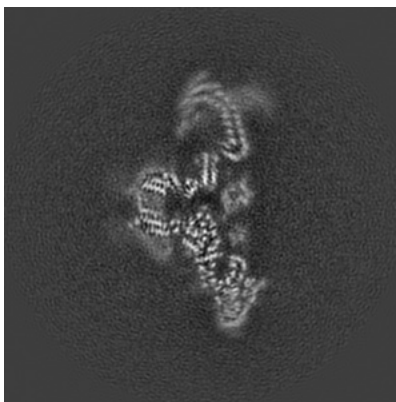
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

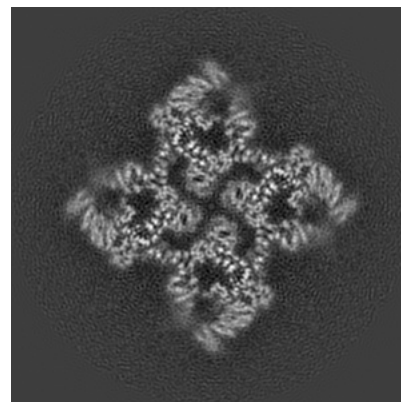
6.3.1 Primary map



X Index: 225

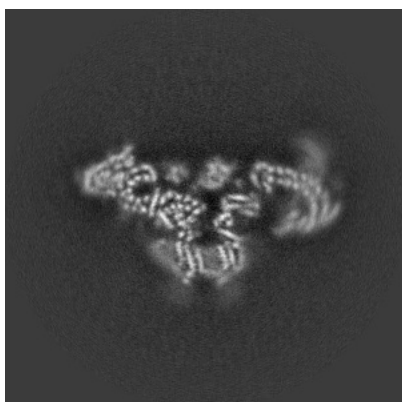


Y Index: 175

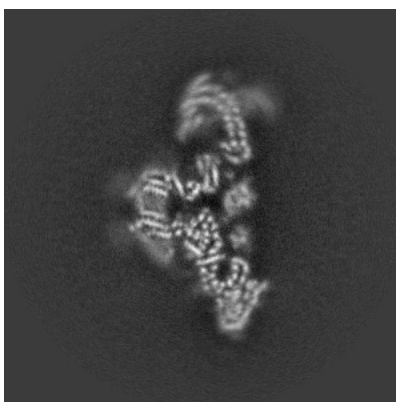


Z Index: 232

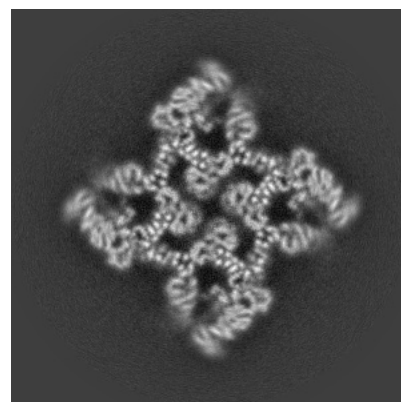
