



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 02:08 PM EDT

PDB ID : 5TAZ  
EMDB ID : EMD-8390  
Title : Structure of rabbit RyR1 (ryanodine 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 : 4.30 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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

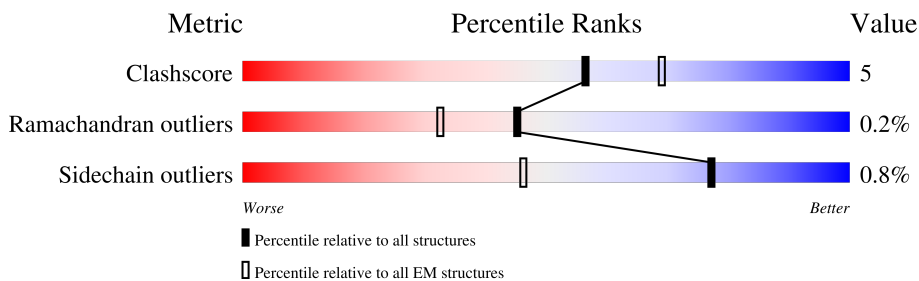
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 121276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

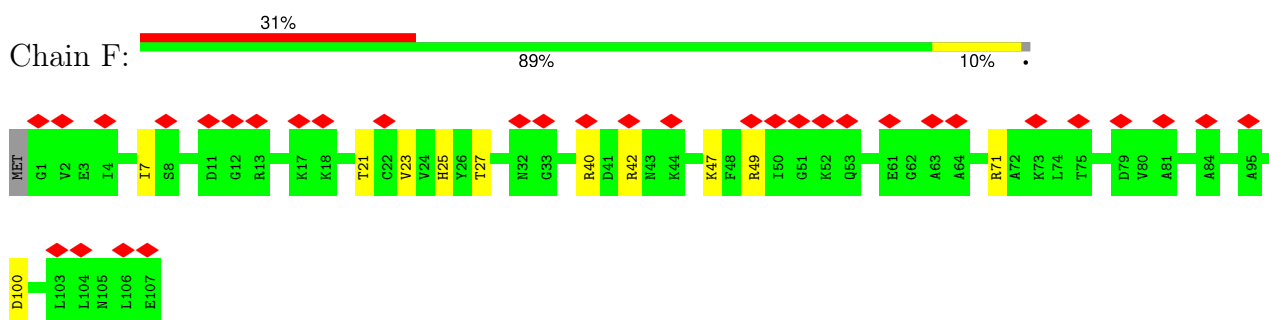
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

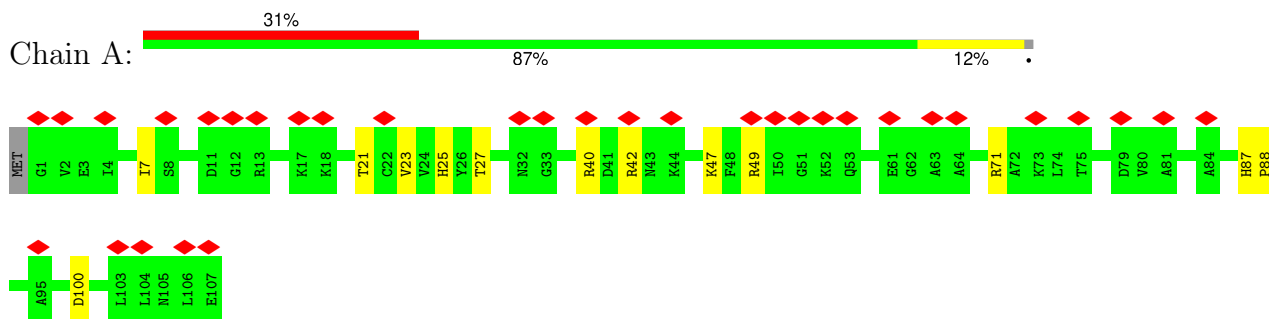
### 3 Residue-property plots [i](#)

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.

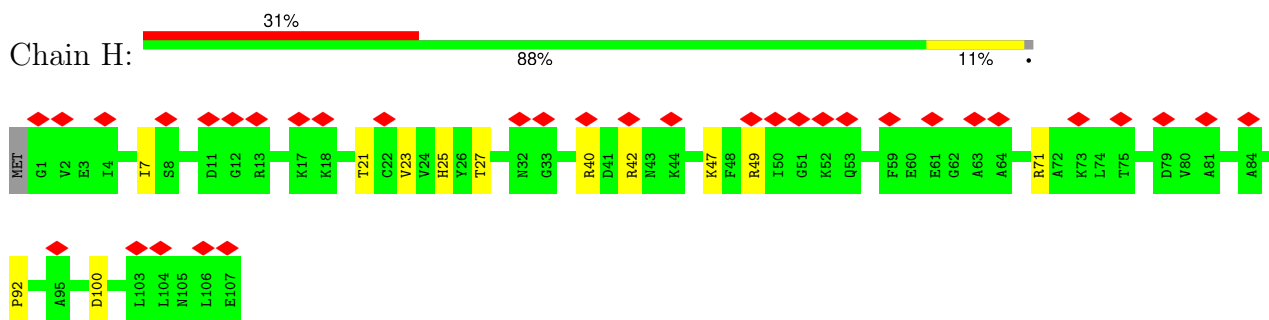
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



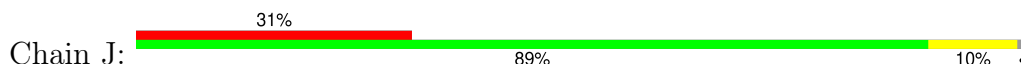
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

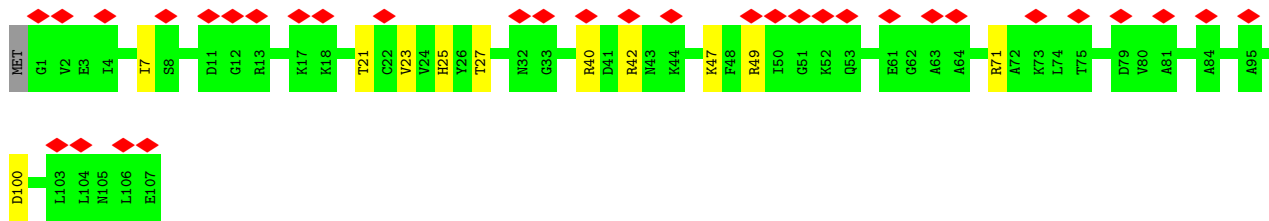


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

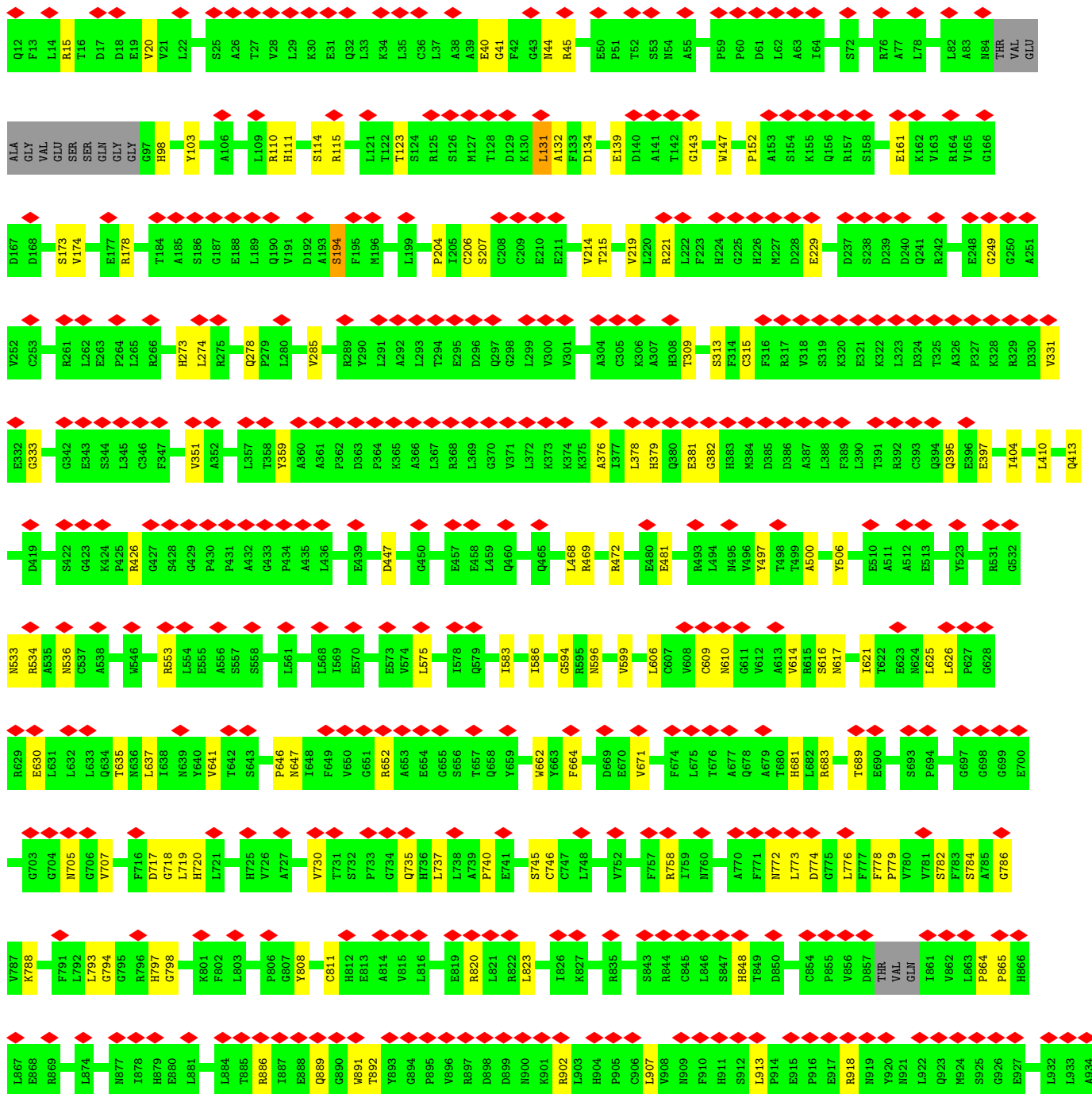
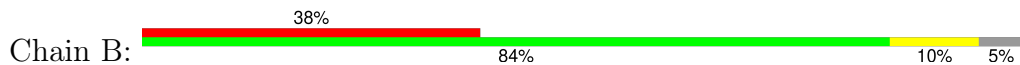


