



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:19 AM UTC

PDB ID : 8VK4 / pdb_00008vk4
EMDB ID : EMD-43304
Title : Structure of mouse RyR1 in complex with S100A1 (high-Ca²⁺/CFF/ATP dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-08
Resolution : 3.56 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

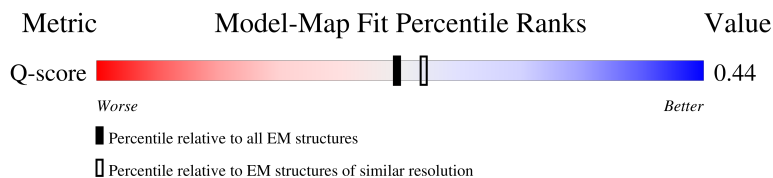
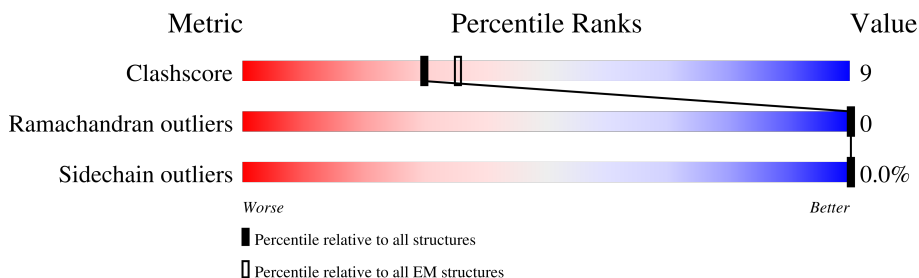
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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	12750 (3.06 - 4.06)

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	E	108	
1	F	108	
1	G	108	
1	H	108	

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Mol	Chain	Length	Quality of chain
2	I	94	
2	J	94	
2	K	94	
2	L	94	
2	M	94	
2	N	94	
2	O	94	
2	P	94	
3	A	5035	
3	B	5035	
3	C	5035	
3	D	5035	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 149304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 2 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	J	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	K	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	L	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	N	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	M	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	O	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	P	93	Total	C	N	O	S	0	0
			729	460	114	152	3		

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		
3	B	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		
3	C	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		

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

Mol	Chain	Residues	Atoms		AltConf
4	I	2	Total	Ca	0
			2	2	
4	J	2	Total	Ca	0
			2	2	
4	D	1	Total	Ca	0
			1	1	
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	K	2	Total	Ca	0
			2	2	
4	L	2	Total	Ca	0
			2	2	
4	N	2	Total	Ca	0
			2	2	
4	M	2	Total	Ca	0
			2	2	
4	O	2	Total	Ca	0
			2	2	
4	P	2	Total	Ca	0
			2	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

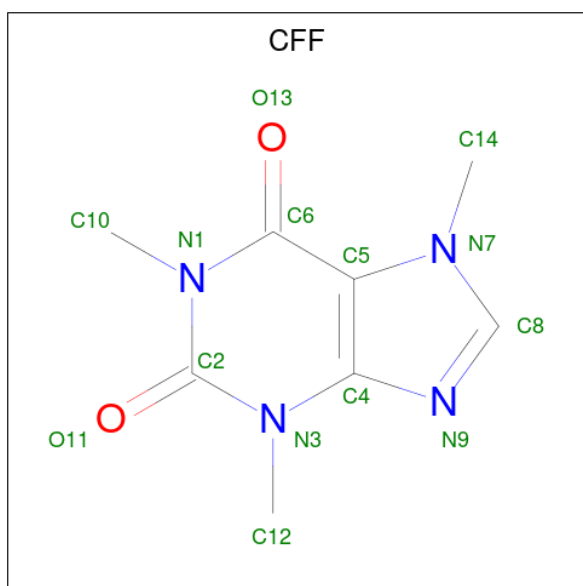
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	

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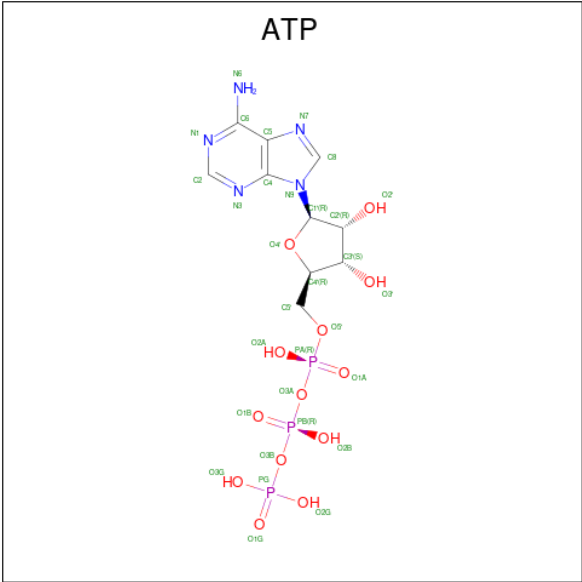
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



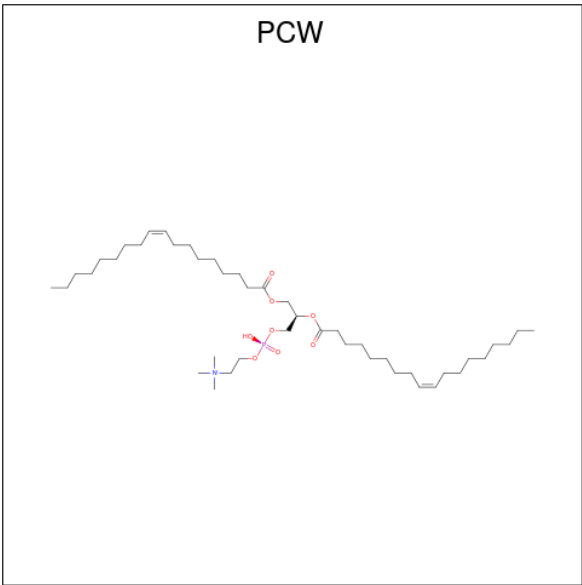
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			14	8	4	2	
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

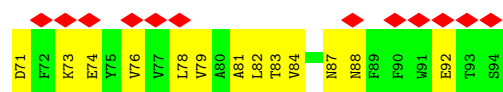


Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10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

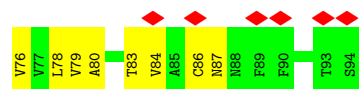
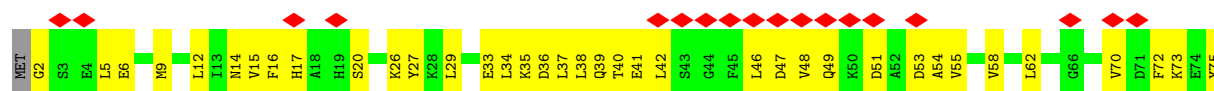
- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



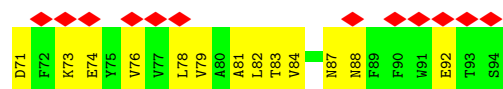
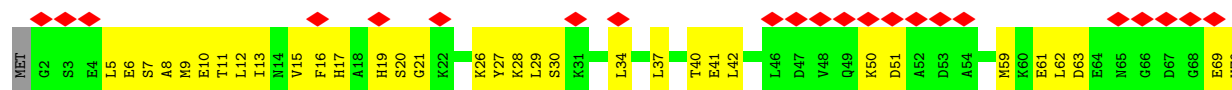
Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	



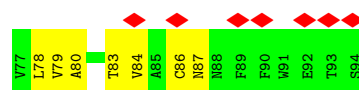
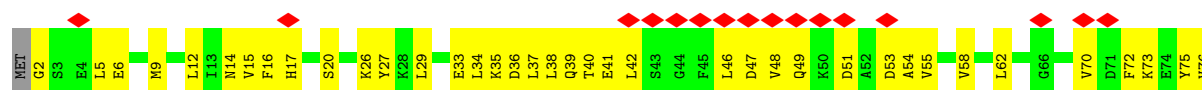
• Molecule 2: Protein S100A1



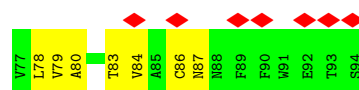
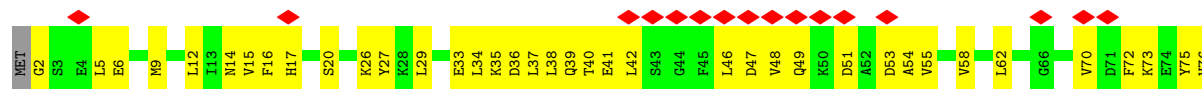
• Molecule 2: Protein S100A1



