



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 09:08 PM EST

PDB ID : 6X33  
EMDB ID : EMD-22016  
Title : Wt pig RyR1 in complex with apoCaM, EGTA condition (class 3, open)  
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.  
Deposited on : 2020-05-21  
Resolution : 4.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

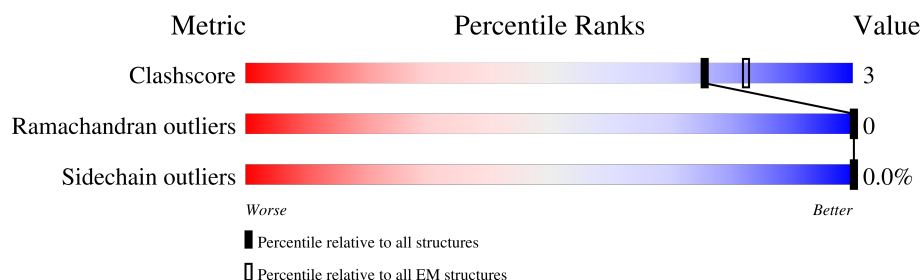
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.





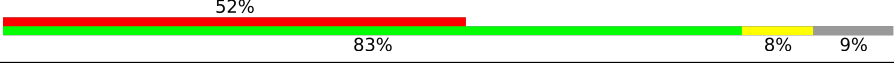
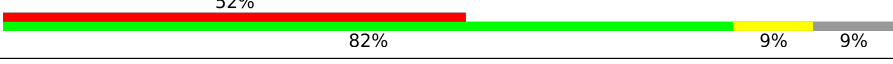
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	107	<div> <div>19%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	107	<div> <div>19%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	G	107	<div> <div>20%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	J	107	<div> <div>19%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	B	3816	<div> <div>32%</div> <div>93%</div> <div>7%</div> </div>
2	E	3816	<div> <div>32%</div> <div>93%</div> <div>7%</div> </div>
2	H	3816	<div> <div>32%</div> <div>93%</div> <div>7%</div> </div>
2	K	3816	<div> <div>32%</div> <div>93%</div> <div>7%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	C	148	
3	F	148	
3	I	148	
3	L	148	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 112372 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	A	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	D	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	G	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	J	106	Total	C	N	O	S	0	0
			727	460	124	139	4		

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	E	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	H	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	K	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	F	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	I	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	L	135	Total	C	N	O	S	0	0
			768	477	138	151	2		

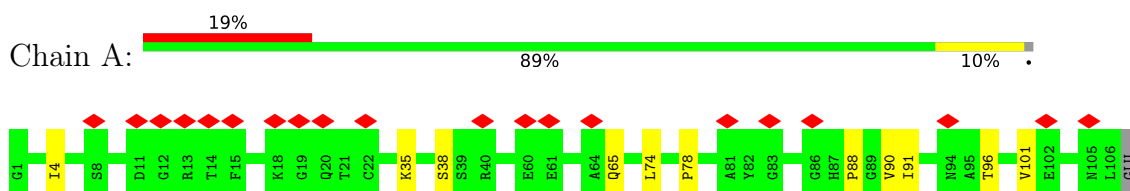
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	E	1	Total 1	Zn 1	0
4	H	1	Total 1	Zn 1	0
4	K	1	Total 1	Zn 1	0

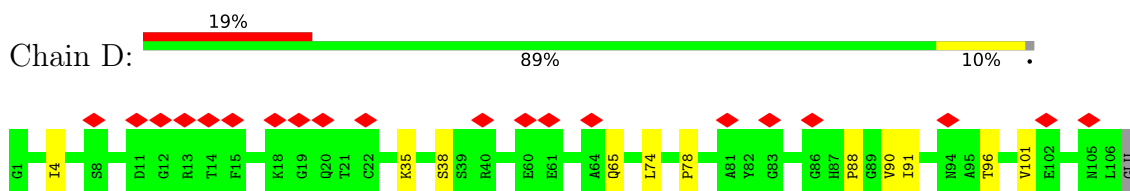
### 3 Residue-property plots

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

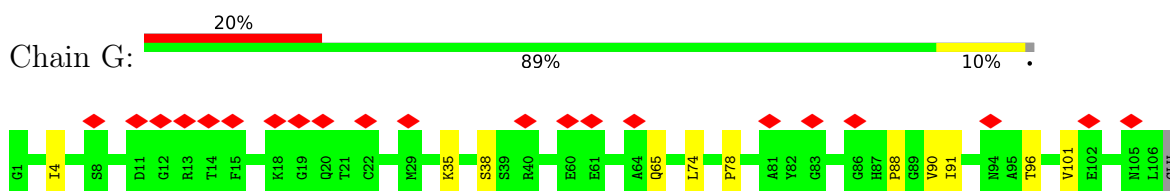
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



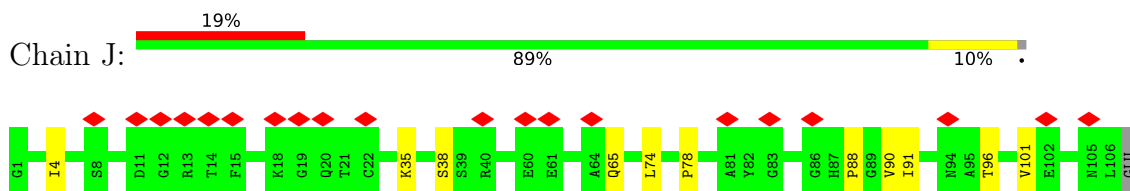
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



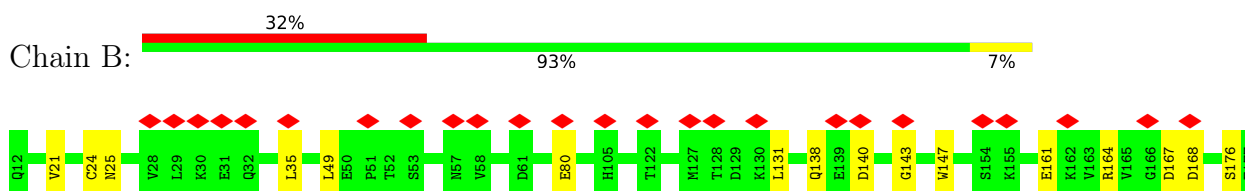
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

