



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 06:39 pm BST

PDB ID : 9S4N / pdb_00009s4n
EMDB ID : EMD-54570
Title : Activated-state RyR1 with activating ligand mixture (Calcium/ACP/Caffeine) in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-28
Resolution : 3.53 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:

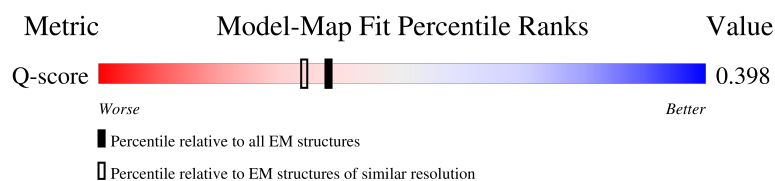
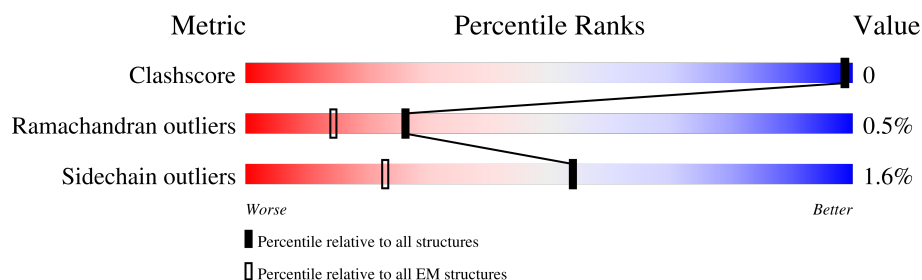
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.53 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.



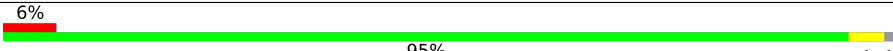
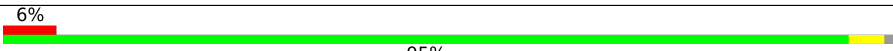
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12947 (3.03 - 4.02)

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	23% 85% 13%
1	B	5037	23% 85% 13%
1	C	5037	23% 85% 13%
1	D	5037	20% 84% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	 6%94%5% •
2	F	108	 6%94%5% •
2	G	108	 6%95%• •
2	H	108	 6%95%• •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 287284 atoms, of which 143000 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
			69821	22323	34733	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69821	22323	34733	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69821	22323	34733	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69821	22323	34733	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		

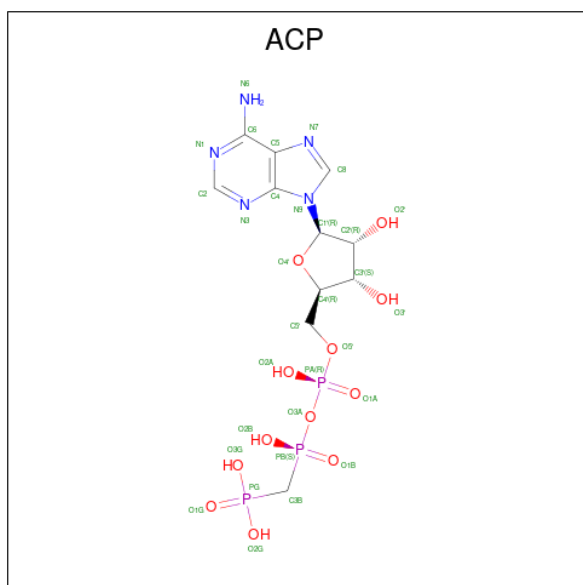
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

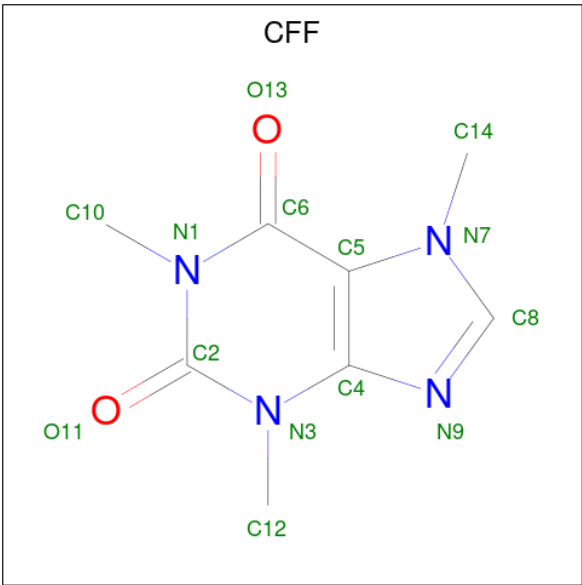
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

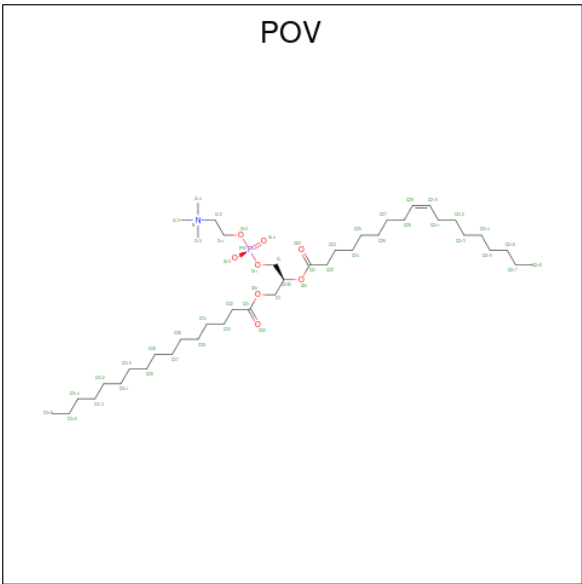
- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	D	1	Total	C	H	N	O	0
			24	8	10	4	2	

- Molecule 7 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).

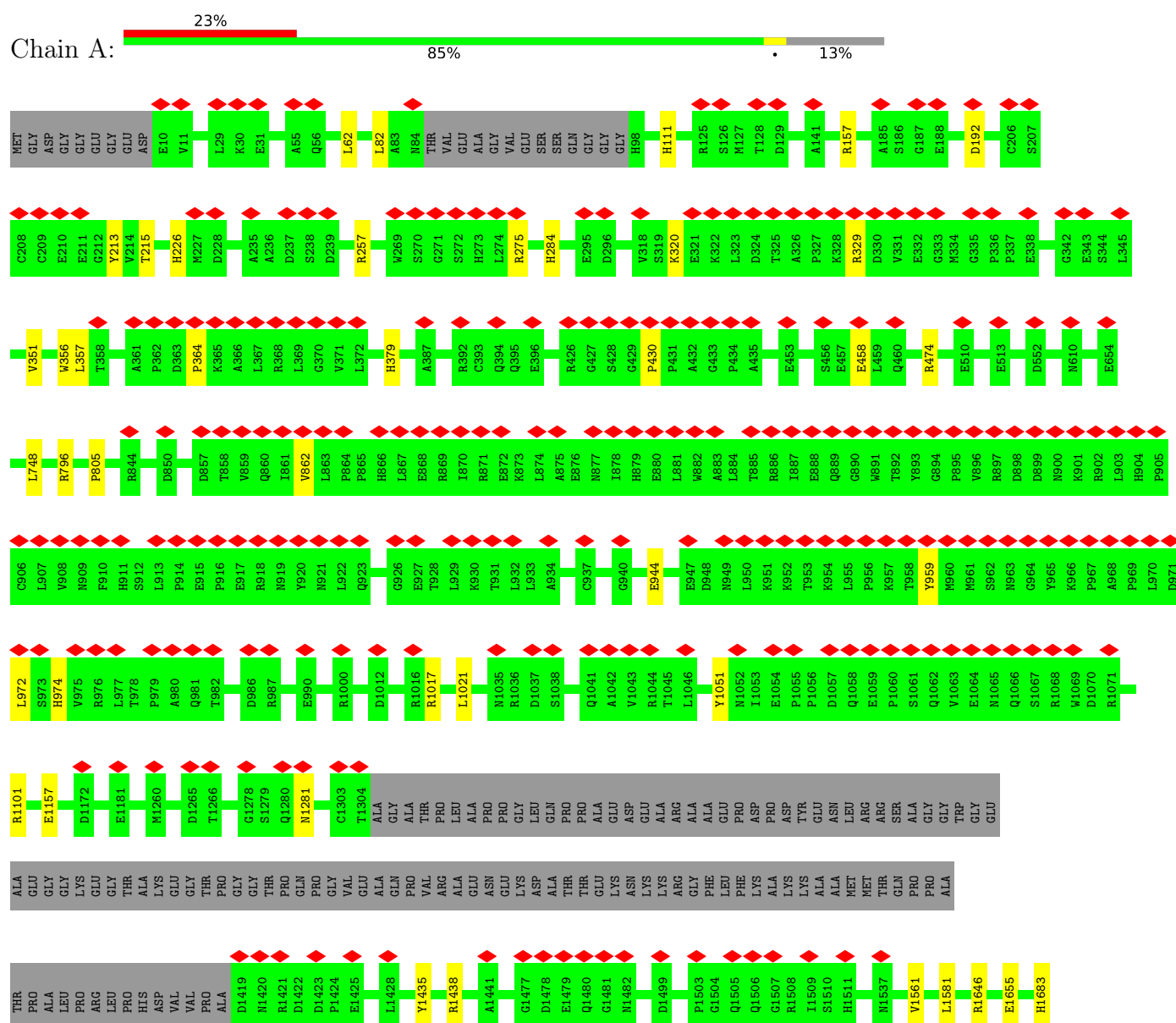


Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
7	C	1	Total 134	C 42	H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

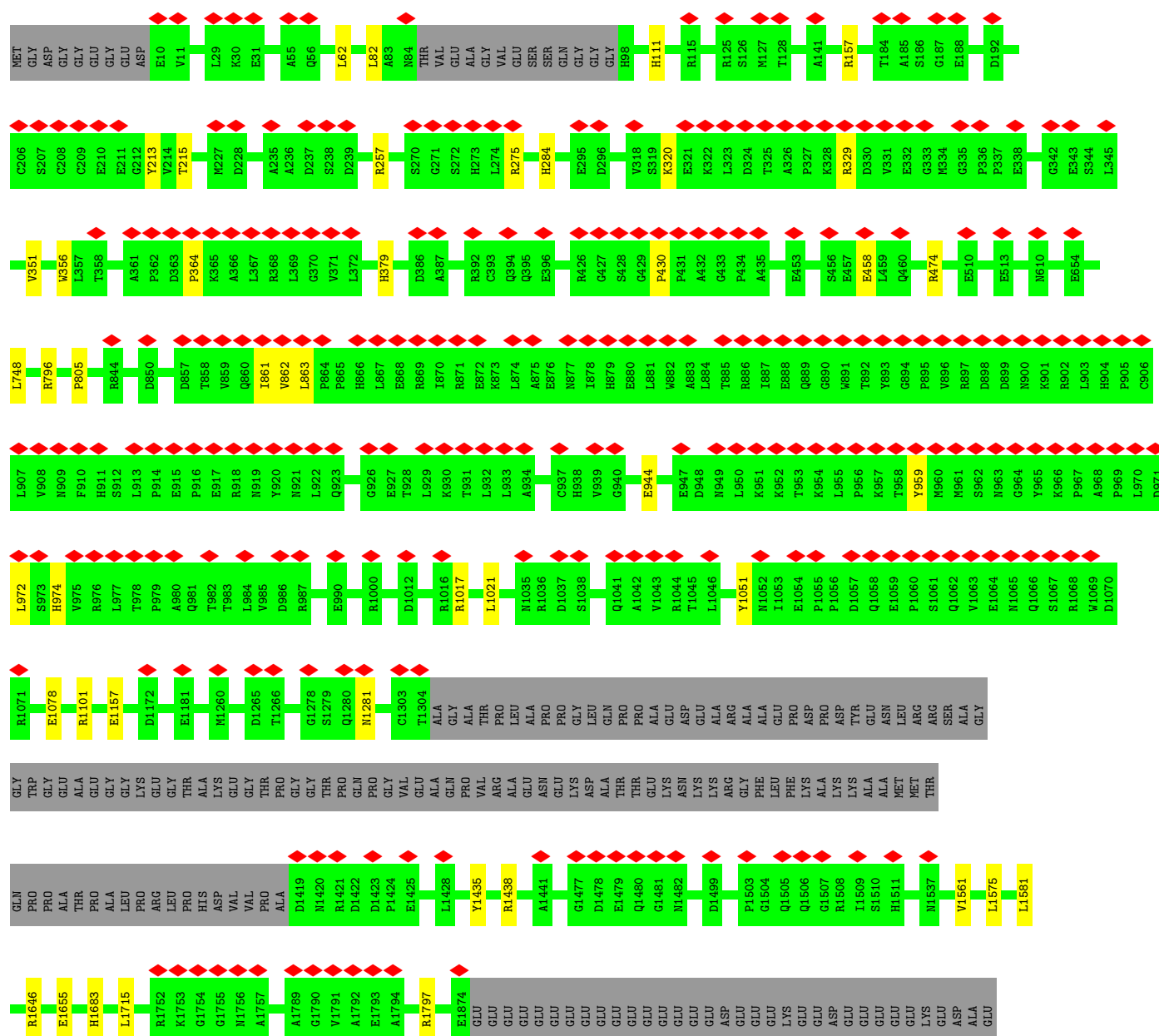
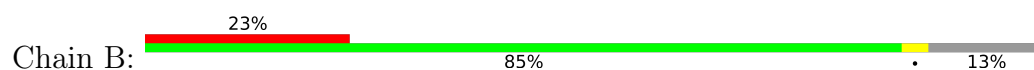
• Molecule 1: Ryanodine receptor 1





