



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 10:45 AM EST

PDB ID : 9E19
EMDB ID : EMD-47386
Title : Structure of RyR1 in the open state in the presence of pentoxifylline
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 4.04 Å (reported)
Based on initial model : 7TZC

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.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

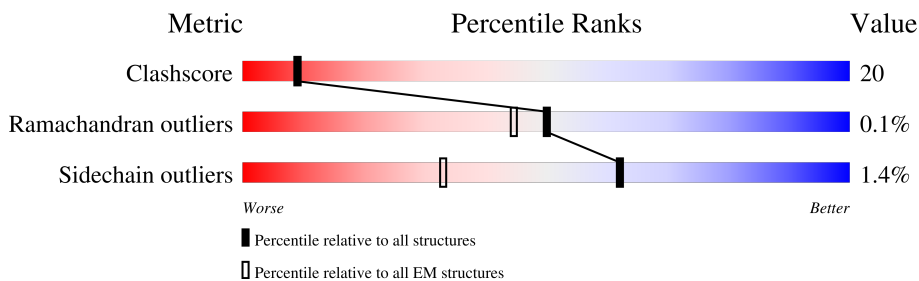
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.04 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 ≥ 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 6 unique types of molecules in this entry. The entry contains 144136 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	35150	22365	6063	6485	237	9	0
1	B	4404	35150	22365	6063	6485	237	9	0
1	D	4404	35150	22365	6063	6485	237	9	0
1	C	4404	35150	22365	6063	6485	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	831	527	146	154	4	0	0
2	H	107	831	527	146	154	4	0	0
2	G	107	831	527	146	154	4	0	0
2	F	107	831	527	146	154	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).

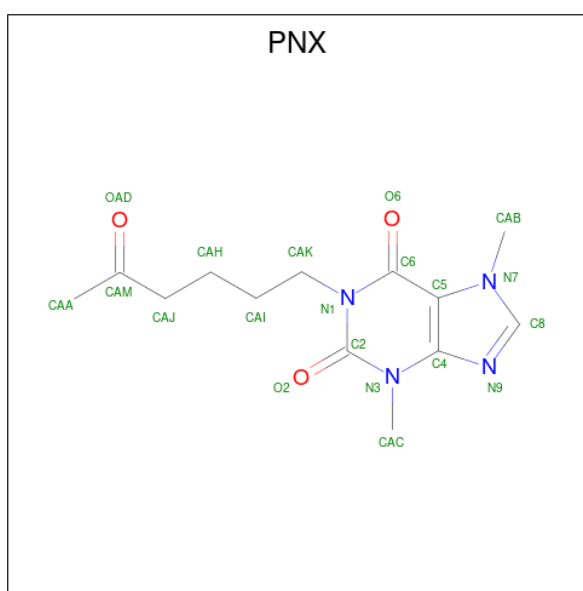
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	Total	Zn	0
			1	1	

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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 3,7-DIMETHYL-1-(5-OXOHEXYL)-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (three-letter code: PNX) (formula: C₁₃H₁₈N₄O₃) (labeled as "Ligand of Interest" by depositor).

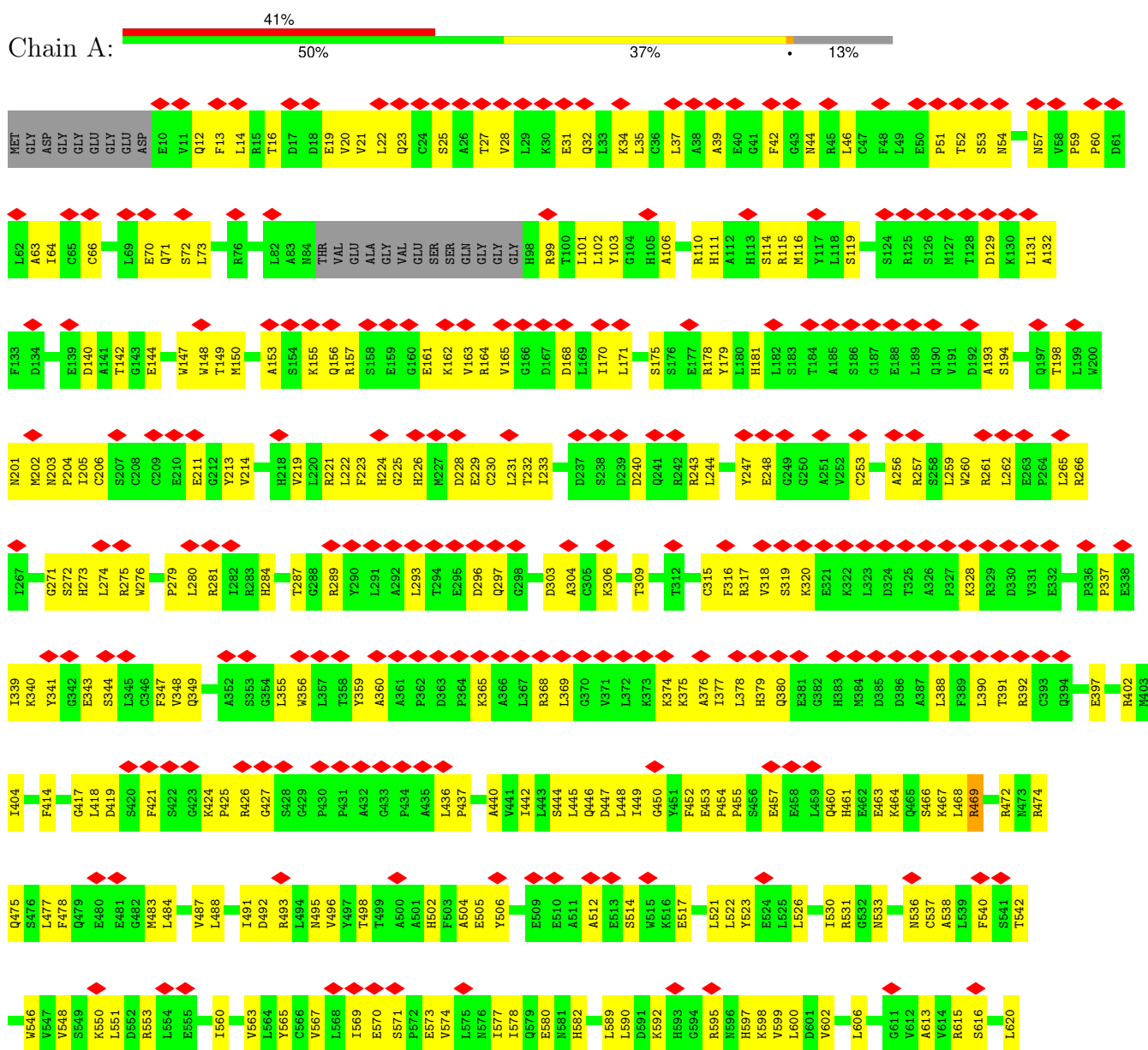


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			20	13	4	3	
6	B	1	Total	C	N	O	0
			20	13	4	3	
6	D	1	Total	C	N	O	0
			20	13	4	3	
6	C	1	Total	C	N	O	0
			20	13	4	3	

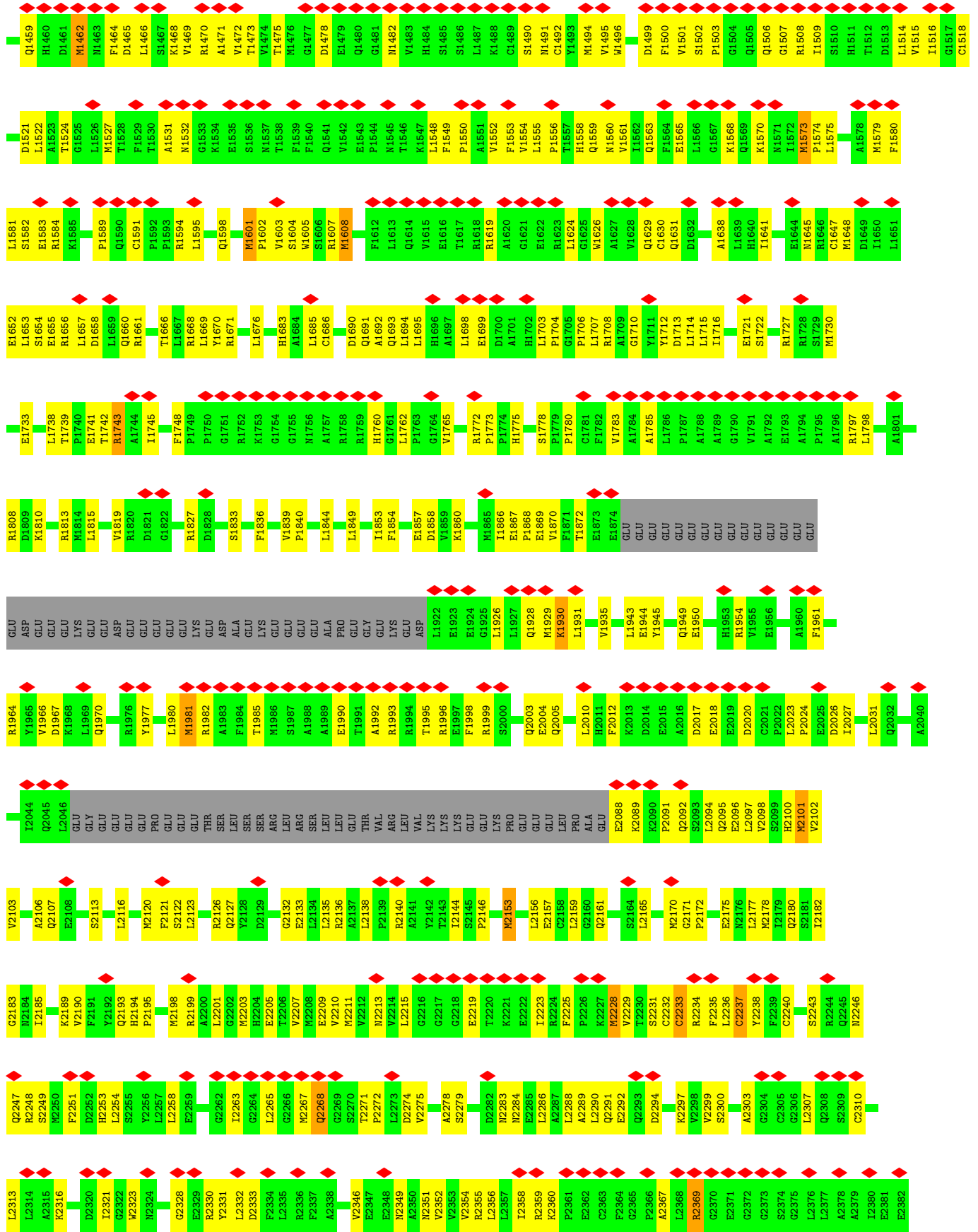
3 Residue-property plots [i](#)

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.

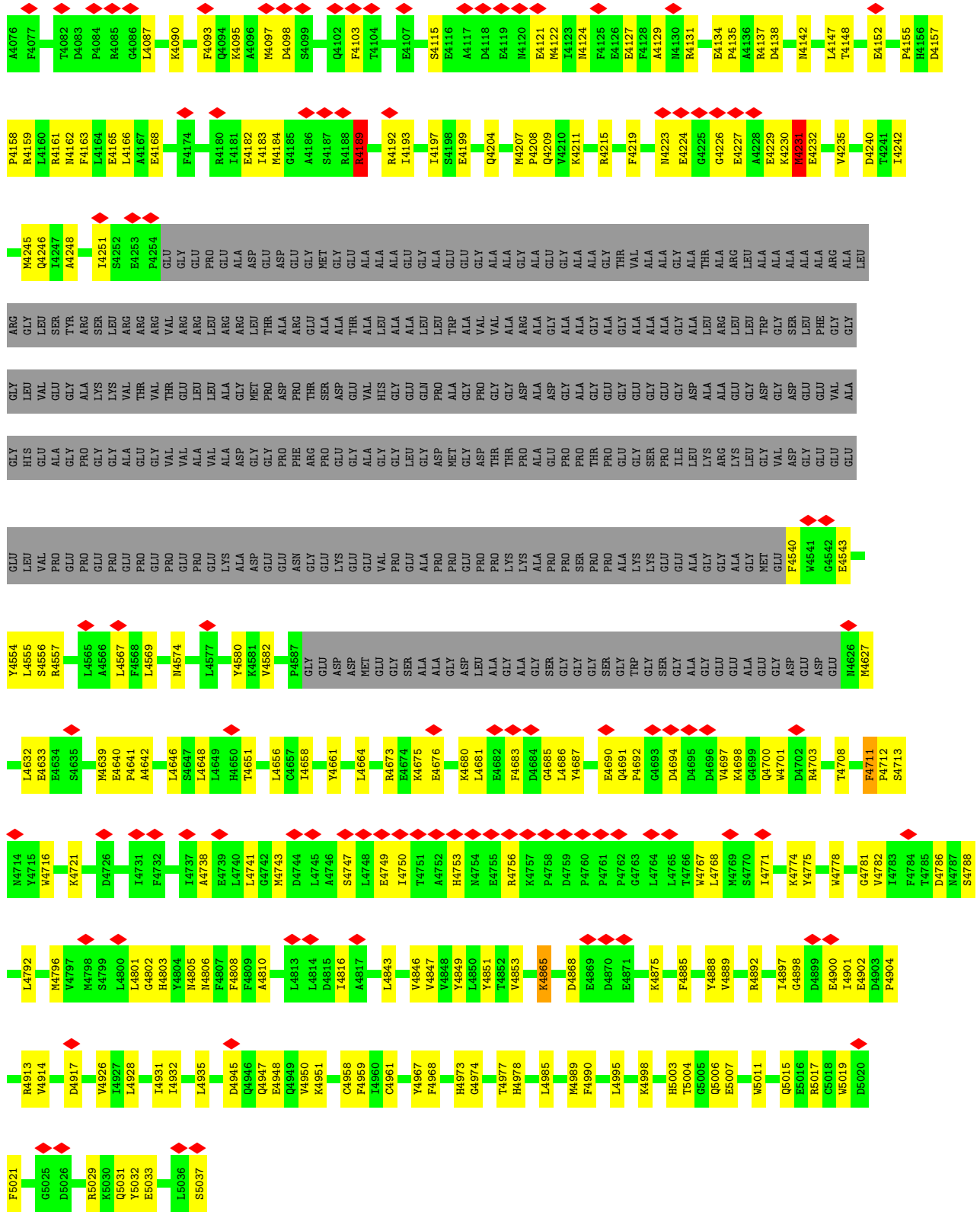
• Molecule 1: Ryanodine receptor 1



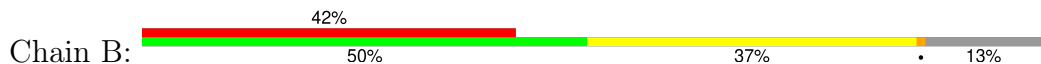
ALA	L1272	V1199	S1136	D1070	V1010	D948	E888	P825	R758	S693	I621
LYS	A1273	G1200	E1137	R1071	Q1011	N949	Q889	I826	I759	P694	T622
LYS	H1274	H1201	F1139	V1072	D1012	L950	G890	K827	N760	P895	E823
ALA	L1275	L1202	G1140	R1073	I1013	K951	G891	R830	P763	P896	M824
ALA	M1276	G1205	R1141	R1076	P1014	K952	T892	R831	V764	G897	L826
SER	M1277	Q1206	P1142	A1077	A1015	T953	T893	E832	F768	C898	R629
ALA	G1278	D1207	W1143	E1078	R1016	K954	G894	G833	E769	G899	E830
GLY	S1279	Q1210	Q1144	K1079	M1017	L955	P895	P834	F771	L631	L632
THR	M1281	L1211	S1145	Y1081	M1018	P956	T896	G835	F772	L633	L633
ALA	S1282	L1212	G1146	Y1082	R1021	T958	D898	G836	L773	M636	M636
ALA	L1283	F1213	D1147	Q1084	L1021	Y959	D899	P837	L774	L637	L637
ALA	L1284	F1214	V1148	W1088	V1022	M960	D900	G838	G775	I638	I638
LYS	E1285	A1215	W1149	R1087	P1023	M961	K901	P842	L776	M639	M639
GLU	M1286	G1150	G1150	W1089	Y1024	S962	R902	S843	L777		
GLY	L1287	C1151	M1152	F1090	R1026	N963	R903	R844	L778		
THR	F1288	I1153	D1154	E1091	L1027	G964	L904	C945	F779		
ALA	L1289	D1155	F1092	F1093	D1028	Y965	H904	C846	V780		
ALA	R1290	L1155	E1093	A1094	E1029	K966	P905	S847	V781		
LYS	L1291	T1156	E1157	A1095	C906	P967	C906	H948	S782		
GLY	S1292	E1157	M1158	V1096	A1030	A968	L907	T949	S783		
PRO	L1293	M1158	T1159	E1099	T1031	P969	V908	T850	A785		
GLY	P1294	T1159	I1160	M1100	K1032	L970	V909	D850	G786		
GLY	F1297	I1161	F1162	R1101	R1033	D971	N909	F851	F787		
THR	H1298	F1162	T1163	V1102	F910	H911	F910	V852	K788		
ALA	L1299	T1163	L1164	G1103	M1035	L972	H911	P853	H789		
GLN	H1300	L1164	M1165	W1104	R1036	S973	S912	C854	V790		
VAL	F1301	G1166	A1105	R1106	D1037	H974	L913	P855	R790		
GLY	R1232	E1167	G1166	A1106	S1038	V975	F914	V856	F791		
VAL	W1237	V1168	L1169	P1107	L1039	R976	E915	D857	L792		
ALA	K1240	L1170	M1170	L1109	C1040	T978	N919	R858	L793		
ALA	Q1244	S1171	D1172	D1112	Q1041	P979	N919	Q860	G794		
GLY	F1245	G1174	S1173	V1113	A1042	A980	N920	I861	G795		
ALA	E1246	S1175	D1172	L1115	R1045	Q81	N921	V862	R796		
GLY	P1247	G1174	G1174	L1115	T1045	T982	N922	L863	H797		
ALA	P1250	S1176	E1176	G1116	L1046	P983	Q923	P864	G798		
ALA	H1251	E1177	T1177	A1117	L1047	L984	M924	P865	K801		
THR	H1254	L1179	A1178	D1118	G1048	V985	S925	H866	F802		
THR	Y1255	F1179	A1178	E1119	Y1049	D866	G926	L867	L803		
GLY	Y1256	R1180	E1181	L1120	Y1051	R987	E927	E868	P804		
GLY	V1257	S1181	L1182	A1121	M1052	L988	T928	I870	P805		
ASN	A1258	E1183	G1126	G1124	I1053	A989	L929	R869	P906		
LYS	R1259	E1183	G1126	F1124	E1054	A989	L929	I871	G807		
LYS	M1260	I1184	H1127	G1124	P1055	G992	T931	E872	Y808		
ARG	D1261	G1185	H1127	G1126	P1056	N994	L932	K873	E741		
ALA	G1262	D1186	G1127	G1126	D1057	A997	L933	L874	L675		
ALA	T1263	F1187	G1128	H1127	Q1058	D998	L935	A875	T676		
GLY	V1264	F1188	Q1130	G1130	E1059	R1000	G936	A876	A677		
ASP	D1265	L1189	R1131	Q1130	P1060	V1001	G937	E876	A678		
PRO	T1266	S1193	H1133	R1131	P1061	A1002	C937	N877	L750		
ASP	P1267	L1194	L1134	L1134	Q1062	Q1003	H938	I878	S751		
TYR	P1268	G1195	G1135	G1135	V1063	W1005	V939	I879	S752		
	R1271	P1196			M1064	W1005	G940	R818	L753		
					Q1066	S1008	N941	E819	P754		
					S1067	A1009	A942	E819	S754		
					R1068		D943	R820	L688		
					W1069		E944	R822	L689		
							A946	L823	E690		
								E824	G691		
									Y692		

