



wwPDB EM Validation Summary Report ⓘ

Feb 25, 2024 – 12:17 PM EST

PDB ID : 6X35
EMDB ID : EMD-22018
Title : Pig R615C RyR1 in complex with CaM, EGTA (class 1, 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

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

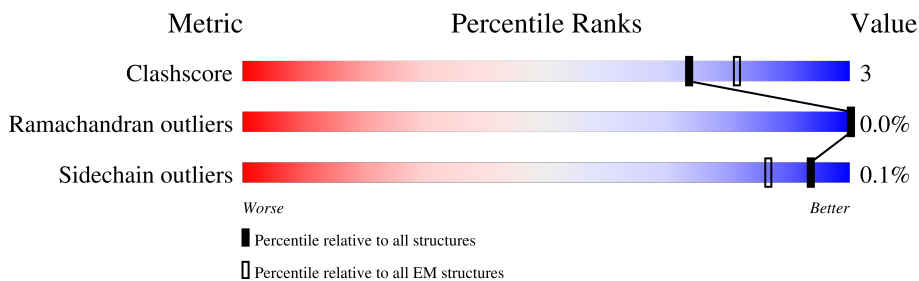
1 Overall quality at a glance

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.






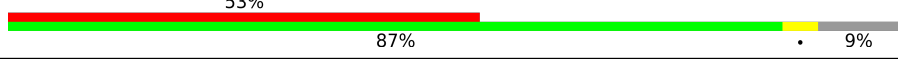
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	110	
1	D	110	
1	G	110	
1	J	110	
2	B	3801	
2	E	3801	
2	H	3801	
2	K	3801	

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

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 111888 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	A	106	740	472	128	137	3	0	0
1	D	106	740	472	128	137	3	0	0
1	G	106	740	472	128	137	3	0	0
1	J	106	740	472	128	137	3	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68106
A	-1	ASN	-	expression tag	UNP P68106
A	0	ALA	-	expression tag	UNP P68106
D	-2	SER	-	expression tag	UNP P68106
D	-1	ASN	-	expression tag	UNP P68106
D	0	ALA	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	ASN	-	expression tag	UNP P68106
G	0	ALA	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	ASN	-	expression tag	UNP P68106
J	0	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	3801	26463	16948	4708	4641	166	6	0
2	E	3801	26463	16948	4708	4641	166	6	0
2	H	3801	26463	16948	4708	4641	166	6	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	3801	26463	16948	4708	4641	166	6	0

- Molecule 3 is a protein called Calmodulin-1.

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

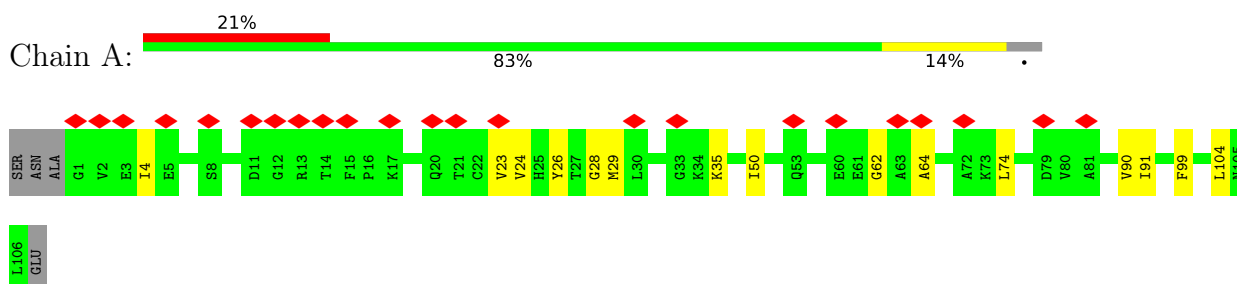
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

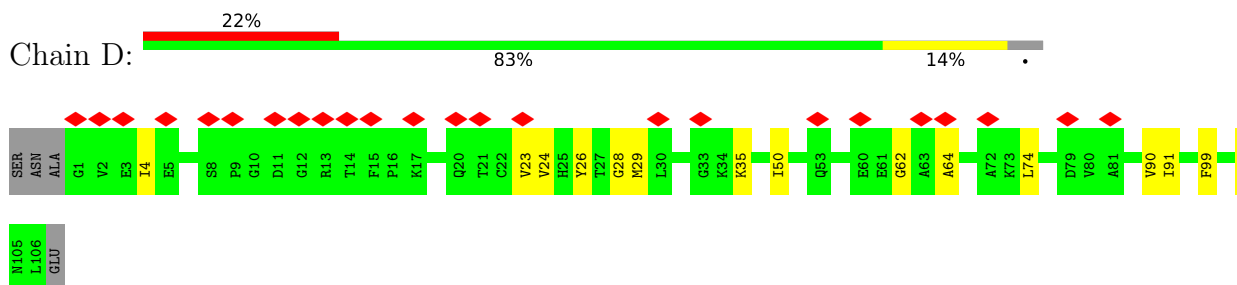
3 Residue-property plots [i](#)

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

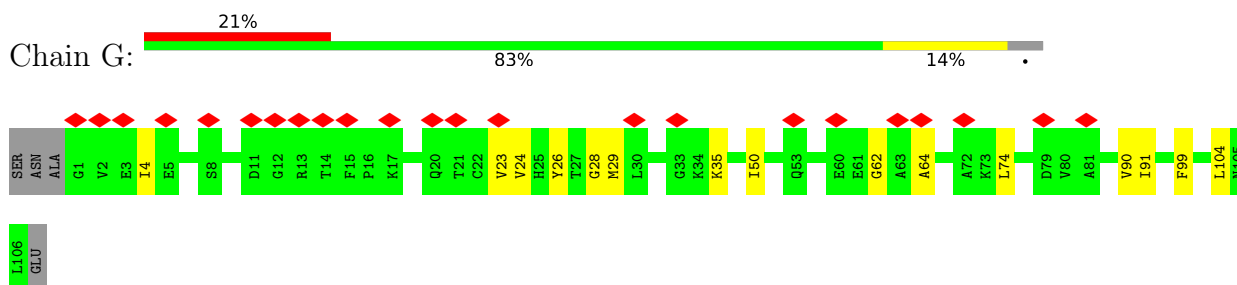
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



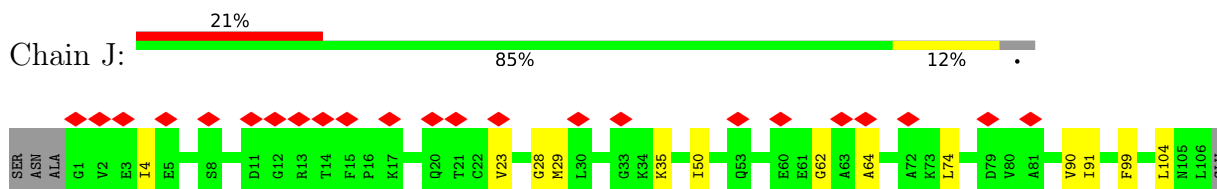
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