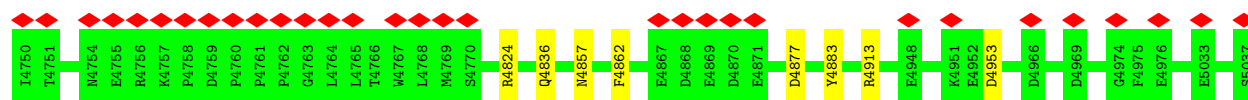


- Molecule 1: Ryanodine receptor 1

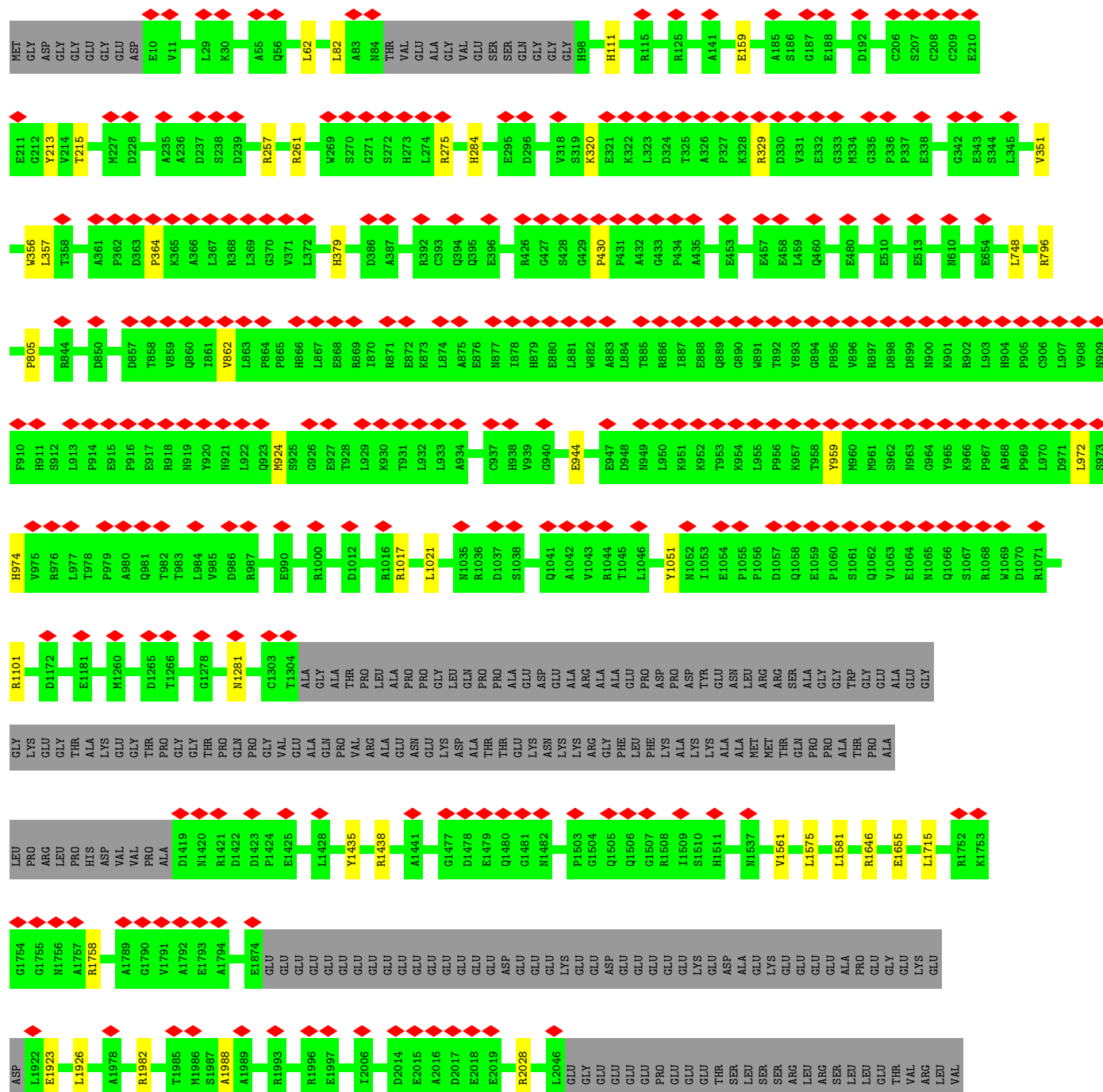
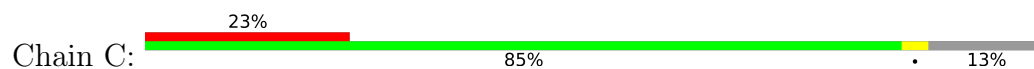


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F2997	F2998	A2999	K3000	I3001	L3002	Y3009	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	K3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	E3035	K3036	E3037	M3038	A3048	R3051	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	D3060	V3065	N3066	A3072	R3073	S3074	L3075	D3076	A3077	R3078							
Y2935	A2936	Y2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	Q2971	E2972	F2973	L2974	A2975	L2976	E2977	A2978	V2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	L2995	K2996		
A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	R2887	K2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	K2896	K2897	G2898	G2899	T2901	H2902	L2903	L2904	L2905	V2906	F2907	Y2908	D2909	T2910	T2911	A2913	K2914	E2915	K2916	A2917	R2918	D2919	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934		
A2815	M2816	I2817	A2818	M2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	ILE	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ASP	N2855	P2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874				
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F2679	W2680	G2681	I2682	F2683	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	M2698	L2710	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754			
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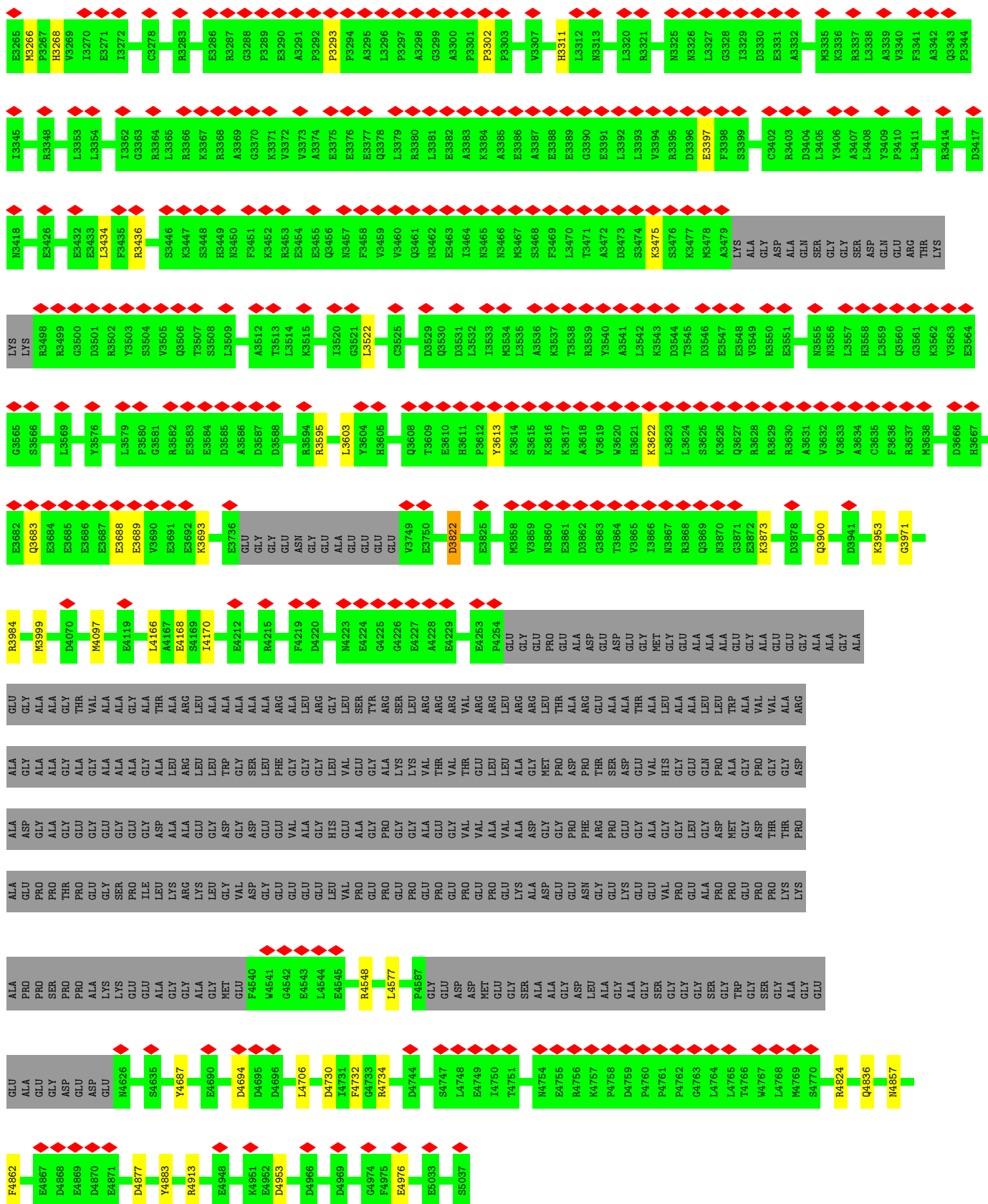




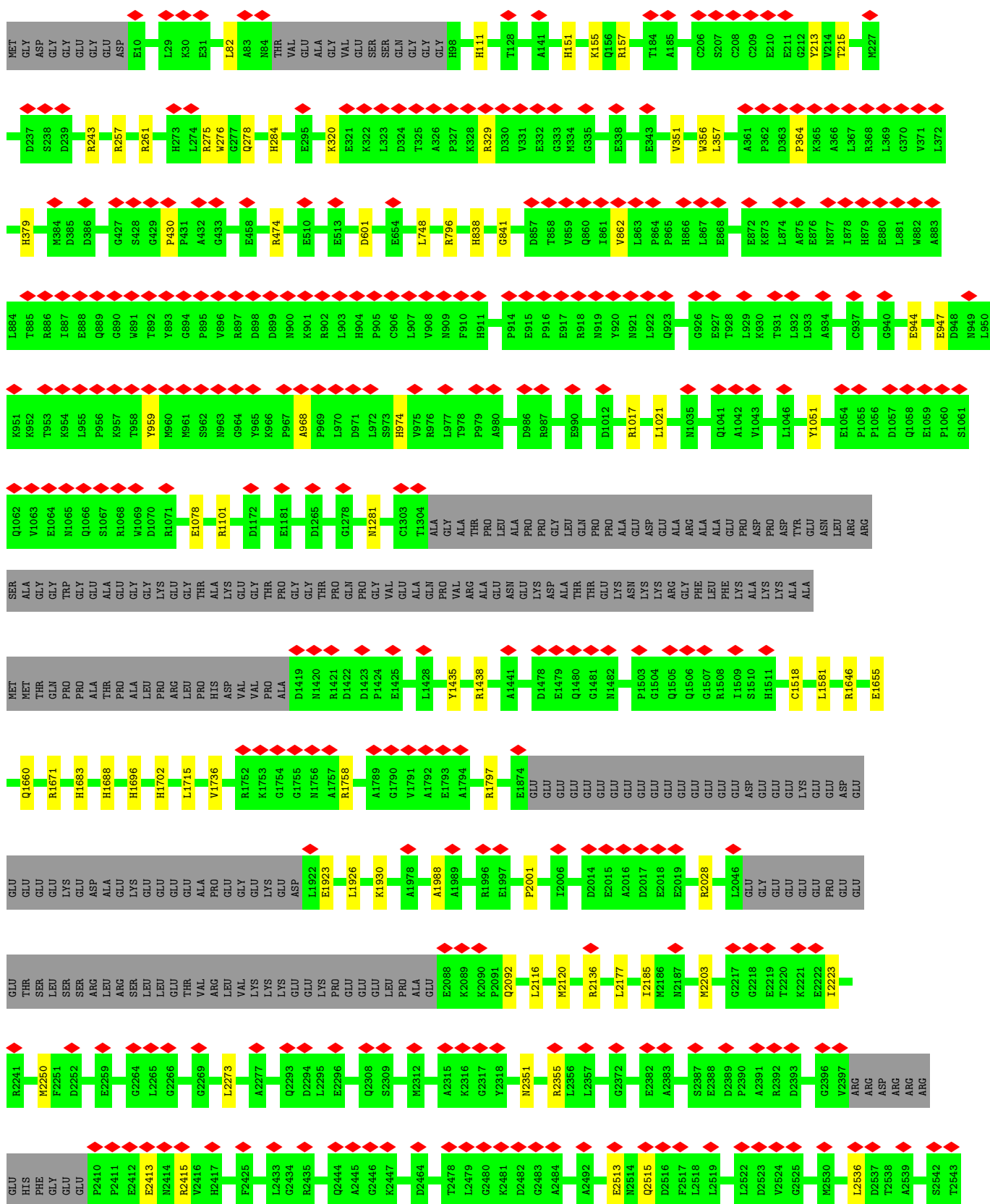
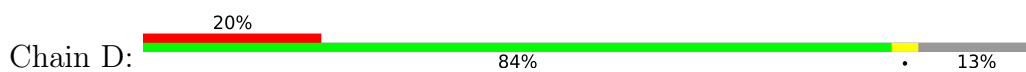
● Molecule 1: Ryanodine receptor 1



