



# wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 04:27 AM EST

PDB ID : 9E1I  
EMDB ID : EMD-47395  
Title : Structure of RyR1 in the open state in the presence of oxopyricid  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2024-10-21  
Resolution : 3.20 Å (reported)  
Based on initial model : 7TZC

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  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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

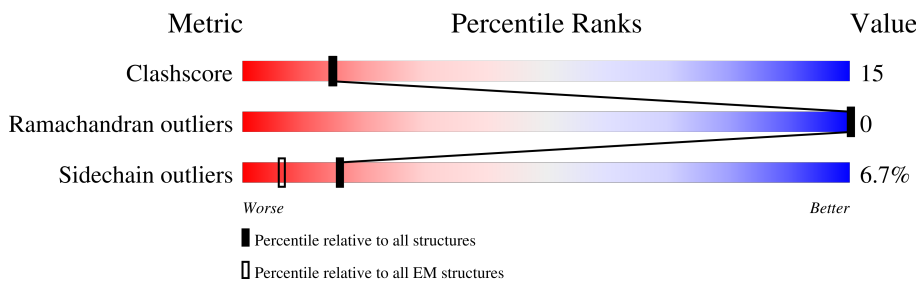
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	5037	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	108	
2	F	108	
2	G	108	
2	H	108	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144120 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	B	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	D	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
1	C	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	H	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	G	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	F	107	Total 831	C 527	N 146	O 154	S 4	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

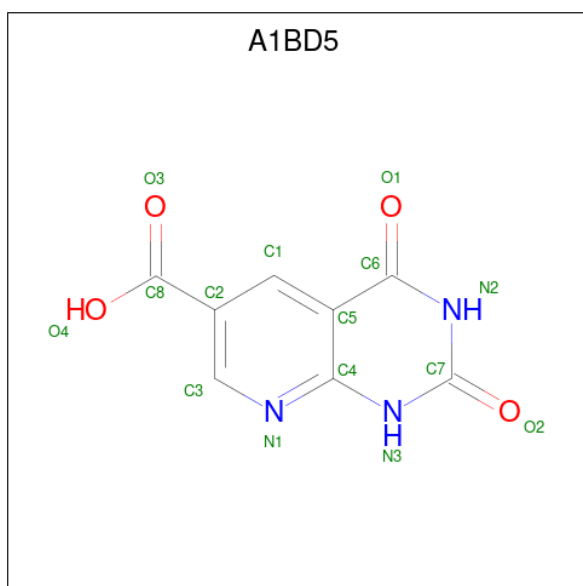
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is oxopyricid (three-letter code: A1BD5) (formula:  $C_8H_5N_3O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	3	4	
6	B	1	Total	C	N	O	0
			15	8	3	4	
6	D	1	Total	C	N	O	0
			15	8	3	4	
6	C	1	Total	C	N	O	0
			15	8	3	4	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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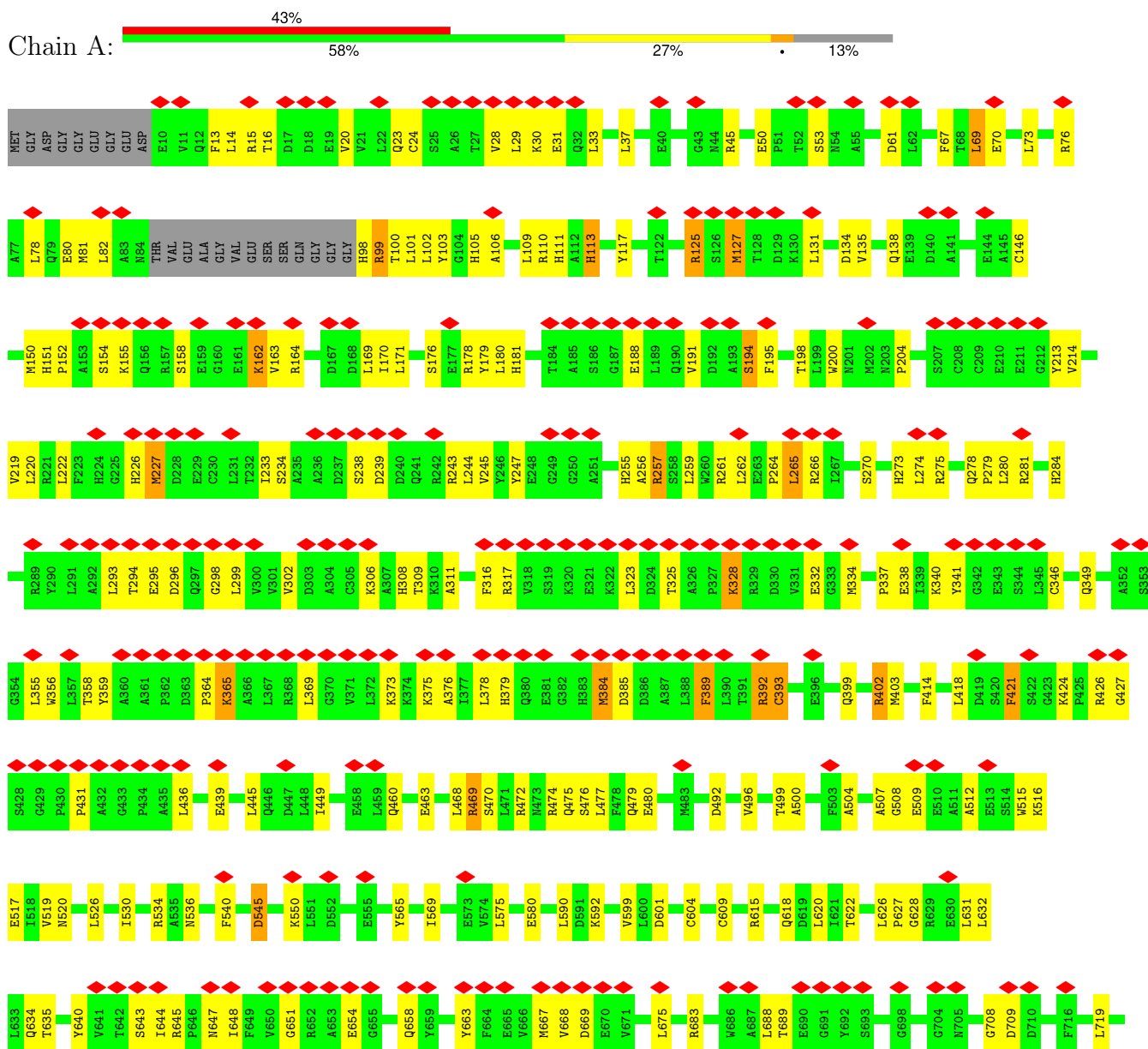
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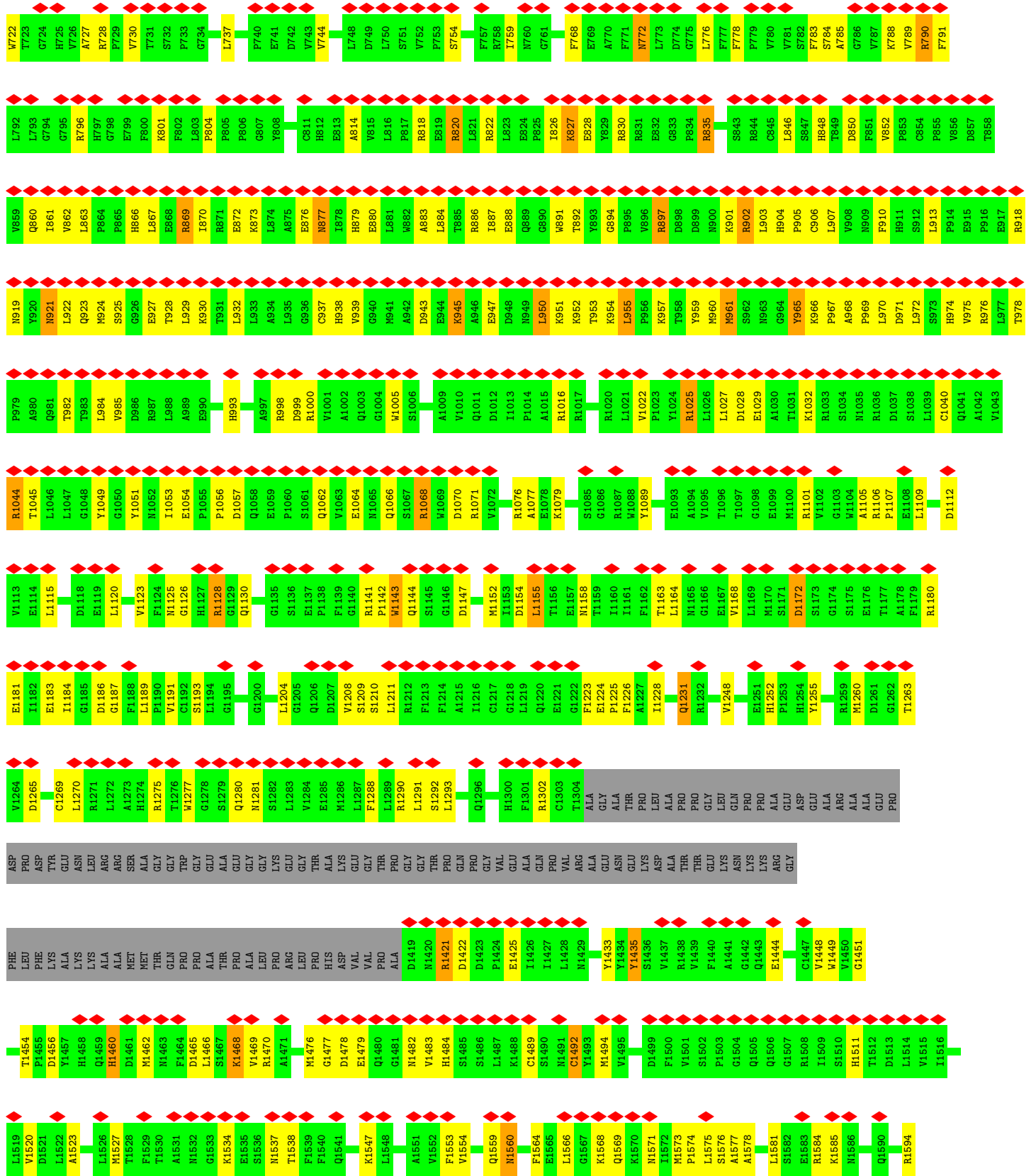
Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total O 1 1	0
7	C	1	Total O 1 1	0

### 3 Residue-property plots

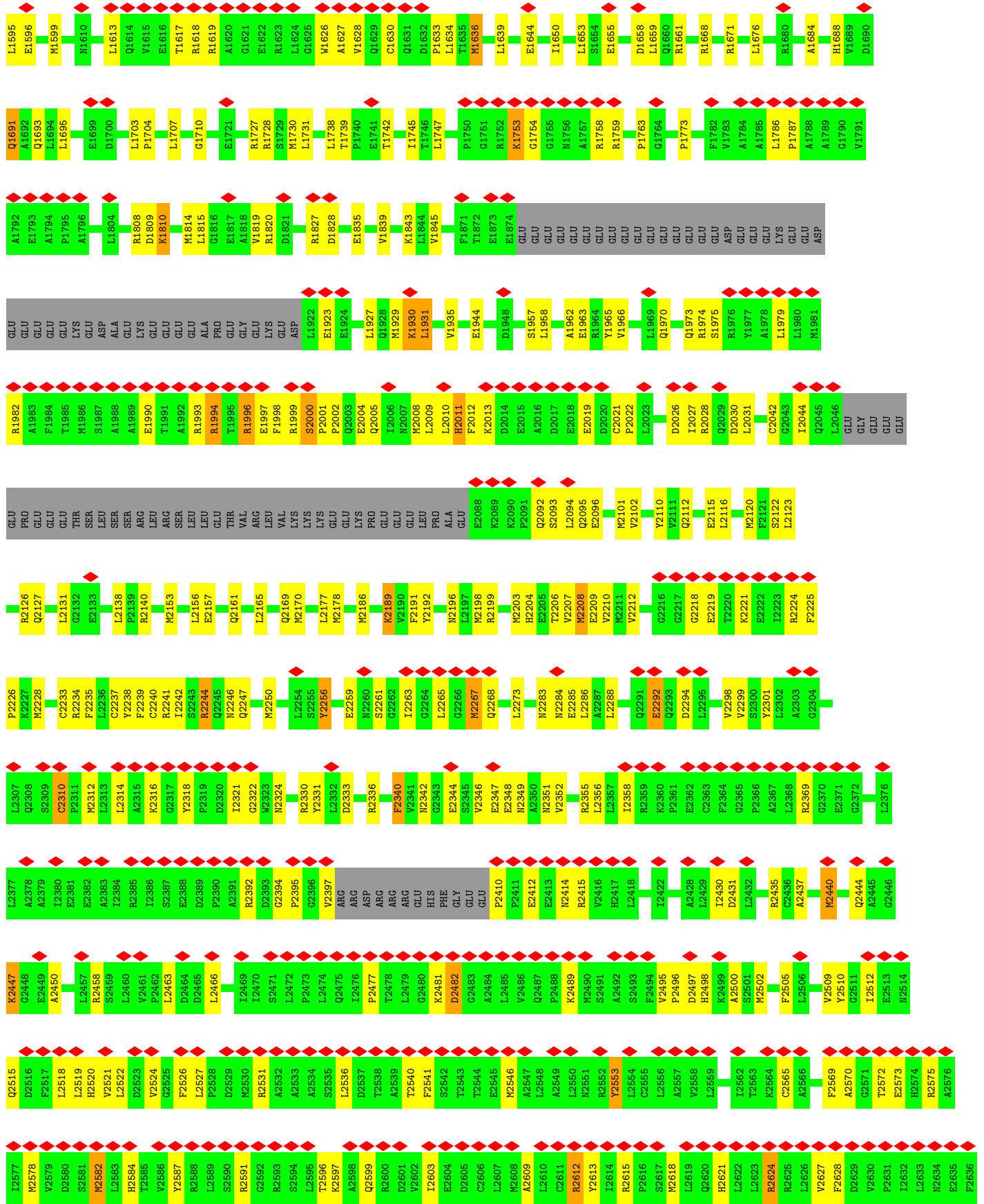
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Ryanodine receptor 1