6.3.2 Raw map



X Index: 224



Y Index: 176

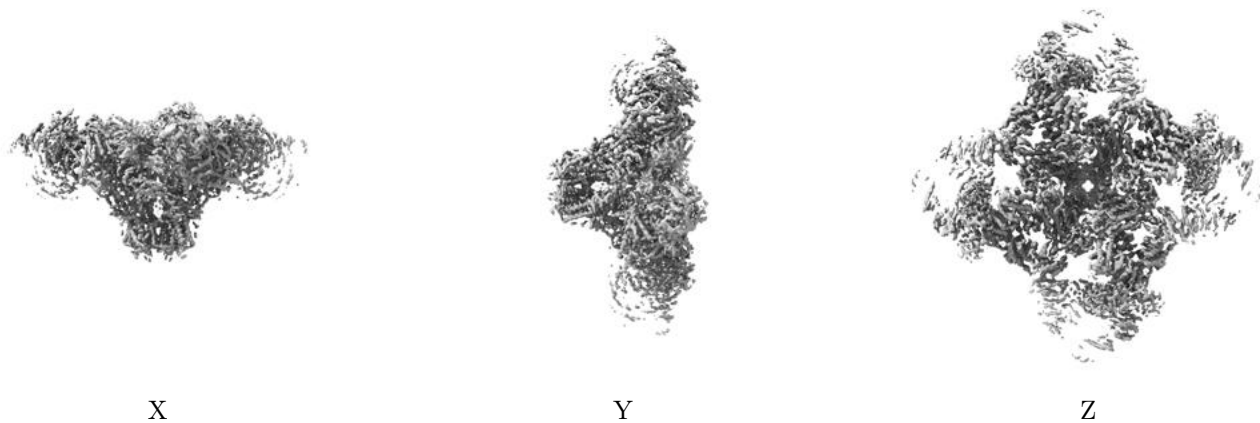


Z Index: 232

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

6.4 Orthogonal 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.

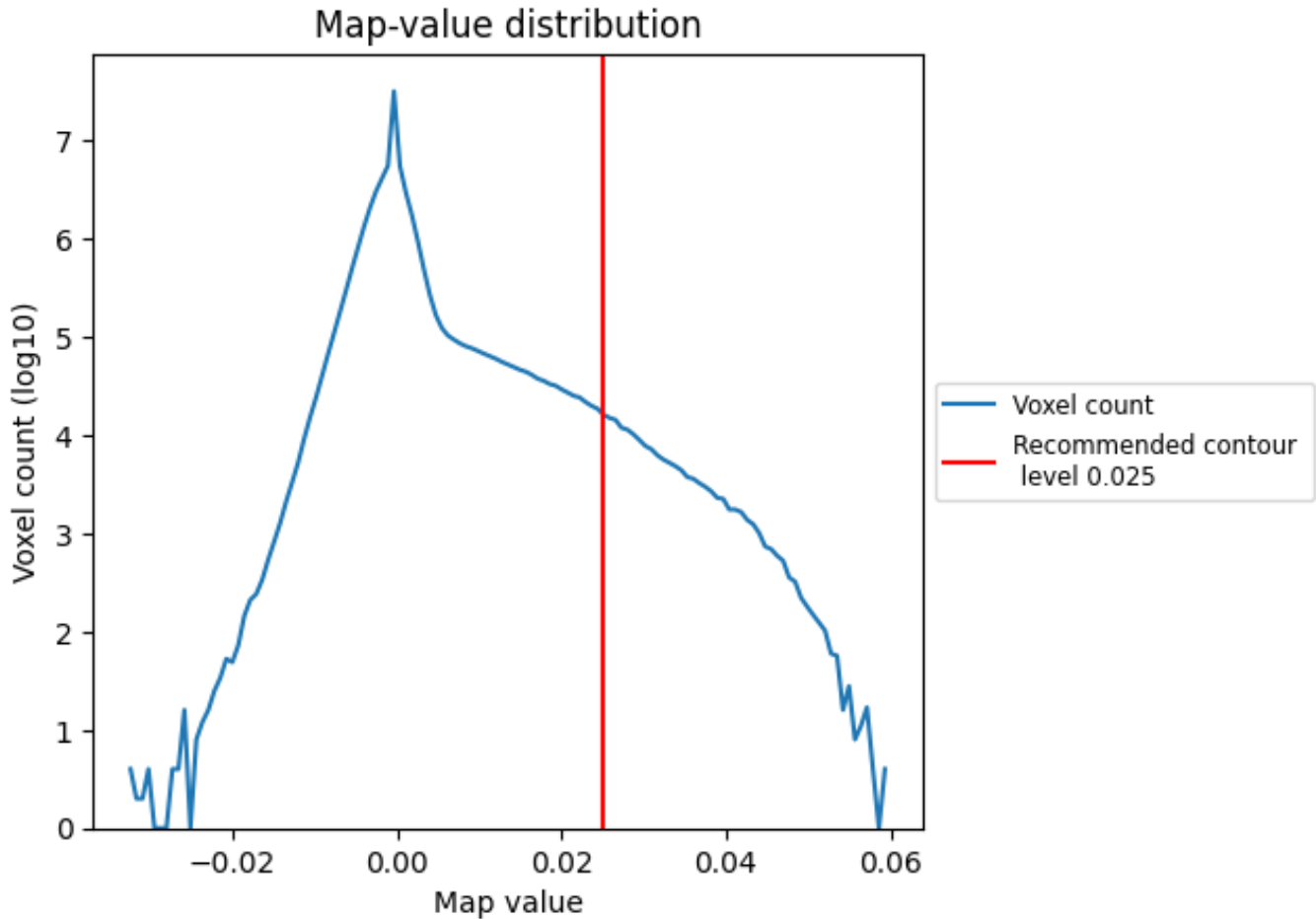
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

