



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 5TAV / pdb_00005tav
EMDB ID : EMD-8386
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
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:

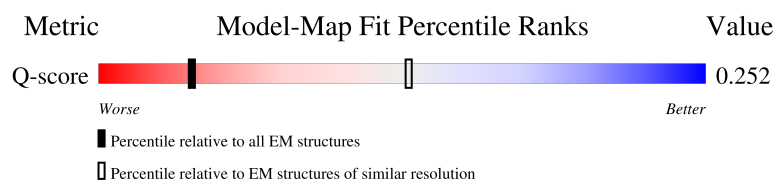
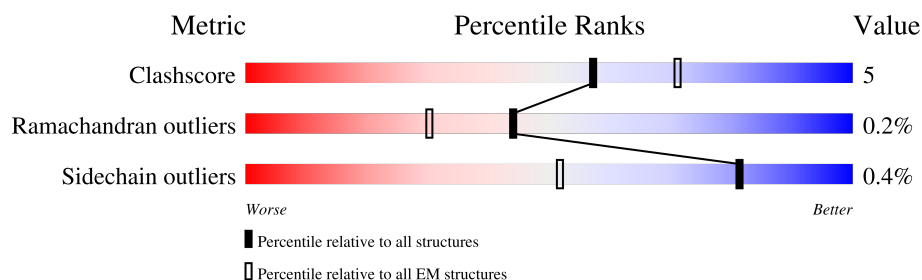
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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%			
			84%11%5%			
2	E	4416	39%			
			84%11%5%			
2	G	4416	39%			
			84%10%5%			
2	I	4416	39%			
			84%11%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.

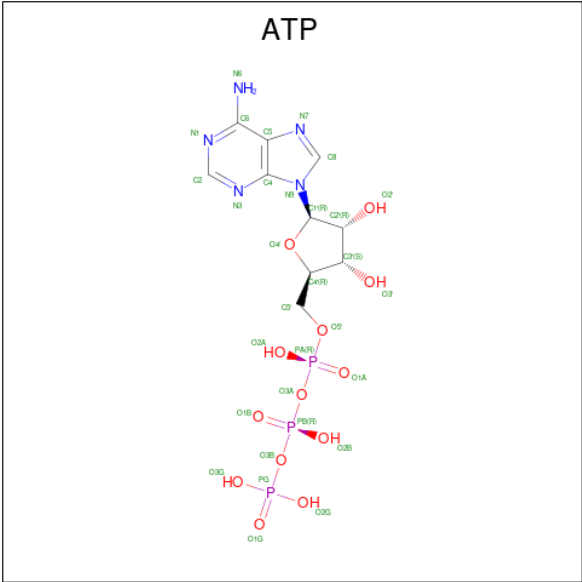
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

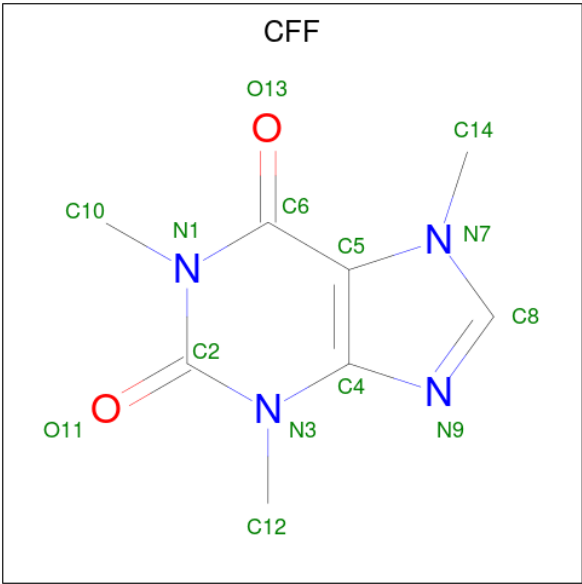
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- 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	E	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	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

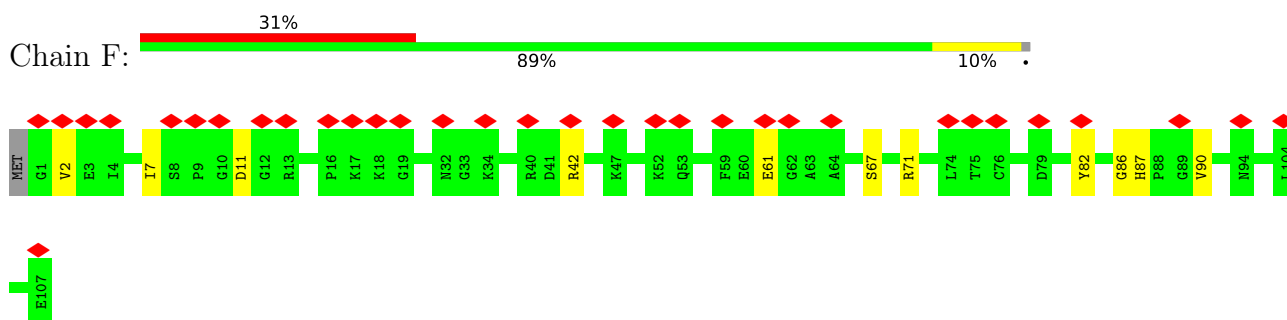
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

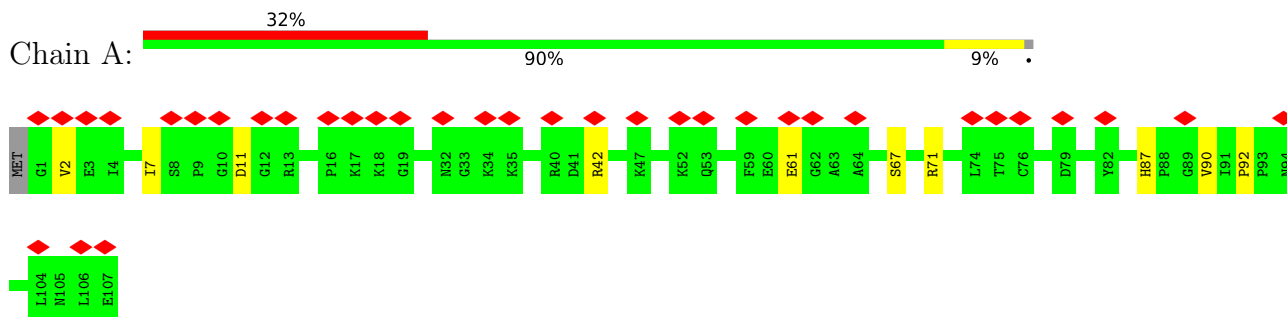
3 Residue-property plots [i](#)

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.

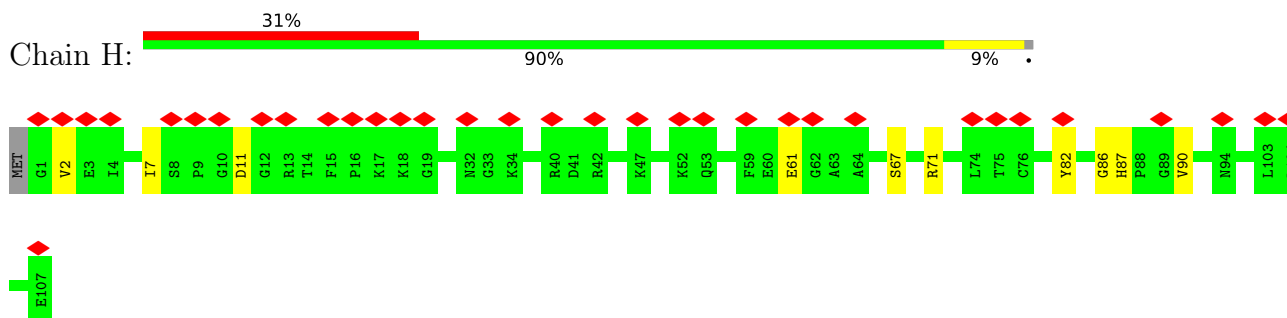
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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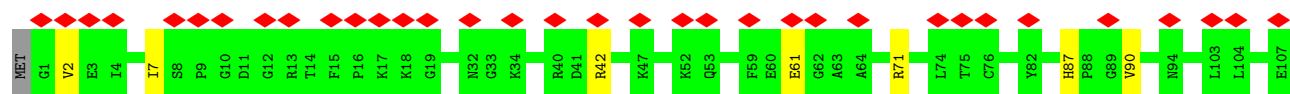


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



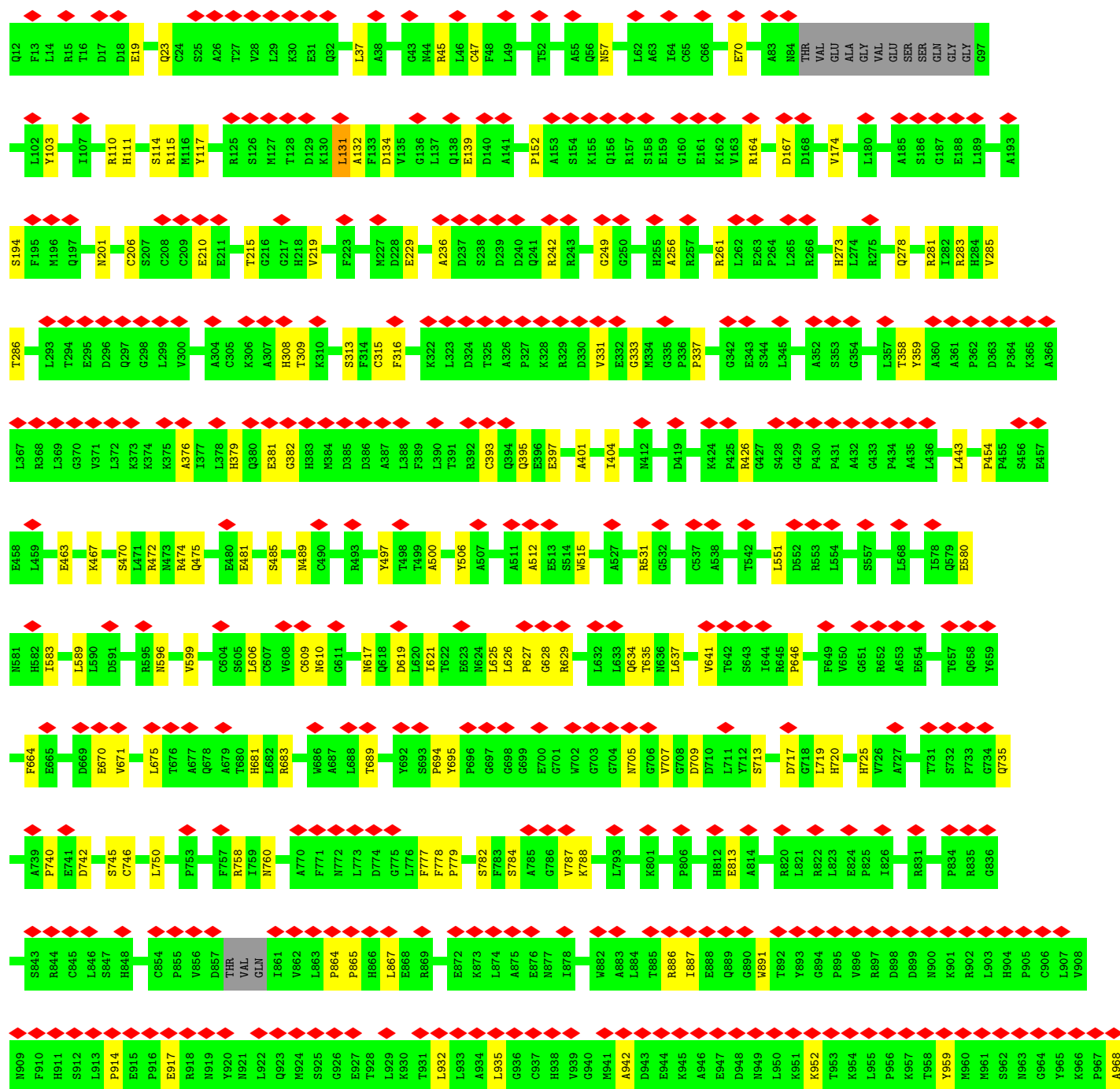
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 2: Ryanodine receptor 1

