



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 06:13 AM UTC

PDB ID : 9EI1 / pdb_00009ei1
EMDB ID : EMD-47395
Title : Structure of RyR1 in the open state in the presence of oxopyridicid
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.20 Å(reported)
Based on initial model : 7TZC

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

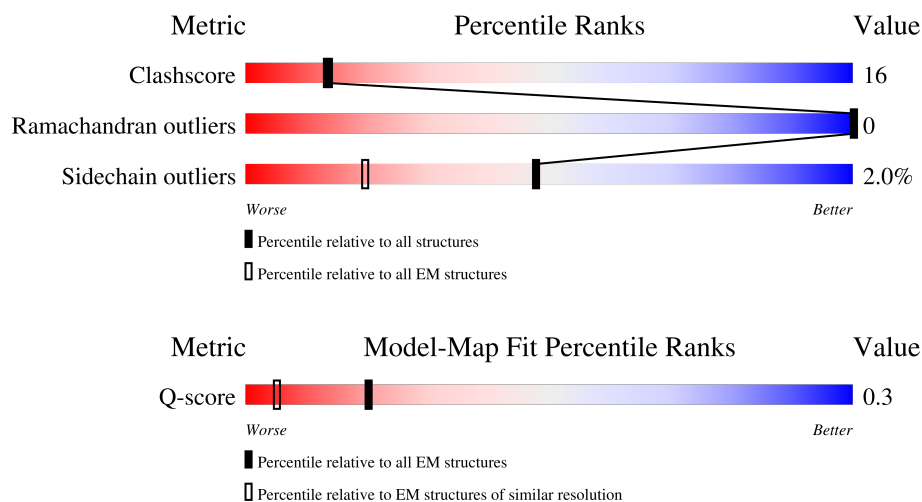
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	5037	43% 58% 28% 13%
1	B	5037	43% 59% 28% 13%
1	C	5037	43% 59% 28% 13%
1	D	5037	43% 59% 28% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	79% 71% 27% ..
2	F	108	77% 72% 26% ..
2	G	108	78% 72% 26% ..
2	H	108	77% 70% 29% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

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

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

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



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

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

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

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

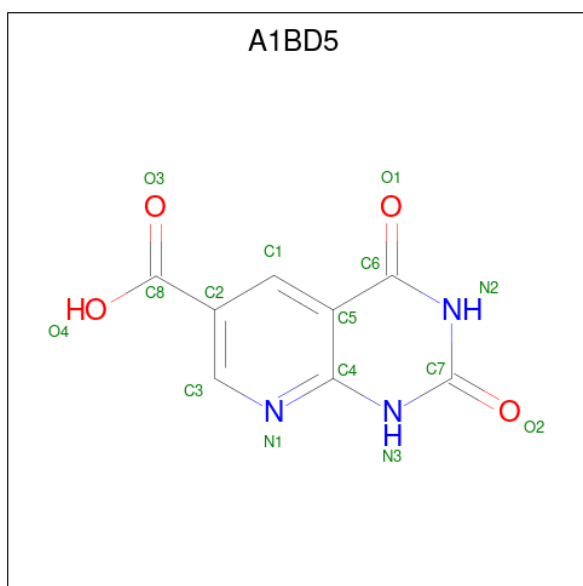
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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

- Molecule 6 is oxopyridicid (CCD ID: A1BD5) (formula: $C_8H_5N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	3	4	
6	B	1	Total	C	N	O	0
			15	8	3	4	
6	D	1	Total	C	N	O	0
			15	8	3	4	
6	C	1	Total	C	N	O	0
			15	8	3	4	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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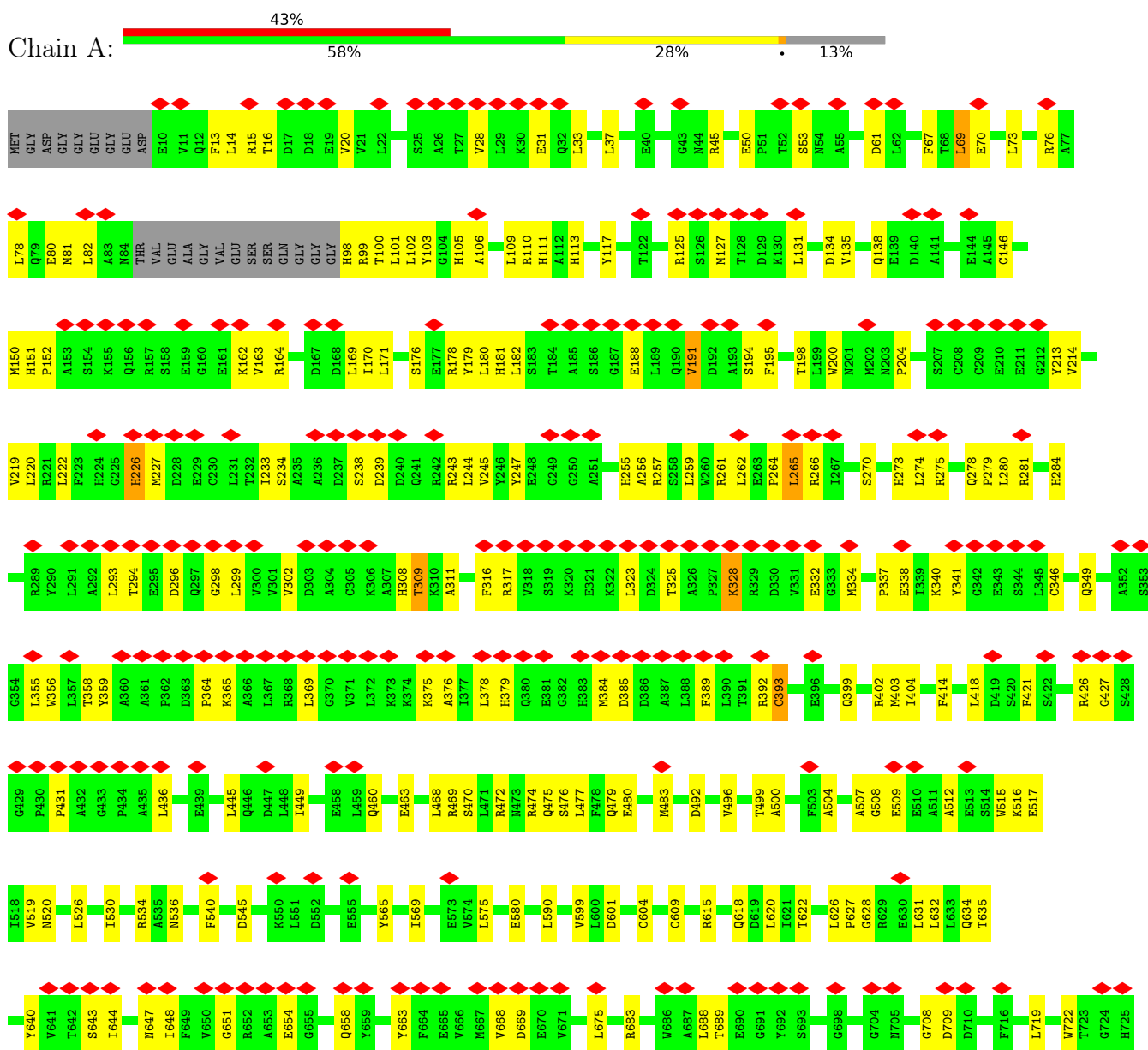
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Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	O 1	0
7	C	1	Total 1	O 1	0

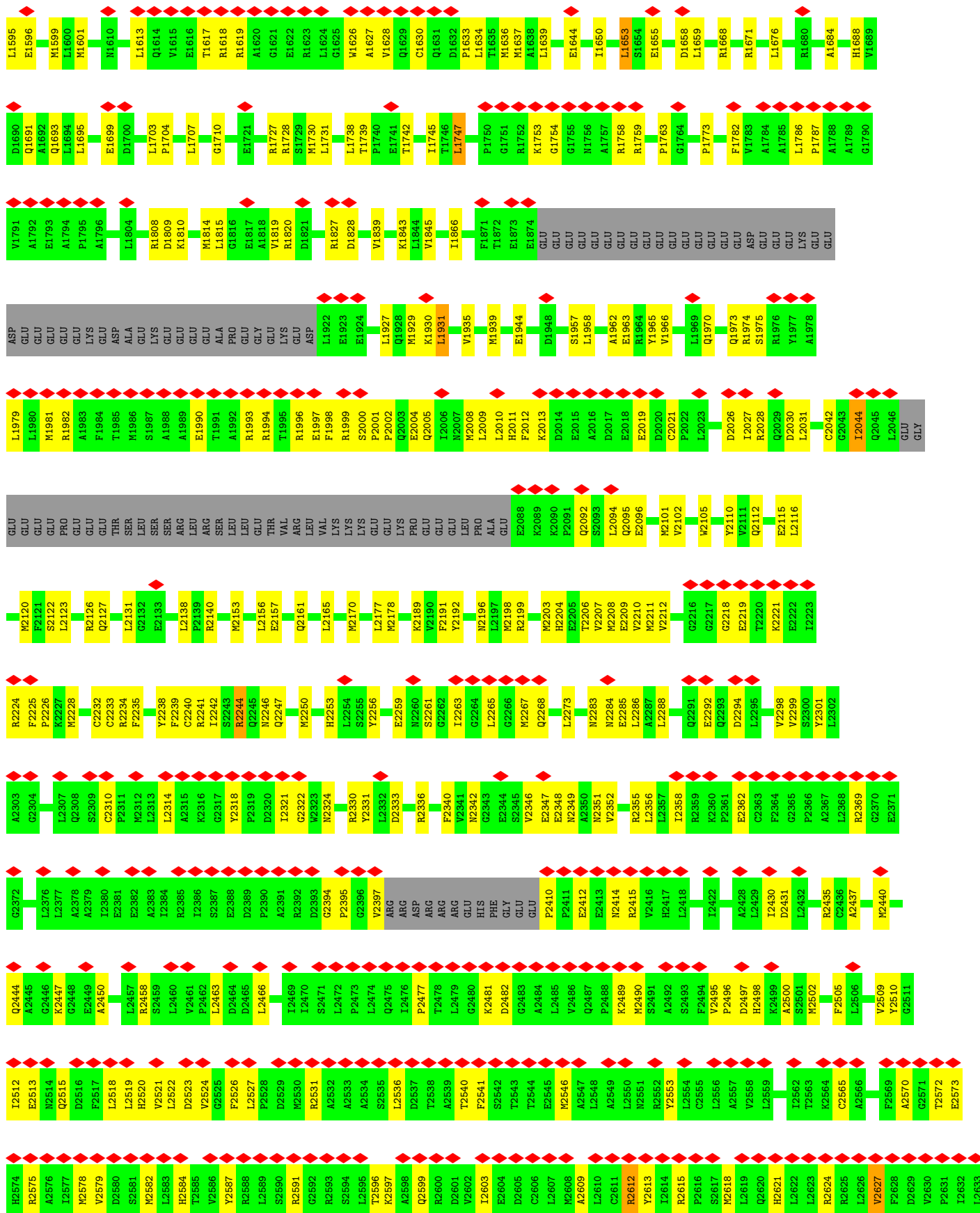
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 1

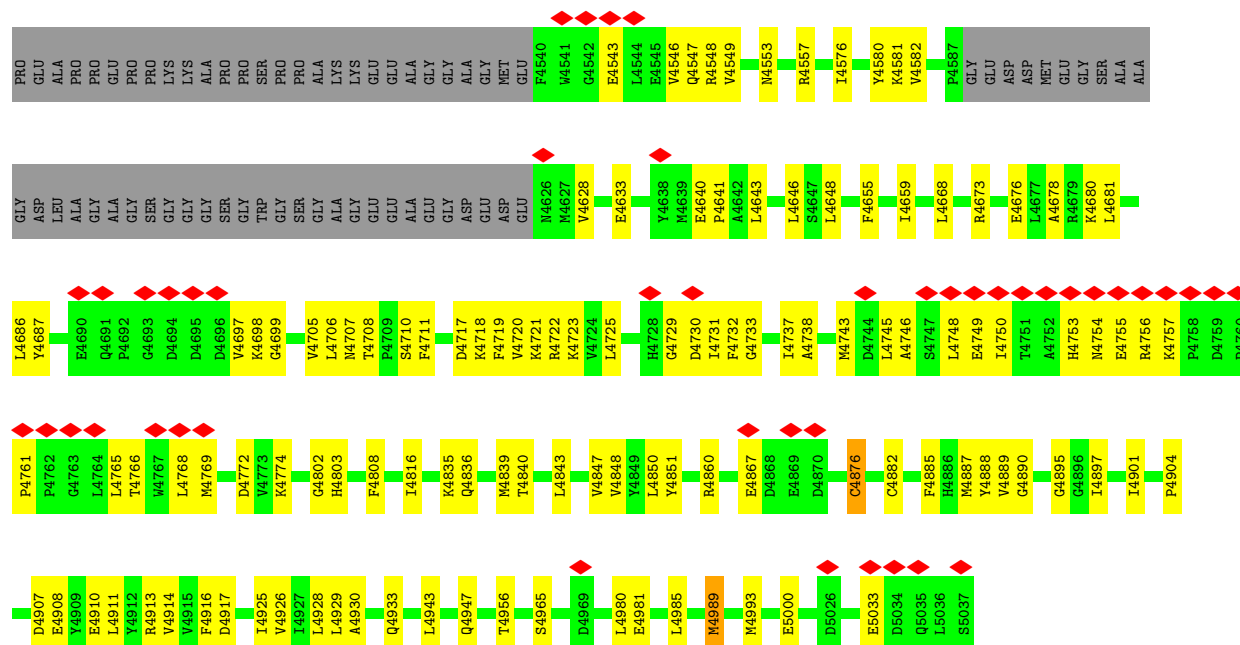




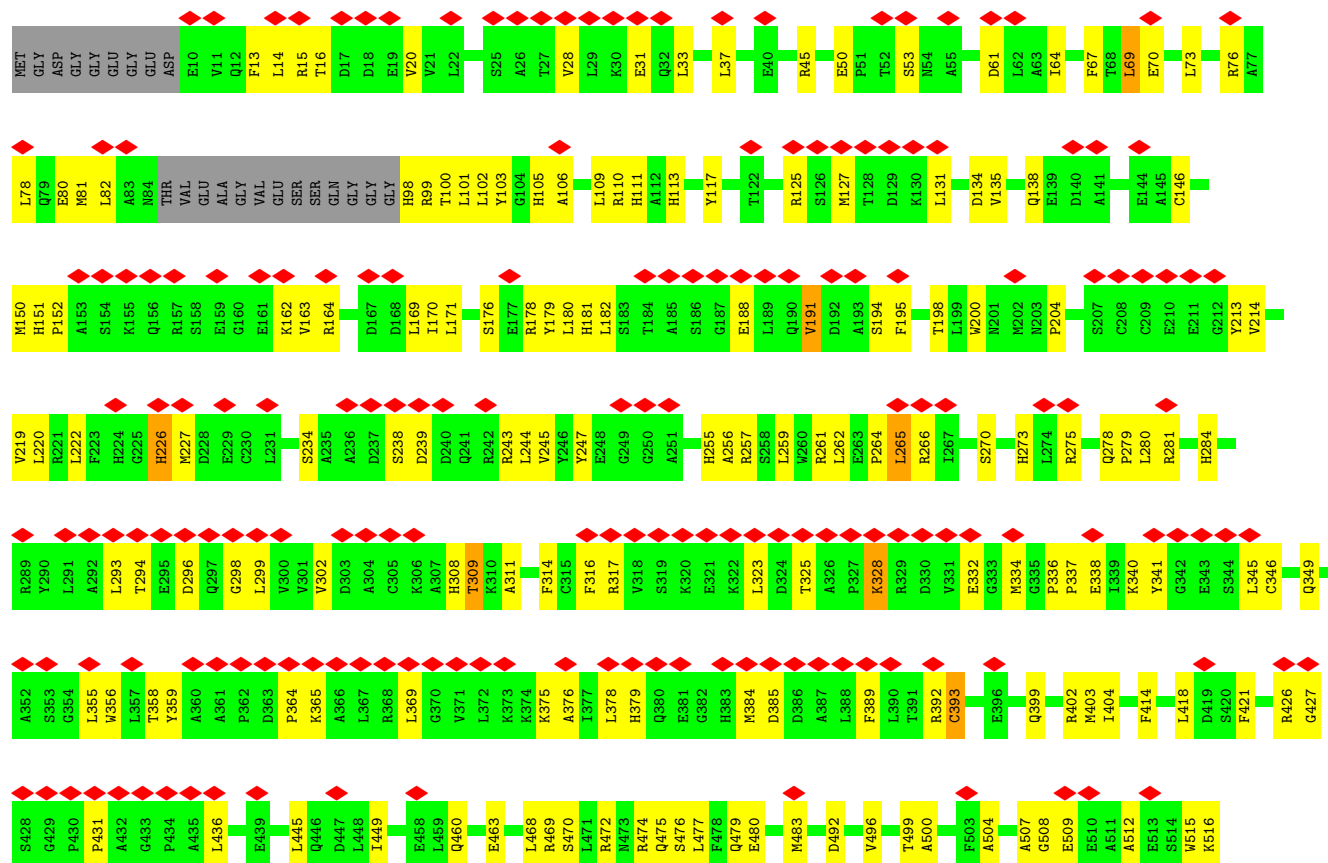
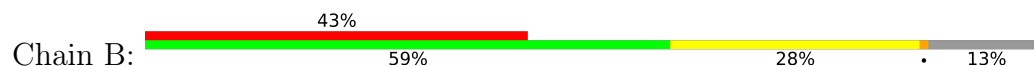


