



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:39 AM UTC

PDB ID : 5TAN / pdb_00005tan
EMDB ID : EMD-8380
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

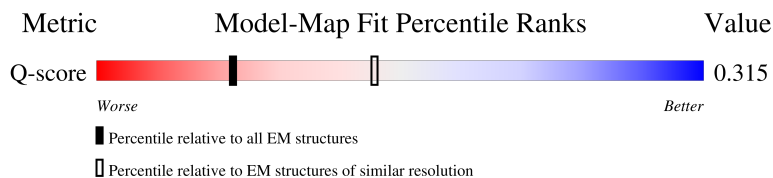
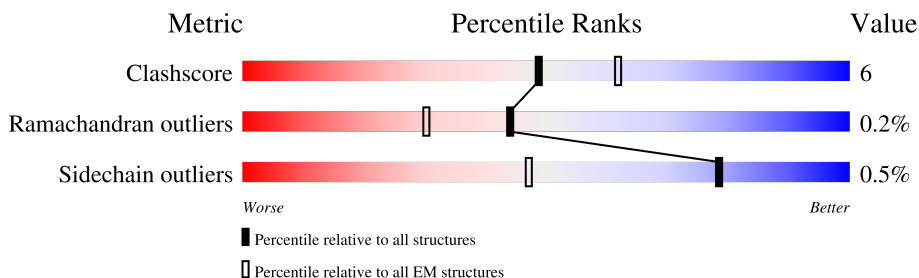
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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.



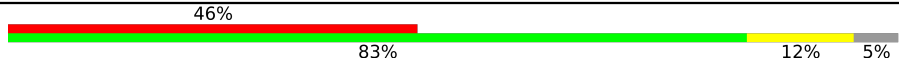



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	108	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">58%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 58%, orange 58%, yellow 79%, green 79%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 5px;"> <div style="text-align: center;">79%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 79%, orange 79%, yellow 99%, green 99%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div>
1	F	108	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">59%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 59%, orange 59%, yellow 79%, green 79%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 5px;"> <div style="text-align: center;">79%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 79%, orange 79%, yellow 99%, green 99%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div>
1	H	108	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">60%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 60%, orange 60%, yellow 79%, green 79%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 5px;"> <div style="text-align: center;">79%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 79%, orange 79%, yellow 99%, green 99%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div>
1	J	108	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">58%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 58%, orange 58%, yellow 79%, green 79%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div> <div style="display: flex; justify-content: space-between; align-items: center; margin-top: 5px;"> <div style="text-align: center;">79%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 79%, orange 79%, yellow 99%, green 99%, grey 100%);"></div> <div style="text-align: right;">20% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

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

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

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

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

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

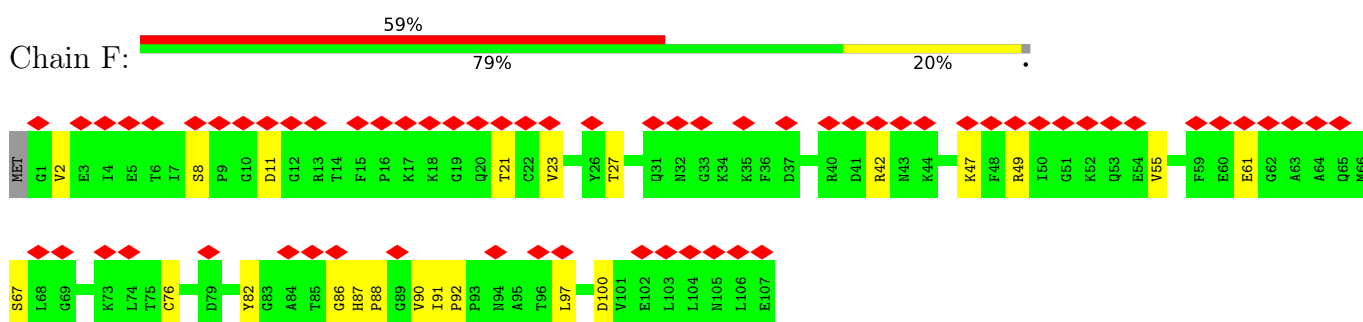
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	

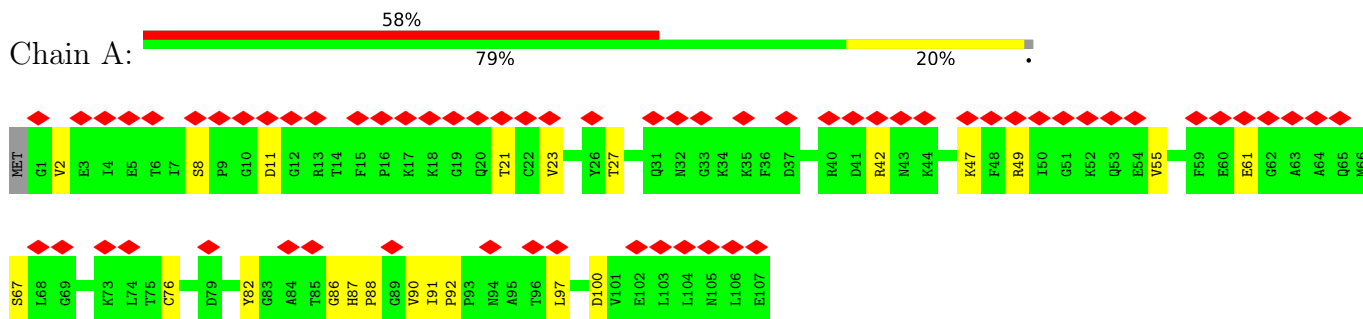
3 Residue-property plots [i](#)

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

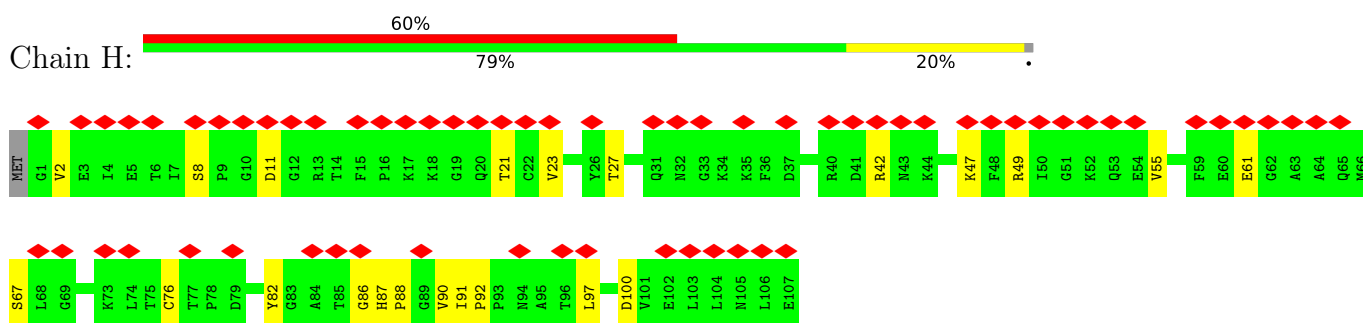
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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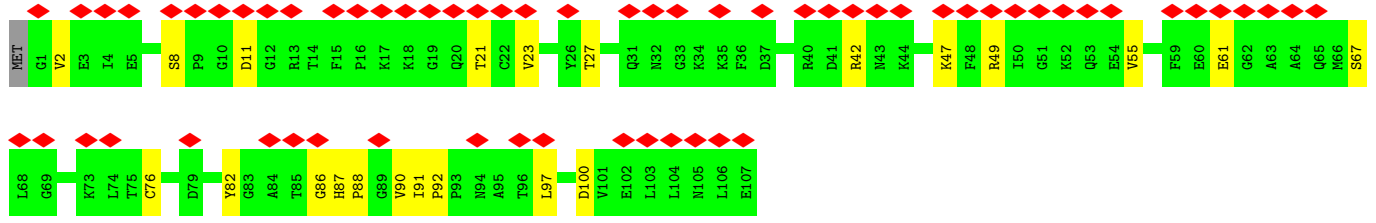


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

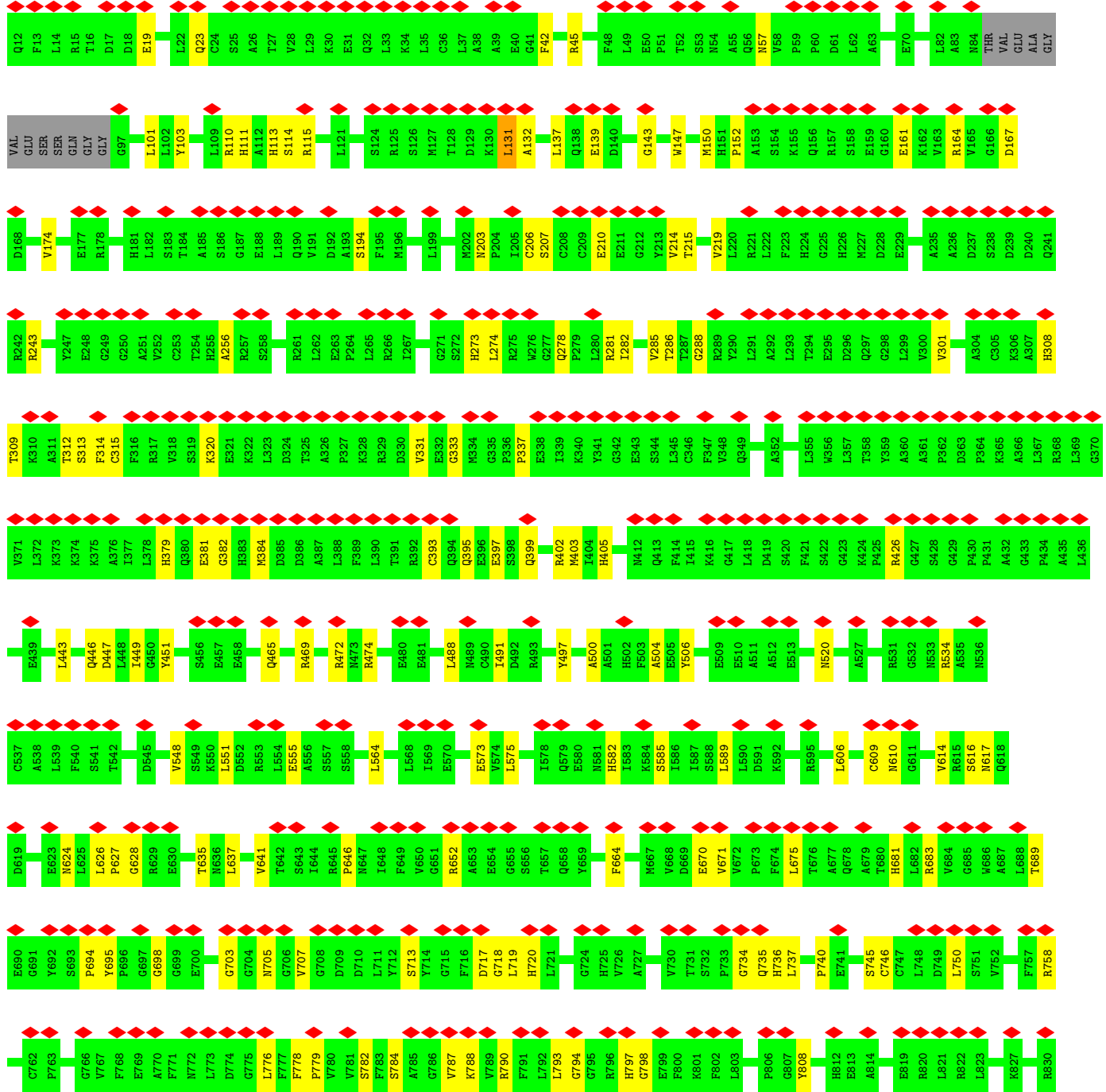
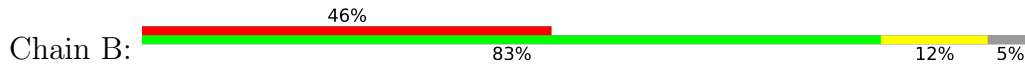