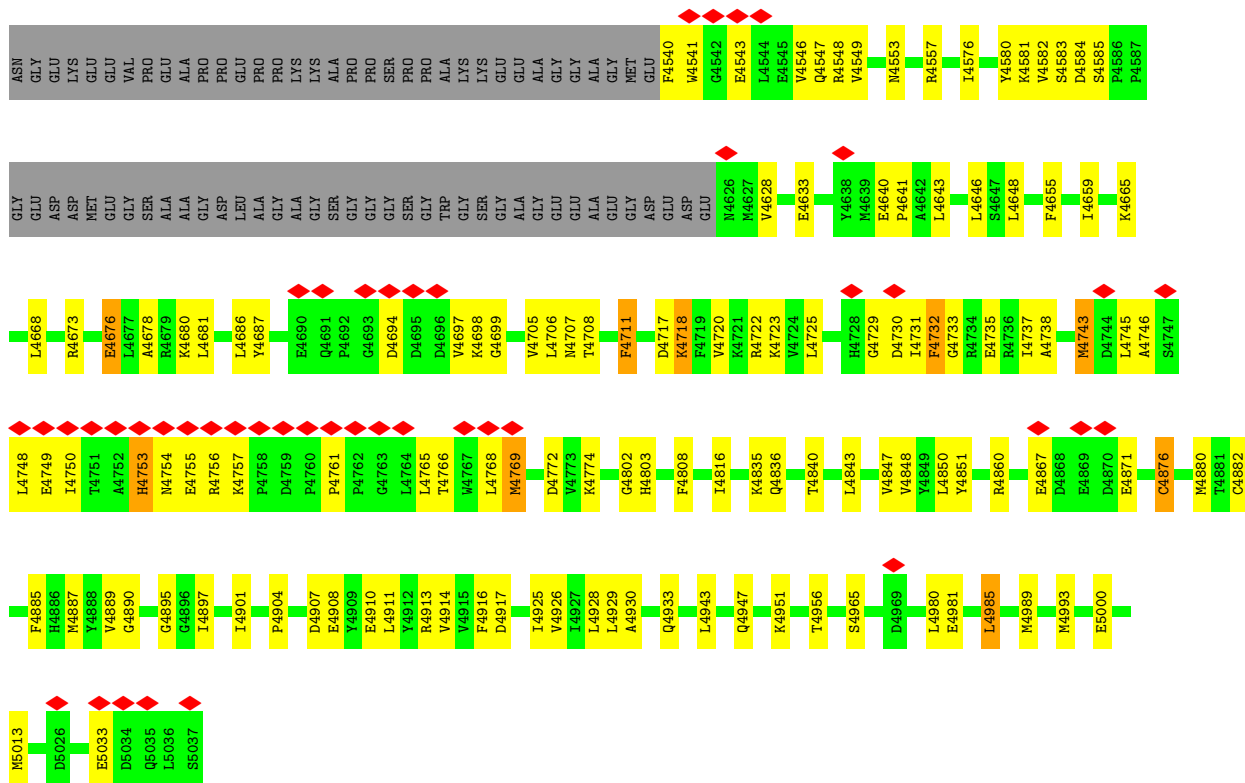




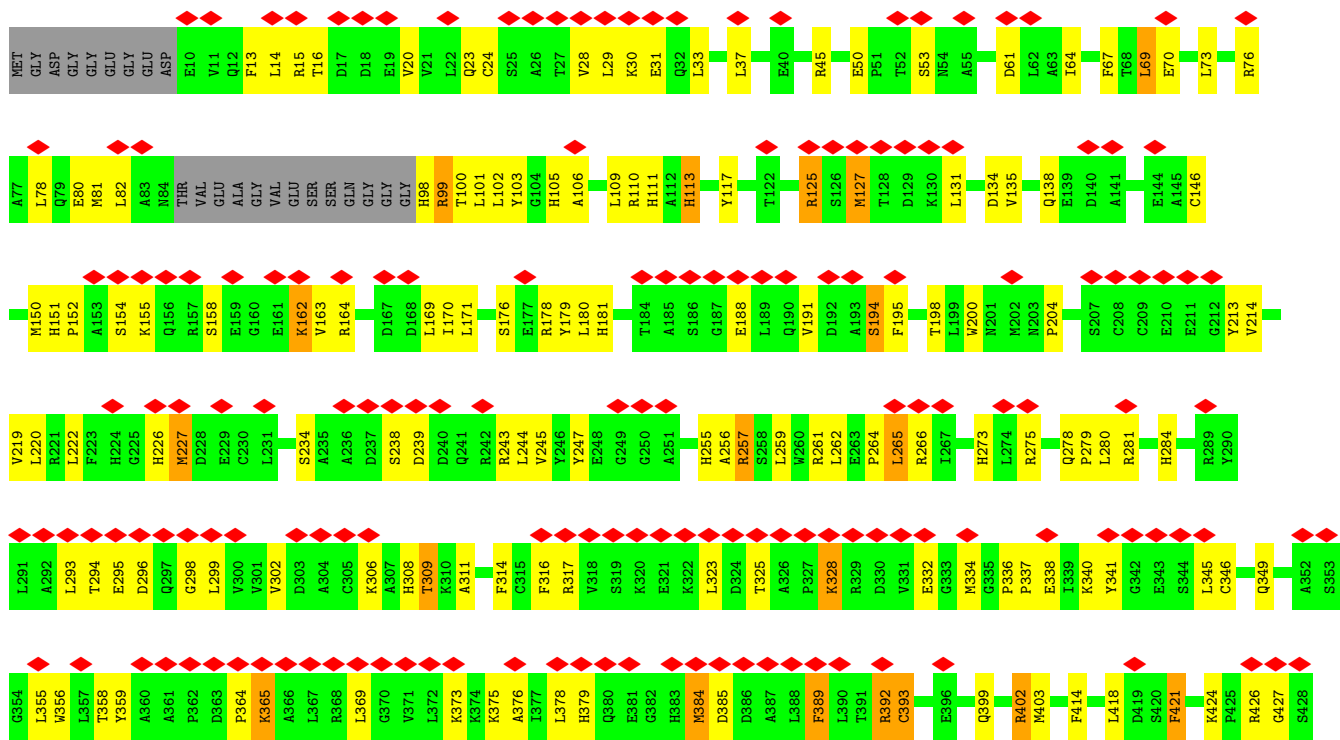


H3357	F3358	I3359	P3360	T3361	P3302	G3363	R3364	L3365	R3366	F3367	G3368	A3369	H3370	G3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	A3382	A3383	K3384	A3385	E3386	A3387	G3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3405	V3406	A3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416																											
P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316	G3317	G3318	R3317	P3318	A3319	M3320	P3321	V3323	A3324	N3325	N3326	L3327	G3328	I3329	E3330	E3331	A3332	T3333	V3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	L3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356																											
E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	A3251	D3252	I3253	G3254	G3255	L3256	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	N3266	P3267	H3268	V3269	I3270	F3271	I3272	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	R3290	A3291	P3292	P3293	P3294	A3295	L3296																												
F2997	F2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	Q2961	L2962	L2963	L2964	R2965	W2966	M2967	D2968	L2969	G3020	Q2971	E2972	L2973	L2974	A2975	H2976	L2977	E2978	M3038	V2980	V2981	S2982	S2983	G2984	R2985	E2986	L2987	L2988	L2989	K2990	H2991	E2992	Q2993	E2994	L2995	K2996																											
F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	P3085	F3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	R3105	M3106	V3107	E3108	M3109	L3110	R3111	L3112	G3113	V3115	S3116																												
T3177	T3178	F3179	M3180	T3181	Y3182	V3183	E3184	L3185	K3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	L3198	A3199	M3200	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	Q3211	F3212	G3213	D3214	D3215	V3216	L3217	D3218	D3219	D3220	V3221	K3222	S3223	P3224	R3225	E3226	R3227	L3228	A3229	P3230	P3231	P3232	P3233	N3234	S3235	V3236																												
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P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	V3307	T3308	S3309	D3310	H3311	L3312	N3313	S3314	L3315	L3316	G3317	G3318	R3317	P3318	A3319	M3320	P3321	V3323	A3324	N3325	N3326	L3327	G3328	I3329	E3330	E3331	A3332	T3333	V3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	L3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356																											
H2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	H2646	H2647	Y2648	E2649	K2650	C2651	K2652	L2653	Y2654	Y2655	C2656	L2657	P2658	T2659	G2660	W2661	A2662	N2663	F2664	Y2666	T2667	S2668	T2669	E2670	V2671	L2672	E2673	L2674	T2675	R2676	K2677	L2678	P2679	W2680	G2681	T2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696																												
R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	A2705	I2706	A2707	G2708	A2709	L2710	P2711	P2712	D2713	Y2714	V2715	D2716	A2717	P2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	ALA	THR	VAL	ASP	PRO	ARG	GLY	Y2885	N2886	P2887	Q2888	P2889	P2890	D2891	L2892	S2893	G2894	S2895	L2896	R2897	L2898	L2899	L2900	A2901	L2902	P2903	L2904	L2905	P2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	E2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936
K2757	F2758	A2759	E2760	Y2761	T2762	K2763	E2764	K2765	W2766	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	Q2778	E2779	N2780	Y2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	Y2793	Y2794	K2795	T2796	R2797	S2798	E2799	K2800	D2801	L2743	E2803	L2804	Y2805	L2746	R2806	P2748	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816																										
I2817	A2818	W2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	ALA	ALA	THR	ASP	PRO	ARG	GLU	GLY	Y2885	N2886	P2887	Q2888	P2889	P2890	D2891	L2892	S2893	G2894	S2895	L2896	R2897	L2898	L2899	L2900	A2901	L2902	P2903	L2904	L2905	P2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	E2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	
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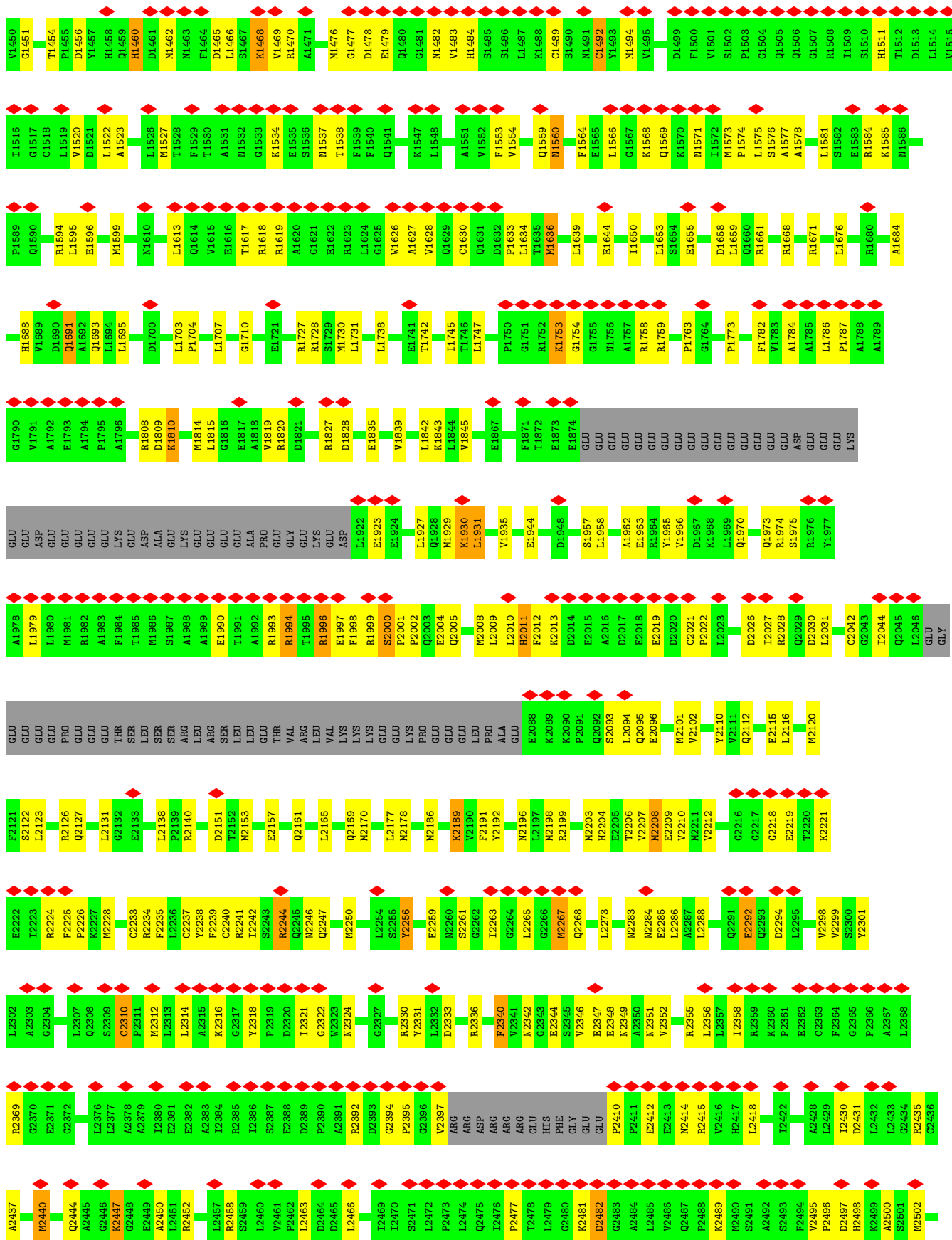
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ARG	GLU	SER	GLU	GLY	MET	GLY	E4152	V4072	L3980	E3861	K3758	D3675	E3598	T3538	M3478	N3418
ALA	ALA	ALA	ASP	GLU	GLY	GLY	H4153	G4073	A3981	D3862	E3769	D3676	E3589	R3539	A3479	N3419
VAL	THR	ALA	VAL	VAL	ALA	ALA	H4156	S4074	R3984	G3863	Q3761	K3679	S3600	Y3540	LYS	R3420
LEU	LEU	LEU	HIS	LEU	ALA	ALA	E4075	A4076	W3986	T3864	R3762	A3880	A3601	A3421	ALA	A3421
ALA	ALA	ALA	GLY	ALA	GLY	GLY	D4157	F4077	D3987	V3865	Q3766	G3681	V3602	H3422	GLY	H3422
ASP	LEU	LEU	ASP	LEU	GLY	GLY	F4078	Q4078	D3987	N3867	R3769	E3682	Y3604	H3423	ASP	H3423
LEU	LEU	LEU	LEU	TRP	GLY	GLY	D4079	D4079	V3995	R3868	L3770	Q3683	Y3604	L3424	GLN	L3424
LEU	LEU	LEU	TRP	ALA	GLY	GLY	M4082	T4082	F3996	Q3869	H3771	E3684	L3606	T3425	SER	T3425
VAL	VAL	VAL	VAL	VAL	ALA	ALA	D4083	P4083	M3999	N3870	L3772	E3686	L3607	F3427	SER	F3427
VAL	VAL	VAL	VAL	VAL	ALA	ALA	R4084	R4084	K4002	G3871	R3773	E3687	Q3608	R3428	ASP	R3428
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	K4090	K4090	K3873	K3873	G3788	E3689	R3549	R3432	GLU	R3432
ALA	ALA	ALA	ALA	ALA	ALA	ALA	D4006	D4006	V3874	V3874	Q3788	E3690	E3610	R3431	ARG	R3431
ALA	ALA	ALA	ALA	ALA	ALA	ALA	S4007	S4007	M3875	M3875	G3791	V3690	H3611	A3431	THR	A3431
ALA	ALA	ALA	ALA	ALA	ALA	ALA	A4186	A4186	A3876	A3876	Q3791	E3691	F3612	E3432	LYS	E3432
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	F4093	F4093	R3878	R3878	K3793	E3693	K3614	L3434	LYS	L3434
ALA	ALA	ALA	ALA	ALA	ALA	ALA	Q4094	Q4094	E4011	E4011	V3794	K3693	S3615	F3435	LYS	F3435
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4012	L4012	F3880	F3880	L3798	D3696	K3616	R3436	LYS	R3436
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4013	L4013	D3883	D3883	L3802	R3707	A3618	R3437	LYS	R3437
ALA	ALA	ALA	ALA	ALA	ALA	ALA	K4014	K4014	L3884	L3884	L3802	R3707	V3619	R3438	LYS	R3438
ALA	ALA	ALA	ALA	ALA	ALA	ALA	E4015	E4015	L3884	L3884	L3802	R3707	V3619	G3439	LYS	G3439
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4016	L4016	L3890	L3890	L3805	T3711	V3620	E3440	LYS	E3440
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4017	L4017	L3890	L3890	V3812	T3711	H3621	I3441	LYS	I3441
ALA	ALA	ALA	ALA	ALA	ALA	ALA	Q4100	Q4100	N3896	N3896	V3812	T3711	K3622	F3442	LYS	F3442
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4019	L4019	F3899	F3899	K3816	K3715	L3623	I3443	LYS	I3443
ALA	ALA	ALA	ALA	ALA	ALA	ALA	Q4020	Q4020	S3931	S3931	L3716	K3715	L3624	Y3444	LYS	Y3444
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4030	L4030	D3932	D3932	L3716	K3715	L3624	N3445	LYS	N3445
ALA	ALA	ALA	ALA	ALA	ALA	ALA	M4039	M4039	F3933	F3933	D3717	D3717	S3625	S3446	LYS	S3446
ALA	ALA	ALA	ALA	ALA	ALA	ALA	L4040	L4040	F3936	F3936	E3825	Y3720	K3626	R3447	LYS	R3447
ALA	ALA	ALA	ALA	ALA	ALA	ALA	A4041	A4041	W3935	W3935	A3834	Y3720	Q3627	S3448	LYS	S3448
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• Molecule 1: Ryanodine receptor 1