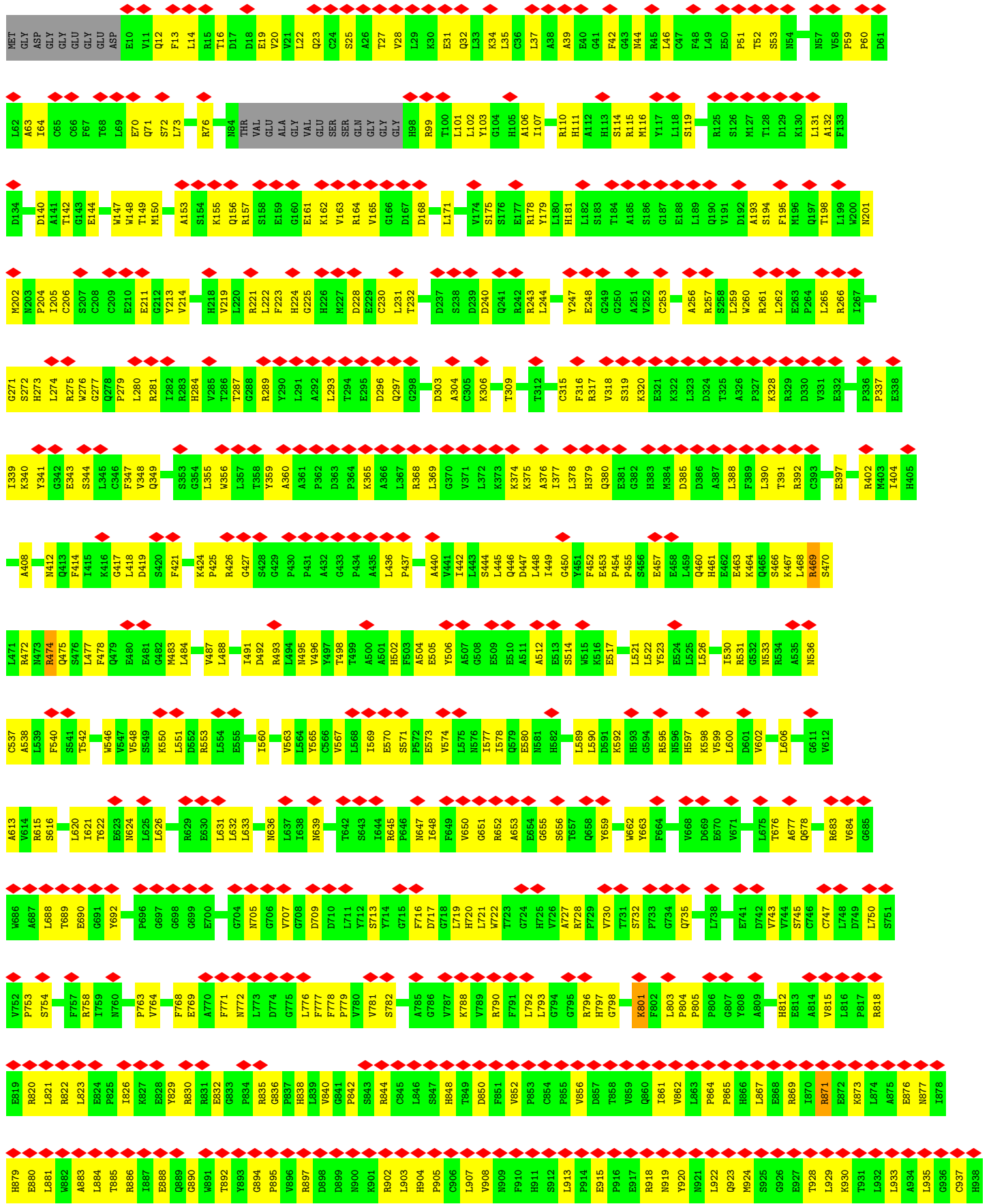


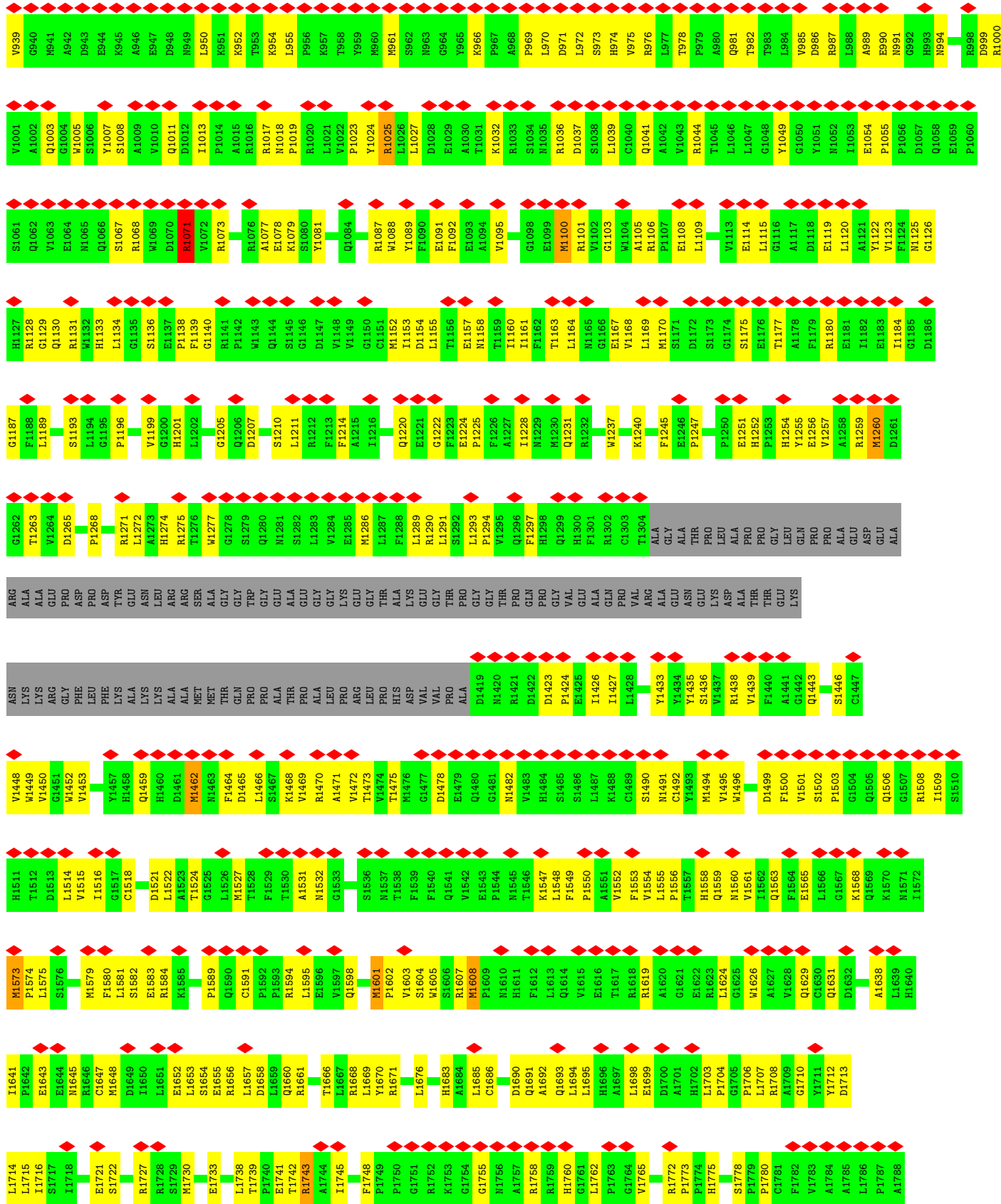
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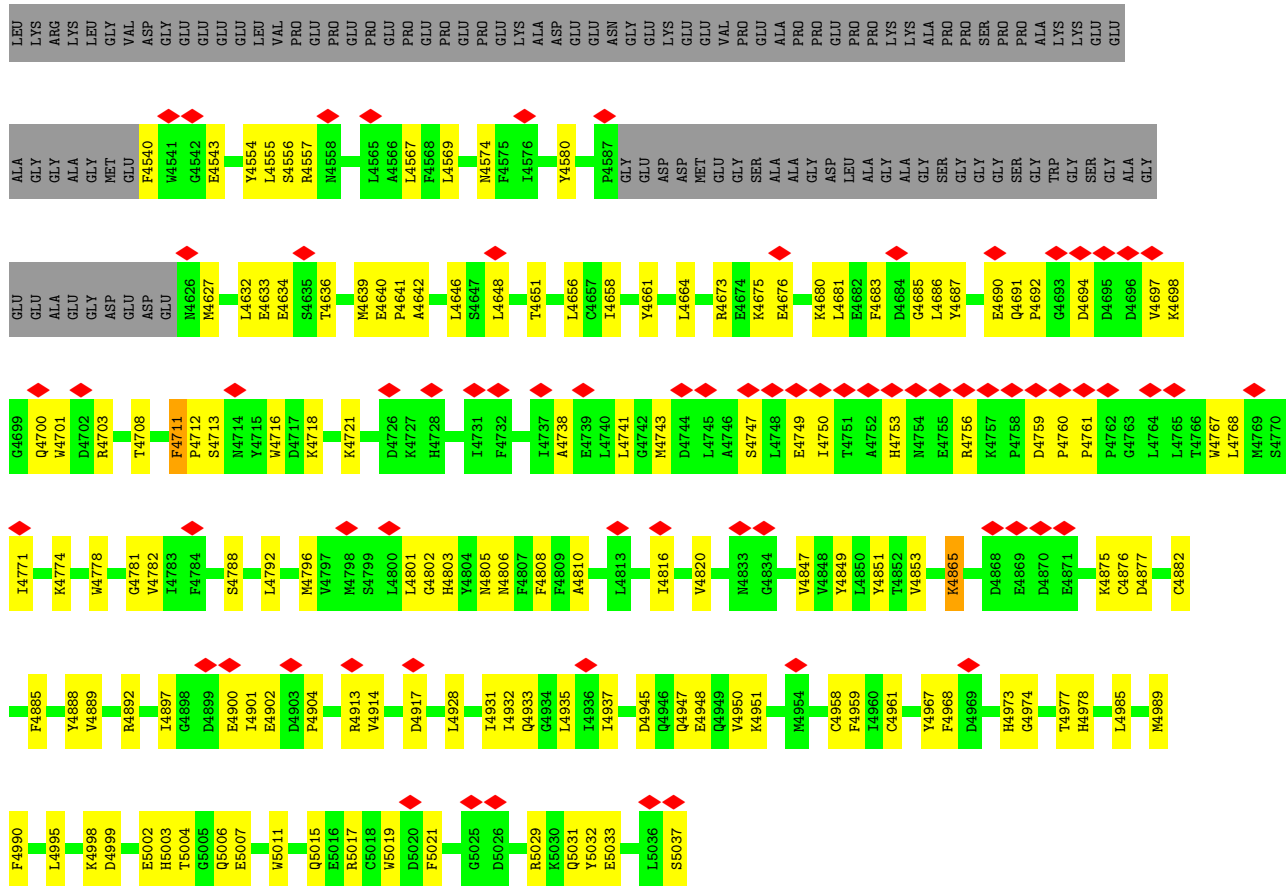
• Molecule 1: Ryanodine receptor 1