Chain B: 39% 84% 11% 5%





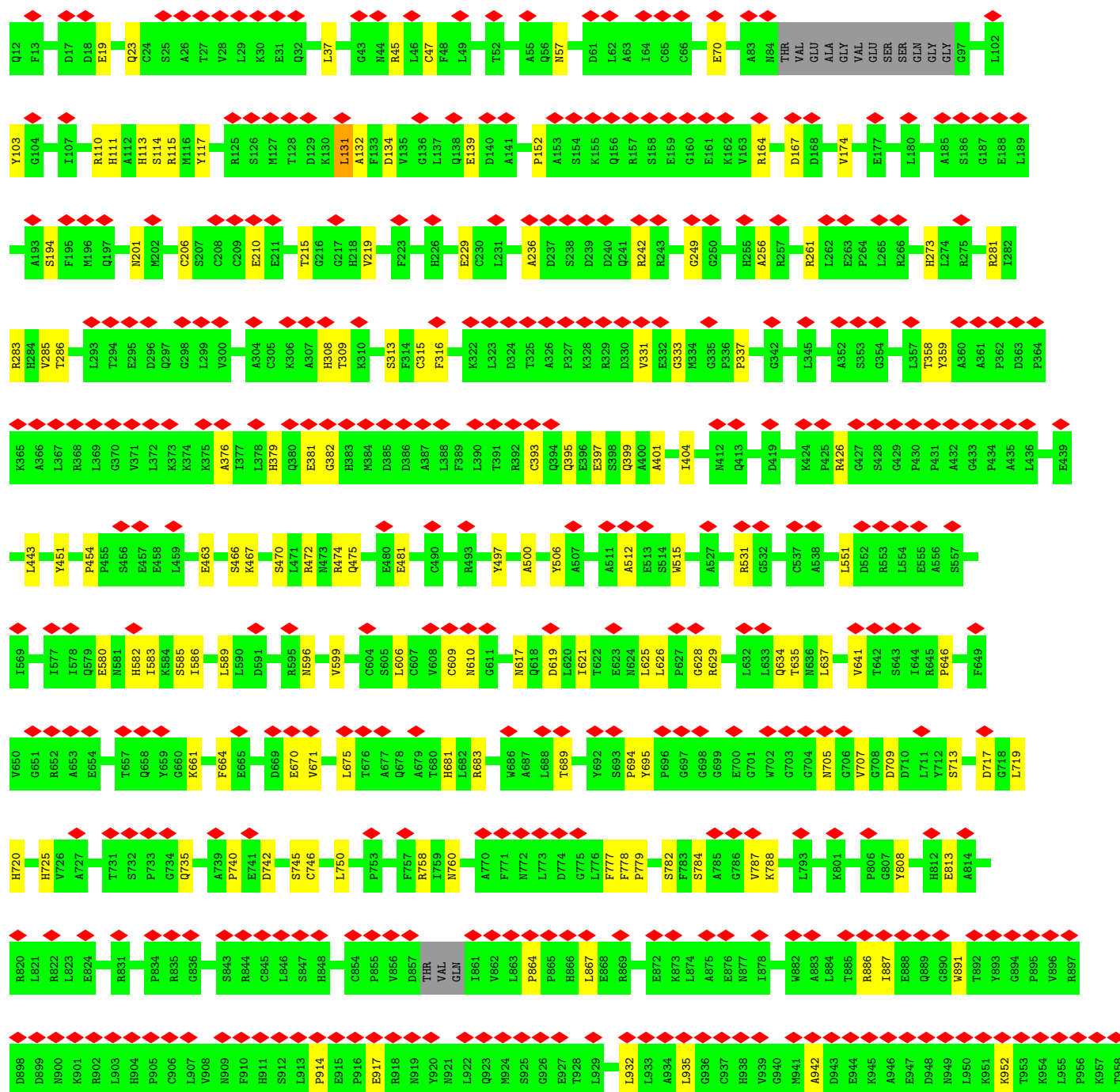
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X3414	X3417	X3423	X3427	X3431	X3432	X3433	X3434	X3435	X3436	X3439	X3440	X3443	X3449	X3453	X3454	X3457	X3458	X3459	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536											
X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3369	X3372	X3373	X3374	X3375	X3376	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3413				
X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3295	X3296	X3297	X3298	X3301	X3302	X3303	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3341	X3342	X3343	X3344	X3345	X3346	X3347	X3348					
X3196	X3197	X3200	X3206	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	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					
X3034	X3035	X3036	X3037	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3143	X3144	X3149	X3152	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3175	X3176	X3179	X3183	X3189	X3190	X3191	X3192	X3193	X3194	X3195										
L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	S2940	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2961	X2965	X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2999	X3005	X3006	X3014	X3019	X3022	X3023	X3027	X3028	X3029	X3032	X3033								
L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	T2884	T2885	W2886	G2887	T2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	X2896	K2897	G2898	G2899	G2900	T2901	H2902	F2903	L2904	L2905	V2906	P2907	V2908	V2909	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2917	R2918	D2919	X3028	X3029	E2921	K2922	A2923	Q2924	E2925
W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	LYS	LYS	THR	ARG	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	GLU	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866			
I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	E2759	E2760	Y2761	T2762	H2763	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	T2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805		
E2347	E2348	N2349	K2350	N2351	V2352	R2355	L2358	L2359	E2362	L2368	E2371	G2372	G2373	S2374	A2378	A2379	I2380	E2381	E2382	D2389	P2390	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	PHE	HIS	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415	T2426	T2430	D2431	G2434											
R2435	P2438	H2441	G2446	K2447	G2448	E2449	L2453	L2460	D2464	D2465	L2466	L2469	I2470	S2471	L2472	Q2475	L2476	P2477	T2478	L2479	X2491	X2492	X2493	Y2502	X2511	X2512	X2513	X2529	X2534	X2535	X2561	X2562	X2569	X2581	X2582	X2583	X2584	X2585	X2597	X2606																			
X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2630	X2648	X2649	X2650	X2651	X2669	X2670	X2671	X2672	X2674	X2675	X2676	X2680	X2681	X2687	X2688	X2689	X2690	X2691	X2692	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746						

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D4684	Y4687	T4688	T4689	E4690	S4691	P4692	G4693	D4694	D4695	D4696	Y4697	K4698	D4699	Q4700	R4703	L4704	L4705	L4706	M4707	M4714	Y4715	M4716	L4725	D4726	D4727	H4728	D4729	D4730	I4731	R4734	I4737	A4738	L4741	C4742	M4743	D4744	L4745	A4746	S4747	L4748	E4749	I4750	T4751	A4752	H4753	M4754	E4755	R4756	P4757	P4758	P4759		
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P4176	Y4177	M4184	G4185	A4186	S4187	R4188	A4189	I4190	E4191	A4192	I4193	Y4194	F4195	E4196	I4197	S4198	E4199	R4202	E4206	R4215	F4219	G4225	G4226	E4227	A4228	E4229	K4230	M4231	E4232	S4236	E4239	D4240	A4248	I4251	S4252	E4253	X4320	X4321	X4322	X4323	X4324	X4325	X4326	X4327	X4328	X4329	X4330	X4331	X4332				
F4093	Q4094	K4095	A4096	M4097	D4098	S4099	K4100	K4101	K4102	F4103	T4104	G4105	P4106	Q4109	F4110	S4113	C4114	S4115	E4116	A4117	D4118	E4119	N4120	E4121	N4122	I4123	N4124	F4125	E4126	E4127	N4130	R4131	F4132	Q4133	R4137	N4142	E4152	H4153	V4154	P4155	H4156	D4157	P4158	R4159	L4160	R4161	N4162	F4163	L4164	E4165	E4172		
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35037

