



wwPDB EM Validation Summary Report ⓘ

Jul 20, 2026 – 04:58 pm BST

PDB ID : 9S16 / pdb_00009s16
EMDB ID : EMD-54445
Title : Apo-state RyR1 in the native membrane solved by "SPA"
Authors : Mikirtumov, V.
Deposited on : 2025-07-17
Resolution : 3.60 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

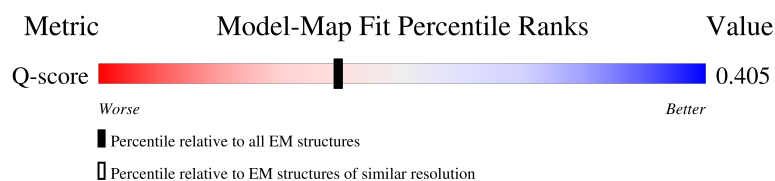
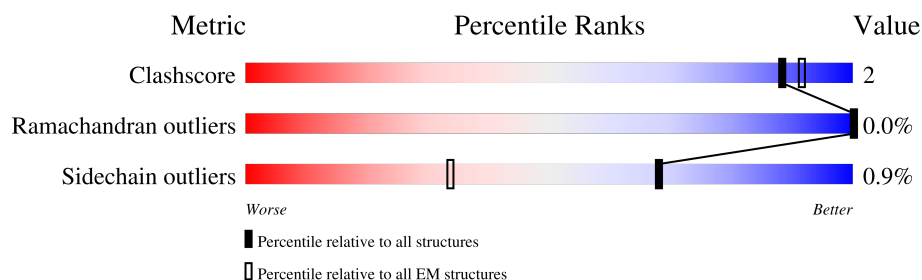
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	25% 81% 6% 13%
1	B	5037	25% 81% 6% 13%
1	C	5037	25% 81% 6% 13%
1	D	5037	25% 81% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	 96%
2	F	108	 96%
2	G	108	 95%
2	H	108	 96%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 287008 atoms, of which 142908 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	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
3	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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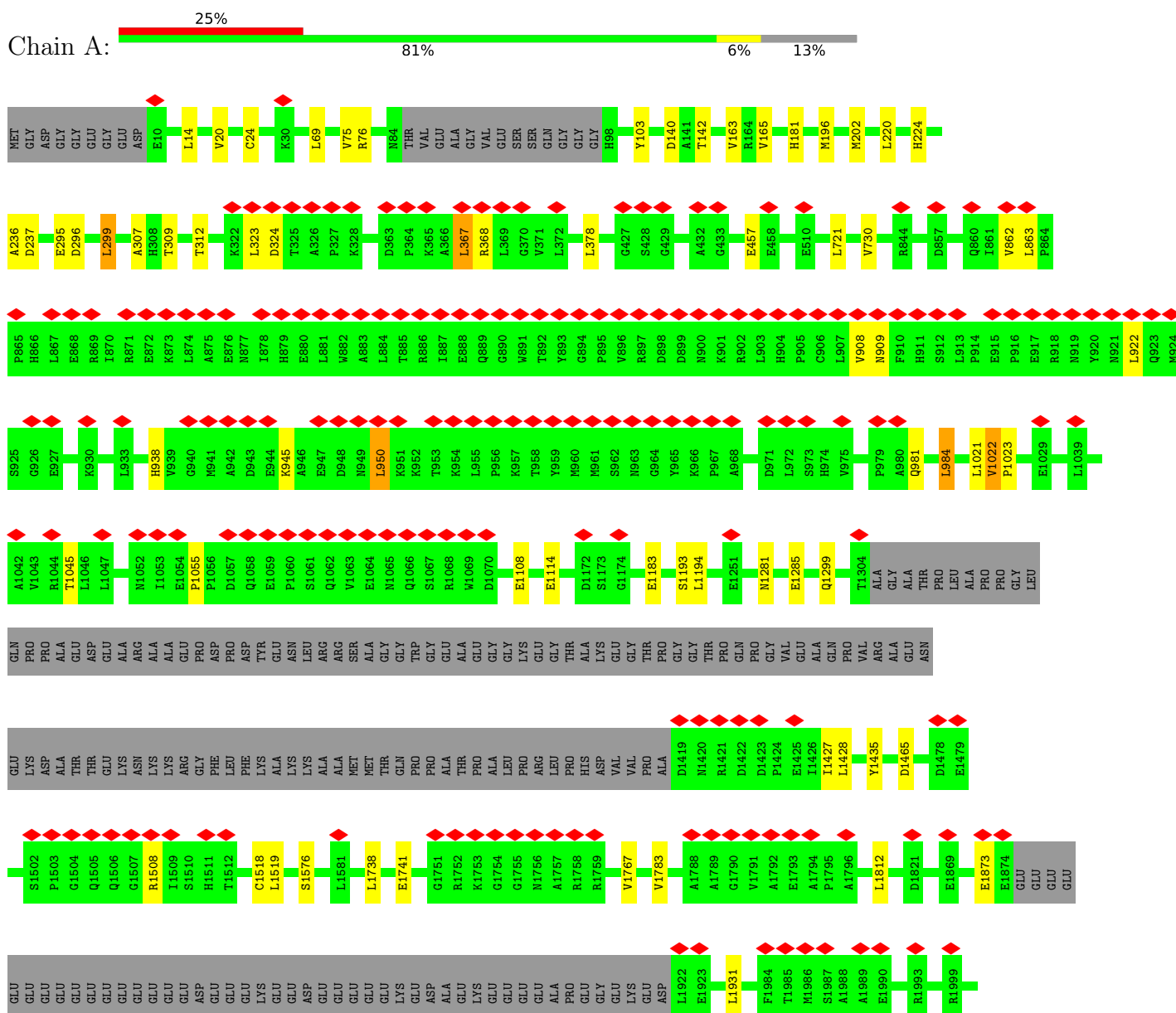
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	D	1	1	1	0

