



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:55 AM UTC

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

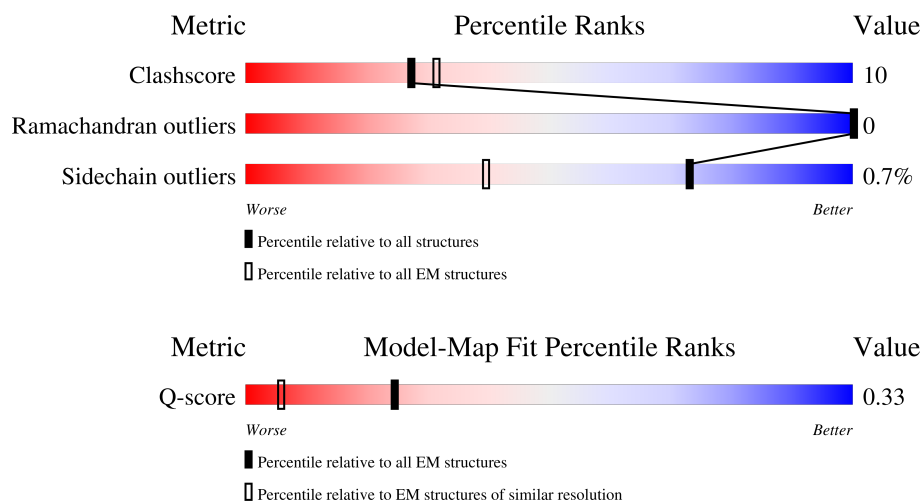
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13929 (2.53 - 3.53)

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	44% 68% 19% 13%
1	B	5037	44% 69% 19% 13%
1	C	5037	44% 69% 19% 13%
1	D	5037	44% 68% 19% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	79% 22% ..
2	F	108	78% 24% .
2	G	108	79% 23% ..
2	H	108	78% 20% ..

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.

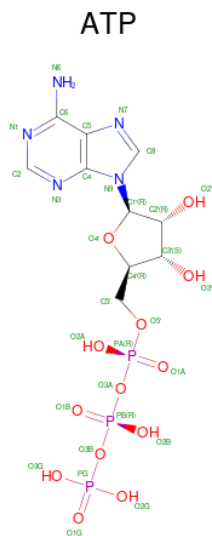
- Molecule 1 is a protein called Ryanodine receptor 1.

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).

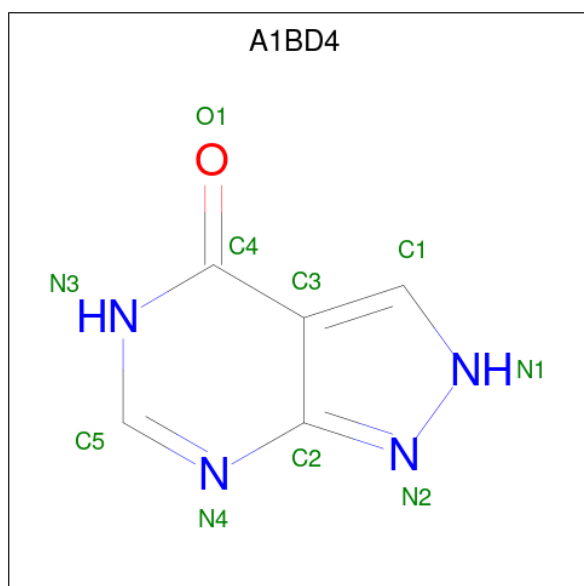
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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

- Molecule 6 is allopurinol (CCD ID: A1BD4) (formula: $C_5H_4N_4O$) (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	

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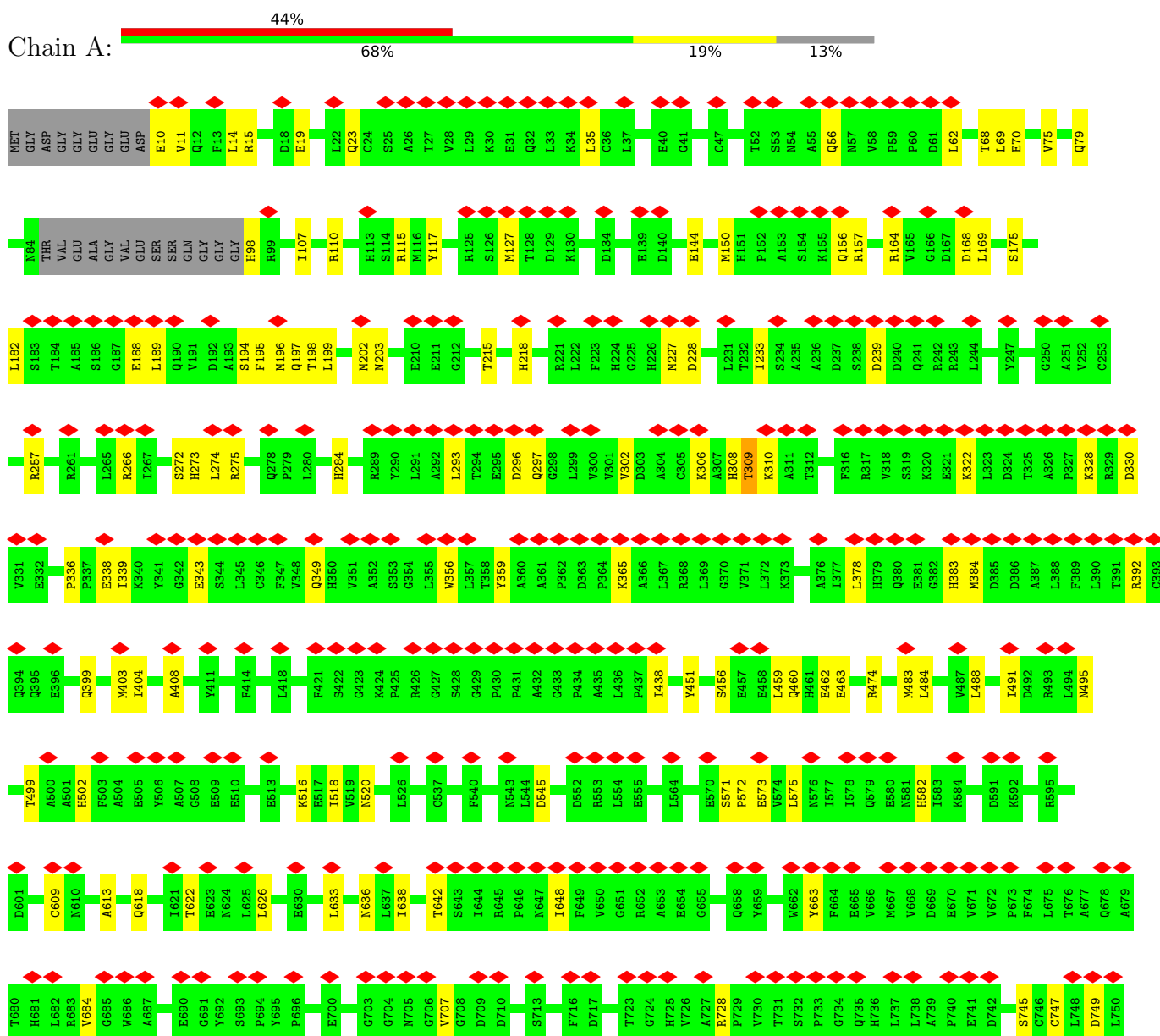
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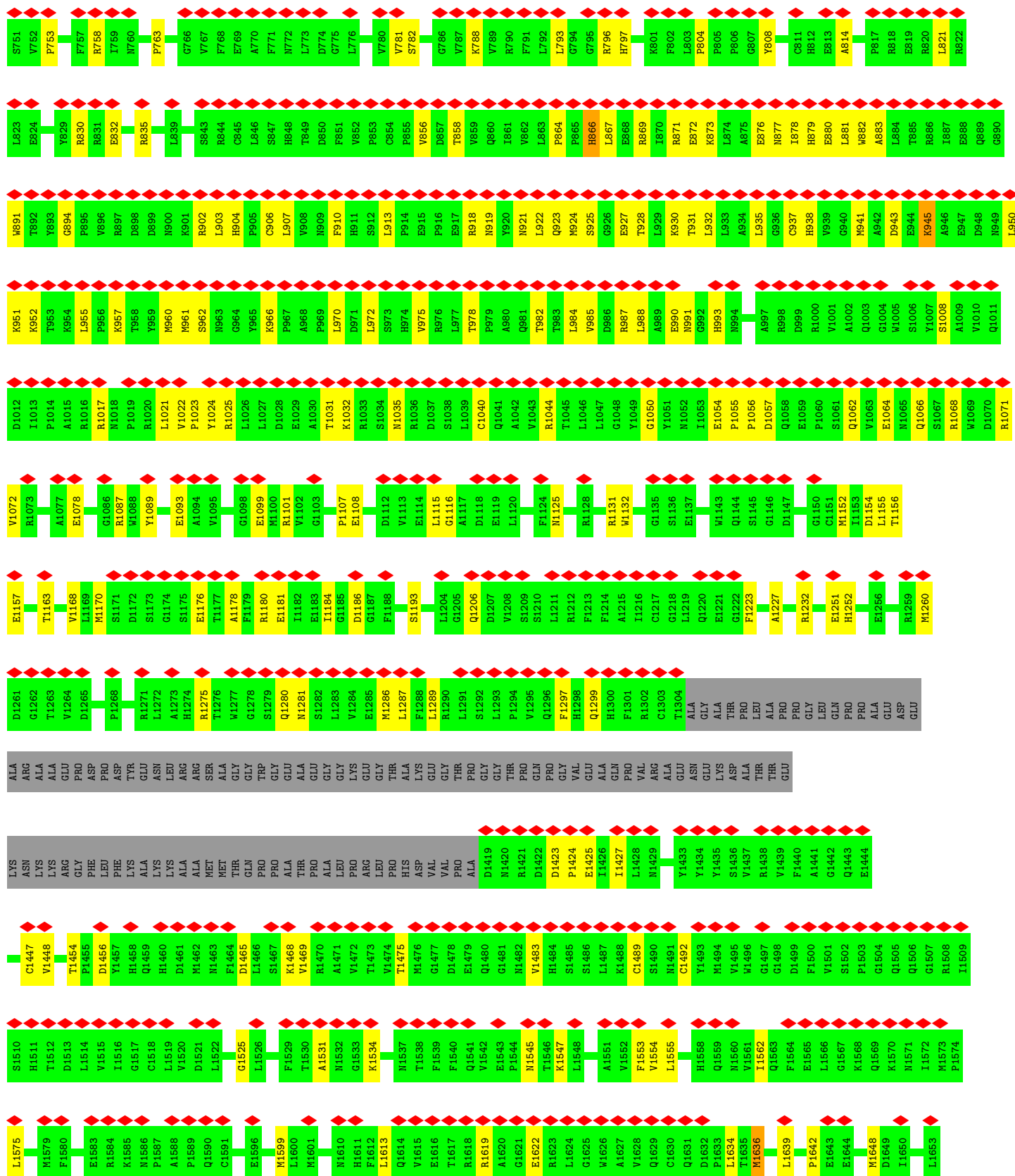
Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	O	0
			2	2	
7	C	2	Total	O	0
			2	2	

3 Residue-property plots

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





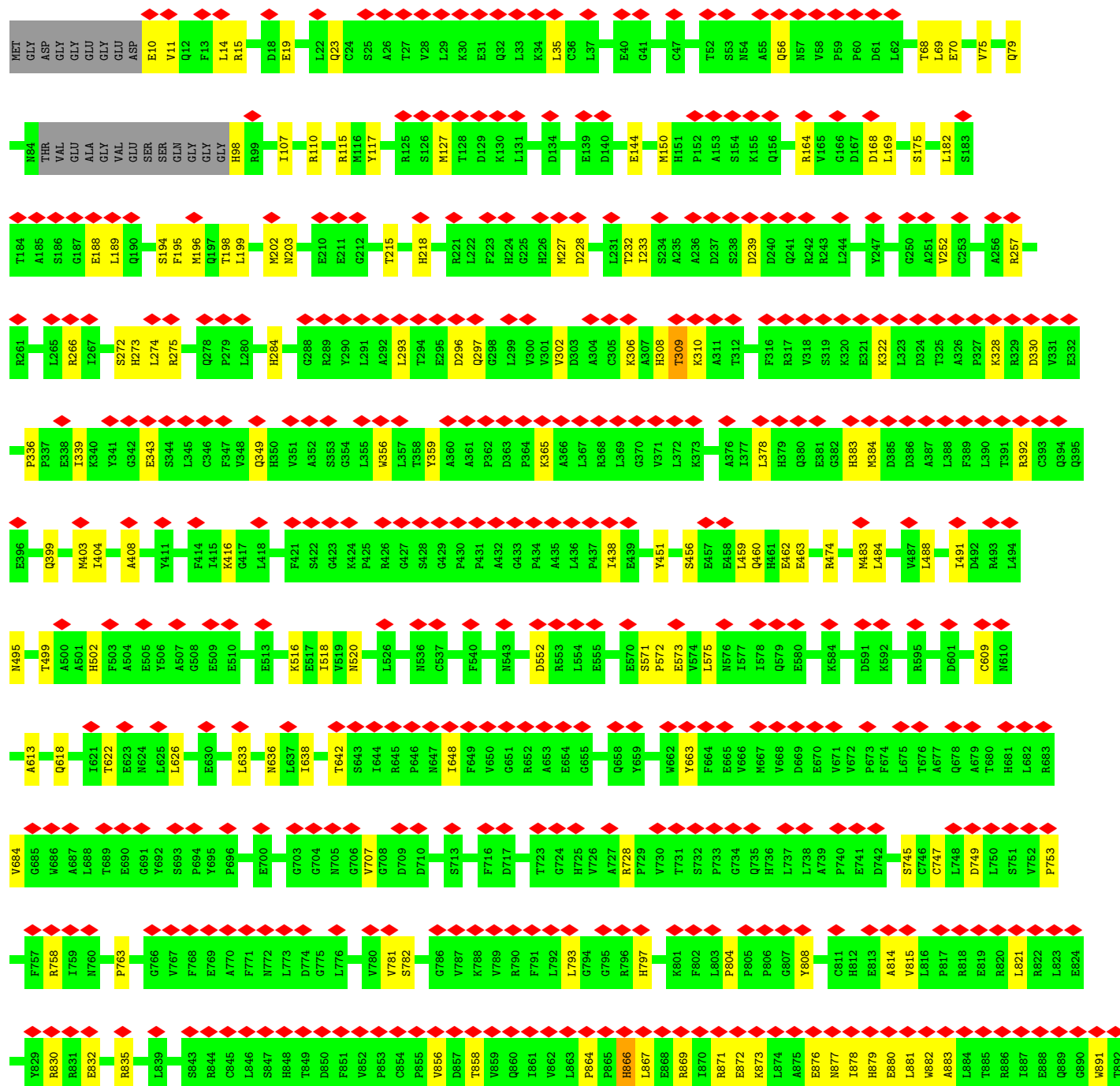
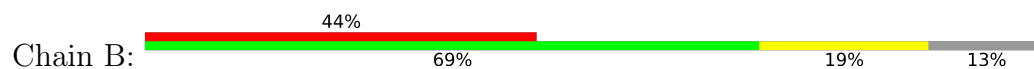