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

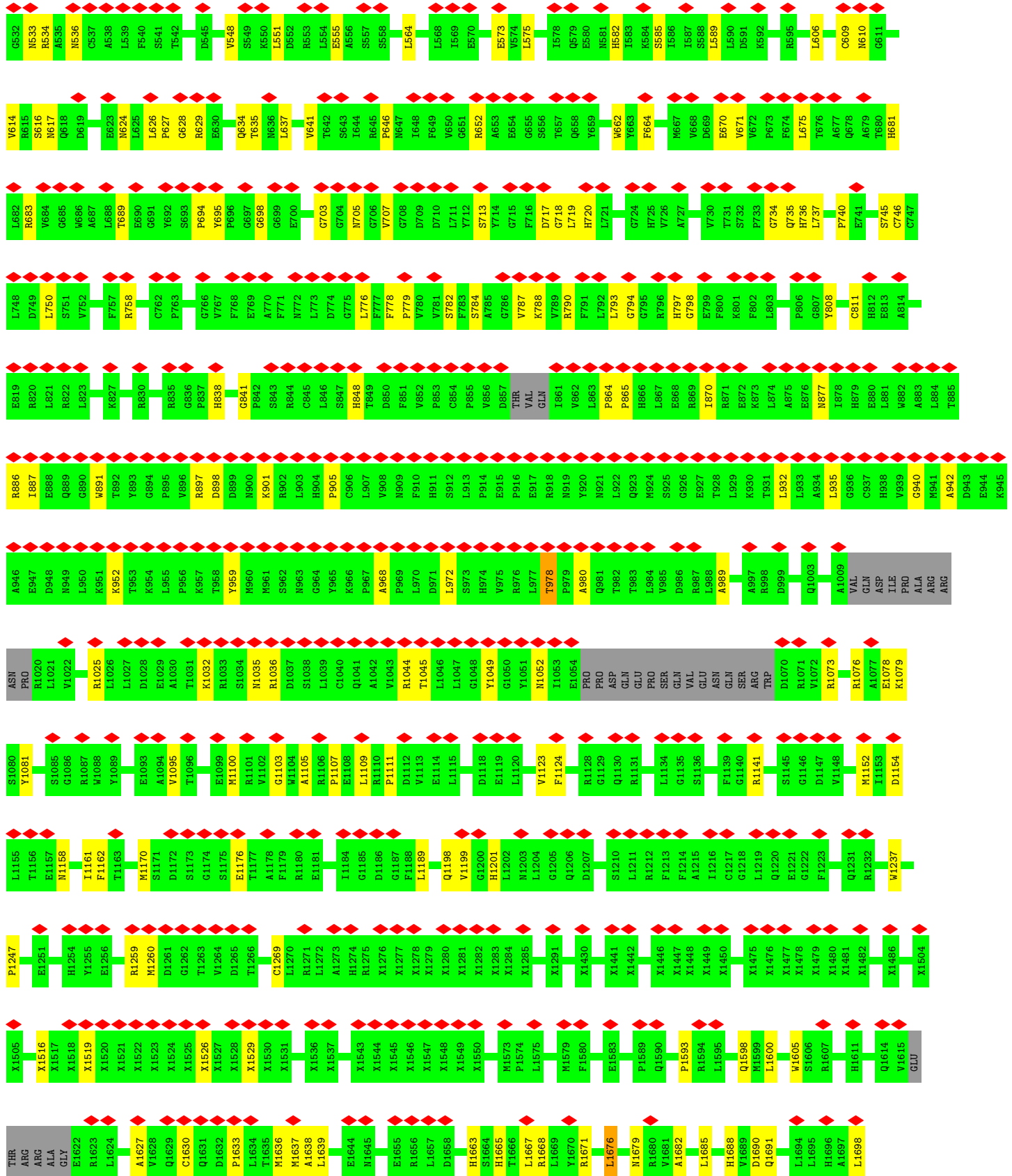


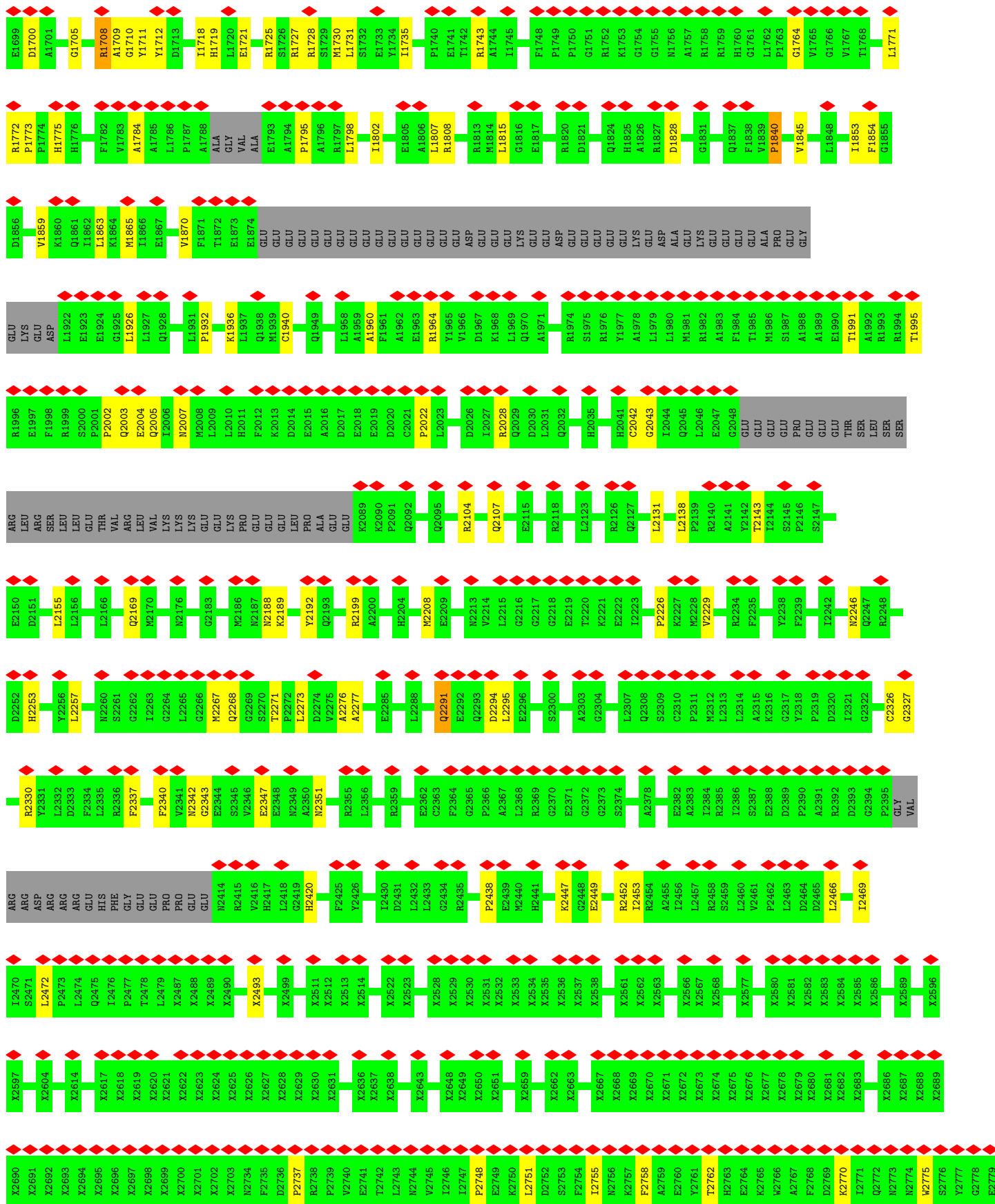


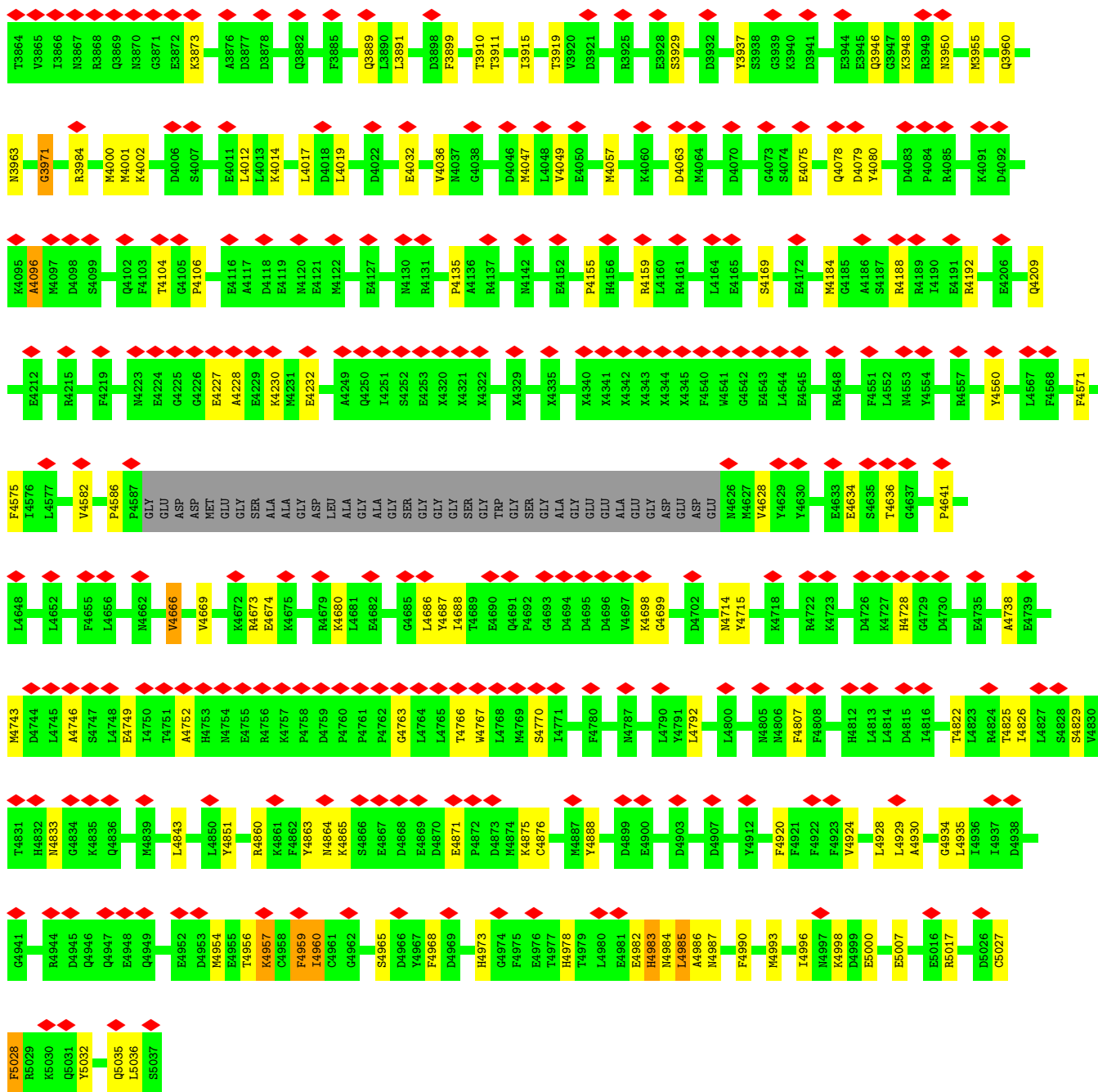
• Molecule 2: Ryanodine receptor 1



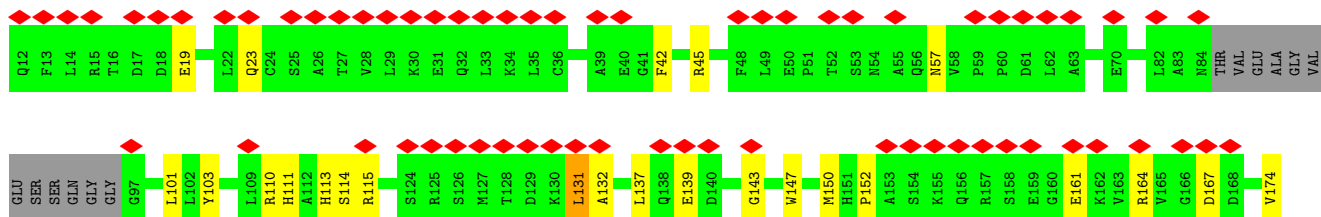
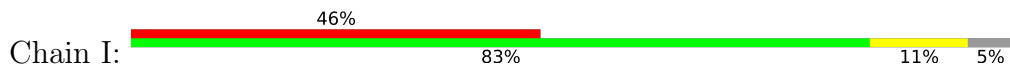
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A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	E2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3003	X3004	X3005			
S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	L2872	A2873	M2874	A2875	A2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	M2884	T2885	M2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2921	K2922		
E2803	I2804	Y2805	R2806	R2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	THR	THR	GLU	LYS	LYS	LYS	THR	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	ARG	GLU	GLY	Y2855	M2856	P2857	Q2858	P2859	P2860	D2861	L2862			
L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	L2793	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	D2800	D2801	K2802
E2347	E2348	M2349	A2350	N2351	R2355	L2356	R2359	K2360	P2361	E2362	F2364	P2365	P2366	L2368	R2369	G2370	E2371	G2372	S2374	A2378	I2384	R2385	I2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415								
W2416	H2417	L2418	G2419	H2420	F2425	Y2426	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	M2440	H2441	K2447	G2448	E2449	R2452	R2453	R2454	A2455	I2456	L2457	R2458	S2459	W2460	P2462	L2463	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	D2474	Q2475	I2476	I2477	T2478	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631						
X2511	X2512	X2513	X2514	X2522	X2523	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2561	X2562	X2563	X2566	X2567	X2568	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2588	X2589	X2589	X2596	X2614	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2631										
X2638	X2643	X2648	X2649	X2650	X2651	X2659	X2662	X2663	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742								