3 Residue-property plots [i](#)

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

- Molecule 1: Ryanodine receptor 1

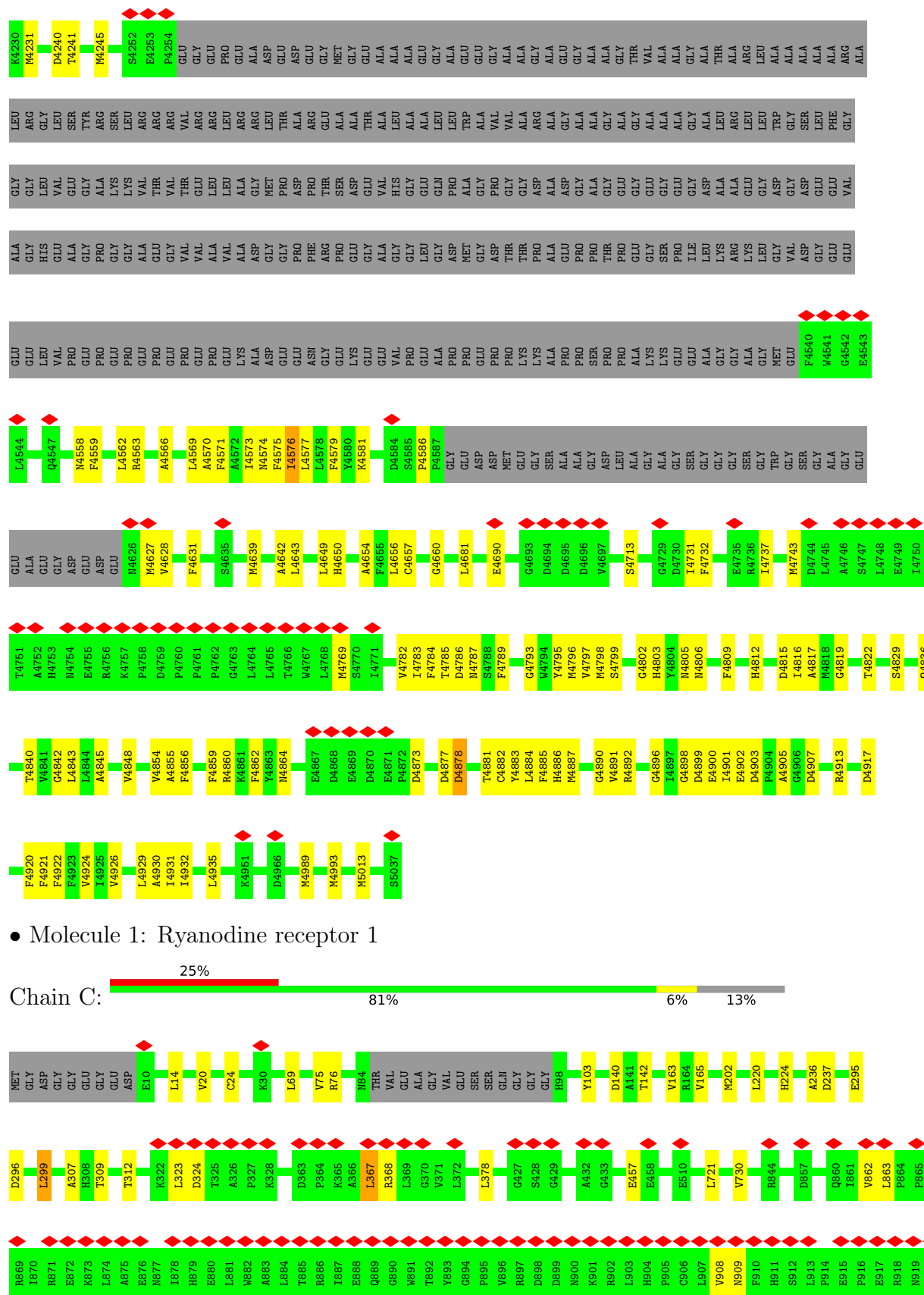


G3126	G3127	G3128	L3129	T3130	Y3131	T3132	T3133	T3134	T3135	L3136	L3137	F3138	V3139	L3140	F3144	G3145	G3146	G3149	H3150	Q3151	F3152	G3153	D3154	R3155	V3156	I3157	L3158	D3159	V3161	Q3162	G3165	G3166	R3167	T3168	G3170	S3171	I3172	V3173	T3174	G3175	T3177	T3178	K3179	N3180	T3181	Y3182	T3183	E3184	K3185	L3186	P3188	A3189							
V3065	N3066	C3067	L3068	H3069	L3070	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	K3105	N3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	R3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125		
L3002	L3003	P3004	L3005	L3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	G3014	L3015	V3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	K3036	E3037	M3038	L3039	L3042	F3043	G3044	K3045	L3046	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	A3063	V3064		
GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	L2964	R2965	V2966	M2967	D2968	L2969	S2970	Q2971	E2972	F2973	L2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	F2990	H2991	E2992	Q2993	E2994	I2995	K2996	F2997	F2998	K3000	I3001		
E2880	N2881	Y2882	H2883	T2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	E2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	T2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	R2918	D2919	R2920	E2921	K2922	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	T2939		
E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLU	THR	ARG	THR	GLU	LYS	LYS	THR	LYS	LYS	THR	LYS	ILE	SER	THR	ALA	THR	ASP	PRO	ARG	GLU	GLY	V2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	H2874	A2875	E2876	Q2877	L2878	A2879		
E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	T2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	T2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	W2818	A2819
R2697	M2698	C2702	A2705	I2706	D2707	G2708	A2709	L2710	P2711	F2712	D2713	Y2714	W2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	W2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	V2745	I2746	L2747	T2748	E2749	K2750	D2751	D2752	S2753	F2754	L2755	W2756	K2757	F2758	A2759				
L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	I2632	L2633	N2634	E2635	F2636	A2637	K2638	L2641	K2642	L2643	R2650	P2658	T2659	G2660	N2663	F2664	G2665	V2666	T2667	S2668	E2671	L2672	H2673	L2674	T2675	K2676	R2677	L2678	F2679	G2681	L2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	Y2696							
D2529	M2530	R2531	A2532	A2533	A2534	S2535	L2536	D2537	T2538	A2539	P2540	F2541	N2551	R2552	Y2553	L2554	V2558	K2564	L2568	F2569	T2572	R2575	M2578	V2579	D2580	H2584	L2589	S2590	R2591	G2592	Q2599	R2600	D2601	V2602	L2603	E2604	L2607	R2612	Y2613	I2614	R2615	S2616	W2617	M2618	L2619														
G2394	P2395	G2396	V2397	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	V2416	E2439	D2465	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	K2489	M2490	D2507	T2512	D2516	F2517	L2518	L2522	D2523	V2524	G2525	F2526	L2527	P2528								
K2090	E2108	D2109	L2123	L2165	V2168	M2198	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	R2224	F2225	R2244	D2252	I2263	G2264	L2265	G2266	M2267	Q2268	G2269	S2309	C2310	P2311	M2312	L2313	L2314	A2315	K2316	D2320	L2377	A2383	I2384	R2385	I2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393													
H2008	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	E2025	G2043	T2044	Q2045	L2046	GLU	GLY	GLU	GLU	GLU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU	E2088	K2089								

ALA	GLY	LEU	M4230	L4059	E3750	L3623	G3560	R3498	V3438	V3372	H3311	M3250
GLY	ARG	ARG	M4231	D4070	V3751	L3624	G3561	R3499	G3439	V3373	L3312	G3191
LEU	GLY	LEU	D4240	S3752	S3752	S3625	G3562	R3499	E3440	A3374	N3313	A3251
ALA	GLU	LEU	T4241	F3753	V3563	K3626	V3563	D3501	E3441	E3375	L3316	I3253
GLY	ARG	THR	M4245	K3756	G3565	Q3627	E3664	R3502	F3442	E3376	G3317	C3193
PRO	ALA	ARG	A4075	A4076	G3565	R3628	G3565	V3503	I3443	E3377	N3318	L3194
GLY	LYS	LEU	F4077	F4078	S3666	R3629	S3666	S3504	Y3444	Q3378	I3319	C3254
ALA	VAL	ARG	D4079	D4079	L3569	R3630	L3569	V3505	Y3445	L3379	L3320	R3196
GLY	THR	ARG	Y4080	Y4080	R3570	A3631	Q3506	Q3506	S3446	R3380	A3198	A3257
VAL	THR	VAL	V3632	V3632	R3570	V3632	T3507	T3507	K3447	L3381	R3321	A3257
VAL	GLU	ARG	V3633	V3633	M3573	V3633	S3508	S3508	K3448	L3382	L3322	E3207
ALA	ARG	ARG	A3574	A3574	A3574	A3574	L3509	L3509	H3449	E3383	A3200	A3199
LEU	LEU	LEU	C3635	C3635	C3577	C3635	T3510	T3510	R3448	L3323	R3322	G3260
VAL	ARG	ARG	F3636	F3636	R3577	F3636	V3511	V3511	N3450	V3324	V3324	A3261
ASP	ALA	ARG	R3637	R3637	G3578	R3637	G3578	G3578	F3451	A3385	N3325	R3262
GLY	LEU	THR	M3638	M3638	L3579	M3638	T3513	T3513	K3452	E3386	L3327	Y3263
GLY	PRO	THR	L3641	L3641	P3580	L3641	L3514	L3514	E3454	A3387	G3328	K3264
ASP	ALA	ARG	E3665	E3665	G3581	E3665	K3515	K3515	Q3456	E3388	I3329	F3205
GLY	GLY	GLY	D3666	D3666	R3582	D3666	K3516	K3516	Q3456	E3389	I3330	M3266
MET	ALA	GLY	E3666	E3666	G3582	E3666	M3517	M3517	Q3456	G3390	D3339	P3267
GLY	GLY	GLY	D3666	D3666	E3583	D3666	L3518	L3518	N3457	E3391	E3331	H3268
GLY	THR	THR	E3670	E3670	E3584	E3670	P3519	P3519	F3458	A3332	A3332	Q3209
ALA	VAL	ALA	E3670	E3670	E3584	E3670	L3520	L3520	V3460	L3392	L3210	I3270
ALA	ALA	ALA	E3670	E3670	E3584	E3670	L3520	L3520	V3460	L3393	L3210	E3271
GLY	ALA	ALA	E3670	E3670	E3584	E3670	L3520	L3520	V3460	L3394	W3334	I3272
GLY	GLY	GLY	E3670	E3670	E3586	E3670	G3521	G3521	Q3461	R3395	M3335	I3273
GLY	GLY	GLY	E3670	E3670	E3586	E3670	M3524	M3524	N3462	D3396	K3336	E3212
GLY	GLY	GLY	E3670	E3670	E3586	E3670	G3525	G3525	E3463	E3397	R3337	E3213
GLY	GLY	GLY	E3670	E3670	E3586	E3670	T3528	T3528	N3465	F3398	A3339	L3274
GLY	GLY	GLY	E3670	E3670	E3586	E3670	D3529	D3529	N3466	V3400	V3340	N3214
GLY	GLY	GLY	E3670	E3670	E3586	E3670	Q3530	Q3530	M3467	L3401	F3341	A3215
GLY	GLY	GLY	E3670	E3670	E3586	E3670	D3531	D3531	S3468	C3402	A3342	P3275
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3532	L3532	F3469	R3403	Q3343	M3276
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3533	L3533	L3470	D3404	F3344	L3277
GLY	GLY	GLY	E3670	E3670	E3586	E3670	M3534	M3534	L3471	L3405	W3346	S3217
GLY	GLY	GLY	E3670	E3670	E3586	E3670	V3596	V3596	T3471	L3405	S3347	V3218
GLY	GLY	GLY	E3670	E3670	E3586	E3670	Q3597	Q3597	A3472	V3406	R3347	Y3219
GLY	GLY	GLY	E3670	E3670	E3586	E3670	E3598	E3598	D3473	A3407	R3348	T3220
GLY	GLY	GLY	E3670	E3670	E3586	E3670	V3599	V3599	S3474	L3408	R3349	S3223
GLY	GLY	GLY	E3670	E3670	E3586	E3670	S3600	S3600	S3475	R3350	R3350	F3224
GLY	GLY	GLY	E3670	E3670	E3586	E3670	A3601	A3601	S3476	Y3409	R3351	R3225
GLY	GLY	GLY	E3670	E3670	E3586	E3670	V3602	V3602	S3477	P3351	R3287	E3226
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3603	L3603	K3477	L3411	G3288	R3227
GLY	GLY	GLY	E3670	E3670	E3586	E3670	Y3604	Y3604	M3478	L3412	A3228	A3228
GLY	GLY	GLY	E3670	E3670	E3586	E3670	H3605	H3605	L3478	L3412	E3352	E3290
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	A3411	L3413	L3353	A3291
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	AL	L3413	L3354	L3230
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	ALA	R3414	H3355	G3231
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLY	Y3415	S3356	P3292
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	ASP	V3416	R3357	R3293
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	ALA	D3417	R3358	P3294
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	ALA	W3423	F3359	R3234
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	S3235	S3235
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	V3236	V3236
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3237	E3237
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3238	E3238
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
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GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
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GLY	GLY	GLY	E3670	E3670	E3586	E3670	L3606	L3606	GLN	F3359	E3239	E3239
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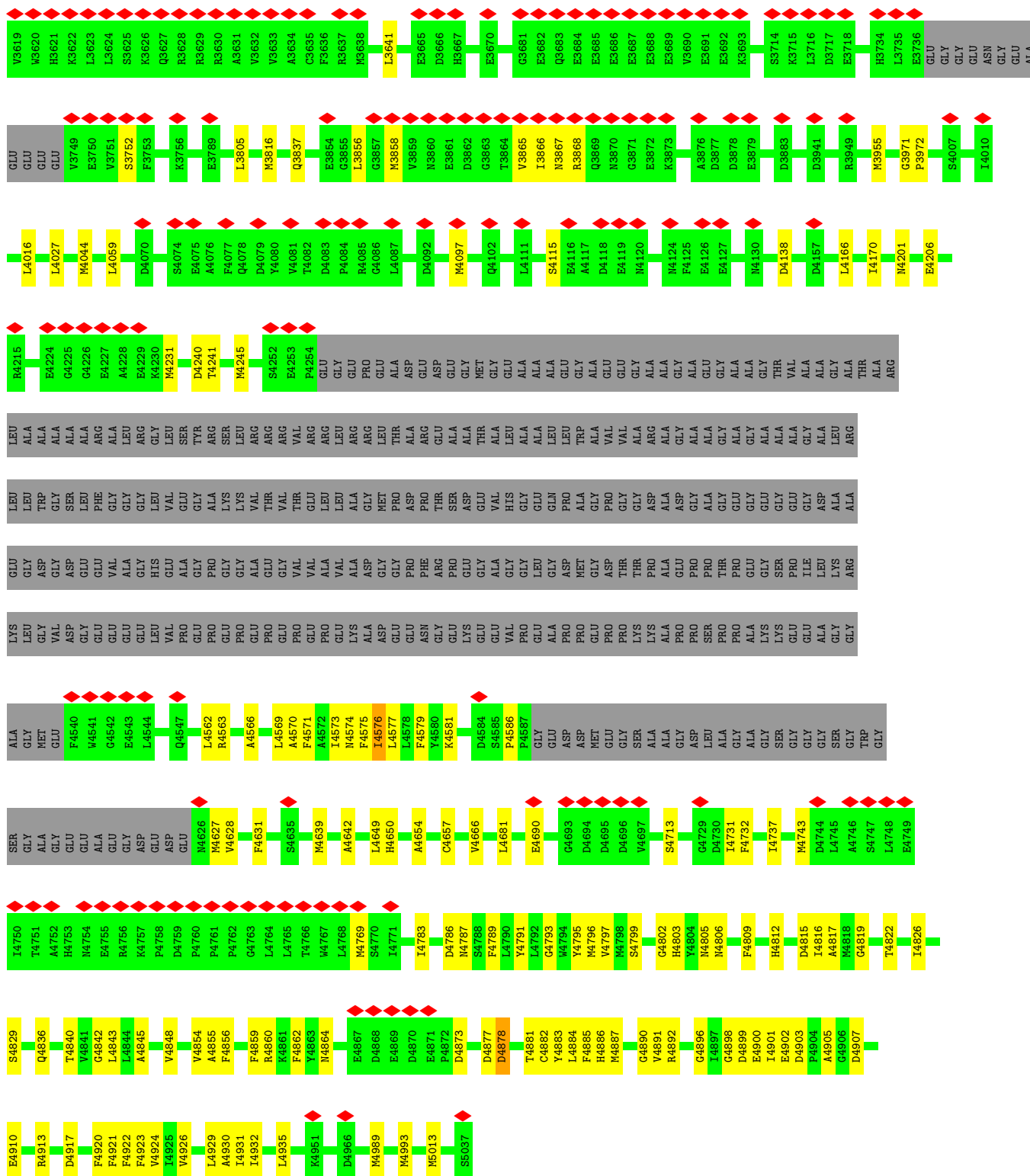