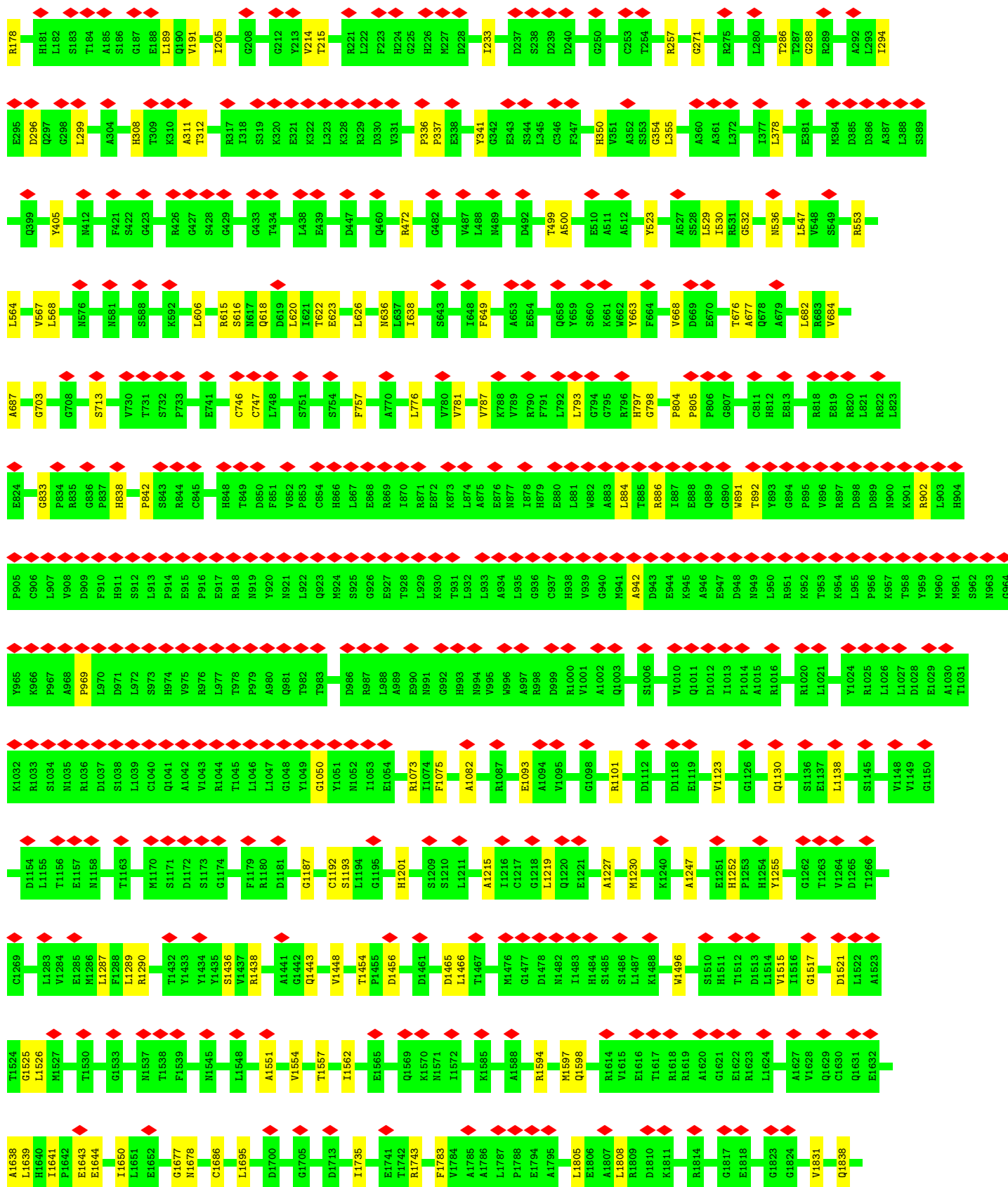


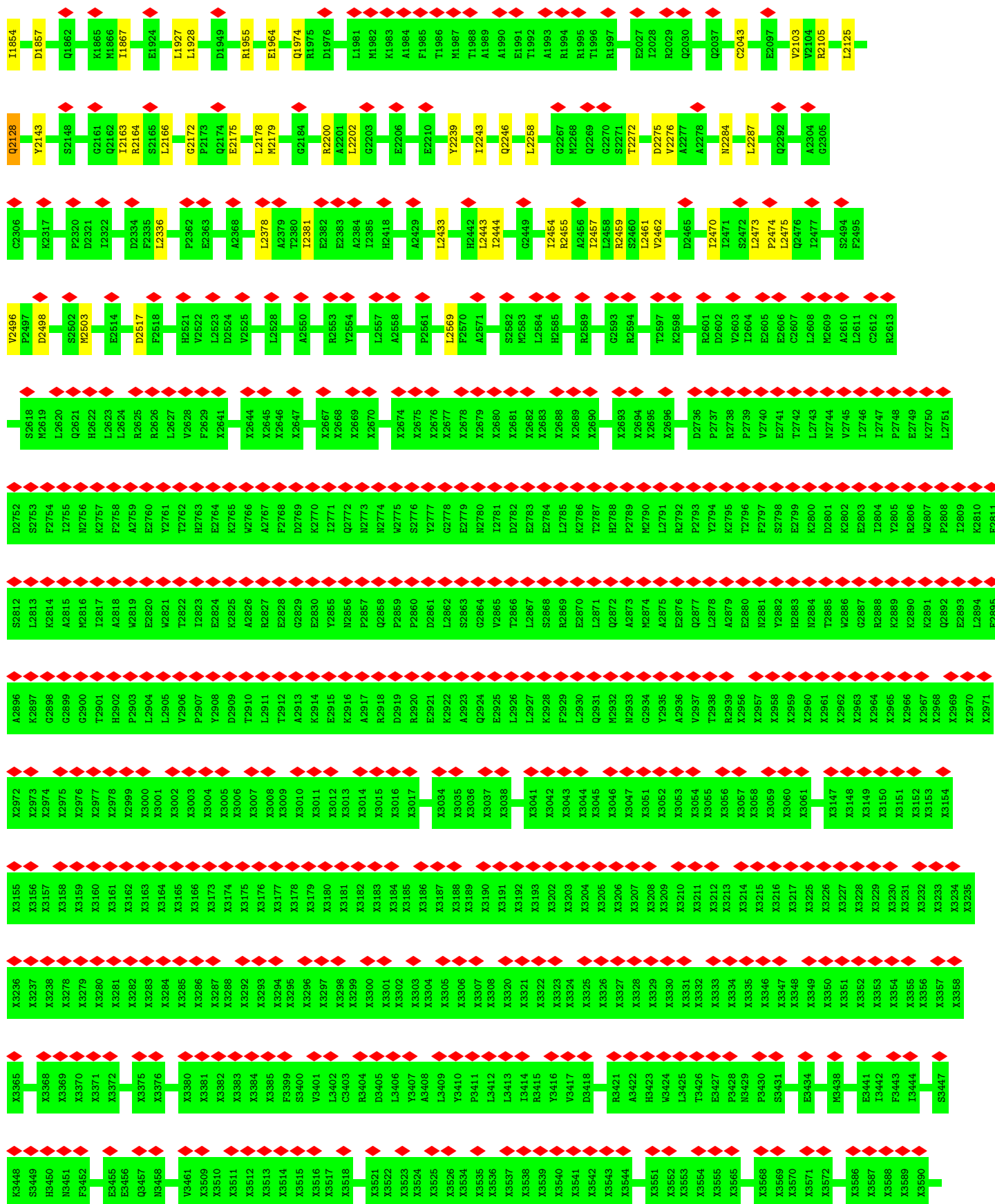
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

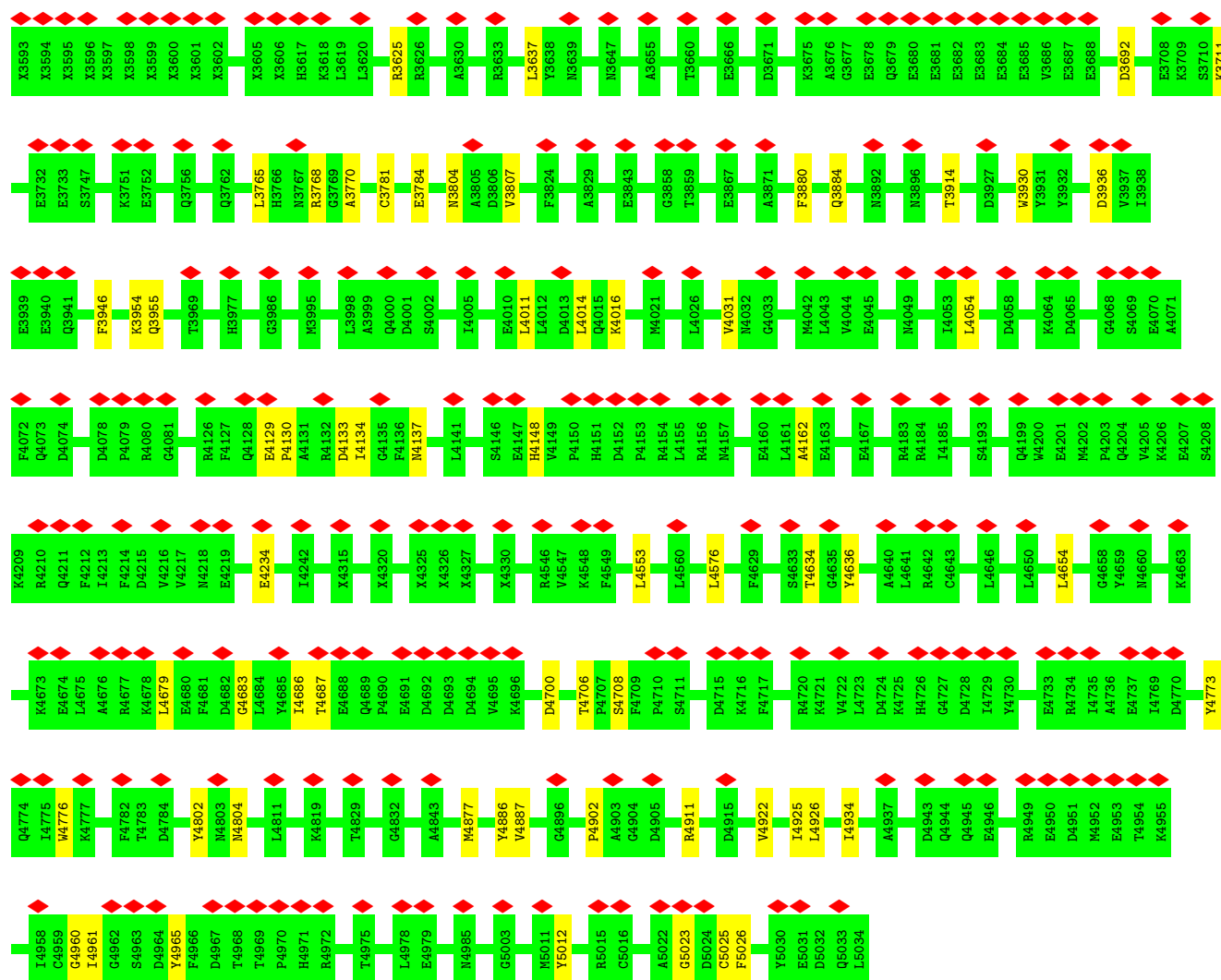


- Molecule 2: Ryanodine Receptor

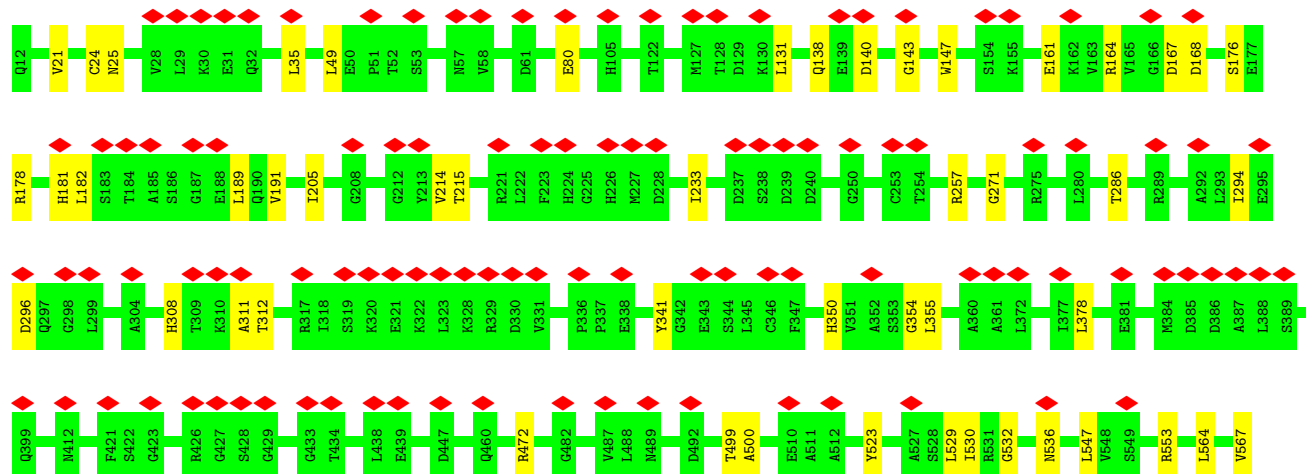
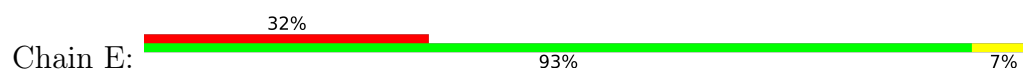