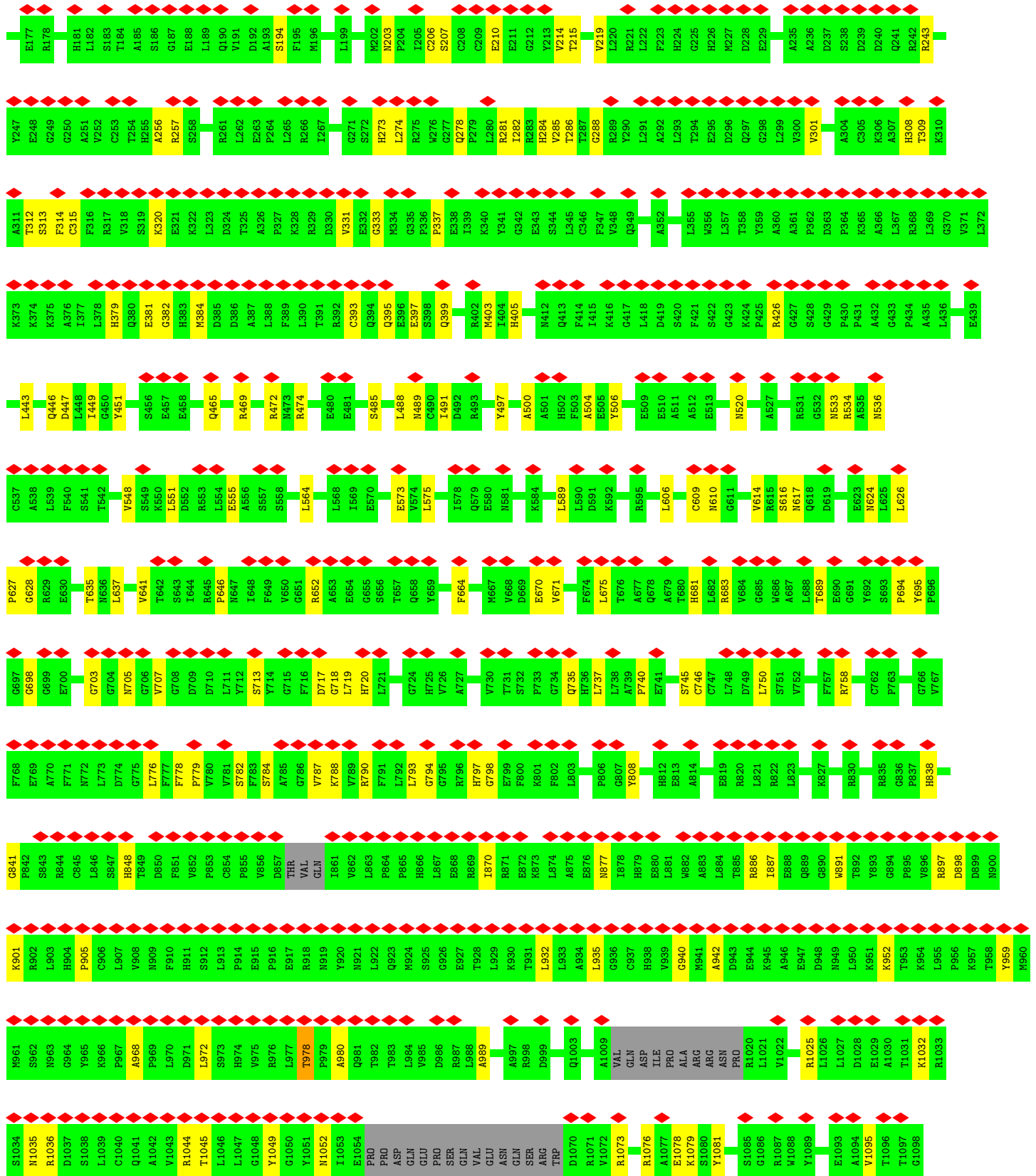


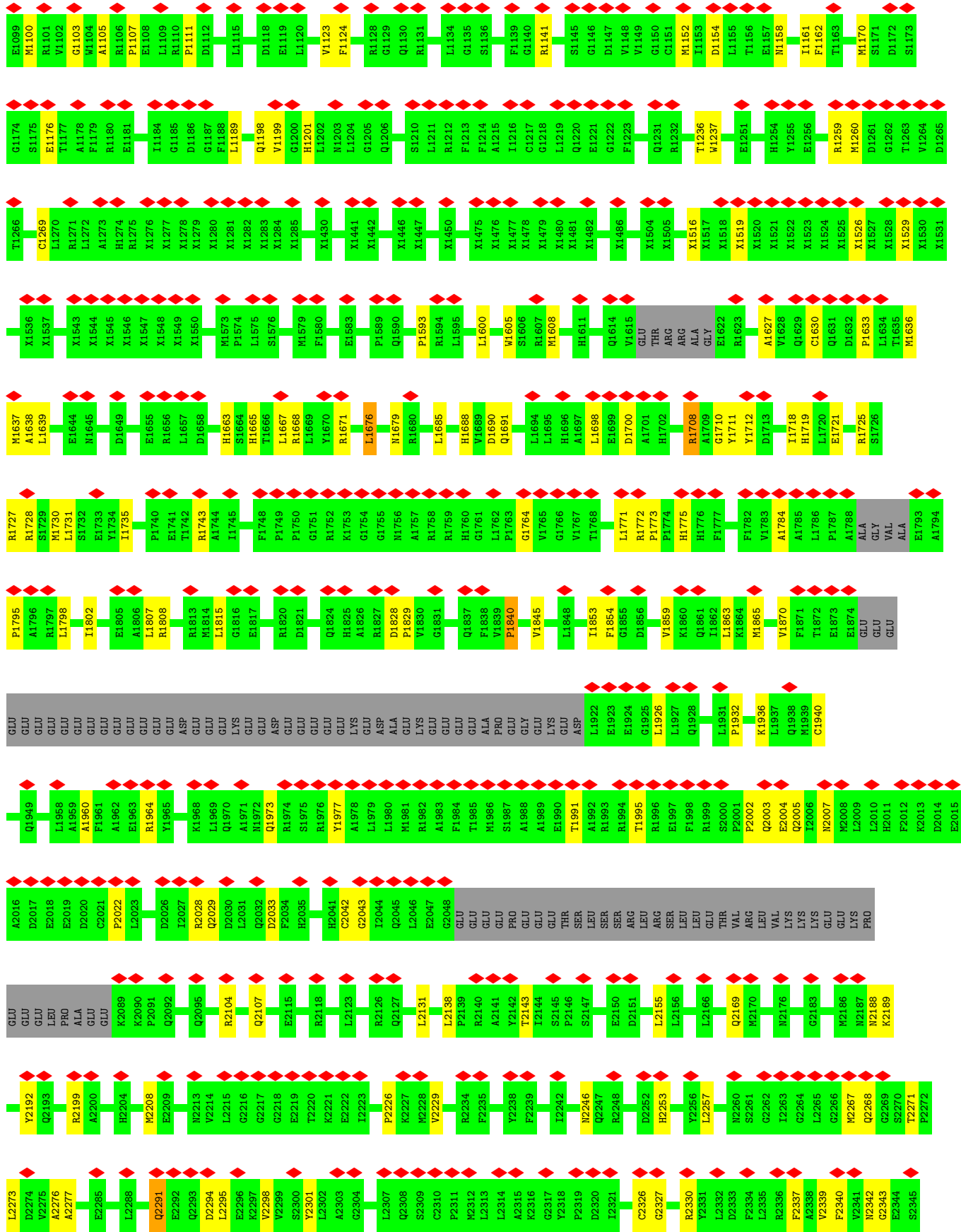




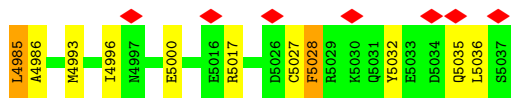
• Molecule 2: Ryanodine receptor 1



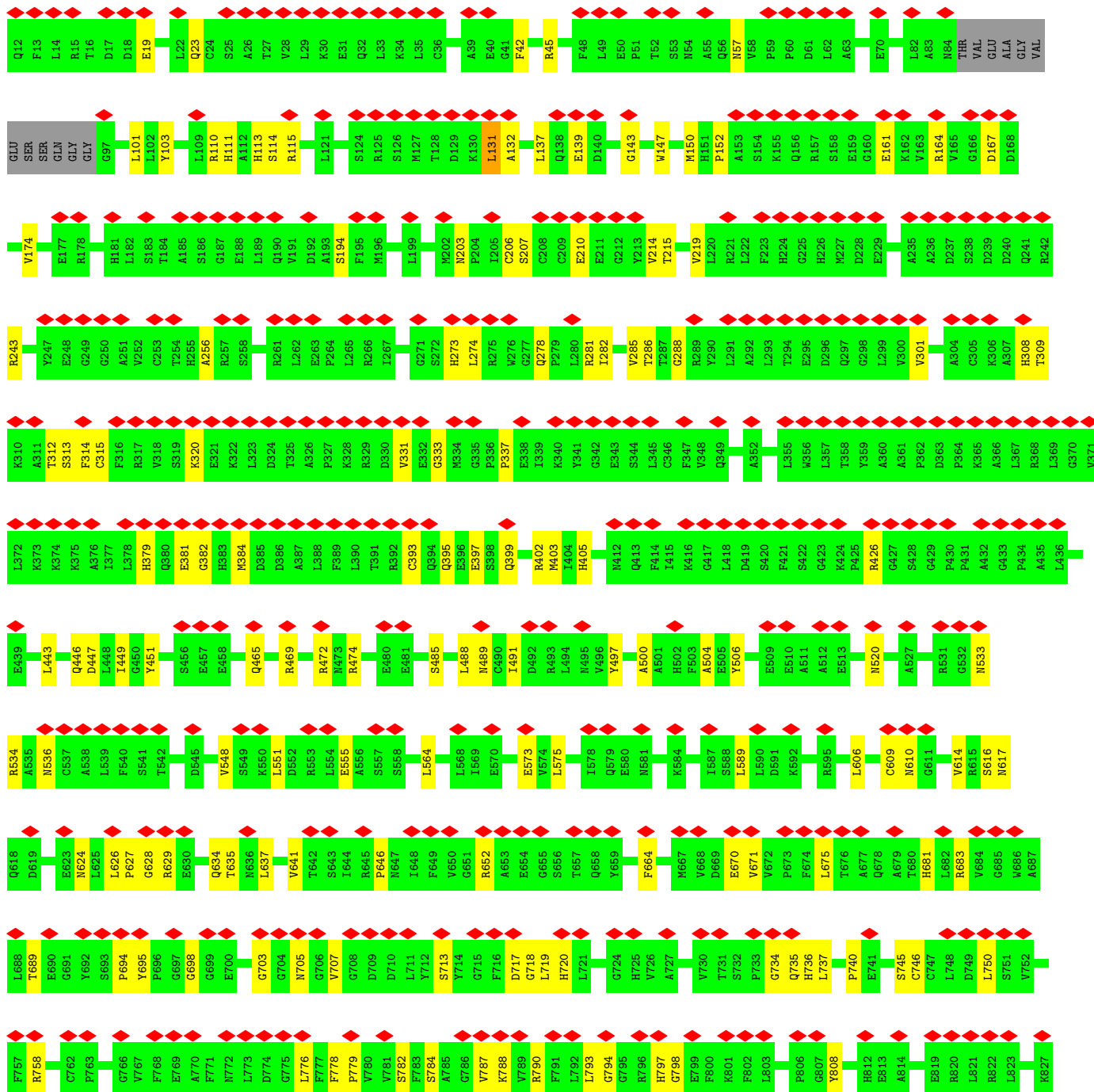
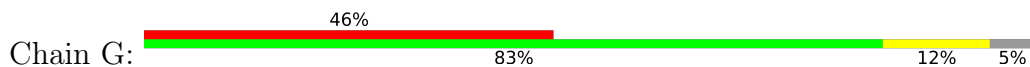