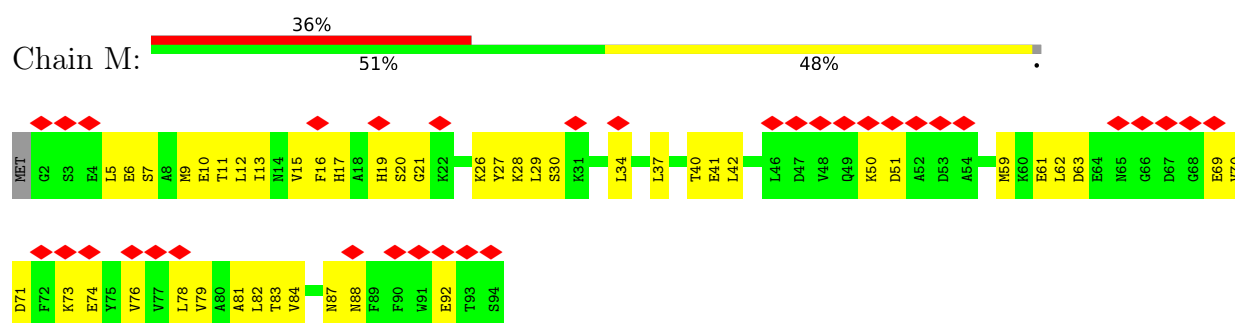
• Molecule 2: Protein S100A1



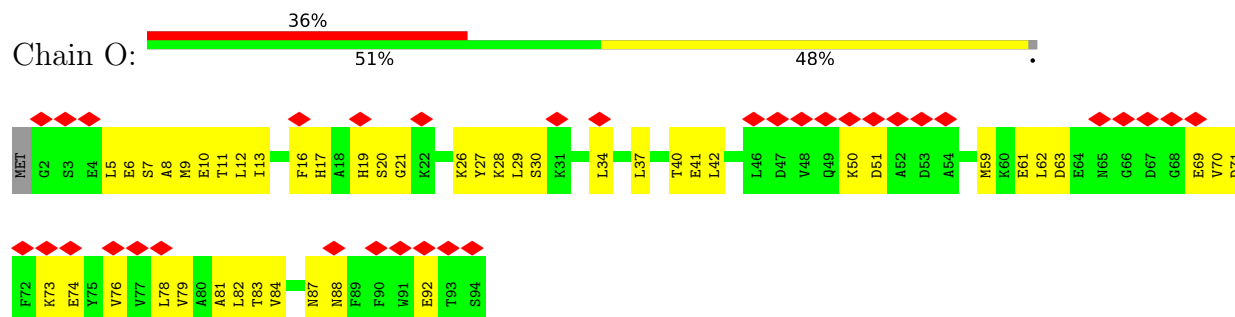
• Molecule 2: Protein S100A1



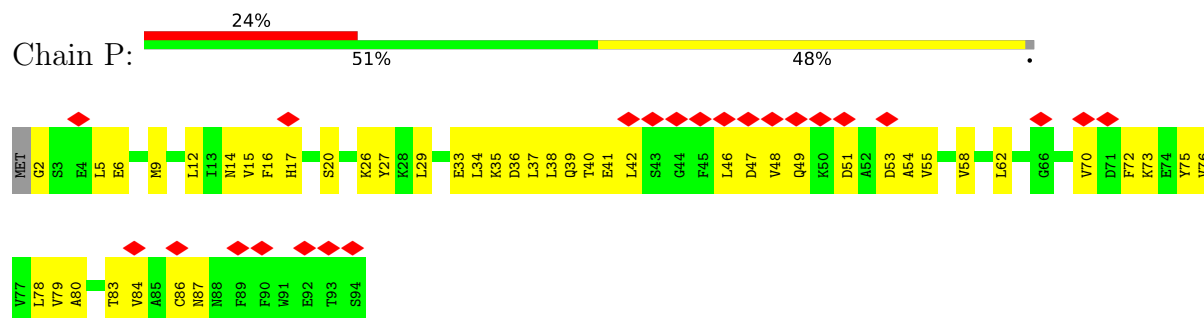
• Molecule 2: Protein S100A1



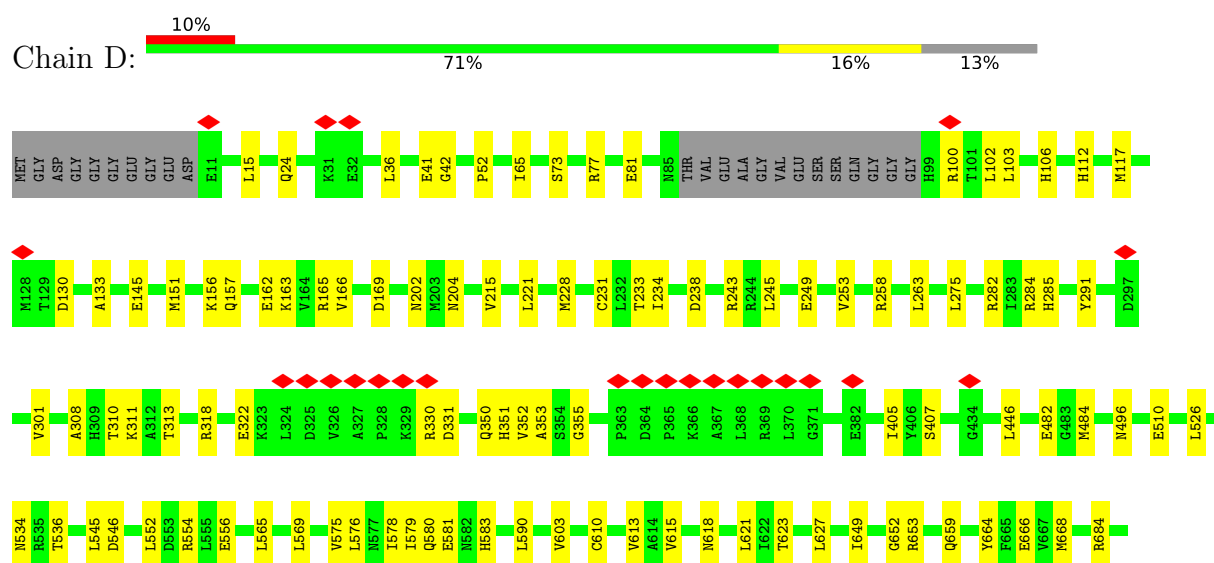
- Molecule 2: Protein S100A1

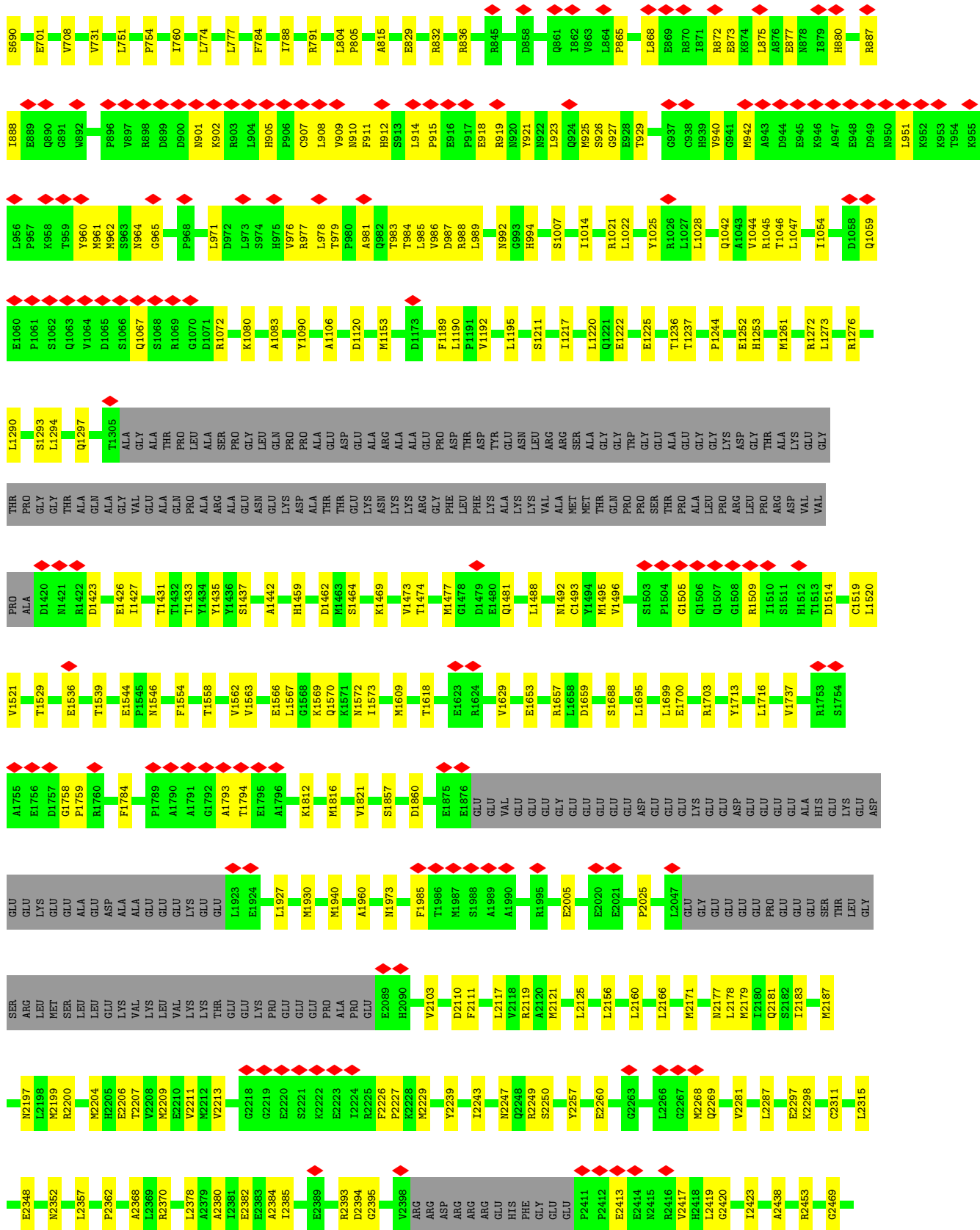


- Molecule 2: Protein S100A1



- Molecule 3: Ryanodine receptor 1

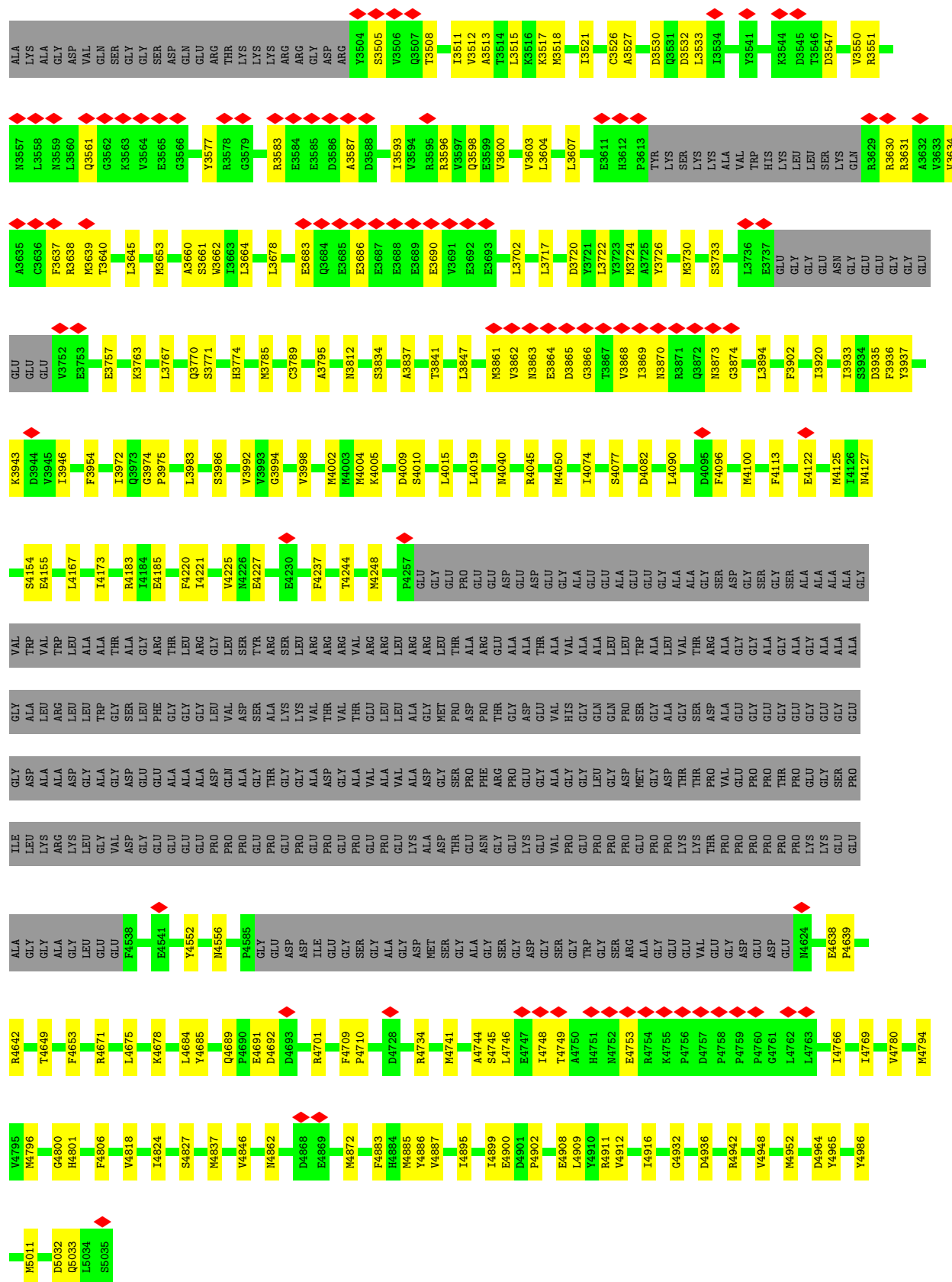








E3398	F3399	S3400	V3401	L3402	C3403	R3404	D3405	L3406	Y3407	A3408	L3409	Y3410	P3411	L3412	L3413	L3414	R3415	R3421		N3431	A3432		L3435		M3438	V3439	G3440	E3441	L3442	F3443	I3444	S3447		N3451	F3452	K3453	R3454	E3455	E3456		N3463	E3464	I3465	R3466	L3467	M3468	S3469	F3470	L3471	L3472	ALA	ASP	ASN	GLY	SER	LYS	MET			
L3317	G3318	N3319	I3320	L3321	R3322	A3323	I3324	V3325	L3330	D3331	S3332	E3333	A3334	M3336	K3337	I3341	L3344	R3415	R3421		N3431	A3432		L3435		M3438	V3439	G3440	E3441	L3442	F3443	I3444	S3447		N3451	F3452	K3453	R3454	E3455	E3456		N3463	E3464	I3465	R3466	L3467	M3468	S3469	F3470	L3471	L3472	ALA	ASP	ASN	GLY	SER	LYS	MET		
Y3220	E3226	E3227	R3228	A3229	I3230	L3233	F3234	N3235	S3236	E3237	E3238	E3239	E3253	I3254	G3255	G3256	L3257	A3262	R3263	M3267	V3270	I3271	E3272	L3275	P3276	L3278	C3279	S3280	Y3281	L3282	R3288	E3291	A3292	P3293	P3294	P3295	A3296	L3297	A3298	A3299	G3300	A3301	T3309	D3310	H3311	H3312	L3316													
L3113	GLY	VAL	SER	GLN	ALA	ARG	THR	GLN	VAL	K3124	G3125	V3126	G3127	Q3128	T3131	V3135	A3136	V3140	L3141	T3142	F3145	D3155	D3156	V3157	I3158	V3164	Y3167	Y3281	S3172	L3176	G3177	R3180	N3181	P3182	Y3183	V3184	E3185	L3187	R3197	V3204	M3107	V3108	E3109	N3212	E3213															
I2975	L2978	V2981	V2982	S2983	S2984	G2985	R2986	V2987	E2988	F2989	F2999	L3003	L3004	R3005	S3028	E3036	M3039	L3047	L3050	H3053	R3054	V3055	V3065	L3069	L3076	D3077	A3078	R3079	M3082	P3086	V3089	K3090	D3103	I3104	E3105	R3106	V3107	E3108	E3109	N3110	L3111	R3112																		
G2900	G2901	S2902	H2903	P2904	L2905	L2906	V2907	P2908	L2909	D2910	T2911	L2912	T2913	A2914	K2915	E2916	K2917	A2918	R2919	D2920	R2921	E2922	K2923	A2924	Q2925	E2926	L2927	L2928	K2929	F2930	L2931	Q2932	M2933	N2934	G2935	Y2936	A2937	V2938	T2939	R2940	G2941	L2942	D2943	M2945	E2946	L2947	D2948	T2949	S2950	L2952	F2958	S2971	Q2972	E2973	F2974					
THR	ARG	LYS	SER	GLN	THR	ALA	GLN	TYR	ASP	PRO	ARG	GLY	Y2856	N2857	P2858	Q2859	P2860	P2861	D2862	L2863	S2864	V2865	V2866	T2867	L2868	S2869	R2870	E2871	L2872	Q2873	A2874	M2875	A2876	E2877	Q2878	L2879	A2880	E2881	N2882	Y2883	H2884	N2885	T2886	V2887	G2888	R2889	K2890	K2891	K2892	Q2893	T2894	S2895	L2895	A2897	K2898	G2899				
E2760	N2761	I2762	D2763	E2764	E2765	L2766	K2767	T2768	H2769	P2790	M2791	L2792	R2793	P2794	Y2795	K2796	T2797	F2798	S2799	E2800	K2801	D2802	K2803	E2804	L2805	Y2806	R2807	P2808	N2809	L2810	K2811	E2812	S2813	L2814	K2815	A2816	M2817	L2818	A2819	W2820	E2821	W2822	T2823	V2824	E2825	K2826	A2827	K2828	E2829	G2830	E2831	GLY	GLY	LYS	THR	GLY	LYS	LYS	LYS	LYS
Y2720	S2721	S2722	K2723	T2724	E2725	K2726	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2735	F2736	D2737	P2738	R2739	P2740	V2741	E2742	T2743	L2744	N2745	V2746	I2747	L2748	P2749	E2750	K2751	L2752	D2753	S2754	R2755	I2756	N2757	K2758	F2759	A2760	E2761	T2762	T2763	H2764	E2765	K2766	W2767	A2768	F2769	D2770	K2771	I2772	Q2773	N2774	N2775	W2776	S2777	Y2778	Q2779		
M2579	M2583	Y2588	R2592	G2593	S2595	A2599	V2603	C2607	M2619	L2623	L2624	R2625	R2626	L2627	V2628	P2641	L2642	K2643	L2644	L2645	K2654	L2658	T2668	L2673	H2674	L2675	T2676	R2677	K2678	L2679	Q2694	E2695	R2698	I2699	M2701	P2702	C2703	I2707	Y2715																					
G2263	L2266	G2267	M2268	Q2269	V2281	L2287	E2297	K2298	C2311	L2314	L2315	Y2319	L2322	E2348	N2352	L2357	P2362	A2368	L2369	R2370	L2378	A2379	A2380	E2382	E2383	A2384	I2385	E2389	R2393	D2394	G2395	V2398	ARG	ASP	ARG	ARG	ARG	GLY	HIS	PHE																				
L2160	L2166	M2171	N2177	L2178	L2179	L2180	Q2181	S2182	I2183	M2187	N2197	L2198	M2199	R2200	M2204	E2205	T2207	V2208	R2209	V2211	M2212	Y2213	G2218	Q2219	E2220	S2221	K2222	I2224	M2229	C2233	Y2239	I2243	N2247	Q2248	R2249	S2250	H2254	L2255	Y2257	E2260																				

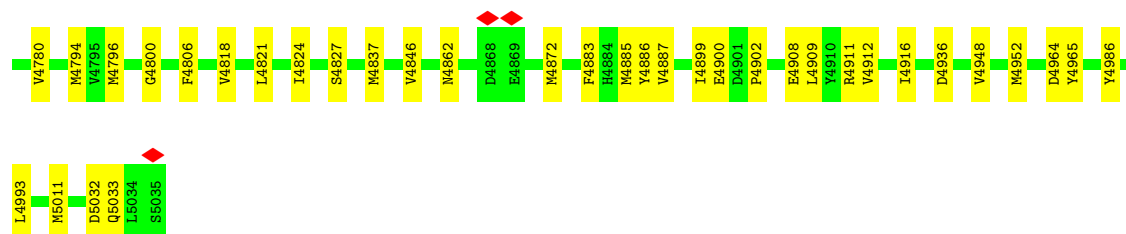


- Molecule 3: Ryanodine receptor 1

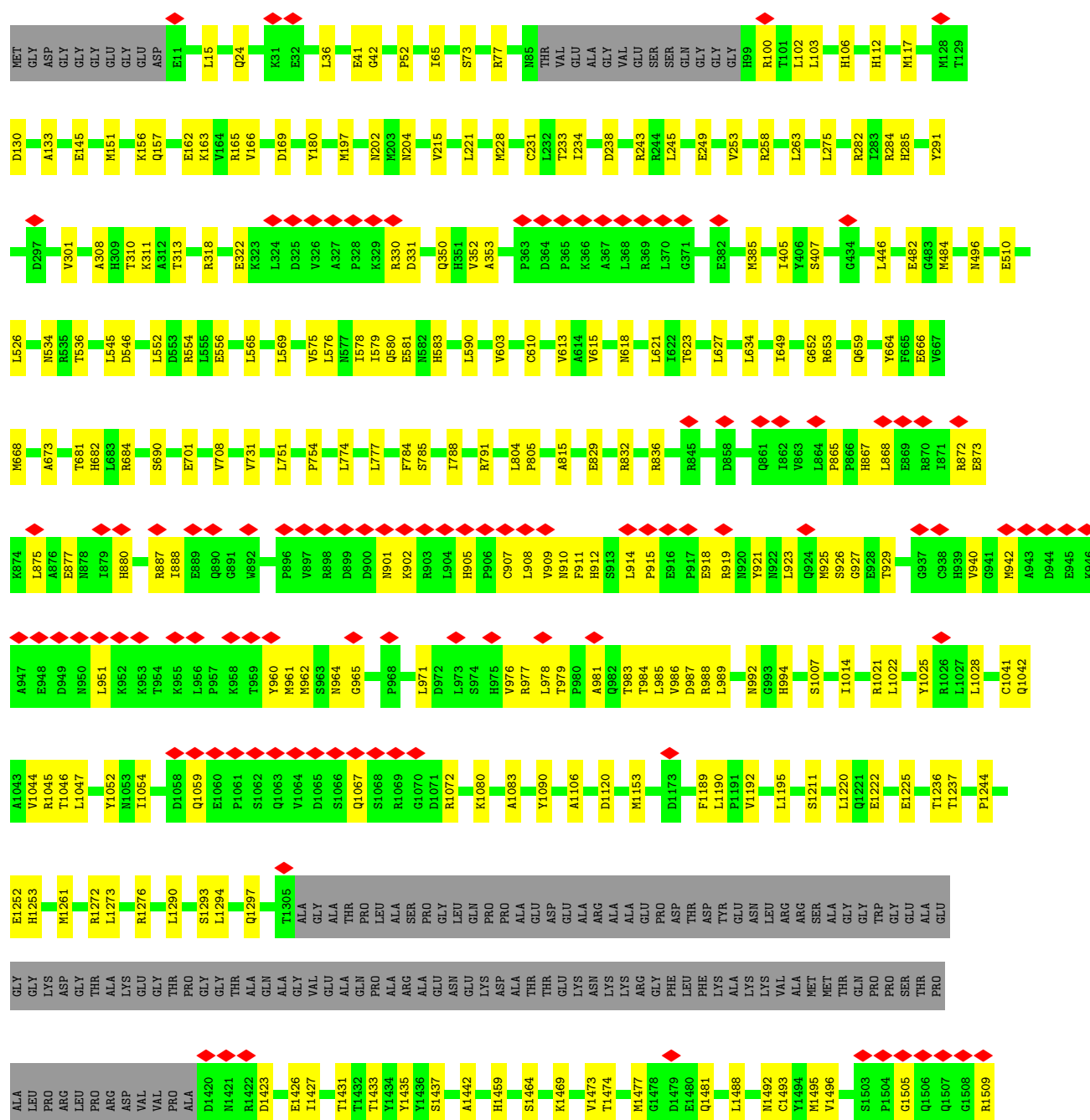








• Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, CFF, PCW, 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	E	0.19	0/847	0.34	0/1142
1	F	0.19	0/847	0.34	0/1142
1	G	0.19	0/847	0.33	0/1142
1	H	0.19	0/847	0.33	0/1142
2	I	0.17	0/739	0.49	0/992
2	J	0.21	0/739	0.53	0/992
2	K	0.17	0/739	0.49	0/992
2	L	0.21	0/739	0.53	0/992
2	M	0.17	0/739	0.49	0/992
2	N	0.21	0/739	0.53	0/992
2	O	0.18	0/739	0.49	0/992
2	P	0.21	0/739	0.53	0/992
3	A	0.20	0/35638	0.36	0/48272
3	B	0.20	0/35638	0.36	0/48272
3	C	0.20	0/35638	0.36	0/48272
3	D	0.20	0/35638	0.36	0/48272
All	All	0.20	0/151852	0.37	0/205592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	E	829	0	826	13	0
1	F	829	0	826	11	0
1	G	829	0	826	11	0
1	H	829	0	826	11	0
2	I	729	0	705	53	0
2	J	729	0	705	56	0
2	K	729	0	705	53	0
2	L	729	0	705	55	0
2	M	729	0	705	53	0
2	N	729	0	705	57	0
2	O	729	0	705	52	0
2	P	729	0	705	55	0
3	A	34849	0	34448	596	0
3	B	34849	0	34448	590	0
3	C	34849	0	34448	594	0
3	D	34849	0	34448	586	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
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	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	14	0	10	0	0
6	B	14	0	10	0	0
6	C	14	0	10	0	0
6	D	14	0	10	0	0
7	A	62	0	24	3	0
7	B	62	0	24	4	0
7	C	62	0	24	4	0
7	D	62	0	24	4	0
8	A	108	0	167	6	0
8	B	108	0	167	5	0
8	C	108	0	167	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	108	0	167	5	0
All	All	149304	0	147540	2692	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 9.