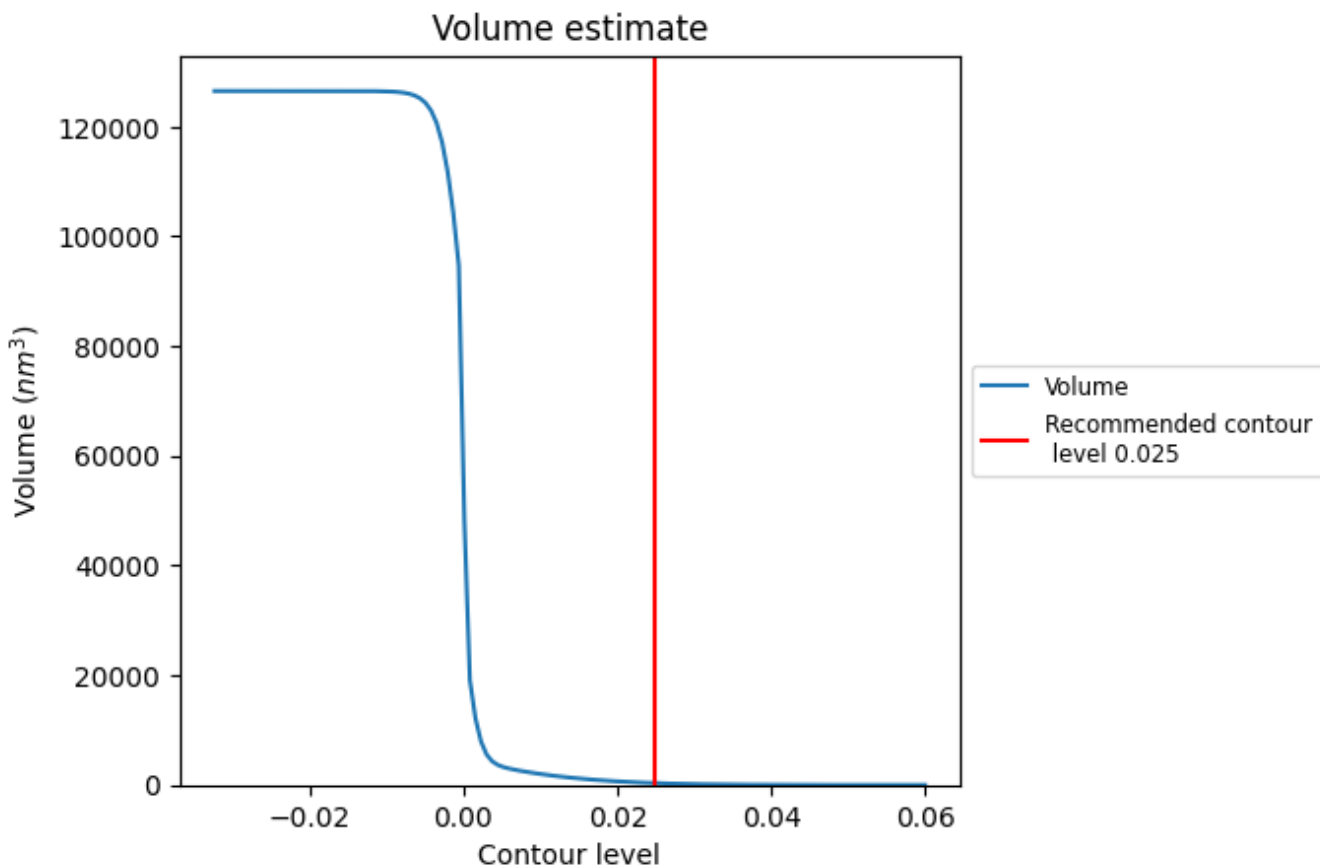
This section contains the results of statistical analysis of the map.

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.