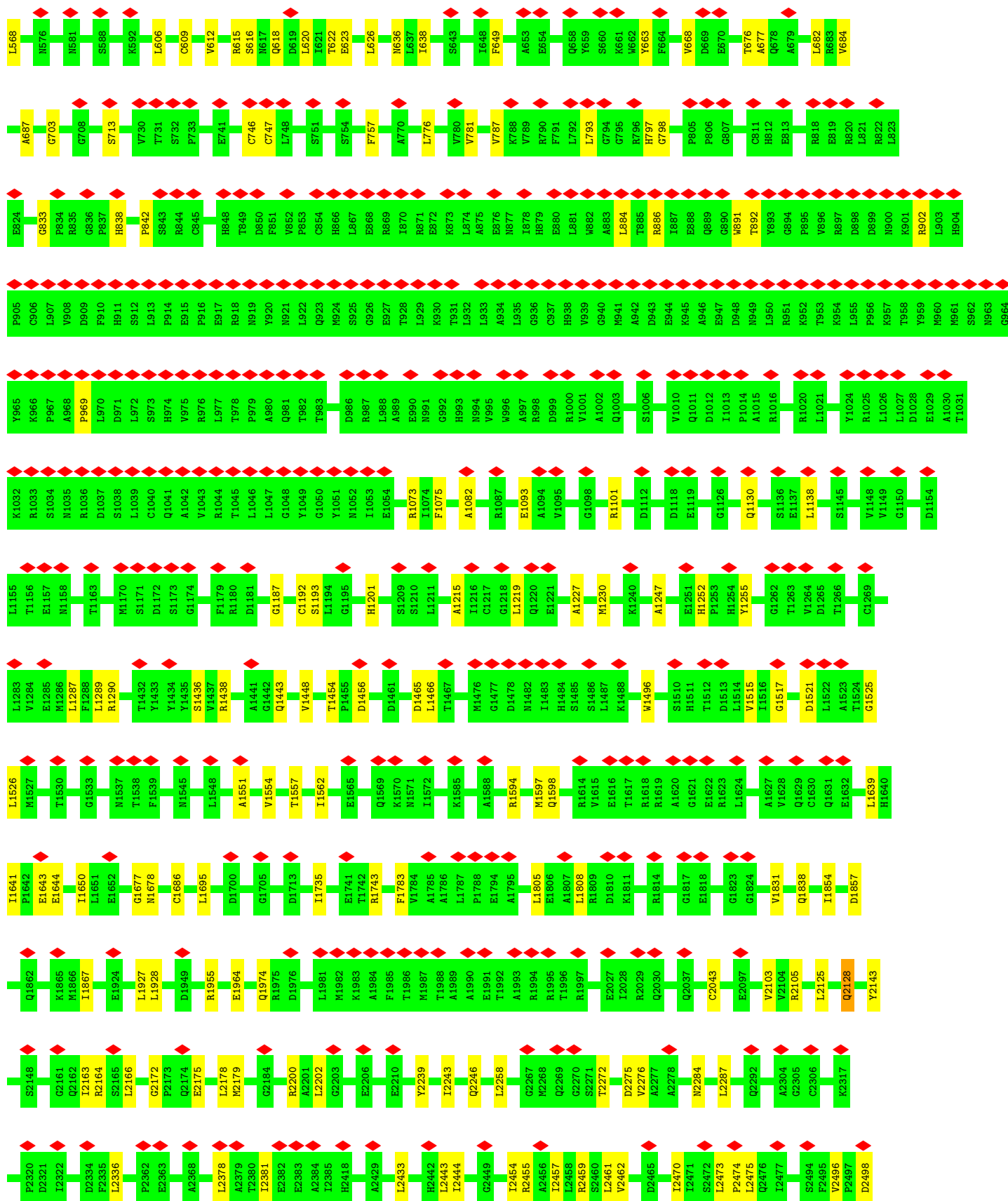






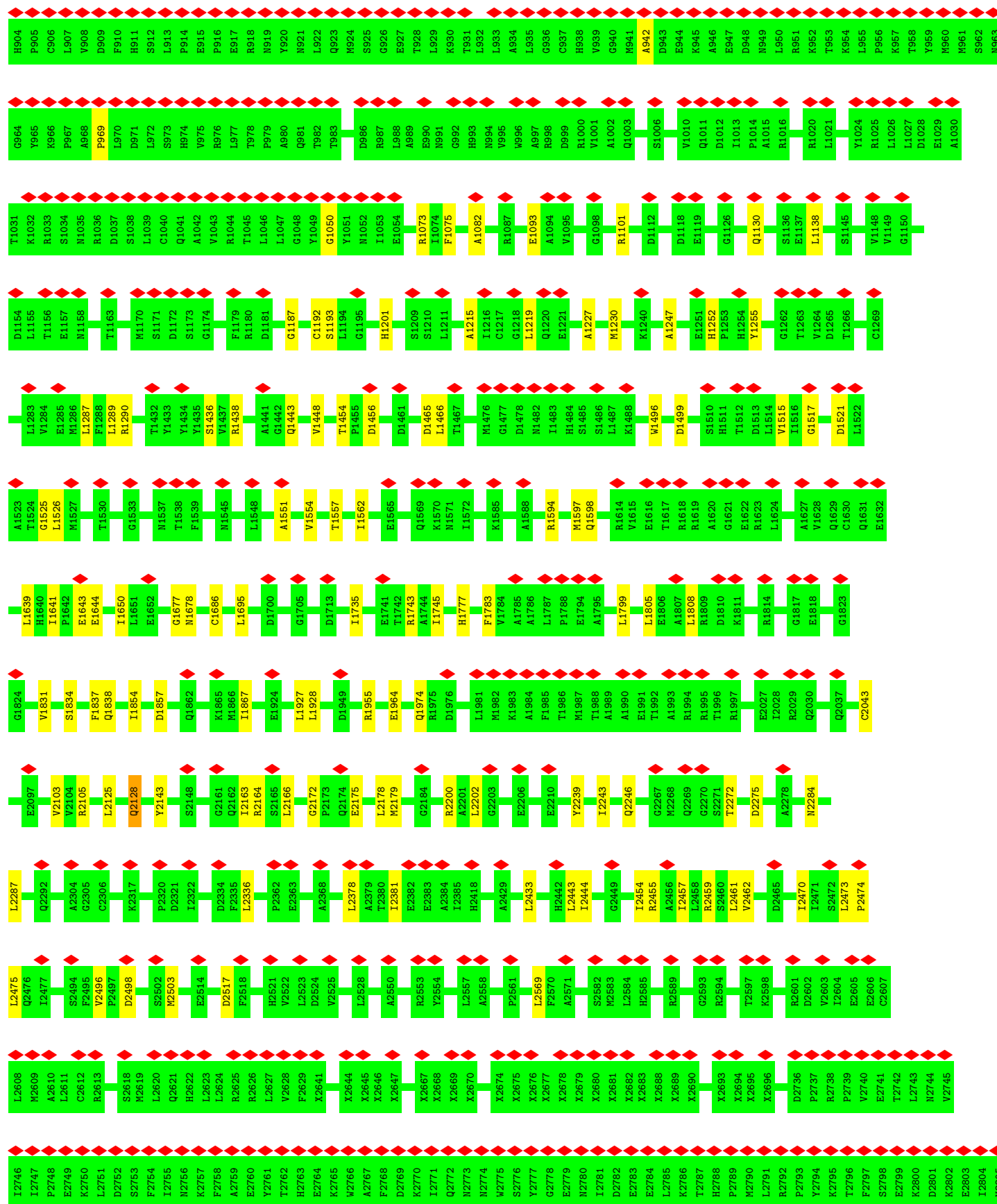
### • Molecule 2: Ryanodine Receptor



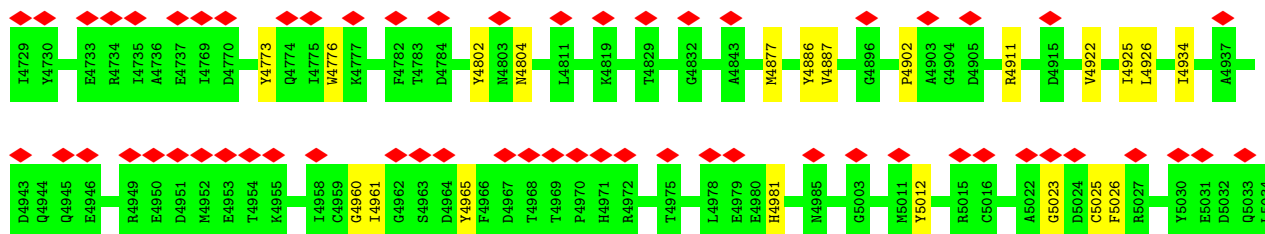


E3939	E3940	Q3941	F3946	K3954	Q3955	T3969	H3977	G3986	M3995	L3998	A3999	Q4000	D4001	S4002	I4005	E4010	L4011	D4012	L4013	L4014	Q4015	K4016	M4021	L4026	V4031	M4032	G4033	M4042	L4043	V4044	E4045	M4049	L4053	L4054	D4058	K4064	D4065	G4068	S4069	E4070	A4071																		
X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3605	X3606	H3617	X3618	L3619	L3620	R3625	R3626	A3630	R3633	L3637	Y3638	X3639	N3647	A3655	T3660	E3666	D3671	K3675	A3676	G3677	E3678	Q3679	E3680	E3681	E3682	E3683	E3684	E3685	V3686	E3687	E3688	D3692	E3708	K3709	S3710	K3711	E3732	E3733														
S3747	K3751	E3752	Q3756	Q3762	L3765	H3766	N3767	R3768	G3769	A3770	C3781	E3784	N3804	A3805	D3806	V3807	F3824	A3829	E3843	G3858	T3859	E3867	A3871	F3880	Q3884	N3892	N3896	T3905	T3906	T3914	D3927	W3930	Y3931	Y3932	D3936	V3937	T3938	S3710	K3711	E3732	E3733																		
N3451	F3452	E3455	E3456	Q3457	N3458	V3461	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3521	X3522	X3523	X3524	X3525	X3526	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3551	X3552	X3553	X3554	X3555	X3565	X3568	X3569	X3570	X3571	X3572	X3586	X3587	X3588	X3589	X3590	X3593	X3594	X3595							
X3369	X3370	X3371	X3372	X3375	X3376	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	F3399	S3400	L3402	C3403	R3404	D3405	L3406	Y3407	A3408	L3409	Y3410	P3411	L3412	L3413	I3414	R3415	Y3416	V3417	D3418	R3421	A3422	H3423	V3424	L3425	T3426	E3427	P3428	N3429	P3430	S3431	E3434	M3438	E3441	T3442	F3443	I3444	S3447	K3448	S3449	H3450					
X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3365	X3368	
X3158	X3159	X3160	X3161	X3162	X3163	X3164	X3165	X3166	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238
X2975	X2976	X2977	X2978	X2989	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3034	X3035	X3036	X3037	X3038	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3147	X3148	X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157			
G2899	Q2900	T2901	H2902	L2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	T2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	A2936	V2937	T2938	R2939	X2956	T2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	
A2815	M2816	L2817	A2818	L2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	Y2855	N2856	P2857	Q2858	T2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	T2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898
N2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	Y2777	Q2778	E2779	N2780	L2781	D2782	E2783	L2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	R2796	P2797	S2798	E2799	K2800	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754			
L2620	Q2621	H2622	L2623	L2624	R2625	R2626	L2627	V2628	F2629	X2641	X2644	X2645	X2646	X2647	X2667	X2668	X2669	X2670	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2688	X2689	X2690	X2693	X2694	X2695	X2696	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754			
S2502	K2503	E2514	D2517	F2518	H2521	V2522	L2523	D2524	V2525	L2528	A2550	K2553	Y2554	L2557	A2558	P2561	L2569	F2570	A2571	S2582	L2583	L2584	H2585	R2589	G2593	R2594	T2597	K2598	R2601	D2602	V2603	L2604	E2605	E2606	C2607	L2608	A2610	L2611	C2612	R2613	S2618	K2619																	

