



wwPDB EM Validation Summary Report ⓘ

Jun 16, 2025 – 05:06 PM EDT

PDB ID : 9E1F / pdb_00009e1f
EMDB ID : EMD-47392
Title : Structure of RyR1 in the primed state in the presence of allopurinol
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.03 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

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

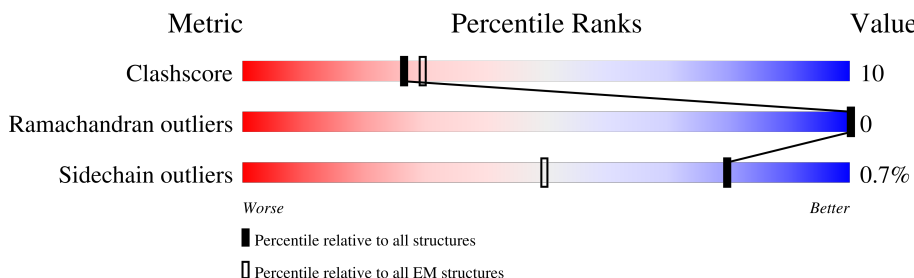
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	<div> <div>44%</div> <div>68%</div> <div>19%</div> <div>13%</div> </div>
1	B	5037	<div> <div>44%</div> <div>69%</div> <div>19%</div> <div>13%</div> </div>
1	C	5037	<div> <div>44%</div> <div>69%</div> <div>19%</div> <div>13%</div> </div>
1	D	5037	<div> <div>44%</div> <div>68%</div> <div>19%</div> <div>13%</div> </div>
2	E	108	<div> <div>79%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
2	F	108	<div> <div>78%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	G	108	<div> <div>79%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
2	H	108	<div> <div>78%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144104 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	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

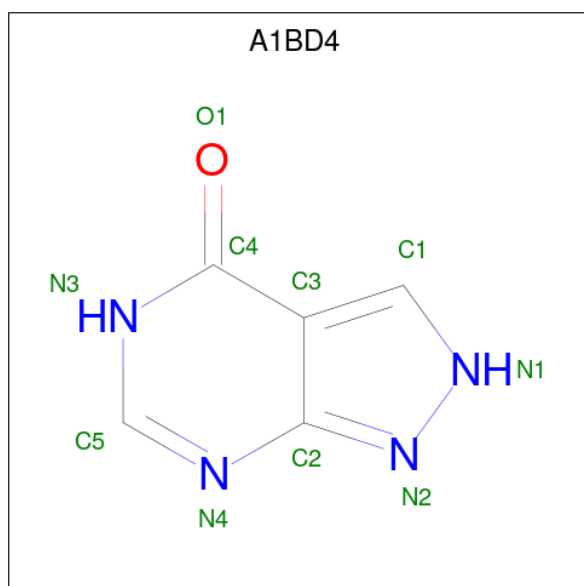
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

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 allopurinol (CCD ID: A1BD4) (formula: C₅H₄N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			10	5	4	1	
6	B	1	Total	C	N	O	0
			10	5	4	1	
6	D	1	Total	C	N	O	0
			10	5	4	1	
6	C	1	Total	C	N	O	0
			10	5	4	1	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	O	0
			2	2	
7	B	2	Total	O	0
			2	2	

Continued on next page...

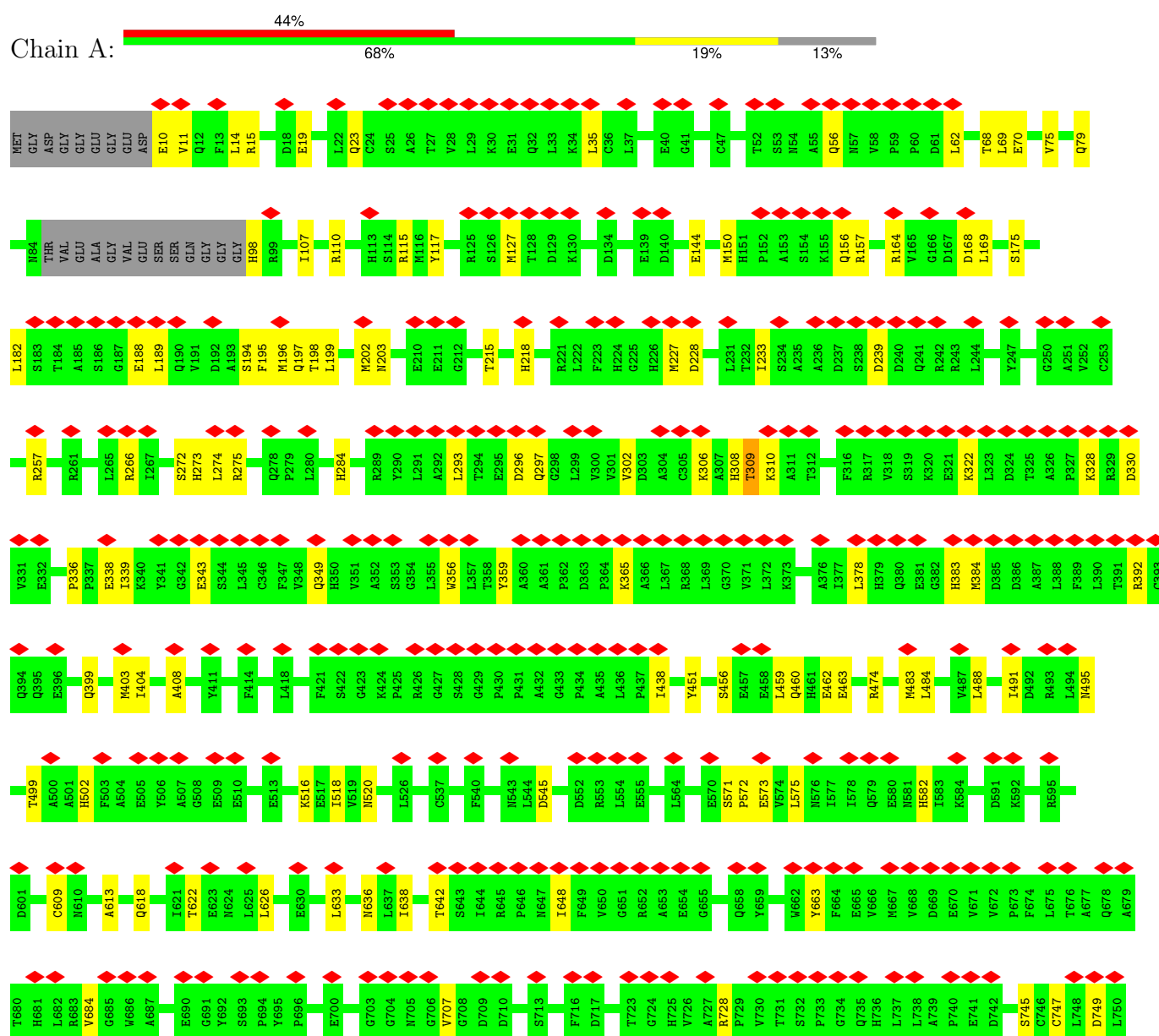
Continued from previous page...

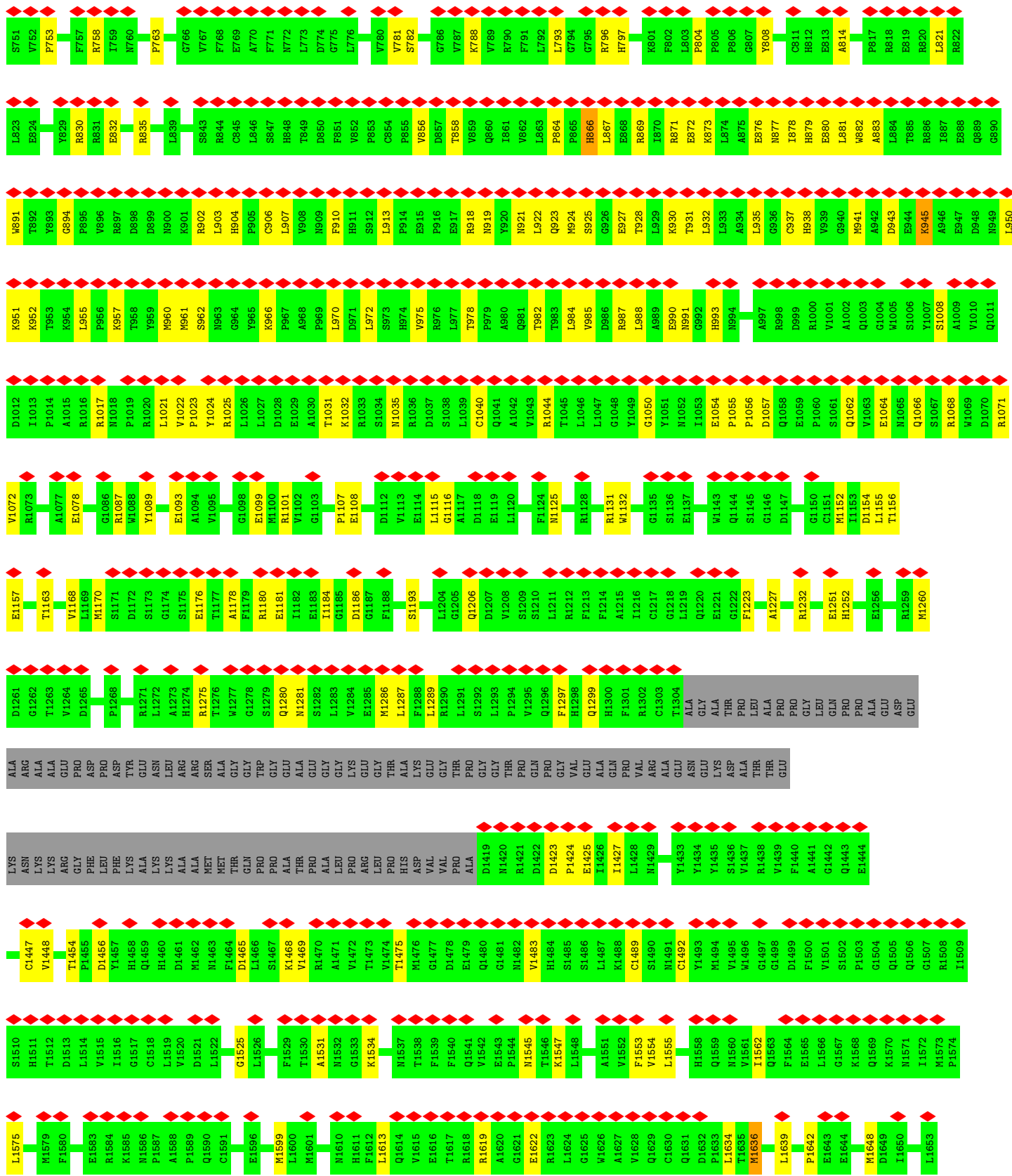
Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	O	0
			2	2	
7	C	2	Total	O	0
			2	2	

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





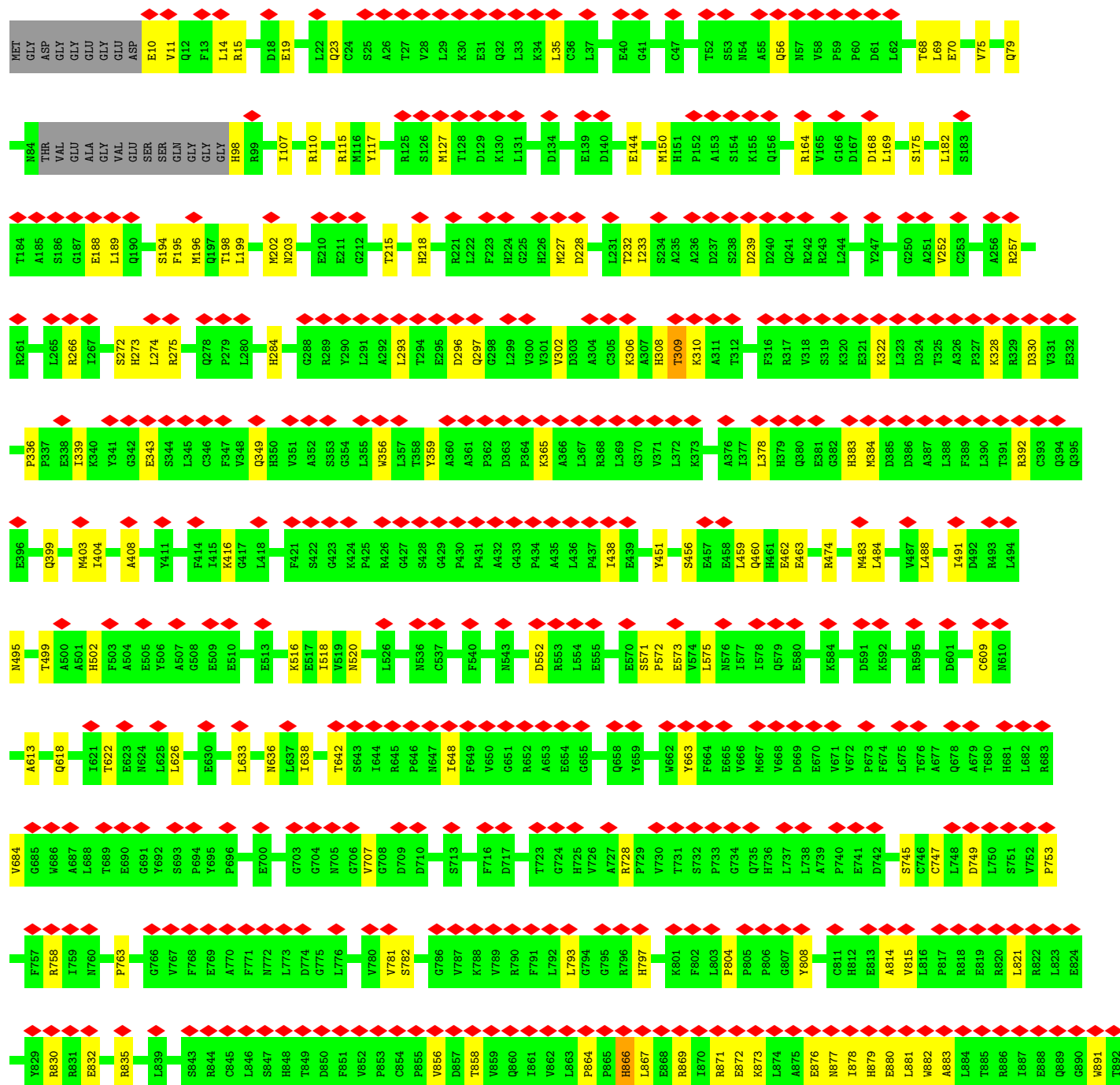
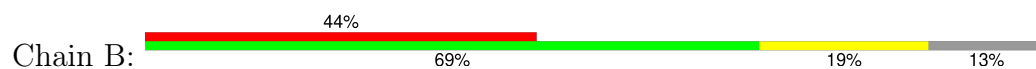