The worst 5 of 2692 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:GLU:OE2	3:A:2694:GLN:NE2	1.72	1.23
3:C:2694:GLN:NE2	2:M:10:GLU:OE2	1.72	1.23
3:D:2694:GLN:NE2	2:O:10:GLU:OE2	1.72	1.22
3:B:2694:GLN:NE2	2:K:10:GLU:OE2	1.72	1.21
3:A:875:LEU:HD11	3:A:1047:LEU:HD21	1.41	1.02

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	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
1	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
1	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	I	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	J	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	K	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	L	91/94 (97%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	N	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	O	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	P	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
3	A	4351/5035 (86%)	4238 (97%)	113 (3%)	0	100	100
3	B	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
3	C	4351/5035 (86%)	4241 (98%)	110 (2%)	0	100	100
3	D	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
All	All	18552/21324 (87%)	18032 (97%)	520 (3%)	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	E	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	I	80/81 (99%)	80 (100%)	0	100	100
2	J	80/81 (99%)	80 (100%)	0	100	100
2	K	80/81 (99%)	80 (100%)	0	100	100
2	L	80/81 (99%)	80 (100%)	0	100	100
2	M	80/81 (99%)	80 (100%)	0	100	100
2	N	80/81 (99%)	80 (100%)	0	100	100
2	O	80/81 (99%)	80 (100%)	0	100	100
2	P	80/81 (99%)	80 (100%)	0	100	100
3	A	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
3	C	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
3	D	3811/4296 (89%)	3809 (100%)	2 (0%)	88	87
All	All	16240/18192 (89%)	16232 (100%)	8 (0%)	100	100

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5011	MET
3	C	3757	GLU
3	B	3757	GLU
3	A	5011	MET
3	B	5011	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1042	GLN
2	L	87	ASN
3	C	1430	ASN
3	C	3147	HIS
3	A	1430	ASN

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 44 ligands modelled in this entry, 24 are monoatomic - leaving 20 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
8	PCW	C	5107	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
8	PCW	A	8007	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
7	ATP	B	8003	-	32,33,33	0.54	0	48,52,52	0.55	0
6	CFF	A	8002	-	15,15,15	0.32	0	23,23,23	0.46	0
8	PCW	B	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	B	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	A	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	A	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	D	8007	-	53,53,53	1.17	4 (7%)	59,61,61	2.30	9 (15%)
8	PCW	D	8006	-	53,53,53	1.16	5 (9%)	59,61,61	2.35	9 (15%)
7	ATP	C	5106	-	32,33,33	0.27	0	48,52,52	0.68	0
8	PCW	B	8007	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
6	CFF	D	8002	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	A	8003	-	32,33,33	0.53	0	48,52,52	0.54	0
6	CFF	C	5103	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	D	8005	-	32,33,33	0.27	0	48,52,52	0.68	0
7	ATP	C	5104	-	32,33,33	0.54	0	48,52,52	0.55	0
8	PCW	C	5101	-	53,53,53	1.17	5 (9%)	59,61,61	2.30	9 (15%)
6	CFF	B	8002	-	15,15,15	0.33	0	23,23,23	0.46	0
7	ATP	D	8003	-	32,33,33	0.53	0	48,52,52	0.55	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
8	PCW	C	5107	-	-	21/57/57/57	-
8	PCW	A	8007	-	-	19/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	8003	-	-	6/22/38/38	0/3/3/3
6	CFF	A	8002	-	-	-	0/2/2/2
8	PCW	B	8006	-	-	21/57/57/57	-
7	ATP	B	8005	-	-	6/22/38/38	0/3/3/3
8	PCW	A	8006	-	-	21/57/57/57	-
7	ATP	A	8005	-	-	6/22/38/38	0/3/3/3
8	PCW	D	8007	-	-	19/57/57/57	-
8	PCW	D	8006	-	-	21/57/57/57	-
7	ATP	C	5106	-	-	6/22/38/38	0/3/3/3
8	PCW	B	8007	-	-	19/57/57/57	-
6	CFF	D	8002	-	-	-	0/2/2/2
7	ATP	A	8003	-	-	6/22/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
7	ATP	D	8005	-	-	6/22/38/38	0/3/3/3
7	ATP	C	5104	-	-	6/22/38/38	0/3/3/3
8	PCW	C	5101	-	-	19/57/57/57	-
6	CFF	B	8002	-	-	-	0/2/2/2
7	ATP	D	8003	-	-	6/22/38/38	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	8006	PCW	O3-C11	3.07	1.42	1.33
8	A	8006	PCW	O3-C11	3.07	1.42	1.33
8	B	8006	PCW	O3-C11	3.07	1.42	1.33
8	C	5107	PCW	O3-C11	3.07	1.42	1.33
8	A	8007	PCW	O3-C11	3.03	1.42	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	8006	PCW	C8-N-C6	11.60	139.44	108.98
8	C	5107	PCW	C8-N-C6	11.60	139.44	108.98
8	D	8006	PCW	C8-N-C6	11.59	139.42	108.98
8	B	8006	PCW	C8-N-C6	11.59	139.42	108.98
8	B	8007	PCW	C8-N-C6	10.98	137.81	108.98

There are no chirality outliers.

5 of 208 torsion outliers are listed below:

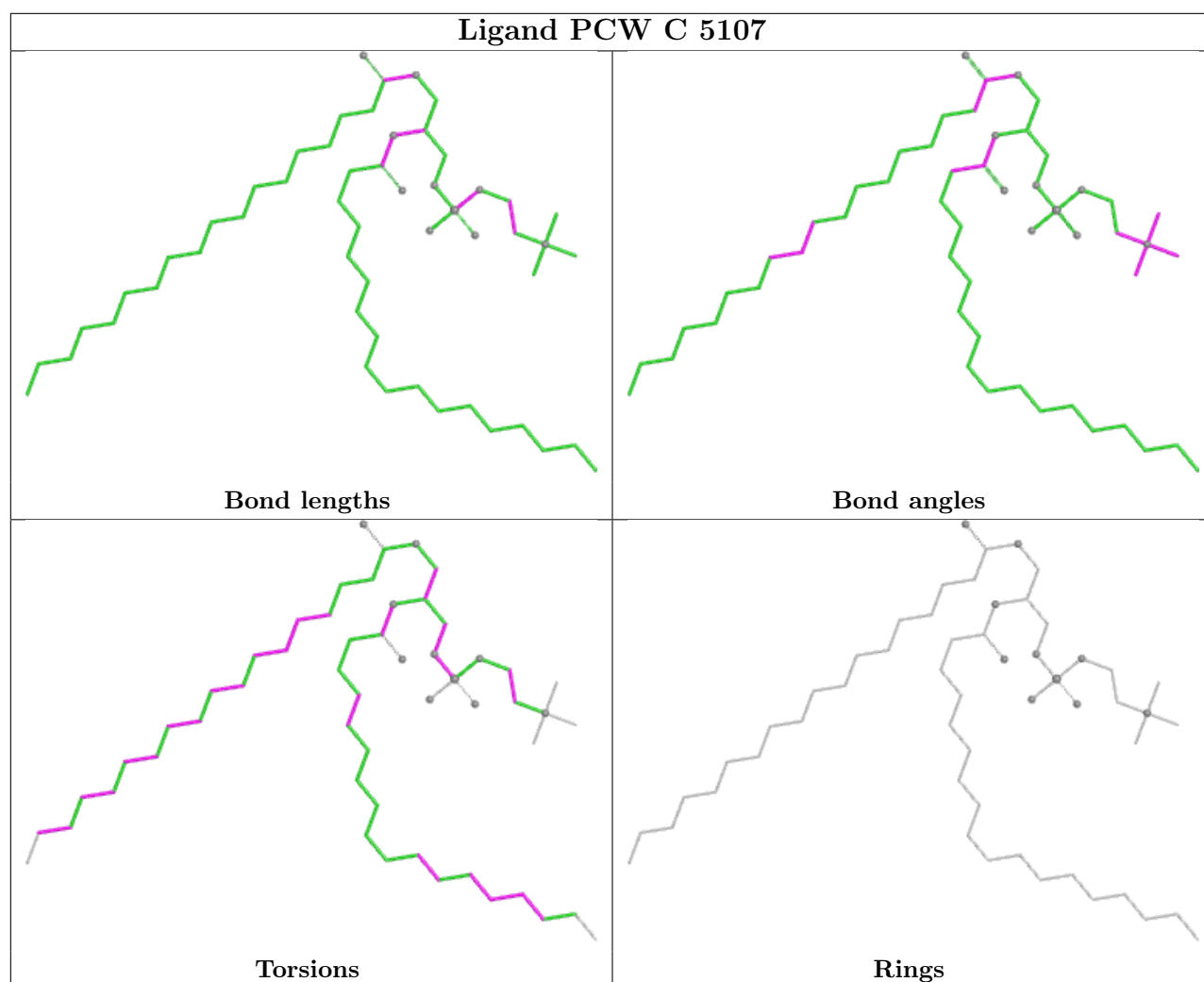
Mol	Chain	Res	Type	Atoms
7	D	8003	ATP	C5'-O5'-PA-O1A
7	D	8003	ATP	C5'-O5'-PA-O3A
7	D	8005	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O3A

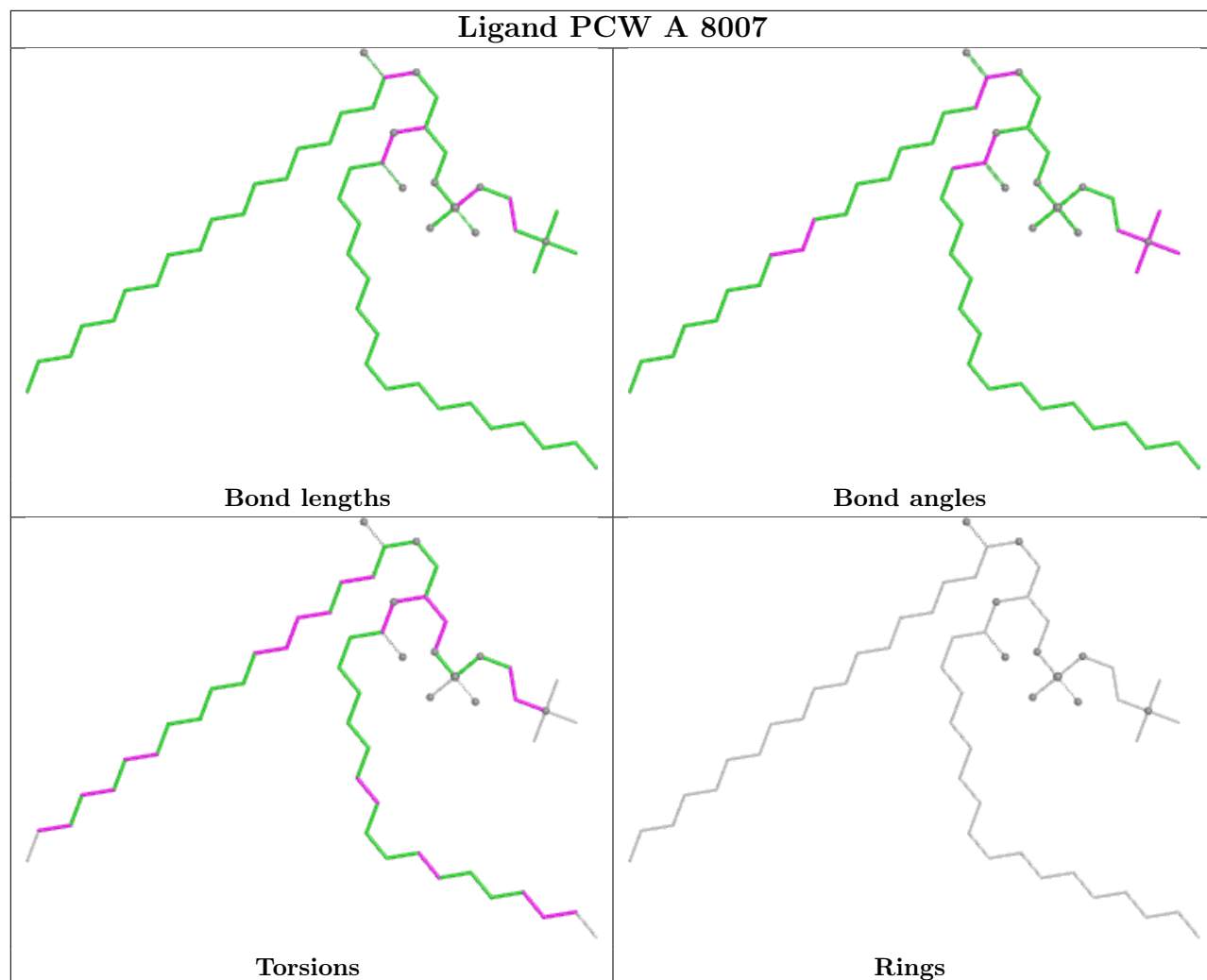
There are no ring outliers.

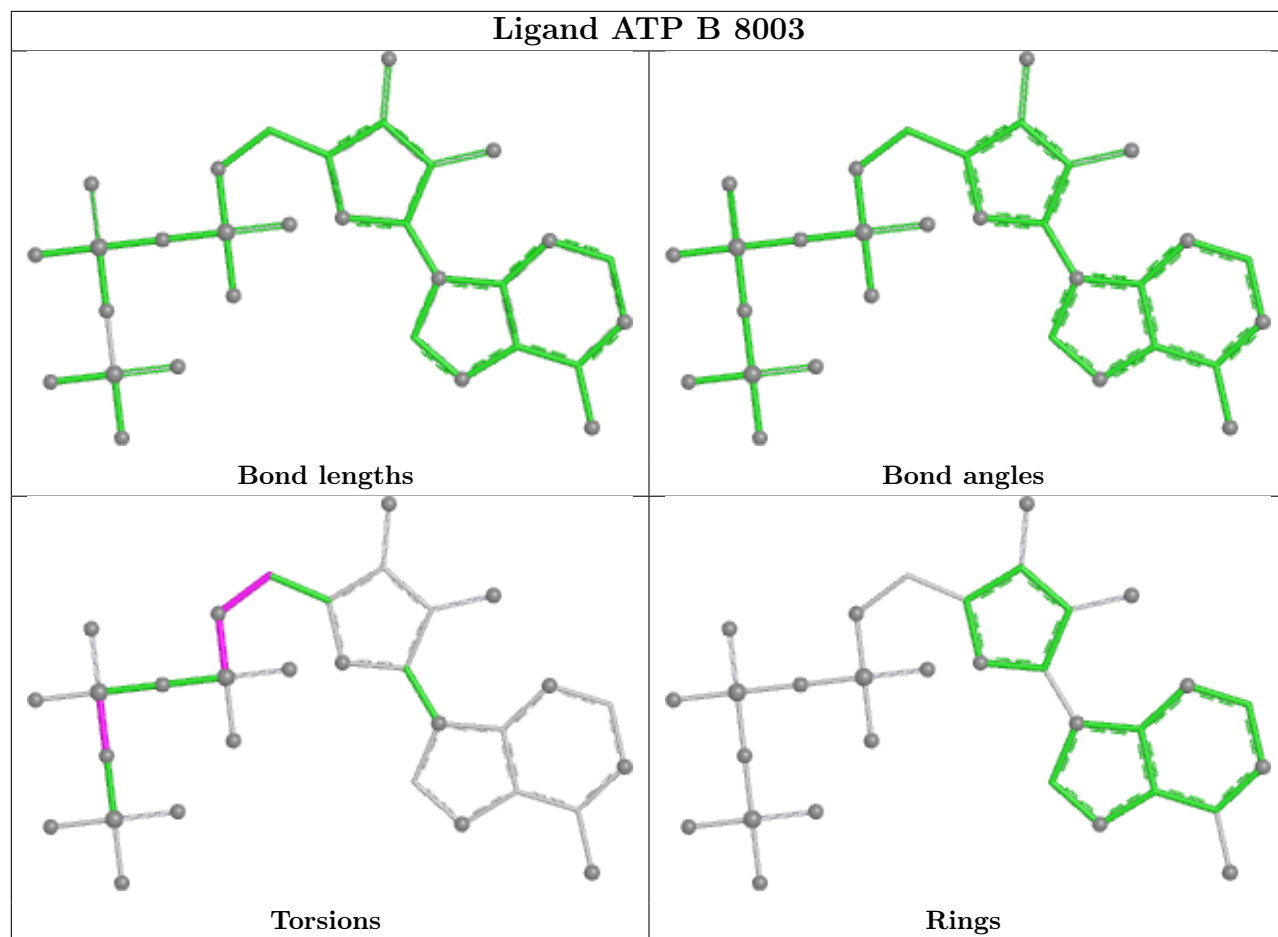
12 monomers are involved in 31 short contacts:

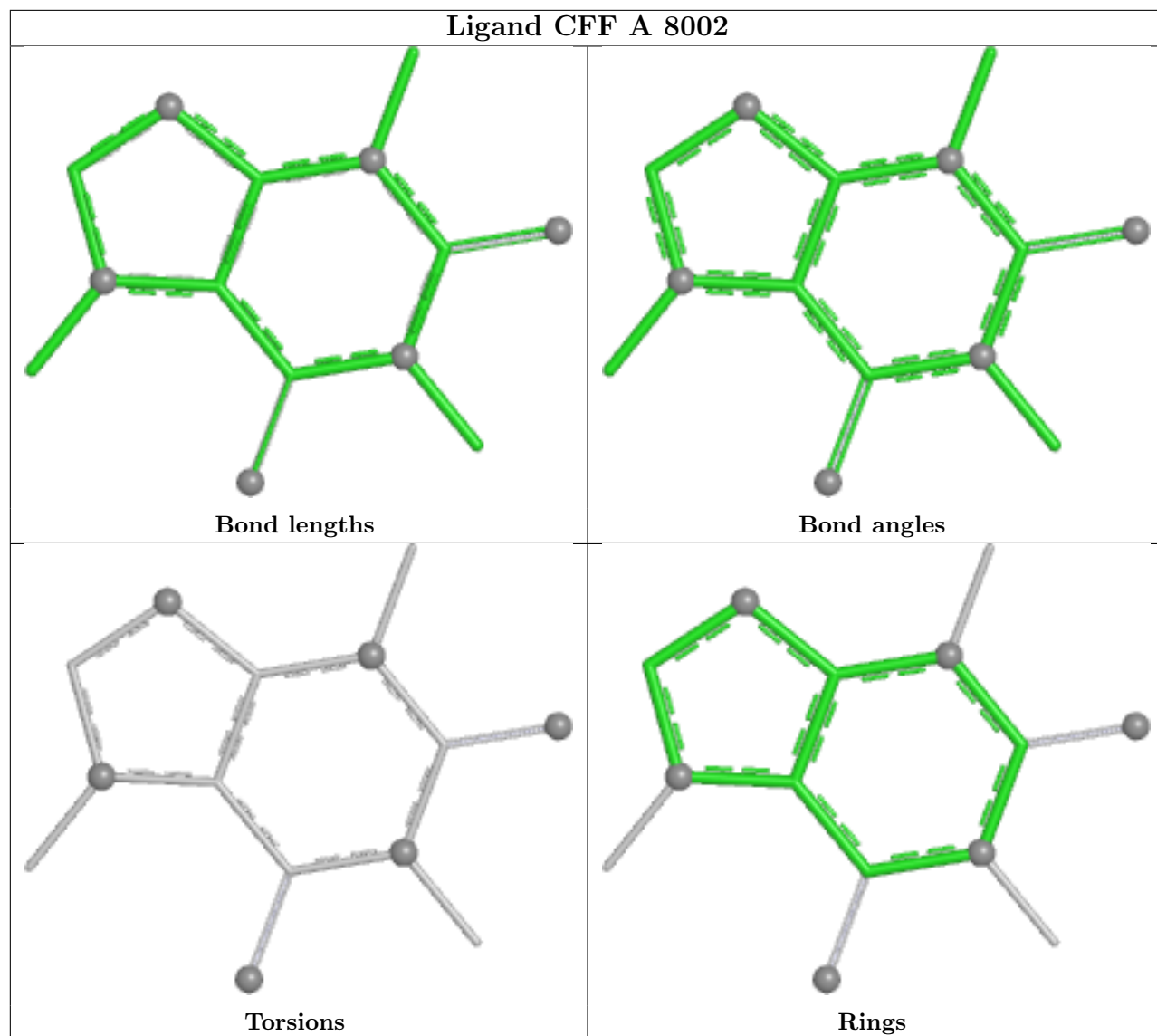
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5107	PCW	1	0
8	A	8007	PCW	4	0
8	B	8006	PCW	1	0
7	B	8005	ATP	4	0
8	A	8006	PCW	2	0
7	A	8005	ATP	3	0
8	D	8007	PCW	4	0
8	D	8006	PCW	1	0
7	C	5106	ATP	4	0
8	B	8007	PCW	4	0
7	D	8005	ATP	4	0
8	C	5101	PCW	3	0

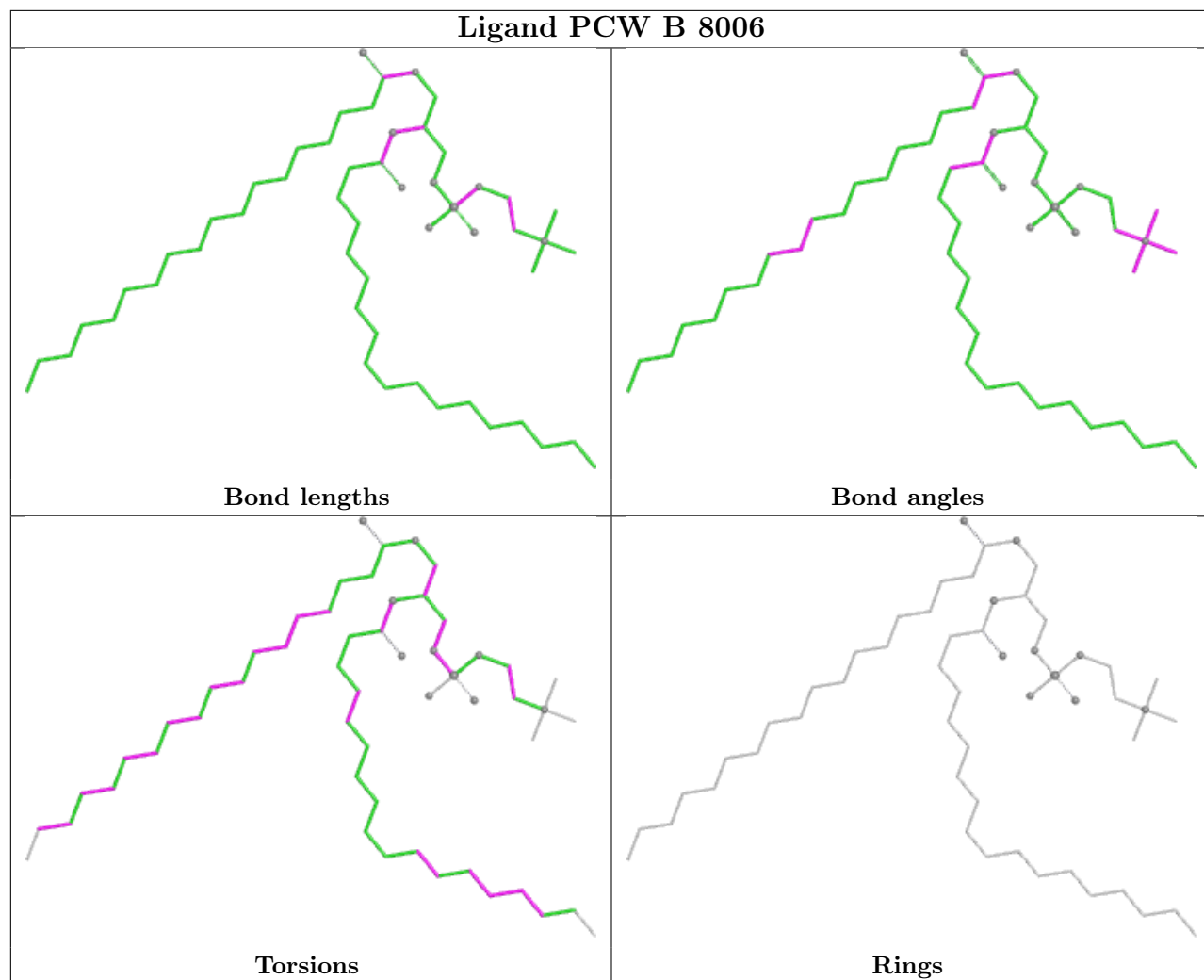
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