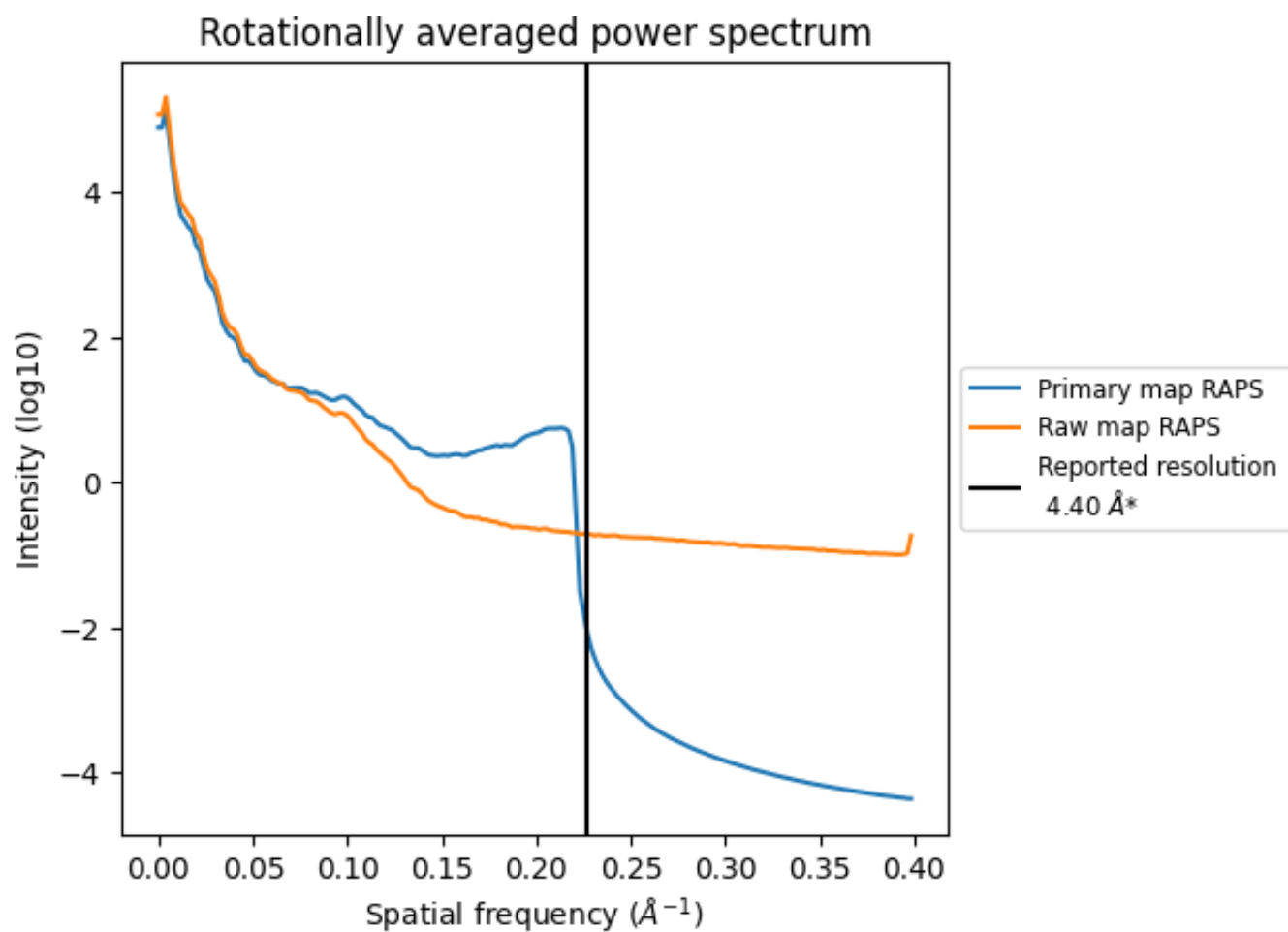
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 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 i

