



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:39 pm GMT

PDB ID : 5GKY
EMDB ID: : EMD-9518
Title : Structure of RyR1 in a closed state (C1 conformer)
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

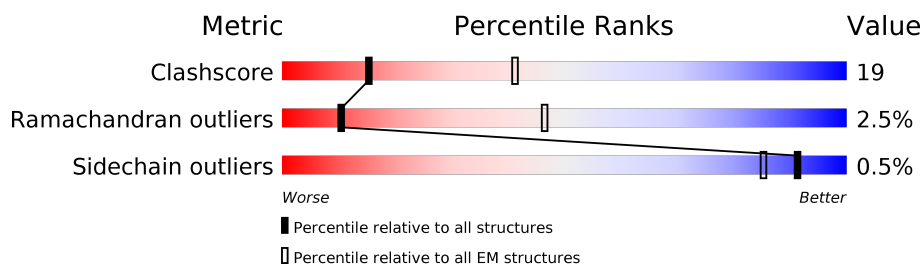
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	5037	46% 26% • 27%
1	C	5037	46% 26% • 27%
1	E	5037	46% 26% • 27%
1	G	5037	46% 25% • 27%
2	B	108	56% 43% •
2	D	108	56% 43% •
2	F	108	56% 43% •
2	H	108	56% 43% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 111036 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
1	A	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	C	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	E	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		
1	G	3660	Total	C	N	O	S	1	0
			26926	17112	4683	4974	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

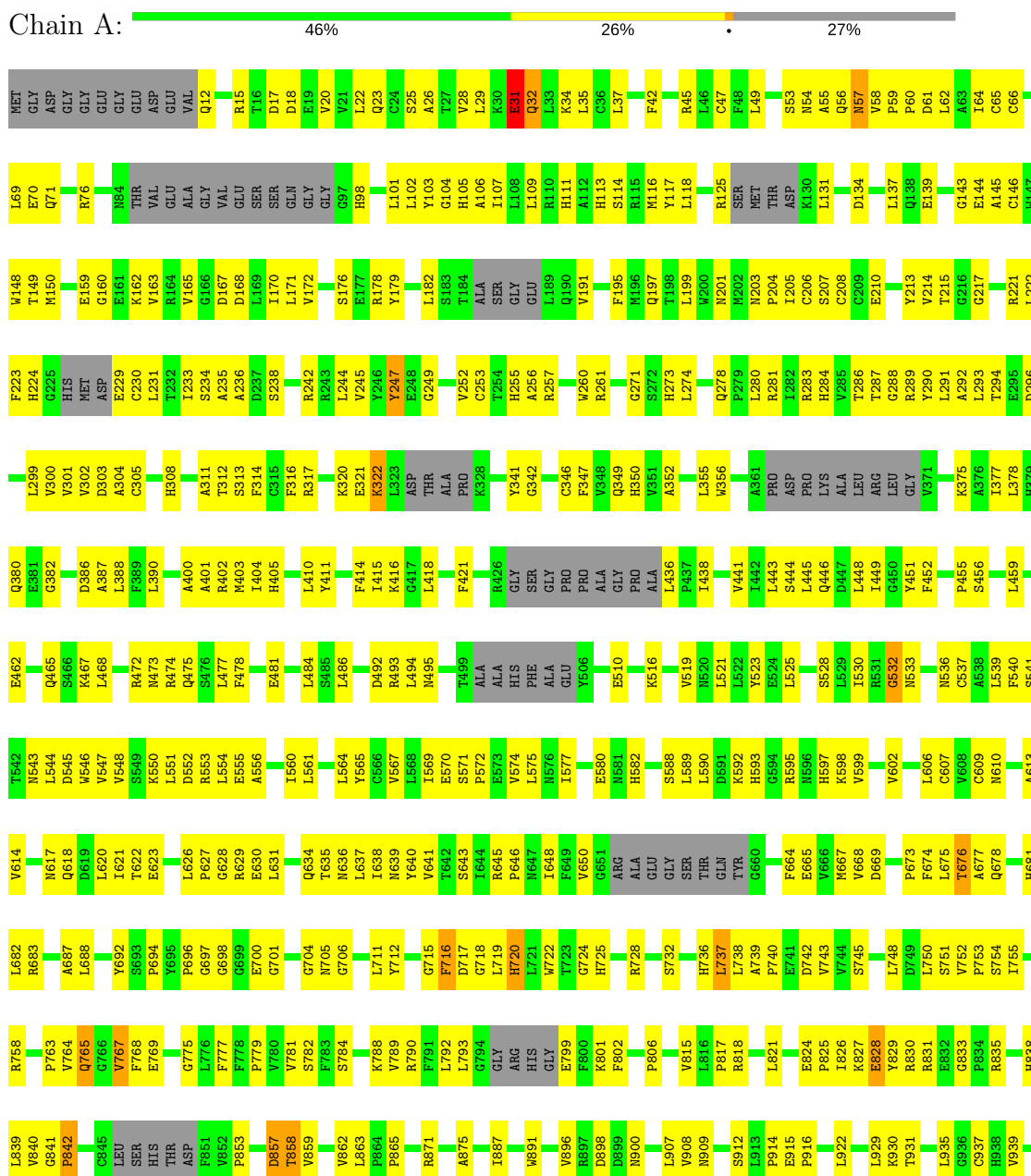
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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



