



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 03:30 PM EDT

PDB ID : 5TAU
EMDB ID : EMD-8385
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 6.20 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

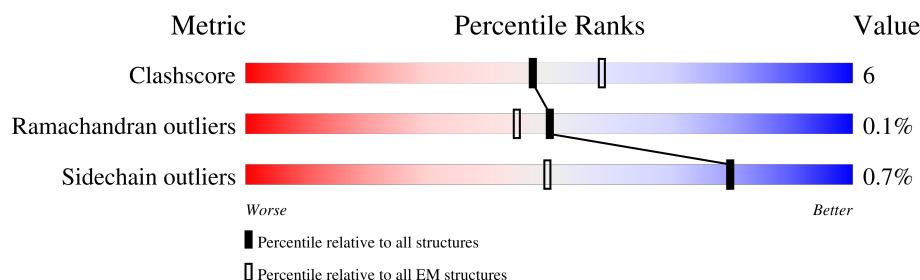
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121436 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.

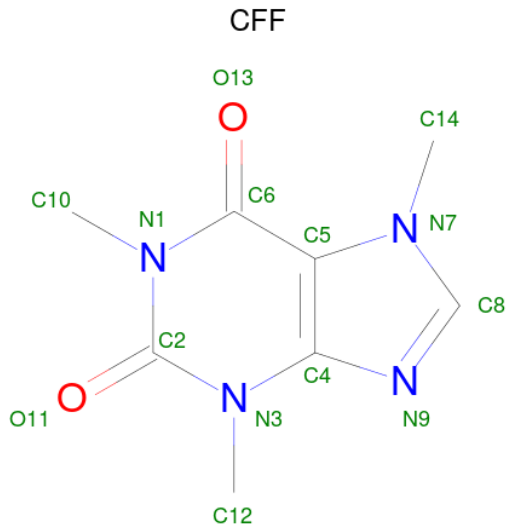
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29495	18683	5227	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

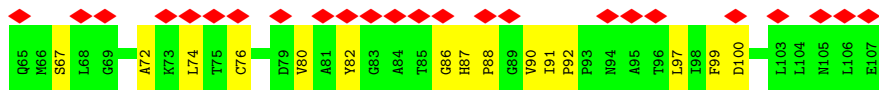
- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



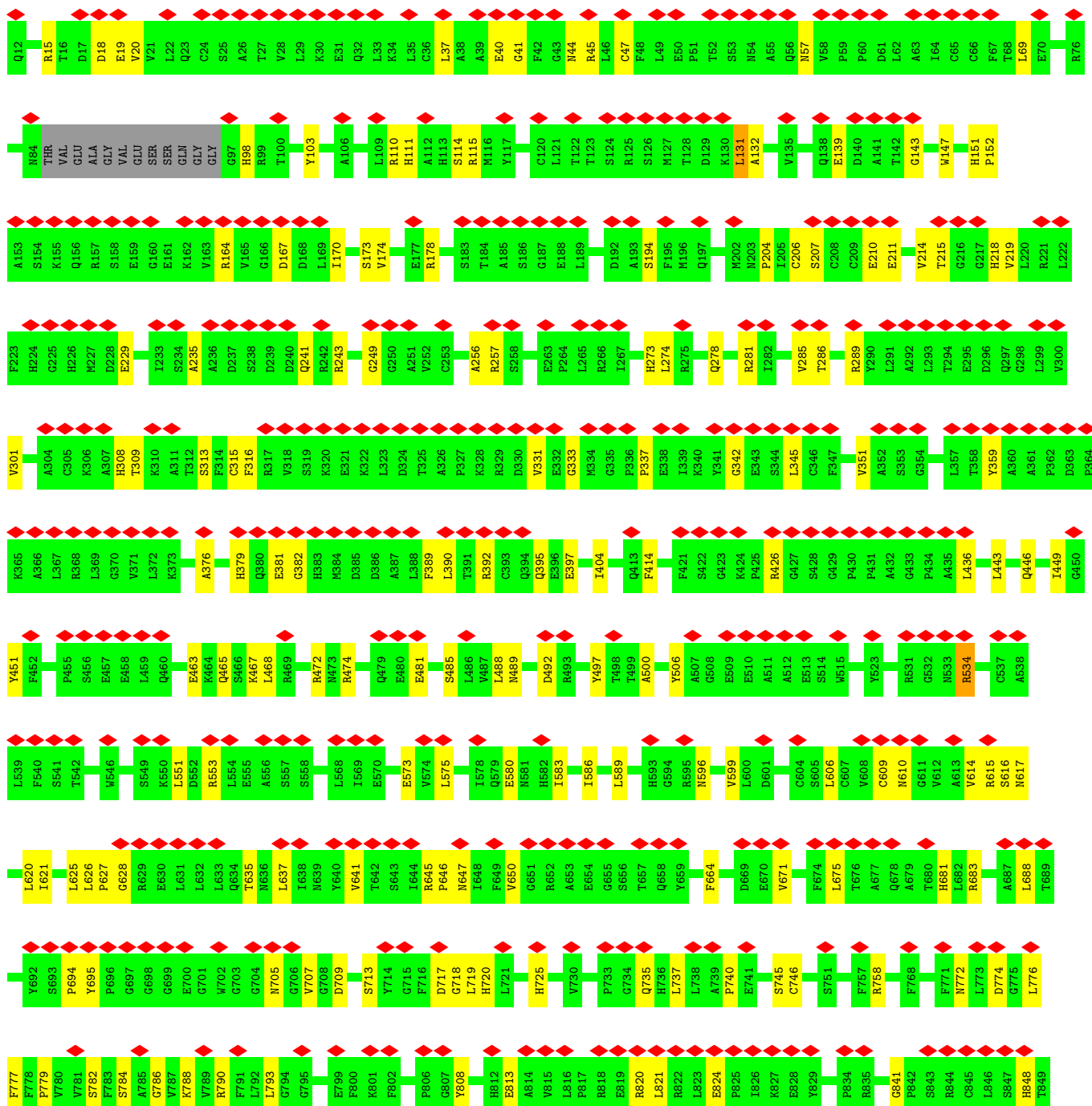
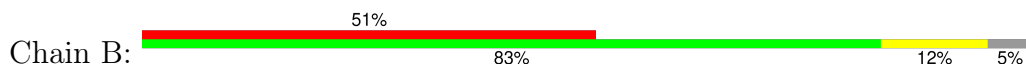
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

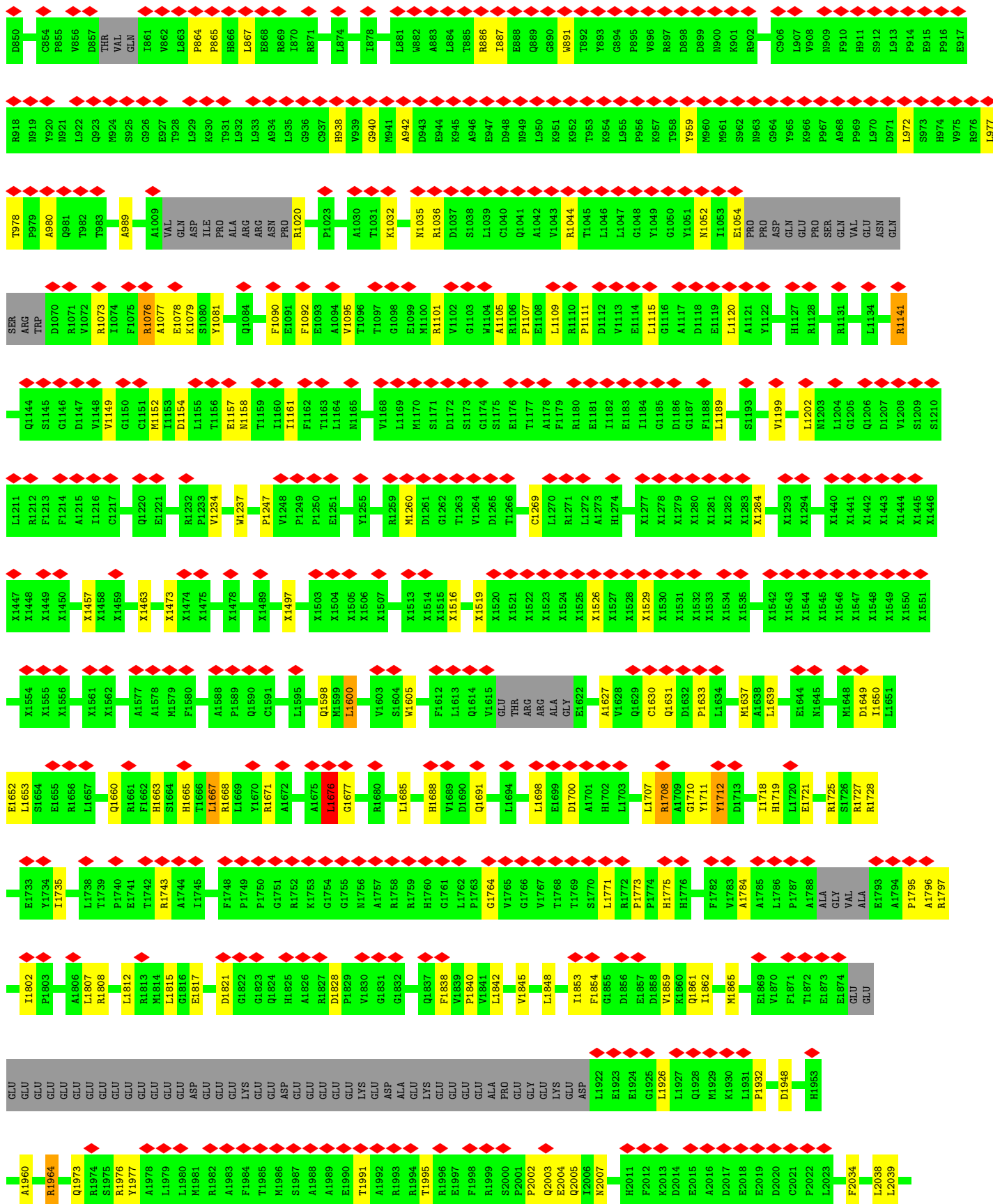
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	