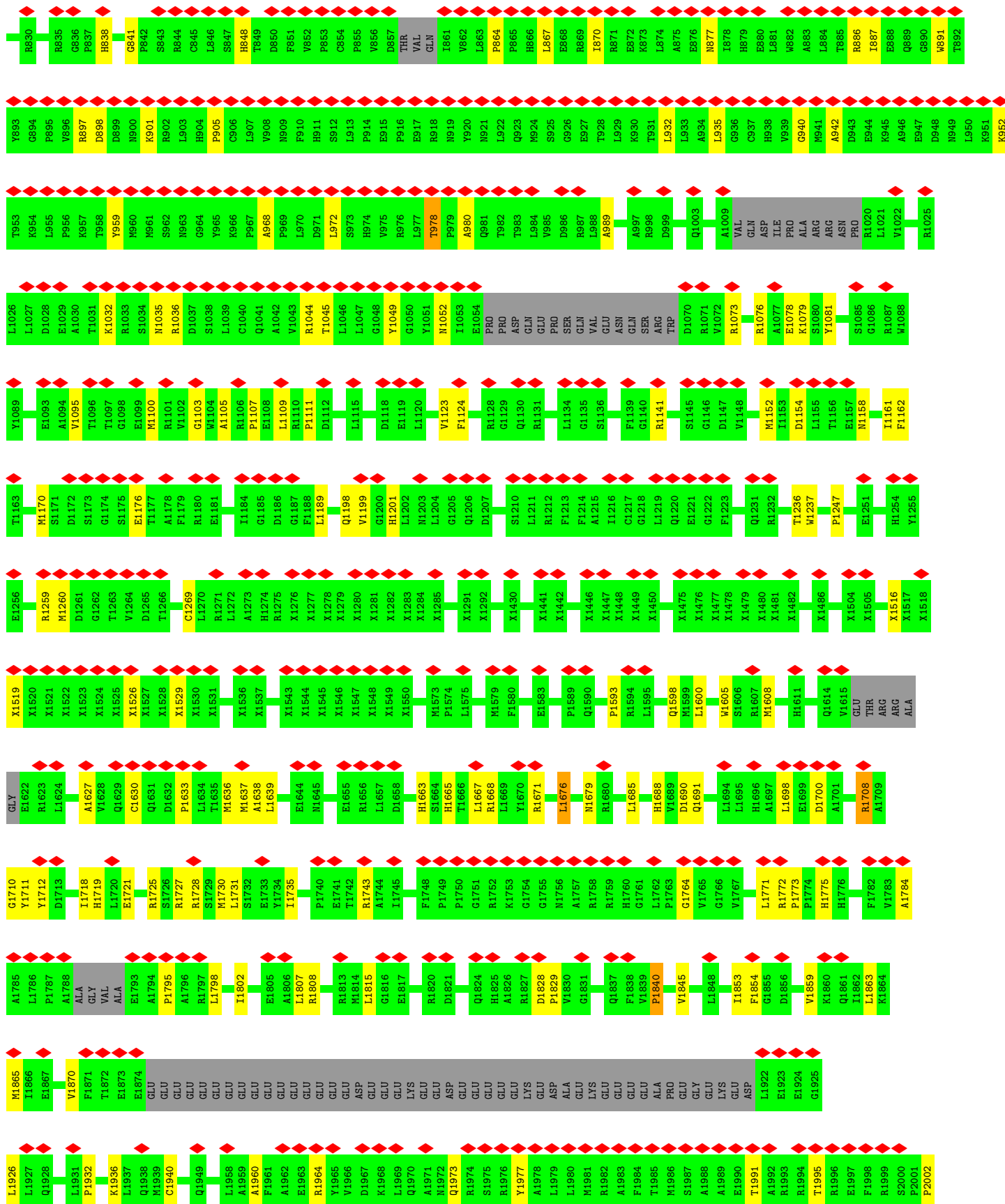


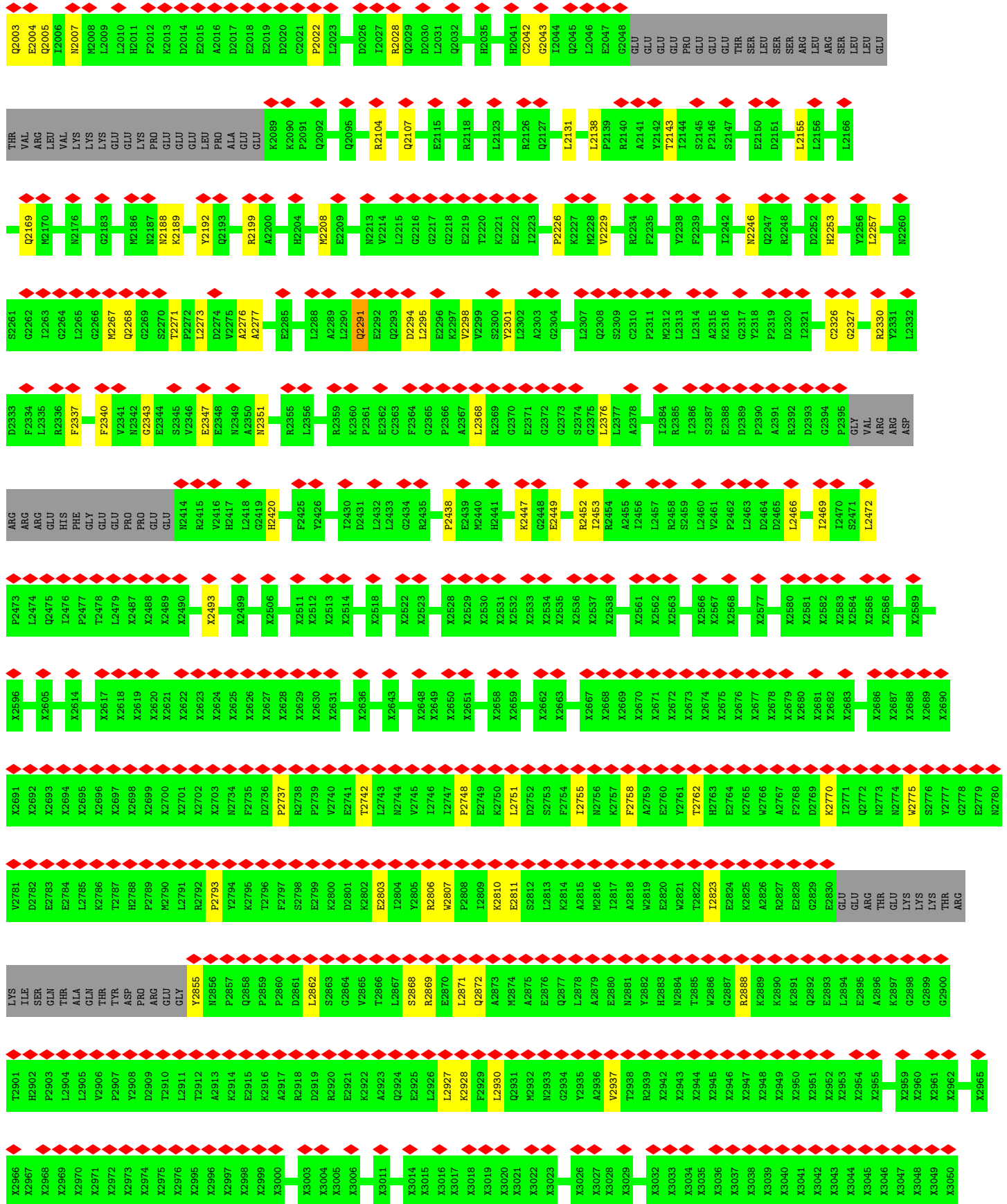
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R2415	V2416	H2417	L2418	G2419	H2420	F2425	Y2426	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	M2440	H2441	K2447	G2448	E2449	R2452	I2453	A2455	I2456	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	Q2476	I2477	P2478	T2478	L2479	X2487	X2488	X2489	X2490	X2493																																
X2499	X2511	X2512	X2513	X2514	X2522	X2523	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2561	X2562	X2563	X2566	X2567	X2568	X2577	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2589	X2596	X2596	X2596	X2614	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630																																
X2631	X2636	X2637	X2638	X2643	X2648	X2649	X2650	X2651	X2659	X2662	X2663	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	X2704	X2705	X2706	X2707	X2708	X2709	X2710	X2711	X2712	X2713	X2714	X2715	X2716	X2717	X2718	X2719	X2720	X2721	X2722	X2723	X2724	X2725	X2726	X2727	X2728	X2729	X2730	X2731	X2732	X2733	X2734	X2735	X2736	X2737	X2738	X2739
V2740	E2741	T2742	L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	S2754	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Z2777	G2778	E2779	N2780	W2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	L2796	S2798	E2799																							
X2800	D2801	X2802	E2803	L2804	Y2805	R2806	X2807	P2808	L2809	K2810	E2811	S2812	L2813	X2814	A2815	M2816	L2817	A2818	X2819	E2820	X2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	X2855	X2856	P2857	Q2858	P2859																								
P2860	D2861	L2862	S2863	G2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	K2892	E2893	L2894	E2895	A2896	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	X2906	P2907	Y2908	D2909	T2910	L2911	T2912	X2913	K2914	E2915	K2916	A2917	R2918	D2919																								
R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2959	X2960	X2961	X2962	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X3000	X3003																												
X3004	X3005	X3006	X3011	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3143																													
X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3151	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3182	X3183	X3184	X3185	X3186	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3201	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215																												
X3216	X3217	X3218	X3219	X3220	X3221	X3222	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	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285																									
X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3323	X3324	X3325	X3326	X3327	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	X3369	X3370	X3371	X3372	X3373	X3374	X3377	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418																										

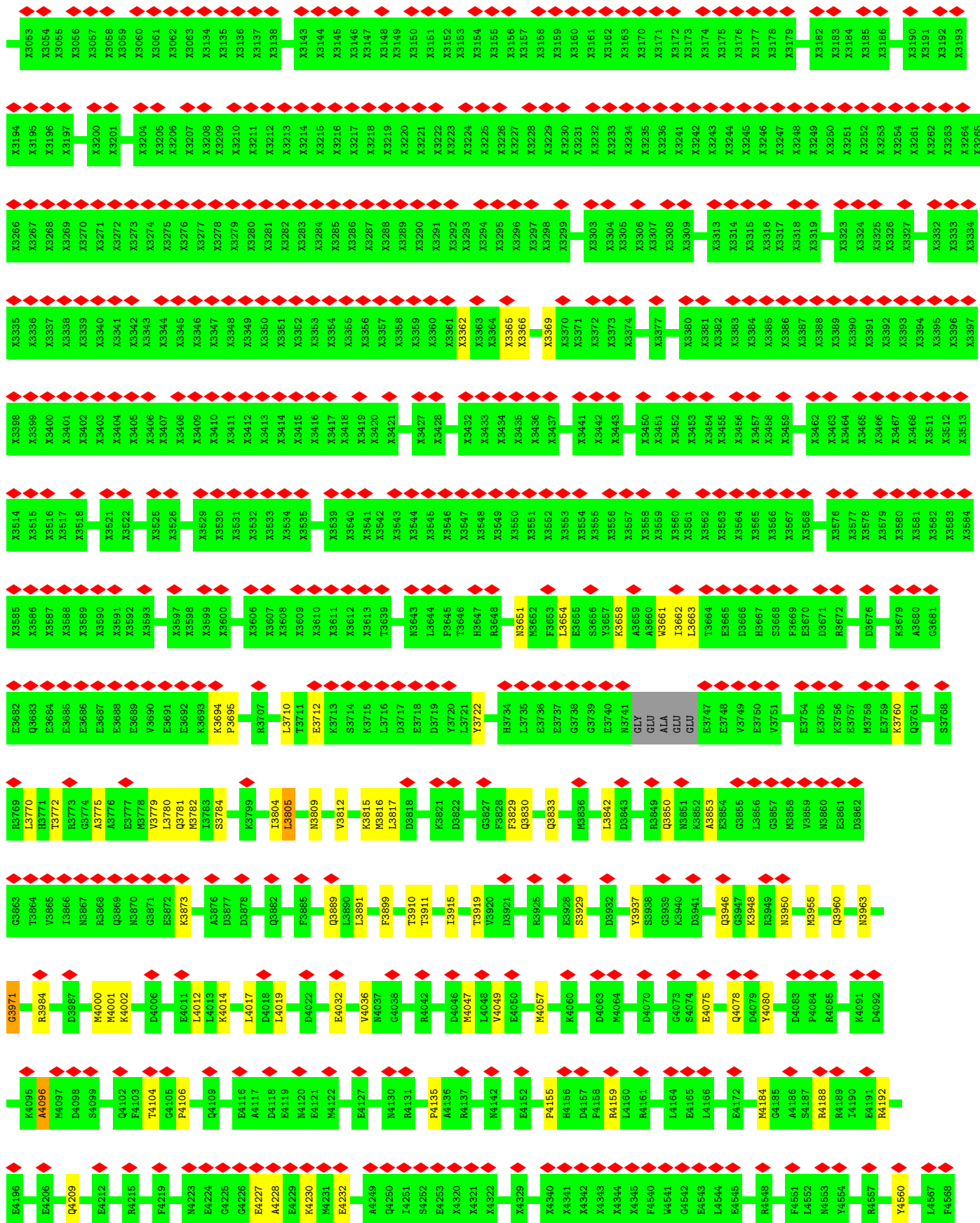


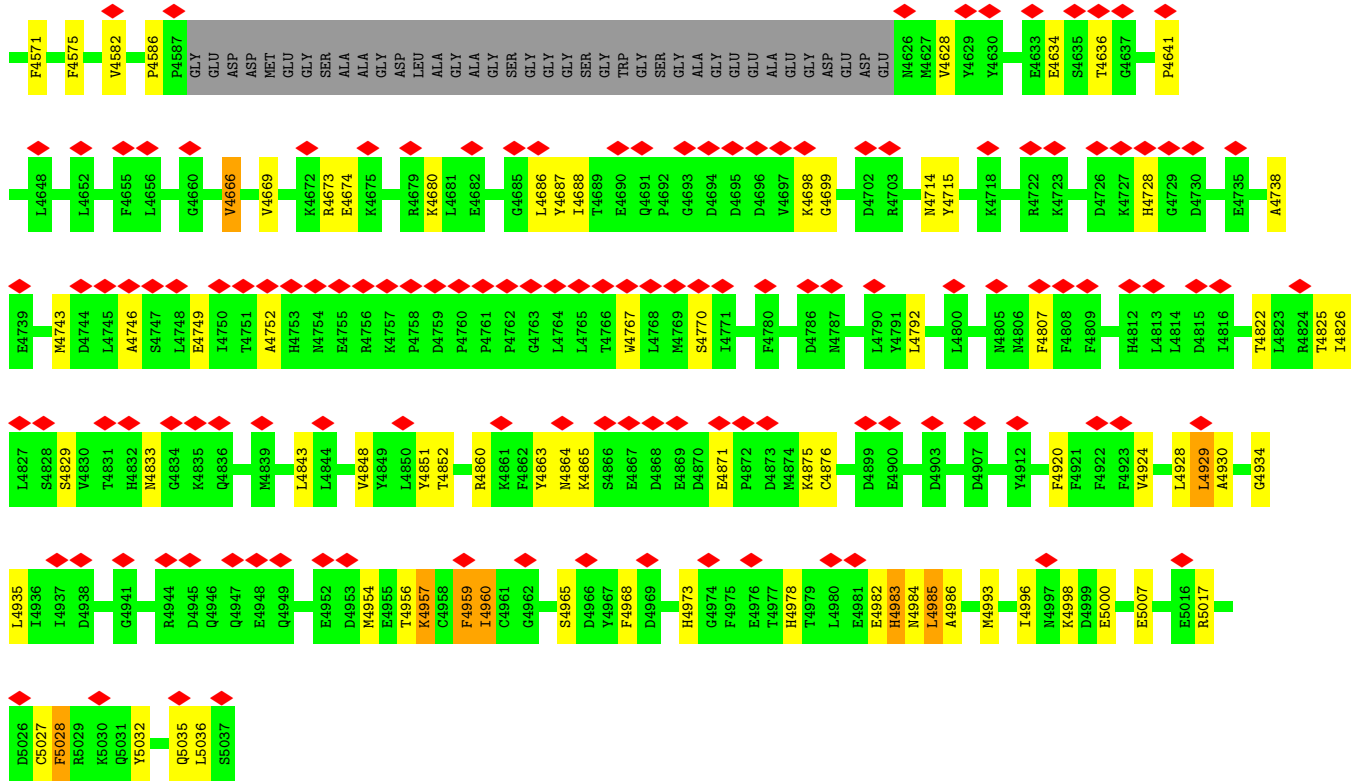
● Molecule 2: Ryanodine receptor 1











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	0.070	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.48	0/1123
2	B	0.23	0/25428	0.53	3/34534 (0.0%)
2	E	0.23	0/25428	0.53	3/34534 (0.0%)
2	G	0.23	0/25428	0.53	4/34534 (0.0%)
2	I	0.23	0/25428	0.53	4/34534 (0.0%)
All	All	0.23	0/105048	0.53	14/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	137	LEU	CA-C-N	-5.93	114.43	121.90
2	G	137	LEU	C-N-CA	-5.93	114.43	121.90
2	B	137	LEU	CA-C-N	-5.93	114.43	121.90
2	B	137	LEU	C-N-CA	-5.93	114.43	121.90
2	E	137	LEU	CA-C-N	-5.93	114.43	121.90

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	13	0
1	J	818	0	824	13	0
2	B	29499	0	24753	315	0
2	E	29499	0	24753	325	0
2	G	29499	0	24753	319	0
2	I	29499	0	24753	309	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102396	1287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1287 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:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	43	77
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	43	77
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	44	77

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
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%)	2481 (100%)	12 (0%)	81	81
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	I	2493/3022 (82%)	2480 (100%)	13 (0%)	81	81
All	All	10324/12444 (83%)	10275 (100%)	49 (0%)	78	81

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	2339	VAL

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Mol	Chain	Res	Type
2	I	4960	ILE
2	I	3663	LEU
2	I	4929	LEU
2	G	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 248 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4109	GLN
2	G	3809	ASN
2	I	725	HIS
2	G	3647	HIS
2	G	4201	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
4	CFF	B	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.75	11 (47%)
4	CFF	G	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.75	11 (47%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.76	10 (20%)
3	ATP	I	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	10 (20%)
4	CFF	E	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.74	11 (47%)
4	CFF	I	5102	-	15,15,15	1.96	7 (46%)	23,23,23	2.74	11 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5101	ATP	C5-C4	4.25	1.46	1.39
3	B	5101	ATP	C5-C4	4.23	1.46	1.39
3	G	5101	ATP	C5-C4	4.23	1.46	1.39
3	I	5101	ATP	C5-C4	4.20	1.46	1.39
4	E	5102	CFF	C6-N1	-3.81	1.32	1.40