M2120	F2121	S2122	L2123	L2124	H2125	R2126	Q2127	Y2128	E2047	S1975	L1825	T1746	H1663	A1588	VAL	ALA	PRO	HIS	F1223	E1137	GLU	A946
E2133	L2134	L2135	R2136	A2137	L2067	E2068	R2139	A2140	A2141	Z2070	R2071	T2142	T2143	S2145	P2146	V2149	E2150	L2151	T2152	M2153	GLN	ASP
L2154	S2155	L2156	E2157	C2158	L2159	G2160	H2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	GLY
L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	GLY
L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	GLY
L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	GLY
L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	GLY
L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	GLY
L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	GLY
L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324	L2325	L2326	L2327	L2328	L2329	GLY
L2330	L2331	L2332	L2333	L2334	L2335	L2336	L2337	L2338	L2339	L2340	L2341	L2342	L2343	L2344	L2345	L2346	L2347	L2348	L2349	L2350	L2351	GLY
L2352	L2353	L2354	L2355	L2356	L2357	L2358	L2359	L2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	GLY
L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	GLY
L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	L2413	L2414	L2415	L2416	L2417	GLY
L2418	L2419	L2420	L2421	L2422	L2423	L2424	L2425	L2426	L2427	L2428	L2429	L2430	L2431	L2432	L2433	L2434	L2435	L2436	L2437	L2438	L2439	GLY
L2440	L2441	L2442	L2443	L2444	L2445	L2446	L2447	L2448	L2449	L2450	L2451	L2452	L2453	L2454	L2455	L2456	L2457	L2458	L2459	L2460	L2461	GLY
L2462	L2463	L2464	L2465	L2466	L2467	L2468	L2469	L2470	L2471	L2472	L2473	L2474	L2475	L2476	L2477	L2478	L2479	L2480	L2481	L2482	L2483	GLY
L2484	L2485	L2486	L2487	L2488	L2489	L2490	L2491	L2492	L2493	L2494	L2495	L2496	L2497	L2498	L2499	L2500	L2501	L2502	L2503	L2504	L2505	GLY
L2506	L2507	L2508	L2509	L2510	L2511	L2512	L2513	L2514	L2515	L2516	L2517	L2518	L2519	L2520	L2521	L2522	L2523	L2524	L2525	L2526	L2527	GLY
L2528	L2529	L2530	L2531	L2532	L2533	L2534	L2535	L2536	L2537	L2538	L2539	L2540	L2541	L2542	L2543	L2544	L2545	L2546	L2547	L2548	L2549	GLY
L2550	L2551	L2552	L2553	L2554	L2555	L2556	L2557	L2558	L2559	L2560	L2561	L2562	L2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	GLY
L2572	L2573	L2574	L2575	L2576	L2577	L2578	L2579	L2580	L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	GLY
L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	GLY
L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	GLY
L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	GLY
L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	GLY
L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	GLY
L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	GLY
L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	GLY
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L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	GLY
L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	GLY
L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	GLY
L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	GLY
L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	GLY
L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	GLY
L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	GLY
L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	GLY
L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	GLY
L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	GLY
L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	GLY
L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	GLY
L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	GLY
L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	GLY
L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	GLY
L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	GLY
L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	GLY
L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	GLY
L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	GLY
L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	GLY
L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	GLY
L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	GLY
L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	GLY
L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	GLY
L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	GLY
L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	GLY
L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	GLY
L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	GLY
L3386	L3387	L																				