L2634	L2635	F2636	A2637	L2638	L2639	F2640	L2641	L2642	L2643	L2644	T2645	H2646	L2647	L2648	L2649	R2650	C2651	L2652	L2653	L2654	L2655	C2656	L2657	L2658	L2659	G2660	L2661	A2662	L2663	F2664	G2665	L2666	L2667	S2668	L2669	E2670	E2671	L2672	L2673	L2674	T2675	R2676	L2677	L2678	F2679	G2680	G2681	L2682	L2683	L2684	S2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	G2693
E2694	L2695	Y2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	L2709	L2710	P2711	P2712	D2713	L2714	L2715	D2716	A2717	L2718	L2719	S2720	S2721	K2722	A2723	E2724	K2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753
F2754	L2755	L2756	K2757	L2758	L2759	E2760	L2761	L2762	L2763	E2764	K2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	N2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813
K2814	A2815	M2816	L2817	L2818	L2819	E2820	L2821	L2822	L2823	E2824	K2825	A2826	L2827	E2828	L2829	E2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873
M2874	A2875	E2876	L2877	L2878	L2879	E2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933
G2934	Y2935	A2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993
E2994	L2995	L2996	L2997	L2998	L2999	K3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053
V3054	S3055	L3056	F3057	L3058	L3059	D3060	A3061	L3062	A3063	L3064	V3065	L3066	L3067	L3068	L3069	L3070	L3071	A3072	L3073	S3074	L3075	D3076	A3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113
K3114	V3115	S3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173
S3174	L3175	G3176	T3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233
N3234	S3235	V3236	E3237	L3238	L3239	C3240	L3241	D3242	L3243	P3244	L3245	L3246	L3247	L3248	L3249	M3250	A3251	D3252	L3253	G3254	G3255	L3256	A3257	E3258	S3259	G3260	A3261	R3262	Y3263	T3264	E3265	M3266	L3267	P3268	H3269	L3270	L3271	L3272	L3273	L3274	L3275	M3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293
P3294	A3295	L3296	P3297	A3298	L3299	A3300	P3301	P3302	L3303	L3304	L3305	A3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353
L3354	H3355	S3356	H3357	L3358	L3359	F3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413

GLY	GLY	ALA	GLU	F4077	K3984	V3859	K3756	L3663	R3594	M3534	S3474	R3414
LEU	ALA	LEU	GLY	Q4078	L3985	N3860	E3757	L3664	R5595	L3535	K3475	Y3415
ASP	LEU	GLY	GLY	D4079	E3861	E3862	E3758	E3665	V3596	A3536	S3476	Y3416
TRP	ALA	GLY	GLY	T4082	V3995	D3862	K3760	D3675	Q3597	K3537	K3477	D3417
ALA	ALA	GLY	GLY	D4083	F3996	D3863	K3761	D3676	V3598	T3538	M3478	R3418
VAL	VAL	ALA	ALA	P4084	M3999	T3864	R3762		V3599	R3539	A3479	R3419
VAL	VAL	ALA	GLY	R4085	K4002	V3865	Q3767	K3679	S3600	Y3540	LYS	R3420
ALA	ALA	GLY	GLY	G4086	L4003	I3866	S3768	A3680	A3601	A3541	GLY	A3421
ARG	ALA	ALA	ALA		A4004	N3867	R3769	G3681	V3602	R3542	ALA	A3421
ASP	ALA	GLY	GLY	K4090	Q4005	R3868	H3770	E3682	L3603	R3543	ALA	H3422
ALA	ALA	ALA	ALA	K4091	D4006	Q3869	H3771	E3683	L3604	L3424	GLN	K3423
ALA	ALA	ALA	ALA	D4092	S4007	N3870	T3772	Q3683	H3605	T3425	SER	L3424
GLY	GLY	GLY	GLY	F4093	S4008	K3871	R3773	E3684	L3606	T3545	GLY	T3425
VAL	VAL	VAL	VAL	Q4094	S4009	E3872	K3778	E3685	L3607	E3426	GLY	E3426
ALA	ALA	ALA	ALA	K4095	Q4009	E3872	K3778	E3686	E3607	E3547	SER	R3427
ALA	ALA	ALA	ALA	A4096	K3873	K3873	K3782	E3687	Q3608	E3548	ASP	R3428
ALA	ALA	ALA	ALA	M4097	E4011	V3874	K3782	E3688	T3609	V3549	GLN	R3428
GLY	GLY	GLY	GLY	L4012	L4013	D3877	A3785	E3689	H3611	R3550	GLU	A3429
ALA	ALA	ALA	ALA	K4014	K4014	D3878	G3788	E3690	P3612	R3551	ARG	R3430
THR	ALA	ALA	ALA	E4015	L4015	E3879	G3788	E3691	Y3613	E3551	THR	R3430
ALA	ALA	ALA	ALA	S4099	L4016	F3880	G3791	E3692	Y3614	F3552	LYS	A3431
ARG	ALA	ALA	ALA	Q4100	L4017	D3883	G3791	E3693	K3614	L3553	LYS	E3432
LEU	ALA	ALA	ALA	K4101	D4018	L3884	V3794	K3693	Q3554	Q3554	LYS	E3433
ALA	ALA	ALA	ALA	K4102	L4019	L3884	L3798	D3696	K3554	R3498	LYS	E3434
ALA	ALA	ALA	ALA	F4103	Q4020	L3890	L3798	D3696	K3555	R3499	LYS	E3434
ALA	ALA	ALA	ALA	T4104	M4023	L3890	L3798	D3696	K3556	R3499	LYS	E3434
ALA	ALA	ALA	ALA	G4105	L4030	N3896	L3805	R3707	K3617	G3500	LYS	E3435
ALA	ALA	ALA	ALA	F4106	L4040	F3899	L3805	R3707	K3617	G3500	LYS	E3435
ALA	ALA	ALA	ALA	E4107	A4041	T3912	V3812	T3711	A3618	R3501	LYS	E3436
ALA	ALA	ALA	ALA	I4108	A4041	V3935	V3812	T3711	V3619	R3502	LYS	E3437
ALA	ALA	ALA	ALA	L4112	V4045	Y3937	K3816	K3715	W3620	Y3503	LYS	E3438
ALA	ALA	ALA	ALA	S4113	E4050	Y3937	K3816	K3715	G3561	S3504	LYS	E3439
ALA	ALA	ALA	ALA	S4114	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3440
ALA	ALA	ALA	ALA	S4115	M4057	Y3937	K3816	K3715	K3562	V3505	LYS	E3441
ALA	ALA	ALA	ALA	E4116	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3442
ALA	ALA	ALA	ALA	A4117	M4057	Y3937	K3816	K3715	K3562	V3505	LYS	E3443
ALA	ALA	ALA	ALA	D4118	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3444
ALA	ALA	ALA	ALA	E4119	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3445
ALA	ALA	ALA	ALA	M4120	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3446
ALA	ALA	ALA	ALA	E4121	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3447
ALA	ALA	ALA	ALA	M4122	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3448
ALA	ALA	ALA	ALA	F4123	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3449
ALA	ALA	ALA	ALA	M4124	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3450
ALA	ALA	ALA	ALA	F4125	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3451
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3452
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3453
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3454
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3455
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3456
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3457
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3458
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ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3460
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3461
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3462
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3463
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ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3465
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ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3468
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ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3471
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3472
ALA	ALA	ALA	ALA	E4126	E4056	Y3937	K3816	K3715	K3562	V3505	LYS	E3473



• Molecule 1: Ryanodine receptor 1







R3225	C3165	K3105	K3045	R2985	E2925	V2865	Y2805	R2625	S2685	R2625	K2564	S2501
E3226	Y3166	M3106	L3046	V2986	L2926	T2866	R2806	L2626	L2686	L2626	C2665	M2502
R3227	R3167	V3107	A3047	E2987	L2927	L2867	W2807	V2627	A2687	V2627	A2666	F2605
A3228	T3168	E3108	A3048	K2988	K2928	S2868	P2808	F2628	H2688	F2628	F2669	L2506
L3229	L3169	N3109	L3049	S2989	F2929	R2869	L2809	D2629	R2689	D2629	A2570	V2509
L3230	C3170	L3110	V3050	P2990	L2930	E2870	K2810	V2630	K2690	V2630	A2570	V2509
G3231	S3171	R3111	R3051	H2991	Q2931	L2871	E2811	P2631	Y2691	P2631	G2571	G2510
L3232	L3172	L3112	H3052	E2992	M2932	Q2872	S2812	L2632	D2692	L2632	T2572	G2511
P3233	G3113	G3113	K3053	Q2993	N2933	A2873	S2813	L2633	Q2693	L2633	E2573	L2512
M3234	S3174	K3114	V3054	E2994	G2934	M2874	K2814	M2634	E2694	M2634	H2574	E2513
S3235	L3175	V3115	S3055	L2995	Y2935	A2875	A2815	E2635	L2695	E2635	R2575	Q2515
V3236	G3176	S3116	L3056	K2996	A2936	E2876	M2816	F2636	Y2696	F2636	A2576	D2516
E3237	T3177	GLN	F3057	F2997	V2937	Q2877	L2817	A2637	R2697	A2637	L2577	F2517
A3238	T3178	ALA	G3058	F2998	T2938	L2878	A2818	K2638	M2698	K2638	M2578	L2518
M3239	K3179	ARG	T3059	F2998	T2938	L2878	A2818	M2639	A2699	M2639	V2579	L2519
C3240	N3180	THR	T3059	A2999	R2939	A2879	W2819	D2640	N2700	D2640	D2580	H2520
C3240	N3180	GLN	D3060	K3000	GLY	E2880	E2820	L2641	P2701	L2641	S2691	V2521
F3241	T3181	VAL	A3061	I3001	LYS	N2881	W2821	K2642	P2701	L2641	M2582	V2521
D3242	Y3182	K3123	A3072	P3062	LYS	Y2882	T2822	K2642	C2702	K2642	M2582	D2522
L3243	V3183	G3124	R3073	L3002	MET	H2883	L2823	L2643	L2703	L2643	L2583	D2522
P3244	E3184	V3125	V3064	P3004	GLU	N2884	E2824	L2644	C2704	L2644	H2694	V2524
V3245	K3185	G3126	V3065	L3005	L2946	T2885	K2825	T2645	A2705	T2645	T2585	G2525
L3246	L3186	Q3127	N3066	I3006	D2947	V2886	A2826	N2646	R2706	N2646	V2586	F2526
R3247	R3187	N3128	C3067	I3006	T2948	W2886	A2826	H2647	L2706	H2647	V2586	F2526
R3248	L3129	L3129	L3068	N3007	T2948	G2887	R2827	R2648	A2707	R2648	R2587	F2528
L3249	T3130	L3129	H3068	Q3008	S2949	R2888	E2828	E2649	Q2708	E2649	R2588	D2529
M3250	Y3131	Y3009	H3069	Y3009	S2950	K2889	G2829	R2650	Q2709	R2650	S2590	M2530
R3251	T3132	T3070	L3070	F3010	L2951	K2890	E2830	R2651	L2710	R2651	R2591	R2531
A3252	T3133	L3071	L3071	T3011	E2952	K2891	GLU	C2651	P2711	C2651	R2591	R2531
G3253	R3134	A3072	A3072	N3012	K2953	Q2892	GLU	W2652	P2711	W2652	G2592	A2532
D3252	L3135	R3073	R3073	H3013	R2954	Q2892	GLU	K2653	P2712	K2653	R2593	A2533
A3254	A3136	S3074	S3074	C3014	F2955	E2893	THR	Y2654	D2713	Y2654	S2594	A2534
G3255	L3136	Y3075	L3075	L3015	A2956	L2894	GLU	Y2655	Y2714	Y2655	S2594	L2535
L3256	A3195	L3076	L3076	Y3016	F2957	E2895	LYS	C2656	V2715	C2656	L2695	L2536
R3257	R3196	L3076	D3076	L3016	F2957	L2895	LYS	D2637	D2716	D2637	T2596	T2537
A3258	L3197	P3138	A3077	F3017	G2958	A2896	LYS	L2657	A2717	L2657	K2597	D2537
S3259	A3198	V3139	R3078	R3017	Q2958	K2897	THR	P2658	Q2717	P2658	A2598	T2538
G3260	S3259	L3140	T3079	L3018	L2960	G2998	ARG	T2659	S2718	T2659	Q2599	A2539
A3261	A3200	T3141	V3080	S3019	F2959	G2899	LYS	R2660	Y2719	R2660	R2600	T2540
R3262	M3201	T3142	M3081	T3020	Q2961	G2900	ILE	G2660	S2720	G2660	D2601	F2541
A3261	K3201	P3021	K3082	P3021	Q2962	T2901	SER	W2661	S2721	W2661	V2602	S2542
R3262	L3143	A3261	K3082	A3022	L2963	T2901	THR	A2662	K2722	A2662	L2603	T2543
Y3263	Y3263	F3144	S3083	K3023	L2964	H2902	ALA	F2664	K2723	F2664	E2604	T2544
T3264	Q3145	Q3084	S3083	K3023	L2964	P2903	GLN	G2665	A2724	G2665	C2605	E2545
E3265	H3146	G3084	P3085	V3024	W2966	L2904	THR	Q2665	E2724	Q2665	C2606	M2546
M3266	L3147	E3086	E3086	G3026	M2967	L2905	T2895	L2785	K2725	L2785	C2606	
F3267	A3148	I3087	D3076	S3027	D2968	V2906	ASP	L2785	LYS	LYS	C2606	
H3268	Q3149	T3087	V3088	S3028	L2969	P2907	PRO	K2786	THR	THR	L2608	A2547
S3269	H3150	Q3149	K3089	G3028	L2969	Y2908	ARG	T2787	VAL	VAL	M2608	L2548
L3270	Q3209	Q3151	K3089	G3029	S2970	D2909	GLU	H2788	ASP	ASP	A2609	A2549
E3271	L3210	F3152	A3090	H3030	Q2971	T2910	GLY	P2789	THR	THR	L2610	L2550
L3272	N3211	G3153	G3091	A3031	E2972	T2910	Y2855	E2670	ALA	ALA	C2611	M2551
T3273	E3212	D3154	L3092	S3032	F2973	L2911	N2856	E2671	GLU	GLU	R2612	R2552
Y3213	Y3213	L3154	L3092	S3032	F2973	T2912	T2857	L2672	GLY	GLY	Y2613	Y2553
N3214	N3214	R3093	S3094	N3033	L2974	T2912	P2857	H2673	M2734	M2734	L2614	L2554
A3215	A3215	V3156	F3095	K3034	A2975	A2913	Q2858	R2673	F2735	F2735	R2615	C2555
M3276	K3276	I3157	F3096	E3035	H2976	K2914	P2859	L2674	D2736	L2674	P2616	L2556
S3217	S3217	L3158	F3096	E3035	L2977	E2915	P2860	T2675	P2737	T2675	S2617	A2557
V3218	V3218	L3157	E3097	K3036	L2977	K2916	D2861	R2676	P2738	R2676	M2618	V2558
C3278	C3278	D3159	E3097	E3037	E2978	A2917	L2862	K2677	R2738	K2677	L2619	L2559
Y3219	Y3219	D3160	S3098	E3037	E2978	R2918	S2863	L2678	P2739	P2739	Q2620	
S3279	S3279	V3161	A3099	M3038	A2979	D2919	G2864	F2679	V2740	F2679	H2621	
Y3280	Y3280	L3161	S3100	I3039	V2980	R2920	E2741	W2680	T2740	W2680	L2622	T2562
L3281	L3281	Q3162	S3100	T3040	V2981	E2921	T2742	L2681	E2741	L2681	L2623	
P3282	P3282	L3163	D3102	S3041	S2982	E2921	L2743	T2682	T2743	T2682	R2624	
R3283	R3283	S3164	T3102	F3043	Q2984	K2922	G2884	F2683	N2744	F2683		
			T3103	F3043	G2984	A2923		D2684		D2684		
			F3104	T3044								

