



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:42 PM UTC

PDB ID : 5TAT / pdb_00005tat
EMDB ID : EMD-8384
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.80 Å(reported)

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:

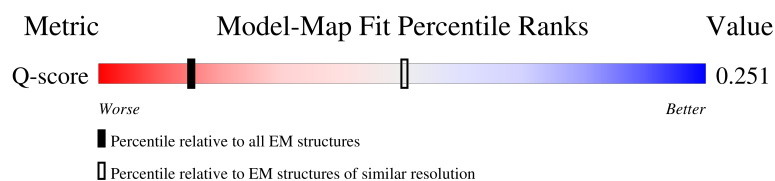
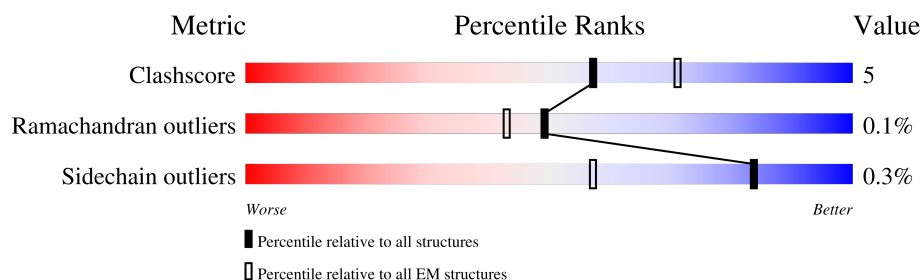
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	108	
1	F	108	
1	H	108	
1	J	108	

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Mol	Chain	Length	Quality of chain			
2	B	4416	39%			
2	E	4416	84%			
2	G	4416	11%			
2	I	4416	5%			

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

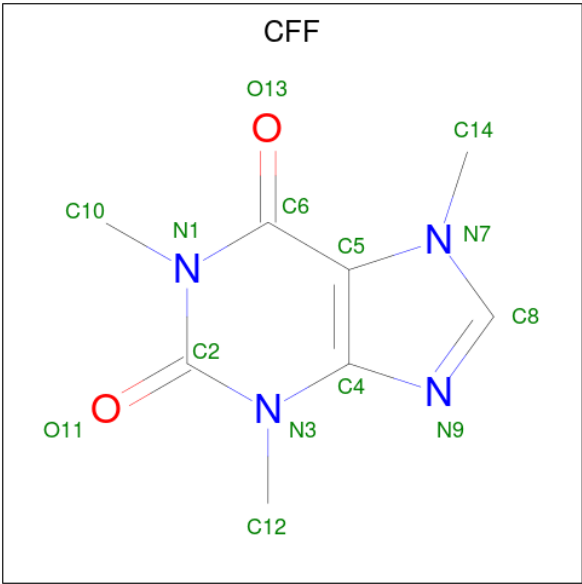
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

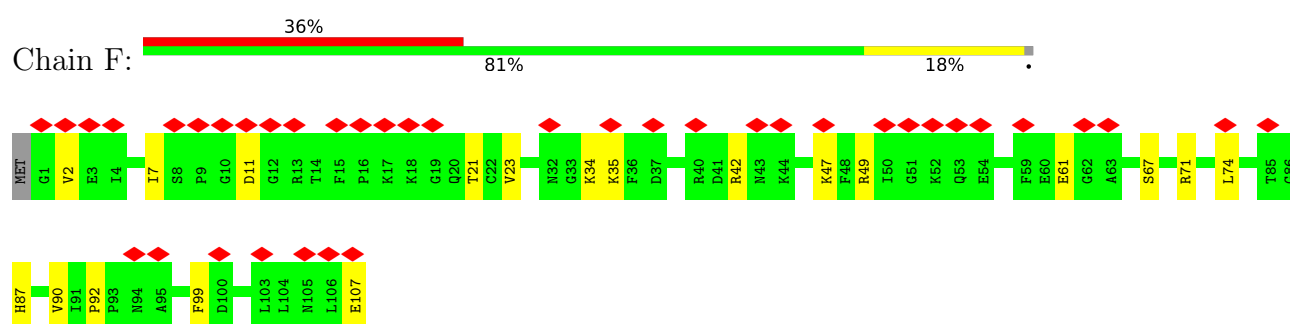
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

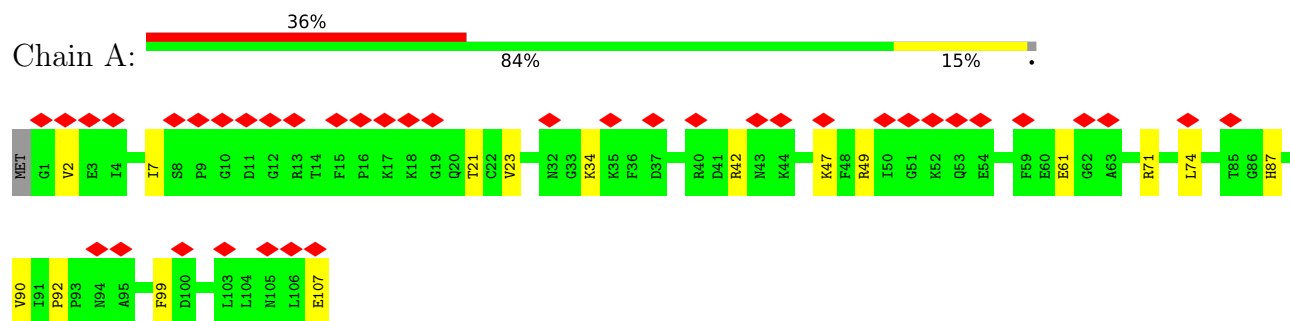
3 Residue-property plots [i](#)

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.

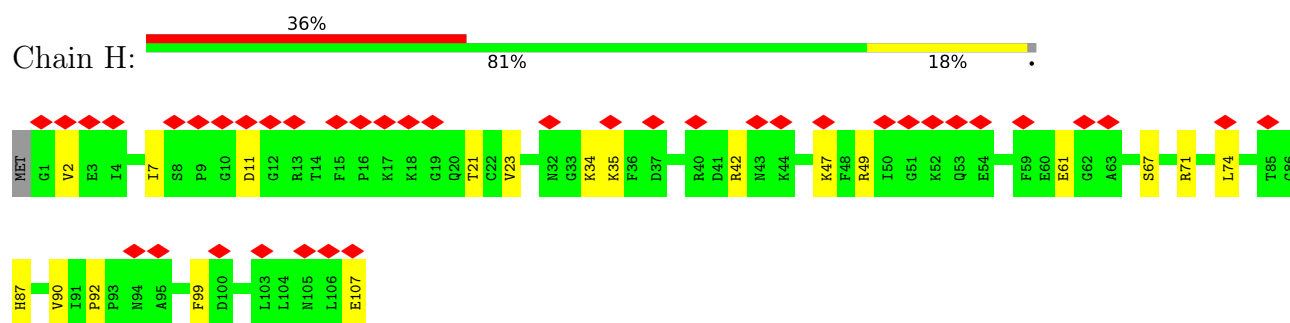
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



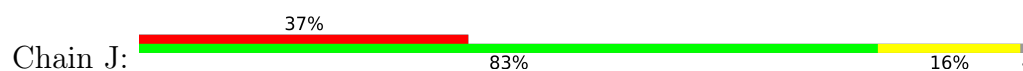
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

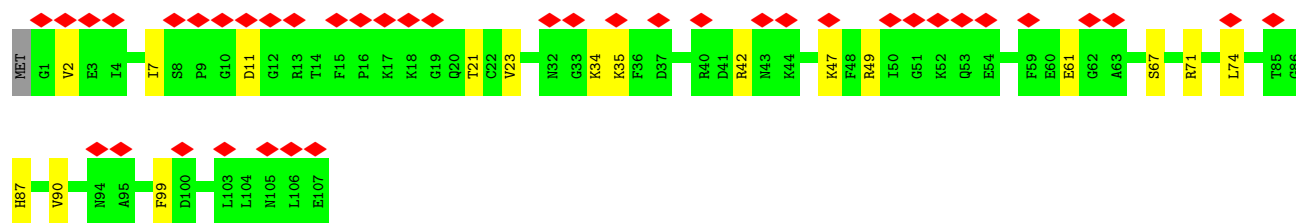


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

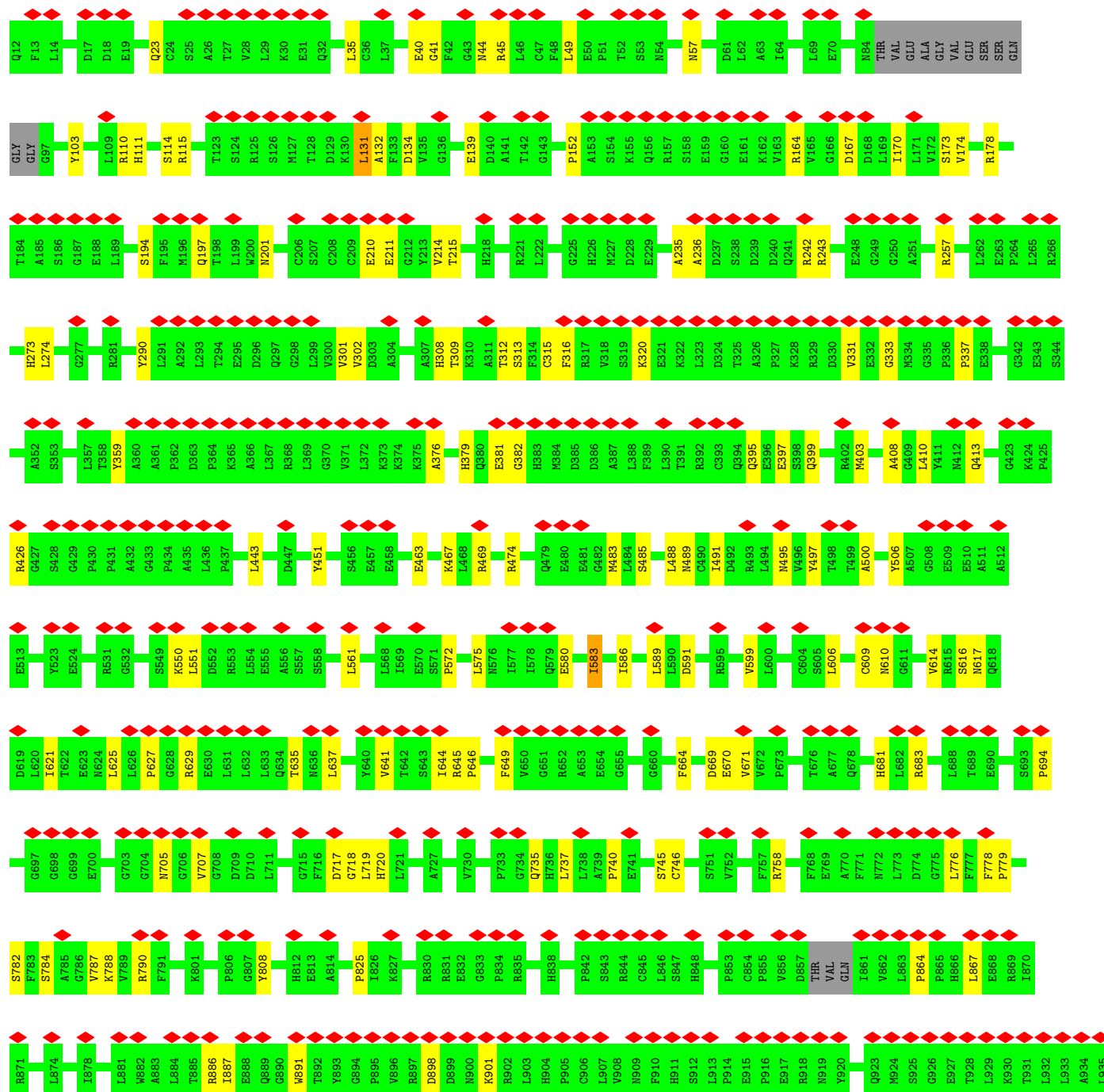
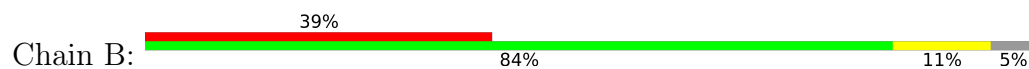