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5102	CFF	C14-N7-C8	-7.71	111.86	126.28
4	B	5102	CFF	C14-N7-C8	-7.70	111.88	126.28
4	I	5102	CFF	C14-N7-C8	-7.68	111.91	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
3	B	5101	ATP	C5-C4-N3	-5.17	119.60	126.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

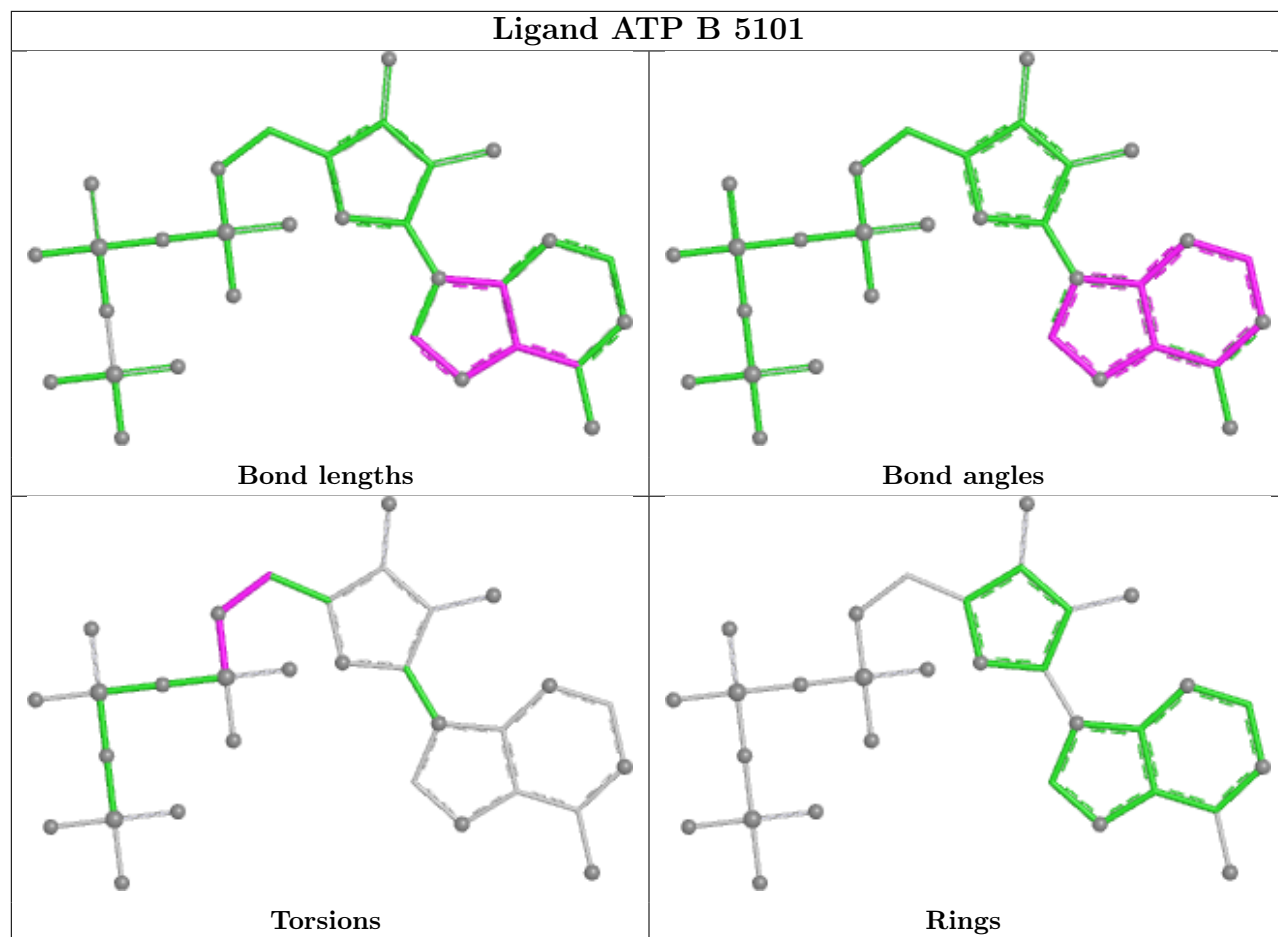
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A

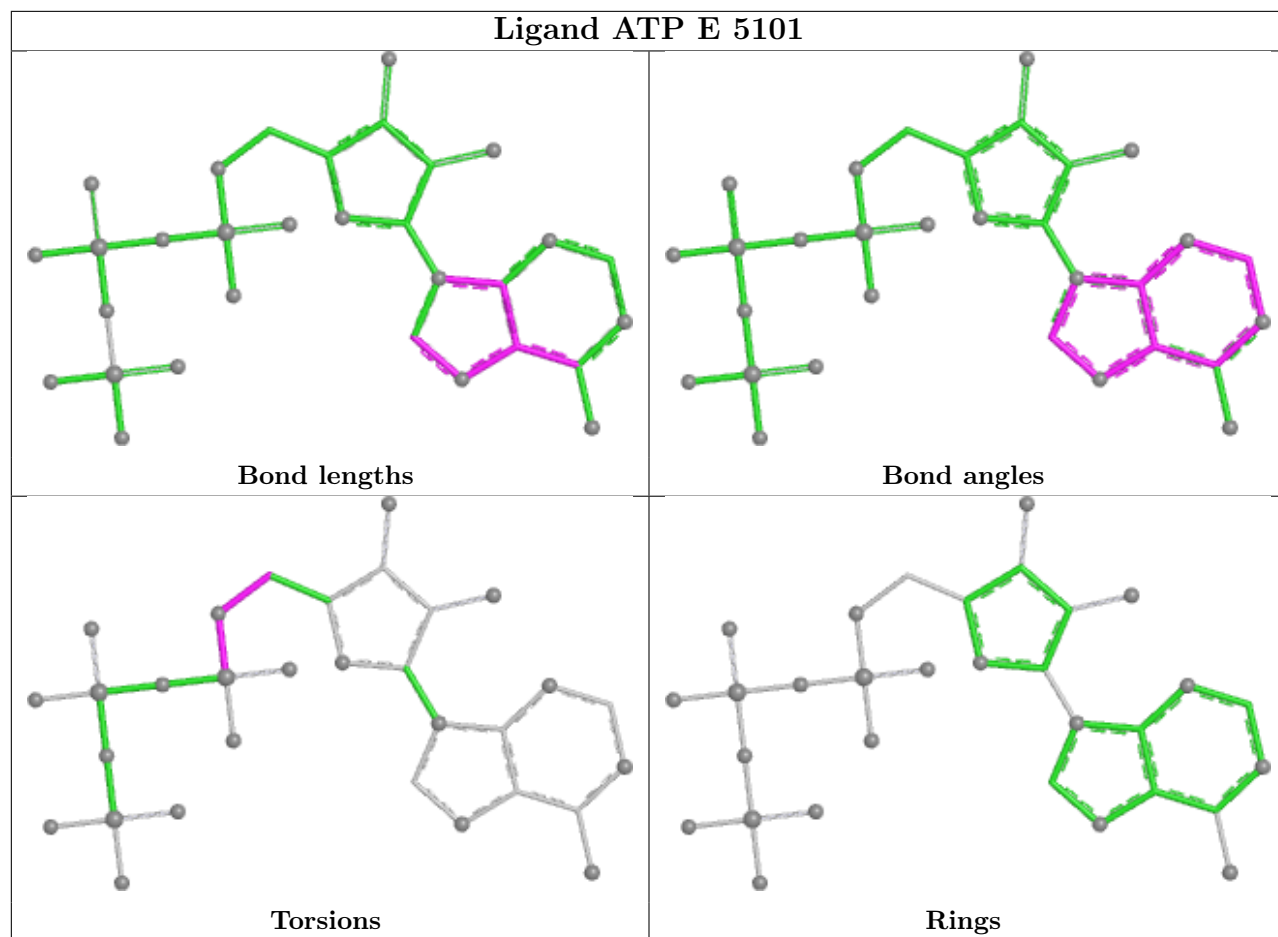
There are no ring outliers.

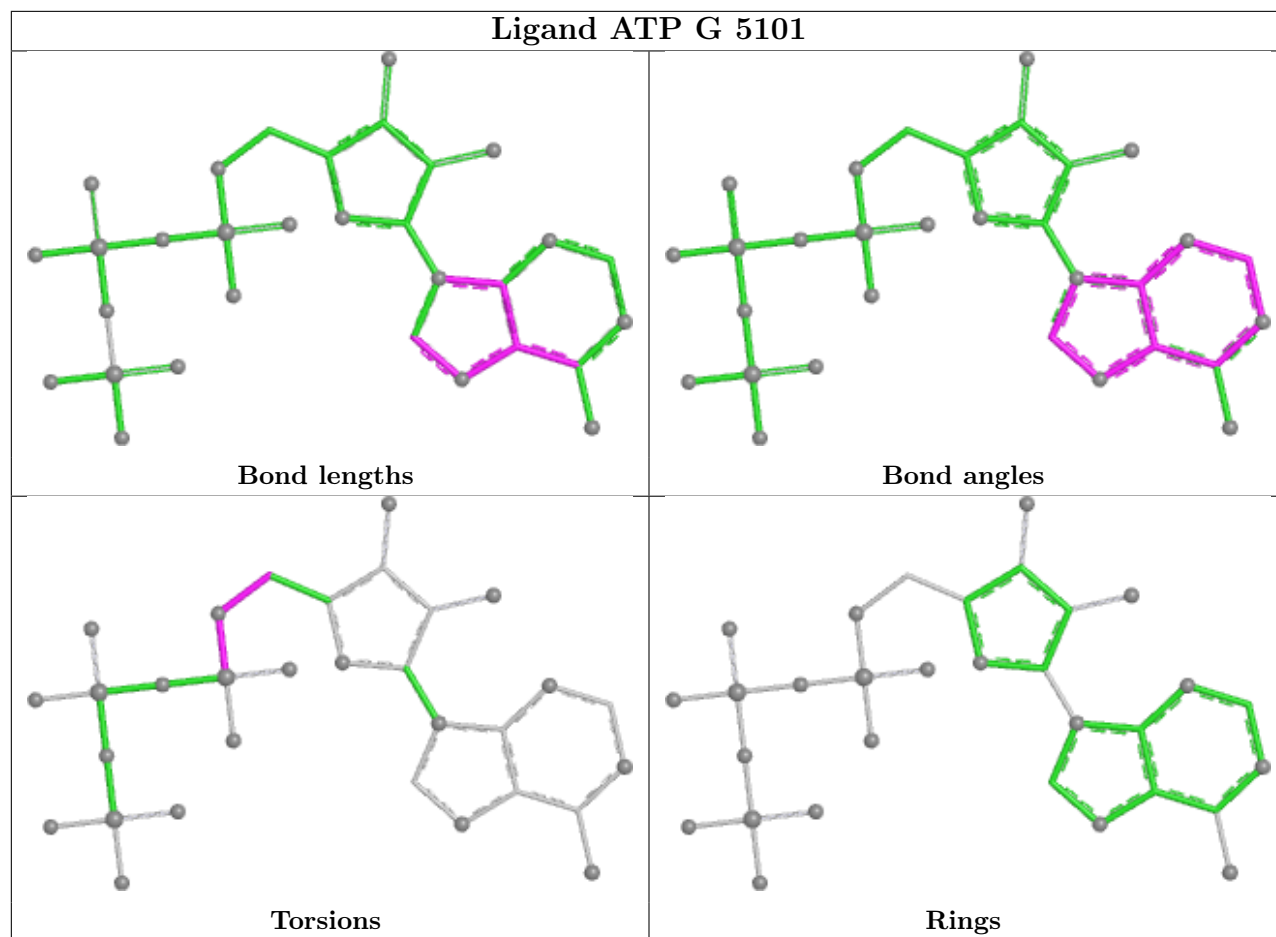
4 monomers are involved in 8 short contacts:

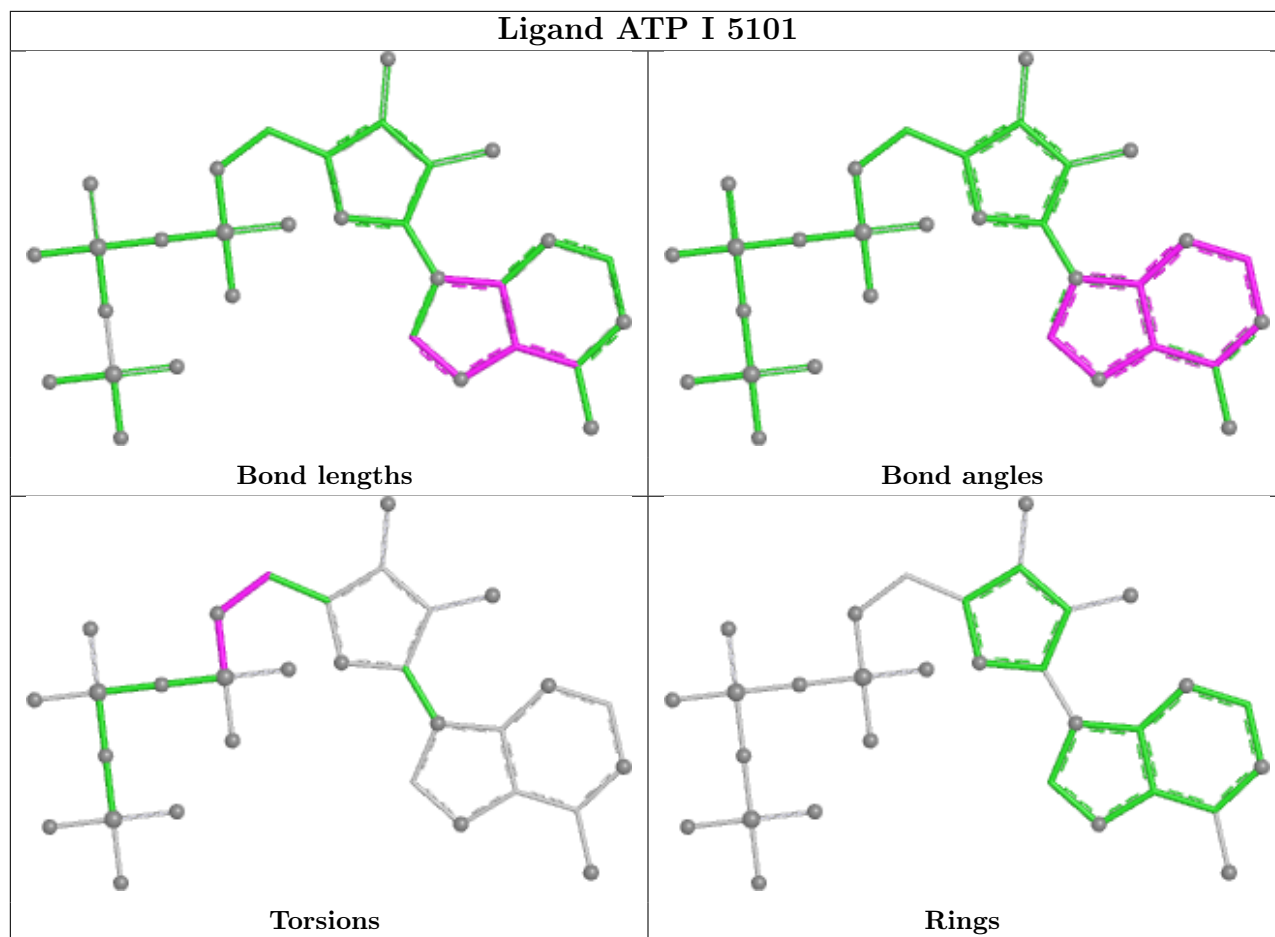
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
3	I	5101	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [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	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93