GLY	Q4133	F4065	G3947	L3842	GLU	P3645	D3585	C3525	N3465	L3405	I3345	K3285
GLU	T4148	L4066	K3948	D3843	ALA	M3652	A3586	A3526	N3466	Y3406	V3346	E3286
ALA	N4149	K4067	T3966	A3846	GLU	F3653	D3587	P3527	M3467	A3407	S3347	R3287
ALA	L4150	K4069	T3966	F3847	GLU	L3654	D3588	P3528	S3468	L3408	R3348	G3288
GLU	S4151	D4070	Q3970	E3848	GLU	E3655	F3589	D3529	F3469	F3409	A3349	F3289
GLY	E4152	V4072	G3971	R3849	GLU	S3656	S3590	Q3530	L3470	P3410	R3350	E3290
ALA			P3972		GLU	Y3657	K3591	D3531	T3471	L3411	P3351	A3291
GLU			C3973	K3852		K3658	T3592	I3532	A3472	L3412	E3352	P3292
GLU			T3974	A3853		A3659	V3593	I3533	D3473	T3413	L3353	P3293
GLY			Q3978	E3854		L3663	F3593	M3534	S3474	R3414	L3354	P3294
ALA			S3979	G3855		T3664	R3595	L3535	K3475	F3415	H3355	A3295
GLY			L3980	L3856		E3655	R3596	A3536	S3476	Y3416	S3356	L3296
ALA			A3981	G3857		D3675	V3597	K3537	K3477	V3417	H3357	P3297
GLU				G3858		D3676	Q3597	T3538	N3478	D3418	F3358	A3298
GLY			R3984	V3859		D3676	F3598	R3539	M3479	N3419	I3359	G3299
ALA			L3985	N3860		K3679	V3599	A3540	A3479	R3420	P3360	A3300
ALA				E3861		A3680	S3600	A3541	LYS	R3421	T3361	A3301
THR			F3996	D3862		G3681	A3601	L3542	ALA	H3422	I3362	P3302
VAL			F3996	G3863		E3682	V3602	K3543	ASP	W3423	G3363	P3303
ALA			M3999	T3864		Q3683	L3603	D3544	GLN	L3424	R3364	C3304
ALA			K4003	V3865		E3684	Y3604	T3545	GLY	T3425	L3365	T3305
ALA			L4002	T3866		E3685	H3605	L3546	GLY	E3426	R3366	A3306
ALA			A4004	N3867		E3686	L3606	E3547	ASP	P3427	K3367	V3307
LEU			D4006	R3868		E3687	E3607	E3548	ASP	N3428	R3368	T3308
ALA			S4007	Q3869		E3688	Q3608	V3549	GLN	A3429	A3369	S3309
ALA			A4008	N3870		E3689	T3609	R3550	GLU	N3430	G3370	D3310
ALA			Q4009	G3871		V3690	E3610	E3551	ARG	A3431	K3371	H3311
ALA			I4010	E3872		E3691	H3611	F3552	THR	E3432	V3372	L3312
ALA			E4011	K3873		E3692	P3612	L3553	LYS	L3433	V3373	L3313
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ALA			L4013	D3877		D3696	K3614	N3555	R3499	F3435	E3375	L3315
ALA			L4014	D3878		D3696	S3615	R3556	R3499	R3436	E3376	L3316
ALA			E4015	E3879		R3707	K3616	L3557	D3501	M3437	E3377	G3317
LEU			L4016	F3880			L3617	H3558	R3502	V3438	Q3378	N3318
LEU			L4017	F3880			A3618	L3559	Y3503	G3439	L3379	I3319
LEU			L4018	F3880			V3619	S3504	S3504	E3440	R3380	L3320
LEU			Q4020	D3883			K3620	G3560	S3505	I3441	L3381	R3321
ARG			A4041	N3886			H3621	G3561	V3505	F3442	E3382	I3322
ARG			I4040	F3889			K3622	K3562	Q3506	I3443	A3383	I3323
ARG			A4041	F3889			L3623	V3563	T3507	Y3444	K3384	V3324
VAL			V4045	T3912			L3624	E3564	S3508	W3445	A3385	N3325
ARG			E4050	T3912			S3625	Q3565	L3509	S3446	E3386	N3326
LEU			E4056	T3930			K3626	S3566	I3510	K3447	A3387	L3327
ARG			E4066	W3935			Q3627	P3567	V3511	S3448	E3388	G3328
LEU			K4060	Y3936			R3628	S3568	A3512	G3390	E3389	I3329
THR			F4061	Y3937			R3629	L3569	T3513	N3450	G3390	D3330
ALA			F4062	L3835			R3630	R3570	L3514	F3451	E3391	E3331
ALA			D4063	F3941			A3631	K3571	K3515	K3452	L3392	A3332
GLU			M4064	T3942			V3632	Q3572	K3516	R3453	L3393	T3333
GLY				I3943			V3633	A3574	L3517	E3454	V3394	W3334
GLY				E3944			A3634	L3575	P3519	E3455	R3395	H3335
MET				Q3946			F3636	R3576	T3520	Q3456	N3396	K3336
							R3637	R3577	G3521	F3458	E3397	R3337
							K3638	G3578	L3522	V3459	F3398	L3338
							T3639	L3579	N3523	V3460	S3399	A3339
							P3640	P3580	Q3461	V3461	V3400	Y3340
							L3641	Q3581	N3462	E3463	L3401	F3341
							N3643	R3582	R3403	E3463	R3403	A3342
							L3644	E3584	I3464	I3464	D3404	Q3343
												P3344

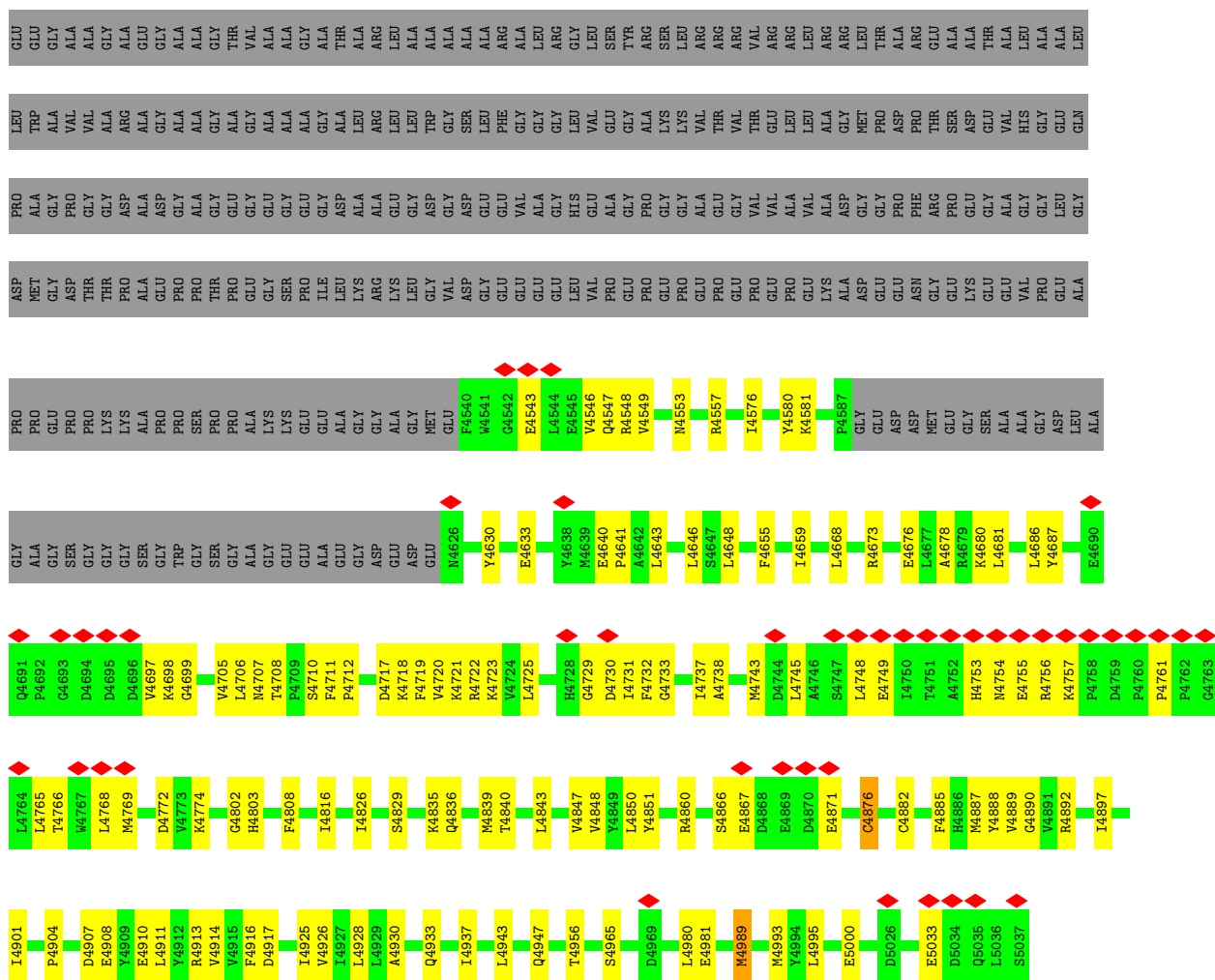




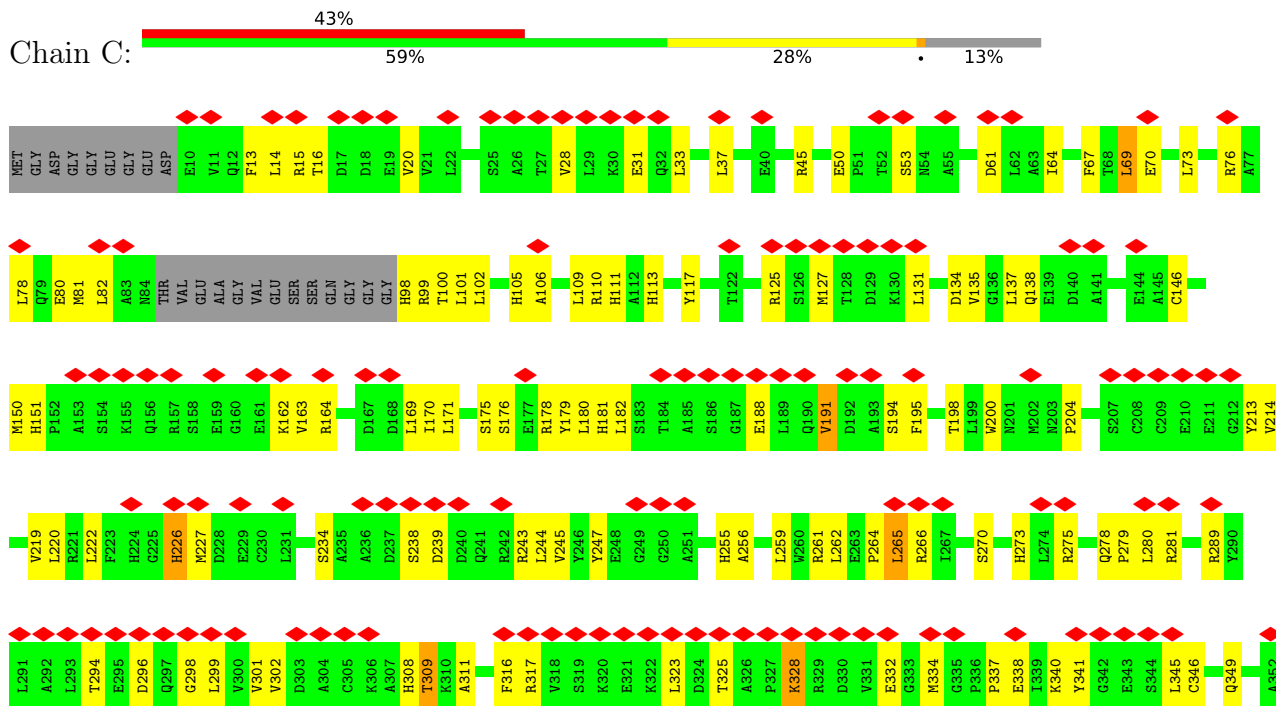


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G3176	S3116	L3056	K2996	K2996	A2936	E2876	M2816	N2756	Y2696	F2636	A2576	Q2515	K2447
T3177	GLN	F3057	F2997	F2997	Y2937	Q2877	L2817	K2757	M2697	A2637	I2577	D2516	G2448
T3178	ALA	G3058	F2998	F2998	T2938	L2878	A2818	F2758	M2698	M2638	M2578	L2518	F2449
T3179	ARG	T3059	A2999	A2999	R2939	A2879	W2819	A2759	A2699	M2639	V2579	L2519	F2448
T3180	THR	D3060	K3000	K3000	GLY	E2880	E2820	E2760	M2700	P2640	D2580	H2520	A2450
T3181	GLN	A3061	I3001	I3001	L3001	E2881	W2821	Y2761	P2701	L2641	S2581	L2521	R2458
T3182	VAL	P3062	L3002	L3002	L3002	Y2882	T2822	T2762	C2702	K2642	S2582	V2522	S2459
V3183	K3123	A3063	L3003	L3003	ASP	H2883	L2823	H2763	L2703	L2643	L2583	D2523	L2460
V3184	G3126	V3064	P3004	P3004	MT	N2884	E2824	E2764	L2704	L2644	T2584	V2524	V2461
K3185	L3005	V3065	L3005	L3005	GLU	T2885	E2825	K2765	C2704	T2645	T2585	G2525	L2463
L3186	I3006	D2947	I3006	I3006	L2946	W2886	K2826	W2766	I2705	N2646	V2586	F2526	D2464
R3187	N3007	T2948	N3007	N3007	T2948	W2887	R2827	A2767	A2707	H2647	Y2587	L2527	D2465
P3188	Q3008	S2949	Q3008	Q3008	S2949	R2888	E2828	F2768	Q2708	Y2648	R2588	P2528	L2466
A3189	Y3009	I2951	Y3009	Y3009	I2951	G2829	G2829	D2769	A2709	E2649	S2590	D2529	T2470
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C3193	N3012	R2954	N3012	N3012	R2954	GLU	GLU	Q2772	P2712	W2652	Q2593	A2532	L2473
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L3199	S3018	L2960	S3018	S3018	L2960	ARG	ARG	Q2778	S2718	T2659	Q2599	T2540	L2479
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H3201	T3020	G2962	T3020	T3020	G2962	SER	SER	N2780	S2720	W2661	D2601	S2542	K2481
P3202	P3021	L2963	P3021	P3021	L2963	GLN	GLN	D2781	K2721	A2662	T2602	T2543	D2482
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G3204	P2903	R2965	P2903	P2903	R2965	GLN	GLN	E2783	A2723	D2605	E2606	E2545	A2484
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GLU		K4143	GLU	GLU		D3588		A3407	S3347	R3287
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GLU		K4145	GLU	GLU		E3590		Y3409	A3349	F3289
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GLU		K4147	GLU	GLU		K3592		L3411	E3352	A3291
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- Molecule 1: Ryanodine receptor 1