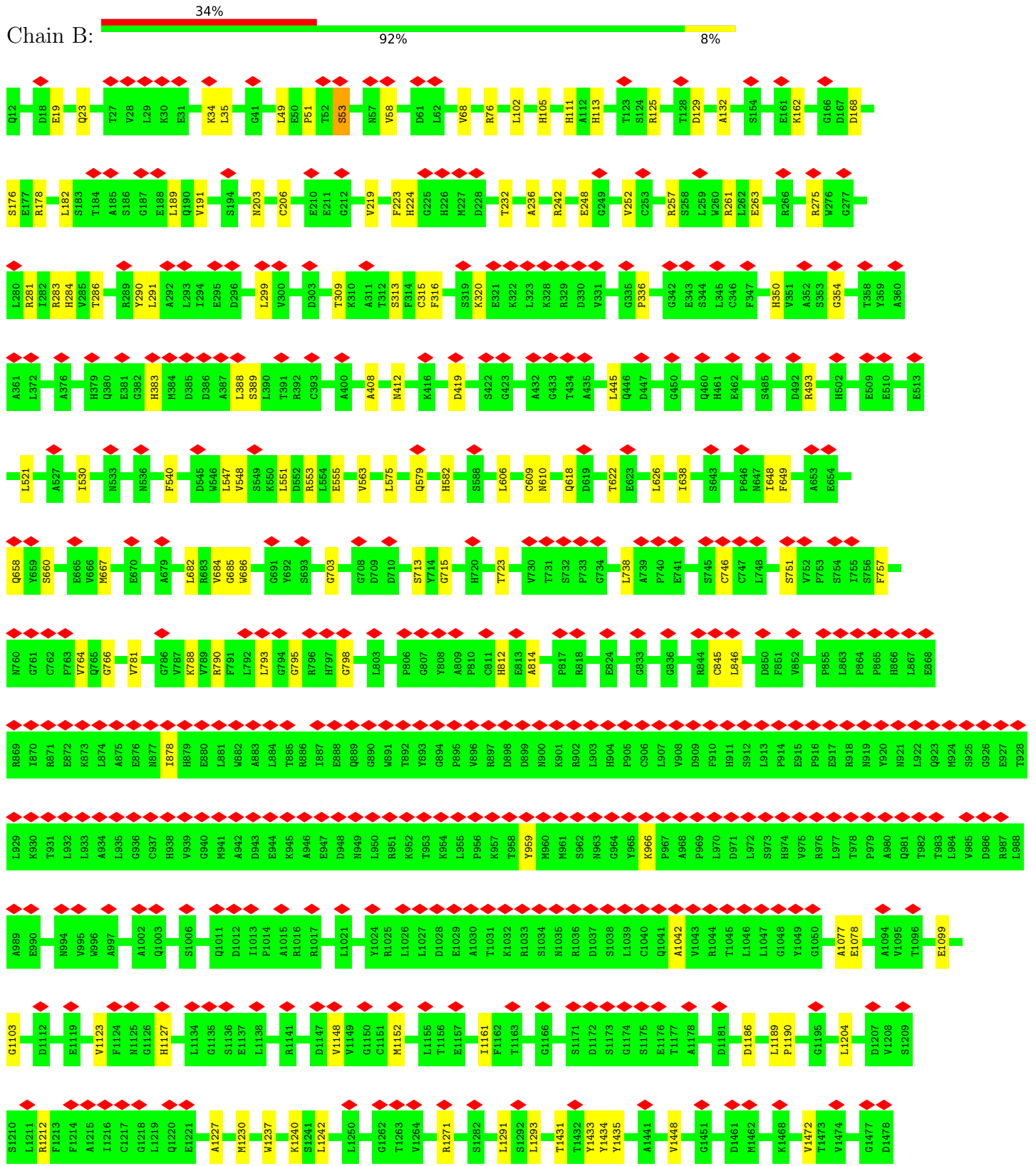
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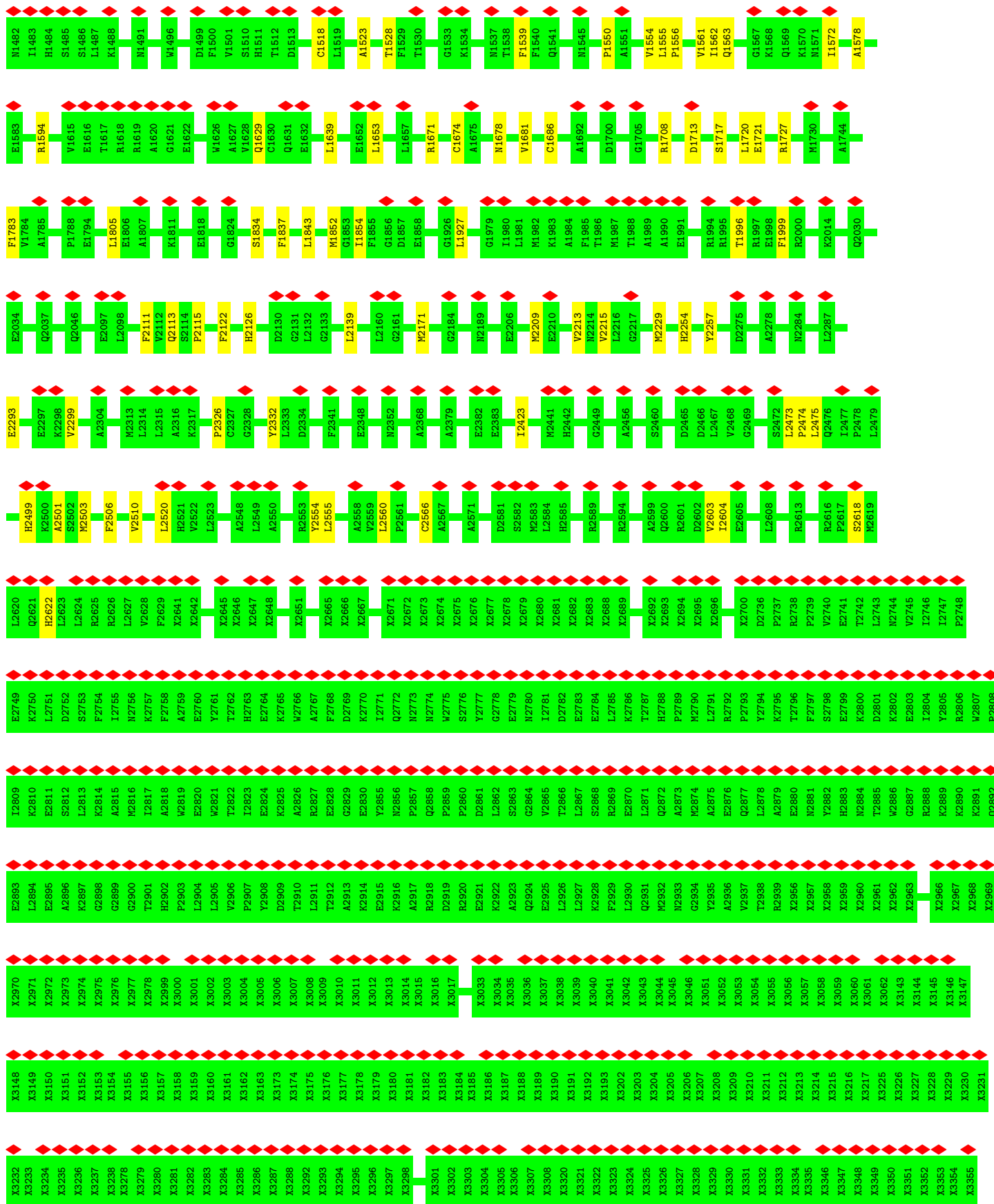


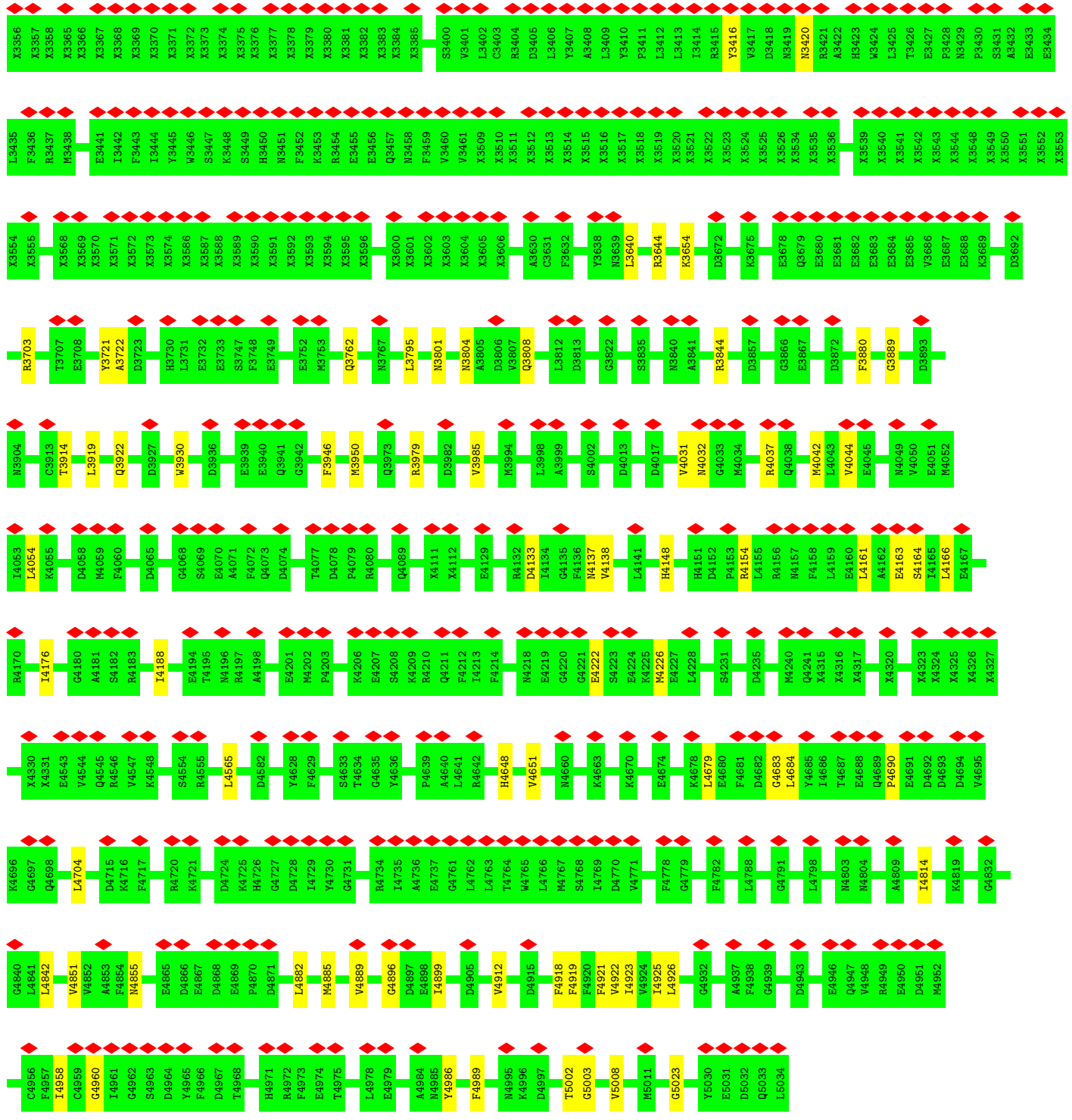
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



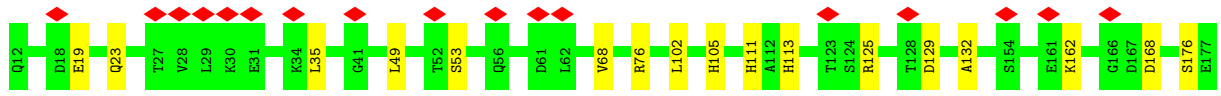
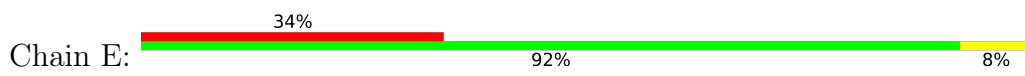
● Molecule 2: Ryanodine Receptor