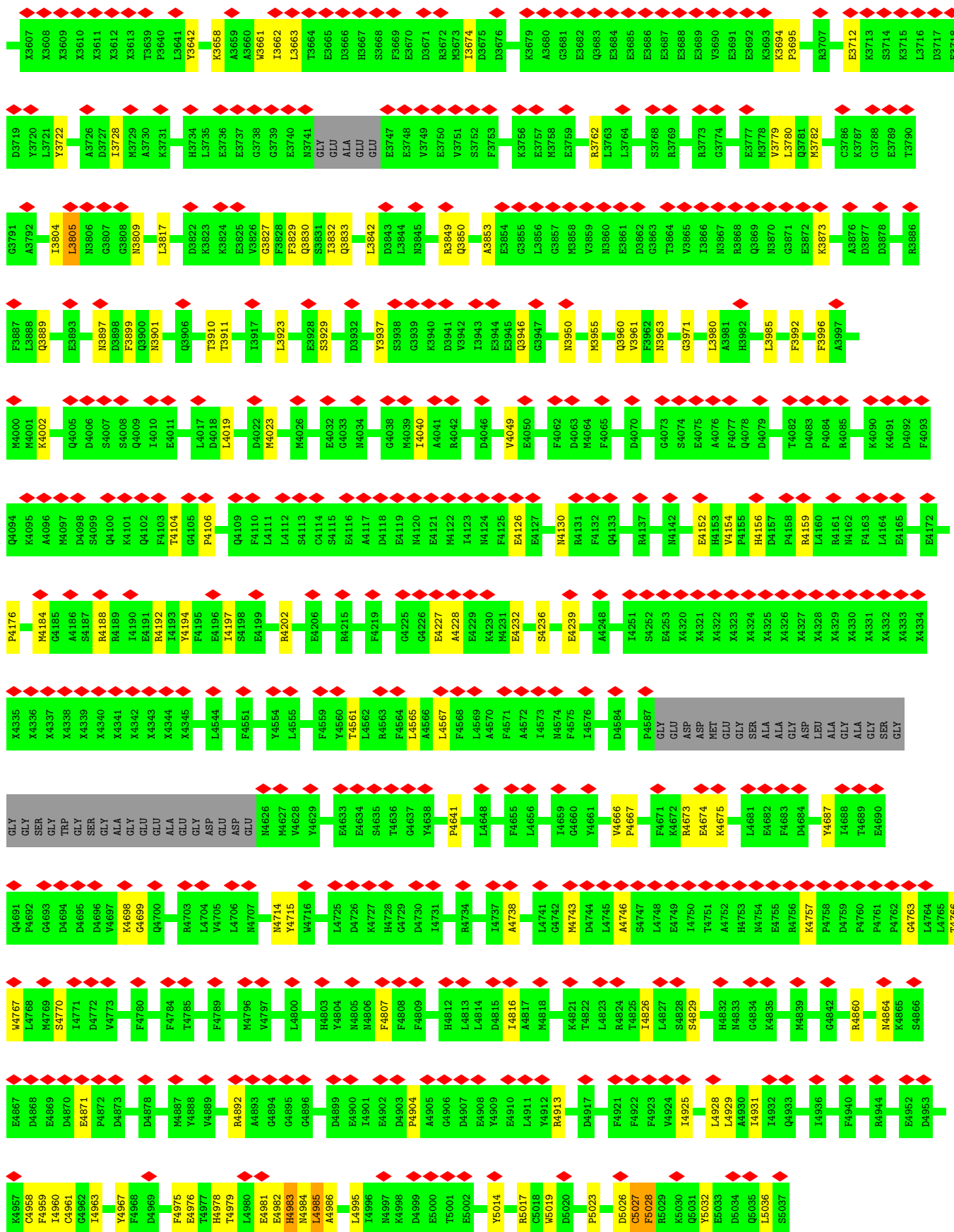
• Molecule 2: Ryanodine receptor 1

Chain E: 39% 84% 11% 5%



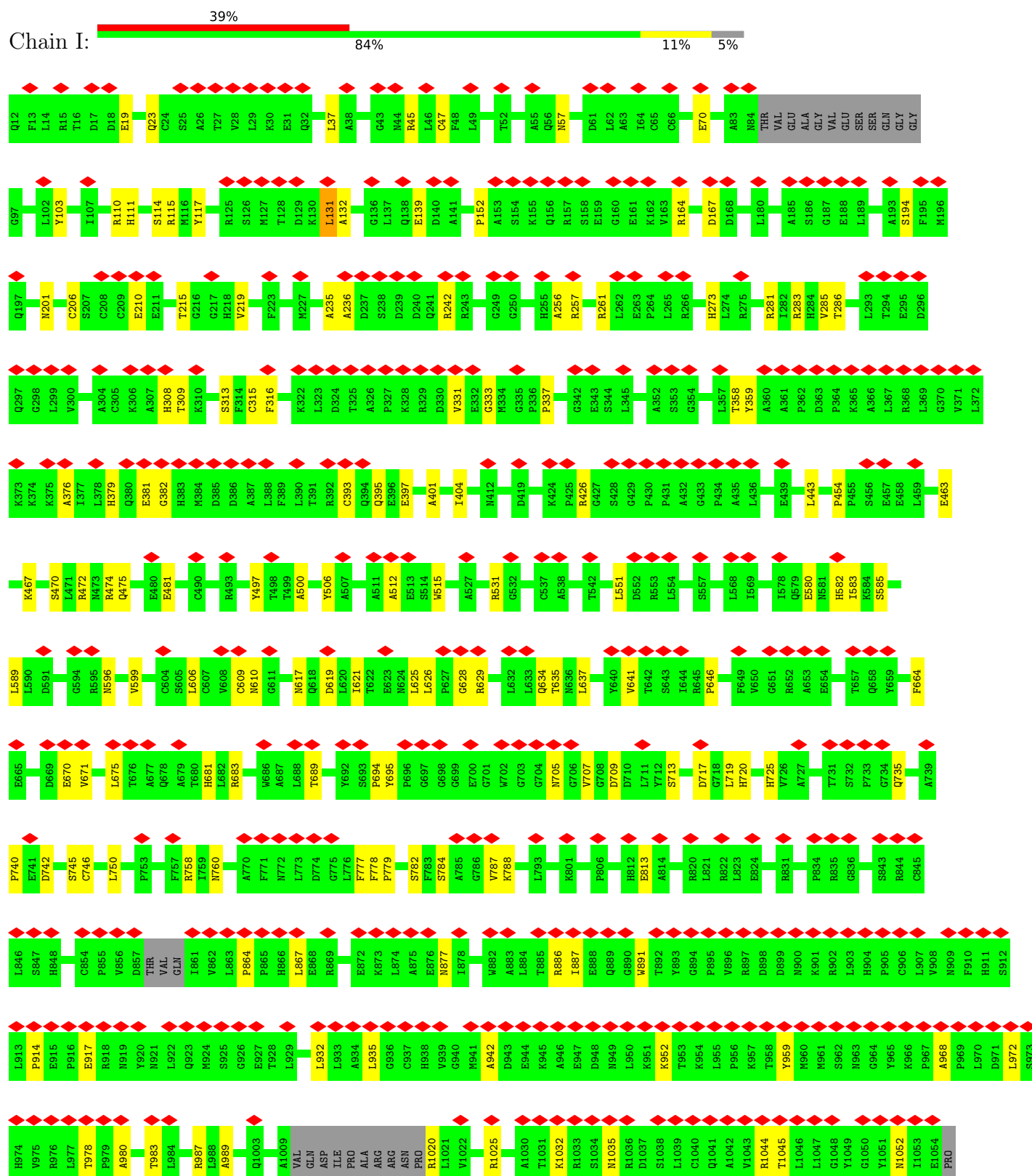


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● Molecule 2: Ryanodine receptor 1

Chain I:





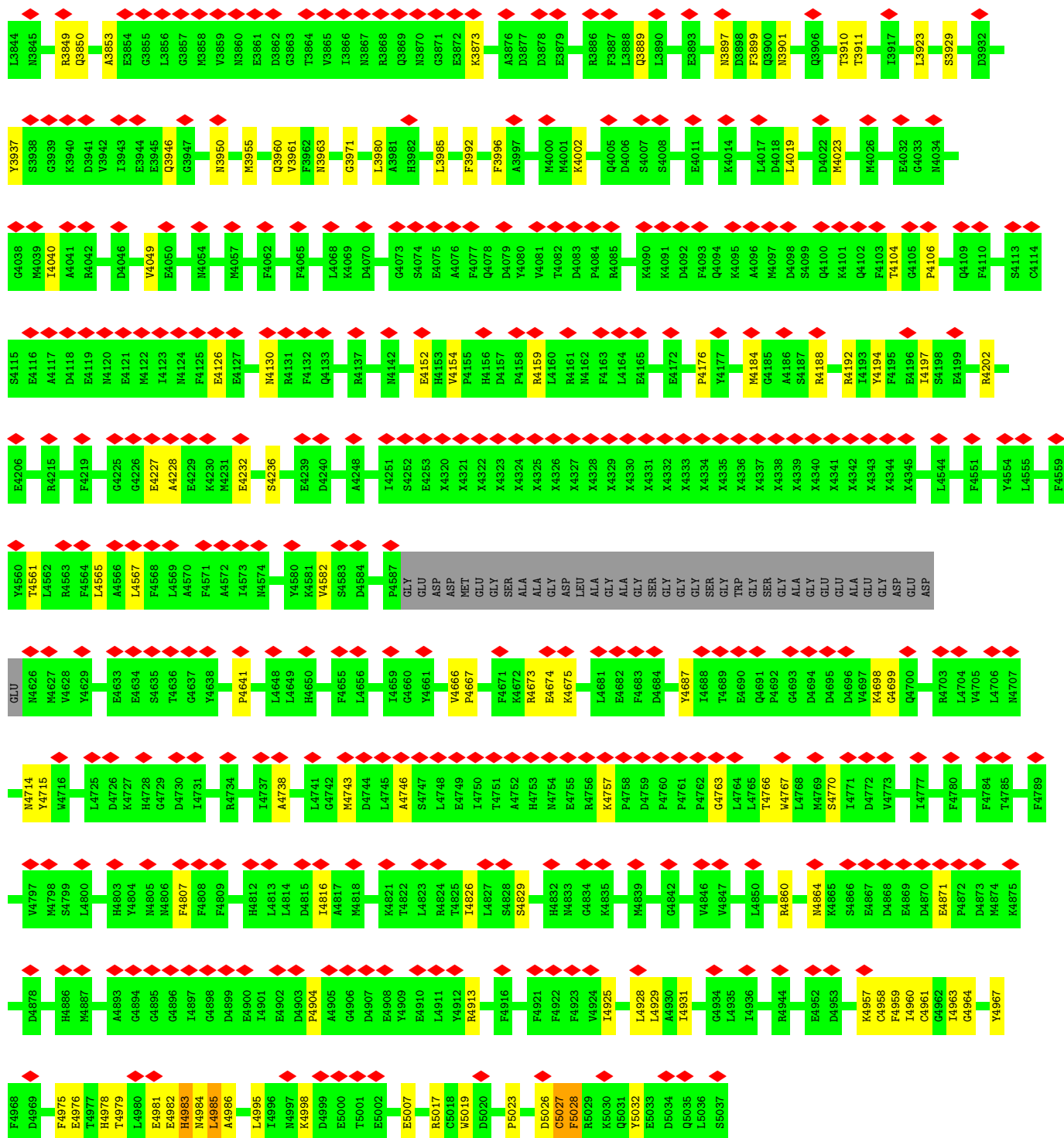




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S973	H974	V975	R976	L977	T978	P979	A980	T983	L984	R987	L988	A989	Q1003	A1009	VAL	GLN	ASP	E1078	PRO	ALA	ARG	ARG	ASN	P80	R1020	L1021	V1022	R1025	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054
Q12	F13	L14	R15	T16	D17	E18	E19	Q23	C24	S25	A26	T27	V28	L29	K30	E31	Q32	L37	A38	G43	M44	R45	L46	C47	F48	L49	T52	A55	Q56	N57	L62	A63	I64	C65	C66	E70	A83	N84	THR	VAL	GLU	ALA	GLY	VAL	GLU	SER	GLN	GLY	G97				
L102	Y103	I107	R110	H111	S114	R115	M116	Y117	R125	S126	V127	M128	D129	K130	L131	A132	F133	D134	V135	G136	L137	Q138	E139	D140	A141	P152	A153	S154	K155	Q156	R157	S158	E159	G160	E161	K162	V163	R164	D167	D168	L180	A185	S186	G187	E188	L189	A193	S194	F195				
M196	Q197	N201	C206	C208	C209	E210	E211	T215	G216	H217	H218	V219	F223	H226	M227	A236	D237	S238	D239	D240	Q241	R242	R243	G249	G250	A256	R257	R261	L262	E263	P264	L265	R266	H273	L274	R275	R283	H284	V285	T286	L293	T294	E295	D296	Q297	G298							
L299	V300	A304	C305	K306	A307	H308	T309	K310	S313	C314	F315	F316	K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	G335	P336	P337	G342	E343	S344	L345	A352	S353	G354	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	K374
K375	A376	T377	L378	H379	Q380	E381	G382	H383	M384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	E395	E396	E397	A401	L404	M412	D419	K424	P425	R426	G427	S428	G429	P430	P431	A432	G433	P434	A435	L436	E439	L443	P454	P455	S456	E457	E458	L459	E463	S466				
K467	S470	L471	R472	N473	R474	Q475	E480	A481	C490	R493	G497	T498	A500	Y506	A507	A511	A512	E513	S514	W515	A527	R531	G532	C537	A538	T542	L551	D552	R553	L554	S557	L568	L569	L578	Q579	E580	N581	H582	L583	K584	S585	L589											
L590	D591	G594	R595	N596	V599	C604	S605	L606	V608	C609	N610	G611	V612	A613	N617	Q618	D619	L620	L621	T622	E623	N624	L625	L626	P627	G628	R629	L632	L633	Q634	T635	N636	L637	Y640	V641	T642	S643	R645	P646	F649	V650	G651	R652	A653	E654	T657	Q658	Y659					
F664	E665	D669	E670	V671	L675	T676	A677	Q678	T680	H681	L682	R683	W686	A687	L688	T689	Y692	S693	P694	F695	P696	G697	G698	G699	E700	G701	W702	G703	G704	W705	G706	V707	D709	D710	L711	V712	S713	D717	G718	L719	H720	H725	V726	A727	T731	S732	F733	G734	Q735				
A739	P740	E741	D742	S745	C746	L750	F753	F757	R758	N760	A770	F771	N772	L773	D774	L776	F777	F778	P779	S782	F783	S784	A785	G786	V787	K788	L793	R801	P806	H812	E813	A814	R820	L821	R822	L823	E824	R831	P834	R835	C836	S843	R844										
C845	L846	S847	H848	C854	P855	V856	D857	THR	VAL	GLN	T861	V862	L863	P864	P865	H866	L867	E868	R869	E872	K873	L874	C937	H938	Y939	G940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972