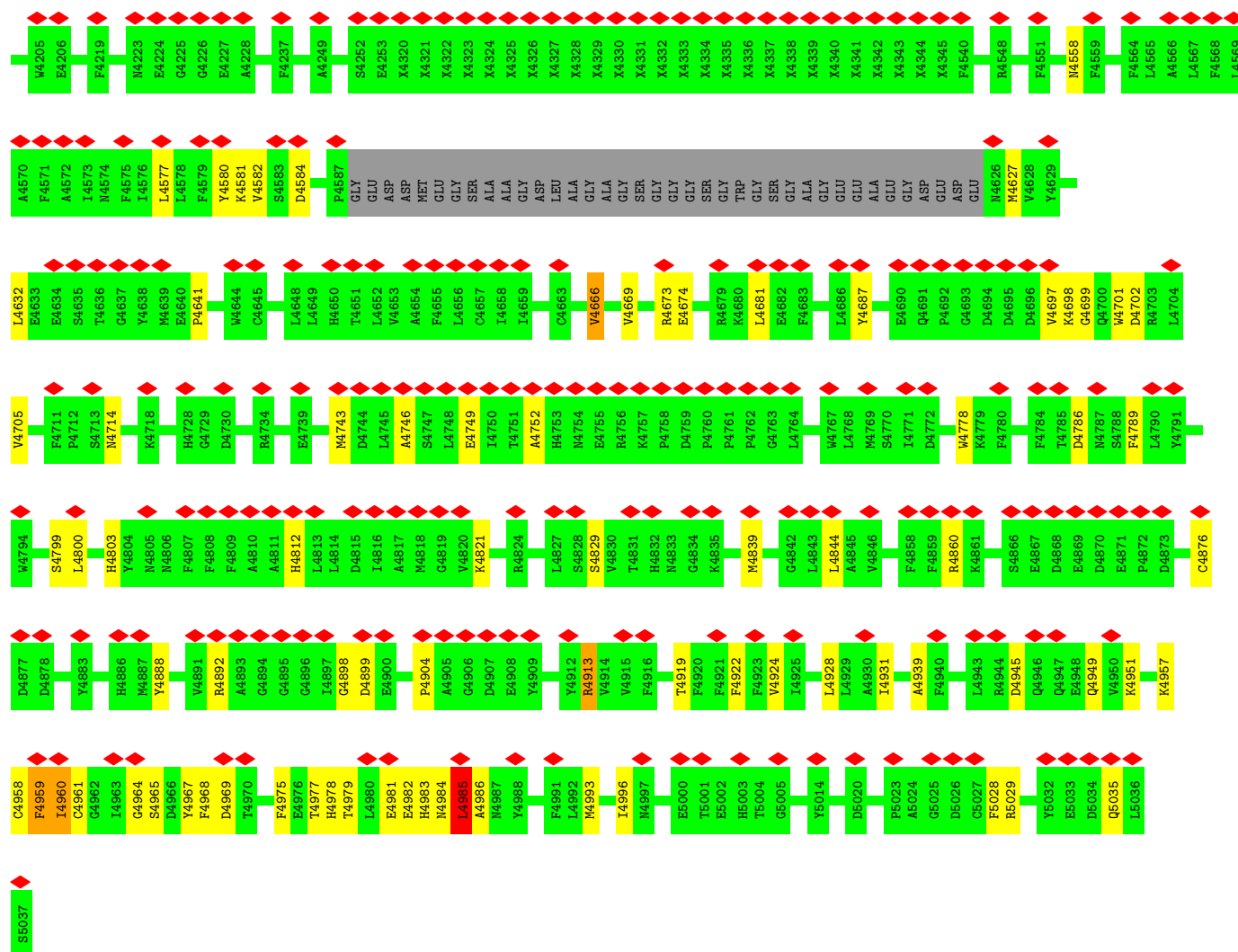
- Molecule 2: Ryanodine receptor 1



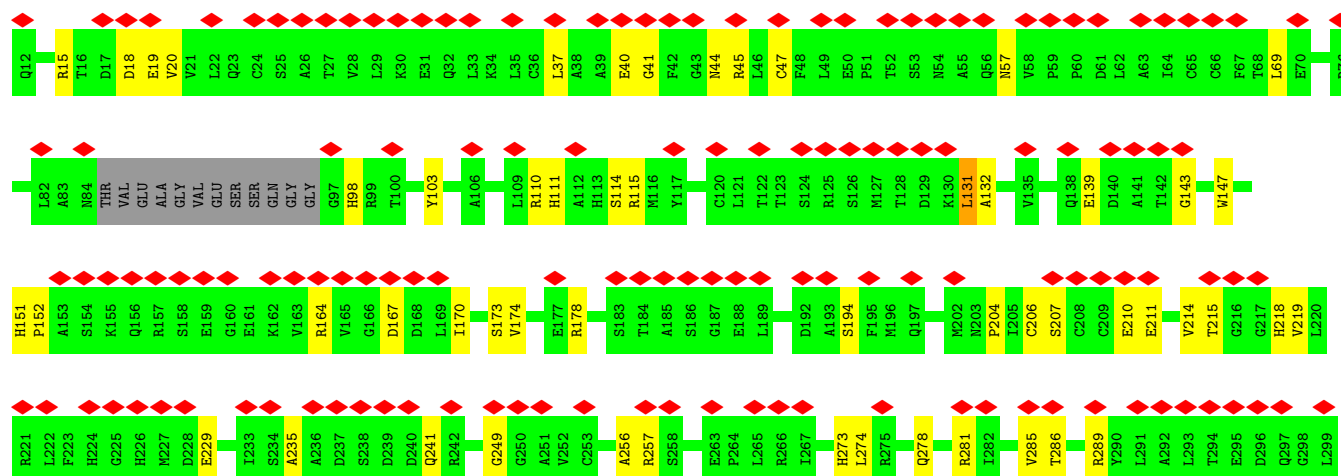
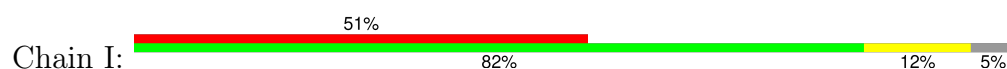


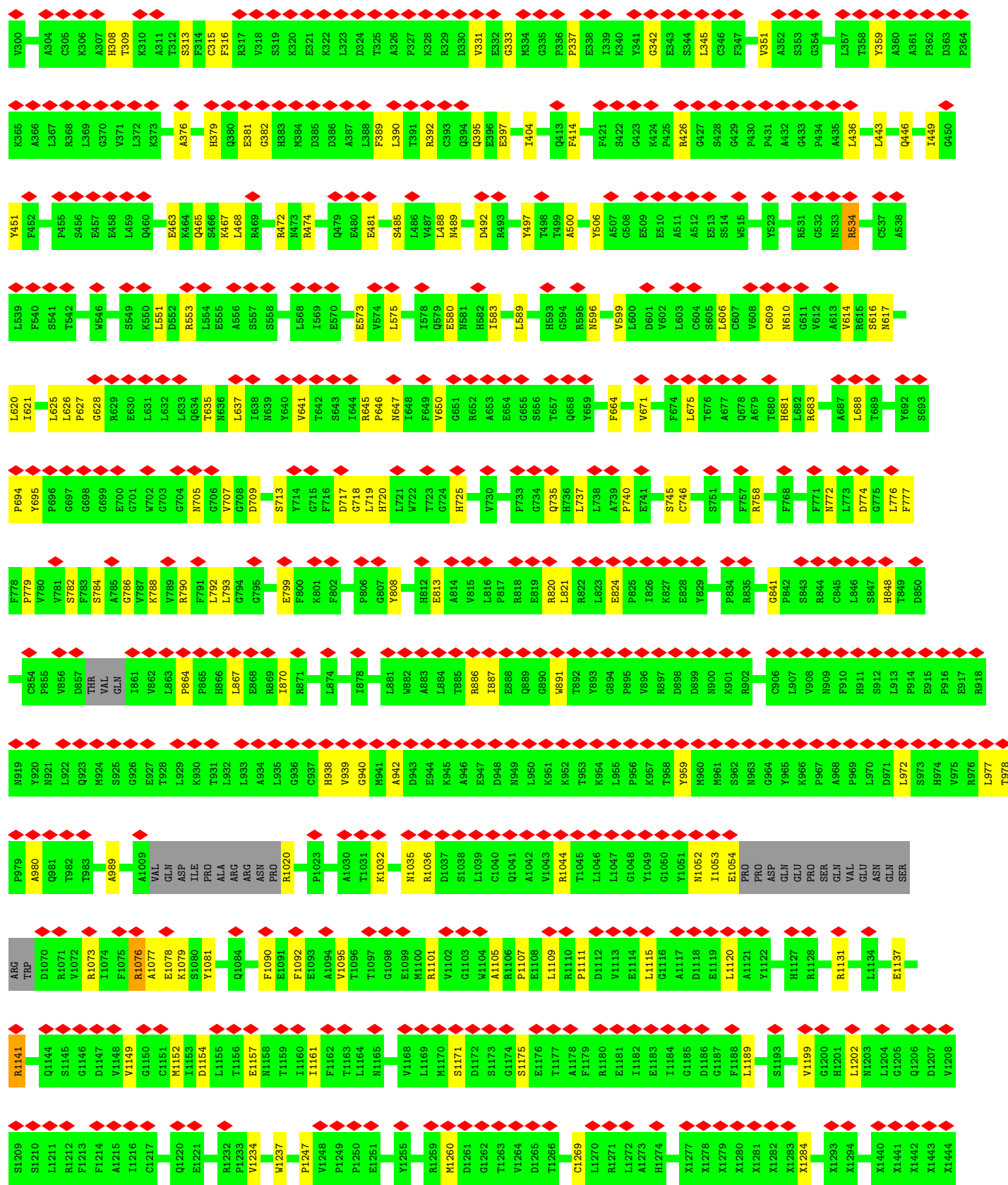
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X2966	X2967	X2968	X2969	X2970	X2971	X2972	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3003	X3006	X3010	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050					
P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2964	X2965	
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SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	Y2855	M2856	P2857	Q2858	P2859	D2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	R2868	E2870	L2871	Q2872	A2873	M2874	E2875	A2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	M2884	T2885	W2886	G2887	L2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	D2899	G2900	T2901	H2902		
C2042	C2043	L2044	Q2045	L2046	E2047	C2048	GLU	GLU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG	ARG	SER	LEU	LEU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	GLU	LYS	PRO	ALA	GLU	X2089	X2090	P2091	Q2092	S2093	D2109	Q2112	X2118	X2119	H2125												
R2126	Q2127	Y2128	D2129	G2130	L2131	G2132	R2136	A2141	S2145	P2146	S2147	E2150	L2155	L2166	M2170	N2187	N2188	K2189	V2190	F2191	Y2192	N2196	R2199	A2200	H2204	N2213	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	K2224	F2225	P2226	K2227	S2231	R2234	F2235	F2239															
R2248	F2251	D2252	H2253	L2254	S2255	L2256	L2257	L2258	E2259	N2260	S2261	Q2262	I2263	G2264	L2265	G2266	M2267	Q2268	G2269	S2270	T2271	L2273	A2276	A2277	E2285	L2286	A2287	L2288	A2289	L2290	Q2291	E2292	Q2293	D2294	L2295	Y2301	G2304	C2305	L2307	Q2308	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316	P2319	D2320									
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P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2415	V2416	G2419	H2420	D2431	P2438	E2439	M2440	H2441	L2442	I2443	K2447	R2452	L2457	R2458	S2459	L2460	L2463	D2464	D2465	L2466	V2467	G2468	I2469	I2470	S2471	L2472	P2473	L2474	Q2475	L2476	P2477	T2478										
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X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	I2776	Y2777	G2778	E2779	N2780	V2781	D2782
E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	V2794	T2795	T2796	F2797	S2798	E2799	K2800	K2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	E2813	K2814	A2815	M2816	L2817	E2818	Y2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	E2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	
SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	Y2855	M2856	P2857	Q2858	P2859	D2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	R2868	E2870	L2871	Q2872	A2873	M2874	E2875	A2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	M2884	T2885	W2886	G2887	L2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	D2899	G2900	T2901	H2902		
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L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	Y3720	M3723	H3729	A3730	K3731	S3732	C3733	H3734	L3735	E3736	E3737	G3738	G3739	E3740	N3741	GLY	ALA	GLU	R3672	M3673	I3674	S3678	K3679	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	X3688	X3689	X3690	X3691	V3690	E3691	E3692	K3693	K3694	P3695	Q3700	H3704	R3707									
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X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324			
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• Molecule 2: Ryanodine receptor 1

