



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:23 AM UTC

PDB ID : 5TAU / pdb_00005tau
EMDB ID : EMD-8385
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 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:

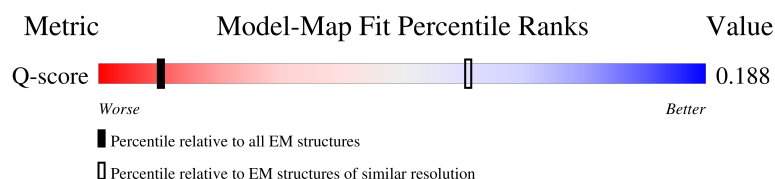
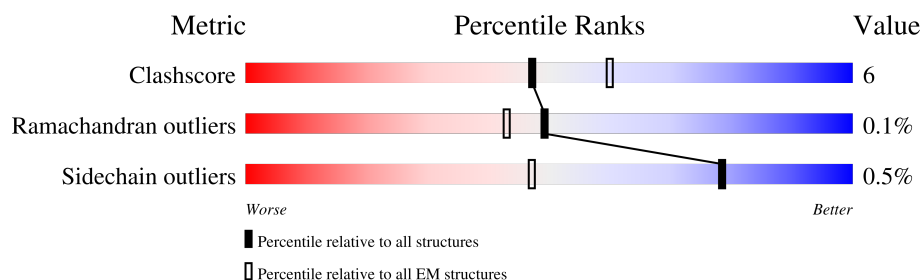
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.20 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	537 (5.70 - 6.70)

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	51% 70% 29%
1	F	108	52% 69% 30%
1	H	108	52% 72% 27%
1	J	108	53% 72% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	4416	51% 82% 12% 5%
2	E	4416	51% 82% 12% 5%
2	G	4416	51% 82% 12% 5%
2	I	4416	51% 82% 13% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121436 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.

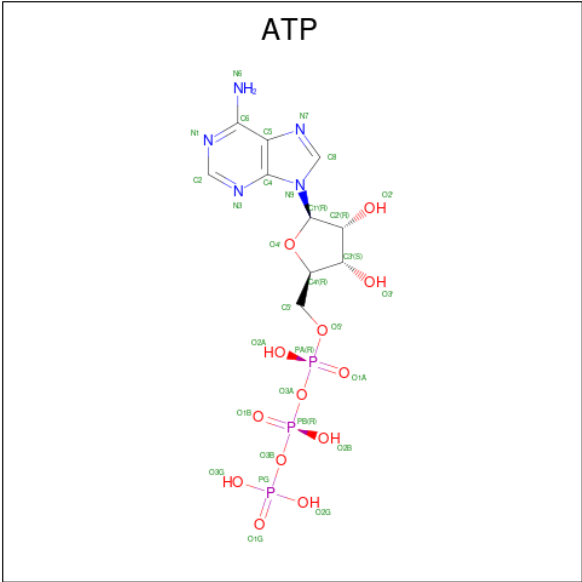
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

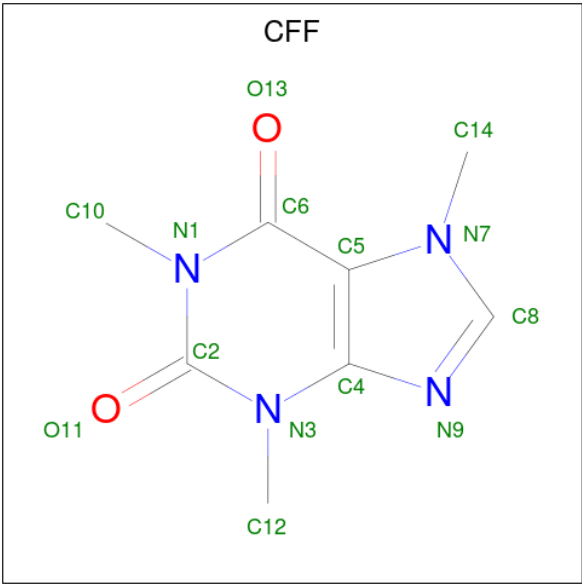
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		

- 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	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	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

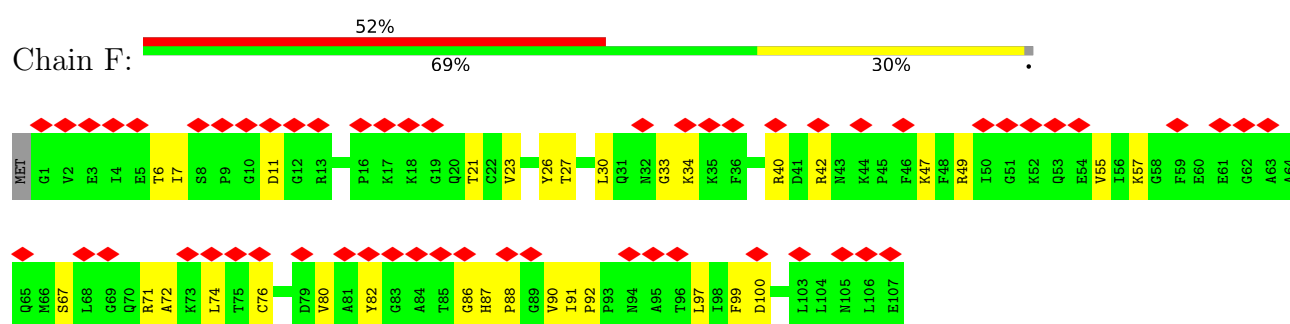
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

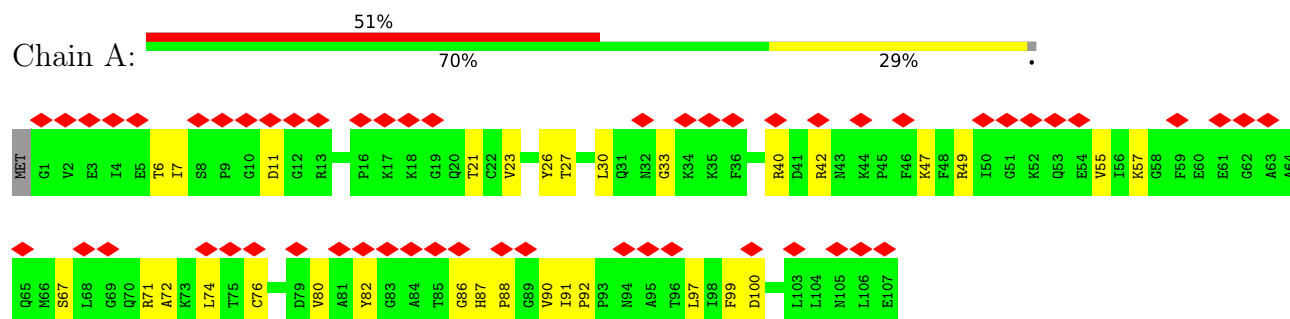
3 Residue-property plots [i](#)

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

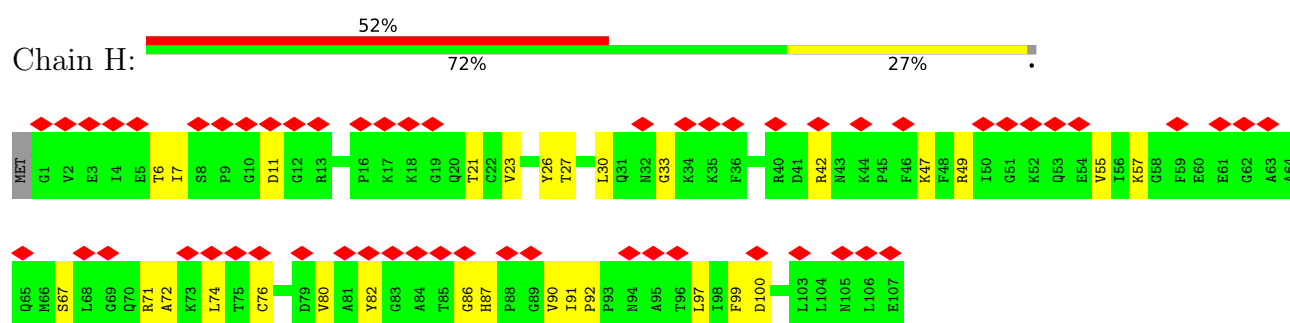
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

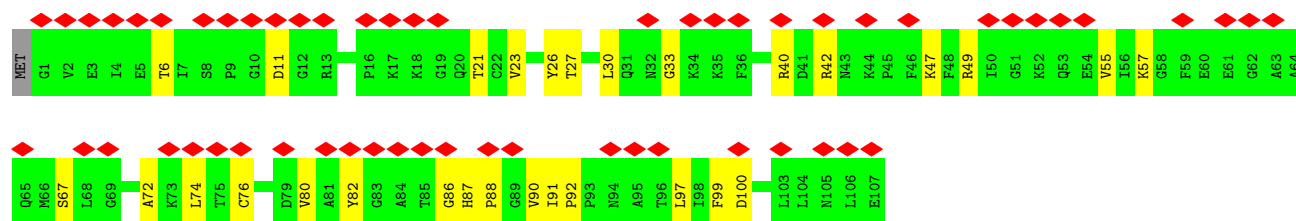


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

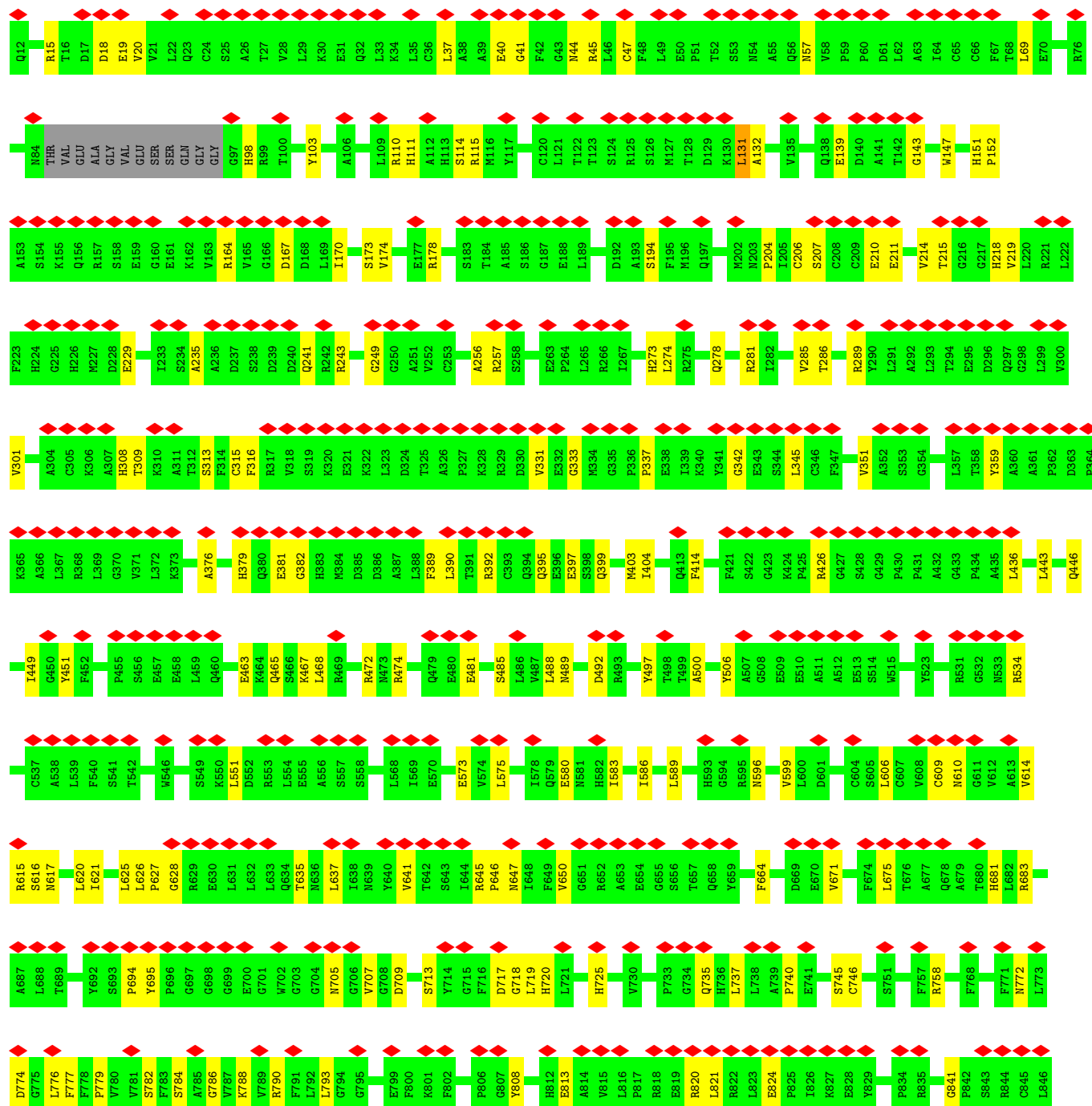
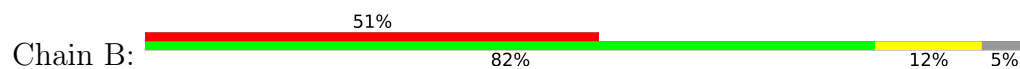