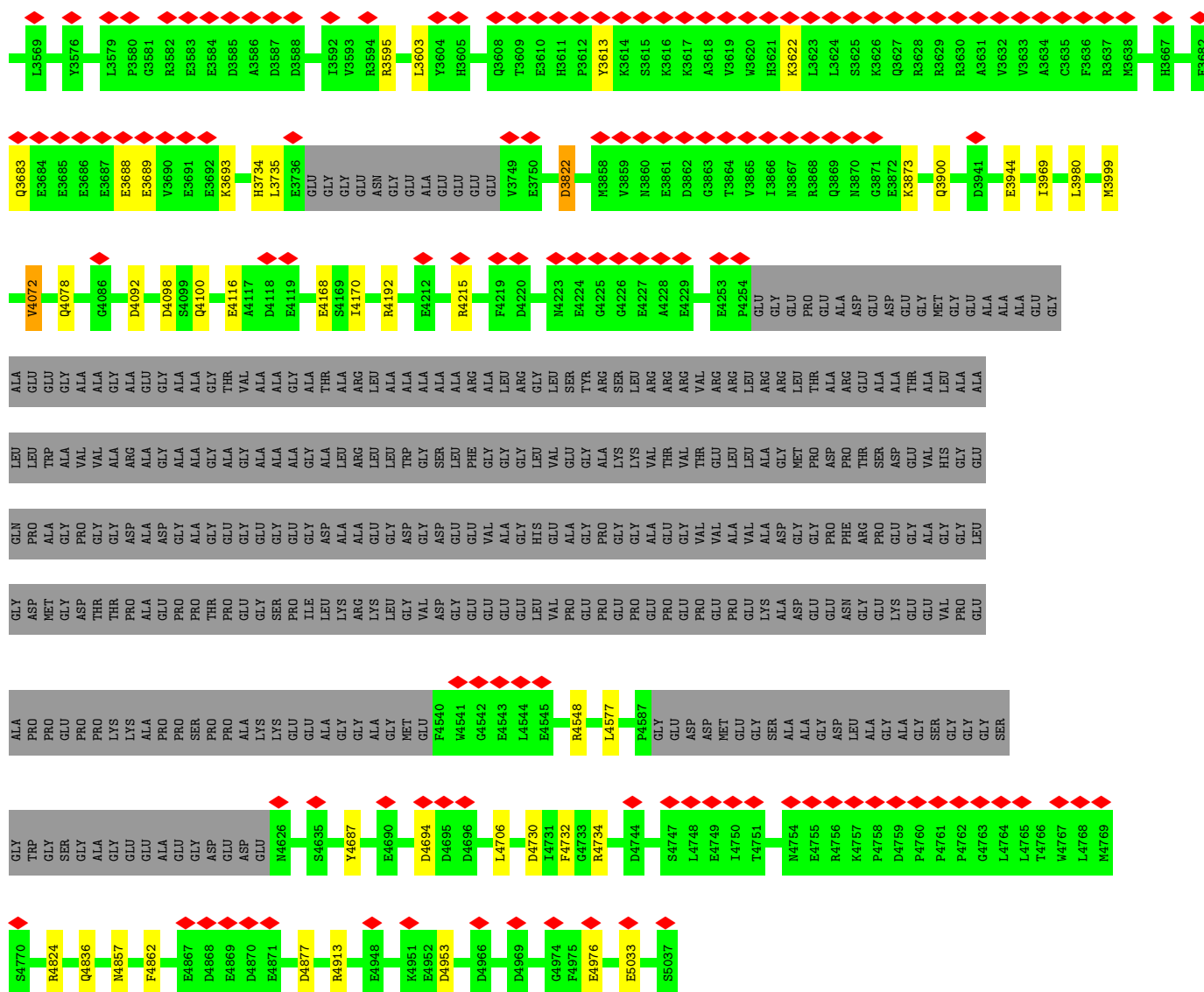




- Molecule 1: Ryanodine receptor 1

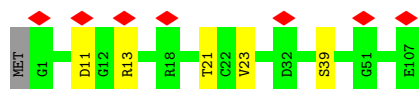


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R3337	L3338	A3339	I3345	R3348	L3353	L3354	R3364	L3365	R3366	K3367	R3368	A3369	G3370	K3371	V3372	V3373	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	L3385	A3386	E3387	E3388	E3389	G3390	P3301	P3302	F3303	V3307	H3311	L3312	N3313	L3320	R3321	N3325	N3326	L3327	G3328	L3329	D3330	E3331	A3332	K3335	K3336									
D3252	I3253	G3254	A3257	E3258	S3259	G3260	A3261	R3262	E3265	M3266	F3267	H3268	E3271	I3272	R3283	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	F3303	V3307	H3311	L3312	N3313	L3320	R3321	N3325	N3326	L3327	G3328	L3329	D3330	E3331	A3332	K3335	K3336										
C3165	Y3166	R3167	I3172	T3176	K3179	Y3182	V3183	E3184	K3185	E3192	R3196	A3199	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3244	D3247										
V3080	H3081	K3082	S3083	I3087	G3091	L3092	R3093	F3096	E3101	E3104	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	Q3127	N3128	L3129	T3133	V3134	A3135	L3136	H3146	I3147	H3150	Q3151	F3152	K3153	D3154	D3155	V3156	I3157	L3158	D3159	S3164												
G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	L2995	K2996	F2997	F2998	A2999	K3000	I3001	Y3009	N3012	H3013	C3014	L3015	Y3016	F3017	L3018	P3021	A3022	K3023	V3024	L3025	G3026	S3027	H3030	A3031	S3032	K3036	E3037	M3038	L3049	H3052	R3053	V3054	S3055	L3056	N3066	A3072	R3073	S3074	L3075	D3076									
D2919	R2920	E2921	K2922	Q2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	F2957	Q2958	F2959	L2964	R2965	D2968	Q2971	E2972	V3064	F2973	T2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983							
P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	M2884	T2885	W2886	E2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2917	R2918	
E2799	K2800	D2801	K2802	L2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	ARG	THR	GLU	L2894	L2895	L2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	A2917	R2918
P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	P2754	L2755	N2756	K2757	P2758	E2759	E2760	Y2761	T2762	K2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	Q2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798
E2649	R2650	C2651	Y2654	Y2655	T2659	G2660	W2661	A2662	N2663	S2668	E2669	R2676	K2677	F2679	G2681	I2682	F2683	A2687	H2688	Y2691	D2692	Q2693	E2694	L2695	V2696	R2697	M2698	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738									
T2544	E2545	R2552	Y2553	L2554	C2555	L2556	A2557	V2558	L2559	R2564	L2568	F2569	A2570	E2573	H2574	L2575	A2576	L2583	H2584	R2588	R2591	Q2592	A2598	Q2599	R2600	V2605	A2609	R2612	Y2613	L2614	R2615	M2618	H2621	R2625	L2628	D2629	E2635	F2636	A2637	V2646	H2647	Y2648																	



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

Chain E: 94% 5% • 6%

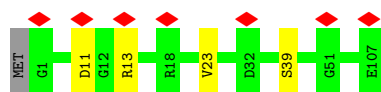


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

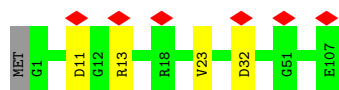
Chain F: 94% 5% • 6%



- 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, C4	Depositor
Number of particles used	37771	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 ($e^-/\text{\AA}^2$)	67.44	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	13.337	Depositor
Minimum map value	0.000	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.262	Depositor
Recommended contour level	1.09	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: CFF, ZN, ACP, POV, CA

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	0.76	2/35885 (0.0%)	1.26	48/48603 (0.1%)
1	B	0.76	1/35885 (0.0%)	1.26	44/48603 (0.1%)
1	C	0.76	2/35885 (0.0%)	1.26	43/48603 (0.1%)
1	D	0.76	4/35885 (0.0%)	1.28	61/48603 (0.1%)
2	E	0.75	0/851	1.33	2/1146 (0.2%)
2	F	0.75	0/851	1.33	3/1146 (0.3%)
2	G	0.75	0/851	1.33	2/1146 (0.2%)
2	H	0.75	0/851	1.36	3/1146 (0.3%)
All	All	0.76	9/146944 (0.0%)	1.27	206/198996 (0.1%)

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	6
1	B	0	7
1	C	0	6
1	D	0	7
All	All	0	26

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2859	PRO	CA-C	6.17	1.55	1.51
1	B	2859	PRO	CA-C	6.02	1.55	1.51
1	A	2859	PRO	CA-C	6.00	1.55	1.51
1	D	2859	PRO	CA-C	5.91	1.55	1.51
1	C	3302	PRO	CA-C	5.26	1.54	1.51

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2773	ASN	CA-CB-CG	6.91	119.50	112.60
1	D	2773	ASN	CA-CB-CG	6.89	119.50	112.60
1	B	4857	ASN	CA-CB-CG	-6.54	106.06	112.60
1	A	4857	ASN	CA-CB-CG	-6.48	106.12	112.60
1	A	192	ASP	CA-CB-CG	6.41	119.01	112.60

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	TYR	Sidechain
1	A	157	ARG	Sidechain
1	A	1982	ARG	Sidechain
1	A	3414	ARG	Sidechain
1	A	959	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	34733	34715	10	0
1	B	35088	34733	34715	8	0
1	C	35088	34733	34715	5	0
1	D	35088	34733	34715	13	0
2	E	832	829	831	0	0
2	F	832	829	831	0	0
2	G	832	829	831	0	0
2	H	832	829	831	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	14	14	0	0
5	B	31	14	14	0	0
5	C	31	14	14	0	0
5	D	31	14	14	0	0
6	A	14	10	10	0	0
6	B	14	10	10	0	0
6	C	14	10	10	0	0
6	D	14	10	10	0	0
7	A	156	246	246	0	0
7	B	104	164	164	1	0
7	C	104	164	164	0	0
7	D	52	82	82	0	0
All	All	144284	143000	142936	35	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 0.

The worst 5 of 35 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:C:4097:MET:HA	1:C:4097:MET:HE2	1.89	0.55
1:A:226:HIS:CD2	1:D:155:LYS:HE2	2.46	0.51
1:D:1715:LEU:C	1:D:1715:LEU:HD23	2.39	0.47
1:A:1715:LEU:C	1:A:1715:LEU:HD23	2.39	0.47
1:B:4097:MET:HE2	1:B:4097:MET:HA	1.96	0.47

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%)	4192 (96%)	161 (4%)	23 (0%)	24	58
1	B	4376/5037 (87%)	4198 (96%)	155 (4%)	23 (0%)	24	58
1	C	4376/5037 (87%)	4183 (96%)	173 (4%)	20 (0%)	24	58
1	D	4376/5037 (87%)	4184 (96%)	173 (4%)	19 (0%)	30	61
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17924/20580 (87%)	17158 (96%)	681 (4%)	85 (0%)	26	58

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3693	LYS
1	C	3693	LYS
1	D	3693	LYS
1	A	862	VAL
1	A	3613	TYR

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%)	3769 (98%)	58 (2%)	57	71
1	B	3827/4276 (90%)	3768 (98%)	59 (2%)	57	71
1	C	3827/4276 (90%)	3766 (98%)	61 (2%)	55	70
1	D	3827/4276 (90%)	3766 (98%)	61 (2%)	55	70
2	E	89/90 (99%)	86 (97%)	3 (3%)	32	58
2	F	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	G	89/90 (99%)	87 (98%)	2 (2%)	45	65
2	H	89/90 (99%)	88 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15664/17464 (90%)	15417 (98%)	247 (2%)	54 70

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4877	ASP
1	D	3434	LEU
1	C	2583	LEU
1	D	3268	HIS
1	D	4953	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1220	GLN
1	D	1837	GLN
1	D	3030	HIS
1	B	1660	GLN
1	B	1300	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	CFF	C	5104	-	15,15,15	0.85	0	23,23,23	0.83	0
7	POV	D	5105	-	51,51,51	0.70	0	57,59,59	0.40	0
7	POV	A	5107	-	51,51,51	0.71	0	57,59,59	0.43	0
5	ACP	B	5103	-	30,33,33	1.36	4 (13%)	45,52,52	1.26	5 (11%)
5	ACP	C	5103	-	30,33,33	1.36	4 (13%)	45,52,52	1.27	6 (13%)
7	POV	B	5106	-	51,51,51	0.69	0	57,59,59	0.41	0
6	CFF	B	5104	-	15,15,15	0.85	0	23,23,23	0.84	0
7	POV	B	5105	-	51,51,51	0.72	0	57,59,59	0.73	2 (3%)
7	POV	C	5106	-	51,51,51	0.68	0	57,59,59	0.43	0
7	POV	A	5105	-	51,51,51	0.75	0	57,59,59	0.71	2 (3%)
5	ACP	D	5103	-	30,33,33	1.36	4 (13%)	45,52,52	1.31	6 (13%)
7	POV	A	5106	-	51,51,51	0.73	0	57,59,59	0.70	2 (3%)
6	CFF	A	5104	-	15,15,15	0.84	0	23,23,23	0.82	0
5	ACP	A	5103	-	30,33,33	1.34	4 (13%)	45,52,52	1.28	6 (13%)
7	POV	C	5105	-	51,51,51	0.74	0	57,59,59	0.74	2 (3%)
6	CFF	D	5104	-	15,15,15	0.78	0	23,23,23	0.85	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
7	POV	D	5105	-	-	9/55/55/55	-
6	CFF	C	5104	-	-	-	0/2/2/2
7	POV	A	5107	-	-	8/55/55/55	-
5	ACP	B	5103	-	-	6/19/38/38	0/3/3/3
5	ACP	C	5103	-	-	6/19/38/38	0/3/3/3
7	POV	B	5106	-	-	7/55/55/55	-
6	CFF	B	5104	-	-	-	0/2/2/2
7	POV	B	5105	-	-	12/55/55/55	-
7	POV	C	5106	-	-	9/55/55/55	-
7	POV	A	5105	-	-	10/55/55/55	-
5	ACP	D	5103	-	-	7/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	A	5106	-	-	11/55/55/55	-
6	CFF	A	5104	-	-	-	0/2/2/2
5	ACP	A	5103	-	-	7/19/38/38	0/3/3/3
7	POV	C	5105	-	-	12/55/55/55	-
6	CFF	D	5104	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	ACP	PB-O2B	-3.22	1.48	1.56
5	B	5103	ACP	PB-O2B	-3.20	1.48	1.56
5	D	5103	ACP	PB-O2B	-3.17	1.48	1.56
5	A	5103	ACP	PB-O2B	-3.11	1.49	1.56
5	B	5103	ACP	PG-O3G	-2.94	1.48	1.54

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	5105	POV	C2-O21-C21	3.71	126.93	117.79
7	B	5105	POV	C2-O21-C21	3.62	126.70	117.79
7	A	5105	POV	C2-O21-C21	3.43	126.23	117.79
7	A	5106	POV	C2-O21-C21	3.42	126.20	117.79
5	D	5103	ACP	C4-C5-N7	2.83	114.06	110.62