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

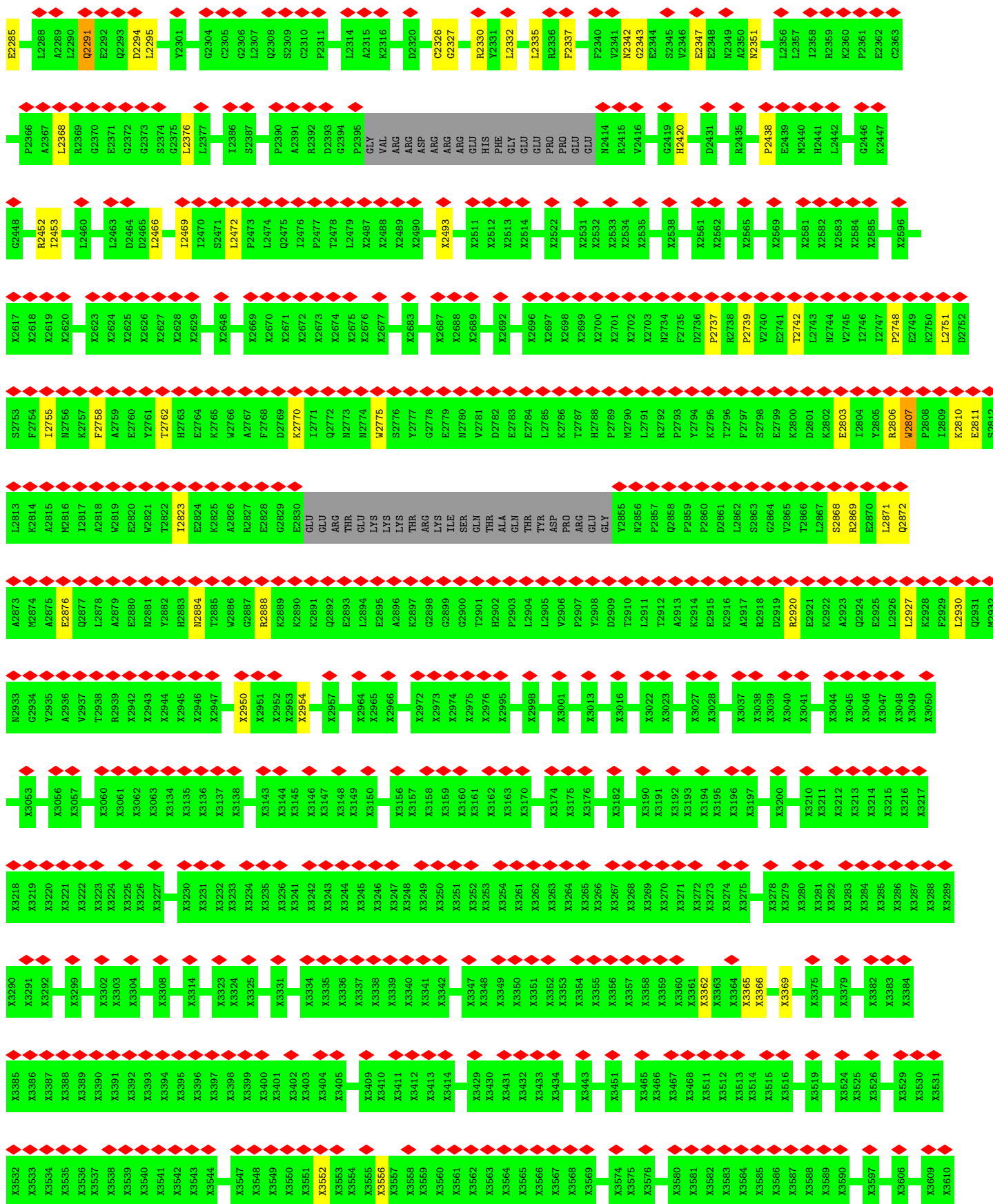




• Molecule 2: Ryanodine receptor 1



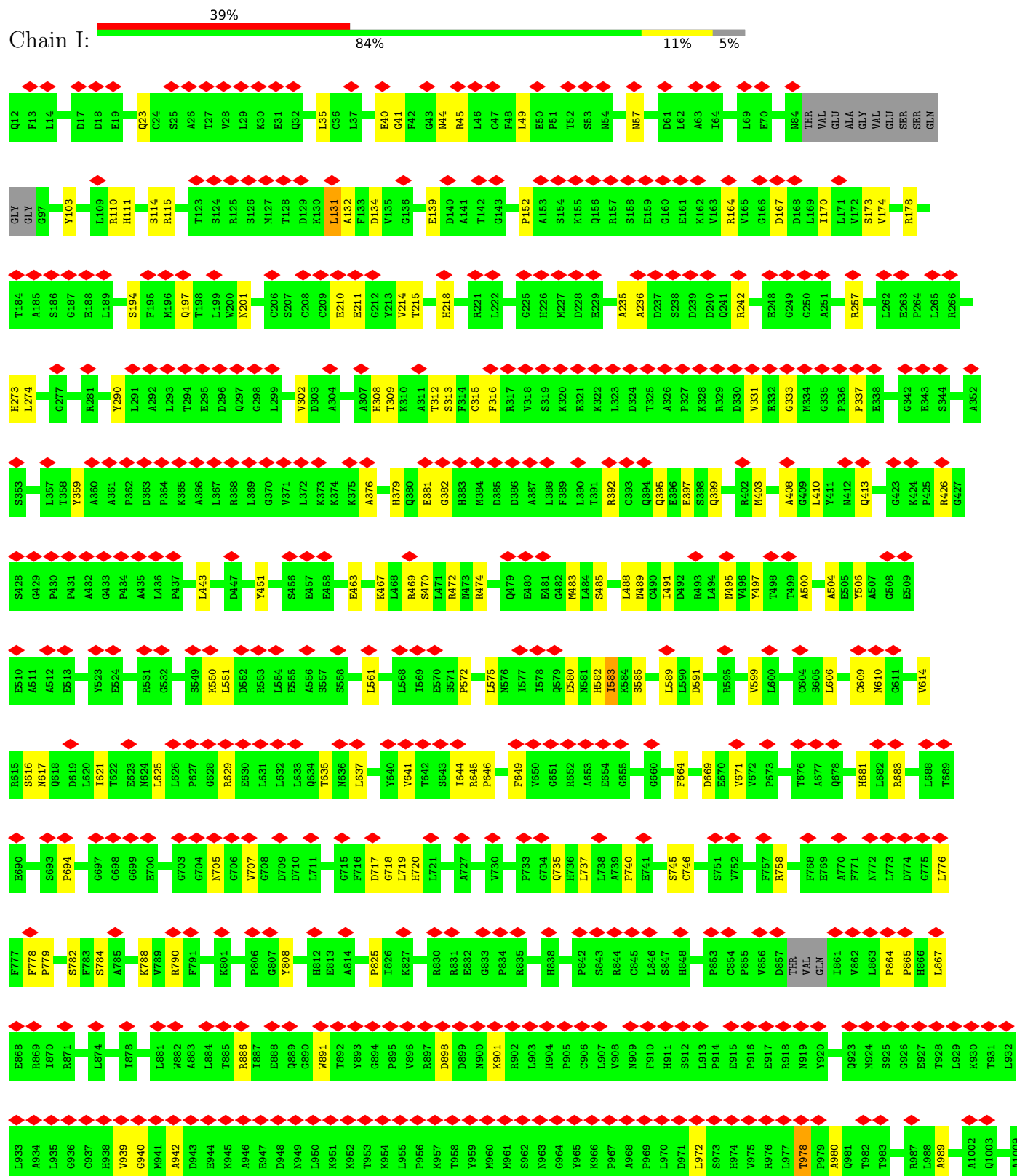


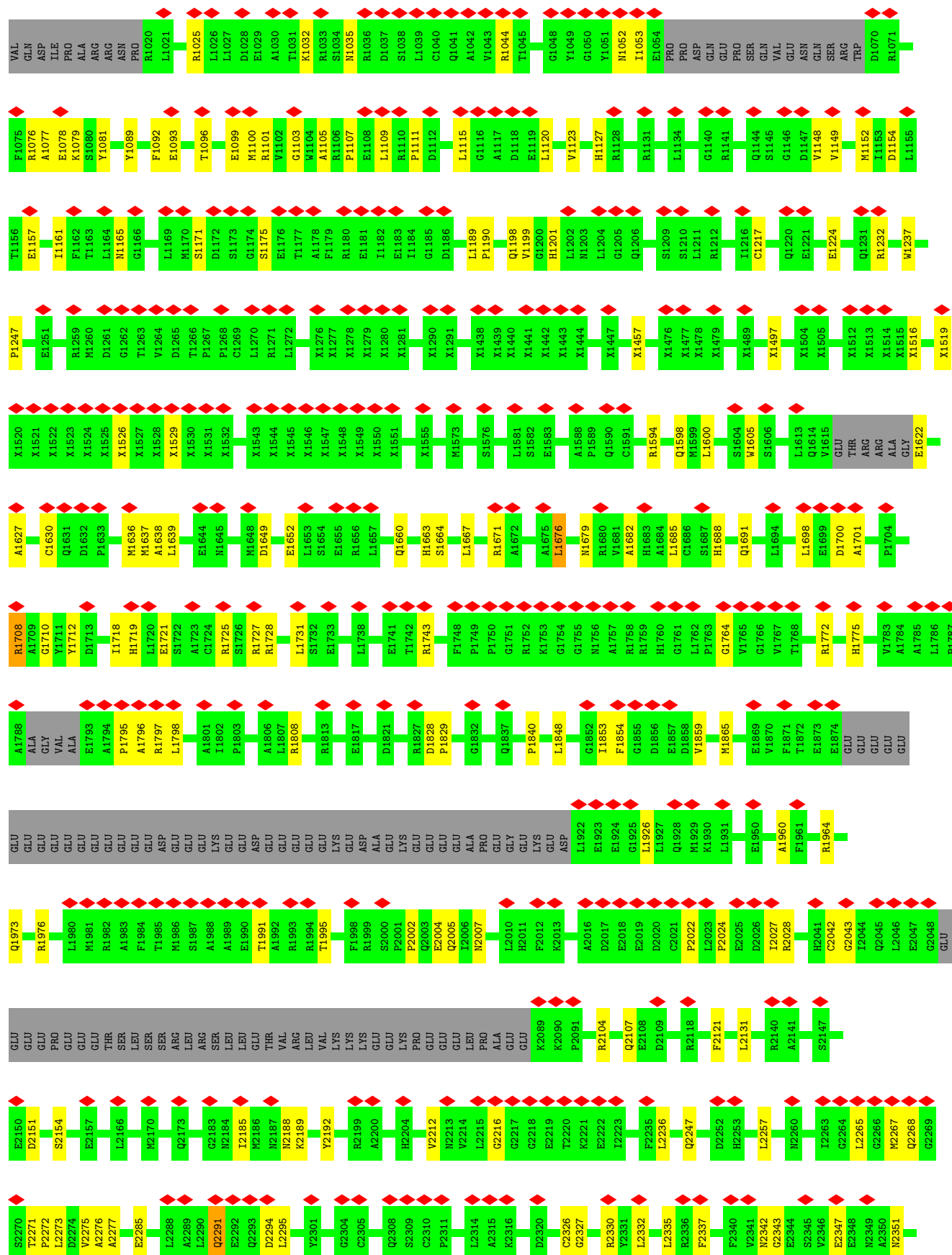




• Molecule 2: Ryanodine receptor 1

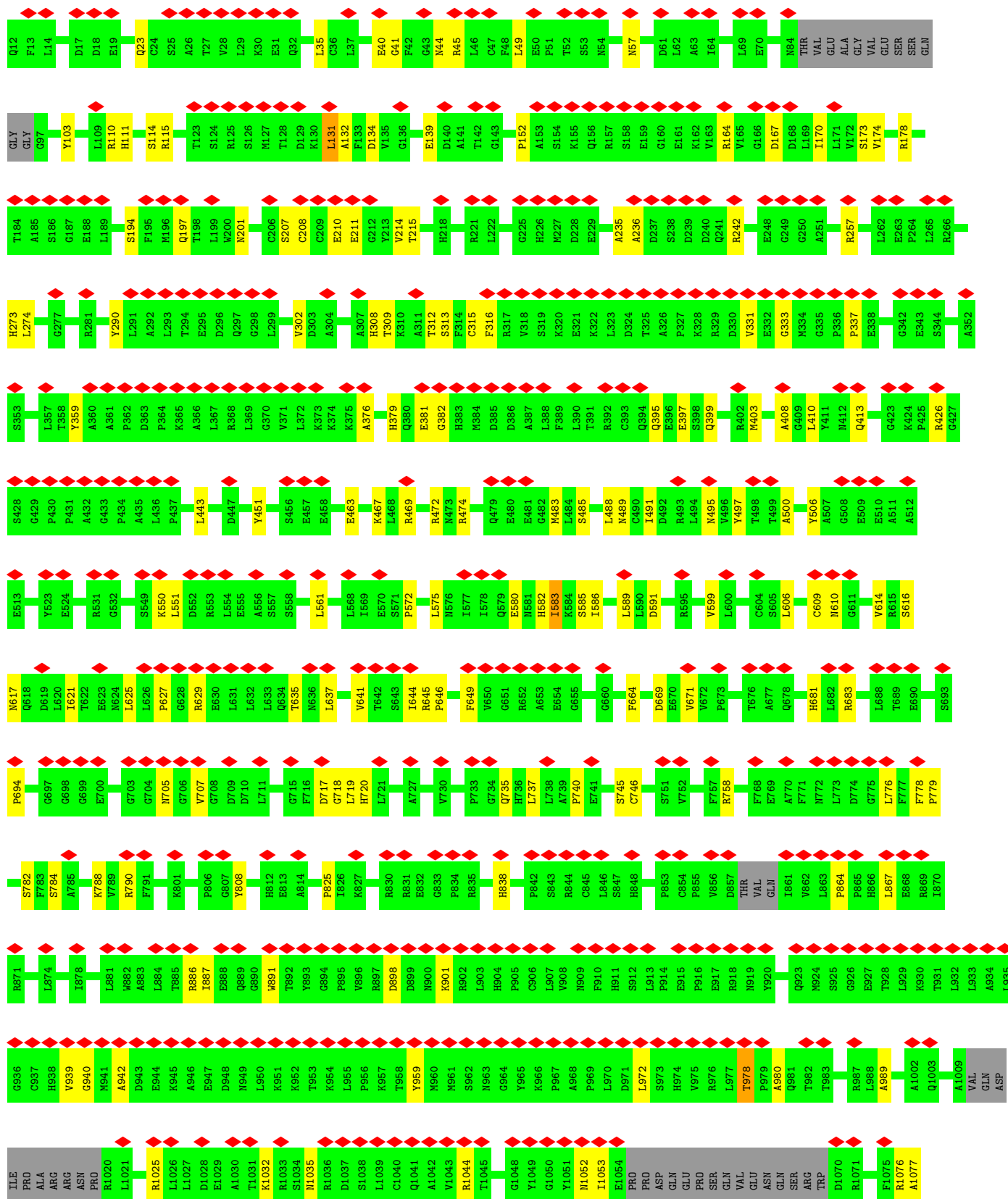
Chain I:





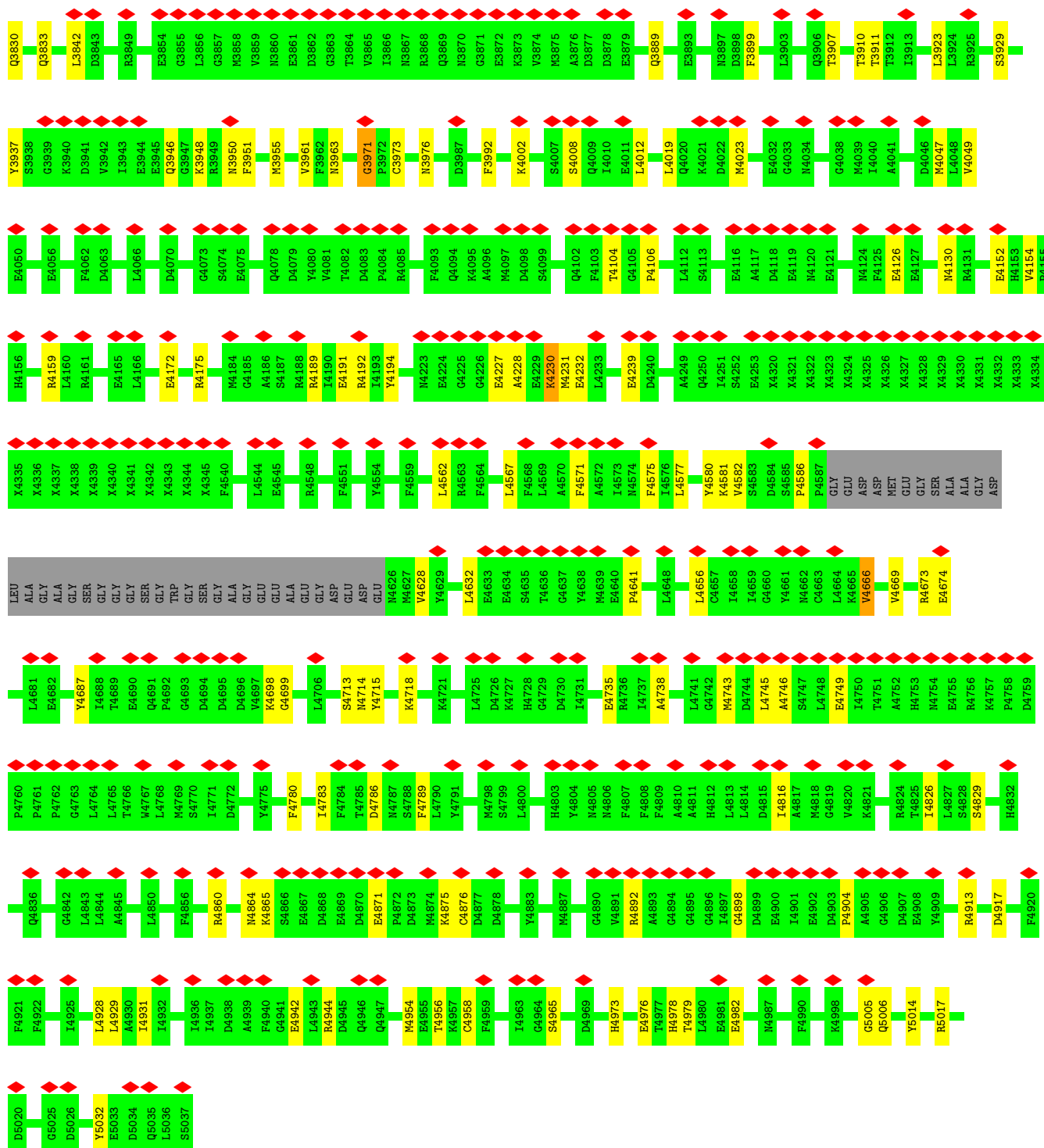
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X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3556	X3557	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3576	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3597					
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X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3302	X3303	X3304	X3308	X3314	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3369	X3372	X3375	X3379			
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X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3174	X3175	X3176	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3210	X3211	X3212	X3213	X3214								
E2925	L2926	L2927	X2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2950	X2951	X2952	X2964	X2965	X2966	X2972	X2973	X2974	X2975	X2976	X2995	X2998	X3001	X3013	X3016	X3022	X3023	X3027	X3028	X3029	X3037	X3038	X3039	X3040	X3041	X3044	X3045										
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Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	GLN	ALA	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	K2860	D2861	L2862	S2863	G2864
V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	E2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	L2766	A2767	D2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	P2793	V2794	K2795	T2796	F2797	E2799	K2800	D2801	L2802	E2803	L2804
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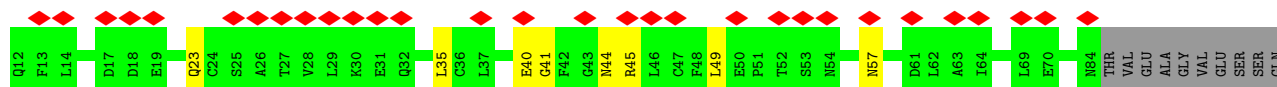


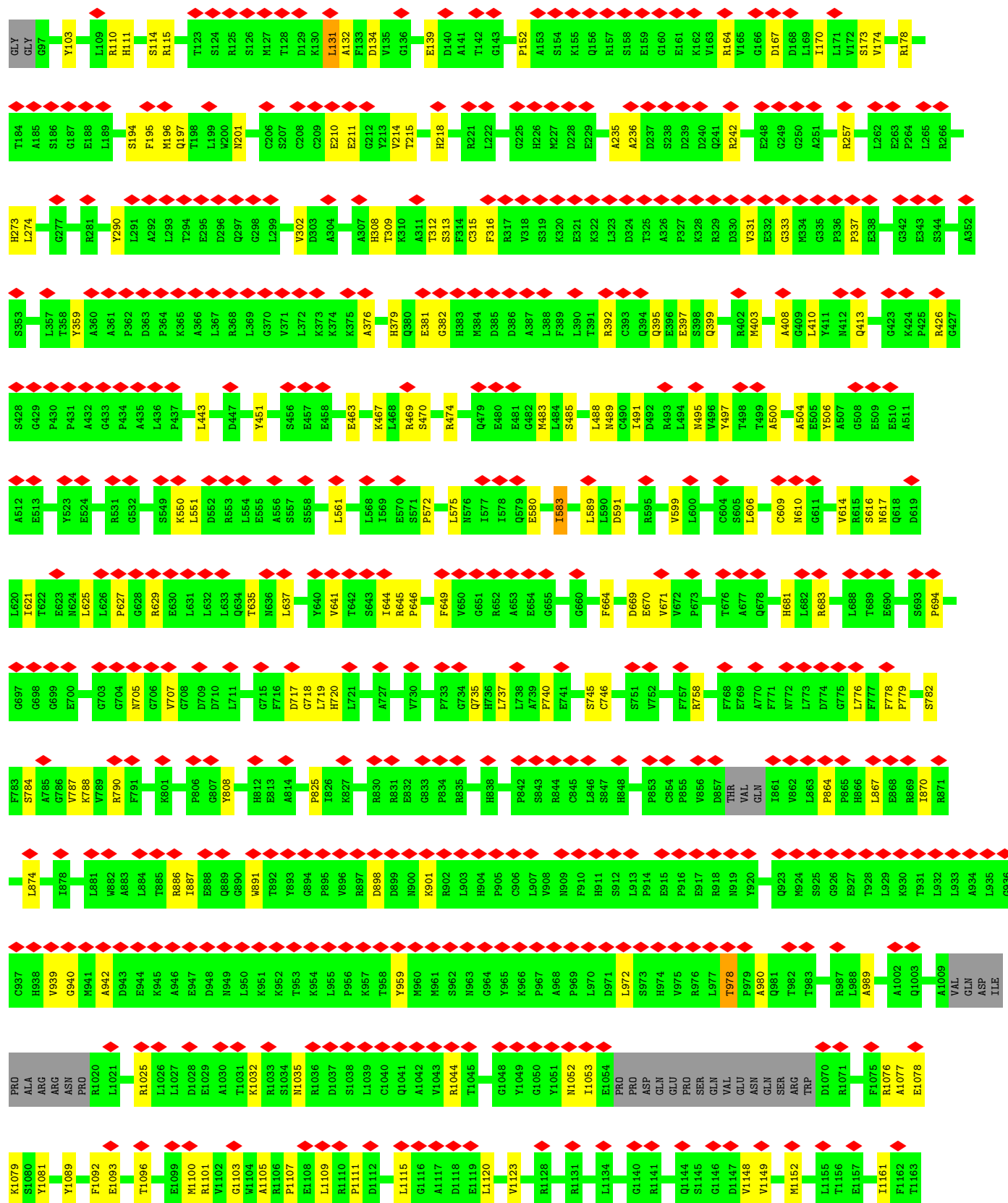
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X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3174	X3175	X3176	X3182	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218									
M2932	N2933	G2934	Y2935	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2950	X2951	X2952	X2957	X2964	X2965	X2966	X2972	X2973	X2974	X2975	X2976	X2995	X2998	X3001	X3013	X3016	X3022	X3023	X3027	X3028	X3037	X3038	X3039	X3040	X3041	X3044	X3045	X3046	X3047	X3048	X3049	X3050														
Q2872	A2873	G2874	M2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931
S2812	L2813	K2814	A2815	M2816	L2817	A2818	N2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	H2902	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	
D2752	S2753	F2754	L2755	N2756	K2757	P2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	D2792	P2793	Y2794	K2795	L2796	F2797	S2798	E2799	D2800	K2801	K2802	E2803	L2804	Y2805	L2806	W2807	P2808	L2809	K2810	E2811
X2617	X2618	X2619	X2620	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2648	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2683	X2687	X2688	X2689	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	L2751									
K2447	G2448	R2452	L2453	L2460	L2463	D2464	L2466	L2469	L2470	S2471	L2472	F2473	L2474	Q2475	L2476	F2477	L2478	L2479	X2487	L2488	X2489	X2490	X2493	X2511	X2512	X2513	X2514	X2522	X2531	X2532	X2533	X2534	X2535	X2538	X2561	X2562	X2565	X2569	X2581	X2582	X2583	X2584	X2585	X2596															