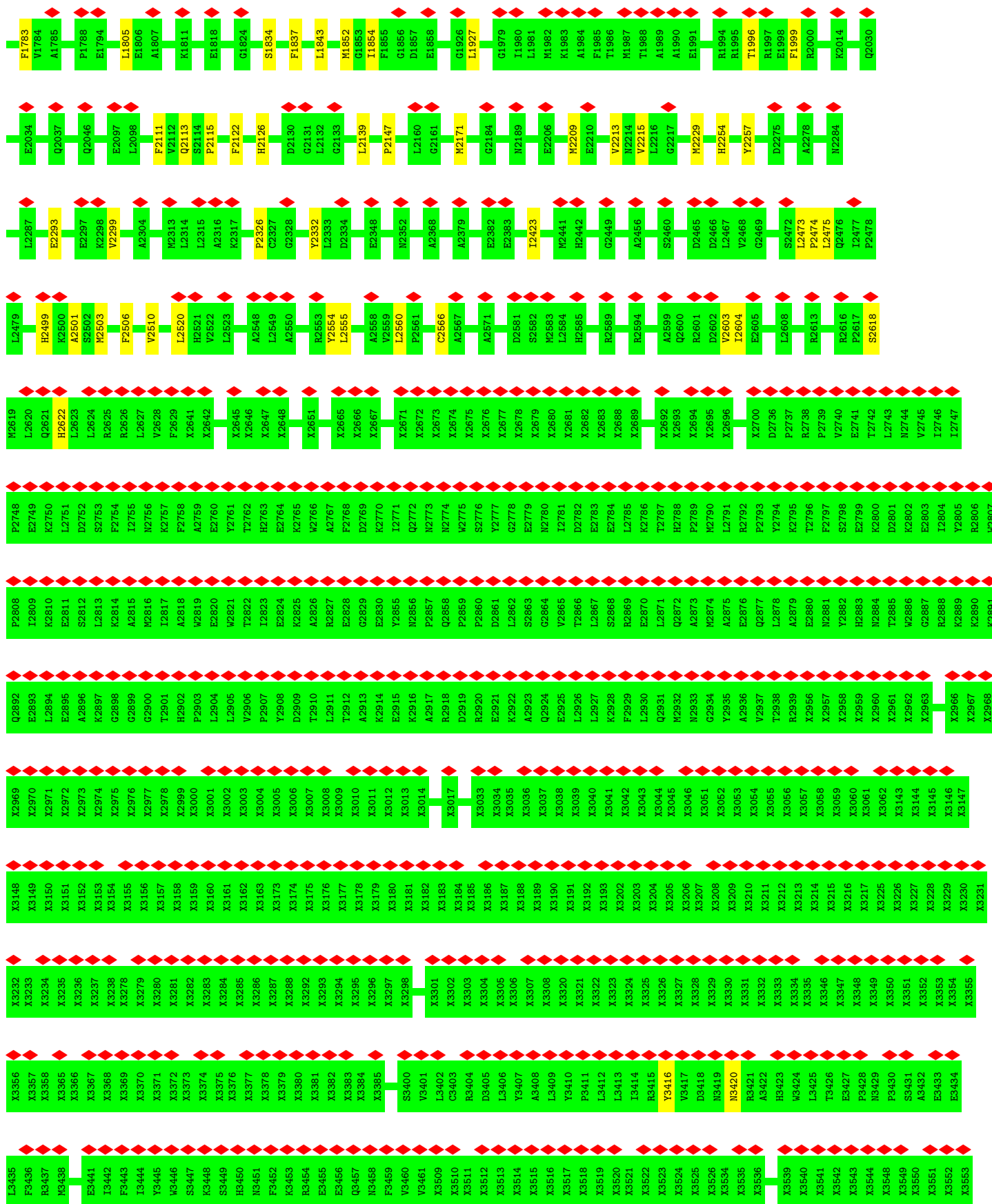


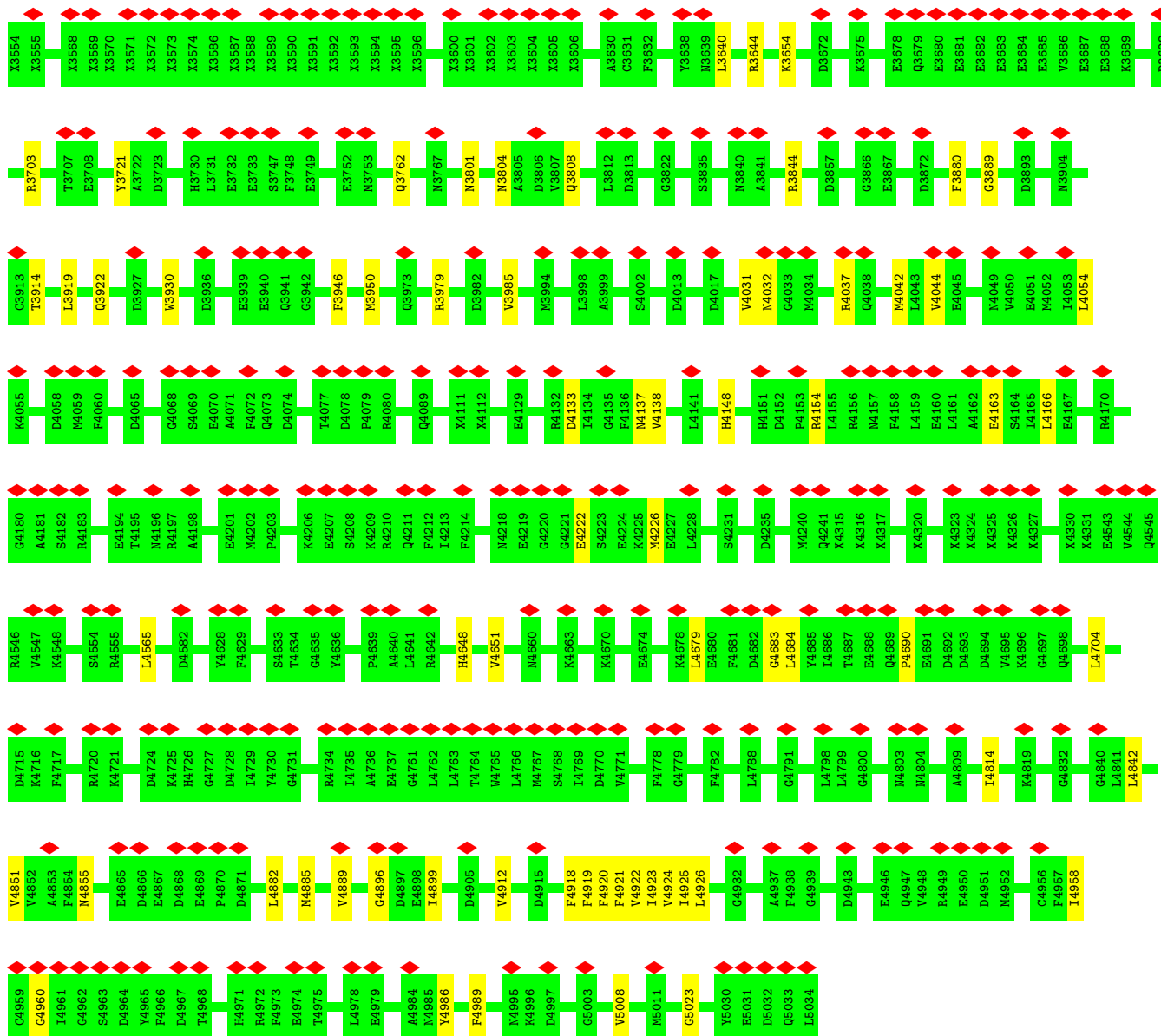




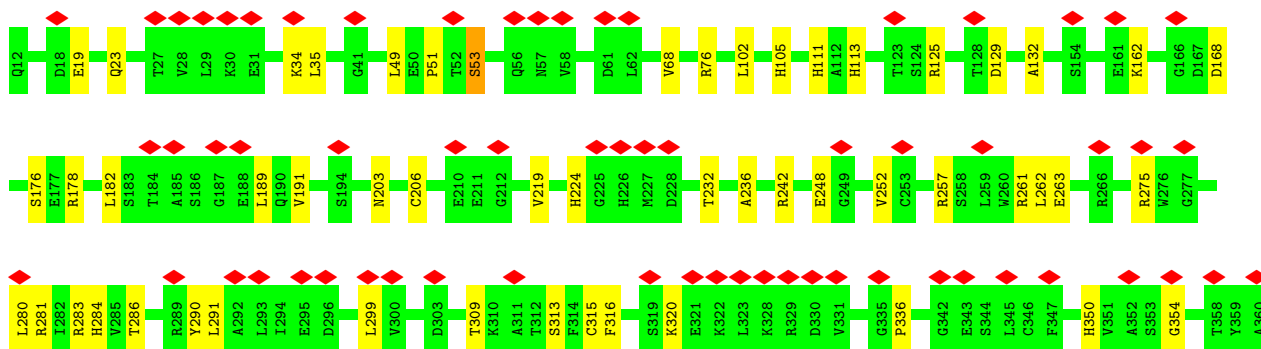
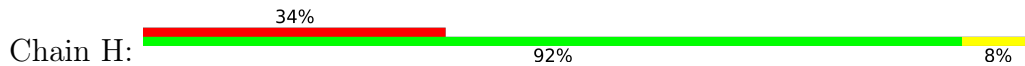
• Molecule 2: Ryanodine Receptor