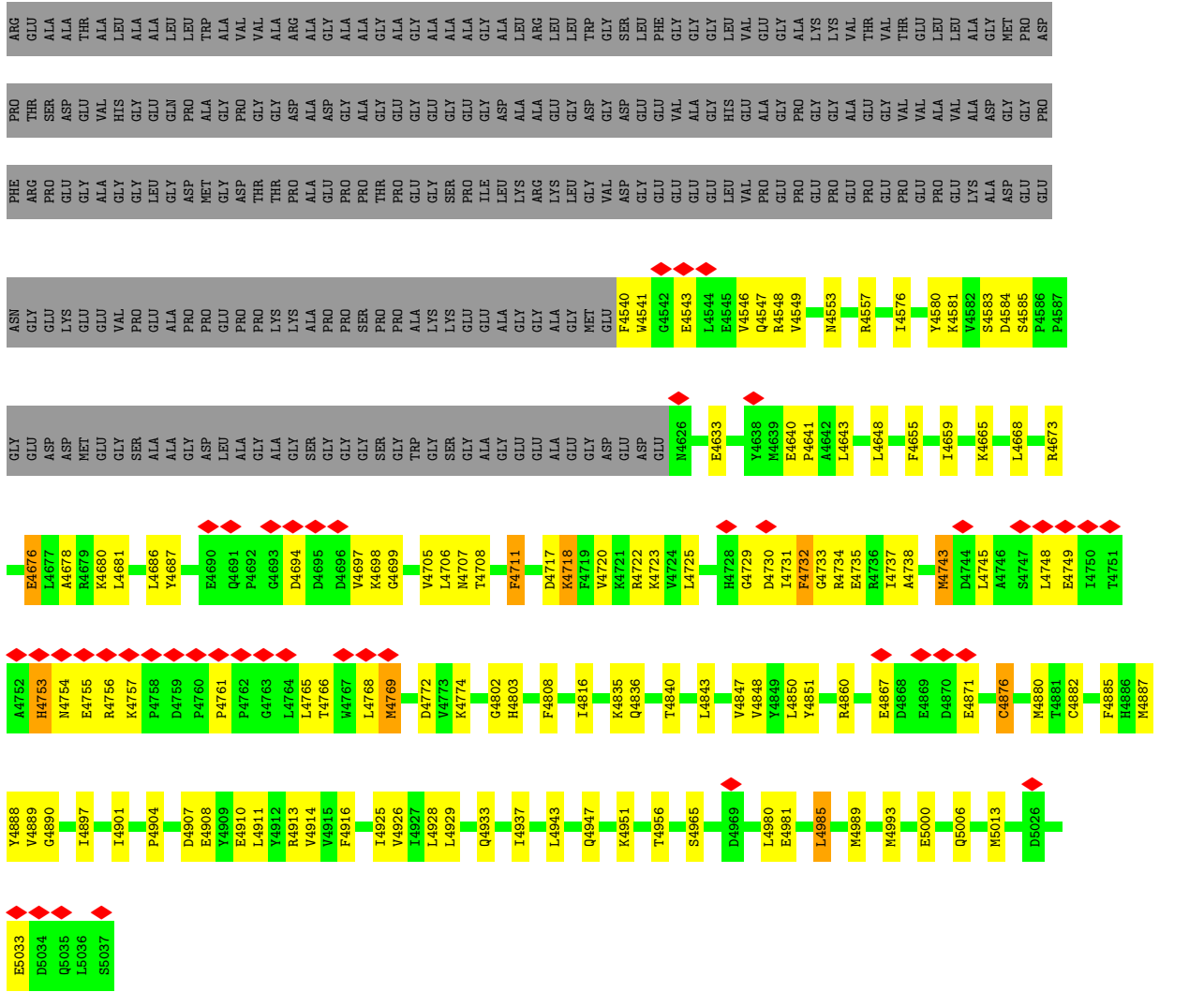




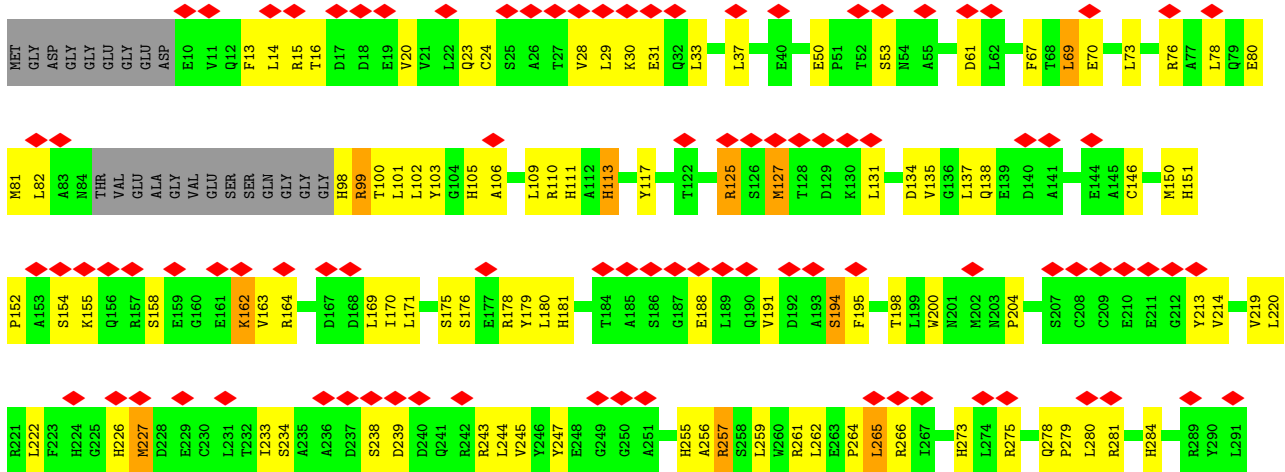
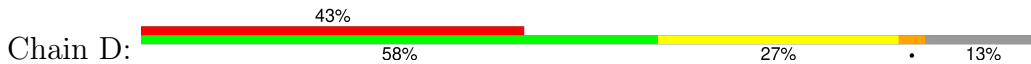
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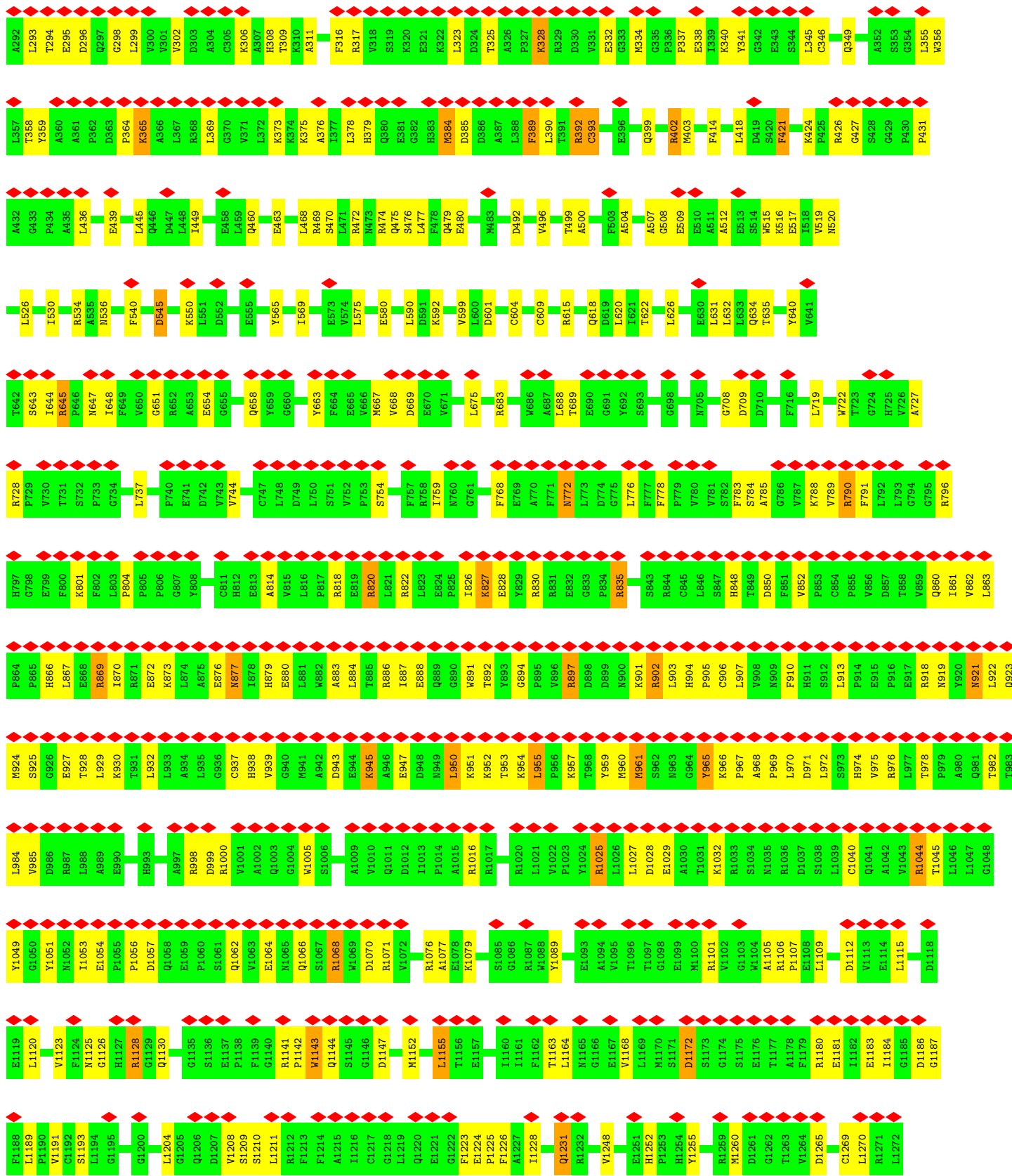
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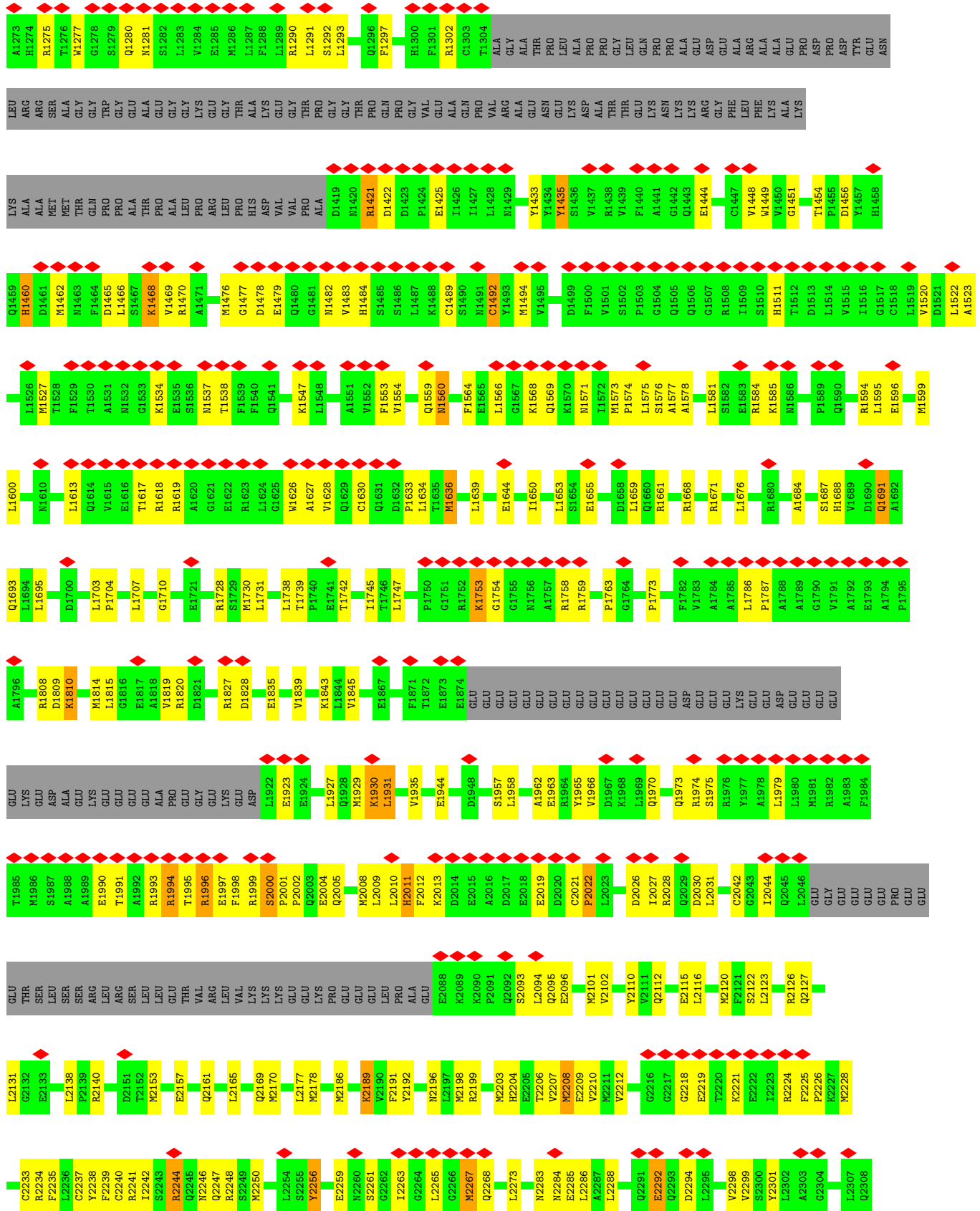




- Molecule 1: Ryanodine receptor 1

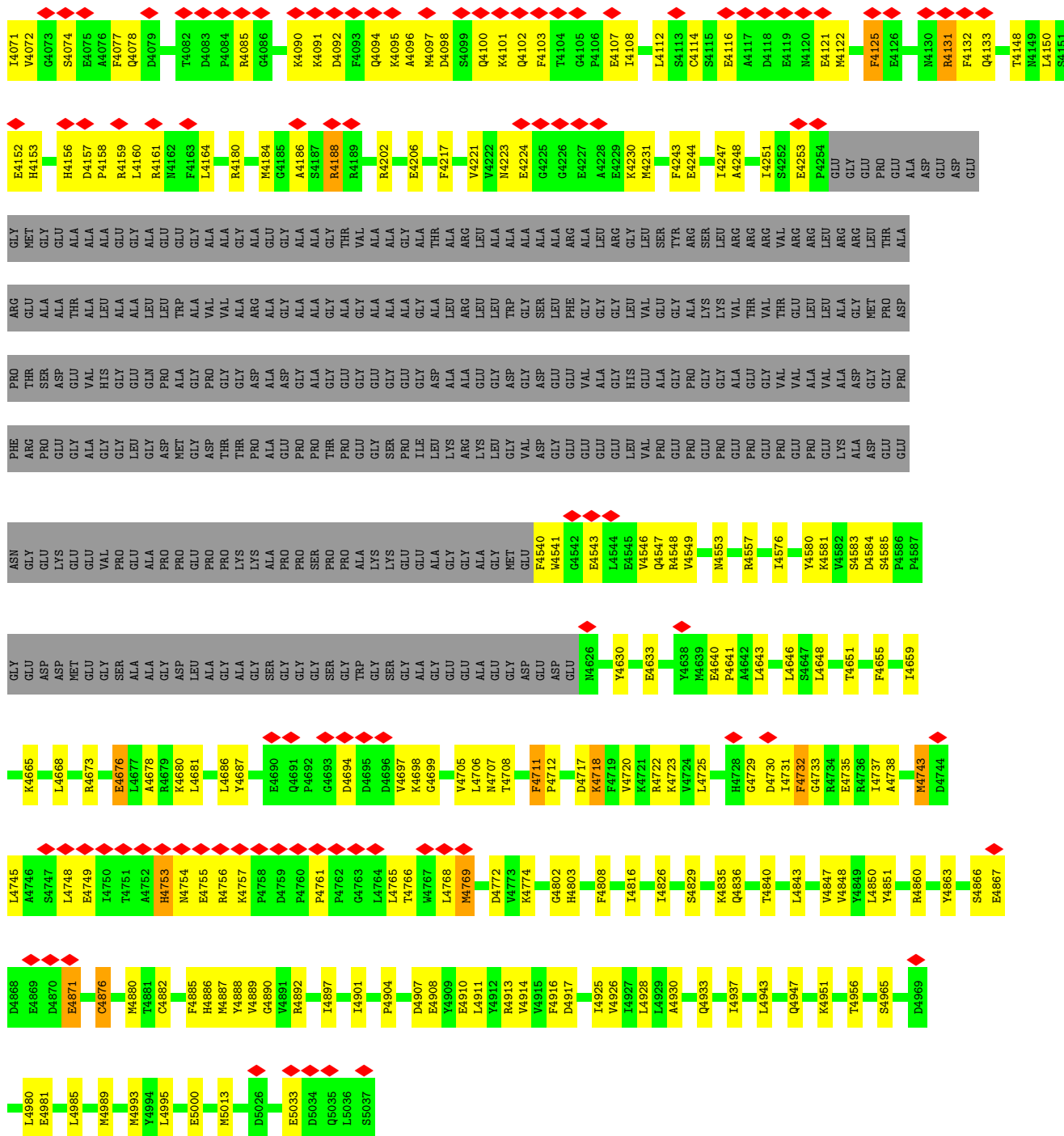




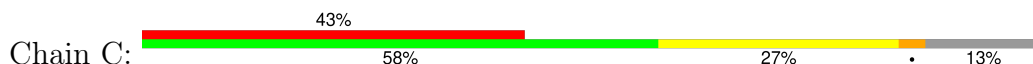


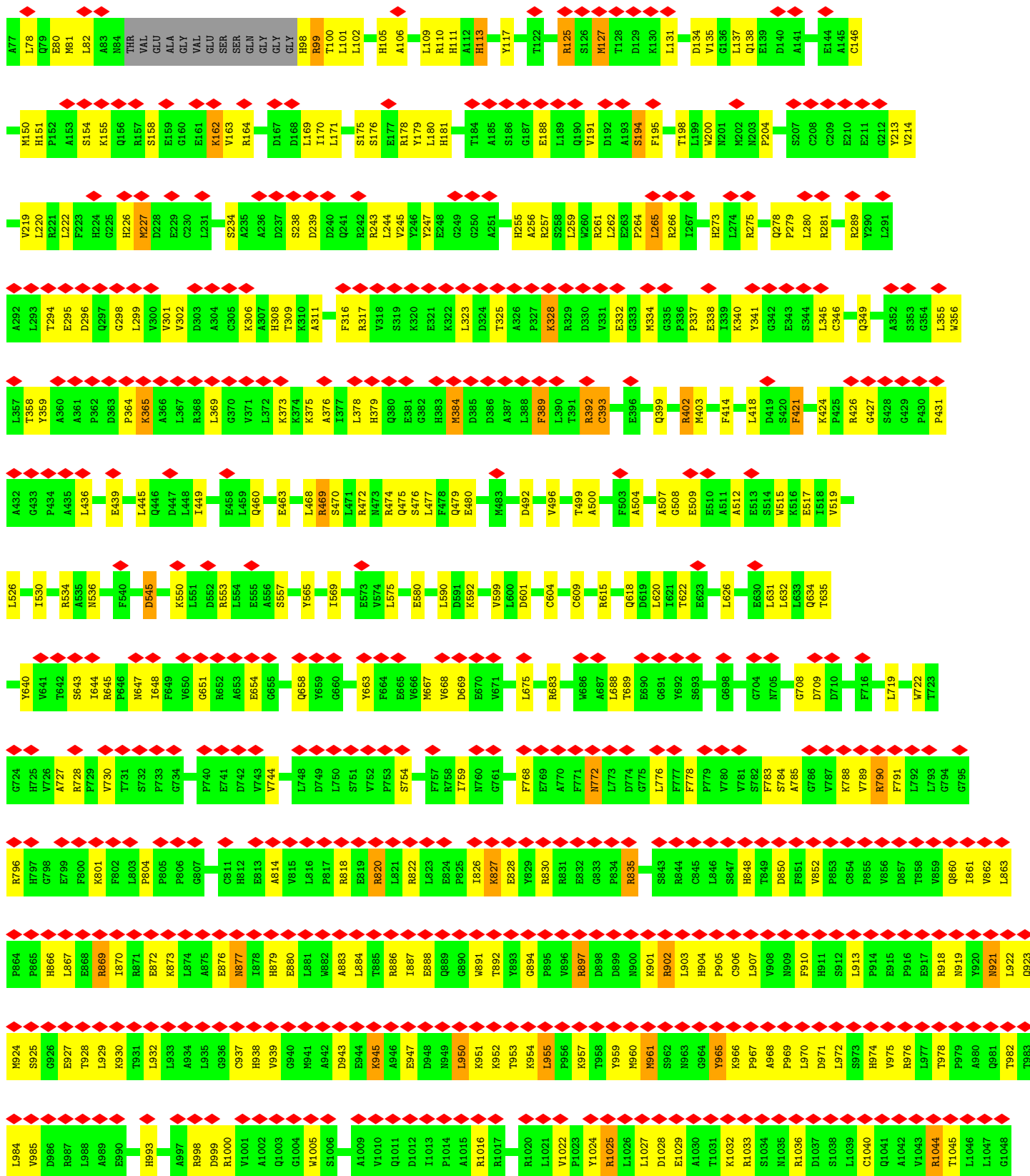
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• Molecule 1: Ryanodine receptor 1