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

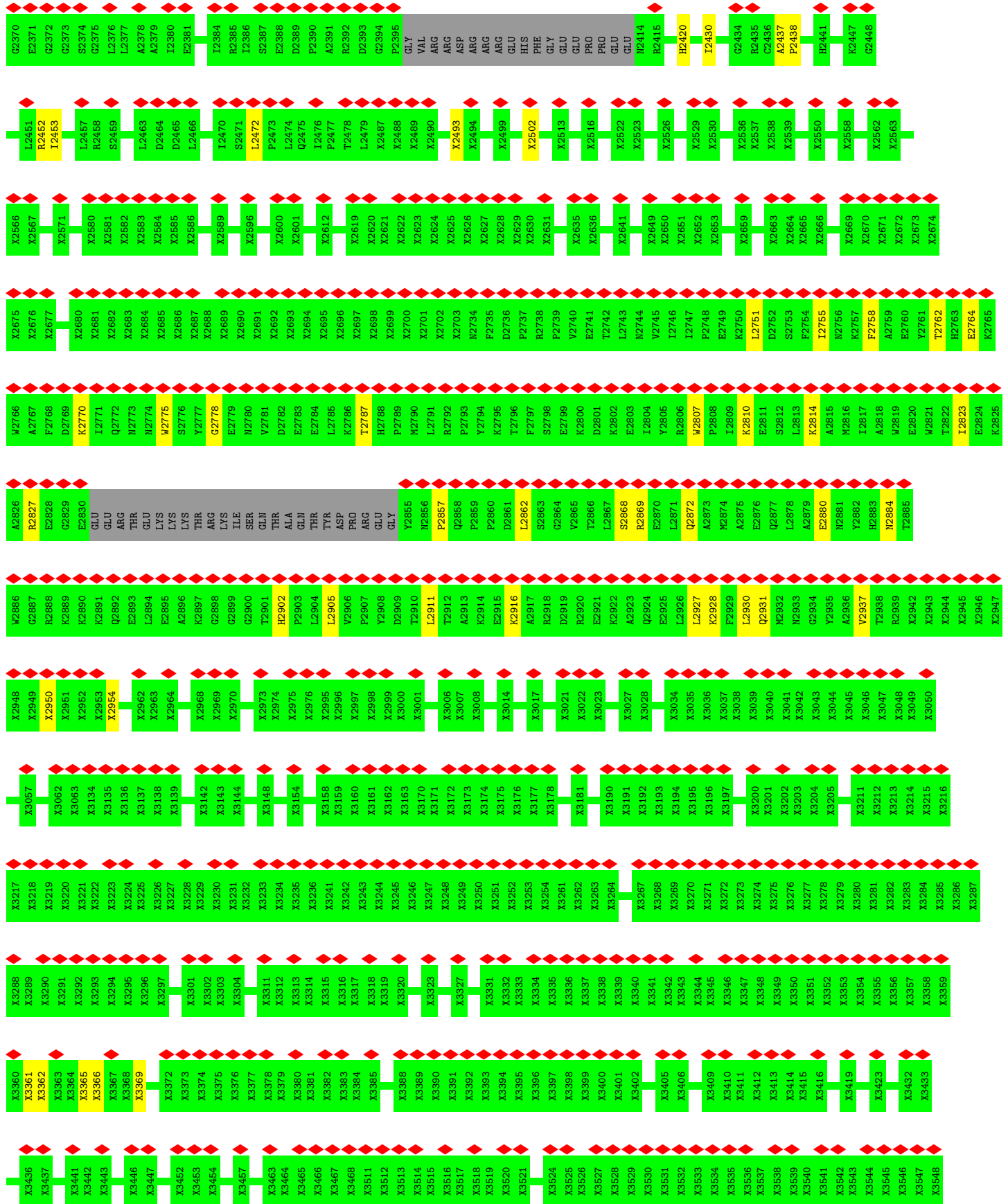




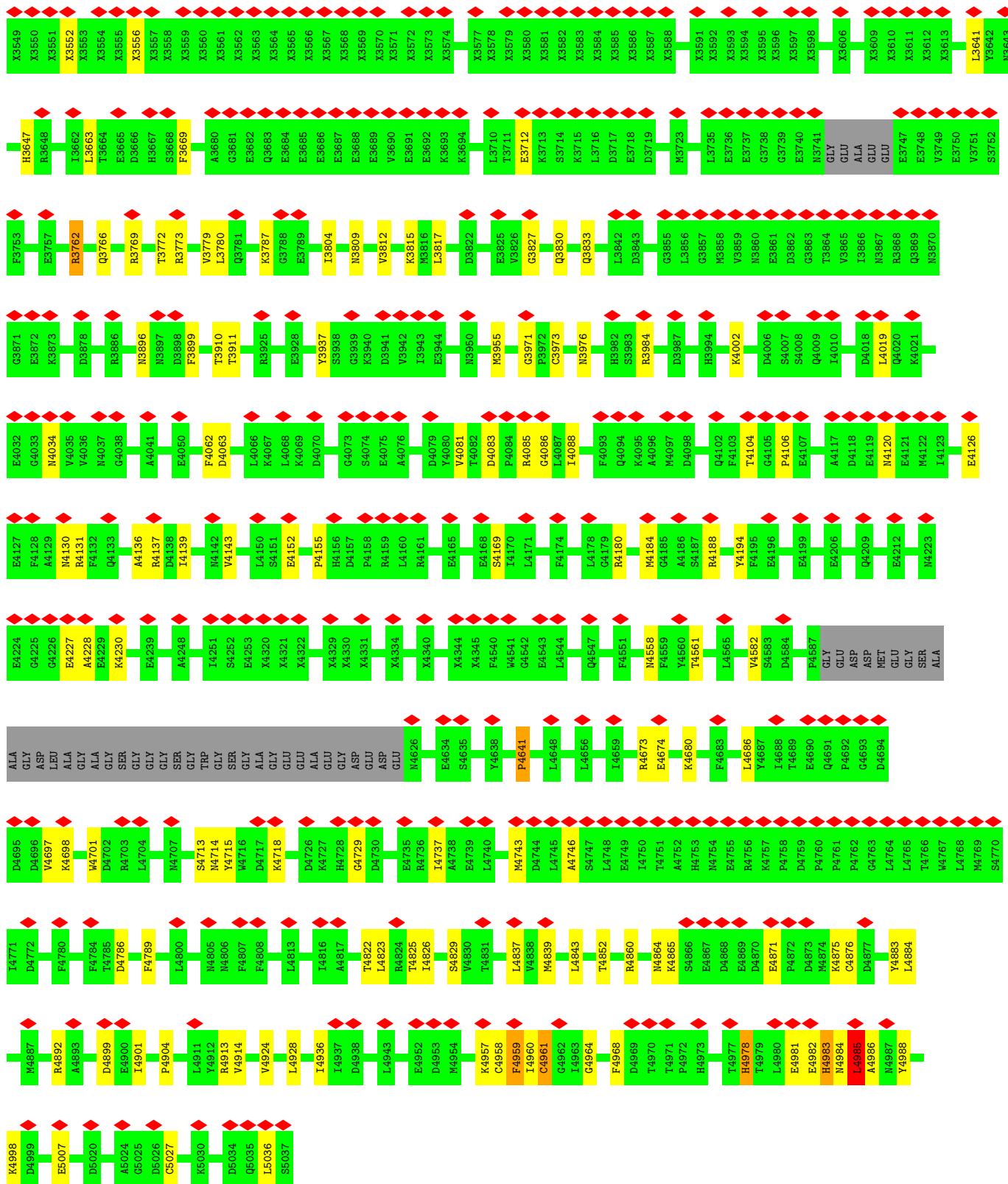
• Molecule 2: Ryanodine receptor 1











• Molecule 2: Ryanodine receptor 1

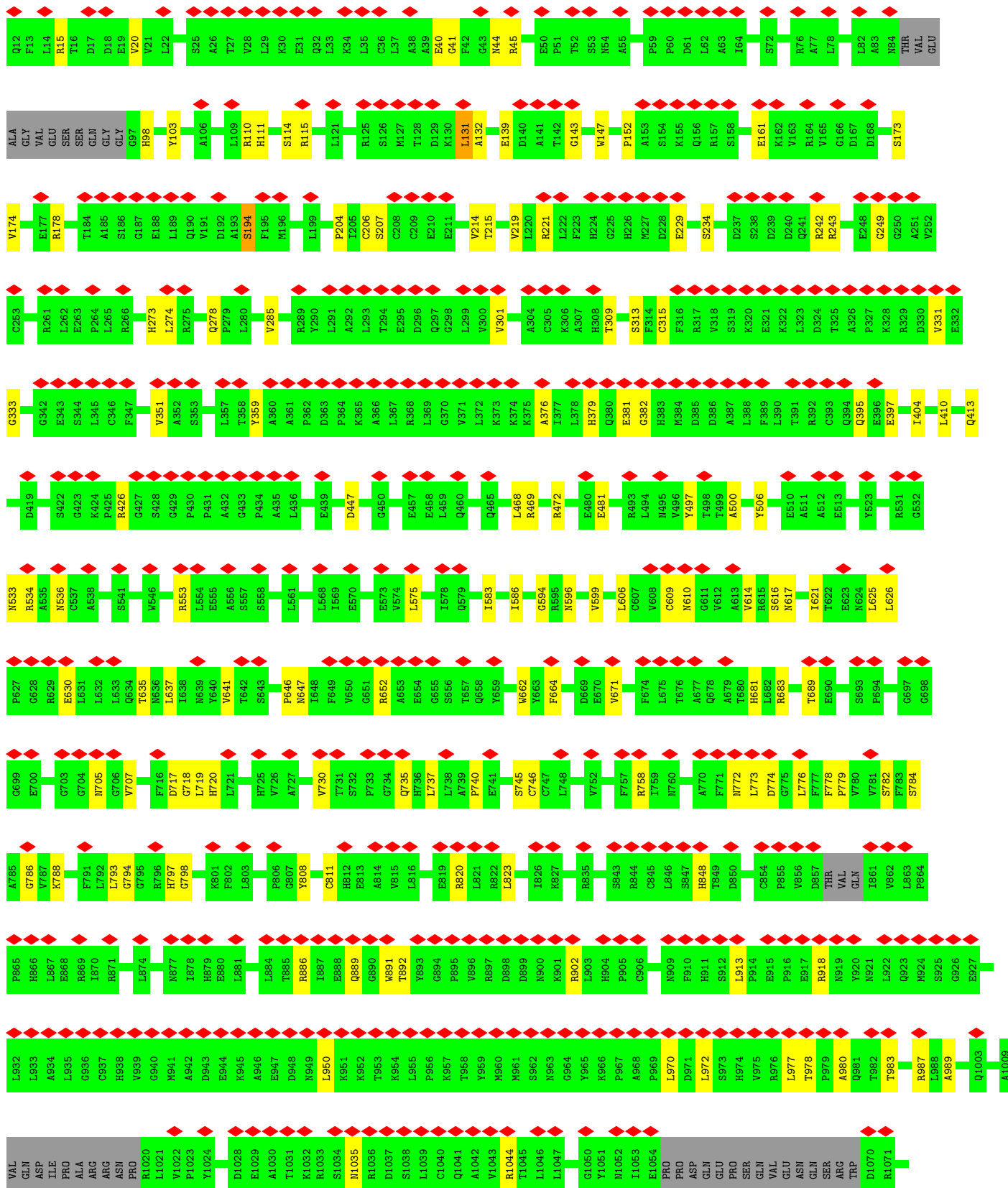
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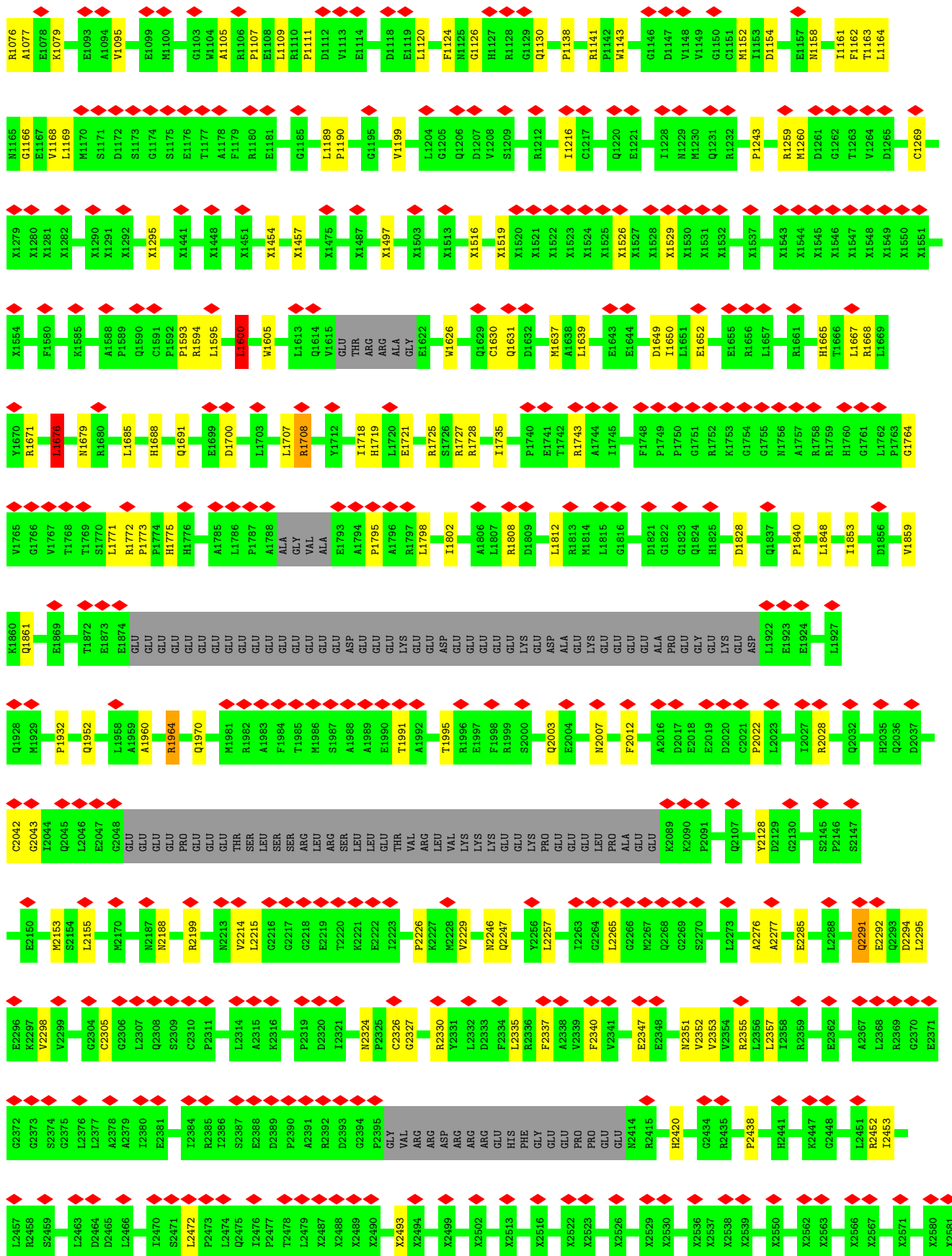
Chain I:

85%

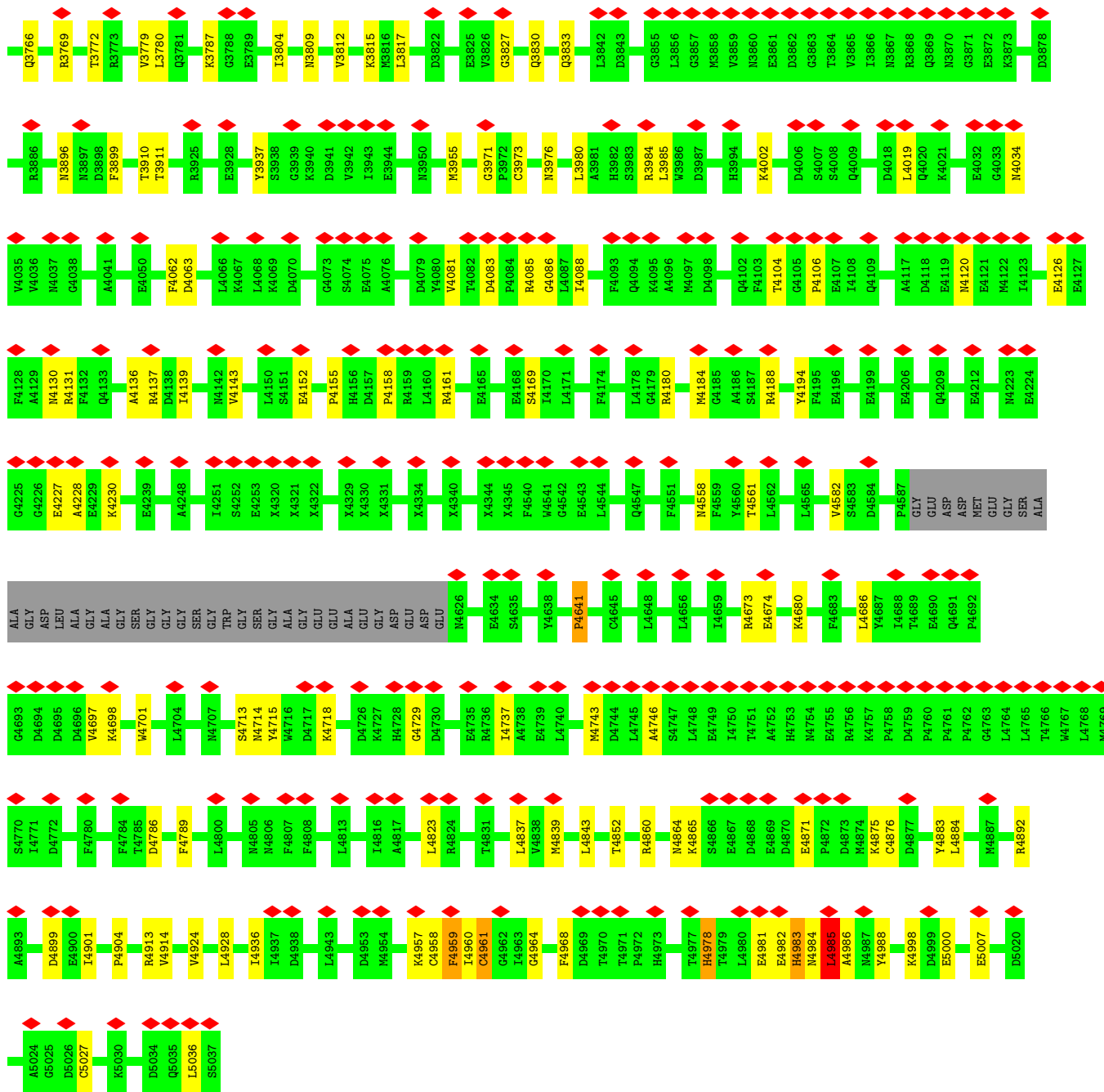
10%

5%

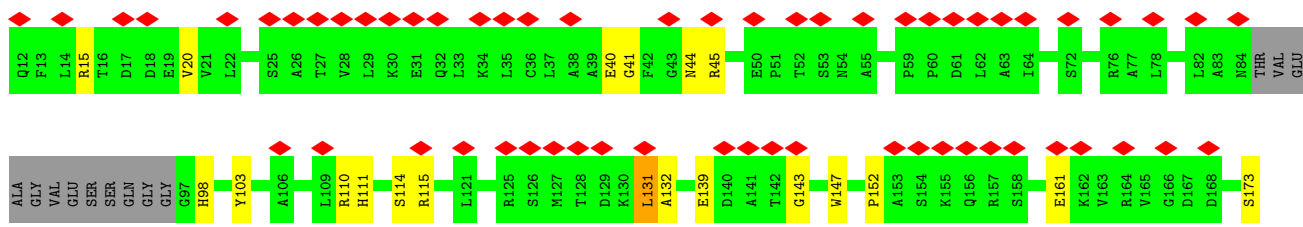
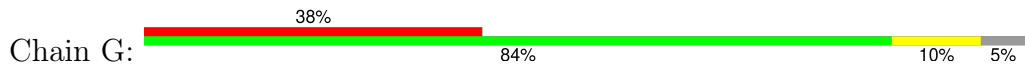


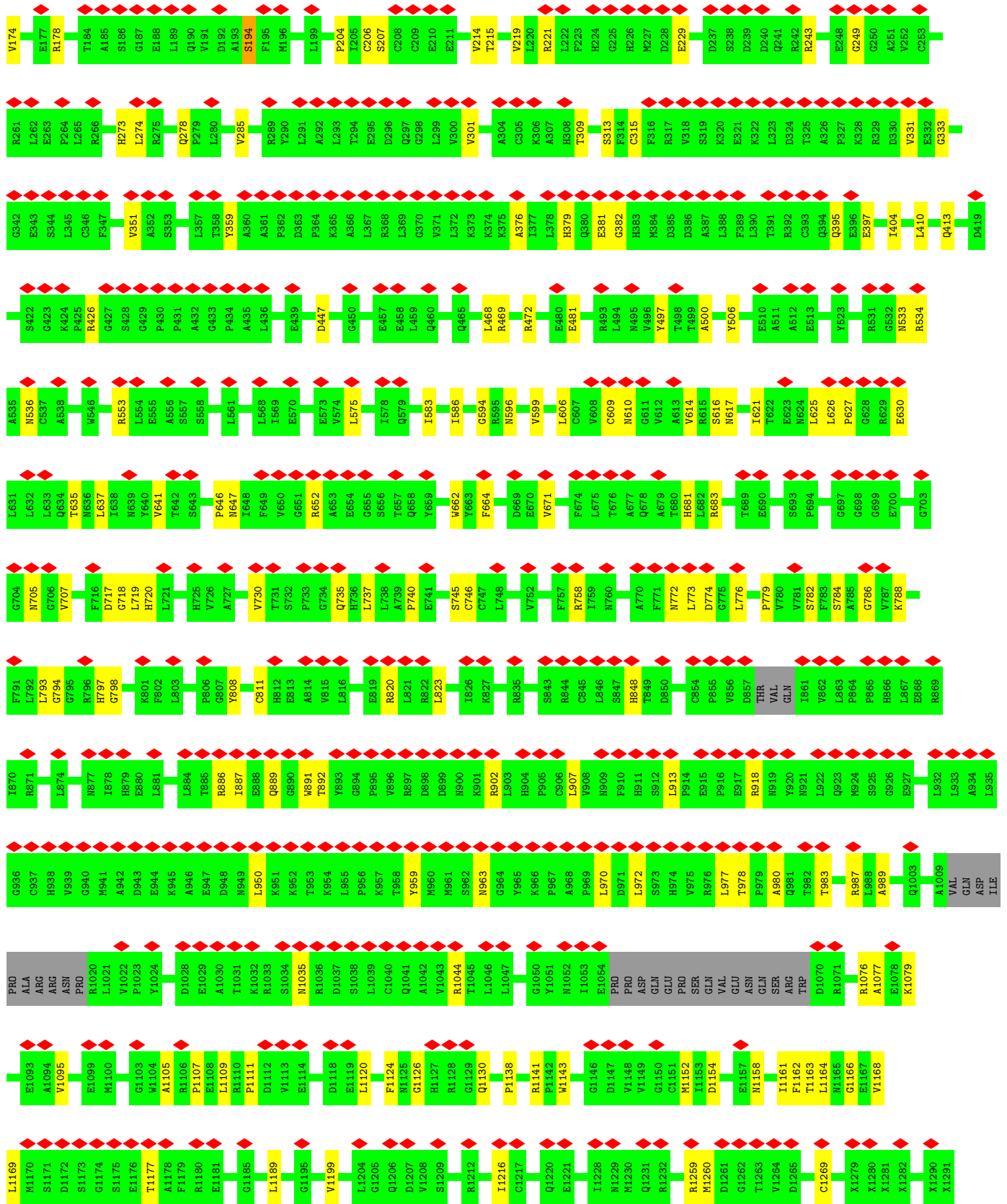


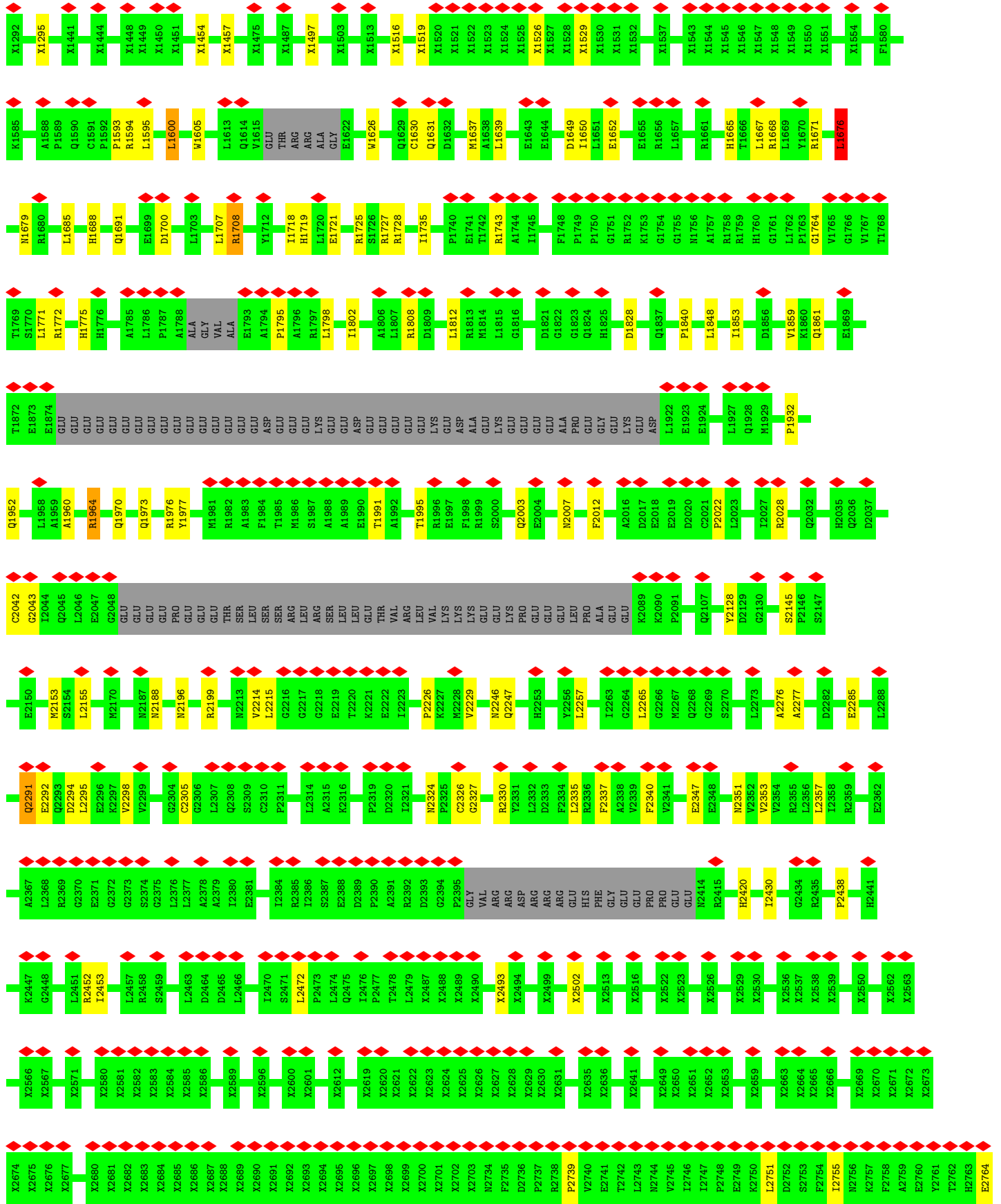
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E2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2705	X2706	X2707	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739	X2740	X2741	X2742	X2743	X2744	X2745	X2746	X2747	X2748	X2749	X2750	X2751	X2752	X2753	X2754	X2755	X2756	X2757	X2758	X2759	X2760	X2761	X2762	X2763	X2764	X2765	X2766	X2767	X2768	X2769	X2770	X2771	X2772																														
N2773	N2774	N2775	S2776	S2777	G2778	E2779	N2780	S2781	D2782	E2783	E2784	L2785	L2786	L2787	T2788	H2788	P2789	M2790	R2791	R2792	P2793	P2794	K2795	T2796	S2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	R2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	E2829	GLU	GLU																																																									
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X3136	X3137	X3138	X3139	X3142	X3143	X3144	X3148	X3154	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3181	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3202	X3203	X3204	X3205	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223																																																																	
X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	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	X3301	X3302	X3303	X3304	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3327	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	X3365	X3366	X3367	X3368																																																															
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• Molecule 2: Ryanodine receptor 1