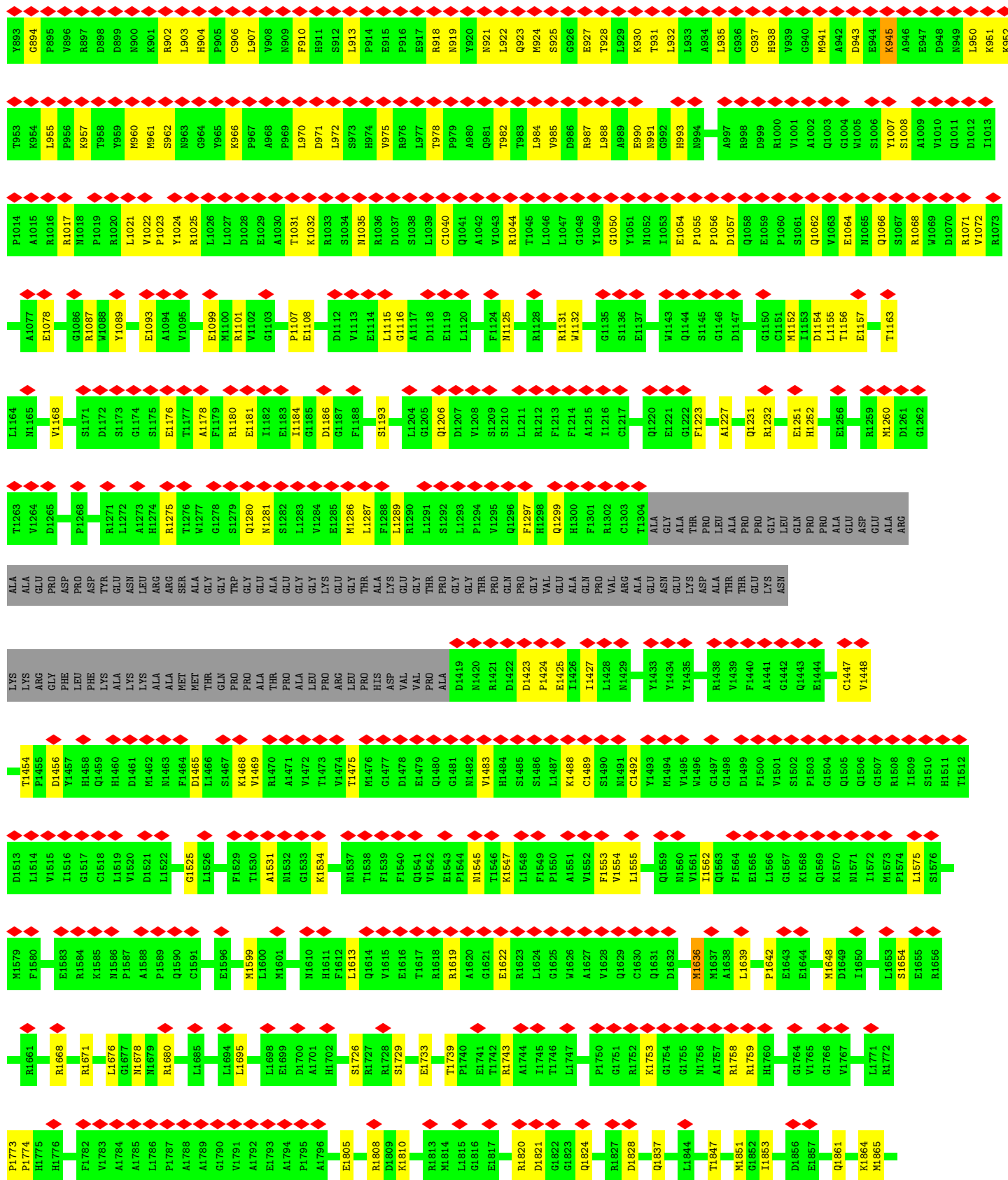
A3431	K3371	H3311	A3251	G3191	V3131	L3071	T3011	I2951	K2891	GLU	P2711
E3432	V3372	L3312	D3252	E3192	T3132	A3072	N3012	E2952	Q2892	GLU	P2712
E3433	V3373	N3313	I3253	C3193	T3133	R3073	H3013	K2953	E2893	THR	D2713
L3434	A3374	S3314	G3254	L3194	V3134	S3074	C3014	R2954	L2894	GLU	V2714
F3435	E3375	L3315	G3255	A3195	A3135	L3075	L3015	F2955	E2895	LYS	V2715
R3436	E3376	L3316	L3256	R3196	A3136	D3076	F3017	A2956	A2896	LYS	D2716
V3437	E3377	L3317	A3257	L3197	L3137	A3077	V3017	F2957	K2897	THR	A2717
V3438	Q3378	N3318	E3258	A3198	R3078	R3078	L3018	Q2958	G2898	ARG	S2718
G3439	L3379	L3319	S3259	A3199	V3139	T3079	S3019	Q2959	G2899	LYS	V2719
E3440	R3380	L3320	G3260	A3200	L3140	V3080	T3020	L2960	G2900	ILE	S2720
I3441	L3381	R3321	A3261	M3201	T3141	M3081	F3021	Q2961	T2901	GLN	S2721
F3442	E3382	I3322	R3262	P3202	T3142	K3082	A3022	Q2962	H2902	THR	K2722
I3443	A3383	I3323	V3263	V3203	L3143	S3083	K3023	L2963	P2903	ALA	A2723
Y3444	K3384	V3324	T3264	A3204	F3144	G3084	V3024	L2964	L2904	THR	A2724
V3445	A3385	N3325	E3265	F3205	Q3145	P3085	L3025	R2965	L2905	TVR	E2725
S3446	E3386	N3326	M3266	L3206	H3146	E3086	G3026	W2966	V2906	ASP	K2725
K3447	A3387	L3327	F3267	E3207	I3147	I3087	S3027	M2967	P2907	PRO	LYS
S3448	E3388	G3328	H3268	P3208	A3148	V3088	G3028	D2968	Y2908	GLU	THR
H3449	E3389	I3329	V3269	Q3209	Q3149	K3089	G3029	I2969	D2909	GLU	VAL
R3450	G3390	D3330	I3270	L3210	H3150	A3090	H3030	S2970	T2910	GLY	ASP
F3451	E3391	E3331	E3271	N3210	Q3151	G3091	S3031	Q2971	L2911	LYS	ALA
K3452	L3392	A3332	I3272	G3212	L3152	L3092	S3032	E2972	L2912	GLY	GLY
R3453	L3393	T3333	T3273	Y3213	G3153	R3093	N3033	F2973	A2913		
E3454	V3394	W3334	L3274	N3214	D3154	S3094	K3034	I2974	Y2794		
F3455	V3395	M3335	P3275	A3215	D3155	F3095	E3035	A2975	K2915		
K3456	R3396	K3336	M3276	C3216	V3156	F3096	K3036	H2976	K2916		
N3457	E3397	R3337	L3277	S3217	I3157	E3097	E3037	L2977	L2917		
F3458	E3398	L3338	C3278	V3218	L3158	S3098	I3038	E2978	A2918		
V3459	S3399	A3339	S3279	Y3219	D3159	A3099	T3039	A2979	D2919		
V3460	V3400	V3340	Y3280	T3220	D3160	S3100	T3040	V2980	R2920		
Q3461	L3401	F3341	L3281	T3221	V3161	E3101	S3041	V2981	E2921		
N3462	K3402	A3342	P3282	K3222	Q3162	D3102	L3042	S2982	K2922		
E3463	R3403	Q3343	A3283	S3223	V3163	I3103	F3043	S2983	A2923		
I3464	D3404	P3344	W3284	P3224	S3164	E3104	C3044	G2984	Q2924		
N3465	L3405	I3345	W3285	R3225	C3165	K3105	K3045	R2985	E2925		
N3466	L3406	V3346	E3286	E3226	V3166	M3106	K3046	V2986	E2926		
K3467	Y3407	S3347	E3287	R3227	F3167	V3107	A3047	E2987	L2927		
S3468	L3408	G3288	G3288	A3228	T3168	E3108	A3048	K2988	K2928		
F3469	Y3409	P3289	P3289	I3229	L3169	N3109	L3049	S2989	F2929		
L3470	P3410	E3290	E3290	L3230	C3170	L3110	V3050	P2990	L2930		
T3471	L3411	A3291	A3291	G3231	S3171	R3111	K3051	H2991	Q2931		
A3472	L3412	P3292	P3292	L3232	T3172	L3112	M2932	E2992	Q2932		
D3473	I3413	P3293	P3293	P3233	Y3173	G3113	R3053	Q2993	N2933		
S3474	R3414	A3294	A3294	N3234	S3174	K3114	V3054	E2994	G2934		
K3475	V3415	L3296	L3296	S3235	L3175	V3115	S3055	I2995	Y2935		
S3476	D3417	V3237	E3237	V3236	G3176	S3116	K2996	K2996	A2936		
K3477	N3418	P3297	P3297	E3237	T3177	GLN	F2997	F2997	V2937		
H3478	N3419	A3298	A3298	E3238	T3178	ALA	F3057	F2998	Y2882		
A3479	R3420	G3299	G3299	M3239	K3179	ARG	G3058	F2998	K2938		
LYS	A3421	A3300	A3300	C3240	N3180	THR	T3059	A2999	R2939		
ALA	H3422	F3241	F3241	F3241	T3181	GLN	GLY	K3000	W2819		
GLY	V3423	D3242	D3242	I3243	Y3182	VAL	LEU	W2886	E2820		
GLN	L3424	E3363	E3363	P3244	V3183	ALA	LYS	W2887	W2821		
SER	T3425	R3365	R3365	V3245	K3185	ARG	ASP	G2887	L2822		
GLY	T3426	K3366	K3366	L3246	G3126	THR	ASP	G2888	T2823		
SER	E3427	R3367	R3367	D3247	Q3127	GLN	GLY	K2889	E2824		
ASP	N3428	A3368	A3368	R3248	N3128	VAL	GLY	T2885	K2825		
	A3429	G3370	G3370	L3249	L3129		GLY	W2887	A2826		
					T3130		GLY	W2887	R2827		
							GLY	W2887	G2829		
							GLY	W2887	K2770		