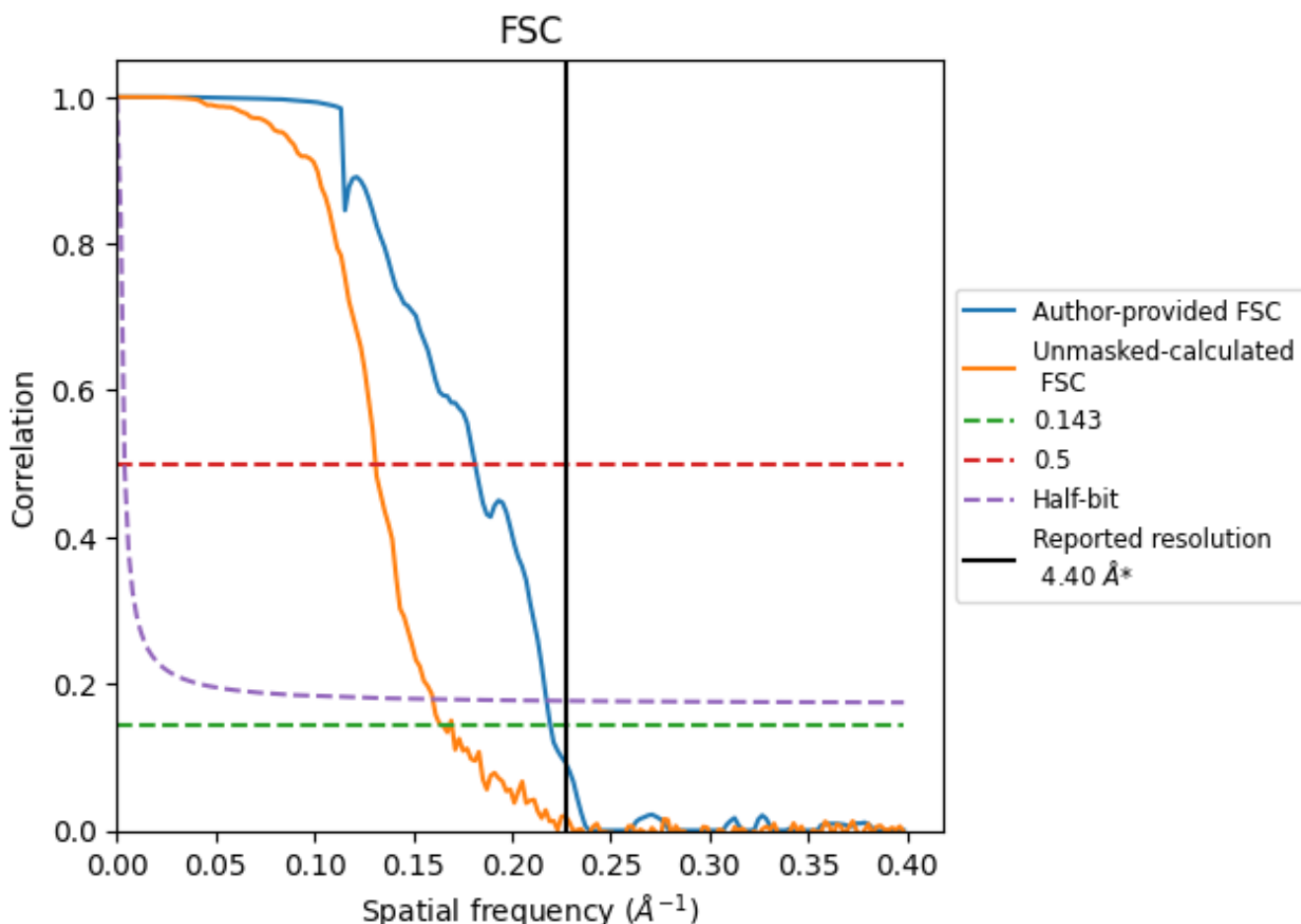


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

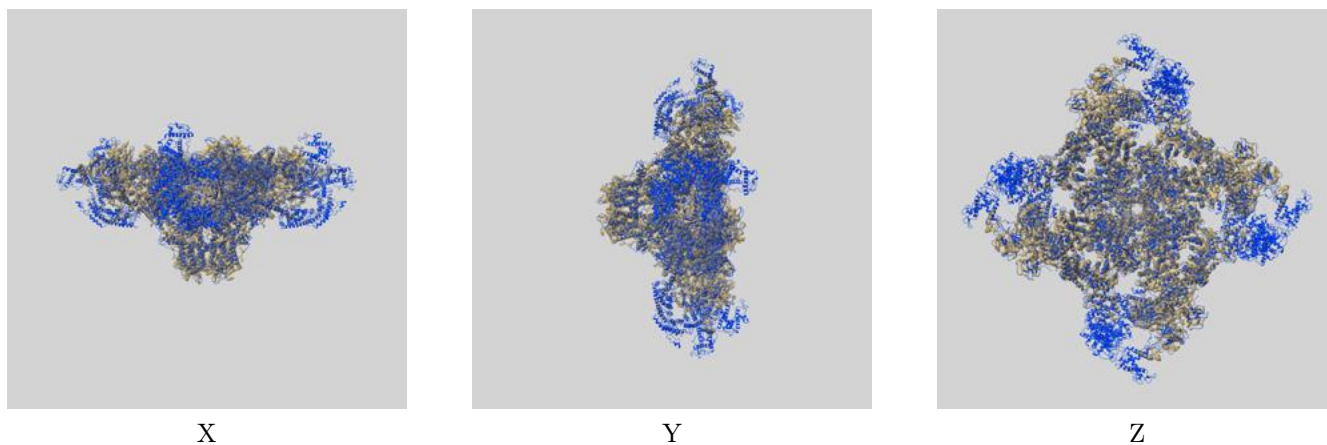
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.56	5.52	4.60
Unmasked-calculated*	6.06	7.64	6.25