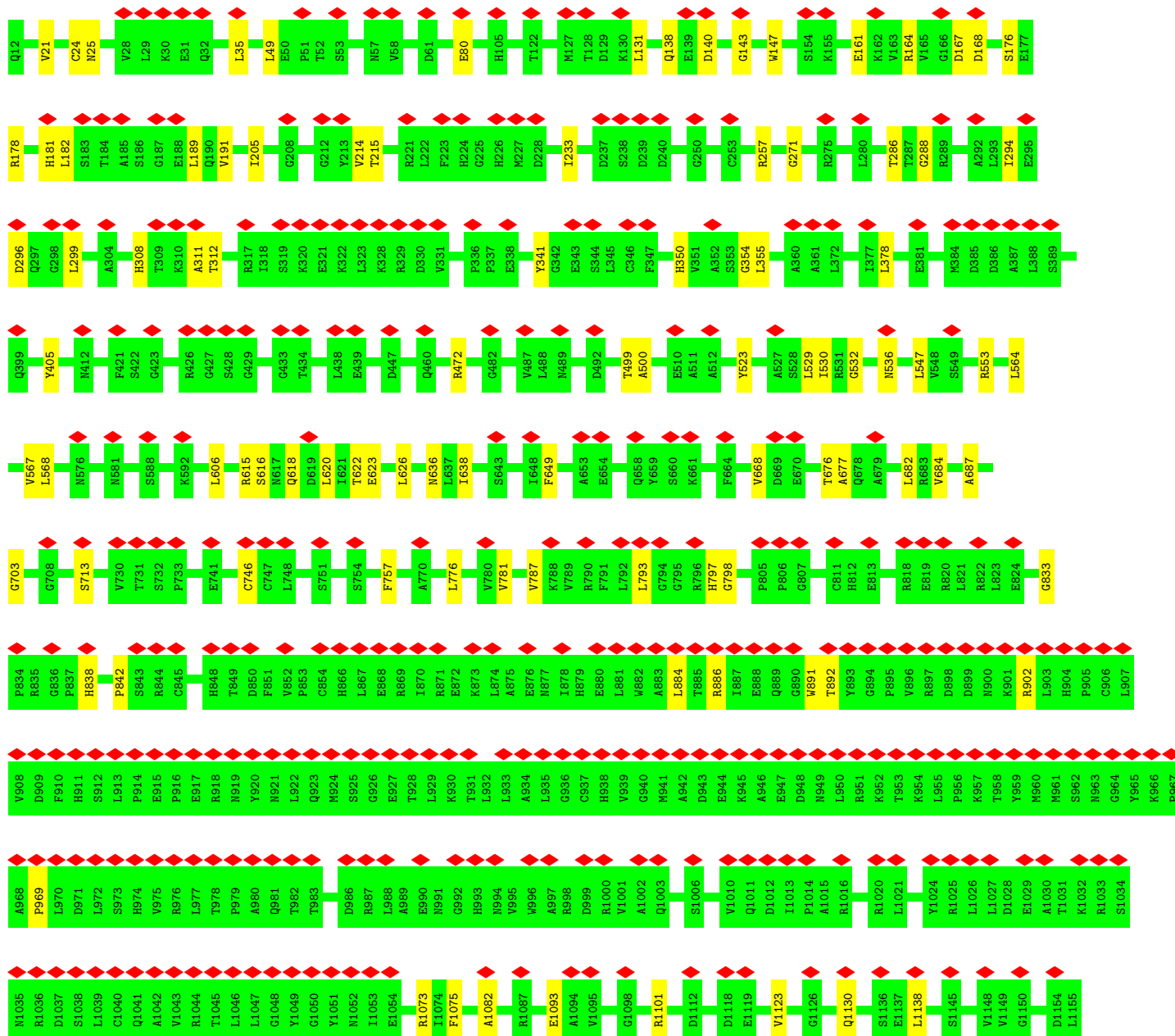
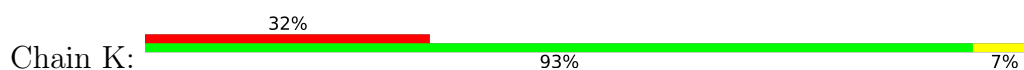