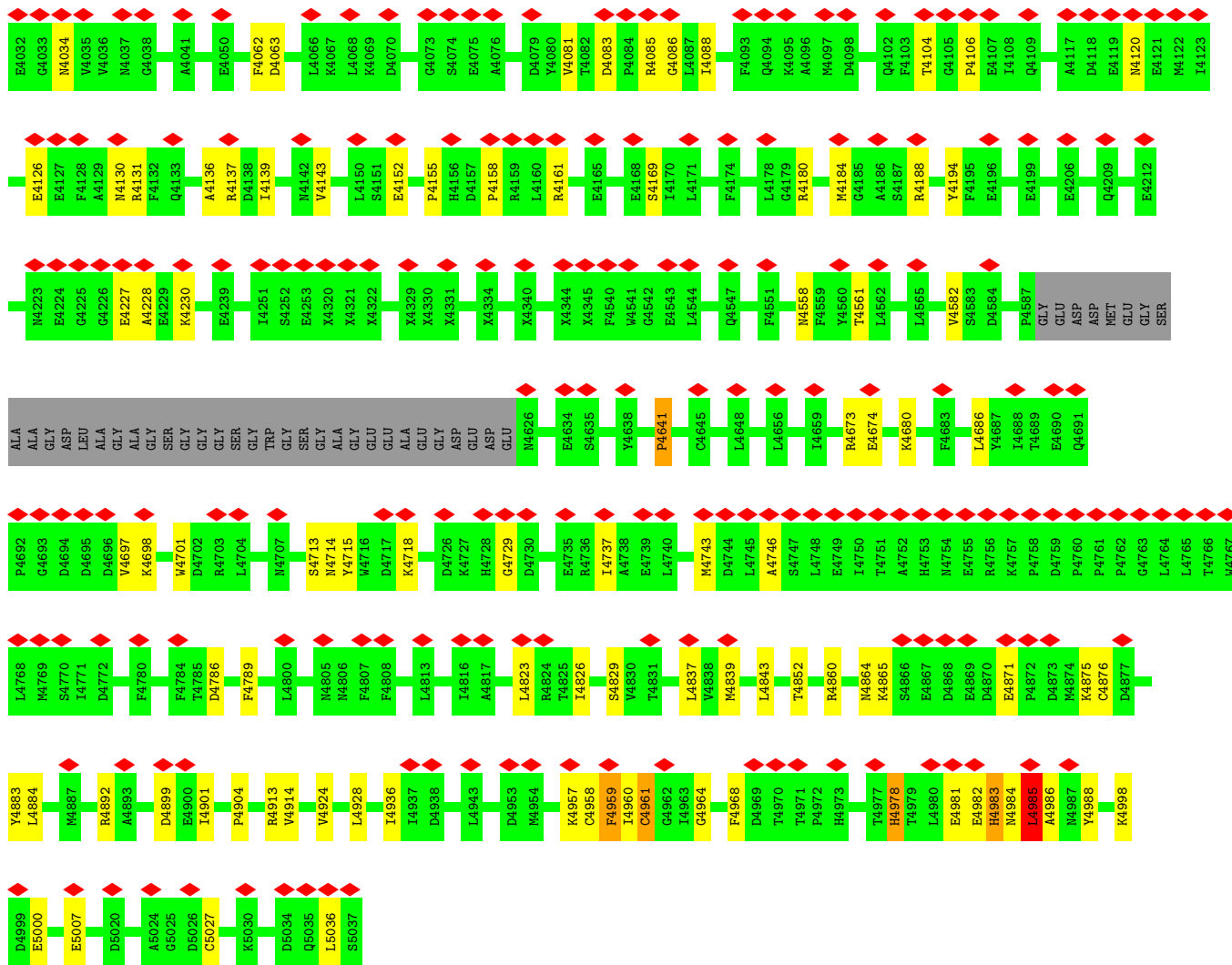




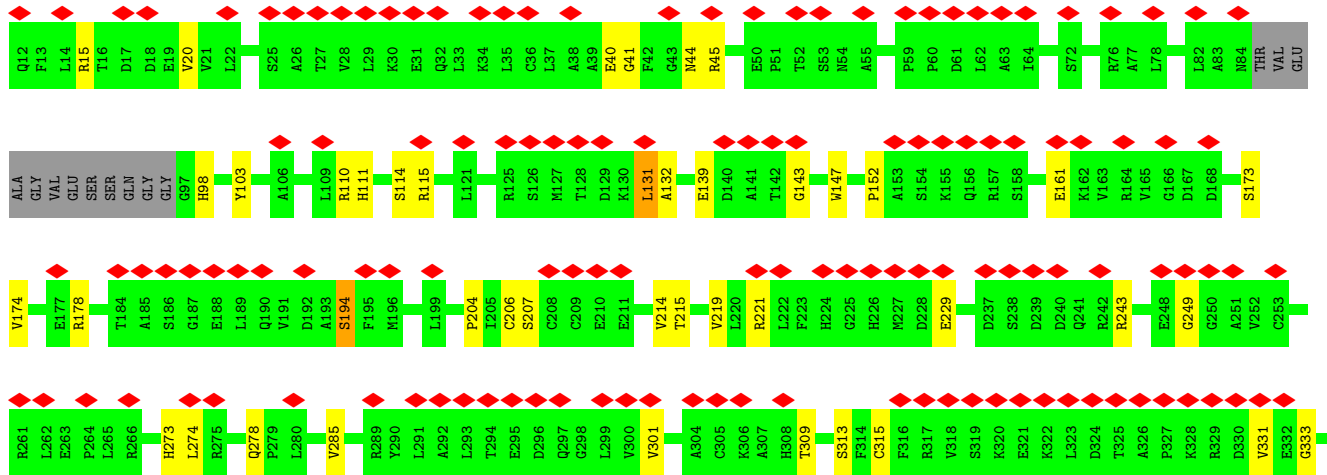
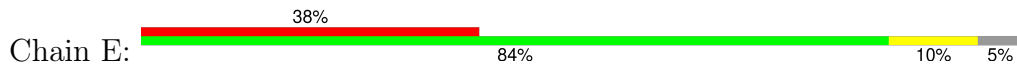


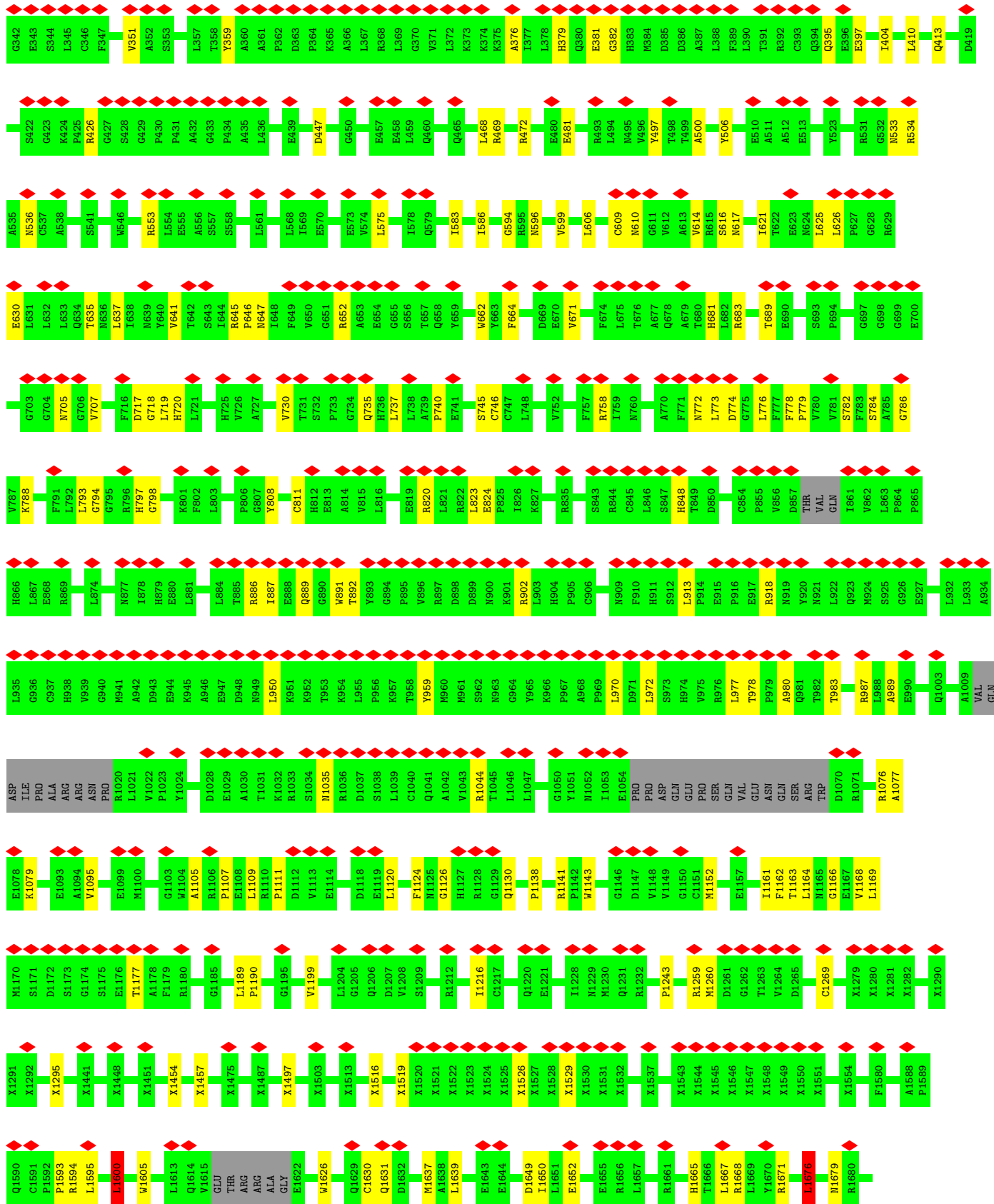
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K2825	A2826	R2827	E2828	E2829	E2830	GLU	GLU	ARG	THR	GLU	GLU	LYS	LYS	LYS	LYS	LYS	THR	ARG	ARG	ILE	SER	GLN	THR	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	R2870	L2871	Q2872	P2808	L2809	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	H2901	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	R2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946																																															
X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2962	X2963	X2964	X2968	X2969	X2970	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3006	X3007	X3008	X3014	X3017	X3021	X3022	X3023	X3027	X3028	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3057	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3142	X3143	X3144	X3148	X3154	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3181	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3202	X3203	X3204	X3205	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	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	X3301	X3302	X3303	X3304	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3327	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	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3423	X3432	X3433	X3436																																																			
X3437	X3441	X3442	X3443	X3444	X3446	X3447	X3452	X3453	X3454	X3457	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	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549																																																																																																								
X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3606	X3609	X3610	X3611	X3612	X3613	L3641	Y3642	N3643																																																																																																										
H3647	R3648	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3689	E3691	E3692	K3693	K3694	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	M3723	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLU	ALA	GLU	GLU	E3747	E3748	V3749	E3750	V3751																																																																																																												
S3752	F3753	E3757	K3760	Q3761	R3762	Q3766	R3769	T3772	R3773	V3779	L3780	Q3781	K3787	G3788	E3789	L3804	L3805	N3809	V3812	K3815	K3816	L3817	D3822	E3825	V3826	G3827	Q3830	Q3833	L3842	D3843	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	V3865	I3866																																																																																																																					
N3867	R3868	Q3869	N3870	G3871	E3872	D3878	R3886	N3896	N3897	D3898	F3899	T3910	T3911	R3925	E3928	Y3937	S3938	G3939	K3940	V3942	L3943	E3944	N3950	M3955	G3971	F3972	C3973	N3976	H3982	S3983	R3984	H3994	K4002	D4006	S4007	S4008	Q4009	D4018	L4019	Q4020	K4021																																																																																																																						