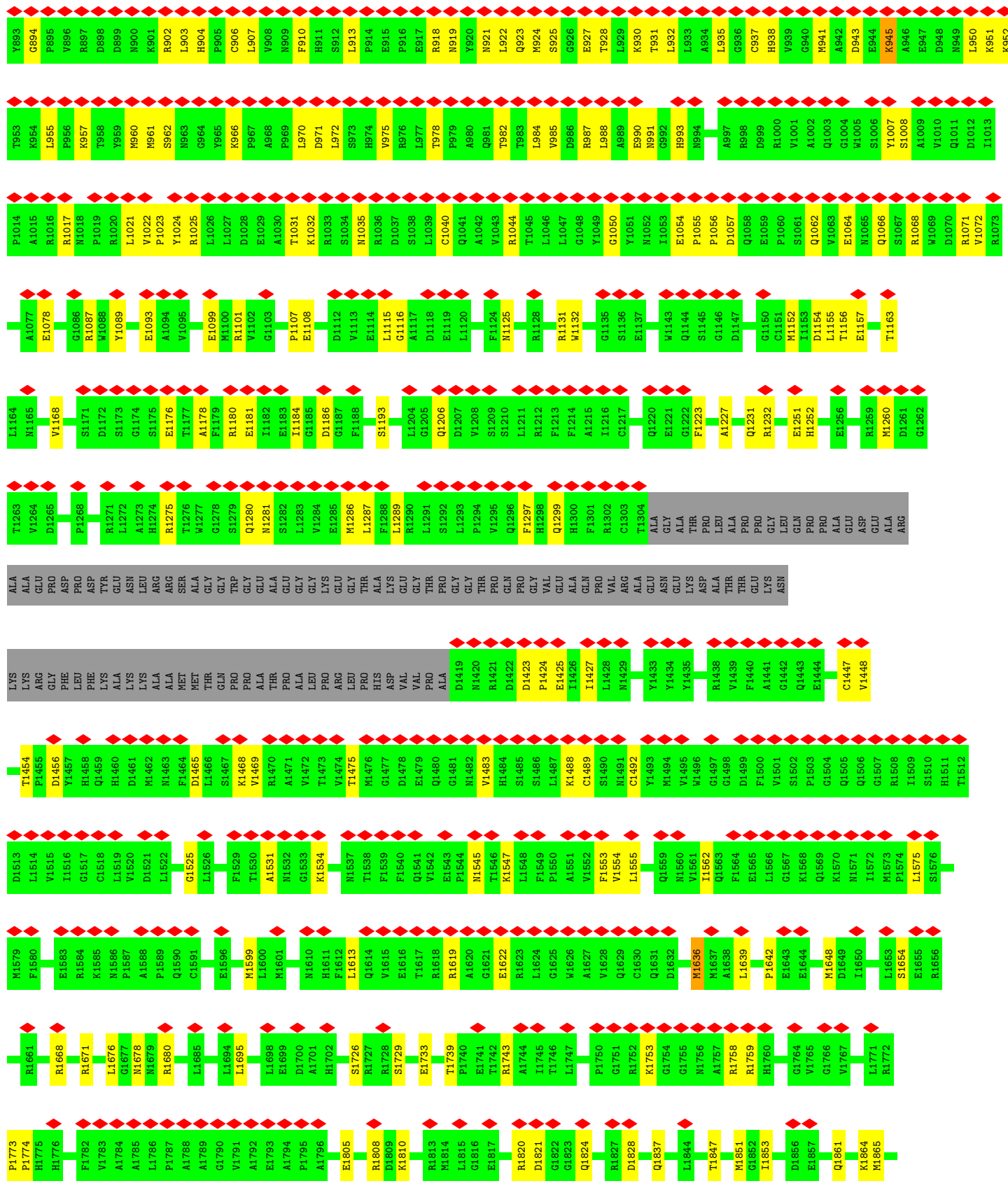
A3431	K3371	H3311	A3251	G3191	V3131	L3071	T3011	I2951	K2891	L2891	F2711
E3432	V3372	L3312	D3252	E3192	T3132	A3072	N3012	E2952	Q2892	Q2772	P2712
E3433	V3373	N3313	I3253	C3193	T3133	R3073	H3013	K2953	E2893	N2773	D2713
L3434	A3374	S3314	G3254	A3194	V3134	S3074	C3014	R2954	L2894	N2774	V2714
F3435	E3375	L3315	G3255	A3195	A3135	L3075	L3015	F2955	E2895	L2775	V2715
R3436	E3376	L3316	L3256	R3196	L3136	D3076	F3017	A2956	A2896	S2776	D2716
V3437	E3377	L3317	A3257	L3197	L3137	A3077	V3017	F2957	K2897	Y2777	A2717
V3438	Q3378	N3318	E3258	A3198	P3138	R3078	L3018	Q2958	G2898	G2778	S2718
G3439	L3379	L3319	S3259	A3199	V3139	T3079	S3019	Q2959	G2899	E2779	V2719
E3440	R3380	L3320	G3260	A3200	L3140	V3080	T3020	L2960	G2900	N2780	S2720
L3441	L3381	R3321	A3261	M3201	T3141	M3081	F3021	Q2961	T2901	V2781	S2721
F3442	E3382	L3322	R3262	P3202	T3142	K3082	A3022	Q2962	H2902	D2782	K2722
I3443	A3383	I3323	V3263	V3203	L3143	S3083	K3023	L2963	P2903	E2783	A2723
Y3444	K3384	V3324	T3264	A3204	F3144	G3084	V3024	L2964	L2904	E2784	E2724
V3445	A3385	N3325	E3265	F3205	Q3145	P3085	L3025	R2965	L2905	L2785	K2725
S3446	E3386	N3326	M3266	L3206	H3146	E3086	G3026	W2966	V2906	K2786	L2786
K3447	A3387	L3327	F3267	E3207	I3147	I3087	S3027	M2967	P2907	T2787	LYS
S3448	E3388	G3328	H3268	P3208	A3148	V3088	G3028	D2968	Y2908	VAL	THR
H3449	E3389	I3329	V3269	Q3209	Q3149	K3089	G3029	I2969	D2909	ASP	ALA
R3450	G3390	D3330	I3270	L3210	H3150	A3090	H3030	S2970	T2910	GLU	ALA
F3451	E3391	E3331	E3271	N3210	Q3151	G3091	S3031	Q2971	L2911	M2790	GLY
K3452	L3392	A3332	I3272	G3212	L3152	L3092	S3032	E2972	L2912	R2792	N2734
R3453	L3393	V3333	T3273	Y3213	G3153	R3093	N3033	F2973	A2913	P2793	F2735
E3454	V3394	W3334	L3274	N3214	D3154	S3094	K3034	I2974	K2914	Y2794	D2736
F3455	R3395	M3335	P3275	A3215	D3155	F3095	E3035	A2975	E2915	K2795	P2737
K3456	D3396	K3336	M3276	C3216	V3156	F3096	K3036	H2976	K2916	T2796	R2738
N3457	R3397	R3337	L3277	S3217	I3157	E3097	E3037	L2977	A2917	F2797	P2739
F3458	E3397	L3338	C3278	V3218	L3158	S3098	I3038	E2978	R2918	S2798	V2740
V3459	F3398	A3339	S3279	Y3219	D3159	A3099	T3039	A2979	D2919	E2799	E2741
V3460	S3399	V3340	Y3280	T3220	D3160	S3100	T3040	V2980	R2920	K2800	T2742
Q3461	V3400	F3341	L3281	T3221	V3161	E3101	S3041	V2981	E2921	D2801	L2743
N3462	L3401	A3342	P3282	K3222	Q3162	I3102	L3042	S2982	K2922	K2802	L2744
E3463	C3402	Q3343	A3283	S3223	V3163	I3103	F3043	S2983	A2923	E2803	V2745
I3464	R3403	P3344	W3284	P3224	S3164	E3104	C3044	G2984	Q2924	L2804	L2746
N3465	D3404	K3345	W3285	R3225	C3165	K3105	K3045	R2985	E2925	Y2805	P2748
L3405	L3405	I3346	E3286	E3226	V3166	M3106	L3046	V2986	L2926	R2806	L2747
Y3406	Y3406	V3347	E3287	R3227	F3167	V3107	A3047	E2987	L2927	W2807	E2749
A3407	A3407	R3348	G3288	A3228	T3168	E3108	A3048	K2988	K2928	P2808	K2750
L3408	L3408	F3289	P3289	I3229	L3169	N3109	L3049	S2989	F2929	L2809	L2751
V3409	V3409	E3290	E3290	L3230	C3170	L3110	P2990	P2990	K2930	K2810	D2752
P3410	P3410	P3351	A3291	G3231	S3171	R3111	R3051	H2991	L2930	E2811	S2753
L3411	L3411	A3291	A3291	G3231	S3171	R3111	R3051	E2992	Q2931	S2812	F2754
L3412	L3412	P3292	P3292	L3232	T3172	L3112	K3052	E2992	G2934	L2813	L2755
I3413	I3413	P3293	P3293	P3233	Y3173	G3113	R3053	Q2993	M2933	K2814	K2756
R3414	R3414	A3294	A3294	N3234	S3174	K3114	V3054	E2994	G2934	A2815	K2757
V3415	V3415	L3295	A3295	S3235	L3175	V3115	S3055	L2995	Y2935	L2816	F2758
F3416	F3416	V3236	V3236	V3236	G3176	S3116	K2996	K2996	A2936	L2817	A2759
D3417	D3417	E3237	E3237	E3237	T3177	GLN	F3057	F2997	V2937	E2818	E2760
N3418	N3418	A3298	A3298	E3238	T3178	ALA	G3058	F2998	K2938	R2819	W2820
R3419	R3419	G3299	G3299	M3239	K3179	ARG	T3059	A2999	T2938	L2820	H2763
L3420	L3420	A3300	A3300	G3240	N3180	THR	D3060	K3000	R2939	W2821	E2764
A3421	A3421	F3301	F3301	F3241	GLN	VAL	A3061	I3001	GLY	ASP	K2765
H3422	H3422	P3302	P3302	D3242	Y3182	K3123	P3062	L3002	LEU	L2823	K2766
W3423	W3423	G3303	G3303	I3243	V3183	G3124	A3063	L3003	L3002	E2824	A2767
L3424	L3424	C3304	C3304	P3244	E3184	V3125	V3064	P3004	LYS	K2825	F2768
T3425	T3425	T3305	T3305	V3245	K3185	G3126	V3065	L3005	ASP	A2826	D2769
E3426	E3426	A3306	A3306	L3246	L3186	Q3127	N3066	I3006	GLY	R2827	K2770
P3427	P3427	V3307	V3307	D3247	R3187	N3128	C3067	N3007	ASP	G2829	
N3428	N3428	T3308	T3308	R3248	P3188	L3129	L3068	Q3008	GLY		
A3429	A3429	S3309	S3309	L3249	A3189	T3130	H3069	Y3009	GLY		
N3430	N3430	D3310	D3310	M3250	L3190		T3070	F3010			





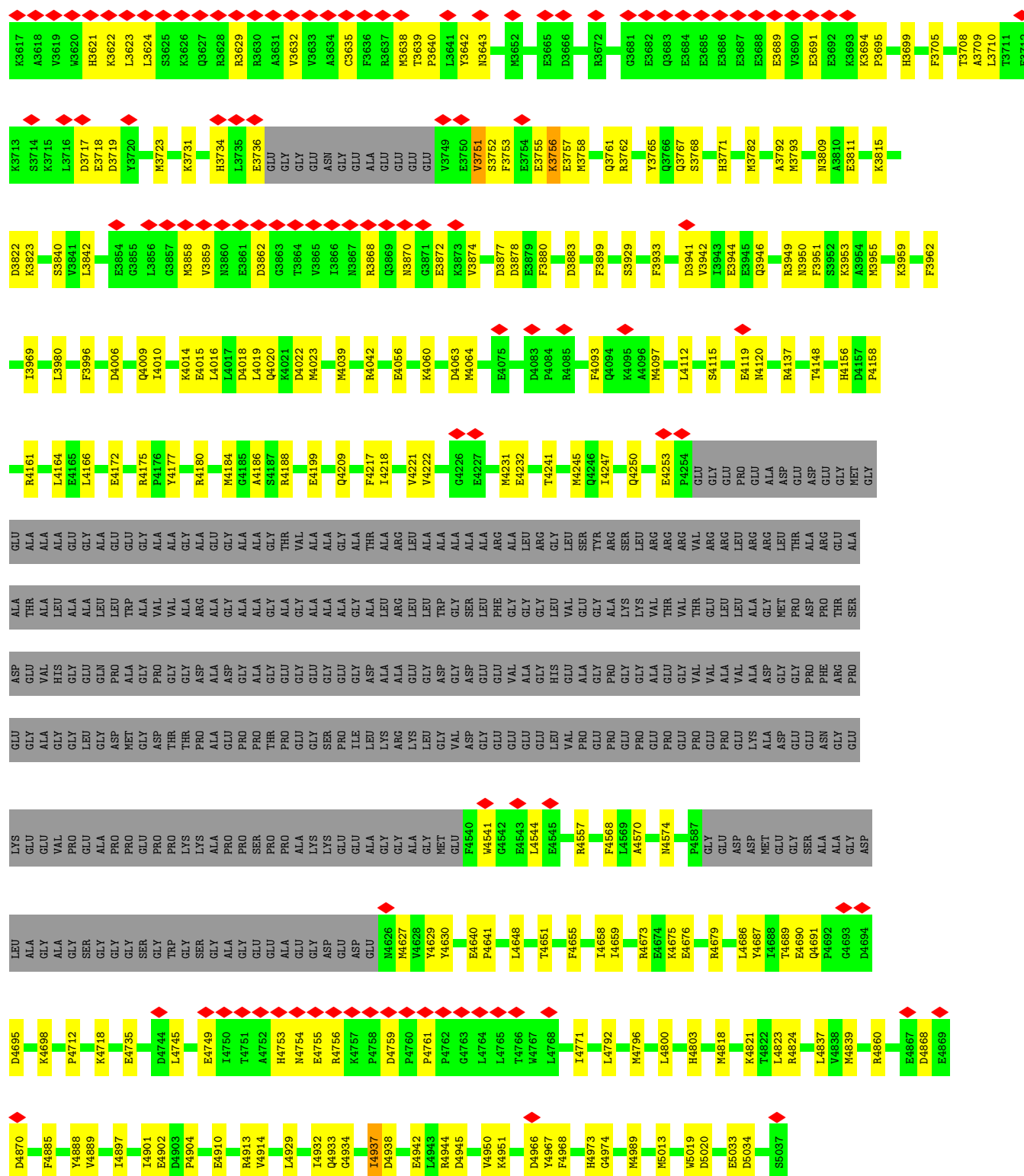
• Molecule 1: Ryanodine receptor 1





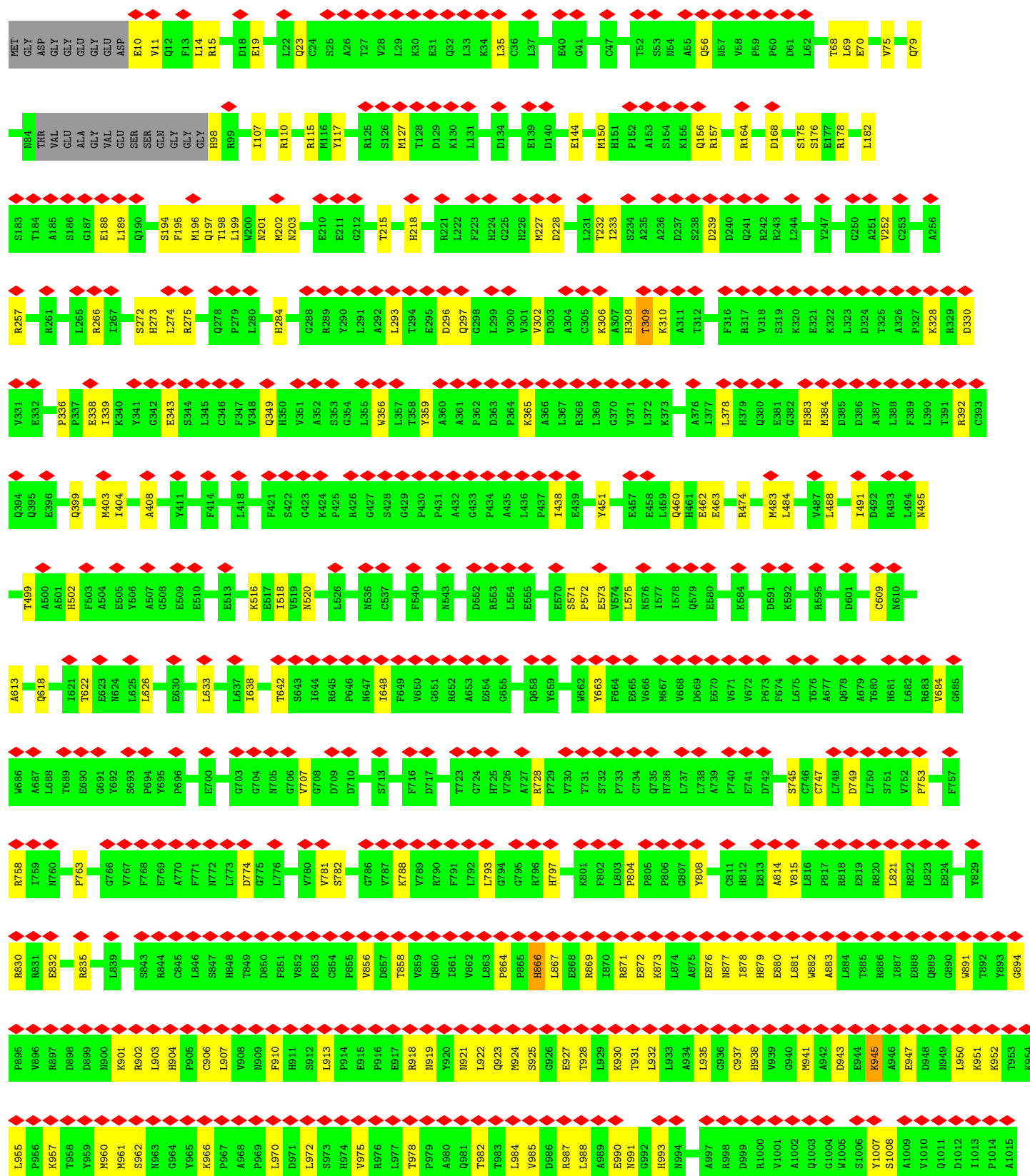
S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	R2790	L2791	R2792	P2793	Y2794	K2795	L2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	L2805	K2806	W2807	L2808	K2809	L2810	E2811	S2812	L2813	K2814	A2815	L2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU
D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	P2739	W2740	E2741	T2742	L2743	N2744	V2745	L2746	D2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	F2767	D2768	D2769	K2770	I2771	Q2772	N2773	N2774	D2775
C2656	L2657	P2658	T2659	G2660	W2661	A2662	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	K2676	K2677	L2678	F2679	W2680	G2681	L2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	N2698	A2699	W2700	P2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	A2709	L2710	P2711	P2712	D2713	V2714	W2715
S2594	L2595	T2596	K2597	A2598	Q2599	R2600	D2601	V2602	L2603	E2604	D2605	C2606	M2608	A2609	L2610	C2611	R2612	Y2613	I2614	R2615	L2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	A2637	K2638	M2639	L2641	K2642	L2643	L2644	T2645	N2646	H2647	L2648	E2649	C2651	Y2655				
M2530	R2531	A2532	A2533	A2534	S2535	L2536	D2537	T2538	A2539	T2540	F2541	S2542	E2545	M2546	A2547	L2548	A2549	L2550	N2551	R2552	Y2553	L2554	C2555	L2556	L2559	T2562	T2563	K2564	C2565	A2566	F2569	A2570	G2571	T2572	E2573	H2574	R2575	A2576	T2577	M2578	V2579	D2580	S2581	L2582	H2584	T2585	V2586	R2587	L2588	L2589	L2592	R2591	G2592	R2593					
D2465	L2466	T2469	S2471	L2470	L2472	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	Q2487	P2488	K2489	M2490	S2491	A2492	S2493	F2494	V2495	P2496	D2497	H2498	K2499	M2502	Y2503	L2504	F2505	L2506	G2511	L2512	E2513	N2514	Q2515	D2516	F2517	L2518	L2519	H2520	V2521	L2522	D2523	V2524	G2525	F2526	P2528	D2529						
G2394	P2395	G2396	V2397	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	N2414	R2415	V2416	H2417	L2418	Q2419	M2423	Y2426	A2427	A2428	L2429	I2430	D2431	L2432	L2433	E2439	M2440	H2441	L2442	G2446	K2447	G2448	E2449	R2452	I2453	R2454	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464									
K2316	G2317	Y2318	P2319	D2320	T2321	G2322	C2326	G2327	R2330	Y2331	L2332	D2333	F2334	V2341	E2348	L2355	L2356	L2357	L2358	K2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	L2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	T2380	E2381	E2382	A2383	L2384	L2385	L2386	S2387	E2388	D2389	P2390	A2391	D2392	D2393					
M2228	V2229	Y2238	L2242	S2243	R2244	H2253	Y2256	L2257	L2258	E2259	G2262	I2263	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2282	N2283	N2284	E2285	L2290	E2291	E2292	Q2293	D2294	L2295	K2297	V2298	W2299	S2300	Y2301	L2302	A2303	G2304	C2305	G2306	L2307	Q2308	S2309	C2310	P2311	M2312	L2313	A2315									
E2108	L2116	M2120	L2123	Q2127	L2155	L2165	L2166	V2167	L2168	Q2169	M2170	Q2173	E2174	E2175	M2176	L2177	M2178	M2186	F2191	Y2192	Q2193	H2194	M2198	L2201	G2202	M2203	M2208	E2209	V2210	M2211	W2212	W2213	V2214	L2215	Q2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	R2224	F2225	K2227														
L2027	R2028	Q2029	D2030	D2033	D2037	Q2045	L2046	GLU	GLY	GLU	R1976	Y1977	A1978	L1979	L1980	M1981	R1982	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	R1993	R1994	R1996	F1997	F1998	R1999	S2000	P2001	Q2005	M2008	L2009	L2010	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	P2022	E2025	D2026										
T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	Q1973	L1969	Q1970	Q1973	R1976	Y1977	A1978	L1979	L1980	M1981	R1982	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	R1993	R1994	R1996	F1997	F1998	R1999	S2000	P2001	Q2005	M2008	L2009	L2010	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	P2022	E2025	D2026						
L1922	E1923	E1924	G1925	L1926	L1927	Q1928	M1929	L1931																																																			





Chain D:

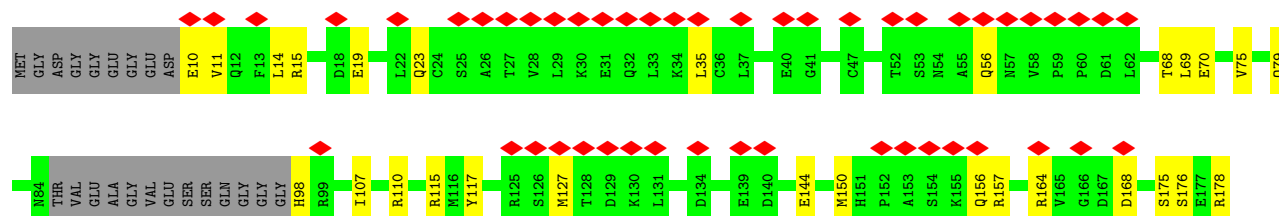


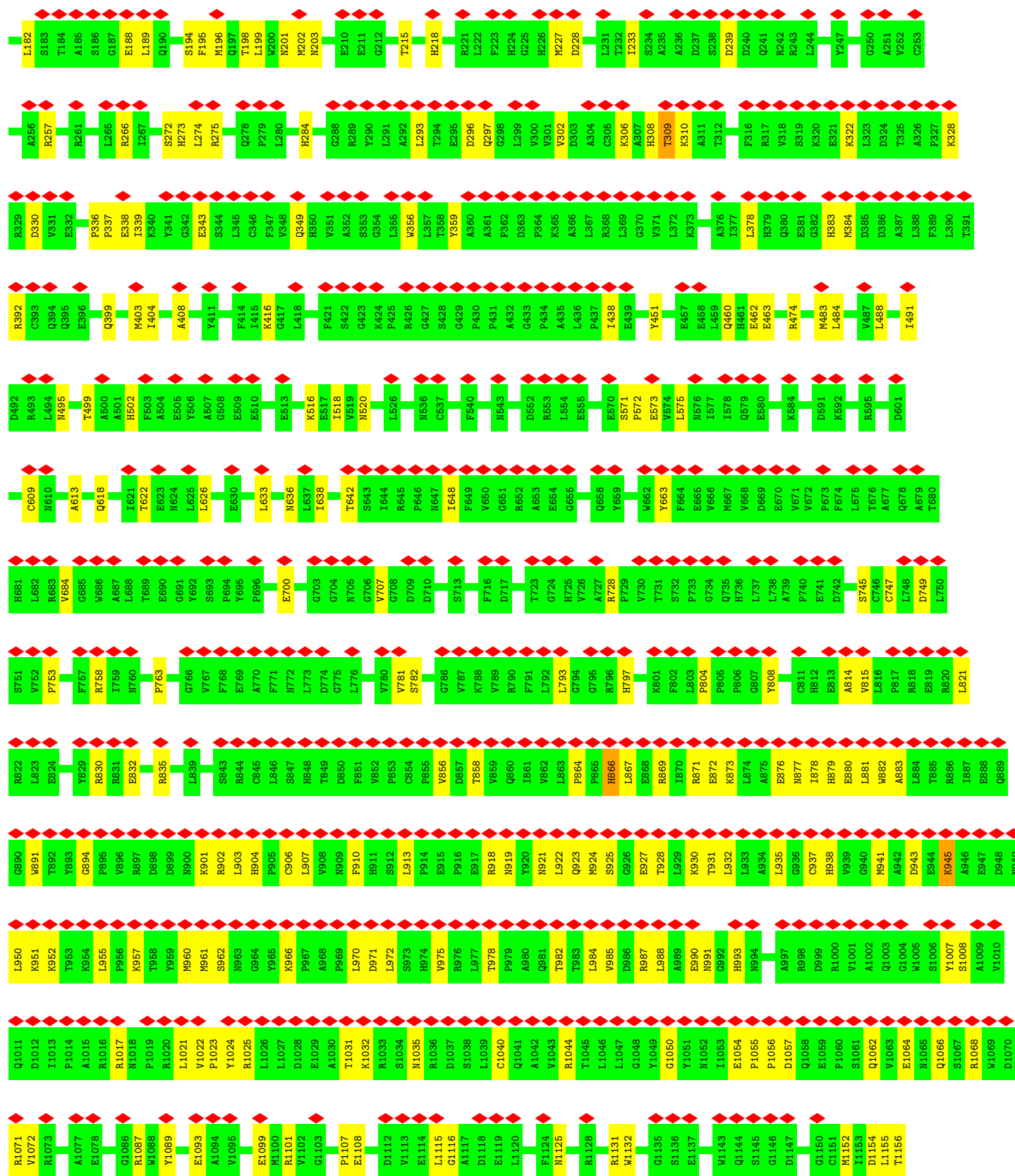


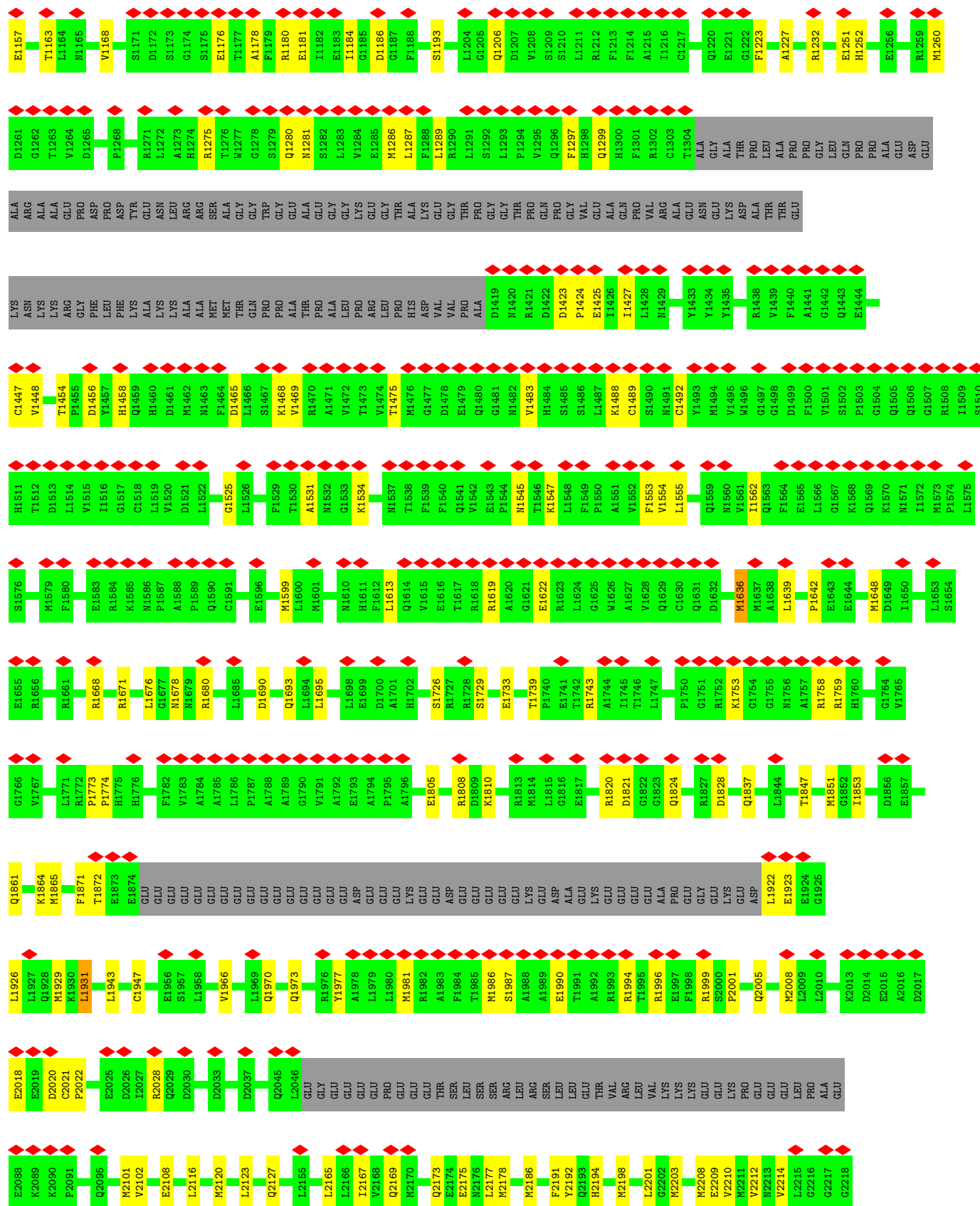




H3699	Q3608	E3548	GLY	R3498	T3308	R3248	P3188	N3128	C3067	N3007	D2947
F3705	T3609	V3549	SER	R3499	S3309	L3249	A3189	L3129	L3068	Q3008	T2948
T3708	E3610	R3550	ASP	G3370	D3310	N3250	L3190	T3130	H3069	Y3009	S2949
A3709	H3611	E3551	GLU	K3371	H3311	A3251	G3191	Y3131	I3070	F3010	S2950
L3710	F3612	F3552	ARG	V3372	L3312	D3252	G3192	T3132	L3071	T3011	I2951
T3711	Y3613	E3553	THR	V3373	N3313	T3253	C3193	T3133	A3072	N3012	E2952
K3712	K3614	Q3554	LYS	A3374	S3314	G3254	L3194	V3134	R3073	H3013	K2953
S3713	S3615	N3555	LYS	E3375	L3315	G3255	A3195	A3135	C3014	C3014	R2954
S3714	K3616	N3556	R3498	E3376	L3316	L3256	L3196	L3136	S3074	L3015	F2955
K3715	K3617	L3557	H3437	E3377	G3317	A3257	L3197	L3137	D3075	L3016	A2956
L3716	A3618	H3558	V3438	Q3378	N3318	E3258	A3198	P3138	A3077	F3017	F2957
D3717	K3619	G3559	G3439	L3379	I3319	E3259	A3199	V3139	R3078	L3018	G2958
E3718	V3620	E3440	E3440	R3380	L3320	G3260	A3200	L3140	F3079	S3019	F2959
D3719	H3621	T3441	T3441	L3381	R3321	A3261	M3201	T3141	V3080	T3020	L2960
Y3720	K3622	F3442	T3442	E3382	I3322	R3262	P3202	T3142	M3081	P3021	Q2961
M3723	L3623	T3443	T3443	A3383	L3323	Y3263	V3203	L3143	K3082	A3022	Q2962
K3731	L3624	Y3444	Y3444	K3384	V3324	T3264	A3204	F3144	S3083	K3023	L2963
H3734	S3625	V3445	V3445	A3385	N3325	E3265	F3205	Q3145	G3084	V3024	L2964
L3735	K3626	S3446	S3446	E3386	N3326	K3266	L3206	H3146	P3085	L3025	R2965
L3736	Q3627	K3447	K3447	L3327	L3327	P3267	E3207	I3147	E3086	G3026	W2966
E3736	R3628	S3448	S3448	E3328	G3328	H3268	P3208	A3148	F3087	S3027	W2967
GLU	R3629	H3449	H3449	E3388	I3329	V3269	Q3209	Q3149	I3088	G3028	D2968
GLY	R3630	N3450	N3450	E3389	D3330	T3270	L3210	H3150	R3089	G3029	I2969
GLY	A3631	F3451	F3451	G3390	E3331	E3271	N3211	Q3151	A3090	H3030	S2970
ASN	V3632	K3452	K3452	E3391	A3332	T3272	E3212	F3152	G3091	A3031	Q2971
GLY	L3633	R3453	R3453	L3392	T3333	T3273	Y3213	G3153	L3092	S3032	E2972
GLY	K3634	E3454	E3454	L3393	W3334	L3274	N3214	D3154	F2973	N3033	F2973
ALA	A3635	E3455	E3455	V3394	M3335	P3275	A3215	D3155	I2974	N3034	I2974
GLU	C3636	Q3456	Q3456	R3396	K3336	N3276	C3216	I3156	F3096	E3035	A2975
GLU	R3637	N3457	N3457	E3397	R3337	L3277	S3217	I3157	E3097	K3036	W2976
GLU	M3638	F3458	F3458	L3338	L3338	C3278	V3218	L3158	S3098	E3037	L2977
E3750	T3639	V3459	V3459	A3339	A3339	S3279	Y3219	D3159	A3099	M3038	E2978
S3752	P3640	V3460	V3460	S3399	V3340	Y3280	T3220	E3160	S3100	I3039	A2979
K3752	L3641	Q3461	Q3461	V3400	F3341	L3281	T3221	V3161	E3101	T3040	V2980
Y3642	Y3642	N3462	N3462	C3402	A3342	P3282	K3222	Q3162	D3102	S3041	V2981
N3643	N3643	I3464	I3464	R3403	Q3343	R3283	S3223	V3163	T3103	L3042	S2982
M3652	M3652	N3465	N3465	D3404	P3344	W3284	P3224	S3164	E3104	F3043	S2983
E3655	E3655	N3466	N3466	L3405	I3345	W3285	R3225	C3165	K3105	C3044	G2984
D3666	D3666	M3467	M3467	Y3406	V3346	E3286	E3226	Y3166	M3106	K3045	R2985
R3672	R3672	S3468	S3468	A3407	S3347	R3287	R3227	V3167	V3107	L3046	V2986
G3681	G3681	L3408	L3408	L3408	R3348	G3288	A3228	T3168	E3108	A3047	E2987
E3682	E3682	F3469	F3469	Y3409	A3349	P3289	I3229	L3169	N3109	A3048	K2988
Q3683	Q3683	L3470	L3470	P3410	R3350	E3290	L3230	C3170	L3110	L3049	S2989
E3684	E3684	T3471	T3471	L3411	P3351	A3291	G3231	S3171	R3111	V3050	P2990
E3685	E3685	A3472	A3472	L3412	P3352	P3292	L3232	I3172	L3112	R3051	H2991
E3686	E3686	D3473	D3473	I3413	L3353	P3293	P3233	Y3173	G3113	H3052	E2992
E3687	E3687	S3474	S3474	R3414	L3354	P3294	N3234	S3174	K3114	R3053	Q2993
E3688	E3688	K3475	K3475	Y3415	H3355	A3295	S3235	L3175	V3115	V3054	E2994
E3689	E3689	S3476	S3476	V3416	S3356	L3296	V3236	G3176	G3116	L3055	I2995
V3690	V3690	D3477	D3477	D3417	H3357	P3297	E3237	T3177	GLN	L3056	K2996
E3691	E3691	N3478	N3478	N3418	F3358	A3298	E3238	T3178	ALA	F3057	F2997
E3692	E3692	LYS	LYS	N3419	I3359	A3299	M3239	K3179	ARG	G3058	F2998
E3693	E3693	ALA	ALA	P3360	P3360	A3300	C3240	N3180	THR	GLN	A2999
K3694	K3694	GLY	GLY	T3361	A3301	P3301	P3241	T3181	VAL	T3059	K3000
P3695	P3695	ASP	ASP	A3421	P3302	P3302	D3242	Y3182	K3123	D3060	I3001
		ALA	ALA	H3422	P3303	G3303	I3243	V3183	G3124	A3061	I3002
		GLN	GLN	V3423	P3304	C3304	P3244	E3184	G3125	P3062	L3003
		SER	SER	L3424	T3305	T3305	P3245	K3185	G3126	A3063	F3004
		GLY	GLY	T3425	A3306	A3306	L3246	L3186	Q3127	V3065	L3005
				E3426	V3307	V3307	D3247	R3187		N3066	I3006
				P3427							

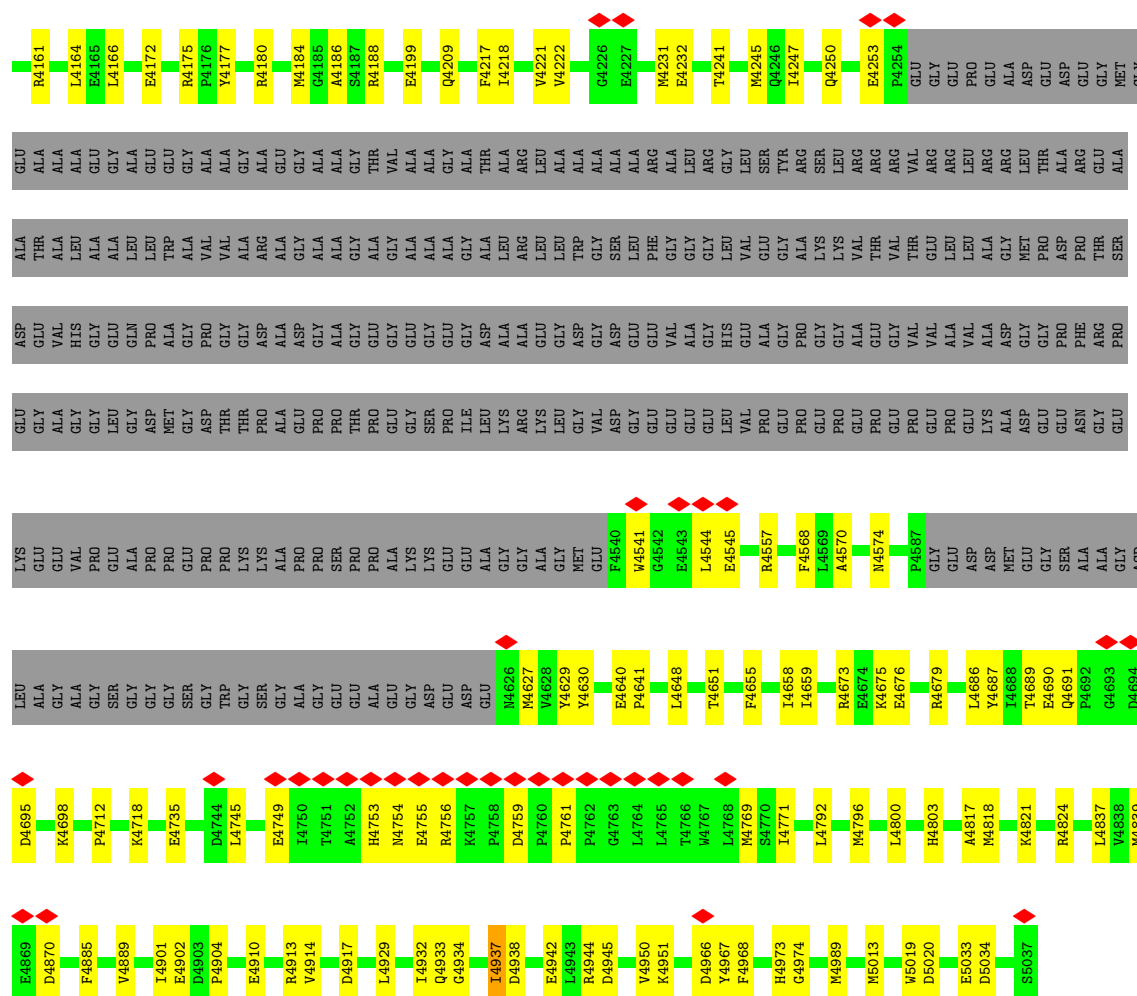




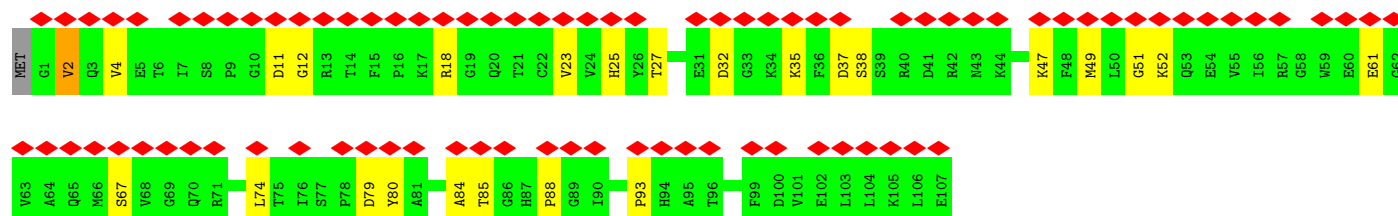
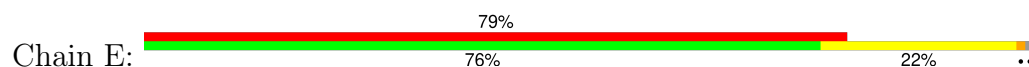