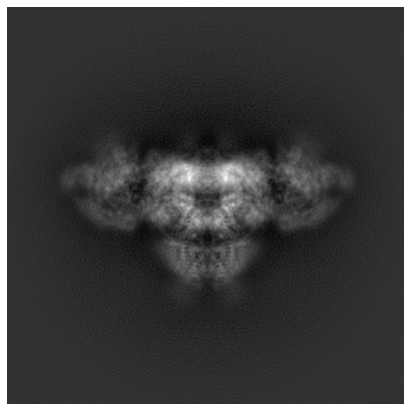
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8380. These allow visual inspection of the internal detail of the map and identification of artifacts.

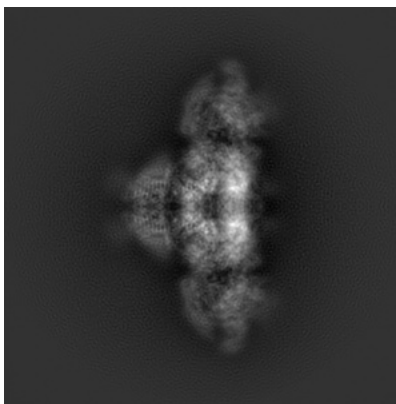
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

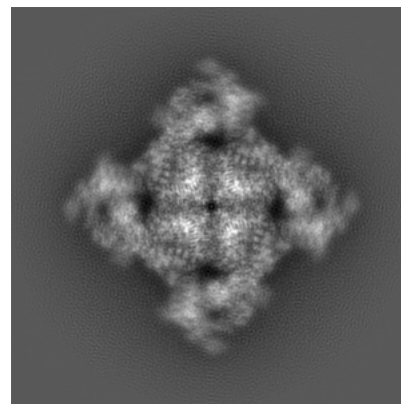
6.1.1 Primary map



X

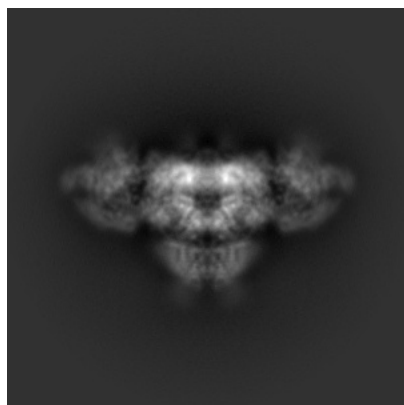


Y

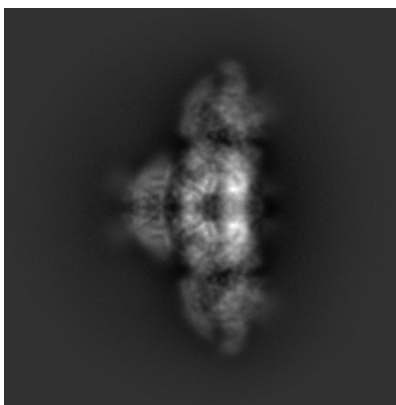


Z

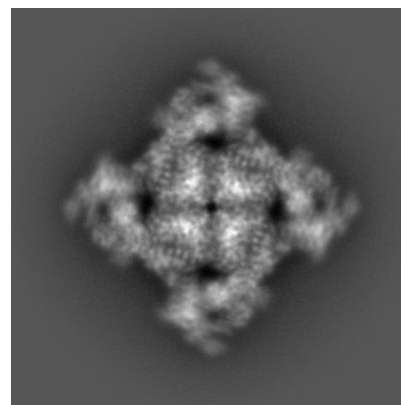
6.1.2 Raw map



X



Y

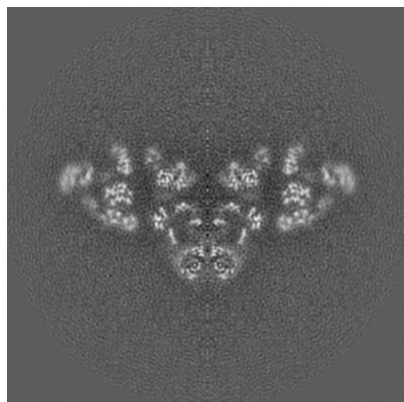


Z

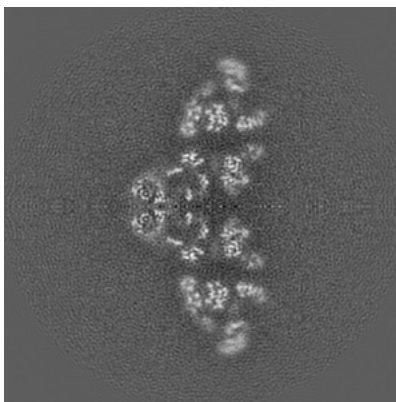
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

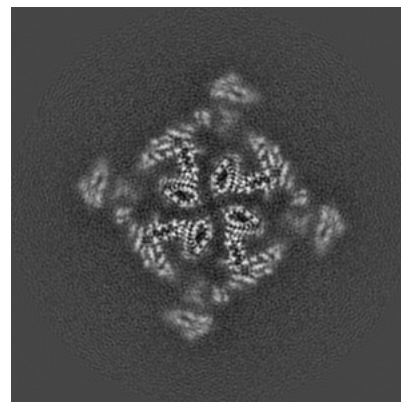
6.2.1 Primary map



X Index: 200

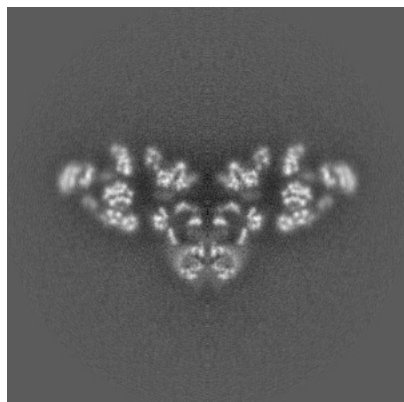


Y Index: 200

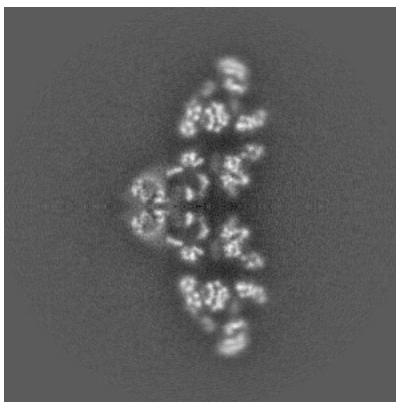


Z Index: 200

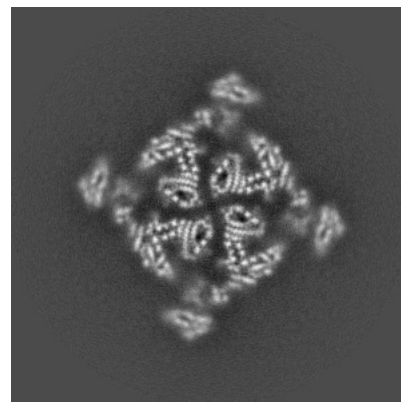
6.2.2 Raw map



X Index: 200



Y Index: 200

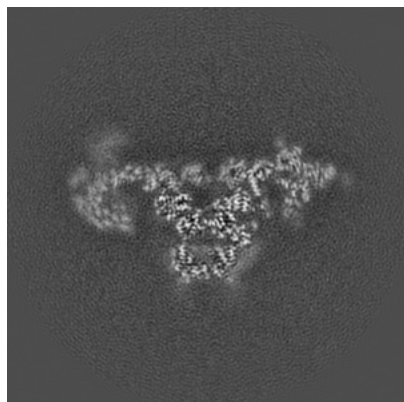


Z Index: 200

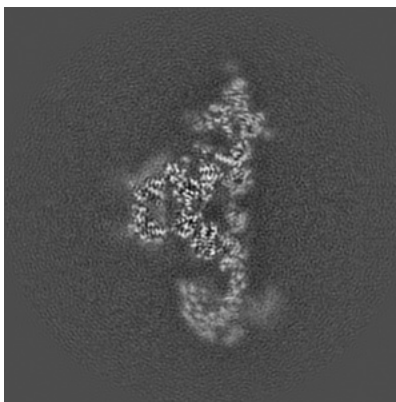
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

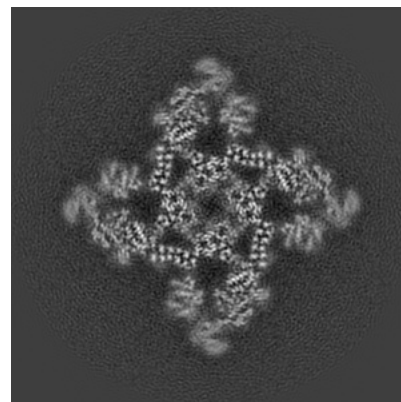
6.3.1 Primary map



X Index: 183

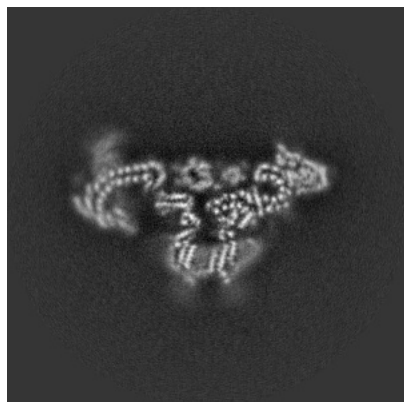


Y Index: 217

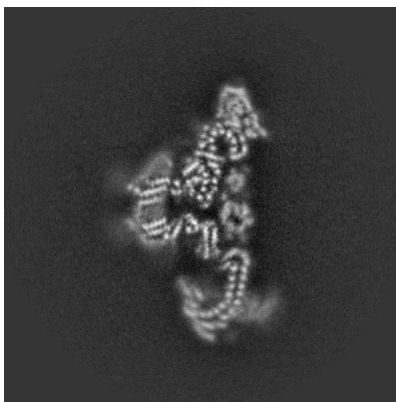


Z Index: 226

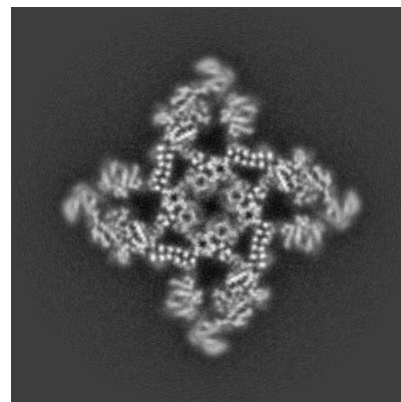
6.3.2 Raw map



X Index: 176



Y Index: 224

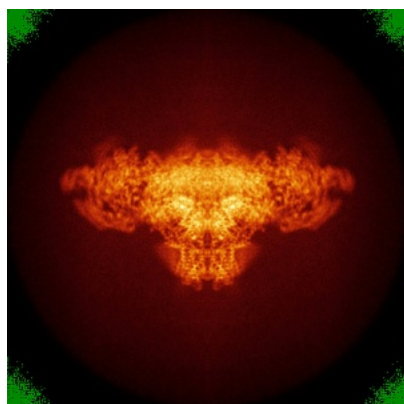


Z Index: 226

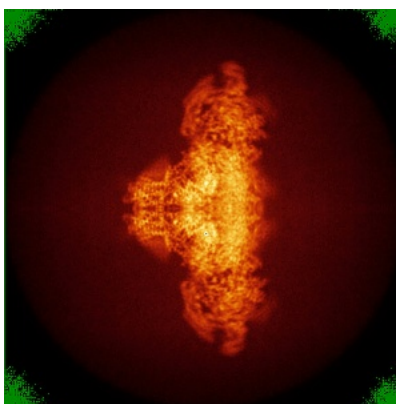
The images above show the largest variance slices of the map in three orthogonal directions.