V3749	E3670	X3440	X3289	X3217	X3049	G2934	M2874	K2814	F2754	X2624
E3750	D3671	X3443	X3290	X3218	X3050	Y2935	M2875	A2815	I2755	X2625
V3751	X3672	X3449	X3291	X3219	X3051	A2936	E2876	A2816	N2756	X2626
S3752	X3673	X3449	X3292	X3220	X3052	V2937	Q2877	I2817	K2757	X2627
F3753	D3675	X3453	X3295	X3221	X3059	T2938	L2878	A2818	F2758	X2628
	D3676	X3454	X3296	X3222	X3060	R2939	A2879	W2819	A2759	X2629
	K3679	X3457	X3297	X3223	X3061	X2942	E2880	E2820	E2760	X2630
	A3680	X3458	X3301	X3224	X3062	X2943	N2881	W2821	Y2761	
	E3682	X3463	X3302	X3227	X3063	X2944	H2882	T2822	T2762	X2648
	E3684	X3466	X3303	X3230	X3134	X2945	H2883	E2824	H2763	X2649
	E3685	X3467	X3312	X3231	X3135	X2946	N2884	E2764	E2764	X2650
	E3686	X3468	X3313	X3232	X3136	X2947	T2885	K2765	K2765	X2651
	E3687	X3469	X3314	X3233	X3137	X2948	W2886	W2766	W2766	
	E3688	X3511	X3315	X3234	X3138	X2949	Q2887	A2767	A2767	X2670
	E3689	X3512	X3316	X3235	X3139	X2950	R2888	F2768	F2768	X2671
	V3690	X3513	X3317	X3236	X3143	X2951	K2889	Q2769	Q2769	X2672
	E3691	X3514	X3318	X3241	X3144	X2952	K2890	K2770	K2770	X2673
	E3692	X3515	X3323	X3242	X3149	X2961	K2891	I2771	I2771	X2674
	K3693	X3518	X3324	X3243	X3152	X2966	Q2892	Q2772	Q2772	X2675
	K3694	X3519	X3325	X3244	X3158	X2967	L2894	N2773	N2773	X2676
	P3695	X3520	X3326	X3245	X3159	X2968	E2895	W2774	W2774	
		X3521	X3327	X3246	X3160	X2969	A2896	W2775	W2775	X2680
		X3522	X3328	X3247	X3161	X2970	K2897	S2776	S2776	X2681
		X3523	X3329	X3248	X3162	X2971	G2898	G2777	G2777	
		X3524	X3330	X3249	X3163	X2972	G2899	G2778	G2778	X2687
		X3525	X3331	X3250	X3164	X2973	G2900	E2779	E2779	X2688
		X3526	X3332	X3251	X3165	X2974	T2901	N2780	N2780	X2689
		X3527	X3333	X3252	X3166	X2975	H2902	V2781	V2781	X2690
		X3528	X3334	X3253	X3167	X2976	P2903	D2782	D2782	X2691
		X3529	X3335	X3254	X3171	X2977	L2904	E2783	E2783	X2692
		X3530	X3336	X3255	X3175	X2978	L2905	E2784	E2784	
		X3531	X3337	X3256	X3176	X2979	L2906	T2785	T2785	X2696
		X3532	X3338	X3257	X3179	X2980	P2907	K2786	K2786	X2698
		X3533	X3339	X3258	X3183	X2989	P2908	ARG	ARG	X2699
		X3534	X3340	X3259	X3189	X3005	Y2908	GLU	GLU	X2700
		X3535	X3341	X3260	X3190	X3006	D2909	GLY	GLY	X2701
		X3536	X3342	X3261	X3191	X3014	T2910	N2855	N2855	X2702
		X3537	X3343	X3262	X3192	X3019	T2911	P2857	P2857	X2703
		X3538	X3344	X3263	X3193	X3022	T2912	Q2858	Q2858	X2734
		X3539	X3345	X3264	X3194	X3023	T2913	P2859	P2859	X2735
		X3540	X3346	X3265	X3195	X3027	K2914	P2860	P2860	D2736
		X3541	X3347	X3266	X3196	X3034	E2915	D2861	D2861	P2737
		X3542	X3348	X3267	X3197	X3035	K2916	L2862	L2862	R2738
		X3543	X3349	X3268	X3200	X3036	E2917	D2863	D2863	P2739
		X3544	X3350	X3269	X3206	X3037	K2918	G2864	G2864	W2740
		X3545	X3351	X3270	X3211	X3043	D2919	V2865	V2865	T2741
		X3546	X3352	X3271	X3212	X3044	R2920	L2866	L2866	T2742
		X3547	X3353	X3272	X3213	X3045	E2921	T2867	T2867	L2743
		X3548	X3354	X3273	X3214	X3046	K2922	L2868	L2868	L2744
		X3549	X3355	X3274	X3215	X3047	E2923	S2869	S2869	W2745
		X3550	X3356	X3275	X3216	X3048	Q2924	R2869	R2869	V2746
		X3551	X3357	X3276	X3217		E2925	E2870	E2870	L2747
		X3552	X3358	X3277	X3218		L2926	L2871	L2871	P2748
		X3553	X3359	X3278	X3219		L2927	W2807	W2807	E2749
		X3554	X3360	X3279	X3220		Q2928	P2808	P2808	K2750
		X3555	X3361	X3280	X3221		F2929	L2810	L2810	L2751
		X3556	X3362	X3281	X3222		Q2930	E2811	E2811	D2752
		X3557	X3363	X3282	X3223		L2931	S2812	S2812	
		X3558	X3364	X3283	X3224		M2932	N2813	N2813	
		X3559	X3365	X3284	X3225					
		X3560	X3366	X3285	X3226					
		X3561	X3367	X3286	X3227					
		X3562	X3368	X3287	X3228					
		X3563	X3369	X3288	X3229					
		X3564	X3370	X3289	X3230					
		X3565	X3371	X3290	X3231					
		X3566	X3372	X3291	X3232					
		X3567	X3373	X3292	X3233					
		X3568	X3374	X3293	X3234					
		X3569	X3375	X3294	X3235					
		X3570	X3376	X3295	X3236					
		X3571	X3377	X3296	X3237					
		X3572	X3378	X3297	X3238					
		X3573	X3379	X3298	X3239					
		X3574	X3380	X3299	X3240					
		X3575	X3381	X3300	X3241					
		X3576	X3382	X3301	X3242					
		X3577	X3383	X3302	X3243					
		X3578	X3384	X3303	X3244					
		X3579	X3385	X3304	X3245					
		X3580	X3386	X3305	X3246					
		X3581	X3387	X3306	X3247					
		X3582	X3388	X3307	X3248					
		X3583	X3389	X3308	X3249					
		X3584	X3390	X3309	X3250					
		X3585	X3391	X3310	X3251					
		X3586	X3392	X3311	X3252					
		X3587	X3393	X3312	X3253					
		X3588	X3394	X3313	X3254					
		X3589	X3395	X3314	X3255					
		X3590	X3396	X3315	X3256					
		X3591	X3397	X3316	X3257					
		X3592	X3398	X3317	X3258					
		X3593	X3399	X3318	X3259					
		X3594	X3400	X3319	X3260					
		X3595	X3401	X3320	X3261					
		X3596	X3402	X3321	X3262					
		X3597	X3403	X3322	X3263					
		X3598	X3404	X3323	X3264					
		X3599	X3405	X3324	X3265					
		X3600	X3406	X3325	X3266					
		X3601	X3407	X3326	X3267					
		X3602	X3408	X3327	X3268					
		X3603	X3409	X3328	X3269					
		X3604	X3410	X3329	X3270					
		X3605	X3411	X3330	X3271					
		X3606	X3412	X3331	X3272					
		X3607	X3413	X3332	X3273					
		X3608	X3414	X3333	X3274					
		X3609	X3415	X3334	X3275					
		X3610	X3416	X3335	X3276					
		X3611	X3417	X3336	X3277					
		X3612	X3418	X3337	X3278					
		X3613	X3419	X3338	X3279					
		X3614	X3420	X3339	X3280					
		X3615	X3421	X3340	X3281					
		X3616	X3422	X3341	X3282					
		X3617	X3423	X3342	X3283					
		X3618	X3424	X3343	X3284					
		X3619	X3425	X3344	X3285					
		X3620	X3426	X3345	X3286					
		X3621	X3427	X3346	X3287					
		X3622	X3428	X3347	X3288					
		X3623	X3429	X3348	X3289					
		X3624	X3430	X3349	X3290					
		X3625	X3431	X3350	X3291					
		X3626	X3432	X3351	X3292					
		X3627	X3433	X3352	X3293					
		X3628	X3434	X3353	X3294					
		X3629	X3435	X3354	X3295					
		X3630	X3436	X3355	X3296					
		X3631	X3437	X3356	X3297					
		X3632	X3438	X3357	X3298					
		X3633	X3439	X3358	X3299					
		X3634	X3440	X3359	X3300					
		X3635	X3441	X3360	X3301					
		X3636	X3442	X3361	X3302					
		X3637	X3443	X3362	X3303					
		X3638	X3444	X3363	X3304					
		X3639	X3445	X3364	X3305					
		X3640	X3446	X3365	X3306					
		X3641	X3447	X3366	X3307					
		X3642	X3448	X3367	X3308					
		X3643	X3449	X3368	X3309					
		X3644	X3450	X3369	X3310					
		X3645	X3451	X3370	X3311					
		X3646	X3452	X3371	X3312					
		X3647	X3453	X3372	X3313					
		X3648	X3454	X3373	X3314					
		X3649	X3455	X3374	X3315					
		X3650	X3456	X3375	X3316					
		X3651	X3457	X3376	X3317					
		X3652	X3458	X3377	X3318					
		X3653	X3459	X3378	X3319					
		X3654	X3460	X3379	X3320					
		X3655	X3461	X3380	X3321					
		X3656	X3462	X3381	X3322					
		X3657	X3463							



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	0.105	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	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: ATP, CFF, 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	0.18	0/834	0.44	0/1123
1	F	0.18	0/834	0.44	0/1123
1	H	0.18	0/834	0.44	0/1123
1	J	0.18	0/834	0.45	0/1123
2	B	0.20	0/25428	0.52	6/34534 (0.0%)
2	E	0.20	0/25428	0.52	6/34534 (0.0%)
2	G	0.20	0/25428	0.52	6/34534 (0.0%)
2	I	0.20	0/25428	0.52	6/34534 (0.0%)
All	All	0.20	0/105048	0.52	24/142628 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2807	TRP	CA-C-N	-7.39	112.52	120.94
2	I	2807	TRP	C-N-CA	-7.39	112.52	120.94
2	B	2807	TRP	CA-C-N	-7.38	112.53	120.94
2	B	2807	TRP	C-N-CA	-7.38	112.53	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2807	TRP	CA-C-N	-7.38	112.53	120.94

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	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	6	0
1	F	818	0	824	6	0
1	H	818	0	824	5	0
1	J	818	0	824	4	0
2	B	29499	0	24746	267	0
2	E	29499	0	24746	272	0
2	G	29499	0	24746	264	0
2	I	29499	0	24746	269	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	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	102368	1082	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 1082 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:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.58	0.92

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%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2916 (90%)	311 (10%)	8 (0%)	43	78
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	43	78
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	44	78

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE

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Mol	Chain	Res	Type
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

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%)	2483 (100%)	10 (0%)	84	83
2	E	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
2	G	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
2	I	2493/3022 (82%)	2483 (100%)	10 (0%)	84	83
All	All	10324/12444 (83%)	10284 (100%)	40 (0%)	81	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4995	LEU
2	G	4154	VAL
2	I	5027	CYS
2	G	1676	LEU
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 227 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4949	GLN

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Mol	Chain	Res	Type
2	G	4691	GLN
2	I	2127	GLN
2	G	4133	GLN
2	G	2127	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	G	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
4	CFF	B	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.78	9 (39%)
4	CFF	I	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.77	9 (39%)
3	ATP	E	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.81	9 (18%)
3	ATP	I	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
3	ATP	B	5101	-	32,33,33	1.38	5 (15%)	48,52,52	1.80	9 (18%)
4	CFF	G	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.79	9 (39%)
4	CFF	E	5102	-	15,15,15	1.84	5 (33%)	23,23,23	2.78	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	G	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	4.53	1.47	1.39
3	I	5101	ATP	C5-C4	4.53	1.47	1.39
3	G	5101	ATP	C5-C4	4.53	1.47	1.39
3	E	5101	ATP	C5-C4	4.52	1.47	1.39
4	I	5102	CFF	C6-N1	-3.89	1.32	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5102	CFF	C14-N7-C8	-7.62	112.02	126.28
4	E	5102	CFF	C14-N7-C8	-7.61	112.03	126.28
4	B	5102	CFF	C14-N7-C8	-7.60	112.05	126.28
4	I	5102	CFF	C14-N7-C8	-7.59	112.08	126.28
3	B	5101	ATP	C5-C4-N3	-5.91	118.58	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