F3010	S2950	K2890	E2830	L2710	E2649	L2589	D2523	L2457	R2385	L2307	E2219
T3011	I2951	K2891	GLU	P2711	R2650	S2590	V2524	R2457	I2386	Q2308	T2220
N3012	E2952	K2892	ARG	D2712	C2651	R2591	G2525	D2458	S2387	S2309	K2221
H3013	K2953	E2893	THR	D2713	W2652	G2592	F2526	S2459	E2388	C2310	E2222
C3014	R2954	L2894	GLU	Y2714		R2593	L2527	L2460	D2389	P2311	L2223
L3015	F2955	W2775	LYS	V2715		S2594	D2529	V2461	P2390	M2312	R2224
Y3016	A2956	A2896	LYS	D2716	C2656	R2594	R2528	P2462	A2391	L2313	F2225
F3017	R2957	G2778	THR	D2717	L2657	L2595	M2530	D2464	R2392	L2314	F2226
L3018	G2958	D2898	ARG	A2718	L2657	T2596	R2531	D2465	R2393	A2315	K2227
S3019	F2959	G2899	LYS	S2719	P2658	K2597	R2532	D2466	G2394	K2316	W2229
T3020	L2960	E2779	ILE	Y2719	G2660	A2598	A2533		G2395	G2317	
P3021	Q2961	M2780	SER	S2720	W2661	R2600	A2534	I2469	P2396	Y2318	Y2238
A3022	Q2962	V2781	GLN	S2721	A2662	D2601	S2535	I2470	G2396	P2319	
K3023	L2963	D2782	THR	K2722	N2663	V2602	L2536	S2471	V2397		I2242
V3024	L2964	E2783	ALA	A2723	F2664	L2603	D2537	L2472	ARG	D2390	S2243
L3025	L2964	E2784	GLN	E2724	G2665	E2604	T2538	P2473	ASP	R2244	
L3025	R2965	L2785	TYR	K2724	V2666	D2605	A2539	L2474	ARG	G2322	H2253
W2966	W2966	K2786	ASP	K2725	T2667	D2606	R2540	L2475	ARG		
G3026	G3026	T2787	PRO	LYS	S2667	D2607	T2541	Q2476	GLU	C2326	
P3027	P2907	H2788	ARG	THR	E2668	M2608	F2541	P2477	HIS	G2327	Y2256
D2968	D2968	P2789	GLU	VAL	E2669	L2609	S2542	T2478	PHE		L2257
G3028	G3028	M2790	ALA	ALA	E2670	L2610	E2545	T2479	GLY	R2330	L2258
G3029	H3030	L2790	GLU	GLU	E2671	C2611	M2546	G2480	GLU	Y2331	E2259
A3031	Q2971	L2791	GLY	GLY	L2672	R2612	A2547	K2481	P2410	L2332	
S2970	E2972	R2792	N2734	F2735	H2673	Y2613	D2547	Q2482	E2412	D2333	G2262
E2972	F2973	K2793	D2736	D2736	L2674	I2614	A2549	P2488	P2411	F2334	I2263
N3033	I2974	Y2794	F2736	F2736	T2675	R2615	L2550	K2489	L2418	V2341	G2264
K3034	A2975	K2795	P2737	P2737	R2676	P2616	R2551	G2483	E2412		L2265
E3035	L2976	P2860	R2796	R2738	K2677	S2617	H2551	A2484	E2413	E2348	G2266
K3036	H2977	L2862	L2862	P2739	L2678	M2618	Y2553	L2485	N2414	M2267	G2267
E3037	E2978	S2798	S2863	V2740	F2679	L2619	Y2554	V2486	R2415	Q2268	Q2268
M3038	Q2978	R2918	G2864	E2741	L2678	L2619	L2554	Q2487	V2416	G2269	G2269
I3039	A2979	D2919	V2740	E2741	E2679	Q2620	L2555	P2488	H2417	L2356	S2269
T3040	V2980	R2920	T2866	T2742	W2680	H2621	L2556	K2489	L2418	L2357	G2270
S3041	V2981	K2800	T2866	L2742	G2681	Q2621	L2556	M2490	G2419	T2271	P2272
L3042	S2982	D2921	L2867	L2743	L2682	L2622		S2491		T2271	L2273
F3043	S2983	K2922	L2867	L2744	F2683	L2623		A2492			
C3044	Q2984	A2923	S2868	V2745	D2684	R2624	C2564	S2493	Y2426		D2282
G3045	R2985	Q2924	E2870	L2746	S2885	R2625	K2564	S2493	A2427	E2362	N2283
L3046	V2986	E2925	L2871	I2747	L2686	L2626	C2565	F2494	A2427	C2363	E2285
A3047	E2987	L2926	Q2872	P2748	A2687	L2627	A2566	V2495	A2428	F2364	
A3048	K2988	L2927	A2873	E2749	H2688	F2628		P2496	A2428	G2365	L2290
L3049	S2989	K2928	M2874	K2750	K2889	F2628	F2569	R2496	L2429	G2366	Q2291
V3050	P2990	F2929	A2875	L2751	K2690	D2629	A2570	H2498	I2430	A2367	E2292
R3051	H2991	L2752	E2876	D2752	K2690	V2630	Q2571	D2498	D2431	L2367	Q2293
H3052	Q2992	Q2931	E2876	S2753	D2691	P2631	T2572	K2499	L2432	L2368	D2294
E2992	E2992	R2932	L2812	F2754	D2692	L2632	E2573		L2433	R2369	L2295
K3053	Q2993	M2933	S2812	F2754	Q2693	L2632	E2573	L2504		G2370	E2296
V3054	E2994	A2879	I2755	T2755	Q2693	L2633	H2574	F2505		E2371	K2297
S3055	I2995	E2880	K2814	N2756	E2694	N2634	R2575	L2506	E2439	G2372	V2297
L3056	A2996	A2815	A2815	N2756	E2694	E2635	A2576		M2440	G2373	W2298
F3057	K2997	M2816	K2757	K2757	Y2696	F2636	L2577	G2511	H2441	Q2375	S2299
G3058	F2997	L2817	F2758	A2759	R2697	A2637	M2578	L2512	L2442	G2375	Y2301
T3059	F2998	A2818	E2760	K2759	M2698	K2638	D2579	E2513	Q2446	L2376	L2302
A2999	A2999	E2819	E2760	A2818	M2699	M2639	D2580	N2514	K2447	L2377	A2303
D3060	R2939	W2819	Y2761	Y2761	M2700	P2640	S2581	Q2515	G2448	A2378	G2304
L3061	GLY	E2820	T2762	T2762	P2701	L2641	S2581	D2516	E2449	A2379	C2305
A3061	LEU	W2821	H2763	H2763	L2701	K2642	L2583	F2517		I2380	G2306
P3062	LYS	E2822	E2764	E2764	C2702	K2642	H2584	L2519	R2452	L2380	
L3062	ASP	T2822	T2764	T2764	L2703	L2643	T2585	L2519	I2453	E2381	
A3063	R2888	I2823	K2765	K2765	C2704	L2644	T2585	H2520	R2454	E2382	
V3064	GLU	E2824	W2766	W2766	A2705	T2645	Y2586	V2521		A2383	
V3065	L2946	K2825	A2767	A2767	L2706	N2646	Y2587	L2522		I2384	
L3065	D2947	A2826	F2768	F2768	G2707	H2647					
C3067	T2948	R2827	G2708	G2708	A2709	Y2648					
L3068	S2949	E2828	A2709	A2709							

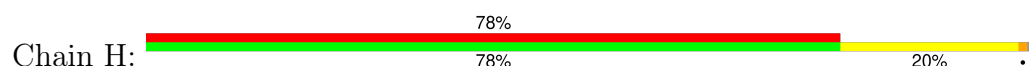
N3809	K3959	T3708	H3611	E3551	GLN	A3431	K3371	H3311	A3251	G3191	Y3131	I33070
A3810	F3962	A3709	P3612	F3552	GLU	E3432	V3372	L3312	D3252	E3192	T3132	L3071
E3811		L3710	Y3613	L3553	ARG	E3433	V3373	N3313	I3253	C3193	T3133	
K3815	I3969	T3711	K3614	Q3554	THR	L3434	A3374	S3314	G3254	L3194	V3134	A3072
D3822	L3960	E3712	S3615	N3555	LYS	F3435	E3375	L3315	G3255	A3195	A3135	S3074
K3823	L3980	K3713	K3616	N3556	LYS	R3436	E3376	L3316	L3256	R3196	L3136	L3075
S3840	F3996	S3714	K3617	L3557	R3498	M3437	E3377	G3317	A3257	L3197	L3137	D3076
V3841		K3715	A3618	H3558	R3499	V3438	Q3378	N3318	E3258	A3198	P3138	A3077
L3842	D4006	L3716	V3619	L3559	G3500	G3439	E3379	I3319	S3259	A3199	V3139	R3078
	Q4009	D3717	W3620	Q3560	D3501	E3440	R3380	L3320	G3260	A3200	L3140	T3079
E3854	L4010	E3718	H3621	Q3561	R3502	I3441	L3381	R3321	A3261	M3201	T3141	V3080
G3855		D3719	K3622	K3562	Y3503	F3442	E3382	I3322	R3262	P3202	T3142	V3081
L3856	M3723	Y3720	L3623	V3563	S3504	I3443	A3383	I3323				K3082
G3857			L3624	E3564	V3505	Y3444	E3384	V3324	Y3263	V3203	L3143	S3083
N3858	K3731		S3625	Q3565	Q3506	W3445	K3384	N3325	T3264	A3204	F3144	
V3859			K3626	S3566	T3507	S3446	A3385	N3326	E3265	F3205	Q3145	G3084
N3860	H3734		Q3627	S3567	S3508	K3447	E3386	L3327	M3266	L3206	H3146	P3085
E3861	L3735		R3628	P3567	S3509	S3448	A3387	L3327	P3267	E3207	I3147	P3086
D3862	E3736		R3629	S3568	L3509	H3449	E3388	G3328	H3268	P3208	A3148	I3087
G3863		GLU	R3630	L3569	V3511	N3450	E3389	I3329	V3269	Q3209	Q3149	V3088
T3864	GLY	GLY	A3631	R3570	A3512	F3451	G3390	D3330	I3270	L3210	H3150	K3089
V3865	GLY	GLY	V3632	Q3572	T3513	K3452	E3391	E3331	E3271	N3211	Q3151	A3090
I3866	ASN	GLU	V3633	M3573	L3514	R3453	L3392	T3333	L3272	Y3213	F3152	G3091
N3867	GLY	GLY	A3634	A3574	K3515	E3454	L3393	W3334	T3273	G3163	G3163	L3092
R3868	ALA	GLU	C3635	L3575	K3516	E3455	V3394	M3335	L3274	N3214	D3154	
Q3869	GLU	GLU	F3636	Y3576	M3517	Q3456	D3396	K3336	P3275	A3215	D3155	F3095
N3870	GLU	GLU	R3637	R3577	L3518	N3457	E3397	R3337	M3276	C3216	V3156	F3096
G3871	GLU	GLU	T3639	G3578	P3519	F3458	E3397	L3338	L3277	S3217	E3097	E3097
K3873	GLU	GLU	P3638	L3579	T3520	V3459	F3398	A3339	C3278	V3218	L3158	S3098
V3874	V3749		P3640	P3580	G3521	Y3460	S3399	V3340	S3279	Y3219	D3159	A3099
	E3750		L3641	G3581	L3522	Q3461	V3400	F3341	Y3280	T3220	D3160	S3100
	V3751		Y3642	C3582	N3523	N3462	L3401	A3342	L3281	T3221	E3101	
D3877	S3762		N3643	R3582	M3524	E3463	C3402	Q3343	P3282	K3222	Q3162	D3102
P4084	F3763			E3583	A3526	I3464	R3403	K3344	W3284	P3224	S3164	E3104
E3879	E3754			E3584	P3527	N3465	D3404	V3346	E3285	R3225	K3105	
F3880	E3755		M3652	D3585	A3526	N3466	L3405	I3345	E3286	C3165	K3106	
	K3756			A3586	T3528	M3467	Y3406	S3347	R3287	Y3167	V3107	
D3883	E3757		E3665	D3587	Q3529	S3468	A3407	R3348	G3288	T3168	E3108	
A4095	M3758		D3666	D3588	Q3530	F3469	L3408	A3349	P3289	L3169	N3109	
F3899				P3589	D3531	L3470	Y3409	R3350	E3290	C3170	L3110	
M4097	Q3761		R3672	E3590	R3531	T3471	P3410	A3350	A3291	S3171	R3111	
	R3762			K3591	L3532	A3472	L3411	R3351	G3231	G3231	L3112	
	Y3765		G3681	K3592	T3533	D3473	L3412	E3352	P3292	L3172		
E4119	Q3766		E3682	M3534	E3533	N3472	I3413	L3353	P3293	Y3173	G3113	
M4120	S3767		Q3683	R3594	L3535	S3474	E3413	L3354	P3294	S3174	K3114	
R4137	S3768		E3684	R3594	A3536	K3475	R3414	H3355	A3295	L3175	V3115	
	H3771		E3685	K3595	K3537	K3476	Y3415	S3356	L3296	G3176	S3116	
T4148			E3686	R3595	T3538	K3477	V3416	H3357	V3236	T3177	GLN	
	M3782		E3687	V3596	R3539	M3478	D3417	F3358	E3237	T3178	ALA	
R3949	A3792		E3688	Q3597	Y3540	N3479	N3418	A3298	E3238	K3179	ARG	
N3950	M3793		E3689	V3598	A3541	P3419	R3419	G3299	M3239	N3180	THR	
F3951			V3690	S3600	L3542	LYS	R3420	A3300	G3240	N3180	GLN	
S3952			E3691	A3601	L3542	GLY	A3421	P3301	P3241	T3181	VAL	
K3953			E3692	K3543	K3543	ASP	A3421	P3302	G3241	R3182	K3123	
A3954			K3693	D3544	D3544	ALA	H3422	P3303	D3242	Y3182	G3124	
M3955			Y3604	T3545	T3545	GLN	W3423	C3304	I3243	V3183	V3125	
			H3605	D3546	D3546	SER	L3424	C3304	P3244	E3184	G3126	
			P3695	H3605	H3605	GLY	T3425	T3305	V3245	K3185	Q3127	
				L3606	L3606	GLY	R3425	A3306	L3246	L3186	G3127	
			E3607	E3547	E3547	SER	E3426	V3307	D3247	R3187	N3128	
			E3608	E3548	E3548	ASP	P3427	V3307	R3248	P3188	L3129	
			Q3608	V3549	V3549		N3428	S3309	R3249	A3189	T3130	
			T3609	R3550	R3550		A3429	D3310		L3190		
			E3610				N3430					

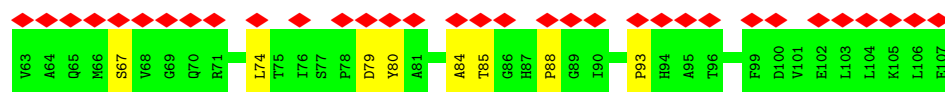


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

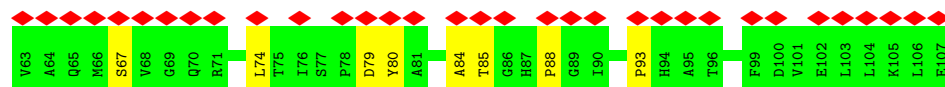
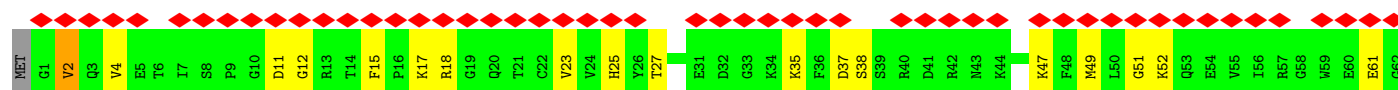
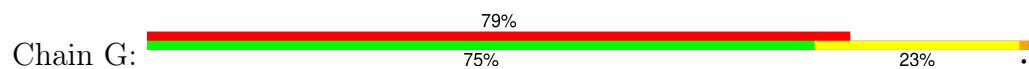


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

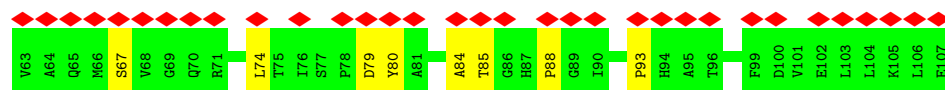
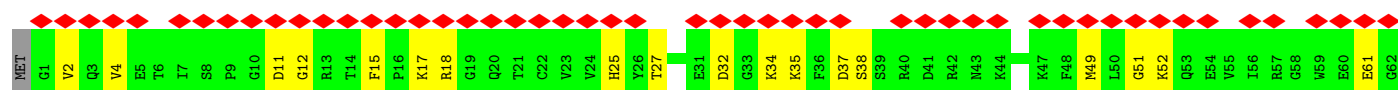
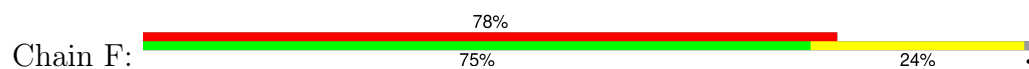




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- 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	41370	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	0.433	Depositor
Minimum map value	-0.213	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, A1BD4, CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/35977	0.36	1/48726 (0.0%)
1	B	0.23	0/35977	0.36	1/48726 (0.0%)
1	C	0.23	0/35977	0.36	1/48726 (0.0%)
1	D	0.23	0/35977	0.36	1/48726 (0.0%)
2	E	0.21	0/850	0.34	0/1146
2	F	0.21	0/850	0.36	0/1146
2	G	0.21	0/850	0.33	0/1146
2	H	0.21	0/850	0.36	0/1146
All	All	0.23	0/147308	0.36	4/199488 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3603	LEU	CA-CB-CG	5.27	134.74	116.30
1	A	3603	LEU	CA-CB-CG	5.26	134.71	116.30
1	D	3603	LEU	CA-CB-CG	5.25	134.69	116.30
1	C	3603	LEU	CA-CB-CG	5.25	134.69	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	34797	698	0
1	B	35150	0	34797	688	0
1	C	35150	0	34797	697	0
1	D	35150	0	34797	697	0
2	E	831	0	831	14	0
2	F	831	0	831	15	0
2	G	831	0	831	14	0
2	H	831	0	831	14	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
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	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	144104	0	142560	2810	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 10.