• Molecule 2: Ryanodine receptor 1

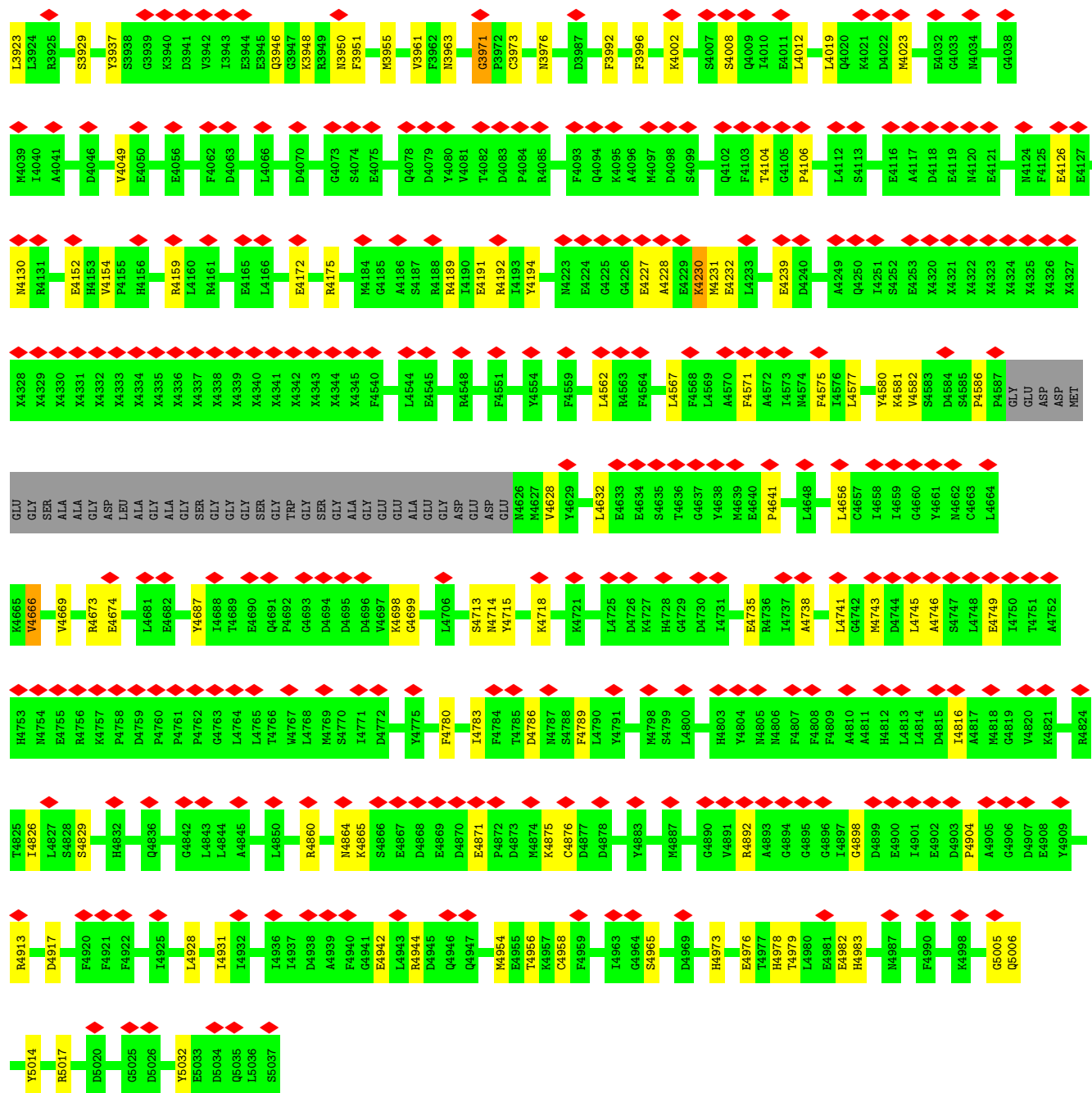
Chain G: 39% 84% 11% 5%







D3822	K3823	K3824	G3827	Q3830	Q3833	L3842	D3843	R3849	E3854	G3855	L3856	G3857	K3858	V3859	N3860	D3862	G3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870	G3871	E3872	K3873	V3874	K3875	D3877	D3878	E3879	Q3889	E3893	N3897	F3899	L3903	Q3906	T3907	T3910	T3912	T3913																
S3732	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	M3758	R3762	S3766	R3769	L3770	H3771	T3772	R3773	V3779	L3780	Q3781	M3782	I3783	S3784	G3788	E3789	T3790	L3798	L3805	N3806	G3807	G3808	N3809	L3817	K3821									
F3653	K3658	W3661	L3662	L3663	T3664	E3665	D3666	H3667	S3668	F3669	R3672	M3673	L3674	D3675	D3676	K3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	V3689	E3690	E3691	E3692	K3693	D3696	Q3700	R3707	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	V3720	Y3722	M3723	A3724	V3725	L3728	M3729										
X3539	X3540	X3541	X3542	X3543	X3544	X3547	X3548	X3549	X3550	X3551	X3552	X3553	X3554	X3555	X3558	X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3574	X3575	X3576	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3597	X3606	X3609	X3610	X3611	X3612	X3613	L3641	V3642	N3643	L3644							
X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3409	X3410	X3411	X3412	X3413	X3414	X3429	X3430	X3431	X3432	X3433	X3434	X3443	X3451	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3519	X3524	X3525	X3526	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538							
X3303	X3304	X3308	X3314	X3323	X3324	X3325	X3331	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3369	X3375	X3379	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391									
X3225	X3226	X3227	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3299	X3302			
X3061	X3062	X3134	X3135	X3136	X3137	X3138	X3143	X3144	X3145	X3146	X3147	X3148	X3149	X3150	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3174	X3175	X3176	X3182	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3200	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224							
R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2950	X2951	X2952	X2957	X2964	X2965	X2966	X2972	X2973	X2974	X2975	X2976	X2995	X2998	X3001	X3013	X3016	X3022	X3023	X3027	X3028	X3029	X3037	X3038	X3039	X3040	X3041	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3060														
A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	K2888	K2889	K2890	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938		
W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	K2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	LYS	LYS	LYS	THR	ARG	THR	LYS	THR	ALA	GLN	THR	E2783	E2784	L2785	K2786	P2787	H2788	P2789	M2790	K2792	P2793	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	L2866	S2867	R2869	E2870	L2871	Q2872	A2873	K2874	A2875	E2876	Q2877	L2878	
A2769	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	P2787	H2788	P2789	M2790	K2792	P2793	P2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	K2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818
X2624	X2625	X2626	X2627	X2628	X2629	X2648	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2683	X2687	X2688	X2689	X2692	X2696	X2697	X2698	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	P2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/834	0.44	0/1123
1	F	0.20	0/834	0.44	0/1123
1	H	0.20	0/834	0.44	0/1123
1	J	0.20	0/834	0.44	0/1123
2	B	0.20	0/25428	0.51	4/34534 (0.0%)
2	E	0.20	0/25428	0.51	4/34534 (0.0%)
2	G	0.20	0/25428	0.51	4/34534 (0.0%)
2	I	0.20	0/25428	0.51	4/34534 (0.0%)
All	All	0.20	0/105048	0.51	16/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

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(°)
2	B	2807	TRP	CA-C-N	-8.18	111.62	120.94
2	B	2807	TRP	C-N-CA	-8.18	111.62	120.94
2	I	2807	TRP	CA-C-N	-8.17	111.63	120.94
2	I	2807	TRP	C-N-CA	-8.17	111.63	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2807	TRP	CA-C-N	-8.17	111.63	120.94

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide

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	818	0	824	10	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	10	0
2	B	29499	0	24741	266	0
2	E	29499	0	24741	264	0
2	G	29499	0	24741	266	0
2	I	29499	0	24741	264	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102348	1073	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 5.

The worst 5 of 1073 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)
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.65
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.30	0.65
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.65

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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	304 (9%)	2 (0%)	48	83
2	E	3235/4416 (73%)	2931 (91%)	302 (9%)	2 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
2	I	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	48	83
All	All	13360/18096 (74%)	12093 (90%)	1259 (9%)	8 (0%)	49	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	4641	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2484 (100%)	9 (0%)	84	83
2	E	2493/3022 (82%)	2484 (100%)	9 (0%)	84	83
2	G	2493/3022 (82%)	2484 (100%)	9 (0%)	84	83
2	I	2493/3022 (82%)	2484 (100%)	9 (0%)	84	83
All	All	10324/12444 (83%)	10288 (100%)	36 (0%)	84	84

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	583	ILE
2	G	4230	LYS
2	G	978	THR
2	G	3663	LEU
2	I	1600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4691	GLN

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Mol	Chain	Res	Type
2	G	4054	ASN
2	E	1688	HIS
2	G	4034	ASN
2	G	1861	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	B	5101	-	32,33,33	1.39	7 (21%)	48,52,52	1.78	9 (18%)
4	CFF	E	5102	-	15,15,15	1.83	5 (33%)	23,23,23	2.81	9 (39%)
3	ATP	G	5101	-	32,33,33	1.39	7 (21%)	48,52,52	1.78	9 (18%)
4	CFF	I	5102	-	15,15,15	1.83	5 (33%)	23,23,23	2.82	9 (39%)
3	ATP	E	5101	-	32,33,33	1.39	7 (21%)	48,52,52	1.78	9 (18%)
4	CFF	G	5102	-	15,15,15	1.83	5 (33%)	23,23,23	2.83	9 (39%)
3	ATP	I	5101	-	32,33,33	1.39	7 (21%)	48,52,52	1.78	9 (18%)
4	CFF	B	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.83	9 (39%)

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	B	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.36	1.46	1.39
3	I	5101	ATP	C5-C4	4.33	1.46	1.39
3	G	5101	ATP	C5-C4	4.31	1.46	1.39
3	E	5101	ATP	C5-C4	4.30	1.46	1.39
4	B	5102	CFF	C6-N1	-3.75	1.32	1.40

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.83	111.63	126.28
4	G	5102	CFF	C14-N7-C8	-7.81	111.67	126.28
4	E	5102	CFF	C14-N7-C8	-7.79	111.70	126.28
4	I	5102	CFF	C14-N7-C8	-7.78	111.72	126.28
3	E	5101	ATP	C5-C4-N3	-5.82	118.70	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

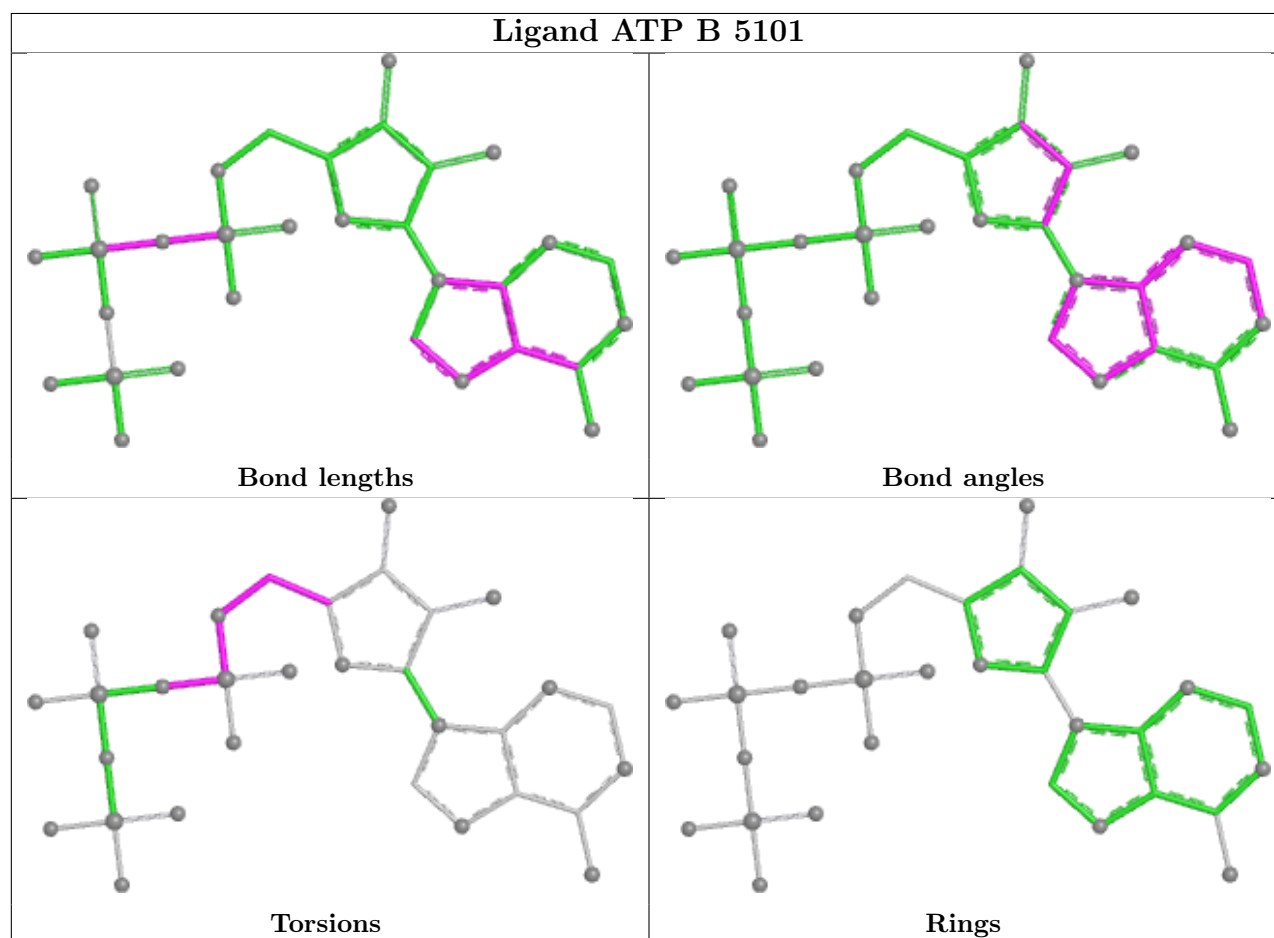
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