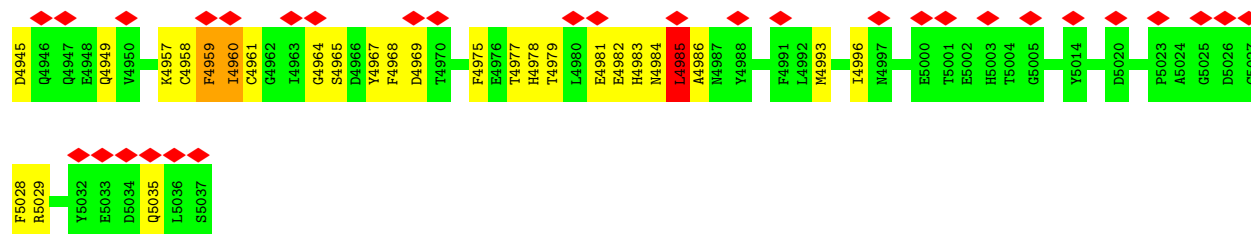






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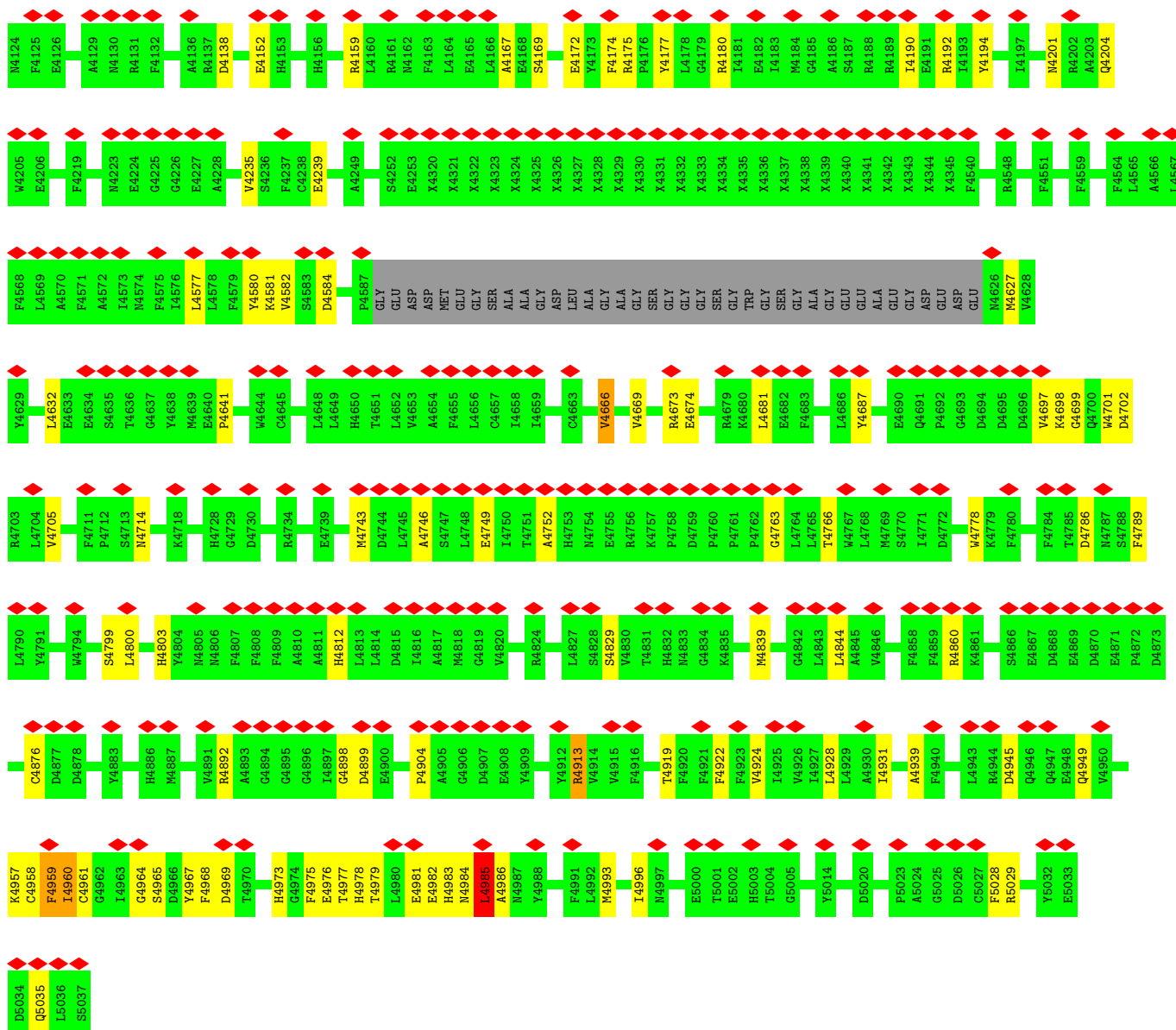




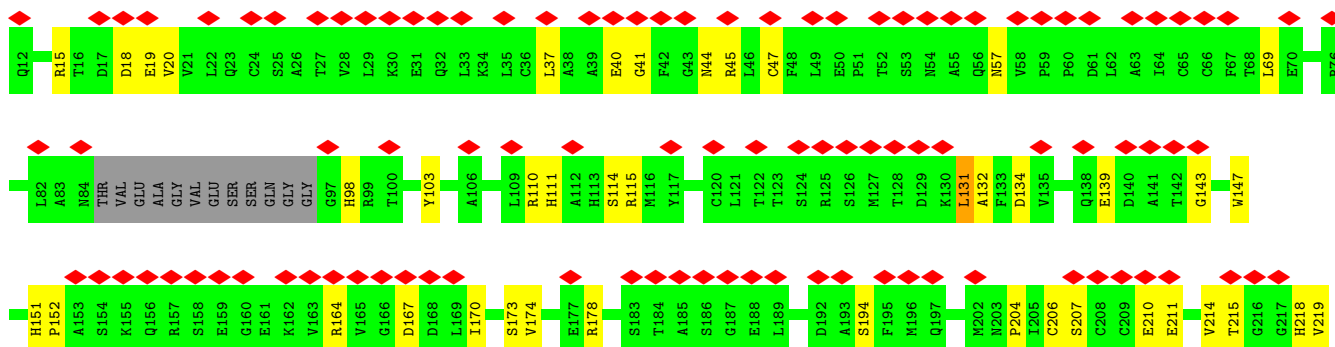
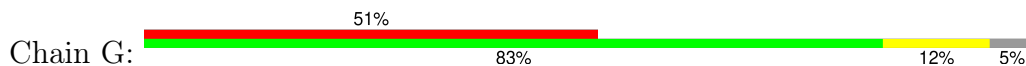


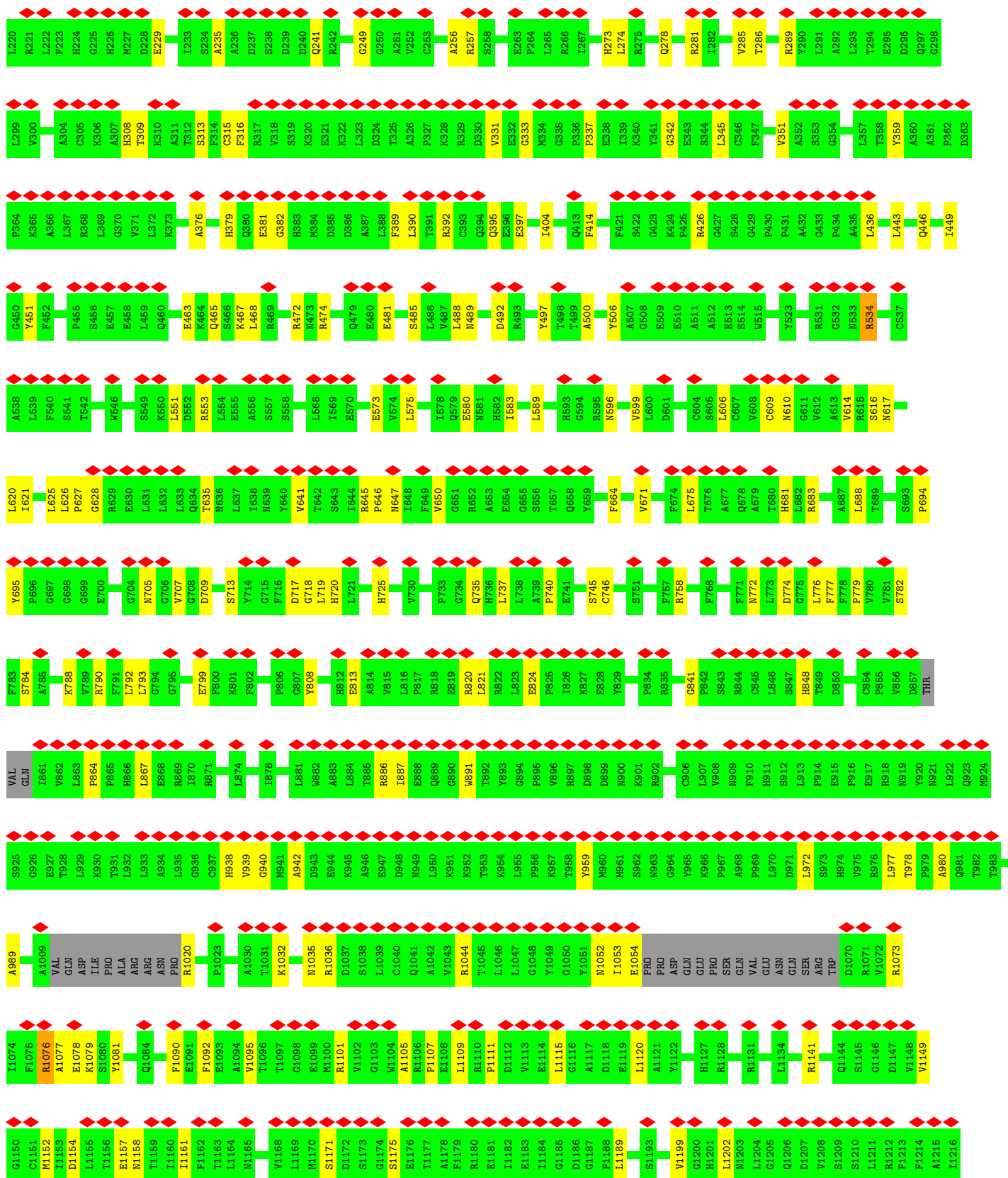
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• Molecule 2: Ryanodine receptor 1

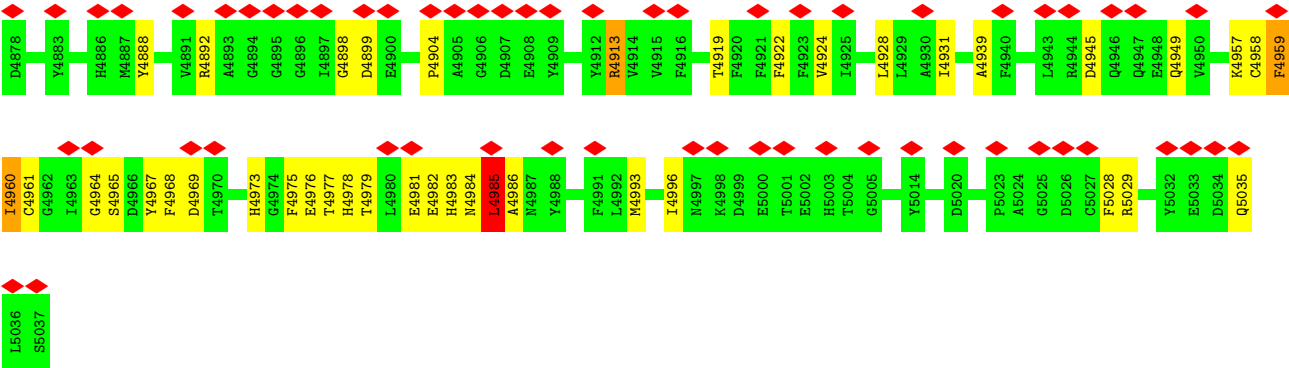






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X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3071	X3072	X3073	X3074	X3075	X3076	X3077	X3078	X3079	X3080	X3081	X3082	X3083	X3084	X3085	X3086	X3087	X3088	X3089	X3090	X3091	X3092	X3093	X3094	X3095	X3096	X3097	X3098	X3099	X3100	X3101	X3102	X3103	X3104	X3105	X3106	X3107	X3108	X3109	X3110	X3111	X3112	X3113	X3114	X3115	X3116	X3117	X3118	X3119	X3120	X3121	X3122	X3123	X3124	X3125	X3126	X3127		
X2971	X2972	X2973	X2974	X2975	X2976	X2977	X2978	X2979	X2980	X2981	X2982	X2983	X2984	X2985	X2986	X2987	X2988	X2989	X2990	X2991	X2992	X2993	X2994	X2995	X2996	X2997	X2998	X2999	X3000	X3003	X3006	X3010	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3052	X3055	X3056	X3059
Y2908	D2909	T2910	L2911	T2912	A2913	X2914	E2915	X2916	E2917	A2918	D2919	X2920	E2921	X2922	A2923	E2924	X2925	L2926	L2927	X2928	F2929	L2930	Q2931	X2932	N2933	G2934	Y2935	X2936	V2937	T2938	X2939	N2940	X2941	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2967	X2968	X2969	X2970										
THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	R2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	Q2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907													
H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	D2800	E2801	K2802	E2803	L2804	Y2805	R2806	V2807	P2808	E2809	L2810	E2811	D2812	L2813	K2814	A2815	M2816	L2817	A2818	N2819	E2820	N2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	T2901	H2902	P2903	L2904	L2905	V2906	P2907											
X2607	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697																
X2489	X2490	X2493	X2502	X2511	X2512	X2513	X2514	X2517	X2521	X2522	X2523	X2524	X2529	X2530	X2531	X2532	X2533	X2536	X2537	X2555	X2556	X2557	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2581	X2582	X2583	X2584	X2585	X2586	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2605	X2606																									
X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	R2738	P2739	E2740	E2741	T2742	L2743	V2744	I2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	D2753	P2754	I2755	N2756	K2757	P2758	A2759	E2760	X2761	T2762	H2763	E2764	K2765	N2766	A2767	P2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	T2777	G2778	E2779	N2780	V2781	D2782	E2783	I2784	L2785	K2786	T2787													





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	0.076	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.032	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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.52	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25424	0.53	8/34530 (0.0%)
2	E	0.29	0/25424	0.53	9/34530 (0.0%)
2	G	0.29	0/25424	0.53	8/34530 (0.0%)
2	I	0.29	0/25424	0.53	8/34530 (0.0%)
All	All	0.29	0/105032	0.53	33/142612 (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 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	LEU	CA-CB-CG	8.24	134.26	115.30
2	E	131	LEU	CA-CB-CG	8.24	134.25	115.30
2	I	131	LEU	CA-CB-CG	8.23	134.24	115.30
2	G	131	LEU	CA-CB-CG	8.23	134.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4985	LEU	CA-CB-CG	7.85	133.36	115.30

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	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	18	0
1	F	818	0	824	20	0
1	H	818	0	824	15	0
1	J	818	0	824	17	0
2	B	29495	0	24734	313	0
2	E	29495	0	24734	312	0
2	G	29495	0	24734	310	0
2	I	29495	0	24734	314	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	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	121436	0	102320	1289	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 6.