The worst 5 of 2810 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:4860:ARG:NH1	1:D:4630:TYR:OH	1.88	1.06
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	1.92	1.01
1:B:4630:TYR:OH	1:C:4860:ARG:NH1	1.97	0.96
1:D:4860:ARG:NH1	1:C:4630:TYR:OH	1.97	0.95
1:D:2765:LYS:HZ3	1:D:2857:PRO:HB2	1.38	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%)	4235 (97%)	150 (3%)	0	100	100
1	B	4385/5037 (87%)	4235 (97%)	150 (3%)	0	100	100
1	C	4385/5037 (87%)	4236 (97%)	149 (3%)	0	100	100
1	D	4385/5037 (87%)	4235 (97%)	150 (3%)	0	100	100
2	E	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17960/20580 (87%)	17355 (97%)	605 (3%)	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%)	3813 (99%)	23 (1%)	84	92
1	B	3836/4276 (90%)	3813 (99%)	23 (1%)	84	92
1	C	3836/4276 (90%)	3813 (99%)	23 (1%)	84	92
1	D	3836/4276 (90%)	3813 (99%)	23 (1%)	84	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	85 (96%)	4 (4%)	23	54
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	63
2	G	89/90 (99%)	85 (96%)	4 (4%)	23	54
2	H	89/90 (99%)	85 (96%)	4 (4%)	23	54
All	All	15700/17464 (90%)	15593 (99%)	107 (1%)	80	90

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4695	ASP
1	D	2862	LEU
1	C	3753	PHE
1	B	4937	ILE
1	D	1636	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	866	HIS
1	C	1300	HIS
1	C	3355	HIS
1	B	981	GLN
1	B	909	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	D	5301	-	28,33,33	0.66	0	34,52,52	0.74	2 (5%)
6	A1BD4	D	5304	-	9,11,11	1.18	1 (11%)	6,15,15	1.31	1 (16%)
6	A1BD4	C	5304	-	9,11,11	1.18	1 (11%)	6,15,15	1.31	1 (16%)
3	ATP	C	5301	-	28,33,33	0.66	0	34,52,52	0.75	2 (5%)
3	ATP	A	5301	-	28,33,33	0.66	0	34,52,52	0.74	2 (5%)
6	A1BD4	B	5304	-	9,11,11	1.16	1 (11%)	6,15,15	1.32	1 (16%)
6	A1BD4	A	5304	-	9,11,11	1.17	1 (11%)	6,15,15	1.33	1 (16%)
3	ATP	B	5301	-	28,33,33	0.66	0	34,52,52	0.74	2 (5%)

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	D	5301	-	-	3/18/38/38	0/3/3/3
6	A1BD4	D	5304	-	-	-	0/2/2/2
6	A1BD4	C	5304	-	-	-	0/2/2/2
3	ATP	C	5301	-	-	3/18/38/38	0/3/3/3
3	ATP	A	5301	-	-	3/18/38/38	0/3/3/3
6	A1BD4	B	5304	-	-	-	0/2/2/2
6	A1BD4	A	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5304	A1BD4	C3-C4	-3.07	1.42	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5304	A1BD4	C3-C4	-3.07	1.42	1.47
6	A	5304	A1BD4	C3-C4	-3.06	1.42	1.47
6	B	5304	A1BD4	C3-C4	-2.99	1.42	1.47

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'	-2.38	107.74	109.92
3	A	5301	ATP	C4'-O4'-C1'	-2.37	107.76	109.92
3	C	5301	ATP	C5-C6-N6	2.36	123.91	120.31
3	D	5301	ATP	C4'-O4'-C1'	-2.35	107.78	109.92
3	A	5301	ATP	C5-C6-N6	2.34	123.88	120.31

There are no chirality outliers.

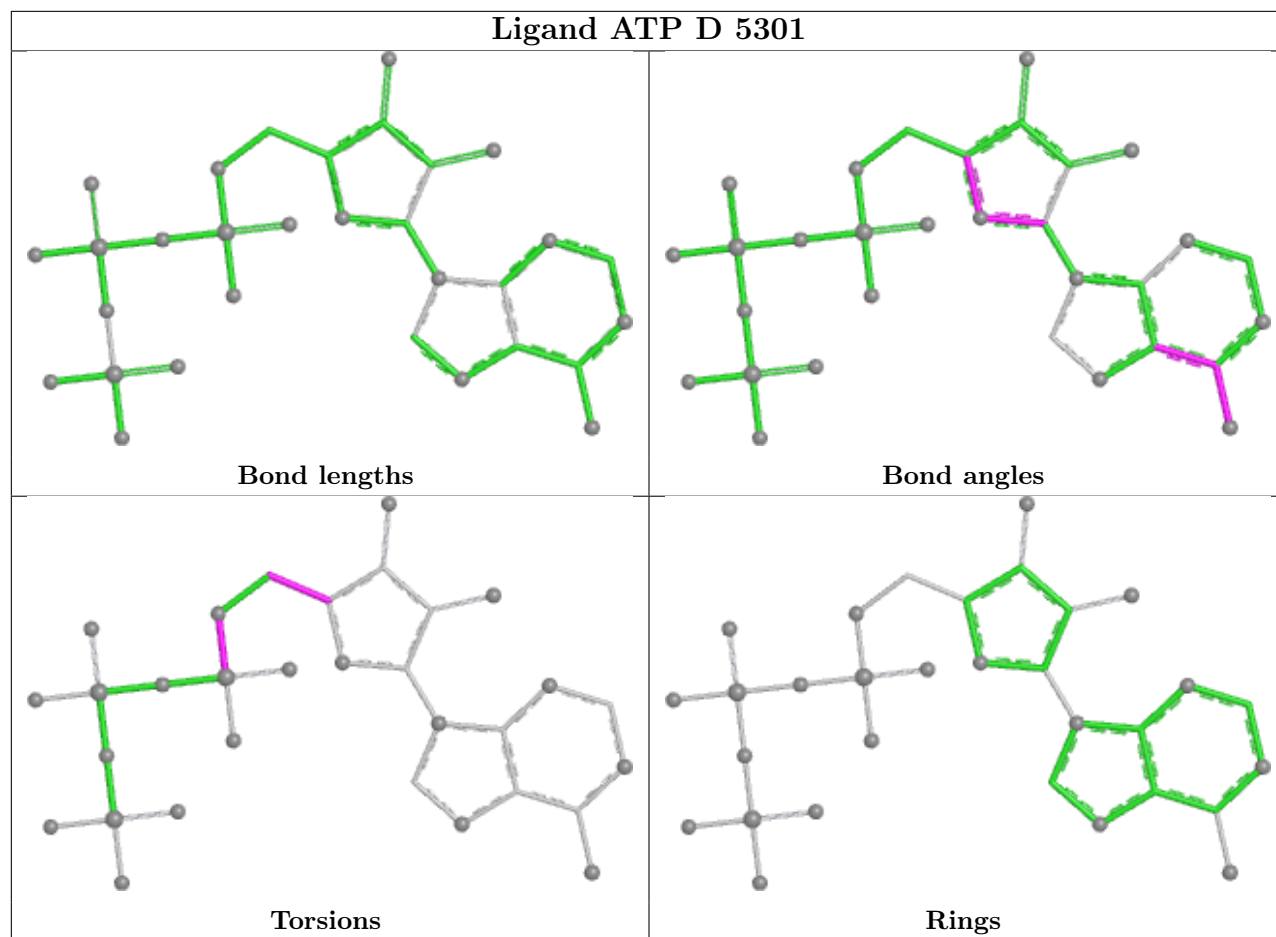
5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	D	5301	ATP	C5'-O5'-PA-O2A

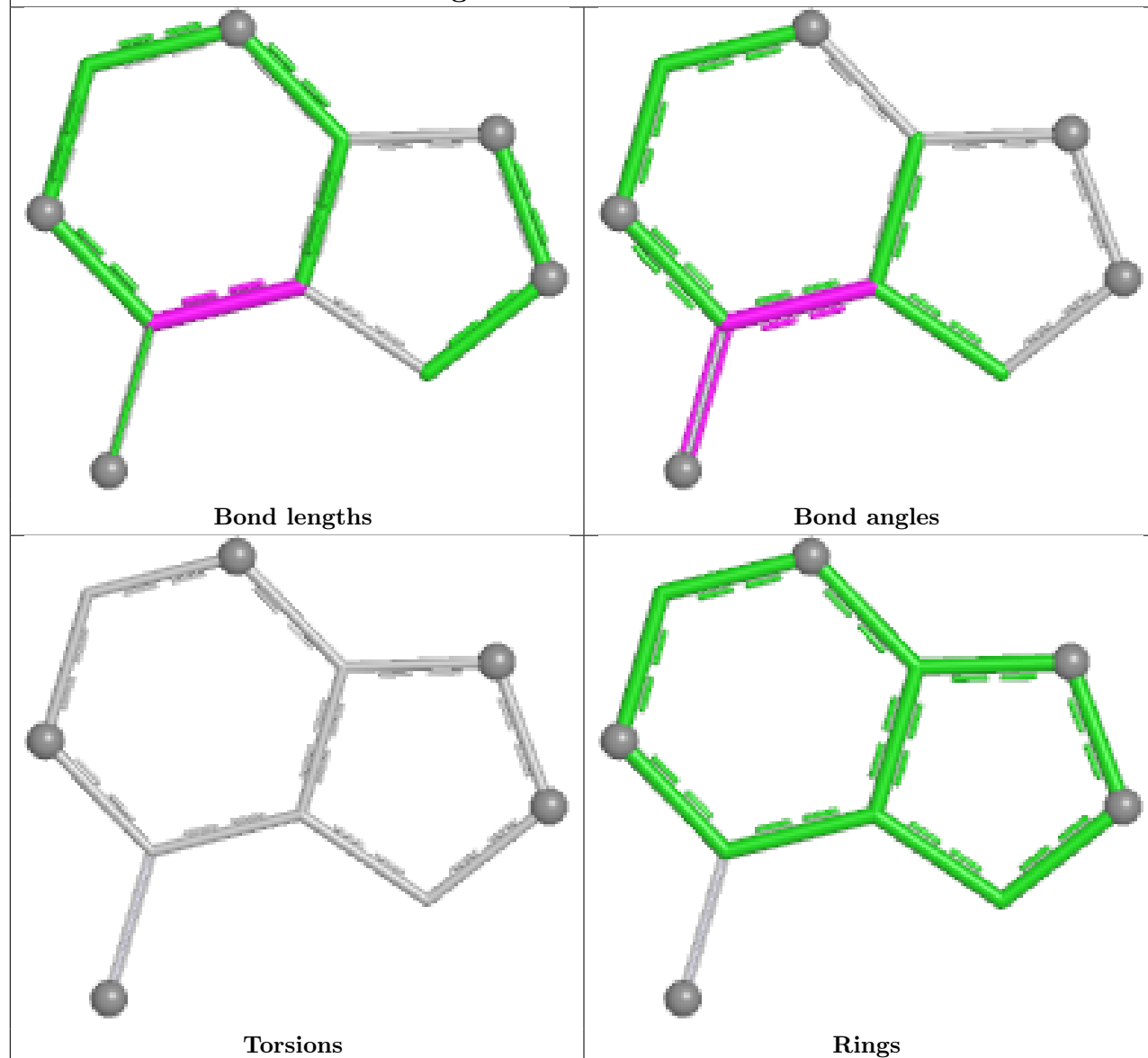
There are no ring outliers.

No monomer is involved in short contacts.

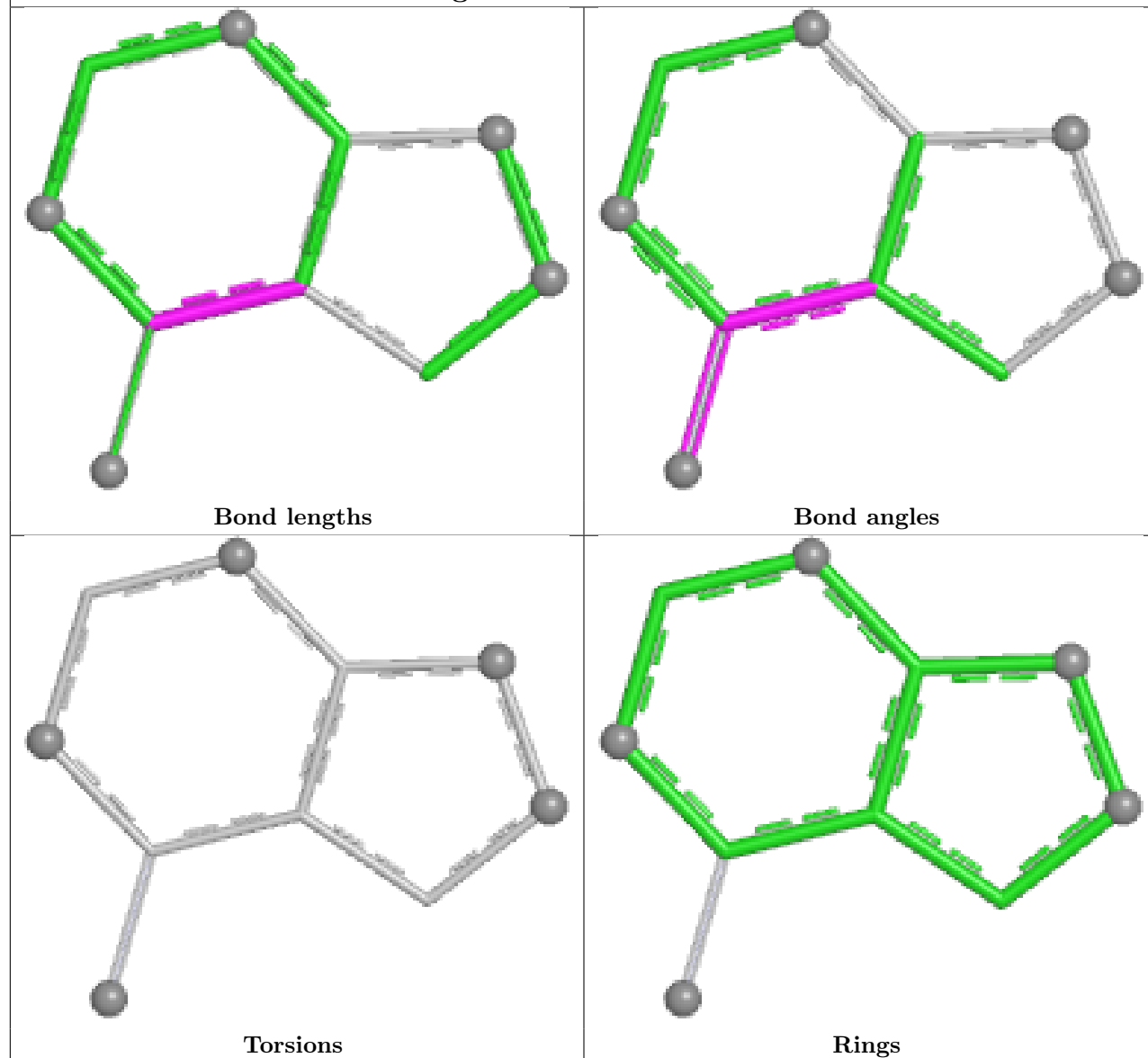
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