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

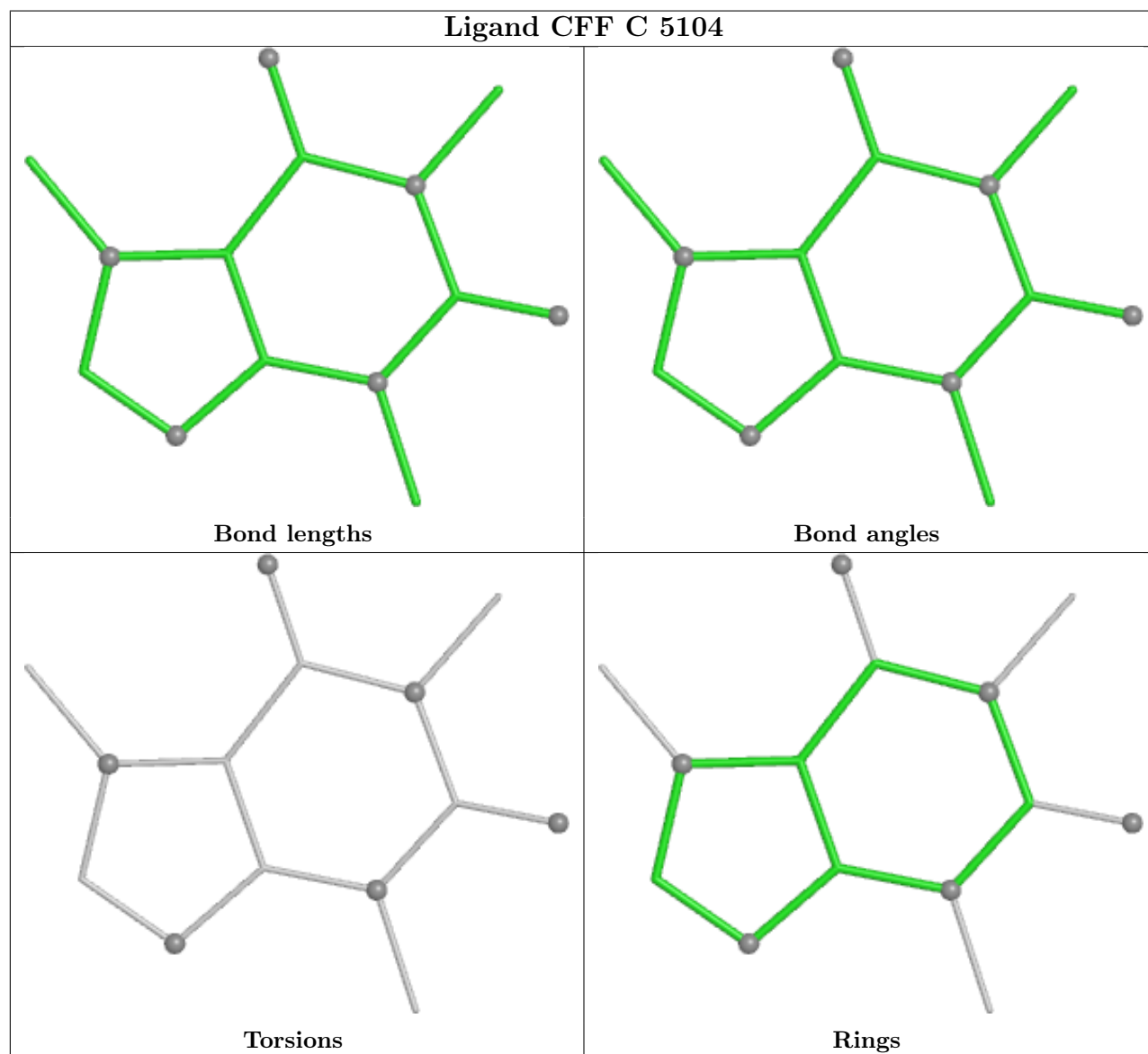
Mol	Chain	Res	Type	Atoms
5	A	5103	ACP	C5'-O5'-PA-O1A
5	A	5103	ACP	C4'-C5'-O5'-PA
5	A	5103	ACP	O4'-C4'-C5'-O5'
5	A	5103	ACP	C3'-C4'-C5'-O5'
5	B	5103	ACP	C5'-O5'-PA-O1A

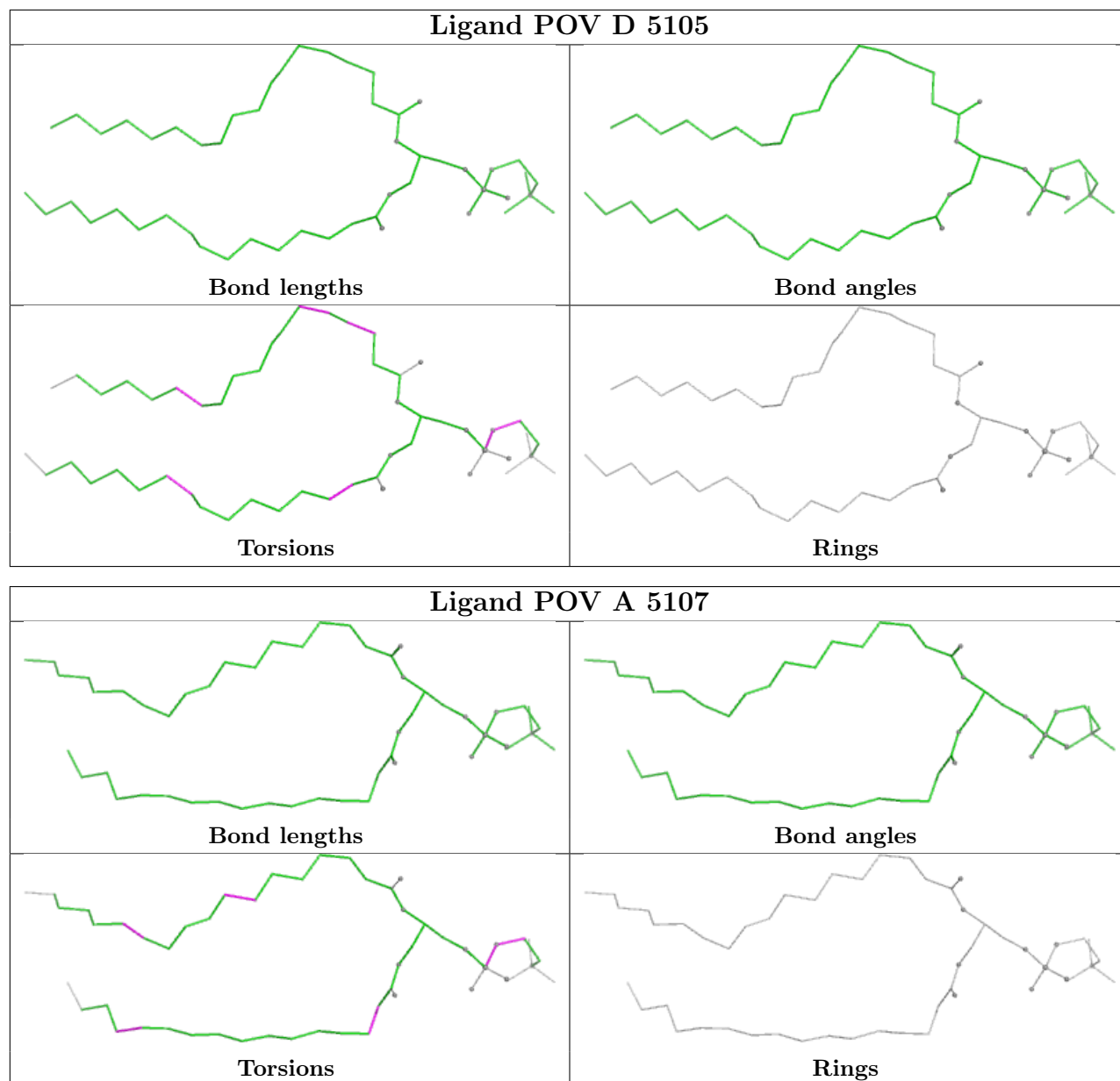
There are no ring outliers.

1 monomer is involved in 1 short contact:

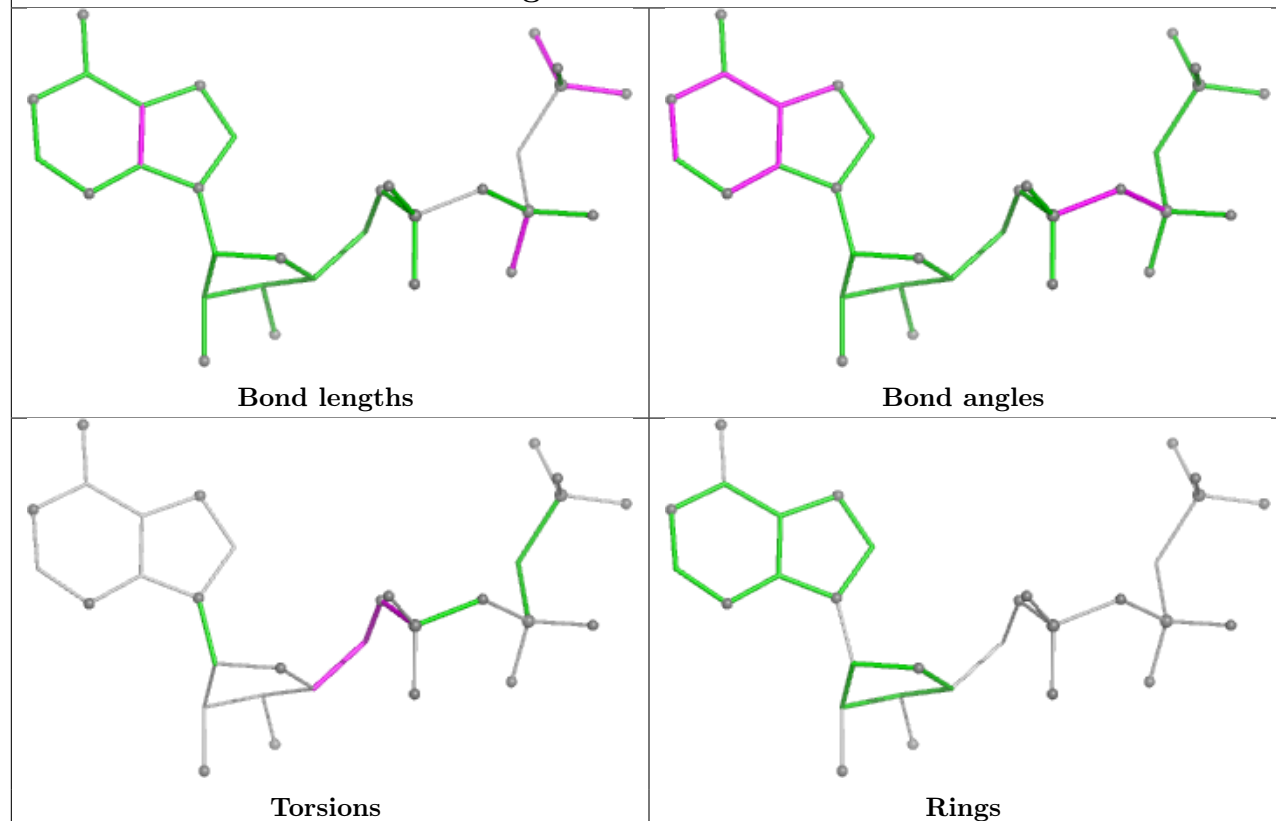
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	5106	POV	1	0

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.