The worst 5 of 1289 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:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.60	0.90
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.60	0.90
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.60	0.89
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.60	0.89
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.86	0.76

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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2926 (90%)	304 (9%)	5 (0%)	44	78
2	E	3235/4416 (73%)	2924 (90%)	306 (10%)	5 (0%)	44	78
2	G	3235/4416 (73%)	2925 (90%)	305 (9%)	5 (0%)	44	78
2	I	3235/4416 (73%)	2922 (90%)	308 (10%)	5 (0%)	44	78
All	All	13360/18096 (74%)	12077 (90%)	1263 (10%)	20 (0%)	50	83

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU

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Mol	Chain	Res	Type
2	I	4985	LEU
2	E	4985	LEU
2	G	4985	LEU
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	2492/3022 (82%)	2473 (99%)	19 (1%)	79	85
2	E	2492/3022 (82%)	2473 (99%)	19 (1%)	79	85
2	G	2492/3022 (82%)	2473 (99%)	19 (1%)	79	85
2	I	2492/3022 (82%)	2473 (99%)	19 (1%)	79	85
All	All	10320/12444 (83%)	10244 (99%)	76 (1%)	80	87

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	131	LEU
2	G	4120	ASN
2	G	553	ARG
2	G	3663	LEU
2	G	4960	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4120	ASN

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Mol	Chain	Res	Type
2	G	3950	ASN
2	G	57	ASN
2	G	1598	GLN
2	G	4120	ASN

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
4	CFF	B	5102	-	8,15,15	2.12	3 (37%)	8,23,23	1.34	1 (12%)
3	ATP	E	5101	-	28,33,33	0.98	1 (3%)	34,52,52	1.21	2 (5%)
4	CFF	I	5102	-	8,15,15	2.13	3 (37%)	8,23,23	1.36	2 (25%)
4	CFF	E	5102	-	8,15,15	2.12	3 (37%)	8,23,23	1.34	1 (12%)
3	ATP	B	5101	-	28,33,33	0.98	1 (3%)	34,52,52	1.21	2 (5%)
4	CFF	G	5102	-	8,15,15	2.12	3 (37%)	8,23,23	1.34	1 (12%)
3	ATP	G	5101	-	28,33,33	0.98	1 (3%)	34,52,52	1.21	2 (5%)
3	ATP	I	5101	-	28,33,33	0.99	1 (3%)	34,52,52	1.21	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C5-C4	-3.55	1.33	1.39
4	B	5102	CFF	C5-C4	-3.55	1.33	1.39
4	E	5102	CFF	C5-C4	-3.55	1.33	1.39
4	I	5102	CFF	C5-C4	-3.54	1.33	1.39
4	I	5102	CFF	C6-N1	-3.30	1.32	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5101	ATP	N3-C2-N1	-3.56	123.83	128.67
3	E	5101	ATP	N3-C2-N1	-3.54	123.87	128.67
3	I	5101	ATP	N3-C2-N1	-3.53	123.88	128.67
3	B	5101	ATP	N3-C2-N1	-3.53	123.88	128.67
3	E	5101	ATP	C4-C5-N7	-2.79	106.39	109.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

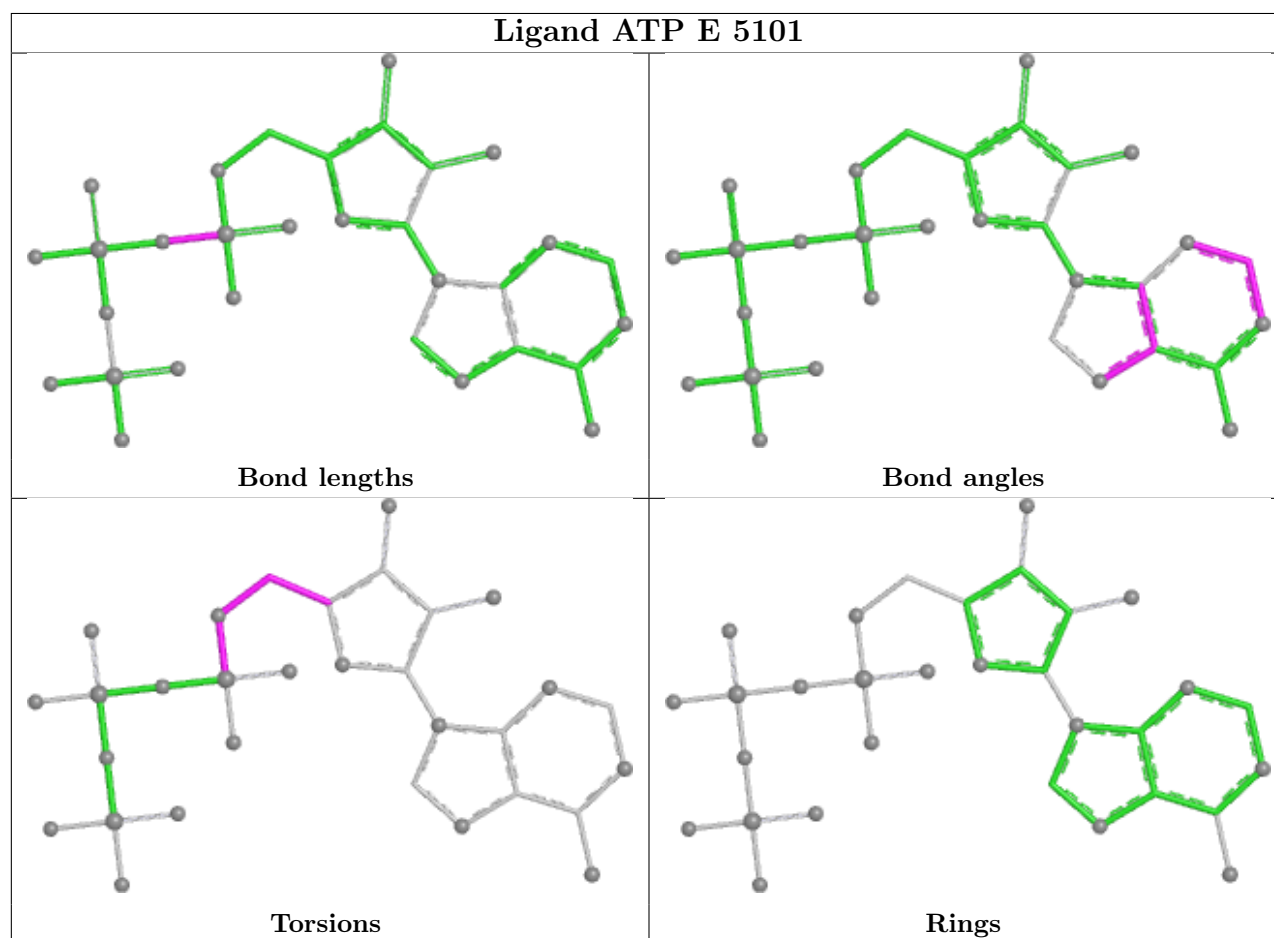
Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

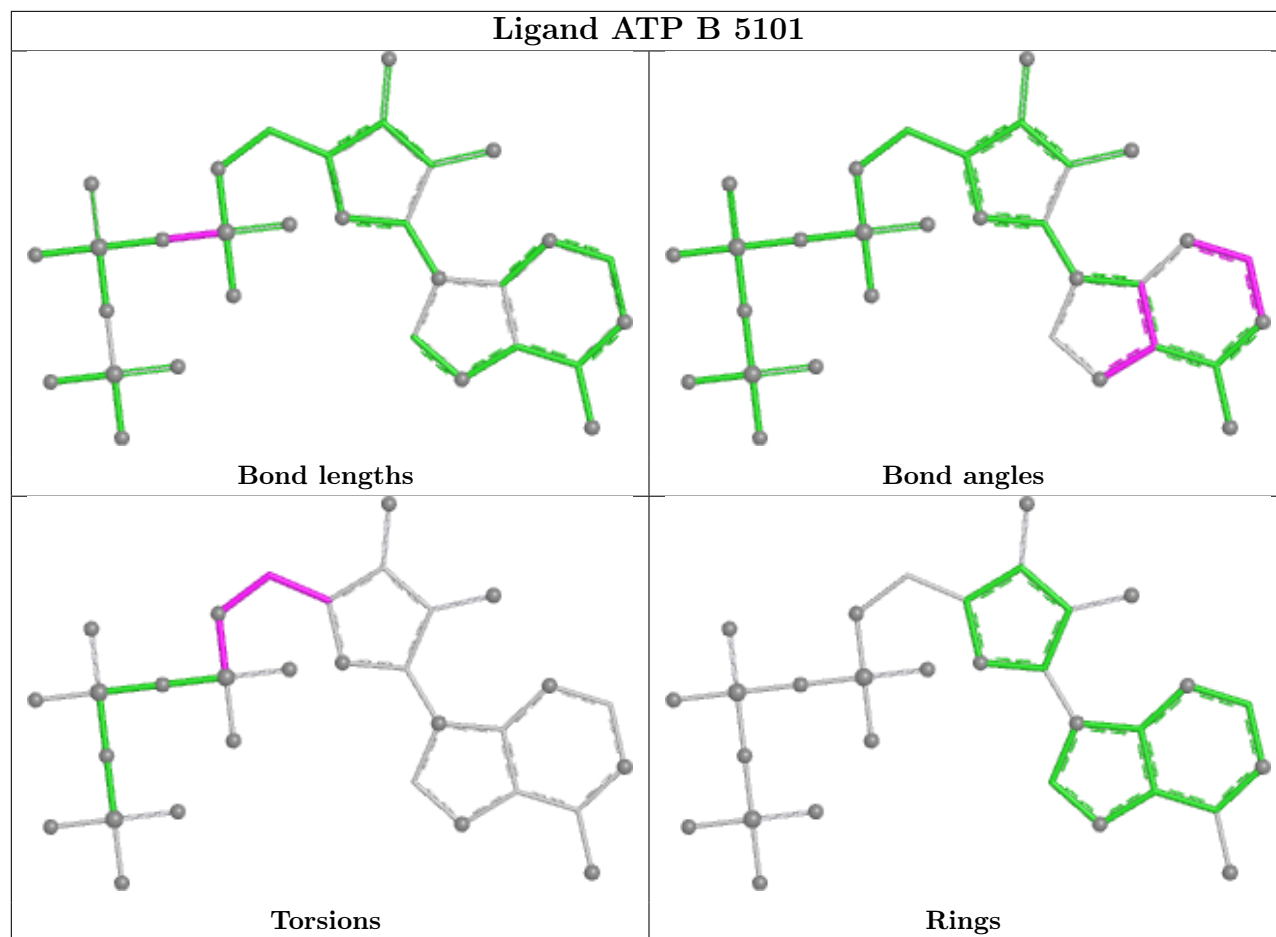
There are no ring outliers.