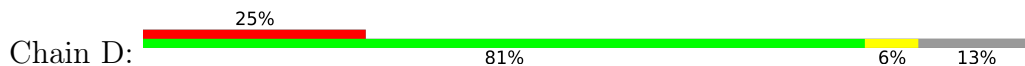








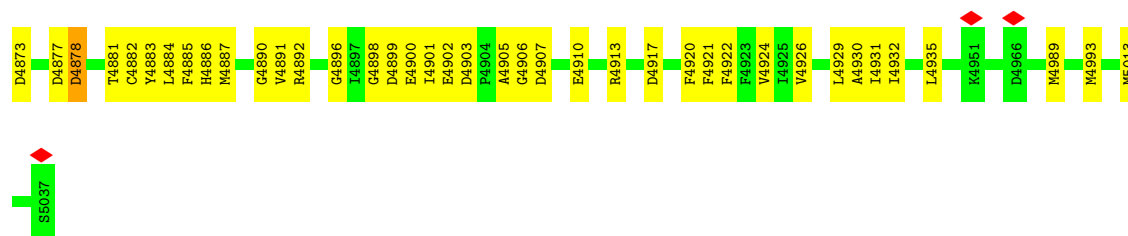
- Molecule 1: Ryanodine receptor 1





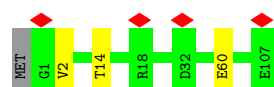
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L4790	V4866	P4586	GLU	GLY	THR	ALA	Q4102	E3854	A3634	M3573	I3510	K3450
V4791	L4681	P4587	VAL	GLY	ALA	ALA	L4111	G3855	C3635	A3574	V3511	F3451
C4792	E4690	GLY	GLU	GLY	LEU	GLU	S4115	L3856	F3636		A3512	K3452
V4793	Q4693	ASP	LEU	GLN	LEU	ALA	E4116	G3857	R3637	R3577	T3513	R3453
V4794	D4694	PRO	ASP	PRO	TRP	GLU	F4117	M3858	K3638	G3578	L3514	E3454
V4795	D4695	VAL	THR	VAL	ALA	ALA	D4118	V3859		P3580	K3515	E3455
V4796	D4696	GLY	THR	GLY	ASP	GLY	E4119	E3860		L3579	K3516	Q3456
V4797	V4697	ALA	THR	ASP	ALA	GLU	F4124	E3861	E3665	R3581	M3517	N3457
V4800	S4713	ALA	ALA	ASP	ALA	GLU	E4125	E3862	D3666	R3582	P3519	F3458
V4801	G4729	LEU	PRO	ASP	ALA	GLY	E4126	T3864	H3667	E3583	G3520	V3459
V4802	D4730	PRO	PRO	ALA	ALA	ALA	E4130	V3865	E3670	E3584	I3520	V3460
V4803	I4731	PRO	PRO	GLY	GLY	GLY	N4138	I3866	G3681	A3586	M3524	Q3461
V4804	F4732	PRO	GLY	GLY	ALA	THR	D4138	E3867	E3682	D3587	C3525	N3462
V4805	E4735	GLY	GLY	GLY	GLY	VAL	L4166	R3868	Q3683	D3588		E3463
V4806	R4736	LEU	SER	GLY	ALA	ALA	L4170	Q3869	E3684	P3589	T3528	I3464
V4807	I4737	ALA	ASP	GLY	GLY	ALA	E4170	E3870	E3685	E3590	D3529	N3466
V4808	M4743	ALA	ASP	ASP	LEU	ALA	T4170	G3871	E3686	K3591	Q3530	N3467
V4809	D4744	ARG	ALA	ALA	LEU	ALA	N4201	E3872	E3687	T3592	D3531	S3468
V4810	L4745	GLY	ARG	ALA	LEU	ALA	E4206	K3873	E3688	V3593	L3532	F3469
V4811	L4746	LEU	LEU	GLY	GLY	ALA	R4215	D3883	E3689	R3594	I3533	L3470
V4812	A4747	GLY	VAL	GLY	GLY	ALA	R4215	E3841	E3691	R3595	M3534	T3471
V4813	S4748	ASP	ASP	SER	GLY	ALA	E4224	R3849	E3692	Q3597	L3535	A3472
V4814	L4748	GLY	GLY	GLY	LEU	ALA	G4225	M3955	K3715	V3599	L3536	D3473
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V4816	I4750	VAL	VAL	GLY	VAL	ALA	E4227	P3972	D3717	A3601	K3537	K3475
V4817	T4751	GLY	GLY	GLY	GLY	ALA	A4228	S4007		V3602	R3539	S3476
V4818	A4752	HIS	GLY	GLY	LEU	GLY	E4229	L4016	H3734	L3603	Y3540	K3477
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V4821	E4755	GLY	GLY	GLY	GLY	TYR	E4241	L4016	L3735	L3606	D3544	ALA
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V4823	K4757	GLY	GLY	GLY	GLY	LYS	T4241	M4044	GLY	Q3608	D3546	ASP
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V4826	P4760	VAL	VAL	THR	THR	ARG	E4253	L4059	GLY	E3611	R3550	ASP
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V4835	L4649	GLY	GLY	GLY	GLY	ALA	GLU	D4079	GLY	W3620	L3559	LYS
V4836	L4650	GLY	GLY	GLY	GLY	ALA	ASP	R4085	GLY	H3621	L3559	LYS
V4837	L4651	GLY	GLY	GLY	GLY	ALA	GLY	L4086	GLY	K3622	Q3560	LYS
V4838	L4652	GLY	GLY	GLY	GLY	ALA	GLY	L4087	GLY	L3623	Q3561	LYS
V4839	L4653	GLY	GLY	GLY	GLY	ALA	GLY	D4092	GLY	L3624	K3562	LYS
V4840	L4654	GLY	GLY	GLY	GLY	ALA	GLY	E3789	GLY	S3625	V3563	LYS
V4841	L4655	GLY	GLY	GLY	GLY	ALA	GLY	L3805	GLY	K3626	E3564	LYS
V4842	L4656	GLY	GLY	GLY	GLY	ALA	GLY	K3816	GLY	Q3627	G3565	LYS
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V4846	L4660	GLY	GLY	GLY	GLY	ALA	GLY		GLY	V3632		LYS
V4847	L4661	GLY	GLY	GLY	GLY	ALA	GLY		GLY	V3633		LYS
V4848	L4662	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4849	L4663	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4850	L4664	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4851	L4665	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4852	L4666	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4853	L4667	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4854	L4668	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4855	L4669	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4856	L4670	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4857	L4671	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4858	L4672	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4859	L4673	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4860	L4674	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4861	L4675	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4862	L4676	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4863	L4677	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4864	L4678	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4865	L4679	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4866	L4680	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4867	L4681	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4868	L4682	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4869	L4683	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4870	L4684	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4871	L4685	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS
V4872	L4686	GLY	GLY	GLY	GLY	ALA	GLY		GLY			LYS