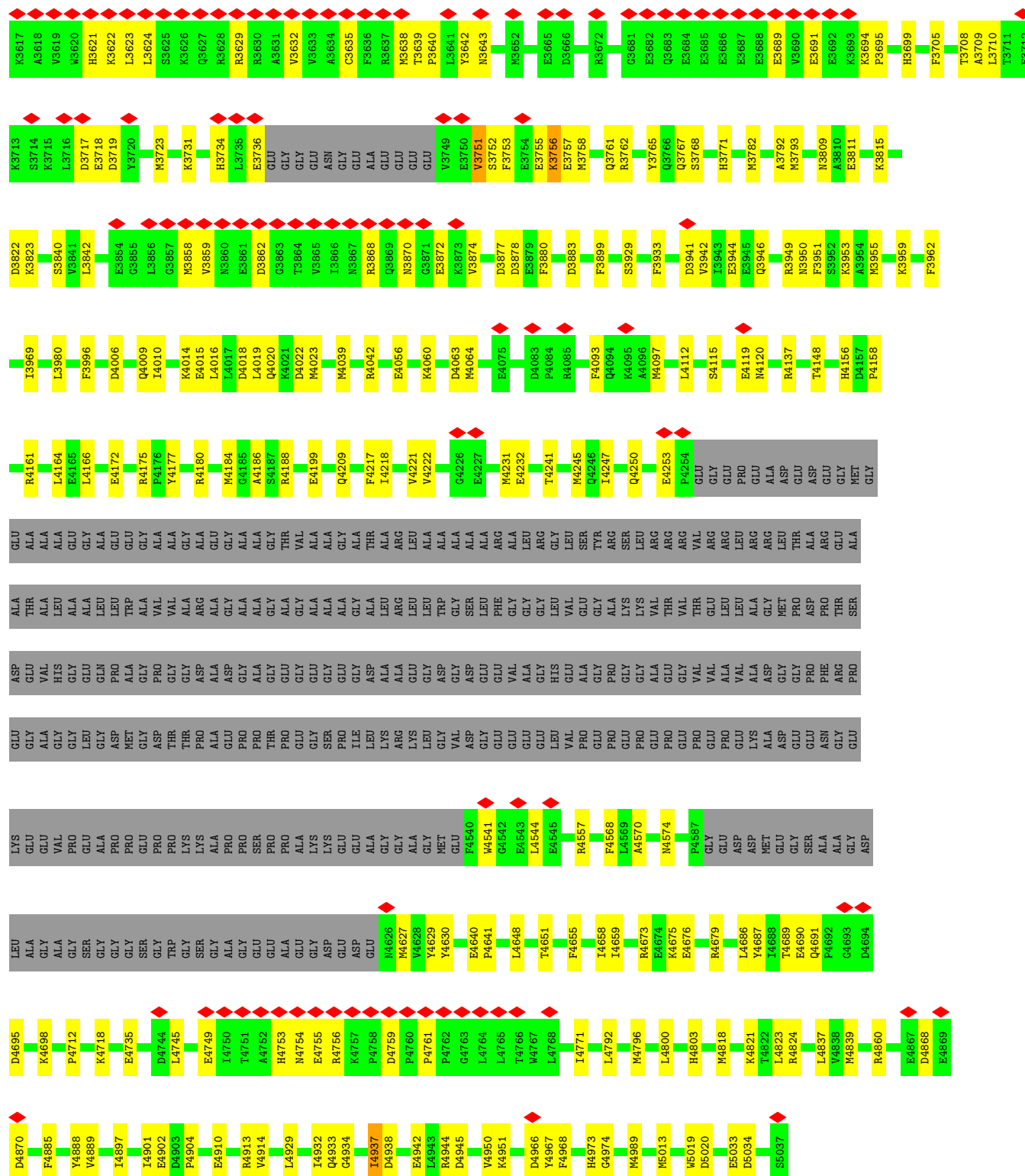
• Molecule 1: Ryanodine receptor 1



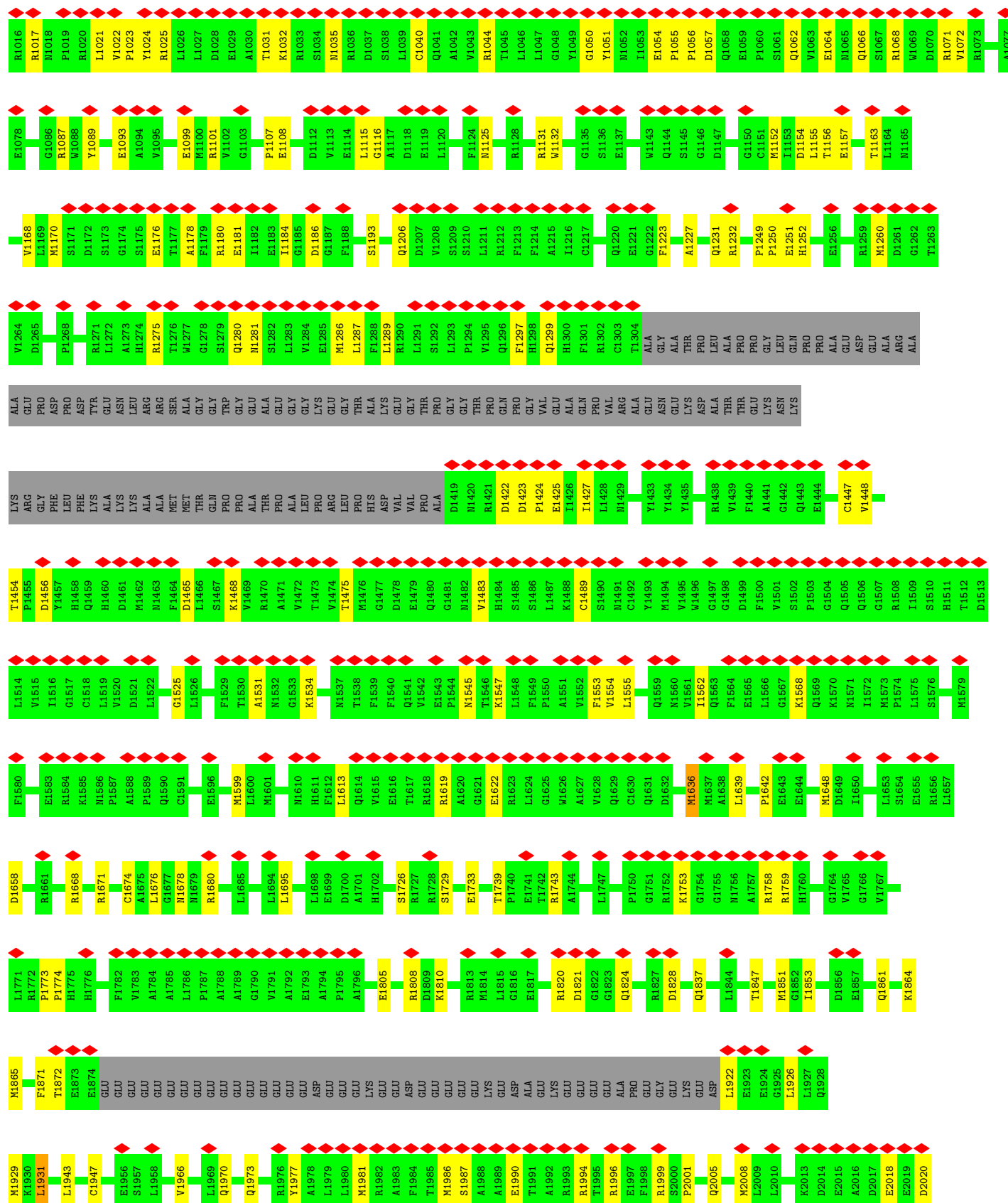




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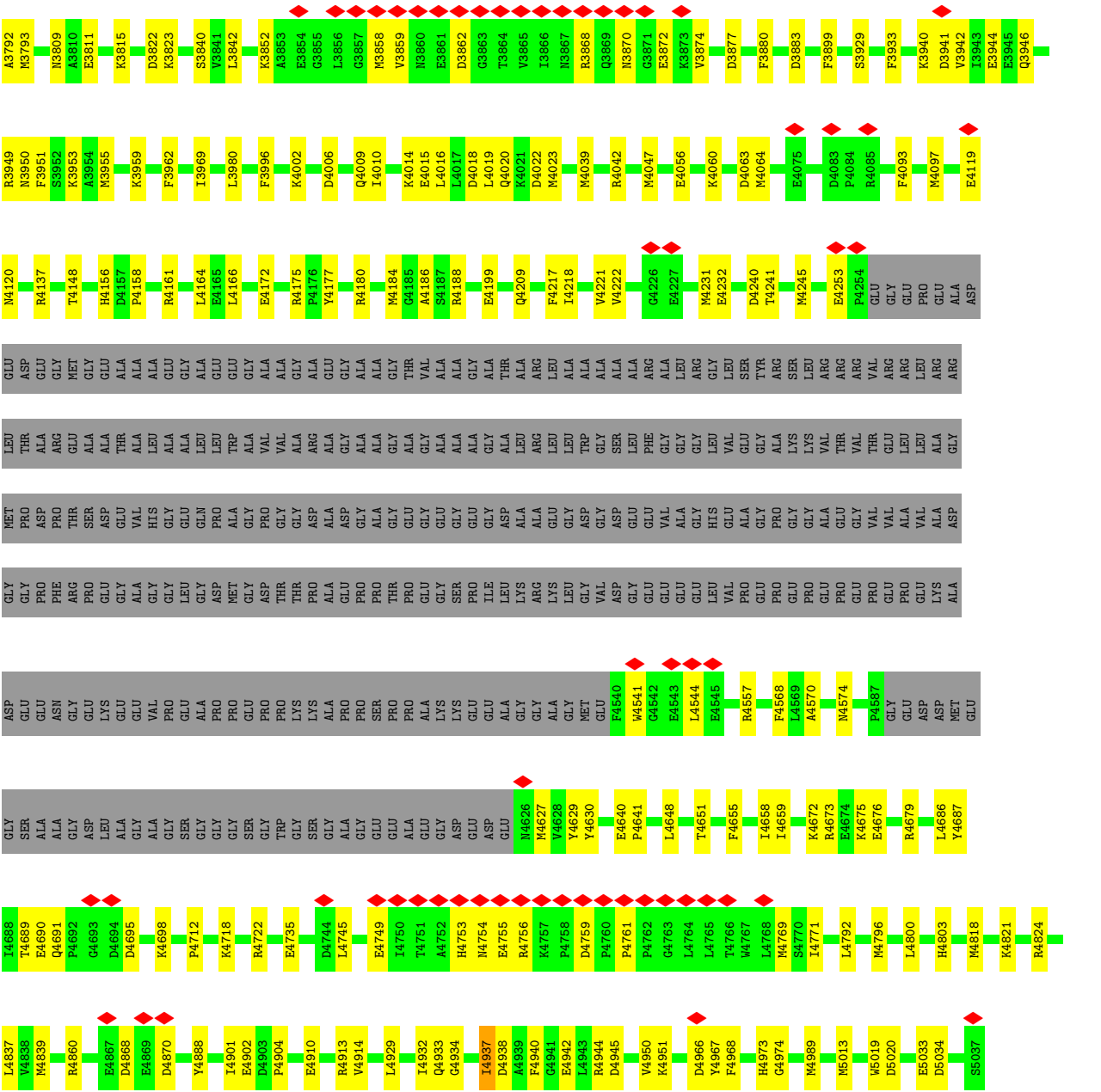




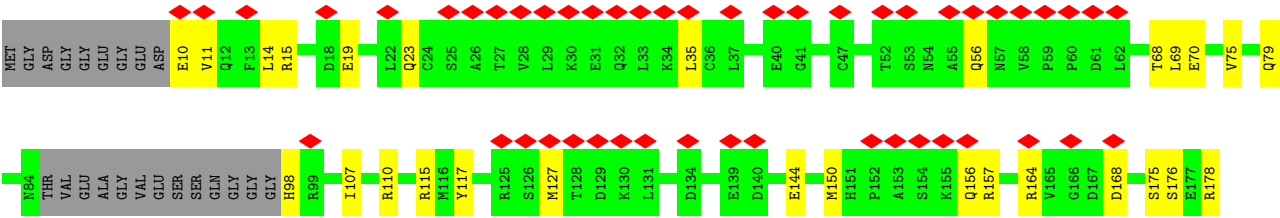


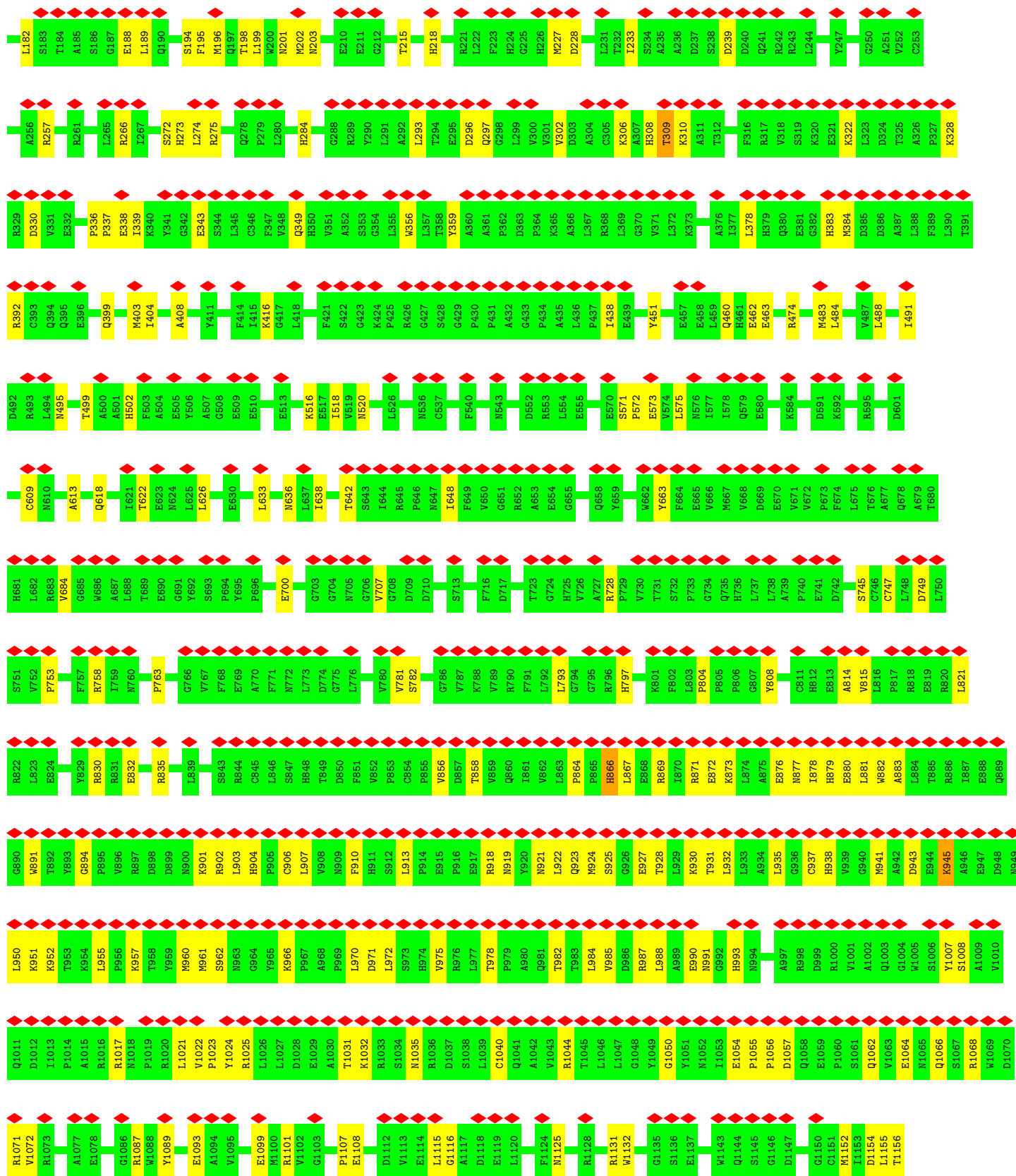


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GLY	R3630	N3450	N3450	G3390	D3330	T3270	L3210	Q3149	R3089	G3028	I2969
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		GLY	GLY	T3425	L3365	A3306	V3245	K3185	G3126	V3065	L3005
				E3426	R3366	V3307	L3246	L3186	Q3127	N3066	I3006
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● Molecule 1: Ryanodine receptor 1

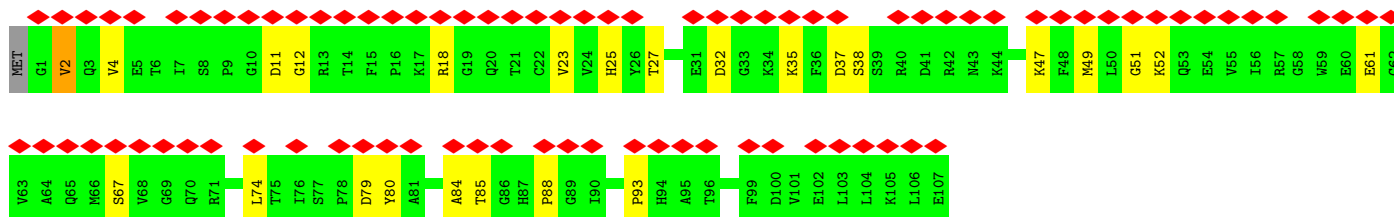


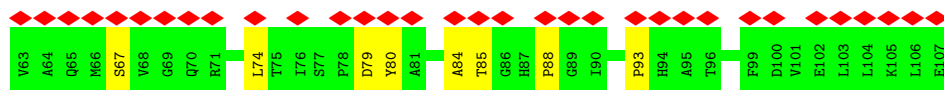




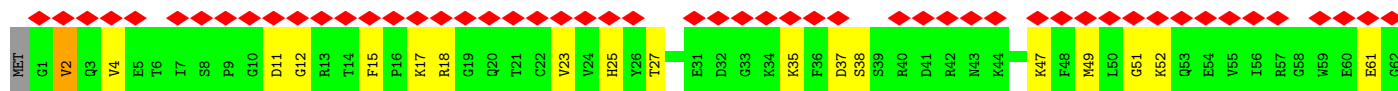
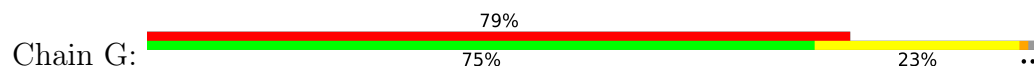
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L2589	S2590	R2591	Q2592	R2593	S2594	L2595	T2596	K2597	A2598	Q2599	R2600	D2601	V2602	I2603	E2604	D2605	C2606	L2607	M2608	A2609	L2610	C2611	R2612	Y2613	I2614	R2615	P2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	L2632	L2633	M2634	E2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	M2646	H2647	Y2648
D2523	V2524	G2525	F2526	L2527	F2528	D2529	M2530	R2531	A2532	A2533	A2534	S2535	L2536	D2537	T2538	A2539	T2540	F2541	S2542	E2545	M2546	A2547	L2548	A2549	L2550	N2551	L2552	Y2553	L2554	C2555	L2556	L2562	T2563	K2564	C2565	A2566	F2569	A2570	Q2571	T2572	E2573	H2574	R2575	A2576	L2577	M2578	V2579	D2580	S2581	M2582	L2583	H2584	T2585	Y2586	Y2587	R2588			
L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	I2469	T2470	S2471	L2472	P2473	L2474	Q2475	T2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	S2491	A2492	S2493	F2494	V2495	P2496	D2497	H2498	K2499	L2504	F2505	L2506	G2511	L2512	E2513	N2514	Q2515	D2516	F2517	L2518	L2519	H2520	V2521	L2522				
R2385	I2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	G2396	V2397	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	V2416	H2417	L2418	G2419	M2423	Y2426	A2427	A2428	L2429	I2430	D2431	L2432	L2433	E2439	M2440	H2441	L2442	G2446	K2447	G2448	E2449	R2452	I2453	R2454								
L2307	Q2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316	G2317	Y2318	P2319	D2320	I2321	G2322	C2326	G2327	R2330	Y2331	L2332	D2333	F2334	V2341	E2348	R2355	L2356	L2357	L2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	G2372	Q2373	S2374	Q2375	L2376	L2377	A2378	A2379	I2380	E2381	E2382	A2383	L2384					
E2219	T2220	K2221	E2222	L2223	R2224	F2225	F2226	K2227	W2228	V2229	Y2238	I2242	S2243	R2244	H2253	Y2256	L2257	L2258	E2259	G2262	L2263	G2264	L2265	G2266	L2267	Q2268	G2269	S2270	T2271	P2272	L2273	D2282	N2283	N2284	E2285	L2290	Q2291	E2292	Q2293	D2294	L2295	E2296	K2297	V2298	S2299	S2300	T2301	L2302	A2303	G2304	C2305	G2306							