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





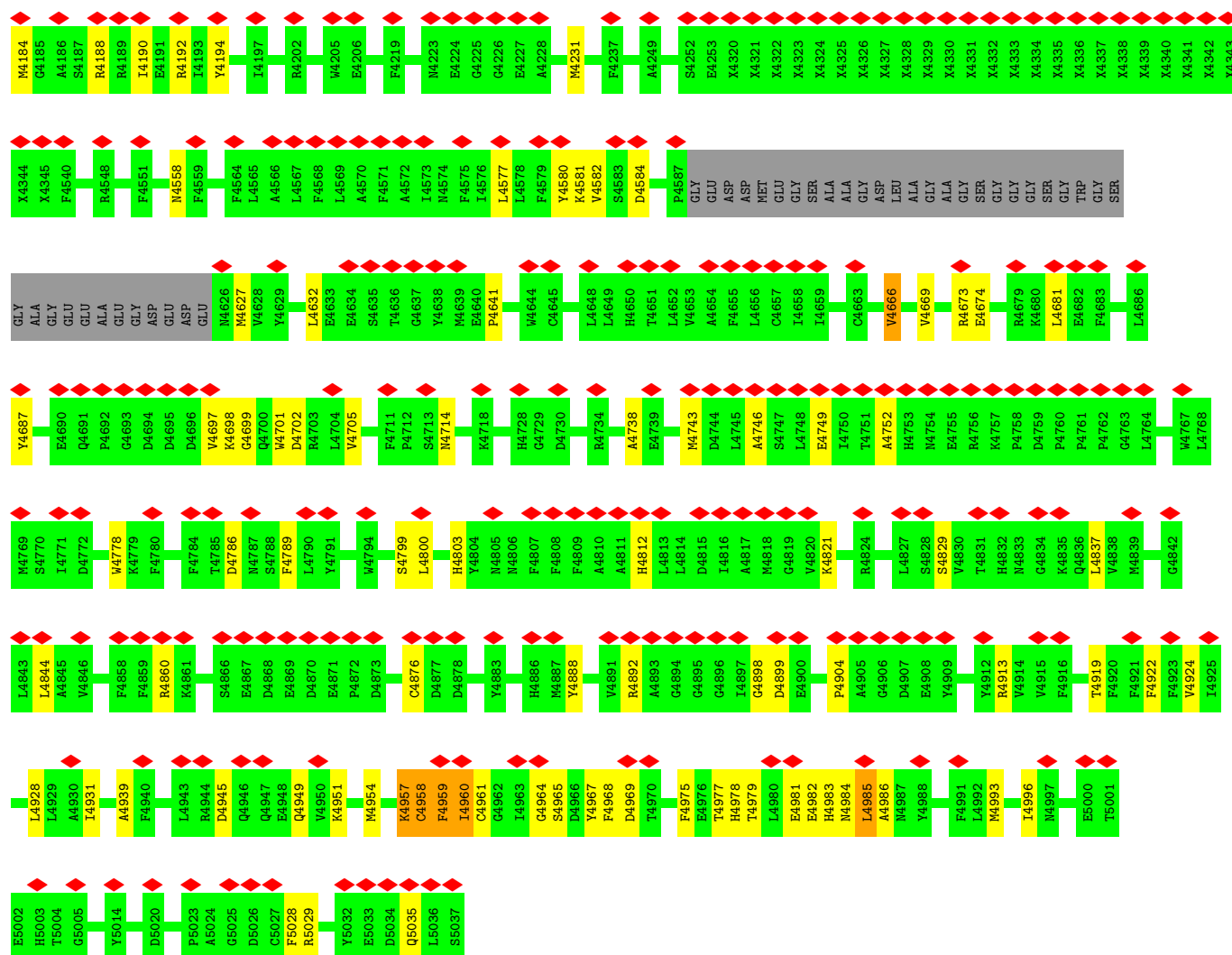
• Molecule 2: Ryanodine receptor 1



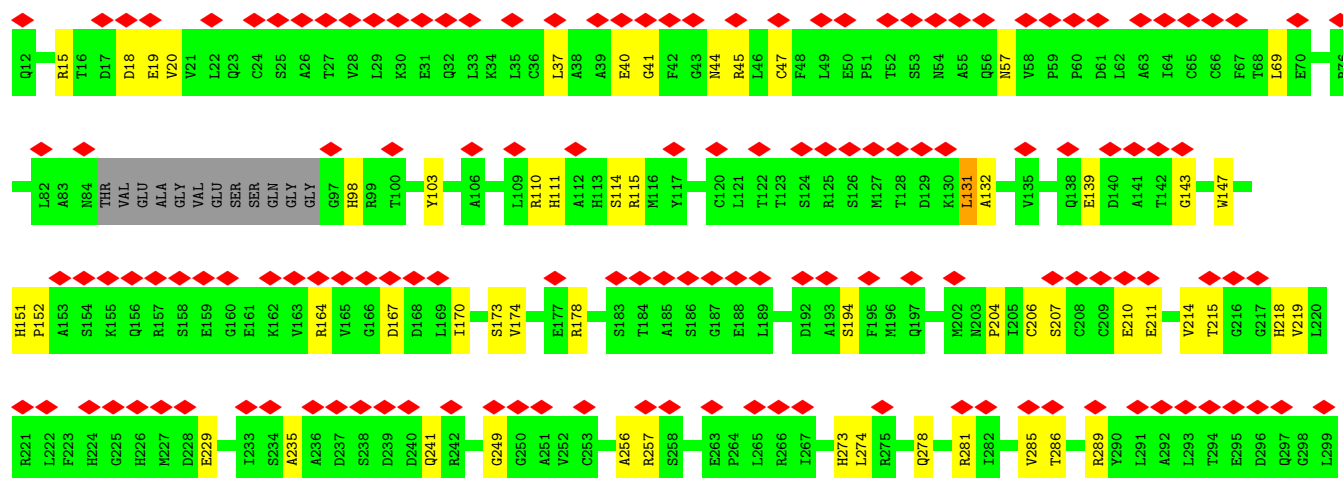
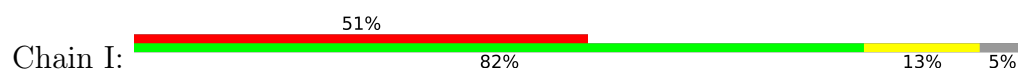
D1948	S847	E1873	A1794	M1648	X1548	D1207	L1134	V975	E915	H2011
D1949	H848	E1874	P1795	D1649	X1444	V1208	R1141	R976	P916	F2012
H1953	T849	GLU	A1796	X1445	X1446	S1209	GLN	L977	E917	K2013
A1960	D850	GLU	R1797	X1446	X1447	S1210	SER	T978	R918	L2006
R1964	GLU	E1733	I1802	X1447	X1448	L1211	TRP	A980	R919	H2017
R1964	GLU	E1734	P1803	X1448	X1449	L1212	D1070	P979	N920	F2018
Q1973	GLU	I1735	E1803	X1450	X1450	F1213	R1071	A981	N921	K2019
A1974	GLU	L1738	X1554	X1457	X1457	F1214	V1072	Q981	N922	L2020
S1975	GLU	L1739	X1555	X1458	X1458	F1215	R1073	T982	L923	H2021
R1976	GLU	T1739	X1556	X1459	X1459	I1216	I1074	T983	Q924	F2022
Y1977	GLU	Q1660	X1561	X1463	X1463	C1217	F1075	A989	M924	L2023
A1978	GLU	F1661	X1562	X1463	X1463	Q1220	A1076	GLN	S925	F2034
L1979	GLU	F1662	A1577	X1463	X1463	E1221	E1077	VAL	G926	
L1980	GLU	H1663	A1578	X1473	X1473	E1221	E1078	GLN	E927	
M1981	GLU	S1664	M1579	X1473	X1473	E1221	D1079	ASP	T928	
G1981	GLU	H1665	F1580	X1474	X1474	E1221	S1080	ASP	L929	
E1981	GLU	T1666	F1580	X1475	X1475	E1221	Y1081	ILE	L930	
R1982	GLU	L1667	A1588	X1478	X1478	E1221	Q1084	PRO	K930	
A1983	GLU	L1668	P1589	X1478	X1478	E1221	E1090	ALA	T931	
F1984	GLU	L1669	Q1590	X1489	X1489	E1221	F1090	ASN	L932	
T1985	GLU	Y1670	C1591	X1497	X1497	E1221	I1160	ARG	L933	
M1986	GLU	A1672	L1595	X1497	X1497	E1221	I1161	PRO	L934	
S1987	GLU	A1675	Q1598	X1503	X1503	E1221	F1162	R1020	L935	
A1988	GLU	L1676	M1599	X1504	X1504	E1221	T1163	PRO	L936	
A1989	GLU	G1677	L1600	X1505	X1505	E1221	L1164	PRO	L937	
F1990	GLU	R1680	V1603	X1506	X1506	E1221	M1165	P1023	G936	
T1991	GLU	L1685	W1605	X1507	X1507	E1221	M1170	A1030	H938	
A1992	GLU	H1688	F1605	X1513	X1513	E1221	S1171	T1031	V939	
R1993	GLU	V1689	F1612	X1514	X1514	E1221	D1172	K1032	G940	
R1994	GLU	D1690	L1613	X1515	X1515	E1221	G1173	N1035	M941	
T1995	GLU	Q1691	Q1614	X1516	X1516	E1221	T1174	R1036	D943	
L1996	GLU	L1694	G1615	X1519	X1519	E1221	E1175	D1037	E944	
R1997	GLU	L1698	GLU	X1520	X1520	E1221	E1176	S1038	K945	
E1997	GLU	L1699	THR	X1521	X1521	E1221	E1177	L1039	L946	
F1998	GLU	E1699	ARG	X1522	X1522	E1221	F1179	C1040	E947	
F1999	GLU	D1700	ALA	X1523	X1523	E1221	R1180	Q1041	D948	
L1999	GLU	A1701	GLY	X1524	X1524	E1221	L1110	A1042	N949	
S2000	GLU	L1702	E1692	X1525	X1525	E1221	P1111	V1043	L950	
S2000	GLU	L1703	A1627	X1526	X1526	E1221	L1112	R1044	K951	
P2001	GLU	L1707	V1628	X1527	X1527	E1221	D1113	T1045	K952	
P2002	GLU	R1708	Q1629	X1528	X1528	E1221	V1113	L1046	T953	
Q2003	GLU	A1709	C1630	X1529	X1529	E1221	E1114	L1047	K954	
E2004	GLU	G1710	Q1631	X1530	X1530	E1221	L1115	L1048	L955	
Q2005	GLU	Y1711	D1632	X1531	X1531	E1221	G1116	Y1049	P956	
L2006	GLU	Y1712	P1633	X1532	X1532	E1221	A1117	G1050	K957	
N2007	GLU	D1713	L1634	X1533	X1533	E1221	D1118	Y1051	T958	
H2011	GLU	L1718	M1637	X1534	X1534	E1221	L1120	N1052	Y959	
F2012	GLU	I1719	A1638	X1535	X1535	E1221	L1121	M1053	M960	
K2013	GLU	L1720	L1639	X1542	X1542	E1221	Y1122	E1054	M961	
D2014	GLU	E1721	E1644	X1543	X1543	E1221	H1127	PRO	N963	
F2015	GLU	L1721	M1645	X1544	X1544	E1221	R1128	ASP	G964	
A2016	GLU	ALA		X1545	X1545	E1221	R1131	GLN	Y965	
M1929	GLU	VAL		X1546	X1546	E1221		GLU	K966	
K1930	GLU	ALA		X1547	X1547	E1221		PRO	P967	
E2018	GLU	E1793				E1221		GLN	A968	
F2019	GLU					E1221		VAL	F910	
D2020	GLU					E1221			H911	
C2021	GLU					E1221			S912	
P2022	GLU					E1221			L913	
L2023	GLU					E1221			P914	
F2034	GLU					E1221			H974	

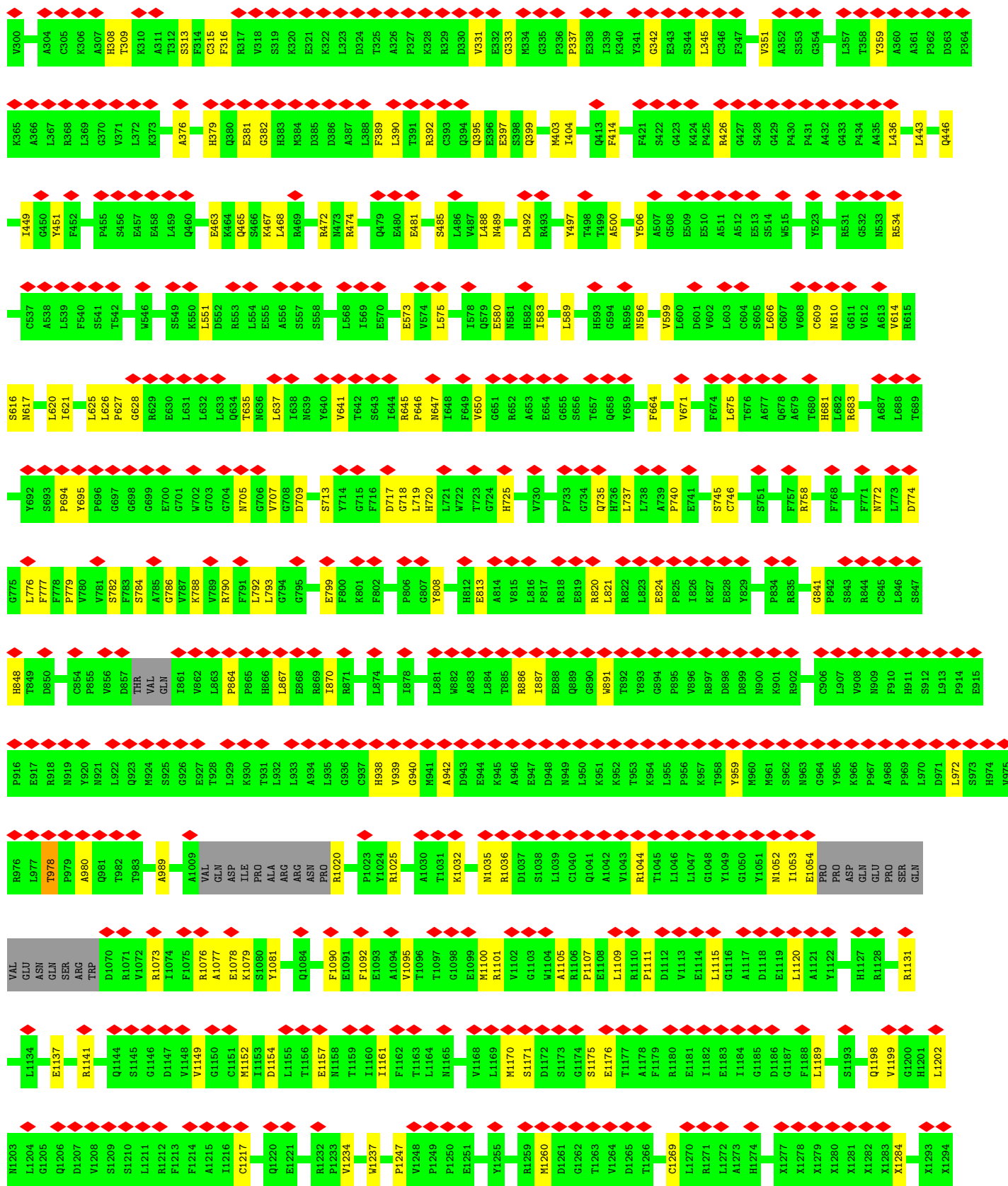


Q4102	L4030	G3857	T3772	P3695	X3600	X3540	X3437	X3377	X3251	X3188
F4103	L4031	M3858	R3773	Q3700	X3601	X3541	X3438	X3378	X3252	X3189
T4104	E4032	V3859	G3774	H3704	X3602	X3542	X3439	X3379	X3253	X3190
G4105	G4033	N3860	A3775	R3707	X3603	X3543	X3440	X3380	X3254	X3191
P4106	G4033	E3861	A3776	L3710	X3604	X3544	X3441	X3381	X3261	X3192
F4110	N4037	D3862	L3780	R3707	X3606	X3546	X3442	X3382	X3262	X3193
S4113	G4036	G3863	Q3781	L3710	X3607	X3547	X3443	X3383	X3263	X3194
C4114	N4037	T3864	S3784	E3712	X3608	X3548	X3444	X3384	X3264	X3195
E4115	G4038	V3865	A3785	R3711	X3609	X3549	X3445	X3385	X3265	X3196
S4116	A4041	N3867	K3787	L3716	X3610	X3550	X3446	X3386	X3266	X3197
A4117	V4049	R3868	G3788	K3714	X3611	X3551	X3450	X3388	X3267	X3198
D4118	E4050	G3869	K3788	K3715	X3612	X3552	X3451	X3389	X3268	X3199
E4119	N3955	N3870	E3789	L3716	X3613	X3553	X3452	X3390	X3269	X3200
N4120	S3956	M3871	D3717	D3717	X3613	X3554	X3453	X3391	X3271	X3201
E4121	K3959	E3872	T3790	E3718	X3614	X3555	X3454	X3392	X3272	X3202
N4122	Q3960	T3802	T3802	D3719	X3615	X3556	X3455	X3393	X3273	X3203
I4123	V3961	L3805	L3805	L3641	X3616	X3557	X3456	X3394	X3274	X3204
N4124	F3962	N3806	N3806	Y3642	X3617	X3558	X3457	X3395	X3275	X3205
F4125	N3963	K3875	G3807	N3643	X3618	X3559	X3458	X3396	X3276	X3206
E4126	E3967	D3877	G3808	L3644	X3619	X3560	X3459	X3397	X3277	X3207
A4129	G3971	D3878	N3809	H3647	X3620	X3561	X3460	X3398	X3278	X3208
N4130	P3972	E3879	K3731	S3656	X3621	X3562	X3461	X3399	X3279	X3209
R4131	C3973	F3880	S3732	G3657	X3622	X3563	X3462	X3400	X3280	X3210
F4132	C3973	T3881	C3733	K3658	X3623	X3564	X3463	X3401	X3281	X3211
A4136	N3976	D3882	H3734	A3659	X3624	X3565	X3464	X3402	X3282	X3212
E4152	A3981	K3815	C3733	A3660	X3625	X3566	X3465	X3403	X3283	X3213
H4153	H3982	M3816	L3735	A3661	X3626	X3567	X3466	X3404	X3284	X3214
H4154	S3983	L3817	L3735	K3662	X3627	X3568	X3467	X3405	X3285	X3215
P4155	R3984	D3822	E3737	L3663	X3628	X3569	X3468	X3406	X3286	X3216
H4156	L3985	K3823	G3738	T3664	X3629	X3570	X3469	X3407	X3287	X3217
F4172	N3986	E3825	E3740	E3665	X3630	X3571	X3511	X3408	X3288	X3218
R4159	F3992	V3826	E3741	H3667	X3631	X3572	X3512	X3409	X3289	X3219
L4160	F3996	F3828	GLY	S3668	X3632	X3573	X3513	X3410	X3290	X3220
R4161	A3997	Q3830	ALA	F3669	X3633	X3574	X3514	X3411	X3291	X3221
N4162	N3997	S3831	GLY	E3670	X3634	X3575	X3515	X3412	X3292	X3222
F4163	F3997	T3832	GLY	D3671	X3635	X3576	X3516	X3413	X3293	X3223
L4164	M4000	L3835	E3747	R3672	X3636	X3577	X3517	X3414	X3294	X3224
E4166	M4001	T3838	E3748	M3673	X3637	X3578	X3518	X3415	X3295	X3225
S4169	K4002	C3839	V3749	I3674	X3638	X3579	X3519	X3416	X3296	X3226
E4172	L4003	S3840	E3750	S3676	X3639	X3580	X3520	X3417	X3297	X3227
V4173	A4004	V3841	V3751	K3679	X3640	X3581	X3521	X3418	X3298	X3228
F4174	Q4005	D3842	S3752	A3680	X3641	X3582	X3522	X3419	X3299	X3229
R4175	D4006	L3843	F3753	G3681	X3642	X3583	X3523	X3420	X3300	X3230
F4176	D4007	F3847	E3754	G3682	X3643	X3584	X3524	X3421	X3301	X3231
Y4177	S4007	E3848	E3755	E3683	X3644	X3585	X3525	X3422	X3302	X3232
A4096	S4008	R3849	K3756	E3684	X3645	X3586	X3526	X3423	X3303	X3233
M4097	Q4009	Q3850	R3762	E3685	X3646	X3587	X3527	X3424	X3304	X3234
L4178	D4018	A3853	Y3765	E3686	X3647	X3588	X3528	X3425	X3305	X3235
Q4179	L4019	E3854	Q3766	E3687	X3648	X3589	X3529	X3426	X3306	X3236
R4180	L4020	G3855	Q3767	E3688	X3649	X3590	X3530	X3427	X3307	X3241
F4181	M4023	G3856	S3768	E3689	X3650	X3591	X3531	X3428	X3308	X3242
E4182	F4182	L3856	R3769	E3690	X3651	X3592	X3532	X3429	X3309	X3243
T4183	F4183	L3857	L3770	E3692	X3652	X3593	X3533	X3430	X3310	X3244
			H3771	E3693	X3653	X3594	X3534	X3431	X3311	X3245
				K3694	X3654	X3595	X3535	X3432	X3312	X3246
					X3655	X3596	X3536	X3433	X3313	X3247
					X3656	X3597	X3537	X3434	X3314	X3248
					X3657	X3598	X3538	X3435	X3315	X3249
					X3658	X3599	X3539	X3436	X3316	X3250