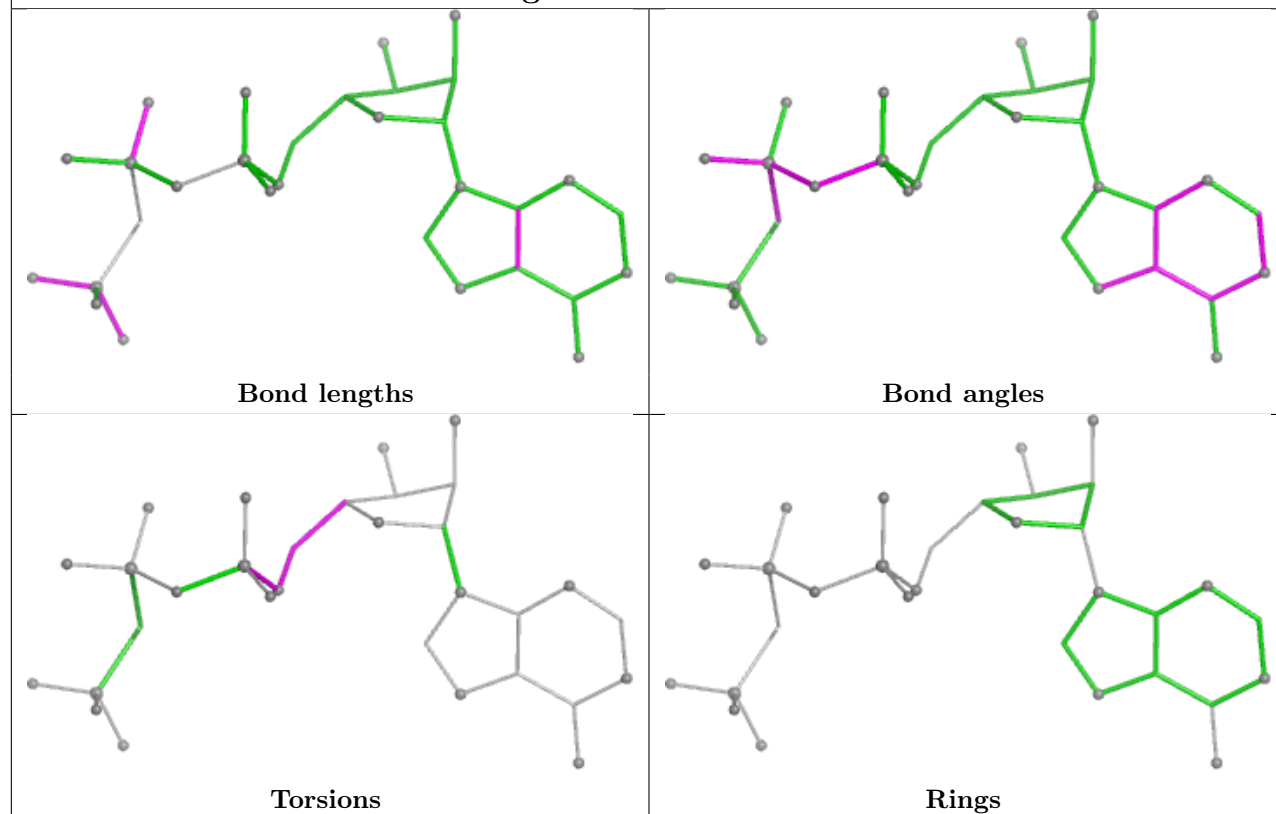


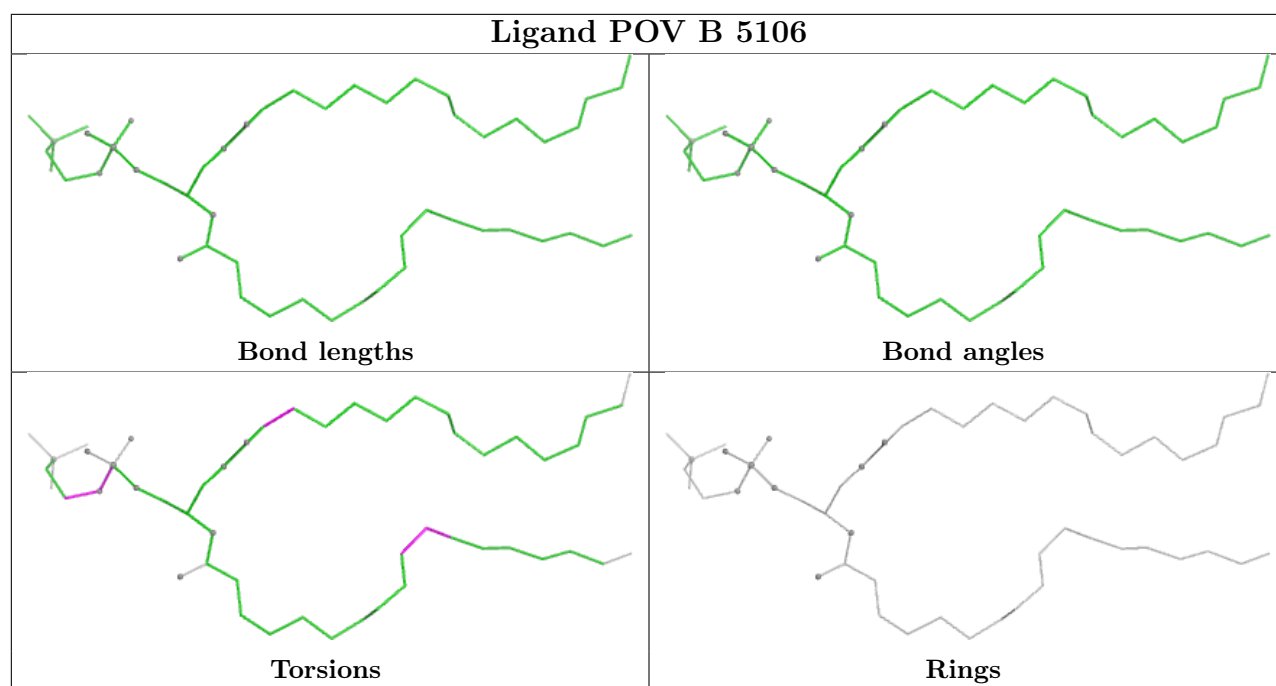


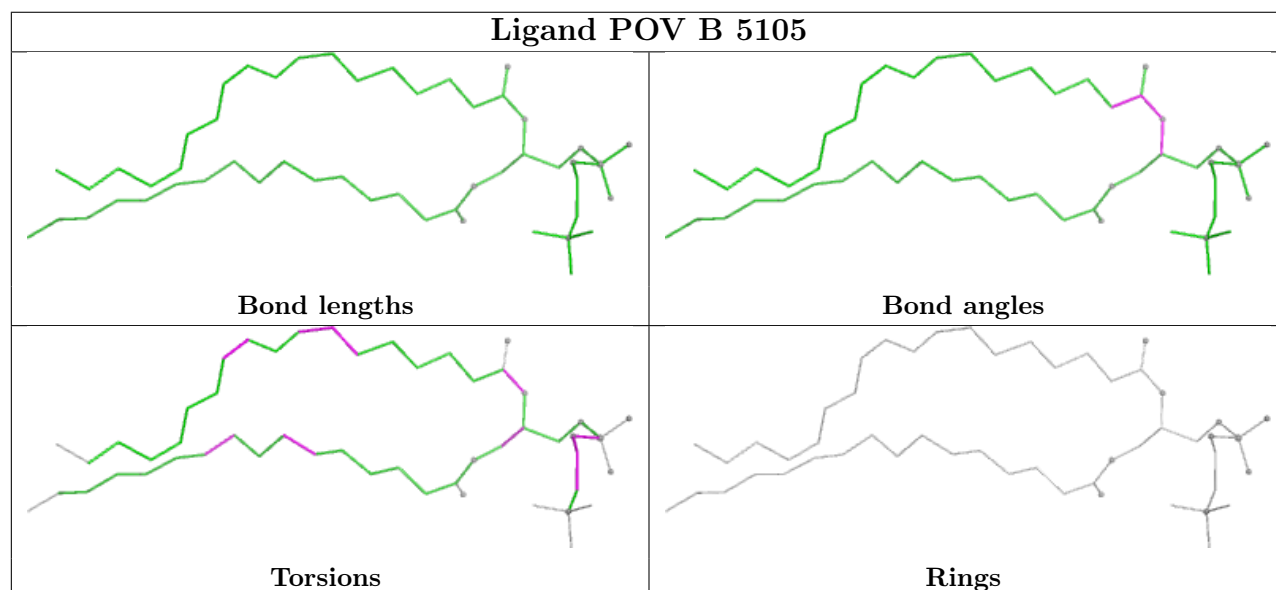
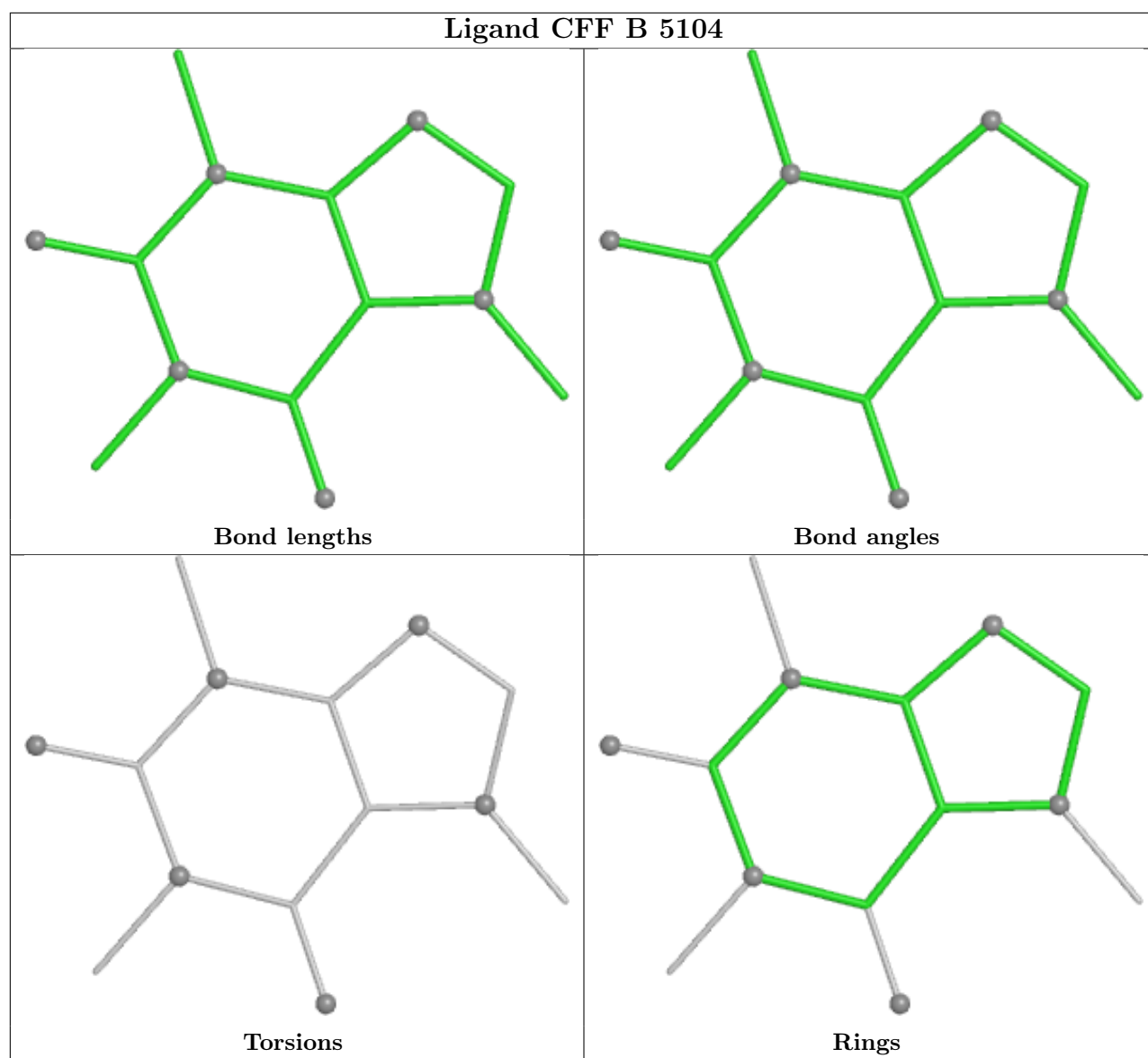
Ligand ACP B 5103

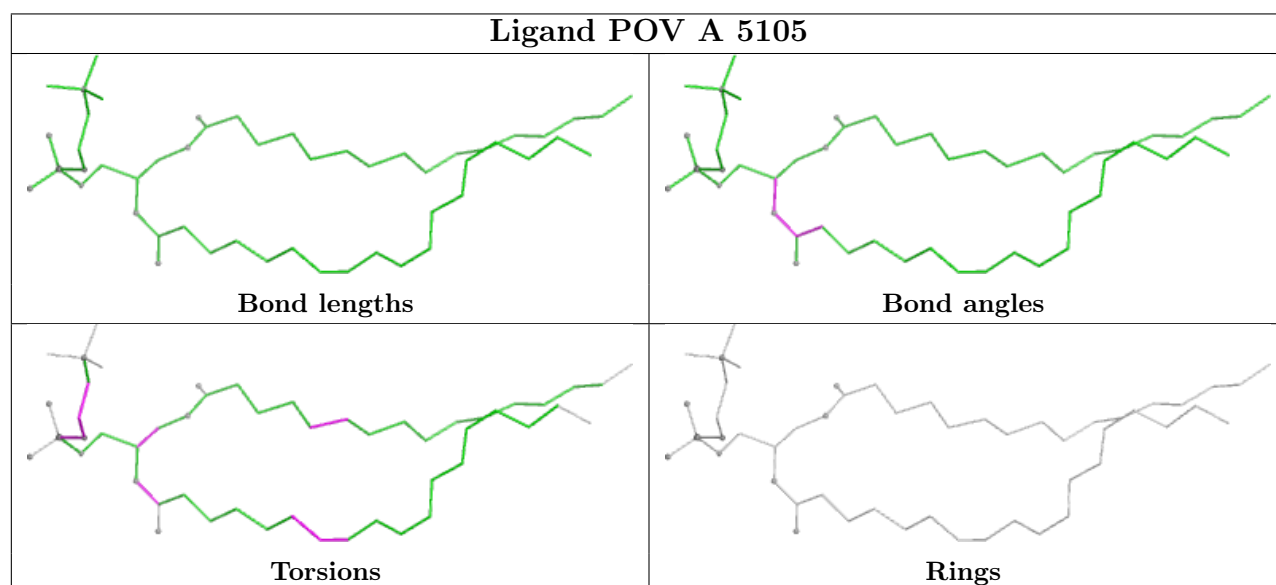
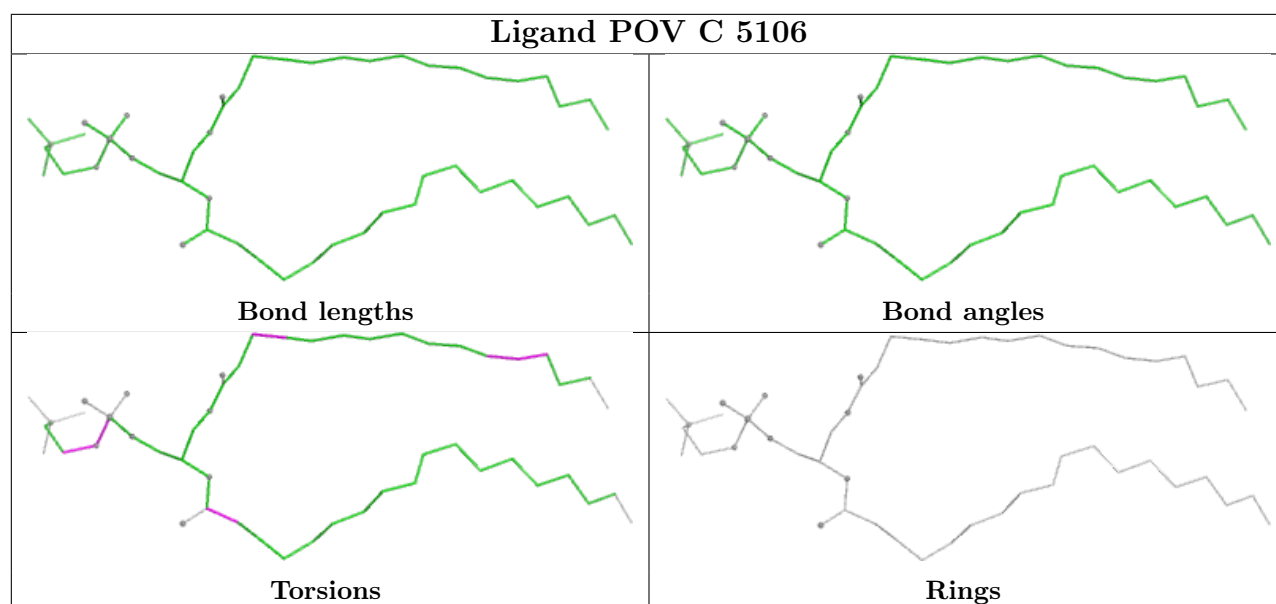