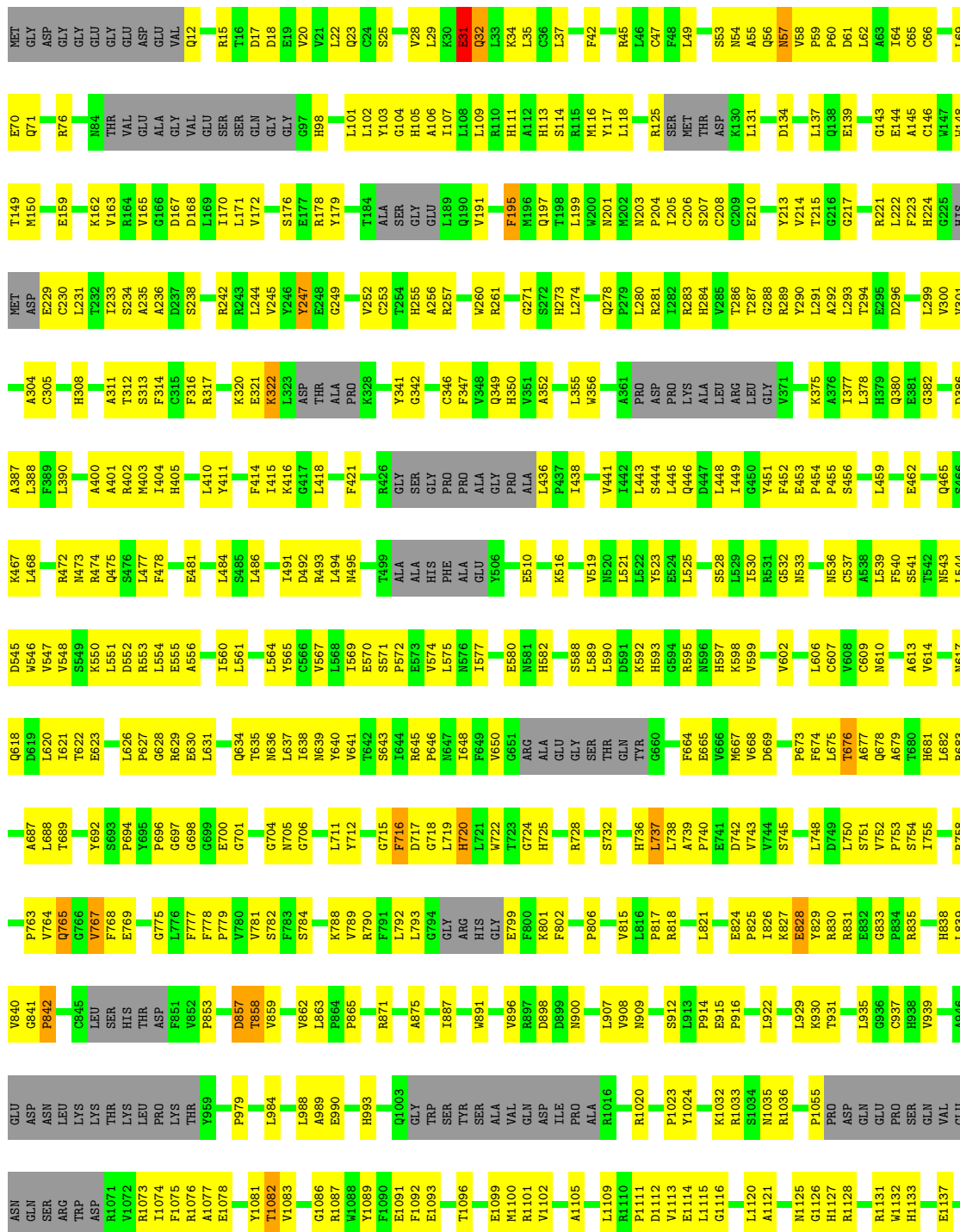






- Molecule 1: Ryanodine receptor 1

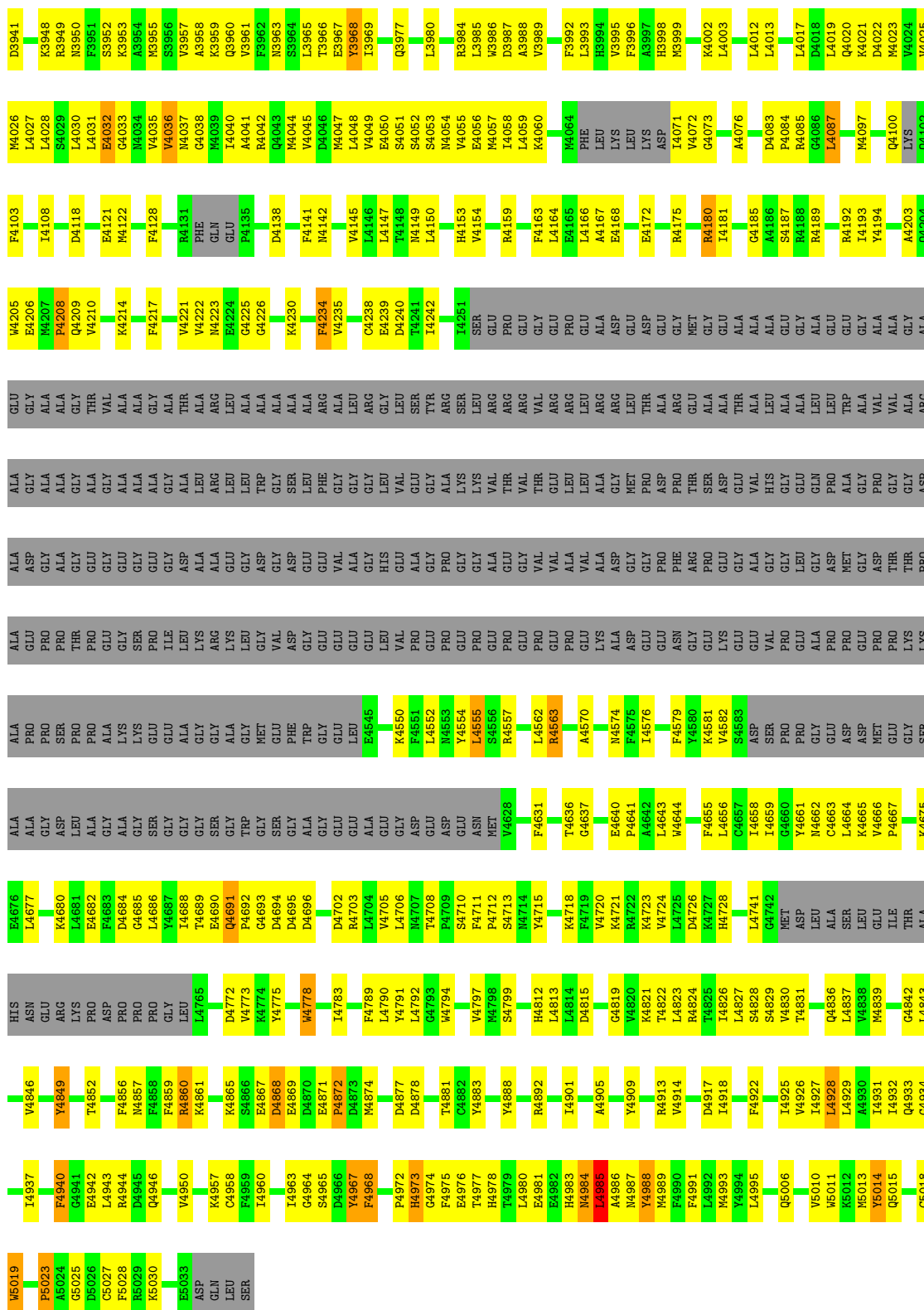
Chain C:  46% 26% . 27%






WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM



- Molecule 1: Ryanodine receptor 1

Chain E:






D2464	D2465	D2466	V2467	I2476	L2307	V2212	Y2128	GLU	GLU	P1829	GLY	Y1670	E1594	GLN	PRO	D2468	D2469	D2470	D2471	D2472	D2473	D2474	D2475	D2476	D2477	D2478	D2479	D2480	D2481	D2482	D2483	D2484	D2485	D2486	D2487	D2488	D2489	D2490	D2491	D2492	D2493	D2494	D2495	D2496	D2497	D2498	D2499	D2500	D2501	D2502	D2503	D2504	D2505	D2506	D2507	D2508	D2509	D2510	D2511	D2512	D2513	D2514	D2515	D2516	D2517	D2518	D2519	D2520	D2521	D2522	D2523	D2524	D2525	D2526	D2527	D2528	D2529	D2530	D2531	D2532	D2533	D2534	D2535	D2536	D2537	D2538	D2539	D2540	D2541	D2542	D2543	D2544	D2545	D2546	D2547	D2548	D2549	D2550	D2551	D2552	D2553	D2554	D2555	D2556	D2557	D2558	D2559	D2560	D2561	D2562	D2563	D2564	D2565	D2566	D2567	D2568	D2569	D2570	D2571	D2572	D2573	D2574	D2575	D2576	D2577	D2578	D2579	D2580	D2581	D2582	D2583	D2584	D2585	D2586	D2587	D2588	D2589	D2590	D2591	D2592	D2593	D2594	D2595	D2596	D2597	D2598	D2599	D2600	D2601	D2602	D2603	D2604	D2605	D2606	D2607	D2608	D2609	D2610	D2611	D2612	D2613	D2614	D2615	D2616	D2617	D2618	D2619	D2620	D2621	D2622	D2623	D2624	D2625	D2626	D2627	D2628	D2629	D2630	D2631	D2632	D2633	D2634	D2635	D2636	D2637	D2638	D2639	D2640	D2641	D2642	D2643	D2644	D2645	D2646	D2647	D2648	D2649	D2650	D2651	D2652	D2653	D2654	D2655	D2656	D2657	D2658	D2659	D2660	D2661	D2662	D2663	D2664	D2665	D2666	D2667	D2668	D2669	D2670	D2671	D2672	D2673	D2674	D2675	D2676	D2677	D2678	D2679	D2680	D2681	D2682	D2683	D2684	D2685	D2686	D2687	D2688	D2689	D2690	D2691	D2692	D2693	D2694	D2695	D2696	D2697	D2698	D2699	D2700	D2701	D2702	D2703	D2704	D2705	D2706	D2707	D2708	D2709	D2710	D2711	D2712	D2713	D2714	D2715	D2716	D2717	D2718	D2719	D2720	D2721	D2722	D2723	D2724	D2725	D2726	D2727	D2728	D2729	D2730	D2731	D2732	D2733	D2734	D2735	D2736	D2737	D2738	D2739	D2740	D2741	D2742	D2743	D2744	D2745	D2746	D2747	D2748	D2749	D2750	D2751	D2752	D2753	D2754	D2755	D2756	D2757	D2758	D2759	D2760	D2761	D2762	D2763	D2764	D2765	D2766	D2767
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PHE GLN GLU	P4135	D4138	F4141	M4044	M4037	M3955	M3956	VAL MET ALA	S3796	L3701	ALA CYS	ALA LEU	ARG MET	P3282	S3217	ALA VAL VAL ASN CYS	ALA VAL VAL ASN CYS	E2870	N2773	PHE GLY VAL
M4039	M4040	M4041	M4042	M4043	M4044	M3957	M3958	D3877	T3797	F3705	PHE MET	TYR GLY	VAL GLN	P3289	S3218	A2875	A2876	E2870	N2774	GLY VAL
M4045	M4046	M4047	M4048	M4049	M4050	M3959	M3960	F3880	K3710	A3709	THR MET	PRO GLY	THR GLN	P3290	S3219	E2877	E2878	E2870	N2775	VAL
M4051	M4052	M4053	M4054	M4055	M4056	M3961	M3962	F3881	L3805	T3711	THR MET	PRO GLY	THR GLN	P3291	S3220	E2879	E2880	E2870	N2776	GLY
M4057	M4058	M4059	M4060	M4061	M4062	M3963	M3964	F3882	L3806	A3712	THR MET	PRO GLY	THR GLN	P3292	S3221	E2881	E2882	E2870	N2777	VAL
M4063	M4064	M4065	M4066	M4067	M4068	M3965	M3966	F3883	L3807	T3713	THR MET	PRO GLY	THR GLN	P3293	S3222	E2883	E2884	E2870	N2778	GLY
M4069	M4070	M4071	M4072	M4073	M4074	M3967	M3968	F3884	L3808	A3714	THR MET	PRO GLY	THR GLN	P3294	S3223	E2885	E2886	E2870	N2779	VAL
M4075	M4076	M4077	M4078	M4079	M4080	M3969	M3970	F3885	L3809	T3715	THR MET	PRO GLY	THR GLN	P3295	S3224	E2887	E2888	E2870	N2780	GLY
M4081	M4082	M4083	M4084	M4085	M4086	M3971	M3972	F3886	L3810	A3716	THR MET	PRO GLY	THR GLN	P3296	S3225	E2889	E2890	E2870	N2781	VAL
M4087	M4088	M4089	M4090	M4091	M4092	M3973	M3974	F3887	L3811	T3717	THR MET	PRO GLY	THR GLN	P3297	S3226	E2891	E2892	E2870	N2782	GLY
M4093	M4094	M4095	M4096	M4097	M4098	M3975	M3976	F3888	L3812	A3718	THR MET	PRO GLY	THR GLN	P3298	S3227	E2893	E2894	E2870	N2783	VAL
M4099	M4100	M4101	M4102	M4103	M4104	M3977	M3978	F3889	L3813	T3719	THR MET	PRO GLY	THR GLN	P3299	S3228	E2895	E2896	E2870	N2784	GLY
M4105	M4106	M4107	M4108	M4109	M4110	M3979	M3980	F3890	L3814	A3720	THR MET	PRO GLY	THR GLN	P3300	S3229	E2897	E2898	E2870	N2785	VAL
M4111	M4112	M4113	M4114	M4115	M4116	M3981	M3982	F3891	L3815	T3721	THR MET	PRO GLY	THR GLN	P3301	S3230	E2899	E2900	E2870	N2786	GLY
M4117	M4118	M4119	M4120	M4121	M4122	M3983	M3984	F3892	L3816	A3722	THR MET	PRO GLY	THR GLN	P3302	S3231	E2901	E2902	E2870	N2787	VAL
M4123	M4124	M4125	M4126	M4127	M4128	M3985	M3986	F3893	L3817	T3723	THR MET	PRO GLY	THR GLN	P3303	S3232	E2903	E2904	E2870	N2788	GLY
M4129	M4130	M4131	M4132	M4133	M4134	M3987	M3988	F3894	L3818	A3724	THR MET	PRO GLY	THR GLN	P3304	S3233	E2905	E2906	E2870	N2789	VAL
M4135	M4136	M4137	M4138	M4139	M4140	M3989	M3990	F3895	L3819	T3725	THR MET	PRO GLY	THR GLN	P3305	S3234	E2907	E2908	E2870	N2790	GLY
M4141	M4142	M4143	M4144	M4145	M4146	M3991	M3992	F3896	L3820	A3726	THR MET	PRO GLY	THR GLN	P3306	S3235	E2909	E2910	E2870	N2791	VAL
M4147	M4148	M4149	M4150	M4151	M4152	M3993	M3994	F3897	L3821	T3727	THR MET	PRO GLY	THR GLN	P3307	S3236	E2911	E2912	E2870	N2792	GLY
M4153	M4154	M4155	M4156	M4157	M4158	M3995	M3996	F3898	L3822	A3728	THR MET	PRO GLY	THR GLN	P3308	S3237	E2913	E2914	E2870	N2793	VAL
M4159	M4160	M4161	M4162	M4163	M4164	M3997	M3998	F3899	L3823	T3729	THR MET	PRO GLY	THR GLN	P3309	S3238	E2915	E2916	E2870	N2794	GLY
M4165	M4166	M4167	M4168	M4169	M4170	M3999	M4000	F3900	L3824	A3730	THR MET	PRO GLY	THR GLN	P3310	S3239	E2917	E2918	E2870	N2795	VAL
M4171	M4172	M4173	M4174	M4175	M4176	M4001	M4002	F3901	L3825	T3731	THR MET	PRO GLY	THR GLN	P3311	S3240	E2919	E2920	E2870	N2796	GLY