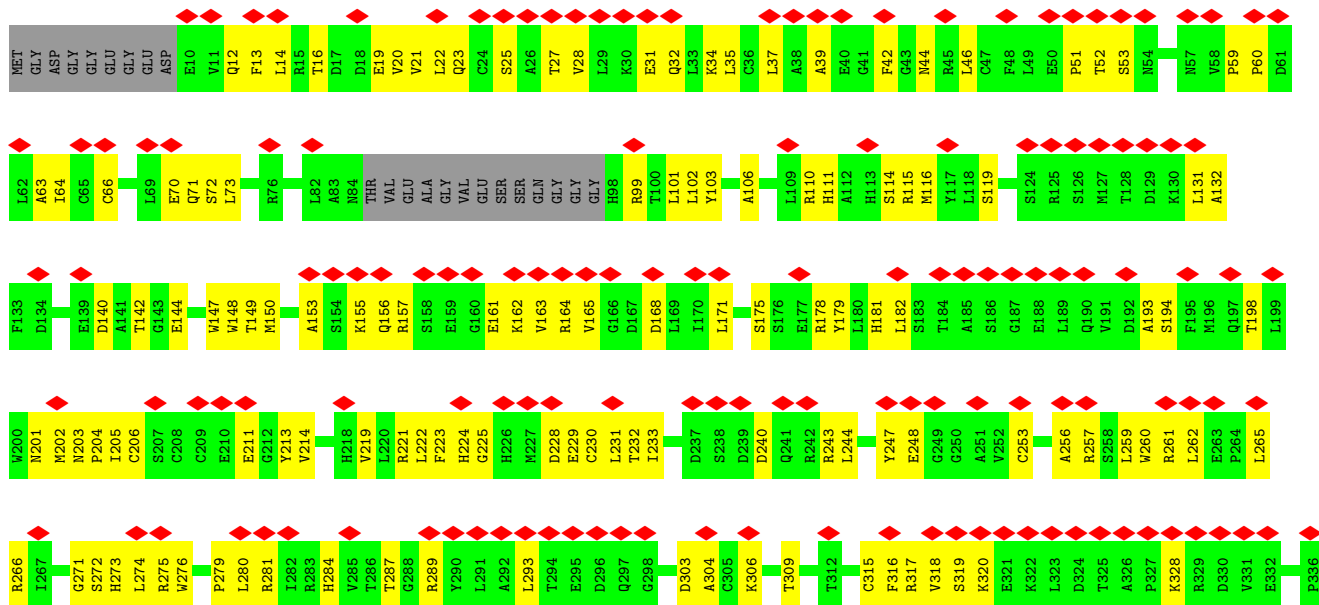


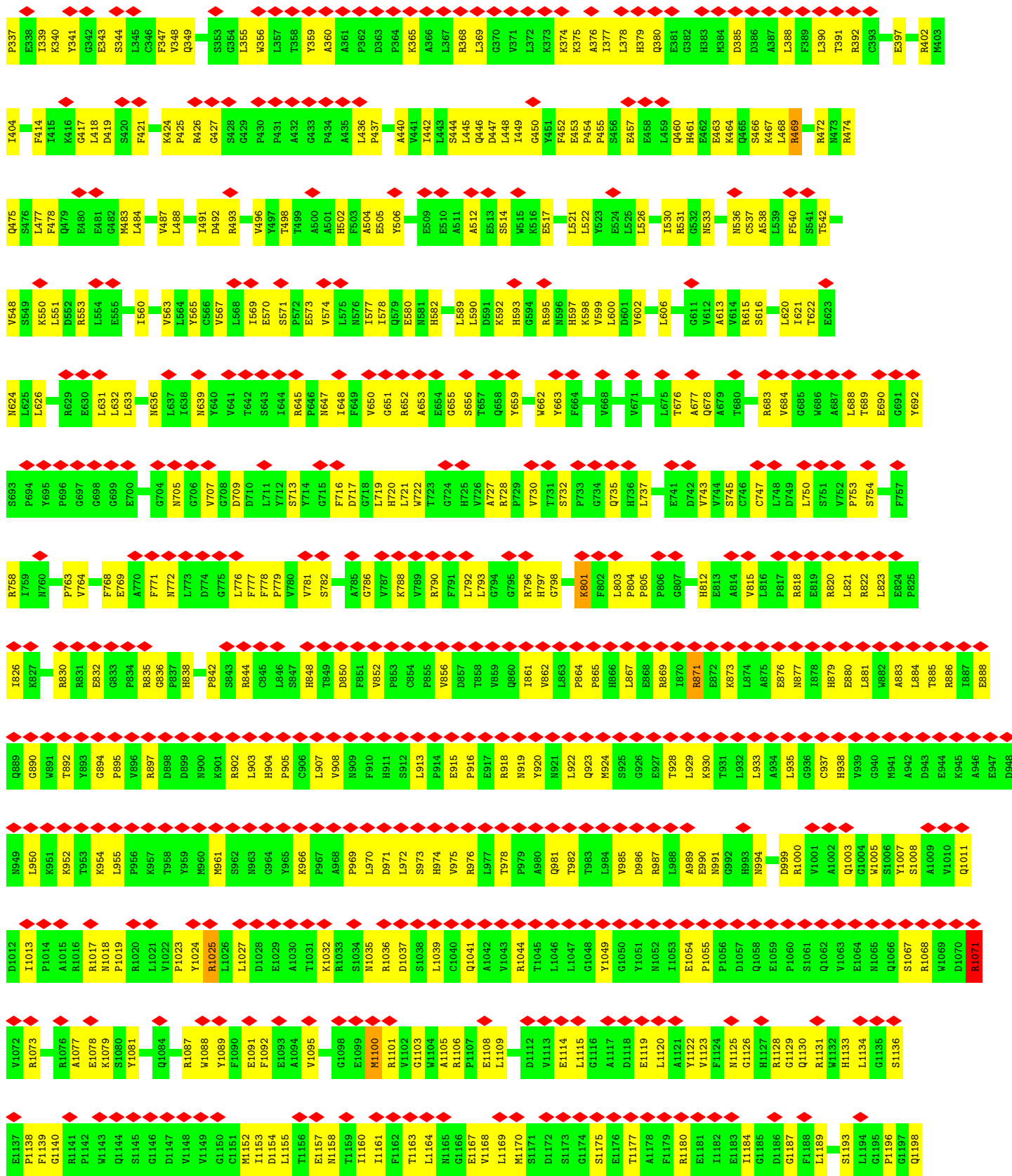


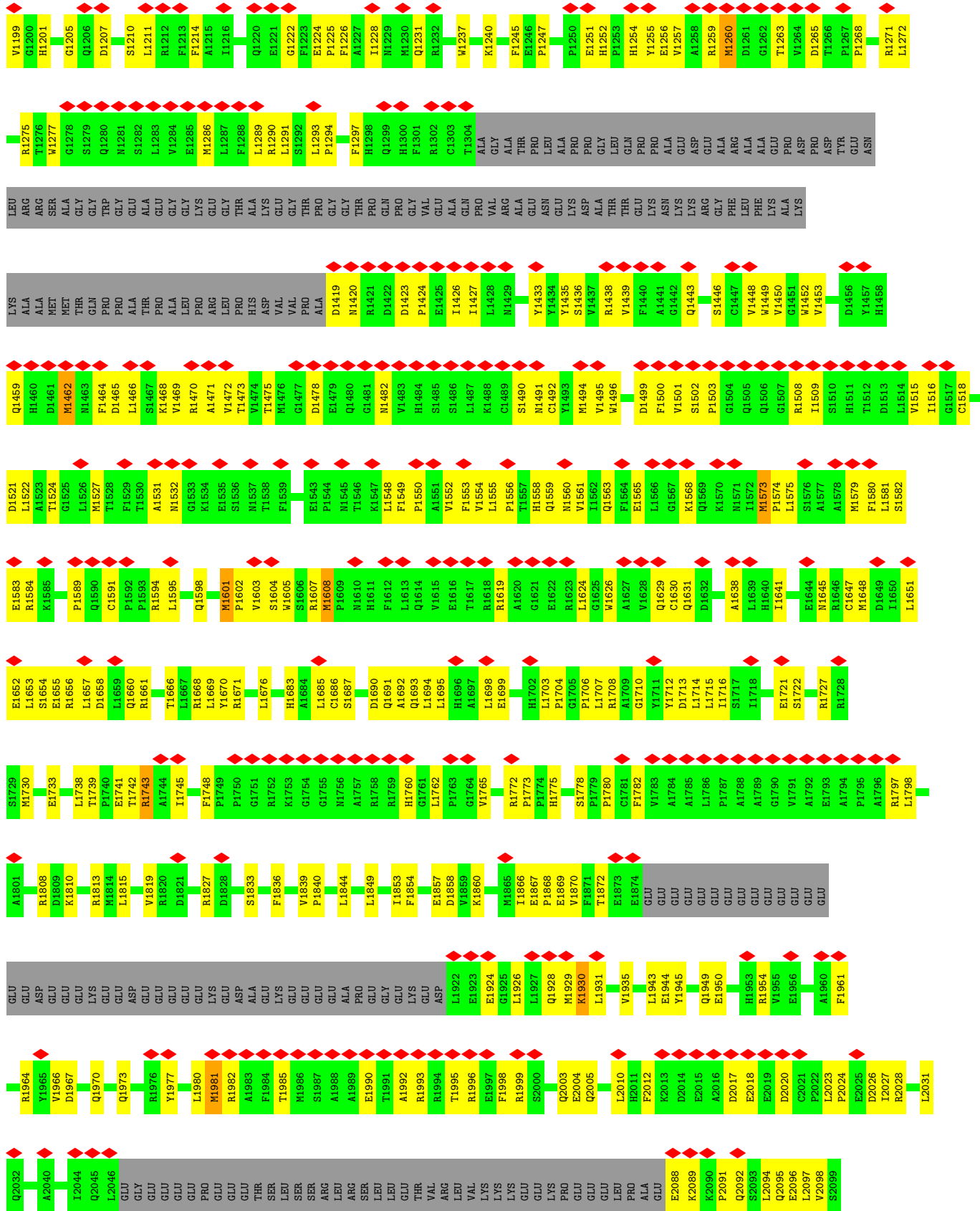
The image displays a grid of amino acid residues from the wwPDB EM Validation Summary Report for EMD-47386, 9E19. Each residue is represented by a colored box containing its 3-letter code and the corresponding amino acid code. The colors indicate the quality of the electron density map for each residue: green for well-resolved, yellow for medium, orange for poor, and grey for missing or unresolvable. Small red diamonds are placed above or below certain boxes to indicate specific validation flags. The residues are arranged in a grid that is approximately 15 columns wide and 25 rows high.



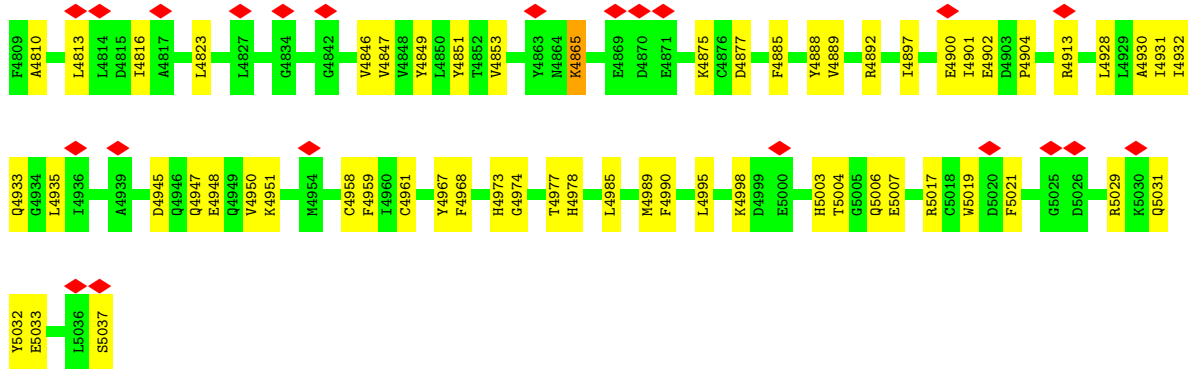
• Molecule 1: Ryanodine receptor 1



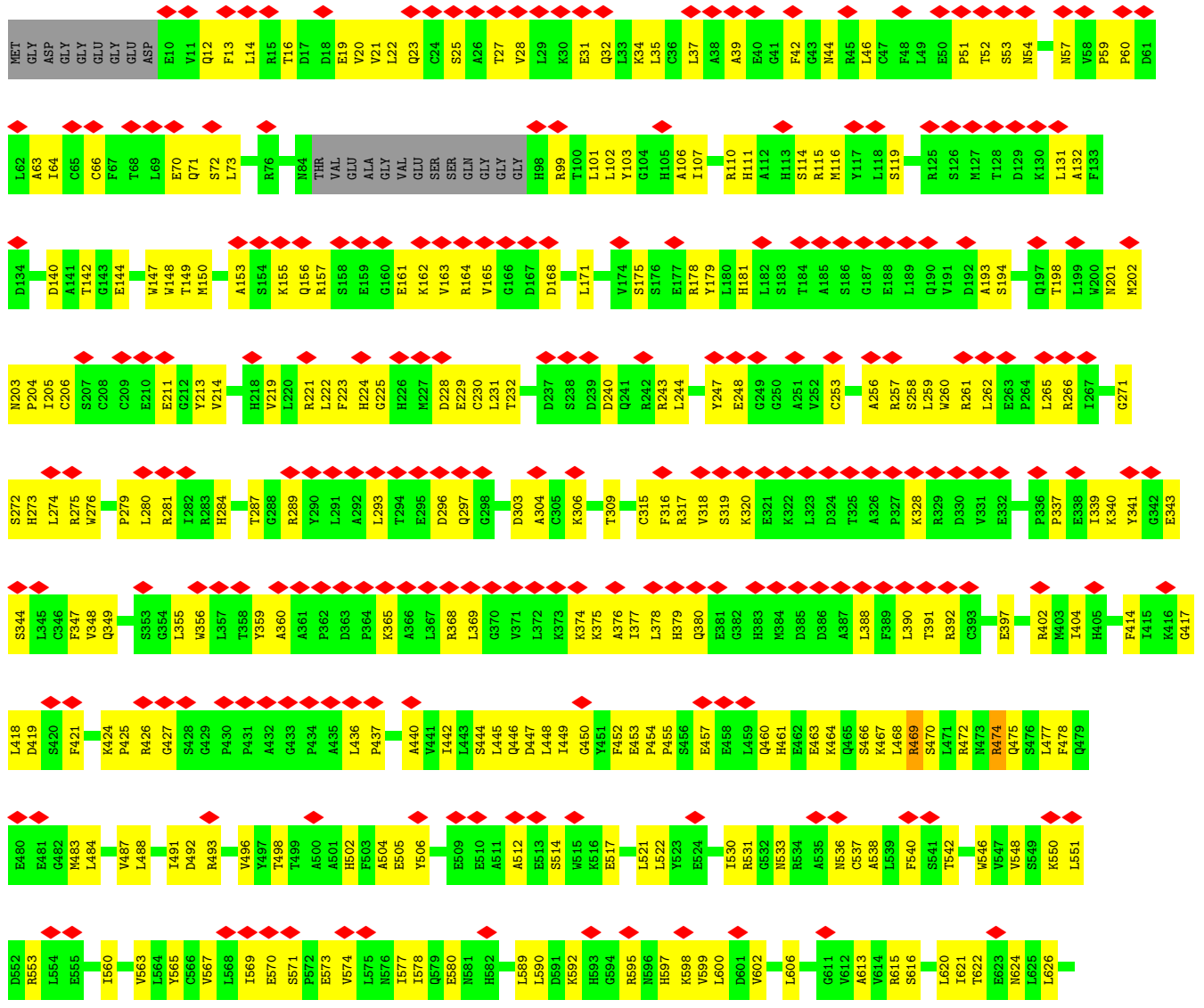
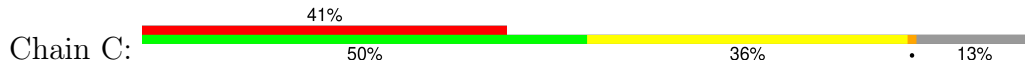


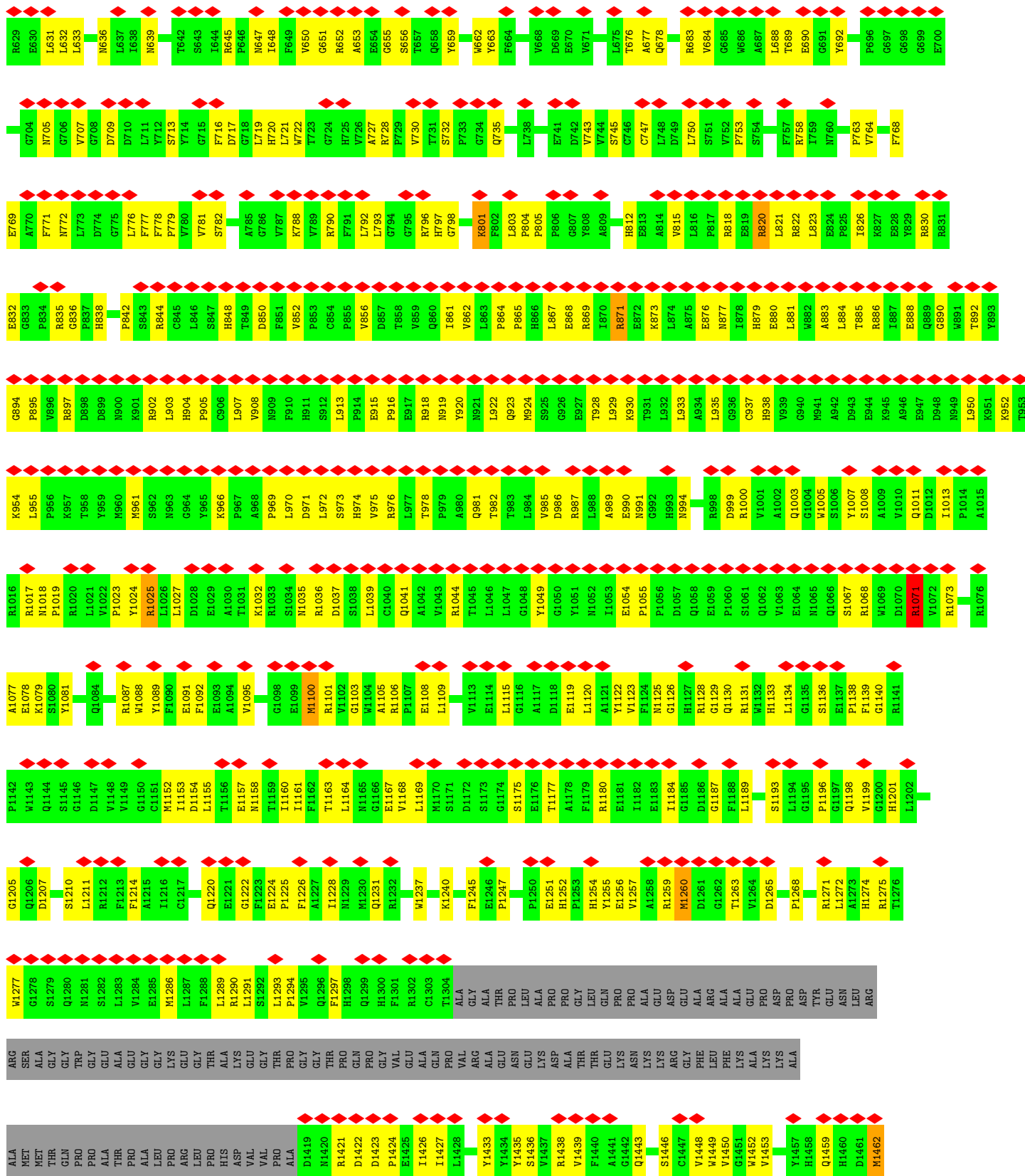


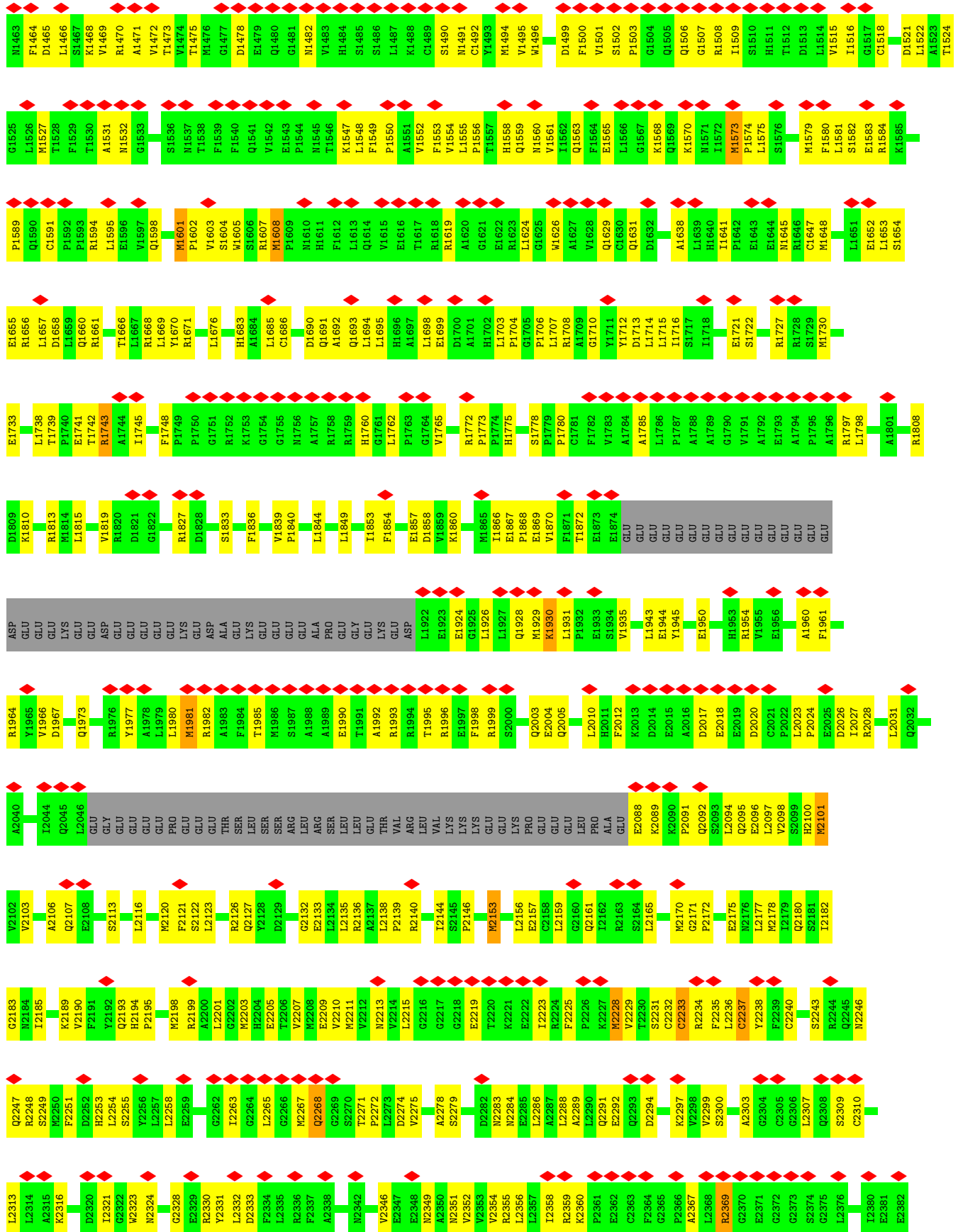
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● Molecule 1: Ryanodine receptor 1