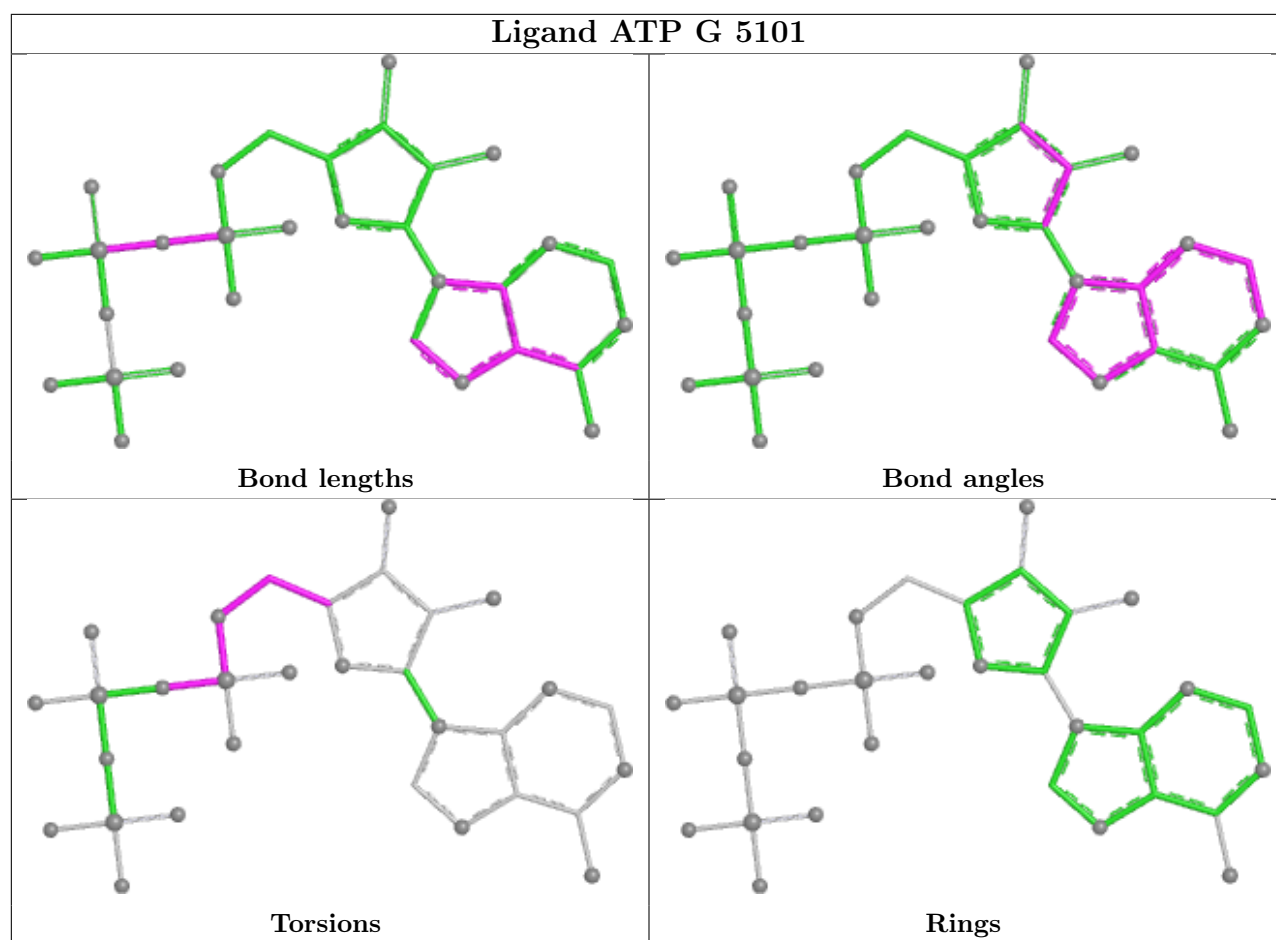
There are no ring outliers.

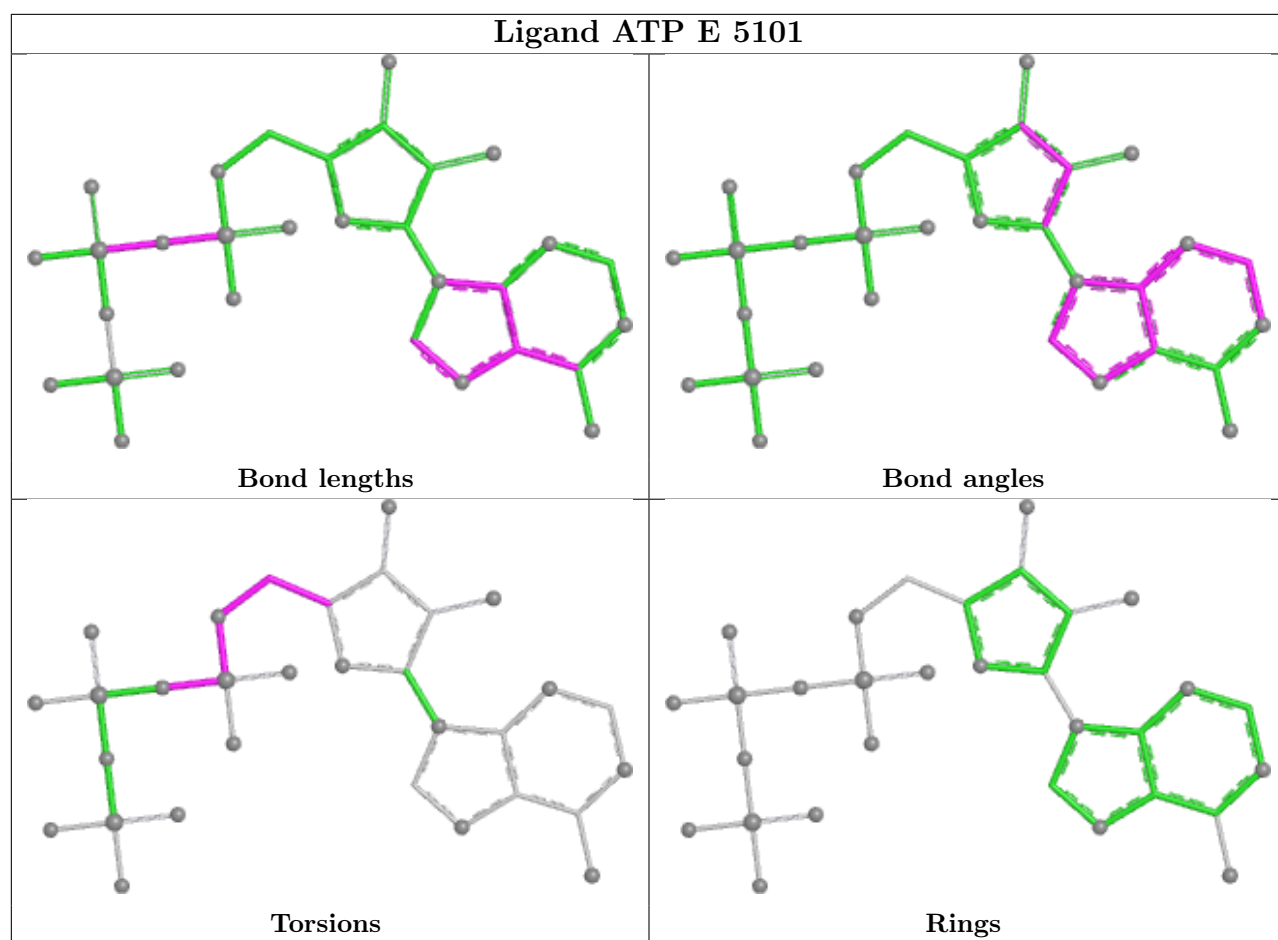
4 monomers are involved in 8 short contacts:

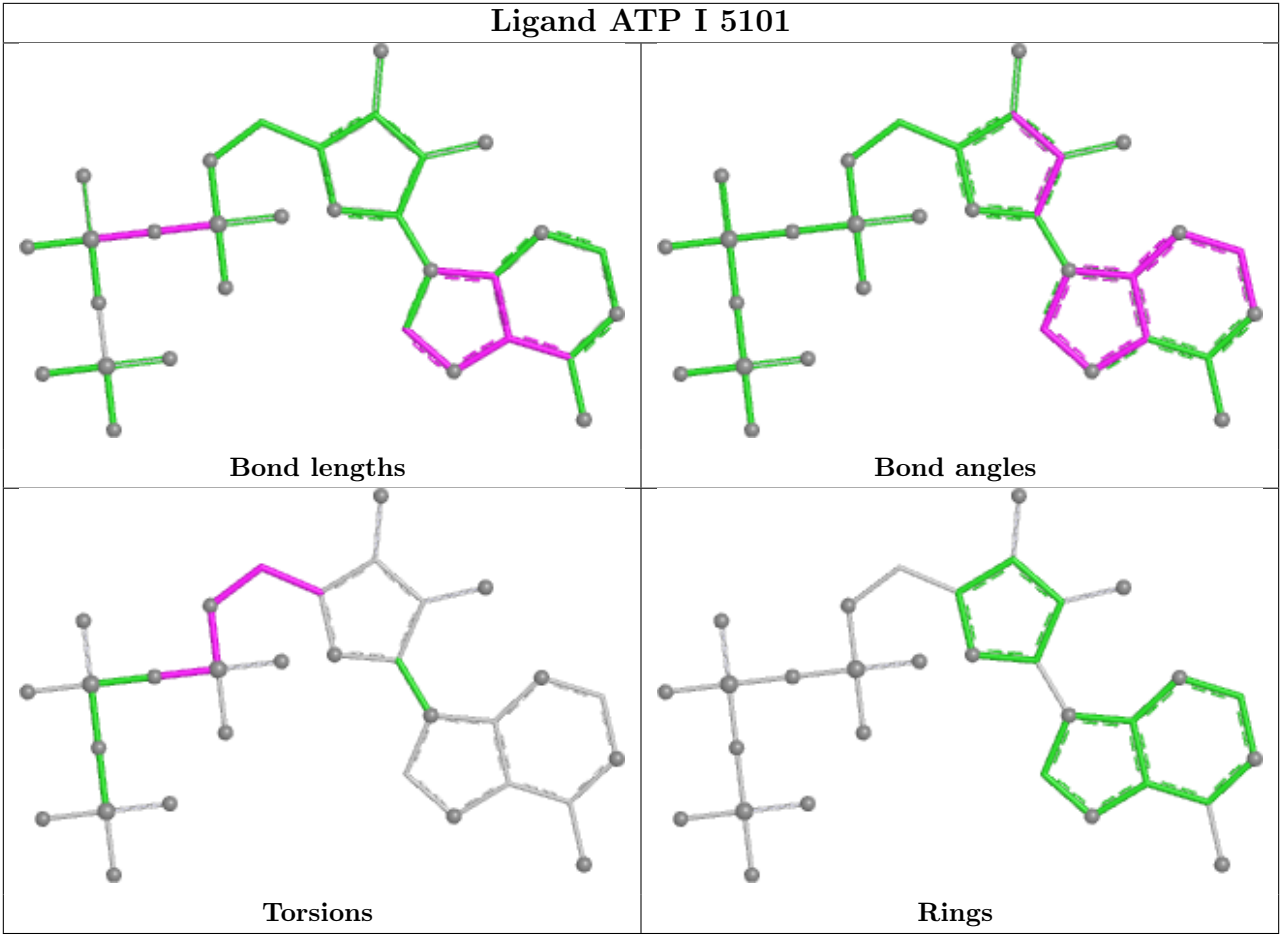
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	2	0
3	G	5101	ATP	2	0
3	E	5101	ATP	2	0
3	I	5101	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.23
1	E	4345:UNK	C	4540:PHE	N	74.23

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Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.22
1	G	4345:UNK	C	4540:PHE	N	74.22
1	I	3613:UNK	C	3639:THR	N	43.91

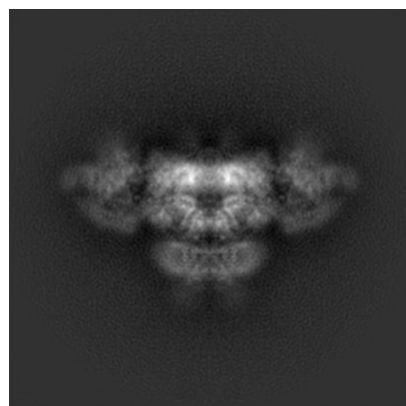
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8384. These allow visual inspection of the internal detail of the map and identification of artifacts.