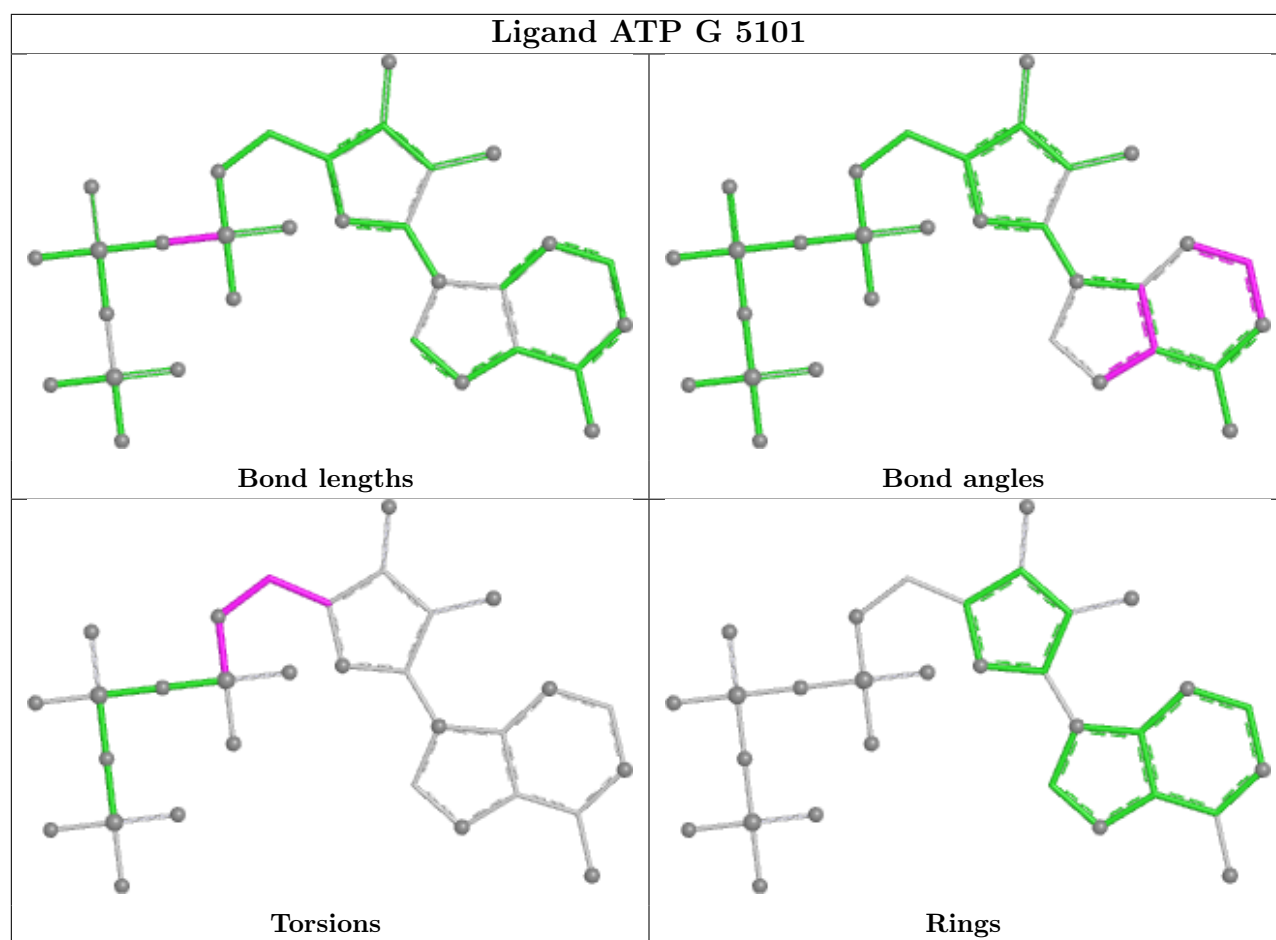
4 monomers are involved in 4 short contacts:

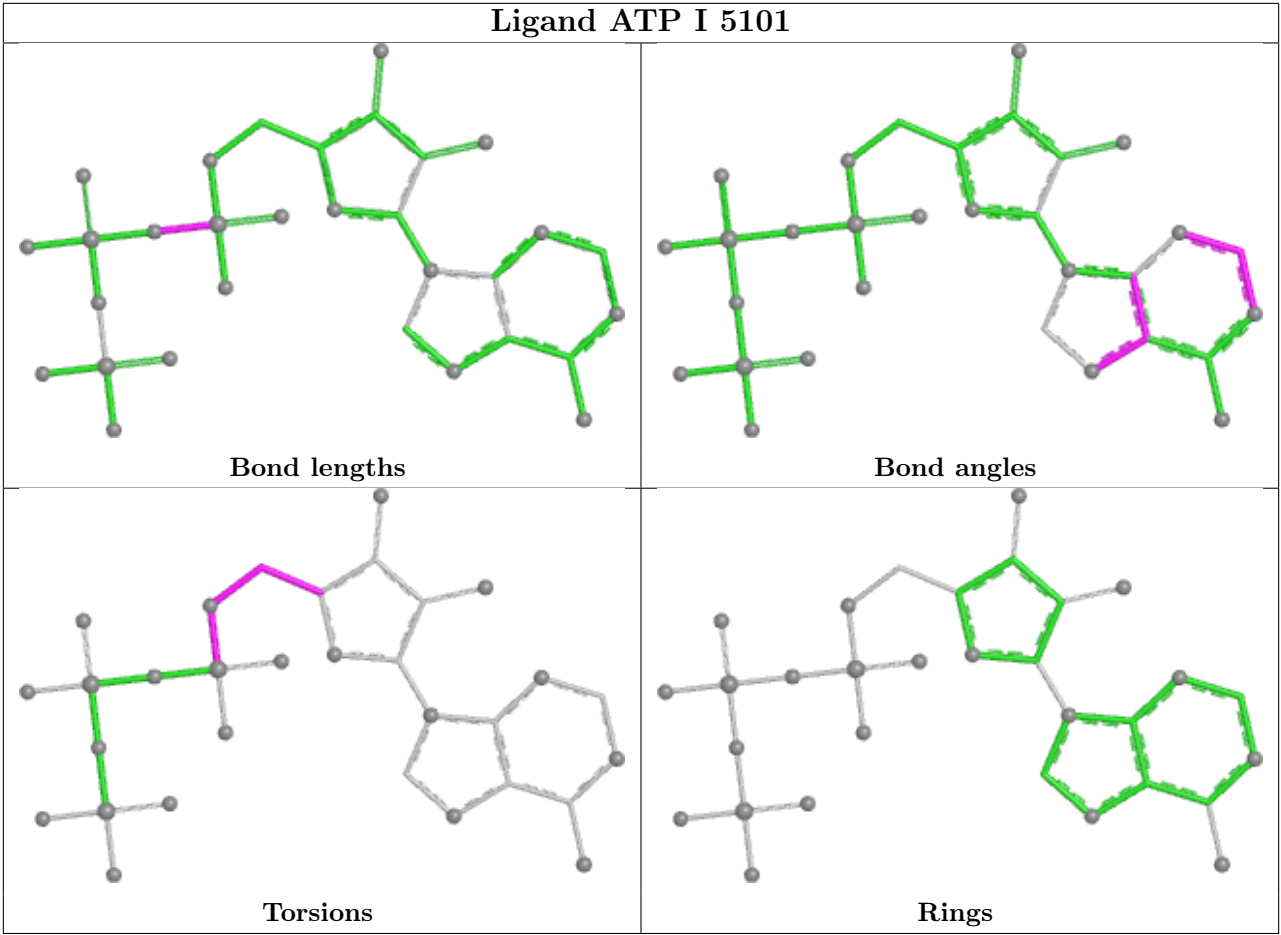
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	1	0

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	I	14
2	E	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	72.97
1	I	4345:UNK	C	4540:PHE	N	72.97

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.97
1	G	4345:UNK	C	4540:PHE	N	72.97
1	B	3613:UNK	C	3639:THR	N	44.25

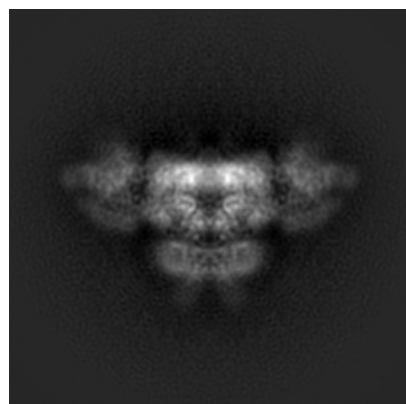
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8385. These allow visual inspection of the internal detail of the map and identification of artifacts.

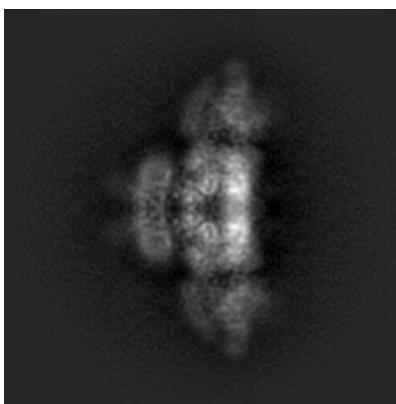
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

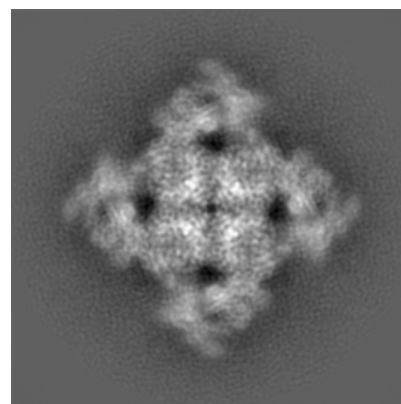
6.1.1 Primary map



X

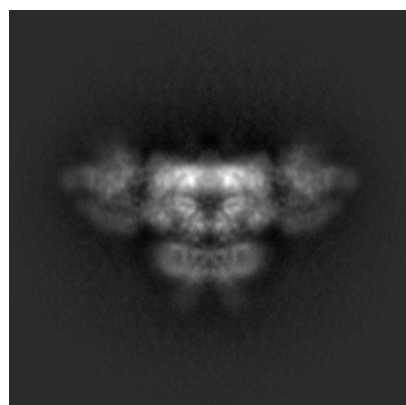


Y

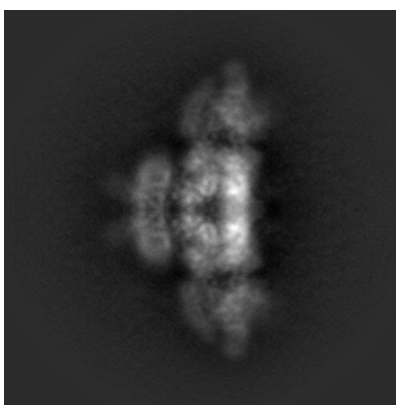


Z

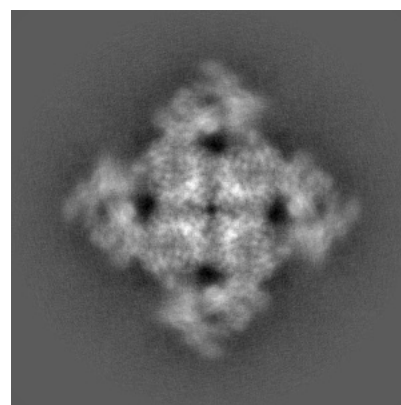
6.1.2 Raw map



X



Y

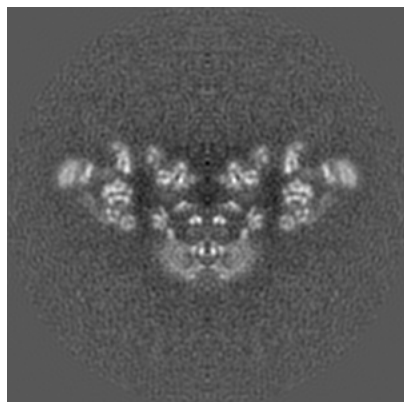


Z

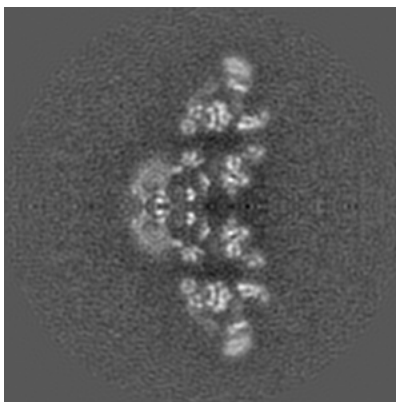
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