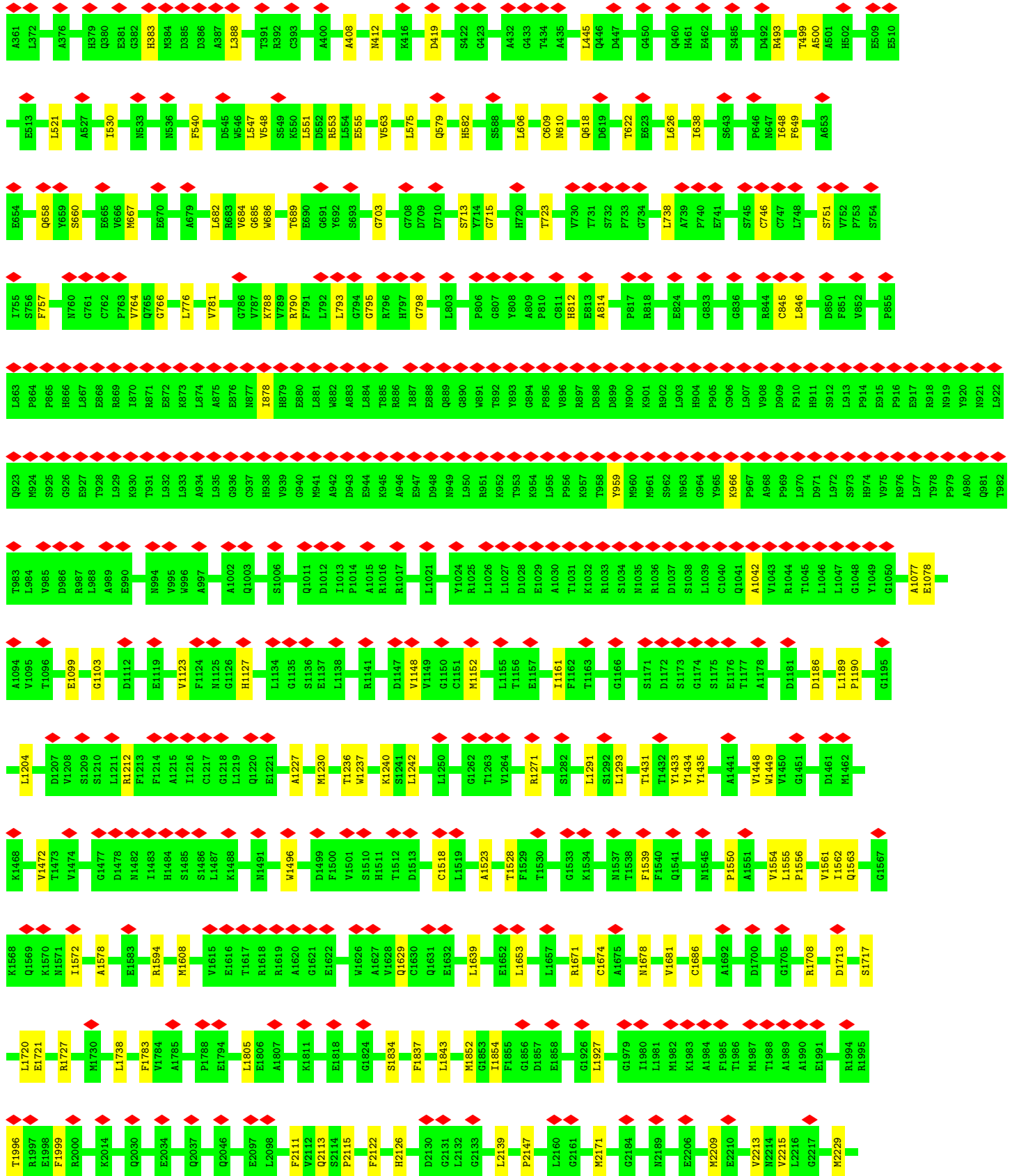


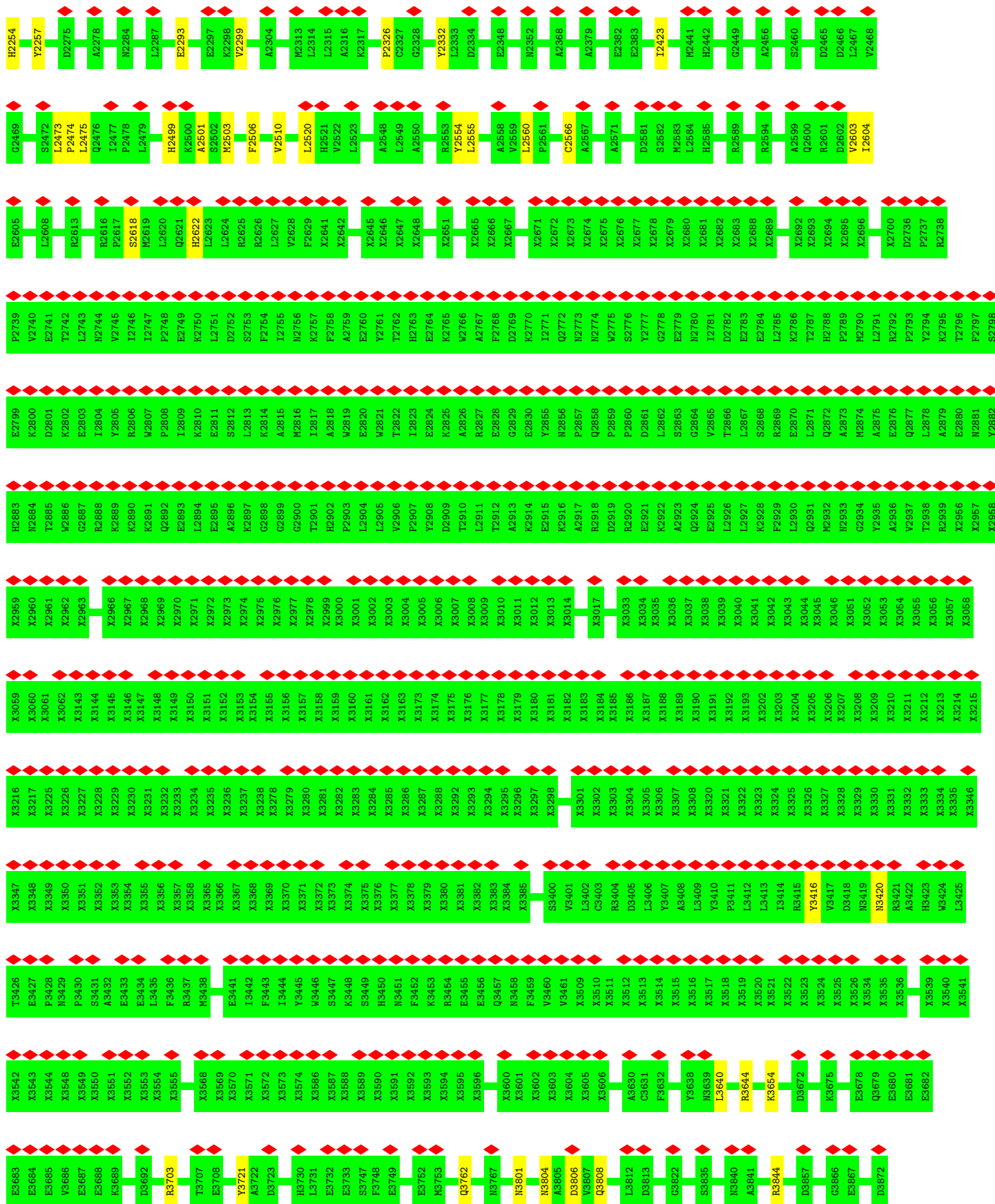


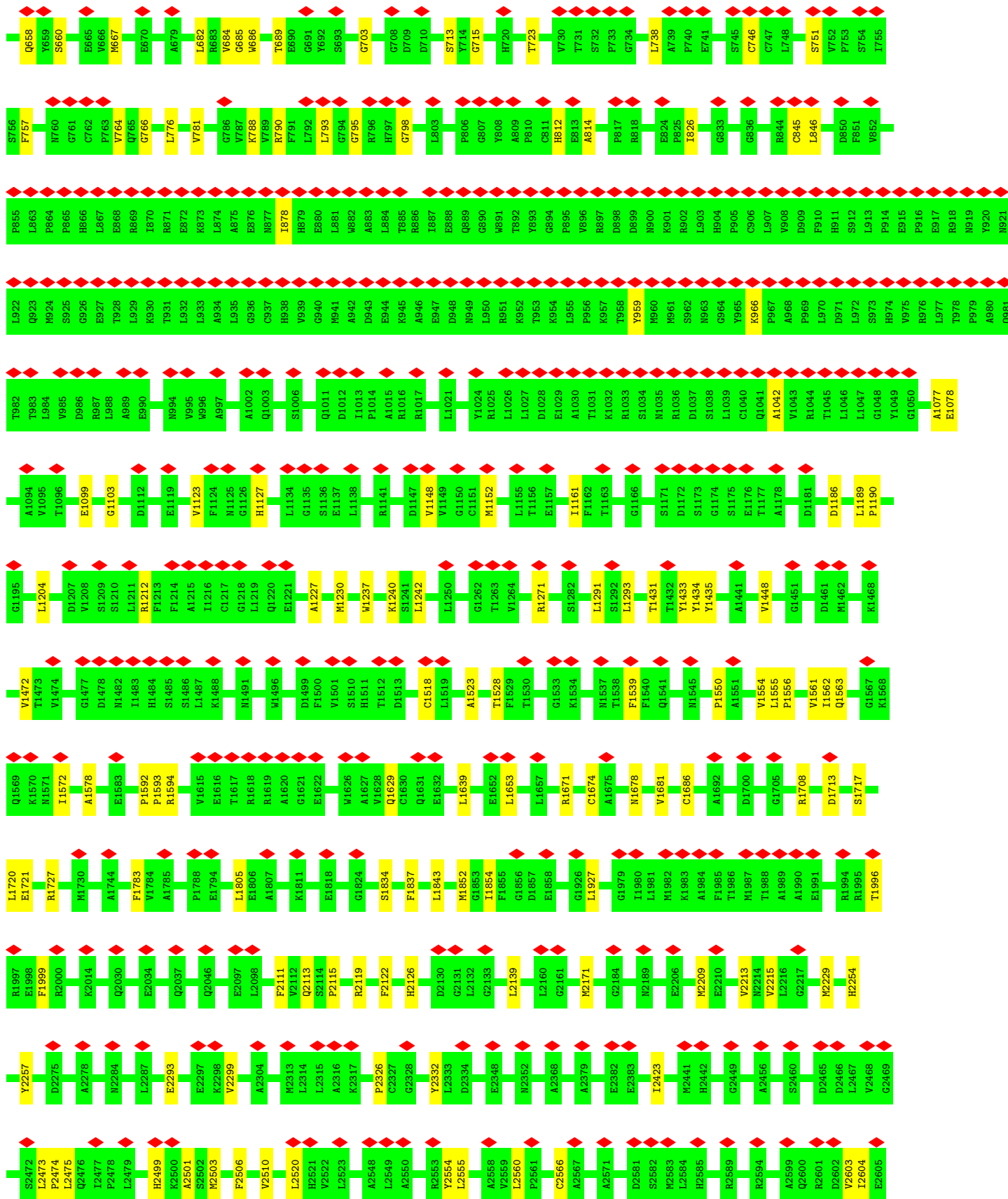


• Molecule 2: Ryanodine Receptor









L2608	L2613	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	F2629	L2641	L2642	L2645	L2646	L2647	L2648	X2651	X2665	X2666	X2667	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2682	X2683	X2688	X2689	X2692	X2693	X2694	X2695	X2696	X2700	D2736	P2737	R2738	P2739																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	L2749	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	F2629	L2641	L2642	X2651	X2665	X2666	X2667	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2682	X2683	X2688	X2689	X2692	X2693	X2694	X2695	X2696	X2700	D2736	P2737	R2738	P2739																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
K2800	D2801	K2802	E2803	L2804	V2805	K2806	L2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	L2822	L2823	E2824	K2825	A2826	R2827	E2828	Q2829	E2830	L2831	N2832	Q2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
M2884	T2885	W2886	Q2887	R2888	K2889	K2890	W2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2916	R2918	D2919	R2920	K2921	K2922	A2923	Q2924	L2925	L2926	L2927	L2928	K2929	L2930	Q2931	M2932	G2933	G2934	Y2935	A2936	V2937	T2938	R2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3017	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601	L3602	L3603	L3604	L3605	L3606	L3607	L3608	L3609	L3610	L3611	L3612	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720	L3721	L3722	L3723	L3724	L3725	L3726	L3727	L3728	L3729	L3730	L3731	L3732	L3733	L3734	L3735	L3736	L3737	L3738	L3739	L3740	L3741	L3742	L3743	L3744	L3745	L3746	L3747	L3748	L3749	L3750	L3751	L3752	L3753	L3754	L3755	L3756	L3757	L3758	L3759	L3760	L3761	L3762	L3763	L3764	L3765	L3766	L3767	L3768	L3769	L3770	L3771	L3772	L3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859	L3860	L3861	L3862	L3863	L3864	L3865	L3866	L3867	L3868	L3869	L3870	L3871	L3872	L3873	L3874	L3875	L3876	L3877	L3878	L3879	L3880	L3881	L3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947	L3948	L3949	L3950	L3951	L3952	L3953	L3954	L3955	L3956	L3957	L3958	L3959	L3960	L3961	L3962	L3963	L3964	L3965	L3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002	L4003	L4004	L4005	L4006	L4007	L4008	L4009	L4010	L4011	L4012	L4013	L4014	L4015	L4016	L4017	L4018	L4019	L4020	L4021	L4022	L4023	L4024	L4025	L4026	L4027	L4028	L4029	L4030	L4031	L4032	L4033	L4034	L4035	L4036	L4037	L4038	L4039	L4040	L4041	L4042	L4043	L4044	L4045	L4046	L4047	L4048	L4049	L4050	L4051	L4052	L4053	L4054	L4055	L4056	L4057	L4058	L4059	L4060	L4061	L4062	L4063	L4064	L4065	L4066	L4067	L4068	L4069	L4070	L4071	L4072	L4073	L4074	L4075	L4076	L4077

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	0.192	Depositor
Minimum map value	-0.147	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (\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 (\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	0/756	0.42	0/1030
1	D	0.25	0/756	0.42	0/1030
1	G	0.25	0/756	0.42	0/1030
1	J	0.25	0/756	0.42	0/1030