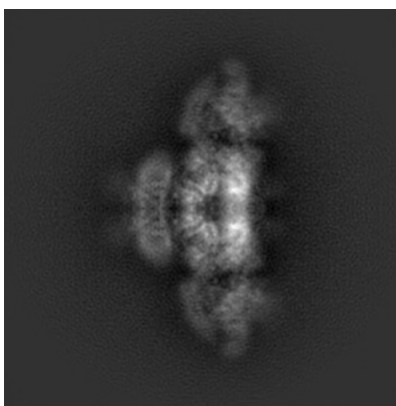
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

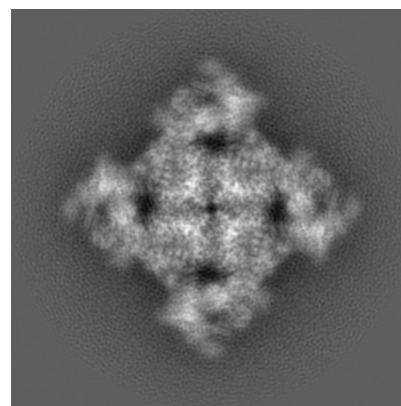
6.1.1 Primary map



X

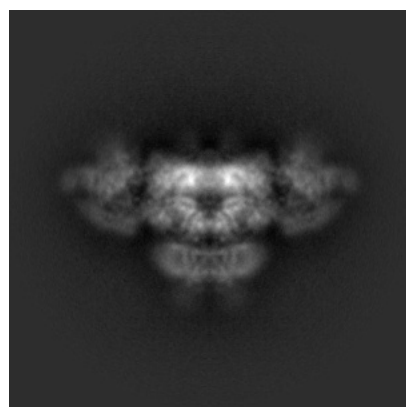


Y

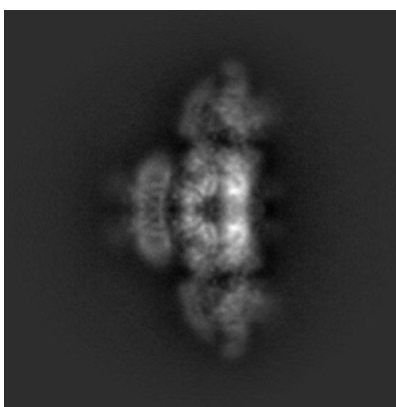


Z

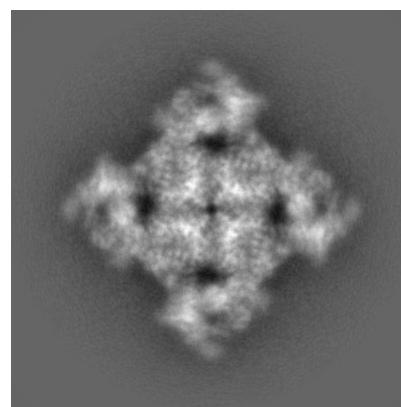
6.1.2 Raw map



X



Y

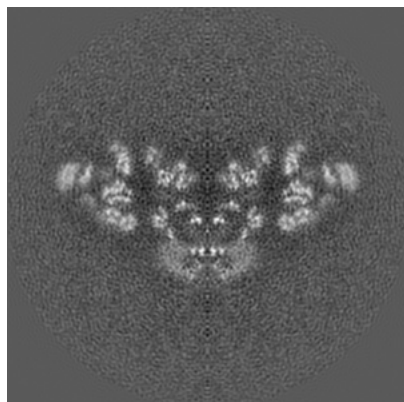


Z

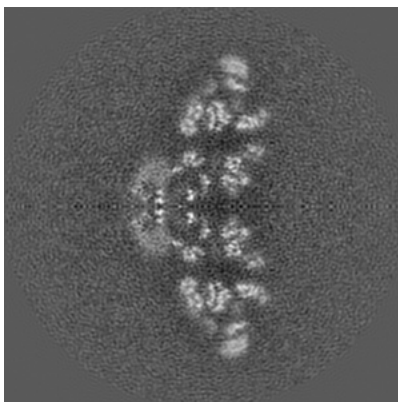
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

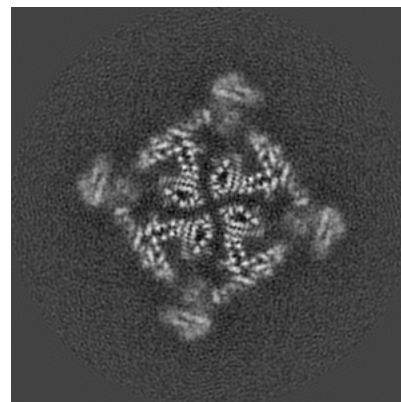
6.2.1 Primary map



X Index: 200

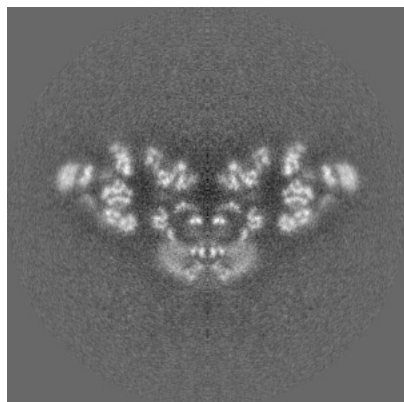


Y Index: 200

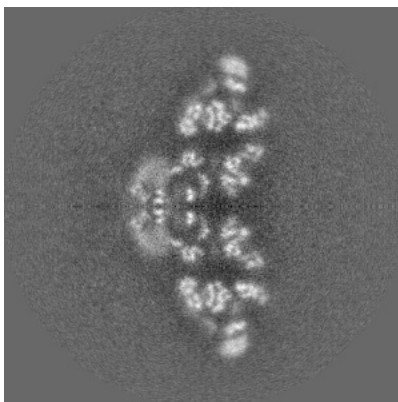


Z Index: 200

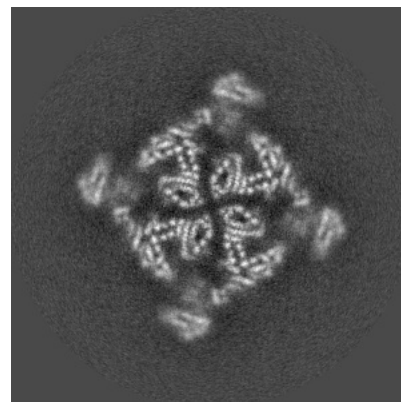
6.2.2 Raw map



X Index: 200



Y Index: 200

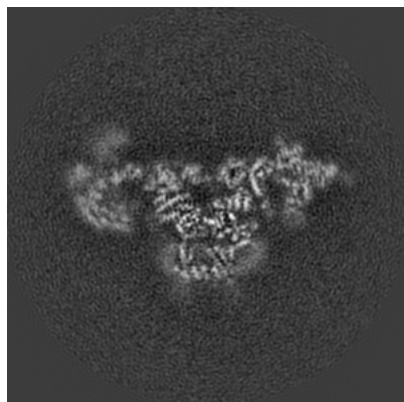


Z Index: 200

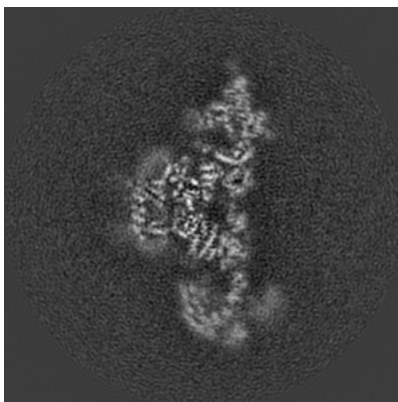
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

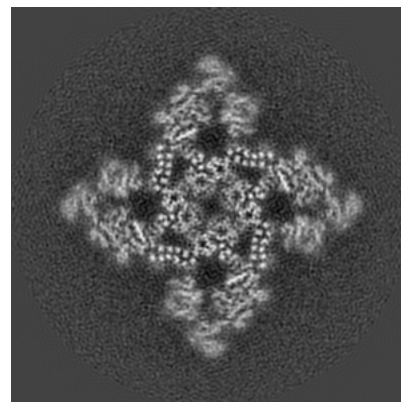
6.3.1 Primary map



X Index: 184

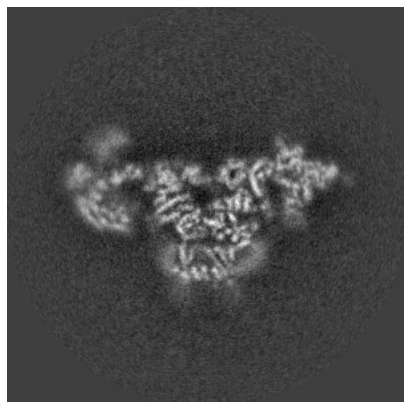


Y Index: 216

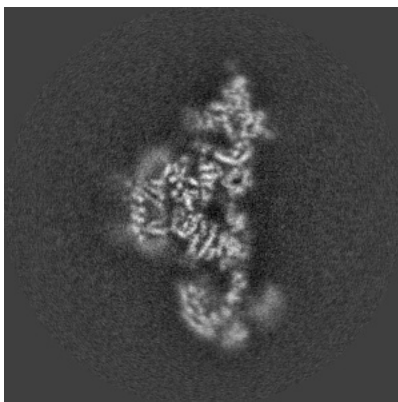


Z Index: 227

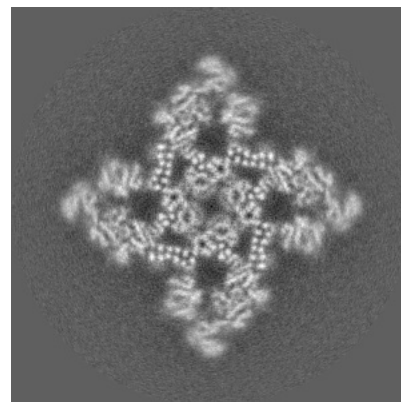
6.3.2 Raw map



X Index: 184



Y Index: 216

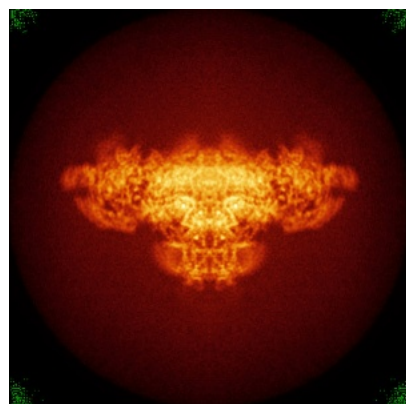


Z Index: 227

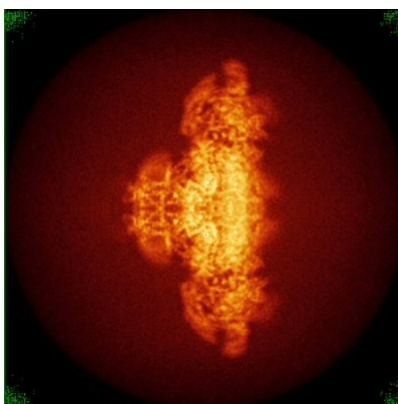
The images above show the largest variance slices of the map in three orthogonal directions.