*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](#)

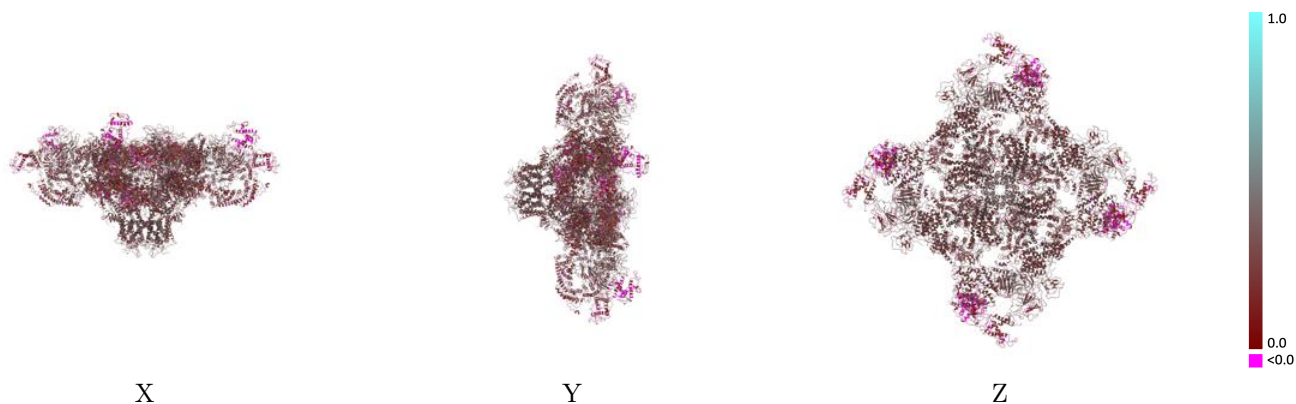
This section contains information regarding the fit between EMDB map EMD-8376 and PDB model 5T9V. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



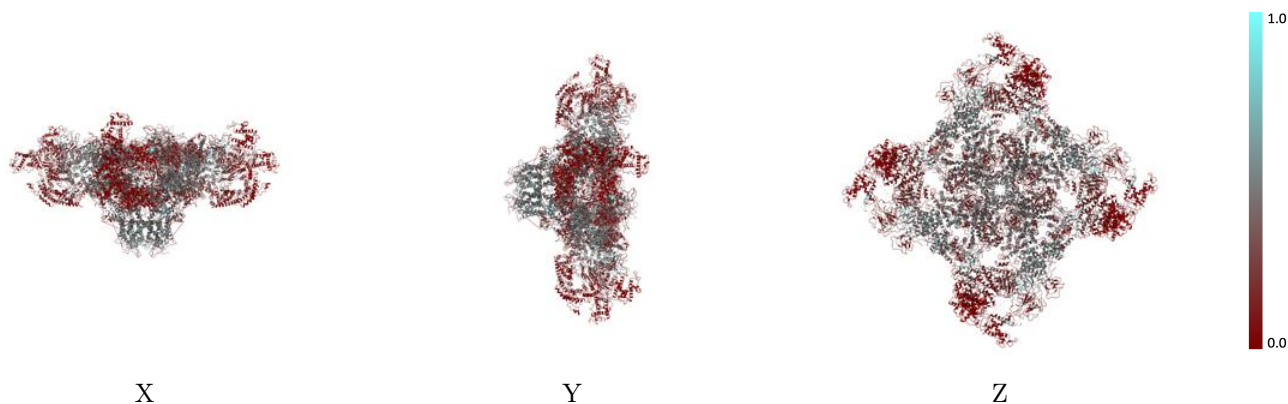
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