• Molecule 2: Ryanodine receptor 1

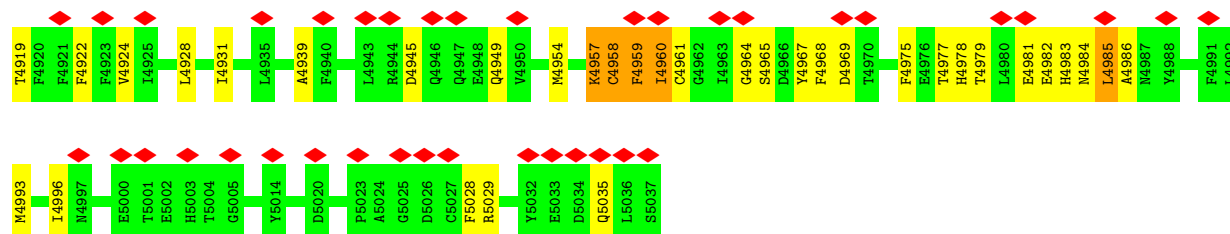




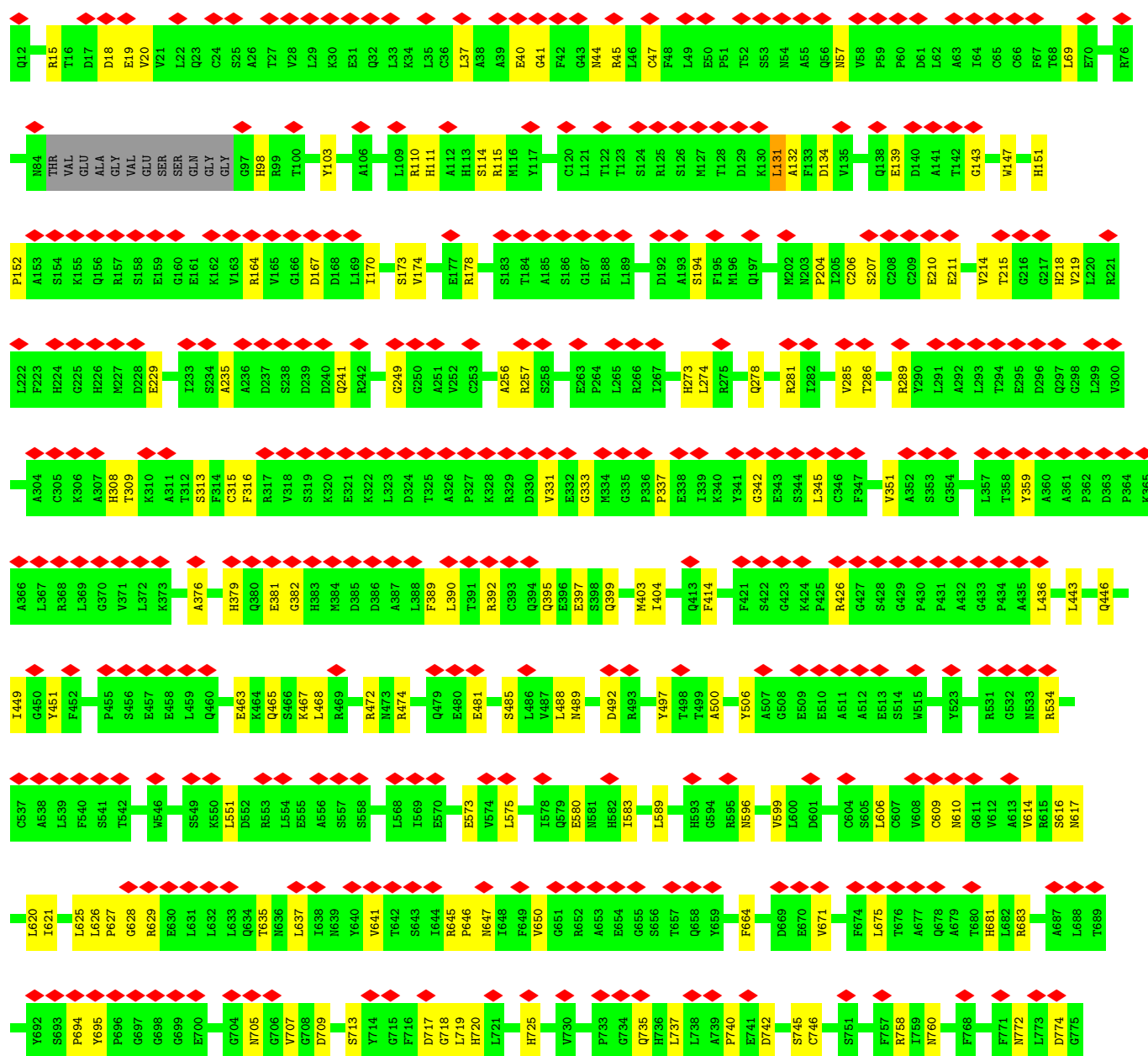
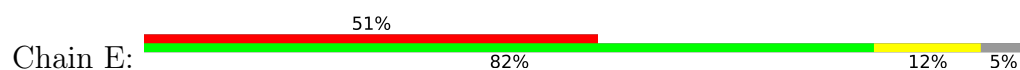


X2569	X25678	F2768	E2828	X2888	X2950	X3036	X3173	X3244	X3310	X3370	X3430	X3533
X2581	X2679	D2769	G2829	K2889	X2951	X3037	X3174	X3245	X3311	X3371	X3431	X3534
X2582	X2680	K2770	E2830	K2890	X2952	X3038	X3175	X3246	X3312	X3372	X3432	X3535
X2583	X2681	I2771	GLU	K2891	X2953	X3039	X3176	X3247	X3313	X3373	X3433	X3536
X2584	X2682	Q2772	ARG	E2892	X2954	X3040	X3177	X3248	X3314	X3374	X3434	X3537
X2585	X2683	Q2773	THR	E2893	X2955	X3041	X3178	X3249	X3315	X3375	X3435	X3538
X2586	X2684	I2774	GLU	L2894	X2956	X3042	X3179	X3250	X3316	X3376	X3436	X3539
	X2685	W2775	LYS	E2895	X2957	X3043		X3251	X3317	X3377	X3437	X3540
	X2686	S2776	LYS	A2896	X2958	X3044	X3188	X3252	X3318	X3378	X3438	X3541
X2595	X2687	Y2777	THR	K2897	X2959	X3045	X3189	X3253	X3319	X3379	X3439	X3542
X2596	X2688	G2778	ARG	G2898	X2960	X3046	X3190	X3254	X3320	X3380	X3440	X3543
X2597	X2689	E2779	LYS	G2899	X2961	X3047	X3191	X3255	X3321	X3381	X3441	X3544
X2598	X2690		ILE	G2900	X2962	X3048	X3192	X3256	X3322	X3382	X3442	X3545
X2599	X2691	W2781	SER	G2901	X2963	X3049	X3193	X3257	X3323	X3383	X3443	X3546
X2600	X2692	D2782	THR	H2902	X2964	X3050	X3194	X3258	X3324	X3384	X3444	X3547
X2601	X2693	E2783	ALA	P2903	X2965	X3051	X3195	X3259	X3325	X3385	X3445	X3548
X2602	X2694	E2784	GLN	L2904	X2966	X3052	X3196	X3260	X3326	X3386	X3446	X3549
	X2695	E2785	THR	L2905	X2967		X3197	X3261	X3327	X3387	X3447	
X2605	X2696	L2786	TYR	V2906	X2968	X3055	X3198	X3262	X3328	X3388	X3450	X3551
X2606	X2697	K2786	ASP	V2907	X2969	X3056	X3199	X3263	X3329	X3389	X3451	X3552
X2607	X2698	T2787	ARG	P2907	X2970	X3057	X3200	X3264	X3330	X3390	X3452	X3553
	X2699	H2788	GLU	Y2908	X2971	X3058	X3201	X3265	X3331	X3391	X3453	X3554
X2617	X2699	P2789	GLY	D2909	X2972	X3059	X3202	X3266	X3332	X3392	X3454	X3555
X2618	X2700	M2790	Y2855	T2910	X2973	X3060	X3203	X3267	X3333	X3393	X3455	X3556
X2619	X2701	L2791	P2856	L2911	X2974	X3061	X3204	X3268	X3334	X3394	X3456	X3557
X2620	X2702	D2792	Q2857	T2912	X2975	X3062	X3205	X3269	X3335	X3395	X3457	X3558
X2621	X2703	X2703	Q2858	A2913	X2976	X3063	X3206	X3270	X3336	X3396	X3458	X3559
X2622	X2704	P2793	P2859	K2914	X2977	X3134	X3207	X3271	X3337	X3397	X3459	X3560
X2623	N2734	Y2794	P2860	E2915	X2978	X3135	X3208	X3272	X3338	X3398	X3460	X3561
X2624	F2735	K2795	D2861	E2916	X2979	X3136	X3209	X3273	X3339	X3399	X3461	X3562
X2625	D2736	T2796	L2862	A2917	X2980	X3137	X3210	X3274	X3340	X3400	X3462	X3563
X2626	P2737	T2797	S2863	R2918	X2981	X3138	X3211	X3275	X3341	X3401	X3463	X3564
X2627	R2738	S2798	G2864	D2919	X2982	X3139	X3212	X3276	X3342	X3402	X3464	X3565
X2628	P2739	E2799	V2865	E2920	X2983	X3140	X3213	X3277	X3343	X3403	X3465	X3566
X2629	X2740	X2800	T2866	E2921	X2984	X3141	X3214	X3278	X3344	X3404	X3466	X3567
	E2741	D2801	L2867	X2922	X2985	X3142	X3215	X3279	X3345	X3405	X3467	X3568
		X2802	S2868	A2923	X2986	X3143	X3216	X3280	X3346	X3406	X3468	X3569
X2644	L2743	E2803	R2869	Q2924	X2987	X3144	X3217	X3281	X3347	X3407	X3511	X3570
X2645	N2744	I2804	E2870	Q2925	X2988	X3145	X3218	X3282	X3348	X3408	X3512	X3571
X2646	V2745	X2805	E2871	L2926	X2989	X3146	X3219	X3283	X3349	X3409	X3513	X3572
X2647	X2746	R2806	Q2872	X2927	X2990	X3147	X3220	X3284	X3350	X3410	X3514	X3573
X2648	I2747	W2807	A2873	K2928	X2991	X3148	X3221	X3285	X3351	X3411	X3515	X3574
X2649	P2748	E2749	M2874	F2929	X2992	X3149	X3222	X3286	X3352	X3412	X3516	X3575
X2650	X2750	K2750	A2875	L2930	X2993	X3150	X3223	X3287	X3353	X3413	X3517	X3576
X2651	L2751	E2811	E2876	Q2931	X2994	X3151	X3224	X3288	X3354	X3414	X3518	X3577
X2652	D2752	S2812	Q2877	M2932	X2995	X3152	X3225	X3289	X3355	X3415	X3519	X3578
X2653	S2753	L2813	L2878	N2933	X2996	X3153	X3226	X3290	X3356	X3416	X3520	X3579
X2654	F2754	X2814	A2879	G2934	X2997	X3154	X3227	X3291	X3357	X3417	X3521	X3580
		A2815	E2880	Y2935	X2998	X3155	X3228	X3292	X3358	X3418	X3522	X3581
X2657	X2755	M2816	N2881	A2936	X2999	X3156	X3229	X3293	X3359	X3419	X3523	X3582
X2658	K2756	L2817	Y2882	V2937	X3000	X3157	X3230	X3294	X3360	X3420	X3524	X3583
X2659	F2757	A2818	H2883	T2938	X3001	X3158	X3231	X3295	X3361	X3421	X3525	X3584
X2670	A2759	X2819	N2884	T2939	X3002	X3159	X3232	X3296	X3362	X3422	X3526	X3585
X2671	E2760	W2819	T2885	R2942	X3003	X3160	X3233	X3297	X3363	X3423	X3527	X3586
X2672	X2761	E2820	W2886	X2943	X3004	X3161	X3234	X3298	X3364	X3424	X3528	X3587
X2673	T2762	W2821	G2887	X2944	X3005	X3162	X3235	X3299	X3365	X3425	X3529	X3588
X2674	H2763	I2823		X2945	X3006	X3163	X3236	X3300	X3366	X3426	X3530	X3589
	E2824	X2825		X2946	X3007	X3170	X3237	X3301	X3367	X3427	X3531	X3590
	K2765	A2826		X2947	X3008	X3171	X3238	X3302	X3368	X3428	X3532	X3591
	W2766	R2827		X2948	X3009	X3172	X3239	X3303	X3369	X3429		X3592