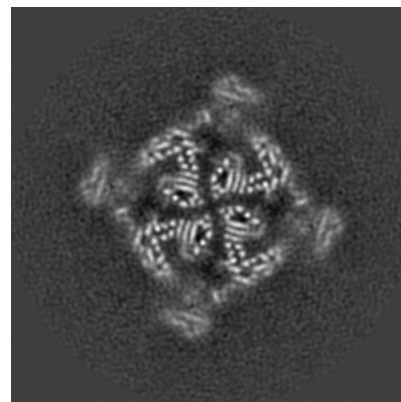
6.2.1 Primary map



X Index: 200

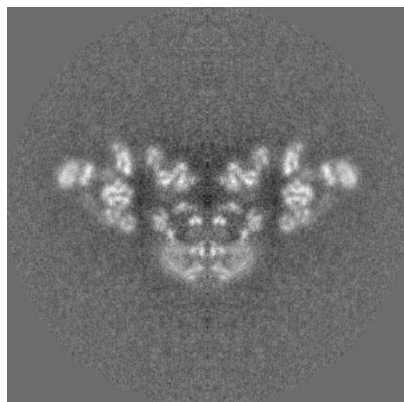


Y Index: 200

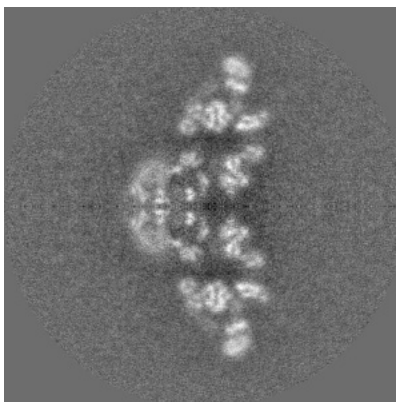


Z Index: 200

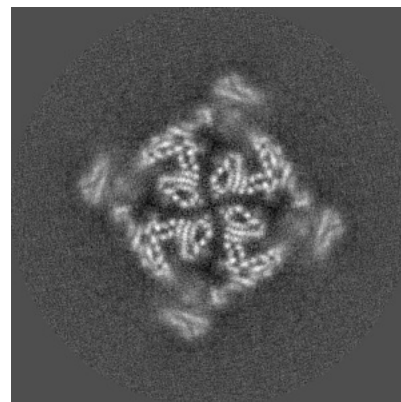
6.2.2 Raw map



X Index: 200



Y Index: 200

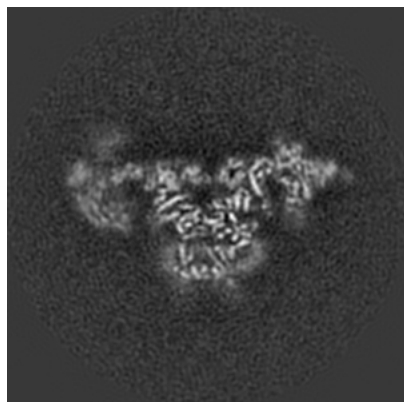


Z Index: 200

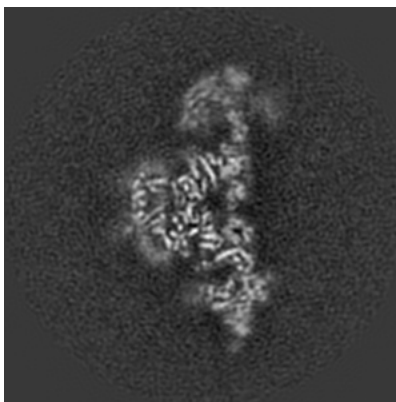
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

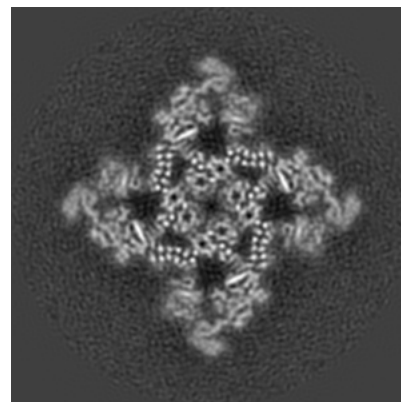
6.3.1 Primary map



X Index: 184

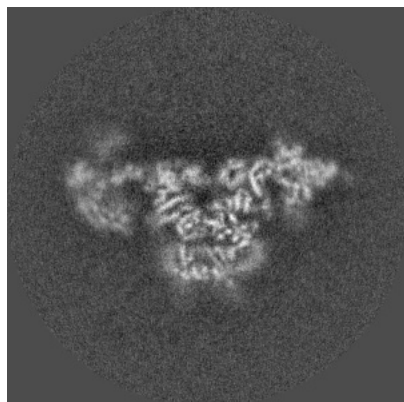


Y Index: 184

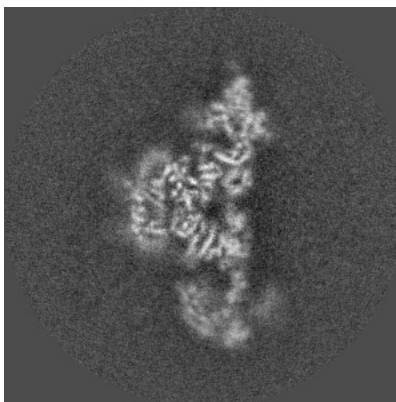


Z Index: 227

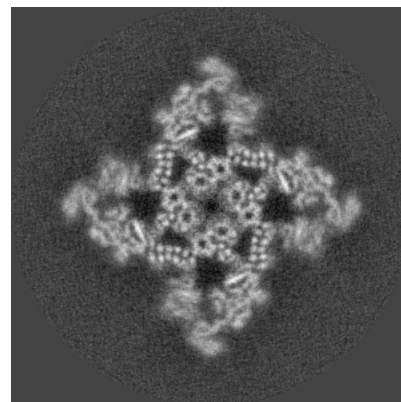
6.3.2 Raw map



X Index: 184



Y Index: 216

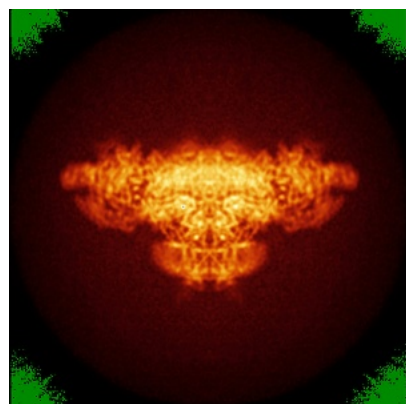


Z Index: 226

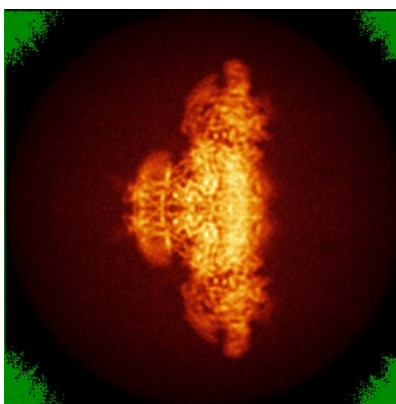
The images above show the largest variance slices of the map in three orthogonal directions.

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

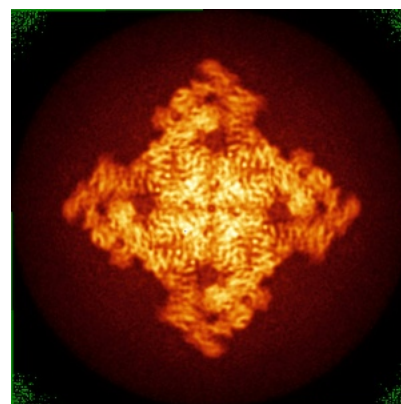
6.4.1 Primary map



X

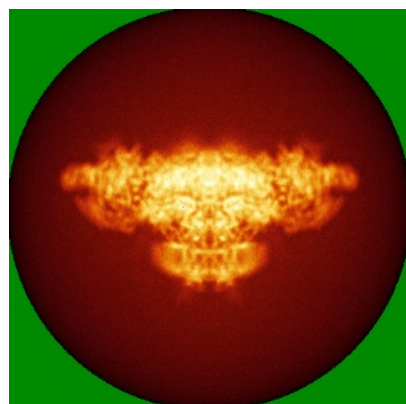


Y

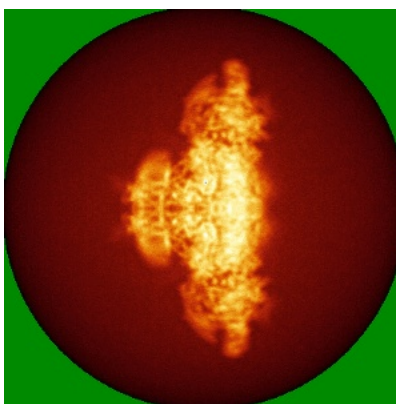


Z

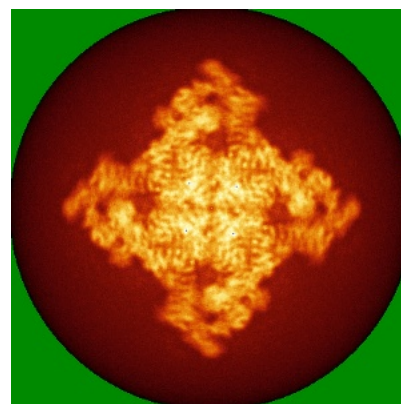
6.4.2 Raw map



X



Y

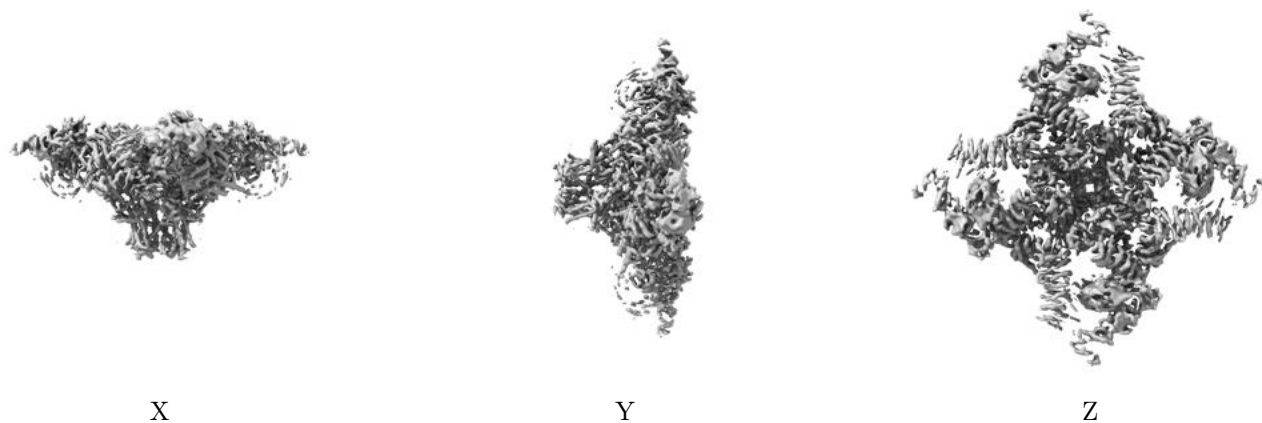


Z

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.

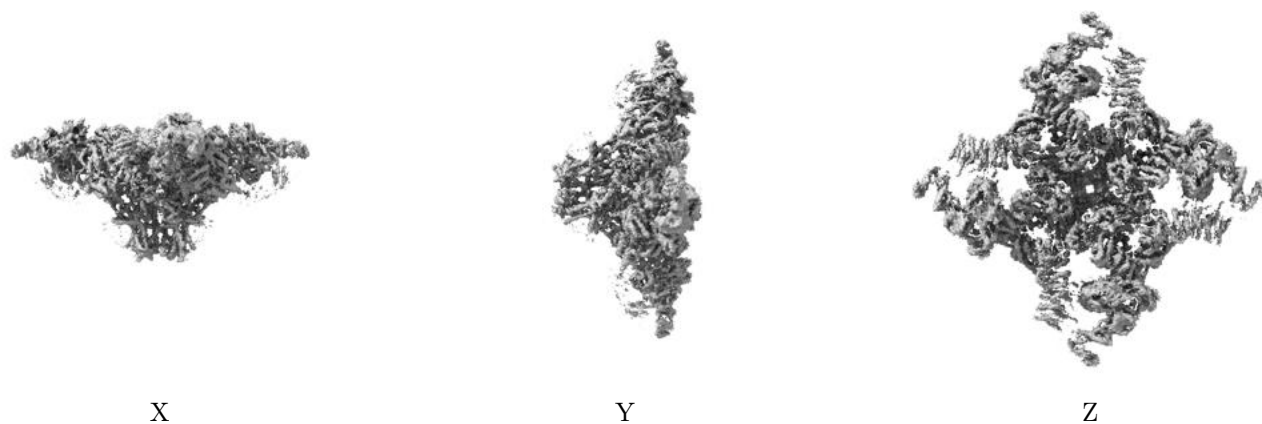
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