M4177	M4178	M4179	M4180	M4181	M4182	M4003	M4004	F3902	L3826	A3732	THR MET	PRO GLY	THR GLN	P3312	S3241	E2921	E2922	E2870	N2797	VAL
M4183	M4184	M4185	M4186	M4187	M4188	M4005	M4006	F3903	L3827	T3733	THR MET	PRO GLY	THR GLN	P3313	S3242	E2923	E2924	E2870	N2798	GLY
M4189	M4190	M4191	M4192	M4193	M4194	M4007	M4008	F3904	L3828	A3734	THR MET	PRO GLY	THR GLN	P3314	S3243	E2925	E2926	E2870	N2799	VAL
M4195	M4196	M4197	M4198	M4199	M4200	M4009	M4010	F3905	L3829	T3735	THR MET	PRO GLY	THR GLN	P3315	S3244	E2927	E2928	E2870	N2800	GLY
M4201	M4202	M4203	M4204	M4205	M4206	M4011	M4012	F3906	L3830	A3736	THR MET	PRO GLY	THR GLN	P3316	S3245	E2929	E2930	E2870	N2801	VAL
M4207	M4208	M4209	M4210	M4211	M4212	M4013	M4014	F3907	L3831	T3737	THR MET	PRO GLY	THR GLN	P3317	S3246	E2931	E2932	E2870	N2802	GLY
M4213	M4214	M4215	M4216	M4217	M4218	M4015	M4016	F3908	L3832	A3738	THR MET	PRO GLY	THR GLN	P3318	S3247	E2933	E2934	E2870	N2803	VAL
M4219	M4220	M4221	M4222	M4223	M4224	M4017	M4018	F3909	L3833	T3739	THR MET	PRO GLY	THR GLN	P3319	S3248	E2935	E2936	E2870	N2804	GLY
M4225	M4226	M4227	M4228	M4229	M4230	M4019	M4020	F3910	L3834	A3740	THR MET	PRO GLY	THR GLN	P3320	S3249	E2937	E2938	E2870	N2805	VAL
M4231	M4232	M4233	M4234	M4235	M4236	M4021	M4022	F3911	L3835	T3741	THR MET	PRO GLY	THR GLN	P3321	S3250	E2939	E2940	E2870	N2806	GLY
M4237	M4238	M4239	M4240	M4241	M4242	M4023	M4024	F3912	L3836	A3742	THR MET	PRO GLY	THR GLN	P3322	S3251	E2941	E2942	E2870	N2807	VAL
M4243	M4244	M4245	M4246	M4247	M4248	M4025	M4026	F3913	L3837	T3743	THR MET	PRO GLY	THR GLN	P3323	S3252	E2943	E2944	E2870	N2808	GLY
M4249	M4250	M4251	M4252	M4253	M4254	M4027	M4028	F3914	L3838	A3744	THR MET	PRO GLY	THR GLN	P3324	S3253	E2945	E2946	E2870	N2809	VAL
M4255	M4256	M4257	M4258	M4259	M4260	M4029	M4030	F3915	L3839	T3745	THR MET	PRO GLY	THR GLN	P3325	S3254	E2947	E2948	E2870	N2810	GLY
M4261	M4262	M4263	M4264	M4265	M4266	M4031	M4032	F3916	L3840	A3746	THR MET	PRO GLY	THR GLN	P3326	S3255	E2949	E2950	E2870	N2811	VAL
M4267	M4268	M4269	M4270	M4271	M4272	M4033	M4034	F3917	L3841	T3747	THR MET	PRO GLY	THR GLN	P3327	S3256	E2951	E2952	E2870	N2812	GLY
M4273	M4274	M4275	M4276	M4277	M4278	M4035	M4036	F3918	L3842	A3748	THR MET	PRO GLY	THR GLN	P3328	S3257	E2953	E2954	E2870	N2813	VAL
M4279	M4280	M4281	M4282	M4283	M4284	M4037	M4038	F3919	L3843	T3749	THR MET	PRO GLY	THR GLN	P3329	S3258	E2955	E2956	E2870	N2814	GLY
M4285	M4286	M4287	M4288	M4289	M4290	M4039	M4040	F3920	L3844	A3750	THR MET	PRO GLY	THR GLN	P3330	S3259	E2957	E2958	E2870	N2815	VAL
M4291	M4292	M4293	M4294	M4295	M4296	M4041	M4042	F3921	L3845	T3751	THR MET	PRO GLY	THR GLN	P3331	S3260	E2959	E2960	E2870	N2816	GLY
M4297	M4298	M4299	M4300	M4301	M4302	M4043	M4044	F3922	L3846	A3752	THR MET	PRO GLY	THR GLN	P3332	S3261	E2961	E2962	E2870	N2817	VAL
M4303	M4304	M4305	M4306	M4307	M4308	M4045	M4046	F3923	L3847	T3753	THR MET	PRO GLY	THR GLN	P3333	S3262	E2963	E2964	E2870	N2818	GLY
M4309	M4310	M4311	M4312	M4313	M4314	M4047	M4048	F3924	L3848	A3754	THR MET	PRO GLY	THR GLN	P3334	S3263	E2965	E2966	E2870	N2819	VAL
M4315	M4316	M4317	M4318	M4319	M4320	M4049	M4050	F3925	L3849	T3755	THR MET	PRO GLY	THR GLN	P3335	S3264	E2967	E2968	E2870	N2820	GLY
M4321	M4322	M4323	M4324	M4325	M4326	M4051	M4052	F3926	L3850	A3756	THR MET	PRO GLY	THR GLN	P3336	S3265	E2969	E2970	E2870	N2821	VAL
M4327	M4328	M4329	M4330	M4331	M4332	M4053	M4054	F3927	L3851	T3757	THR MET	PRO GLY	THR GLN	P3337	S3266	E2971	E2972	E2870	N2822	GLY
M4333	M4334	M4335	M4336	M4337	M4338	M4055	M4056	F3928	L3852	A3758	THR MET	PRO GLY	THR GLN	P3338	S3267	E2973	E2974	E2870	N2823	VAL
M4339	M4340	M4341	M4342	M4343	M4344	M4057	M4058	F3929	L3853	T3759	THR MET	PRO GLY	THR GLN	P3339	S3268	E2975	E2976	E2870	N2824	GLY
M4345	M4346	M4347	M4348	M4349	M4350	M4059	M4060	F3930	L3854	A3760	THR MET	PRO GLY	THR GLN	P3340	S3269	E2977	E2978	E2870	N2825	VAL
M4351	M4352	M4353	M4354	M4355	M4356	M4061	M4062	F3931	L3855	T3761	THR MET	PRO GLY	THR GLN	P3341	S3270	E2979	E2980	E2870	N2826	GLY
M4357	M4358	M4359	M4360	M4361	M4362	M4063	M4064	F3932	L3856	A3762	THR MET	PRO GLY	THR GLN	P3342	S3271	E2981	E2982	E2870	N2827	VAL
M4363	M4364	M4365	M4366	M4367	M4368	M4065	M4066	F3933	L3857	T3763	THR MET	PRO GLY	THR GLN	P3343	S3272	E2983	E2984	E2870	N2828	GLY
M4369	M4370	M4371	M4372	M4373	M4374	M4067	M4068	F3934	L3858	A3764	THR MET	PRO GLY	THR GLN	P3344	S3273	E2985	E2986	E2870	N2829	VAL
M4375	M4376	M4377	M4378	M4379	M4380	M4069	M4070	F3935	L3859	T3765	THR MET	PRO GLY	THR GLN	P3345	S3274	E2987	E2988	E2870	N2830	GLY
M4381	M4382	M4383	M4384	M4385	M4386	M4071	M4072	F3936	L3860	A3766	THR MET	PRO GLY	THR GLN	P3346	S3275	E2989	E2990	E2870	N2831	VAL
M4387	M4388	M4389	M4390	M4391	M4392	M4073	M4074	F3937	L3861	T3767	THR MET	PRO GLY	THR GLN	P3347	S3276	E2991	E2992	E2870	N2832	GLY
M4393	M4394	M4395	M4396	M4397	M4398	M4075	M4076	F3938	L3862	A3768	THR MET	PRO GLY	THR GLN	P3348	S3277	E2993	E2994	E2870	N2833	VAL
M4399	M4400	M4401	M4402	M4403	M4404	M4077	M4078	F3939	L3863	T3769	THR MET	PRO GLY	THR GLN	P3349	S3278	E2995	E2996	E2870	N2834	GLY
M4405	M4406	M4407	M4408	M4409	M4410	M4079	M4080	F3940	L3864	A3770	THR MET	PRO GLY	THR GLN	P3350	S3279					