K3809	K3959	T3708	H3611	E3551	GLN	A3431	K3371	H3311	A3251	G3191	Y3131	I3070
A3810	A3709	A3709	P3612	F3552	GLU	E3432	V3372	L3312	D3252	E3192	T3132	L3071
E3811	F3962	L3710	Y3613	L3553	ARG	E3433	V3373	N3313	I3253	C3193	T3133	
K3815		T3711	K3614	Q3554	THR	L3434	A3374	S3314	G3254	L3194	V3134	R3073
D3822	I3969	E3712	S3615	N3555	LYS	F3435	E3375	L3315	G3255	A3195	A3135	S3074
K3823	L3980	K3713	K3616	K3556		R3436	E3376	L3316	L3256	R3196	L3136	L3075
S3840		S3714	K3617	L3557	R3498	K3437	E3377	G3317	A3257	L3197	L3137	D3076
V3841	F3996	L3715	A3618	H3558	R3499	V3438	Q3378	N3318	E3258	A3198	P3138	A3077
L3842		L3716	V3619	L3559	G3500	G3439	L3379	I3319	S3259	A3199	V3139	R3078
	D4006	D3717	W3620	Q3560	D3501	E3440	R3380	L3320	G3260	A3200	L3140	T3079
Q4009		E3718	H3621	G3561	R3502	I3441	L3381	R3321	A3261	M3201	T3141	V3080
I4010		D3719	K3622	K3562	Y3503	F3442	E3382	I3322	R3262	P3202	T3142	V3081
		Y3720	L3623	V3563	S3504	I3443	A3383	I3323	Y3263	V3203	L3143	K3082
K3723		M3723	L3624	E3564	V3505	Y3444	K3384	N3324	T3264	A3204	F3144	S3083
K3731			S3625	G3565	Q3506	W3445	A3385	N3325	E3265	F3205	Q3145	G3084
H3734			K3626	S3566	T3507	S3446	E3386	N3326	M3266	L3206	H3146	P3085
L3735			Q3627	P3567	S3508	K3447	A3387	L3327	P3267	E3207	I3147	E3086
E3736			R3628	S3568	L3509	S3448	E3388	G3328	H3268	P3208	A3148	I3087
			R3629	L3569	I3510	K3449	E3389	I3329	V3269	Q3209	Q3149	V3088
GLU			R3630	R3570	V3511	N3450	E3390	D3330	I3270	L3210	H3150	V3088
GLY			A3631	W3571	A3512	F3451	G3391	E3331	E3271	N3211	Q3151	K3089
GLY			V3632	Q3572	L3513	K3452	E3391	A3332	I3272	E3212	F3152	A3090
ASN			V3633	M3573	K3453	R3453	L3392	T3333	T3273	Y3213	G3153	G3091
GLY			A3634	A3574	E3454	E3454	L3393	W3334	L3274	N3214	D3154	L3092
ALA			C3635	L3575	E3455	E3455	V3394	M3335	P3275	A3215	D3154	
GLU			F3636	Y3576	Q3456	K3457	D3396	K3336	M3276	C3216	D3156	F3095
GLU			R3637	R3577	N3457	N3457	E3397	R3337	L3277	S3217	I3157	F3096
GLU			M3638	G3578	F3458	F3458	E3397	L3338	C3278	S3217	I3157	E3097
GLU			T3639	L3579	V3459	V3459	F3398	A3339	S3279	V3218	L3158	S3098
GLU			P3640	L3579	V3460	V3460	S3399	S3399	Y3219	A3099	D3159	A3099
V3749			L3641	P3580	G3521	Q3461	V3400	V3340	Y3280	T3220	D3160	S3100
E3750			Y3642	G3581	L3522	Q3461	V3400	F3341	L3281	T3221	E3101	E3101
V3751			Y3642	N3523	N3523	N3462	L3401	A3342	P3282	K3222	Q3162	
S3752			N3643	M3524	M3524	E3463	C3402	Q3343	R3283	S3223	T3103	
E3753				C3525	C3525	I3464	R3403	Q3343	R3283	P3224	E3104	
E3754			M3652	A3526	A3526	N3466	D3404	I3345	W3285	R3225	E3104	
K3756				P3527	P3527	N3467	L3405	V3346	E3286	C3165	K3105	
M3758			E3665	T3528	T3528	M3467	Y3406	S3347	R3287	E3226	K3106	
			D3666	D3587	D3587	S3468	A3407	R3348	G3288	R3227	V3107	
				D3588	D3588	F3469	L3408	R3348	A3228	T3168	E3108	
				P3589	P3589	L3470	Y3409	A3349	P3289	L3169	N3109	
				E3590	E3590	T3471	P3410	R3350	I3229	L3169		
				L3592	L3592	A3472	L3411	A3350	E3290	C3170	L3110	
				K3591	K3591	A3472	L3412	R3351	A3291	R3170	R3111	
				L3592	L3592	D3473	L3412	E3352	P3292	G3231	L3112	
				V3593	V3593	S3474	I3413	L3353	P3293	P3233	Y3173	
				K3594	K3594	K3475	R3414	L3354	P3294	N3234	S3174	
				R3595	R3595	S3476	Y3415	H3355	A3295	S3235	K3114	
				V3596	V3596	K3477	V3416	S3356	L3296	V3236	L3175	
				E3597	E3597	K3477	V3416	H3357	P3297	G3176	G3176	
				E3598	E3598	M3478	D3417	F3358	E3237	T3177	T3177	
				V3599	V3599	A3479	N3418	A3298	E3238	K3178	ARG	
				S3600	S3600	LYS	R3419	I3359	G3299	K3179	THR	
				A3601	A3601	ALA	R3420	P3360	A3300	N3180	GLN	
				K3543	K3543	ASP	A3421	T3361	P3301	T3181	VAL	
				D3544	D3544	ALA	H3422	I3362	P3241	K3123		
				T3545	T3545	GLN	W3423	G3363	P3302	Y3182		
				D3546	D3546	SER	L3424	R3364	I3243	V3183		
				L3605	L3605	GLY	T3425	L3365	C3304	G3124		
				E3607	E3607	GLY	E3426	R3366	T3305	V3125		
				E3607	E3607	SER	F3427	K3367	A3306	G3126		
				V3549	V3549	ASP	N3428	R3368	V3245	Q3127		
				R3550	R3550		A3429	A3369	T3307	L3186		
									V3309	R3187		
									D3310	P3188		
										A3189		
										L3190		

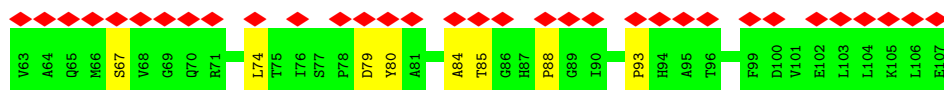
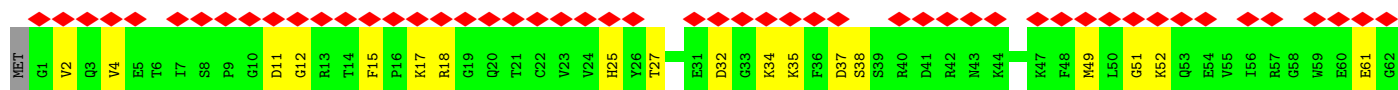
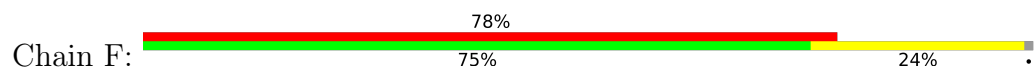




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• 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: A1BD4, CA, ATP, 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%)	78	85
1	B	3836/4276 (90%)	3813 (99%)	23 (1%)	78	85
1	C	3836/4276 (90%)	3813 (99%)	23 (1%)	78	85
1	D	3836/4276 (90%)	3813 (99%)	23 (1%)	78	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	89/90 (99%)	85 (96%)	4 (4%)	24	56
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	63
2	G	89/90 (99%)	85 (96%)	4 (4%)	24	56
2	H	89/90 (99%)	85 (96%)	4 (4%)	24	56
All	All	15700/17464 (90%)	15593 (99%)	107 (1%)	73	84

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
6	A1BD4	A	5304	-	11,11,11	1.06	0	11,15,15	3.93	4 (36%)
3	ATP	A	5301	-	32,33,33	0.35	0	48,52,52	0.38	0
6	A1BD4	B	5304	-	11,11,11	1.07	0	11,15,15	3.93	4 (36%)
6	A1BD4	D	5304	-	11,11,11	1.07	0	11,15,15	3.94	4 (36%)
6	A1BD4	C	5304	-	11,11,11	1.07	0	11,15,15	3.93	4 (36%)
3	ATP	C	5301	-	32,33,33	0.35	0	48,52,52	0.38	0
3	ATP	D	5301	-	32,33,33	0.35	0	48,52,52	0.38	0
3	ATP	B	5301	-	32,33,33	0.34	0	48,52,52	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1BD4	A	5304	-	-	-	0/2/2/2
3	ATP	A	5301	-	-	5/22/38/38	0/3/3/3
6	A1BD4	B	5304	-	-	-	0/2/2/2
6	A1BD4	D	5304	-	-	-	0/2/2/2
6	A1BD4	C	5304	-	-	-	0/2/2/2
3	ATP	C	5301	-	-	5/22/38/38	0/3/3/3
3	ATP	D	5301	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5304	A1BD4	C3-C2-N2	-10.07	106.50	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5304	A1BD4	C3-C2-N2	-10.04	106.52	112.20
6	D	5304	A1BD4	C3-C2-N2	-10.04	106.52	112.20
6	C	5304	A1BD4	C3-C2-N2	-10.04	106.52	112.20
6	D	5304	A1BD4	C2-N2-N1	5.35	111.37	102.58

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

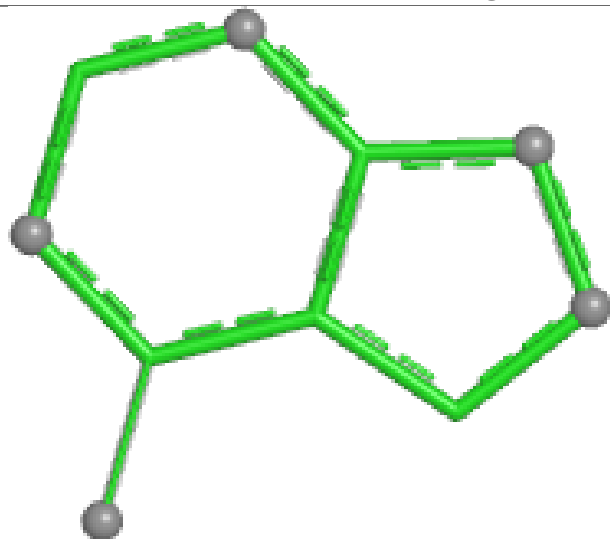
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	D	5301	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

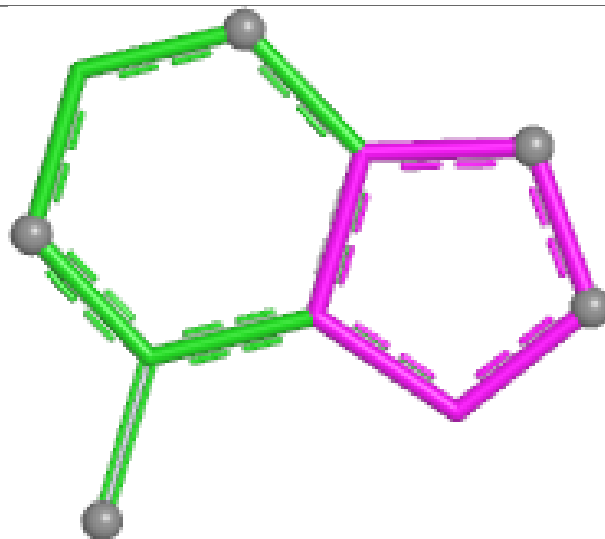
No monomer is involved in short contacts.

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.