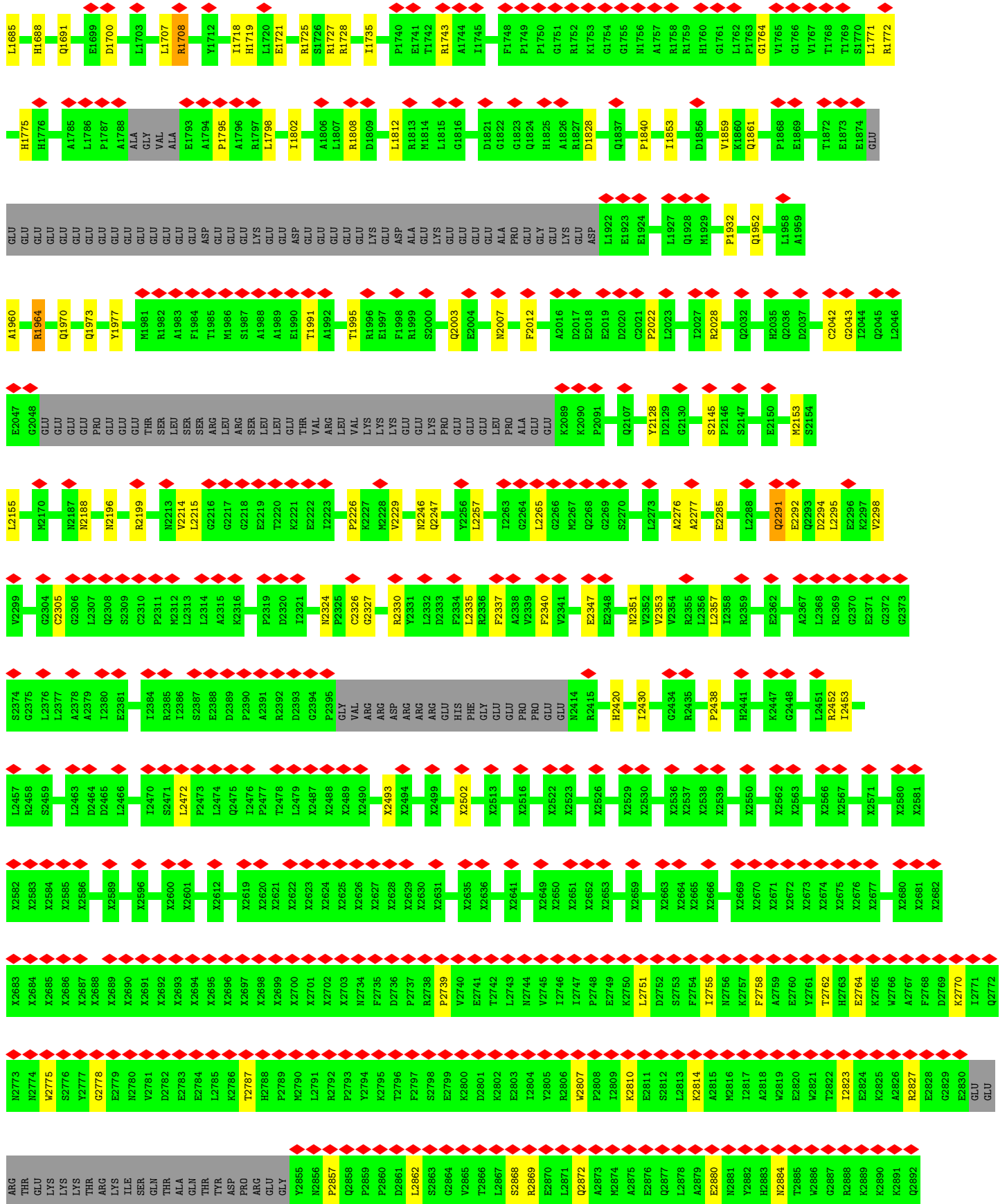




• Molecule 2: Ryanodine receptor 1







E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	H2901	F2902	L2904	L2905	V2906	F2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	H2932	H2933	G2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954																																																																																																																																																																																																																																																																																																																																																	
X2962	X2963	X2964	X2968	X2969	X2970	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3006	X3007	X3008	X3014	X3017	X3021	X3022	X3023	X3027	X3028	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3057	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3142	X3143	X3144	X3148	X3154	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3181	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3202	X3203	X3204	X3205	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223																																																																																																																																																																																																																																																																																																								
X3224	X3225	X3226	X3227	X3228	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	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	X3301	X3302	X3303	X3304	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3327	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368																																																																																																																																																																																																																																																																																																																																																					
X3369	X3370	X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3423	X3432	X3433	X3436	X3437	X3441	X3442	X3443	X3446																																																																																																																																																																																																																																																																																																																																																							
X3447	X3452	X3453	X3454	X3457	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	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556																																																																																																																																																																																																																																																																																																																																																			
X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3591	X3592	X3593	X3594	X3595	X3596	X3597	X3598	X3606	X3609	X3610	X3611	X3612	X3613	L3641	T3642	N3643	H3647	R3648	T3662	L3663	E3665																																																																																																																																																																																																																																																																																																																																																								
D3666	H3667	S3668	F3669	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	E3690	E3691	K3694	P3695	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	M3723	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLU	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3757	K3760																																																																																																																																																																																																																																																																																																																																																										
Q3761	R3762	Q3766	R3769	T3772	R3773	V3779	L3780	Q3781	K3787	G3788	E3789	L3804	L3805	N3809	V3812	K3815	L3817	D3822	E3825	V3826	Q3827	Q3830	Q3833	L3842	D3843	G3855	L3856	G3857	M3858	V3859	N3860	E3861	D3862	G3863	G3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	D3873	D3876	D3877	D3878	D3879	D3880	D3881	D3882	D3883	D3884	D3885	D3886	D3887	D3888	D3889	D3890	D3891	D3892	D3893	D3894	D3895	D3896	D3897	D3898	D3899	D3900	D3901	D3902	D3903	D3904	D3905	D3906	D3907	D3908	D3909	D3910	D3911	D3912	D3913	D3914	D3915	D3916	D3917	D3918	D3919	D3920	D3921	D3922	D3923	D3924	D3925	D3926	D3927	D3928	D3929	D3930	D3931	D3932	D3933	D3934	D3935	D3936	D3937	D3938	D3939	D3940	D3941	D3942	D3943	D3944	D3945	D3946	D3947	D3948	D3949	D3950	D3951	D3952	D3953	D3954	D3955	D3956	D3957	D3958	D3959	D3960	D3961	D3962	D3963	D3964	D3965	D3966	D3967	D3968	D3969	D3970	D3971	D3972	D3973	D3974	D3975	D3976	D3977	D3978	D3979	D3980	D3981	D3982	D3983	D3984	D3985	D3986	D3987	D3988	D3989	D3990	D3991	D3992	D3993	D3994	D3995	D3996	D3997	D3998	D3999	D4000	D4001	D4002	D4003	D4004	D4005	D4006	D4007	D4008	D4009	D4010	D4011	D4012	D4013	D4014	D4015	D4016	D4017	D4018	D4019	D4020	D4021	D4022	D4023	D4024	D4025	D4026	D4027	D4028	D4029	D4030	D4031	D4032	D4033	D4034	D4035	D4036	D4037	D4038	D4039	D4040	D4041	D4042	D4043	D4044	D4045	D4046	D4047	D4048	D4049	D4050	D4051	D4052	D4053	D4054	D4055	D4056	D4057	D4058	D4059	D4060	D4061	D4062	D4063	D4064	D4065	D4066	D4067	D4068	D4069	D4070	D4071	D4072	D4073	D4074	D4075	D4076	D4077	D4078	D4079	D4080	D4081	D4082	D4083	D4084	D4085	D4086	D4087	D4088	D4089	D4090	D4091	D4092	D4093	D4094	D4095	D4096	D4097	D4098	D4099	D4100	D4101	D4102	D4103	D4104	D4105	D4106	D4107	D4108	D4109	D4110	D4111	D4112	D4113	D4114	D4115	D4116	D4117	D4118	D4119	D4120	D4121	D4122	D4123	D4124	D4125	D4126	D4127	D4128	D4129	D4130	D4131	D4132	D4133	D4134	D4135	D4136	D4137	D4138	D4139	D4140	D4141	D4142	D4143	D4144	D4145	D4146	D4147	D4148	D4149	D4150	D4151	D4152	D4153	D4154	D4155	D4156	D4157	D4158	D4159	D4160	D4161	D4162	D4163	D4164	D4165	D4166	D4167	D4168	D4169	D4170	D4171	D4172	D4173	D4174	D4175	D4176	D4177	D4178	D4179	D4180	D4181	D4182	D4183	D4184	D4185	D4186	D4187	D4188	D4189	D4190	D4191	D4192	D4193	D4194	D4195	D4196	D4197	D4198	D4199	D4200	D4201	D4202	D4203	D4204	D4205	D4206	D4207	D4208	D4209	D4210	D4211	D4212	D4213	D4214	D4215	D4216	D4217	D4218	D4219	D4220	D4221	D4222	D4223	D4224	D4225	D4226



## 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	0.147	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.30	0/834	0.54	0/1123
1	F	0.30	0/834	0.54	0/1123
1	H	0.30	0/834	0.54	0/1123
1	J	0.30	0/834	0.54	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.91	133.50	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.45	115.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1600	LEU	CA-CB-CG	6.81	130.95	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	194	SER	Peptide
2	B	808	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	7	0
1	F	818	0	824	6	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29499	0	24749	265	0
2	E	29499	0	24749	262	0
2	G	29499	0	24749	265	0
2	I	29499	0	24748	262	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102291	1047	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 5.

The worst 5 of 1047 close contacts within the same asymmetric unit are listed below, sorted by



their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.18	1.32
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.18	1.32
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.18	1.30
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.18	1.30
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.67	1.02

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%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	44	78
2	E	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	44	78
2	G	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	44	78
2	I	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	44	78
All	All	13360/18096 (74%)	11973 (90%)	1363 (10%)	24 (0%)	45	78

5 of 24 Ramachandran outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1708	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	79	85
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	79	85
All	All	10324/12444 (83%)	10238 (99%)	86 (1%)	77	85

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	4120	ASN
2	E	1964	ARG
2	G	4137	ARG
2	E	534	ARG
2	E	3805	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1679	ASN
2	E	1775	HIS
2	E	3960	GLN
2	I	725	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	I	413	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 8 ligands modelled in this entry, 8 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	14
2	I	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Number of breaks
2	G	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.83
1	I	4345:UNK	C	4540:PHE	N	73.83
1	G	4345:UNK	C	4540:PHE	N	73.83
1	E	4345:UNK	C	4540:PHE	N	73.83
1	B	3613:UNK	C	3639:THR	N	45.16

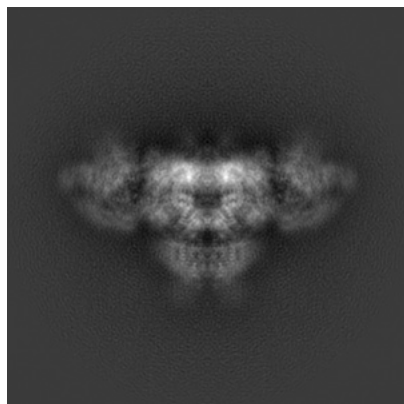
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8390. These allow visual inspection of the internal detail of the map and identification of artifacts.