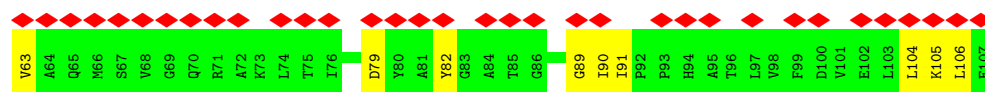


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ALA	W1277	S1193	N1125	P1055	E990	T870	F802	V730	S843	T358	G434	Y359
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TRP	S1279	G1195	H1127	D1057	H993	E872	P804	S732	N647	A535	A361	A360
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LYS	V1284	E1137	E1137	V1063	A1002	L878	E813	D742	R652	L551	Q447	A366
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GLY	L1286	F1138	F1138	E1065	Q1004	E880	V815	V744	E654	R553	I449	R368
THR	L1287	G1139	G1139	Q1066	G1004	E881	L816	L748	G655	L554	E458	L369
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PRO	S1292	S1145	S1145	R1070	Q1010	R886	R821	P753	Y663	Y565	L468	K375
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THR	Q1296	D1147	D1147	V1072	D1012	E888	R822	S754	E665	E573	L471	A376
PRO	L1297	M1152	M1152	R1076	I1013	Q889	L823	F757	V668	V574	M472	L378
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VAL	F1301	T1156	T1156	K1079	R1016	T892	R826	N760	E670	S476	Q475	Q380
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VAL	ALA	R1087	R1087	P1022	P1022	R896	R831	A770	R683	D601	M483	D385
ARG	ALA	W1088	W1088	P1023	P1023	R897	E832	F771	W886	C604	D492	D386
ASN	PRO	Y1089	Y1089	Y1024	Y1024	D898	G833	N772	A687	C609	Y496	A387
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LYS	ALA	A1094	A1094	L1026	L1026	R900	R835	D774	L688	Q618	A500	F389
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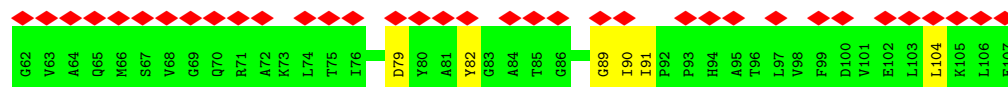
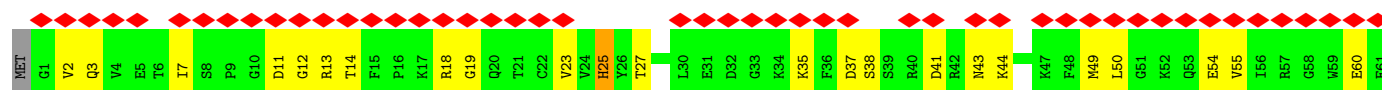
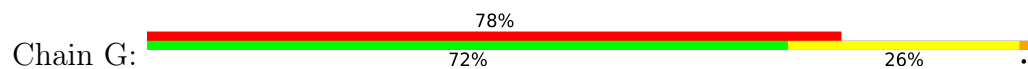




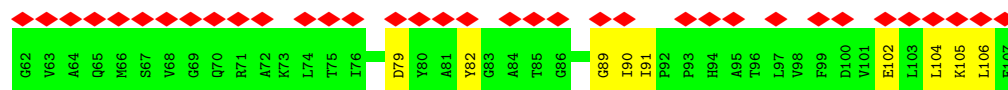
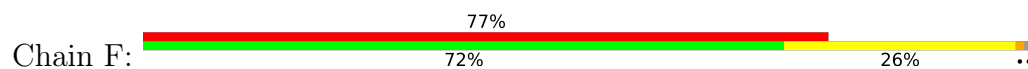
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	D4083	L3985	D3676	D3676	S3600	Y3540	T3360	A3300	C3240
R4180	P4084	V3995	K3679	K3679	A3601	A3541	T3361	P3301	P3241
M4184	R4085	F3996	A3680	A3680	V3602	L3542	I3362	P3302	D3242
C4185	G4086	K3963	G3681	G3681	L3603	K3543	G3363	P3303	I3243
A4186	K4090	T3964	S3768	S3768	Y3604	D3544	R3364	C3304	P3244
S4187	K4091	V3865	R3769	R3769	H3605	T3545	L3365	T3305	V3245
R4188	L4092	I3866	H3770	H3771	L3606	D3546	R3366	A3306	L3246
R4189	D4093	T3772	E3684	E3684	E3607	E3547	K3367	V3307	D3247
	F4093	R3773	E3685	E3685	Q3608	E3548	R3368	T3308	R3248
	Q4094	M3778	E3686	E3686	T3609	V3549	A3369	S3309	L3249
K4095	S4008	G3787	E3687	E3687	E3610	E3550	G3370	D3310	H3250
A4096	Q4009	I3782	E3688	E3688	H3611	E3551	K3371	H3311	A3251
M4097	I4010	S3784	V3690	V3690	P3612	P3552	V3372	L3312	D3252
D4098	E4011	K3785	E3691	E3691	L3553	L3553	V3373	N3313	I3253
S4099	L4012	C3786	K3787	K3787	Q3554	Q3554	A3374	S3314	G3254
Q4100	L4013	G3788	E3692	E3692	N3555	N3555	E3375	L3315	G3255
K4101	K4014	G3791	K3696	K3696	K3616	K3556	E3376	L3316	L3256
E4015	L4015	V3794	D3696	D3696	K3617	L3557	E3377	G3317	A3257
F4217	L4016	V3794	R3707	R3707	A3618	H3558	Q3378	N3318	E3258
V4221	F4102	I3802	L3710	L3710	V3620	K3559	L3379	I3319	S3259
N4223	Q4103	L3805	T3711	T3711	H3621	G3561	R3380	L3320	G3260
E4224	L4017	L3805	E3712	E3712	K3622	K3562	L3381	R3321	A3261
G4225	D4104	M3816	K3713	K3713	L3623	V3563	E3382	I3322	R3262
Q4226	T4104	K3821	S3714	S3714	L3624	E3564	K3384	I3323	Y3263
E4227	L4018	D3822	K3715	K3715	S3625	E3564	A3385	V3324	T3264
E4229	Q4020	K3822	L3716	L3716	K3626	S3566	E3386	N3325	G3265
K4230	M4023	D3823	D3717	D3717	P3627	P3567	A3387	N3326	H3266
M4231	I4040	K3823	M3729	M3729	R3628	S3568	L3387	G3327	P3267
F4234	A4041	K3824	A3730	A3730	R3629	A3512	E3388	I3328	H3268
F4243	V4045	A3834	K3731	K3731	V3630	L3513	E3389	I3329	V3269
E4244	E4050	L3835	H3734	H3734	K3571	K3514	G3390	D3330	I3270
T4247	F4061	T3835	L3735	L3735	Q3572	K3515	E3391	E3331	E3271
A4248	D4063	D3843	E3736	E3736	K3573	K3516	L3392	A3332	I3272
I4251	F4062	D3843	GLU	GLU	A3574	M3517	L3393	T3333	T3273
E4252	M4064	D3844	GLY	GLY	K3575	L3518	V3394	W3334	L3274
P4254	F4065	E3847	GLY	GLY	T3576	P3519	E3395	K3335	P3275
GLU	L4066	R3848	ASN	ASN	R3577	K3521	D3396	Q3336	H3276
GLY	K4067	R3849	GLY	GLY	M3638	Q3578	E3397	R3337	L3277
GLY	L4068		GLY	GLY	T3639	L3522	F3398	L3338	C3278
PRO	K4069		GLY	GLY	P3640	N3523	S3399	A3339	S3279
GLU	L4070		ALA	ALA	F3580	M3524	V3400	V3340	L3281
ALA	D4070		GLU	GLU	G3581	C3525	L3401	F3341	L3280
ASP	I4071		GLU	GLU	N3643	A3526	C3402	A3342	P3282
GLU	T4133		GLU	GLU	L3644	P3527	R3403	Q3343	R3283
	T4148				P3645	E3463	D3404	I3464	W3284
N4149	E4152				N3651	N3465	L3405	F3344	W3285
L4150					F3655	K3467	Y3406	V3345	E3286
S4151					F3655	S3468	A3407	V3346	R3287
E4152					E3655	L3585	L3408	S3347	G3288
						A3586	Y3409	R3348	P3289
						D3587	P3410	R3350	E3290
						L3654	L3411	P3351	



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.428	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.68, 423.68, 423.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8275, 0.8275, 0.8275	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BD5, ZN, CA, ATP

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	0.17	0/35977	0.43	3/48726 (0.0%)
1	B	0.18	0/35977	0.43	3/48726 (0.0%)
1	C	0.18	0/35977	0.43	3/48726 (0.0%)
1	D	0.18	0/35977	0.43	3/48726 (0.0%)
2	E	0.17	0/850	0.41	0/1146
2	F	0.17	0/850	0.42	0/1146
2	G	0.17	0/850	0.42	0/1146
2	H	0.15	0/850	0.40	0/1146
All	All	0.18	0/147308	0.43	12/199488 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	MET	CA-CB-CG	5.94	125.98	114.10
1	A	227	MET	CA-CB-CG	5.93	125.95	114.10
1	B	227	MET	CA-CB-CG	5.92	125.93	114.10
1	D	227	MET	CA-CB-CG	5.90	125.90	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	226	HIS	CA-C-N	5.43	131.91	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2244	ARG	Sidechain
1	B	2244	ARG	Sidechain
1	C	2244	ARG	Sidechain
1	D	2244	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34794	1162	0
1	B	35150	0	34792	1148	0
1	C	35150	0	34792	1134	0
1	D	35150	0	34792	1145	0
2	E	831	0	831	26	0
2	F	831	0	831	23	0
2	G	831	0	831	27	0
2	H	831	0	831	31	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144120	0	142542	4552	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 16.

The worst 5 of 4552 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3477:LYS:HE3	1:B:1141:ARG:CZ	1.20	1.58
1:A:3477:LYS:CE	1:B:1141:ARG:NH1	1.69	1.54
1:A:3477:LYS:CE	1:B:1141:ARG:HD3	1.33	1.53
1:A:1141:ARG:NH1	1:D:3477:LYS:CE	1.70	1.43
1:A:3477:LYS:CE	1:B:1141:ARG:CZ	1.93	1.38

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4385/5037 (87%)	4306 (98%)	79 (2%)	0	100	100
1	B	4385/5037 (87%)	4305 (98%)	80 (2%)	0	100	100
1	C	4385/5037 (87%)	4307 (98%)	78 (2%)	0	100	100
1	D	4385/5037 (87%)	4304 (98%)	81 (2%)	0	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
All	All	17960/20580 (87%)	17635 (98%)	325 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	3836/4276 (90%)	3760 (98%)	76 (2%)	48	72
1	B	3836/4276 (90%)	3760 (98%)	76 (2%)	48	72
1	C	3836/4276 (90%)	3759 (98%)	77 (2%)	48	72
1	D	3836/4276 (90%)	3758 (98%)	78 (2%)	48	72
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	71
2	F	89/90 (99%)	85 (96%)	4 (4%)	24	58
2	G	89/90 (99%)	85 (96%)	4 (4%)	24	58
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	71
All	All	15700/17464 (90%)	15381 (98%)	319 (2%)	48	72

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3874	VAL
1	C	2827	ARG
1	D	4756	ARG
1	C	1231[B]	GLN
1	C	3394	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2780	ASN
1	C	1035	ASN
1	D	3013	HIS
1	D	4162	ASN
1	C	2092	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	A1BD5	A	5304	-	16,16,16	0.96	1 (6%)	21,23,23	0.77	0
3	ATP	A	5301	-	32,33,33	0.31	0	48,52,52	0.38	0
6	A1BD5	B	5304	-	16,16,16	0.94	1 (6%)	21,23,23	0.77	0
6	A1BD5	C	5304	-	16,16,16	0.94	1 (6%)	21,23,23	0.76	0
3	ATP	C	5301	-	32,33,33	0.31	0	48,52,52	0.38	0
3	ATP	B	5301	-	32,33,33	0.31	0	48,52,52	0.39	0
3	ATP	D	5301	-	32,33,33	0.31	0	48,52,52	0.38	0
6	A1BD5	D	5304	-	16,16,16	0.93	1 (6%)	21,23,23	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1BD5	A	5304	-	-	4/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	3/22/38/38	0/3/3/3
6	A1BD5	B	5304	-	-	4/4/4/4	0/2/2/2
6	A1BD5	C	5304	-	-	4/4/4/4	0/2/2/2
3	ATP	C	5301	-	-	3/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	3/22/38/38	0/3/3/3
3	ATP	D	5301	-	-	3/22/38/38	0/3/3/3
6	A1BD5	D	5304	-	-	4/4/4/4	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5304	A1BD5	C1-C2	-2.21	1.36	1.39
6	B	5304	A1BD5	C1-C2	-2.18	1.36	1.39
6	D	5304	A1BD5	C1-C2	-2.14	1.36	1.39
6	C	5304	A1BD5	C1-C2	-2.14	1.36	1.39

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

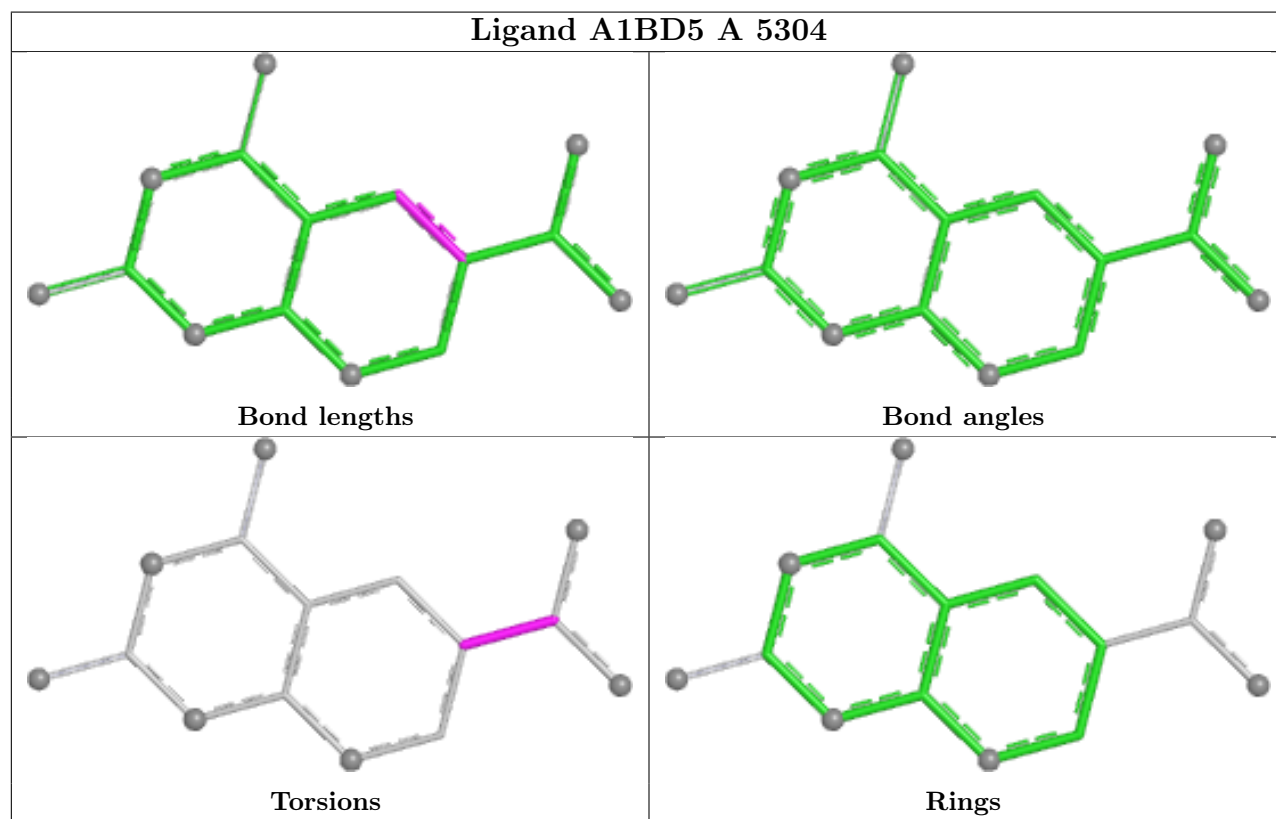
Mol	Chain	Res	Type	Atoms
6	A	5304	A1BD5	C3-C2-C8-O3
6	A	5304	A1BD5	C3-C2-C8-O4
6	B	5304	A1BD5	C3-C2-C8-O3
6	B	5304	A1BD5	C3-C2-C8-O4
6	D	5304	A1BD5	C3-C2-C8-O3

There are no ring outliers.