2	B	0.24	0/25212	0.37	0/34385
2	E	0.23	0/25212	0.37	0/34385
2	H	0.23	0/25212	0.37	0/34385
2	K	0.24	0/25212	0.37	0/34385
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	0.24	0/106960	0.37	0/145896

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	740	0	689	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	740	0	689	8	0
1	G	740	0	689	8	0
1	J	740	0	689	7	0
2	B	26463	0	22978	161	0
2	E	26463	0	22978	161	0
2	H	26463	0	22978	165	0
2	K	26463	0	22978	165	0
3	C	768	0	486	4	0
3	F	768	0	486	4	0
3	I	768	0	486	4	0
3	L	768	0	486	4	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	111888	0	96612	687	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 687 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:H:579:GLN:H	2:H:582:HIS:HD2	1.39	0.70
2:K:4565:LEU:HG	2:K:4814:ILE:HD12	1.73	0.70
2:B:579:GLN:H	2:B:582:HIS:HD2	1.39	0.70
2:E:579:GLN:H	2:E:582:HIS:HD2	1.39	0.70
2:K:579:GLN:H	2:K:582:HIS:HD2	1.39	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	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	D	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	G	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
1	J	104/110 (94%)	95 (91%)	9 (9%)	0	100	100
2	B	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
2	E	3380/3801 (89%)	3327 (98%)	53 (2%)	0	100	100
2	H	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
2	K	3380/3801 (89%)	3327 (98%)	52 (2%)	1 (0%)	100	100
3	C	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	F	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	I	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	L	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
All	All	14444/16236 (89%)	14176 (98%)	265 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	51	PRO
2	B	51	PRO
2	K	51	PRO

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	69/90 (77%)	69 (100%)	0	100	100
1	D	69/90 (77%)	69 (100%)	0	100	100
1	G	69/90 (77%)	69 (100%)	0	100	100
1	J	69/90 (77%)	69 (100%)	0	100	100
2	B	2218/3020 (73%)	2215 (100%)	3 (0%)	93	97
2	E	2218/3020 (73%)	2216 (100%)	2 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	2218/3020 (73%)	2216 (100%)	2 (0%)	93	97
2	K	2218/3020 (73%)	2215 (100%)	3 (0%)	93	97
3	C	29/126 (23%)	29 (100%)	0	100	100
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	9264/12944 (72%)	9254 (100%)	10 (0%)	93	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	53	SER
2	K	58	VAL
2	K	125	ARG
2	E	53	SER
2	E	125	ARG

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	3420	ASN
2	K	203	ASN
2	H	23	GLN
2	K	23	GLN
2	E	3804	ASN

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 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	57
2	E	57
2	H	57
2	K	57

The worst 5 of 228 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	51.63
1	E	4331:UNK	C	4543:GLU	N	51.63
1	H	4331:UNK	C	4543:GLU	N	51.63
1	K	4331:UNK	C	4543:GLU	N	51.63
1	B	1050:GLY	C	1071:ARG	N	45.66

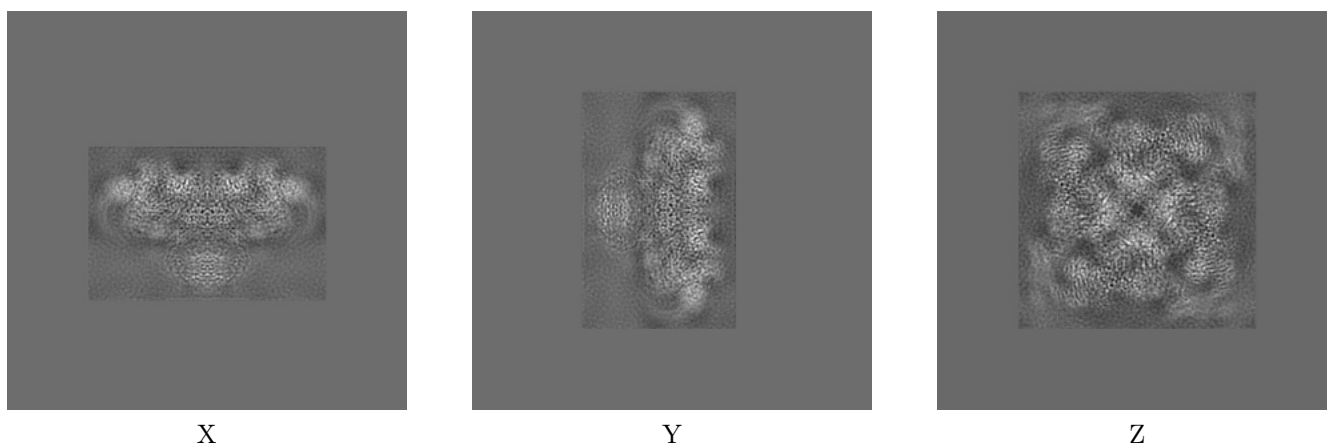
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22018. 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](#)