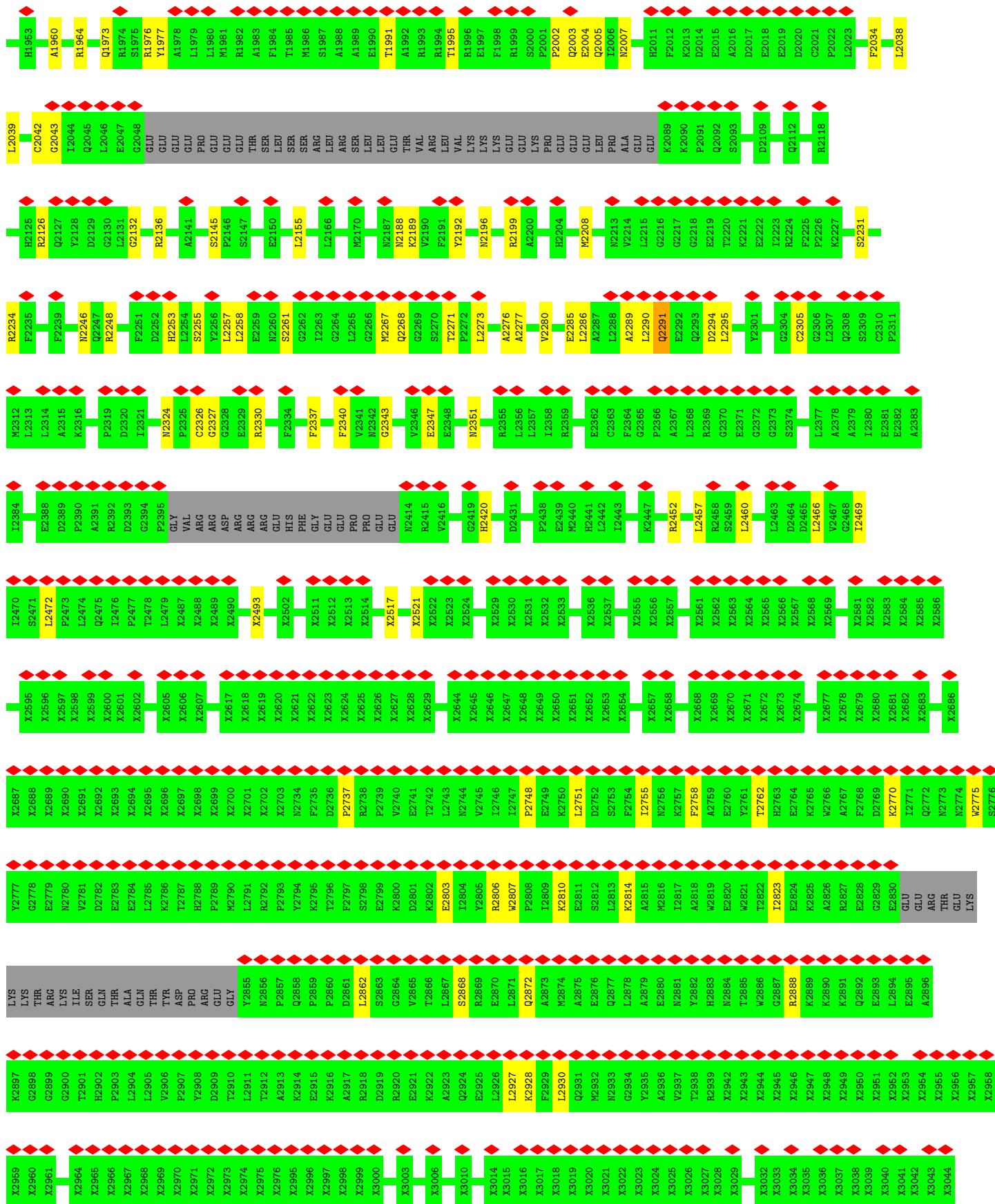




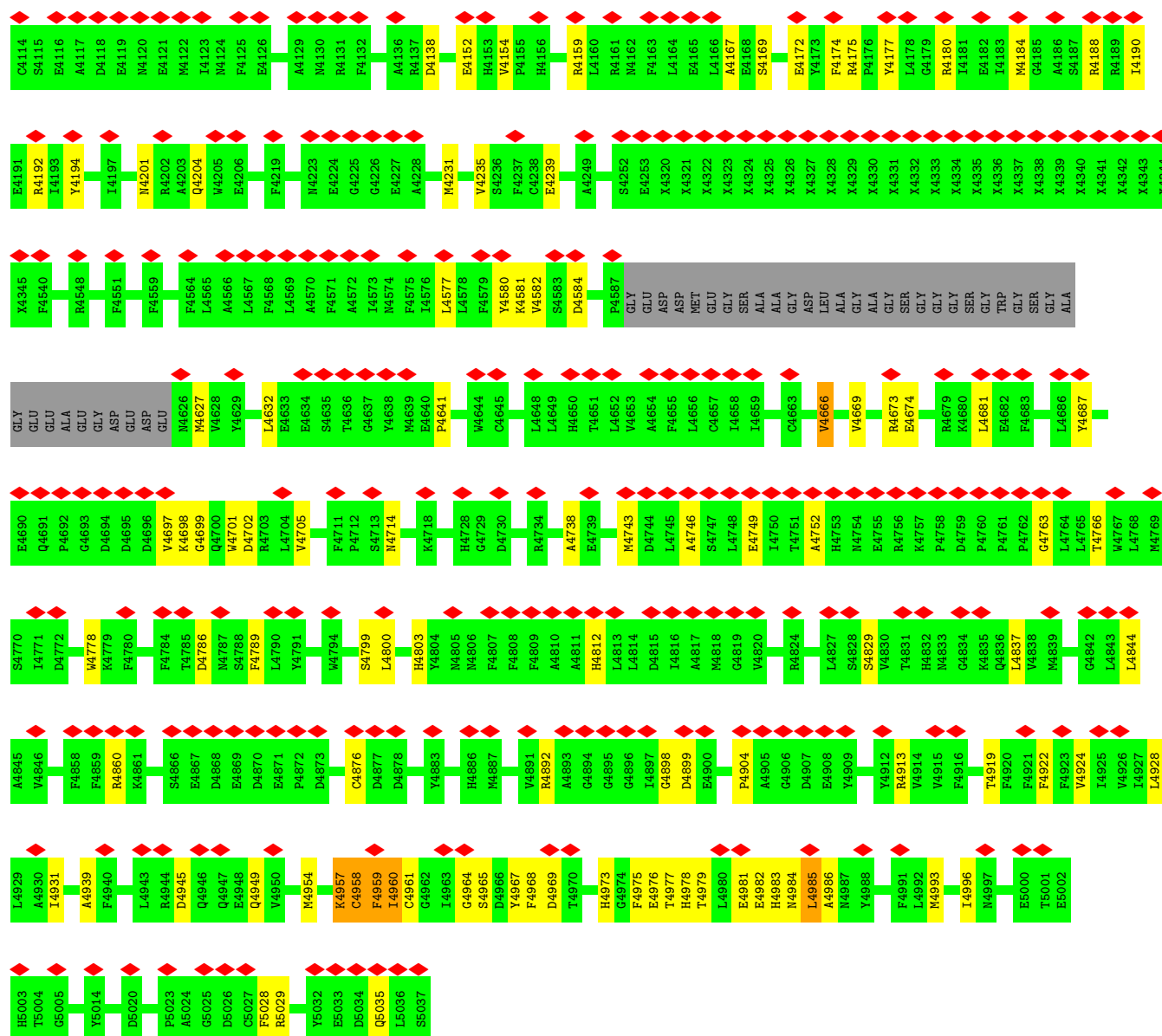
• Molecule 2: Ryanodine receptor 1



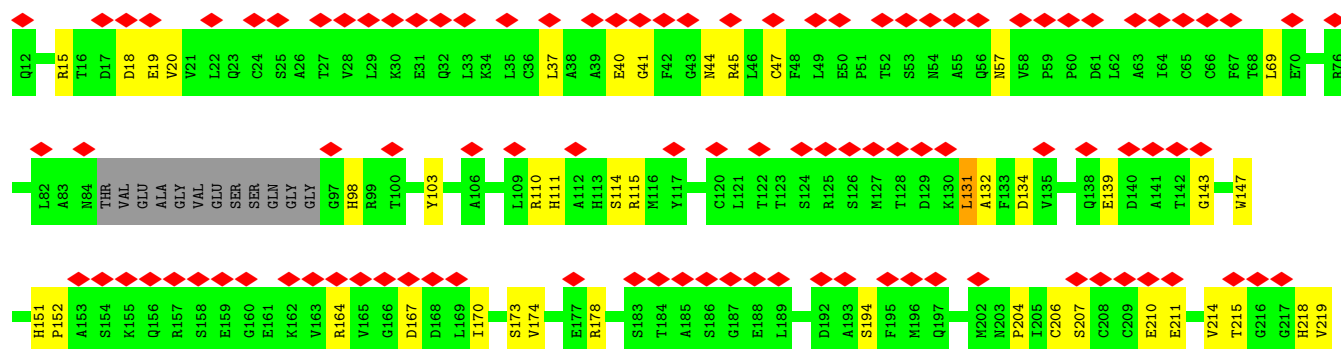
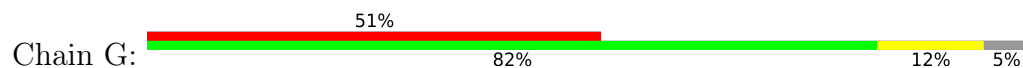
GLU	L1794	L1725	D1649	X1549	X1444	V1208	R1141	SER	A980	Y920	C964	L776
GLU	P1795	S1726	I1650	X1550	X1445	S1209	Q1144	ARG	Q981	N921	P855	F777
GLU	A1796	R1727	E1651	X1551	X1446	S1210	Q1145	THR	T982	L922	V856	F778
GLU	R1797	R1728	L1653	X1554	X1447	L1211	G1146	D1070	T983	Q923	D857	P779
GLU	I1802	E1733	S1654	X1555	X1448	R1212	D1147	R1071	A989	N924	VAL	V780
GLU	P1803	Y1734	E1655	X1556	X1449	F1213	D1148	V1072	A1009	S925	GLN	V781
GLU	A1806	I1735	R1656	X1557	X1450	F1214	V1149	R1073	VAL	Q926	S783	S784
GLU	R1807	L1738	D1657	X1561	X1457	A1215	V1150	F1074	GLN	E927	A785	K788
GLU	R1808	T1739	L1659	X1562	X1458	I1216	G1151	R1075	ASP	T928	V862	V789
GLU	L1812	E1741	Q1660	X1566	X1459	C1217	M1152	A1077	ILE	L929	L863	R790
GLU	R1813	T1742	R1661	X1567	X1463	Q1220	D1154	E1078	PRO	K930	P864	F791
GLU	M1814	H1662	H1663	X1568	X1473	E1221	L1153	S1080	ALA	T931	P865	L867
GLU	L1815	S1664	S1664	X1569	X1474	R1232	L1155	Y1081	ARG	L932	H866	G795
GLU	D1821	H1665	T1666	X1570	X1475	P1233	L1156	Q1084	ASN	A934	E568	E799
GLU	G1822	L1667	R1667	X1578	X1478	V1234	E1157	F1090	PRO	L935	R869	F800
GLU	G1823	R1668	L1668	X1588	X1479	W1237	M1158	E1091	R1020	G936	R871	K801
GLU	Q1824	L1669	L1669	P1589	X1489	P1247	I1160	F1092	P1023	Q937	L874	F802
GLU	H1825	Y1670	Y1670	Q1590	X1497	V1248	I1161	A1094	Y1024	H938	I878	P806
GLU	A1826	R1671	A1672	C1591	X1503	P1249	F1163	V1095	R1025	V939	L881	G807
GLU	R1827	L1676	L1676	L1595	X1504	E1251	L1164	T1096	A1030	G940	L882	Y808
GLU	L1828	G1677	G1677	L1600	X1505	Y1255	M1165	T1097	T1031	M941	A883	E813
GLU	P1829	L1680	L1680	L1605	X1506	W1259	W1169	G1098	K1032	A942	L884	A814
GLU	V1830	R1680	R1680	W1605	X1507	R1259	M1170	M1100	N1035	E944	T885	V815
GLU	G1831	L1685	L1685	W1605	X1513	M1260	S1171	V1102	R1036	K945	T886	L816
GLU	G1832	H1688	H1688	F1612	X1514	D1261	D1172	G1103	D1037	E947	I887	P817
GLU	Q1837	Y1689	Y1689	L1613	X1515	G1262	S1173	G1104	S1038	D948	T887	L818
GLU	V1839	L1690	L1690	Q1614	X1516	T1263	G1174	A1105	L1039	N949	E888	R818
GLU	L1840	Q1691	Q1691	V1615	X1519	V1264	S1175	R1106	C1040	L950	Q889	E819
GLU	L1842	L1694	L1694	W1615	X1520	D1265	E1176	F1107	Q1041	K951	Q890	R820
GLU	V1845	L1698	L1698	THR	X1521	T1266	T1177	E1108	A1042	K952	W891	L821
GLU	L1848	E1699	E1699	ARG	X1522	C1269	A1178	L1109	V1043	T953	T892	R822
GLU	I1853	L1700	L1700	ALA	X1523	L1270	F1179	P1111	R1044	K954	L823	L823
GLU	F1854	D1700	D1700	GLY	X1524	R1271	R1180	D1112	T1045	L955	L824	E824
GLU	G1855	A1701	A1701	E1622	X1525	L1272	E1181	V1113	L1046	P956	P825	F825
GLU	D1856	H1702	H1702	L1633	X1526	A1273	I1182	E1114	L1047	K957	I826	K827
GLU	E1857	L1707	L1707	L1634	X1527	H1274	E1183	L1115	Y1049	T958	K827	E828
GLU	P1859	R1708	R1708	M1637	X1528	X1277	I1184	G1116	G1050	M960	E828	Y829
GLU	L1860	A1709	A1709	L1639	X1529	X1278	G1185	A1117	Y1051	M961	N900	Y829
GLU	Q1861	G1710	G1710	L1639	X1530	X1279	D1186	D1118	M1052	S962	K901	P834
GLU	M1862	Y1711	Y1711	L1639	X1531	X1280	F1187	E1119	I1053	N963	R902	R835
GLU	M1865	Y1712	Y1712	E1644	X1532	X1281	L1189	E1119	E1054	G964	C906	G841
GLU	E1869	D1713	D1713	M1645	X1533	X1282	S1193	A1121	PRO	Y965	L907	P842
GLU	V1870	I1718	I1718	L1648	X1534	X1283	Q1198	Y1122	ASP	K966	V908	S843
GLU	T1871	H1719	H1719	L1648	X1542	X1284	G1200	R1128	GLN	P967	N909	R844
GLU	T1872	L1720	L1720	E1644	X1543	X1293	H1201	R1131	PRO	A968	F910	C845
GLU	E1873	E1721	E1721	M1645	X1544	X1294	L1202	L1134	SER	P969	H911	L846
GLU	ALA	ALA	ALA	M1648	X1545	X1440	M1203	E1137	VAL	D971	S912	S847
GLU	GLY	GLY	GLY	M1648	X1546	X1441	L1204	GLN	GLN	L972	L913	H848
GLU	VAL	VAL	VAL	M1648	X1547	X1442	G1205	GLN	GLN	S973	P914	T849
GLU	ALA	ALA	ALA	M1648	X1548	X1443	Q1206	GLN	GLN	H974	E915	D850
GLU	E1793	E1793	E1793	E1793	X1549	X1444	D1207	GLN	GLN	V975	P916	
GLU										R976	E917	
GLU										L977	R918	
GLU										T978	N919	
GLU										P979		