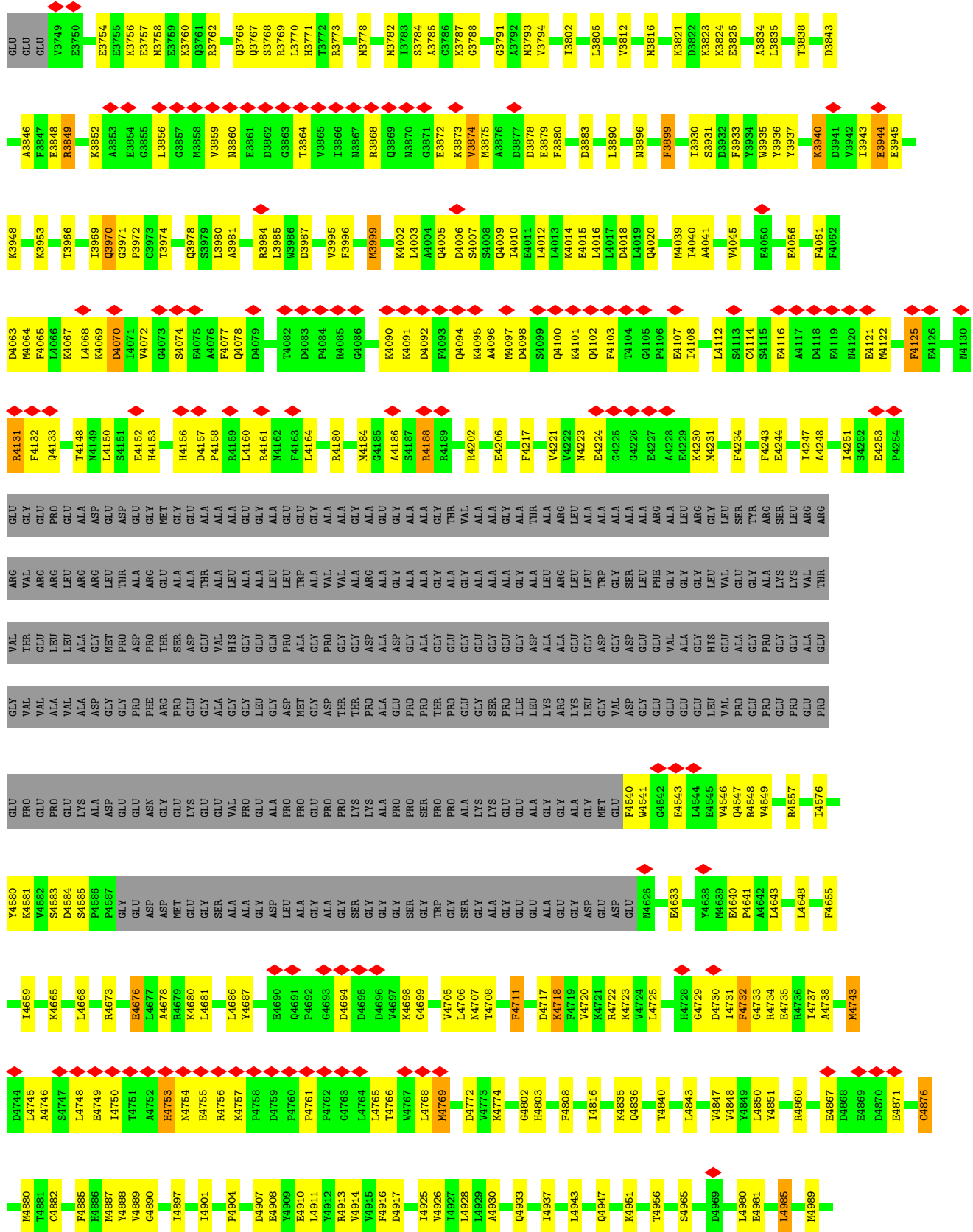


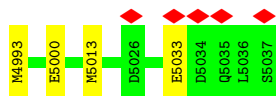




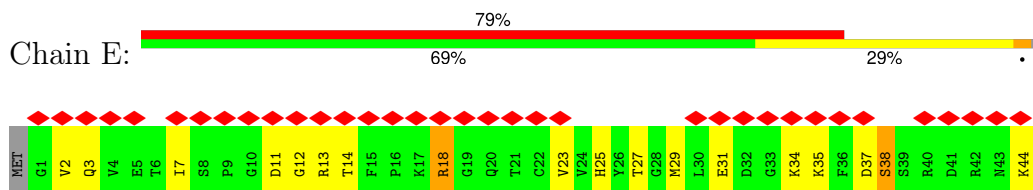
THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	LEU	LEU	THR	GLU	VAL	ARG	LEU	VAL	LYS	LYS	LYS	GLU	GLU	LYS	GLU	GLU	PRO	PRO	ALA	ALA	GLU	E2088	K2089	K2090	F2091	F2092	S2093	L2094	O2095	E2096	M2101	V2102	Y2110	Y2111	Q2112	E2115	L2116	M2120	F2121	S2122	L2123	R2126	Q2127	L2131	G2132	E2133	L2138	P2139	R2140	D2151	T2152	M2153	E2157	Q2161	L2165	L2169	R2241	S2242	R2243	R2244	Q2245	N2246	O2247	R2248	S2249	M2250	L2254	M2176	M2186	K2189	F2190	F2191	Y2192	N2196	L2197	M2198	R2199	M2203	H2204	E2205	T2206	V2207	M2208	E2209	V2210	M2211	V2212	G2216	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	K2227	M2228	V2229	T2230	C2233	R2234	F2235	L2236	C2237	F2238	C2240	R2241	S2242	R2243	R2244	Q2245	N2246	O2247	R2248	S2249	M2250	L2254	M2176	M2186	K2189	F2190	F2191	Y2192	N2196	L2197	M2198	R2199	M2203	H2204	E2205	T2206	V2207	M2208	E2209	V2210	M2211	V2212	G2216	G2217	G2218	E2219	T2220	K2221	E2222	L2223	R2224	F2225	P2226	K2227	M2228	V2229	Q2308	S2309	C2310	A2311	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	L2321	G2322	V2323	N2324	G2327	R2330	Y2331	D2332	L2333	R2336	F2340	V2341	N2342	G2343	E2344	S2345	V2346	E2347	E2348	N2349	A2350	N2351	V2352	R2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	D2366	P2366	A2367	L2368	R2369	G2370	E2371	G2372	L2376	L2377	A2378	A2379	I2380	E2381	E2382	A2383	L2384	R2385	L2386	S2387	E2388	D2389	P2390	G2392	A2391	R2392	D2393	G2394	P2395	G2396	V2397	ARG	ARG	ASP	ARG	ARG	ARG	GLU	GLU	HIS	PHE	GLY	GLU	GLU	P2410	P2411	E2412	E2413	N2414	R2415	V2416	H2417	L2418	L2422	A2428	L2429	L2430	D2431	L2432	L2433	G2434	R2435	C2436	A2437	M2440	Q2444	K2445	G2446	K2447	G2448	E2449	A2450	L2451	R2452	L2457	L2459	H2459	R2459	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	I2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2484	V2486	Q2487	P2488	K2489	N2490	S2491	A2492	S2493	F2494	V2495	F2496	D2497	H2498	K2499	A2500	S2501	H2502	F2505	L2506	V2509	Y2510	G2511	I2512	E2513	N2514	Q2515	D2516	P2517	L2518	L2519	H2520	V2521	L2522	D2523	V2524	G2525	F2526	L2527	F2528	R2588	L2589	S2590	R2591	G2592	R2593	S2594	L2595	K2596	K2597	A2598	Q2599	R2600	D2601	V2602	L2603	E2604	D2605	C2606	L2607	H2608	A2609	L2610	C2611	R2612	Y2613	L2614	R2615	P2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	L2627	F2628	D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	N2646	H2647	V2648	E2649	R2650	C2651	V2652	K2653	Y2654	V2655	C2656	L2657	P2658	T2659	G2660	M2661	A2662	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	V2679	H2680	G2681	L2682	L2683	R2684	F2685	L2686	A2687	H2688	K2689	Y2691	D2692	Q2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	A2705	L2706	A2707	G2708	A2709	L2710	P2711	D2712	D2713	K2714	Y2714	V2715	D2716	L2717	L2718	S2719	Y2719	S2720	S2721	K2722	A2723	E2724	E2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	M2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	M2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	M2774	V2775	S2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	H2807	P2808	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	V2818	V2819	E2820	T2822	L2823	E2824	K2825	A2826	R2827	E2828	K2889	E2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	D2908	D2909	T2910	L2911	L2912	A2913	K2914	E2915	K2916	R2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931
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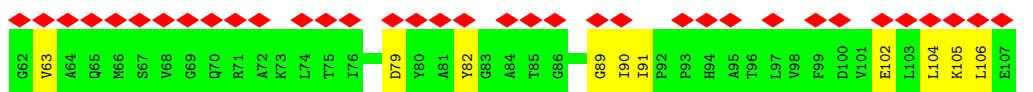
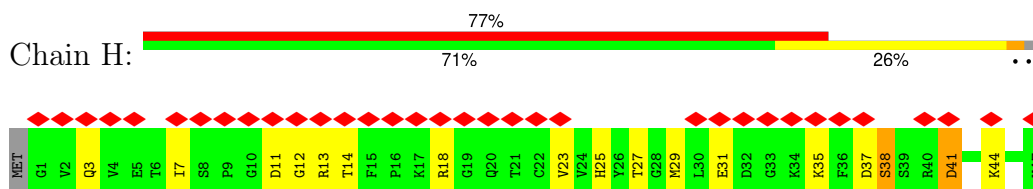




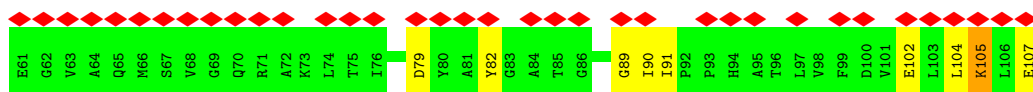
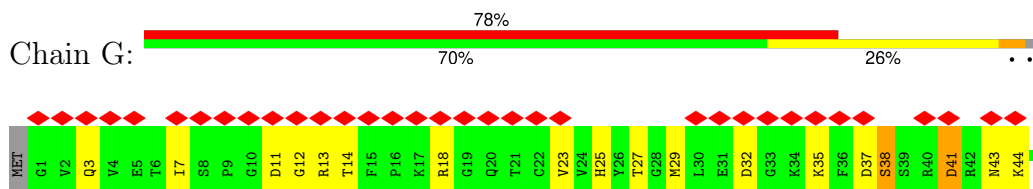
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



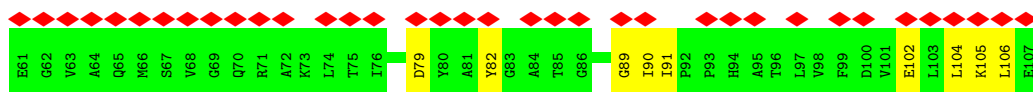
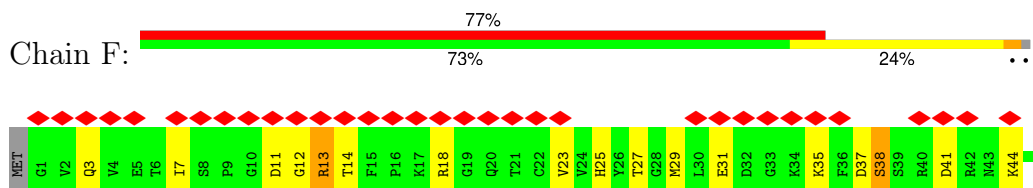
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.68, 423.68, 423.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8275, 0.8275, 0.8275	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: ATP, A1BD5, ZN, CA

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	0.28	1/35977 (0.0%)	0.54	7/48726 (0.0%)
1	B	0.28	1/35977 (0.0%)	0.54	7/48726 (0.0%)
1	C	0.28	1/35977 (0.0%)	0.54	7/48726 (0.0%)
1	D	0.28	1/35977 (0.0%)	0.54	7/48726 (0.0%)
2	E	0.31	0/850	0.61	0/1146
2	F	0.30	0/850	0.62	0/1146
2	G	0.32	0/850	0.62	0/1146
2	H	0.30	0/850	0.61	0/1146
All	All	0.28	4/147308 (0.0%)	0.54	28/199488 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2237	CYS	CB-SG	6.17	1.92	1.82
1	C	2237	CYS	CB-SG	6.17	1.92	1.82
1	A	2237	CYS	CB-SG	6.15	1.92	1.82
1	D	2237	CYS	CB-SG	6.14	1.92	1.82

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	MET	CA-CB-CG	7.46	125.98	113.30
1	A	227	MET	CA-CB-CG	7.44	125.95	113.30
1	B	227	MET	CA-CB-CG	7.43	125.93	113.30
1	D	227	MET	CA-CB-CG	7.41	125.90	113.30
1	D	2905	LEU	CA-CB-CG	6.32	129.83	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2244	ARG	Sidechain
1	B	2244	ARG	Sidechain
1	C	2244	ARG	Sidechain
1	D	2244	ARG	Sidechain

## 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	35150	0	34794	1088	0
1	B	35150	0	34792	1077	0
1	C	35150	0	34792	1066	0
1	D	35150	0	34792	1074	0
2	E	831	0	831	25	0
2	F	831	0	831	21	0
2	G	831	0	831	27	0
2	H	831	0	831	27	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144120	0	142542	4265	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 15.

The worst 5 of 4265 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)
1:A:3477:LYS:HE3	1:B:1141:ARG:CZ	1.20	1.58
1:A:3477:LYS:CE	1:B:1141:ARG:NH1	1.69	1.54
1:A:3477:LYS:CE	1:B:1141:ARG:HD3	1.33	1.53
1:A:1141:ARG:NH1	1:D:3477:LYS:CE	1.70	1.43
1:A:3477:LYS:CE	1:B:1141:ARG:CZ	1.93	1.38

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	4385/5037 (87%)	4306 (98%)	79 (2%)	0	100	100
1	B	4385/5037 (87%)	4305 (98%)	80 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	4385/5037 (87%)	4307 (98%)	78 (2%)	0	100	100
1	D	4385/5037 (87%)	4304 (98%)	81 (2%)	0	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
All	All	17960/20580 (87%)	17635 (98%)	325 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	3836/4276 (90%)	3577 (93%)	259 (7%)	13	43
1	B	3836/4276 (90%)	3575 (93%)	261 (7%)	13	43
1	C	3836/4276 (90%)	3577 (93%)	259 (7%)	13	43
1	D	3836/4276 (90%)	3577 (93%)	259 (7%)	13	43
2	E	89/90 (99%)	83 (93%)	6 (7%)	13	44
2	F	89/90 (99%)	83 (93%)	6 (7%)	13	44
2	G	89/90 (99%)	81 (91%)	8 (9%)	8	30
2	H	89/90 (99%)	84 (94%)	5 (6%)	17	50
All	All	15700/17464 (90%)	14637 (93%)	1063 (7%)	16	43

5 of 1063 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2582	MET
1	C	2825	LYS
1	C	2578	MET
1	C	4541	TRP

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Mol	Chain	Res	Type
1	B	2256	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2284	ASN
1	C	2324	ASN
1	C	3325	ASN
1	B	2324	ASN
1	B	2284	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	$\# Z  > 2$
6	A1BD5	D	5304	-	16,16,16	0.93	1 (6%)	21,23,23	0.76	0
3	ATP	D	5301	-	28,33,33	0.63	0	34,52,52	0.81	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	A1BD5	B	5304	-	16,16,16	0.94	1 (6%)	21,23,23	0.77	0
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	0.82	2 (5%)
6	A1BD5	A	5304	-	16,16,16	0.96	1 (6%)	21,23,23	0.77	0
3	ATP	A	5301	-	28,33,33	0.63	0	34,52,52	0.81	2 (5%)
3	ATP	C	5301	-	28,33,33	0.63	0	34,52,52	0.81	2 (5%)
6	A1BD5	C	5304	-	16,16,16	0.94	1 (6%)	21,23,23	0.76	0

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
6	A1BD5	D	5304	-	-	4/4/4/4	0/2/2/2
3	ATP	D	5301	-	-	2/18/38/38	0/3/3/3
6	A1BD5	B	5304	-	-	4/4/4/4	0/2/2/2
3	ATP	B	5301	-	-	2/18/38/38	0/3/3/3
6	A1BD5	A	5304	-	-	4/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	2/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	2/18/38/38	0/3/3/3
6	A1BD5	C	5304	-	-	4/4/4/4	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5304	A1BD5	C1-C2	-2.21	1.36	1.39
6	B	5304	A1BD5	C1-C2	-2.18	1.36	1.39
6	D	5304	A1BD5	C1-C2	-2.14	1.36	1.39
6	C	5304	A1BD5	C1-C2	-2.14	1.36	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	C4'-O4'-C1'	-3.22	106.97	109.92
3	A	5301	ATP	C4'-O4'-C1'	-3.18	107.02	109.92
3	C	5301	ATP	C4'-O4'-C1'	-3.15	107.04	109.92
3	D	5301	ATP	C4'-O4'-C1'	-3.13	107.05	109.92
3	C	5301	ATP	C5-C6-N6	2.34	123.87	120.31