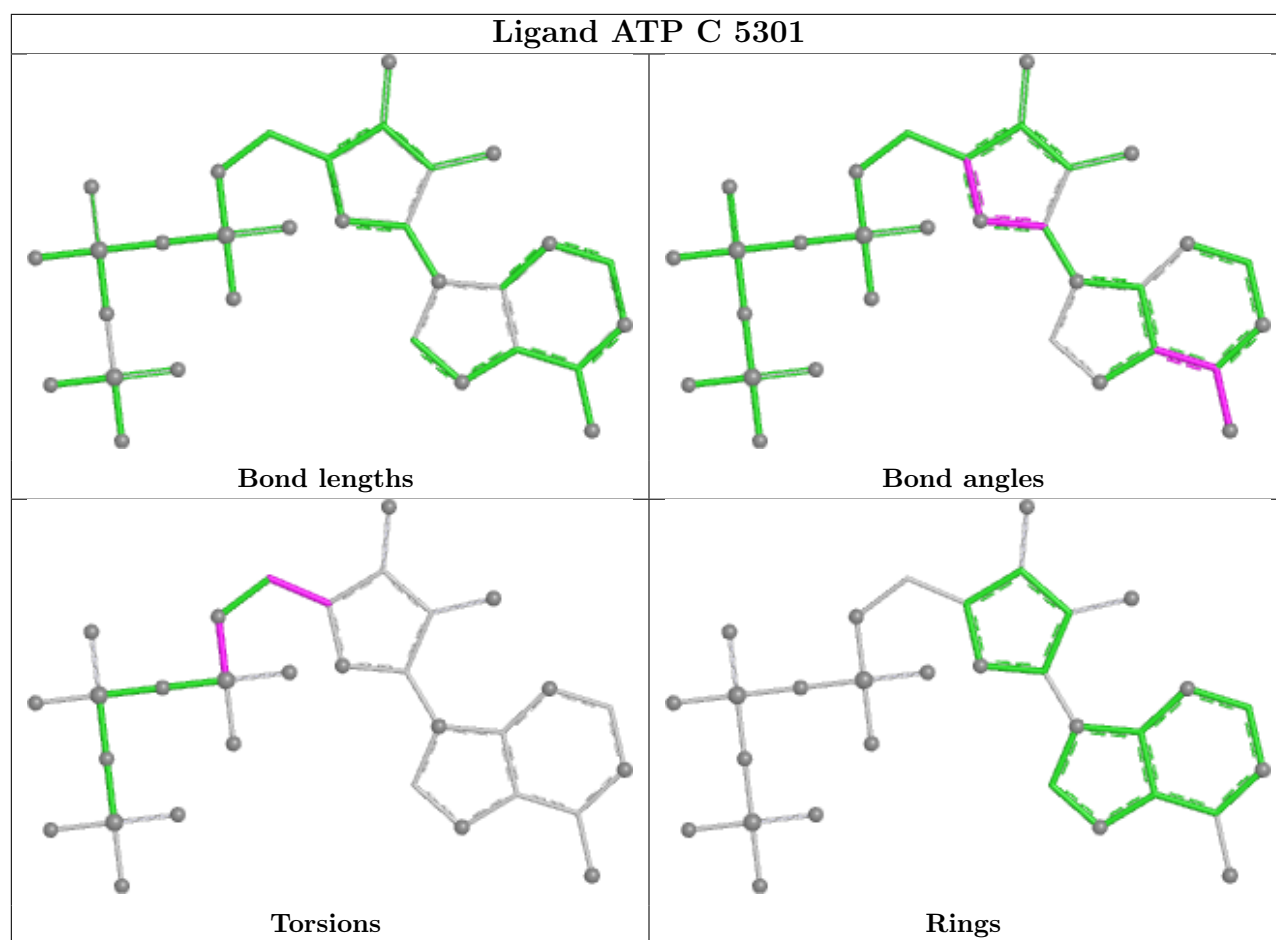


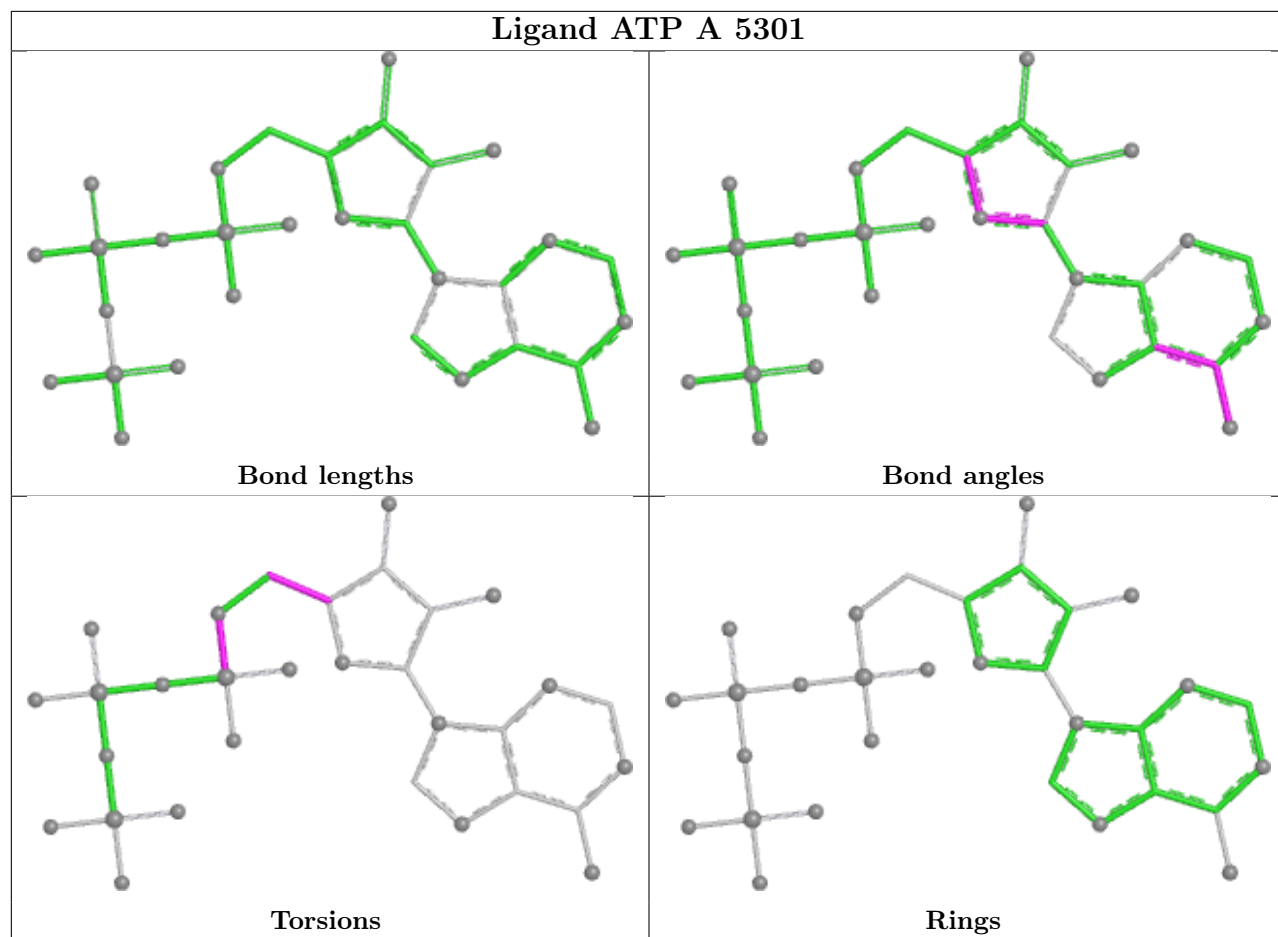
Ligand A1BD4 D 5304



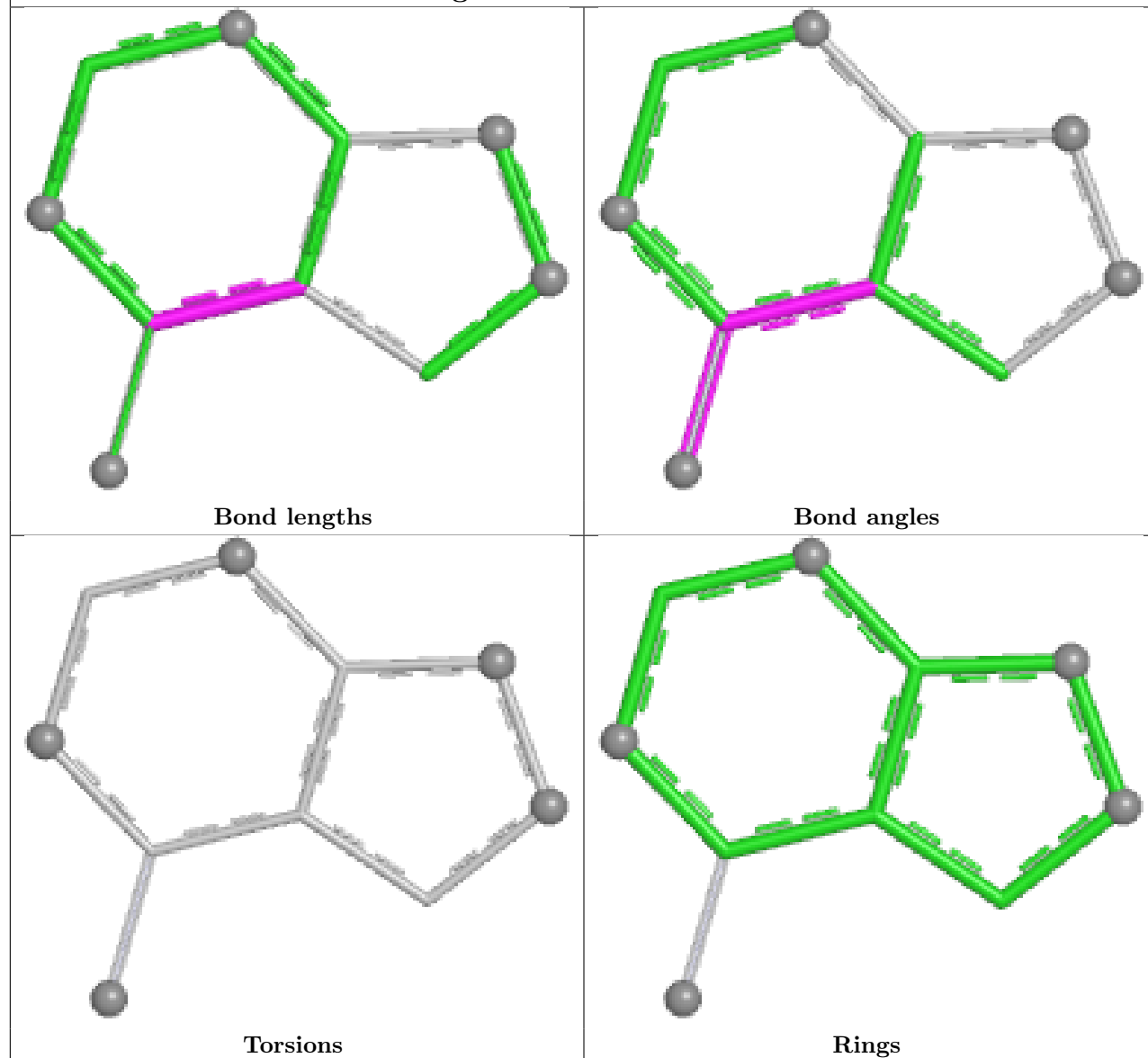
Ligand A1BD4 C 5304



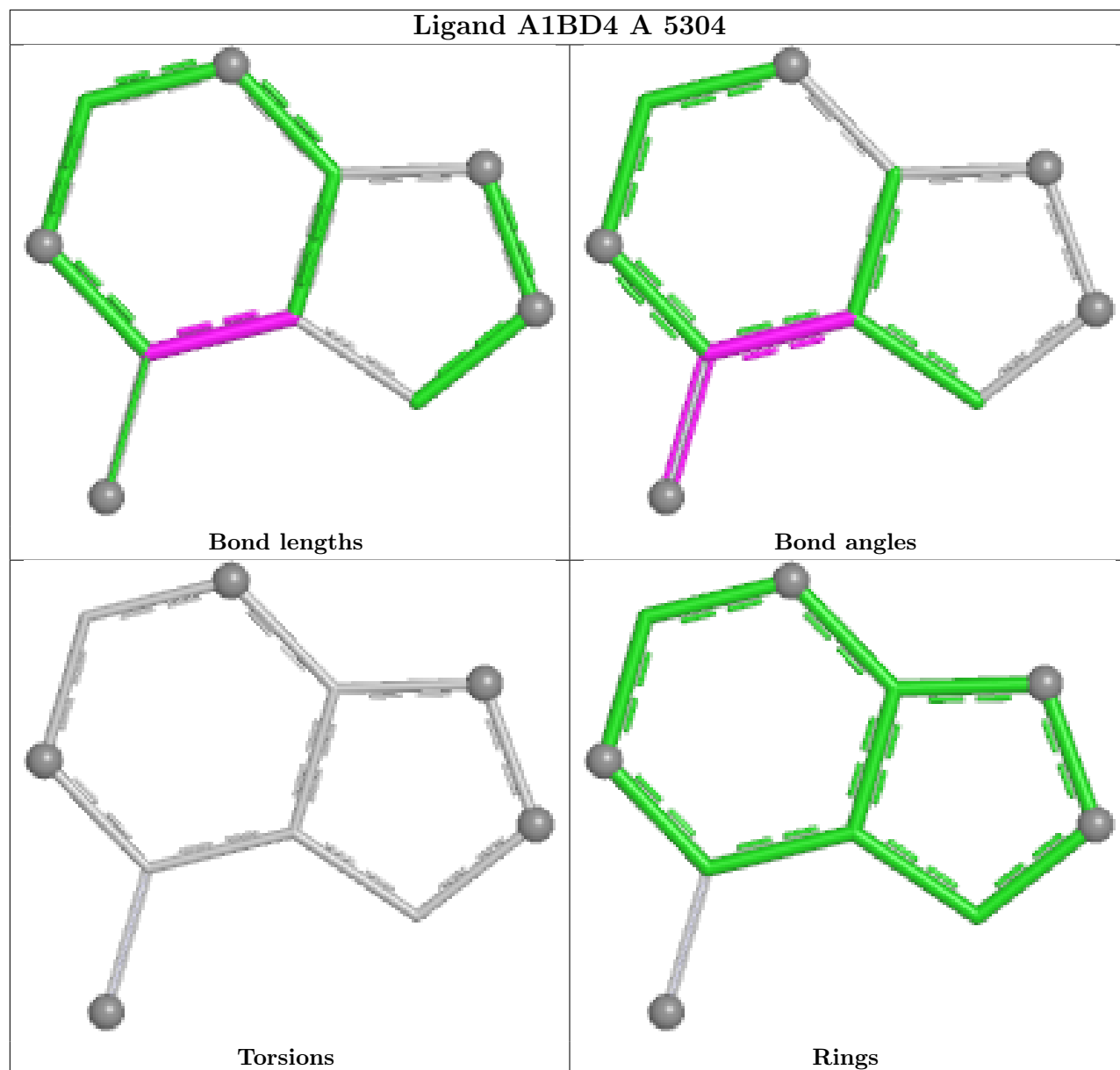


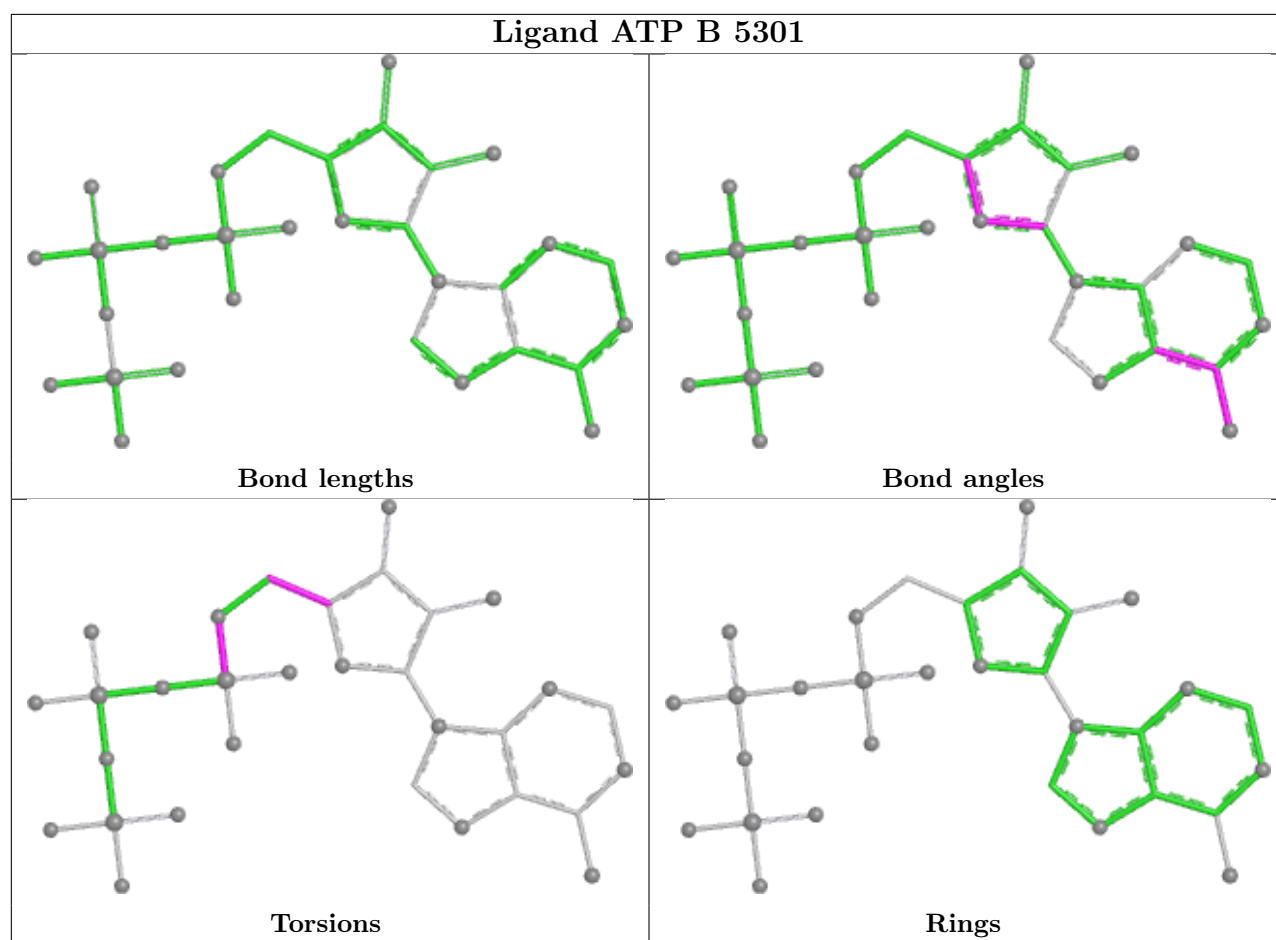


Ligand A1BD4 B 5304



Ligand A1BD4 A 5304





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.

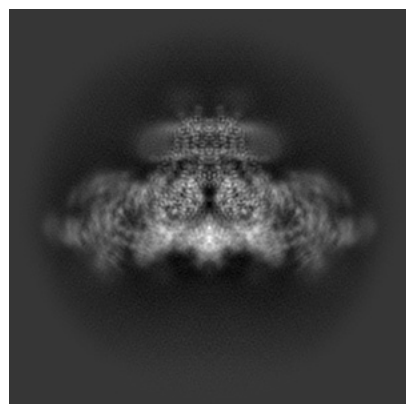
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47392. These allow visual inspection of the internal detail of the map and identification of artifacts.

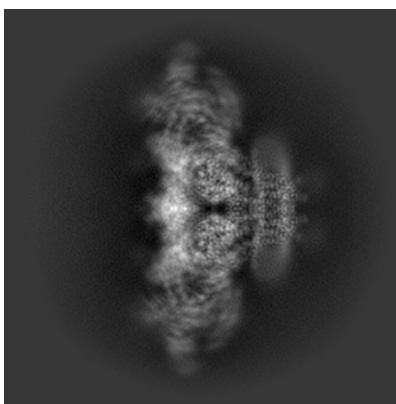
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

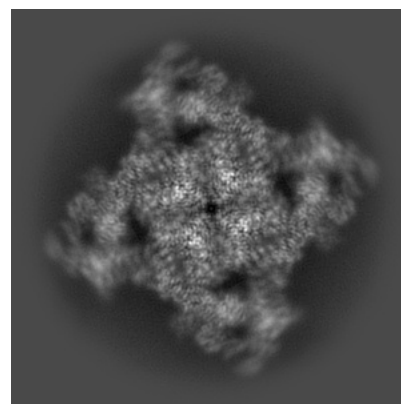
6.1.1 Primary map



X

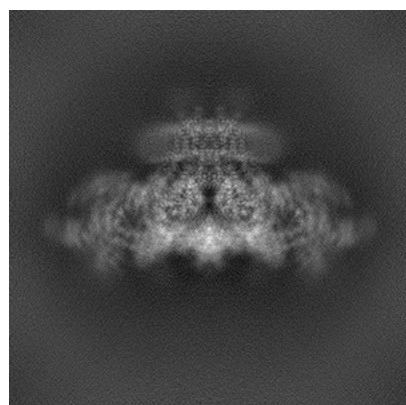


Y

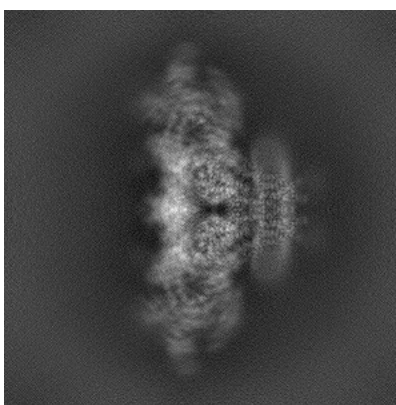


Z

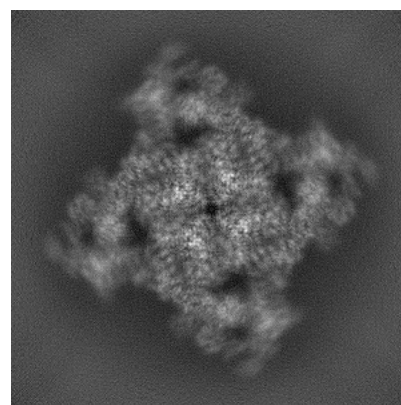
6.1.2 Raw map



X



Y

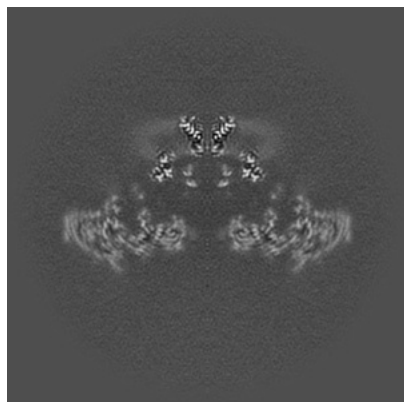


Z

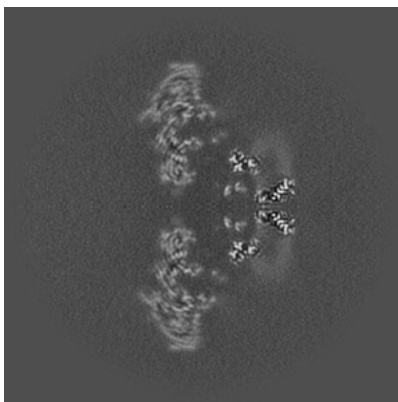
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