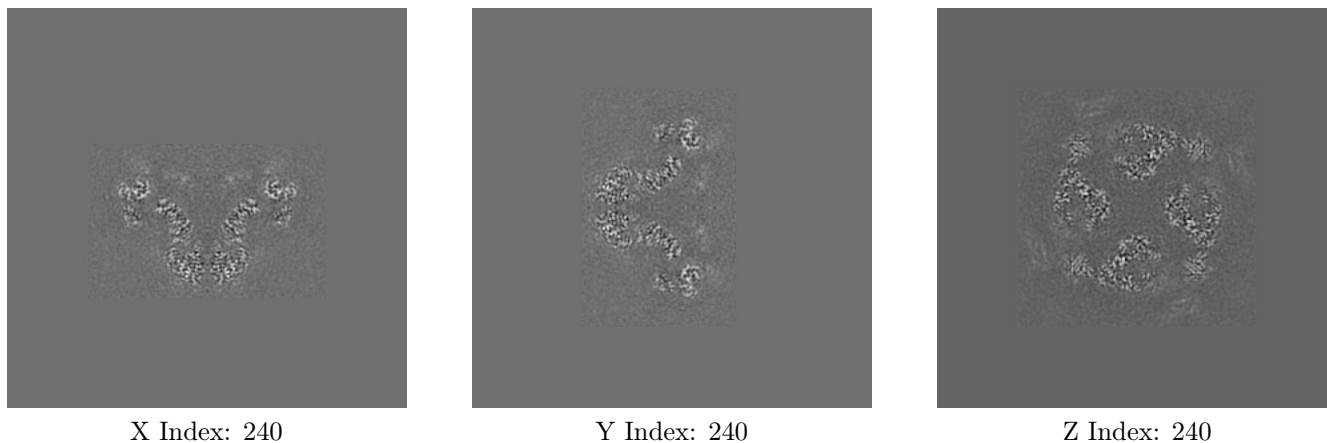
6.1.1 Primary map



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

6.2 Central slices [i](#)

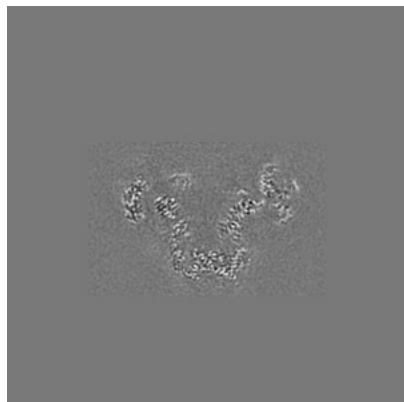
6.2.1 Primary map



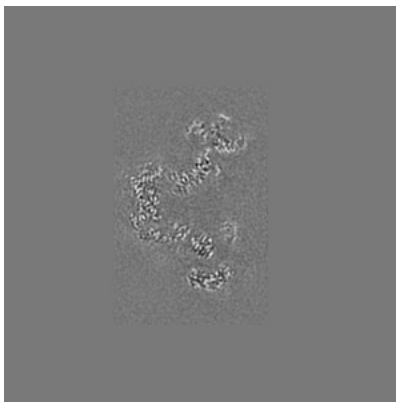
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

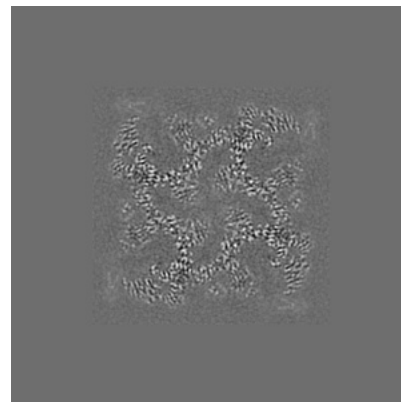
6.3.1 Primary map



X Index: 233



Y Index: 247

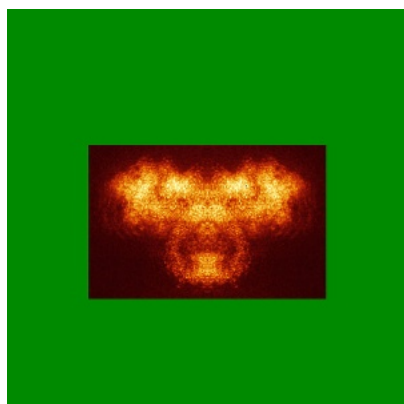


Z Index: 268

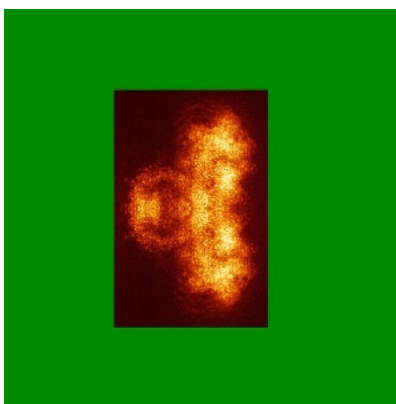
The images above show the largest variance slices of the map in three orthogonal directions.

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

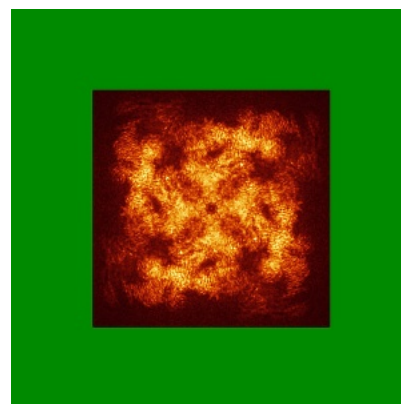
6.4.1 Primary map



X



Y

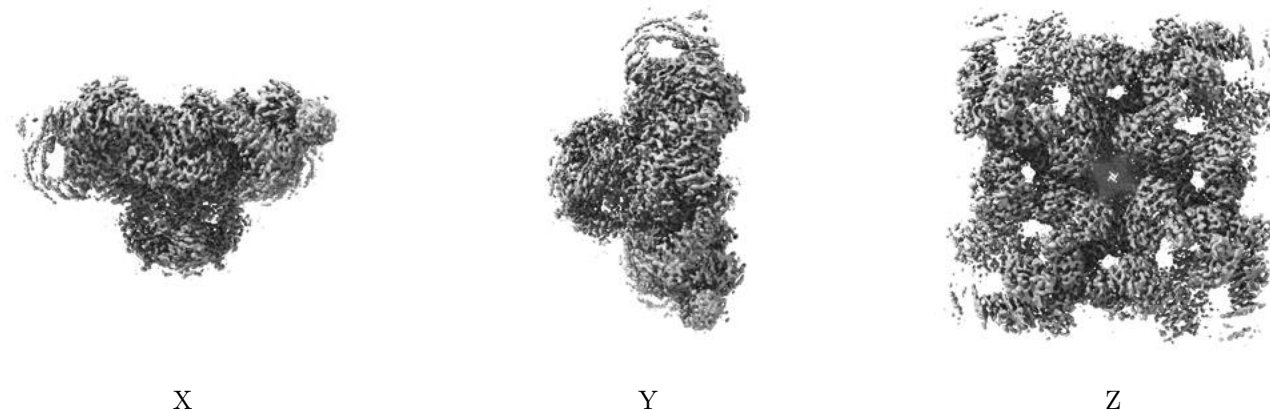


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

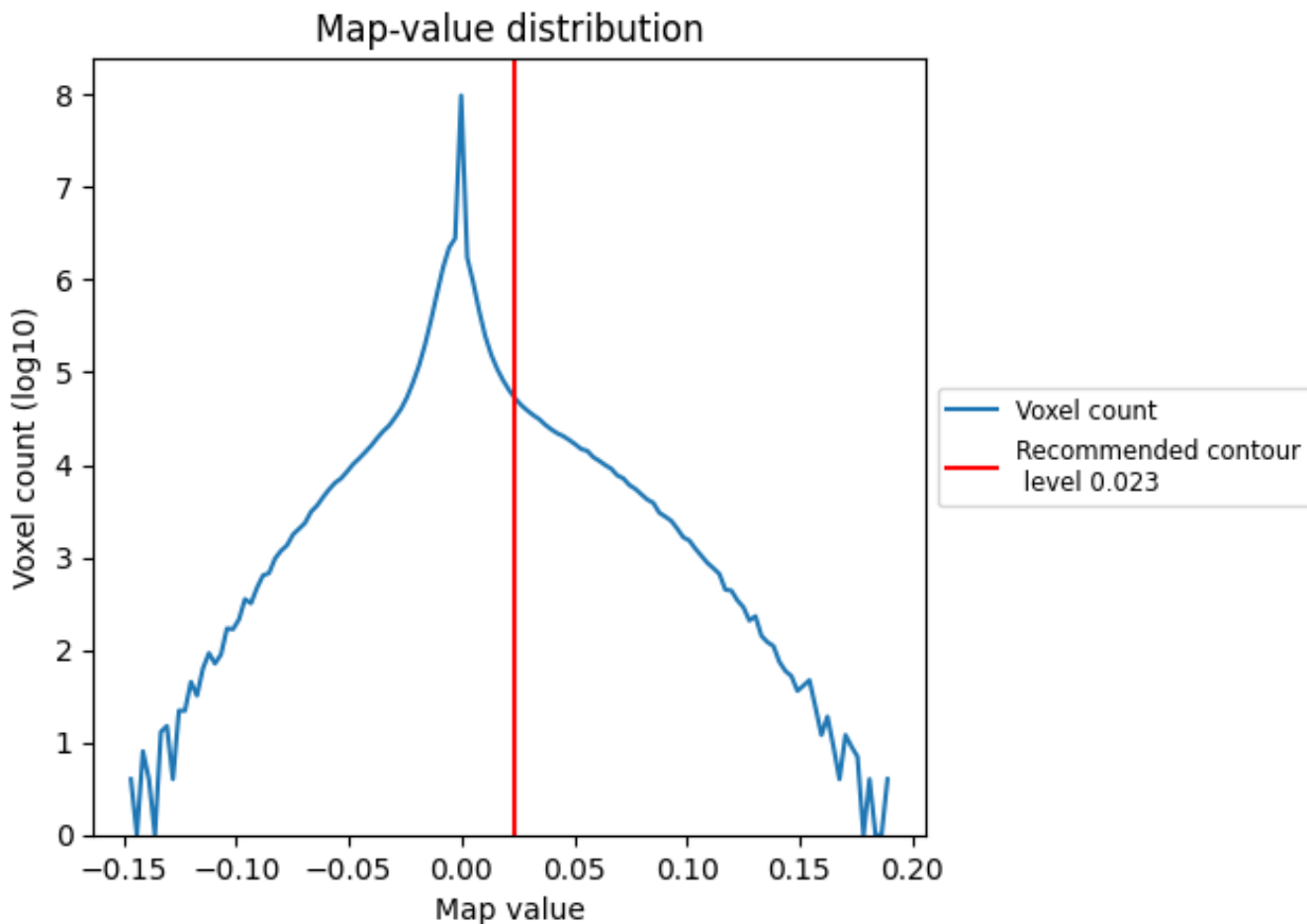
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