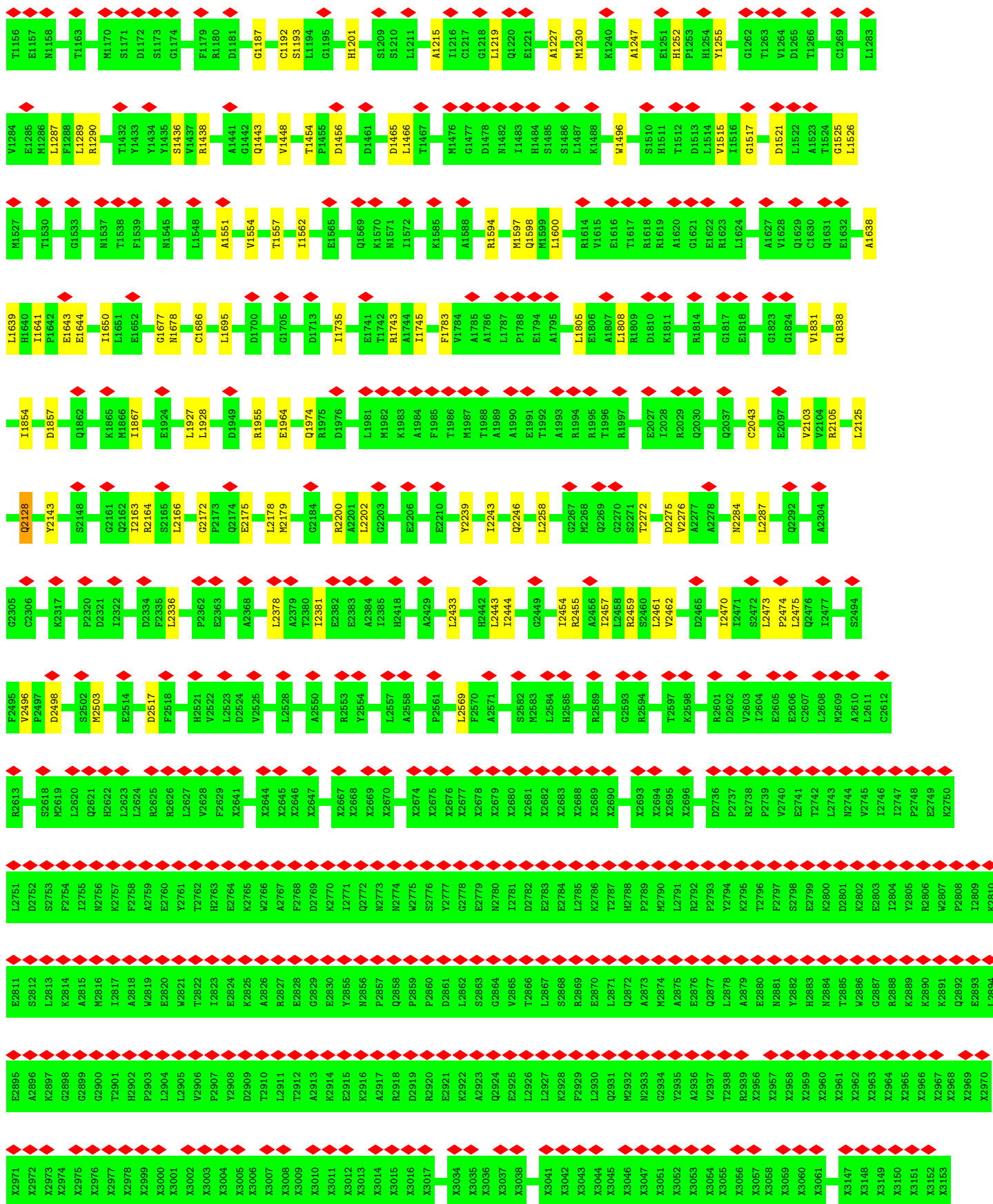


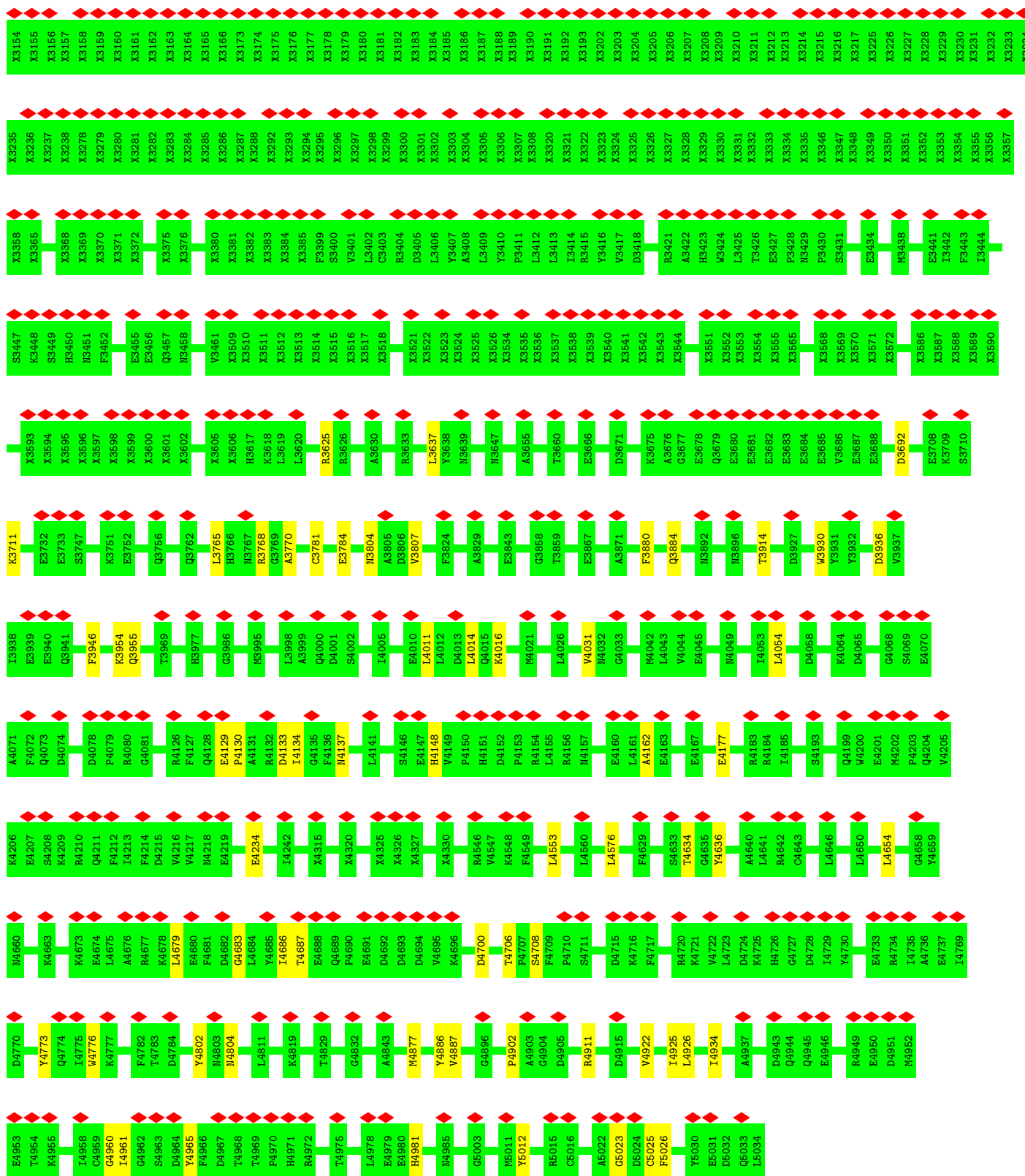
L4646	L4650	L4654	G4658	Y4659	N4660	K4663	K4673	E4674	L4675	A4676	R4677	K4678	L4679	F4681	D4682	C4683	L4684	Y4685	L4686	D4687	E4688	Q4689	F4690	E4691	D4692	D4693	D4694	V4695	K4696	D4700	T4706	P4707	S4708	P4709	P4710	S4711	D4715	K4716	F4717	R4720	K4721	V4722	L4723	D4724	K4725	H4726	G4727	D4728											
S4193	Q4199	V4200	E4201	M4202	Q4203	Q4204	V4205	K4206	E4207	S4208	K4209	R4210	Q4211	F4212	L4213	F4214	D4215	V4216	V4217	N4218	E4219	E4234	I4242	X4315	X4320	X4325	X4326	X4327	X4330	R4546	V4547	K4548	F4549	L4553	L4560	L4576	F4629	S4633	T4634	Y4636	A4640	L4641	R4642	C4643															
D4058	K4064	D4065	G4068	S4069	E4070	A4071	F4072	Q4073	D4074	D4078	P4079	R4080	G4081	R4126	F4127	Q4128	E4129	P4130	A4131	D4132	L4133	I4134	G4135	F4136	N4137	L4141	S4146	E4147	H4148	P4150	H4151	D4152	P4153	R4154	L4155	R4156	N4157	E4160	L4161	A4162	E4163	E4167	E4177	R4183	R4184	L4185													
E3687	E3688	D3692	E3708	K3709	S3710	K3711	E3732	E3733	E3737	S3747	K3751	E3752	Q3756	Q3762	L3765	H3766	H3767	R3768	G3769	S3770	C3781	E3784	N3804	A3805	D3806	V3807	A3829	C3834	E3843	Q3858	T3859	E3867	A3871	F3880	Q3884	N3892	N3896	T3914	K3675	A3676	G3677	E3678	Q3679	E3680	E3681	E3682	E3683	E3684	E3685	V3686									
X3586	X3587	X3588	X3589	X3590	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3605	X3606	H3617	K3618	L3619	L3620	S3621	K3622	Q3623	R3624	R3625	R3626	A3630	R3633	L3637	Y3638	N3639	N3647	A3655	T3660	E3666	D3671	K3675	A3676	G3677	E3678	Q3679	E3680	E3681	E3682	E3683	E3684	E3685	V3686											
E3441	I3442	F3443	I3444	S3447	K3448	S3449	H3450	N3451	F3452	E3455	E3456	Q3457	N3458	V3461	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3521	X3522	X3523	X3524	X3525	X3526	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3551	X3552	X3553	X3554	X3555	X3556	X3568	X3569	X3570	X3571	X3572							
X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3368	X3369	X3370	X3371	X3372	X3375	X3376	X3380	X3381	X3382	X3383	X3384	X3385	F3389	S3400	V3401	C3403	R3404	D3405	L3406	Y3407	A3408	L3409	Y3410	F3411	L3412	L3413	T3414	R3415	Y3416	Y3417	D3418	R3421	A3422	H3423	W3424	L3425	T3426	E3427	P3428	N3429	F3430	S3431	E3434	Y3438								
X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3346	X3347	X3348	X3349	X3350	X3351	X3352
X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3164	X3165	X3166	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3225	X3226	X3227	X3228	X3229
X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3007	X3008	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3034	X3035	X3036	X3037	X3038	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3051	X3052	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3147	X3148			
K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	A2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	A2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965



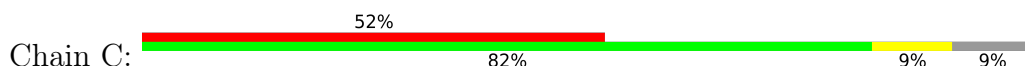
• Molecule 2: Ryanodine Receptor

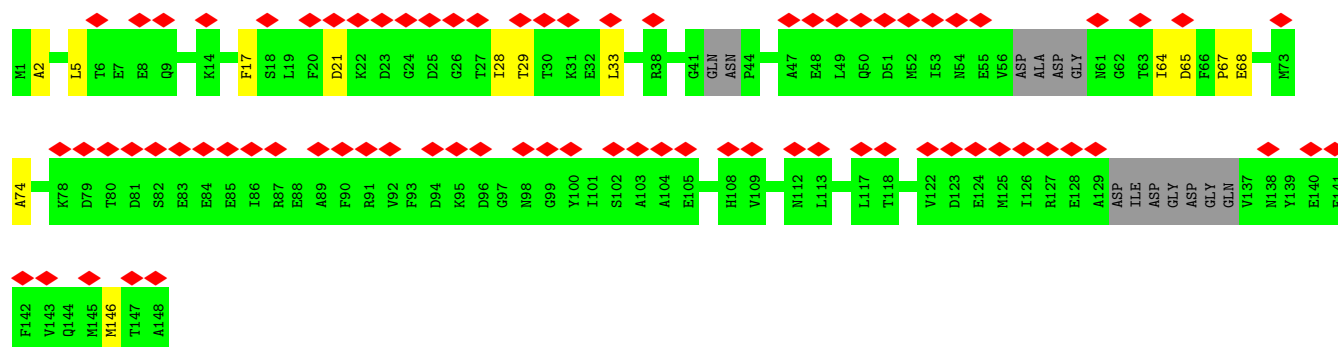




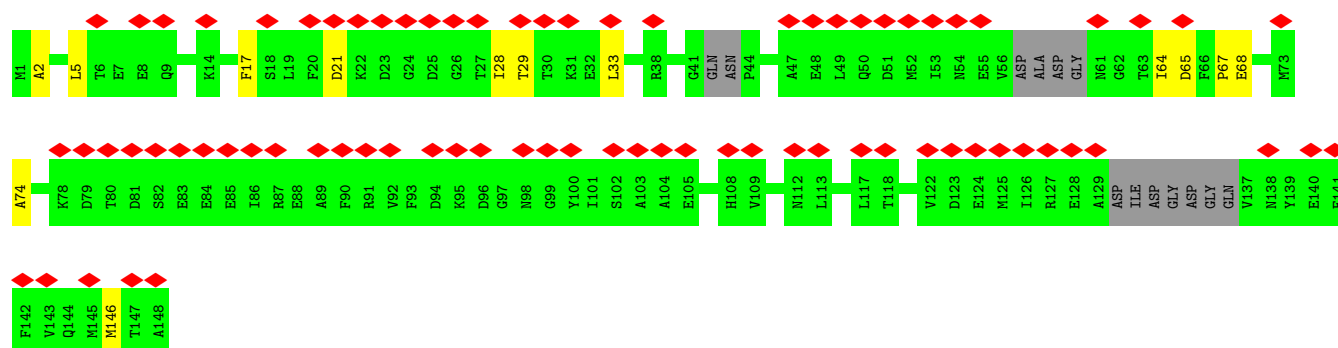
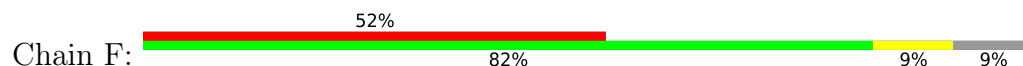


- Molecule 3: Calmodulin-1

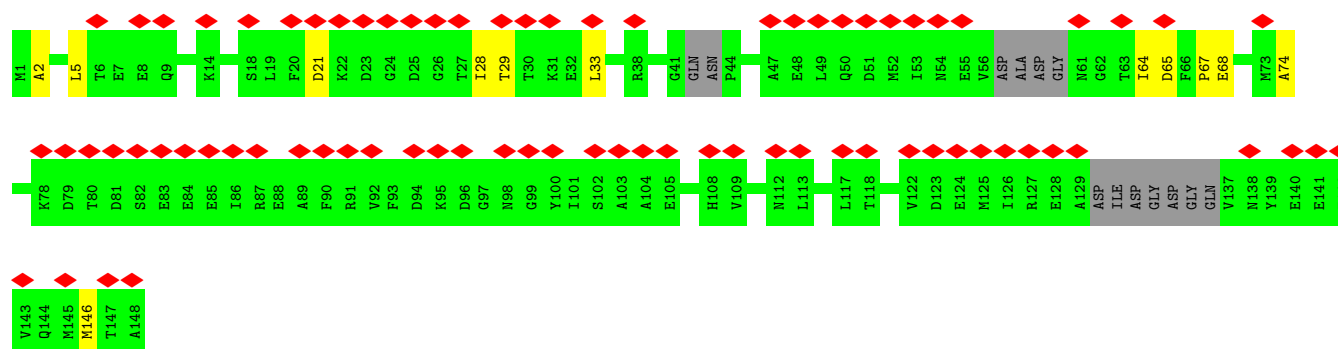
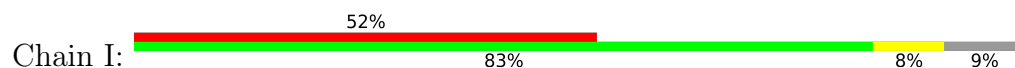