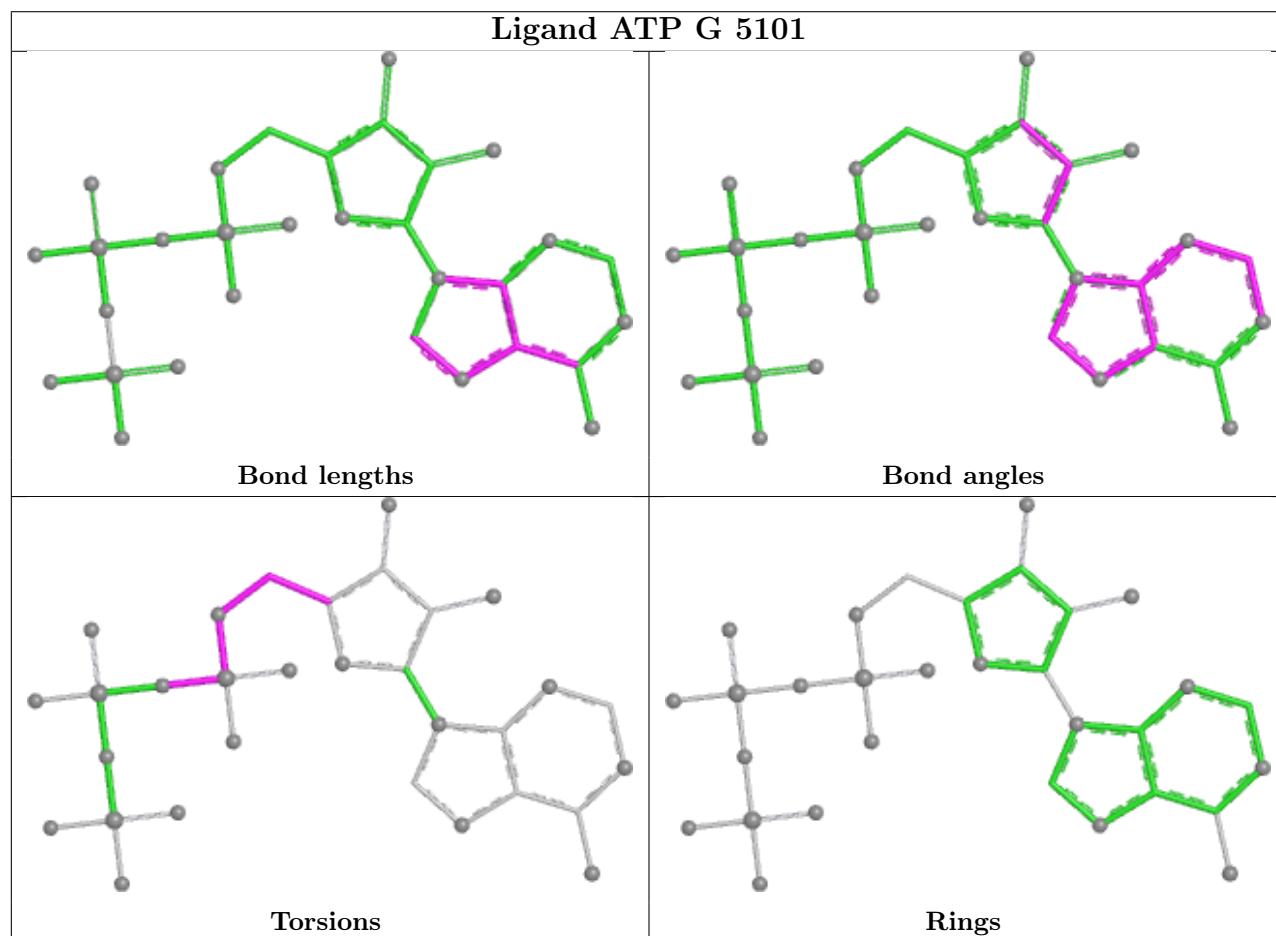
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	PB-O3A-PA-O5'
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A

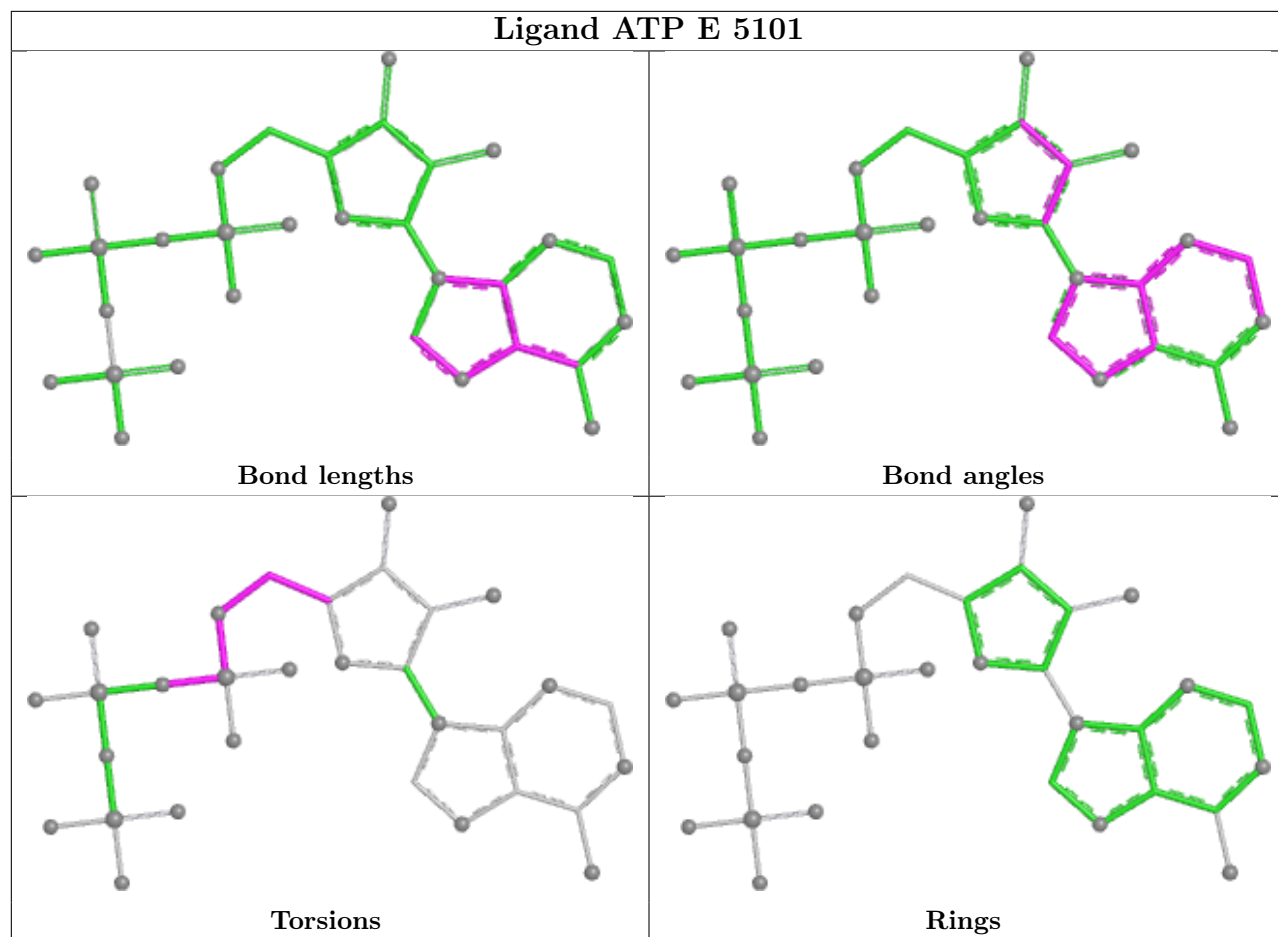
There are no ring outliers.

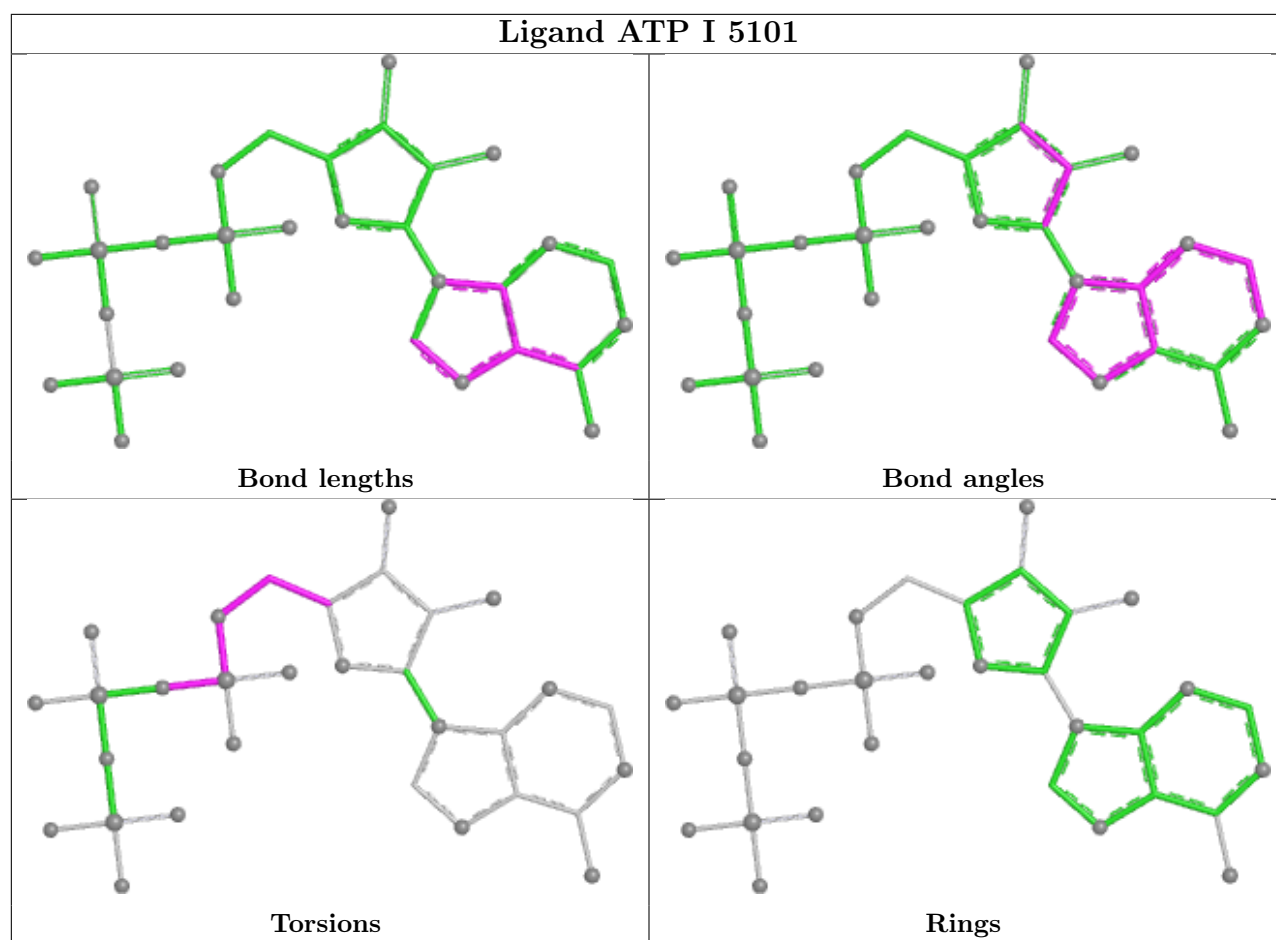
1 monomer is involved in 1 short contact:

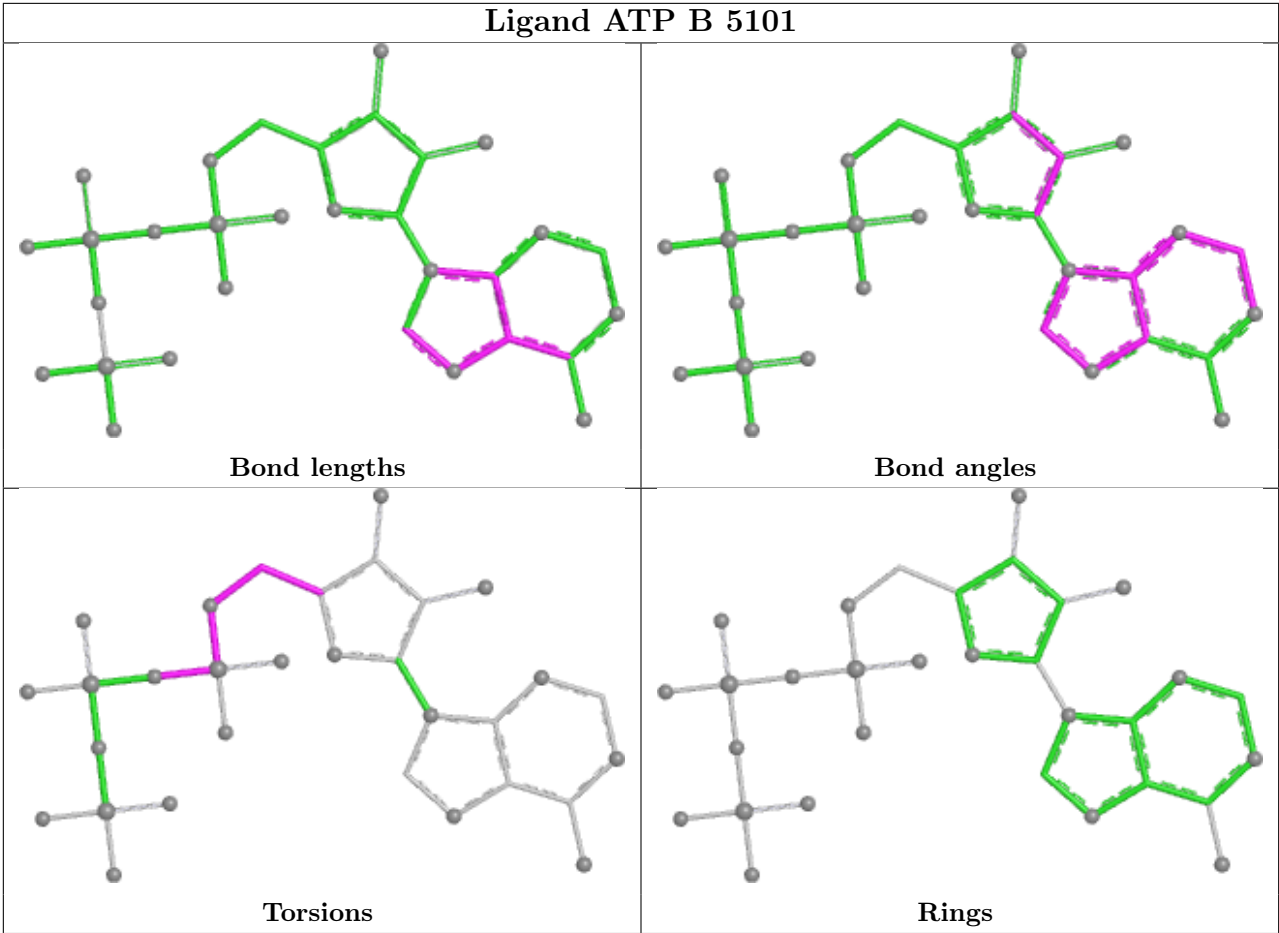
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5102	CFF	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63