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

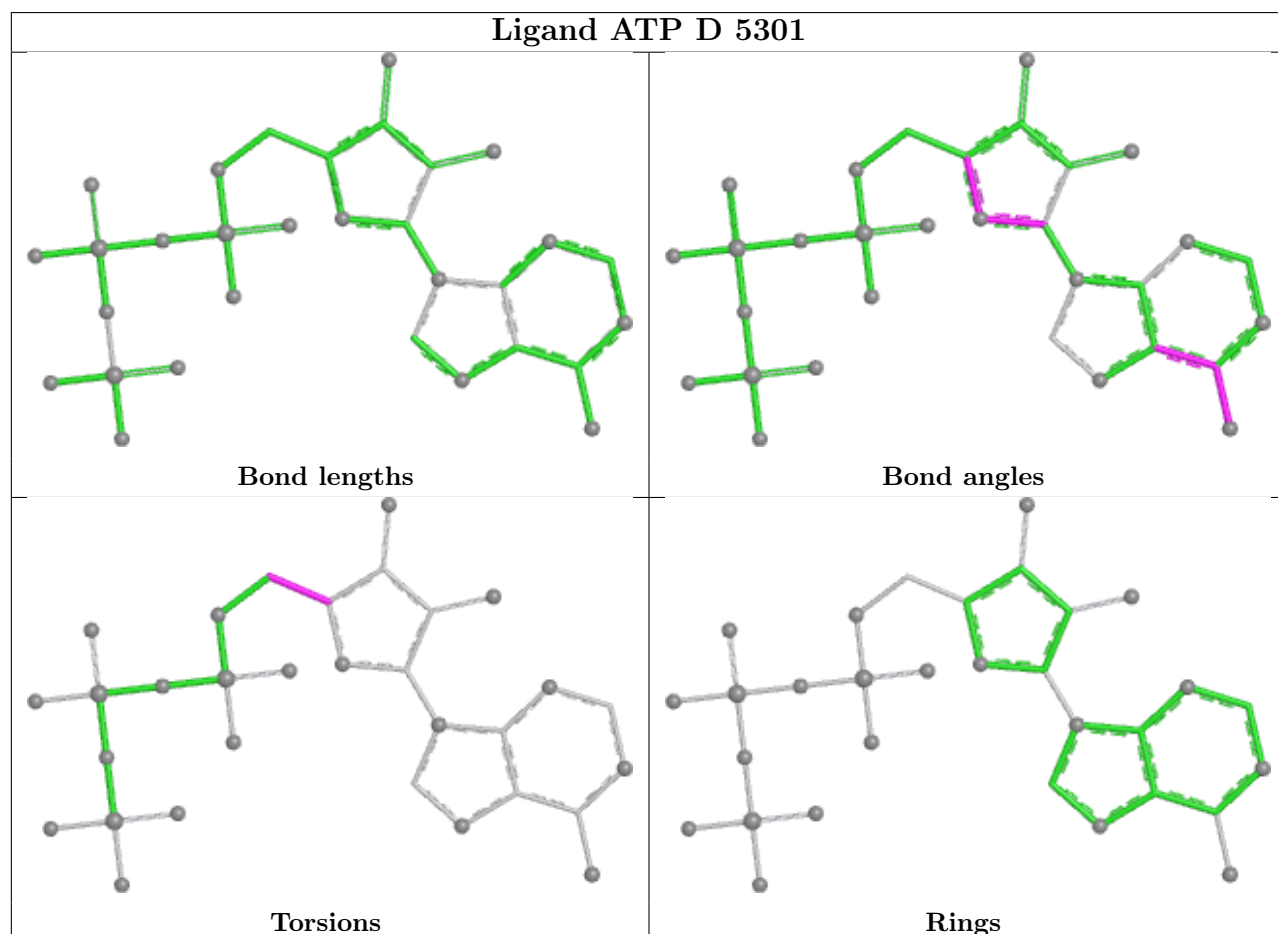
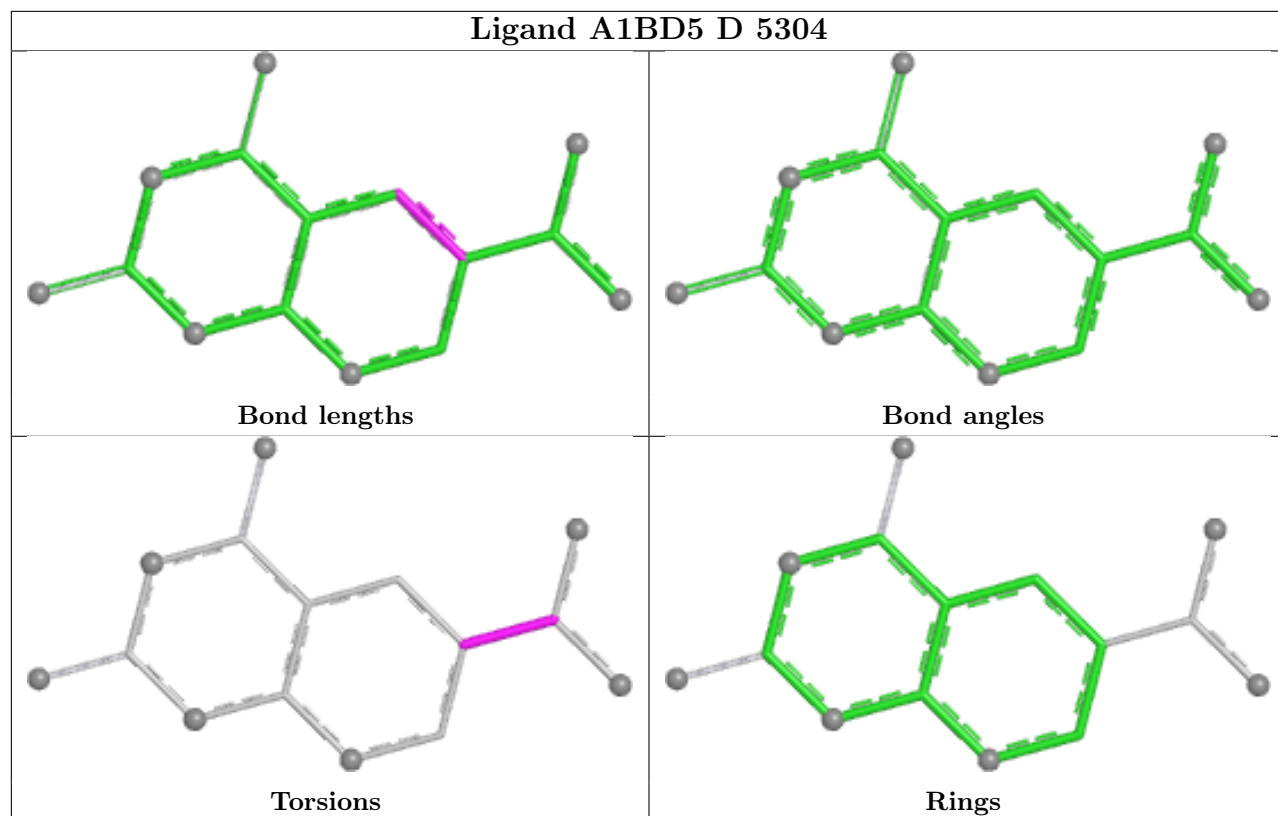
Mol	Chain	Res	Type	Atoms
6	A	5304	A1BD5	C3-C2-C8-O3
6	A	5304	A1BD5	C3-C2-C8-O4
6	B	5304	A1BD5	C3-C2-C8-O3
6	B	5304	A1BD5	C3-C2-C8-O4
6	D	5304	A1BD5	C3-C2-C8-O3

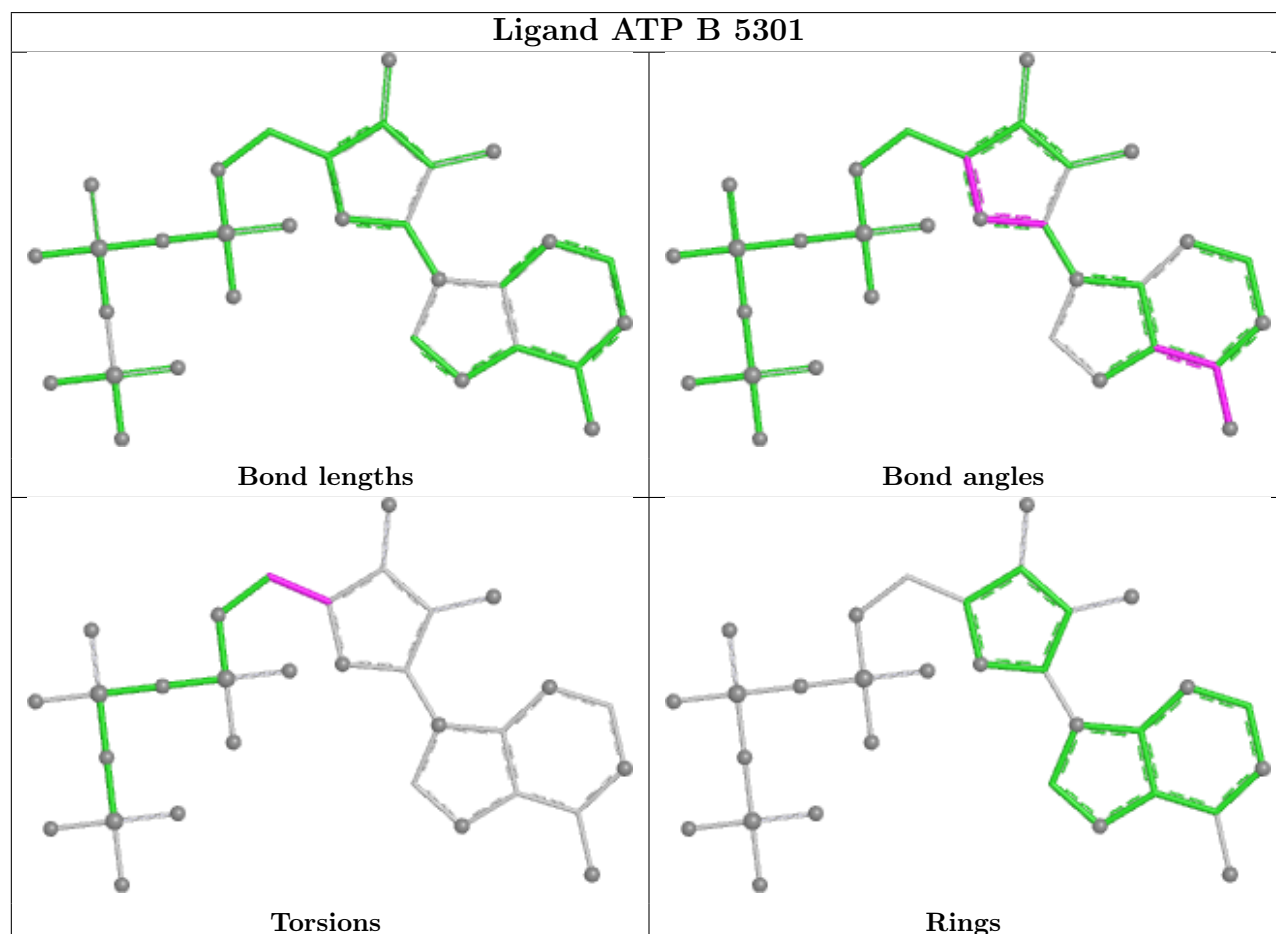
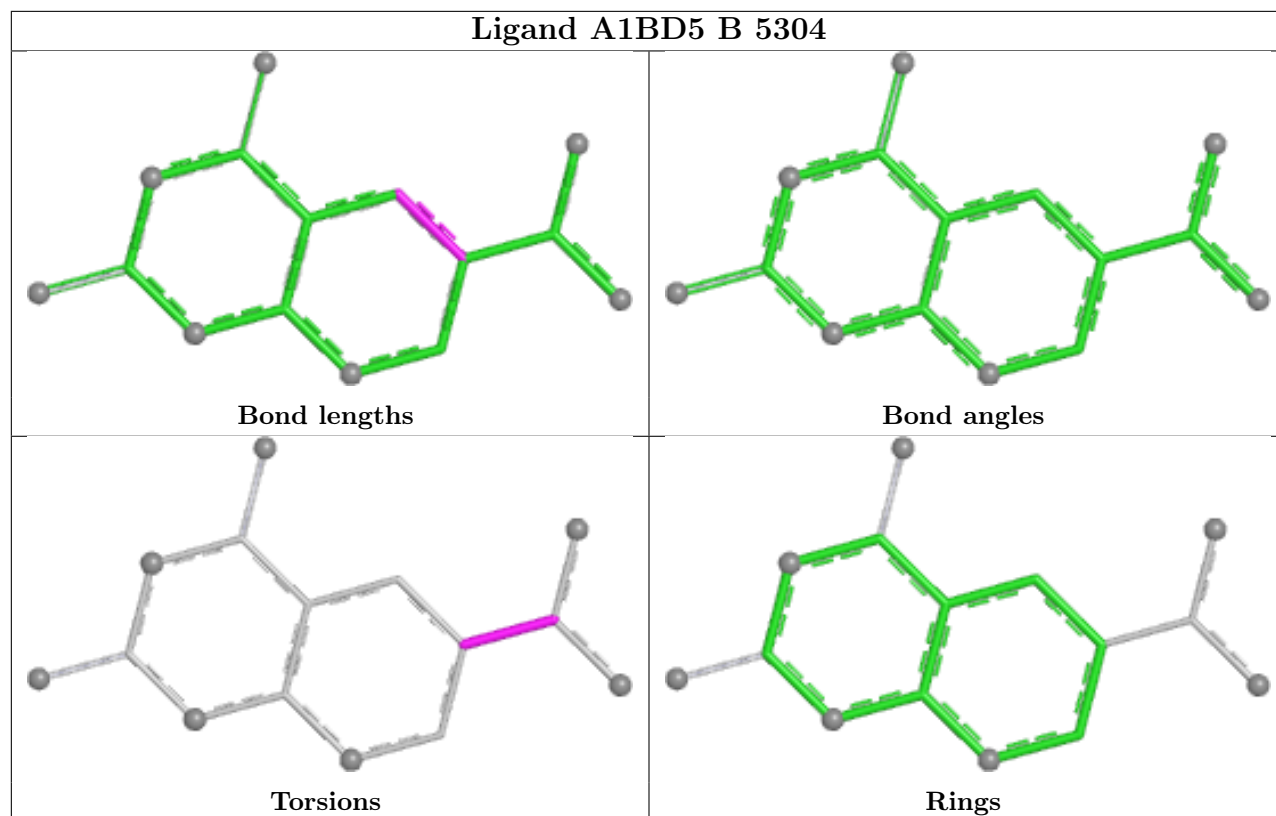
There are no ring outliers.

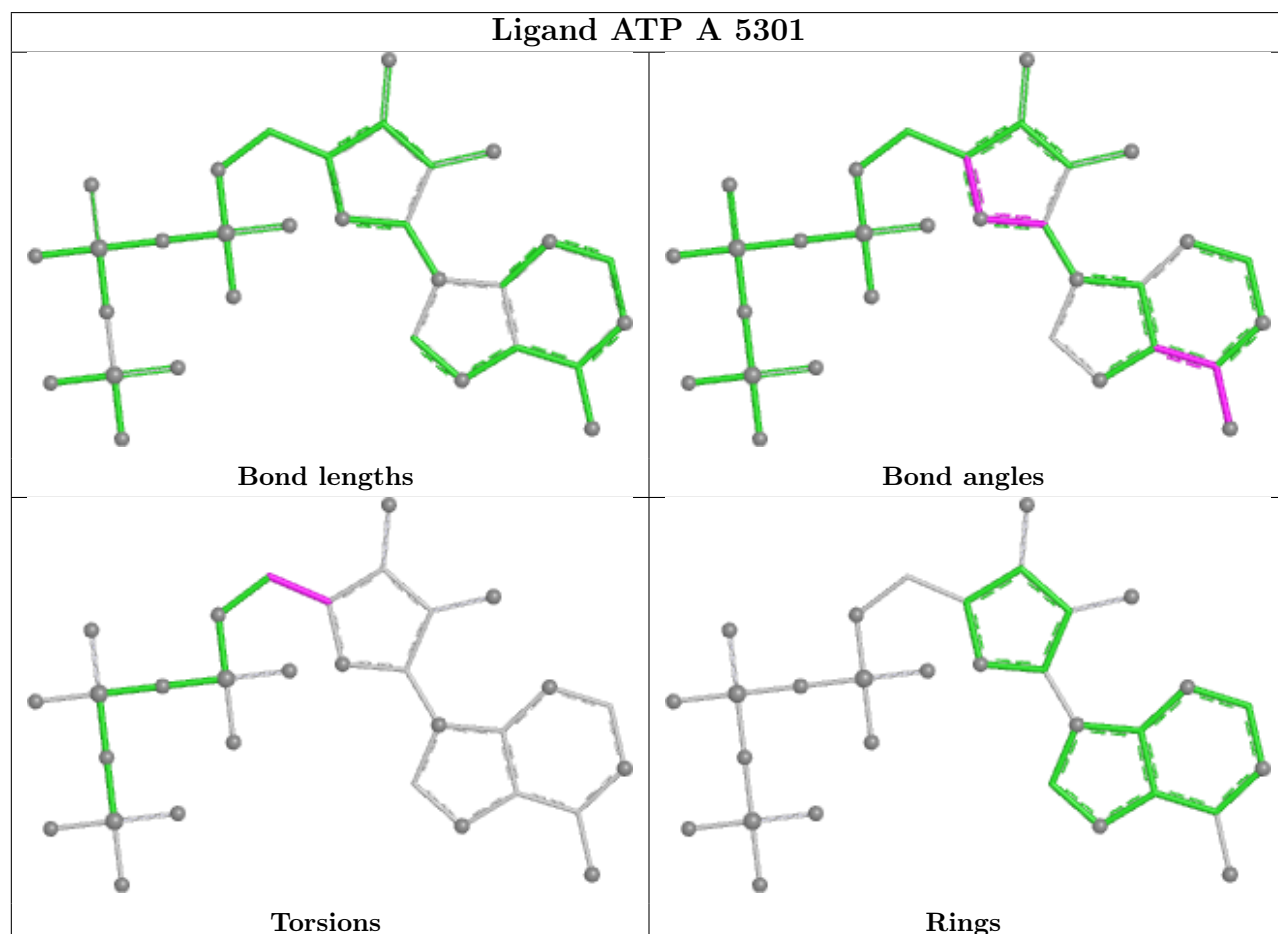
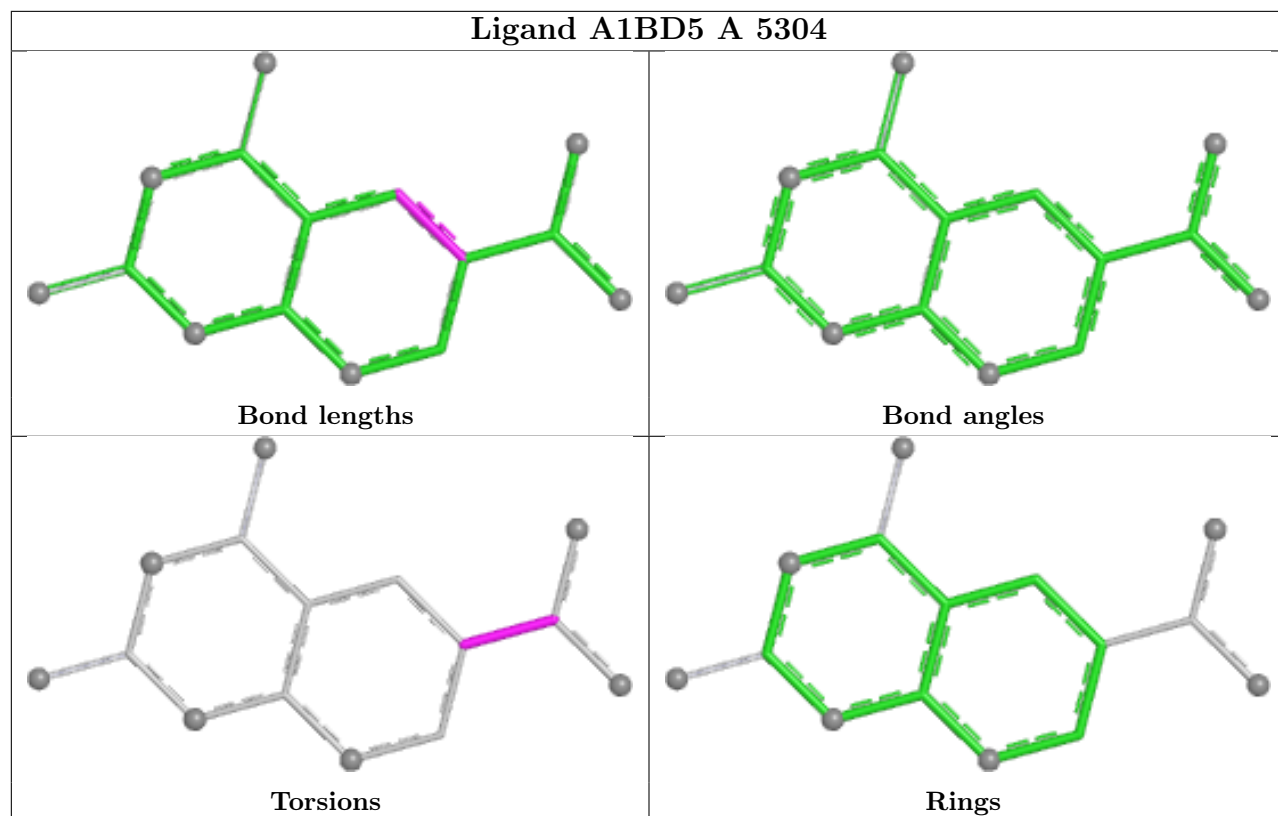
3 monomers are involved in 3 short contacts:

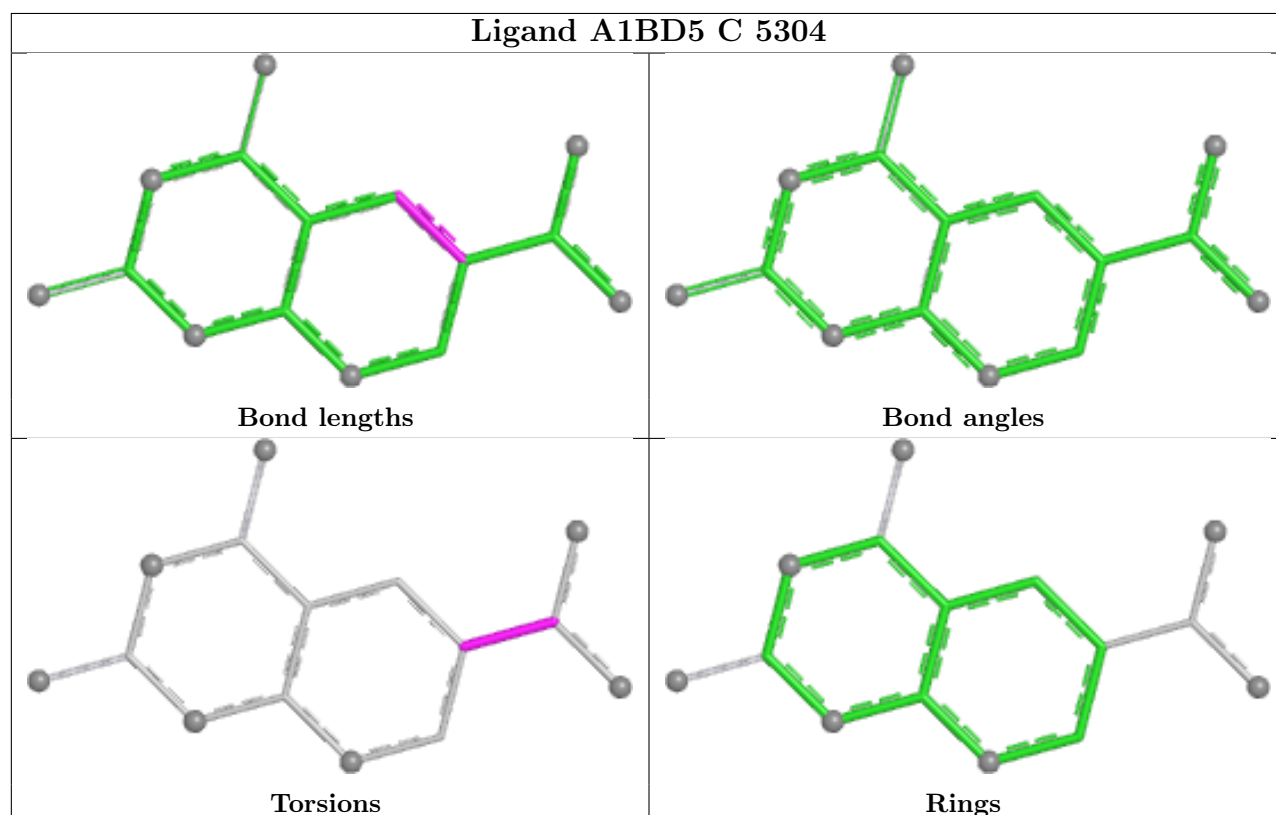
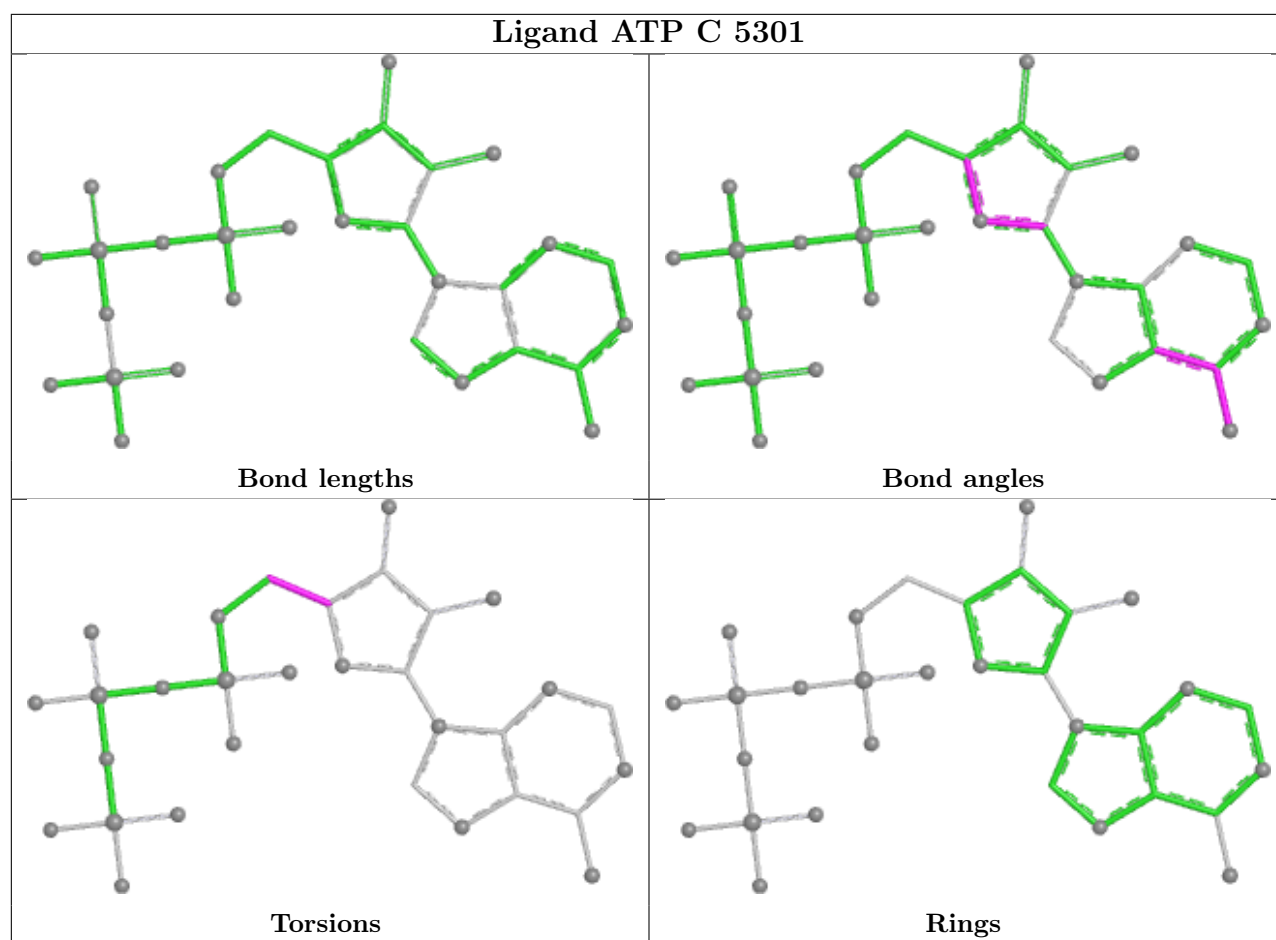
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0
3	C	5301	ATP	1	0

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](#)

There are no chain breaks in this entry.

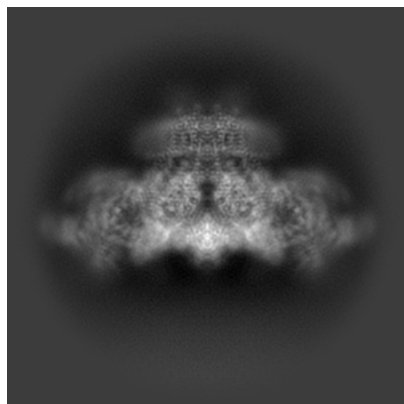
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47395. These allow visual inspection of the internal detail of the map and identification of artifacts.

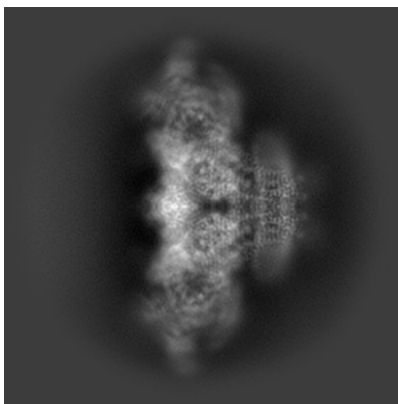
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

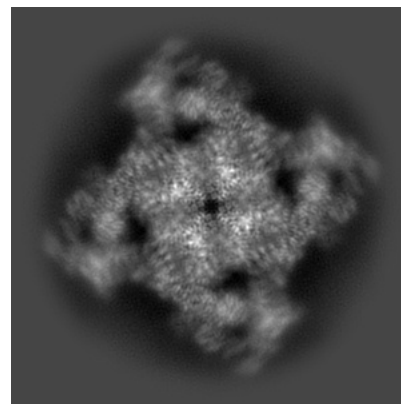
#### 6.1.1 Primary map



X

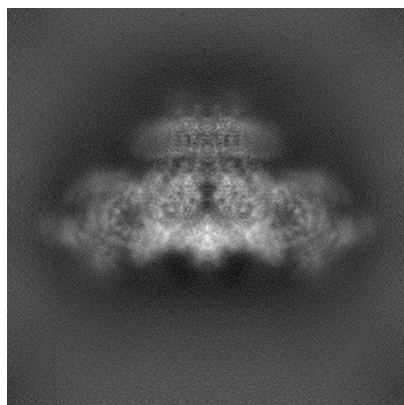


Y

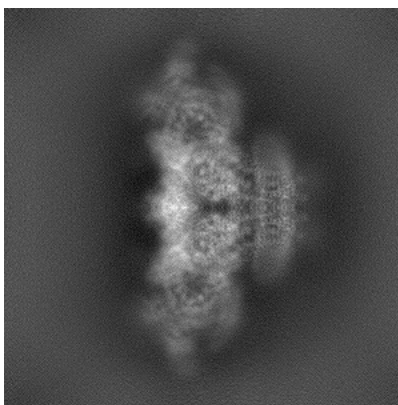


Z

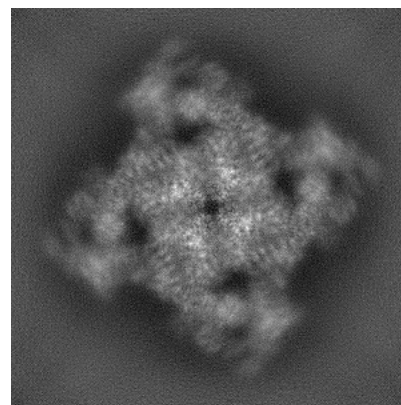
#### 6.1.2 Raw map



X



Y

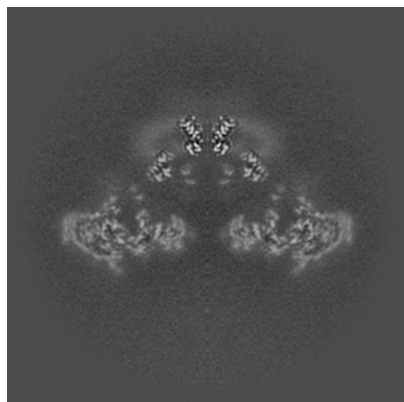


Z

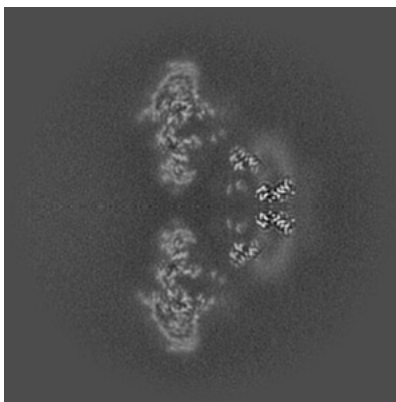
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

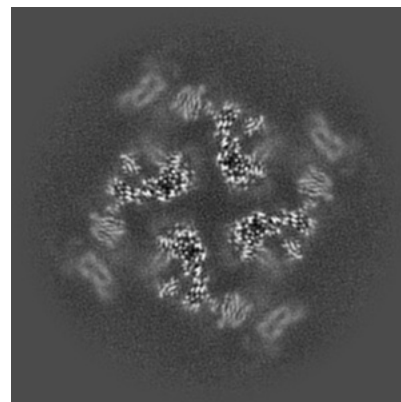
### 6.2.1 Primary map



X Index: 256

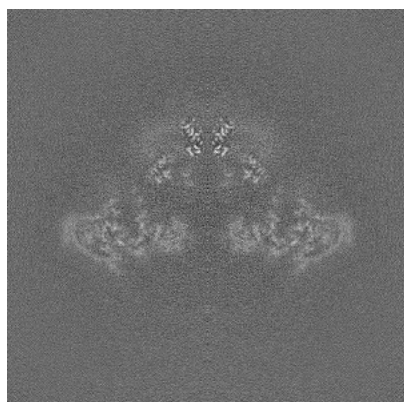


Y Index: 256

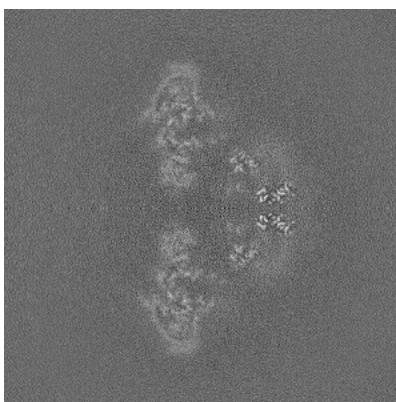


Z Index: 256

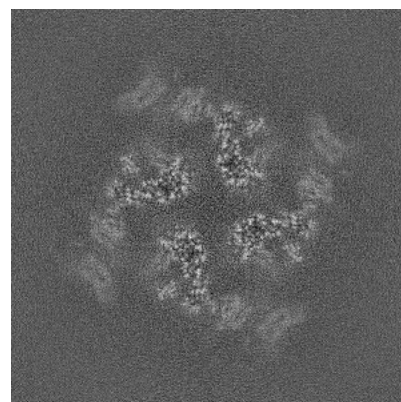
### 6.2.2 Raw map



X Index: 256



Y Index: 256

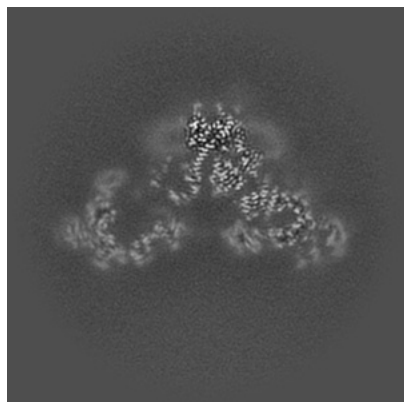


Z Index: 256

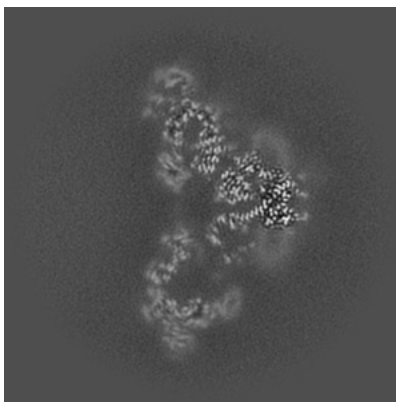
The images above show central slices of the map in three orthogonal directions.