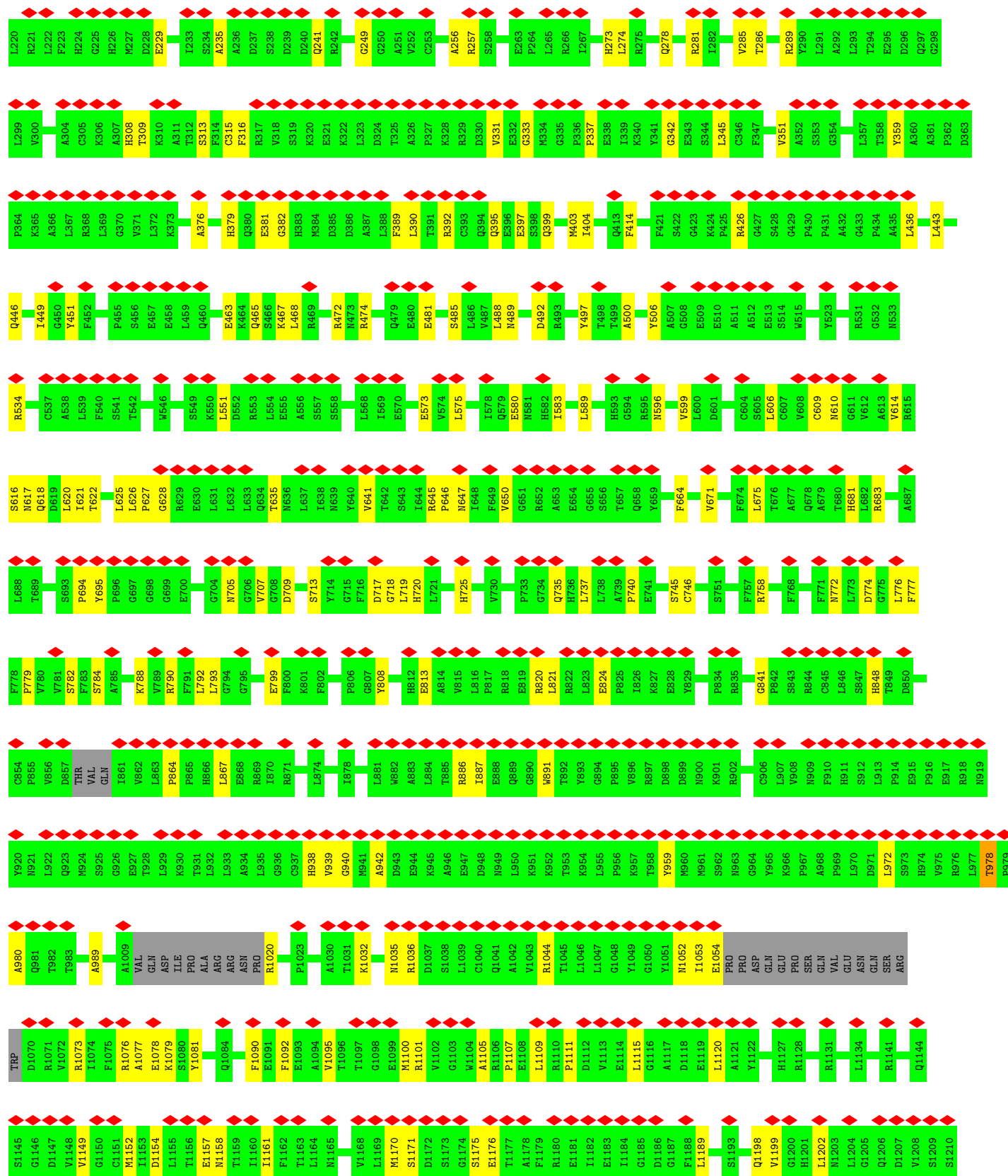


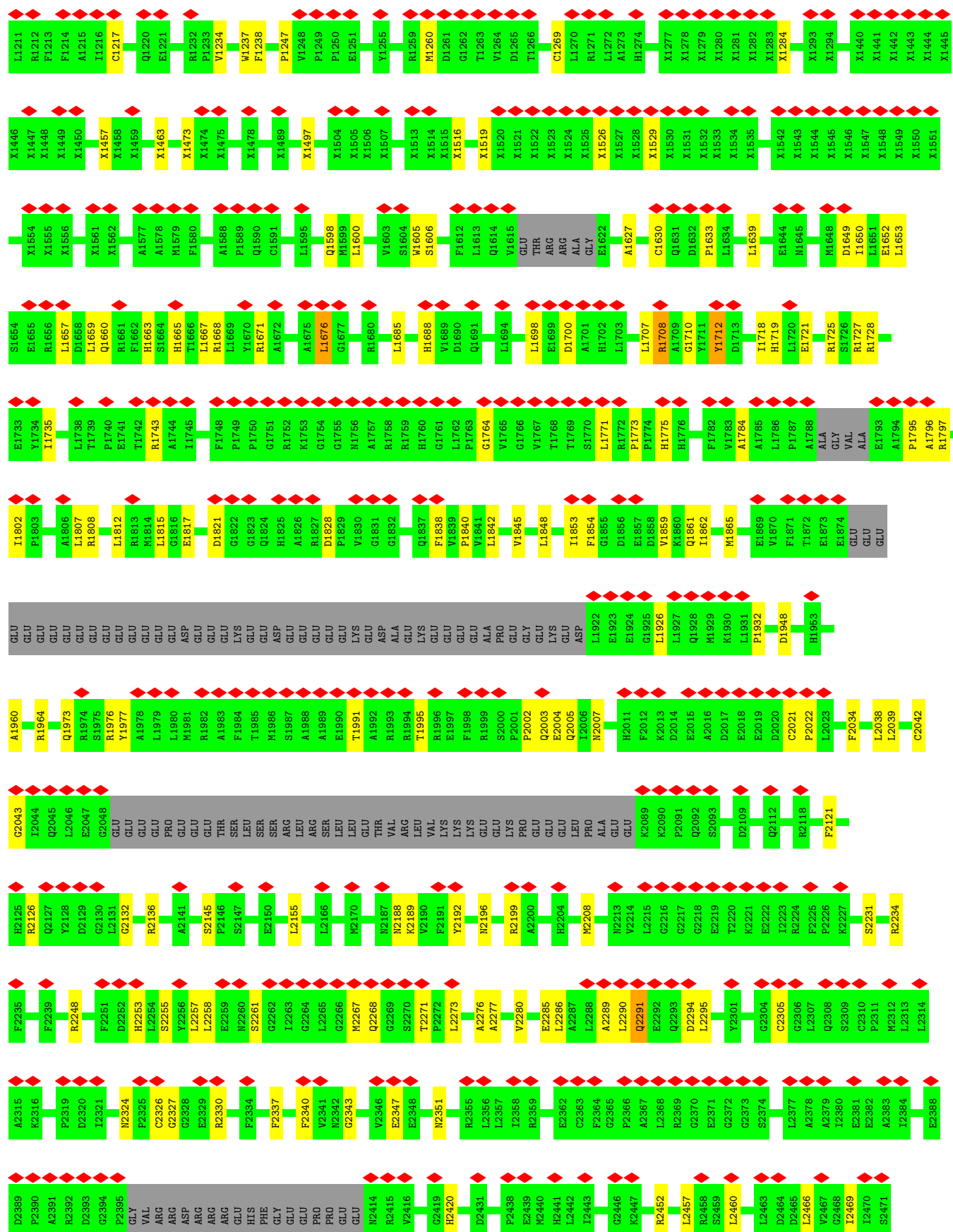
G4038	G3939	D3862	L3780	H5704	X3439	X3379	X3319	X3253	X3189	X3045
L4041	D3940	G3863	Q3781	R3707	X3440	X3380	X3320	X3254	X3190	X3046
V4049	D3941	T3864	A3784	L3710	X3441	X3381	X3321	X3261	X3191	X3047
E4050	V3942	V3865	S3785	T3711	X3442	X3382	X3322	X3262	X3192	X3048
	E3944	N3867	C3786	E3712	X3443	X3383	X3323	X3263	X3193	X3049
S4053	M3955	N3868	K3787	K3713	X3444	X3384	X3324	X3264	X3194	X3050
M4054	K3959	Q3869	K3788	S3714	X3445	X3385	X3325	X3265	X3195	X3051
M4057	Q3960	N3870	E3789	K3715	X3446	X3386	X3326	X3266	X3196	X3052
L4058	V3961	G3871	T3790	L3716	X3447	X3387	X3327	X3267	X3197	
	N3963	E3872	I3802	D3717	X3450	X3388	X3328	X3268	X3198	X3055
F4062	E3967	K3873	L3805	E3718	X3451	X3389	X3329	X3269	X3199	X3056
L4063	N3806	N3874	N3806	D3719	X3452	X3390	X3330	X3270	X3200	X3057
M4064	G3807	A3876	L3641	V3720	X3453	X3391	X3331	X3271	X3201	X3058
F4065	G3808	D3877	Y3642		X3454	X3392	X3332	X3272	X3202	X3059
	G3808	D3878	Y3642		X3455	X3393	X3333	X3273	X3203	X3060
	N3809	E3879	N3643		X3456	X3394	X3334	X3274	X3204	X3061
K4069	N3976	Q3882	H3647		X3457	X3395	X3335	X3275	X3205	X3062
D4070	Q3977	F3885	S3656		X3458	X3396	X3336	X3276	X3206	X3063
L4071	H3981	R3886	Y3657		X3459	X3397	X3337	X3277	X3207	X3064
G4073	H3982	F3885	K3658		X3460	X3398	X3338	X3278	X3208	X3065
S4074	S3983	R3886	A3659		X3461	X3399	X3339	X3279	X3209	X3066
E4075	R3984	Q3889	A3660		X3462	X3400	X3340	X3280	X3210	X3067
L4076	A4076	L3890	Y3661		X3463	X3401	X3341	X3281	X3211	X3068
F4077	M3986	L3891	I3662		X3464	X3402	X3342	X3282	X3212	X3069
Q4078	F3992	E3892	L3663		X3465	X3403	X3343	X3283	X3213	X3070
D4079	F3992	C3892	Y3664		X3466	X3404	X3344	X3284	X3214	X3071
F4080	F3996	E3893	T3664		X3467	X3405	X3345	X3285	X3215	X3072
V4081	F3996	G3894	F3628		X3468	X3406	X3346	X3286	X3216	X3073
T4082	A3997	H3895	D3666		X3469	X3407	X3347	X3287	X3217	X3074
D4083	N3897	N3896	H3667		X3470	X3408	X3348	X3288	X3218	X3075
P4084	M4000	D3898	Y3668		X3471	X3409	X3349	X3289	X3219	X3076
R4085	M4001	F3899	S3668		X3472	X3410	X3350	X3290	X3220	X3077
G4086	K4002	Q3900	X3512		X3473	X3411	X3351	X3291	X3221	X3078
L4087	L4003	N3901	X3514		X3474	X3412	X3352	X3292	X3222	X3079
	A4004	R3904	X3516		X3475	X3413	X3353	X3293	X3223	X3080
	Q4005	T3838	X3517		X3476	X3414	X3354	X3294	X3224	X3081
K4090	D4006	C3839	X3518		X3477	X3415	X3355	X3295	X3225	X3082
R4091	D4006	S3840	X3519		X3478	X3416	X3356	X3296	X3226	X3083
D4092	S4007	V3751	X3520		X3479	X3417	X3357	X3297	X3227	X3084
F4093	S4007	S3752	X3521		X3480	X3418	X3358	X3298	X3228	X3085
Q4094	S4008	F3753	X3522		X3481	X3419	X3359	X3299	X3229	X3086
K4095	Q4009	E3754	X3523		X3482	X3420	X3360	X3300	X3230	X3087
		E3755	X3524		X3483	X3421	X3361	X3301	X3231	X3088
		K3756	X3525		X3484	X3422	X3362	X3302	X3232	X3089
		R3762	X3526		X3485	X3423	X3363	X3303	X3233	X3090
		Q3765	X3527		X3486	X3424	X3364	X3304	X3234	X3091
		Y3766	X3528		X3487	X3425	X3365	X3305	X3235	X3092
		Q3767	X3529		X3488	X3426	X3366	X3306	X3236	X3093
		S3768	X3530		X3489	X3427	X3367	X3307	X3237	X3094
		G3769	X3531		X3490	X3428	X3368	X3308	X3238	X3095
		L3770	X3532		X3491	X3429	X3369	X3309	X3239	X3096
		H3771	X3533		X3492	X3430	X3370	X3310	X3240	X3097
		T3772	X3534		X3493	X3431	X3371	X3311	X3241	X3098
		R3773	X3535		X3494	X3432	X3372	X3312	X3242	X3099
		G3774	X3536		X3495	X3433	X3373	X3313	X3243	X3100
		A3775	X3537		X3496	X3434	X3374	X3314	X3244	X3101
		A3776	X3538		X3497	X3435	X3375	X3315	X3245	X3102
			X3539		X3498	X3436	X3376	X3316	X3246	X3103
			X3540		X3499	X3437	X3377	X3317	X3247	X3104
			X3601		X3500	X3438	X3378	X3318	X3248	X3105
									X3249	X3106
									X3250	X3107
									X3251	X3108
									X3252	X3109
										X3188



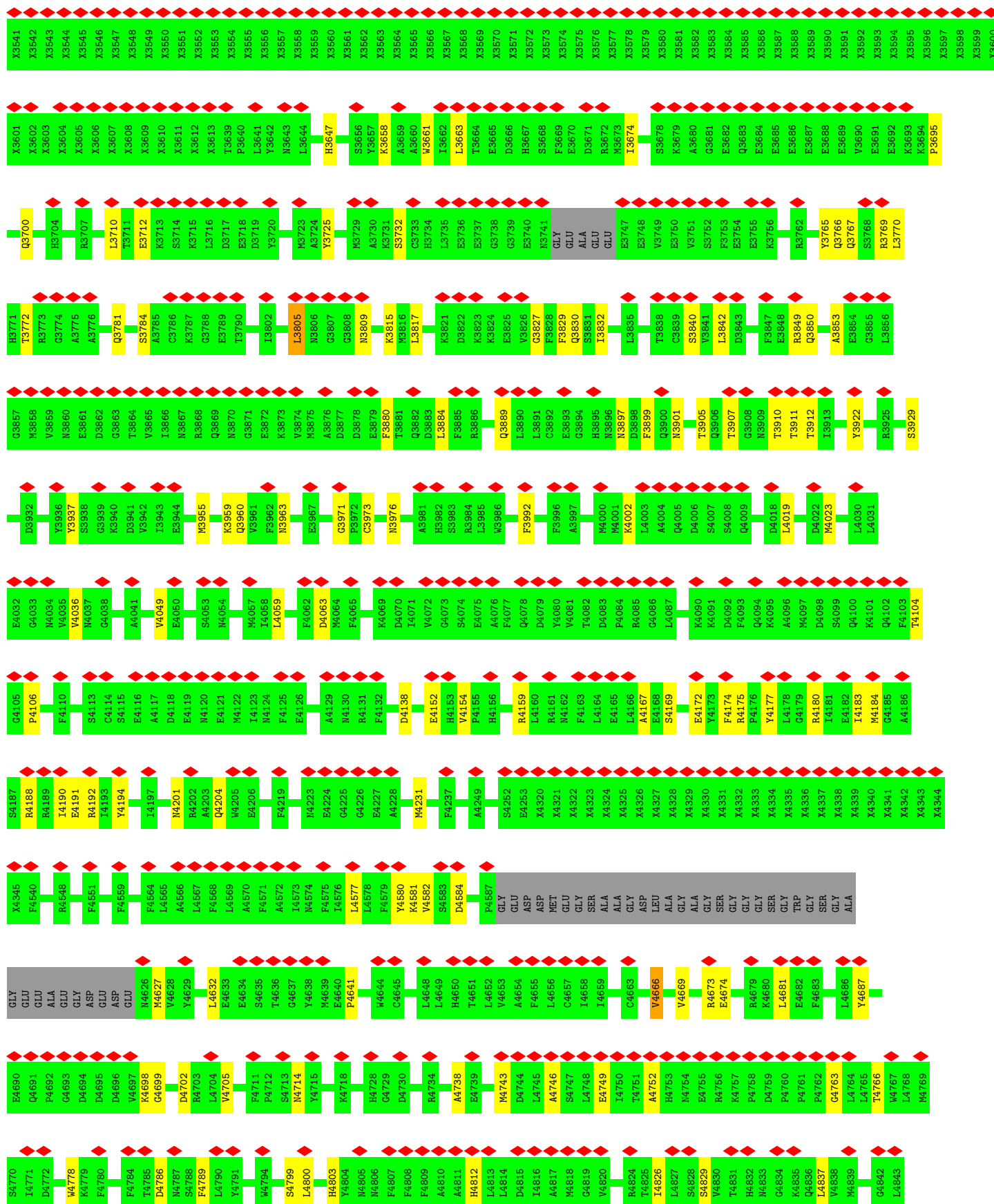
• Molecule 2: Ryanodine receptor 1

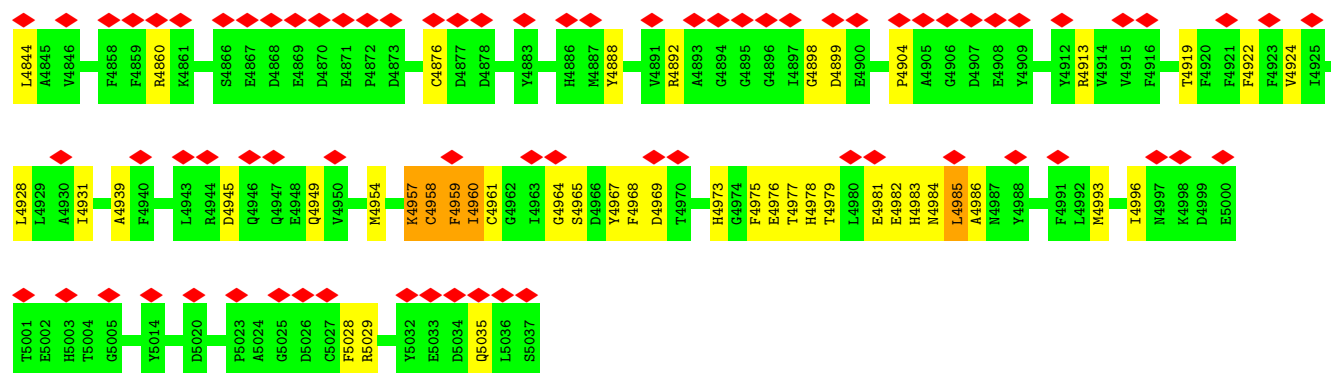






X3438	X3439	X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3447	X3450	X3451	X3452	X3453	X3454	X3455	X3456	X3457	X3458	X3459	X3460	X3461	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540																					
X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437																				
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																				
X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317																				
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	X3237	X3238	X3239	X3240	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251																
X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3083	X3086	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3003	X3006	X3010	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045
X2960	X2961	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	X3003	X3006	X3010	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045								
G2898	G2899	G2900	T2901	G2902	G2903	L2904	L2905	L2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	X2914	E2915	X2916	A2917	D2918	D2919	R2920	E2921	X2922	A2923	Q2924	E2925	L2926	X2927	X2928	P2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959																		
LYS	THR	ARG	ARG	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	S2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	G2886	R2887	L2888	R2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897																				
G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2802	E2803	L2804	Y2805	R2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	A2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	S2776	Y2777																				
X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	L2742	T2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	L2755	N2756	K2757	P2758	A2759	E2760	N2761	T2762	X2763	E2764	K2765	D2766	A2767	P2768	D2769	L2770	K2771	Q2772	N2773	D2774	W2775	S2776	Y2777																				
X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2605	X2606	X2607	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2657	X2658	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687																										
L2472	P2473	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	X2489	X2490	X2493	X2502	X2511	X2512	X2513	X2514	X2517	X2521	X2522	X2523	X2524	X2529	X2530	X2531	X2532	X2533	X2536	X2537	X2555	X2556	X2557	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2581	X2582	X2583	X2584	X2585	X2586	X2595																															





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	0.076	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.032	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: CFF, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/834	0.47	0/1123
1	F	0.19	0/834	0.46	0/1123
1	H	0.19	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.20	0/25424	0.52	4/34530 (0.0%)
2	E	0.20	0/25424	0.52	4/34530 (0.0%)
2	G	0.20	0/25424	0.52	4/34530 (0.0%)
2	I	0.20	0/25424	0.52	4/34530 (0.0%)
All	All	0.20	0/105032	0.51	16/142612 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4958	CYS	CA-C-N	5.46	131.97	121.54
2	E	4958	CYS	C-N-CA	5.46	131.97	121.54
2	I	4958	CYS	CA-C-N	5.44	131.93	121.54
2	I	4958	CYS	C-N-CA	5.44	131.93	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4958	CYS	CA-C-N	5.43	131.91	121.54

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	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	19	0
1	F	818	0	824	20	0
1	H	818	0	824	16	0
1	J	818	0	824	17	0
2	B	29495	0	24734	325	0
2	E	29495	0	24734	324	0
2	G	29495	0	24734	323	0
2	I	29495	0	24734	327	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	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
All	All	121436	0	102320	1341	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 1341 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:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.60	0.90
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.60	0.90
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.60	0.89
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.60	0.89
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.86	0.76

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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2926 (90%)	304 (9%)	5 (0%)	43	78
2	E	3235/4416 (73%)	2924 (90%)	306 (10%)	5 (0%)	43	78
2	G	3235/4416 (73%)	2925 (90%)	305 (9%)	5 (0%)	43	78
2	I	3235/4416 (73%)	2922 (90%)	308 (10%)	5 (0%)	43	78
All	All	13360/18096 (74%)	12077 (90%)	1263 (10%)	20 (0%)	49	83

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	E	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	G	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
2	I	2492/3022 (82%)	2480 (100%)	12 (0%)	81	83
All	All	10320/12444 (83%)	10272 (100%)	48 (0%)	78	83

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	1676	LEU
2	E	4960	ILE
2	E	3663	LEU
2	E	4837	LEU
2	G	978	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	582	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	3976	ASN
2	G	5003	HIS
2	E	797	HIS
2	E	2127	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	E	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
3	ATP	G	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
4	CFF	B	5102	-	15,15,15	1.87	5 (33%)	23,23,23	2.79	8 (34%)
4	CFF	E	5102	-	15,15,15	1.88	6 (40%)	23,23,23	2.78	8 (34%)
3	ATP	I	5101	-	32,33,33	1.40	4 (12%)	48,52,52	1.80	8 (16%)
3	ATP	B	5101	-	32,33,33	1.39	4 (12%)	48,52,52	1.80	8 (16%)
4	CFF	I	5102	-	15,15,15	1.88	5 (33%)	23,23,23	2.79	8 (34%)
4	CFF	G	5102	-	15,15,15	1.87	5 (33%)	23,23,23	2.79	8 (34%)

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	E	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.44	1.47	1.39
3	I	5101	ATP	C5-C4	4.44	1.47	1.39
3	E	5101	ATP	C5-C4	4.42	1.47	1.39
3	G	5101	ATP	C5-C4	4.42	1.47	1.39
4	I	5102	CFF	C6-N1	-3.77	1.32	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.59	112.07	126.28
4	B	5102	CFF	C14-N7-C8	-7.57	112.11	126.28
4	I	5102	CFF	C14-N7-C8	-7.57	112.11	126.28
4	E	5102	CFF	C14-N7-C8	-7.55	112.14	126.28
3	E	5101	ATP	C5-C4-N3	-5.80	118.73	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