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

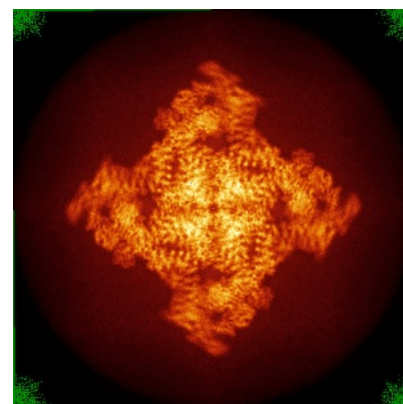
6.4.1 Primary map



X

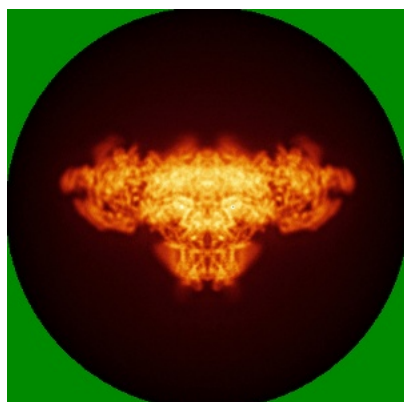


Y

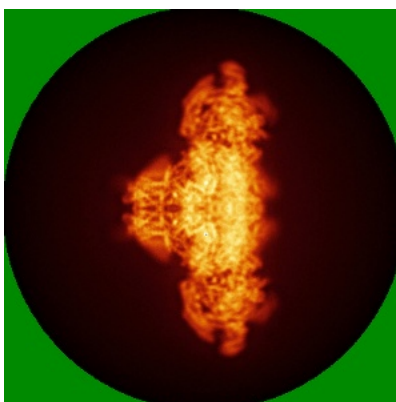


Z

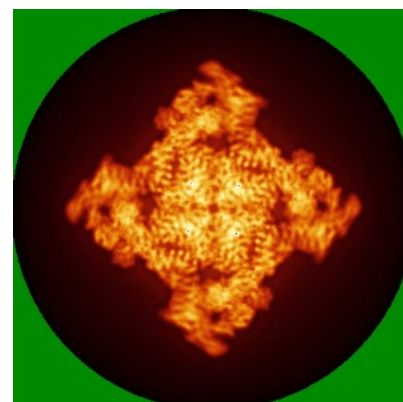
6.4.2 Raw map



X



Y

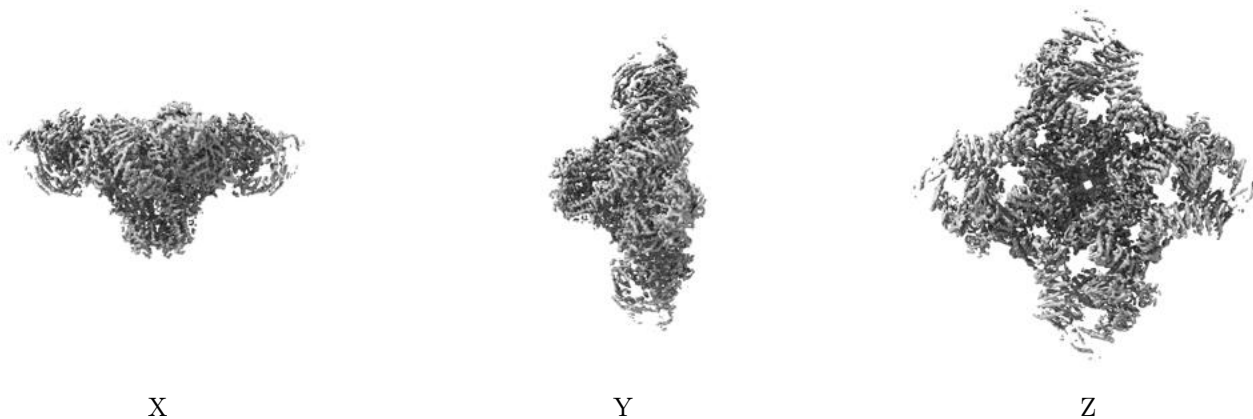


Z

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 0.025. 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.

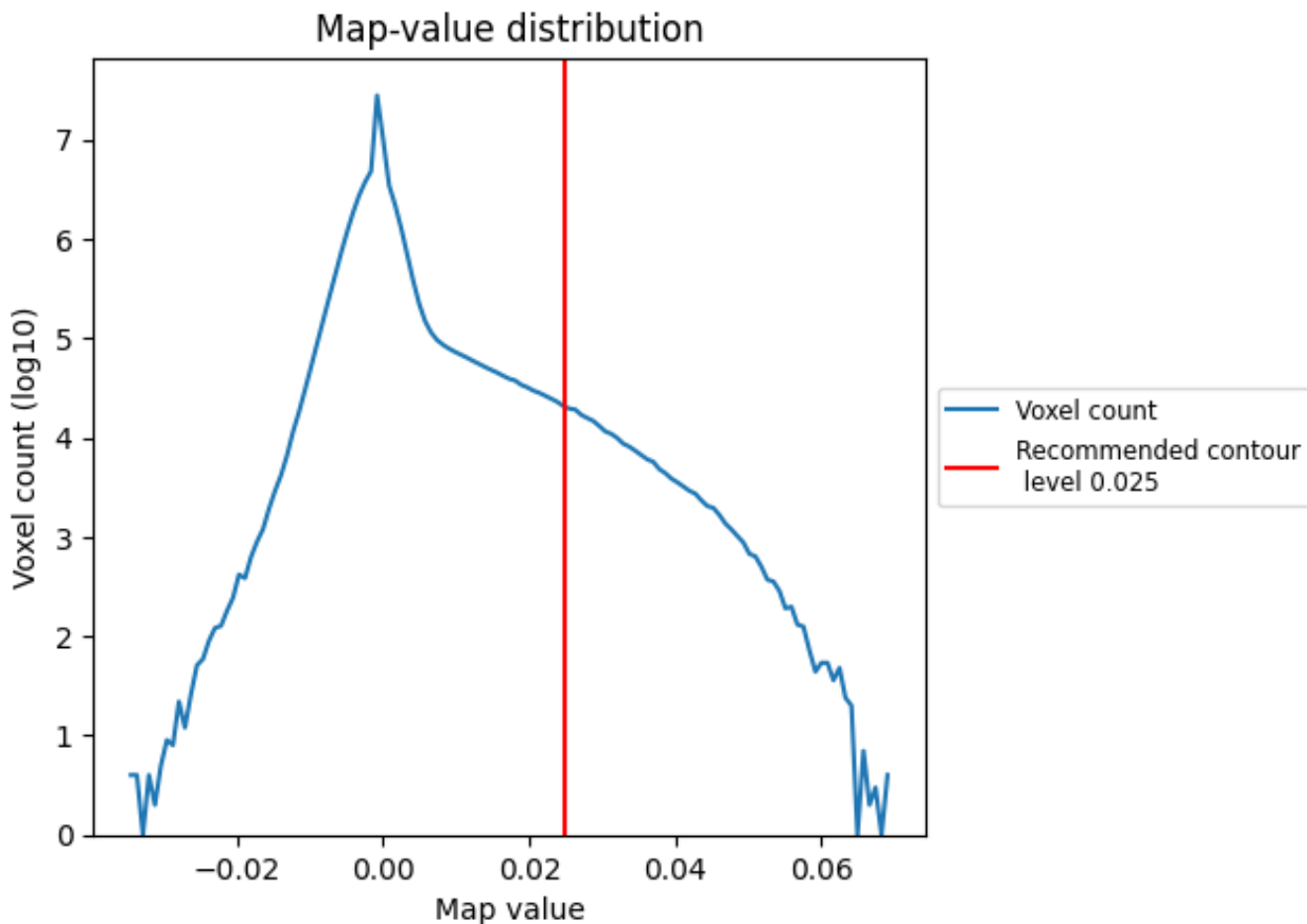
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

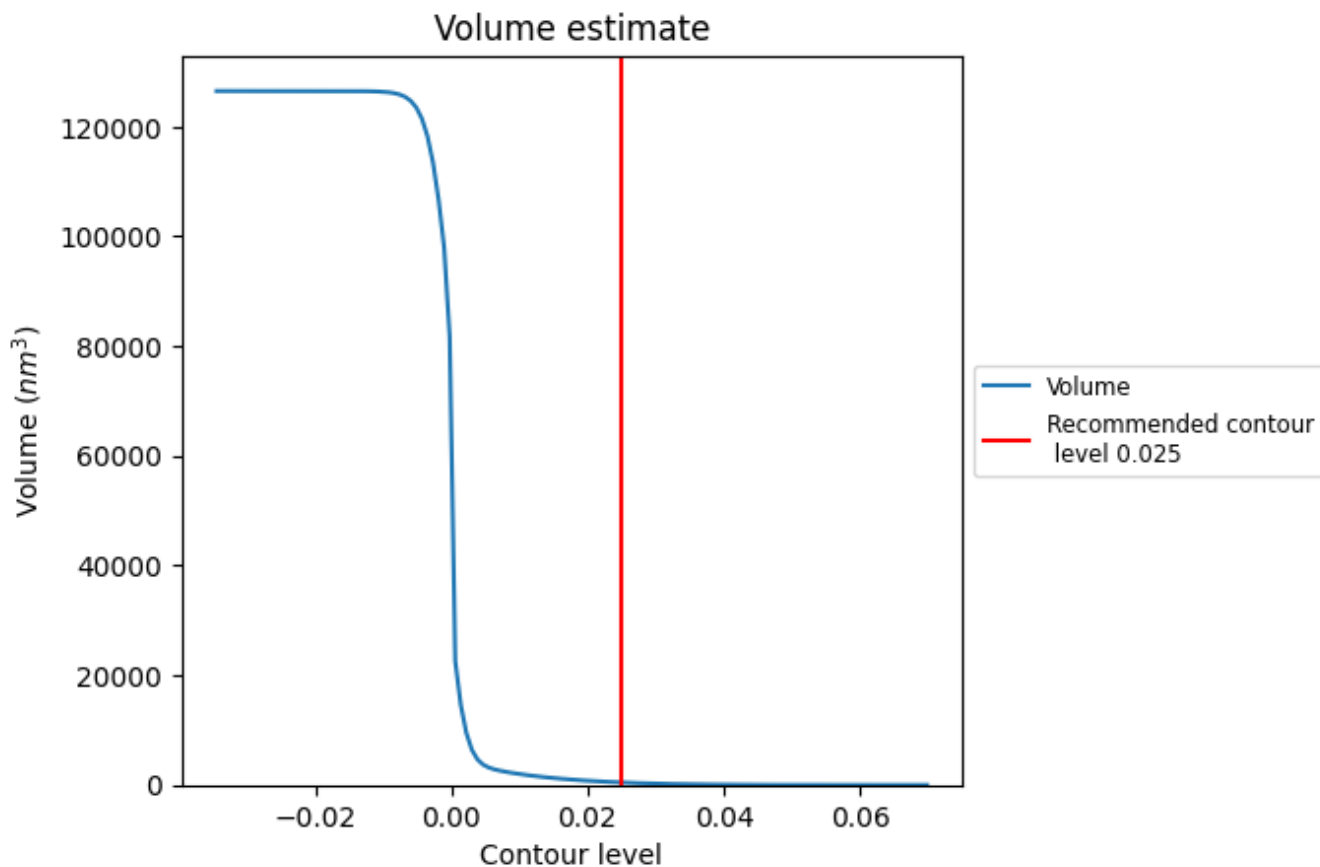
This section contains the results of statistical analysis of the map.

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.

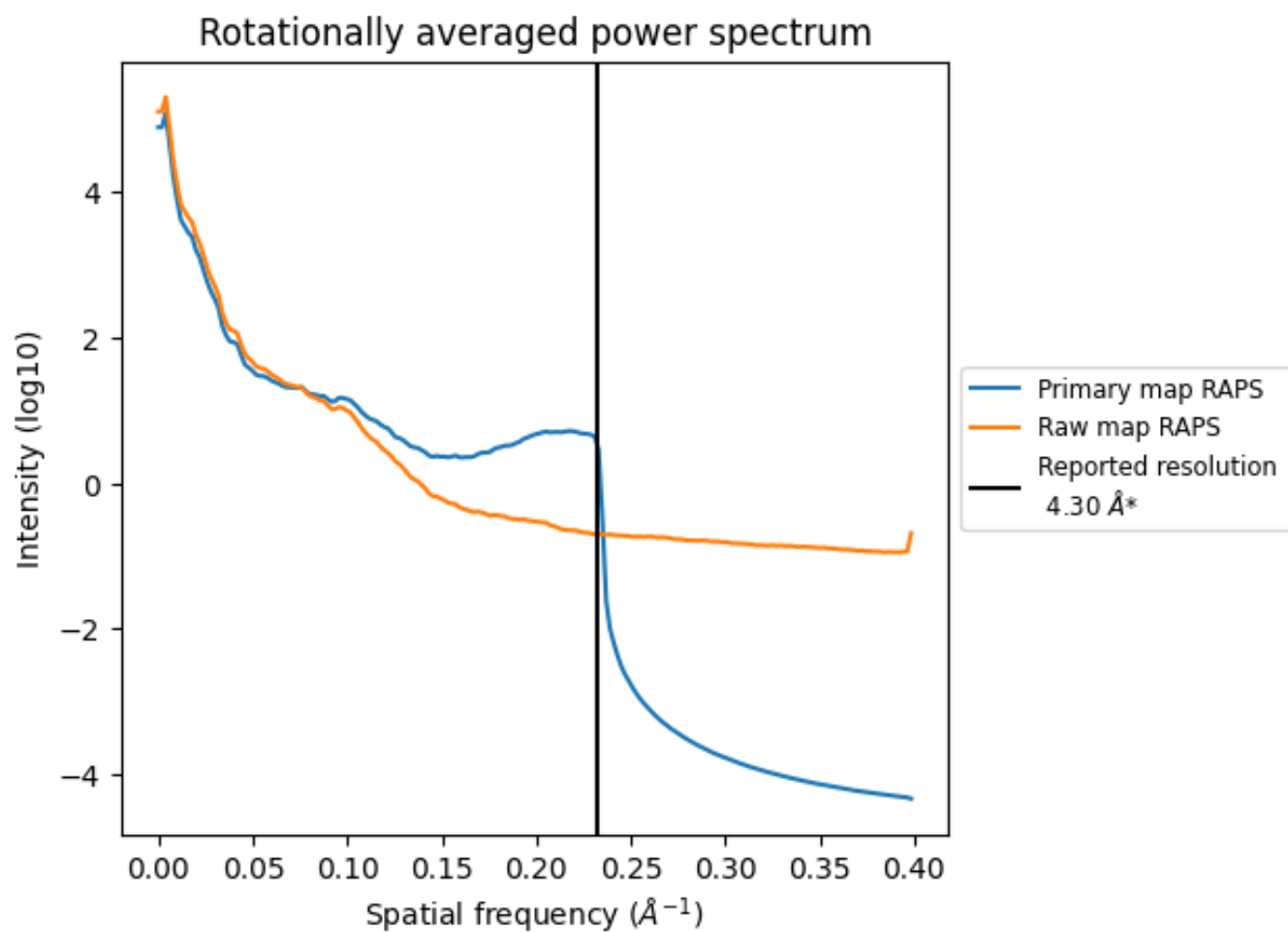
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 452 nm^3 ; this corresponds to an approximate mass of 408 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