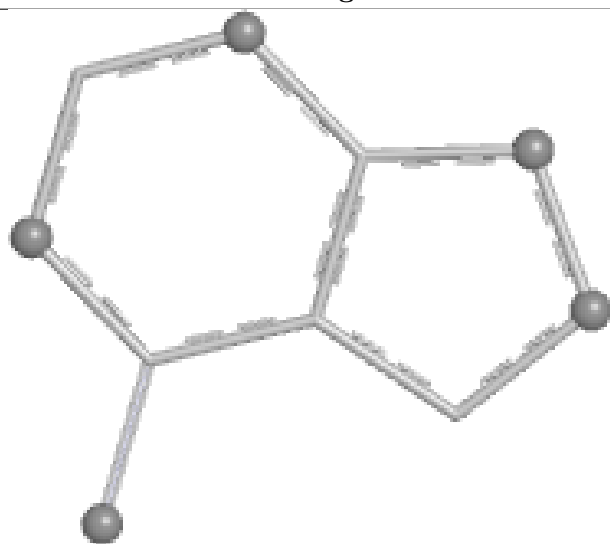
Ligand A1BD4 A 5304



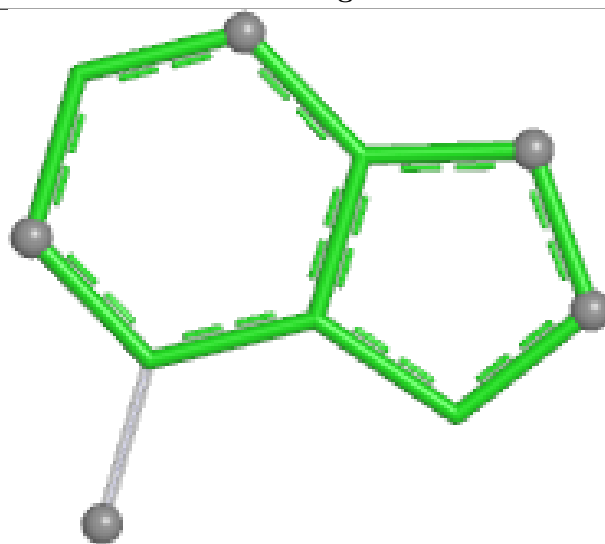
Bond lengths



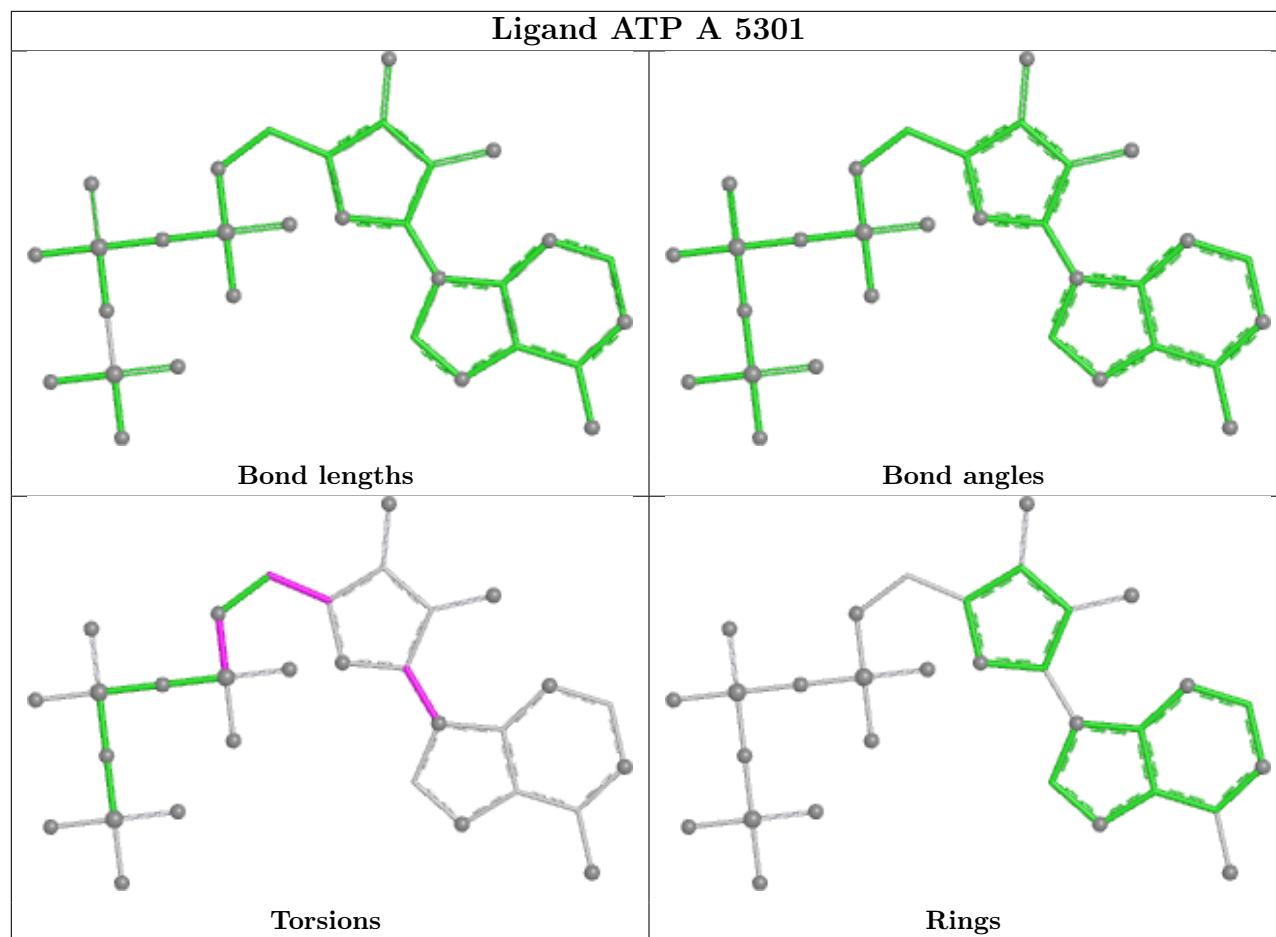
Bond angles



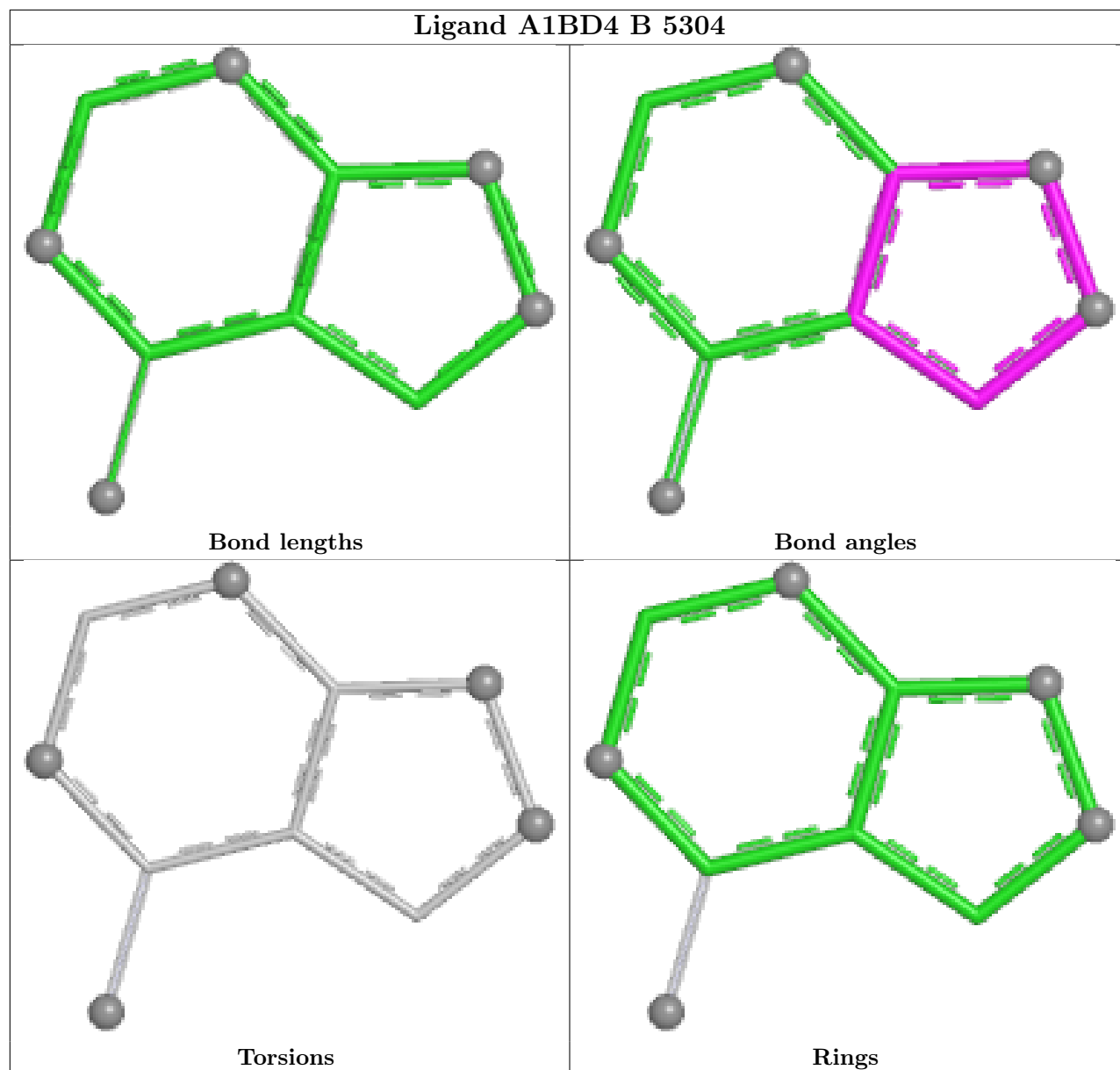
Torsions



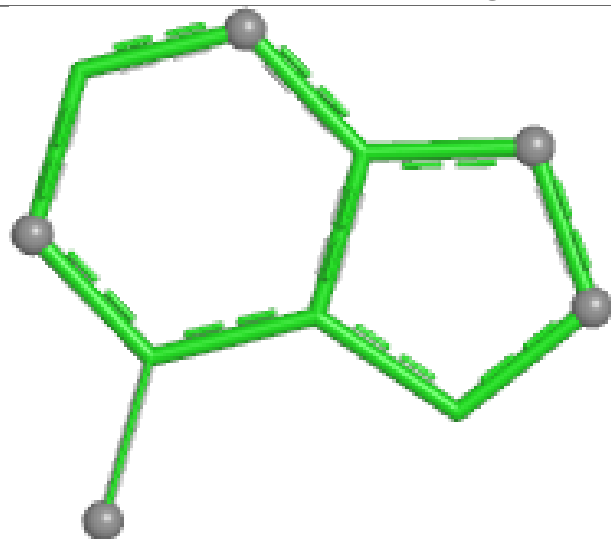
Rings



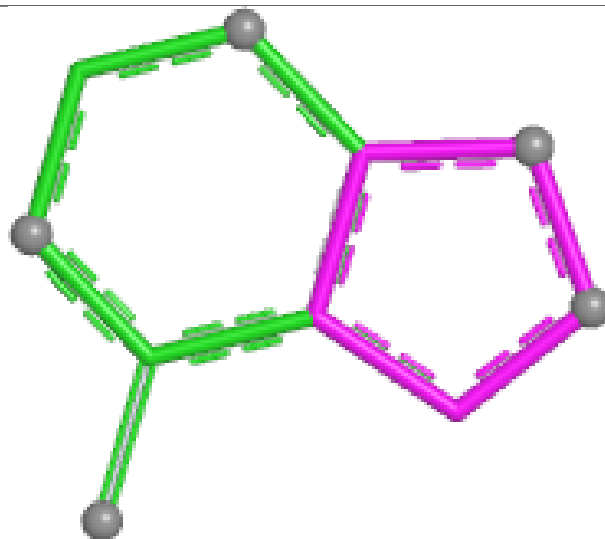
Ligand A1BD4 B 5304



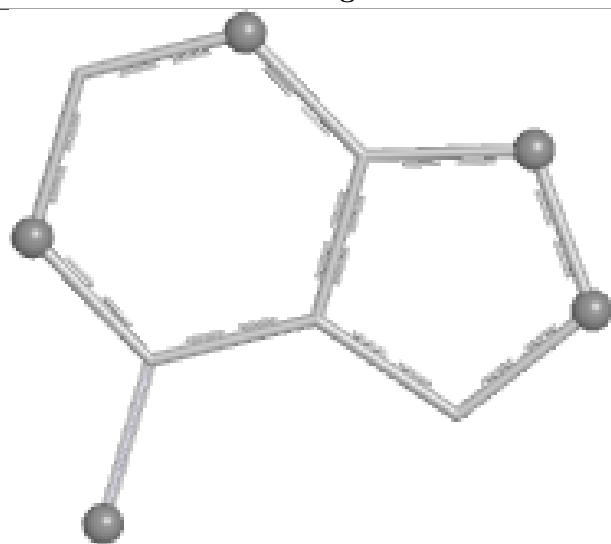
Ligand A1BD4 D 5304



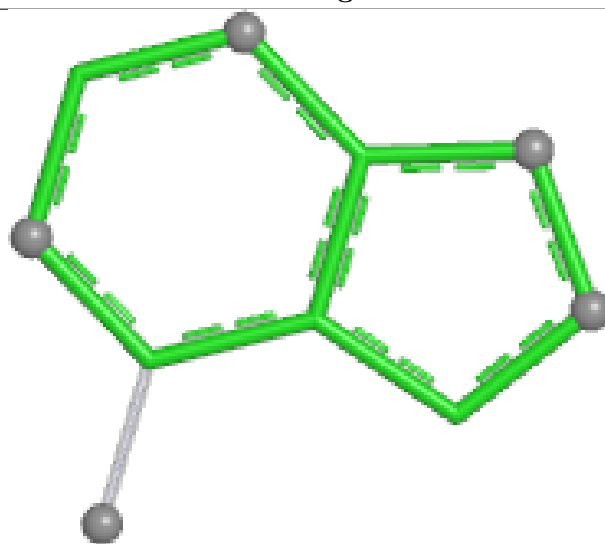
Bond lengths



Bond angles

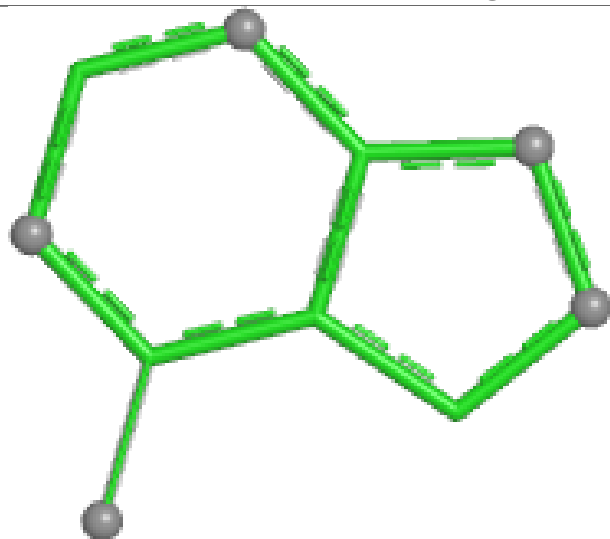


Torsions

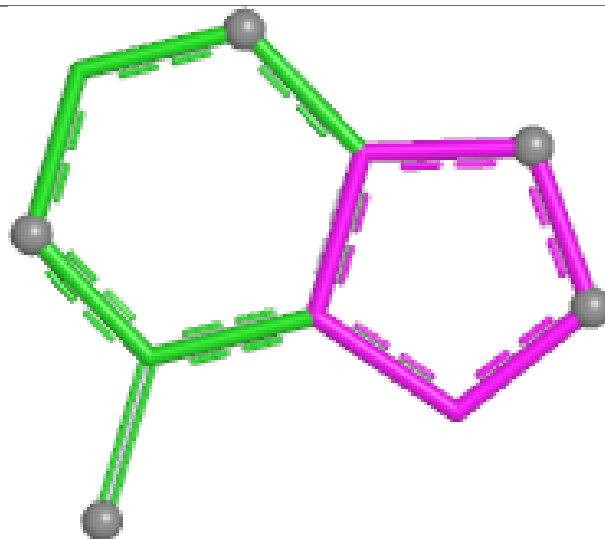


Rings

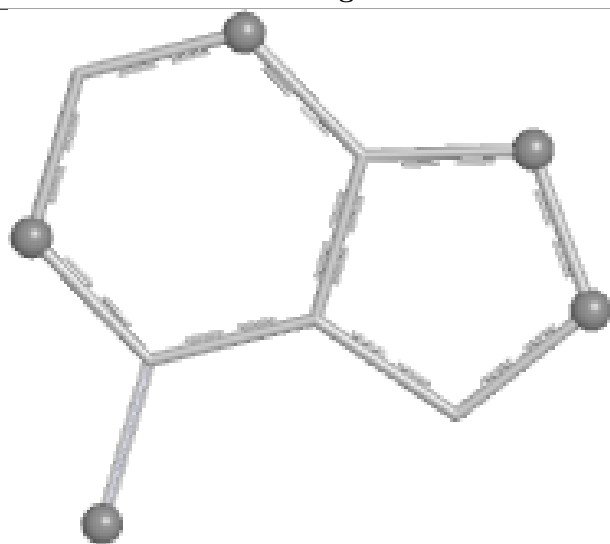
Ligand A1BD4 C 5304



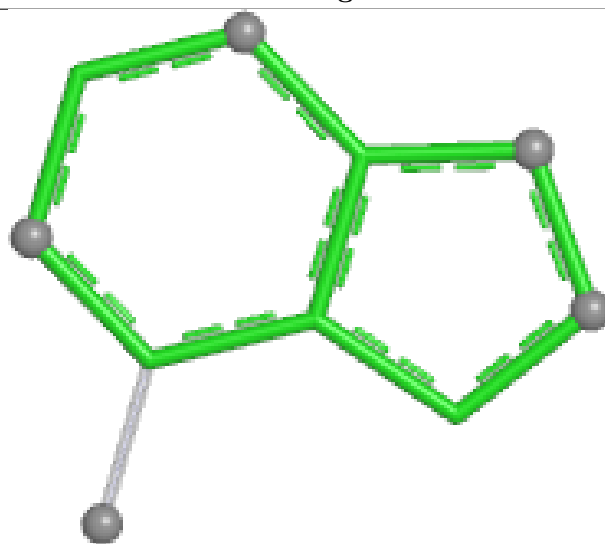
Bond lengths



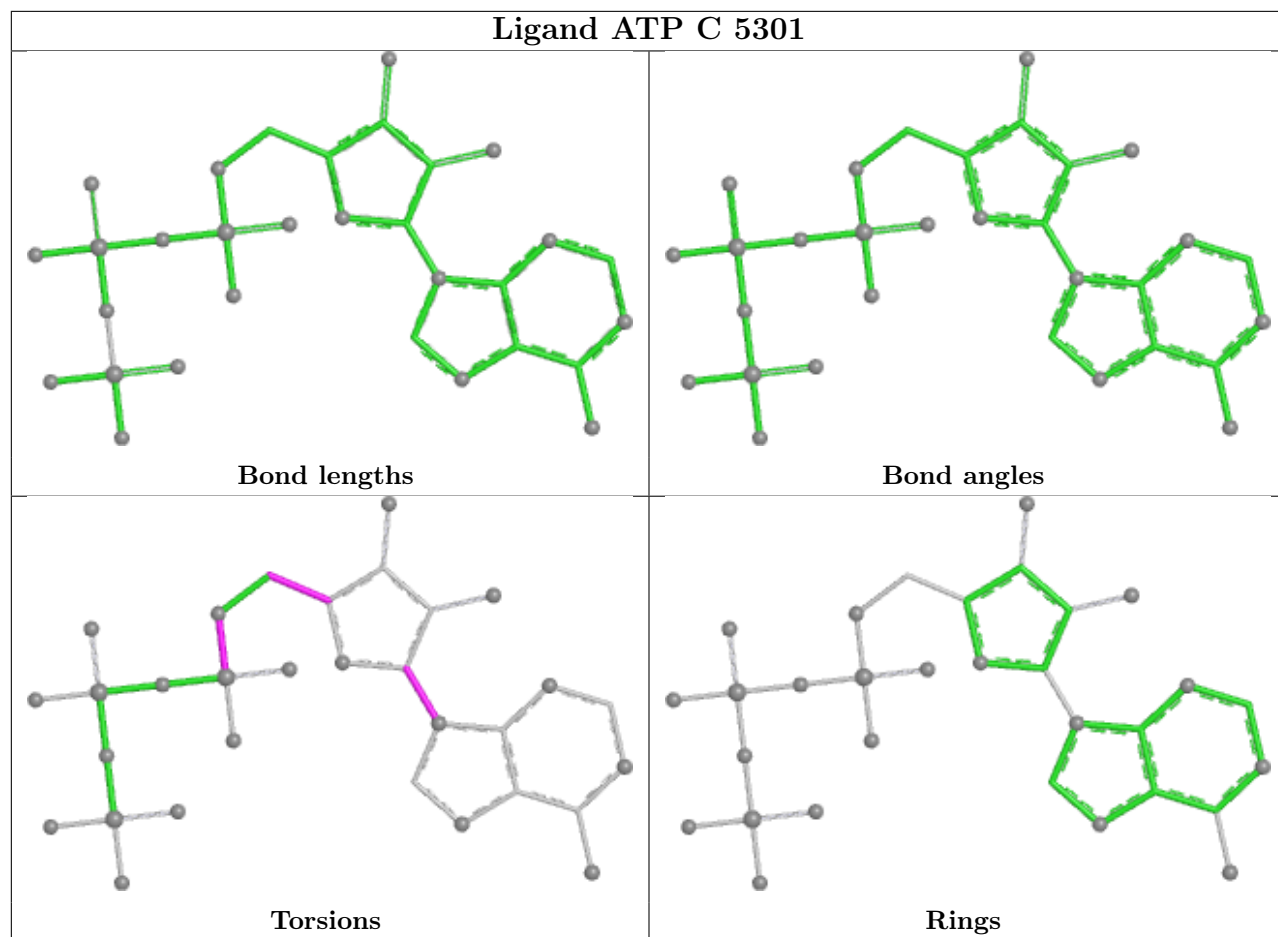
Bond angles

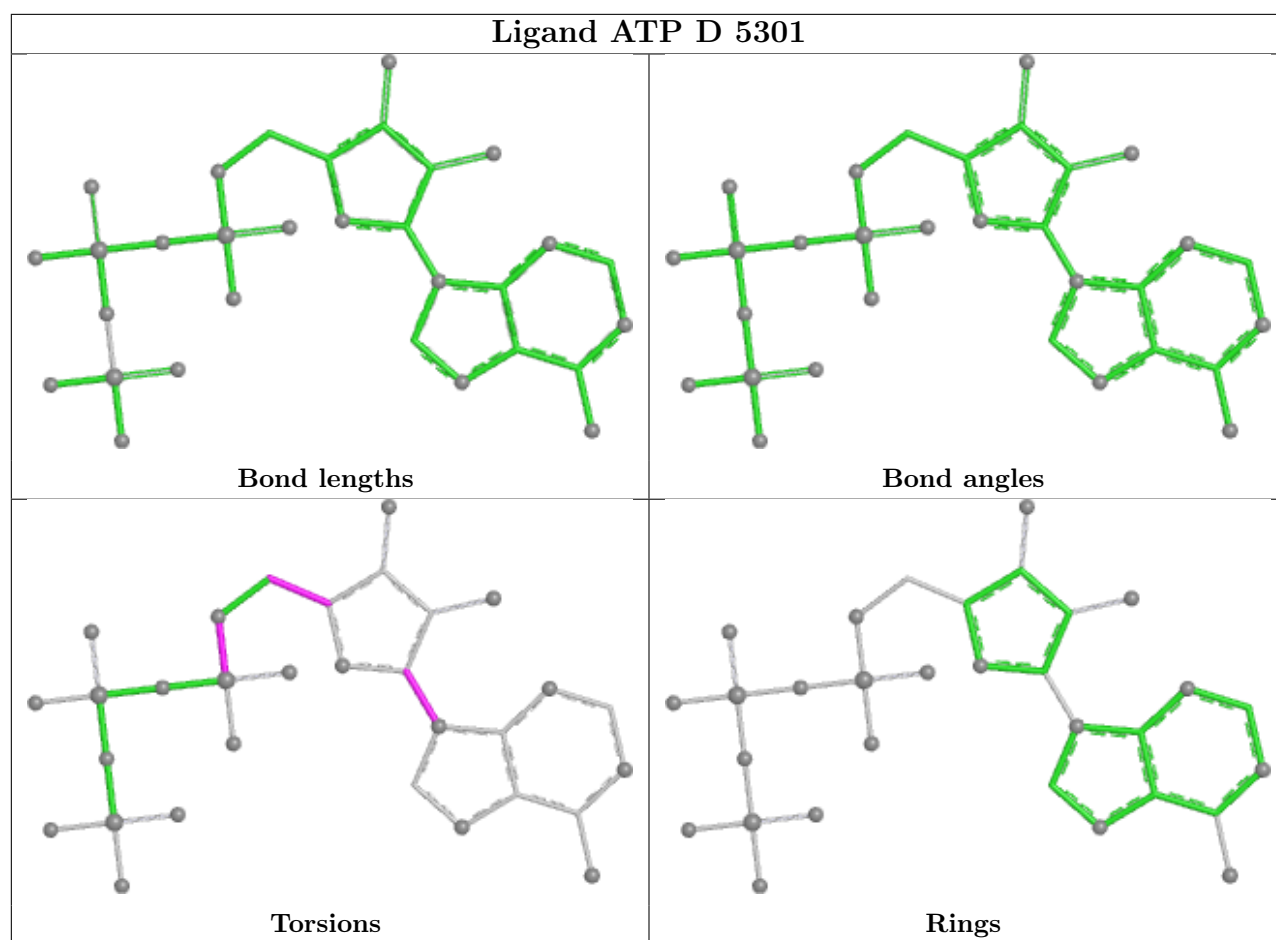


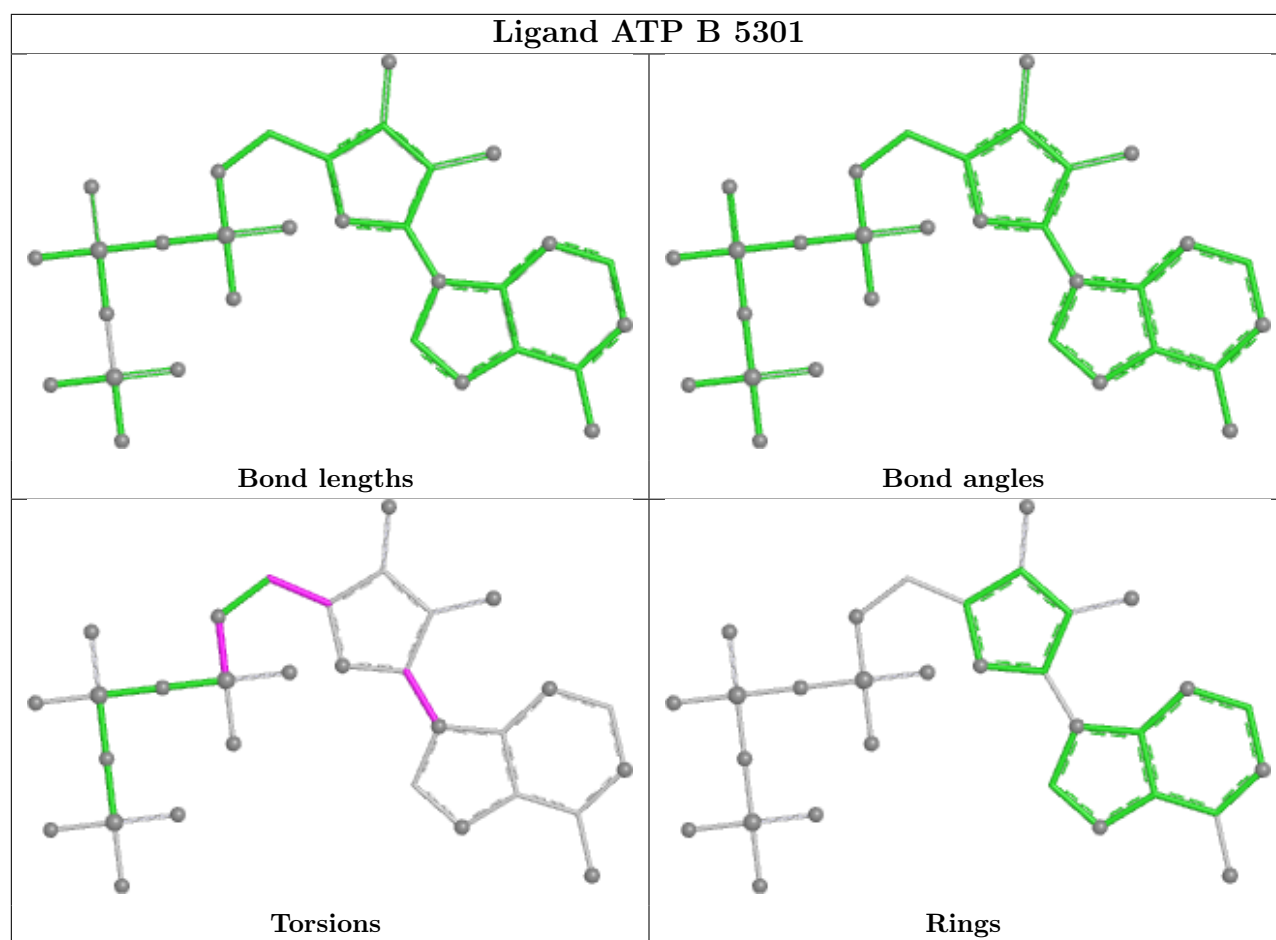
Torsions



Rings







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.

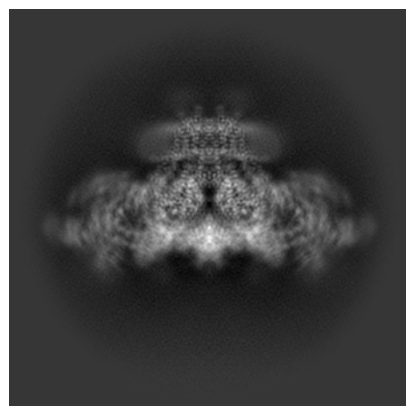