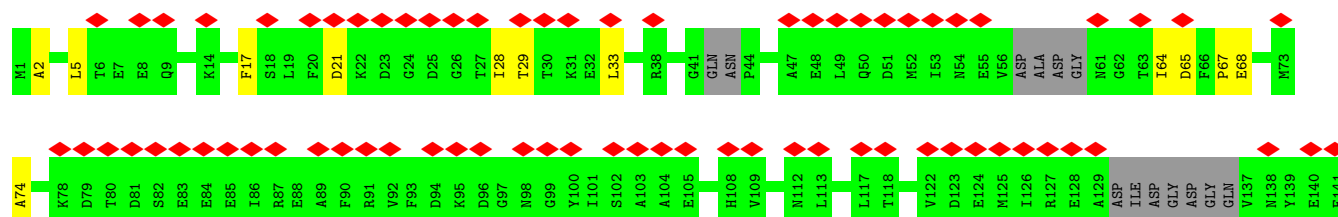
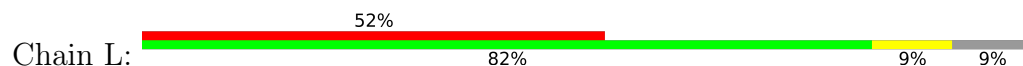
- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1



F142	V143	Q144	M145	M146	T147	A148
------	------	------	------	------	------	------

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size ( $\text{\AA}$ )	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	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: 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	0.25	0/743	0.42	0/1014
1	D	0.25	0/743	0.42	0/1014
1	G	0.25	0/743	0.42	0/1014
1	J	0.25	0/743	0.42	0/1014
2	B	0.23	0/25353	0.38	0/34606
2	E	0.23	0/25353	0.38	0/34606
2	H	0.23	0/25353	0.38	0/34606
2	K	0.23	0/25353	0.38	0/34606
3	C	0.24	0/772	0.36	0/1059
3	F	0.24	0/772	0.36	0/1059
3	I	0.24	0/772	0.36	0/1059
3	L	0.24	0/772	0.36	0/1059
All	All	0.23	0/107472	0.38	0/146716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	727	0	651	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	727	0	651	8	0
1	G	727	0	651	8	0
1	J	727	0	651	8	0
2	B	26597	0	22867	156	0
2	E	26597	0	22867	153	0
2	H	26597	0	22867	157	0
2	K	26597	0	22867	157	0
3	C	768	0	486	9	0
3	F	768	0	486	9	0
3	I	768	0	486	8	0
3	L	768	0	486	9	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
All	All	112372	0	96016	654	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 3.

The worst 5 of 654 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:886:ARG:HB2	2:E:891:TRP:HB2	1.73	0.71
2:B:886:ARG:HB2	2:B:891:TRP:HB2	1.73	0.71
2:H:886:ARG:HB2	2:H:891:TRP:HB2	1.73	0.71
2:K:886:ARG:HB2	2:K:891:TRP:HB2	1.73	0.71
2:E:4706:THR:HG21	2:E:4773:TYR:HB2	1.74	0.70

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	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	D	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	G	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	J	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
2	B	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	E	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	H	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	K	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
3	C	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	F	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	I	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	L	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
All	All	14508/16284 (89%)	14228 (98%)	280 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	66/88 (75%)	66 (100%)	0	100	100
1	D	66/88 (75%)	66 (100%)	0	100	100
1	G	66/88 (75%)	66 (100%)	0	100	100
1	J	66/88 (75%)	66 (100%)	0	100	100
2	B	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	E	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	H	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	K	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
3	C	29/126 (23%)	29 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	29/126 (23%)	29 (100%)	0	100	100
3	I	29/126 (23%)	29 (100%)	0	100	100
3	L	29/126 (23%)	29 (100%)	0	100	100
All	All	9268/12956 (72%)	9264 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2128	GLN
2	E	2128	GLN
2	H	2128	GLN
2	K	2128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	3955	GLN
2	K	2128	GLN
2	H	838	HIS
2	K	838	HIS
2	E	4981	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	56
2	E	56
2	H	56
2	K	56

The worst 5 of 224 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4331:UNK	C	4543:GLU	N	51.24
1	E	4331:UNK	C	4543:GLU	N	51.24
1	H	4331:UNK	C	4543:GLU	N	51.24
1	K	4331:UNK	C	4543:GLU	N	51.24
1	B	1054:GLU	C	1071:ARG	N	36.98

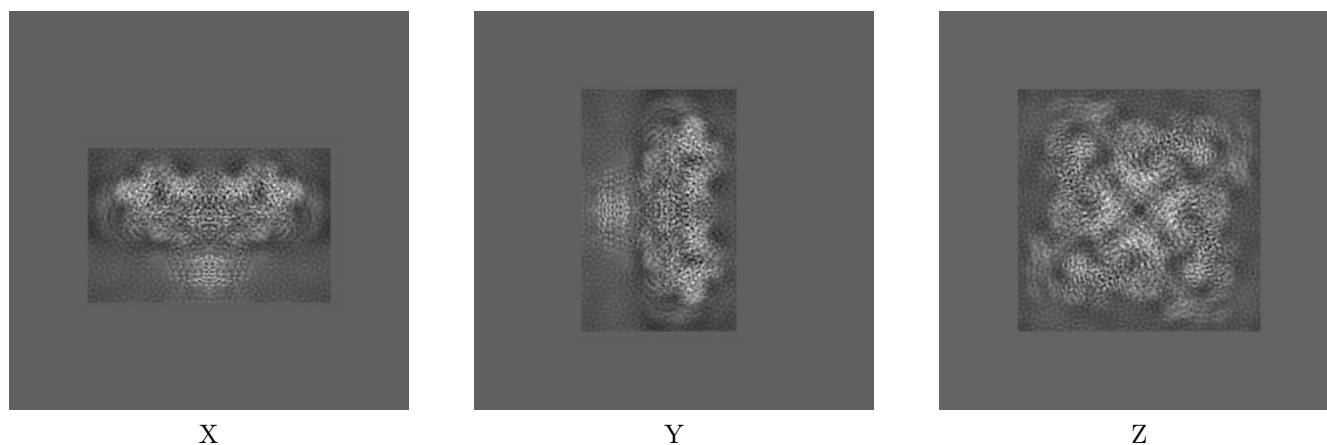
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22016. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

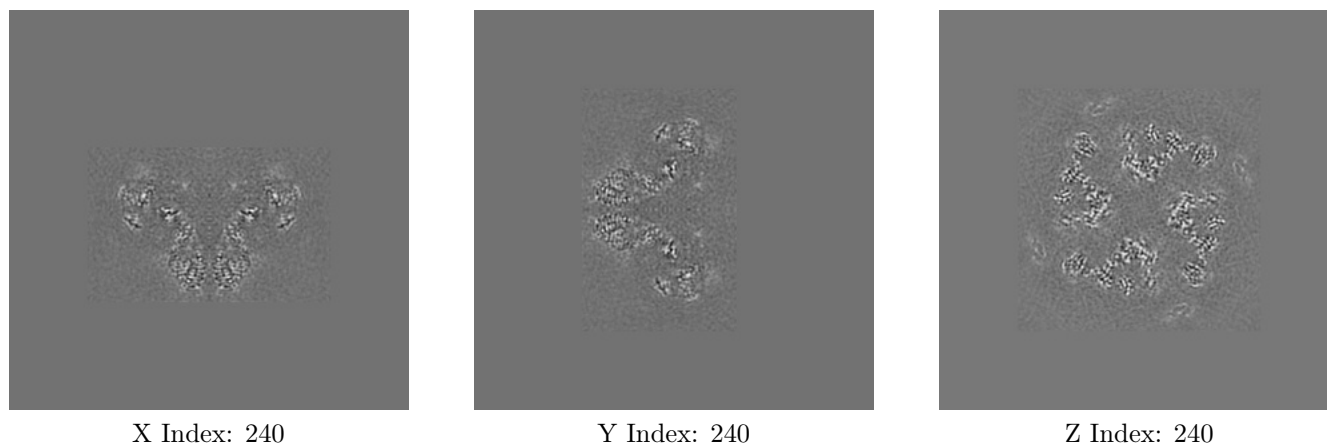
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

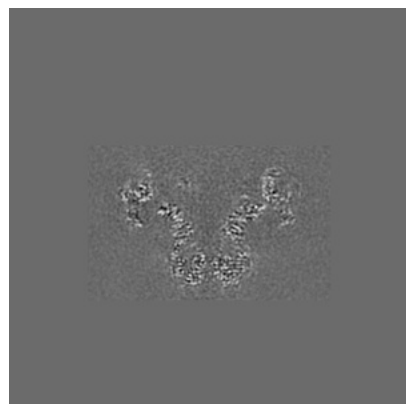
#### 6.2.1 Primary map



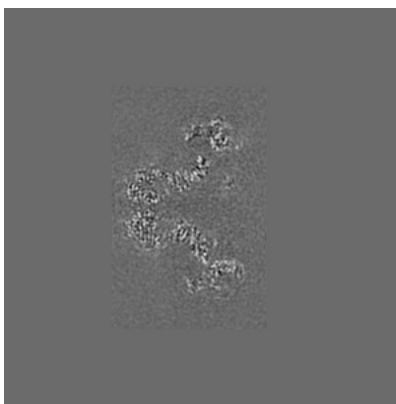
The images above show central slices of the map in three orthogonal directions.