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

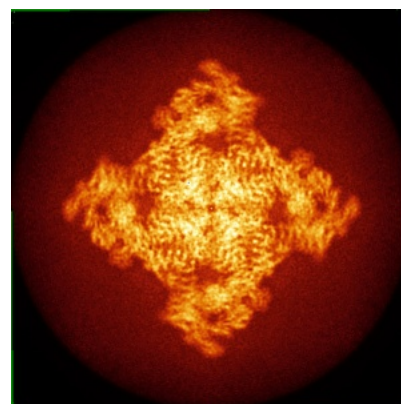
6.4.1 Primary map



X

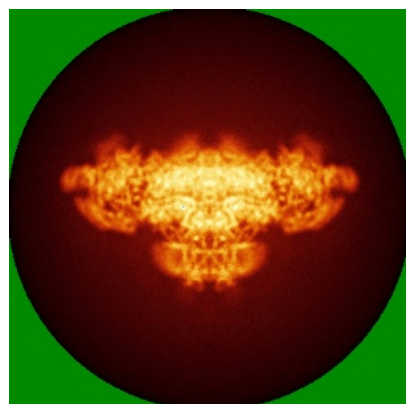


Y

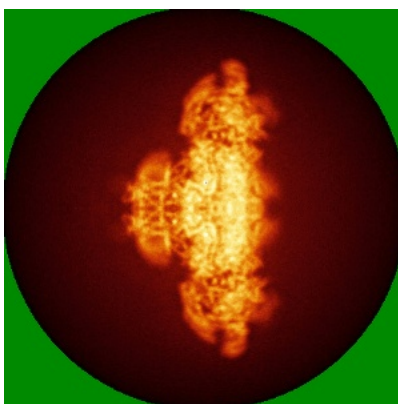


Z

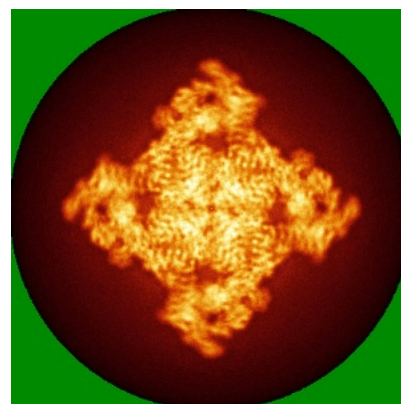
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

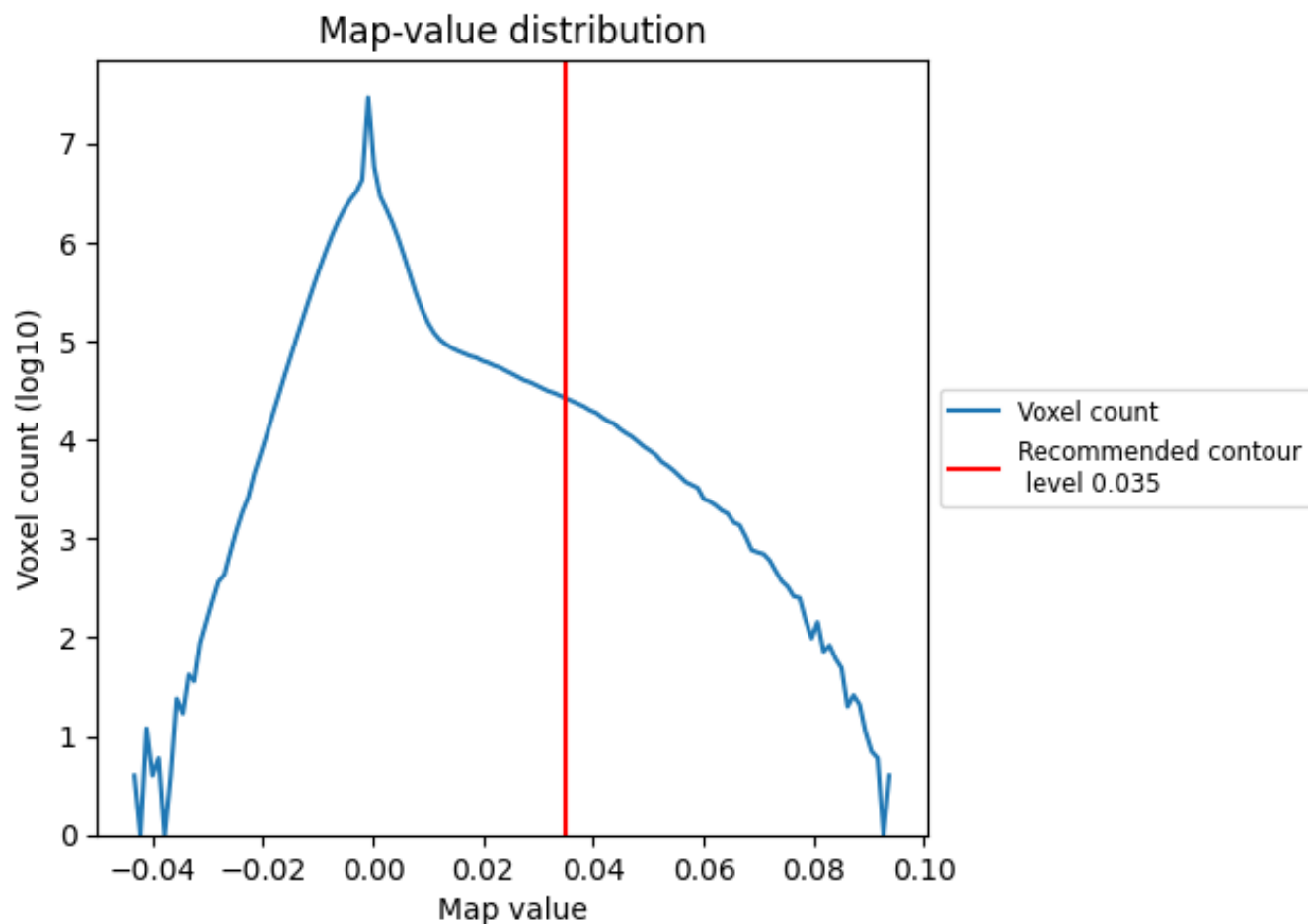
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

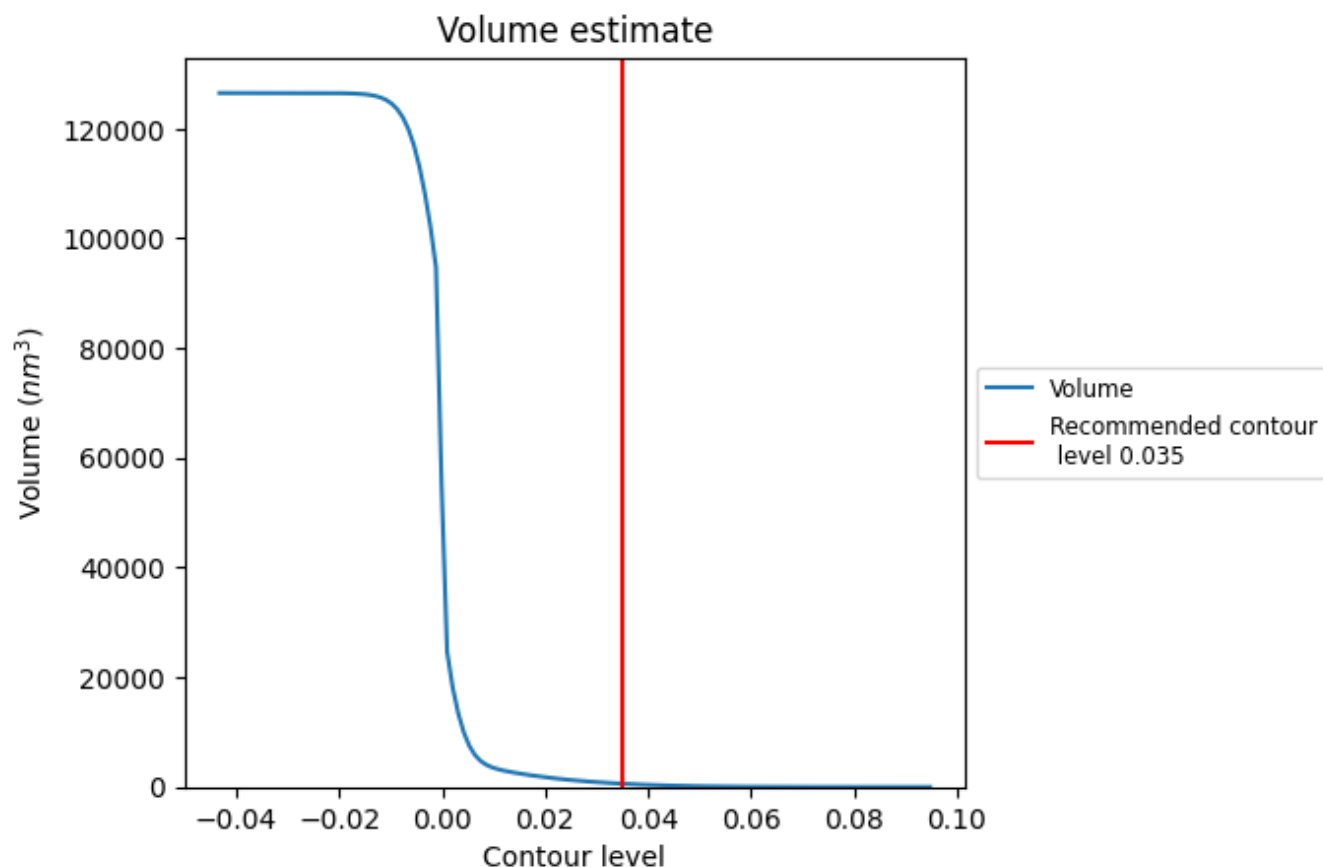
This section contains the results of statistical analysis of the map.

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.

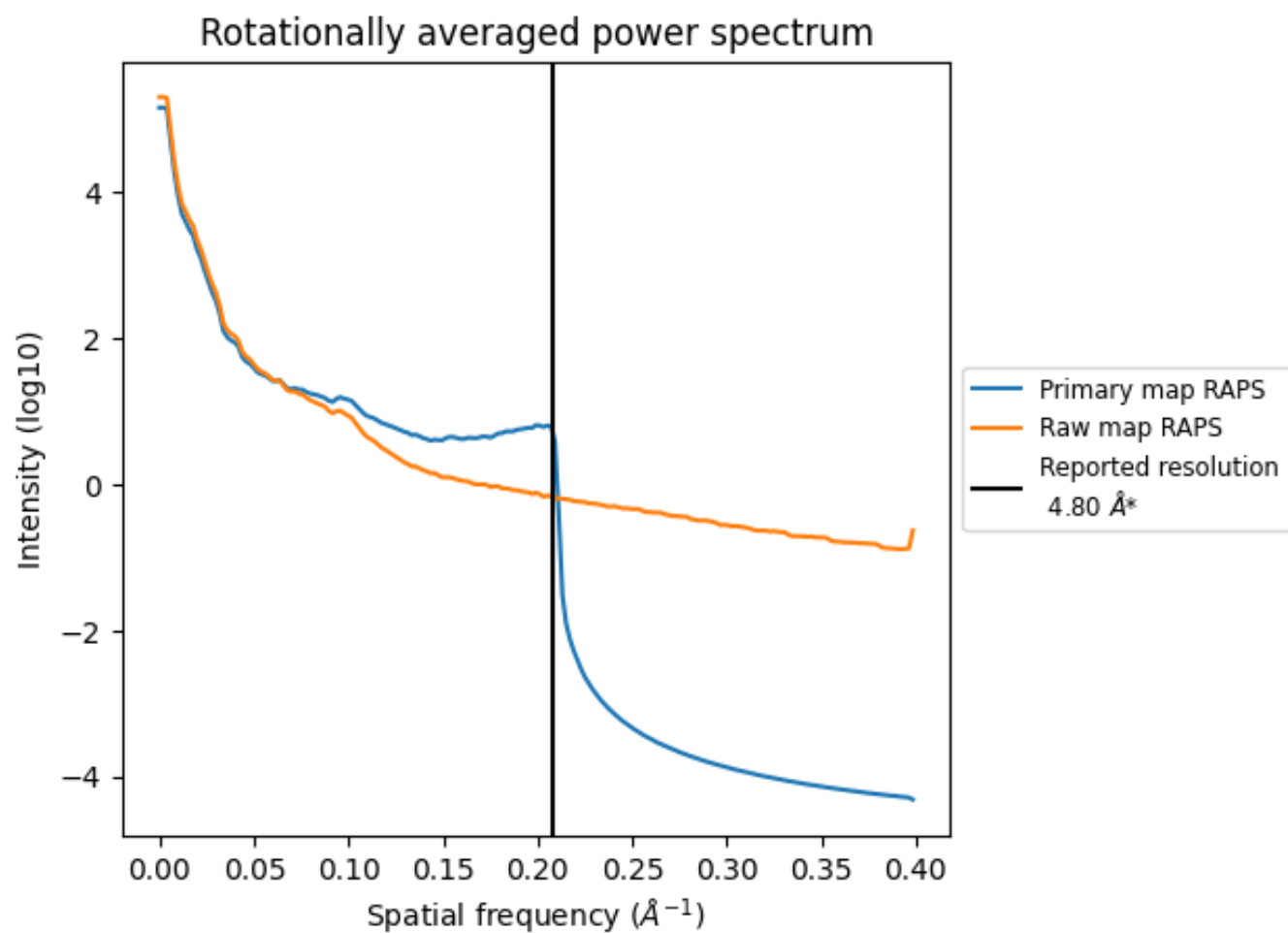
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm^3 ; this corresponds to an approximate mass of 539 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 ⓘ