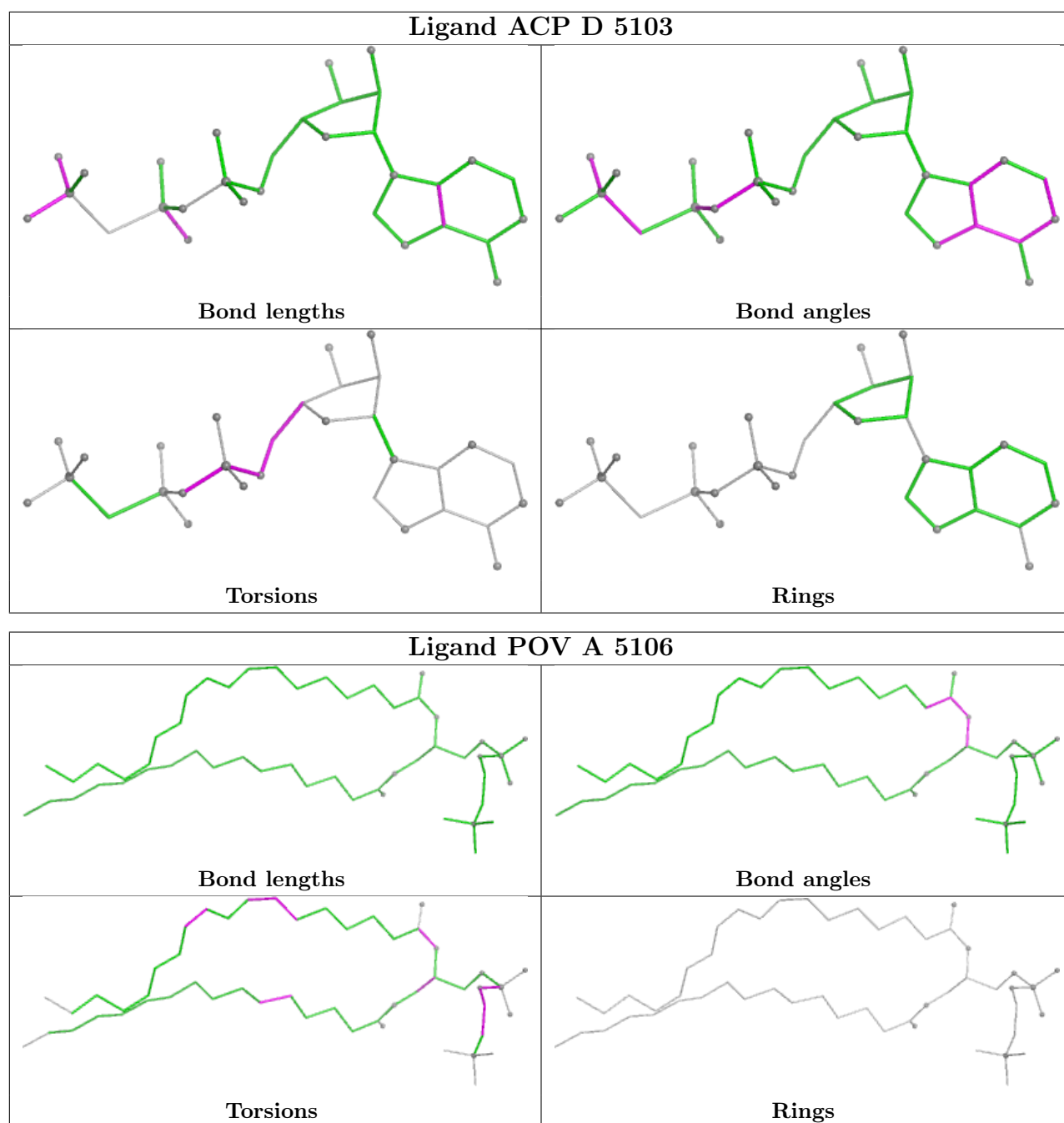
Ligand ACP C 5103

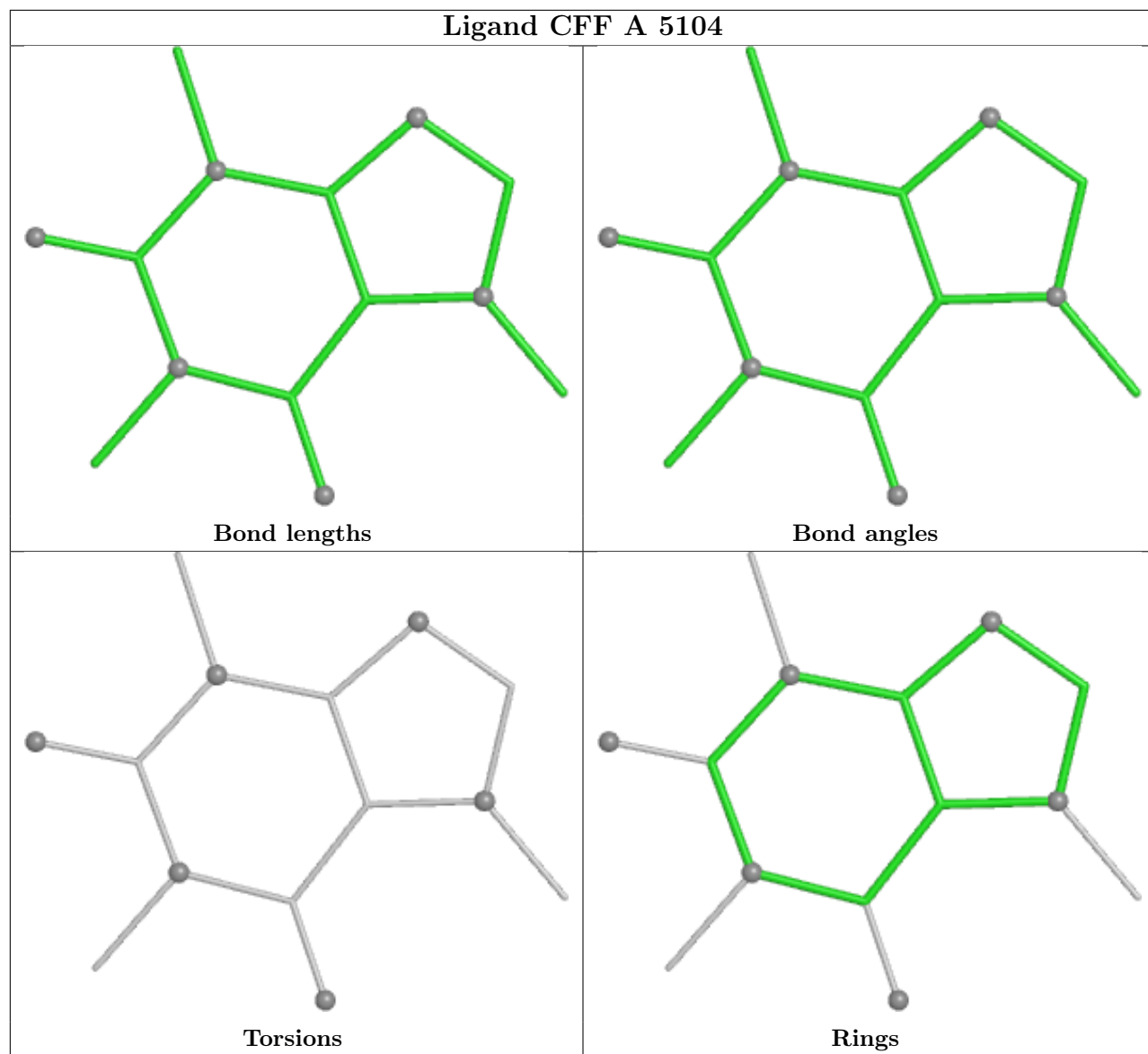


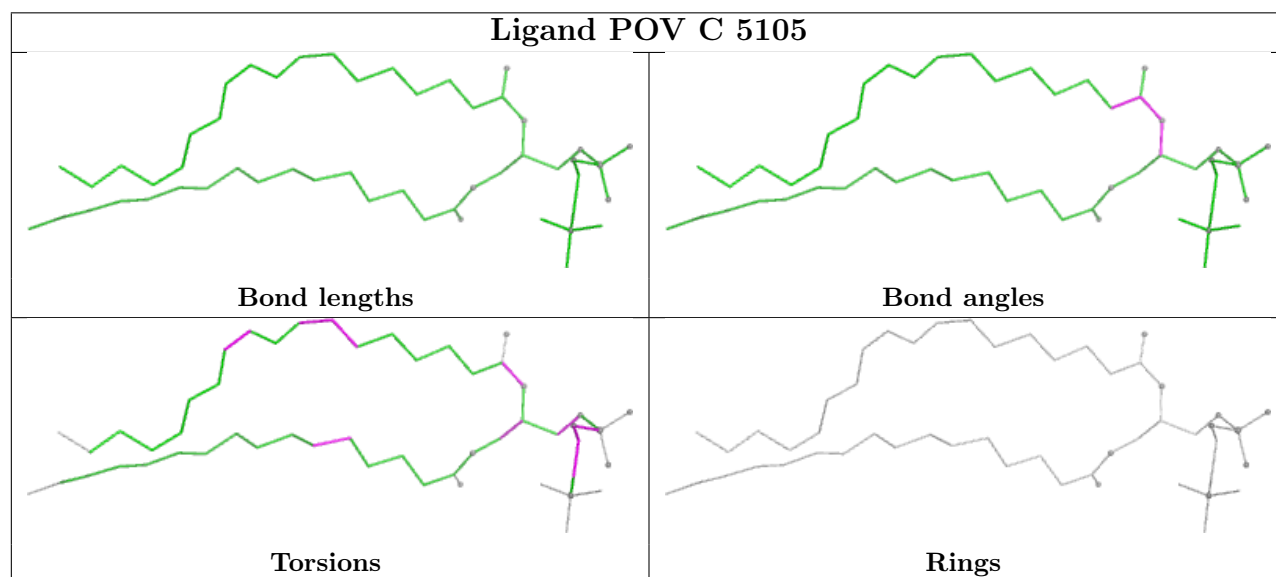
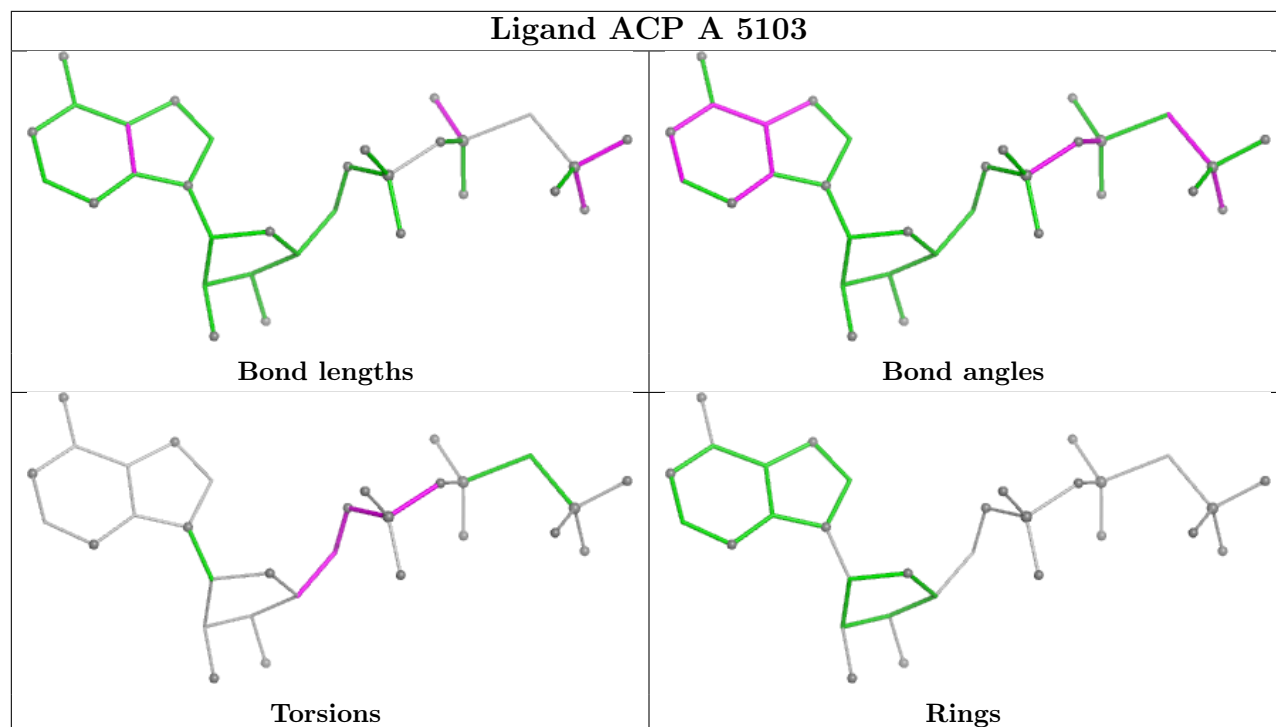


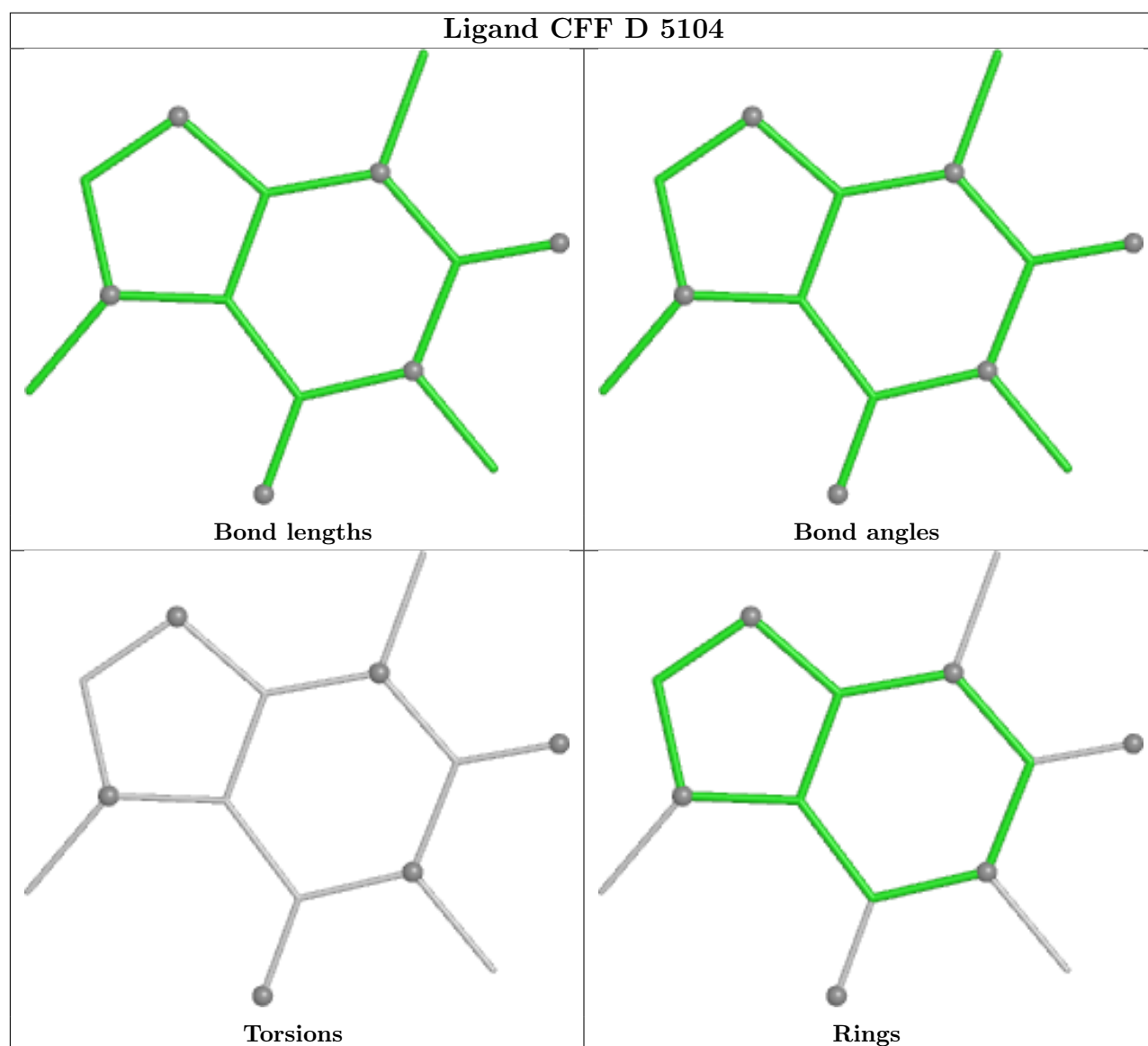












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

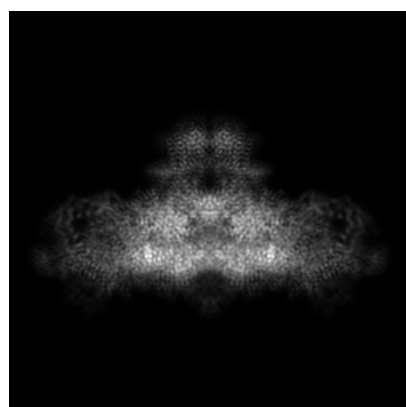
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54570. These allow visual inspection of the internal detail of the map and identification of artifacts.