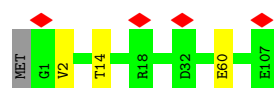
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 96%



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

Chain F: 96%



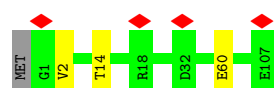
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 95%



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

Chain H: 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	25786	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 ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.271	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.269	Depositor
Recommended contour level	1.12	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.50	31/35885 (0.1%)	0.61	175/48603 (0.4%)
1	B	0.51	31/35885 (0.1%)	0.63	185/48603 (0.4%)
1	C	0.50	30/35885 (0.1%)	0.62	174/48603 (0.4%)
1	D	0.50	31/35885 (0.1%)	0.61	173/48603 (0.4%)
2	E	0.13	0/851	0.35	0/1146
2	F	0.14	0/851	0.36	0/1146
2	G	0.13	0/851	0.35	0/1146
2	H	0.13	0/851	0.35	0/1146
All	All	0.50	123/146944 (0.1%)	0.61	707/198996 (0.4%)

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

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4812	HIS	CE1-NE2	-8.87	1.23	1.32
1	A	4812	HIS	CE1-NE2	-8.85	1.23	1.32
1	A	4803	HIS	ND1-CE1	-8.80	1.23	1.32
1	B	4886	HIS	ND1-CE1	-8.79	1.23	1.32
1	D	4886	HIS	ND1-CE1	-8.77	1.23	1.32

The worst 5 of 707 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4784	PHE	CA-CB-CG	7.70	121.50	113.80
1	B	4922	PHE	CA-CB-CG	7.64	121.44	113.80
1	D	4922	PHE	CA-CB-CG	7.63	121.44	113.80
1	A	4922	PHE	CA-CB-CG	7.62	121.42	113.80
1	C	4922	PHE	CA-CB-CG	7.62	121.42	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4913	ARG	Sidechain
1	B	4913	ARG	Sidechain
1	C	4913	ARG	Sidechain
1	D	4913	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	35088	34734	34715	135	0
1	B	35088	34734	34715	135	0
1	C	35088	34734	34715	135	0
1	D	35088	34734	34715	140	0
2	E	832	829	831	1	0
2	F	832	829	831	1	0
2	G	832	829	831	1	0
2	H	832	829	831	1	0
3	A	104	164	164	0	0
3	B	104	164	164	0	0
3	C	104	164	164	0	0
3	D	104	164	164	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
All	All	144100	142908	142840	549	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 2.

The worst 5 of 549 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:B:3534:MET:HE2	1:B:3534:MET:HA	1.61	0.82
1:A:3534:MET:HE2	1:A:3534:MET:HA	1.61	0.82
1:C:3534:MET:HA	1:C:3534:MET:HE2	1.61	0.80
1:D:3534:MET:HE2	1:D:3534:MET:HA	1.61	0.80
1:C:4059:LEU:HD22	1:C:4170:ILE:HD13	1.70	0.74

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	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
1	B	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
1	C	4376/5037 (87%)	4236 (97%)	139 (3%)	1 (0%)	100	100
1	D	4376/5037 (87%)	4237 (97%)	138 (3%)	1 (0%)	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
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%)	103 (98%)	2 (2%)	0	100	100
All	All	17924/20580 (87%)	17359 (97%)	561 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3478	MET

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Mol	Chain	Res	Type
1	B	3478	MET
1	C	3478	MET
1	D	3478	MET

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	3827/4276 (90%)	3793 (99%)	34 (1%)	70	76
1	B	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
1	C	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
1	D	3827/4276 (90%)	3792 (99%)	35 (1%)	70	76
2	E	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	G	89/90 (99%)	86 (97%)	3 (3%)	32	57
2	H	89/90 (99%)	87 (98%)	2 (2%)	45	65
All	All	15664/17464 (90%)	15516 (99%)	148 (1%)	68	76

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1022	VAL
2	G	2	VAL
1	D	1576	SER
1	D	3752	SER
1	B	1465	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	350	HIS
1	C	3030	HIS

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Mol	Chain	Res	Type
1	D	3651	ASN
1	C	797	HIS
1	C	1775	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	POV	B	5101	-	51,51,51	0.72	0	57,59,59	0.50	0
3	POV	D	5102	-	51,51,51	0.72	0	57,59,59	0.49	0
3	POV	A	5102	-	51,51,51	0.70	0	57,59,59	0.52	0
3	POV	C	5101	-	51,51,51	0.75	1 (1%)	57,59,59	0.65	1 (1%)
3	POV	C	5102	-	51,51,51	0.71	0	57,59,59	0.50	0
3	POV	A	5101	-	51,51,51	0.74	1 (1%)	57,59,59	0.65	1 (1%)
3	POV	B	5102	-	51,51,51	0.74	0	57,59,59	0.64	2 (3%)
3	POV	D	5101	-	51,51,51	0.73	0	57,59,59	0.71	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	B	5101	-	-	9/55/55/55	-
3	POV	D	5102	-	-	9/55/55/55	-
3	POV	A	5102	-	-	8/55/55/55	-
3	POV	C	5101	-	-	12/55/55/55	-
3	POV	C	5102	-	-	10/55/55/55	-
3	POV	A	5101	-	-	14/55/55/55	-
3	POV	B	5102	-	-	14/55/55/55	-
3	POV	D	5101	-	-	13/55/55/55	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5101	POV	C3-C2	2.03	1.56	1.50
3	A	5101	POV	C3-C2	2.00	1.56	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	POV	C2-O21-C21	3.34	126.02	117.79
3	A	5101	POV	C2-O21-C21	3.10	125.42	117.79
3	C	5101	POV	C2-O21-C21	3.10	125.42	117.79
3	B	5102	POV	C2-O21-C21	3.05	125.29	117.79
3	B	5102	POV	O21-C21-C22	2.18	116.21	111.50

There are no chirality outliers.

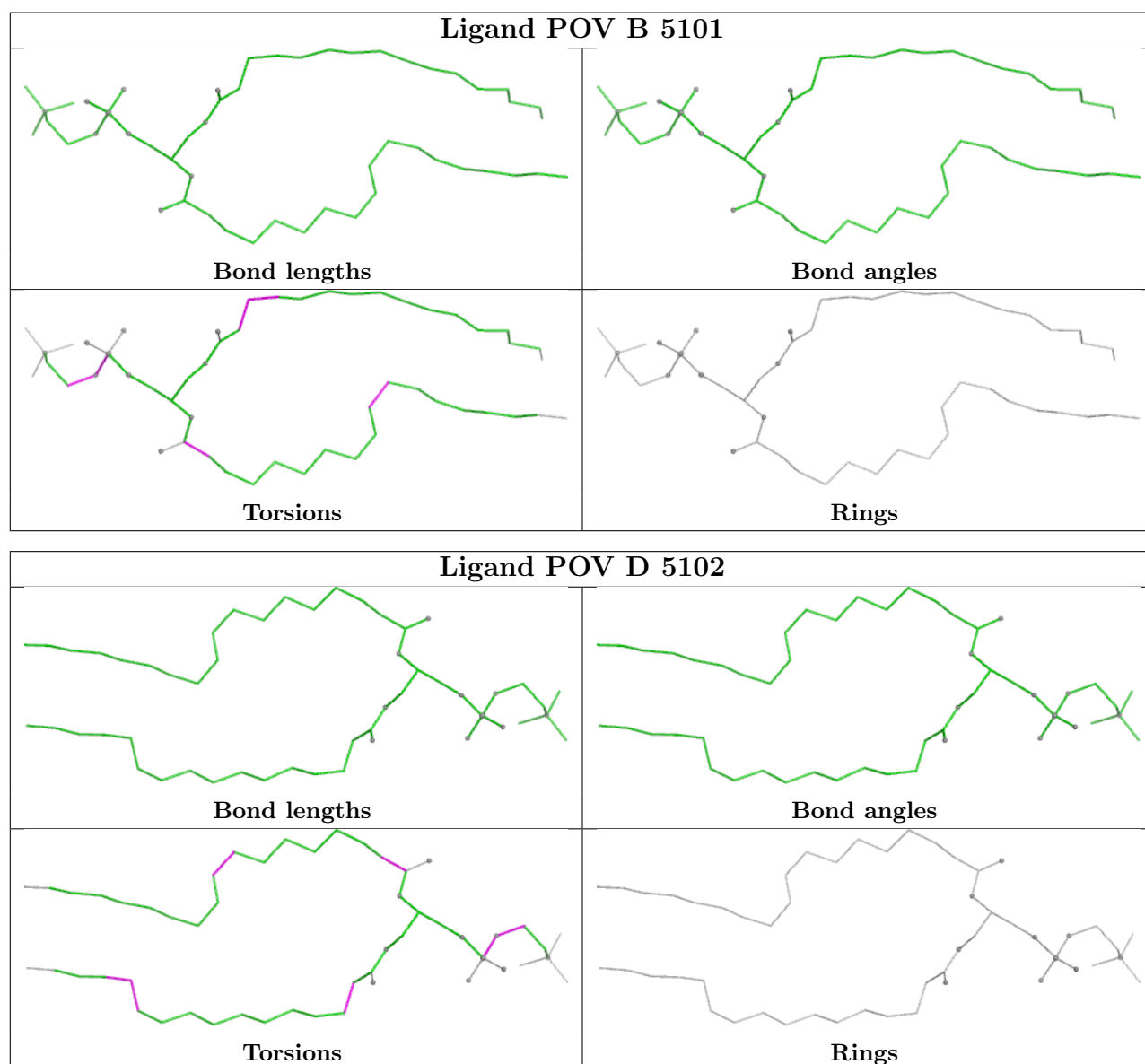
5 of 89 torsion outliers are listed below:

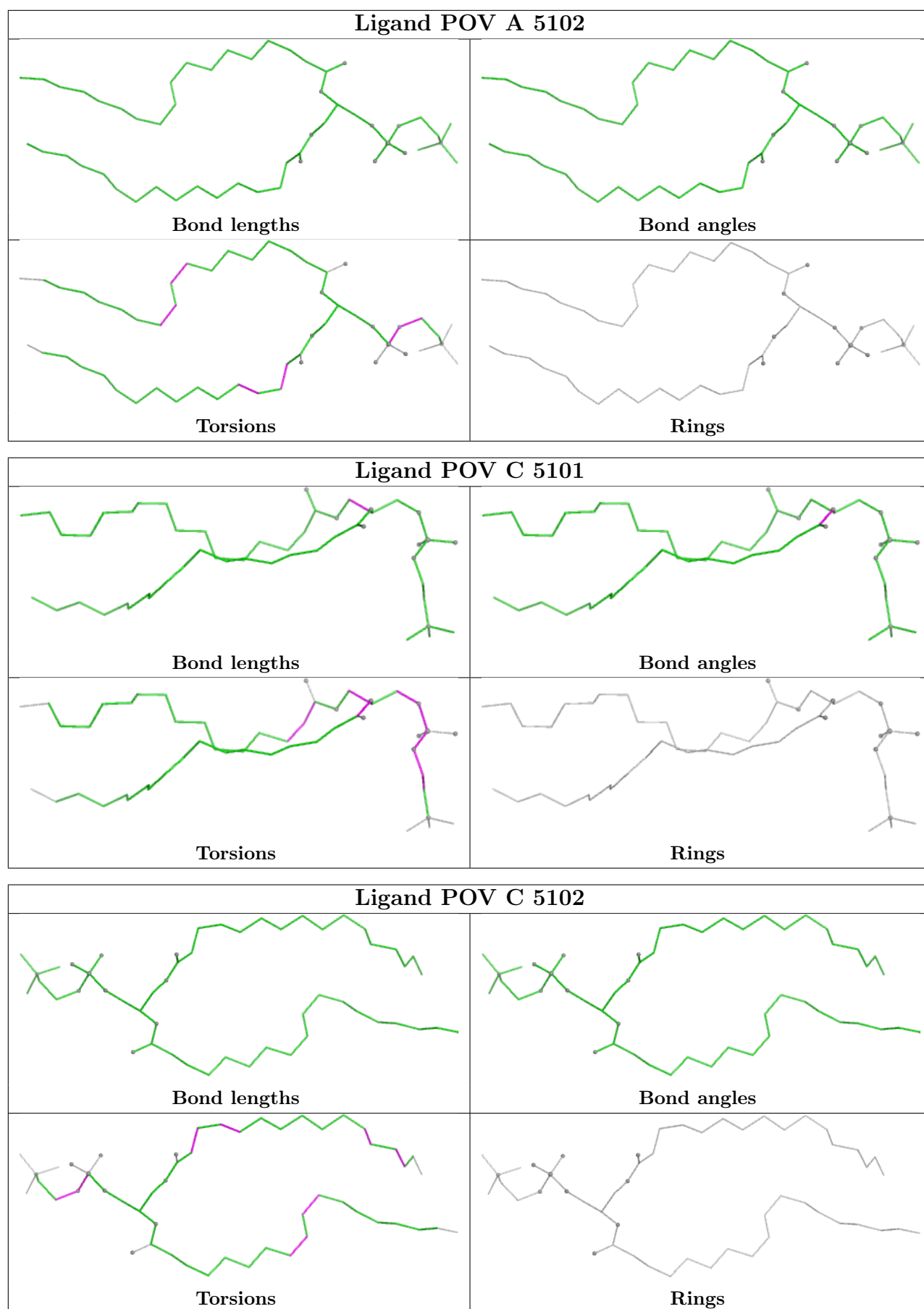
Mol	Chain	Res	Type	Atoms
3	A	5101	POV	C11-O12-P-O11
3	A	5101	POV	C11-O12-P-O14
3	A	5101	POV	C2-C1-O11-P
3	A	5101	POV	C12-C11-O12-P
3	A	5101	POV	C22-C21-O21-C2

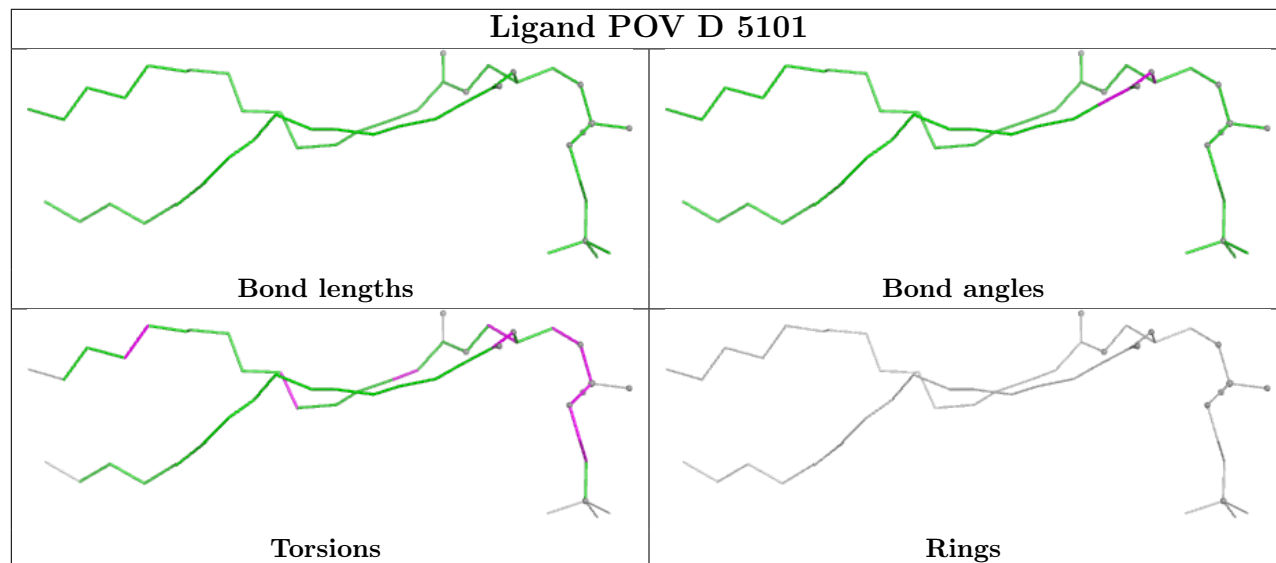
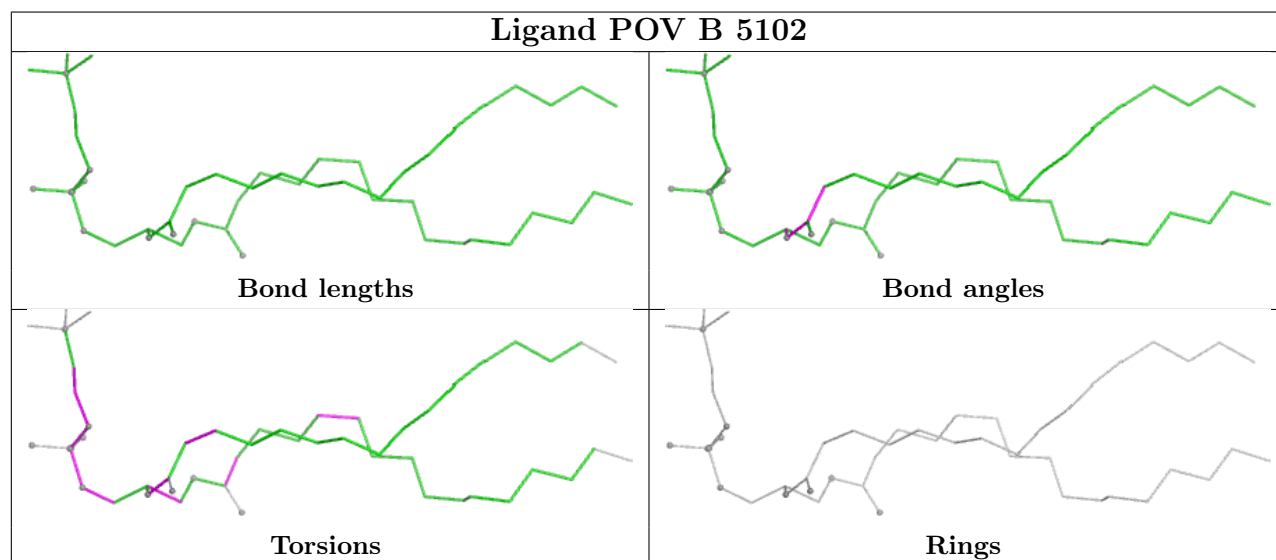
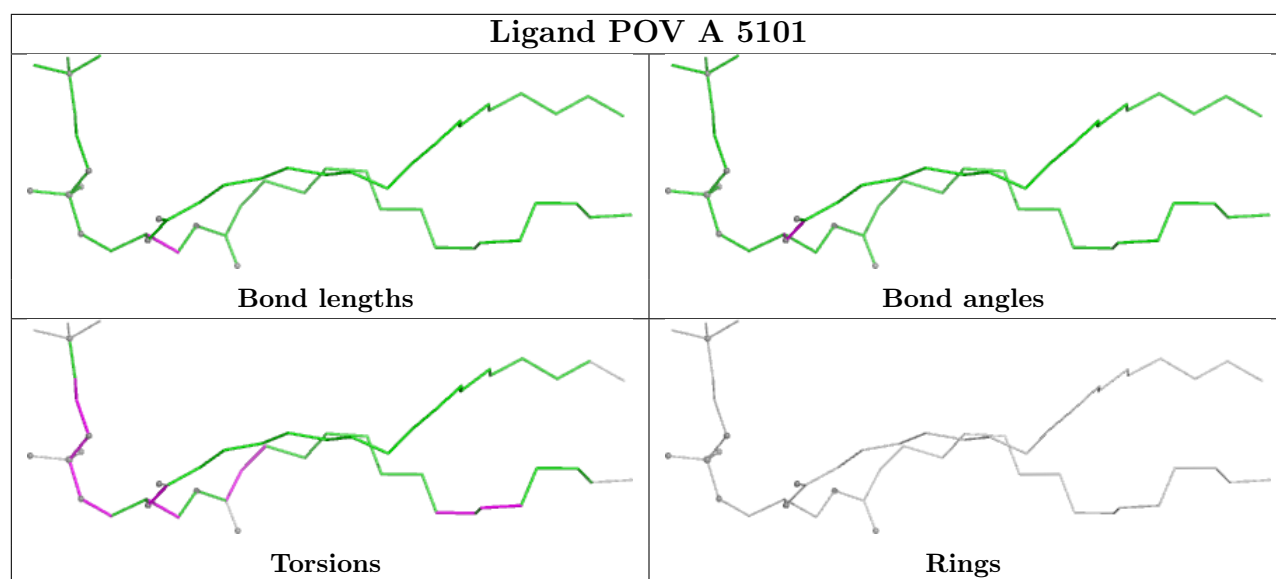
There are no ring outliers.