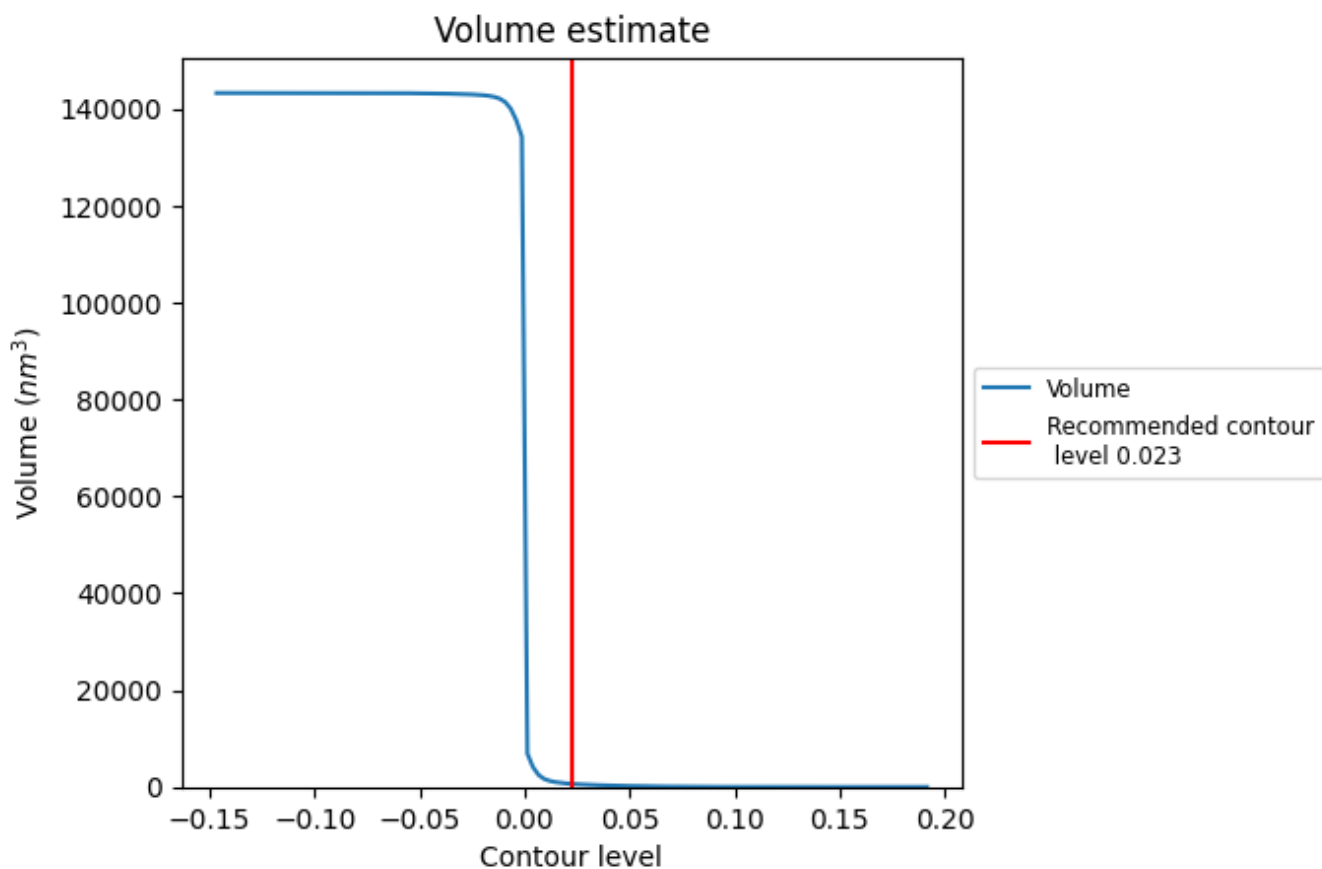
This section contains the results of statistical analysis of the map.

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.

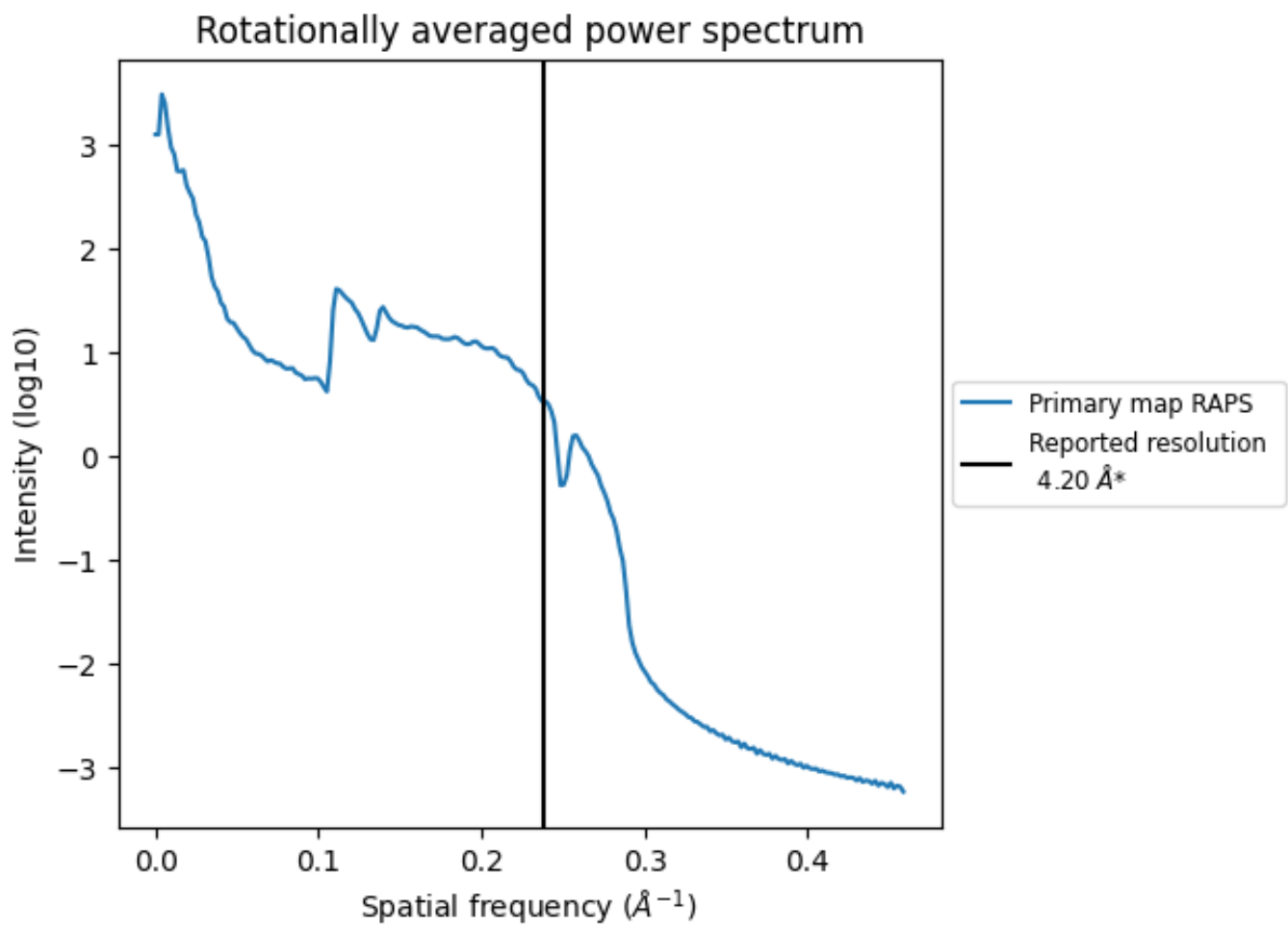
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 622 nm^3 ; this corresponds to an approximate mass of 562 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 0.238\AA^{-1}