[illegible]

- Molecule 1: Ryanodine receptor 1

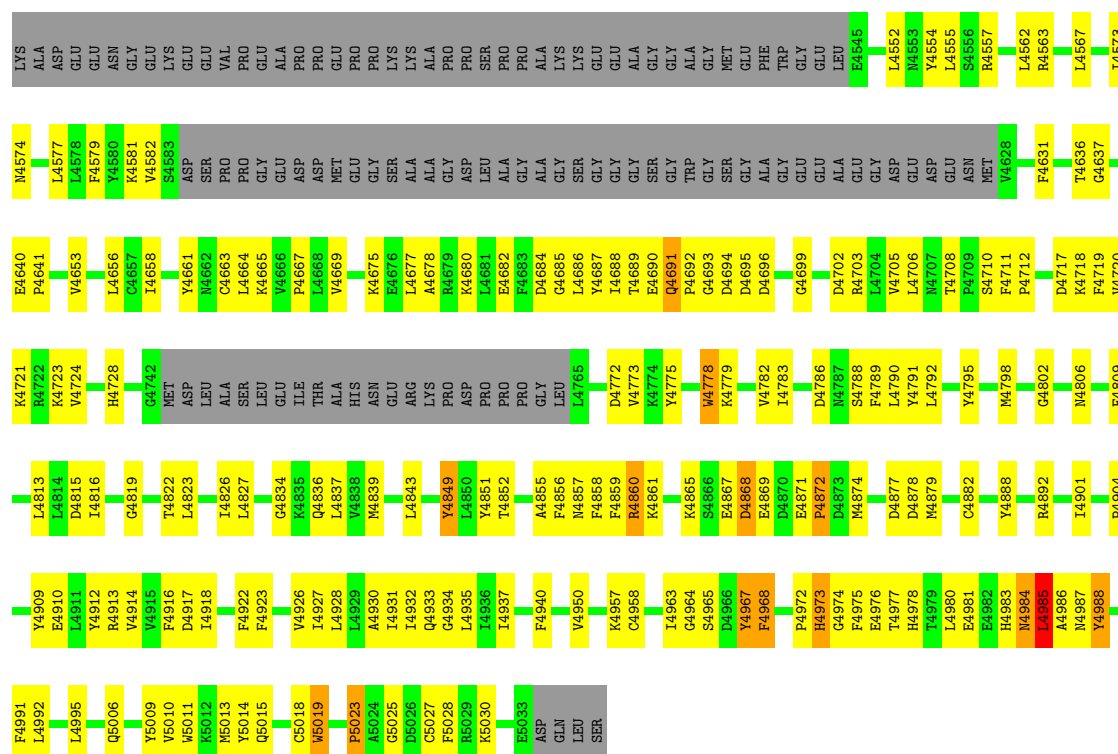
Chain G:  46% 25% . 27%

T149	E70	MET
M150	Q71	GLY
E159	R76	ASP
K162	N84	GLY
V163	THR	GLU
I164	VAL	GLY
V165	GLU	GLY
G166	ALA	ASP
D167	GLY	GLU
D168	VAL	VAL
L169	GLU	Q12
I170	SER	
L171	SER	R15
V172	GLN	T16
	GLY	D17
	GLY	D18
S176	G97	E19
E177	H98	V20
L178		V21
Y179	L101	L22
	L102	Q24
L182	L103	S25
S183	G104	A26
T184	H105	T27
ALA	A106	V28
SER	L107	L29
GLY	L108	K30
GLU	L109	R31
L189	H110	Q32
Q190	H111	L33
V191	A112	K34
	H113	L35
F195	S114	C36
M196	R115	L37
Q197	M116	
T198	Y117	F42
L199	L118	
W200	R125	R45
N201	SER	L46
K202	MET	C47
N203	THR	F48
T204	MET	L49
T205	ASP	
C206	K130	S53
S207	L131	N54
C208		A55
C209	D134	Q56
E210		N57
	L137	V58
Y213	Q138	P59
T214	E139	P60
T215		D61
G216	G143	L62
G217	E144	A63
	A145	I64
R221	C146	C65
L222	W147	
F223	L148	L66
T224		