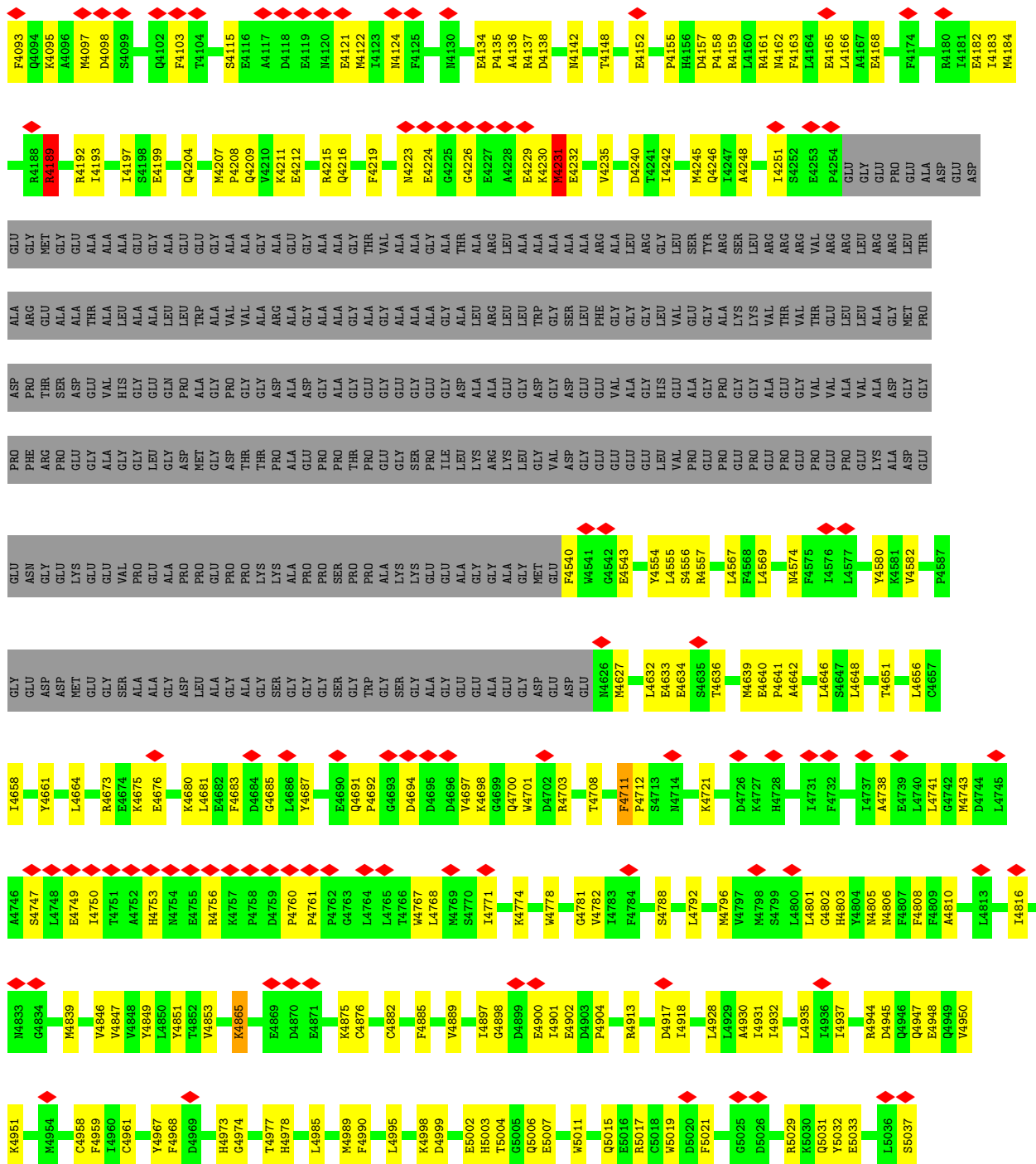




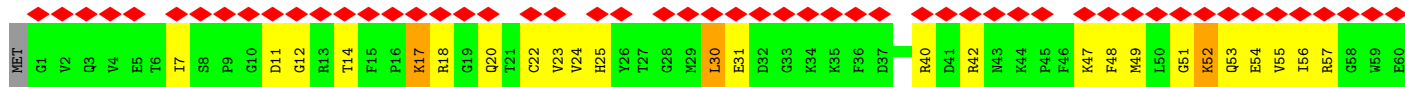
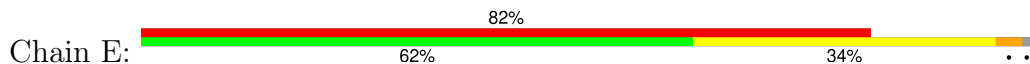


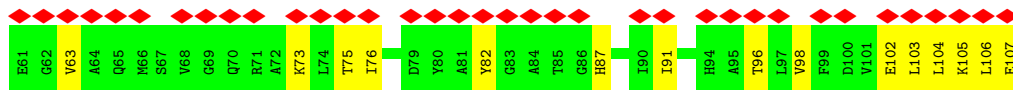
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L2522	D2523	V2524	G2525	F2526	L2527	P2528	D2529	M2530	R2531	A2532	A2533	A2534	S2535	L2536	D2537	T2538	A2539	T2540	F2541	S2542	T2543	L2544	E2545	M2546	A2547	L2548	R2552	Y2553	L2556	A2557	L2558	L2559	P2560	L2561	I2562	T2563	K2564	C2565	A2566	F2569	A2570	G2571	T2572	E2573	H2574	R2575	A2576	I2577	M2578	V2579	D2580	S2581	L2582	L2583	H2584	T2585				
R2588	L2589	S2590	R2591	G2592	R2593	S2594	L2595	T2596	K2597	A2598	Q2599	R2600	D2601	V2602	L2603	E2604	D2605	C2606	L2607	M2608	A2609	L2610	C2611	E2612	L2614	R2615	P2616	M2618	L2619	Q2620	F2621	H2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	F2631	I2632	L2633	N2634	E2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	M2646				
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G2708	A2709	L2710	P2711	Q2712	D2713	Y2714	V2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	LYS	ALA	THR	VAL	ASP	ALA	GLU	N2734	D2735	F2736	P2737	L2738	P2739	V2740	E2741	L2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	H2762	H2763	E2764	K2765	W2766	A2767			
F2768	D2769	K2770	I2771	M2772	Q2773	N2774	W2775	Y2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	R2806	V2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	V2819	E2820	Y2821	T2822	I2823	E2824	K2825	A2826	R2827			
E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	M2856	Q2858	P2859	F2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	Y2883	M2884	T2885	W2886	G2887				
R2888	K2889	R2890	K2891	E2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	Y2906	P2907	Y2908	D2909	T2910	L2911	T2912	F2913	Y2914	K2915	E2916	K2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	K2929	F2929	L2930	Q2931	M2932	G2933	G2934	Y2935	A2936	Y2937	T2938	G2939	I3001	L3002	L3003	P3004	L3005	I3006	L2946	D2947
T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	P2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	I2995	K2996	F2997	P2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	N3007	
Q3008	Y3009	F3010	T3011	M3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	G3032	N3033	K3034	E3035	K3036	E3037	M3038	L3039	T3040	S3041	L3042	F3043	C3044	K3045	V3046	E2987	A3047	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	L3063	A3064	V3065	N3066	C3067	
L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	M3080	K3082	S3083	G3084	E3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	L3125	L3126	G3127	Q3128	F3129	A3130

L3190	G3191	E3192	G3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	P3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	E3226	R3227	A3228	E3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	L3246	R3248	L3249						
M3250	A3251	D3252	G3253	G3254	L3255	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	M3266	P3267	H3268	V3269	I3270	E3271	I3272	T3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	L3229	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	V3307	S3309				
D3310	H3311	L3312	N3313	S3314	L3315	L3316	G3317	N3318	L3319	L3320	R3321	I3322	I3323	V3324	N3325	M3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	W3334	M3335	K3336	R3337	L3338	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	A3349	R3350	P3351	L3354	S3355	H3356	H3357	F3358	I3359	V3415	V3416	D3417	N3418	G3419	R3420	H3422	W3423	L3424	P3427	N3428	A3429	R3430	S3431		
K3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	R3380	L3381	E3382	A3383	K3384	A3385	E3386	L3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	R3397	F3398	S3399	V3400	L3401	C3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	P3410	L3411	L3412	I3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	H3422	W3423	L3424	P3427	N3428	A3429	R3430	S3431						
E3432	E3433	L3434	F3435	R3436	M3437	V3438	G3439	I3441	F3442	L3443	Y3444	W3445	S3446	K3447	S3448	H3449	N3450	F3451	R3452	E3453	E3454	A3455	Q3456	N3457	F3458	V3459	V3460	Q3461	E3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	D3472	D3473	S3474	K3475	S3476	M3477	A3479	LYS	ALA	GLY	ASP	GLN	ALA	SER	SER	GLY	GLY	ASP	GLN	A3431				
GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	V3503	S3504	V3505	Q3506	T3507	S3508	L3509	V3511	A3512	T3513	L3514	K3515	L3516	M3517	L3518	P3519	I3520	G3521	L3522	N3523	M3524	C3525	A3526	F3527	L3528	D3529	Q3530	D3531	L3532	M3533	Q3534	A3535	K3537	T3538	R3539	Y3540	L3605	L3606	E3607	L3608	T3609	E3610	H3611	Y3612	E3613	E3614	S3615						
F3552	L3553	Q3554	N3555	R3556	L3557	H3558	L3559	Q3560	G3561	K3562	E3563	Q3564	G3565	S3566	P3567	S3568	W3571	Q3572	M3573	R3577	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	R3587	D3588	P3589	E3590	S3591	L3592	V3593	R3594	R3595	V3596	E3598	V3599	S3600	A3601	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	Y3612	E3613	E3614	S3615							
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E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	D3696	P3697	L3698	H3699	Q3700	L3701	R3707	L3710	T3711	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	L3721	Y3725	L3728	M3729	A3730	K3731	S3732	C3733	H3734	L3735	E3736	GLU	GLY	GLY	ASN	GLY	GLU	ALA	GLU	GLU	GLU	GLU	V3749	E3750	V3751									
S3752	F3753	E3754	E3755	K3756	E3757	M3758	R3762	S3768	R3769	L3770	H3771	T3772	R3773	G3774	A3775	V3779	C3786	K3787	G3788	M3793	V3794	T3797	I3802	S3803	F3804	L3805	E3811	L3817	D3818	Y3819	K3821	D3822	K3823	K3824	E3825	V3826	F3829	Q3830	L3835	T3838	L3842	D3843	L3844	N3845	E3848	N3850	K3851	M3852	F3859	G3908	N3909	T3910	L3913	L3916	L3917	V3920	Q3927	E3928	S3929	L3930	S3931	D3932
F3933	L4016	L4017	D4018	L4019	Q4020	K4021	D4022	M4023	V4024	E3943	E3944	Q3945	Q3946	G3947	K3948	R3949	F3951	M3955	S3956	V3957	A3958	K3959	Q3960	V3961	F3962	N3963	L3965	T3966	E3967	Y3968	L3969	Q3970	L3980	A3981	L3985	W3986	V3989	G3990	G3991	F3992	L3993	H3994	V3995	F3996	A3997	H3998	M3999	M4000	M4001	K4002	L4003	Q4009	L4012	K4090								

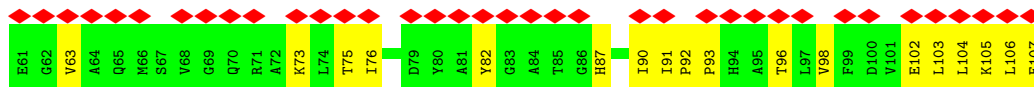
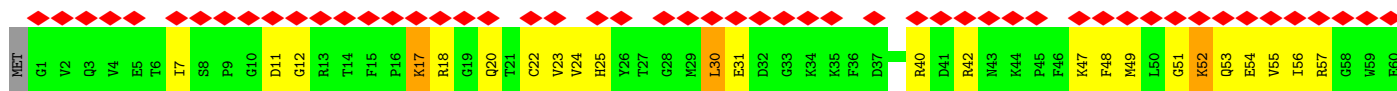
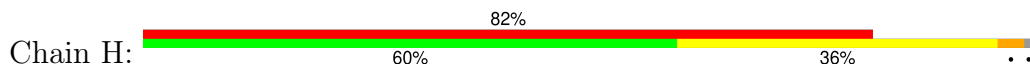


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

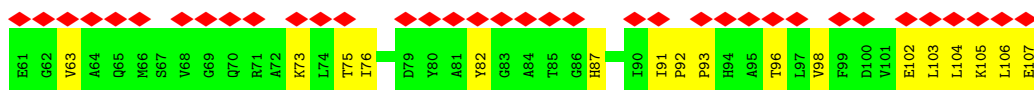
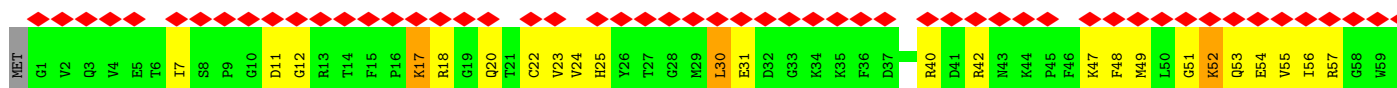
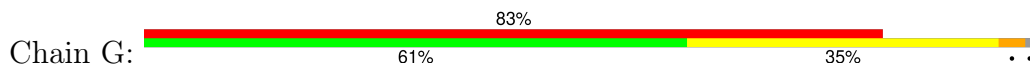




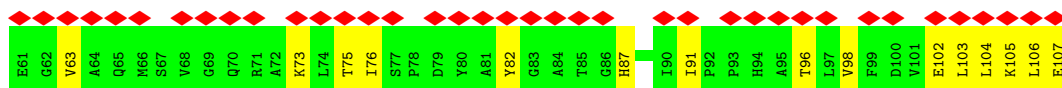
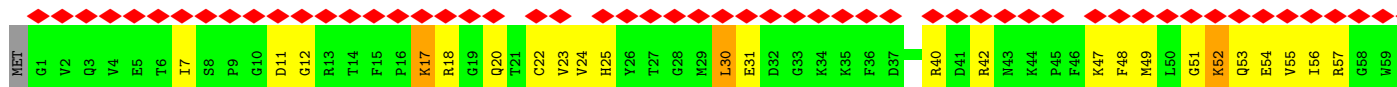
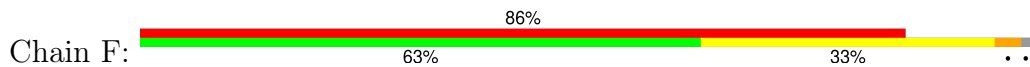
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• 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	3336	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	0.283	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	2/35977 (0.0%)	0.54	14/48726 (0.0%)
1	B	0.27	2/35977 (0.0%)	0.54	14/48726 (0.0%)
1	C	0.27	2/35977 (0.0%)	0.54	14/48726 (0.0%)
1	D	0.27	2/35977 (0.0%)	0.54	14/48726 (0.0%)
2	E	0.27	0/850	0.59	1/1146 (0.1%)
2	F	0.27	0/850	0.59	1/1146 (0.1%)
2	G	0.27	0/850	0.59	1/1146 (0.1%)
2	H	0.27	0/850	0.59	1/1146 (0.1%)
All	All	0.27	8/147308 (0.0%)	0.55	60/199488 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2233	CYS	CB-SG	-5.92	1.72	1.81
1	C	2233	CYS	CB-SG	-5.91	1.72	1.81
1	A	2233	CYS	CB-SG	-5.91	1.72	1.81
1	B	2233	CYS	CB-SG	-5.90	1.72	1.81
1	A	2237	CYS	CB-SG	5.70	1.92	1.82

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2578	MET	CB-CG-SD	8.49	137.88	112.40
1	A	2578	MET	CB-CG-SD	8.48	137.85	112.40
1	B	2578	MET	CB-CG-SD	8.48	137.85	112.40
1	C	2578	MET	CB-CG-SD	8.48	137.83	112.40
1	A	1071	ARG	CA-CB-CG	7.34	129.54	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1608	MET	Peptide
1	A	4189	ARG	Sidechain
1	B	1608	MET	Peptide
1	B	4189	ARG	Sidechain
1	D	1608	MET	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	35150	0	34793	1452	0
1	B	35150	0	34793	1463	0
1	C	35150	0	34793	1445	0
1	D	35150	0	34793	1424	0
2	E	831	0	831	31	0
2	F	831	0	831	27	0
2	G	831	0	831	29	0
2	H	831	0	831	30	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	18	2	0
6	B	20	0	18	2	0
6	C	20	0	18	1	0
6	D	20	0	18	1	0
All	All	144136	0	142616	5816	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 20.