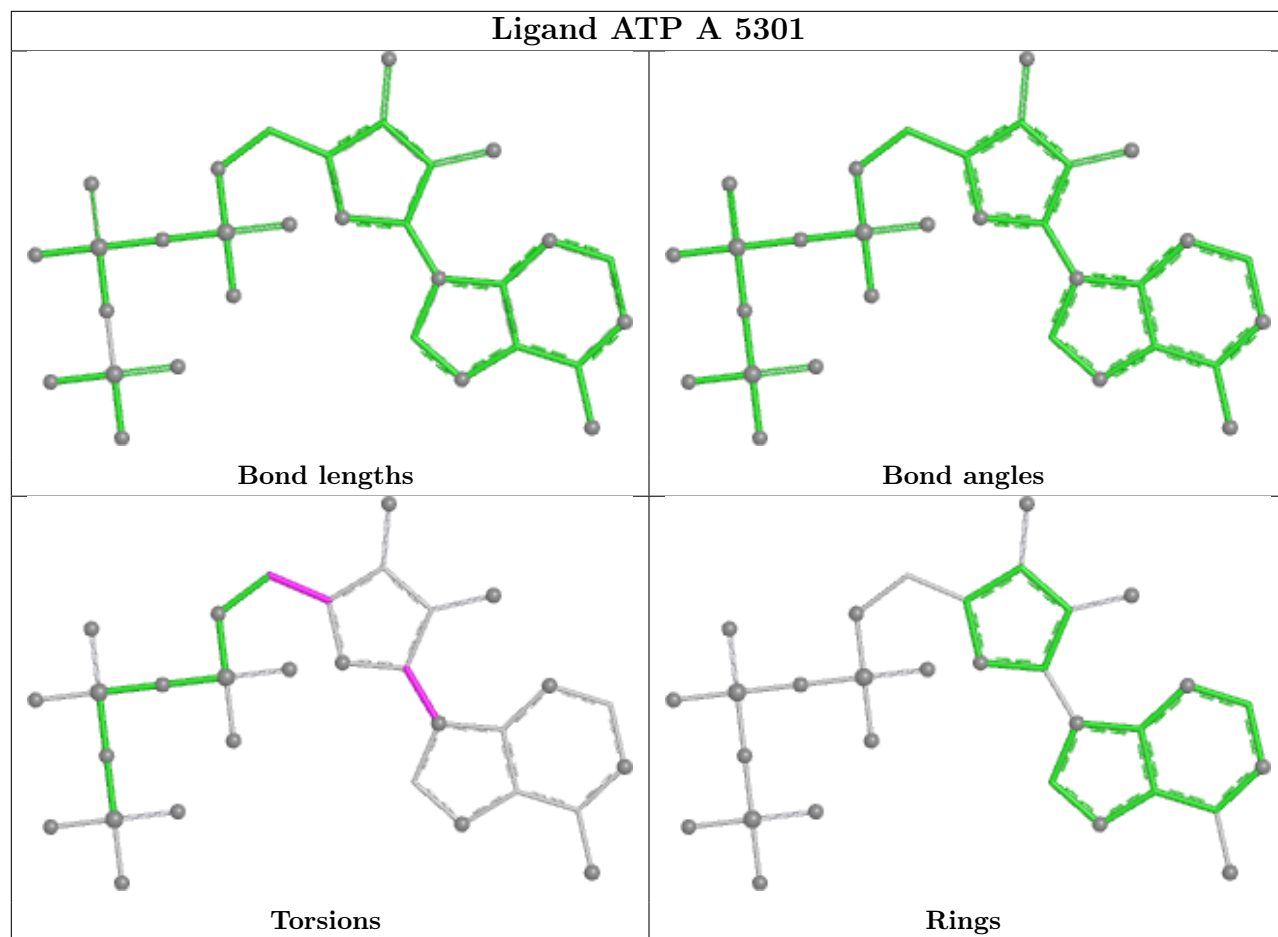
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	1	0
3	C	5301	ATP	1	0
3	B	5301	ATP	1	0

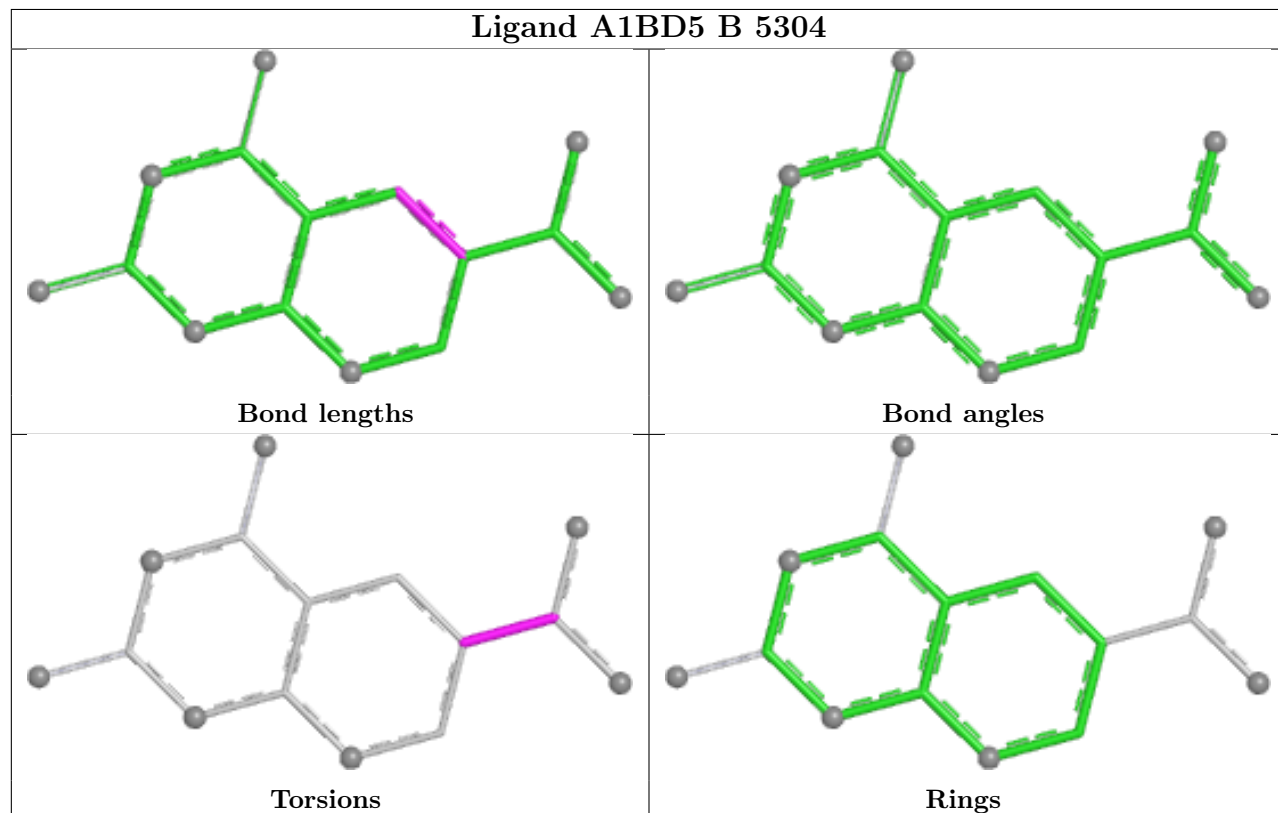
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