PRO	GLY	F1510	ASP	ASP	ASP	Q1144	GLN	ASP	V840	L682	M617	N543	Q465	G382	V300	R225
GLN	GLN	D1147	THR	ASN	G841	P763	SER	ASN	G841	R683	Q618	L544	S466	D386	V301	HIS
PRO	PRO	M1230	THR	LEU	P842	V764	THR	LEU	P842	A687	D619	D545	S467	D387	V302	MET
GLN	GLN	Q1231	THR	LVS	C845	Q765	THR	LVS	C845	L688	L620	N546	L468	A387	V303	ASP
ALA	ALA	R1232	THR	THR	SER	V766	THR	THR	SER	V682	T621	V548	R472	F388	C305	C230
ALA	ALA	T1235	PRO	LVS	HIS	F768	LEU	LVS	HIS	V682	T622	S549	M473	L390	H308	L231
PRO	PRO	T1236	LEU	LEU	THR	E769	LEU	LEU	THR	S693	E623	K550	R474	A400		T232
LEU	LEU	W1237	PRO	PRO	THR	P694	PRO	PRO	THR	P694	L626	L551	R474	A401		L233
ALA	ALA	F1238	LVS	LVS	ASP	G775	THR	THR	ASP	P696	P627	D552	S476	R402	A311	S234
ARG	ARG	T1156	THR	THR	P851	L776	THR	THR	P851	G697	G628	R553	L477	R402	T312	A235
ALA	ALA	E1157	THR	THR	V852	F777	THR	THR	V852	G698	G629	E555	F478	M403	S313	A236
GLY	GLY	Q1244	Y959	Y959	P853	F779	THR	THR	P853	G699	E630	A556	E481	L404	F314	D237
LEU	LEU	F1245	P979	P979	D857	V780	THR	THR	D857	G701	L631			H405	G315	S238
GLN	GLN	I1160	L984	L984	T858	V781	THR	THR	T858	G701	L560			L410	F316	R242
PRO	PRO	I1161	L984	L984	V859	S782	THR	THR	V859	G701	L561			Y411	R317	R242
ALA	ALA	T1162	L988	L988	L863	G704	THR	THR	L863	G704	L564			F414	K320	R243
THR	THR	L1164	A989	A989	P865	N705	THR	THR	P865	N705	V665			I415	E321	L244
ASP	ASP	P1253	E990	E990	S784	G706	THR	THR	S784	G706	V666			K416	K322	V245
ASP	ASP	H1252	H993	H993	K788	L711	THR	THR	K788	L711	C866			D492	K322	V246
GLU	GLU	T1253	Y1098	Y1098	V789	L712	THR	THR	V789	L712	V567			R493	ASP	Y247
ALA	ALA	E1255	F1090	F1090	R790	L712	THR	THR	R790	L712	L568			G417	THR	E248
ALA	ALA	V1257	Q1003	Q1003	F791	L712	THR	THR	F791	L712	N495			L418	ALA	G249
ALA	ALA	A1258	GLY	GLY	L792	G715	THR	THR	L792	G715	E570			F421	PRO	V252
GLU	GLU	R1259	TRP	TRP	L793	F716	THR	THR	L793	F716	S571			K328		C253
PRO	PRO	M1260	SER	SER	G794	L719	THR	THR	G794	L719	P572			Y341		T254
GLY	GLY	D1261	THR	THR	ARG	H720	THR	THR	ARG	H720	E573			G342		H255
LEU	LEU	Y1457	SER	SER	HIS	L721	THR	THR	HIS	L721	L575			GLY		A256
THR	THR	ASP	ALA	ALA	V896	L722	THR	THR	V896	L722	N576			GLY		R257
VAL	VAL	VAL	VAL	VAL	H897	L723	THR	THR	H897	L723	L577			PRO		V260
ASP	ASP	ASP	GLN	GLN	E799	G724	THR	THR	E799	G724	V650			ALA		R261
PRO	PRO	ASN	ASP	ASP	K801	H725	THR	THR	K801	H725	E580			GLY		
PRO	PRO	PRO	ILE	ILE	F802	R728	THR	THR	F802	R728	N581			PRO		G271
ALA	ALA	ALA	ALA	ALA	P806	S732	THR	THR	P806	S732	H582			ALA		S272
ALA	ALA	F1188	L1016	L1016	L907	V815	THR	THR	L907	V815	S588			L436		H273
LEU	LEU	L1189	R1020	R1020	V908	L816	THR	THR	V908	L816	L589			P437		L274
ARG	ARG	F1190	P1111	P1111	N909	H736	THR	THR	N909	H736	L590			I438		Q278
ARG	ARG	V1191	D1112	D1112	S912	L737	THR	THR	S912	L737	D591			V441		P279
GLY	GLY	S1193	V1113	V1113	L913	L738	THR	THR	L913	L738	X592			L442		L280
GLY	GLY	L1194	P1023	P1023	P914	A739	THR	THR	P914	A739	H593			L443		R281
GLY	GLY	G1195	L1115	L1115	E915	P740	THR	THR	E915	P740	G594			S444		T282
ALA	ALA	V1199	G1116	G1116	P916	E741	THR	THR	P916	E741	R595			L445		R283
GLU	GLU	E1285	L1120	L1120	L922	D742	THR	THR	L922	D742	R596			Q446		R284
GLY	GLY	M1286	A1121	A1121	L922	P825	THR	THR	L922	P825	H597			L446		V285
GLY	GLY	L1287	N1035	N1035	V743	V743	THR	THR	V743	V743	X598			L448		T286
LVS	LVS	F1288	R1036	R1036	I826	V744	THR	THR	I826	V744	V599			I449		T287
GLY	GLY	L1289	K1032	K1032	K827	S745	THR	THR	K827	S745	R591			LEU		G288
GLY	GLY	R1290	R1033	R1033	E828	V745	THR	THR	E828	V745	G450			LEU		R289
GLY	GLY	L1291	P1055	P1055	Y829	L748	THR	THR	Y829	L748	G532			GLY		Y290
THR	THR	S1210	ASP	ASP	R830	D749	THR	THR	R830	D749	N533			F452		
ALA	ALA	L1211	GLN	GLN	R831	L750	THR	THR	R831	L750	L606			P455		L291
ASP	ASP	F1212	GLU	GLU	G936	S751	THR	THR	G936	S751	C507			S456		A292
VAL	VAL	F1213	PRO	PRO	G833	P676	THR	THR	G833	P676	V608			K375		L293
GLY	GLY	Q1220	SER	SER	H838	P753	THR	THR	H838	P753	C609			I377		T294
THR	THR	F1223	GLN	GLN	V939	S754	THR	THR	V939	S754	N610			L459		E295
PRO	PRO	F1223	VAL	VAL	A946	I755	THR	THR	A946	I755	P540			H379		D296
GLY	GLY	F1226	ASN	ASN	GLU	R758	THR	THR	GLU	R758	S541			E462		
THR	THR		ASN	ASN							T542					L299