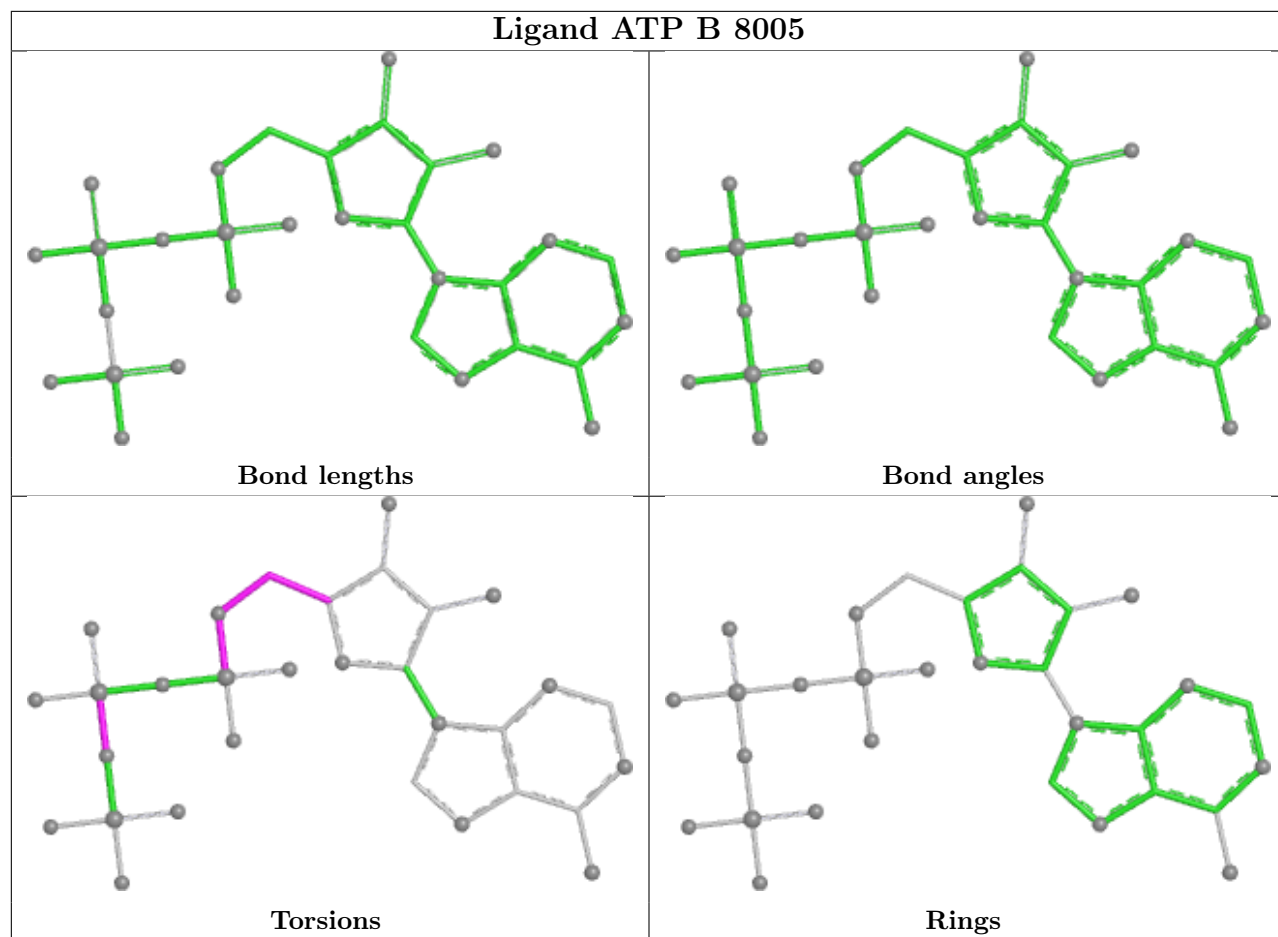


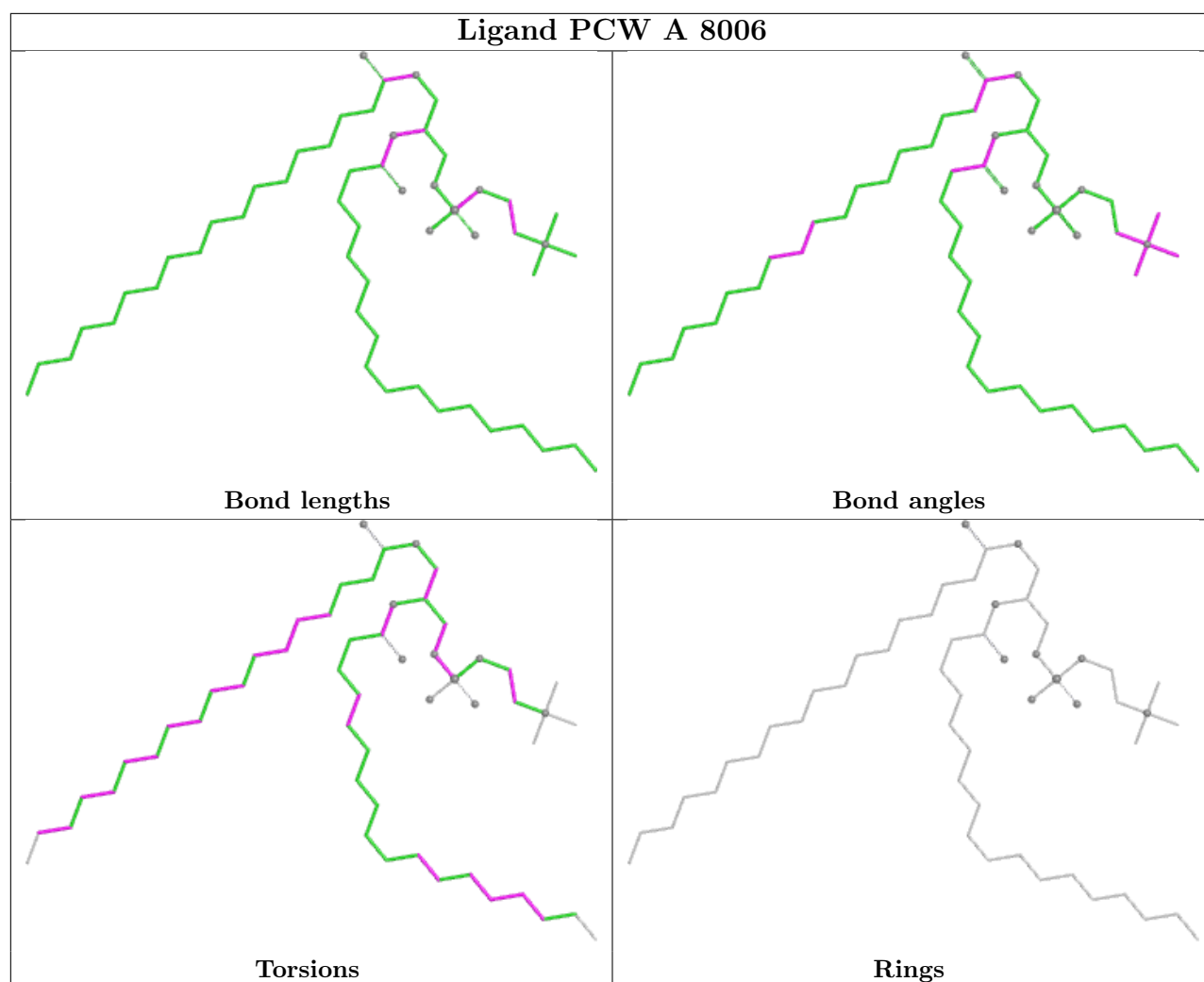


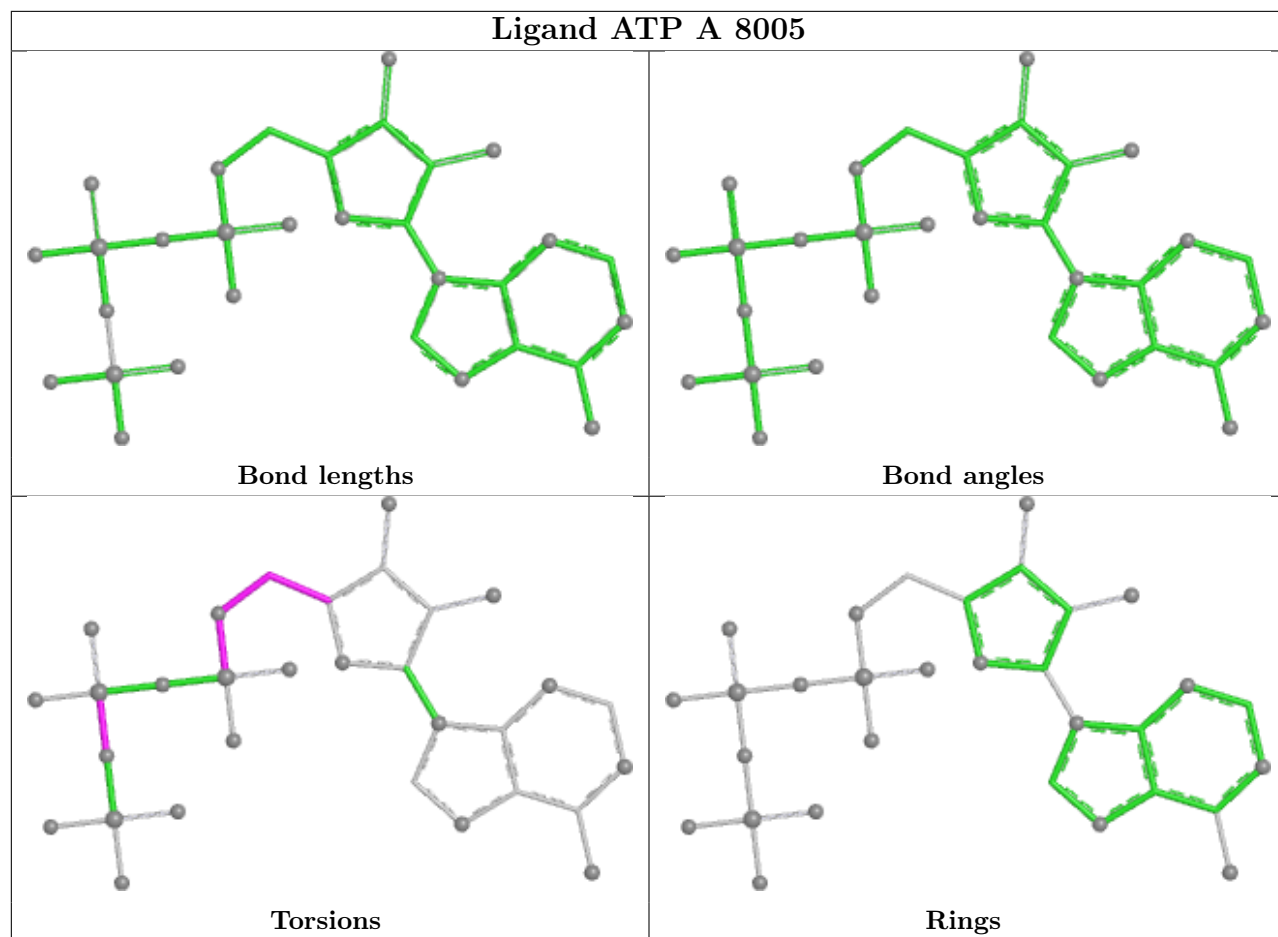


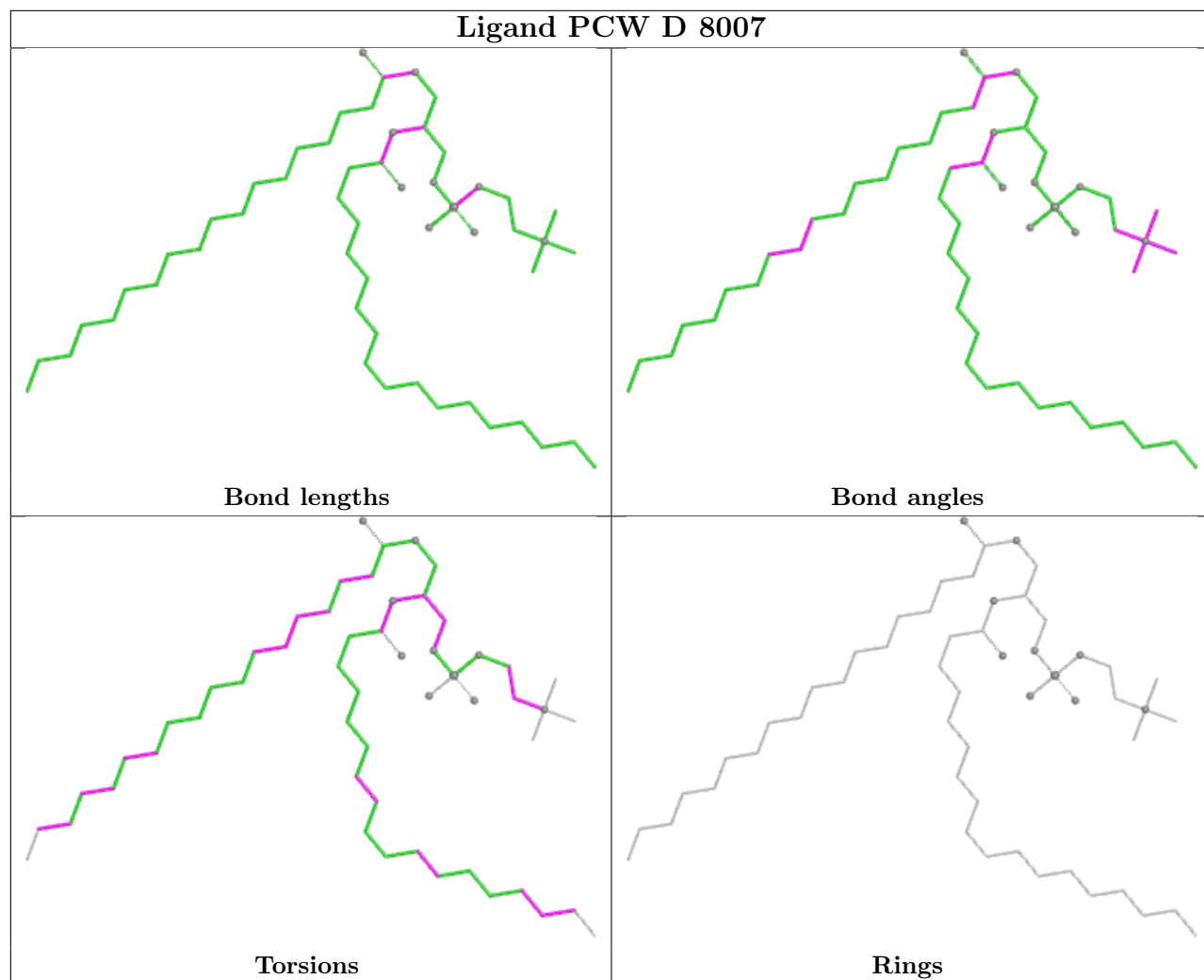


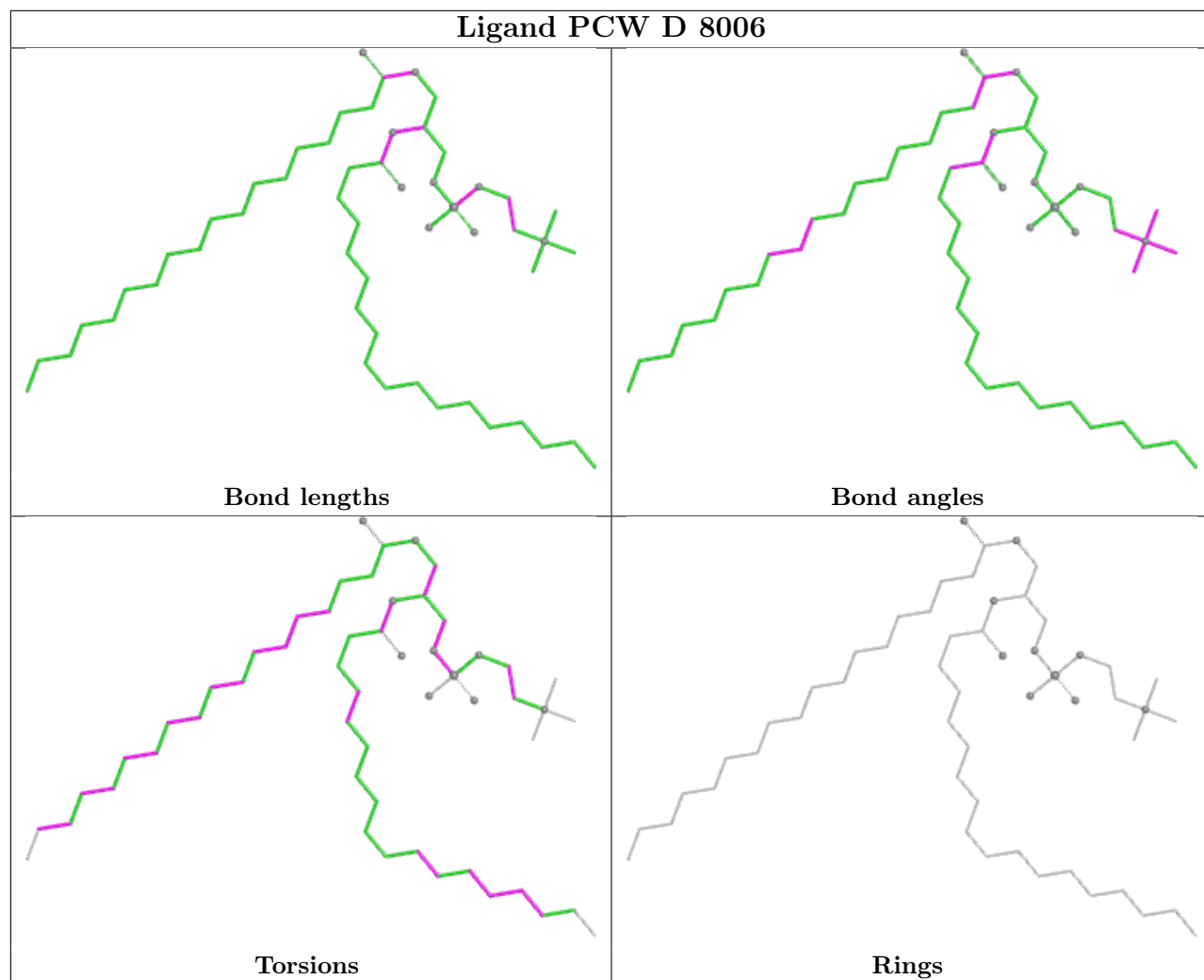


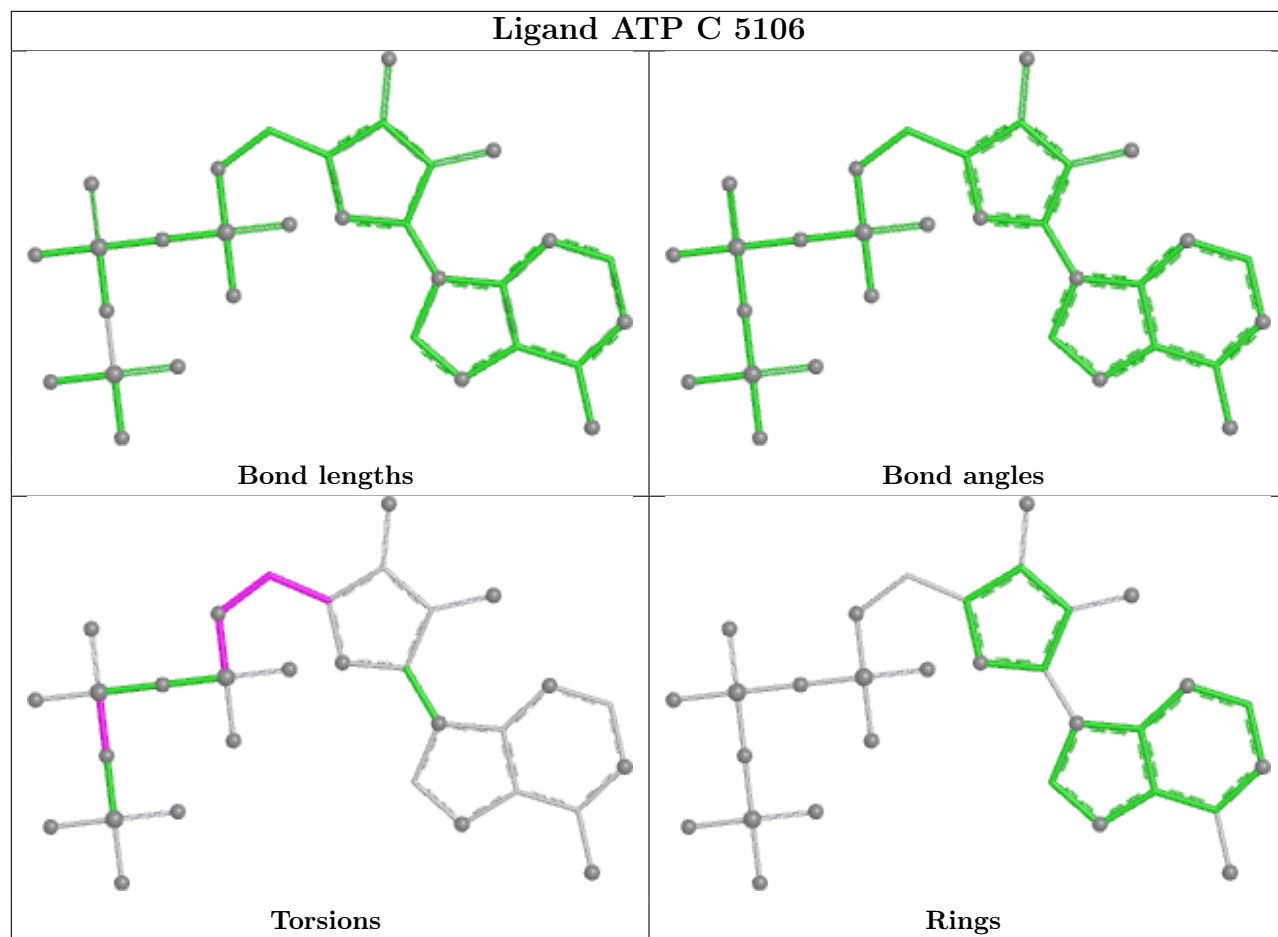


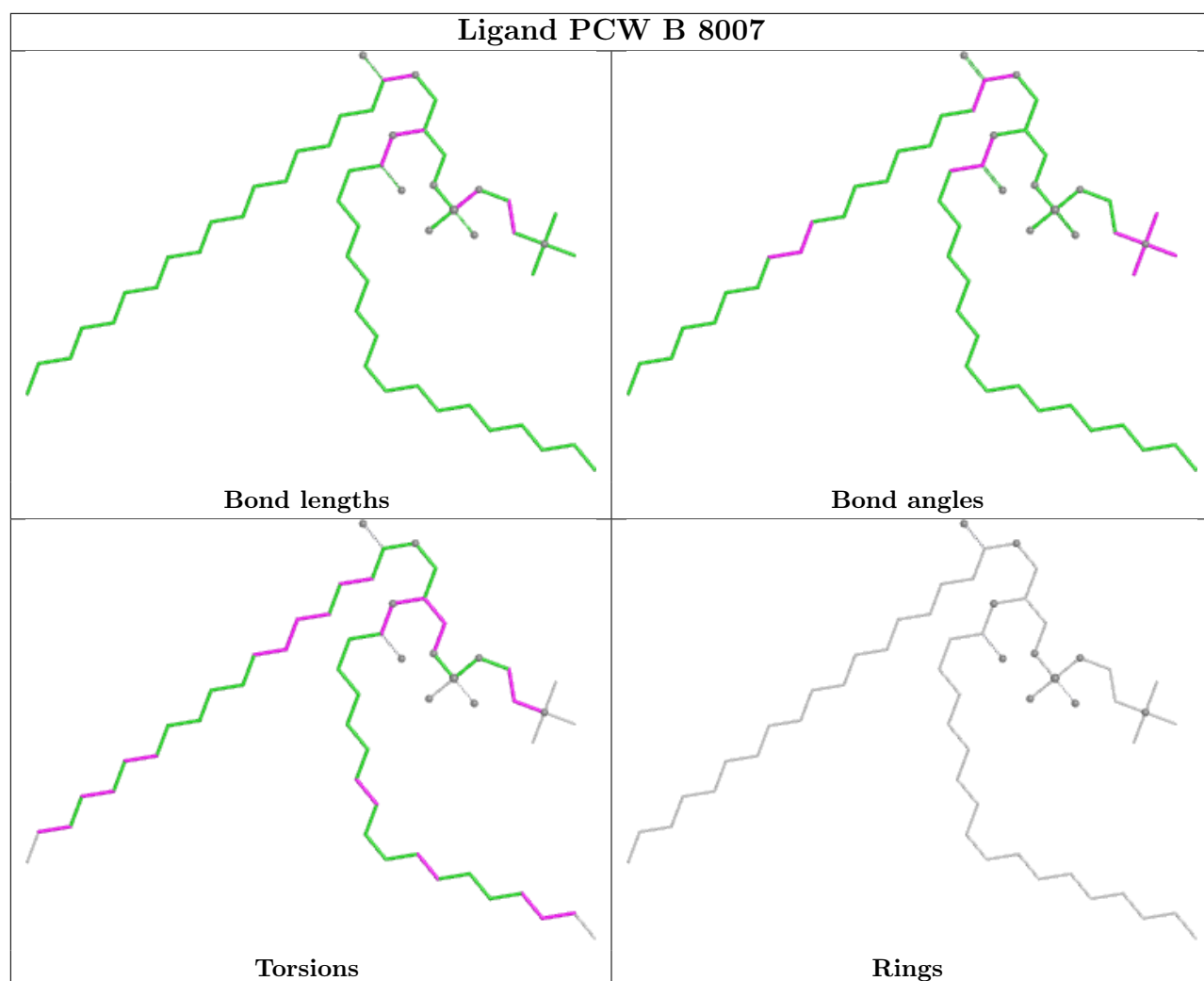


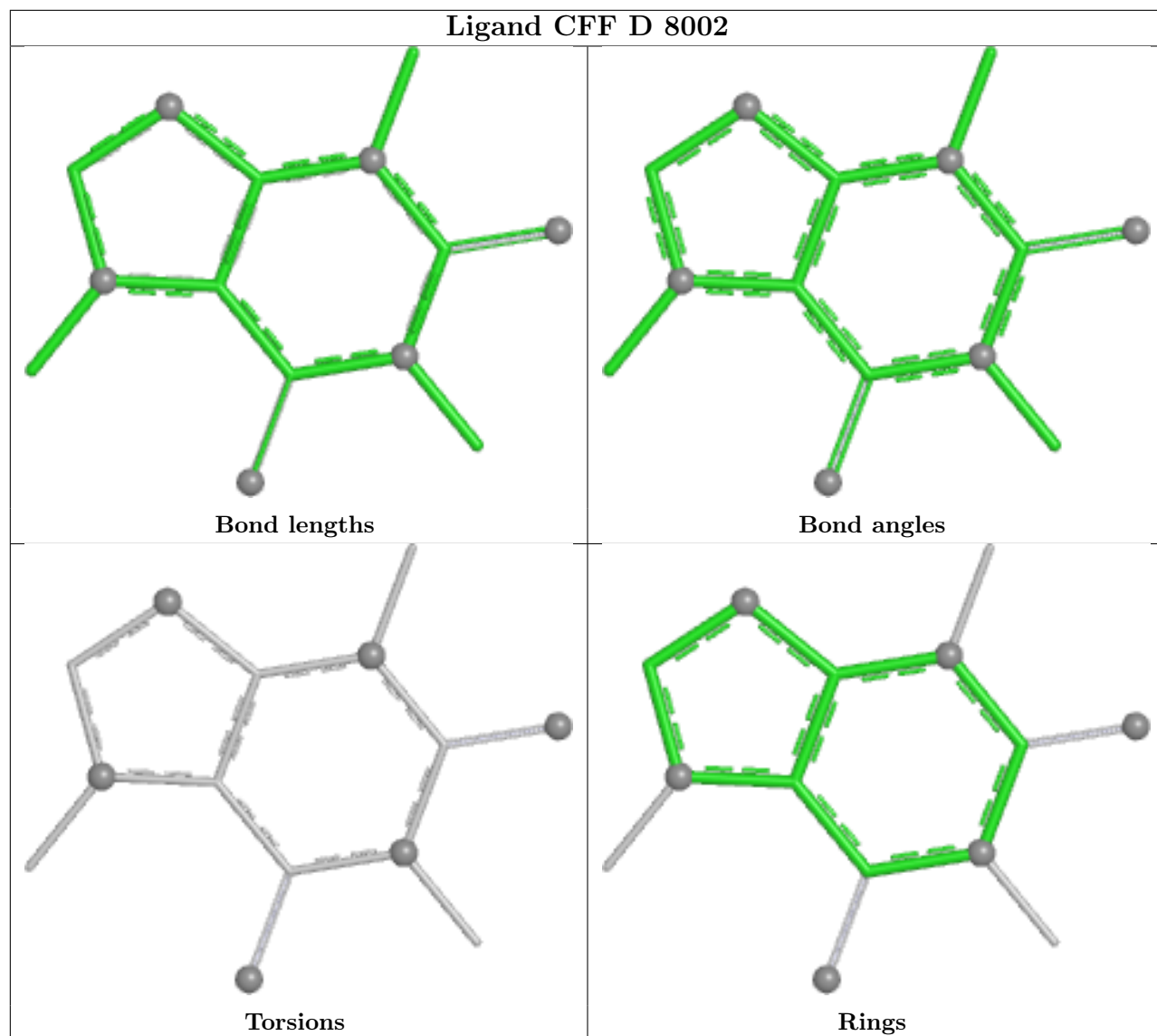


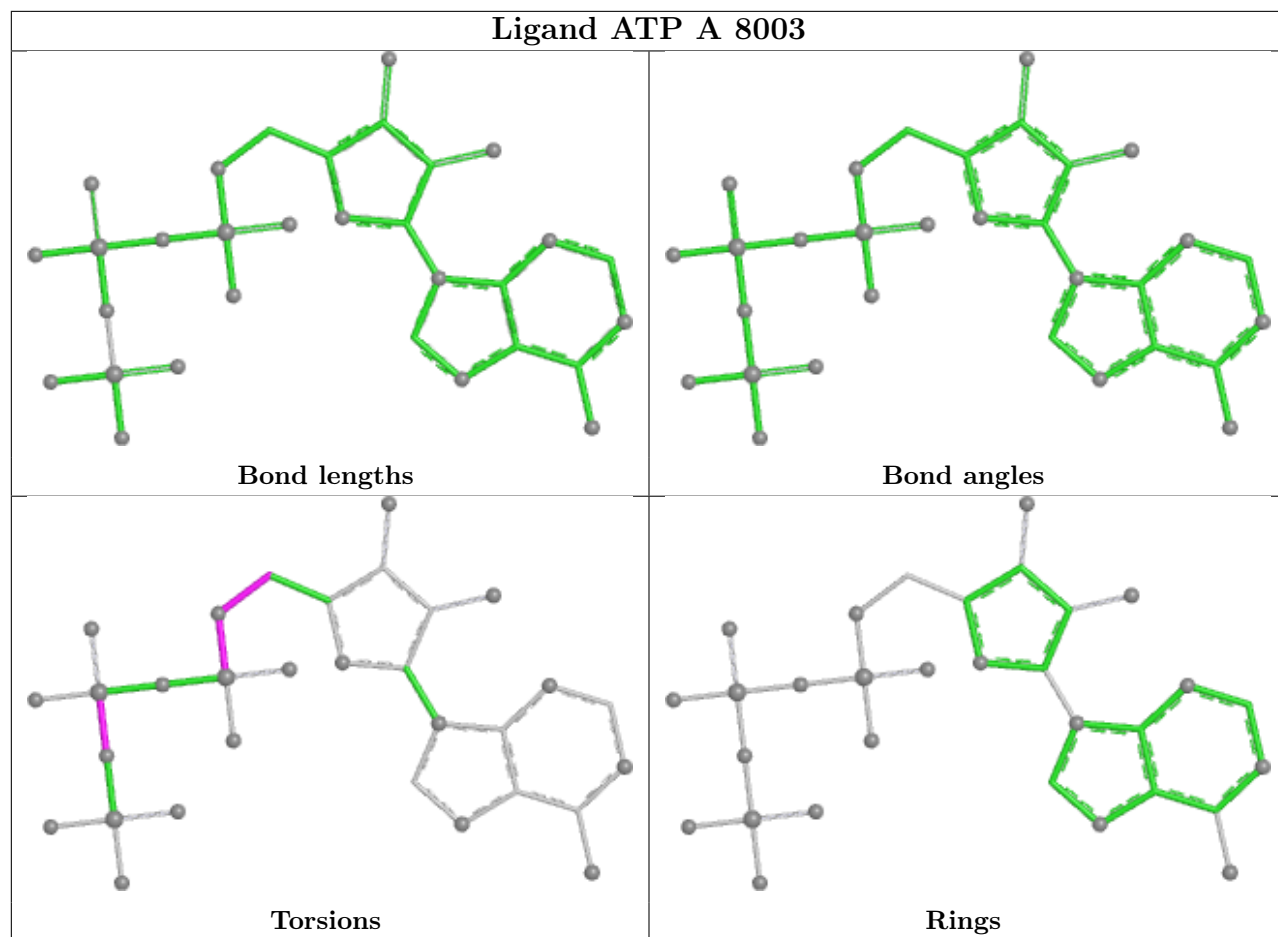


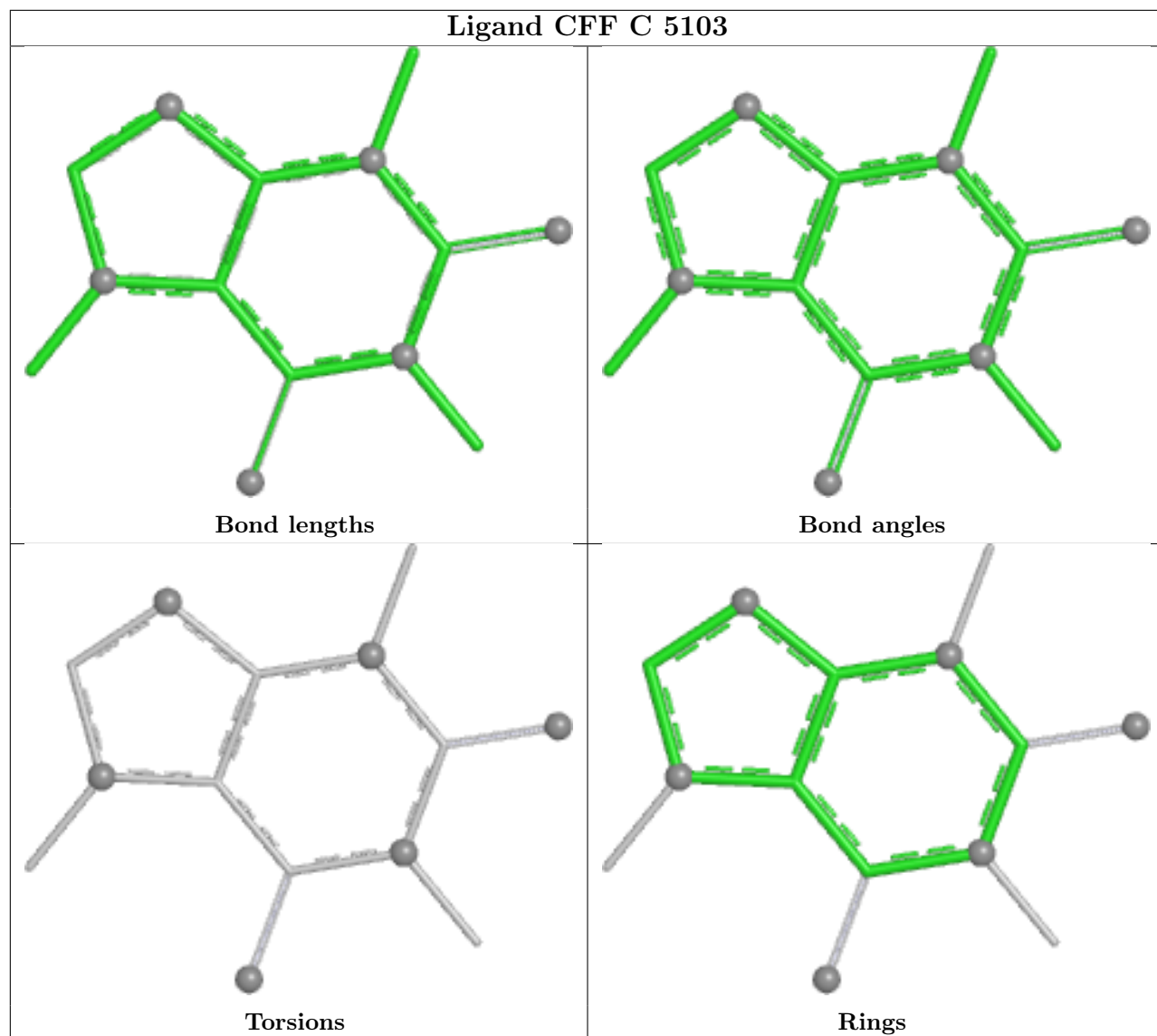


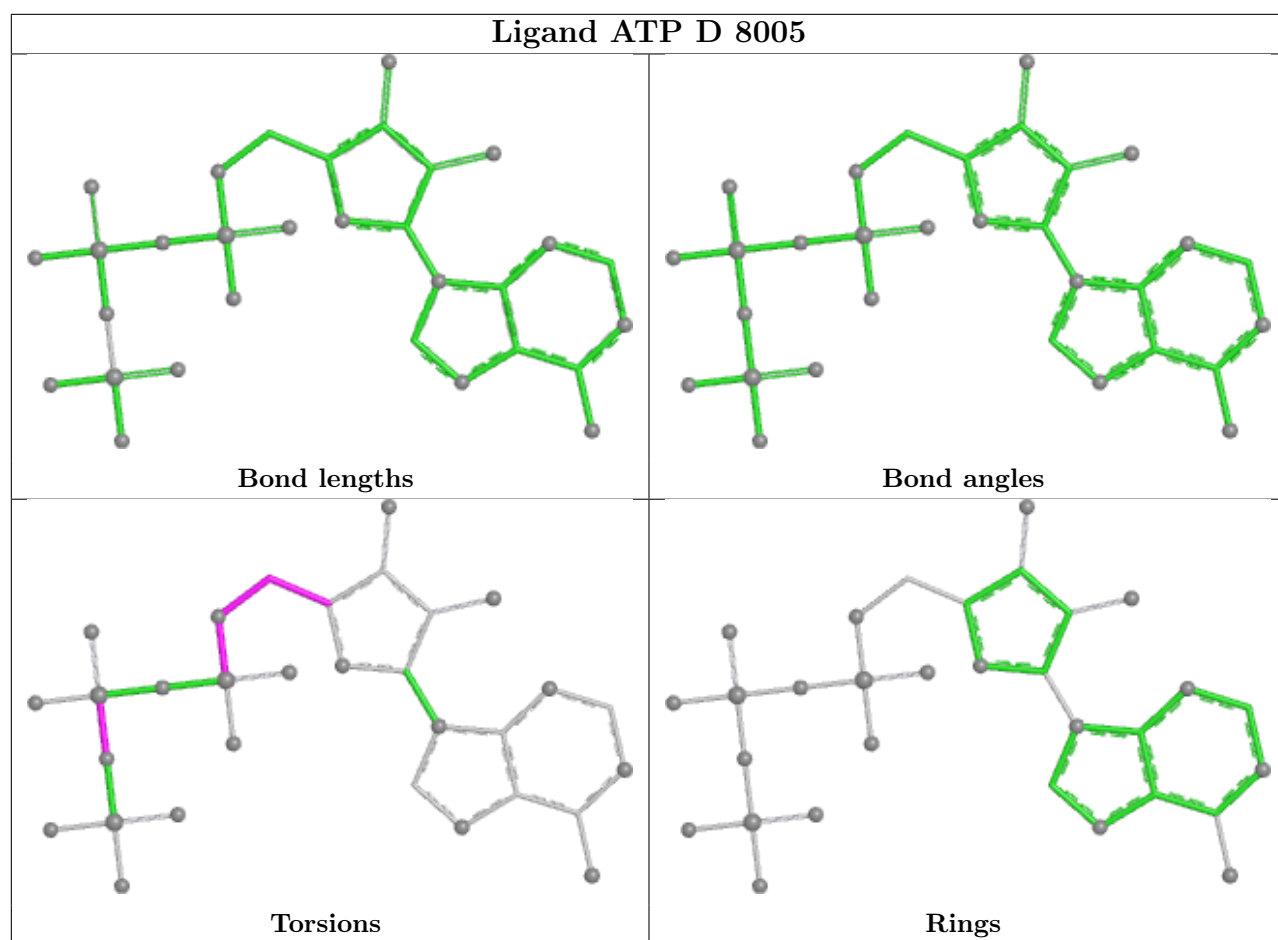


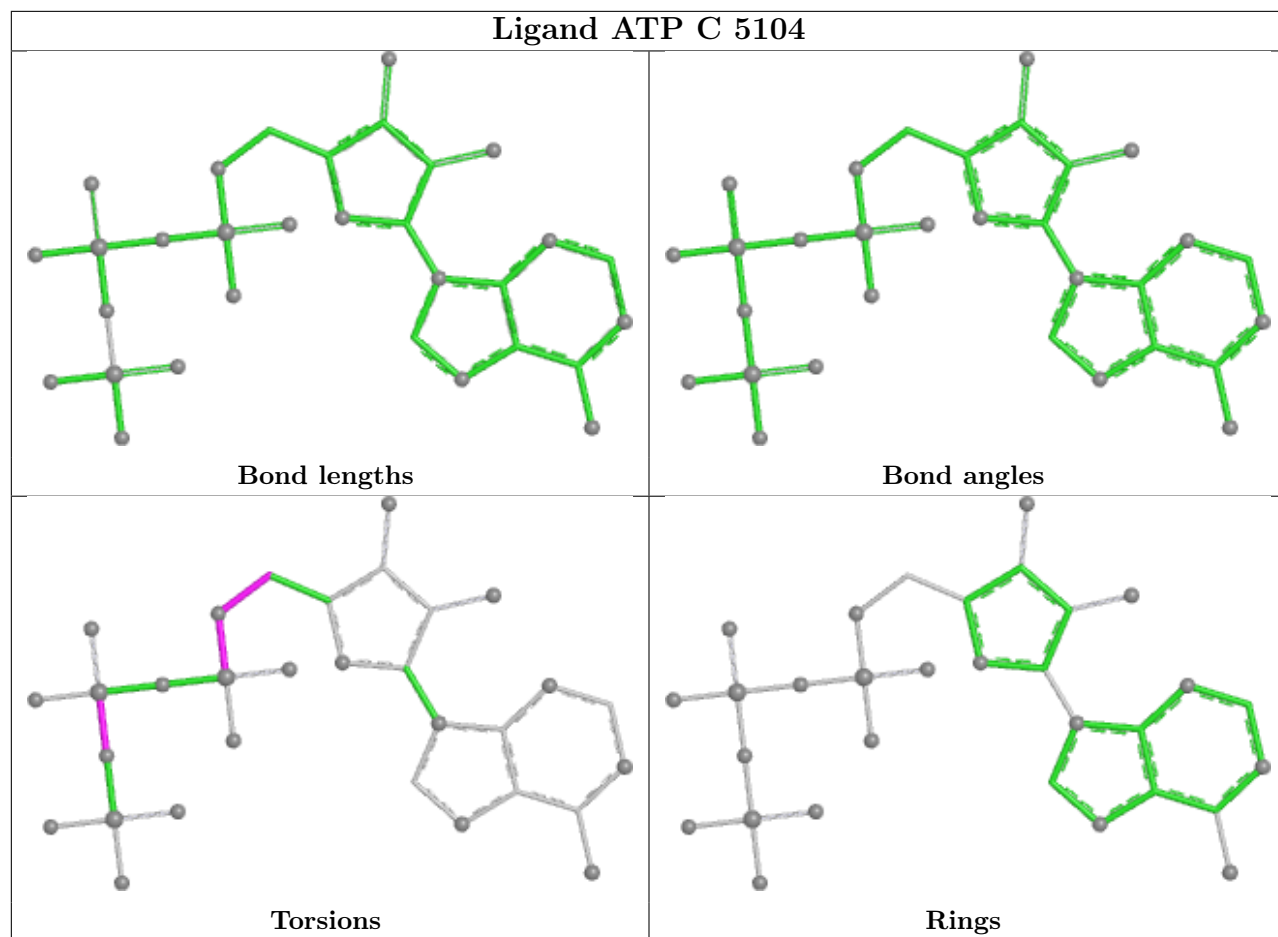


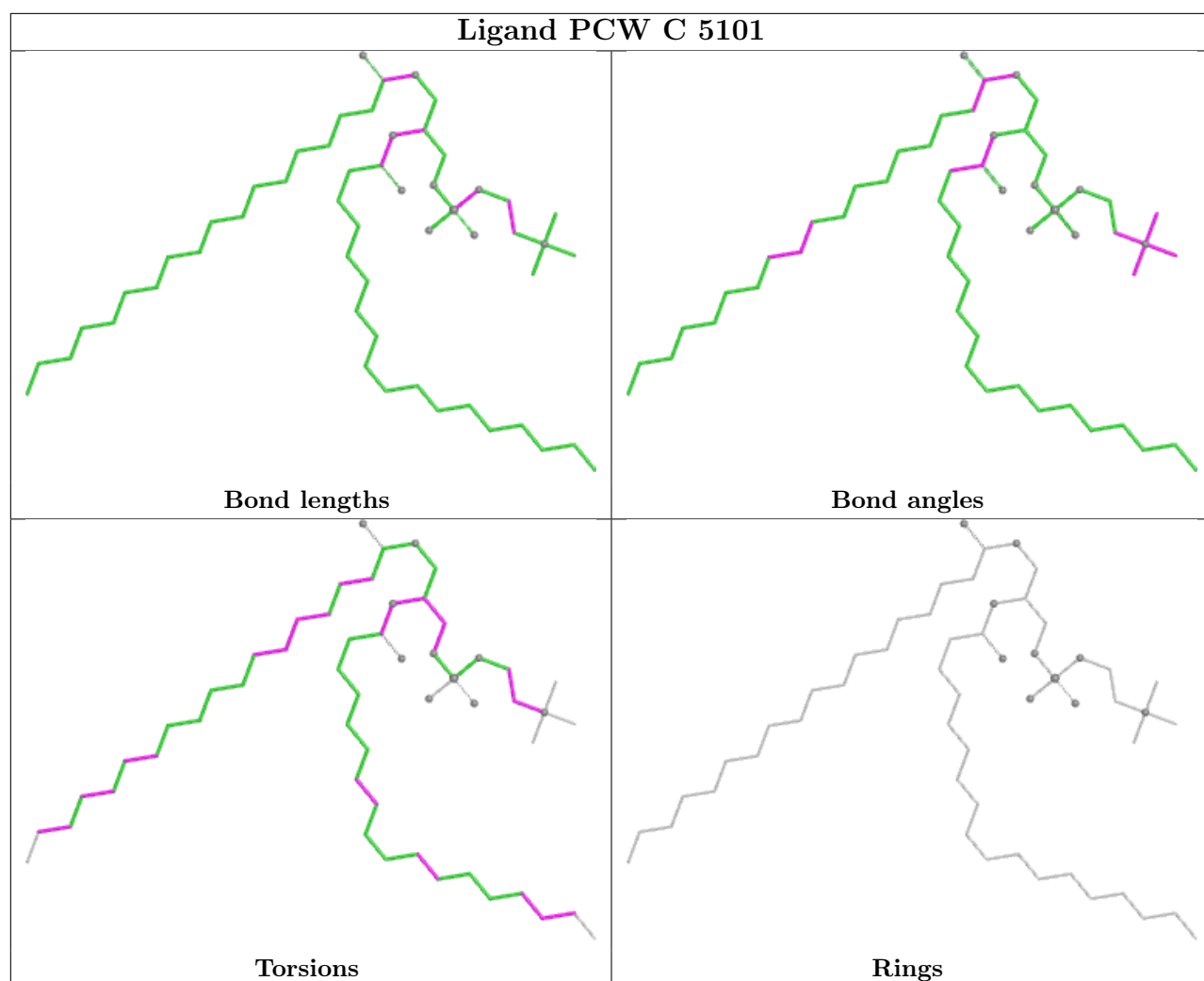


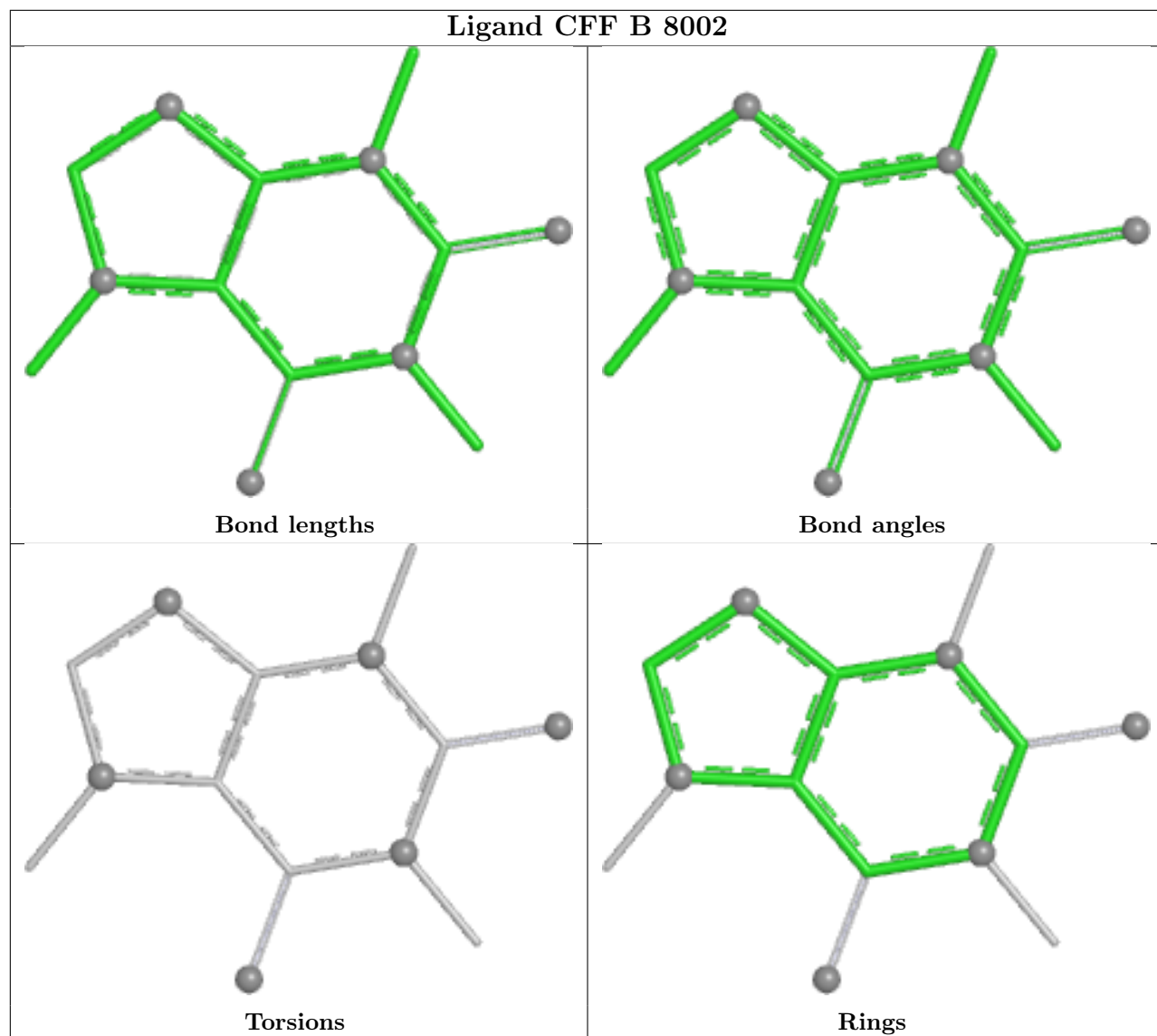