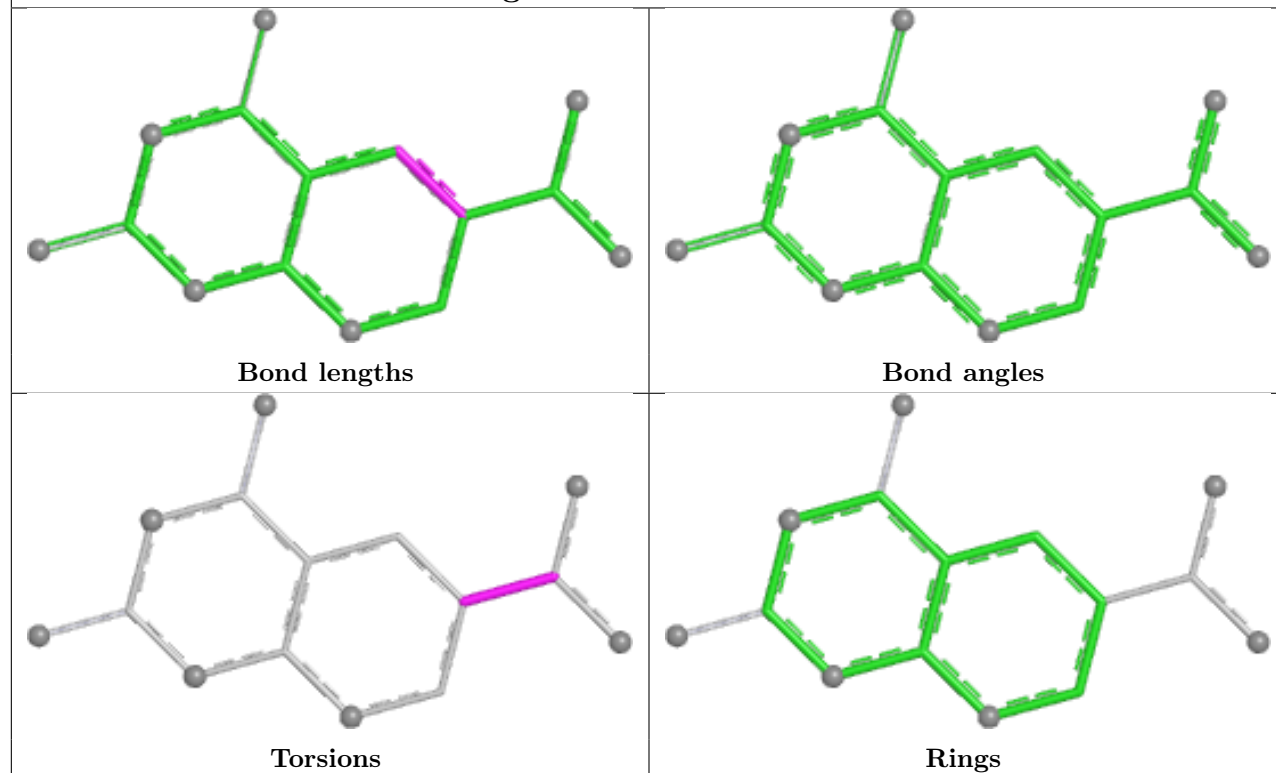
Ligand ATP A 5301



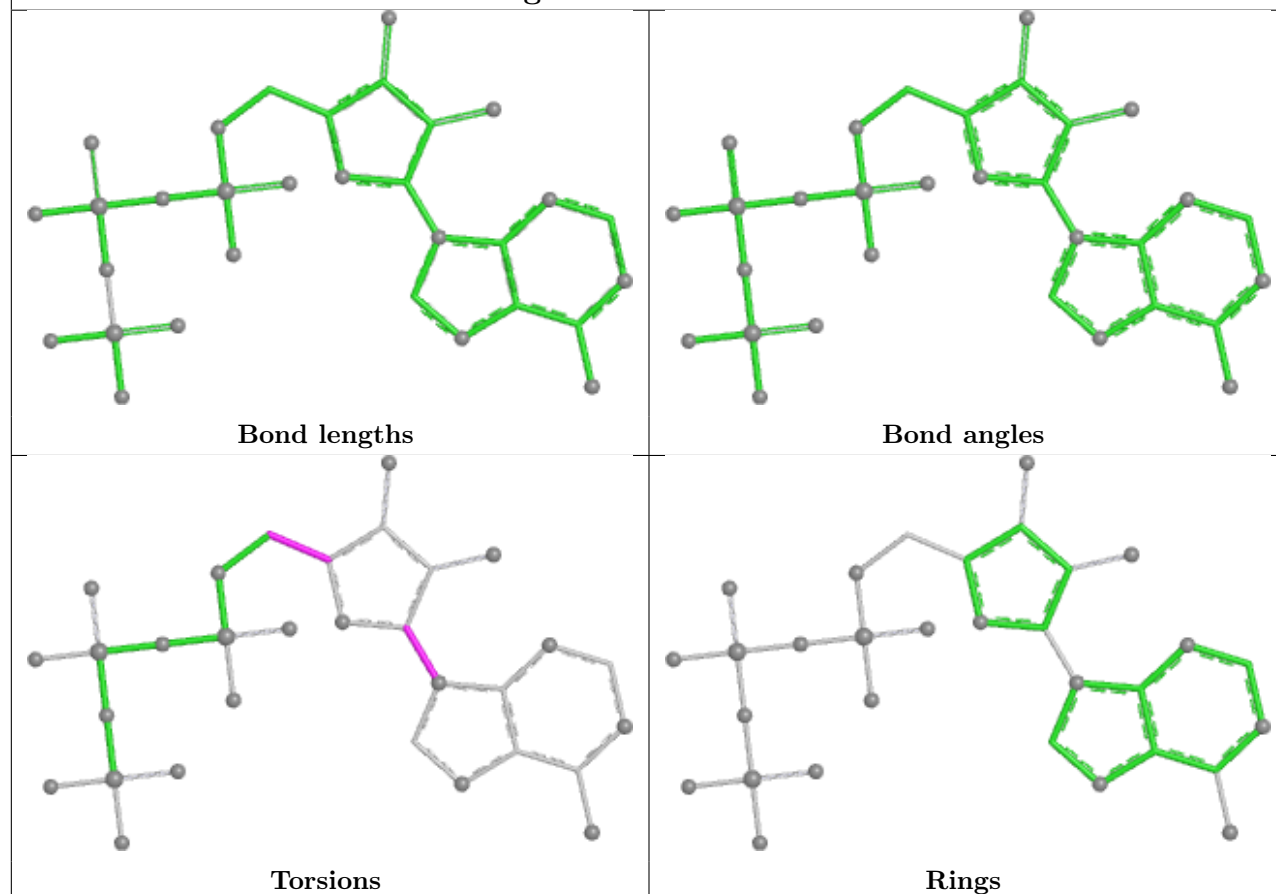
Ligand A1BD5 B 5304

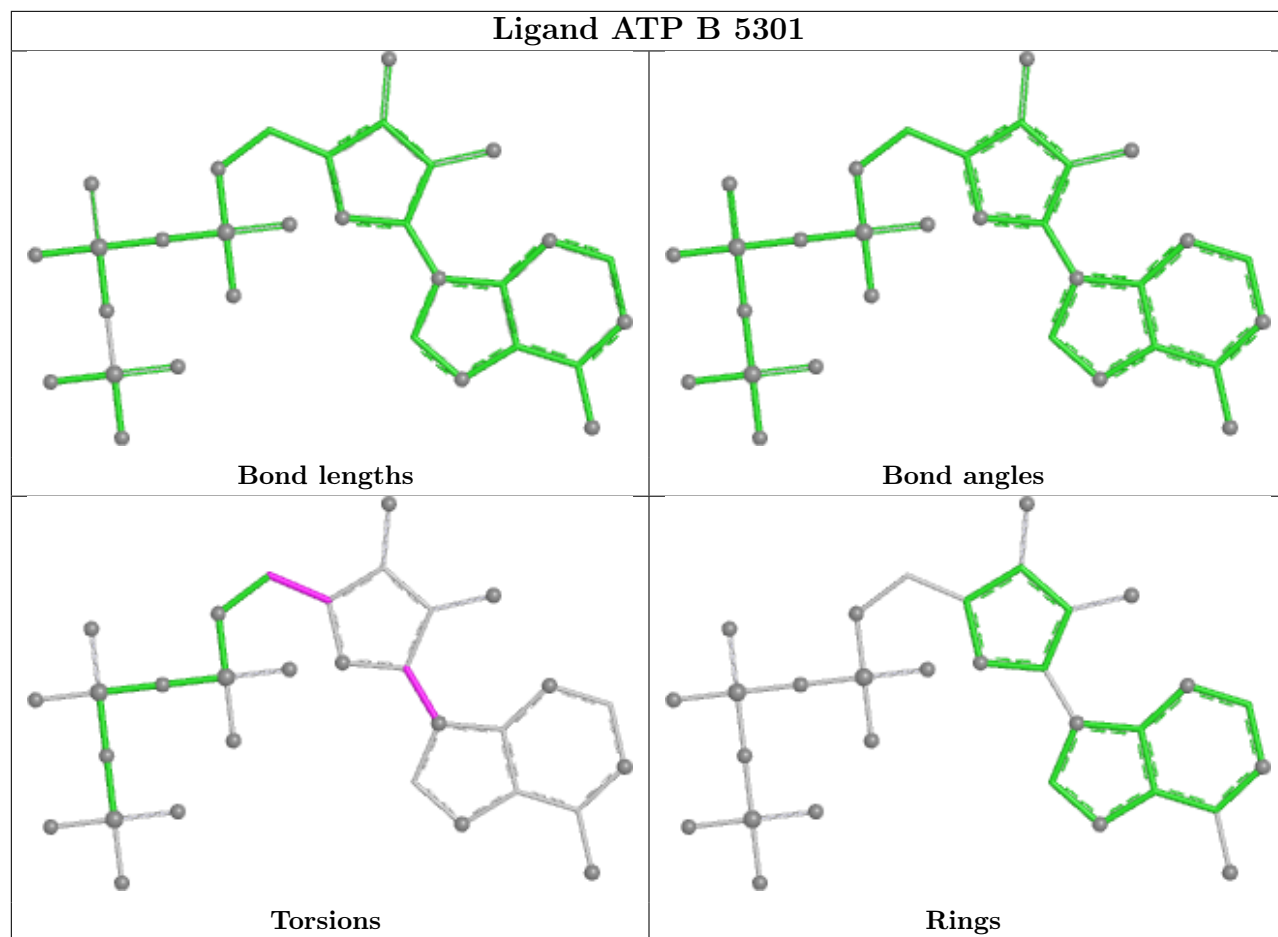


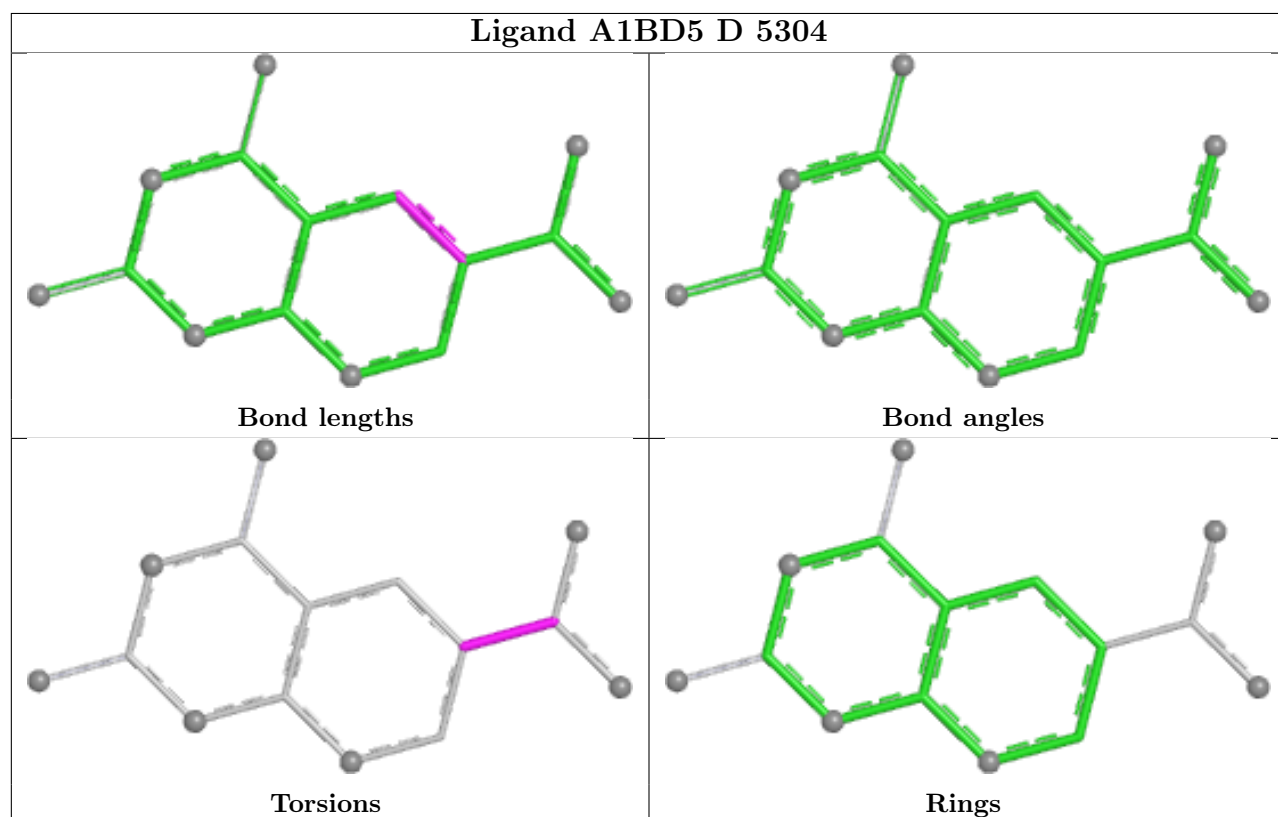
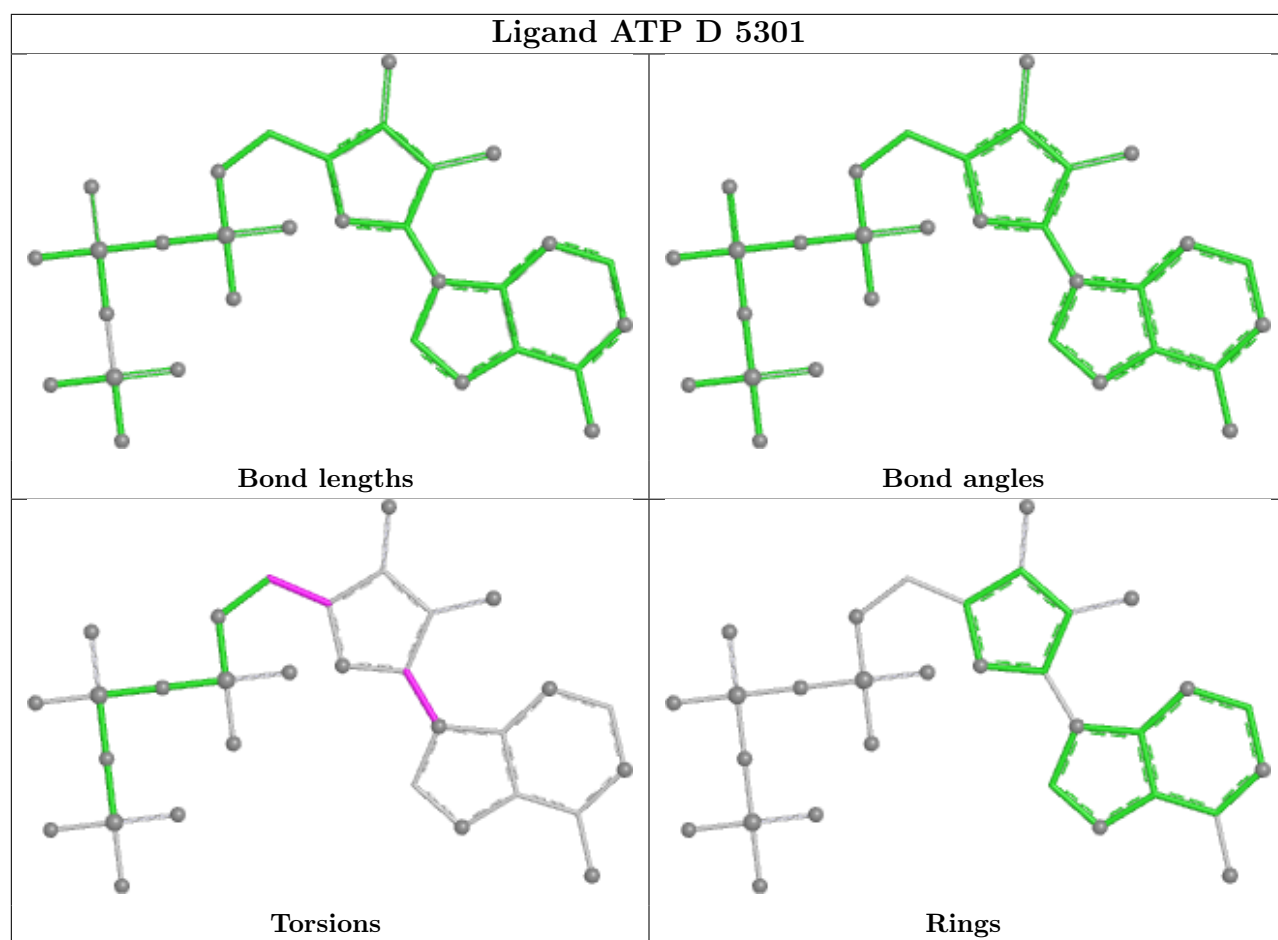
Ligand A1BD5 C 5304



Ligand ATP C 5301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

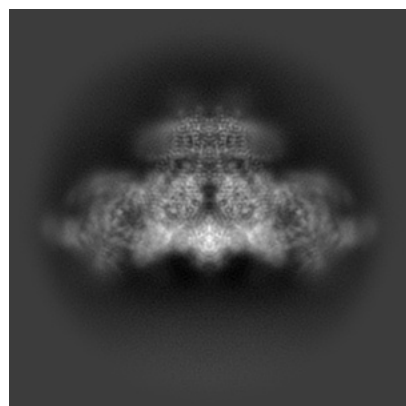
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47395. These allow visual inspection of the internal detail of the map and identification of artifacts.

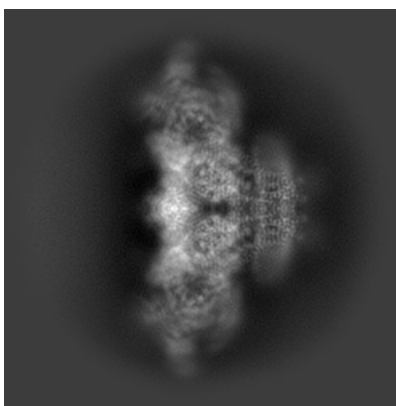
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

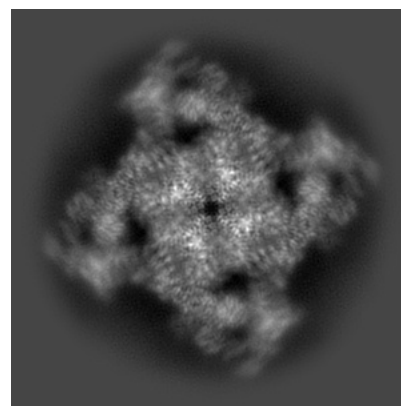
6.1.1 Primary map



X

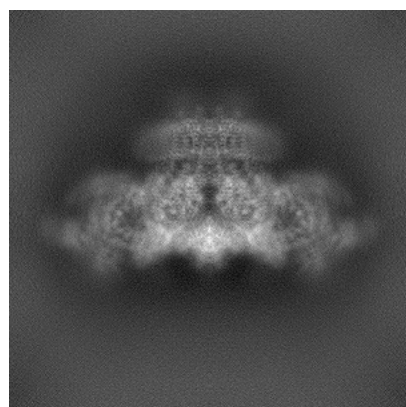


Y

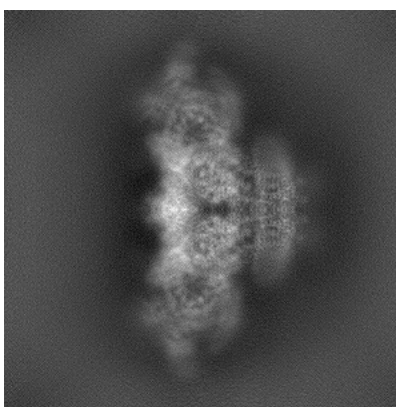


Z

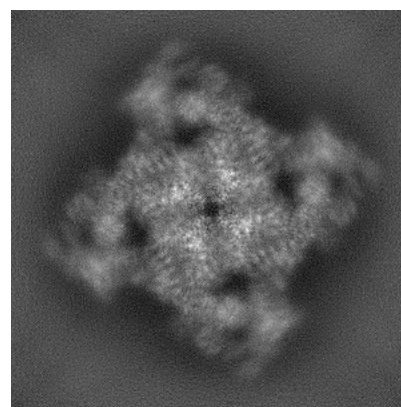
6.1.2 Raw map



X



Y

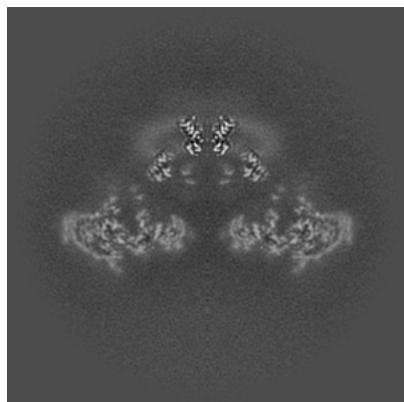


Z

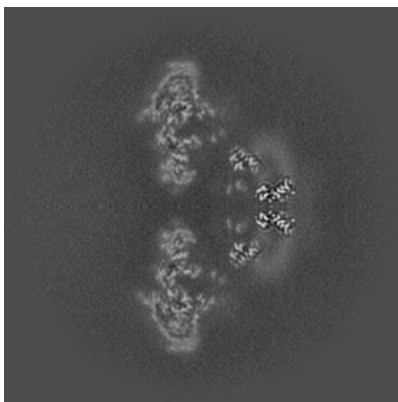
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

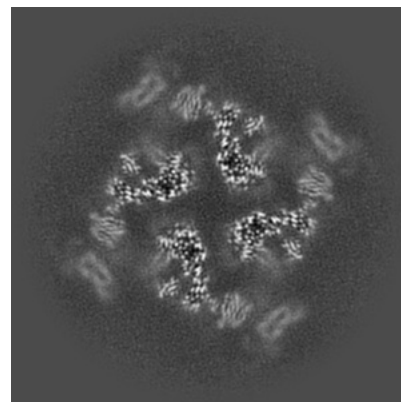
6.2.1 Primary map



X Index: 256

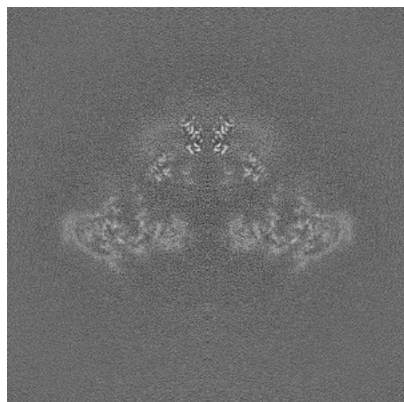


Y Index: 256

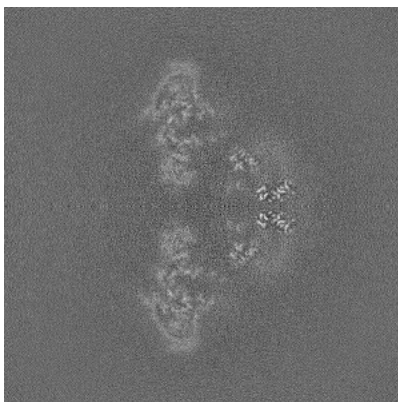


Z Index: 256

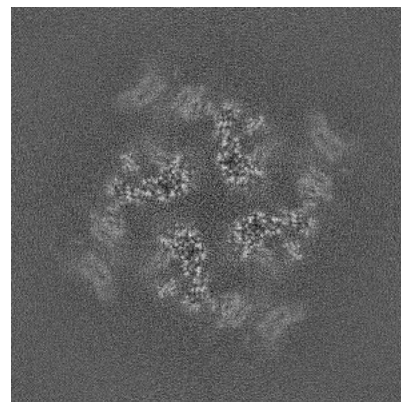
6.2.2 Raw map



X Index: 256



Y Index: 256

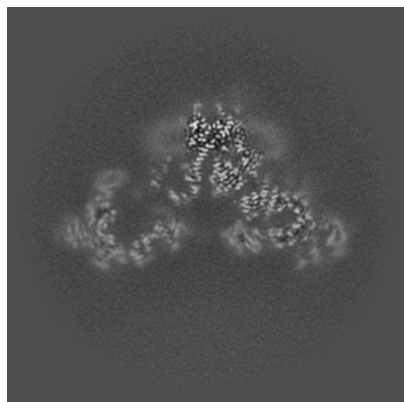


Z Index: 256

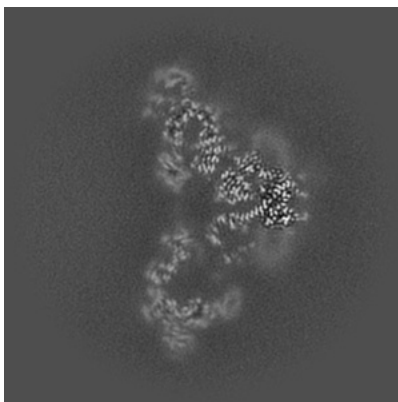
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