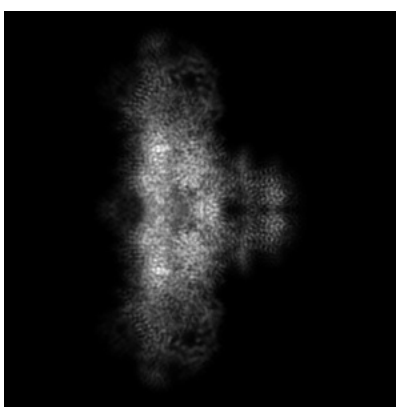
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

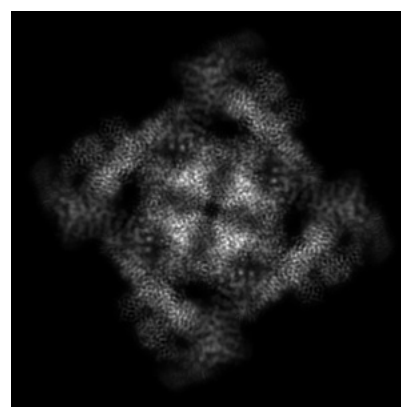
6.1.1 Primary map



X



Y



Z

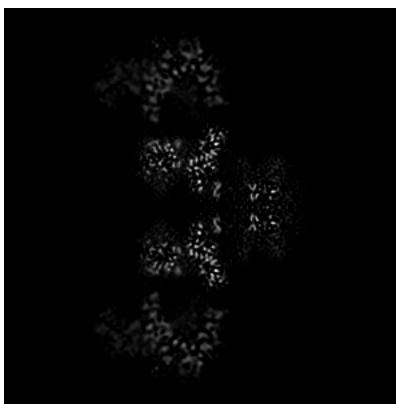
The images above show the map projected in three orthogonal directions.

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](#)

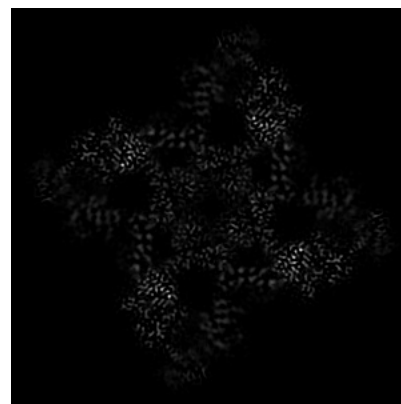
6.3.1 Primary map



X Index: 173



Y Index: 127

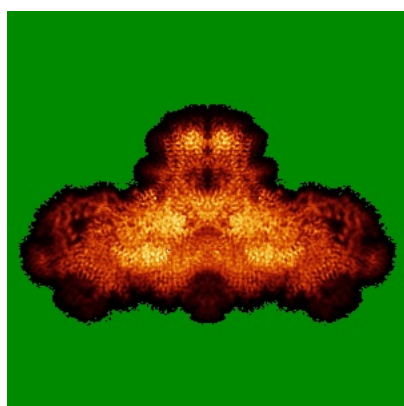


Z Index: 117

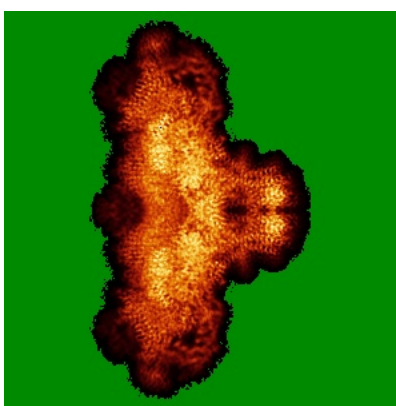
The images above show the largest variance slices of the map in three orthogonal directions.

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

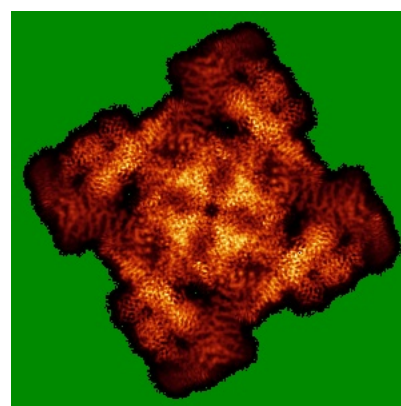
6.4.1 Primary map



X



Y

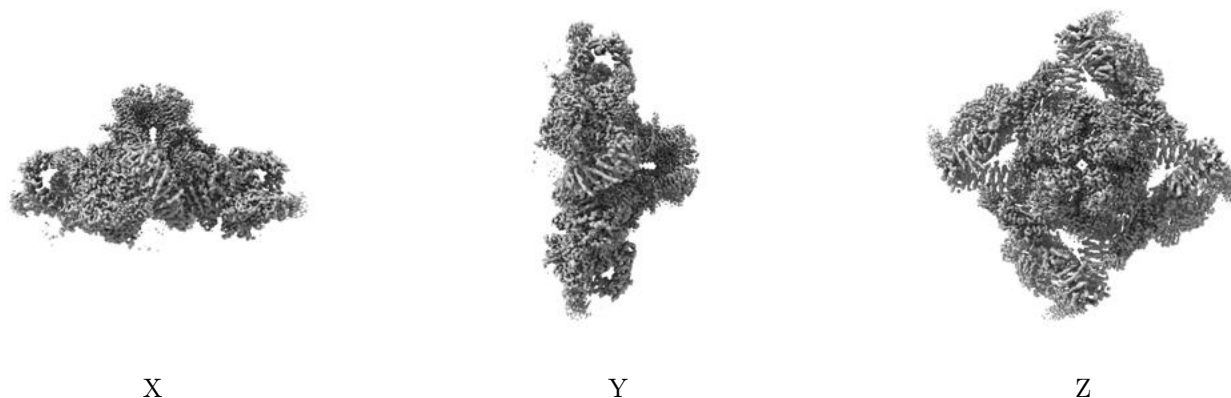


Z

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

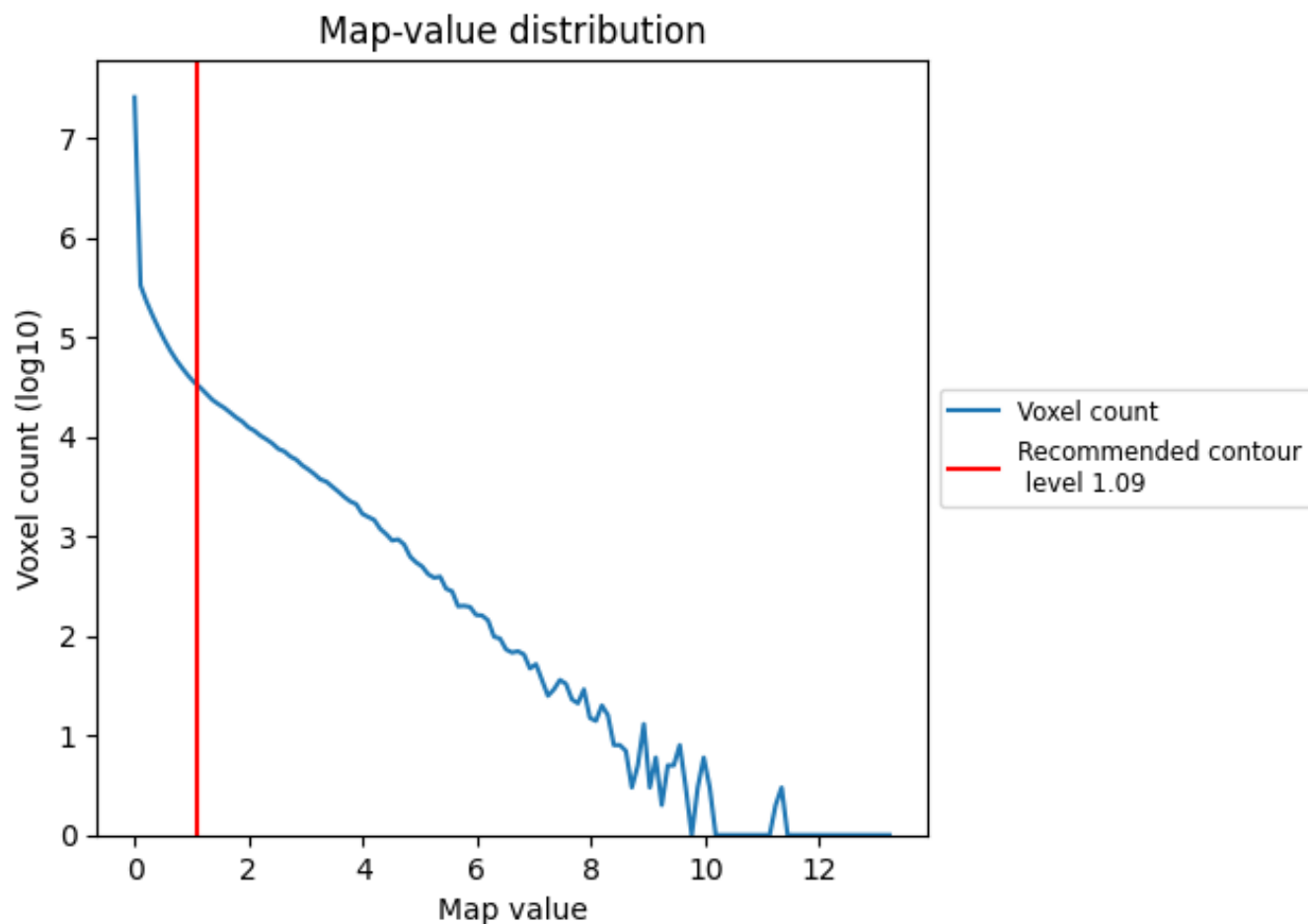
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

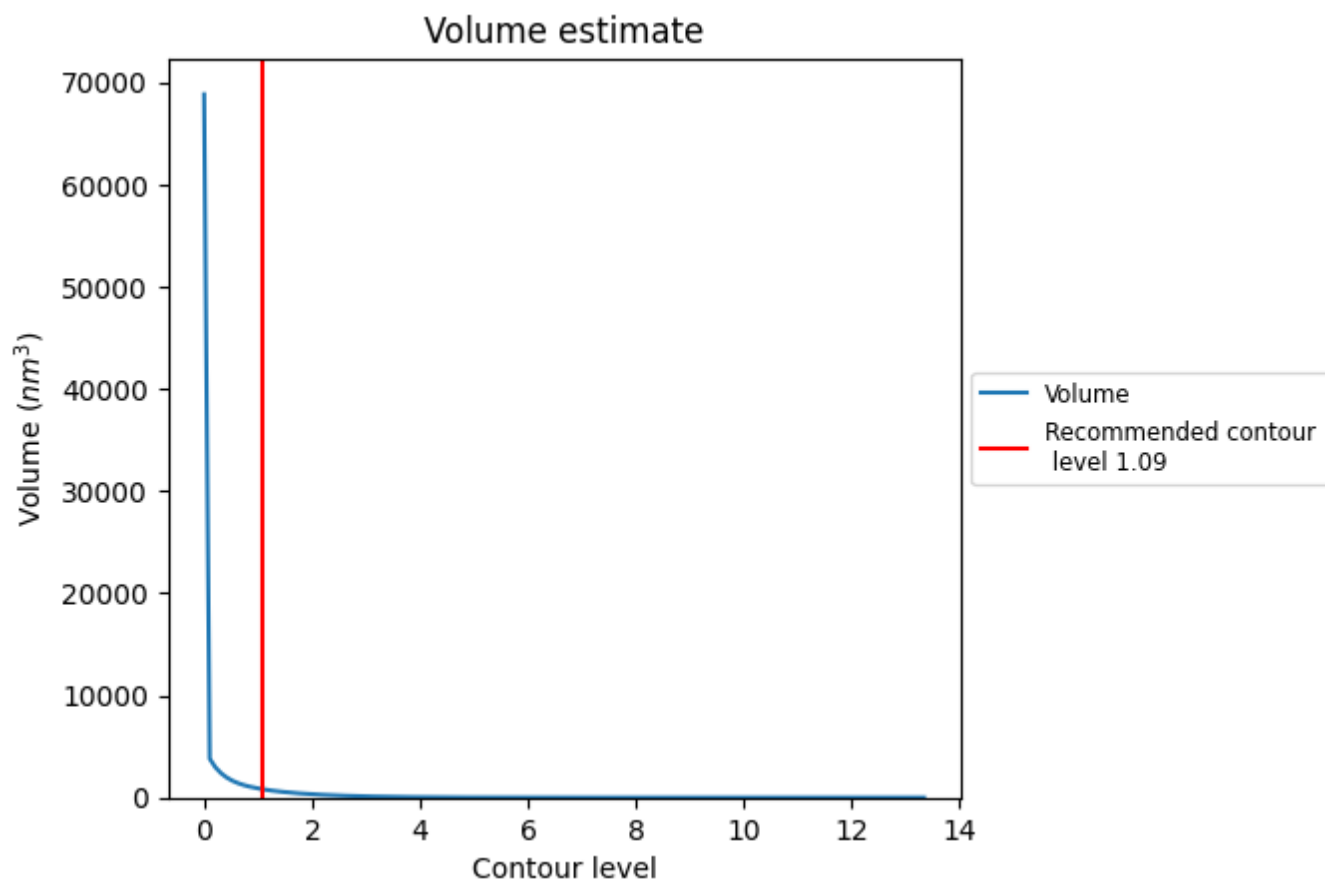
This section contains the results of statistical analysis of the map.