No monomer is involved in short contacts.

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







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.

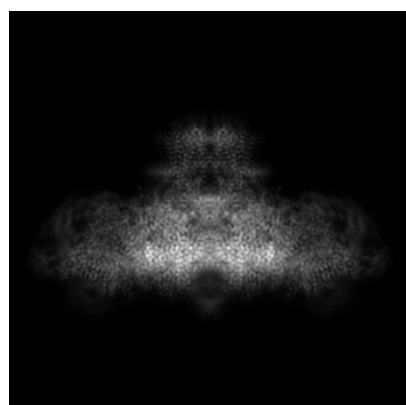
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54445. These allow visual inspection of the internal detail of the map and identification of artifacts.

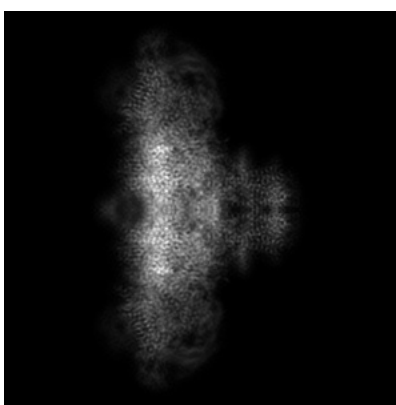
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

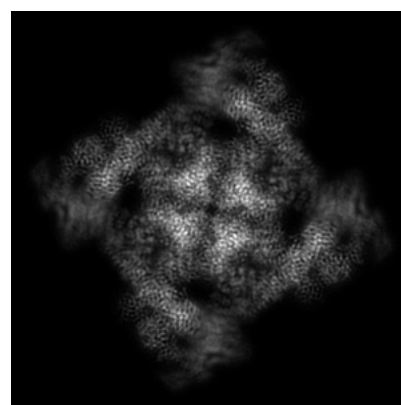
6.1.1 Primary map



X



Y



Z

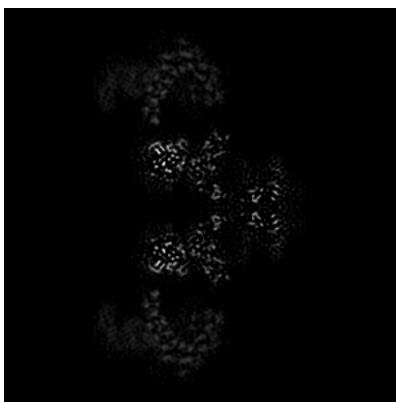
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

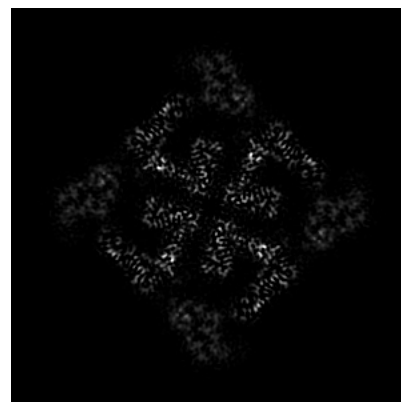
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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: 173



Y Index: 127

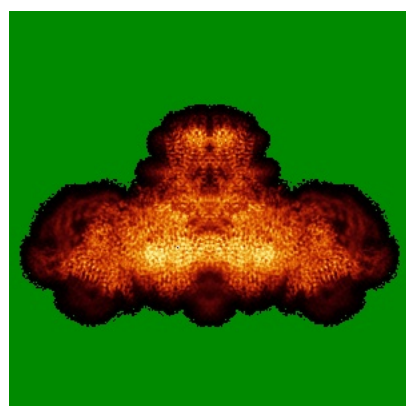


Z Index: 118

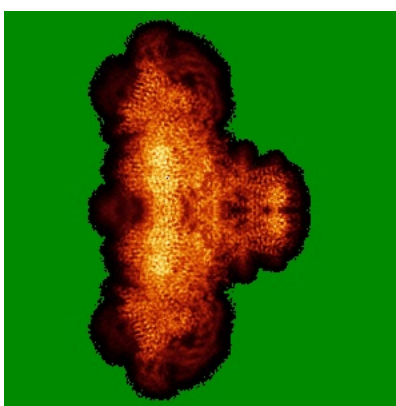
The images above show the largest variance slices of the map in three orthogonal directions.

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

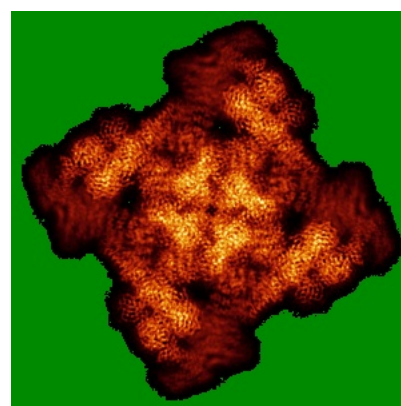
6.4.1 Primary map



X



Y

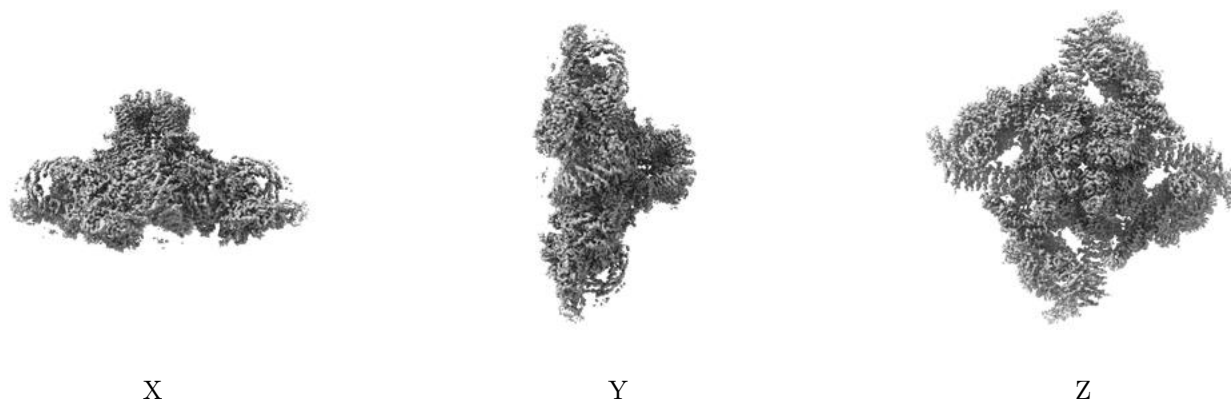


Z

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 1.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