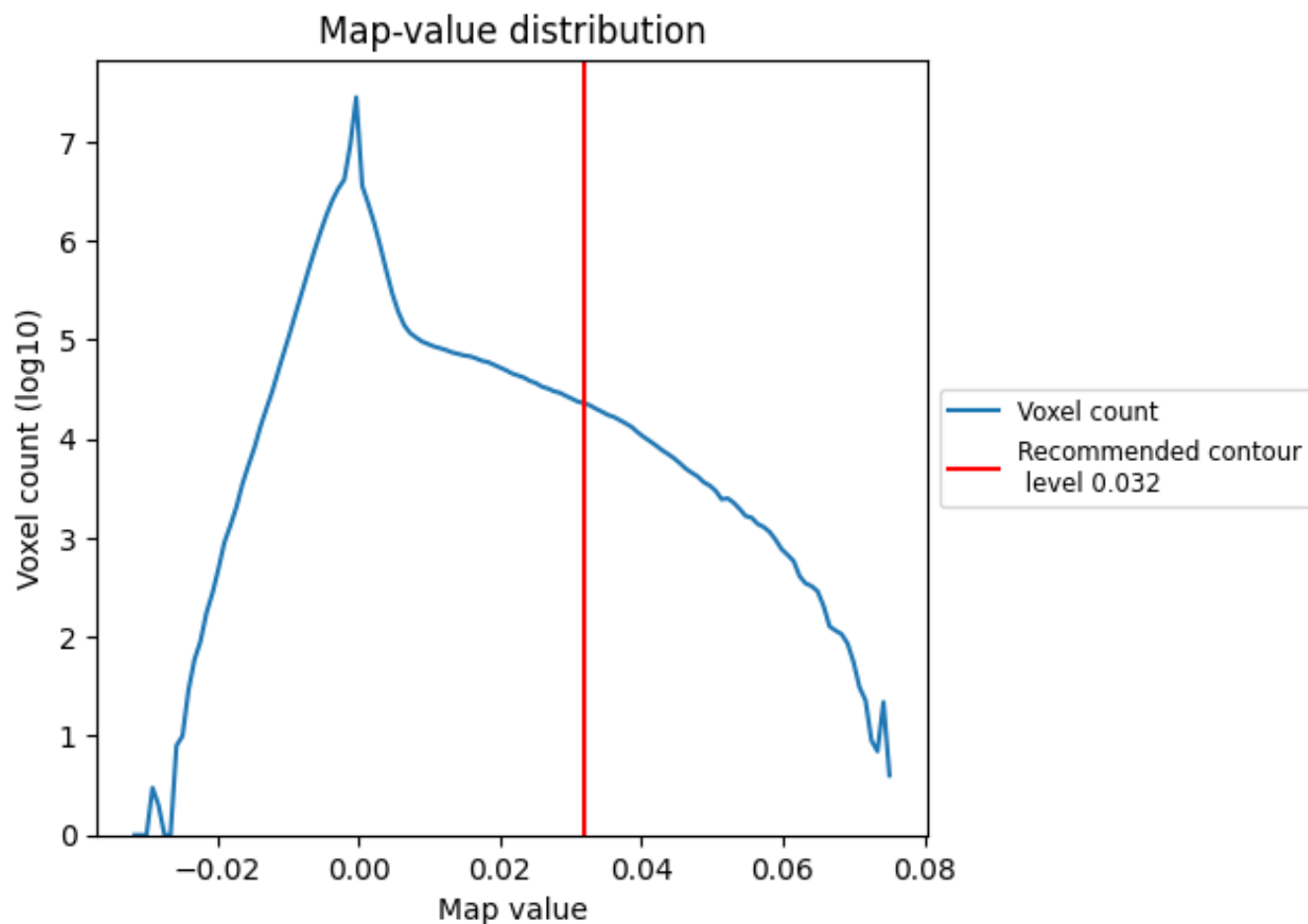
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

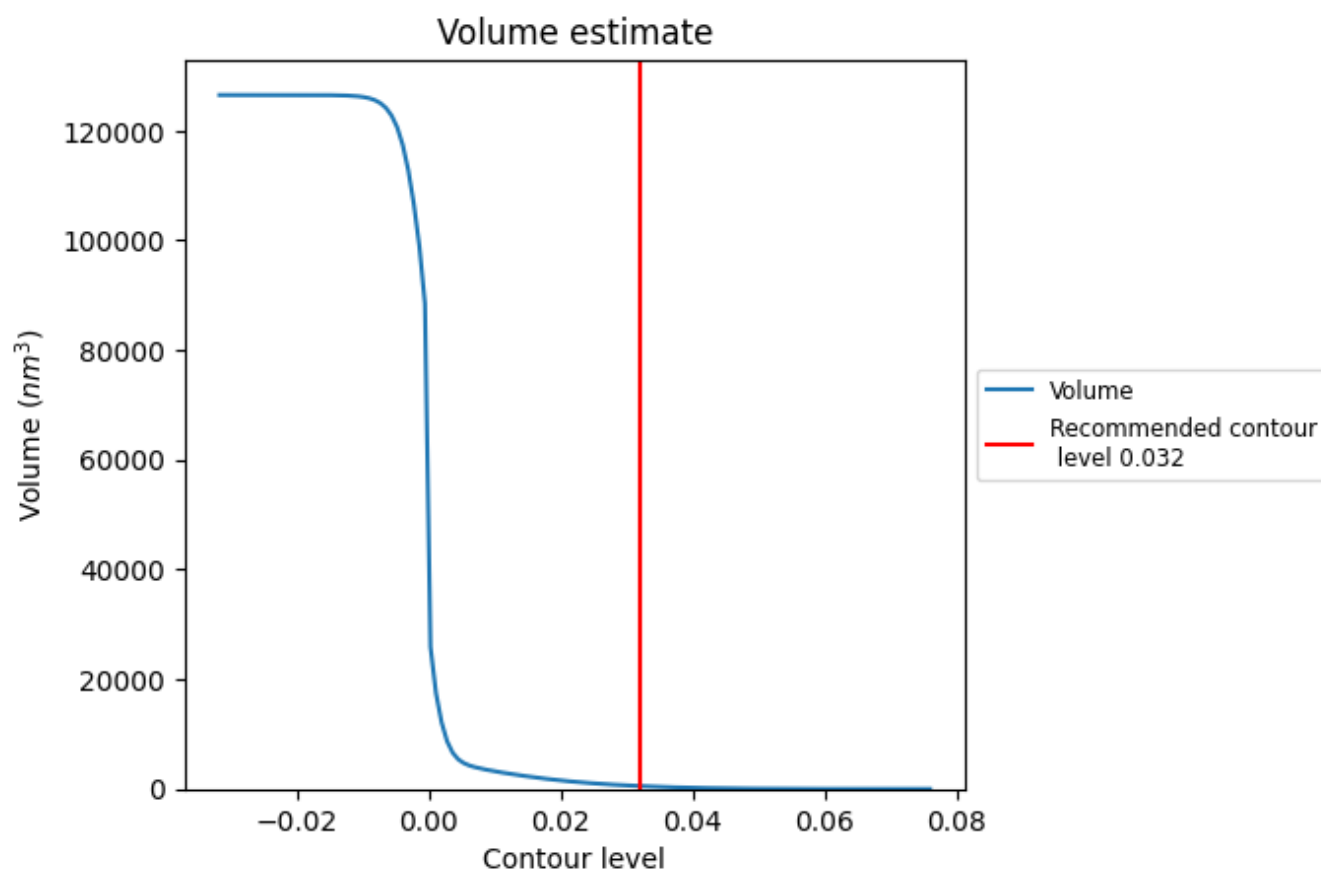
This section contains the results of statistical analysis of the map.

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.

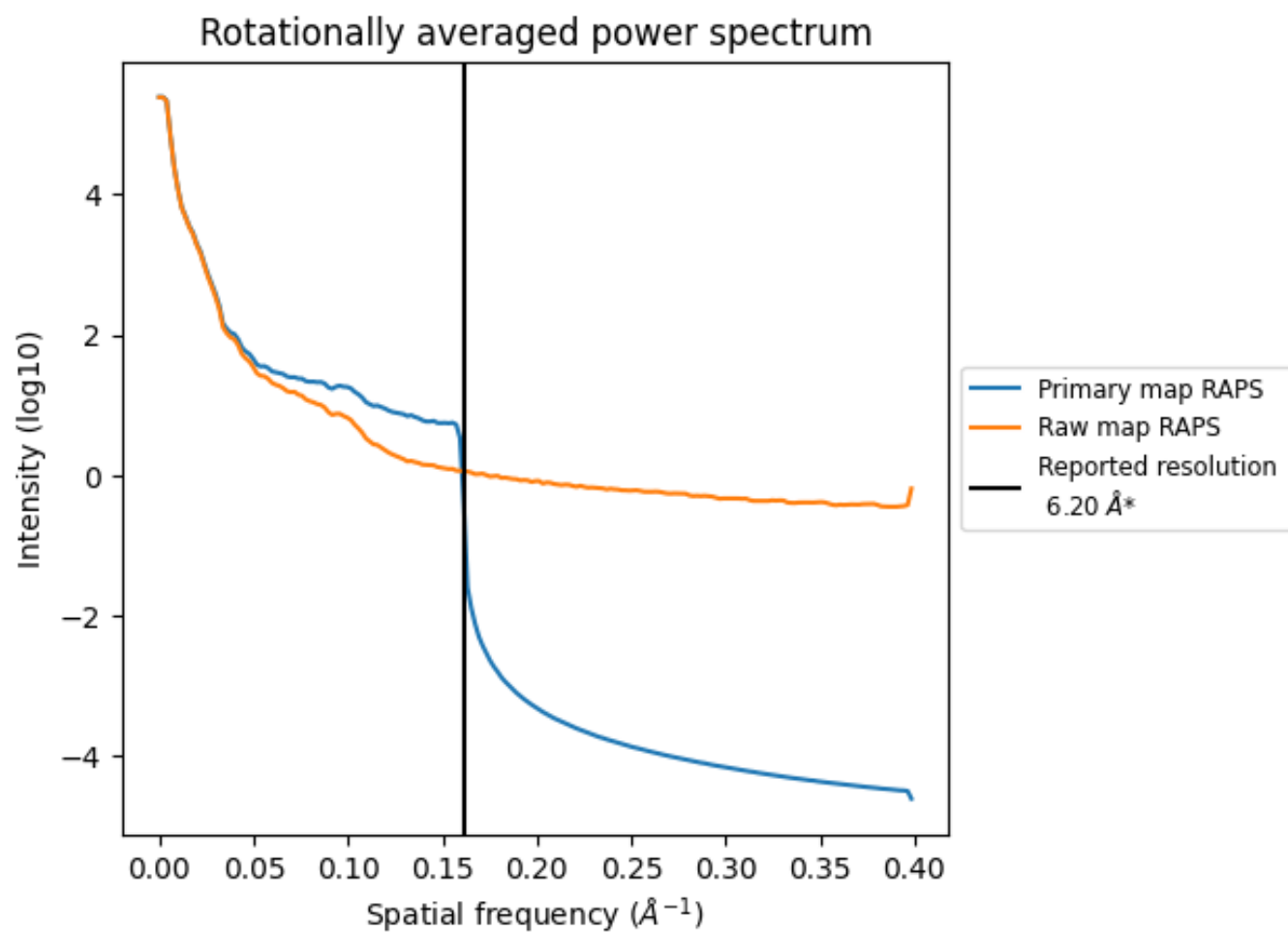
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 482 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 ⓘ