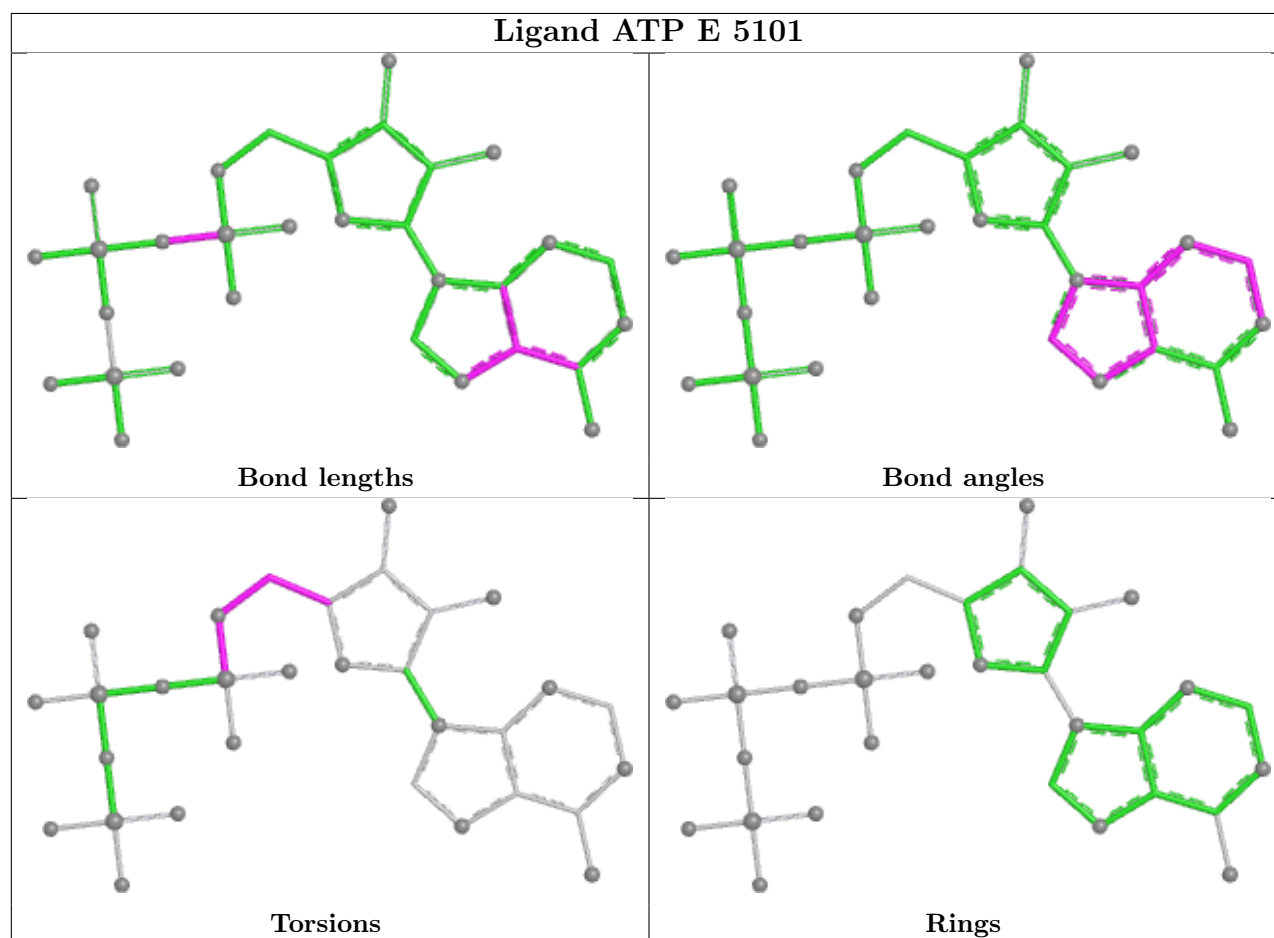
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

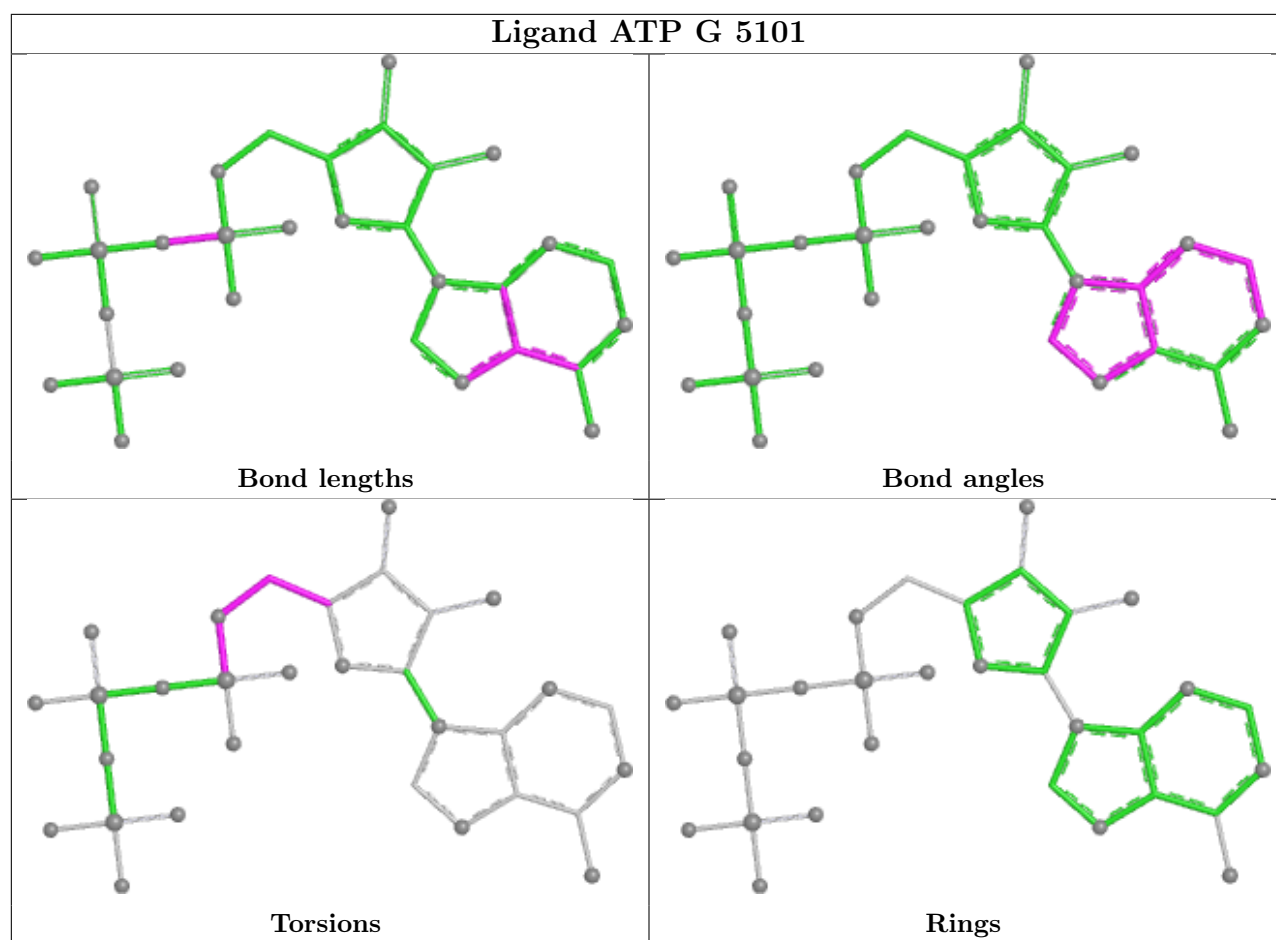
There are no ring outliers.

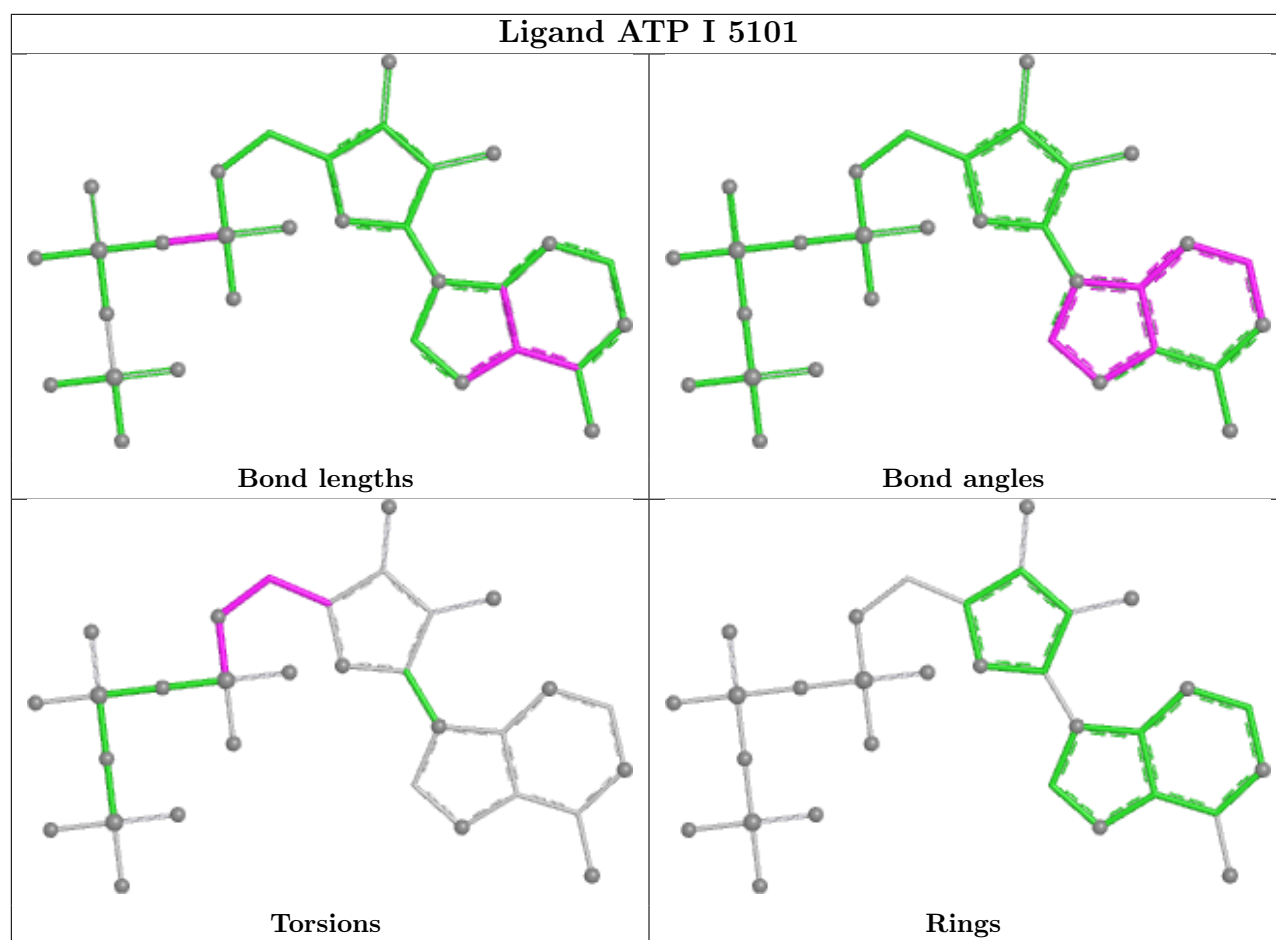
4 monomers are involved in 8 short contacts:

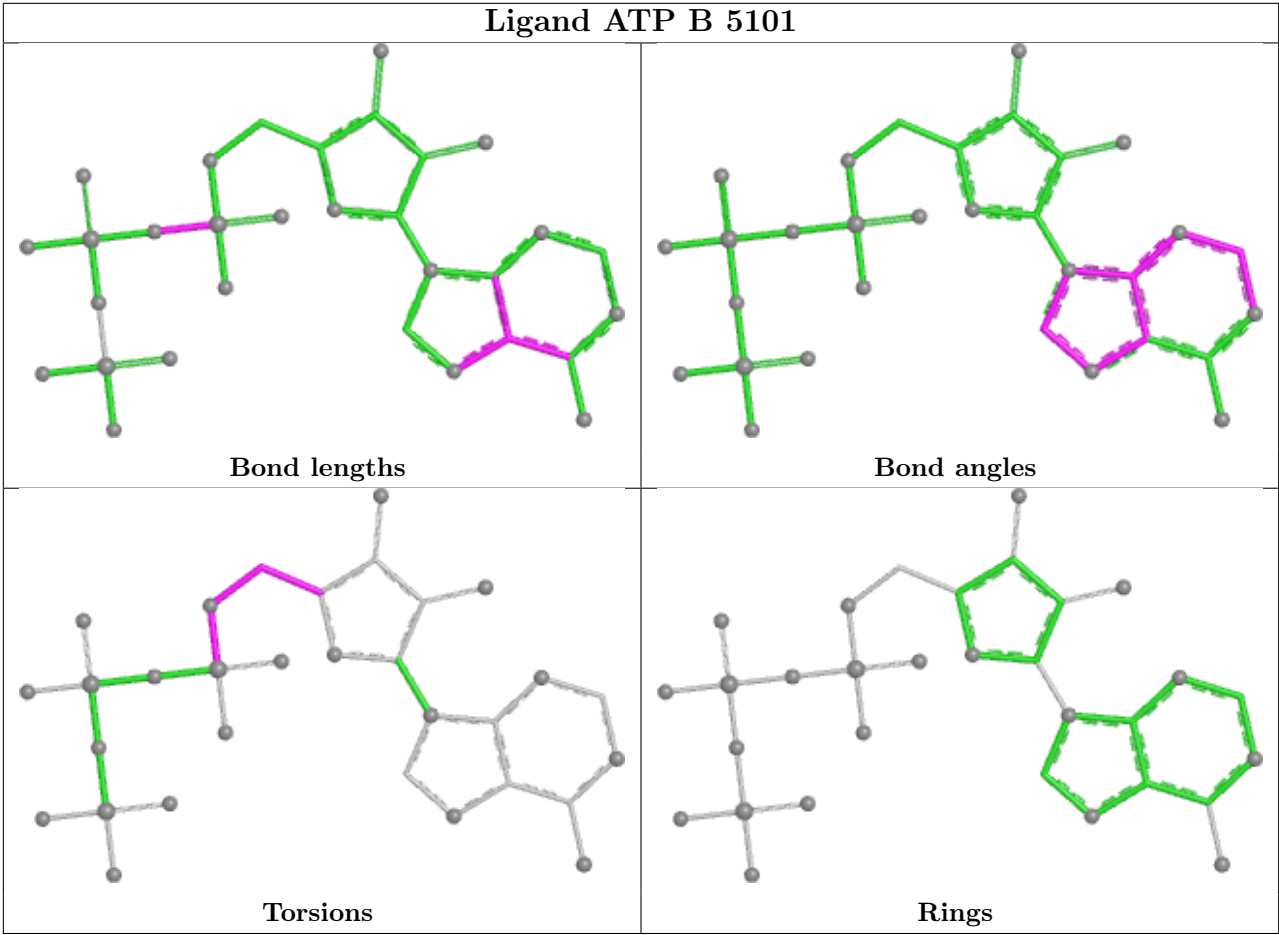
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	0
3	B	5101	ATP	2	0

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	I	14
2	E	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.97
1	I	4345:UNK	C	4540:PHE	N	72.97

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.97
1	G	4345:UNK	C	4540:PHE	N	72.97
1	B	3613:UNK	C	3639:THR	N	44.25

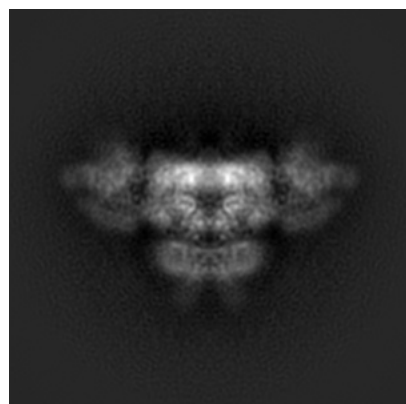
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8385. These allow visual inspection of the internal detail of the map and identification of artifacts.