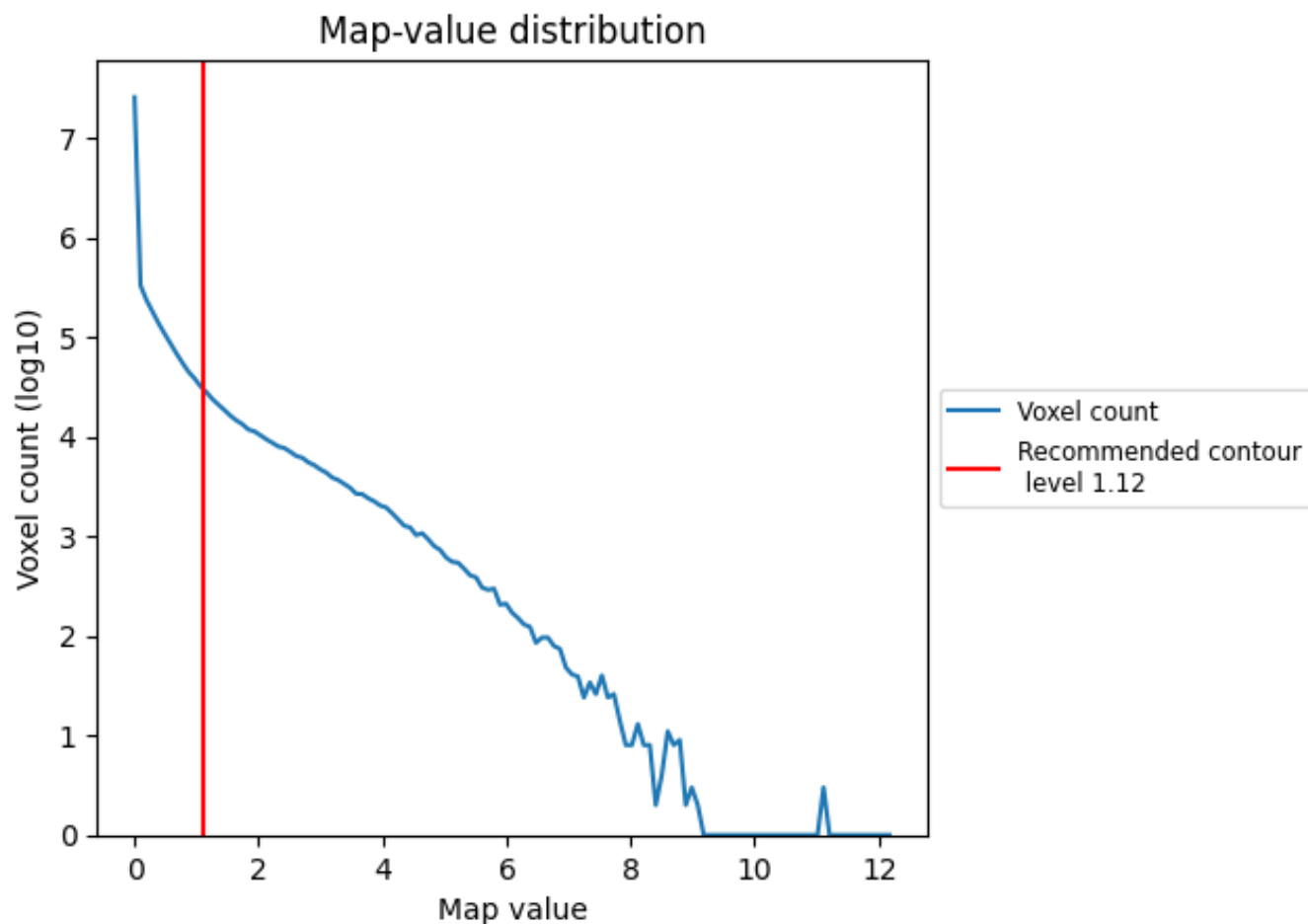
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

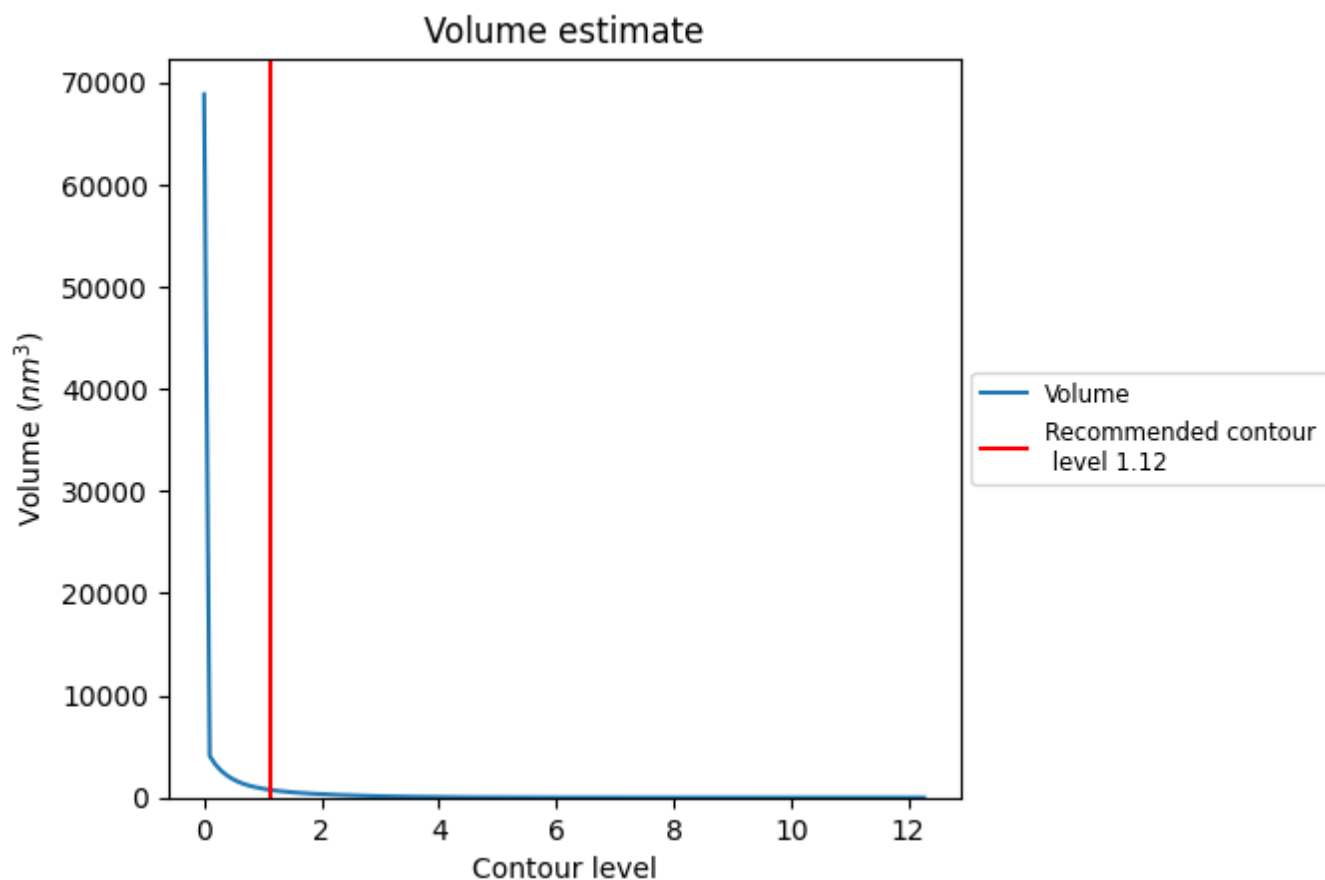
This section contains the results of statistical analysis of the map.

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.

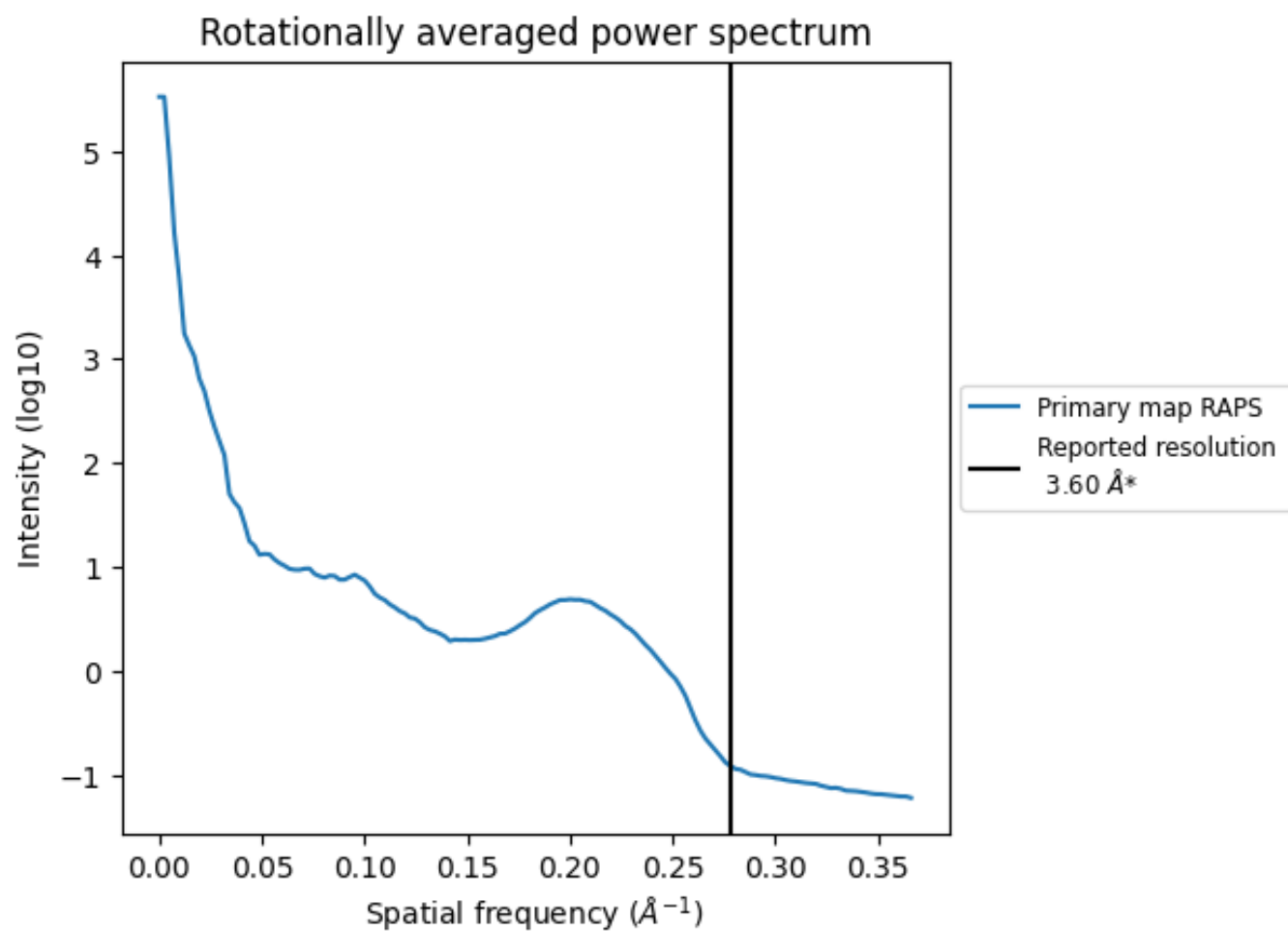
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 759 nm^3 ; this corresponds to an approximate mass of 686 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 0.278 Å⁻¹