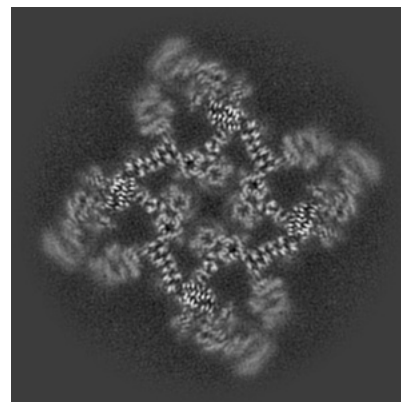
6.3.1 Primary map



X Index: 270

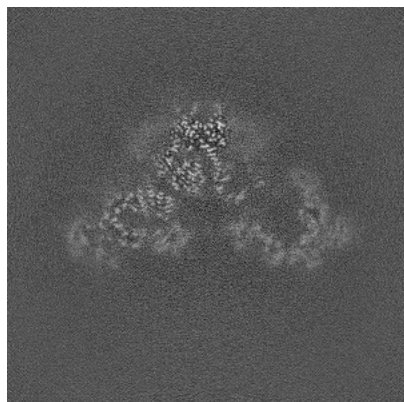


Y Index: 242

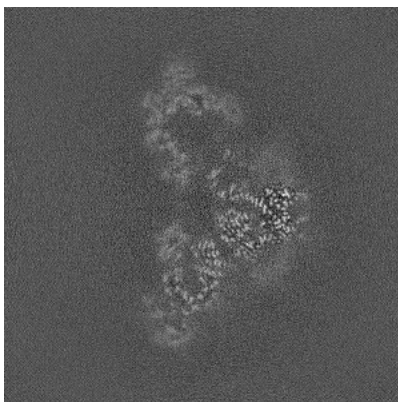


Z Index: 227

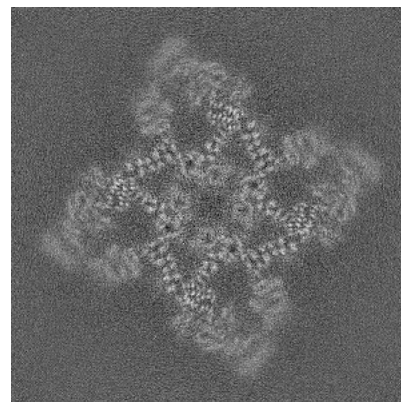
6.3.2 Raw map



X Index: 242



Y Index: 270

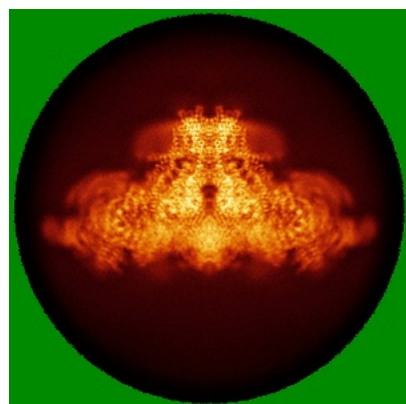


Z Index: 227

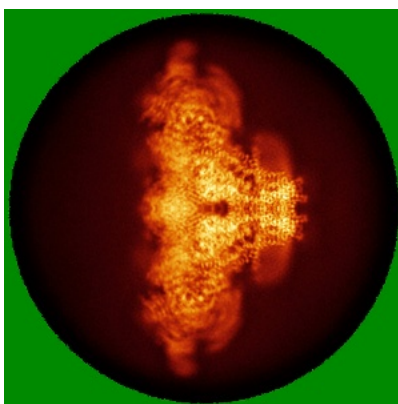
The images above show the largest variance slices of the map in three orthogonal directions.

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

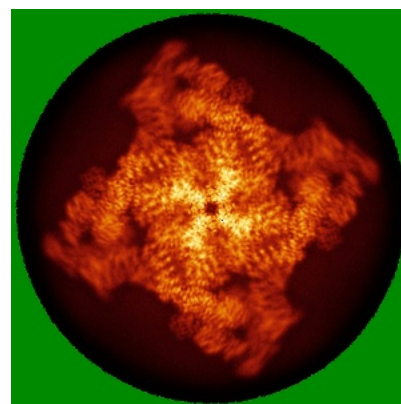
6.4.1 Primary map



X

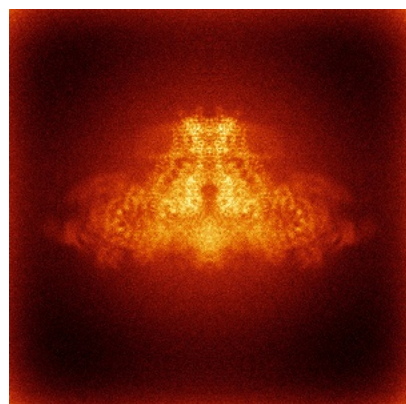


Y

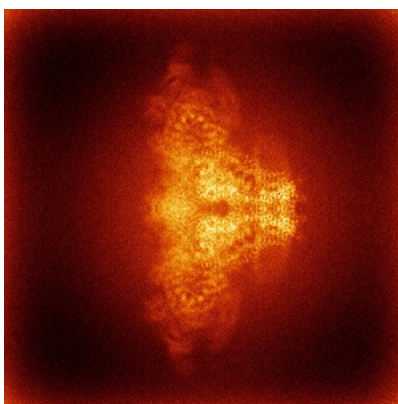


Z

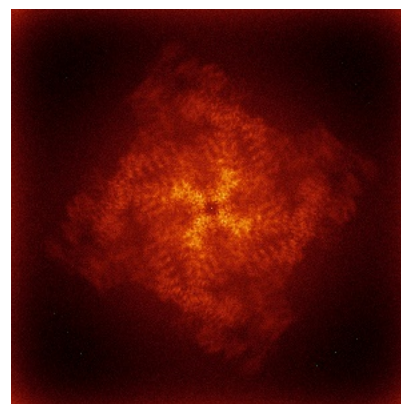
6.4.2 Raw map



X



Y

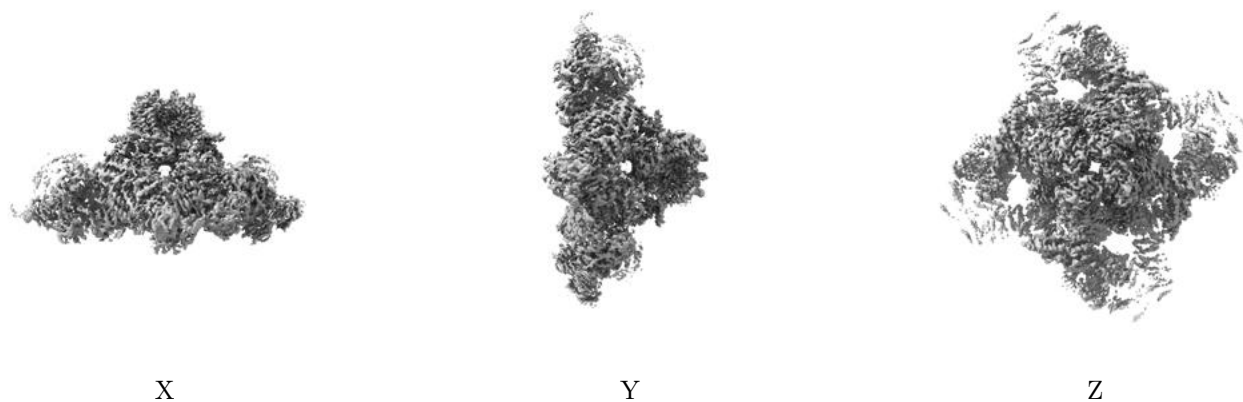


Z

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.

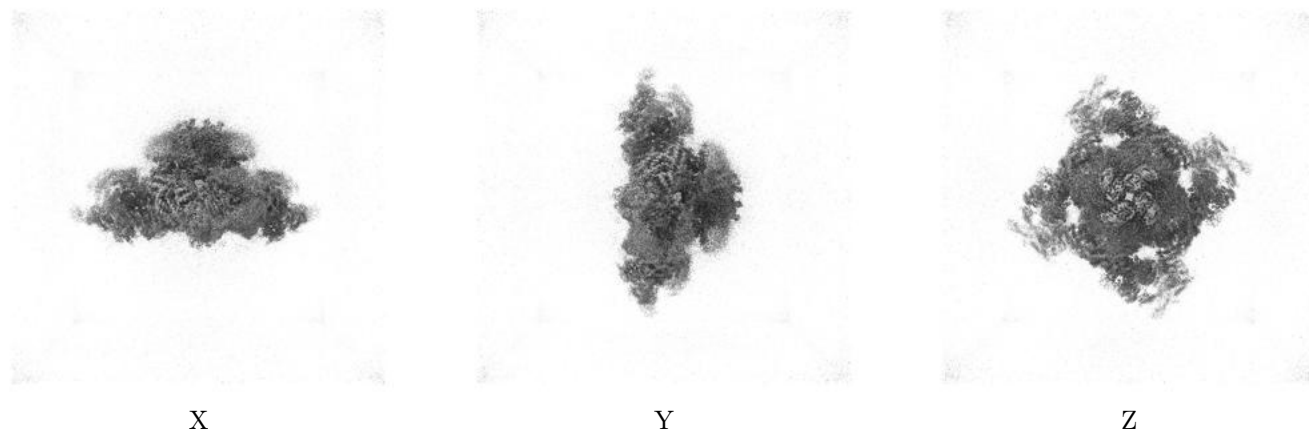
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

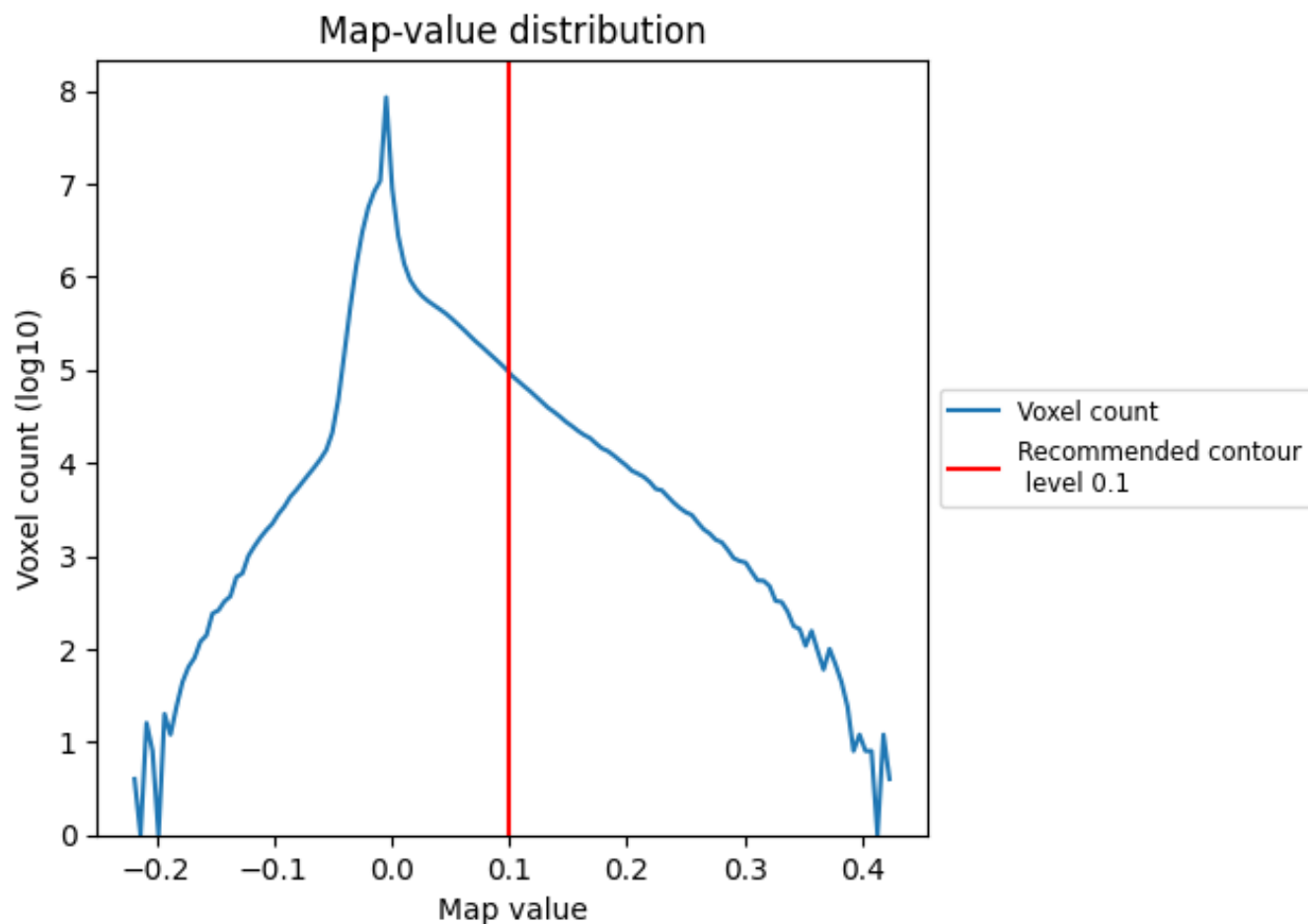
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

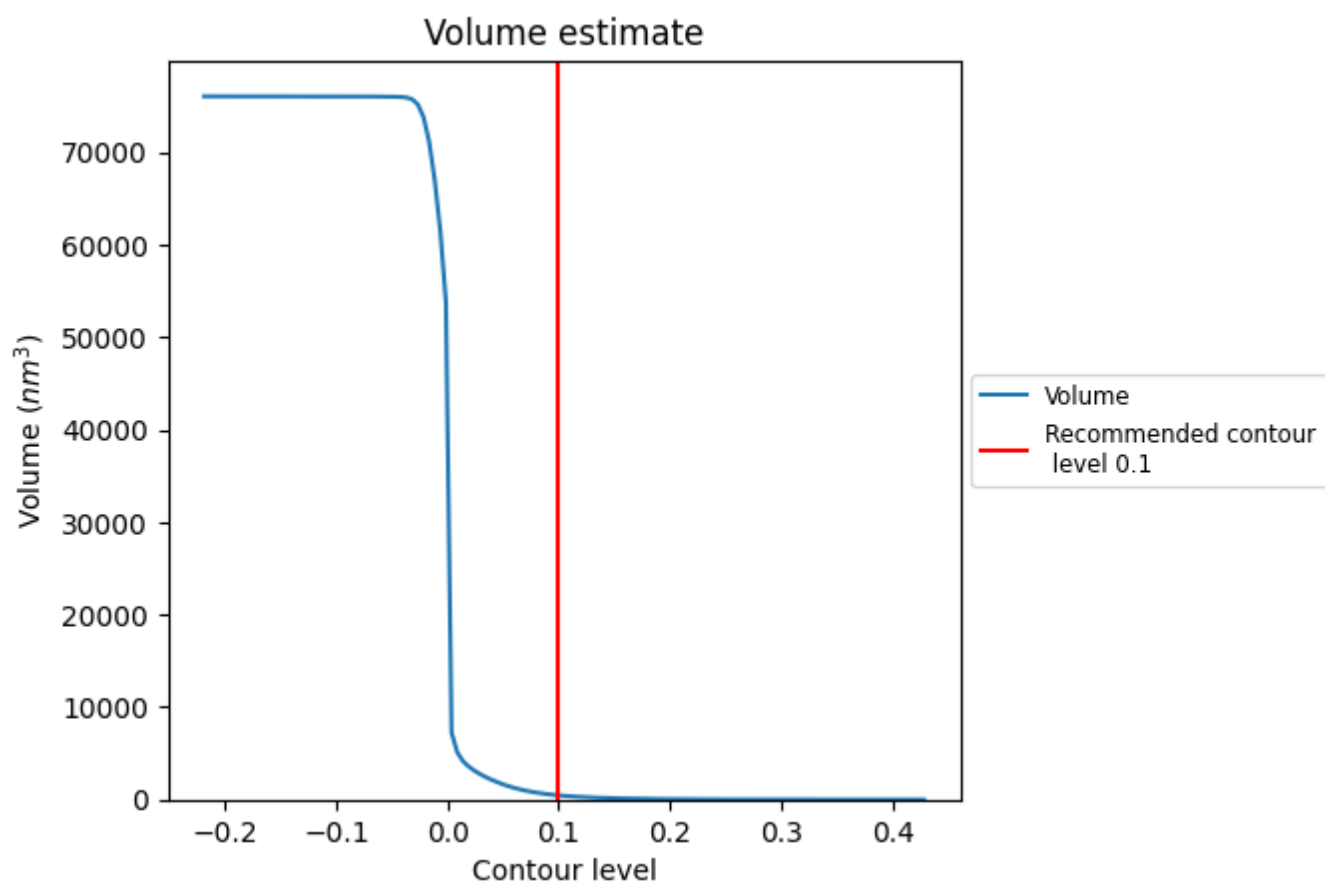
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