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.

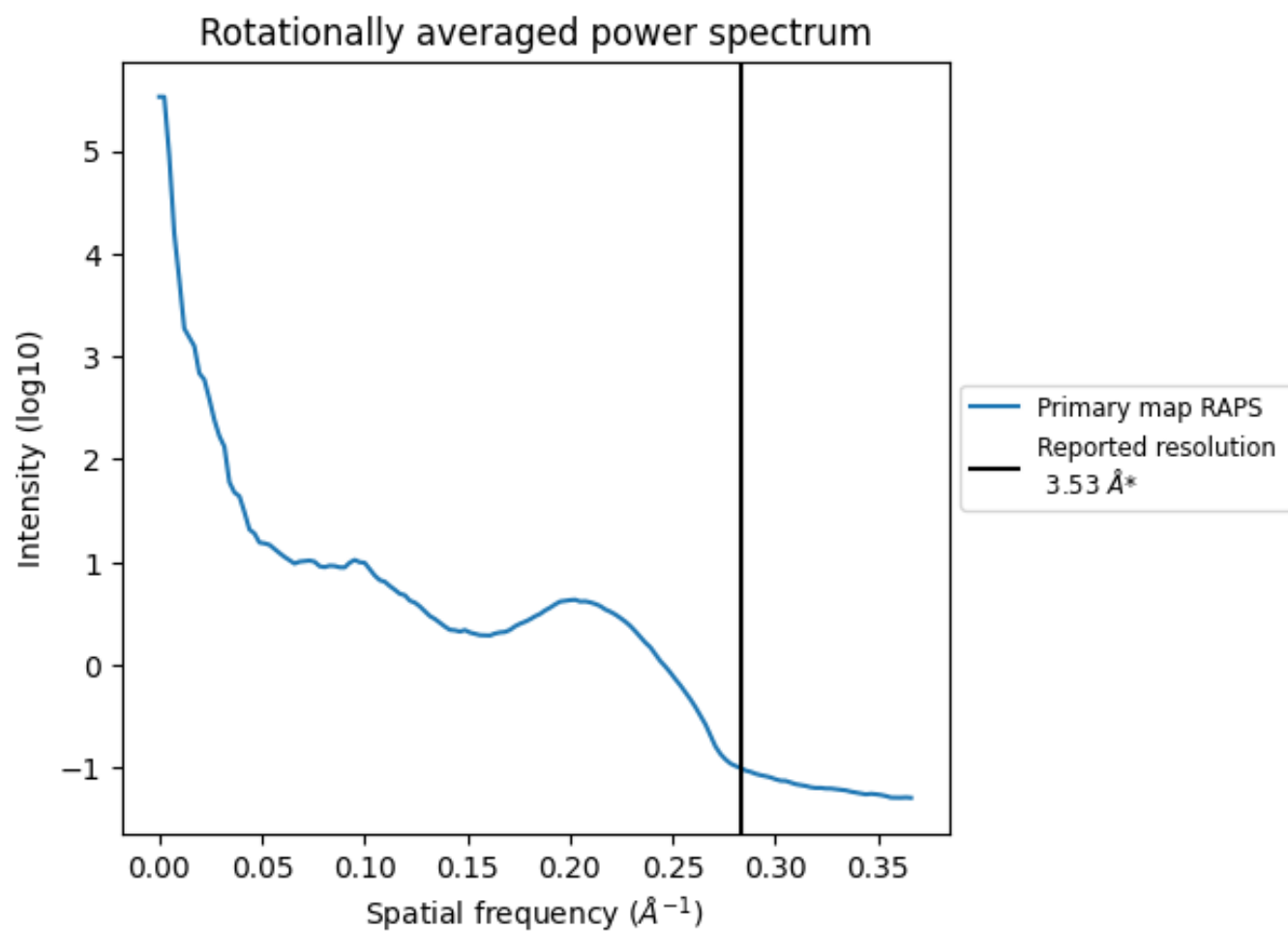
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 812 nm^3 ; this corresponds to an approximate mass of 734 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 0.283 Å⁻¹

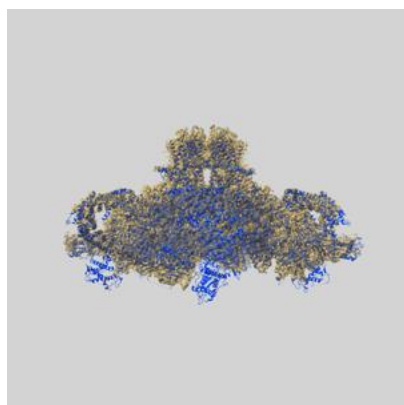
8 Fourier-Shell correlation

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

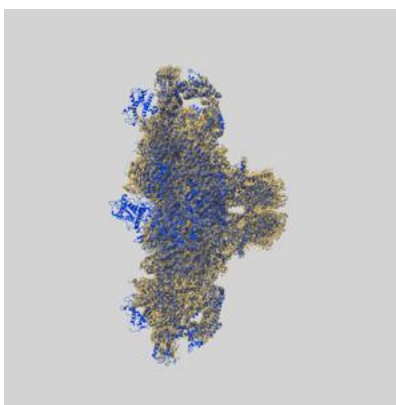
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54570 and PDB model 9S4N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

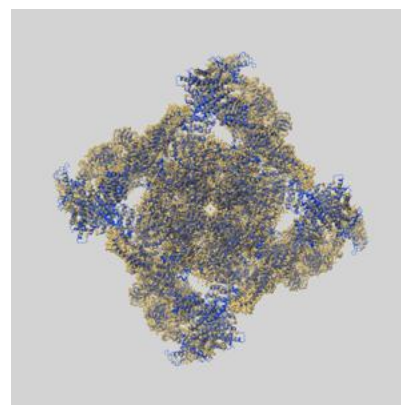
9.1 Map-model overlay [i](#)



X



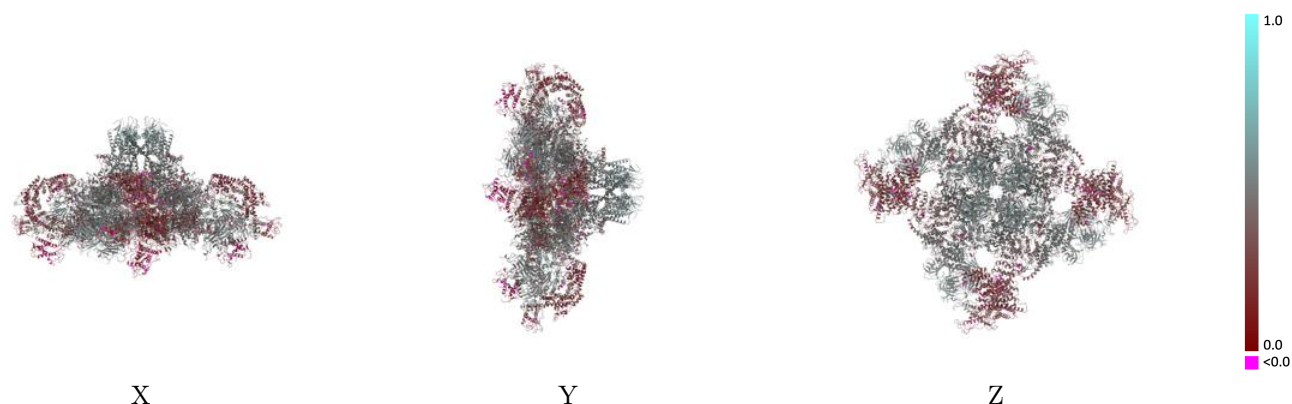
Y



Z

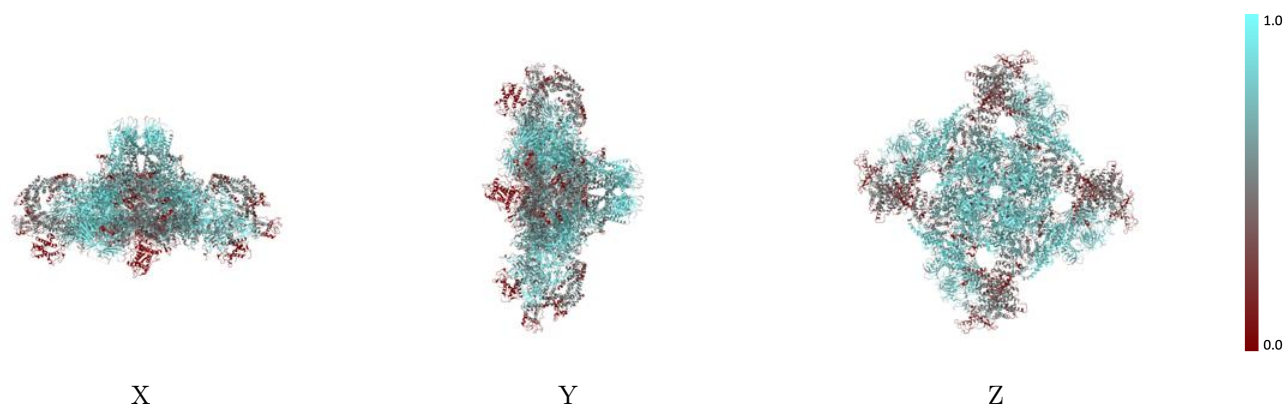
The images above show the 3D surface view of the map at the recommended contour level 1.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



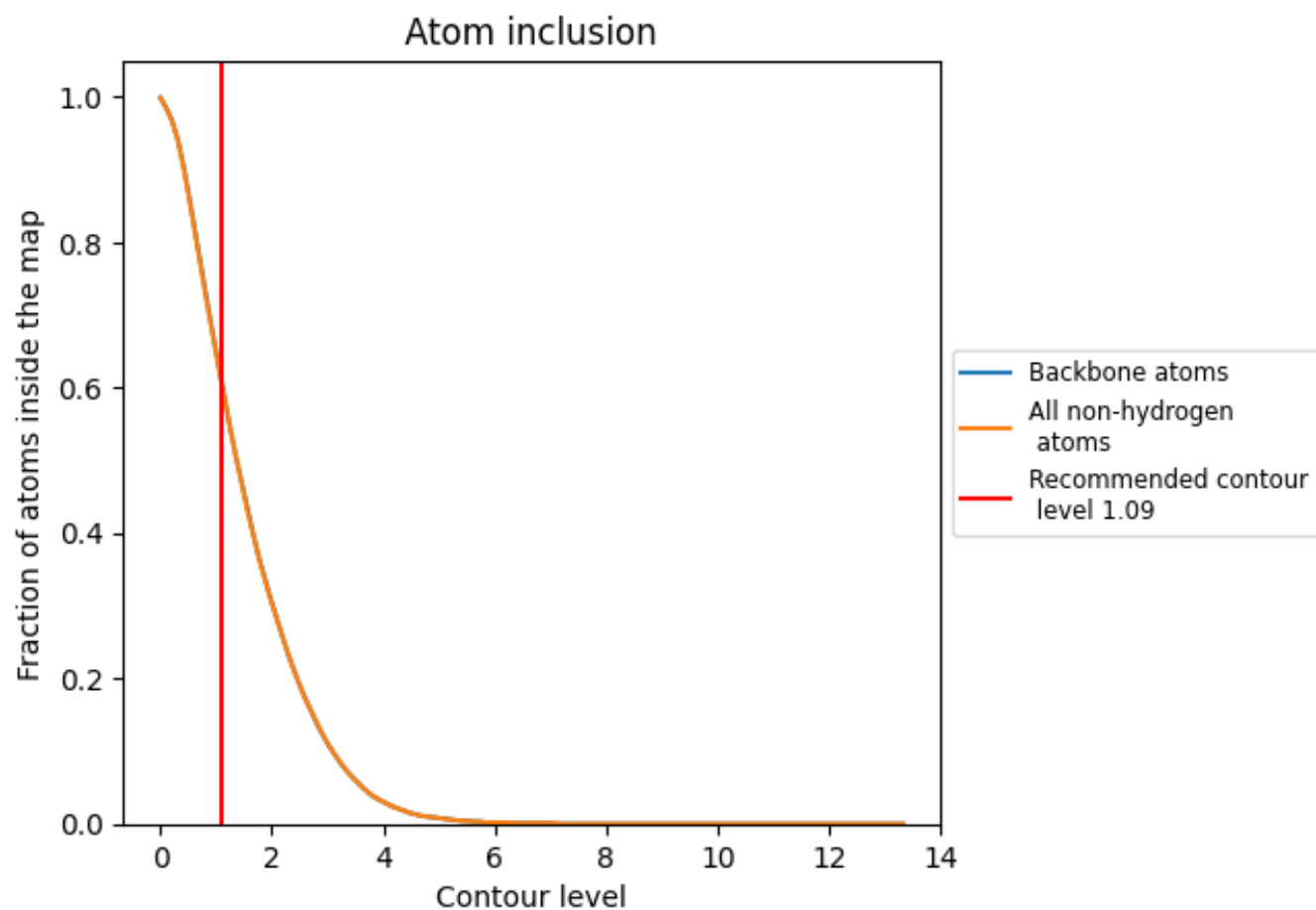
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 61% 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 (1.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.3980
A	0.6070	0.3940
B	0.6060	0.3940
C	0.6080	0.3940
D	0.6390	0.3990
E	0.7230	0.4900
F	0.7220	0.4910
G	0.7220	0.4930
H	0.7480	0.4960

1.0

0.0

<0.0