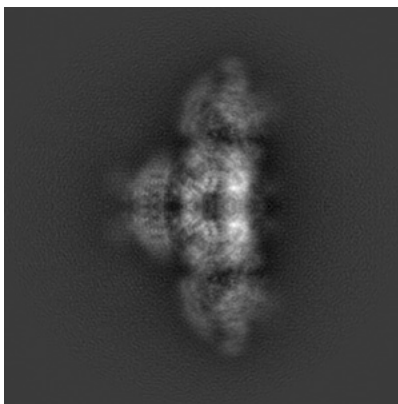
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

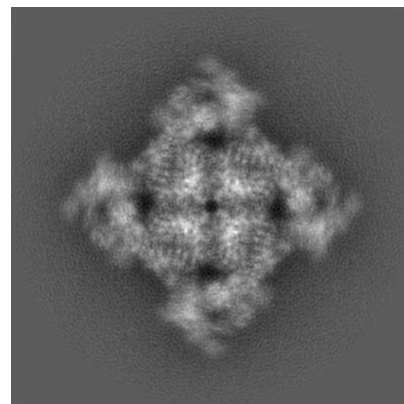
#### 6.1.1 Primary map



X

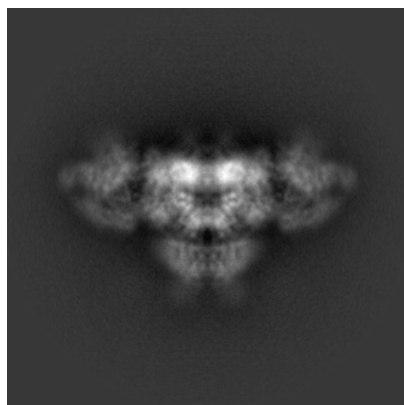


Y

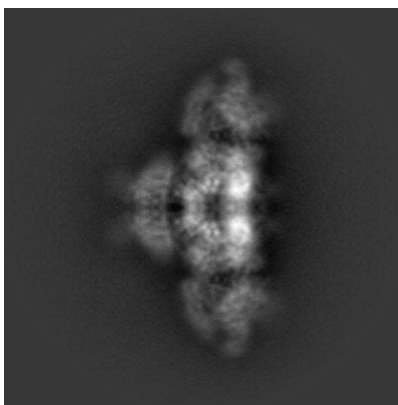


Z

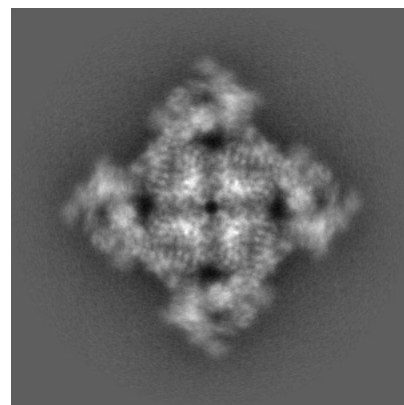
#### 6.1.2 Raw map



X



Y



Z

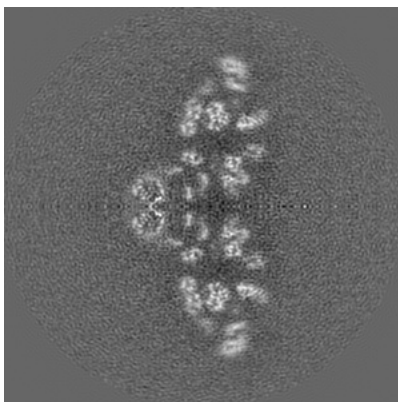
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

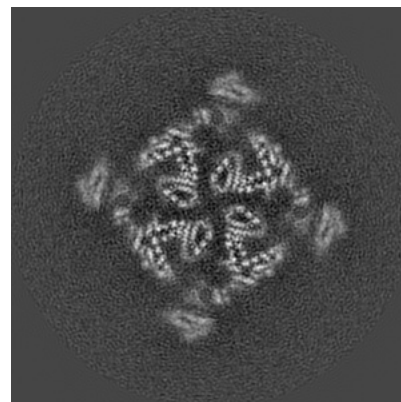
### 6.2.1 Primary map



X Index: 200

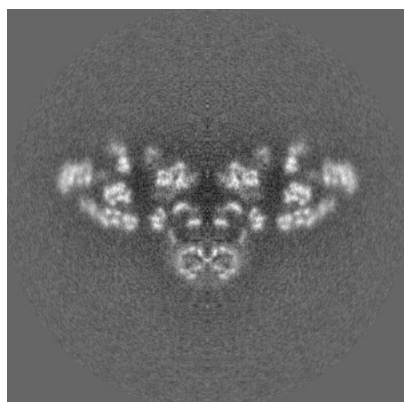


Y Index: 200

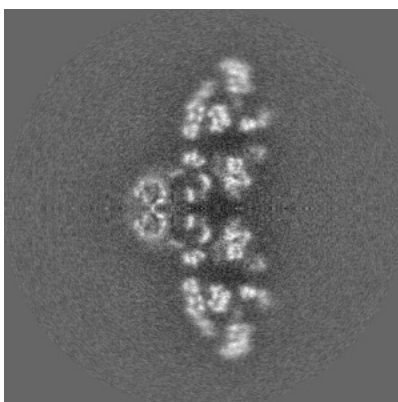


Z Index: 200

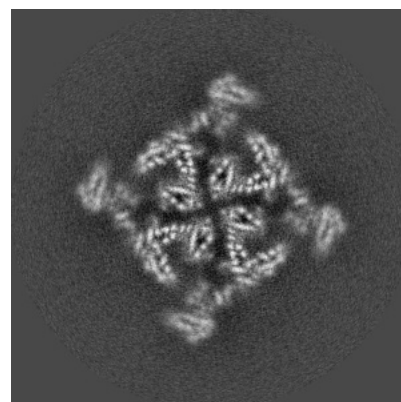
### 6.2.2 Raw map



X Index: 200



Y Index: 200

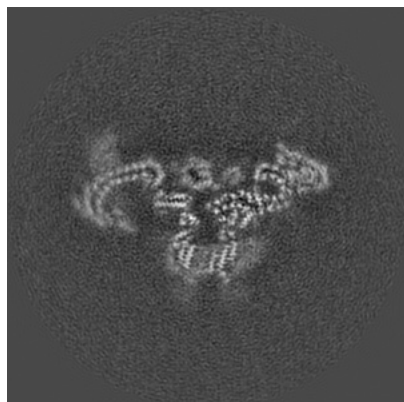


Z Index: 200

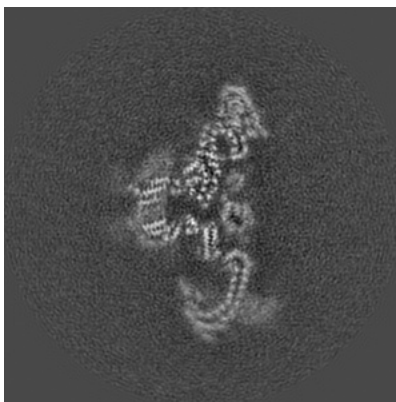
The images above show central slices of the map in three orthogonal directions.

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

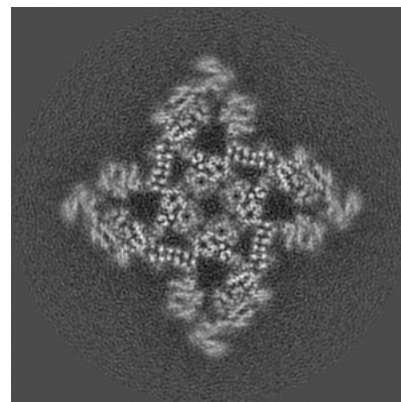
### 6.3.1 Primary map



X Index: 175

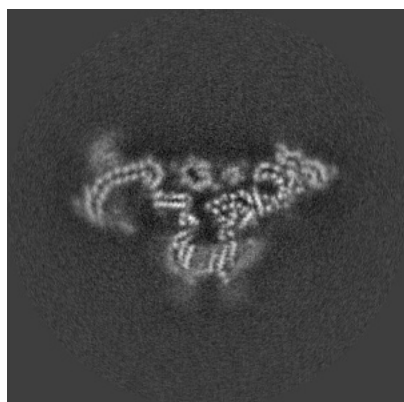


Y Index: 225

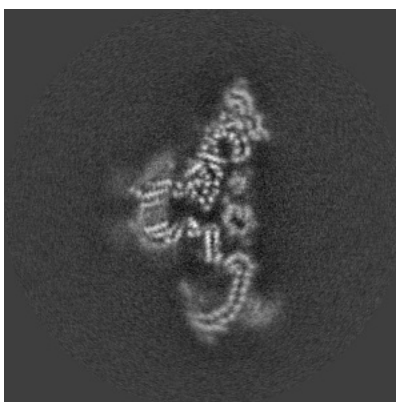


Z Index: 227

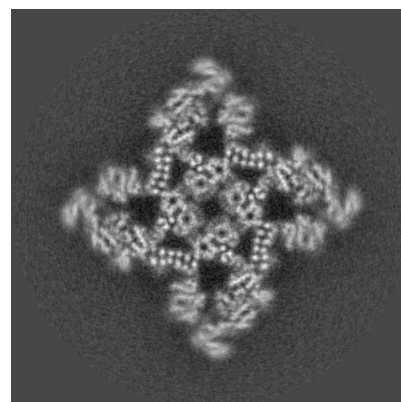
### 6.3.2 Raw map



X Index: 175



Y Index: 225

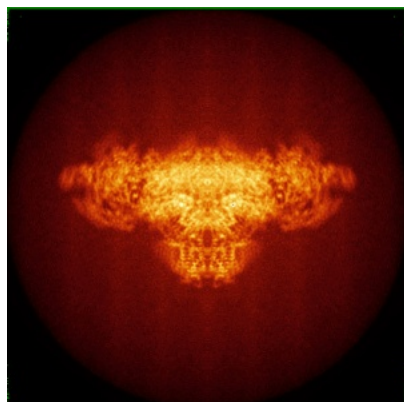


Z Index: 229

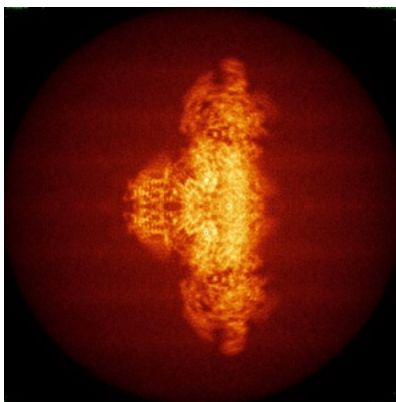
The images above show the largest variance slices of the map in three orthogonal directions.

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

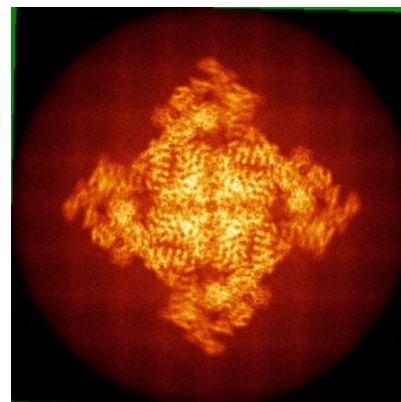
### 6.4.1 Primary map



X

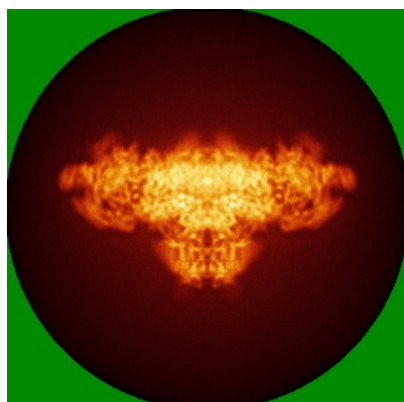


Y

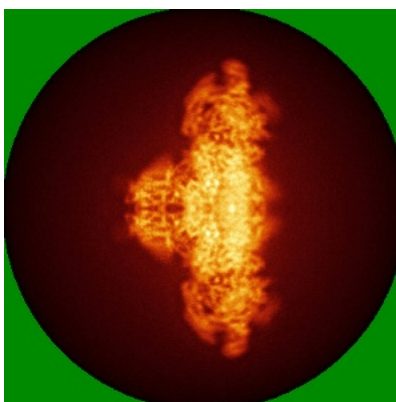


Z

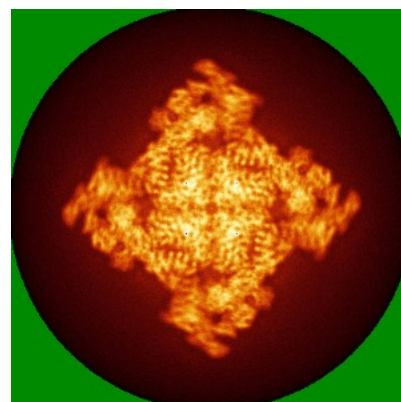
### 6.4.2 Raw map



X



Y



Z

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



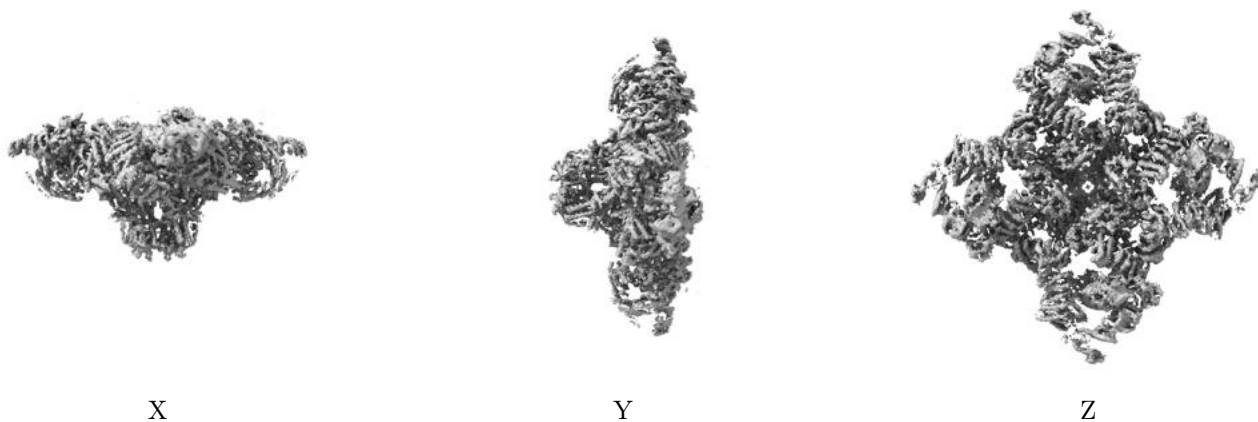
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