The worst 5 of 5816 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:B:2639:MET:HG2	1:B:2640:PRO:HD3	1.47	0.97
1:C:2639:MET:HG2	1:C:2640:PRO:HD3	1.47	0.96
1:D:2639:MET:HG2	1:D:2640:PRO:HD3	1.47	0.96
1:A:2639:MET:HG2	1:A:2640:PRO:HD3	1.47	0.96
1:A:2821:TRP:NE1	1:A:2874:MET:SD	2.46	0.89

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%)	4260 (97%)	121 (3%)	4 (0%)	48 81
1	B	4385/5037 (87%)	4260 (97%)	121 (3%)	4 (0%)	48 81
1	C	4385/5037 (87%)	4260 (97%)	121 (3%)	4 (0%)	48 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	4385/5037 (87%)	4261 (97%)	120 (3%)	4 (0%)	48	81
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17960/20580 (87%)	17449 (97%)	495 (3%)	16 (0%)	50	81

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL
1	A	3300	ALA
1	A	4711	PHE
1	B	908	VAL
1	B	3300	ALA

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%)	3776 (98%)	60 (2%)	58	74
1	B	3836/4276 (90%)	3776 (98%)	60 (2%)	58	74
1	C	3836/4276 (90%)	3776 (98%)	60 (2%)	58	74
1	D	3836/4276 (90%)	3776 (98%)	60 (2%)	58	74
2	E	89/90 (99%)	86 (97%)	3 (3%)	32	54
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	54
2	G	89/90 (99%)	86 (97%)	3 (3%)	32	54
2	H	89/90 (99%)	86 (97%)	3 (3%)	32	54
All	All	15700/17464 (90%)	15448 (98%)	252 (2%)	62	74

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3201	MET
1	C	2369[B]	ARG
1	D	1260	MET
1	C	2268[B]	GLN
1	C	3283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	866	HIS
1	D	3734	HIS
1	D	1252	HIS
1	D	2971	GLN
1	C	156	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	5301	-	28,33,33	0.62	0	34,52,52	0.95	2 (5%)
3	ATP	D	5301	-	28,33,33	0.62	0	34,52,52	0.94	2 (5%)
6	PNX	C	5304	-	13,21,21	1.35	2 (15%)	13,30,30	1.06	1 (7%)
6	PNX	A	5304	-	13,21,21	1.36	2 (15%)	13,30,30	1.06	1 (7%)
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	0.95	2 (5%)
3	ATP	C	5301	-	28,33,33	0.61	0	34,52,52	0.95	2 (5%)
6	PNX	D	5304	-	13,21,21	1.36	2 (15%)	13,30,30	1.07	1 (7%)
6	PNX	B	5304	-	13,21,21	1.37	2 (15%)	13,30,30	1.07	1 (7%)

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	A	5301	-	-	4/18/38/38	0/3/3/3
3	ATP	D	5301	-	-	4/18/38/38	0/3/3/3
6	PNX	C	5304	-	-	4/7/7/7	0/2/2/2
6	PNX	A	5304	-	-	4/7/7/7	0/2/2/2
3	ATP	B	5301	-	-	4/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	4/18/38/38	0/3/3/3
6	PNX	D	5304	-	-	4/7/7/7	0/2/2/2
6	PNX	B	5304	-	-	4/7/7/7	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5304	PNX	C6-N1	-3.10	1.32	1.38
6	A	5304	PNX	C6-N1	-3.08	1.33	1.38
6	D	5304	PNX	C6-N1	-3.06	1.33	1.38
6	C	5304	PNX	C6-N1	-3.04	1.33	1.38
6	D	5304	PNX	O6-C6	-2.41	1.18	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	C4'-O4'-C1'	-4.29	106.00	109.92
3	A	5301	ATP	C4'-O4'-C1'	-4.26	106.02	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5301	ATP	C4'-O4'-C1'	-4.24	106.04	109.92
3	D	5301	ATP	C4'-O4'-C1'	-4.24	106.05	109.92
6	B	5304	PNX	C4-C5-C6	-2.69	117.91	119.96

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

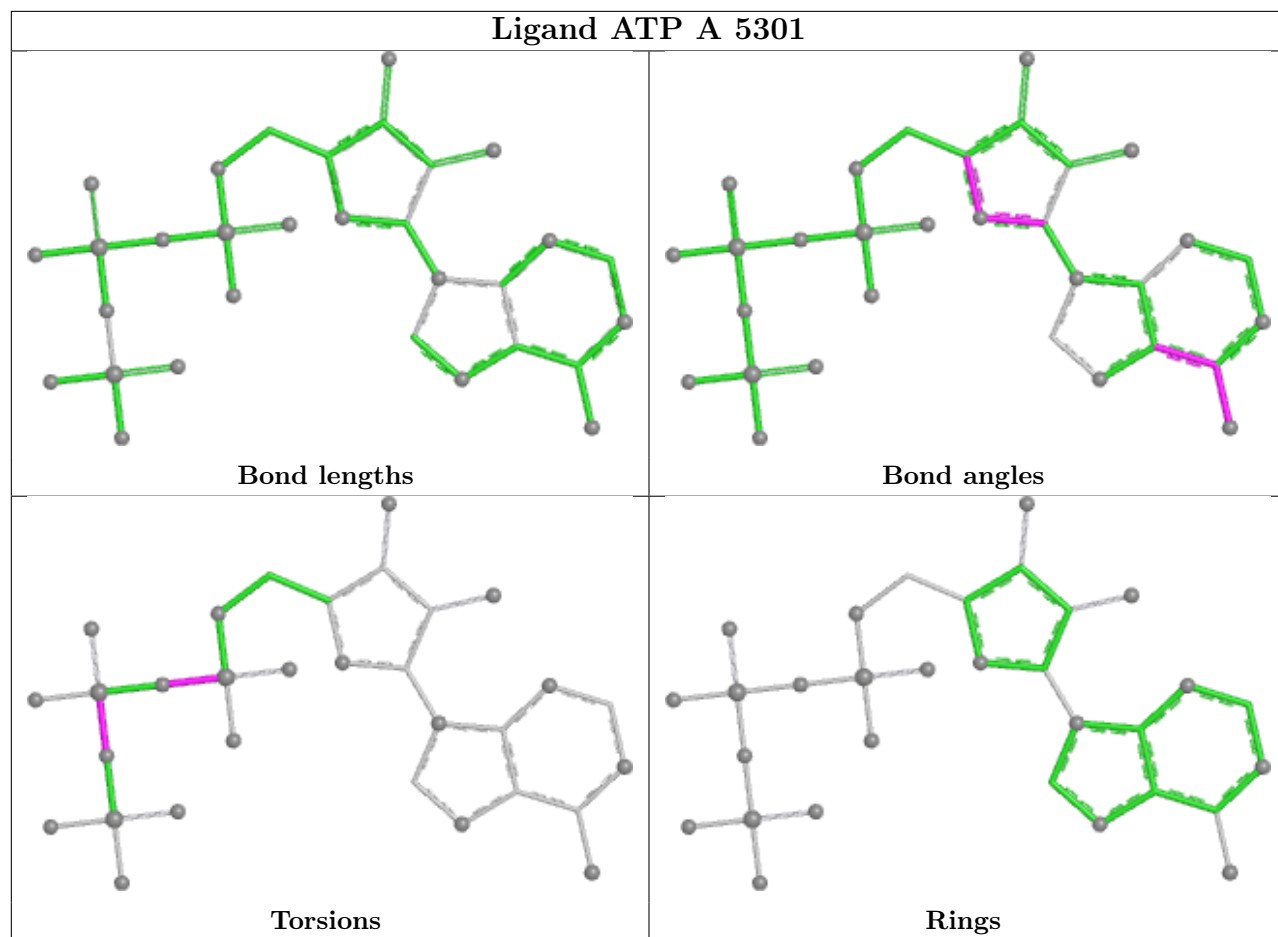
Mol	Chain	Res	Type	Atoms
6	A	5304	PNX	CAI-CAH-CAJ-CAM
6	B	5304	PNX	CAI-CAH-CAJ-CAM
6	D	5304	PNX	CAI-CAH-CAJ-CAM
6	C	5304	PNX	CAI-CAH-CAJ-CAM
6	A	5304	PNX	CAH-CAJ-CAM-OAD

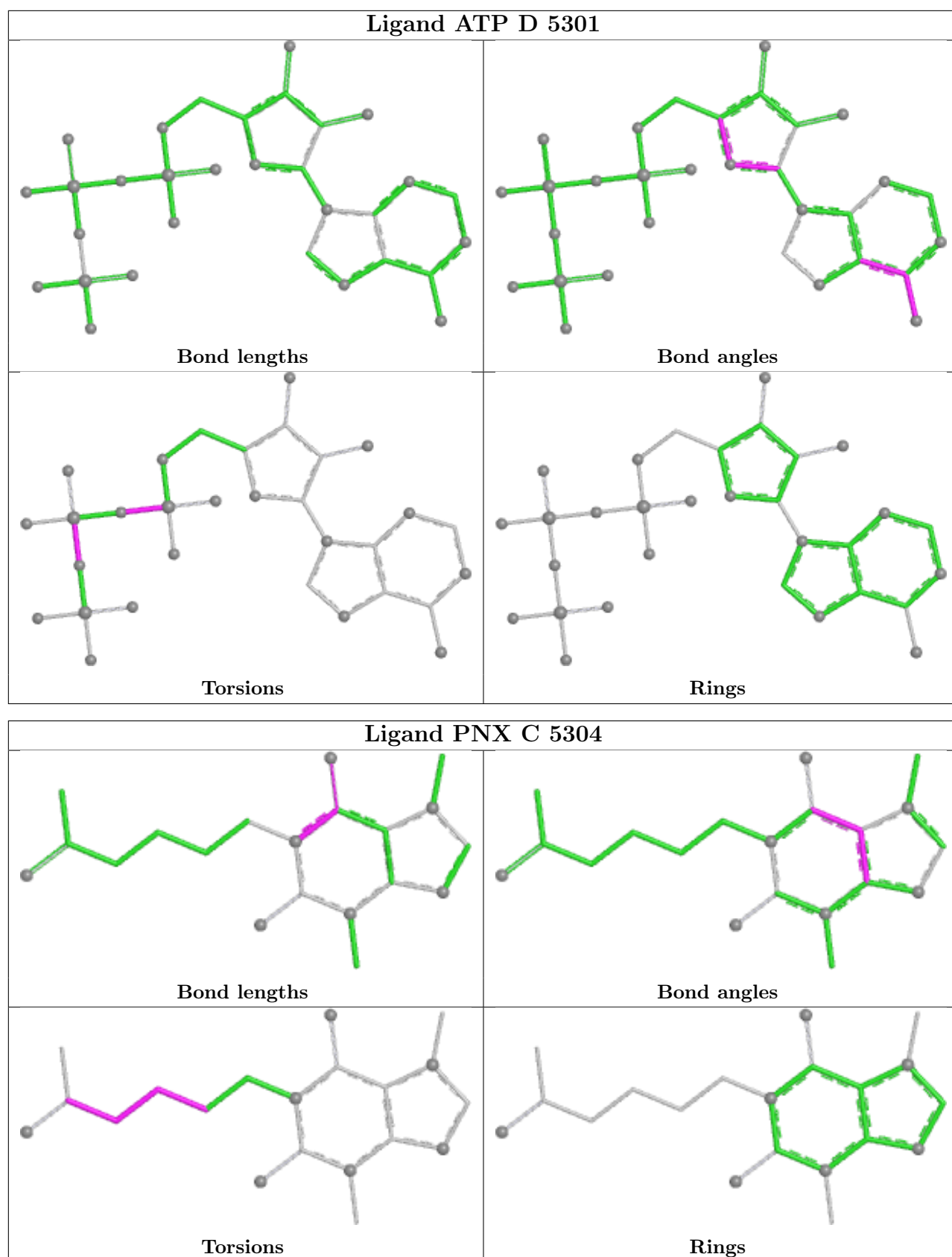
There are no ring outliers.

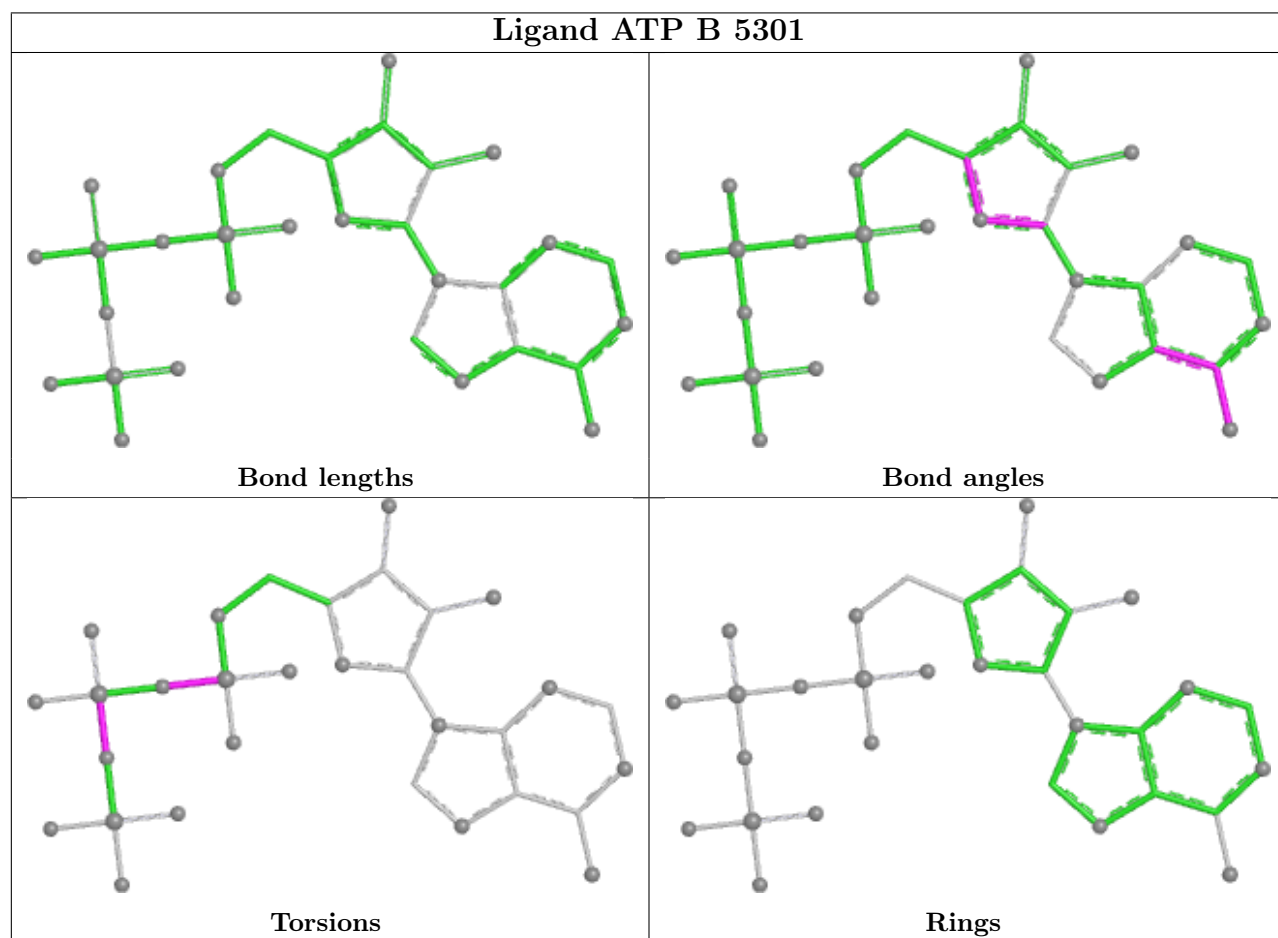
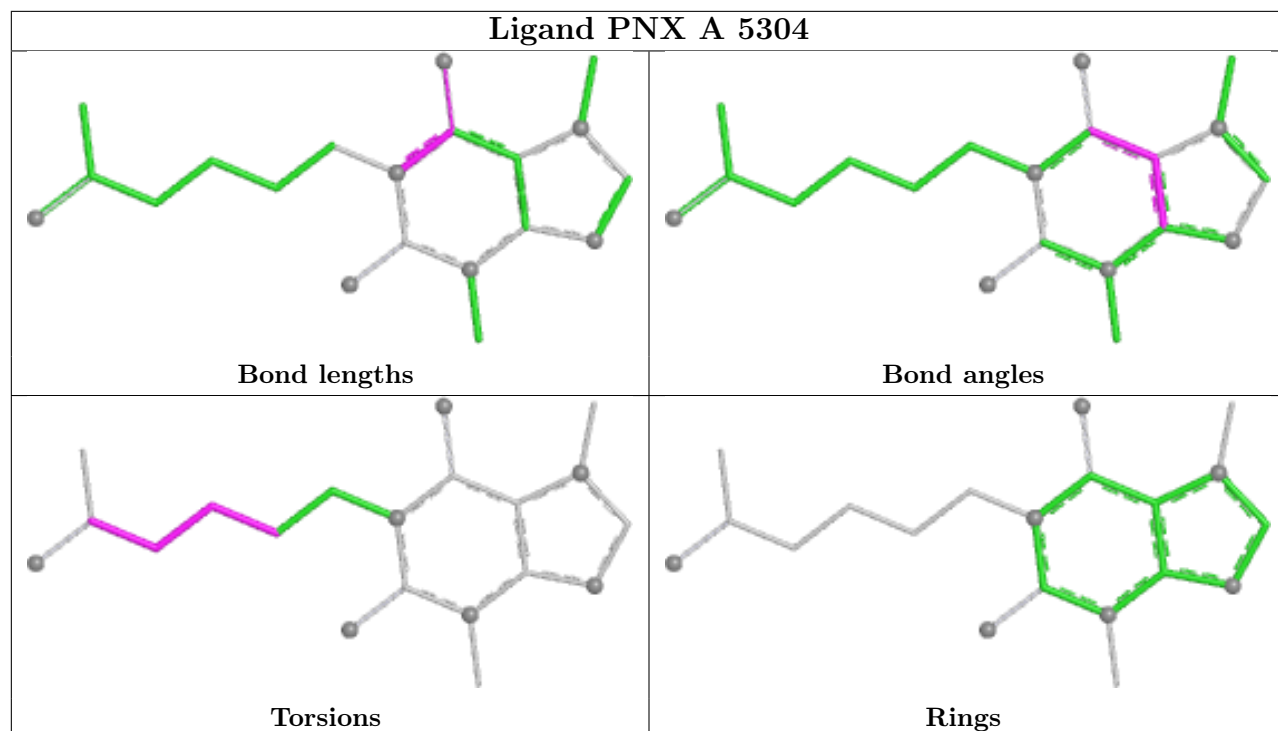
4 monomers are involved in 6 short contacts:

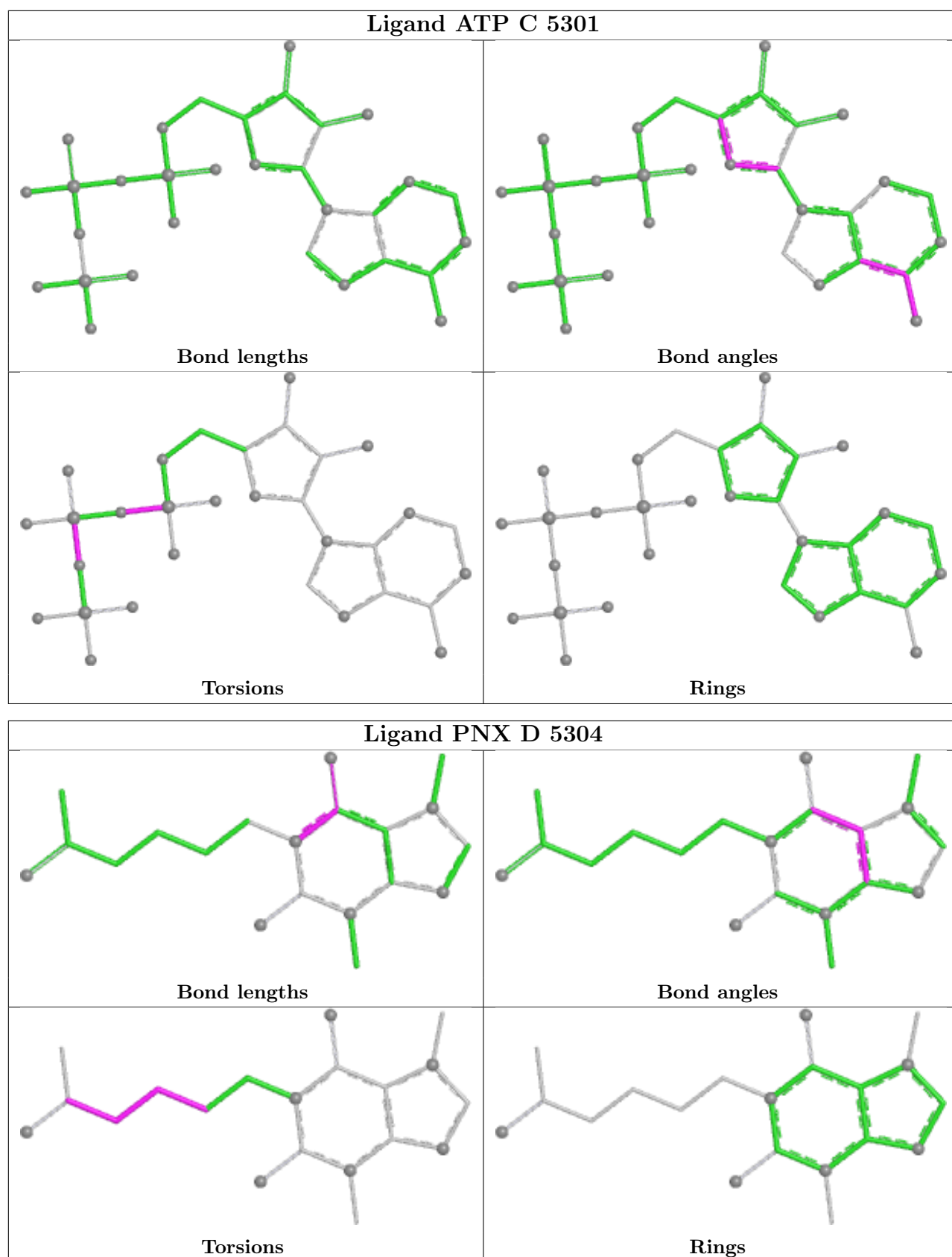
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5304	PNX	1	0
6	A	5304	PNX	2	0
6	D	5304	PNX	1	0
6	B	5304	PNX	2	0

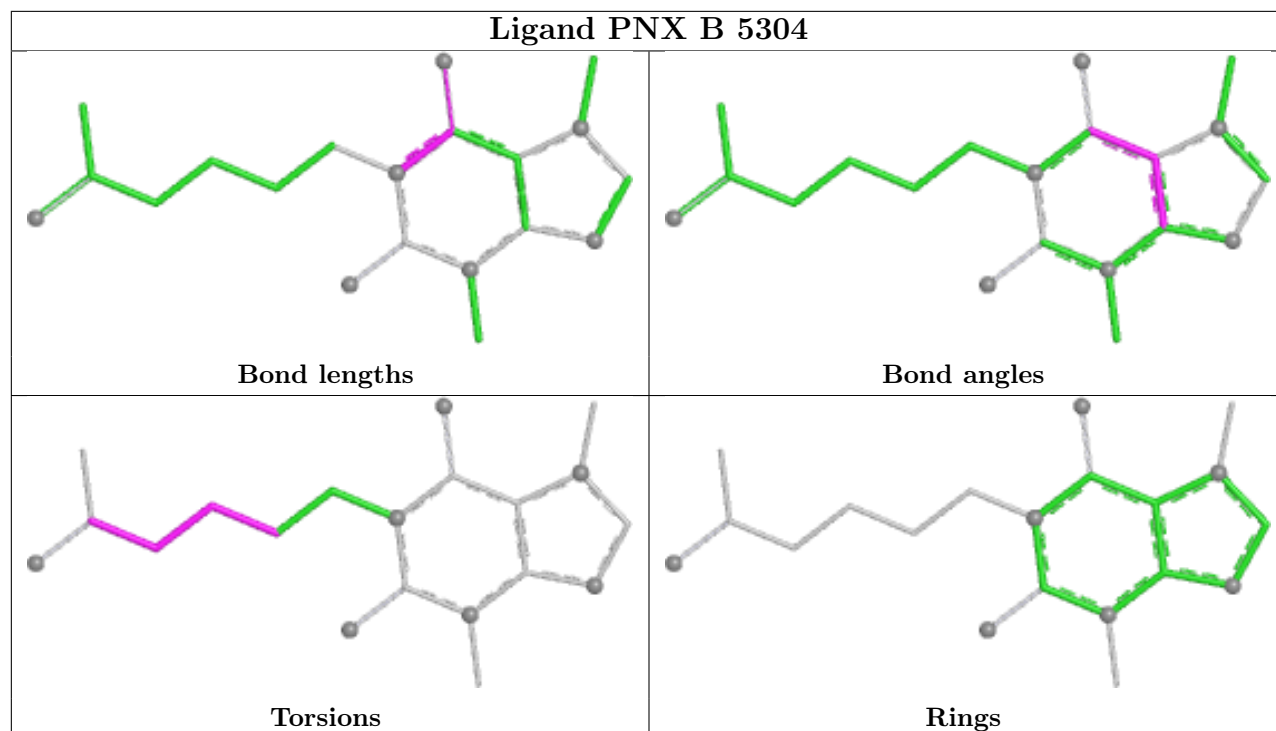
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

There are no chain breaks in this entry.

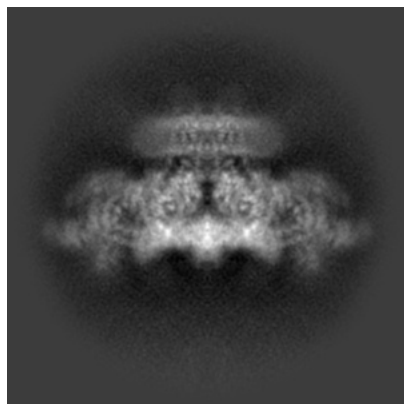
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47386. These allow visual inspection of the internal detail of the map and identification of artifacts.

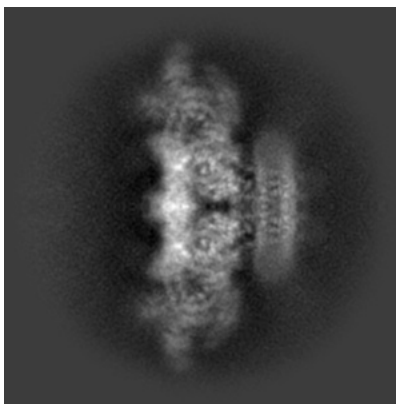
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

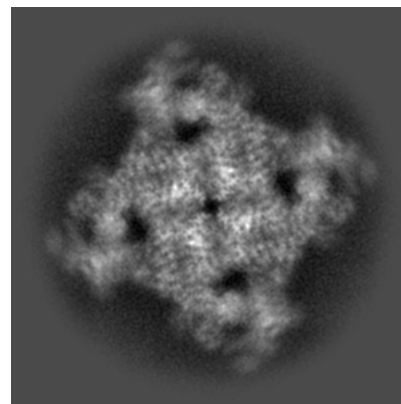
6.1.1 Primary map



X

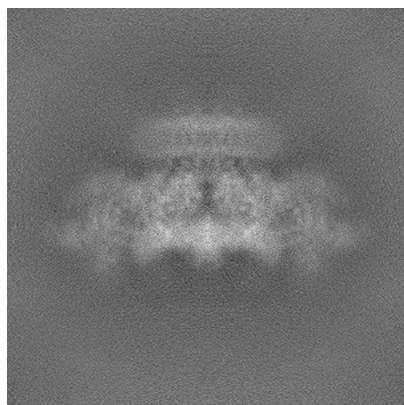


Y

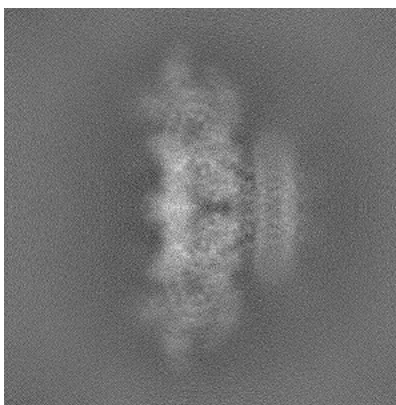


Z

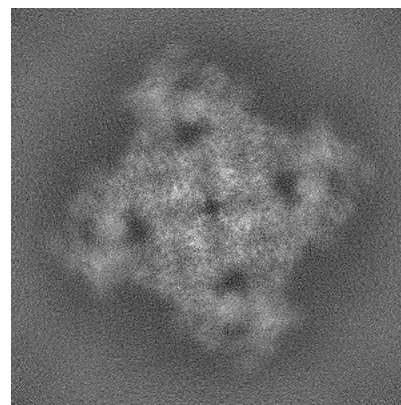
6.1.2 Raw map



X



Y

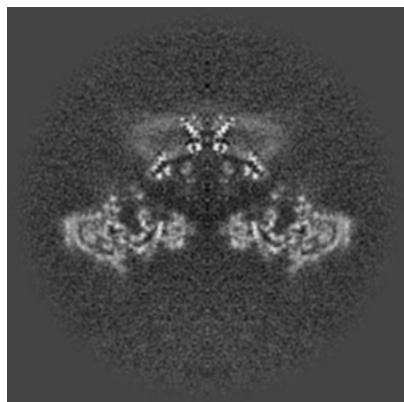


Z

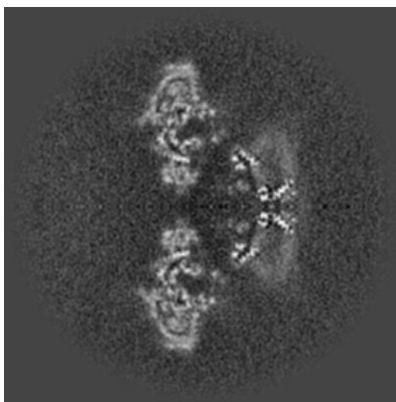
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

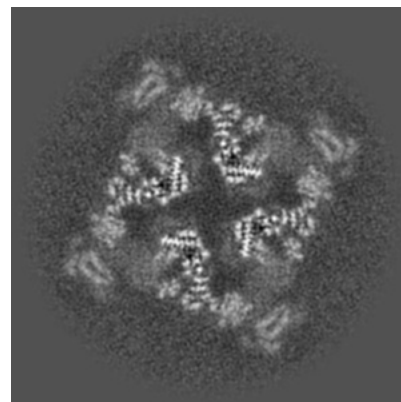
6.2.1 Primary map



X Index: 256

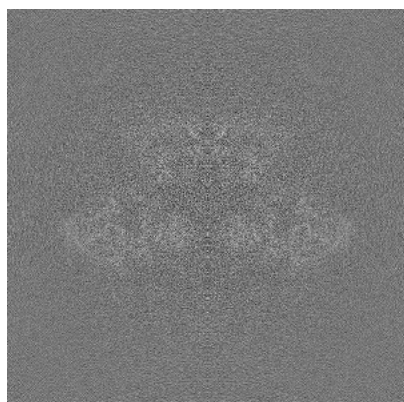


Y Index: 256

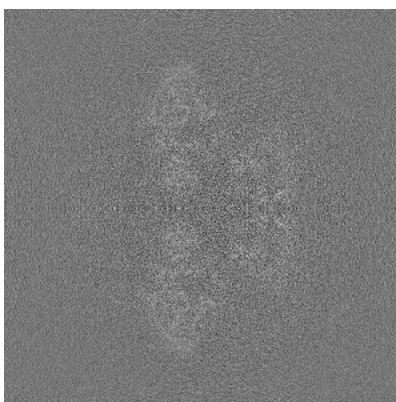


Z Index: 256

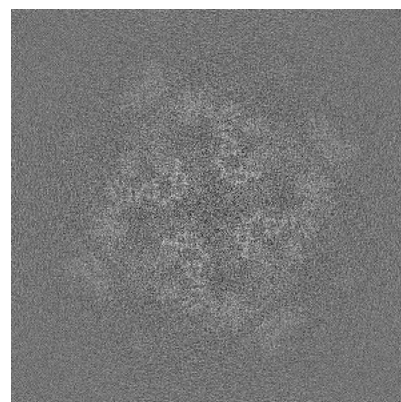
6.2.2 Raw map



X Index: 256



Y Index: 256

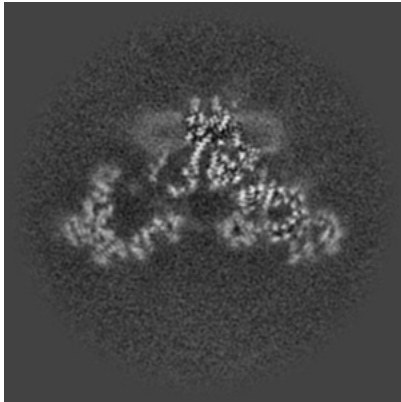


Z Index: 256

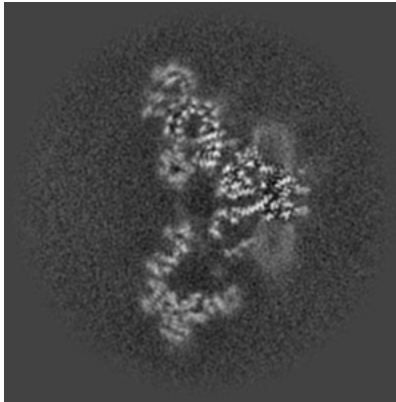
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