6 Map visualisation [i](#)

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.

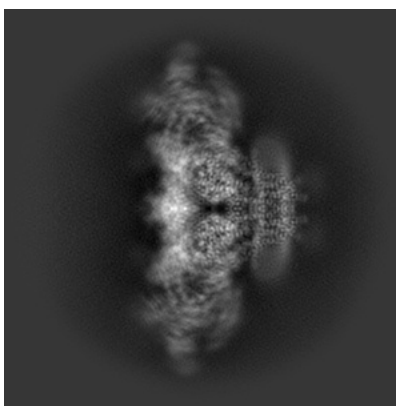
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

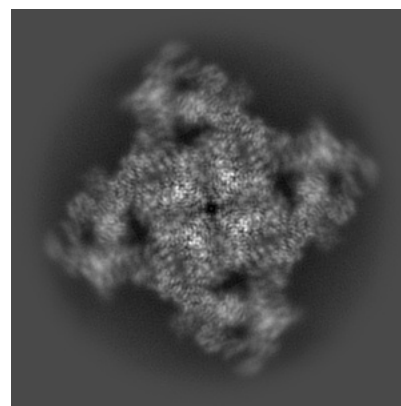
6.1.1 Primary map



X

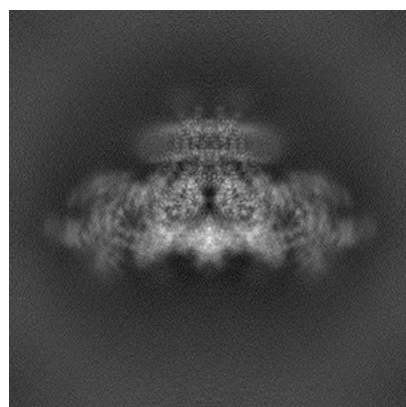


Y

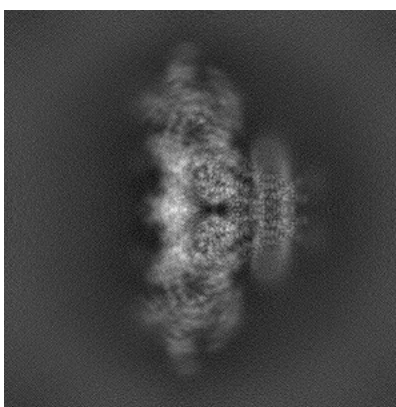


Z

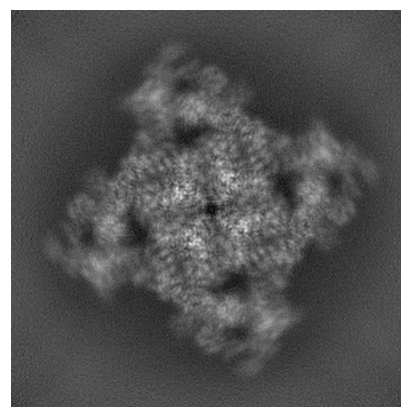
6.1.2 Raw map



X



Y

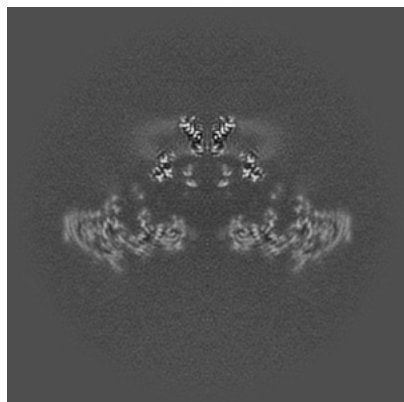


Z

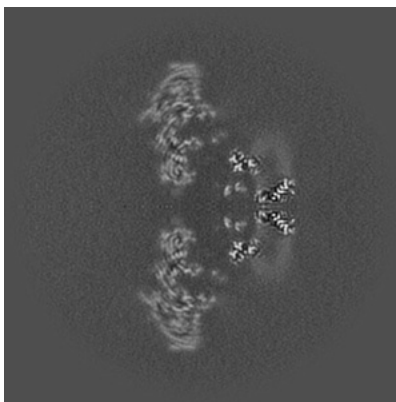
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

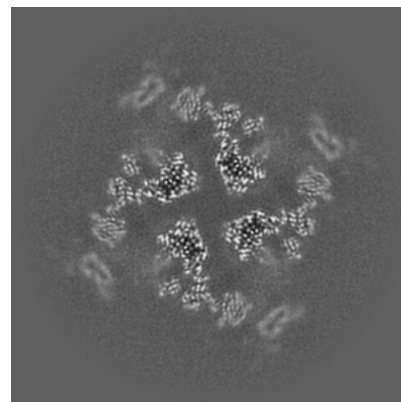
6.2.1 Primary map



X Index: 256

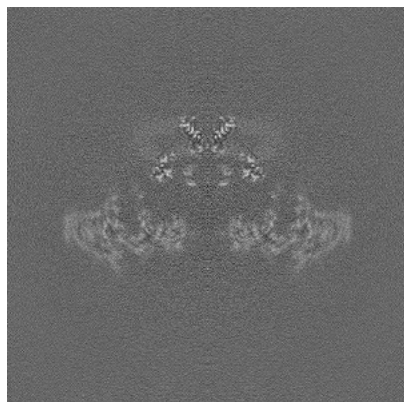


Y Index: 256

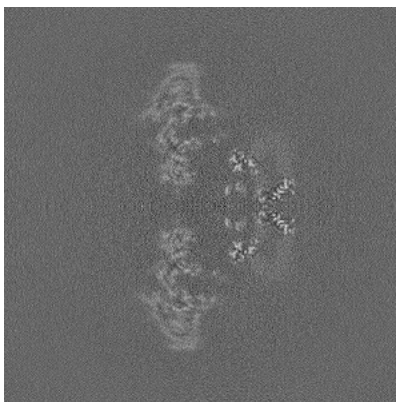


Z Index: 256

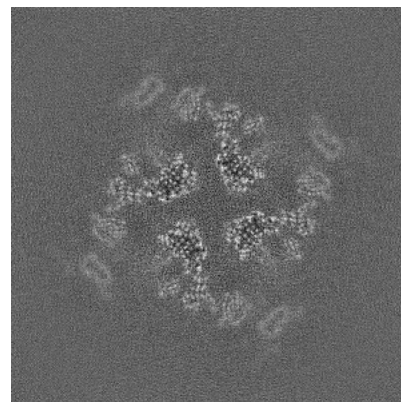
6.2.2 Raw map



X Index: 256



Y Index: 256

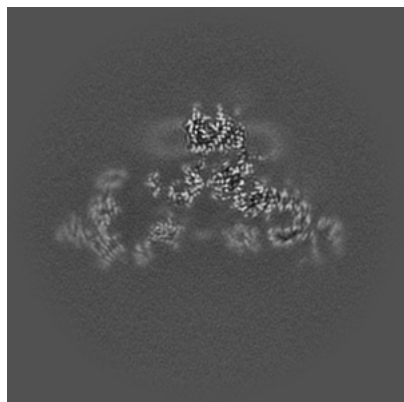


Z Index: 256

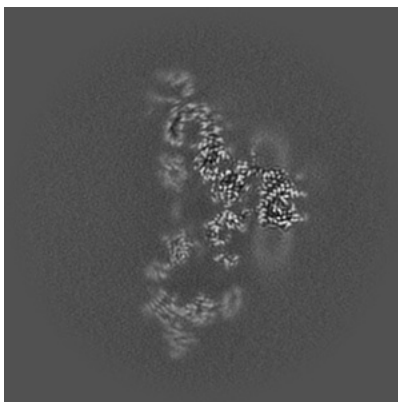
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