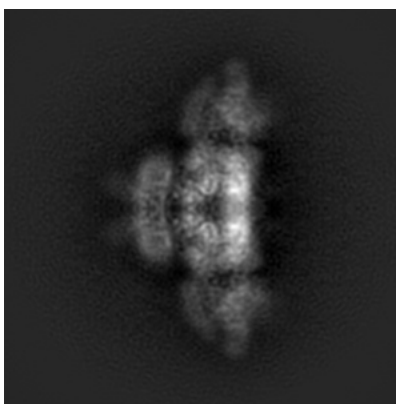
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

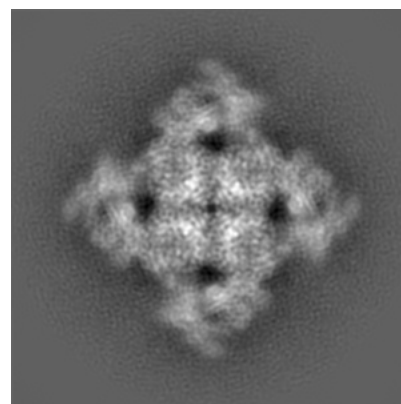
6.1.1 Primary map



X

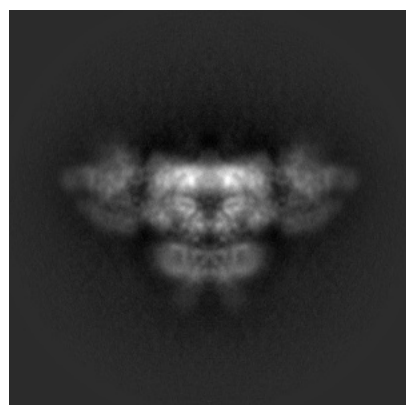


Y

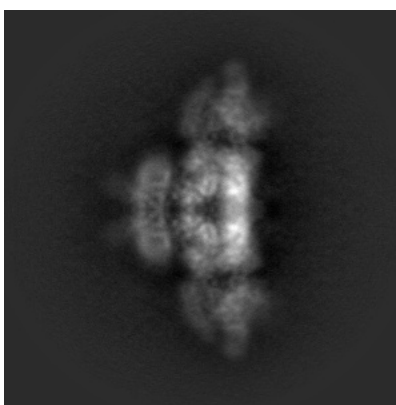


Z

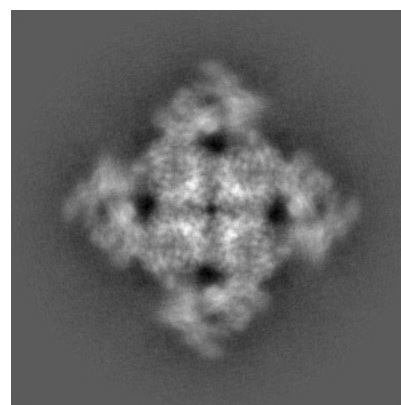
6.1.2 Raw map



X



Y

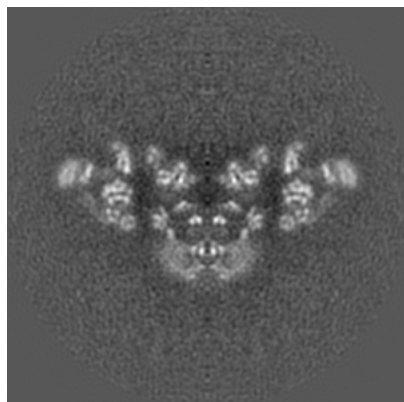


Z

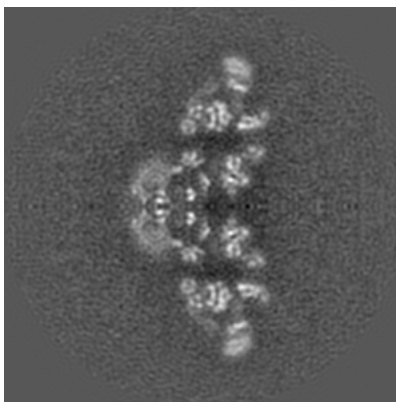
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

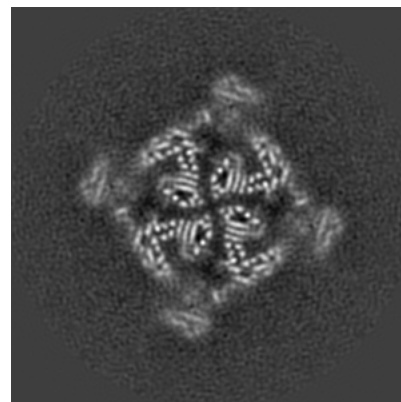
6.2.1 Primary map



X Index: 200

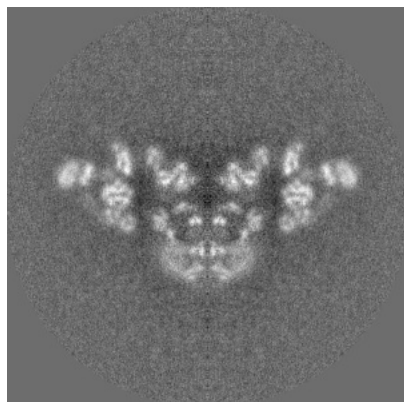


Y Index: 200

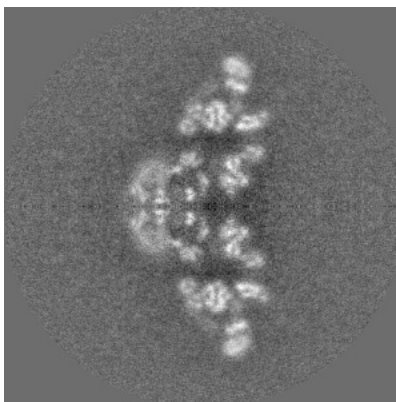


Z Index: 200

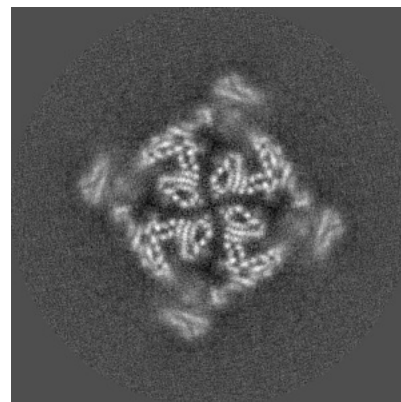
6.2.2 Raw map



X Index: 200



Y Index: 200

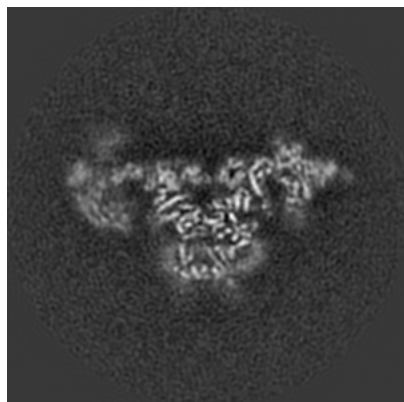


Z Index: 200

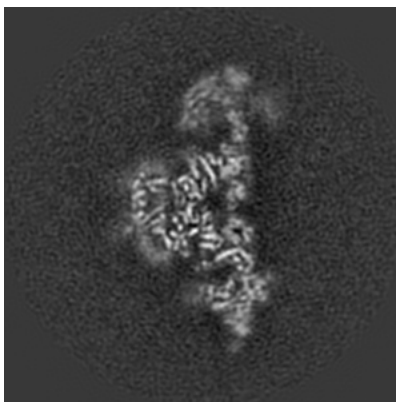
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

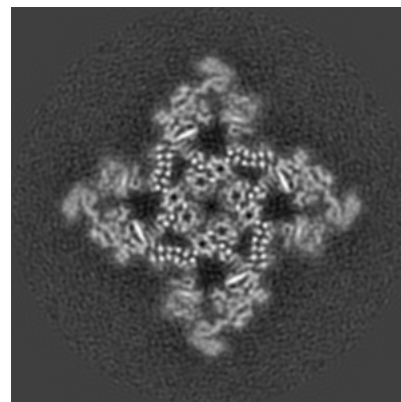
6.3.1 Primary map



X Index: 184

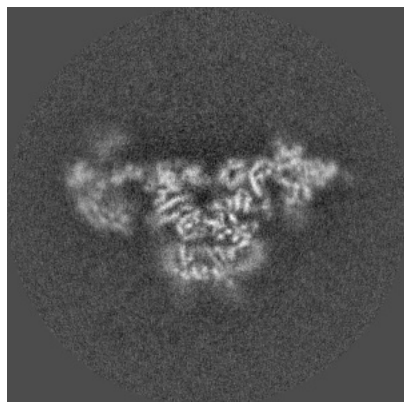


Y Index: 184

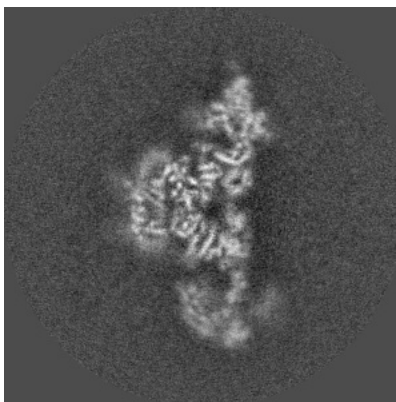


Z Index: 227

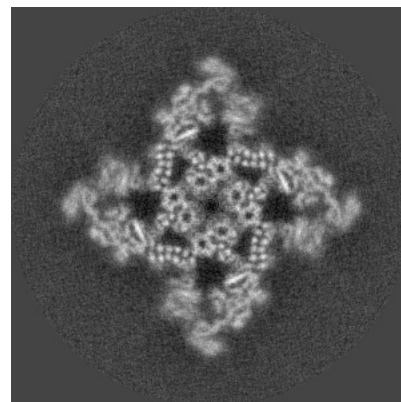
6.3.2 Raw map



X Index: 184



Y Index: 216

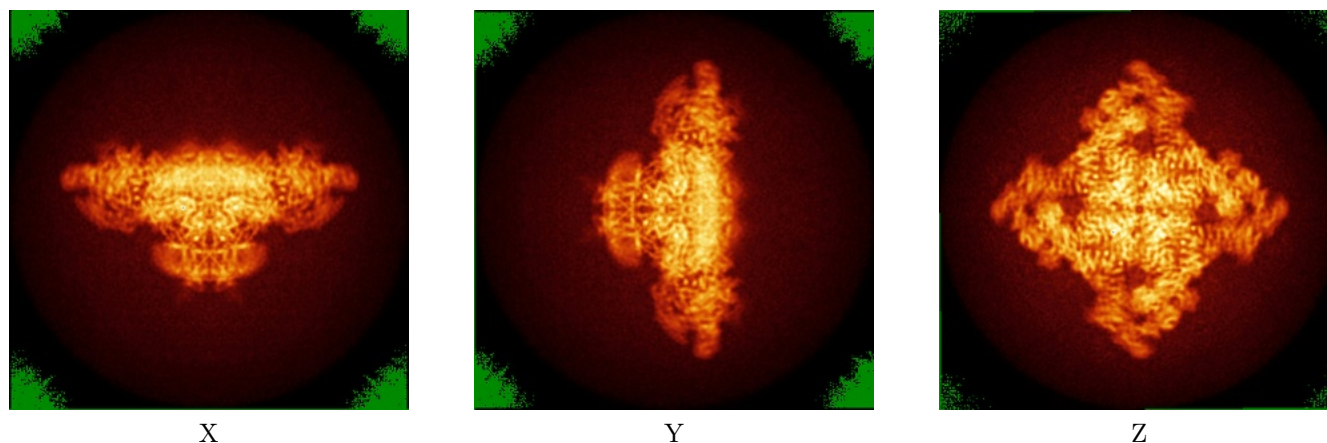


Z Index: 226

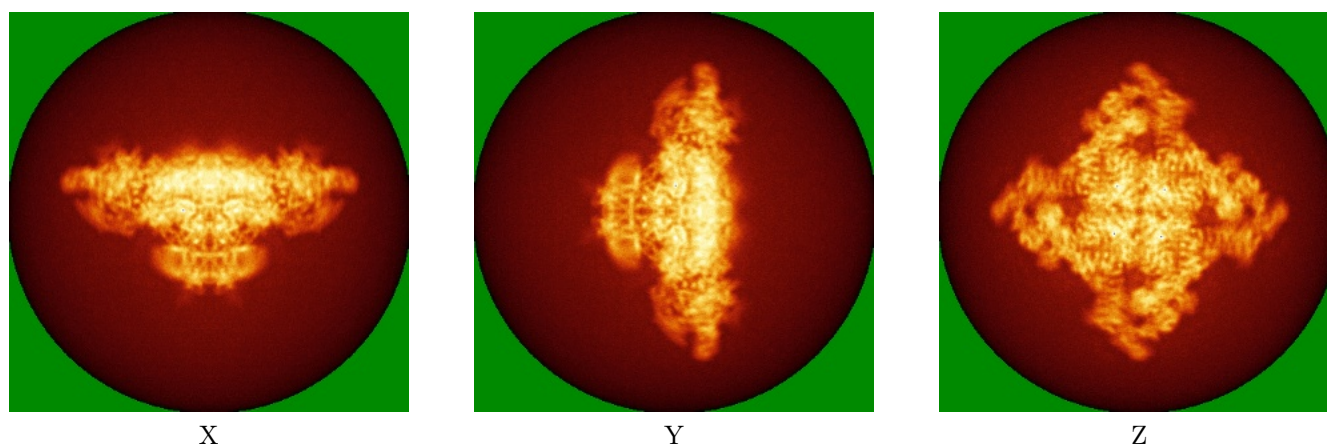
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

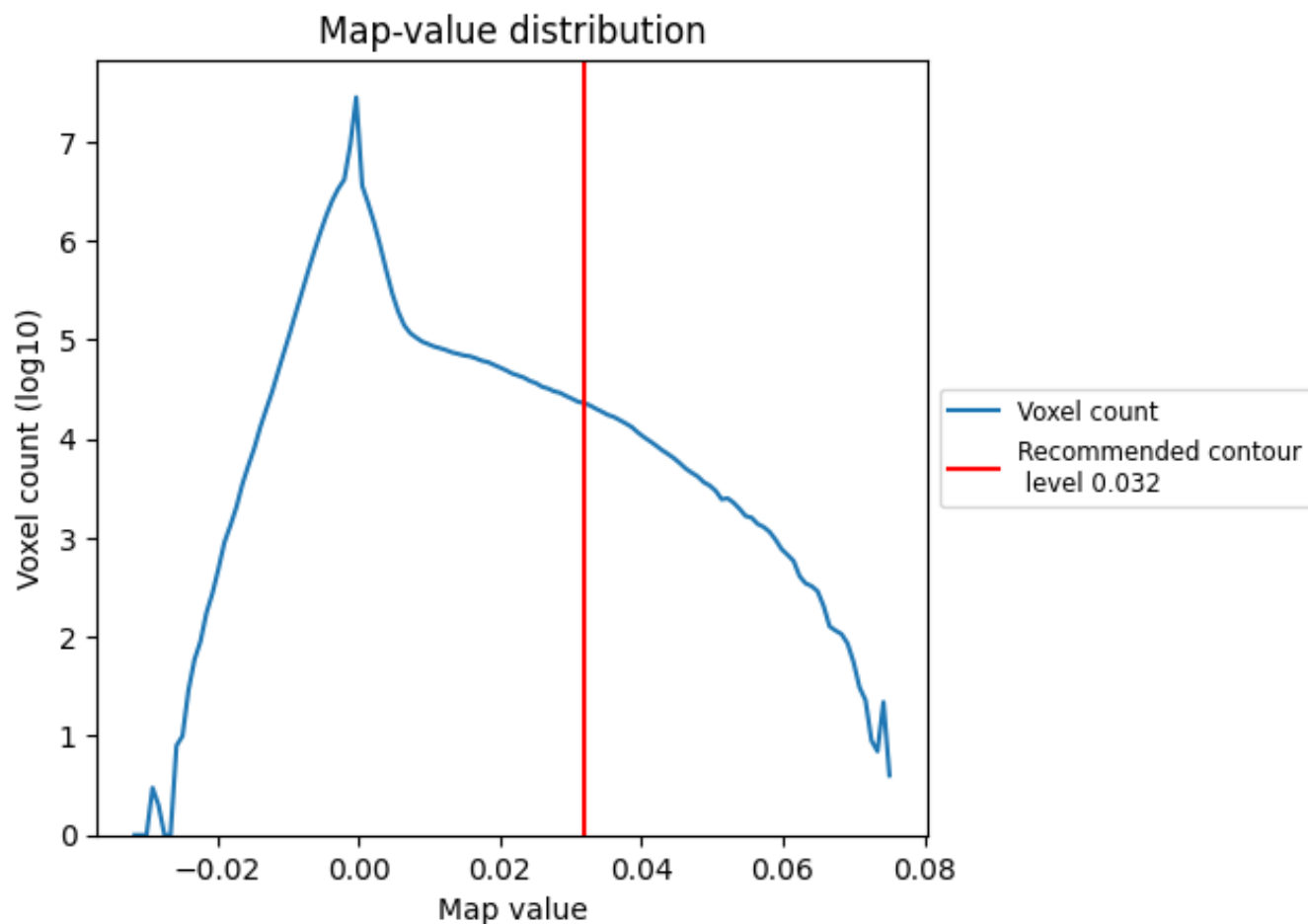
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

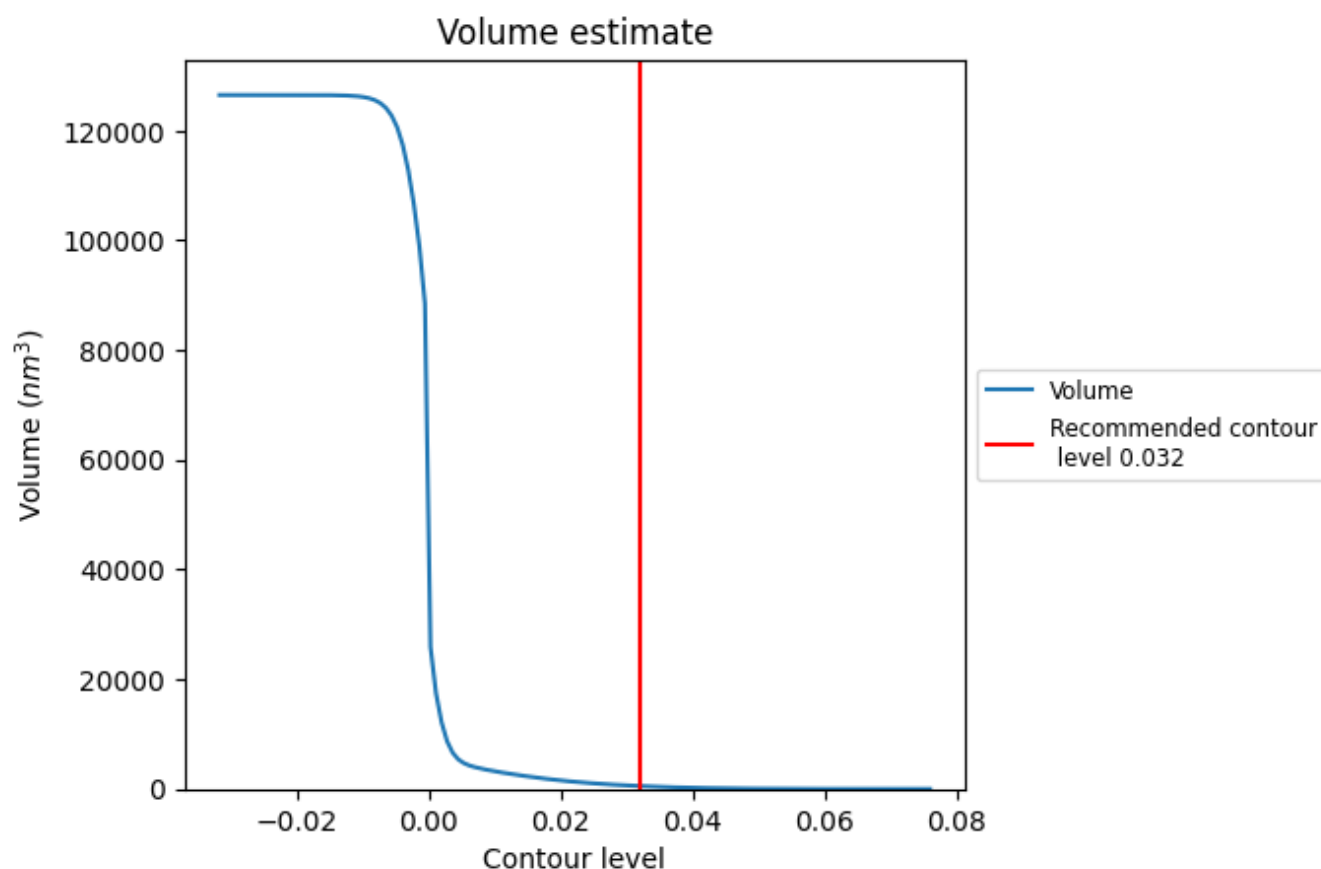
This section contains the results of statistical analysis of the map.