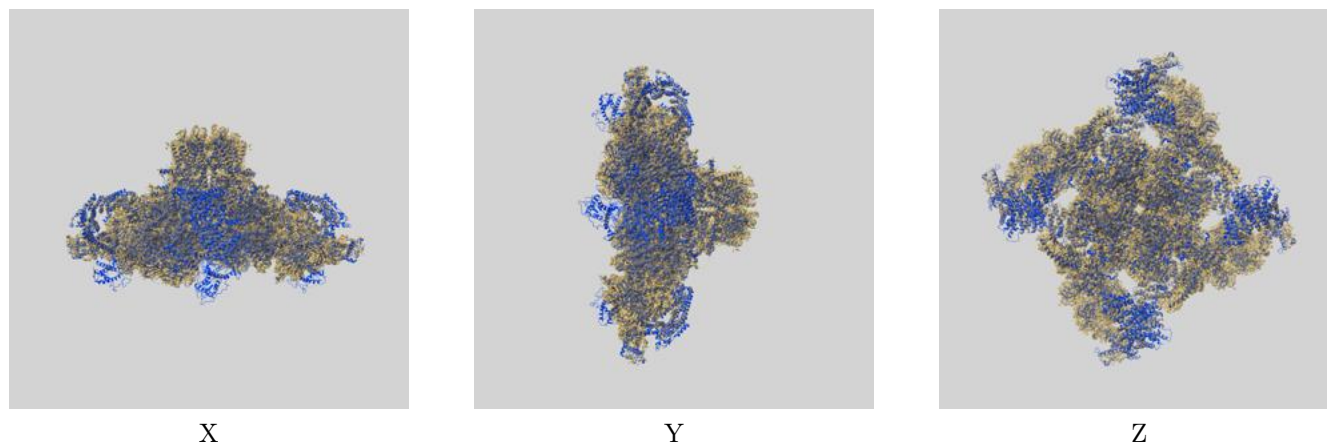
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

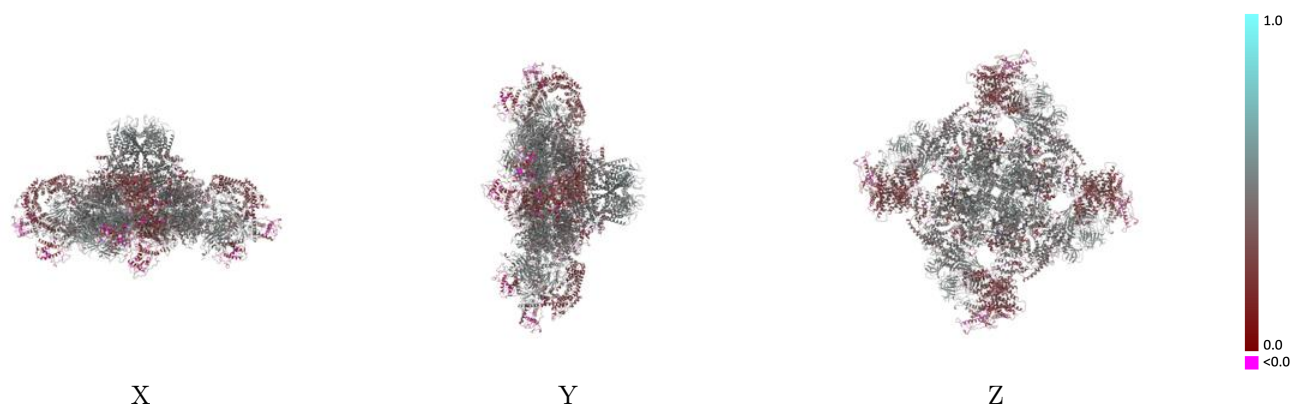
This section contains information regarding the fit between EMDB map EMD-54445 and PDB model 9S16. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



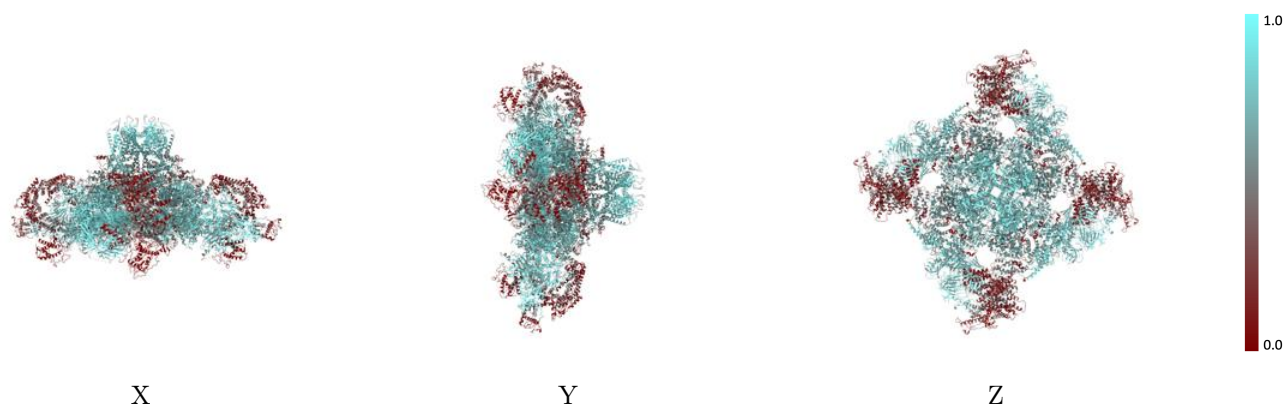
The images above show the 3D surface view of the map at the recommended contour level 1.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



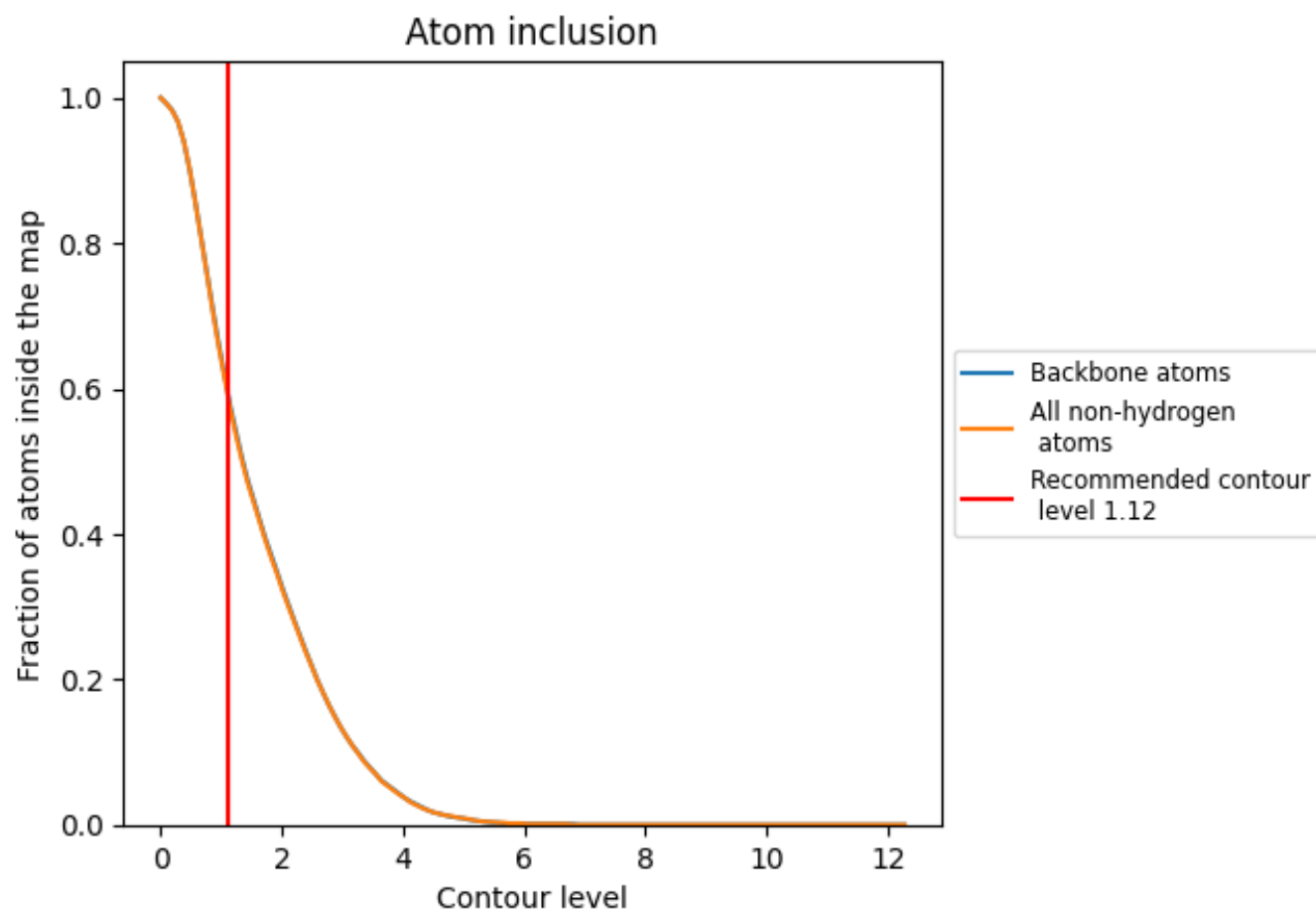
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 58% 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 (1.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5850	0.4050
A	0.5850	0.4040
B	0.5830	0.4040
C	0.5840	0.4040
D	0.5970	0.4020
E	0.7520	0.4880
F	0.7510	0.4890
G	0.7480	0.4910
H	0.7650	0.4850