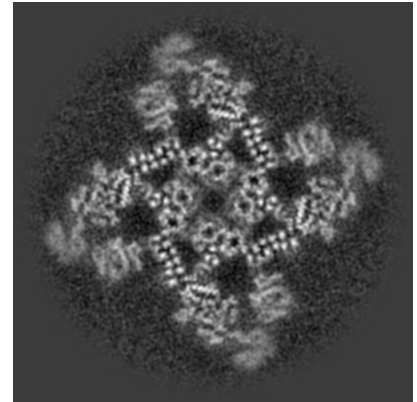
6.3.1 Primary map



X Index: 269

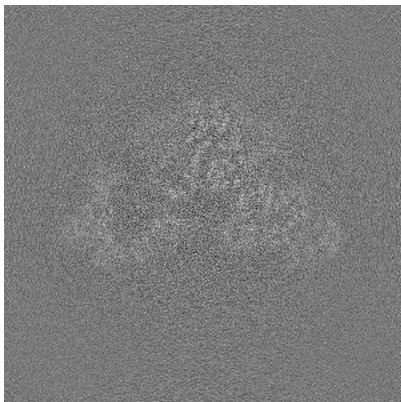


Y Index: 243

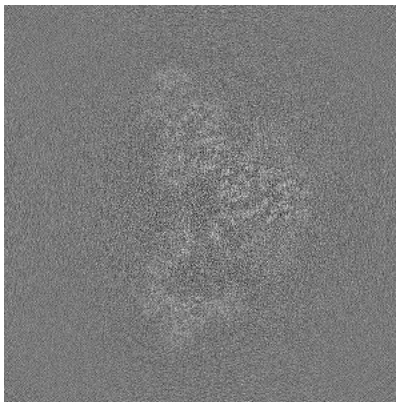


Z Index: 229

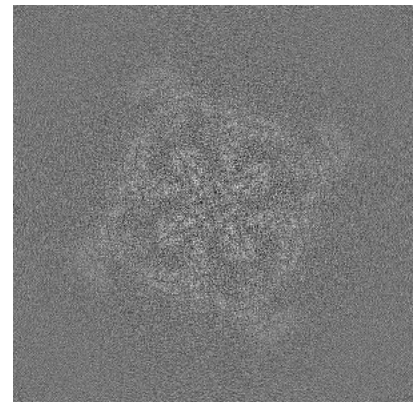
6.3.2 Raw map



X Index: 270



Y Index: 242

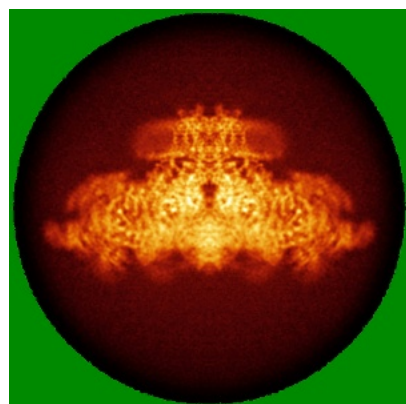


Z Index: 275

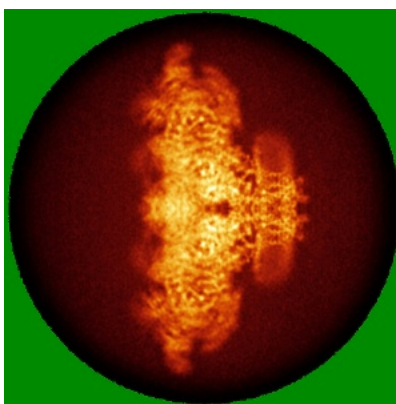
The images above show the largest variance slices of the map in three orthogonal directions.

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

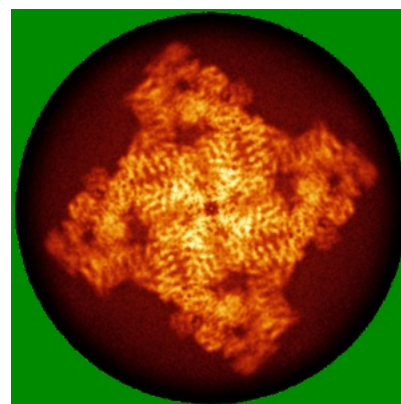
6.4.1 Primary map



X

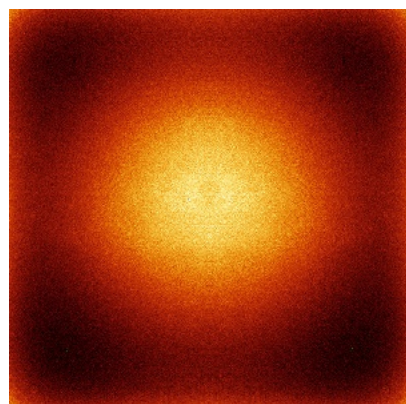


Y

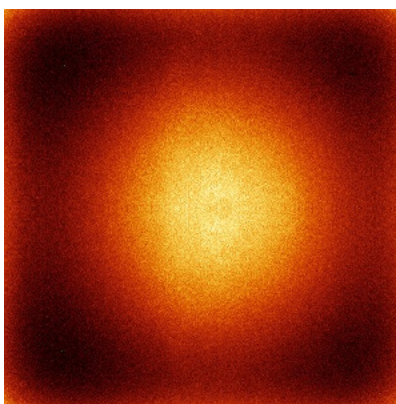


Z

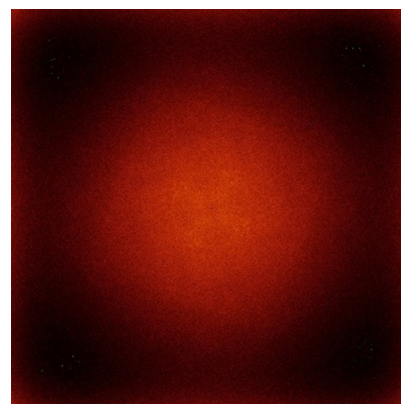
6.4.2 Raw map



X



Y

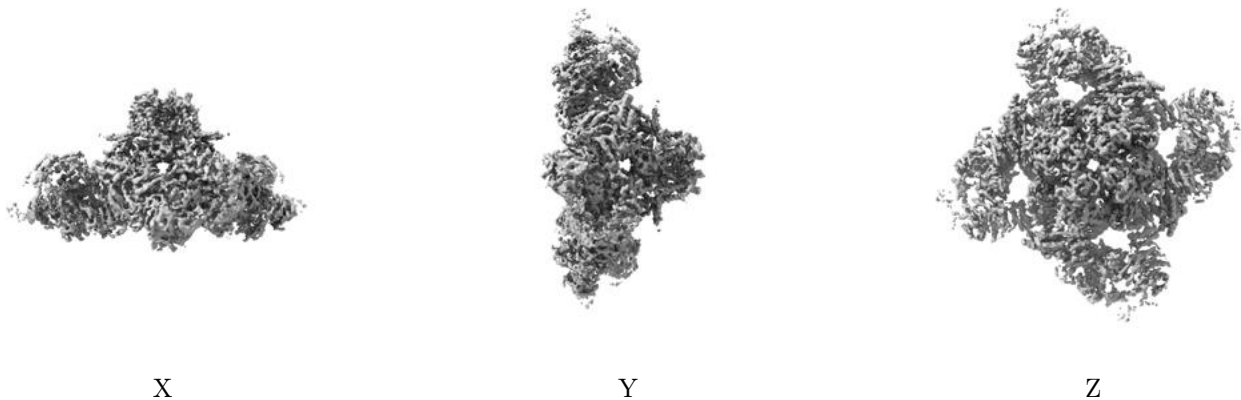


Z

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.

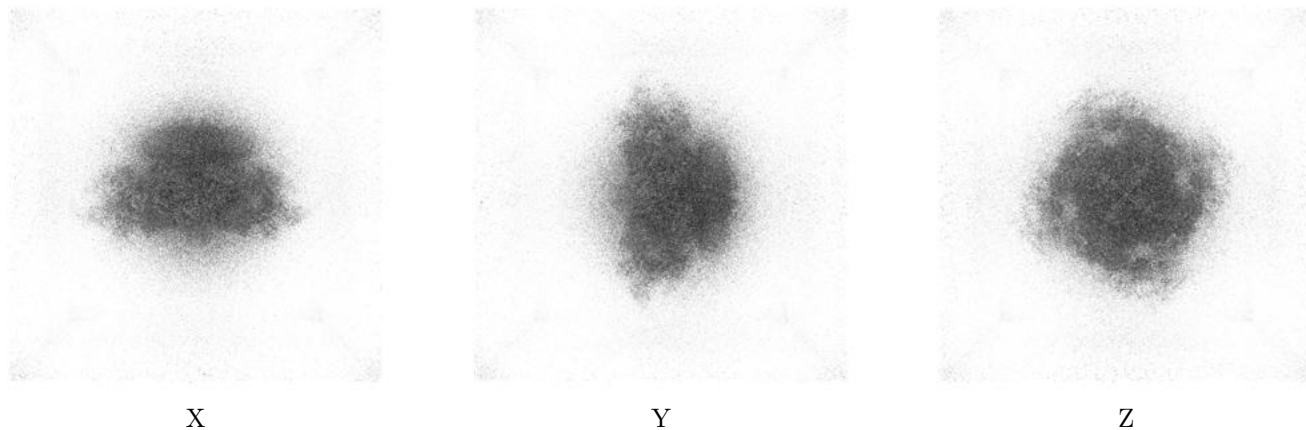
6.5 Orthogonal surface views [i](#)

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.

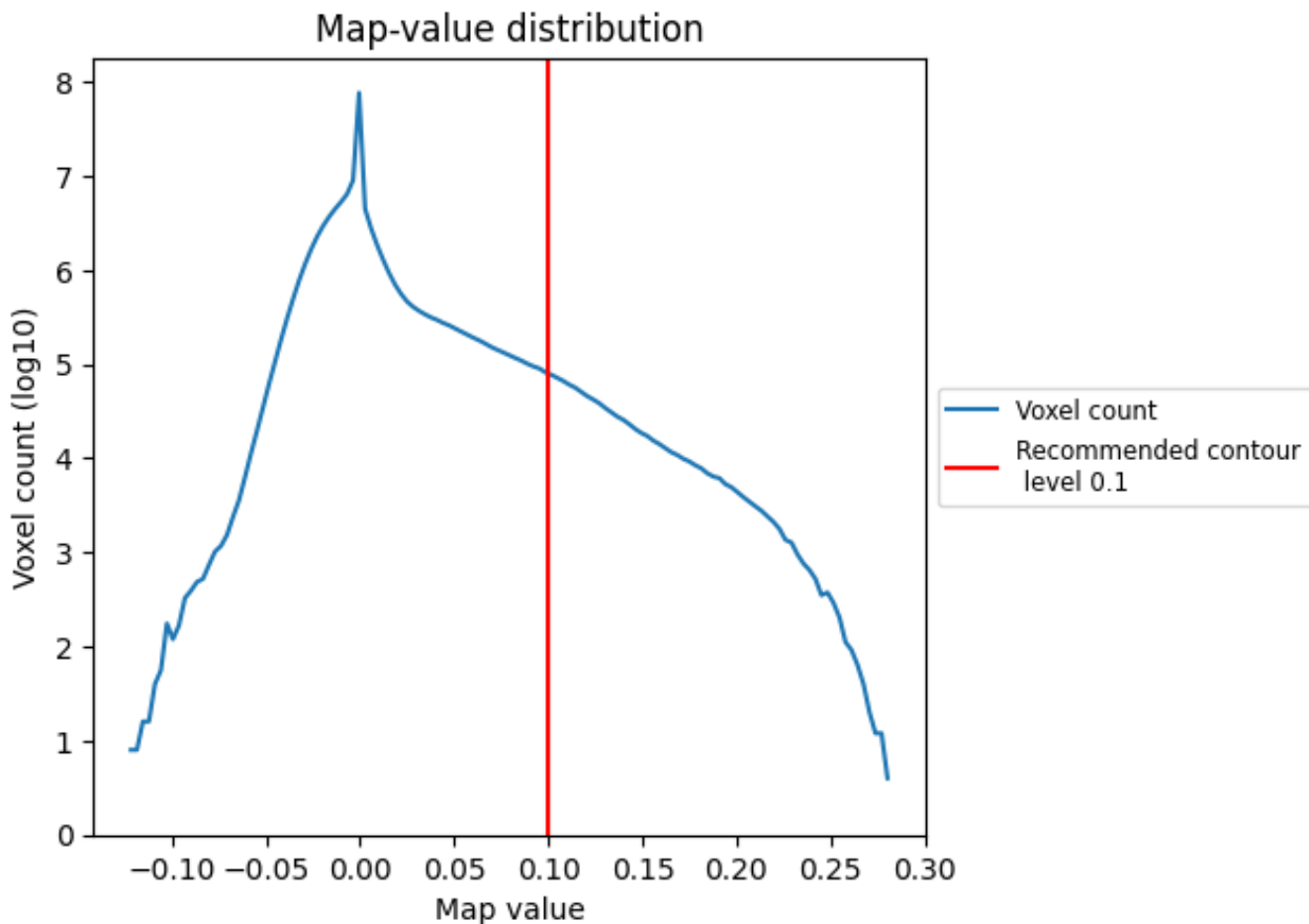
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

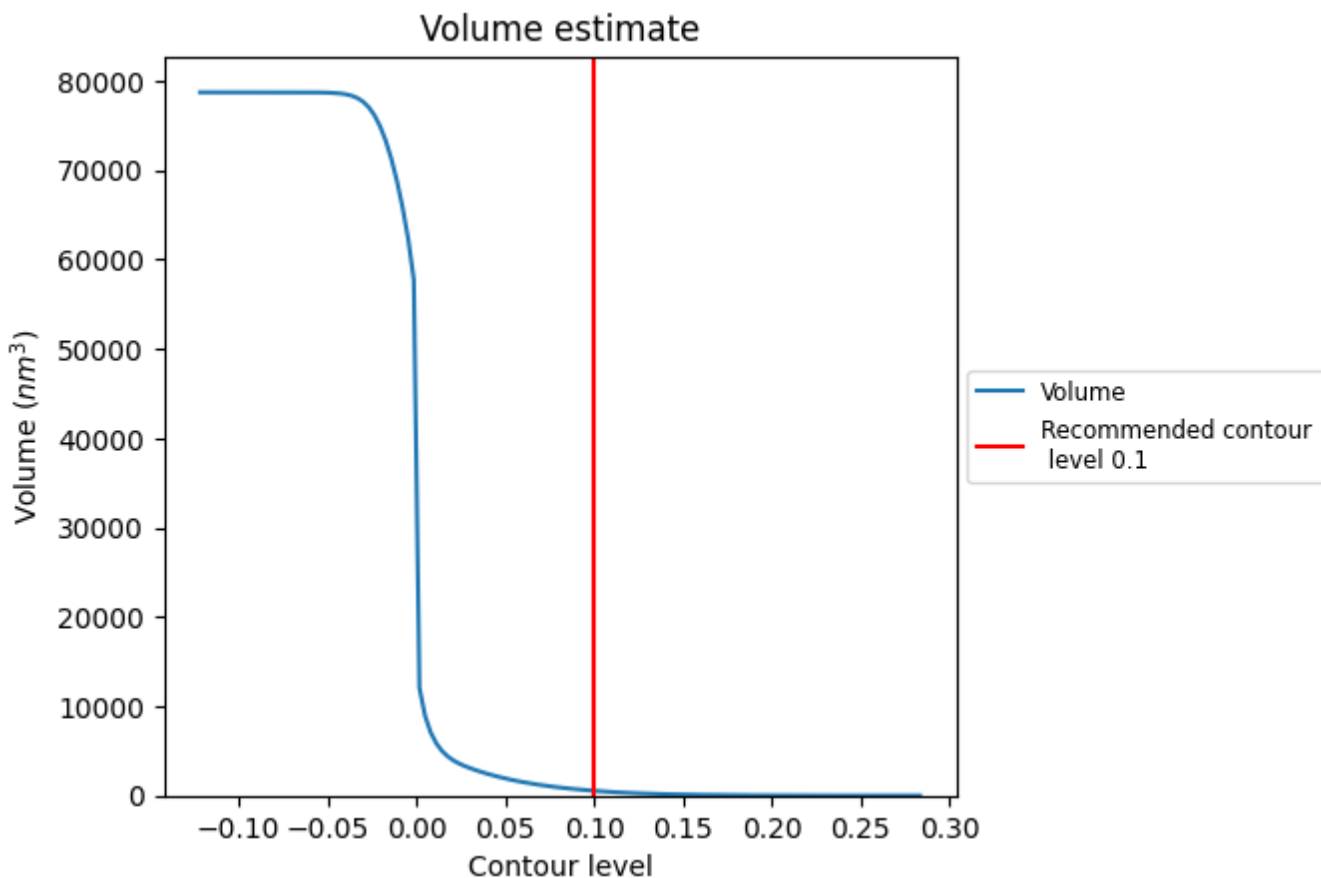
This section contains the results of statistical analysis of the map.