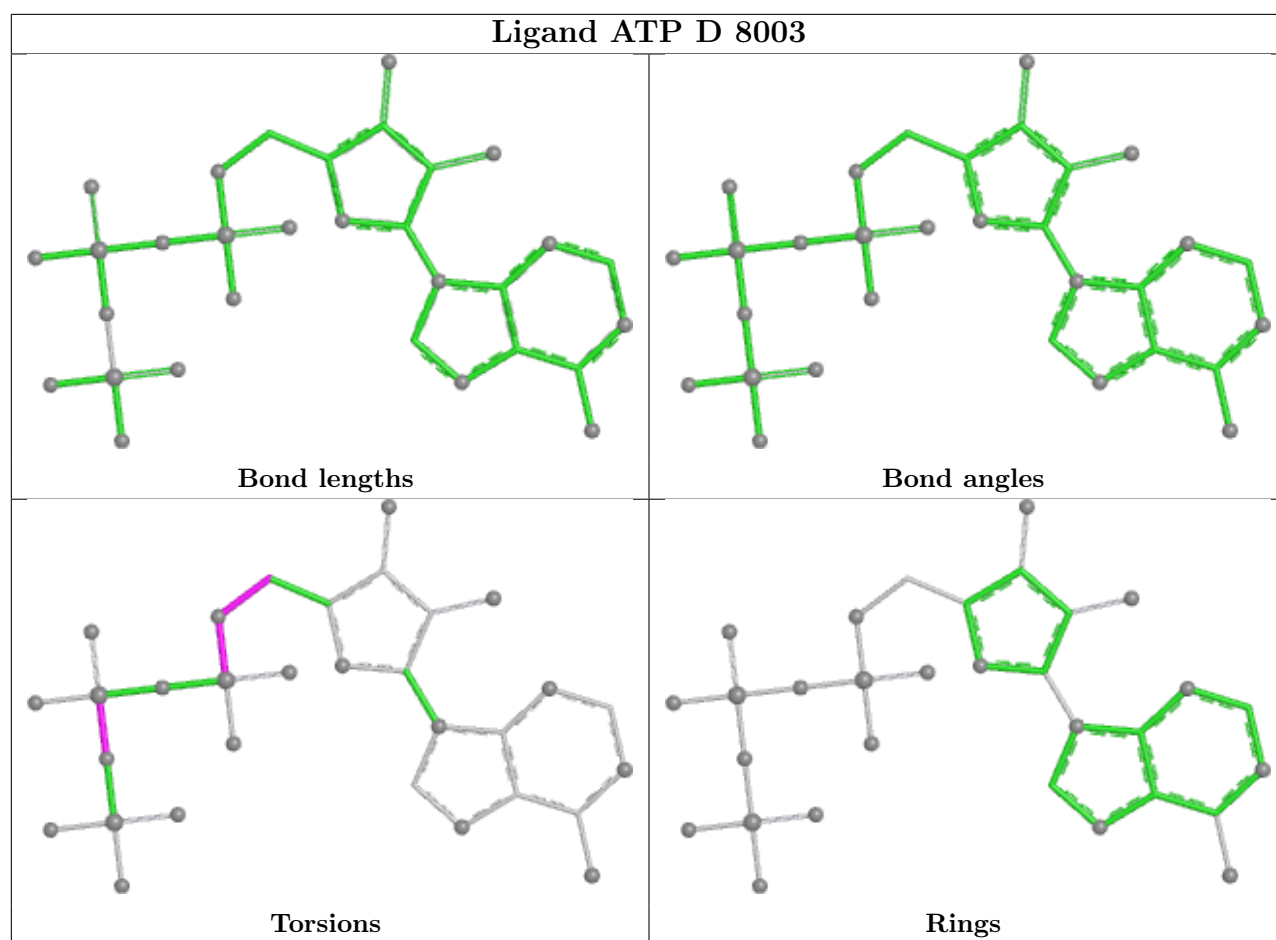












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

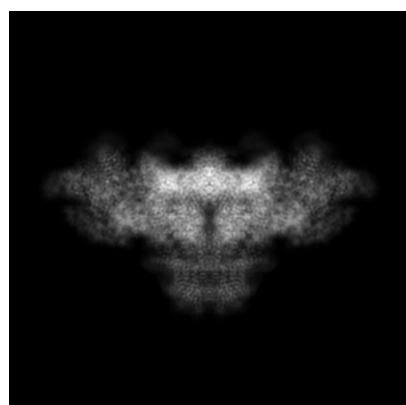
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43304. These allow visual inspection of the internal detail of the map and identification of artifacts.

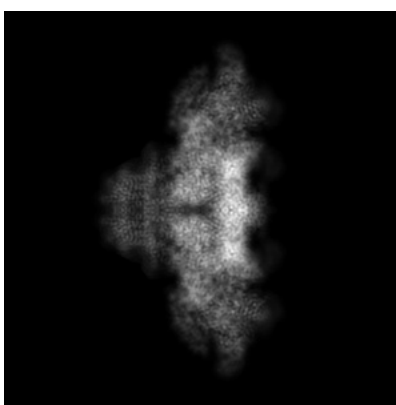
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

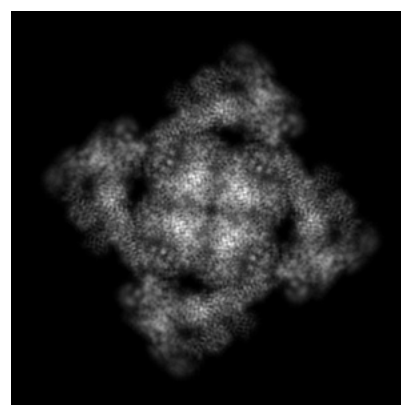
6.1.1 Primary map



X



Y



Z

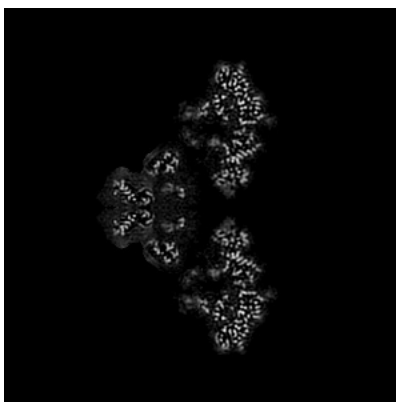
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

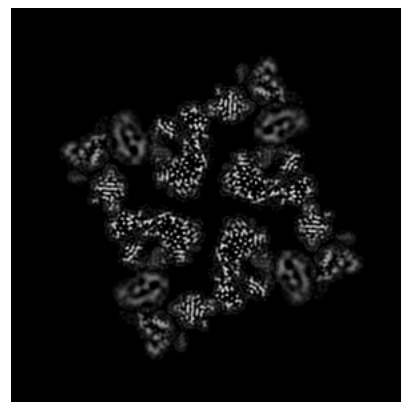