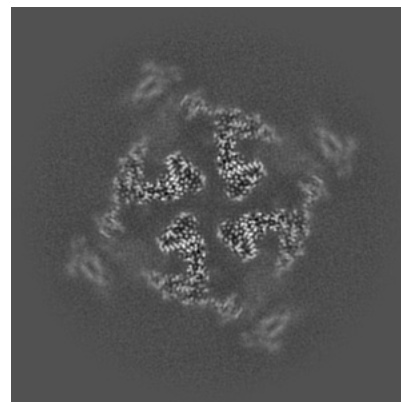
6.3.1 Primary map



X Index: 273

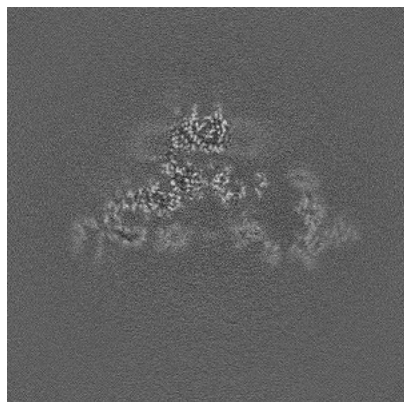


Y Index: 239

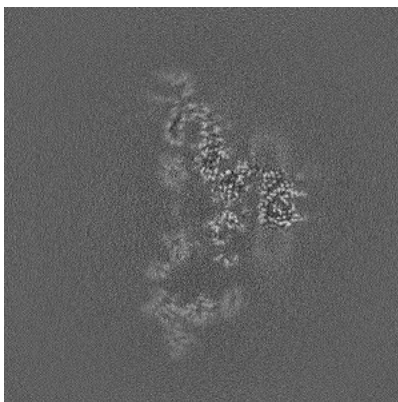


Z Index: 264

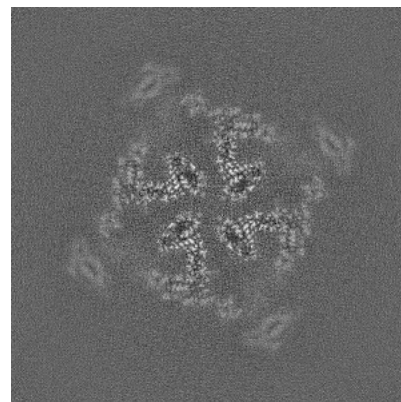
6.3.2 Raw map



X Index: 239



Y Index: 239

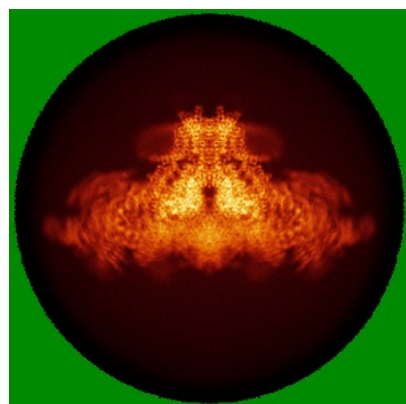


Z Index: 266

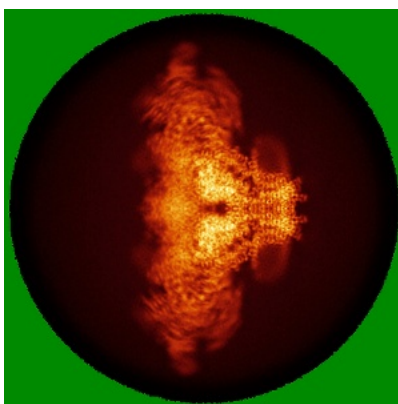
The images above show the largest variance slices of the map in three orthogonal directions.

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

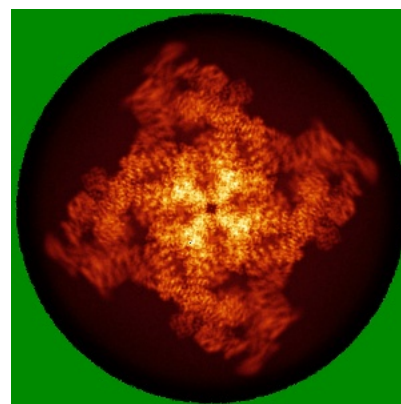
6.4.1 Primary map



X

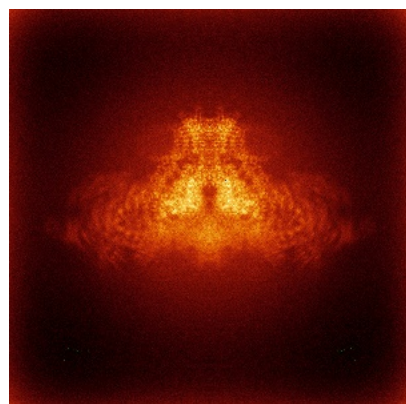


Y

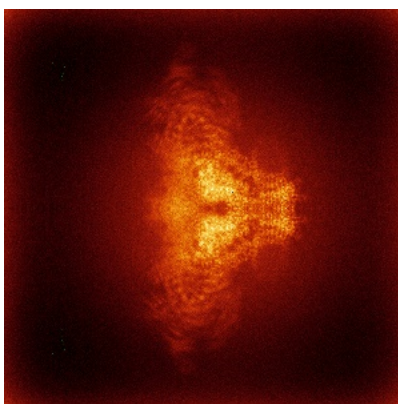


Z

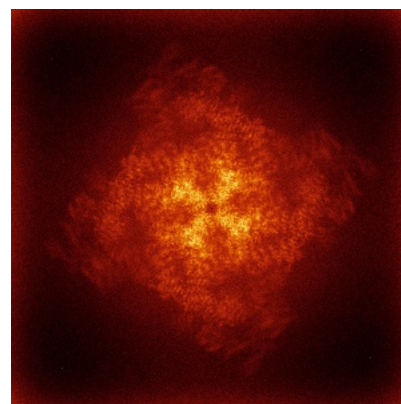
6.4.2 Raw map



X



Y

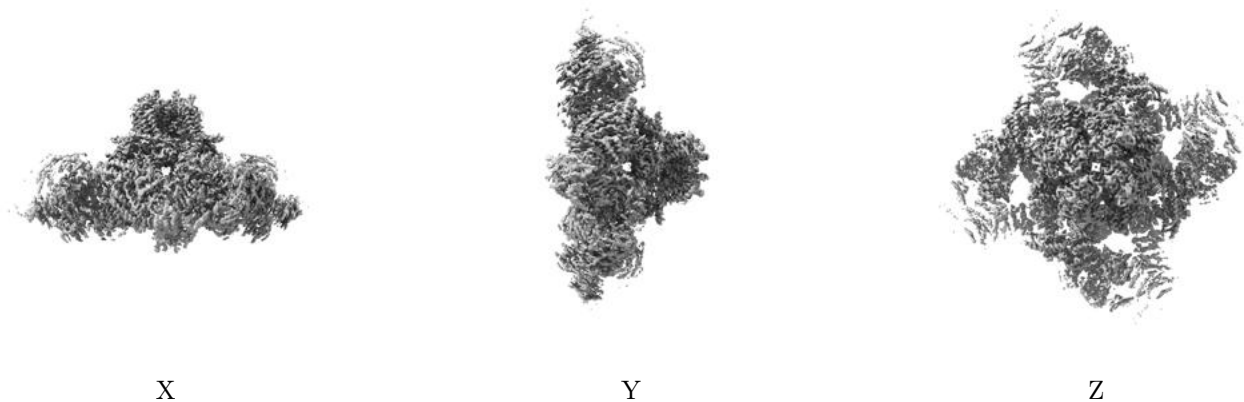


Z

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.

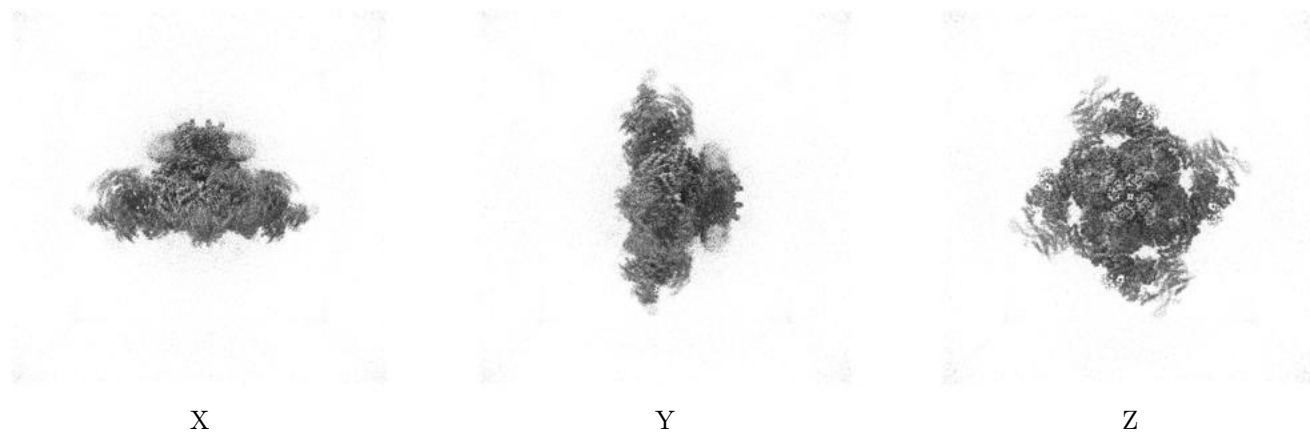
6.5 Orthogonal surface views [i](#)

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.

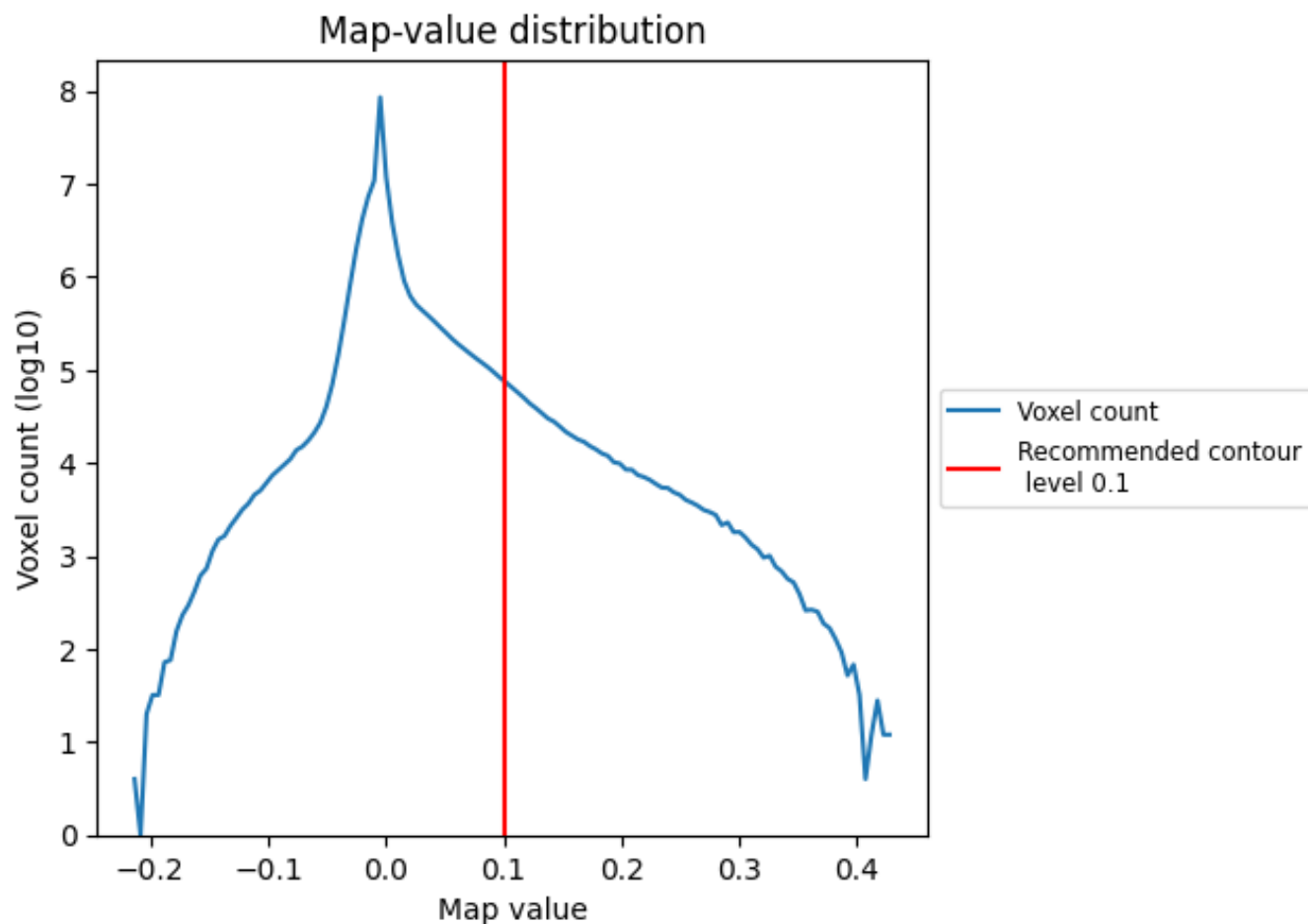
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

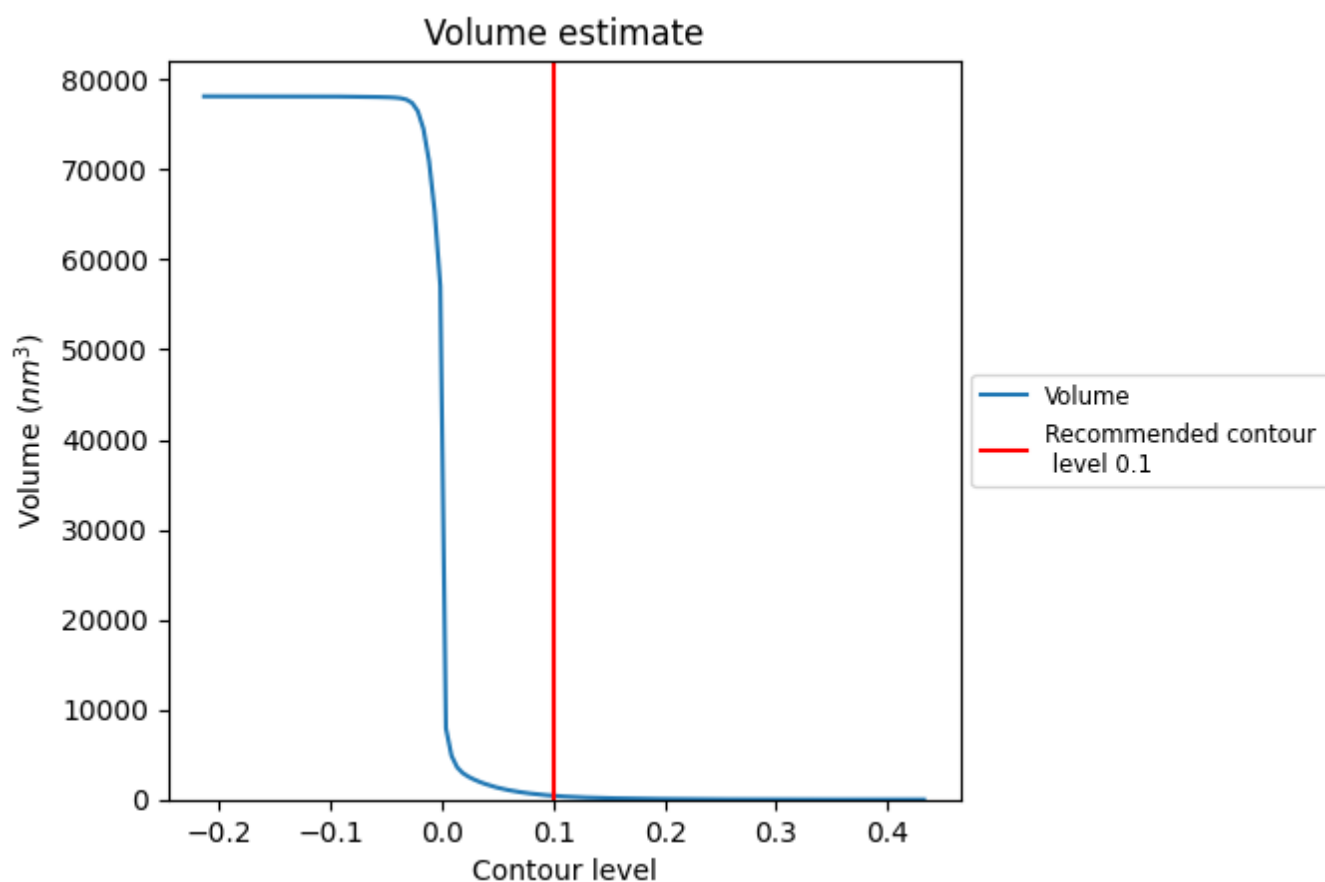
This section contains the results of statistical analysis of the map.