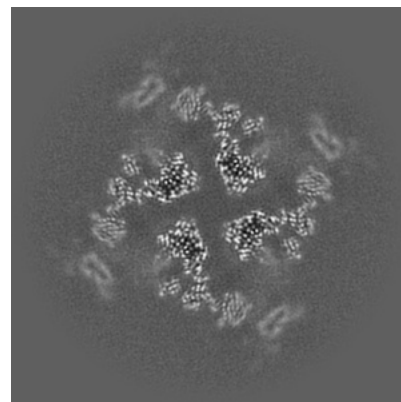
6.2.1 Primary map



X Index: 256

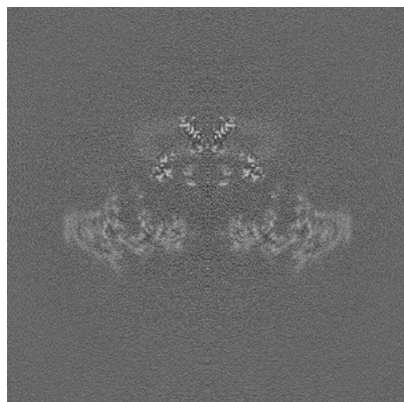


Y Index: 256

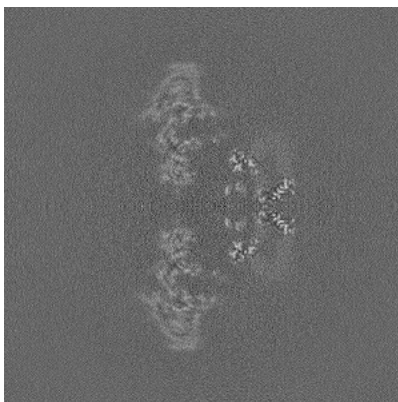


Z Index: 256

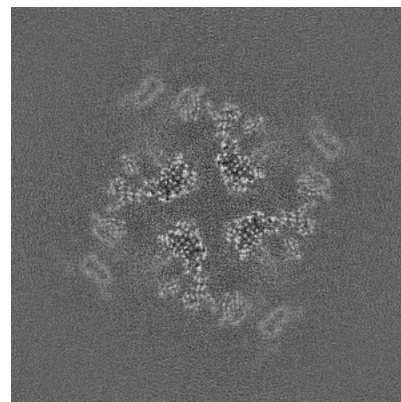
6.2.2 Raw map



X Index: 256



Y Index: 256

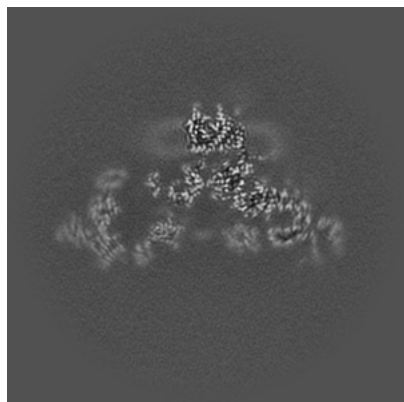


Z Index: 256

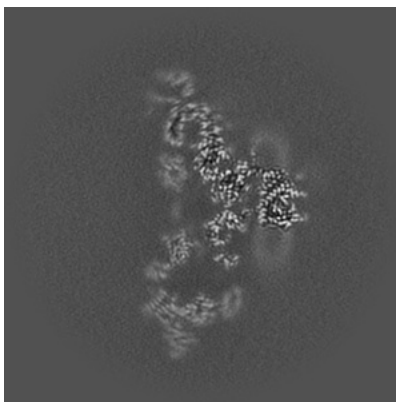
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

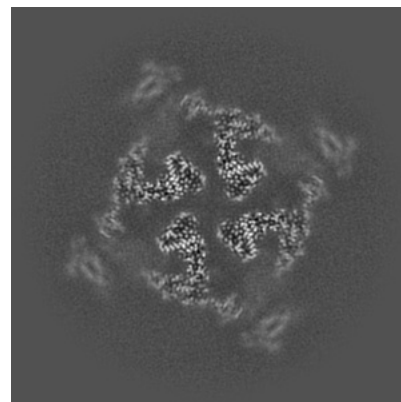
6.3.1 Primary map



X Index: 273

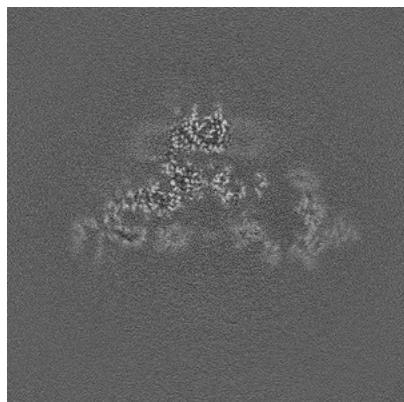


Y Index: 239

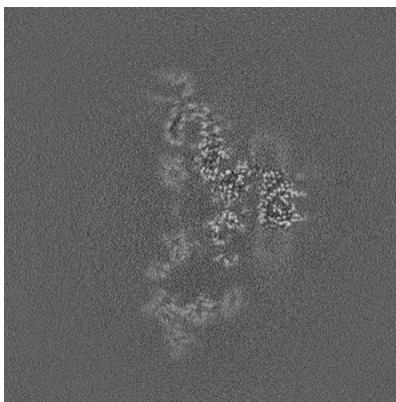


Z Index: 264

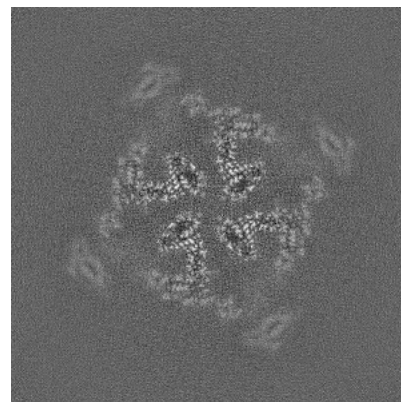
6.3.2 Raw map



X Index: 239



Y Index: 239

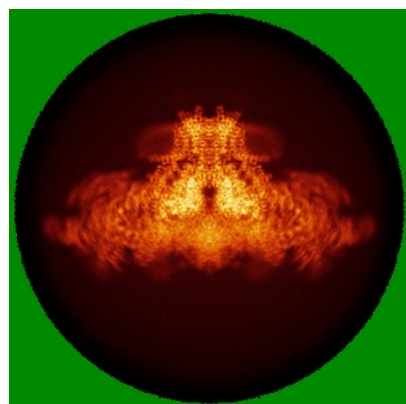


Z Index: 266

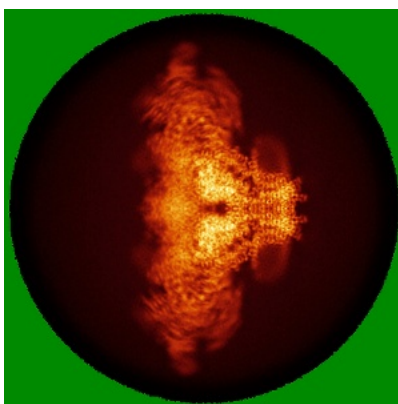
The images above show the largest variance slices of the map in three orthogonal directions.

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

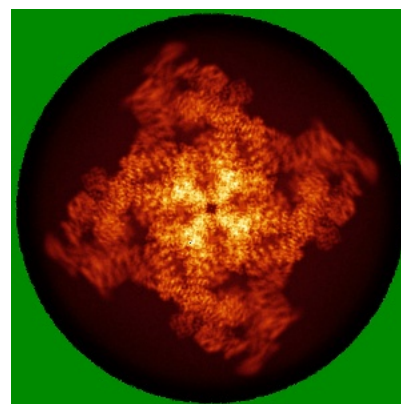
6.4.1 Primary map



X

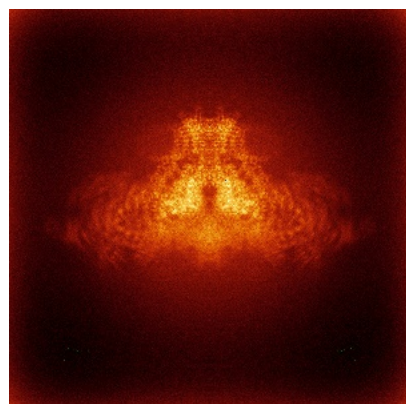


Y

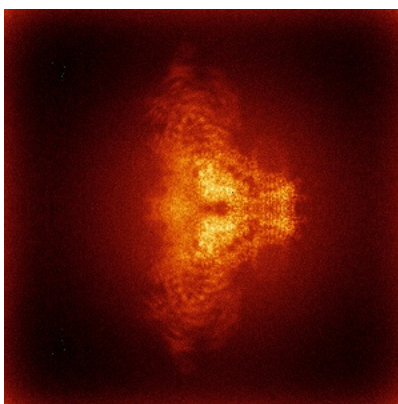


Z

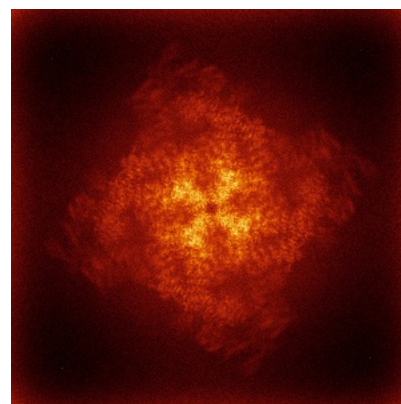
6.4.2 Raw map



X



Y

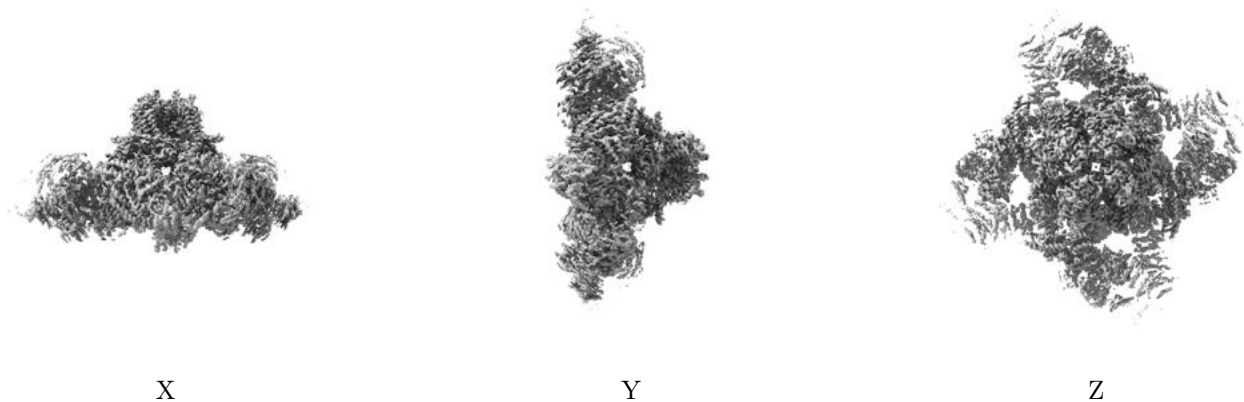


Z

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.

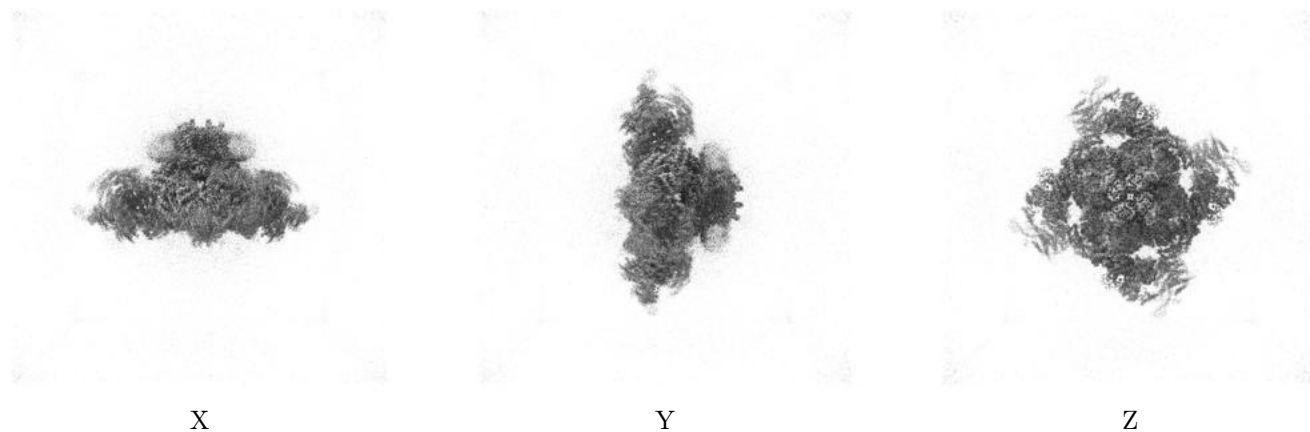
6.5 Orthogonal surface views [i](#)

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.

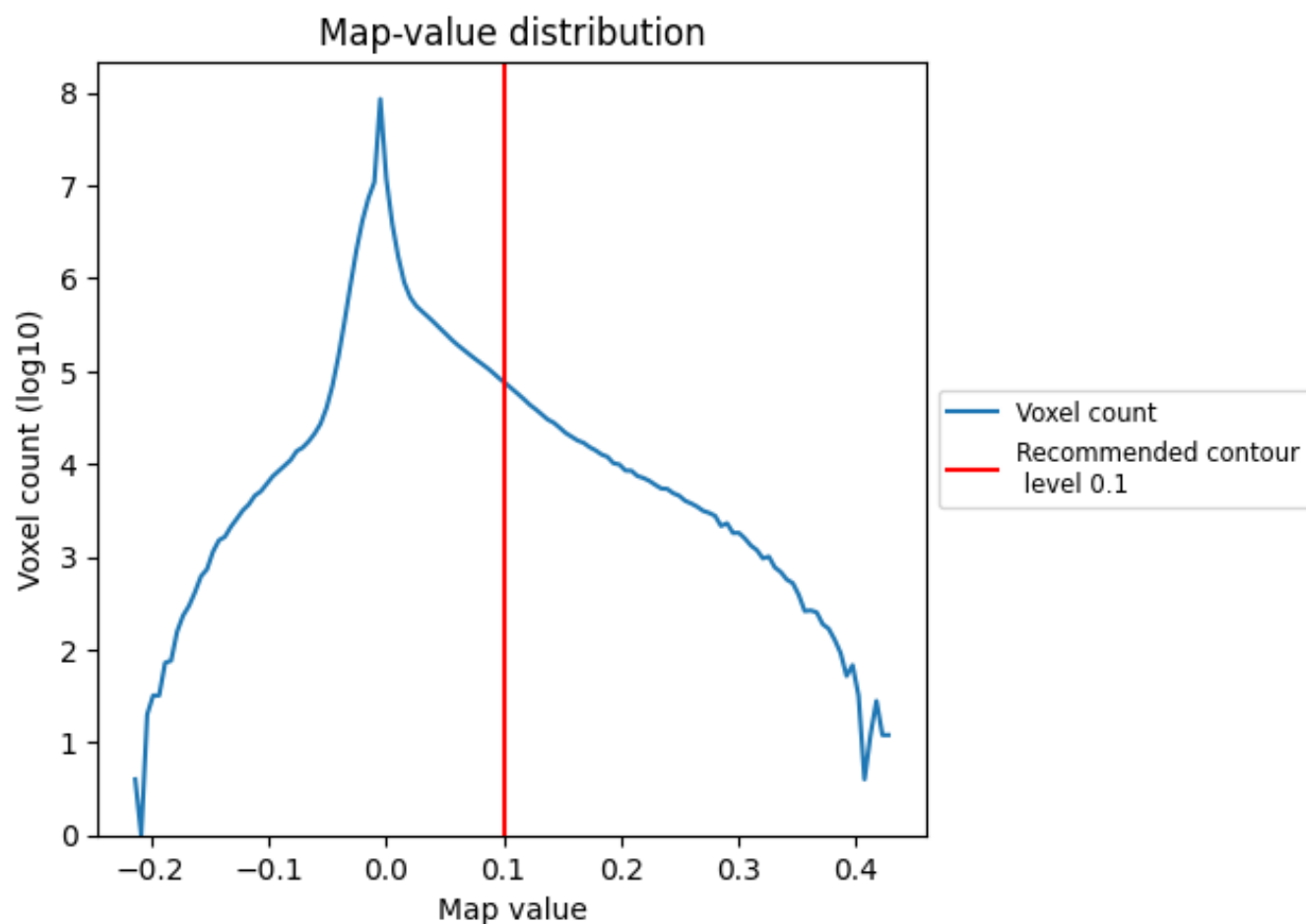
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

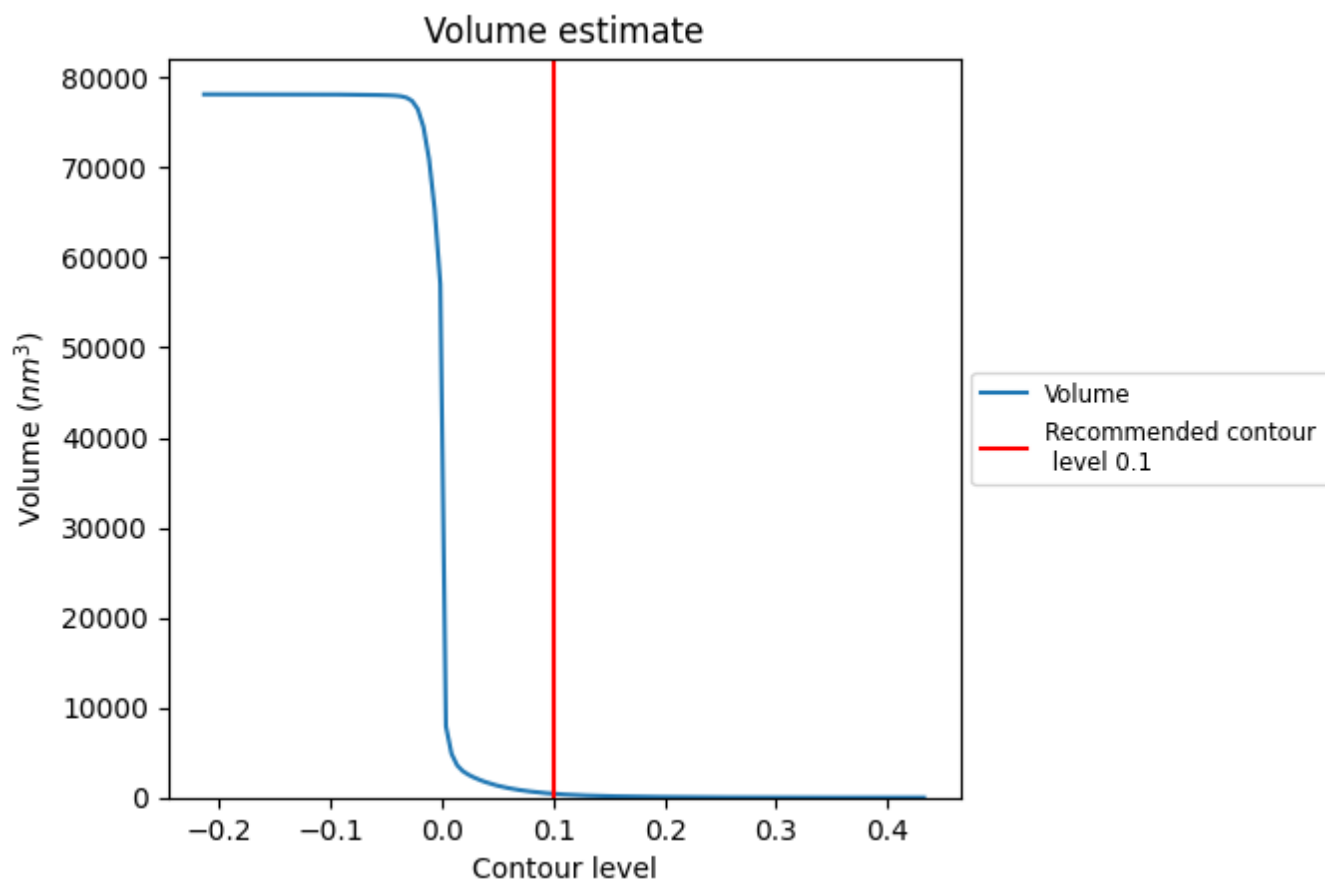
This section contains the results of statistical analysis of the map.