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

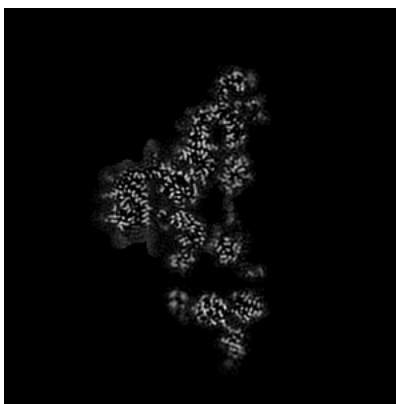
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

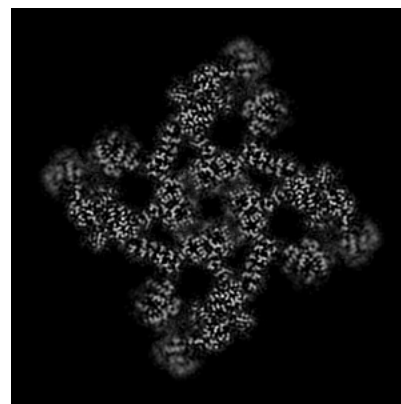
6.3.1 Primary map



X Index: 274



Y Index: 274

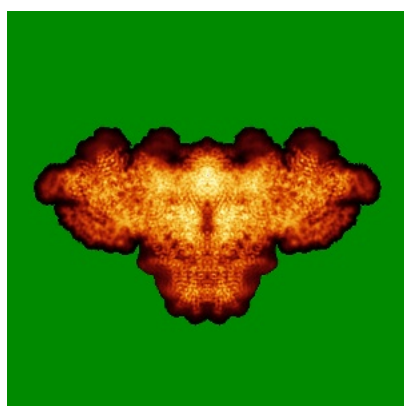


Z Index: 285

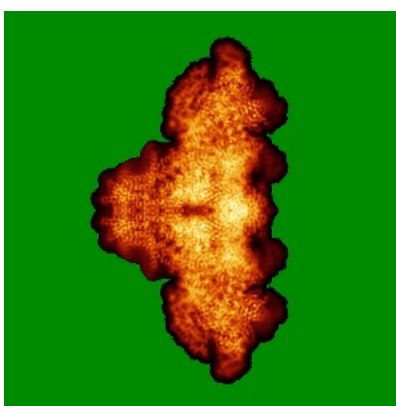
The images above show the largest variance slices of the map in three orthogonal directions.

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

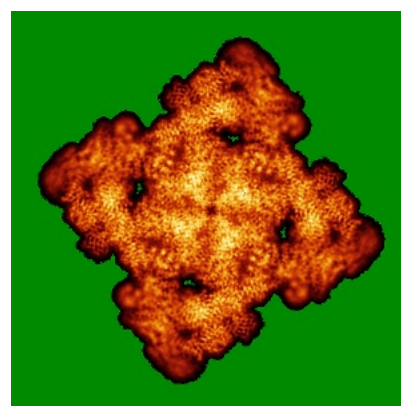
6.4.1 Primary map



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

This section was not generated.