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

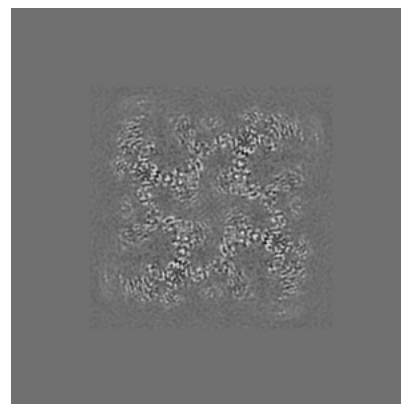
### 6.3.1 Primary map



X Index: 236



Y Index: 236



Z Index: 265

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

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

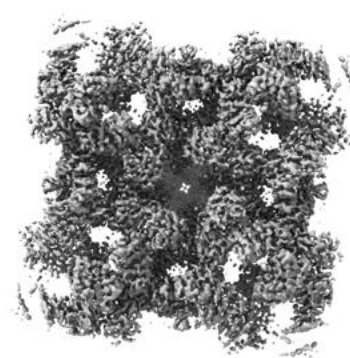
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

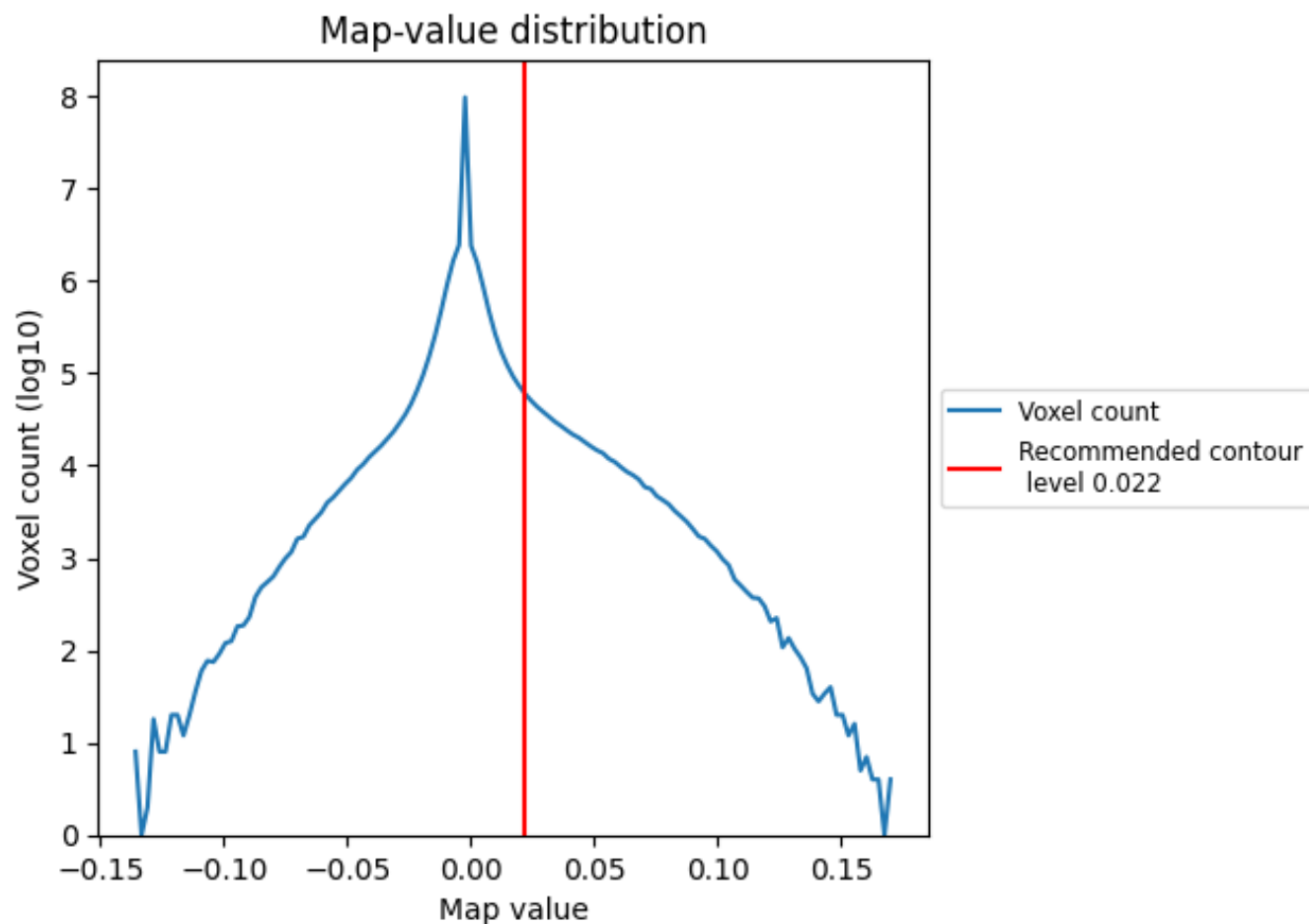
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

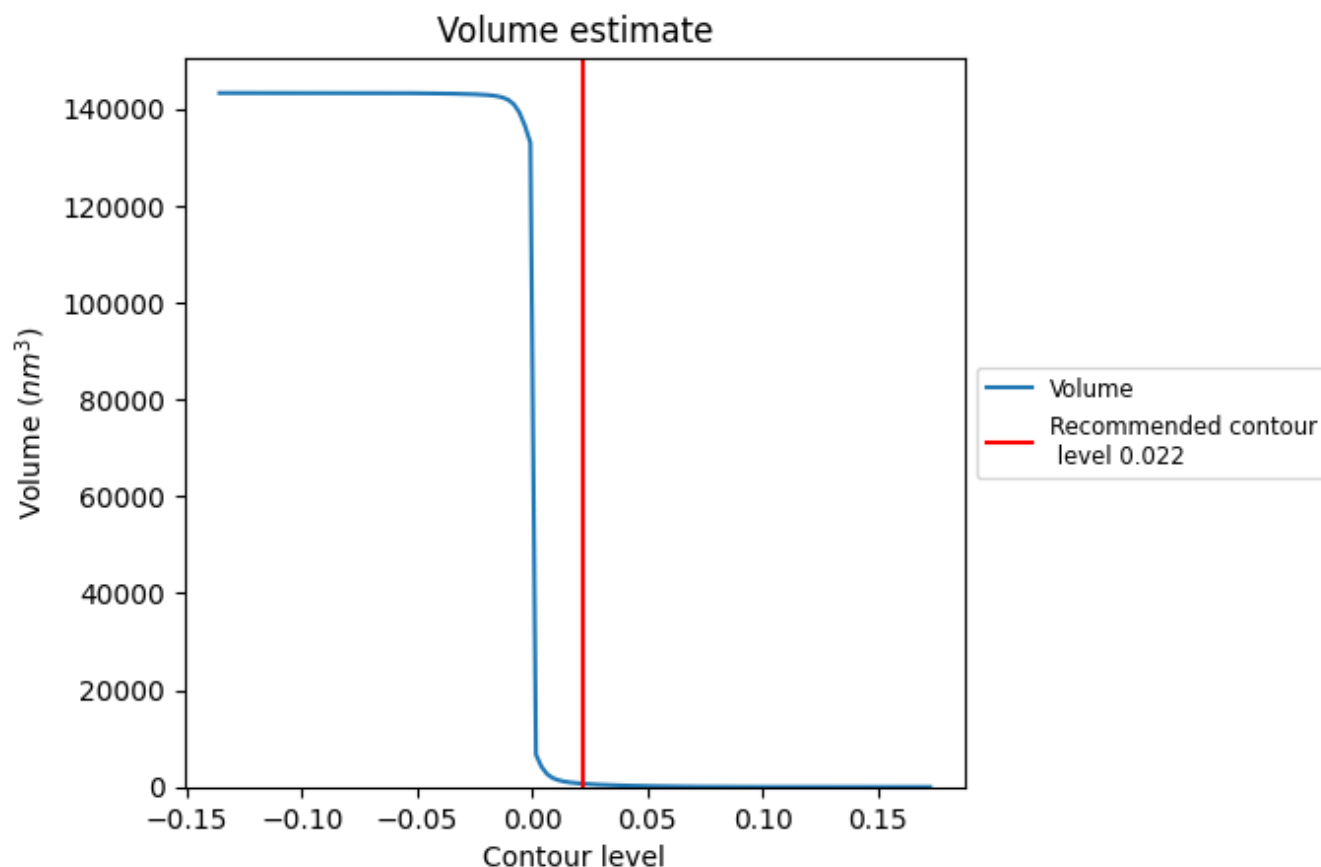
This section contains the results of statistical analysis of the map.

### 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.

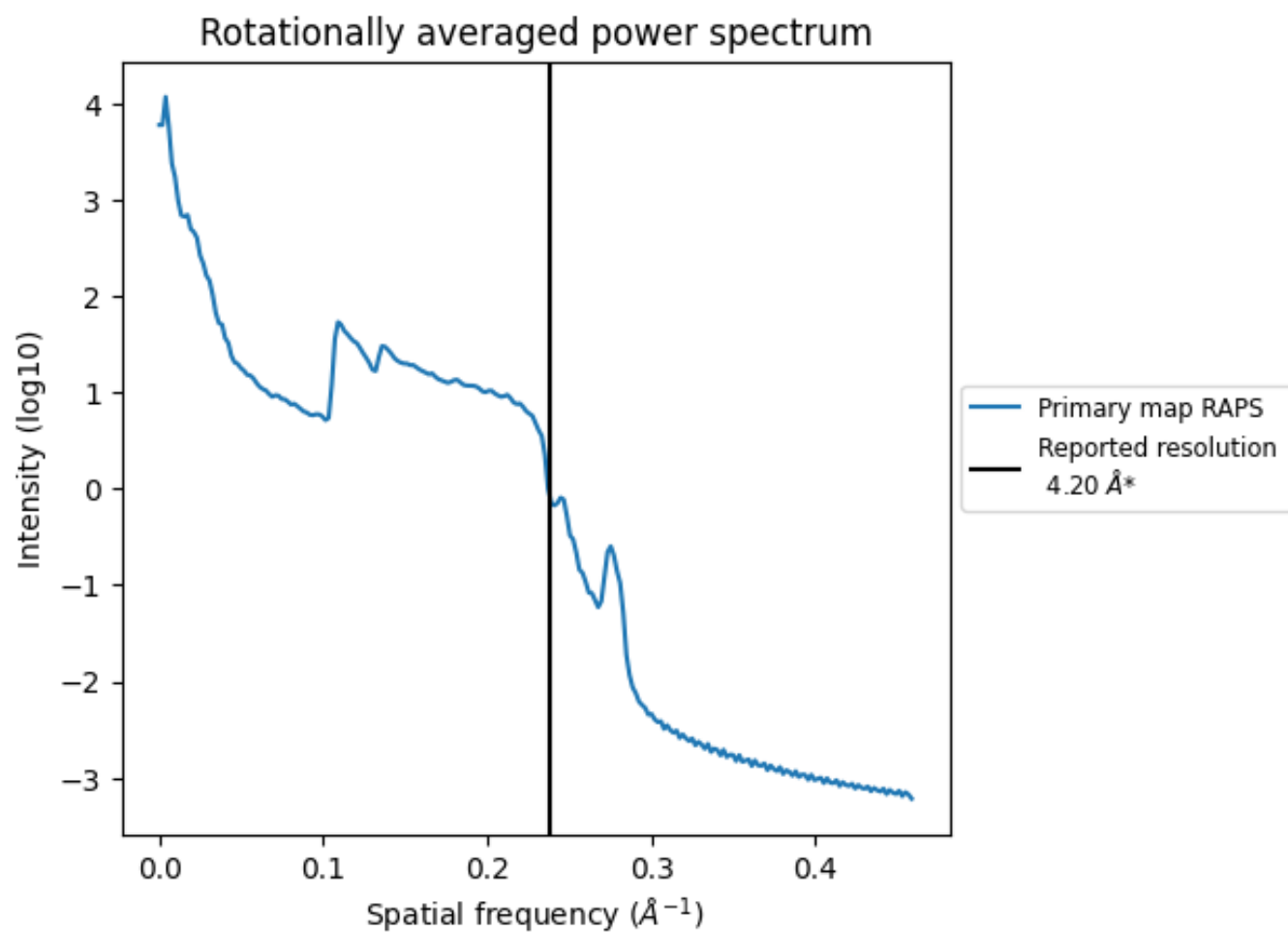
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm<sup>3</sup>; this corresponds to an approximate mass of 607 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 0.238 Å<sup>-1</sup>