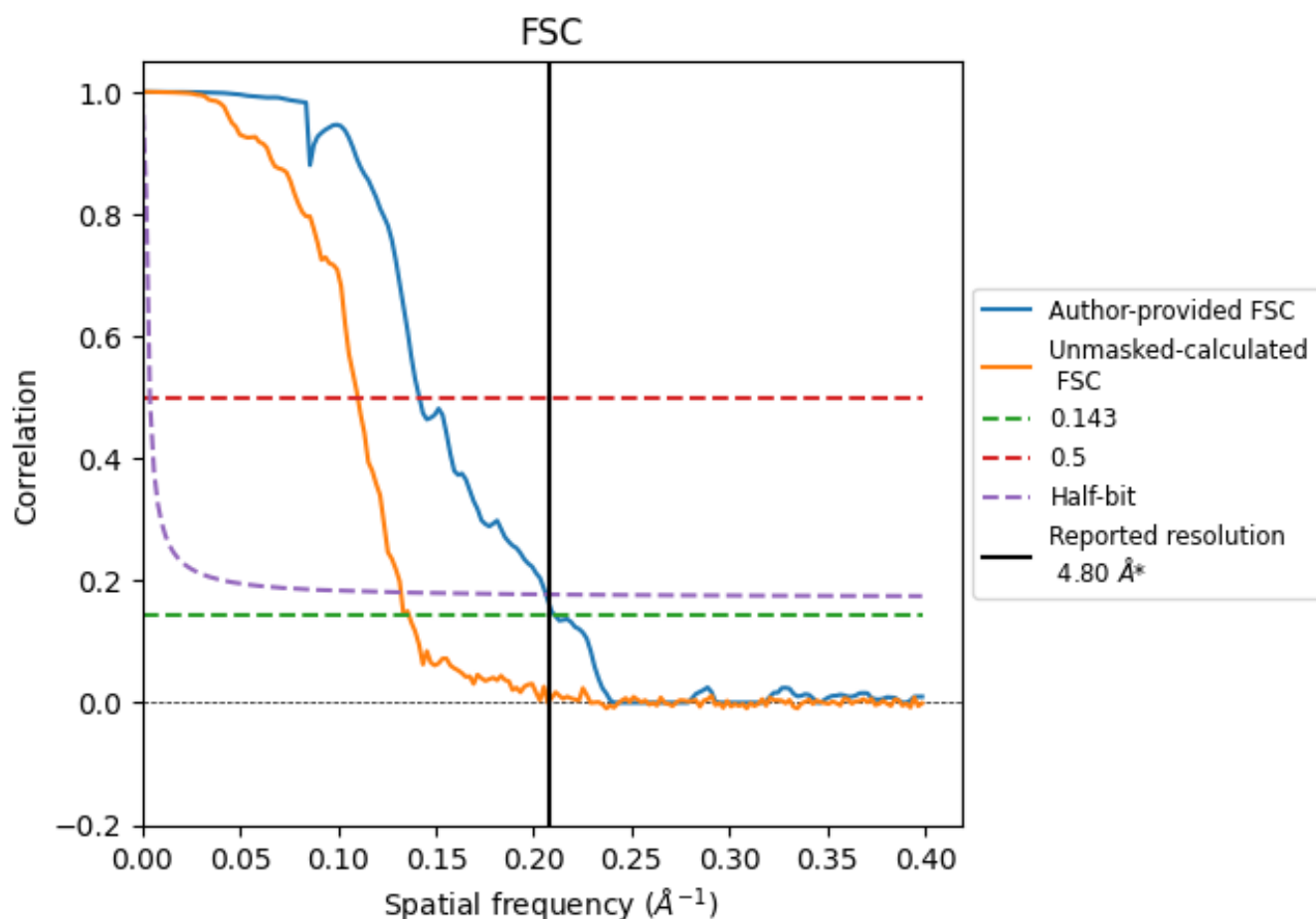


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 $0.208 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

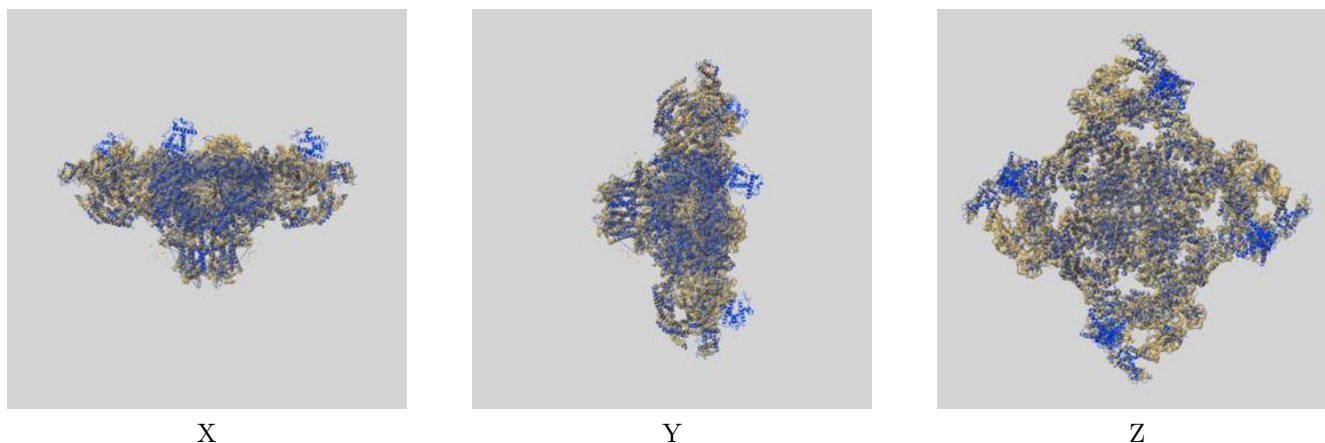
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.07	4.85
Unmasked-calculated*	7.34	9.09	7.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

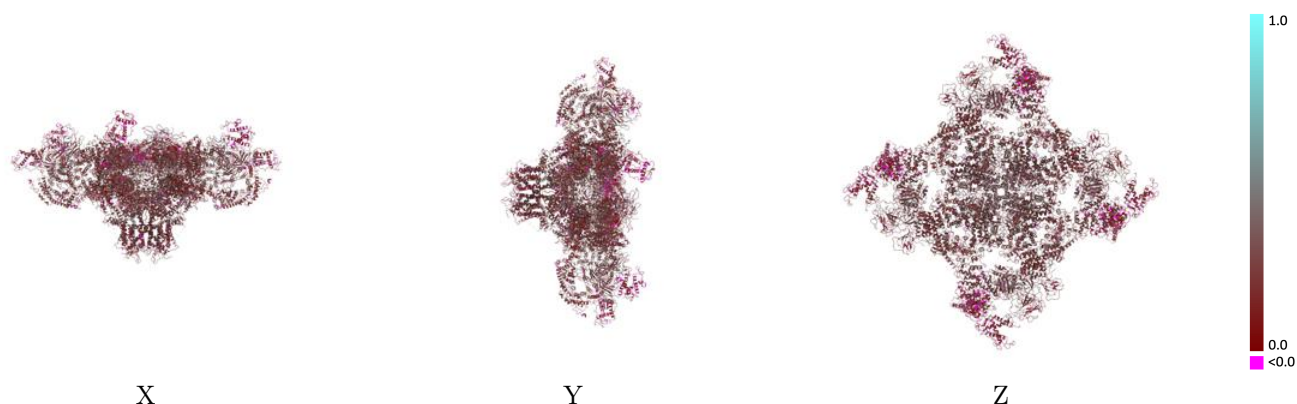
This section contains information regarding the fit between EMDB map EMD-8384 and PDB model 5TAT. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



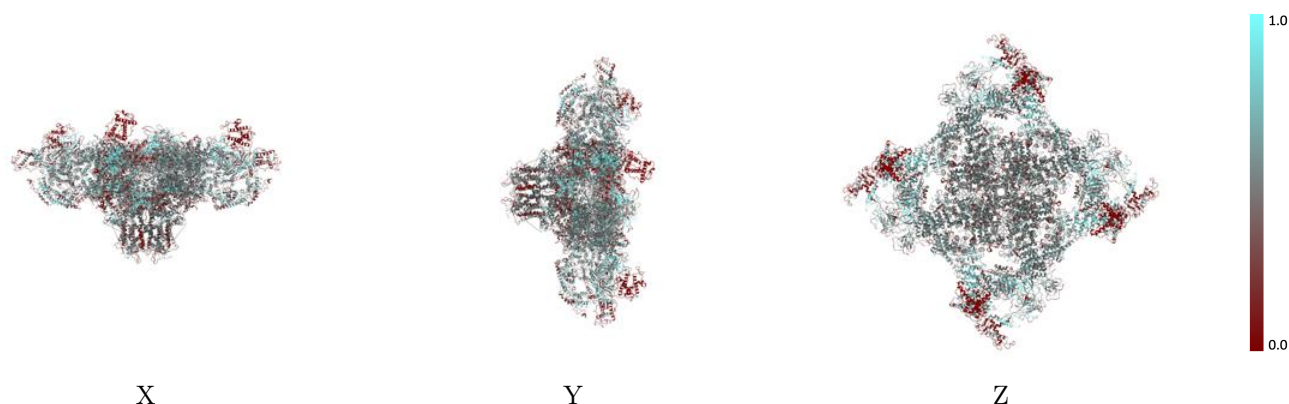
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



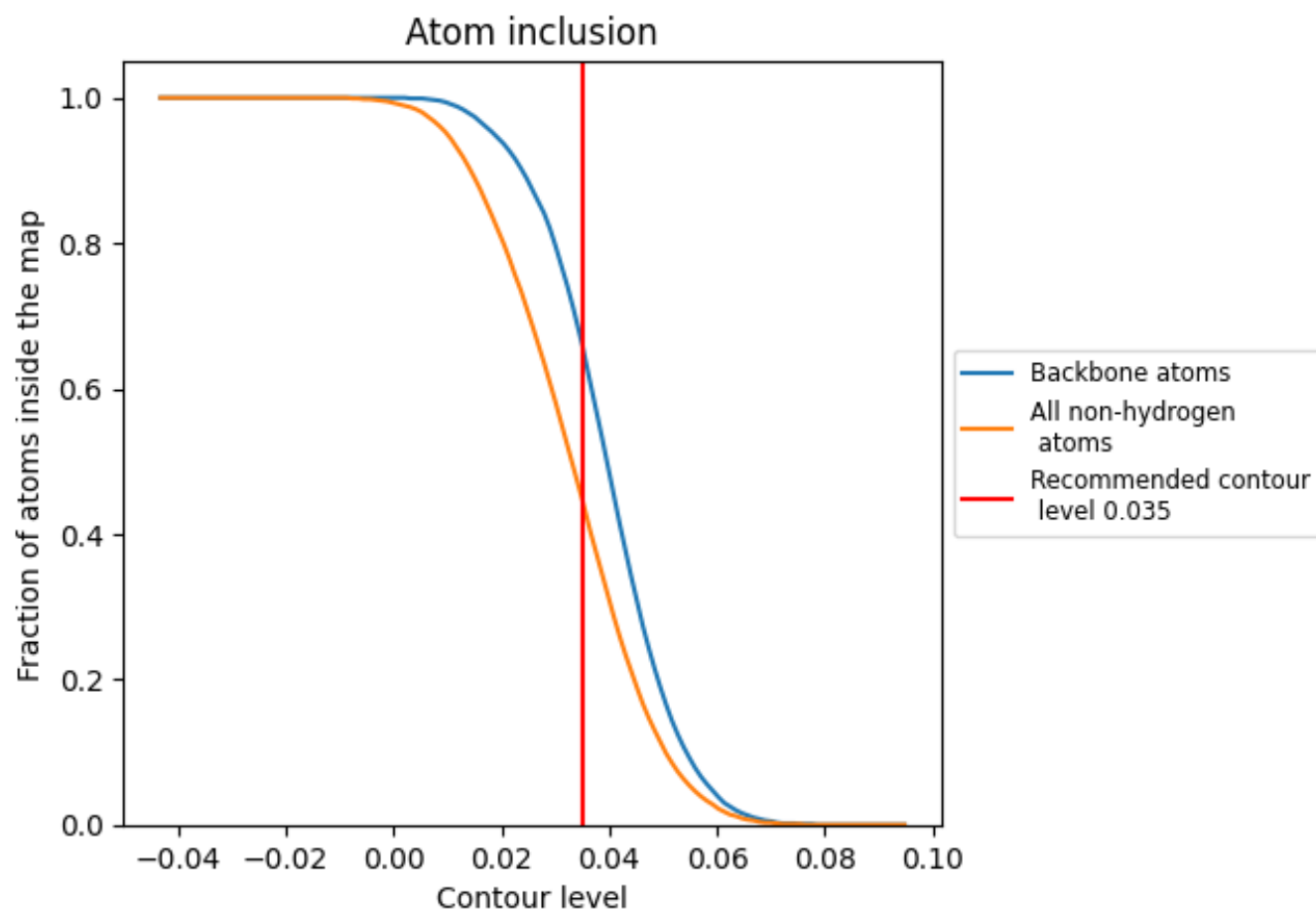
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4470	0.2510
A	0.4490	0.2490
B	0.4470	0.2510
E	0.4470	0.2510
F	0.4490	0.2530
G	0.4470	0.2510
H	0.4450	0.2510
I	0.4480	0.2520
J	0.4440	0.2510

1.0

0.0

<0.0