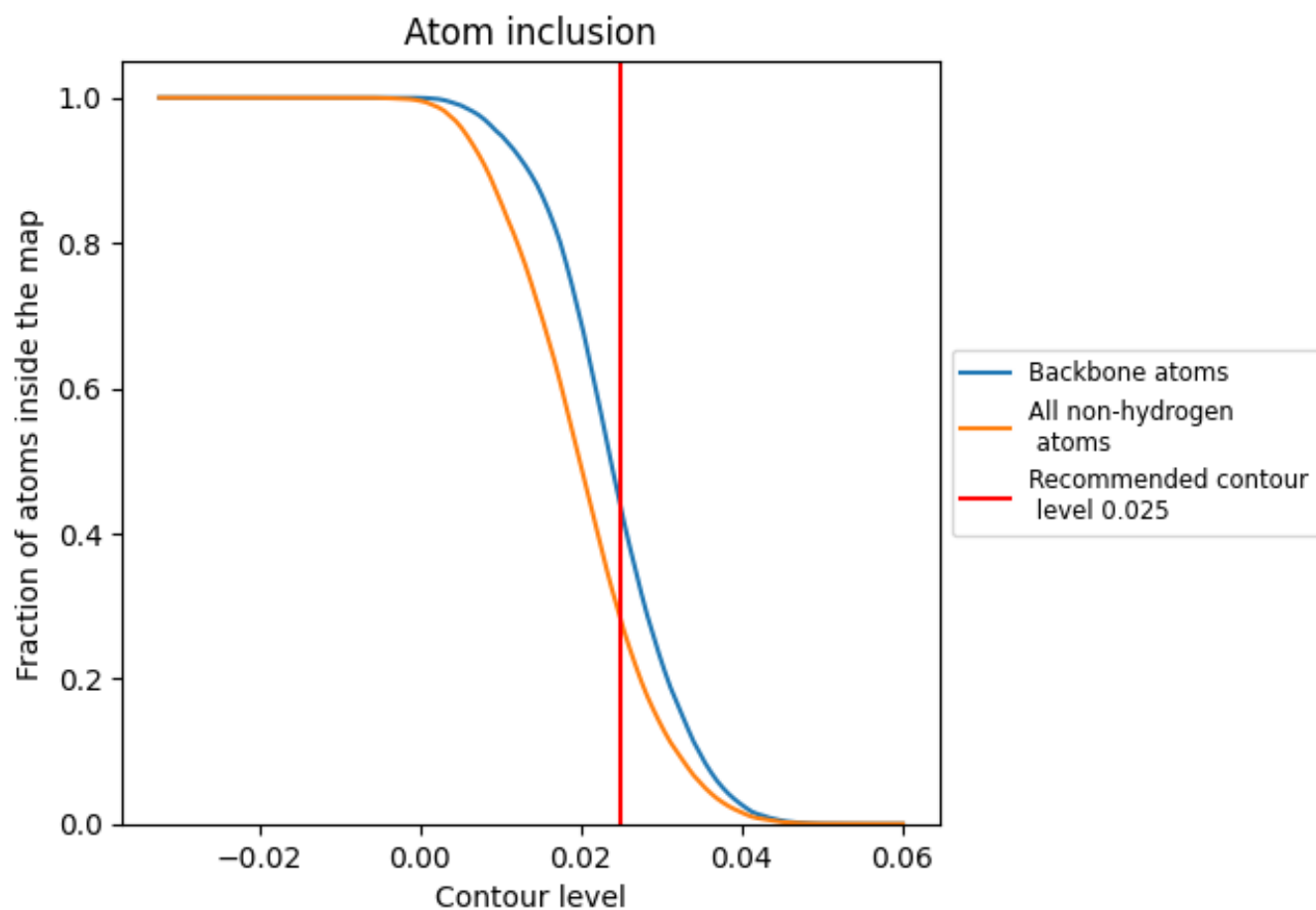
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 43% of all backbone atoms, 28% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2799	 0.2680
A	 0.2692	 0.3040
B	 0.2808	 0.2690
E	 0.2796	 0.2650
F	 0.2680	 0.3070
G	 0.2801	 0.2680
H	 0.2705	 0.3040
I	 0.2803	 0.2660
J	 0.2717	 0.3050