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

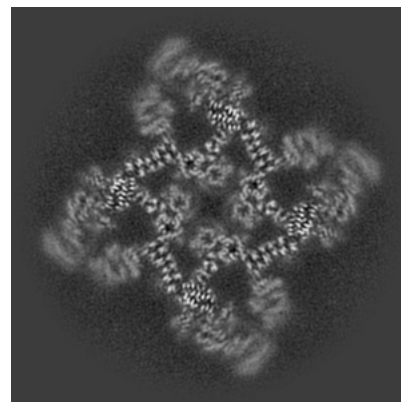
### 6.3.1 Primary map



X Index: 270

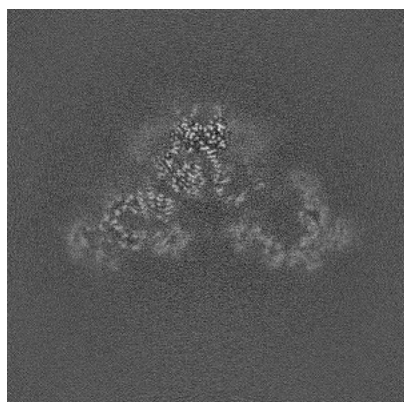


Y Index: 242

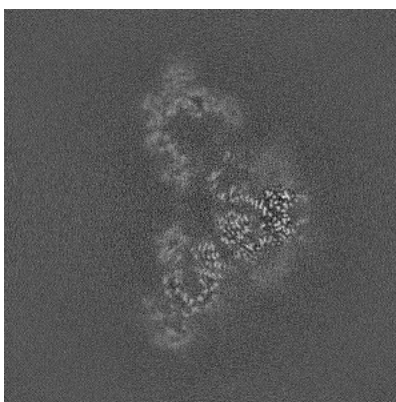


Z Index: 227

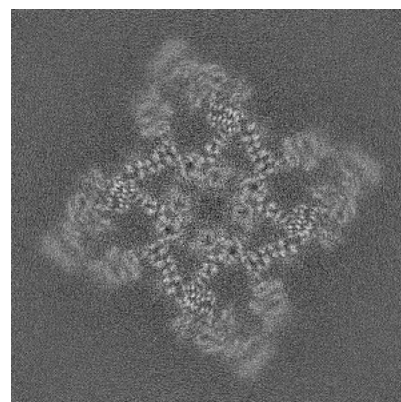
### 6.3.2 Raw map



X Index: 242



Y Index: 270

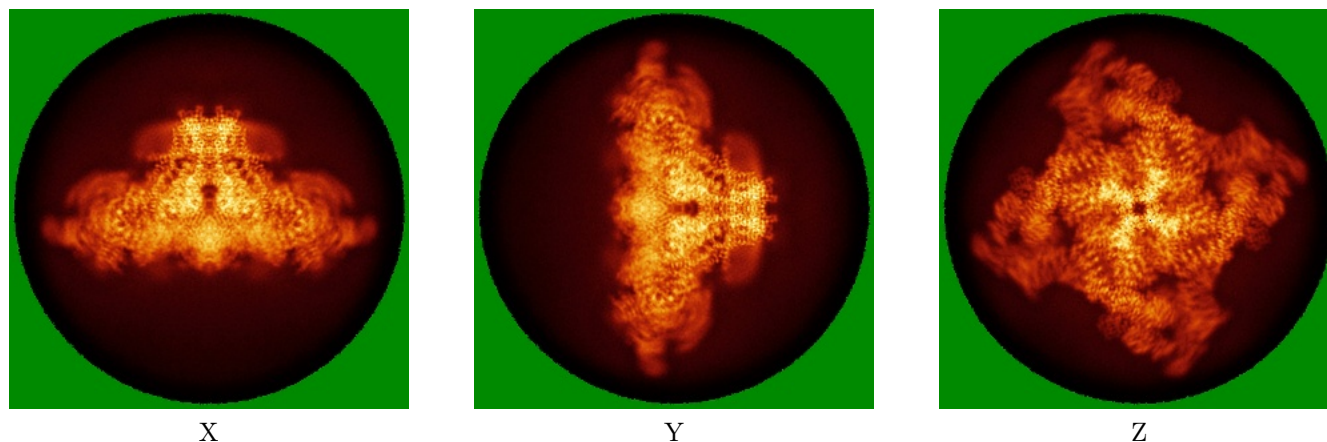


Z Index: 227

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

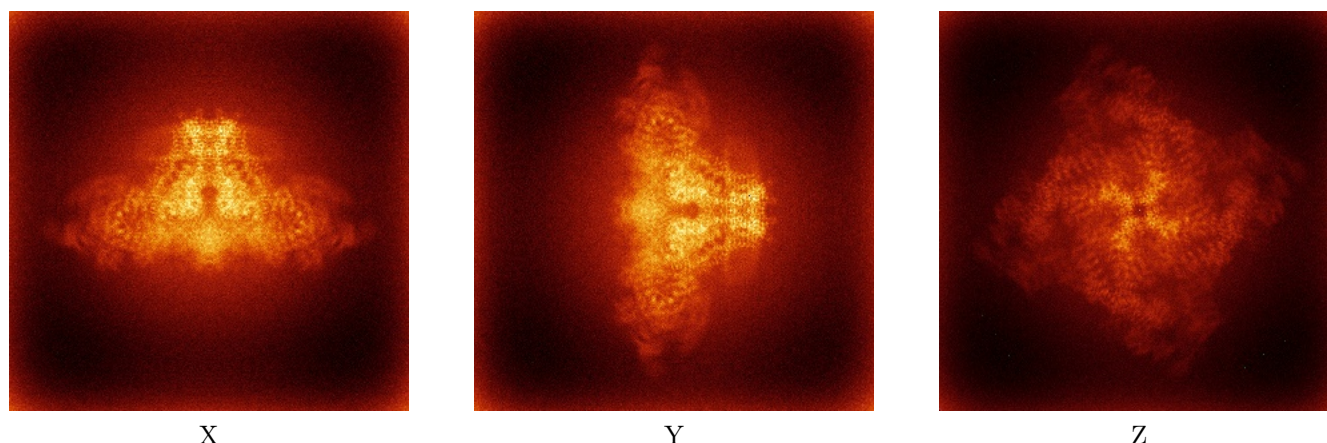


X

Y

Z

### 6.4.2 Raw map



X

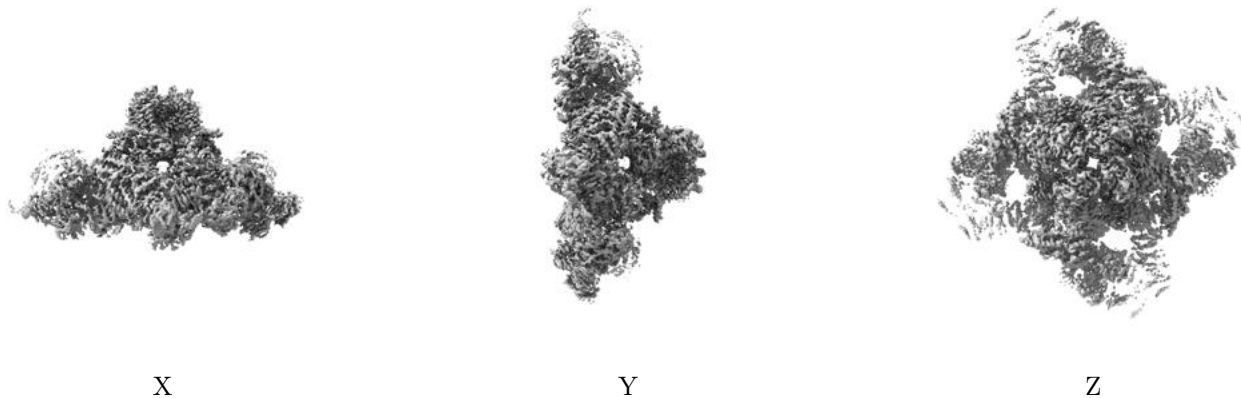
Y

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.

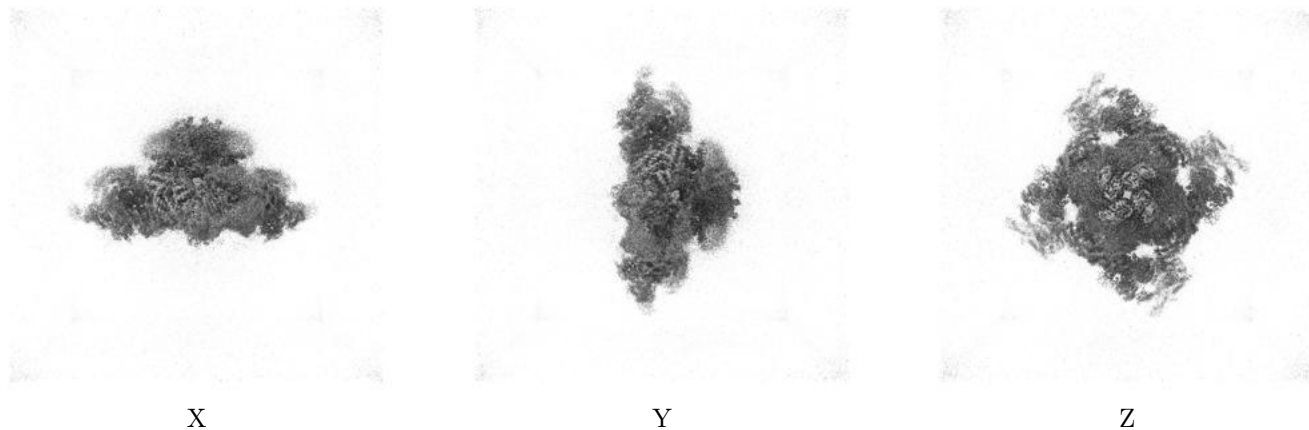
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

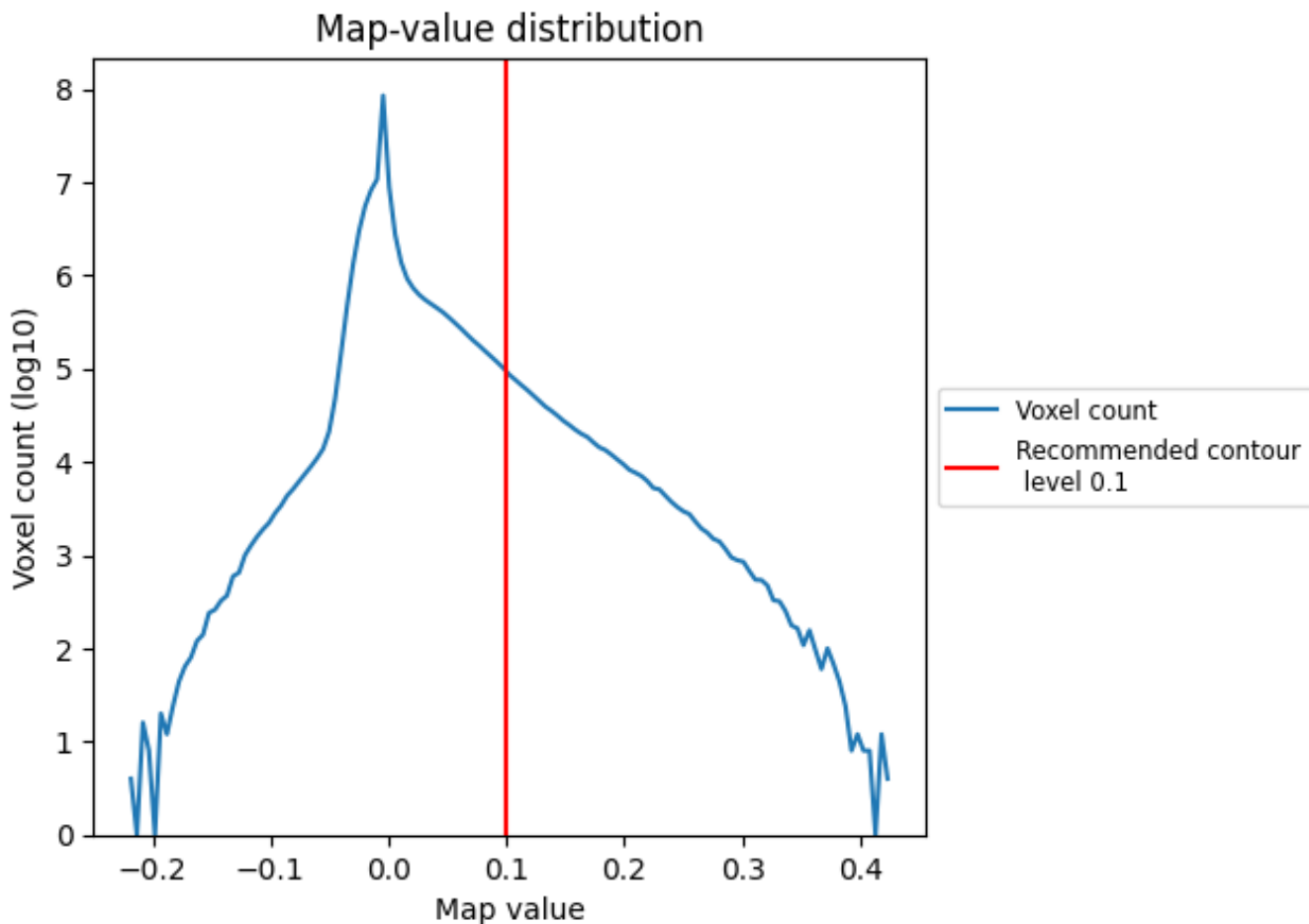
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

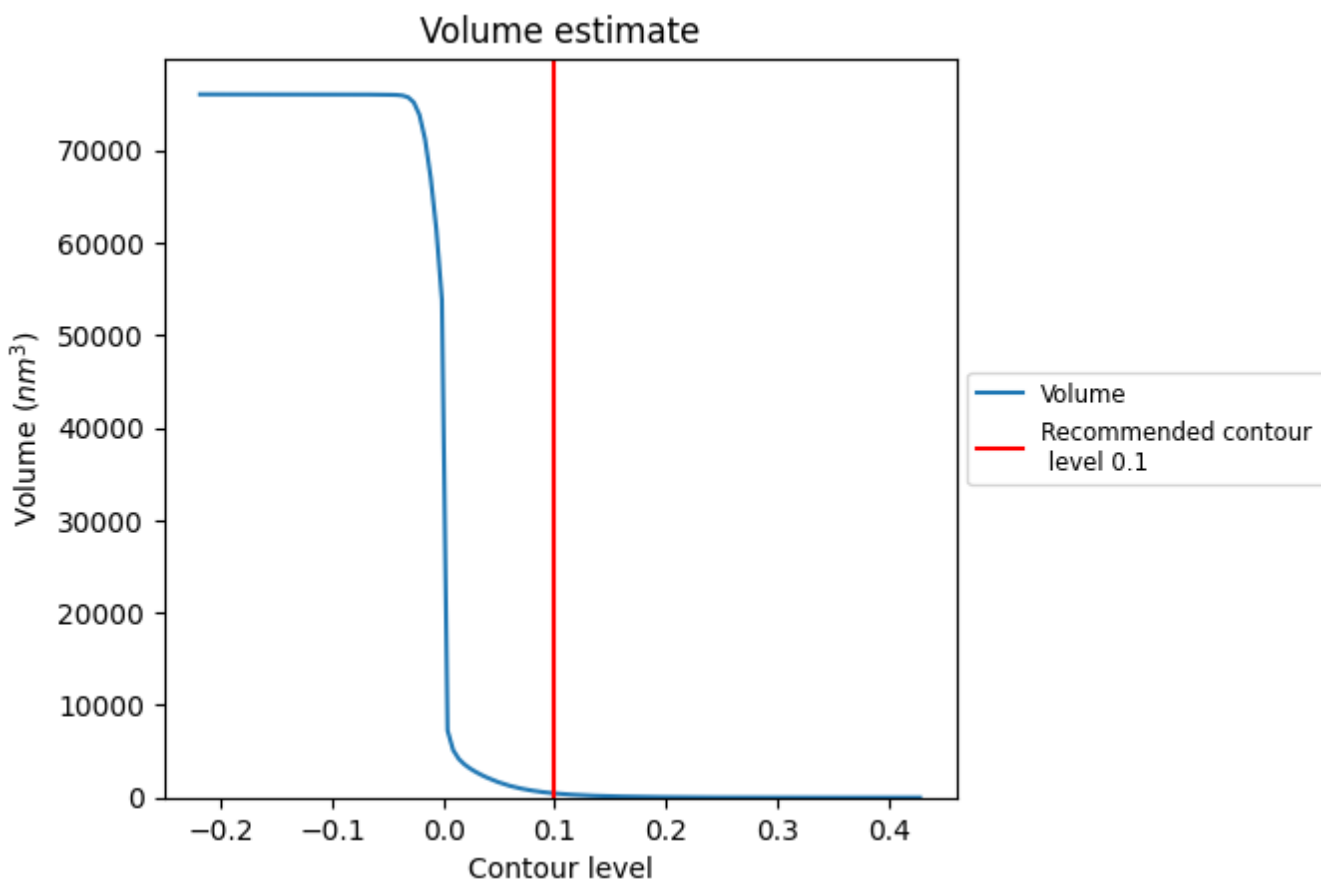
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