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.

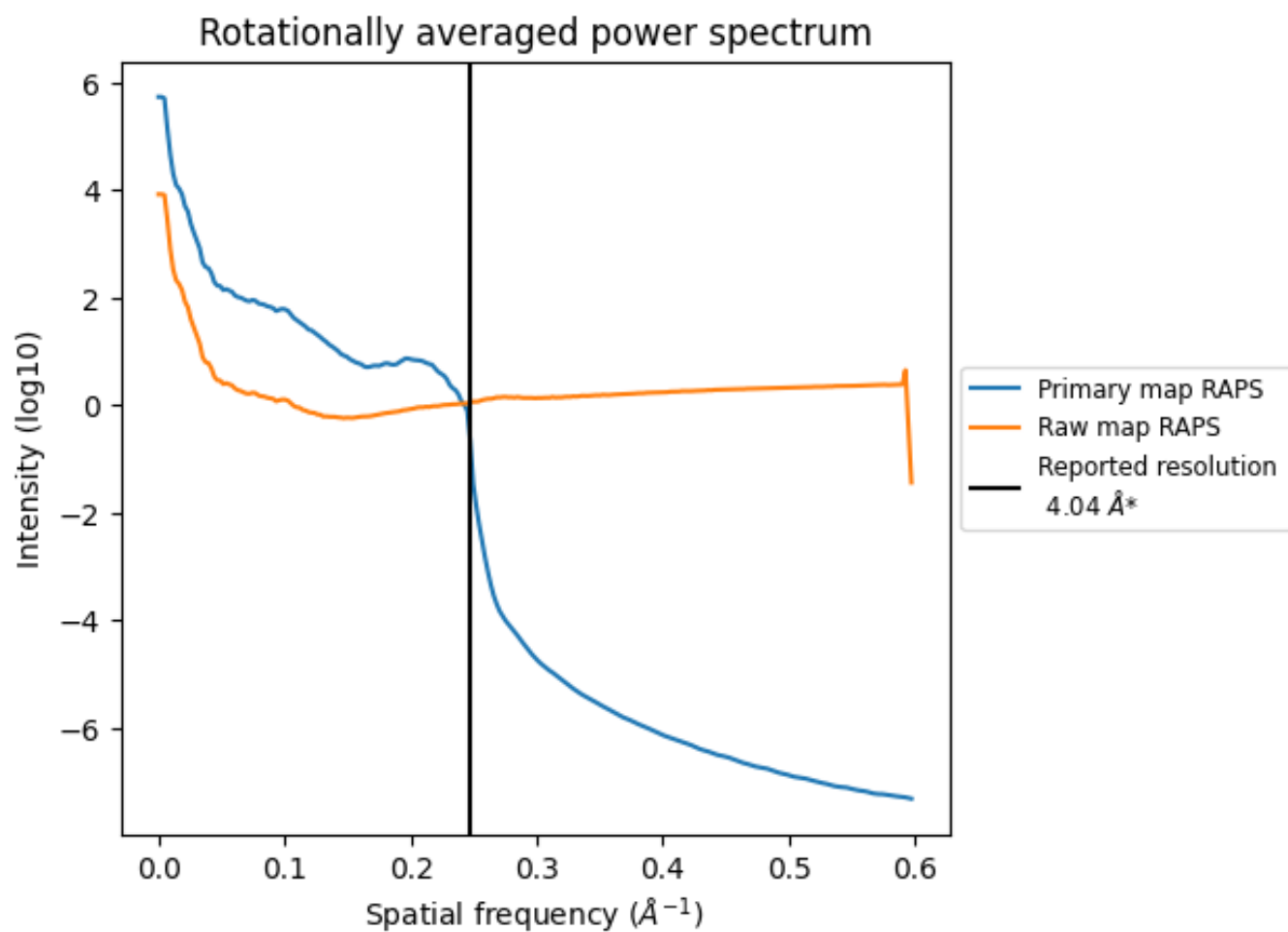
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 534 nm³; this corresponds to an approximate mass of 482 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](#)

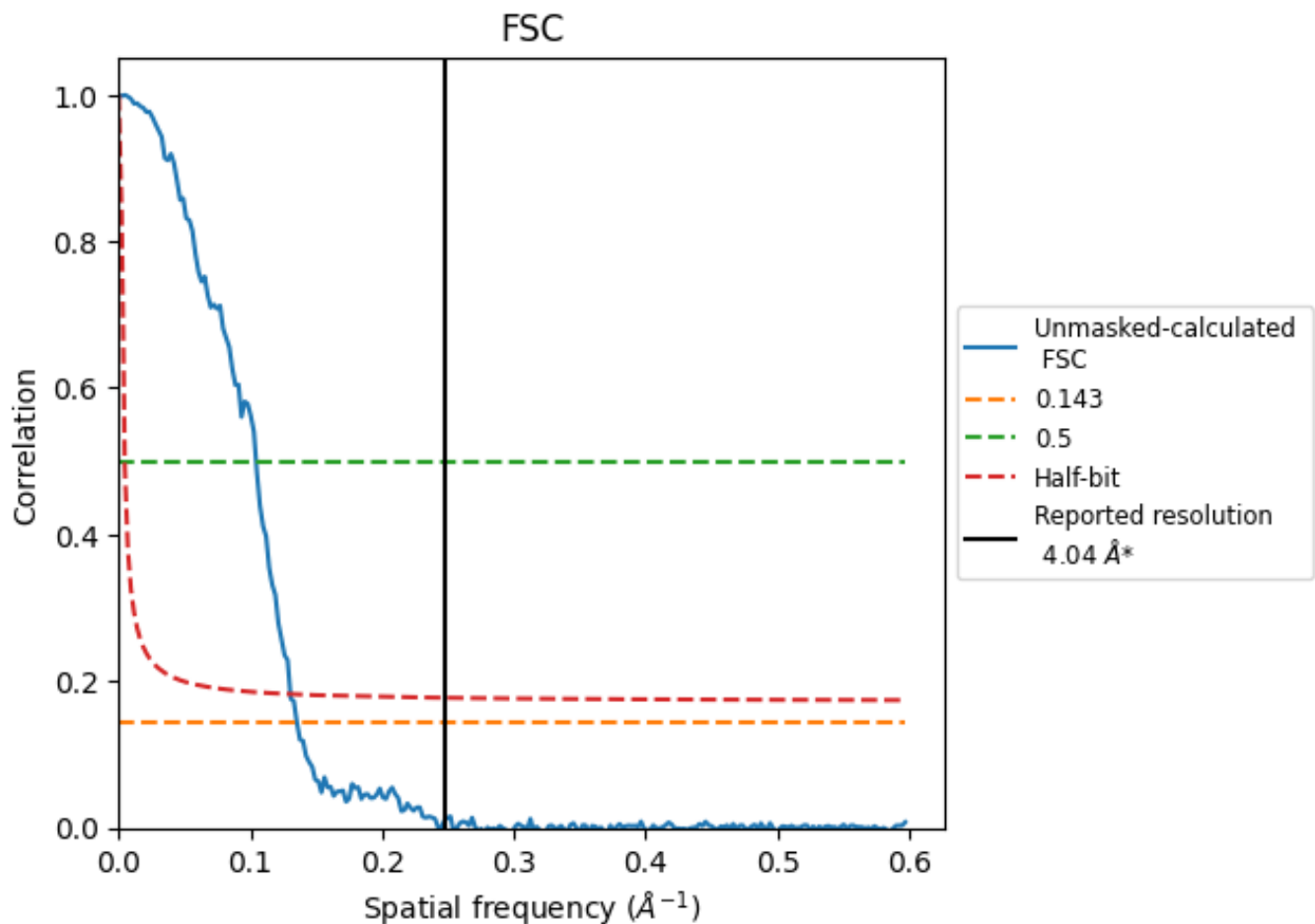


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

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 0.248 Å⁻¹

8.2 Resolution estimates [i](#)

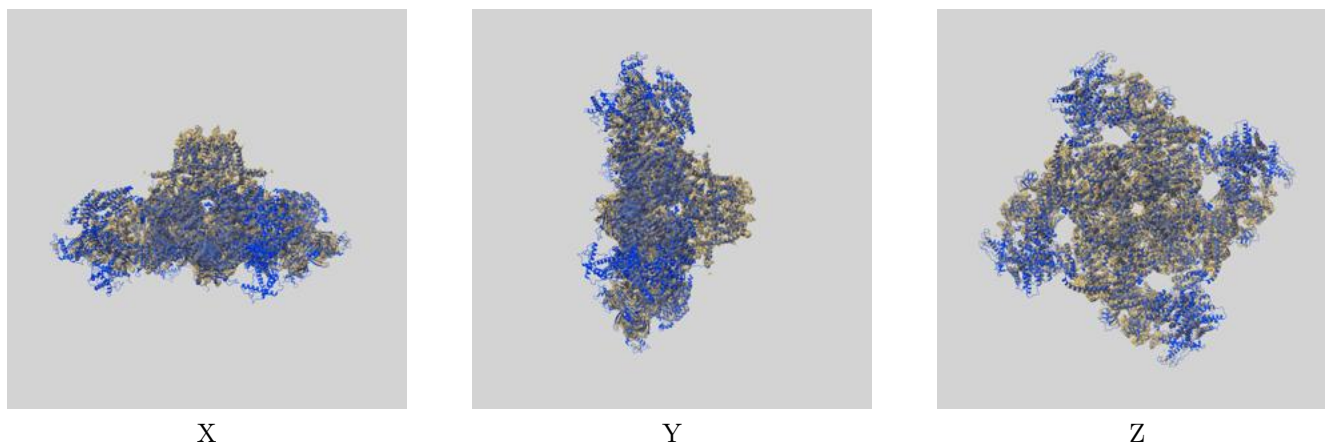
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.04	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.39	9.58	7.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.39 differs from the reported value 4.04 by more than 10 %

9 Map-model fit [i](#)

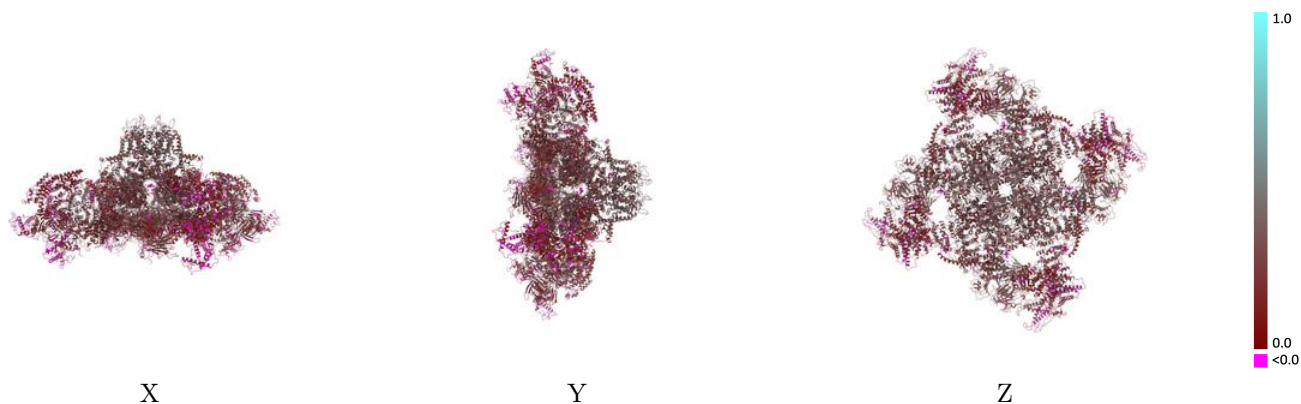
This section contains information regarding the fit between EMDB map EMD-47386 and PDB model 9E19. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



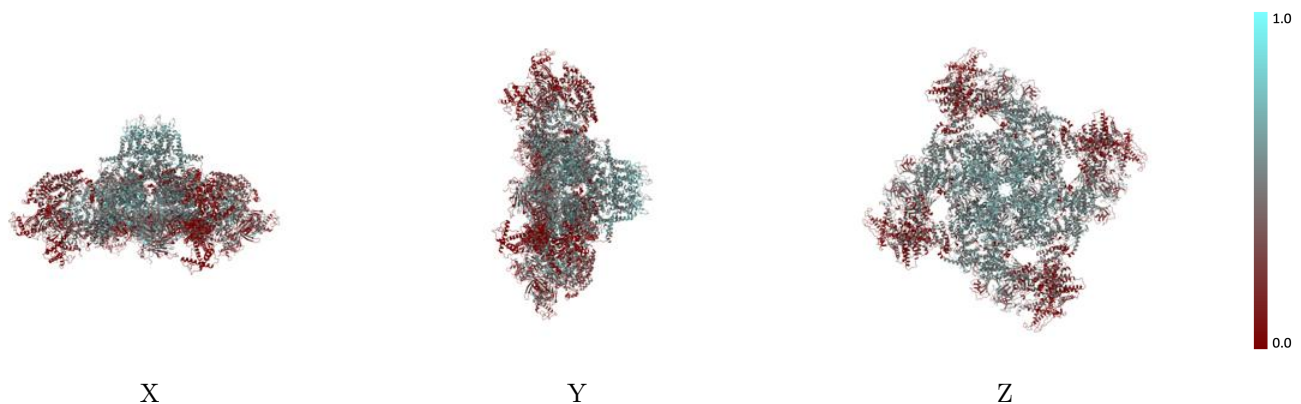
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



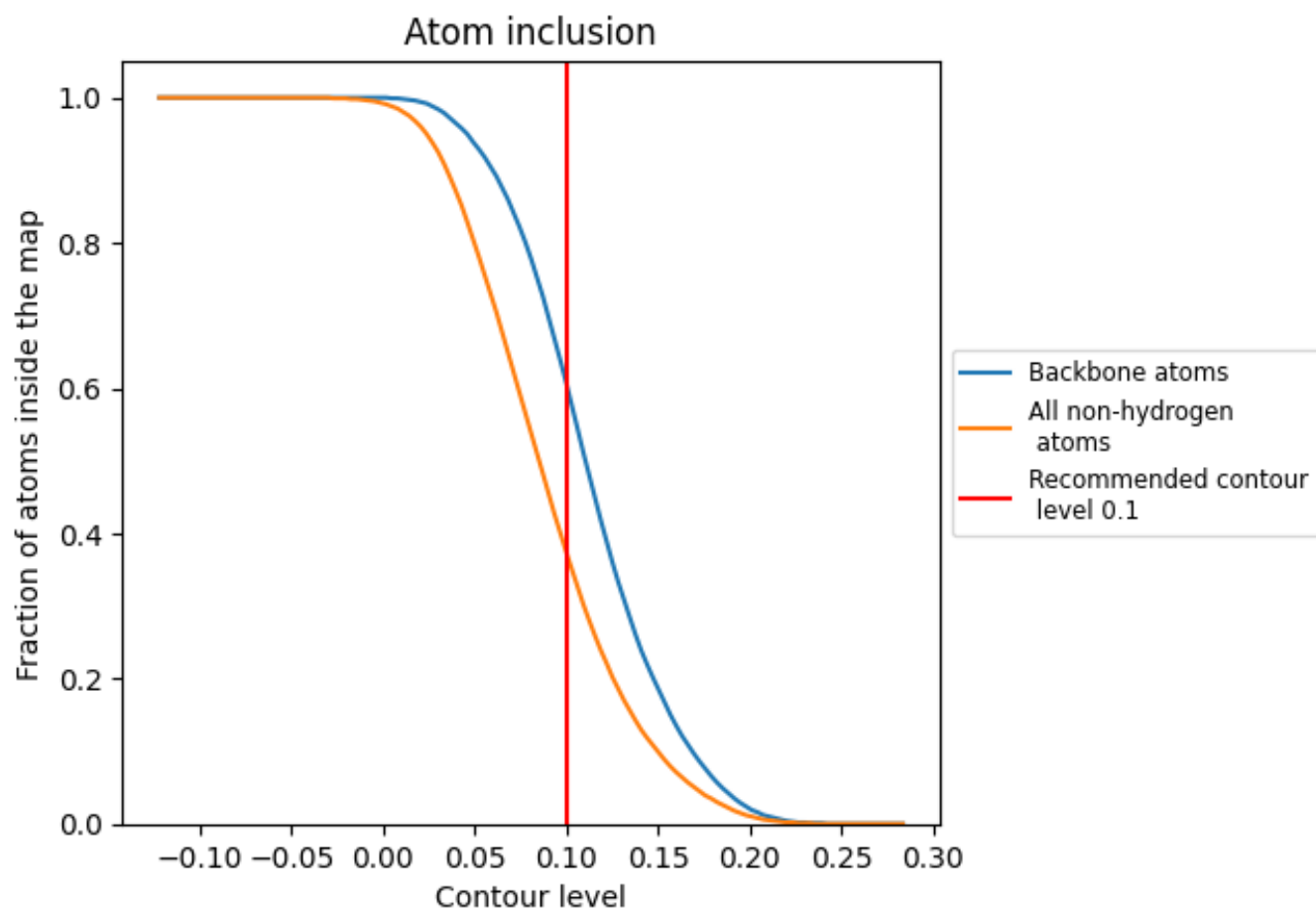
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 61% of all backbone atoms, 37% 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	 0.3740	 0.2250
A	 0.3800	 0.2270
B	 0.3770	 0.2240
C	 0.3780	 0.2240
D	 0.3790	 0.2250
E	 0.1930	 0.2270
F	 0.1950	 0.2210
G	 0.1980	 0.2260
H	 0.1910	 0.2270