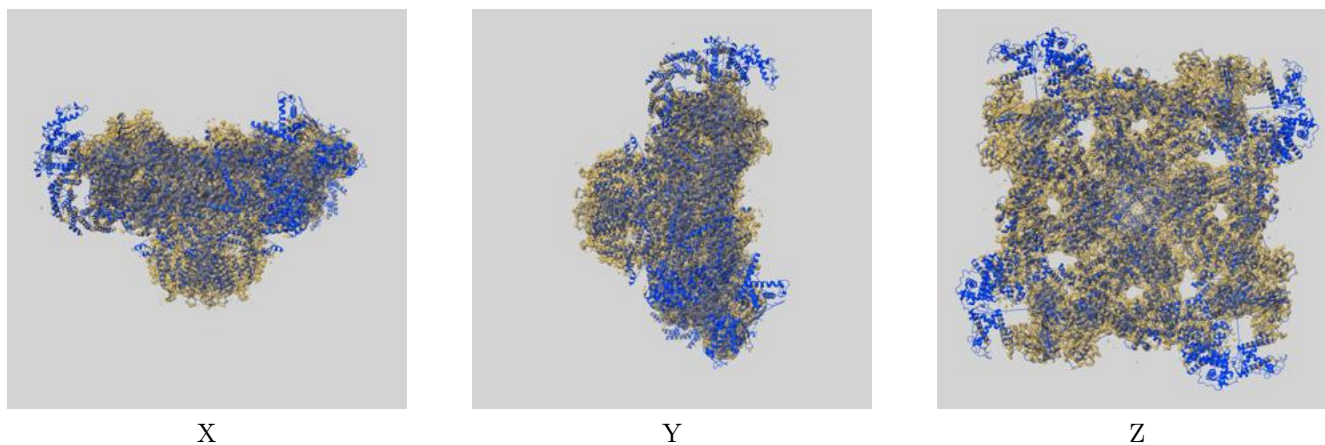
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

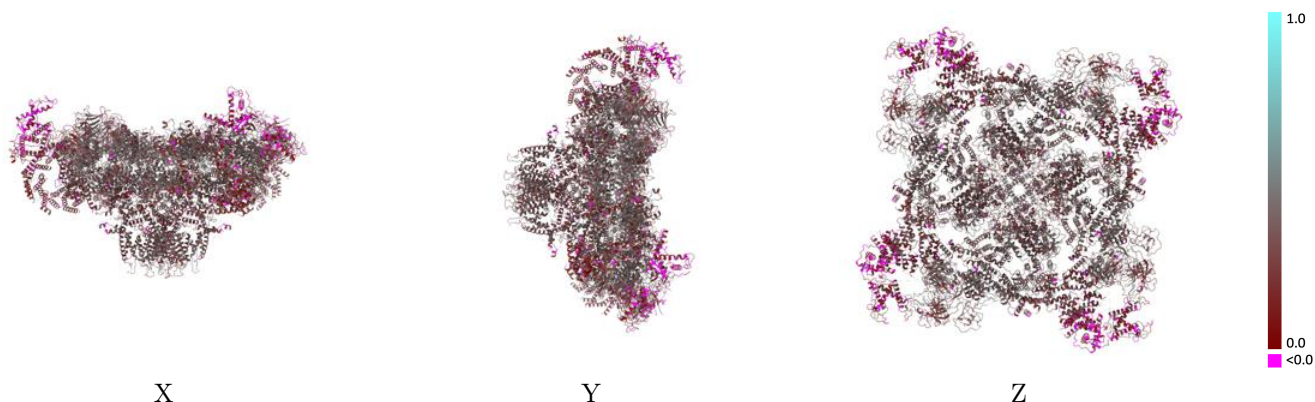
This section contains information regarding the fit between EMDB map EMD-22018 and PDB model 6X35. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



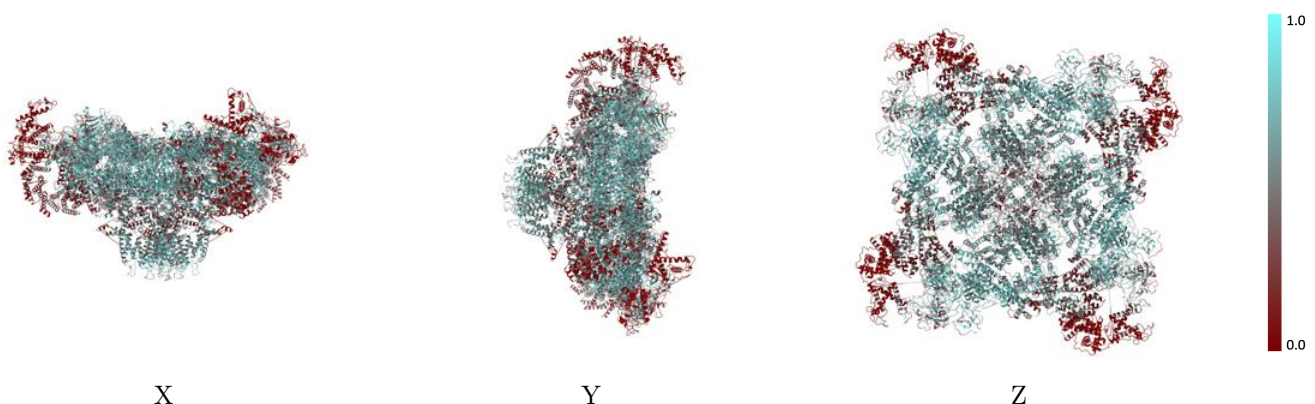
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



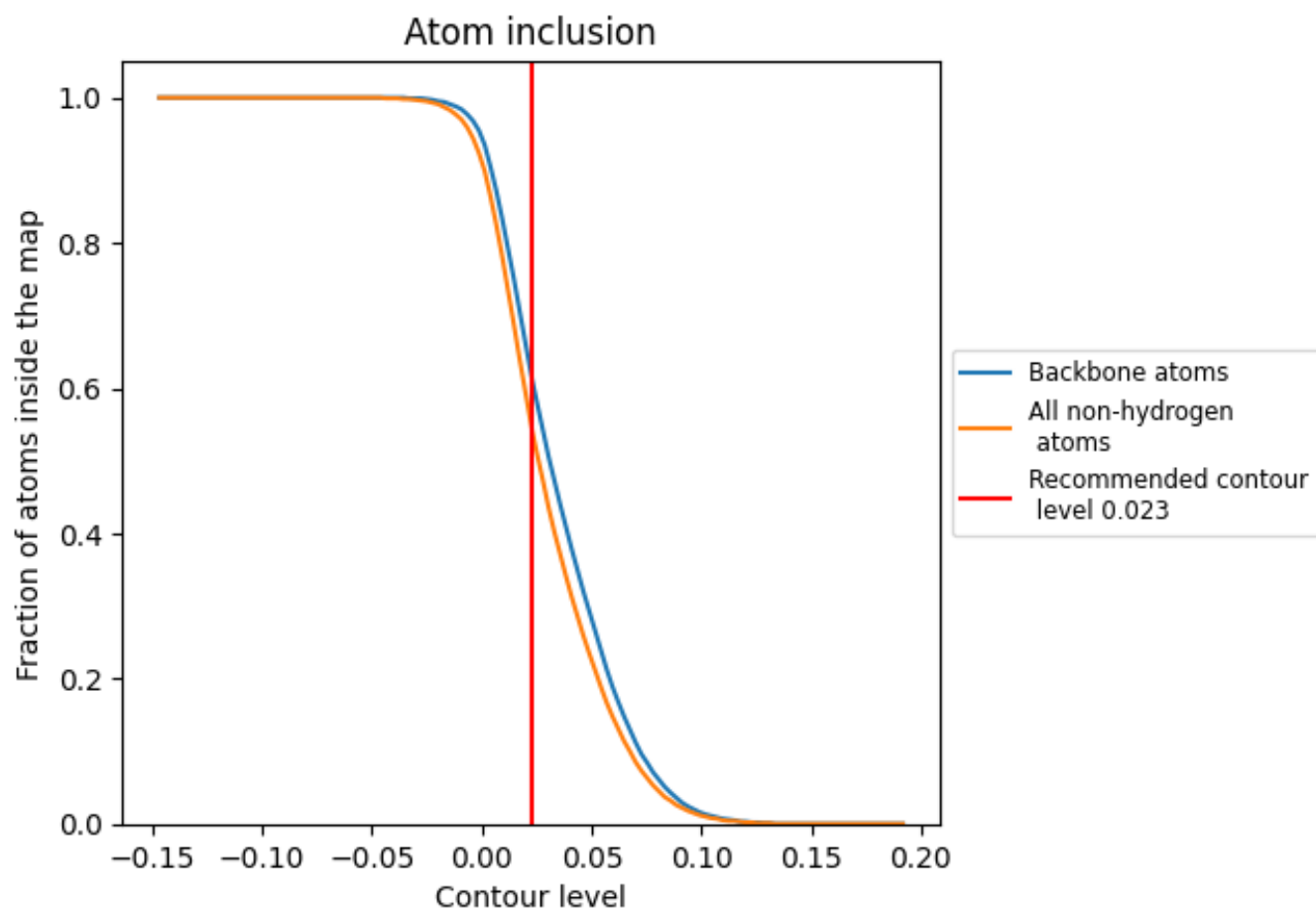
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 54% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.3310
A	0.5930	0.3570
B	0.5440	0.3310
C	0.3760	0.2830
D	0.5900	0.3560
E	0.5440	0.3310
F	0.3760	0.2810
G	0.5910	0.3590
H	0.5440	0.3320
I	0.3750	0.2790
J	0.5910	0.3570
K	0.5440	0.3320
L	0.3760	0.2820