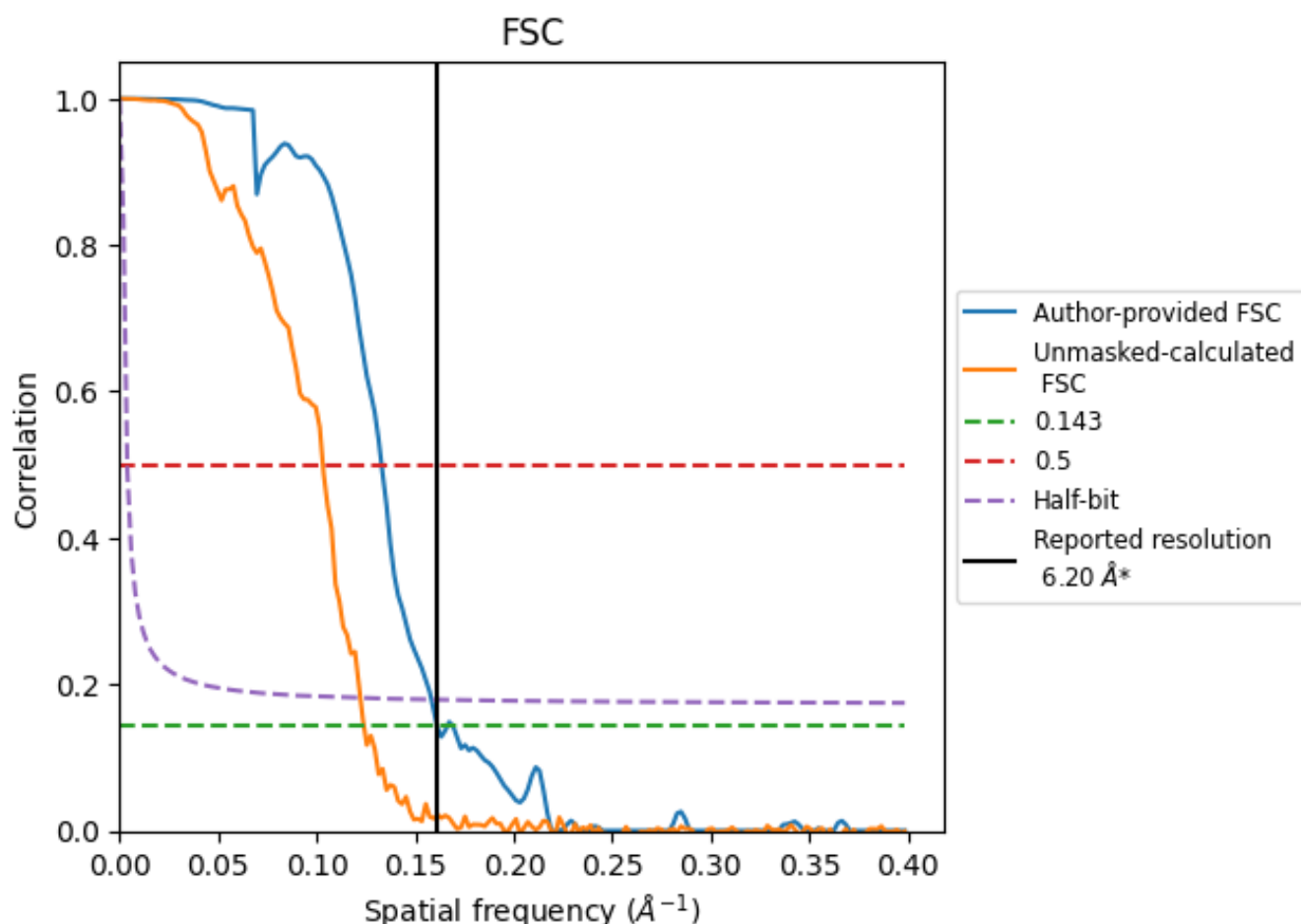


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

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 0.161 Å⁻¹

8.2 Resolution estimates [i](#)

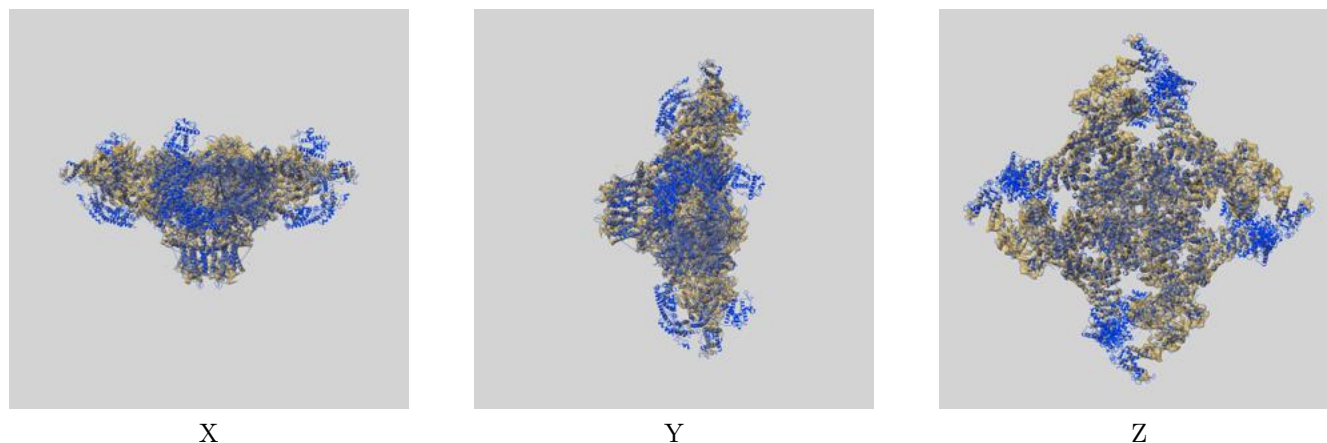
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.21	7.52	6.32
Unmasked-calculated*	8.06	9.69	8.18

*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 8.06 differs from the reported value 6.2 by more than 10 %

9 Map-model fit [i](#)

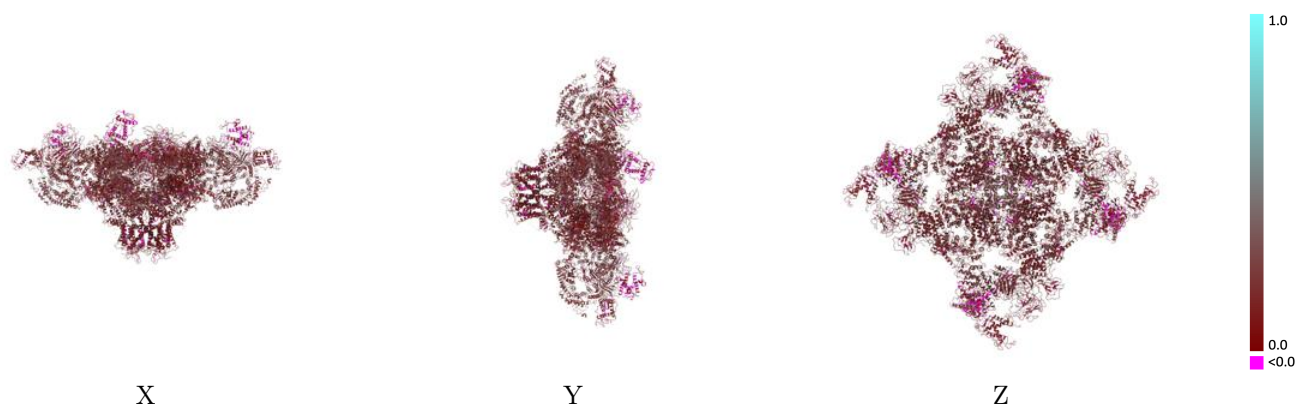
This section contains information regarding the fit between EMDB map EMD-8385 and PDB model 5TAU. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



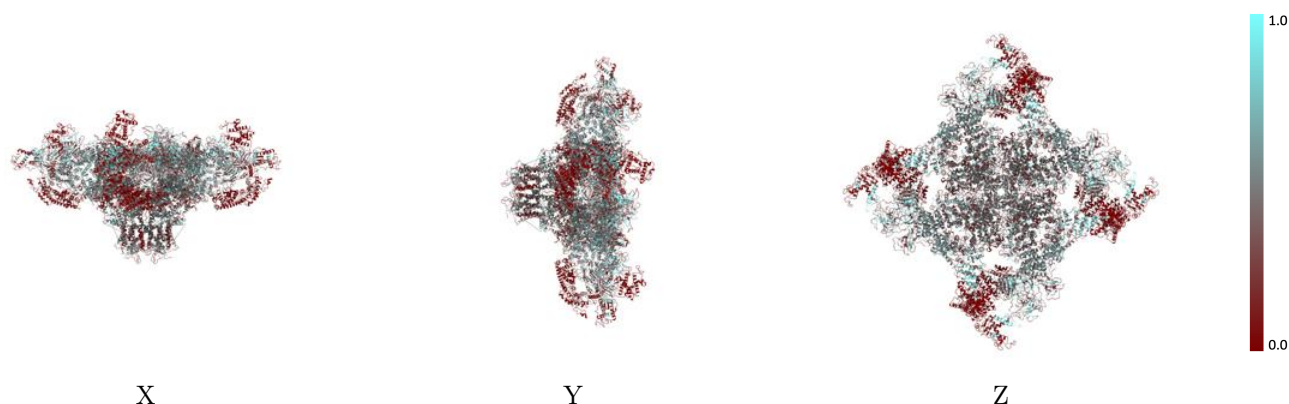
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



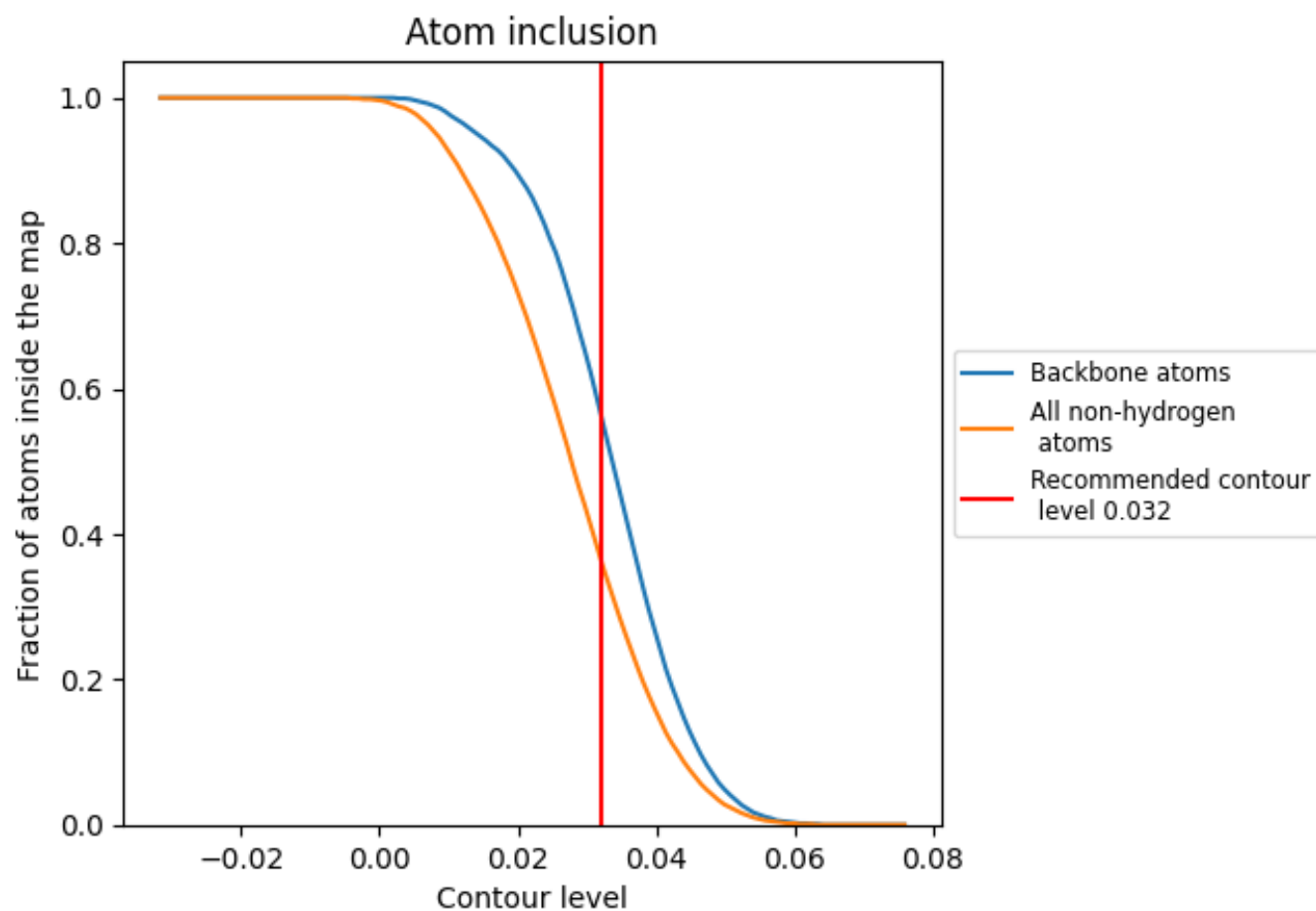
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 37% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3660	<div></div> 0.1880
A	<div></div> 0.3960	<div></div> 0.1860
B	<div></div> 0.3640	<div></div> 0.1880
E	<div></div> 0.3640	<div></div> 0.1880
F	<div></div> 0.3980	<div></div> 0.1900
G	<div></div> 0.3650	<div></div> 0.1880
H	<div></div> 0.3930	<div></div> 0.1880
I	<div></div> 0.3650	<div></div> 0.1880
J	<div></div> 0.3870	<div></div> 0.1880

1.0

0.0

<0.0