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.

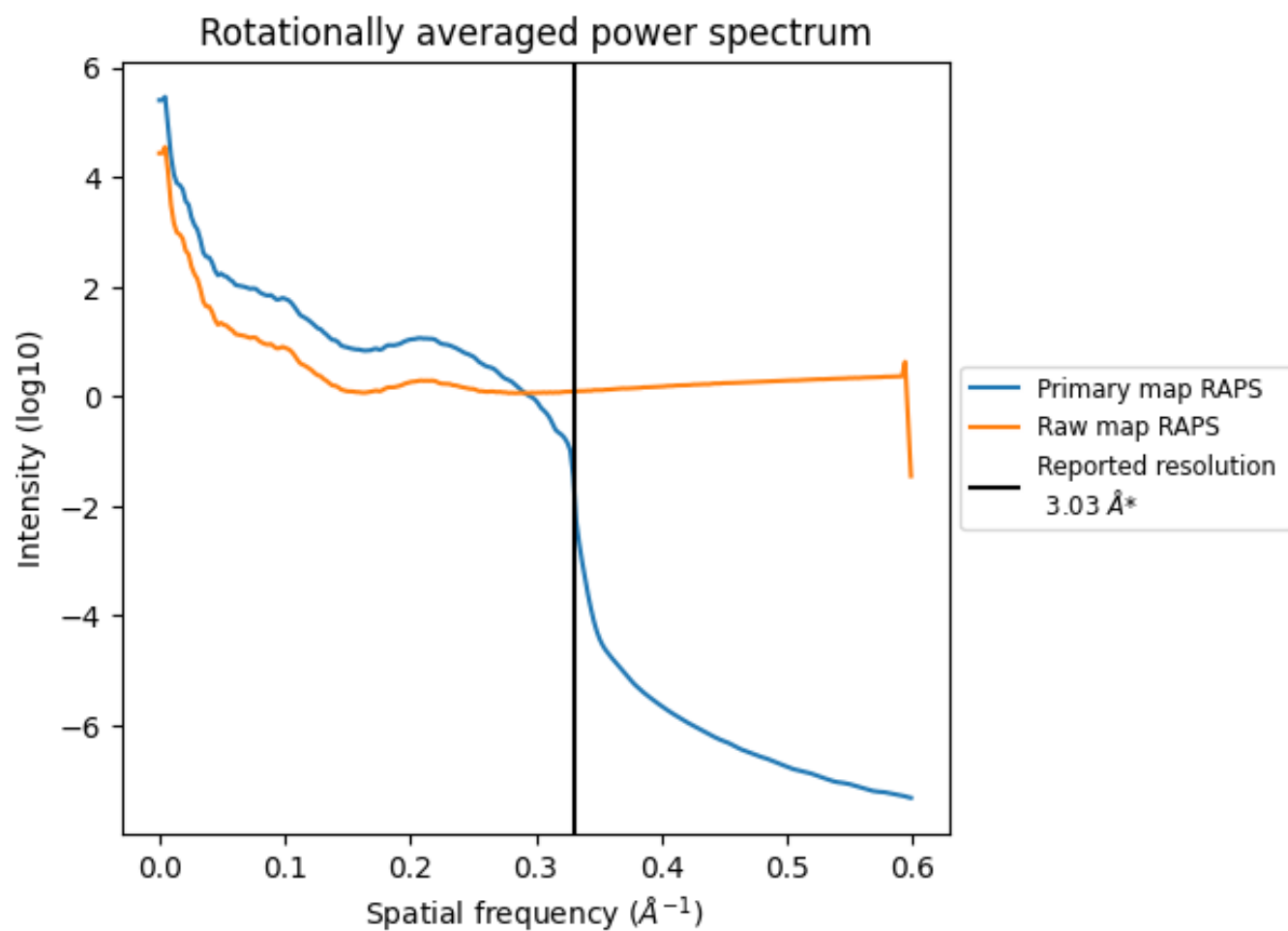
7.2 Volume estimate [i](#)



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 ⓘ

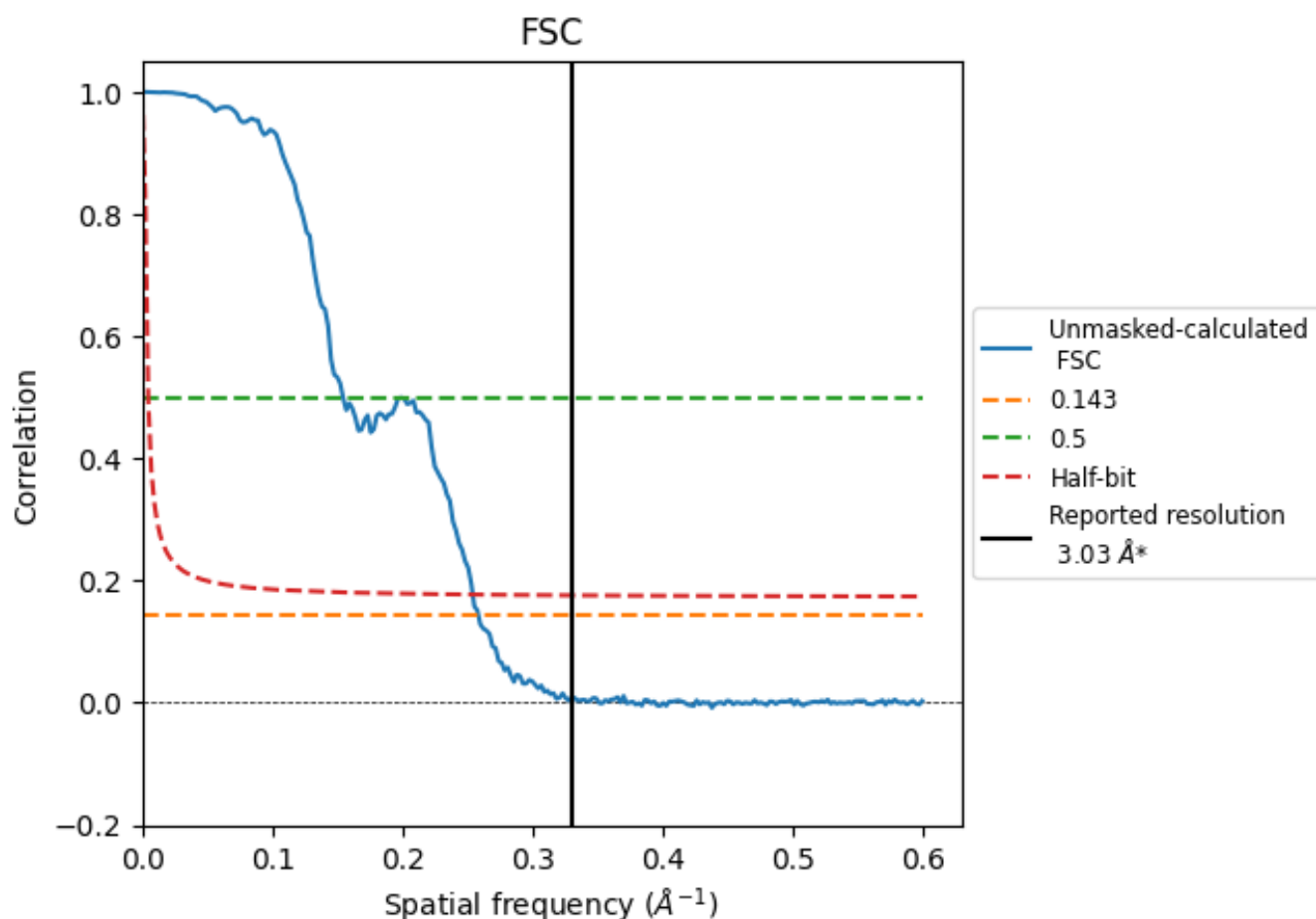


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8.2 Resolution estimates [i](#)

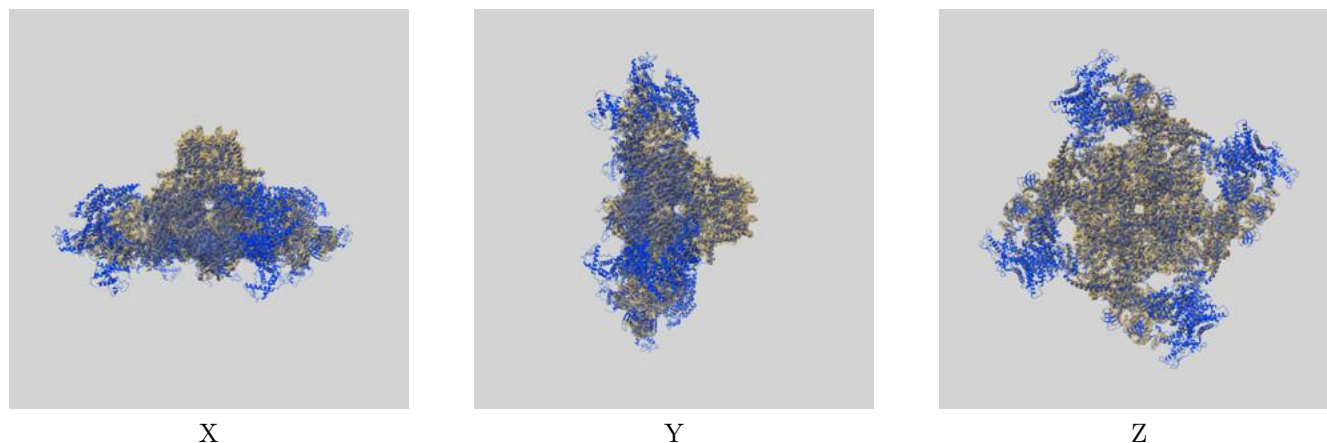
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	6.49	3.94

*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](#)

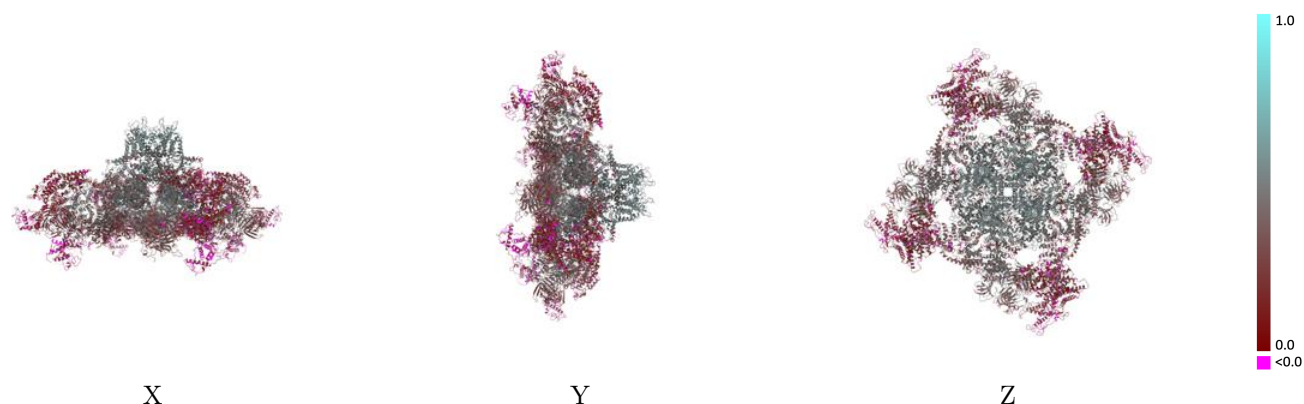
This section contains information regarding the fit between EMDB map EMD-47392 and PDB model 9E1F. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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](#)

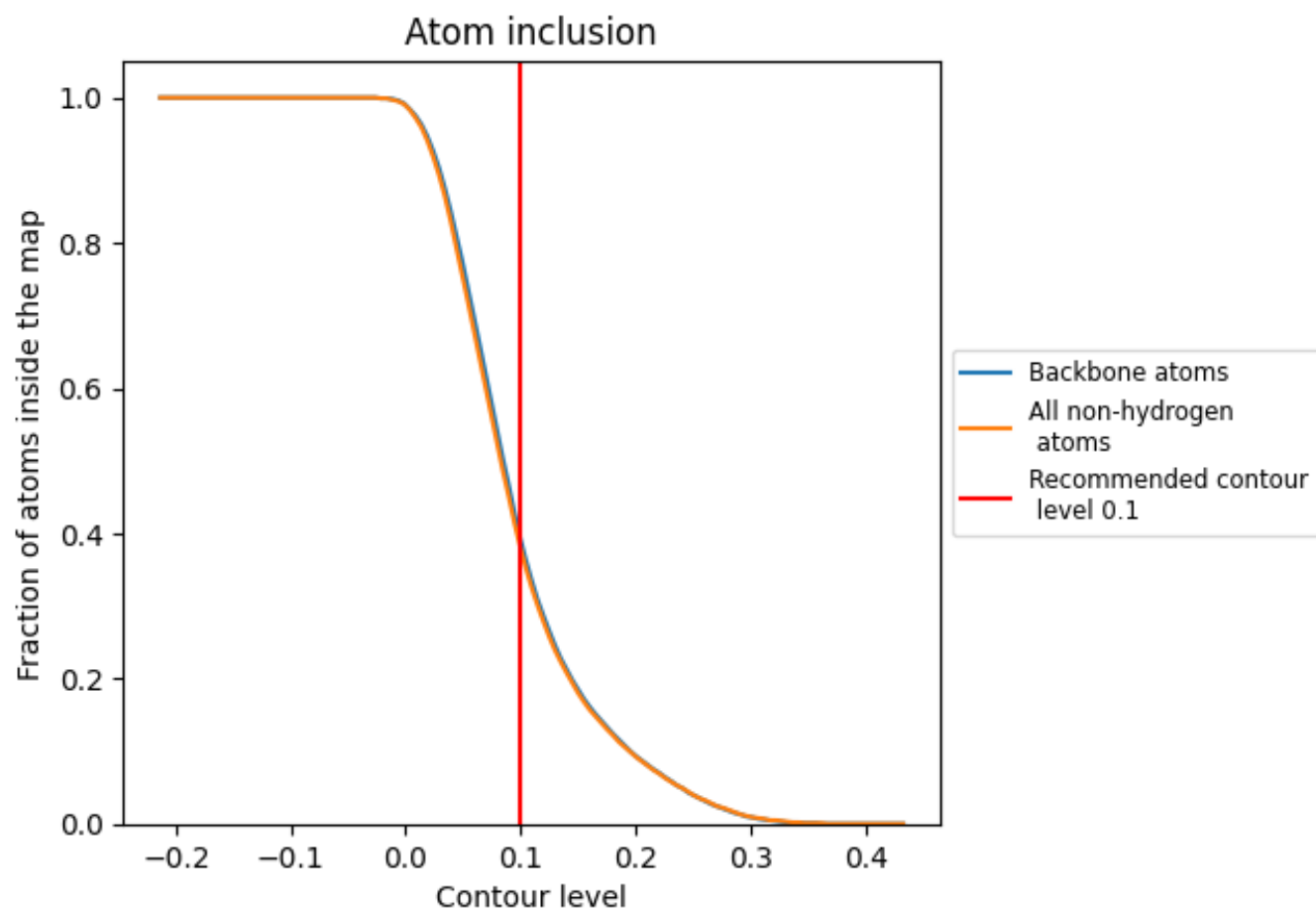


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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

1.0

0.0

<0.0