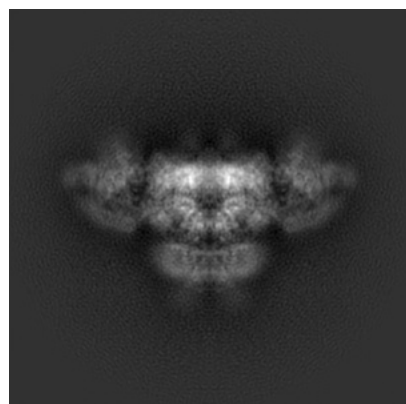
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8386. These allow visual inspection of the internal detail of the map and identification of artifacts.

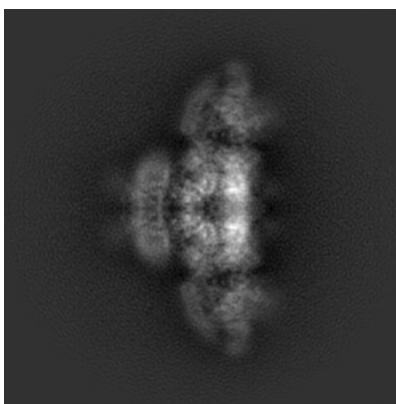
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

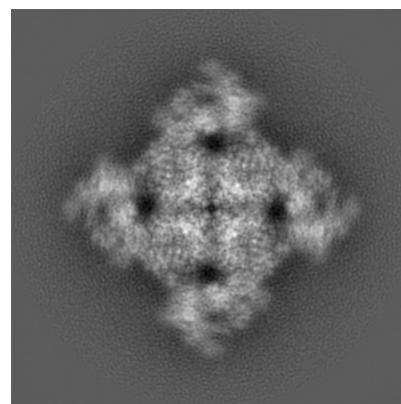
6.1.1 Primary map



X

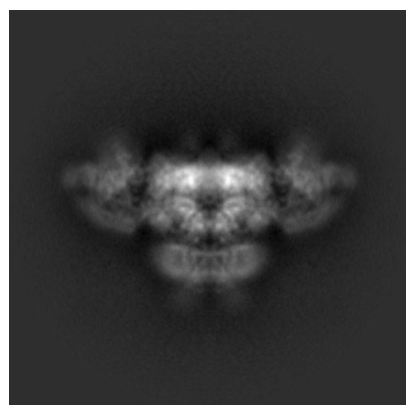


Y

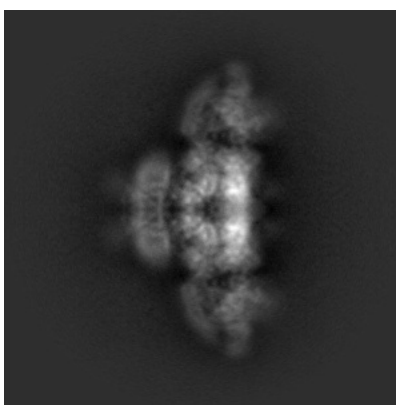


Z

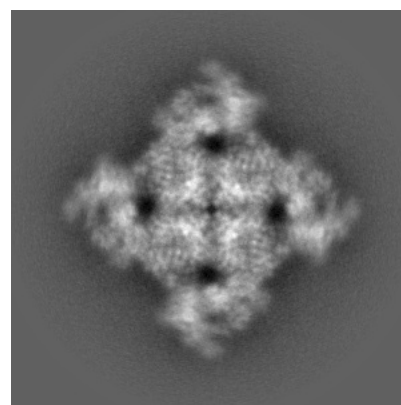
6.1.2 Raw map



X



Y



Z

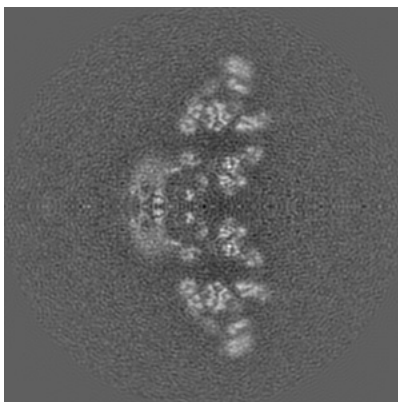
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

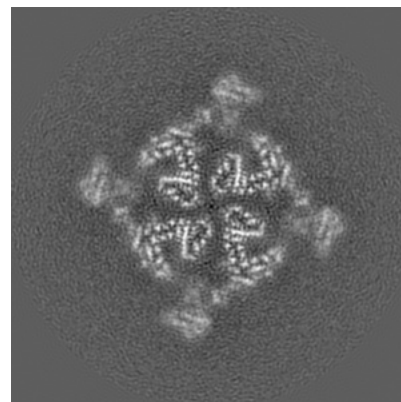
6.2.1 Primary map



X Index: 200

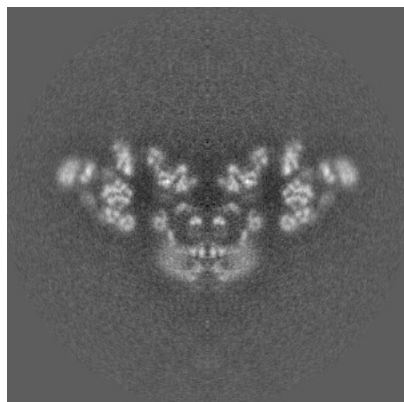


Y Index: 200

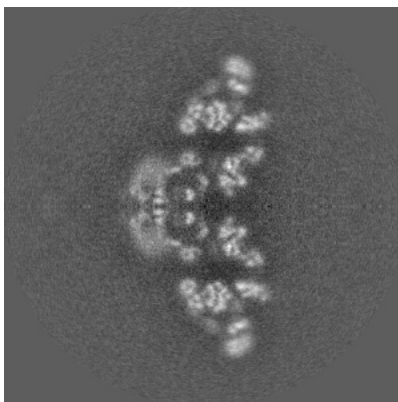


Z Index: 200

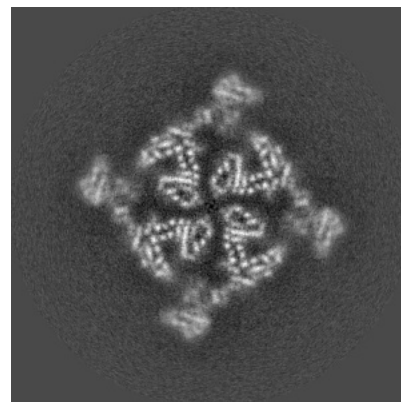
6.2.2 Raw map



X Index: 200



Y Index: 200

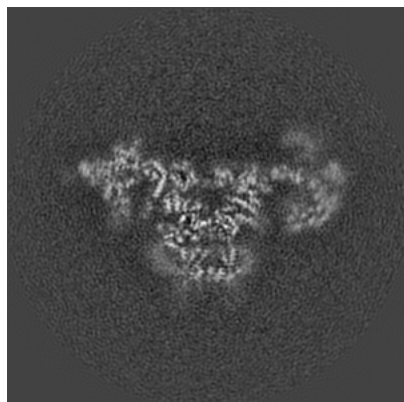


Z Index: 200

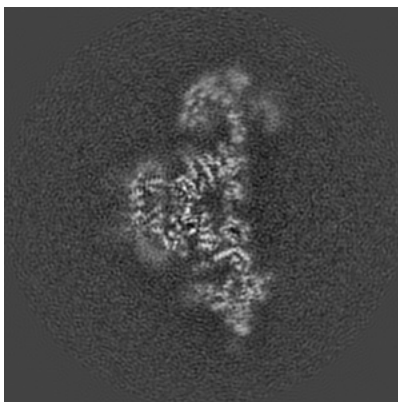
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