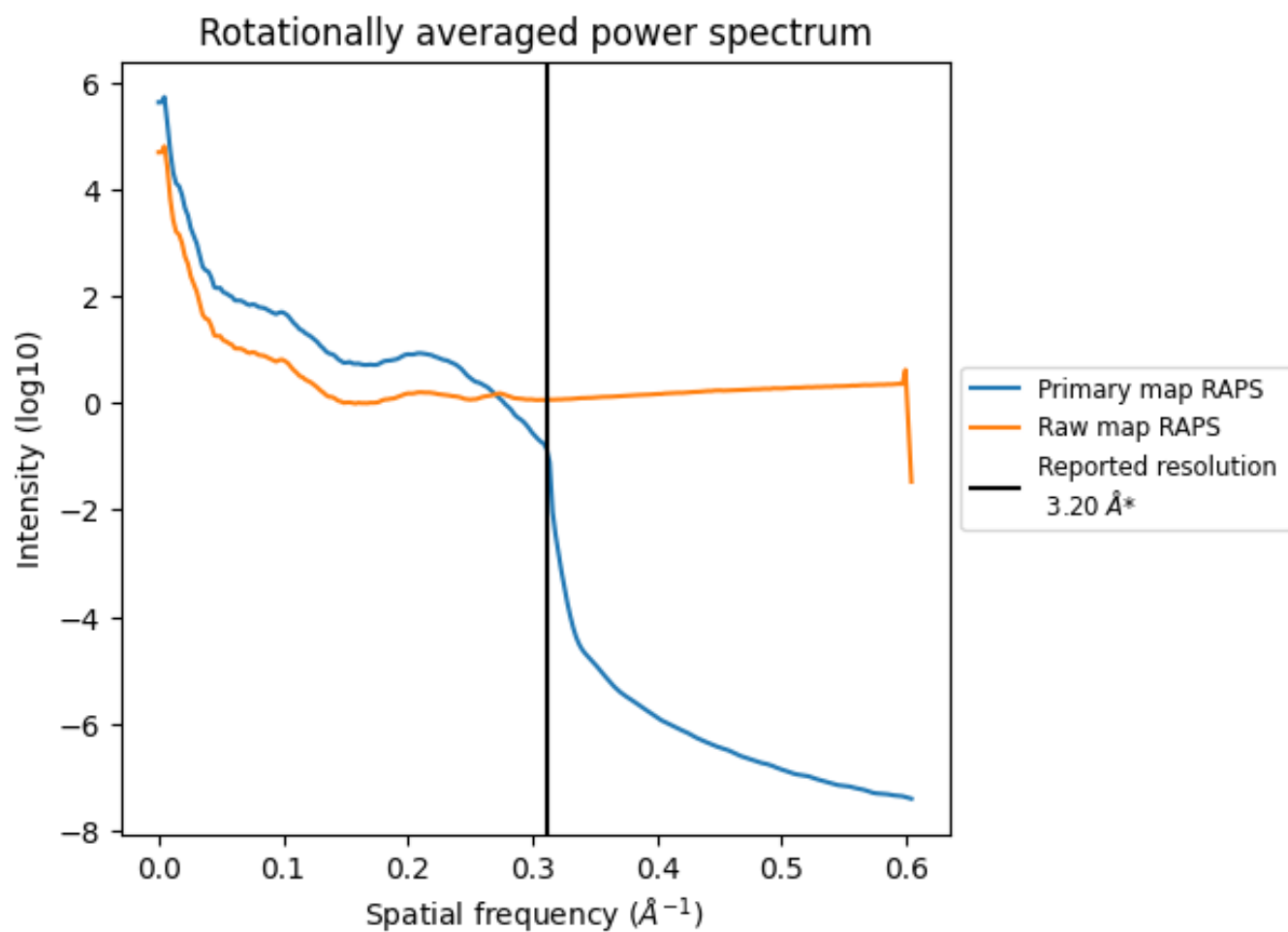


The volume at the recommended contour level is 452  $\text{nm}^3$ ; this corresponds to an approximate mass of 409 kDa.

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

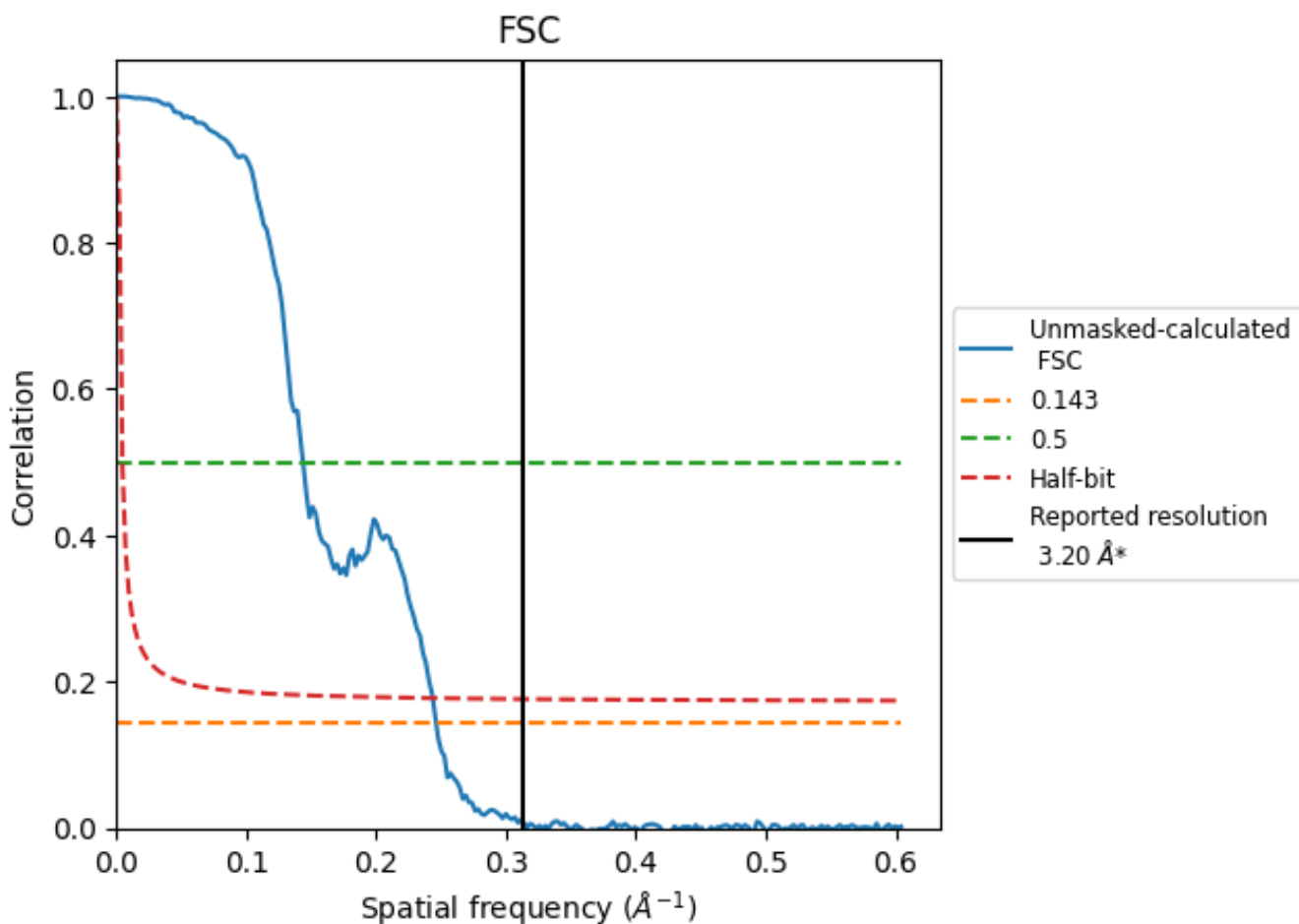


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

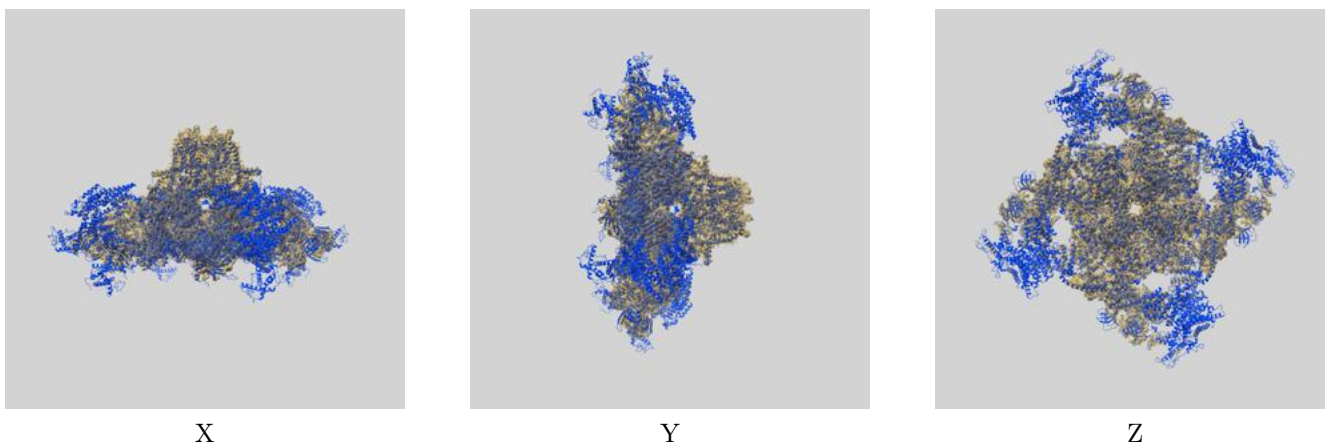
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.96	4.11

\*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 4.06 differs from the reported value 3.2 by more than 10 %

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

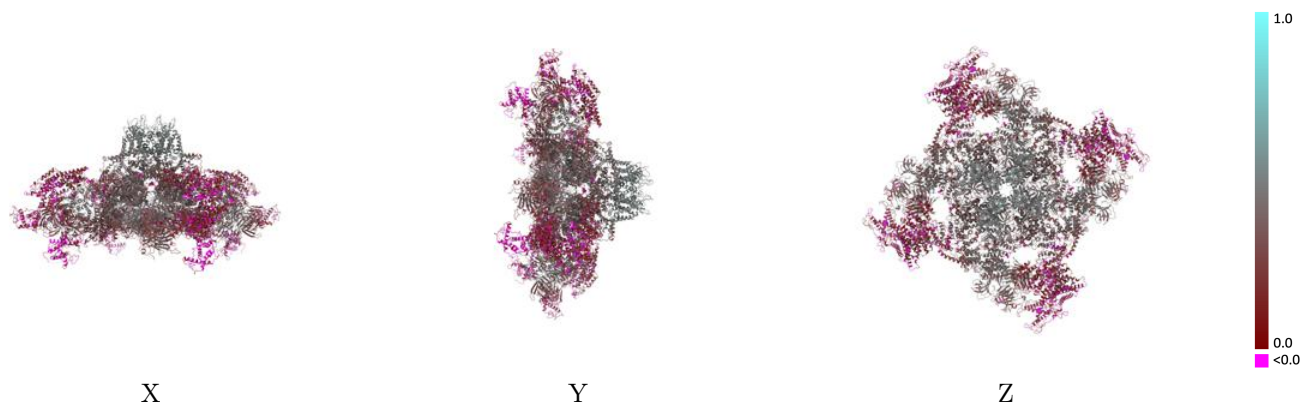
This section contains information regarding the fit between EMDB map EMD-47395 and PDB model 9E1I. Per-residue inclusion information can be found in section 3 on page 7.

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



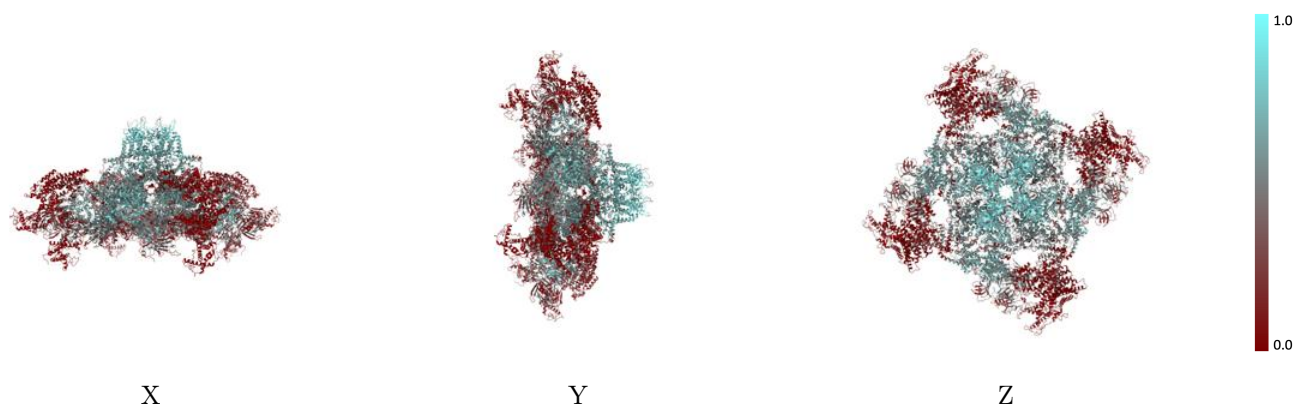
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



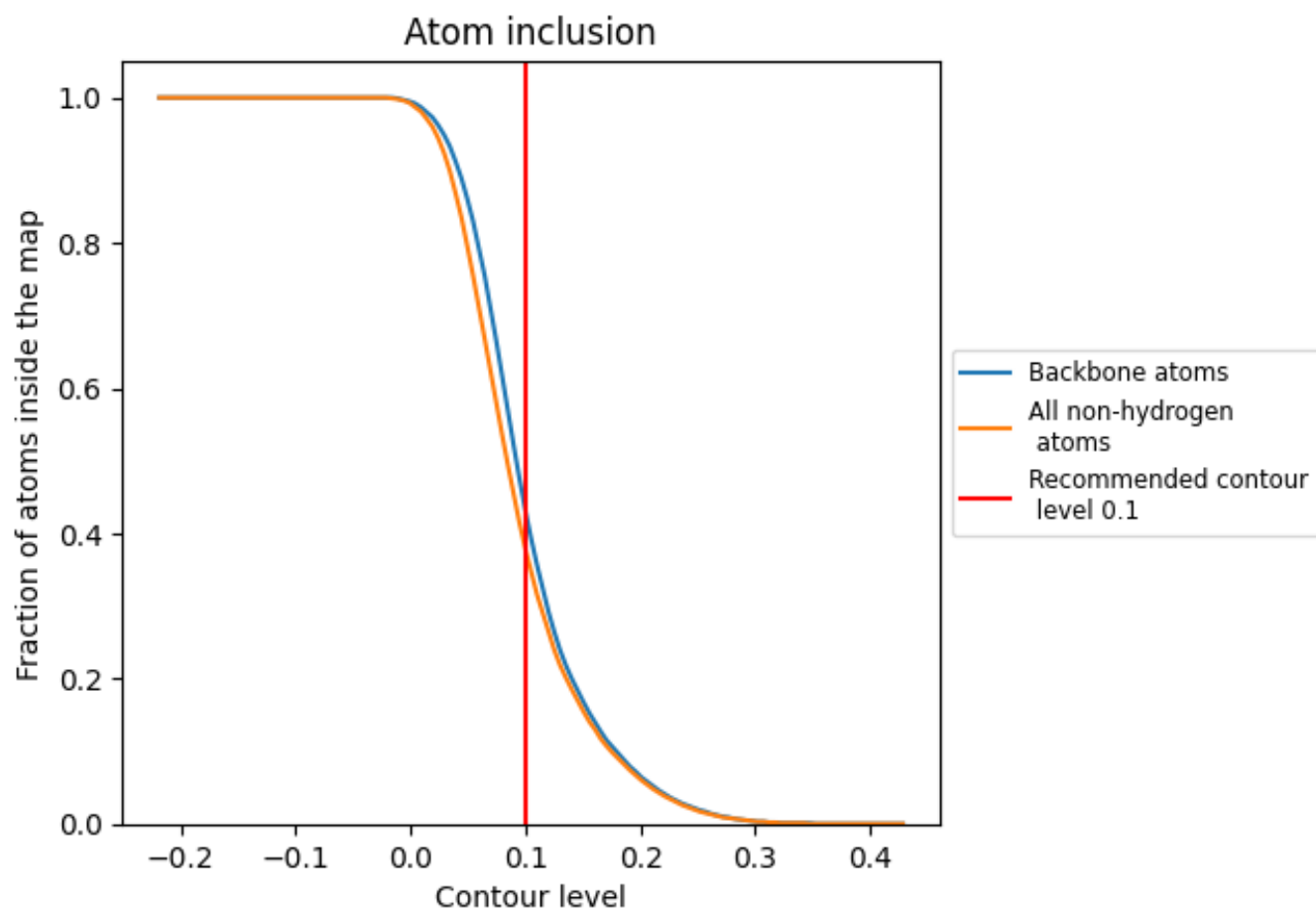
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 38% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3780	0.3000
A	0.3910	0.2990
B	0.3900	0.2980
C	0.3890	0.2970
D	0.3890	0.2980
E	0.2210	0.3870
F	0.2250	0.3860
G	0.2250	0.3850
H	0.2250	0.3880