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.

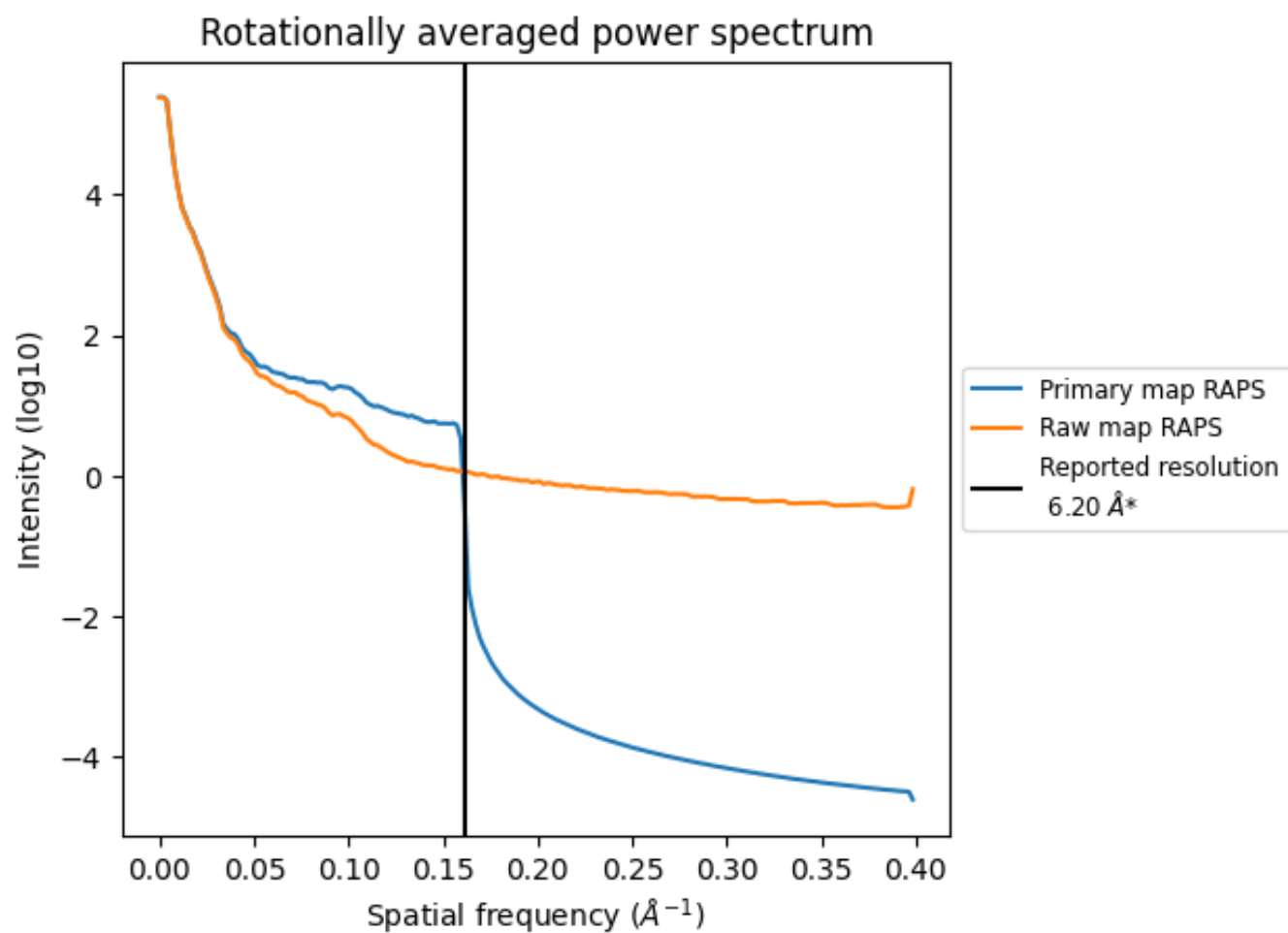
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 482 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 ⓘ

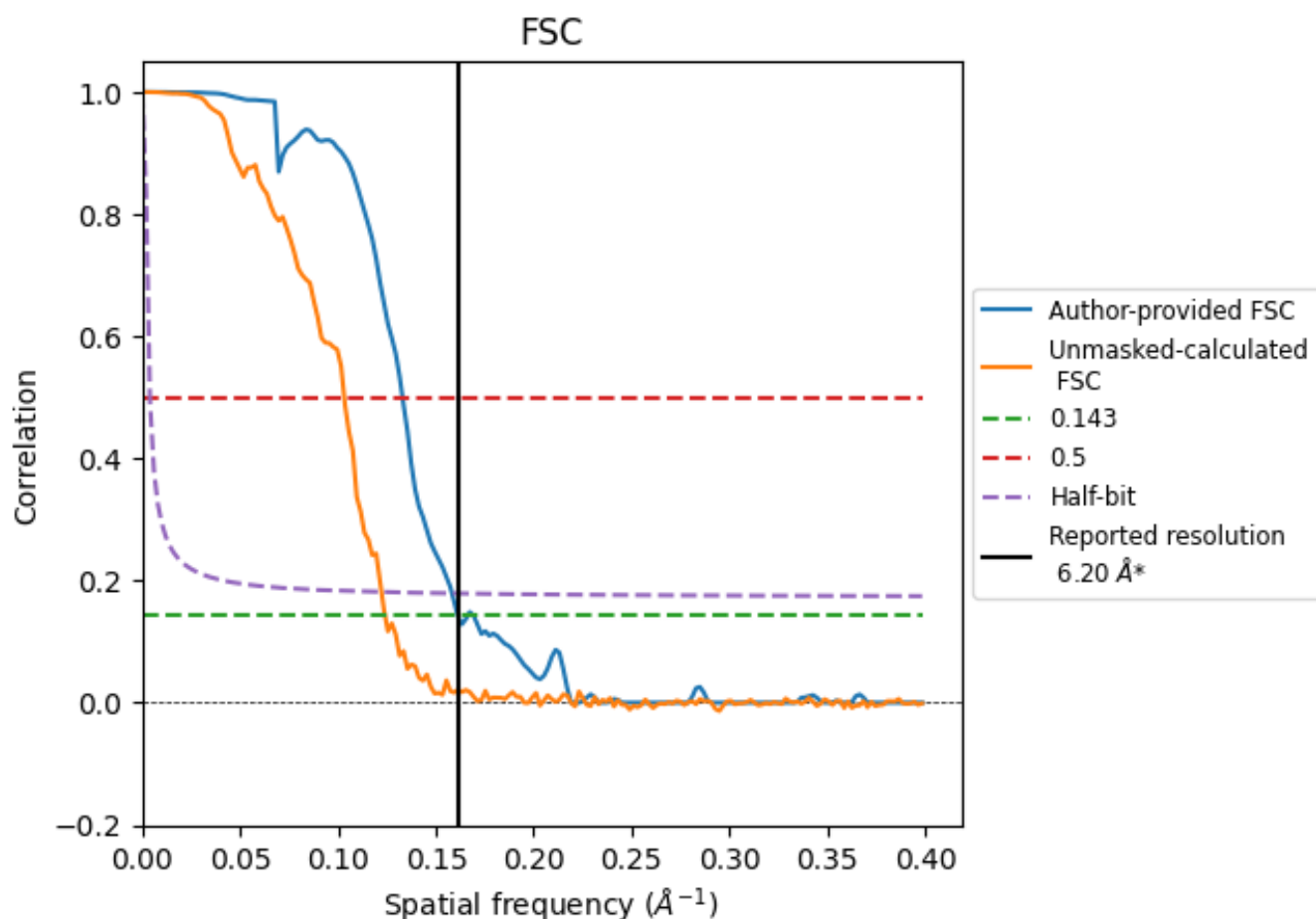


*Reported resolution corresponds to spatial frequency of 0.161 $\text{\AA}^{-1}$

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 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.21	7.52	6.32
Unmasked-calculated*	8.06	9.69	8.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.06 differs from the reported value 6.2 by more than 10 %

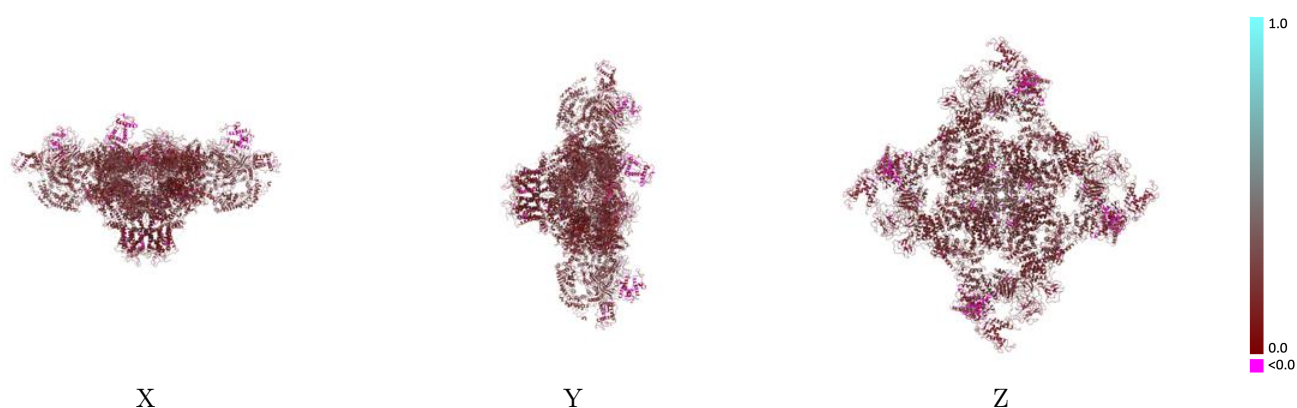
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8385 and PDB model 5TAU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

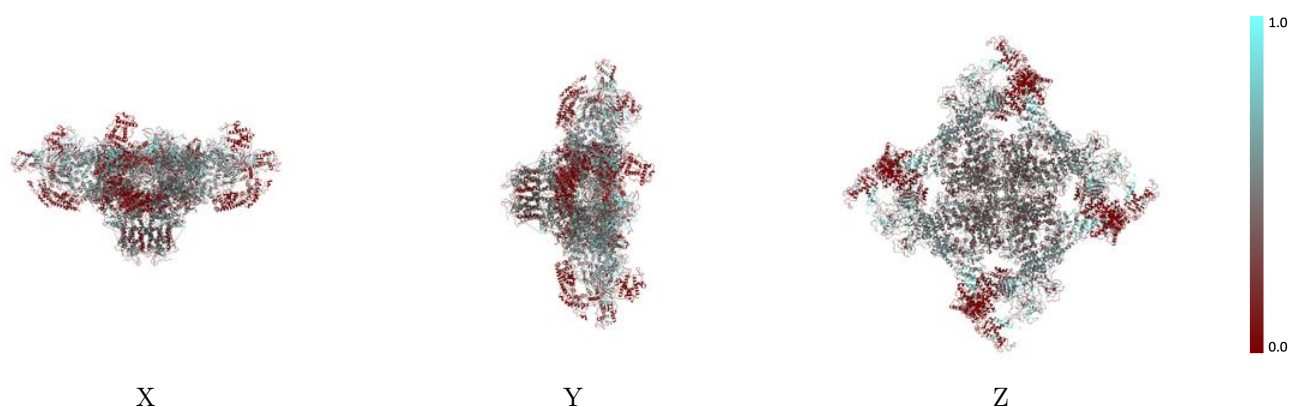
This section was not generated.

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



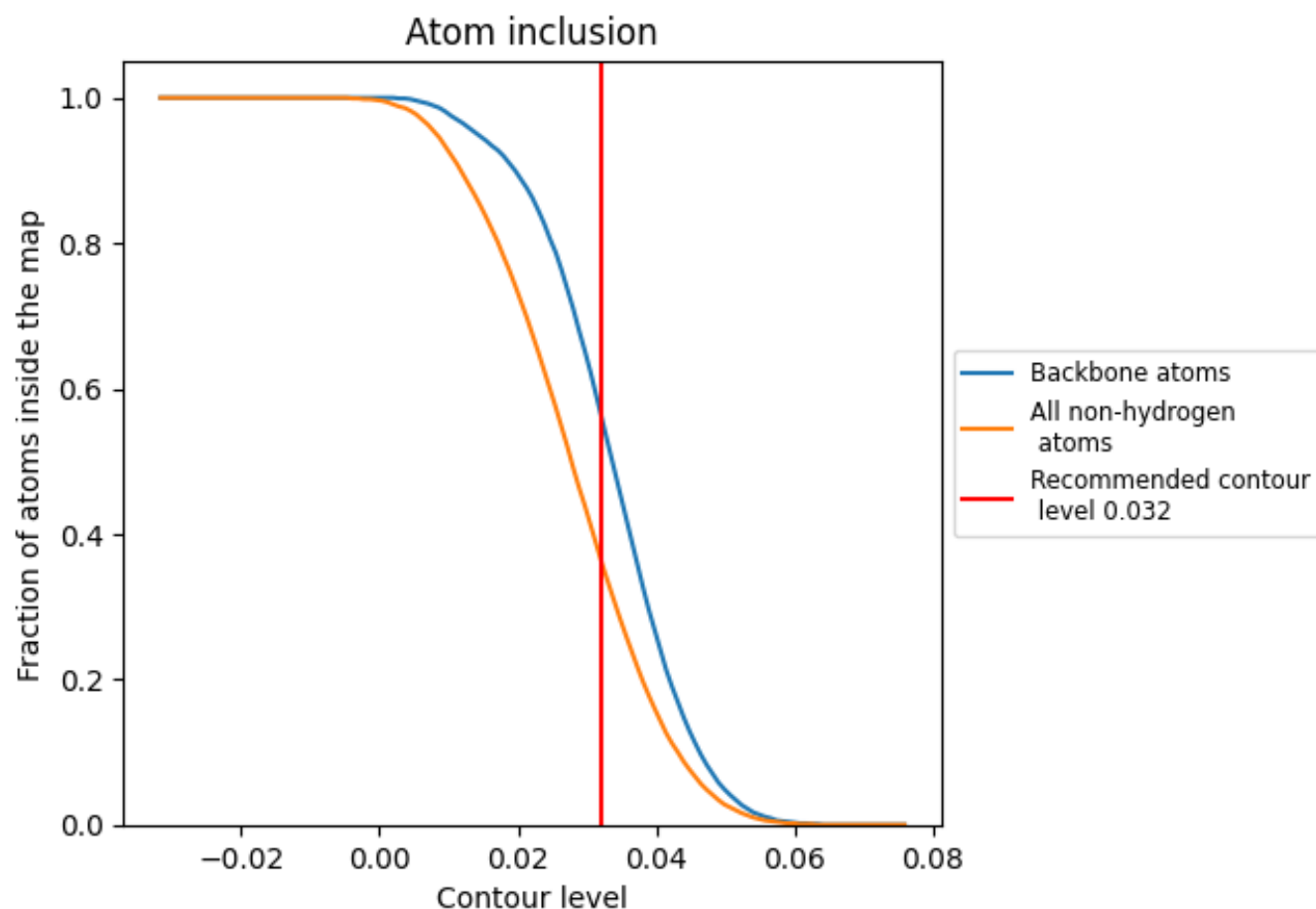
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3660	0.1880
A	0.3960	0.1860
B	0.3640	0.1880
E	0.3640	0.1880
F	0.3980	0.1900
G	0.3650	0.1880
H	0.3930	0.1880
I	0.3650	0.1880
J	0.3870	0.1880

1.0

0.0

<0.0