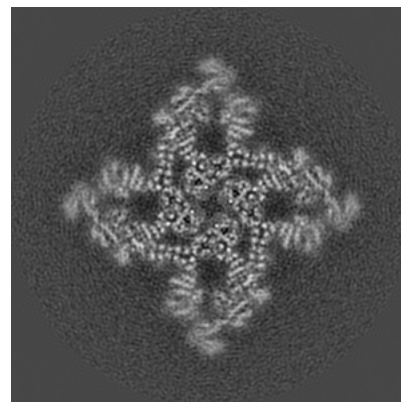
6.3.1 Primary map



X Index: 216

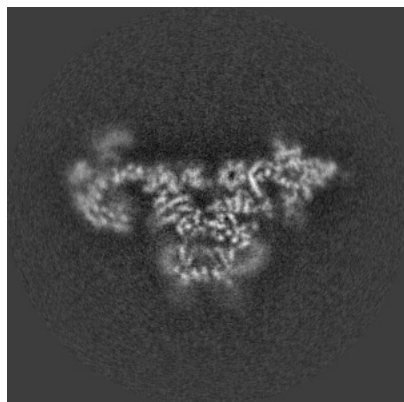


Y Index: 184

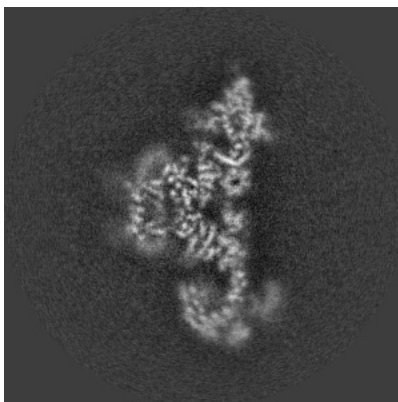


Z Index: 228

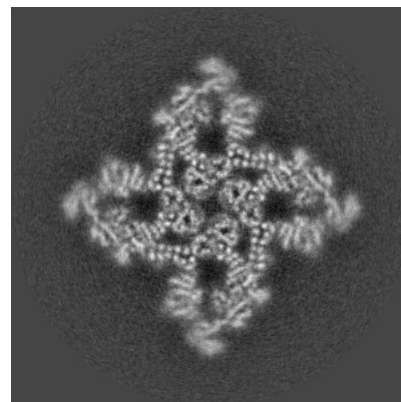
6.3.2 Raw map



X Index: 183



Y Index: 217

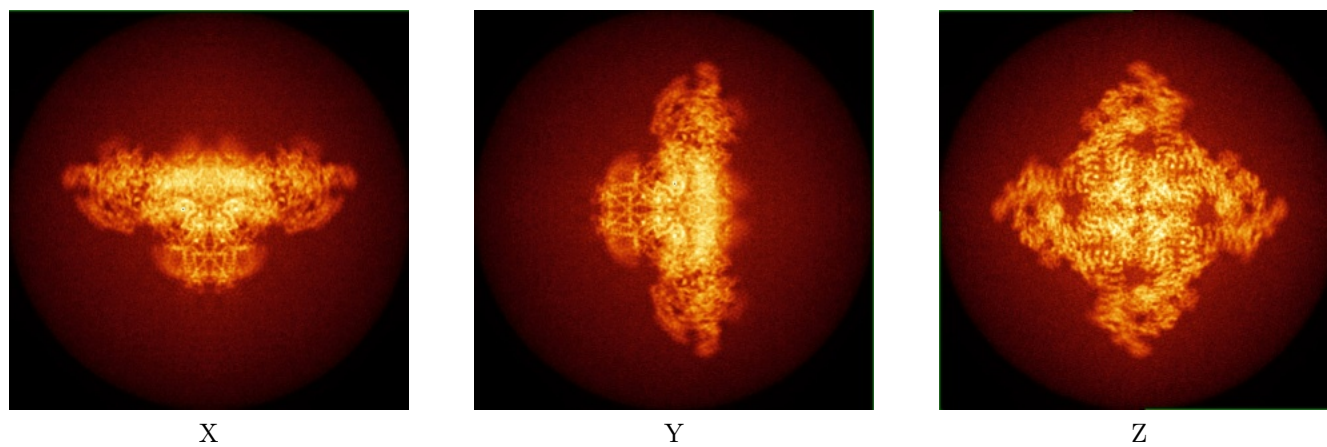


Z Index: 228

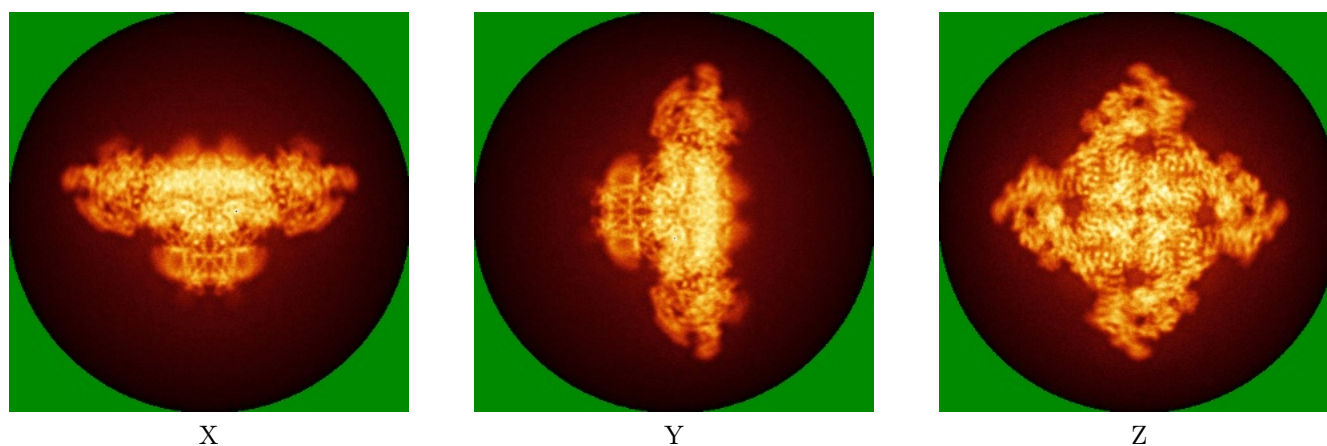
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

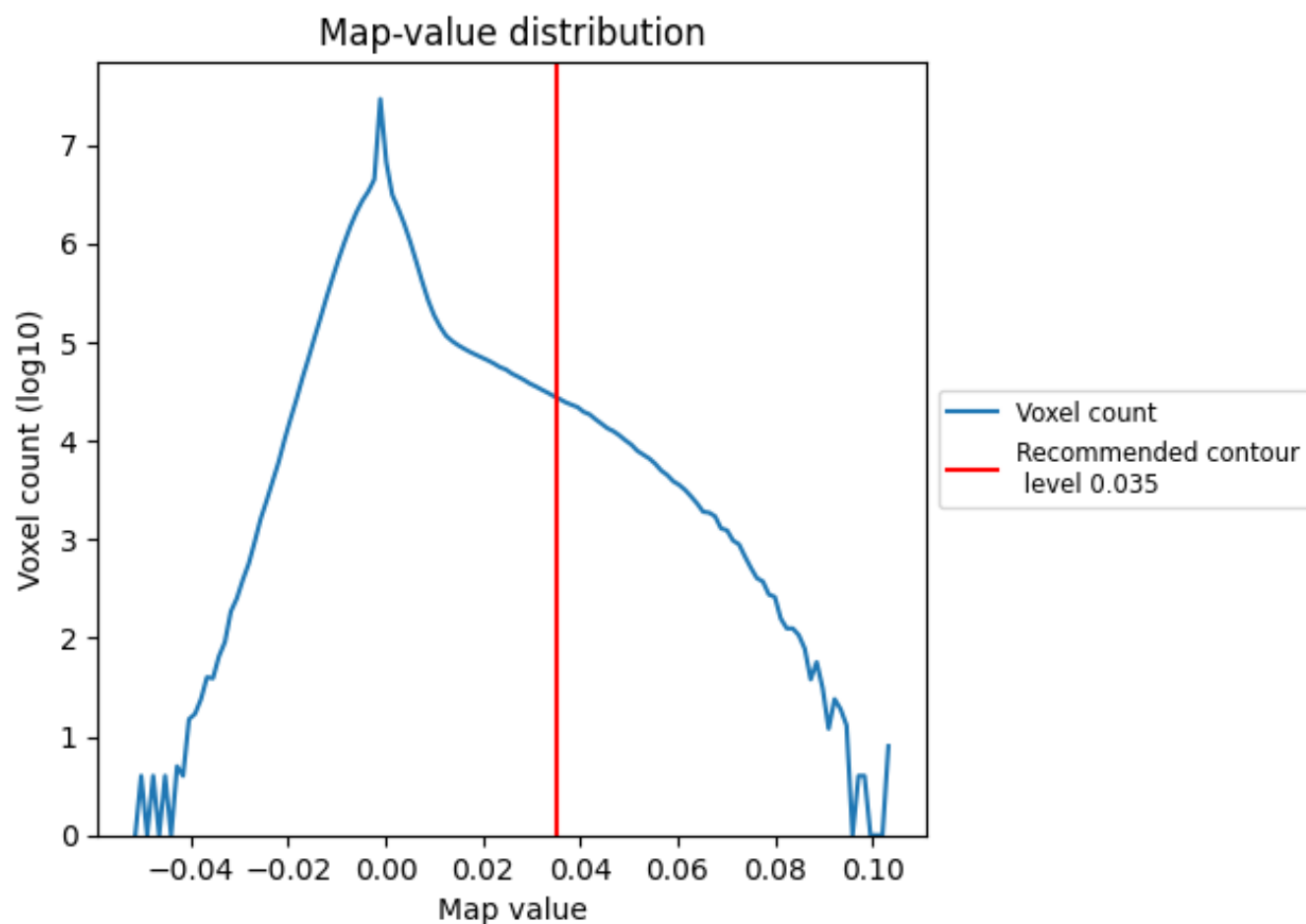
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

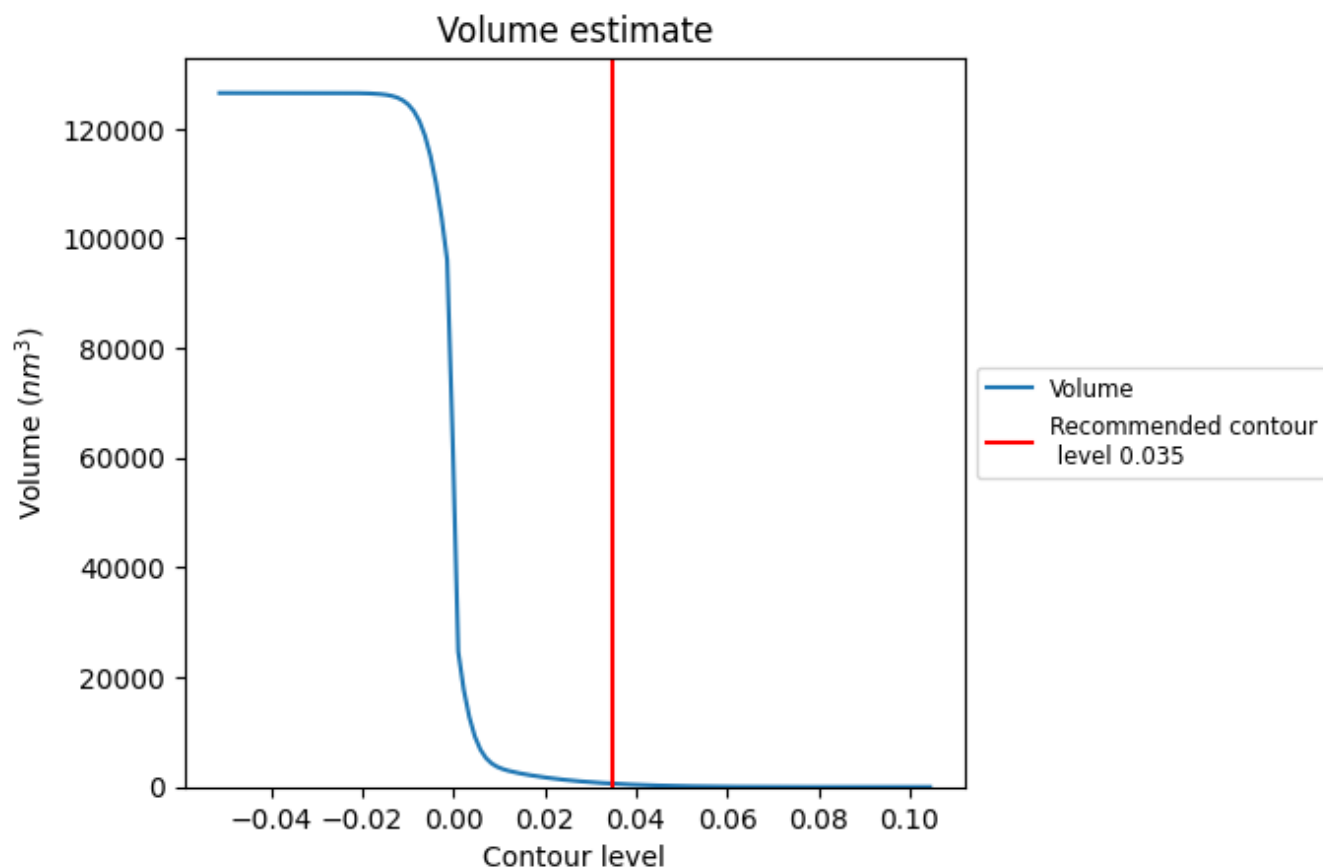
This section contains the results of statistical analysis of the map.

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.