[illegible]



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

Chain B: 56% 43%



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

Chain D: 56% 43%



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

Chain F: 56% 43%

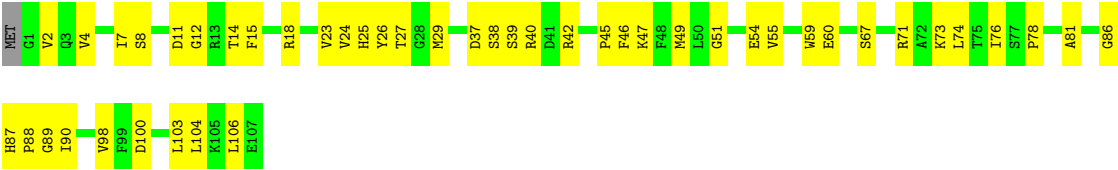


● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:

56%

43%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	119000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.85	25/27395 (0.1%)	0.86	68/37119 (0.2%)
1	C	0.85	27/27395 (0.1%)	0.86	64/37119 (0.2%)
1	E	0.85	24/27395 (0.1%)	0.86	63/37119 (0.2%)
1	G	0.84	26/27395 (0.1%)	0.85	59/37119 (0.2%)
2	B	0.64	0/851	0.68	0/1146
2	D	0.64	0/851	0.68	0/1146
2	F	0.64	0/851	0.68	0/1146
2	H	0.66	0/851	0.69	0/1146
All	All	0.84	102/112984 (0.1%)	0.85	254/153060 (0.2%)

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	17
1	C	0	17
1	E	0	17
1	G	0	16
All	All	0	67

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2853	GLU	CD-OE1	17.93	1.45	1.25
1	E	2853	GLU	CD-OE1	17.88	1.45	1.25
1	G	2853	GLU	CD-OE1	17.49	1.44	1.25
1	C	2853	GLU	CD-OE1	17.32	1.44	1.25
1	G	4988	TYR	CG-CD1	-9.48	1.26	1.39

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	4032	GLU	OE1-CD-OE2	-7.83	113.91	123.30
1	G	4985	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	G	2118	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	3773	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	4563	ARG	NE-CZ-NH2	7.46	124.03	120.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1187	GLY	Mainchain
1	A	31	GLU	Mainchain,Peptide
1	A	322	LYS	Peptide
1	A	841	GLY	Mainchain,Peptide
1	A	857	ASP	Mainchain,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	26926	0	24467	1003	0
1	C	26926	0	24467	1022	0
1	E	26926	0	24467	1004	0
1	G	26926	0	24467	952	0
2	B	832	0	831	41	0
2	D	832	0	831	41	0
2	F	832	0	831	41	0
2	H	832	0	831	40	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111036	0	101192	3945	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 19.

The worst 5 of 3945 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:G:1808:ARG:NH1	1:G:1858:ASP:OD2	1.79	1.16
1:E:1808:ARG:NH1	1:E:1858:ASP:OD2	1.79	1.16
1:C:1808:ARG:NH1	1:C:1858:ASP:OD2	1.79	1.15
1:A:1808:ARG:NH1	1:A:1858:ASP:OD2	1.79	1.14
1:A:1243:PRO:HD2	1:A:1458:HIS:HB3	1.20	1.10

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	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	6	44
1	C	3499/5037 (70%)	3211 (92%)	201 (6%)	87 (2%)	6	44
1	E	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	6	44
1	G	3499/5037 (70%)	3211 (92%)	199 (6%)	89 (2%)	6	44
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	D	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	7 (7%)	1 (1%)	18	61
All	All	14416/20580 (70%)	13232 (92%)	829 (6%)	355 (2%)	10	44

5 of 355 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	737	LEU
1	A	858	THR

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	916	PRO

5.3.2 Protein sidechains ⓘ

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	2503/4276 (58%)	2489 (99%)	14 (1%)	89	95
1	C	2504/4276 (59%)	2490 (99%)	14 (1%)	89	95
1	E	2504/4276 (59%)	2490 (99%)	14 (1%)	89	95
1	G	2502/4276 (58%)	2489 (100%)	13 (0%)	91	96
2	B	89/90 (99%)	89 (100%)	0	100	100
2	D	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10369/17464 (59%)	10314 (100%)	55 (0%)	91	96

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1096	THR
1	E	510	GLU
1	G	1055	PRO
1	C	2066	LEU
1	C	4972	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4153	HIS
1	E	593	HIS
1	G	3851	ASN

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Mol	Chain	Res	Type
1	C	4650	HIS
1	E	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.