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.

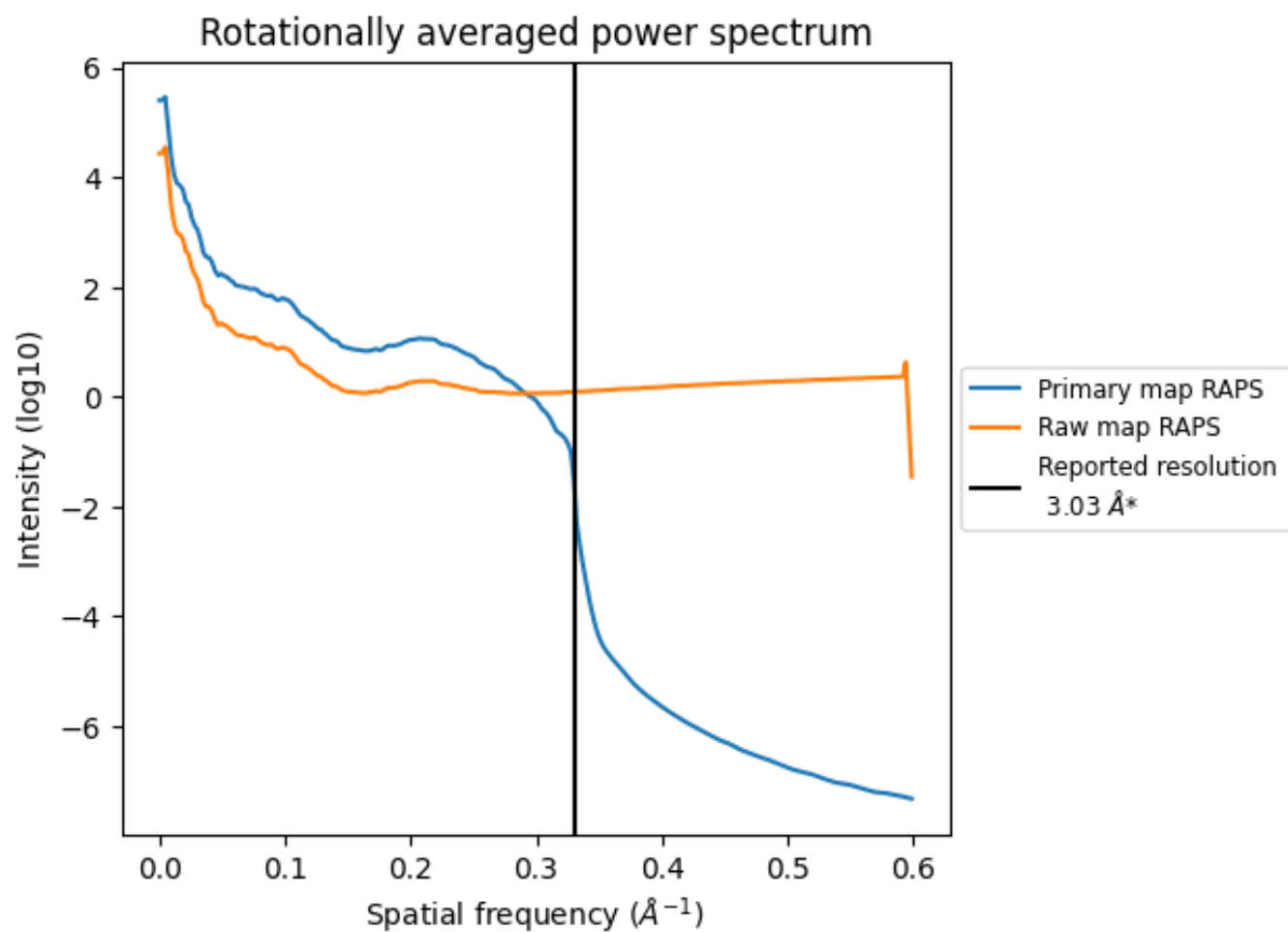
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 424 nm³; this corresponds to an approximate mass of 383 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 ⓘ

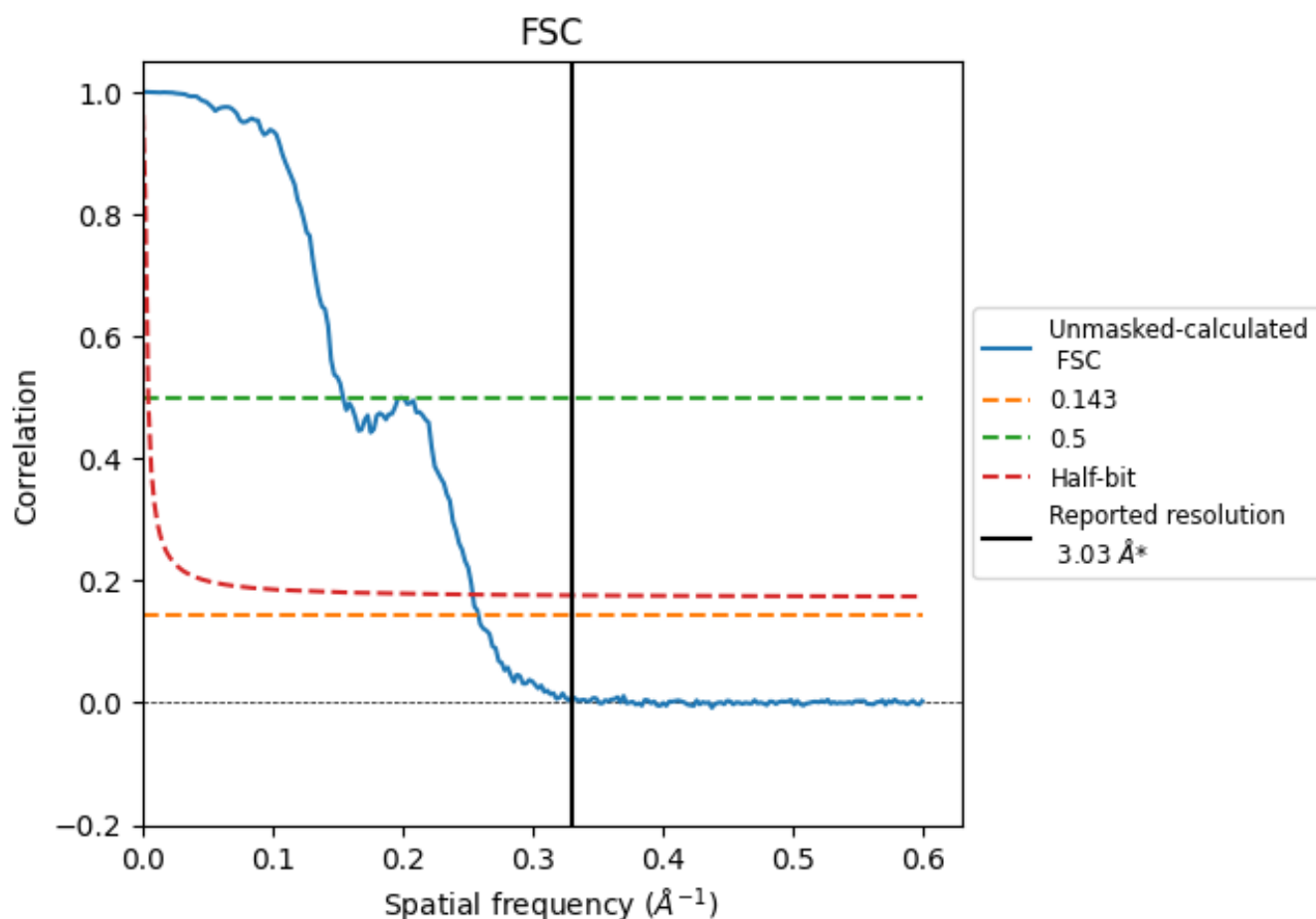


*Reported resolution corresponds to spatial frequency of 0.330 \AA^{-1}

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 0.330 Å⁻¹

8.2 Resolution estimates [i](#)

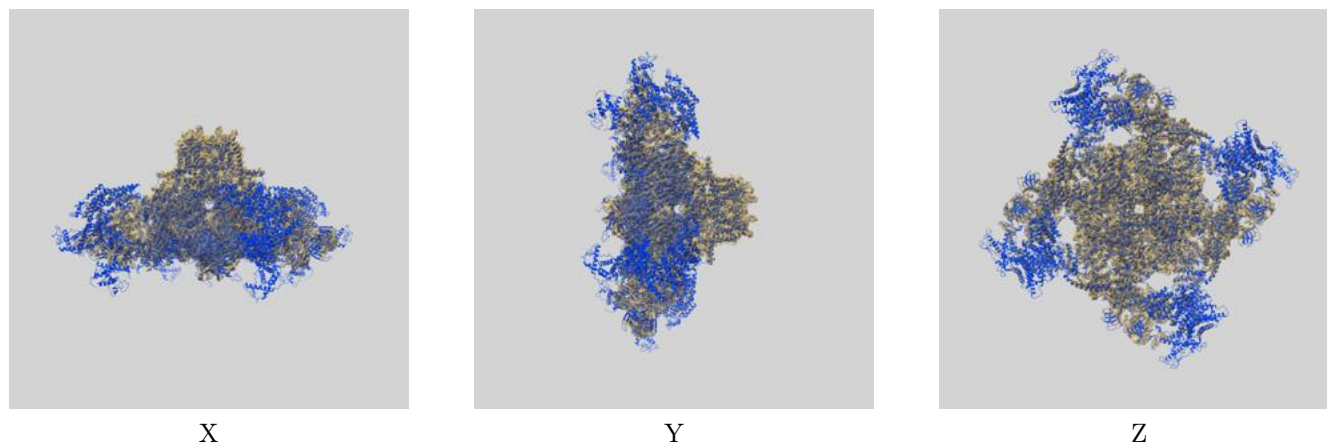
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	6.49	3.94

*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 3.87 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

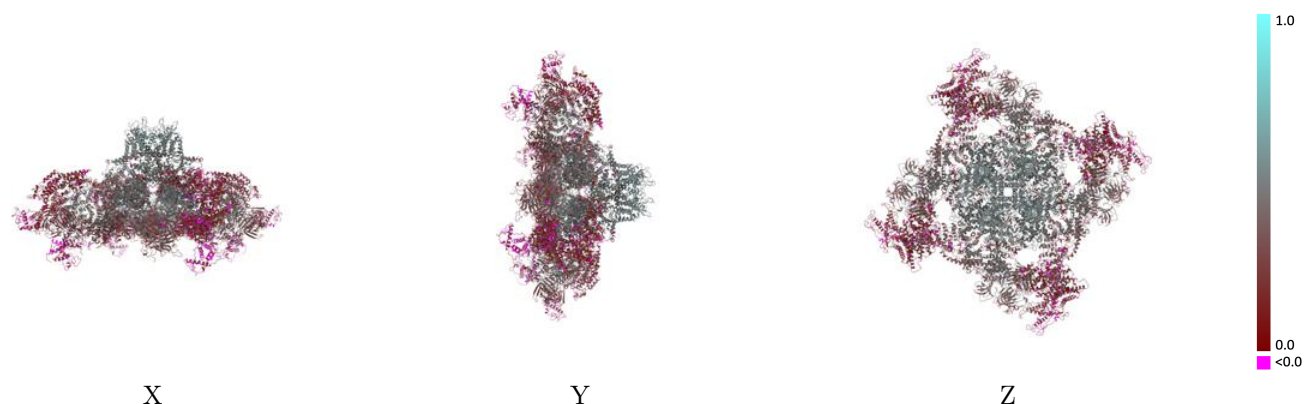
This section contains information regarding the fit between EMDB map EMD-47392 and PDB model 9E1F. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



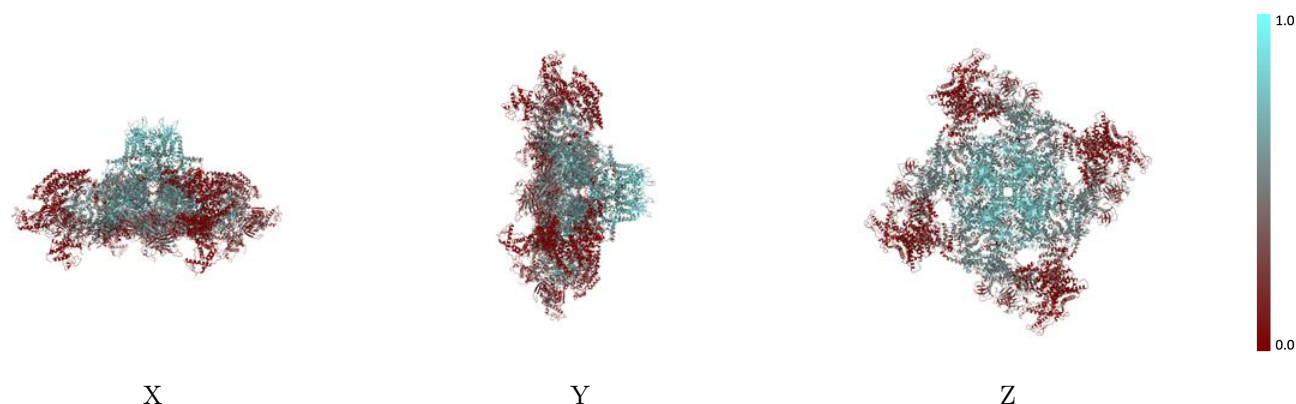
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



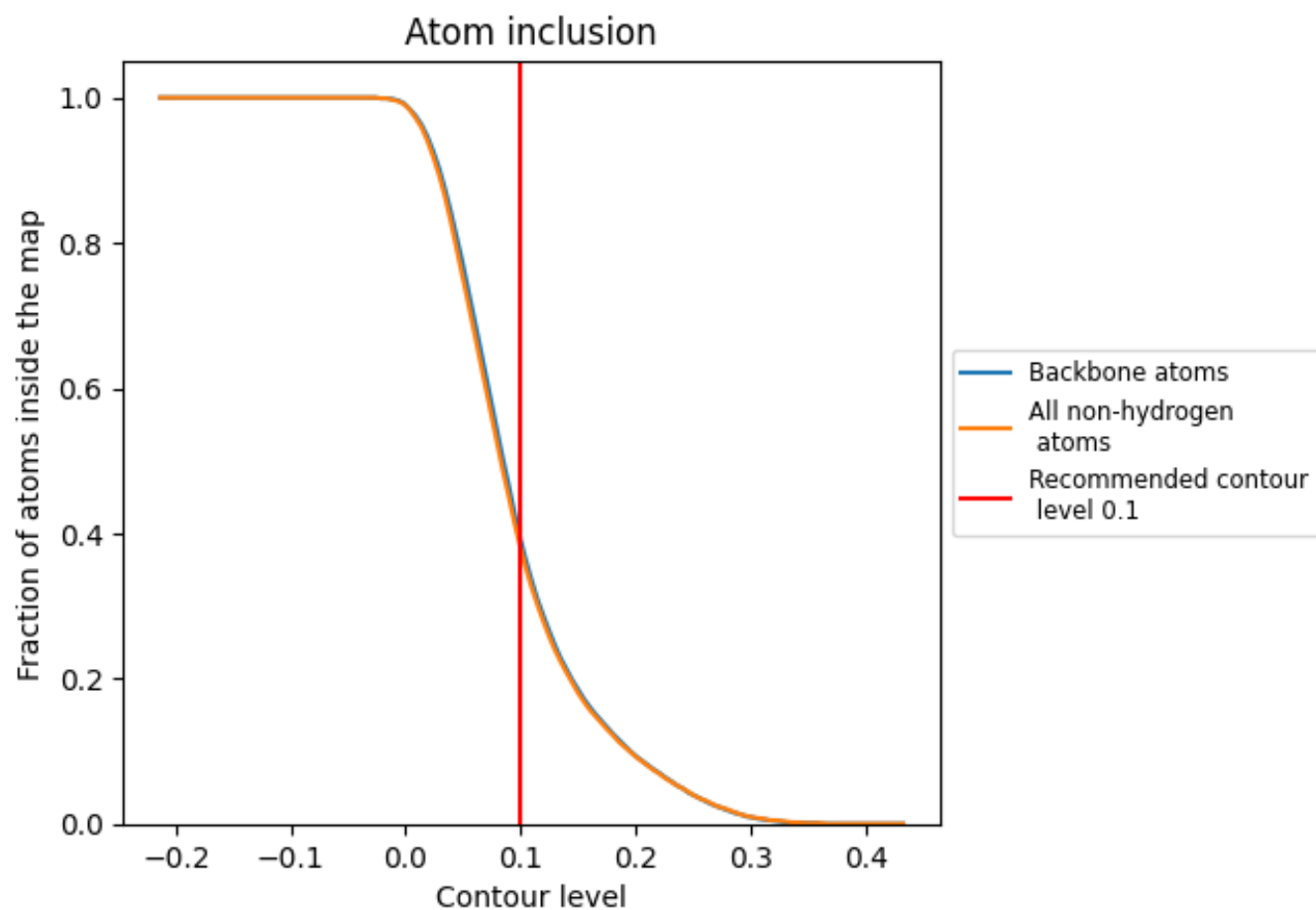
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 39% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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	<div></div> 0.3790	<div></div> 0.3300
A	<div></div> 0.3890	<div></div> 0.3290
B	<div></div> 0.3890	<div></div> 0.3290
C	<div></div> 0.3890	<div></div> 0.3290
D	<div></div> 0.3890	<div></div> 0.3290
E	<div></div> 0.2370	<div></div> 0.3640
F	<div></div> 0.2380	<div></div> 0.3570
G	<div></div> 0.2380	<div></div> 0.3570
H	<div></div> 0.2400	<div></div> 0.3580

1.0

0.0

<0.0