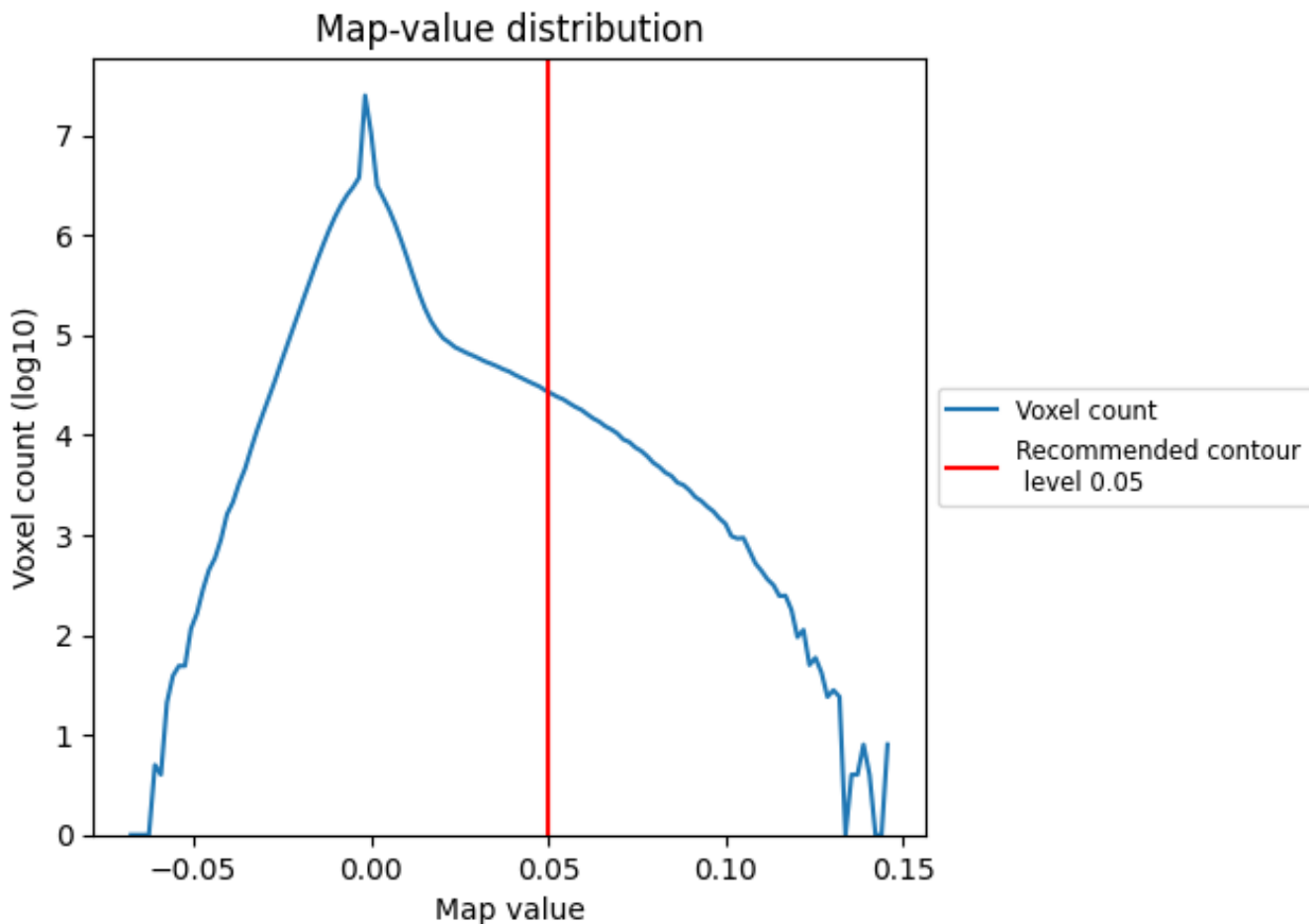
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

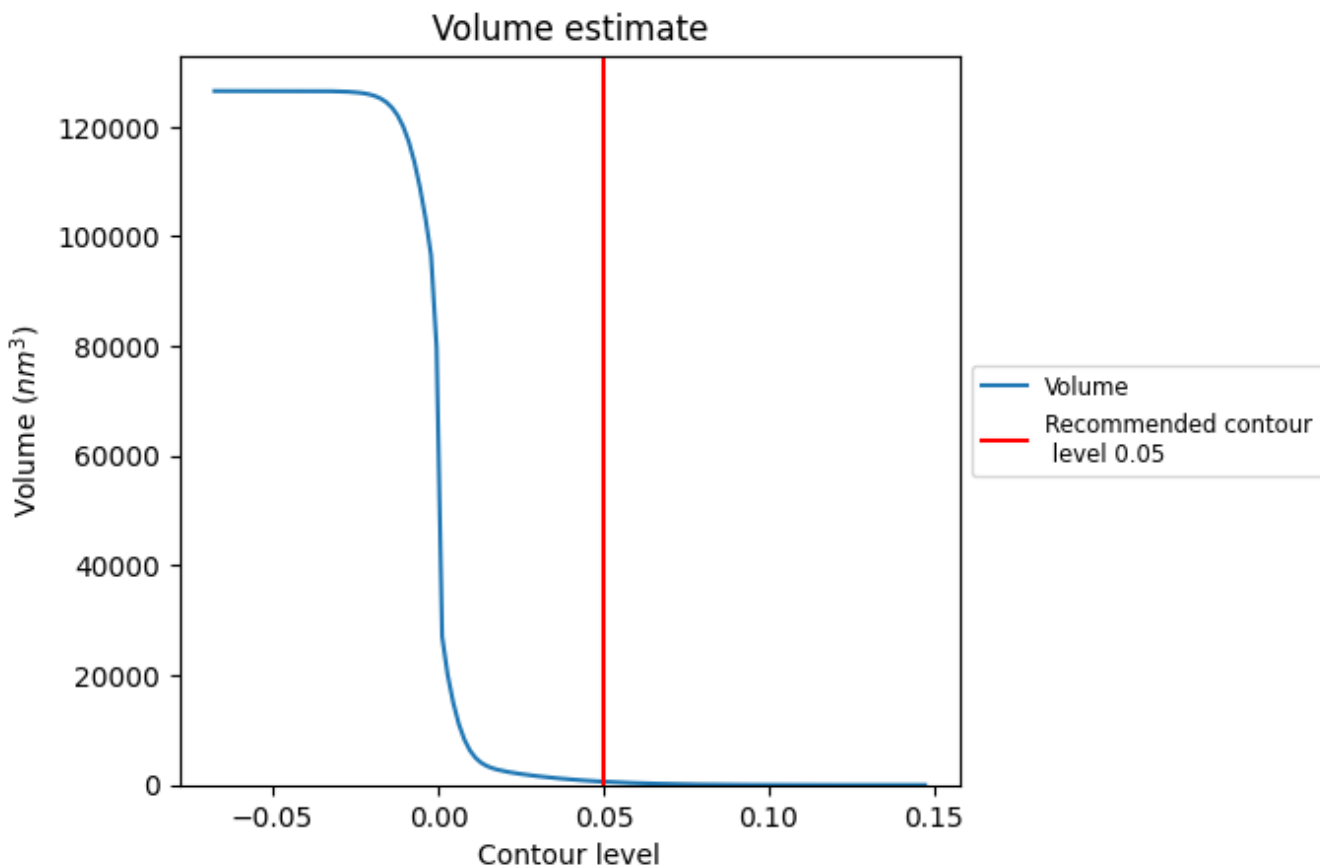
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

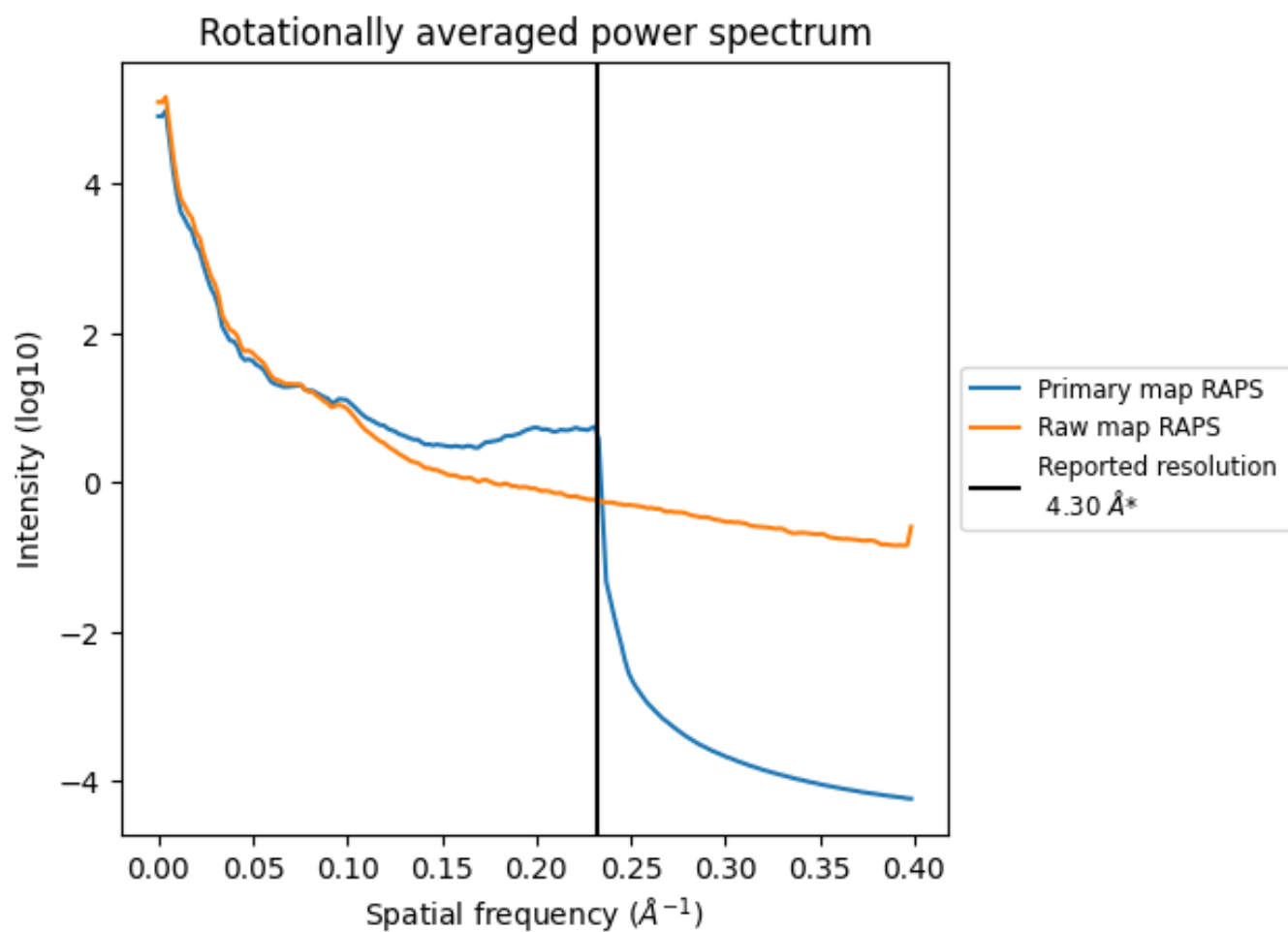
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 603  $\text{nm}^3$ ; this corresponds to an approximate mass of 545 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