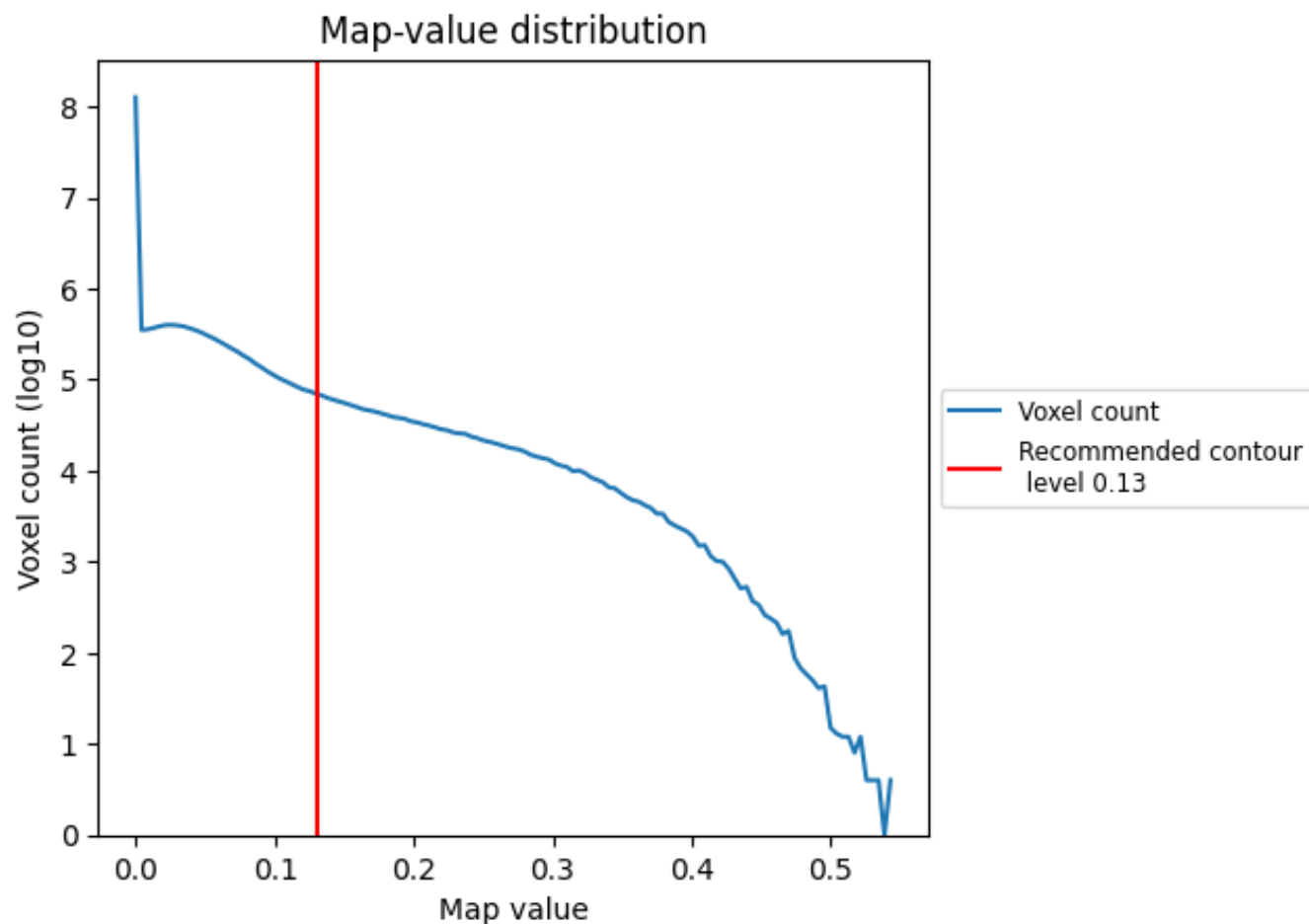
6.6 Mask visualisation

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

7 Map analysis [i](#)

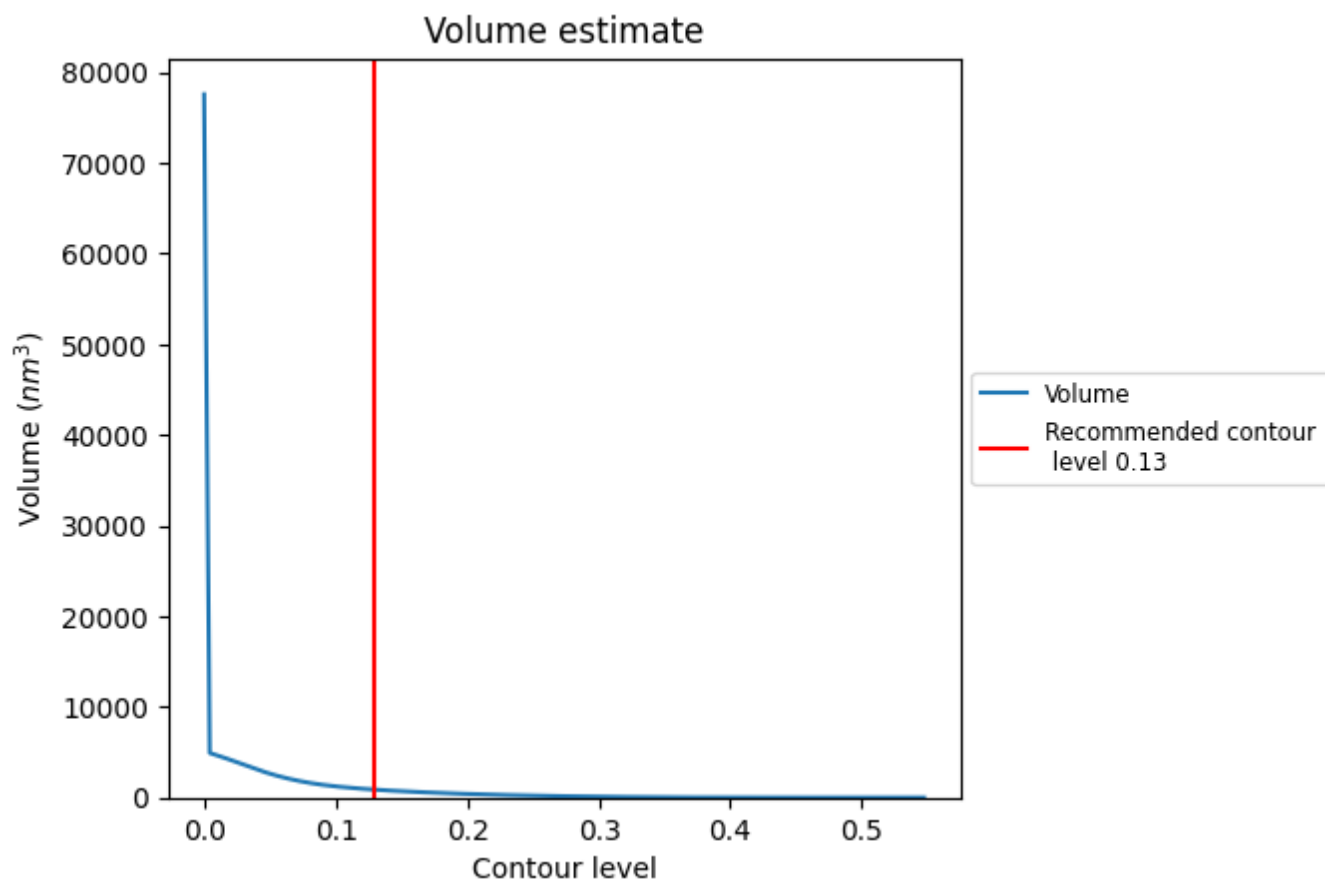
This section contains the results of statistical analysis of the map.

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.

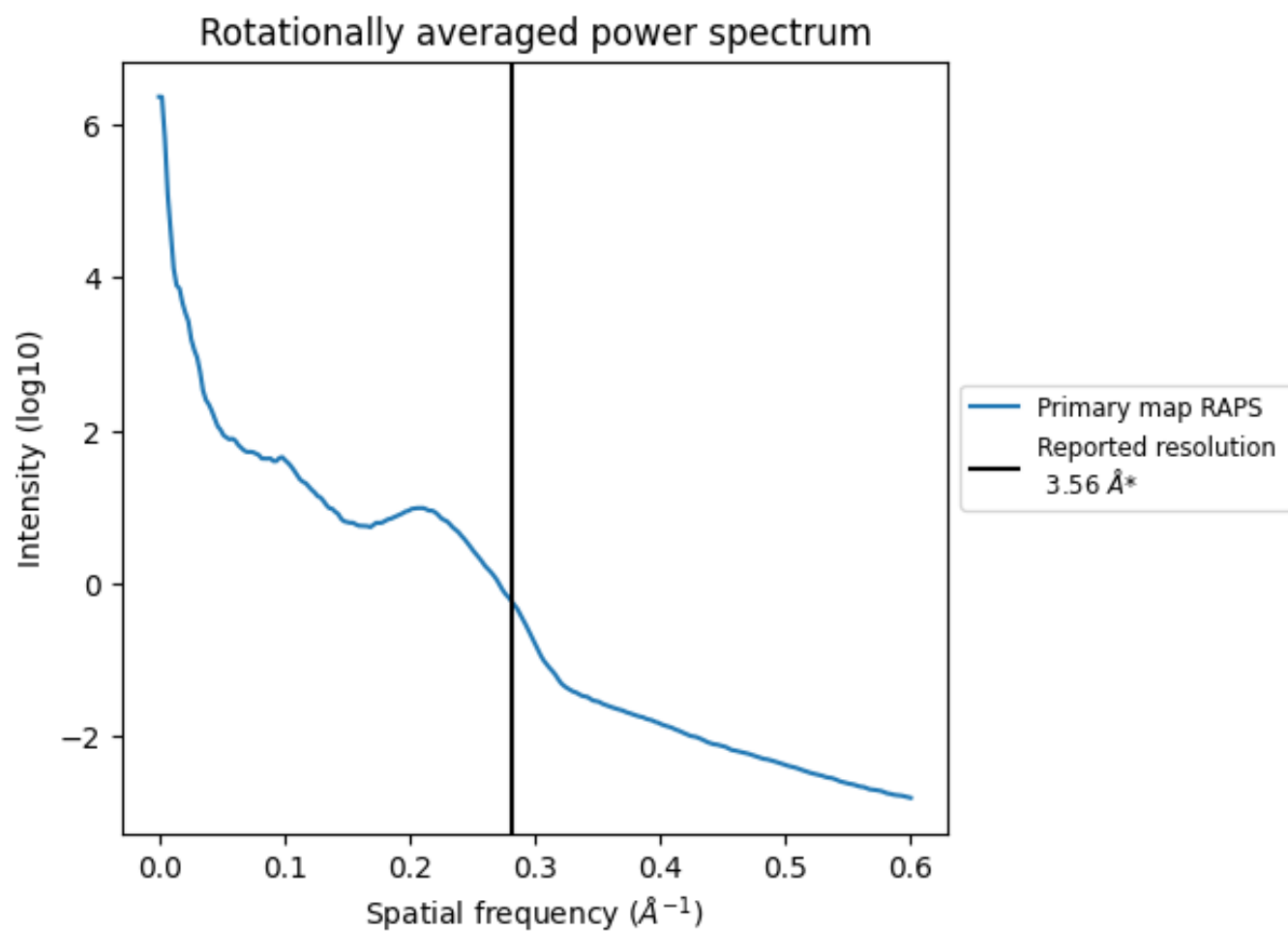
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 870 nm³; this corresponds to an approximate mass of 786 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 0.281 Å⁻¹

8 Fourier-Shell correlation

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

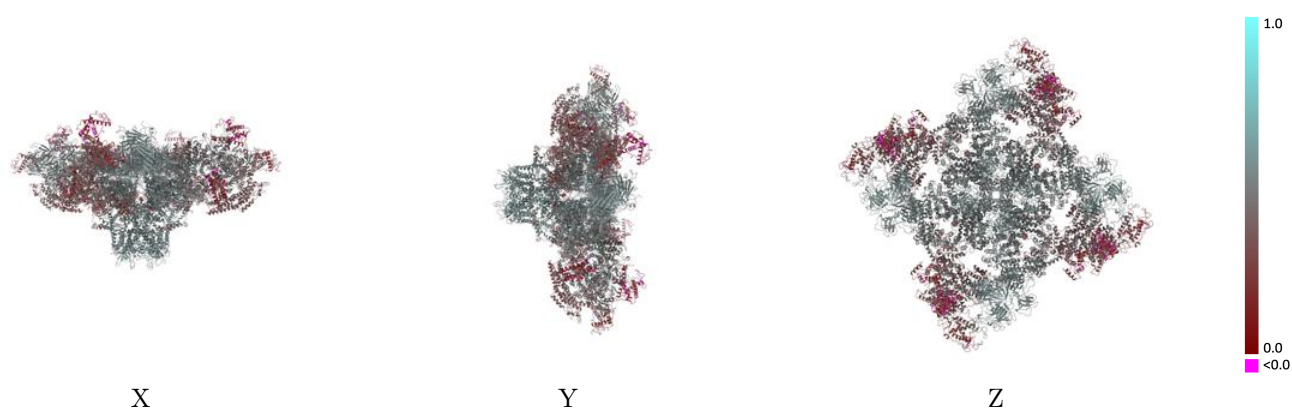
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-43304 and PDB model 8VK4. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

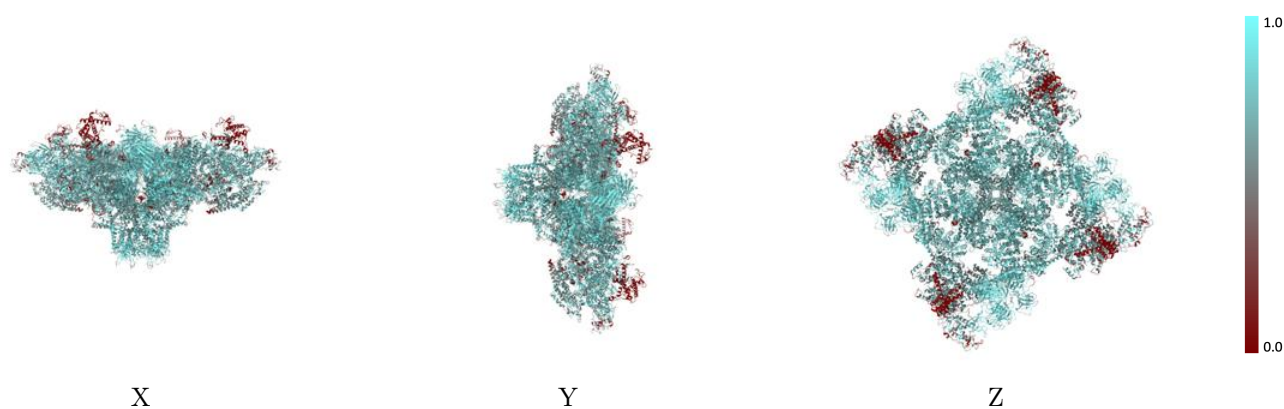
This section was not generated.

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



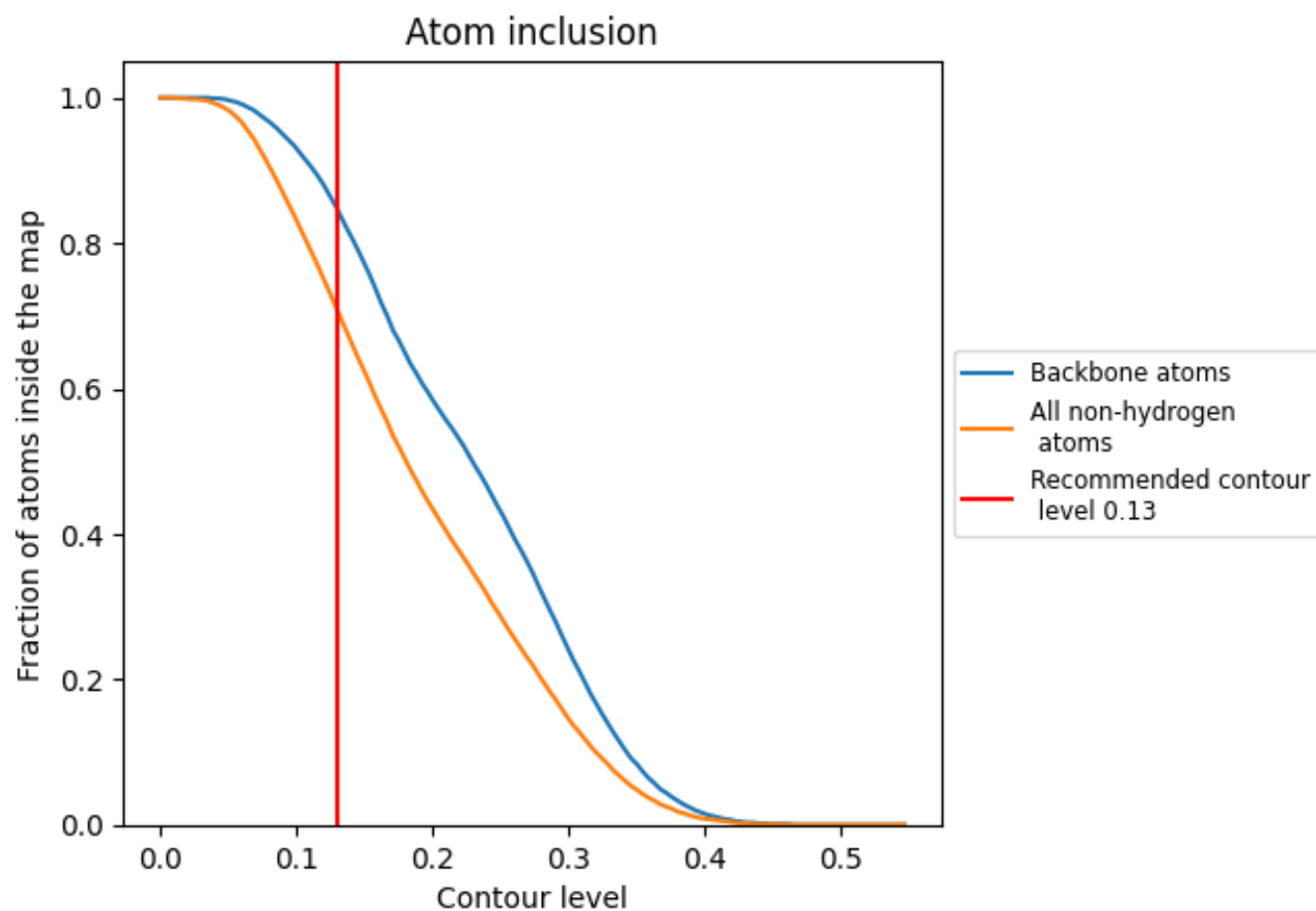
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4400
A	0.7140	0.4500
B	0.7140	0.4490
C	0.7140	0.4500
D	0.7140	0.4500
E	0.7630	0.5070
F	0.7700	0.5060
G	0.7670	0.5050
H	0.7690	0.5070
I	0.4960	0.1660
J	0.5800	0.1760
K	0.4990	0.1680
L	0.5820	0.1770
M	0.5000	0.1690
N	0.5820	0.1790
O	0.4970	0.1650
P	0.5810	0.1770