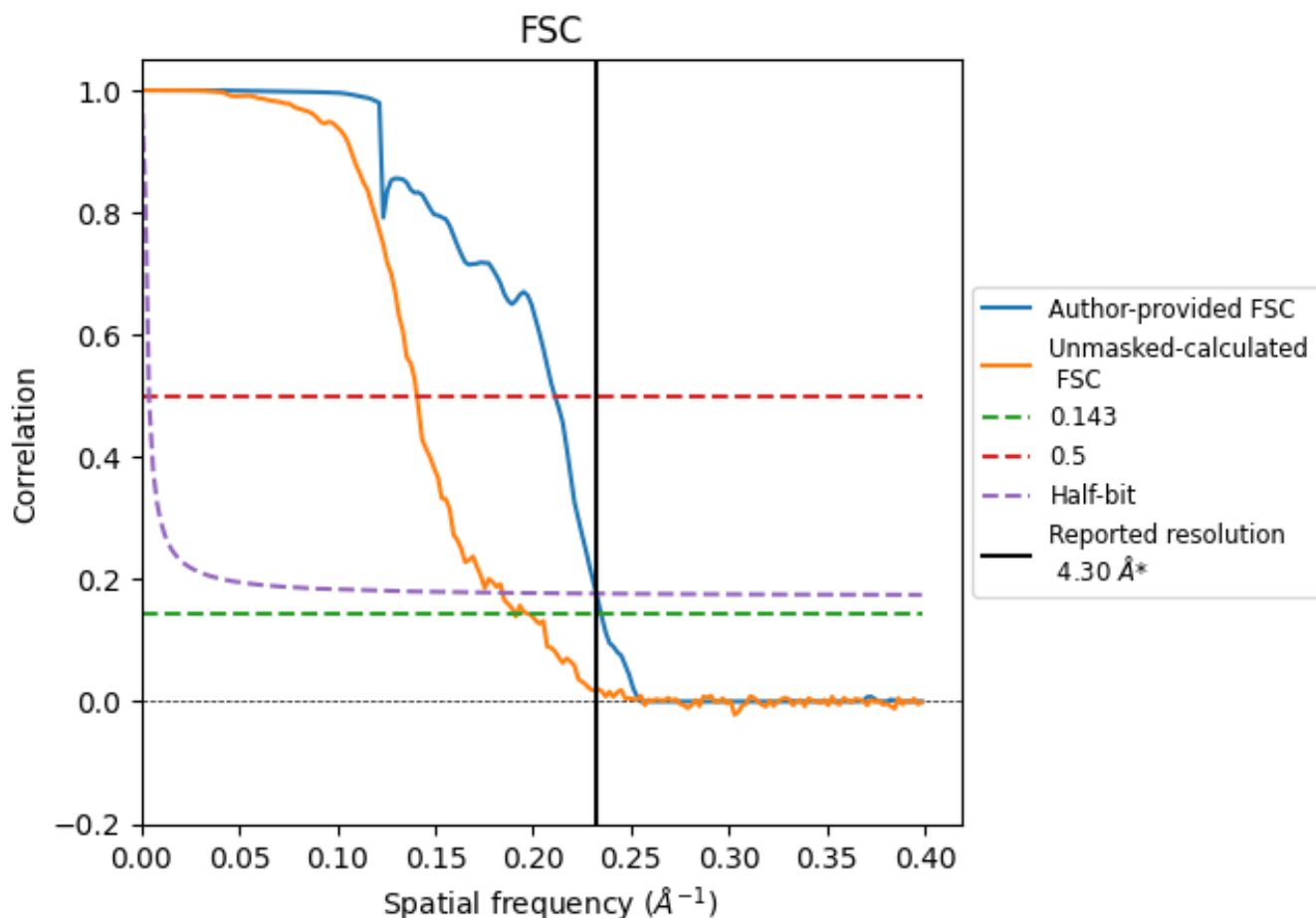


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

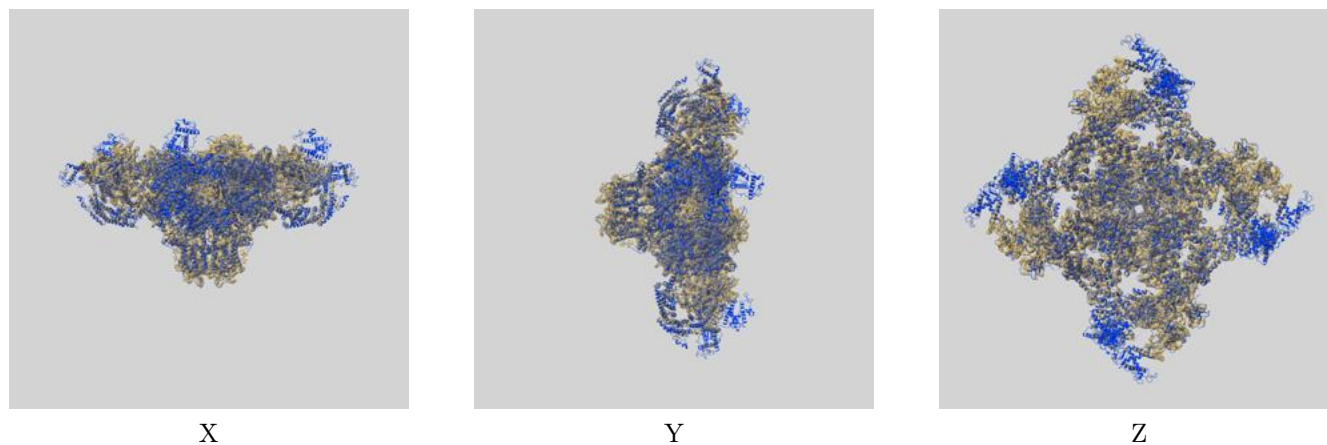
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	4.74	4.31
Unmasked-calculated*	5.24	7.11	5.43

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

9 Map-model fit [i](#)

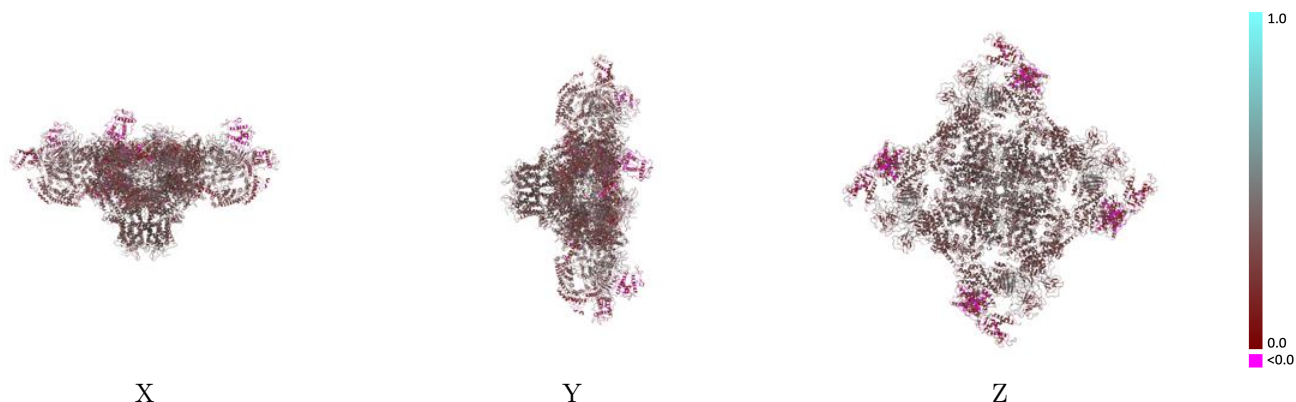
This section contains information regarding the fit between EMDB map EMD-8380 and PDB model 5TAN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



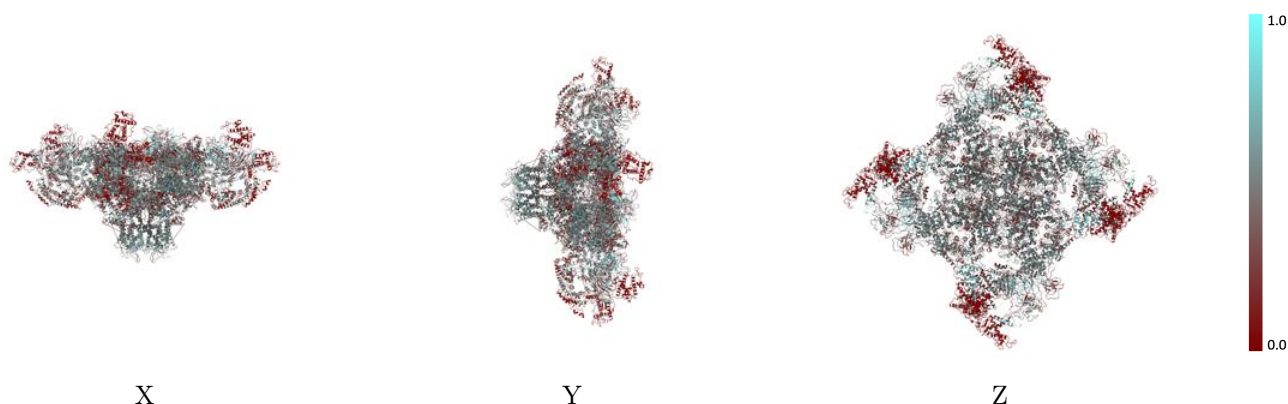
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



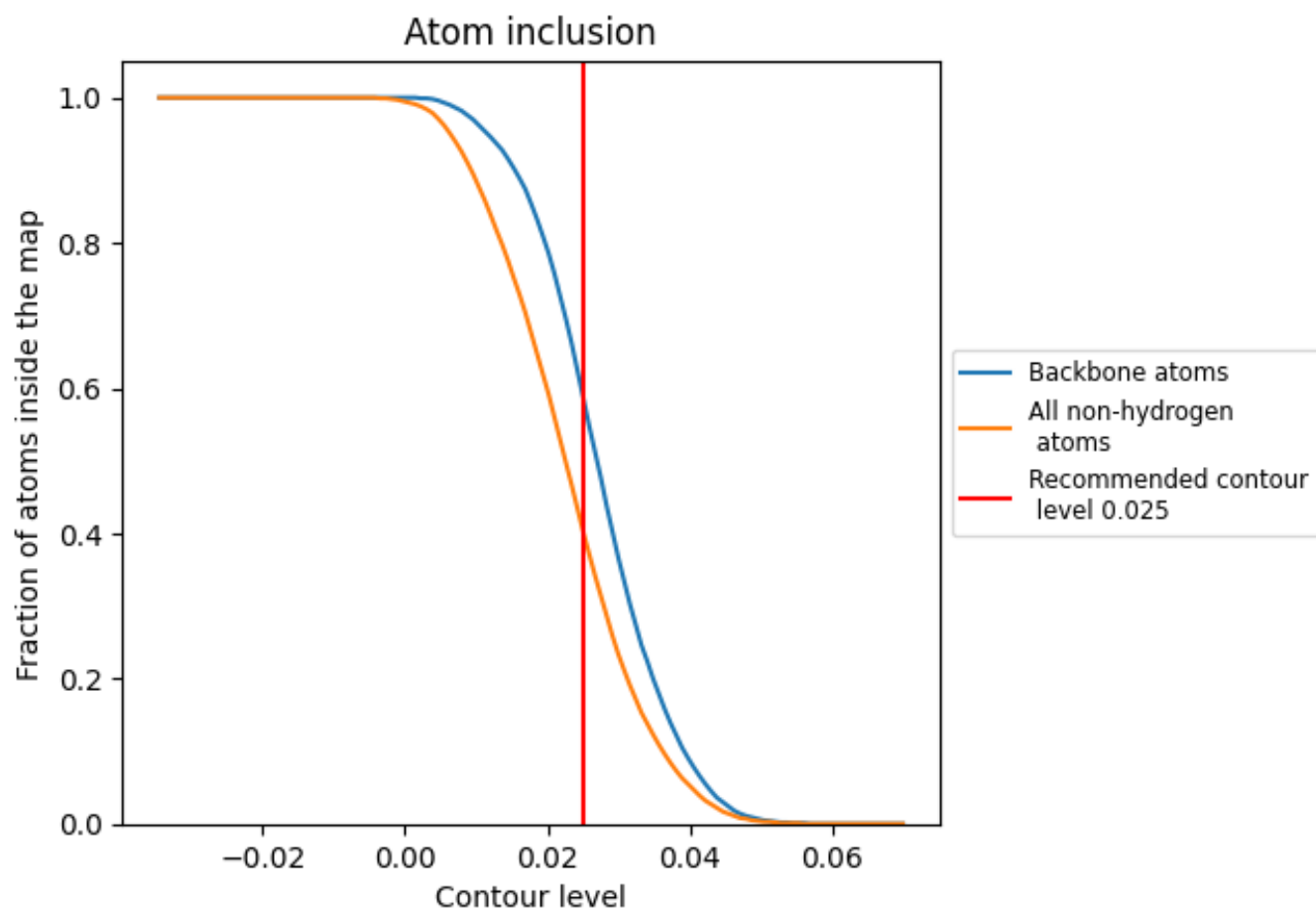
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

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

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

Chain	Atom inclusion	Q-score
All	0.4020	0.3150
A	0.3500	0.3180
B	0.4040	0.3140
E	0.4030	0.3140
F	0.3450	0.3230
G	0.4030	0.3140
H	0.3470	0.3230
I	0.4040	0.3140
J	0.3500	0.3190