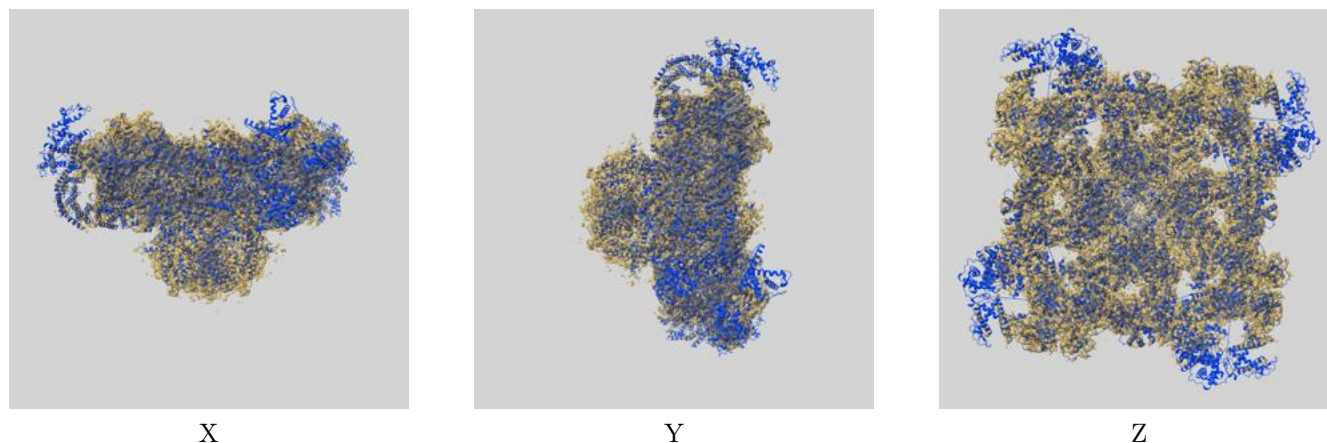
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

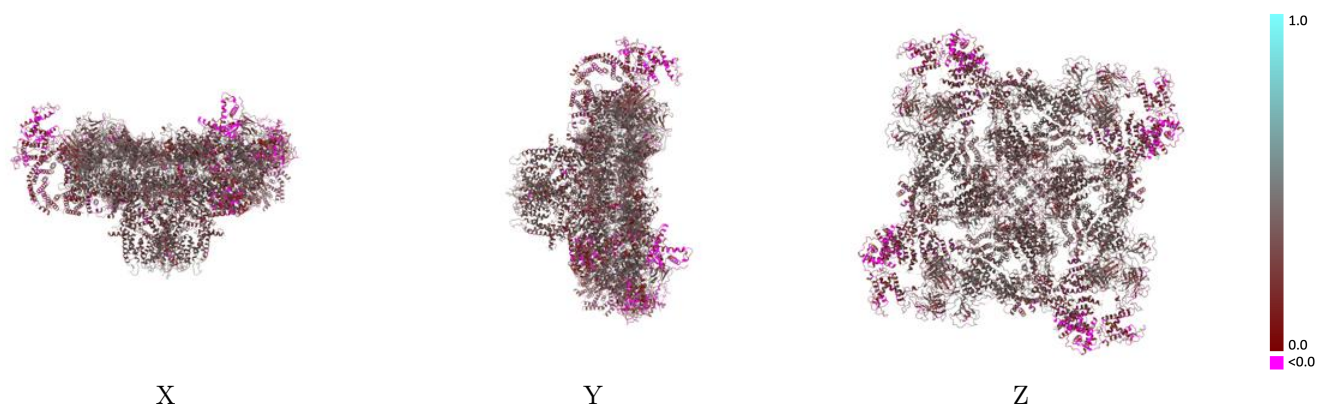
This section contains information regarding the fit between EMDB map EMD-22016 and PDB model 6X33. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



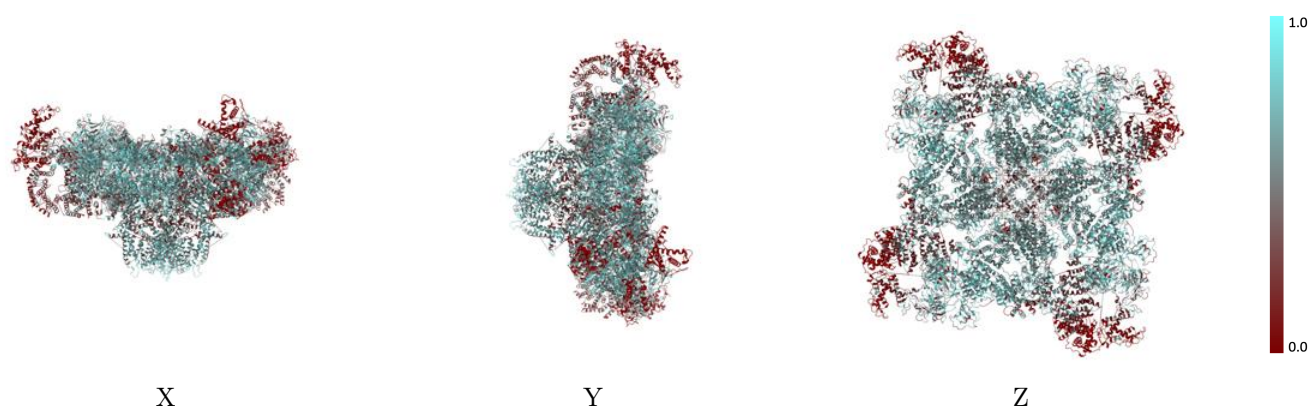
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



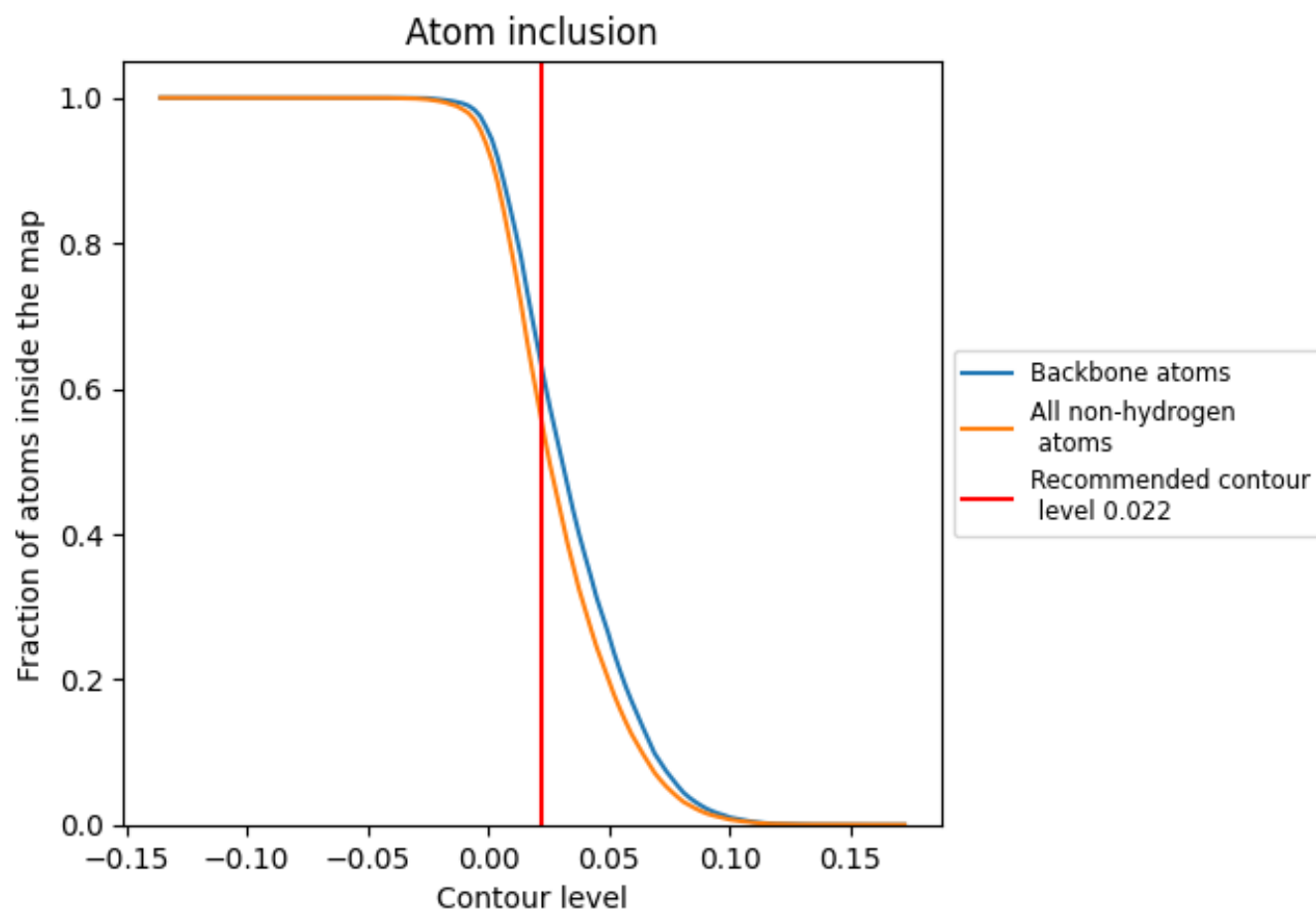
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 56% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5584	<div></div> 0.3230
A	<div></div> 0.6019	<div></div> 0.3810
B	<div></div> 0.5615	<div></div> 0.3230
C	<div></div> 0.4112	<div></div> 0.2760
D	<div></div> 0.6019	<div></div> 0.3780
E	<div></div> 0.5615	<div></div> 0.3230
F	<div></div> 0.4112	<div></div> 0.2740
G	<div></div> 0.6006	<div></div> 0.3780
H	<div></div> 0.5615	<div></div> 0.3230
I	<div></div> 0.4112	<div></div> 0.2720
J	<div></div> 0.6019	<div></div> 0.3790
K	<div></div> 0.5616	<div></div> 0.3220
L	<div></div> 0.4112	<div></div> 0.2750