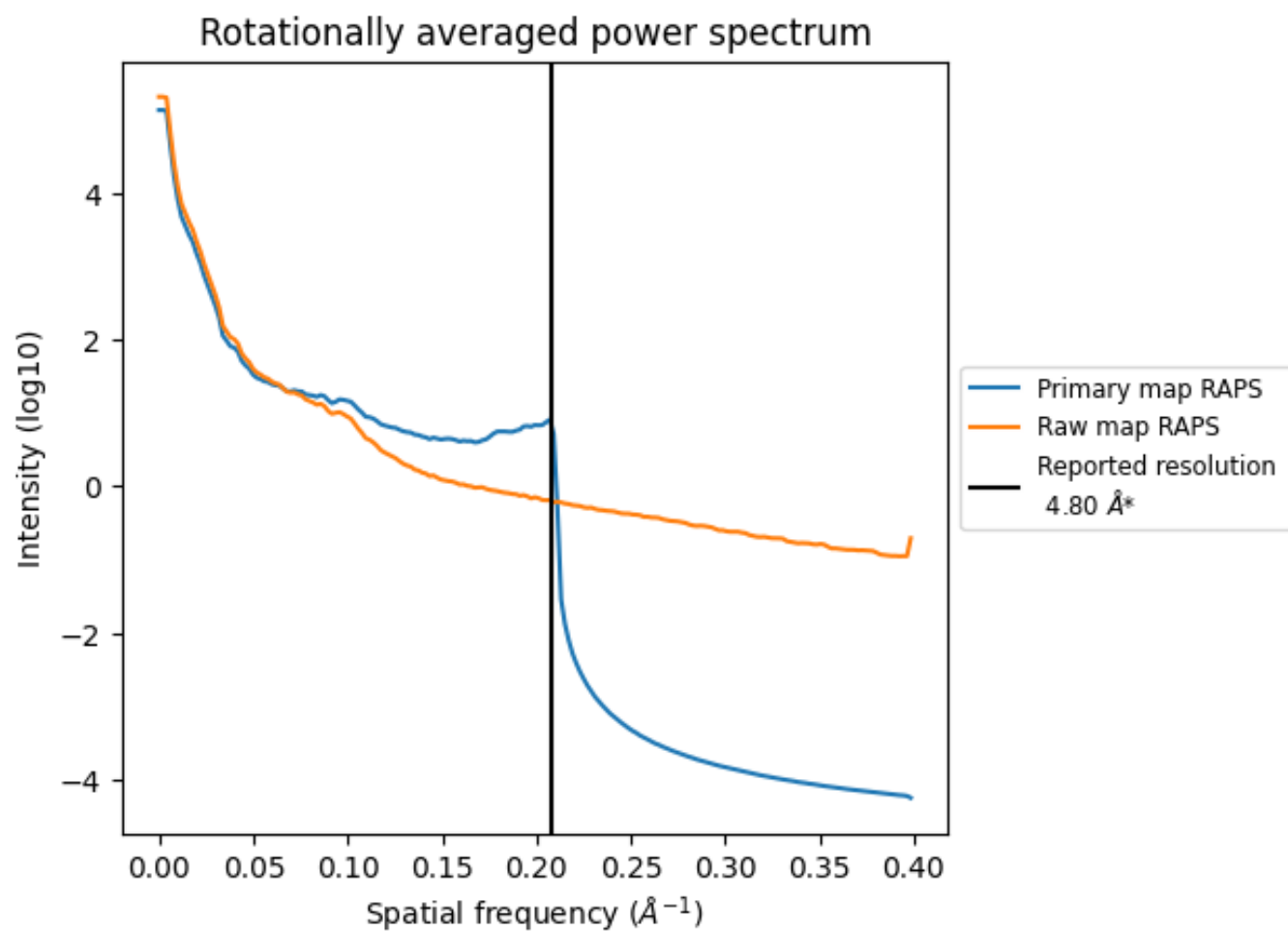
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 605 nm³; this corresponds to an approximate mass of 547 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 ⓘ

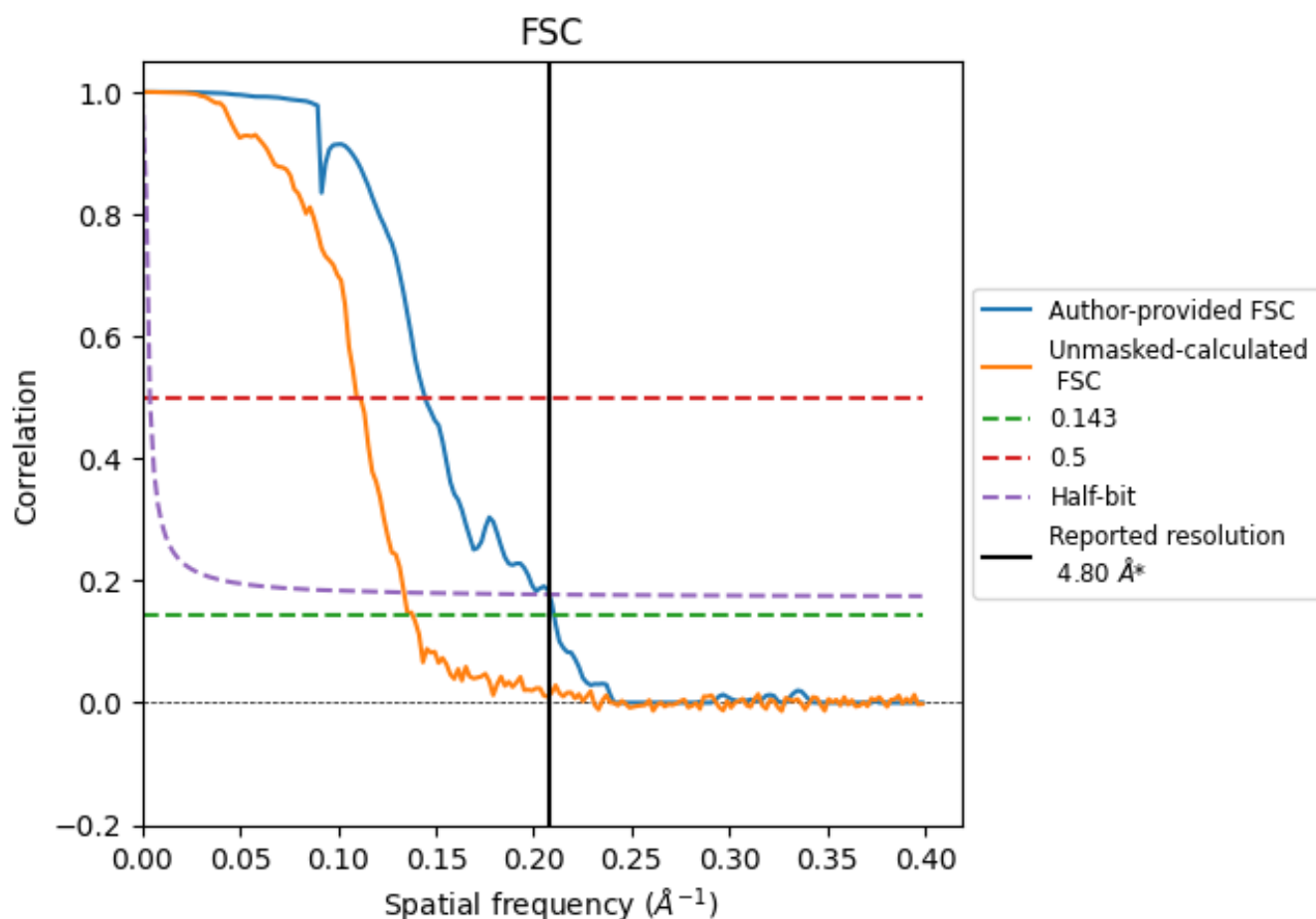


*Reported resolution corresponds to spatial frequency of 0.208 $\text{\AA}^{-1}$

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

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	4.76	6.92	4.81
Unmasked-calculated*	7.24	9.13	7.48

*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 7.24 differs from the reported value 4.8 by more than 10 %

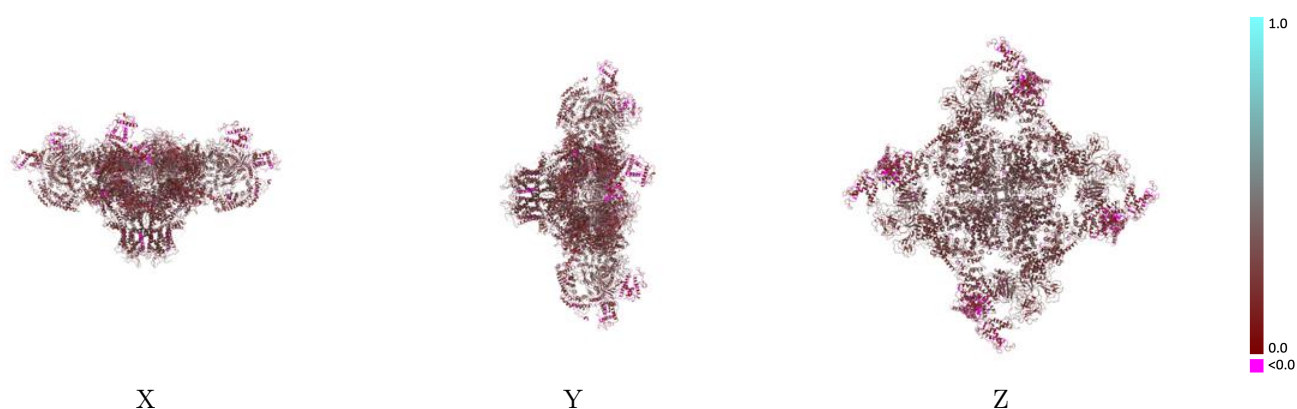
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8386 and PDB model 5TAV. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

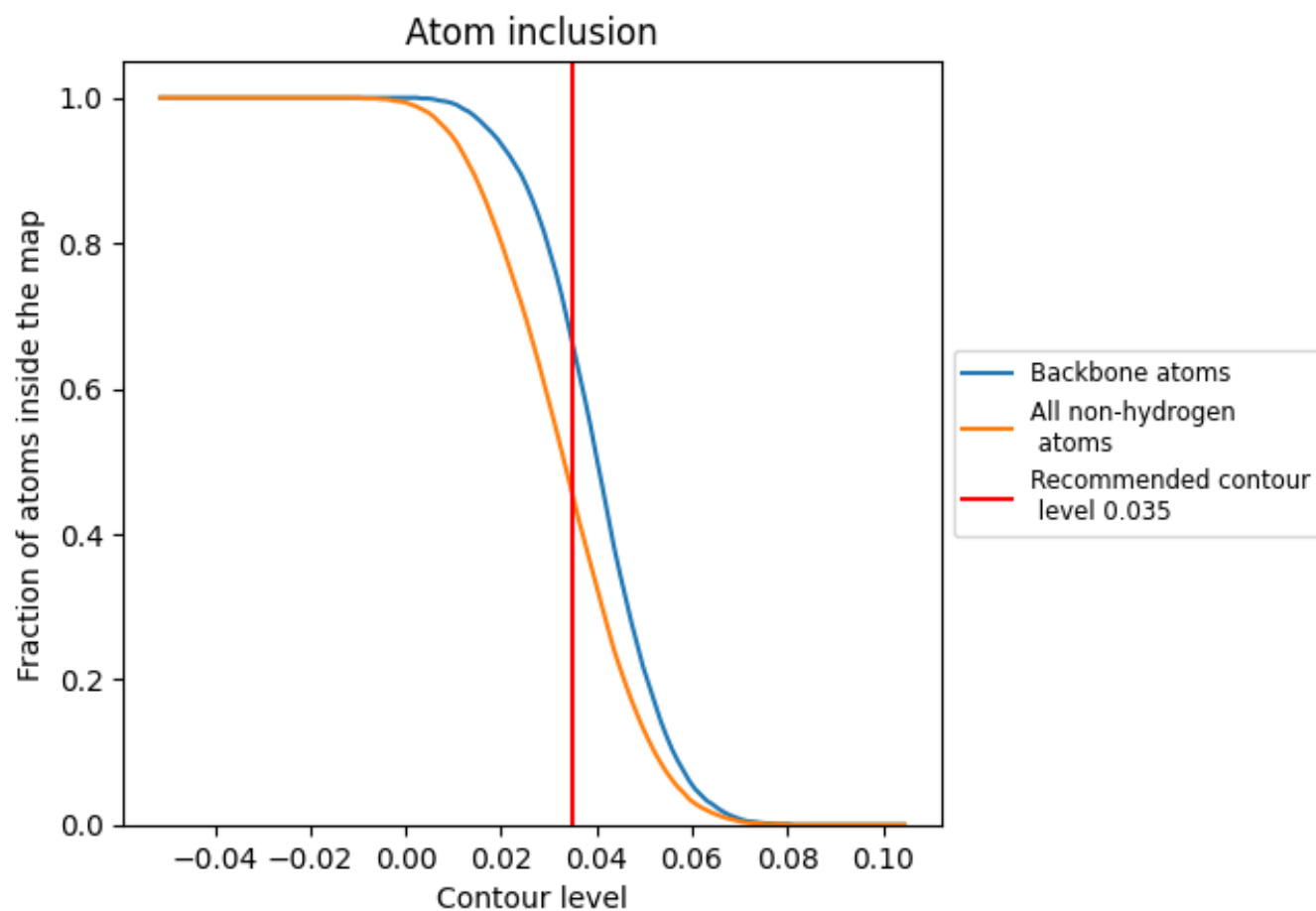


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	0.4530	0.2520
A	0.4630	0.2710
B	0.4530	0.2520
E	0.4520	0.2520
F	0.4650	0.2720
G	0.4520	0.2510
H	0.4620	0.2720
I	0.4530	0.2520
J	0.4620	0.2720

1.0

0.0

<0.0