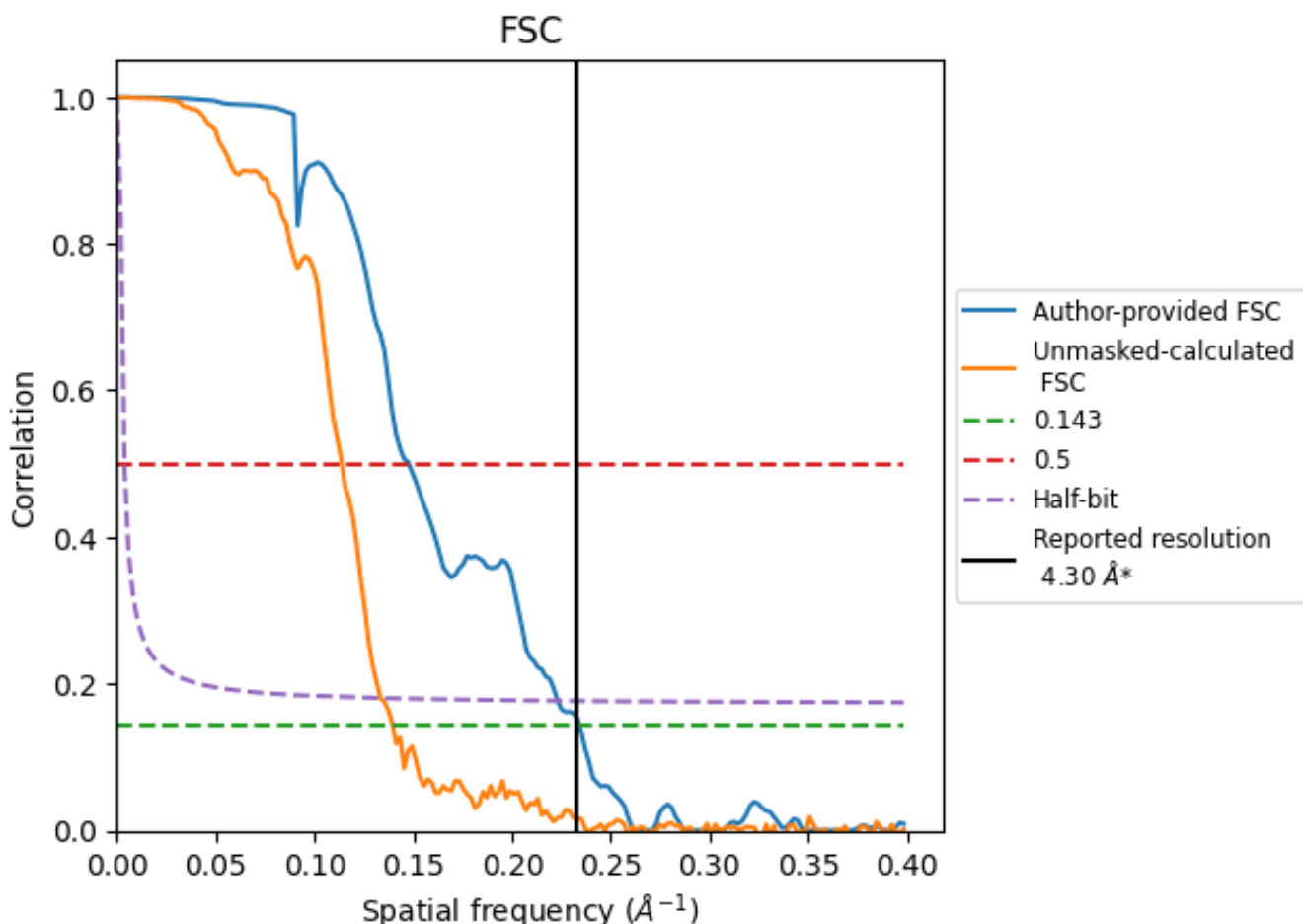


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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  $0.233 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

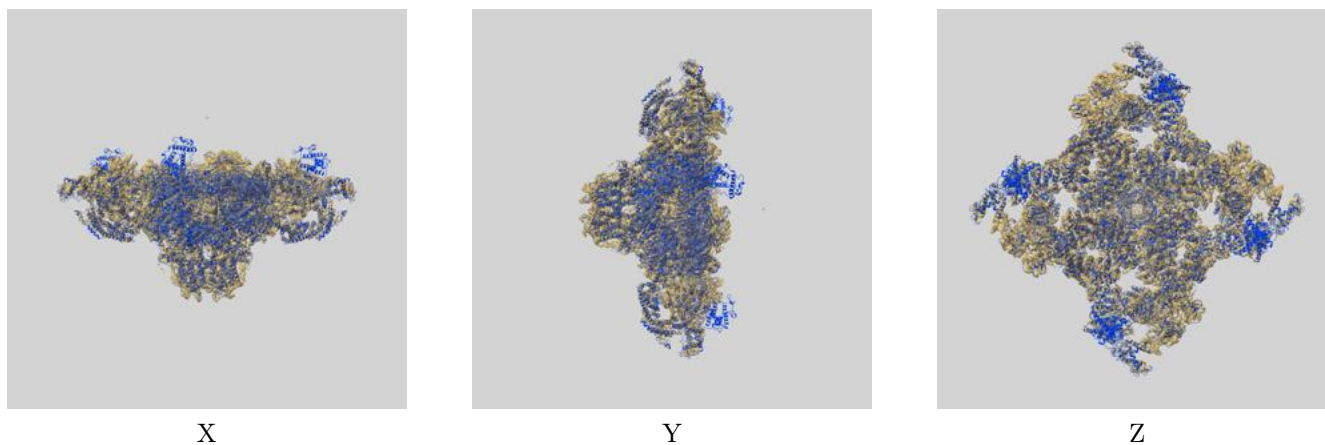
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	6.77	4.48
Unmasked-calculated*	7.16	8.77	7.49

\*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 7.16 differs from the reported value 4.3 by more than 10 %

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

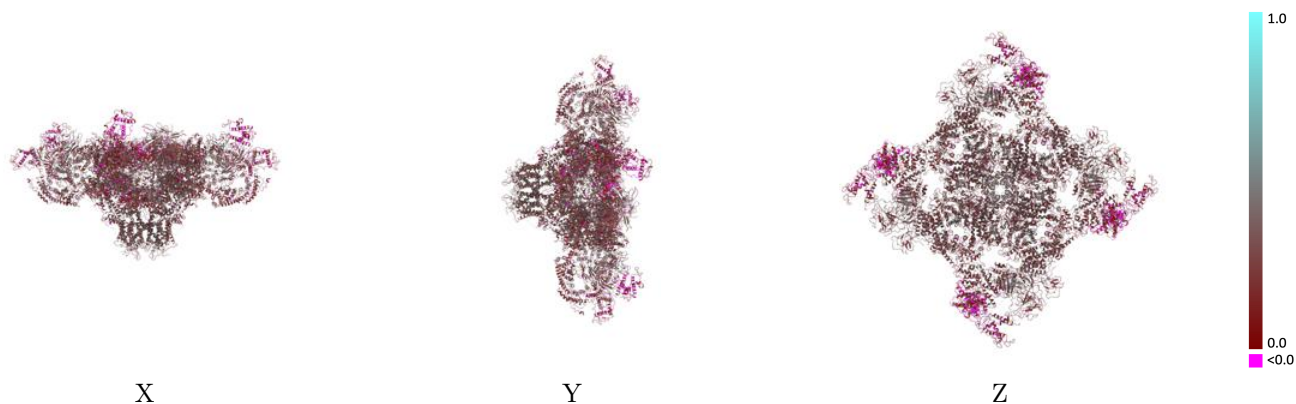
This section contains information regarding the fit between EMDB map EMD-8390 and PDB model 5TAZ. Per-residue inclusion information can be found in section 3 on page 5.

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



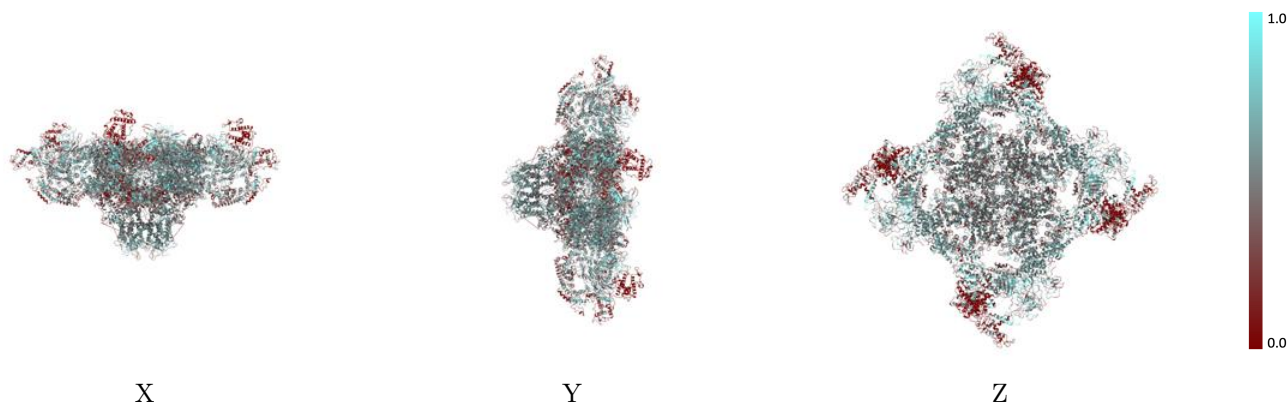
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

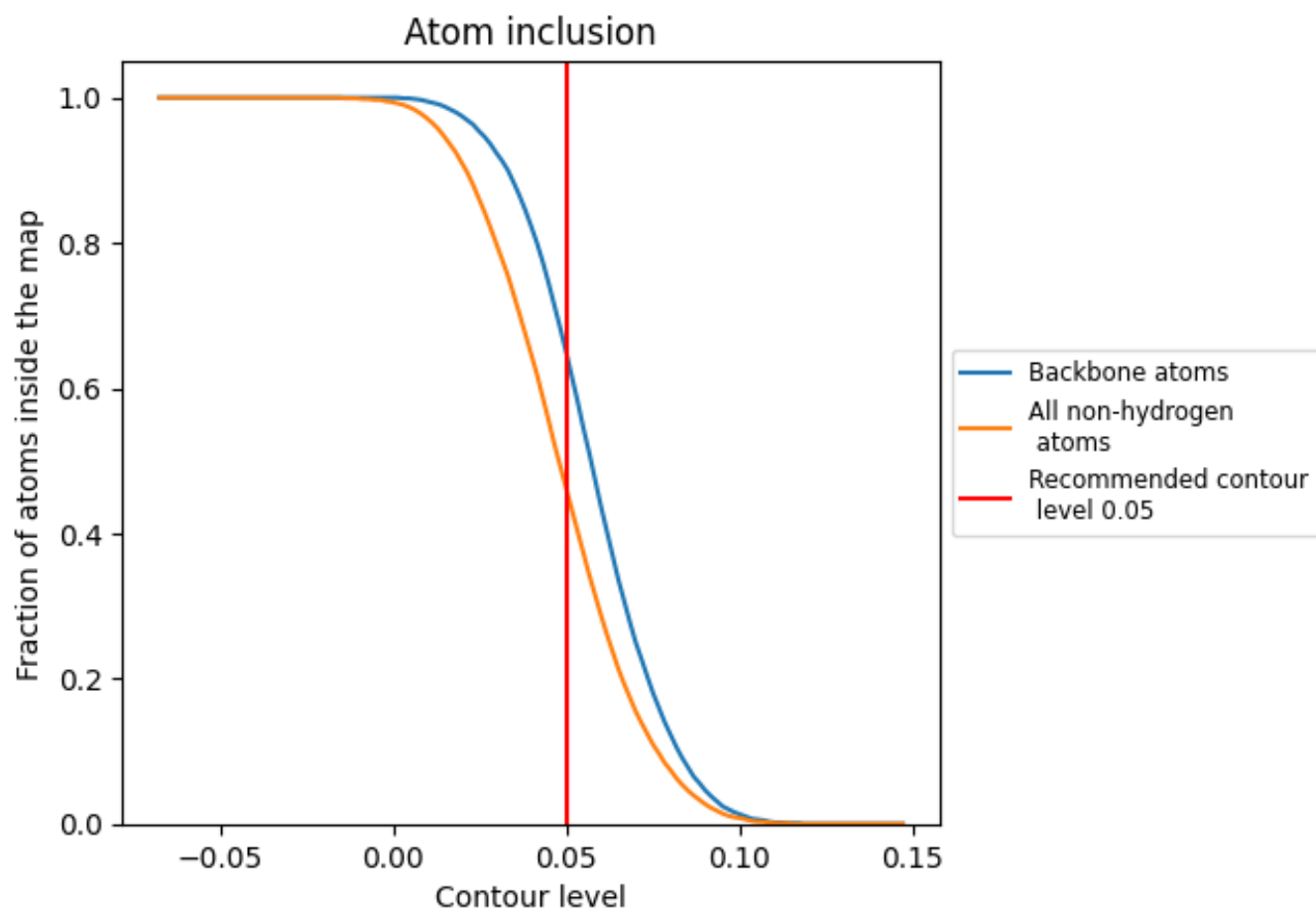
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.05).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 46% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.2730
A	0.4880	0.2880
B	0.4610	0.2730
E	0.4610	0.2730
F	0.4860	0.2930
G	0.4610	0.2730
H	0.4850	0.2930
I	0.4610	0.2730
J	0.4910	0.2910