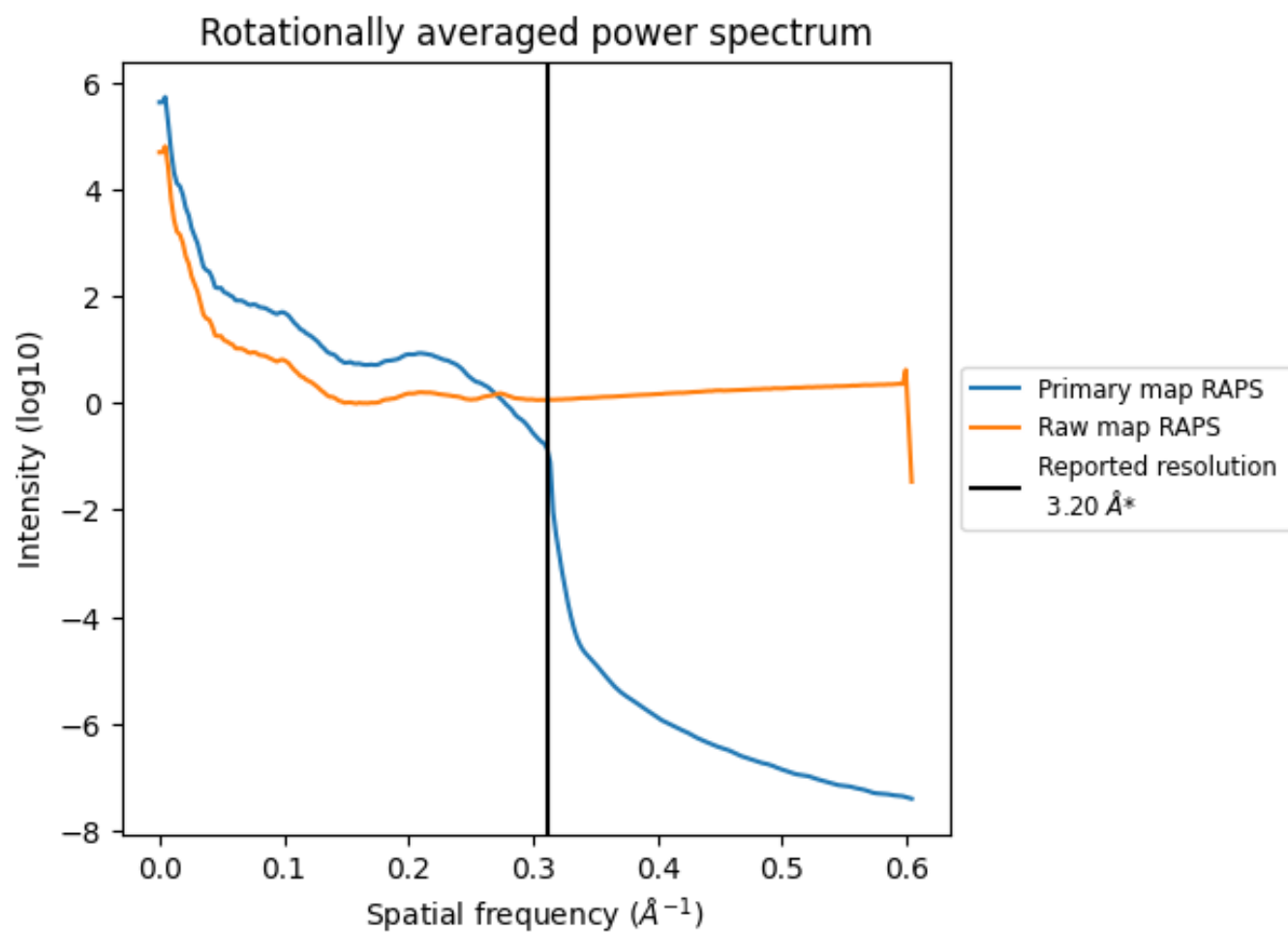
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 409 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 ⓘ

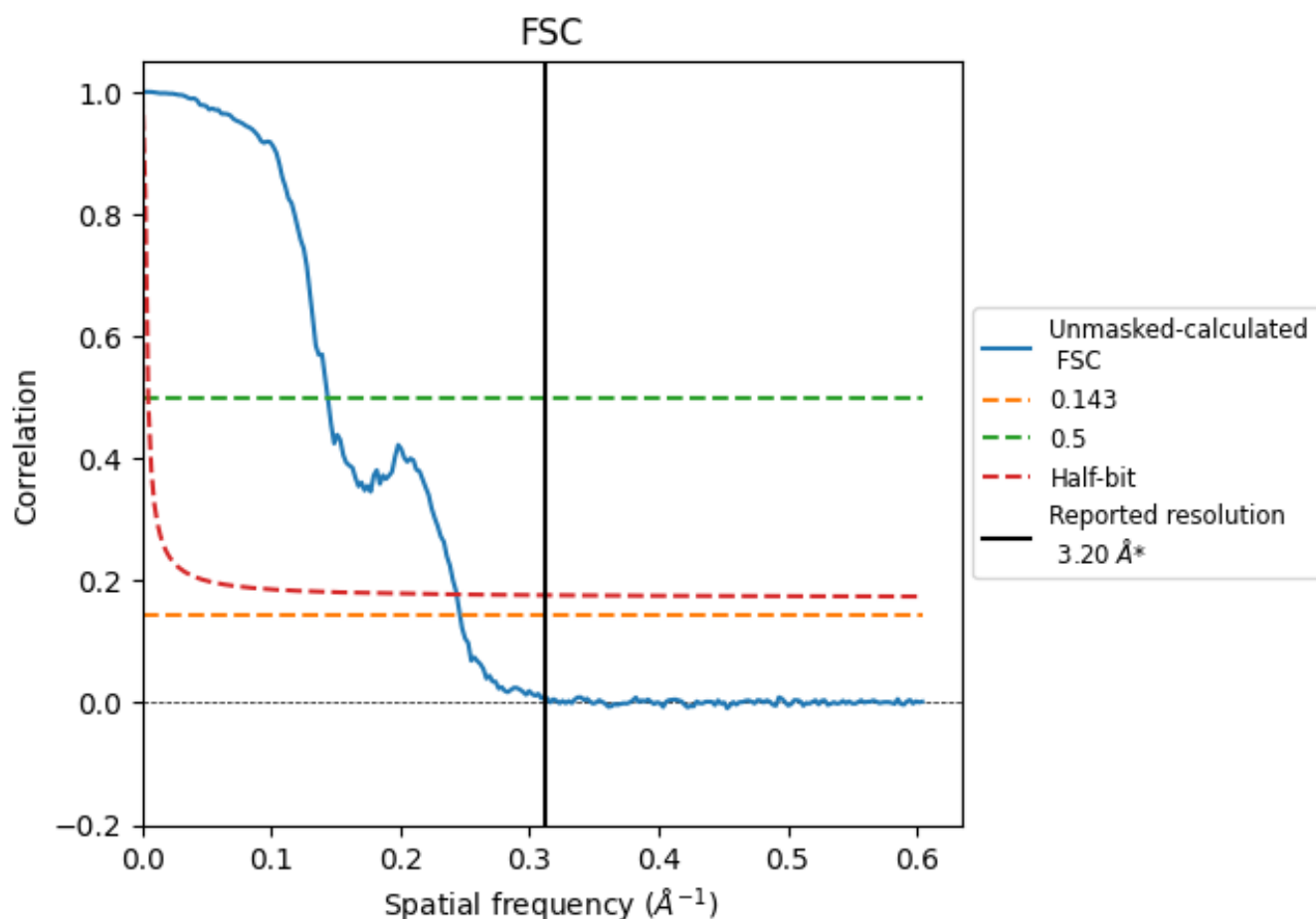


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

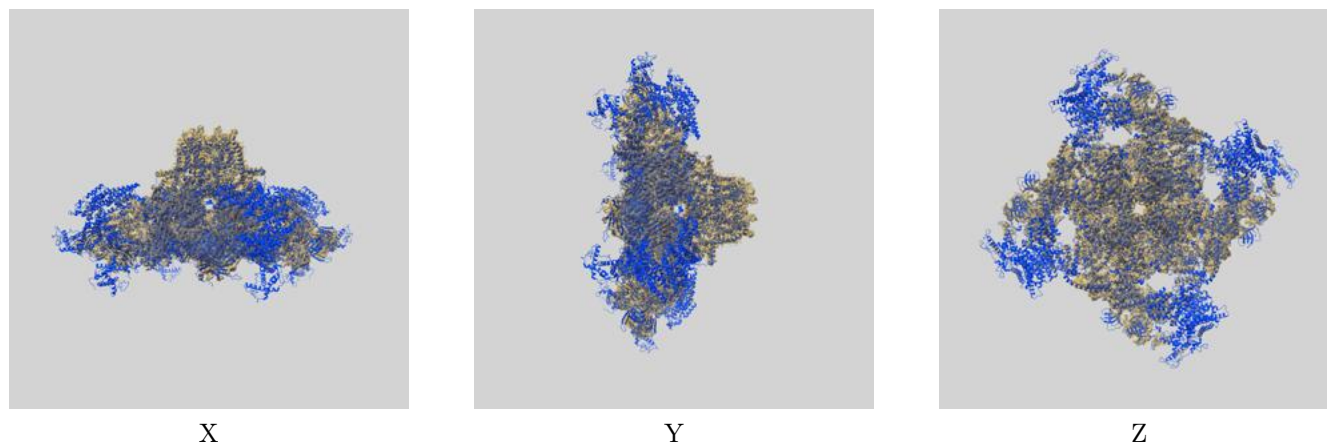
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	6.96	4.11

*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 4.06 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

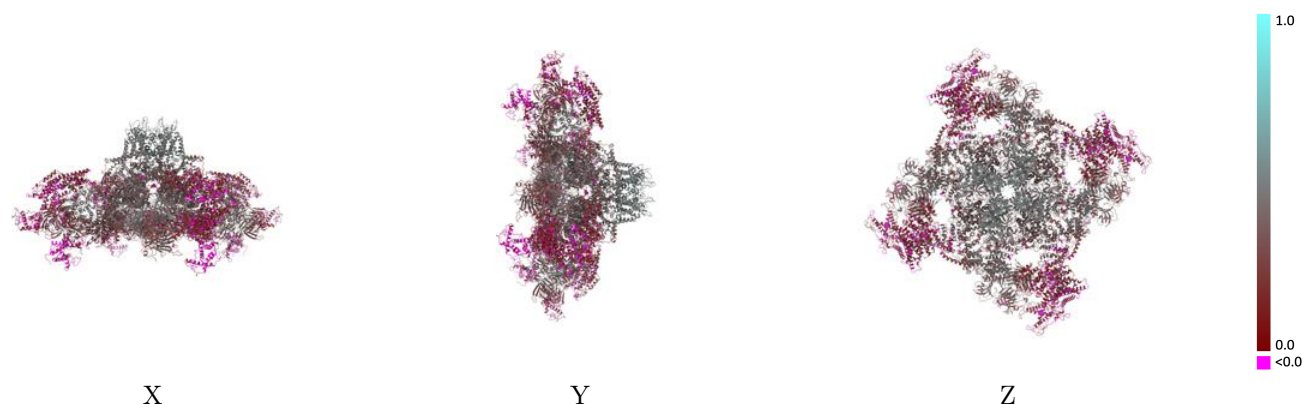
This section contains information regarding the fit between EMDB map EMD-47395 and PDB model 9E1I. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



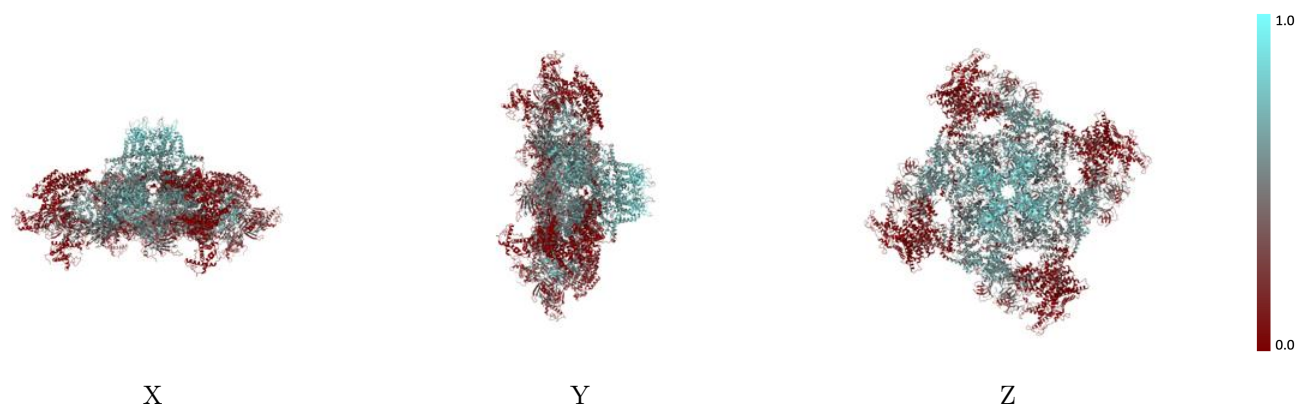
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



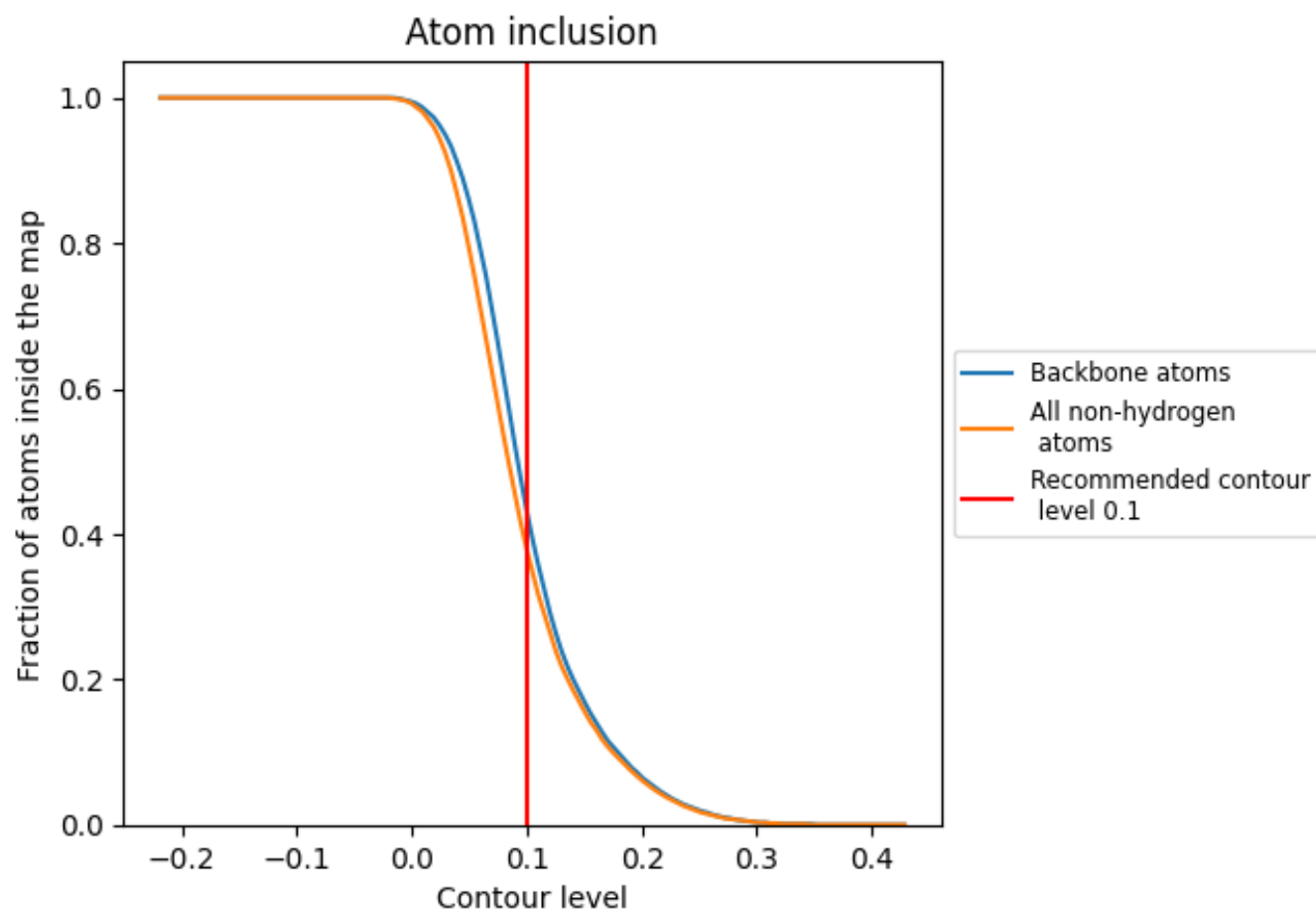
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3780	0.3000
A	0.3910	0.2990
B	0.3900	0.2980
C	0.3890	0.2970
D	0.3890	0.2980
E	0.2210	0.3870
F	0.2250	0.3860
G	0.2250	0.3850
H	0.2250	0.3880

1.0

0.0

<0.0