



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 04:14 PM EDT

PDB ID : 9ZNA / pdb_00009zna
EMDB ID : EMD-74441
Title : Structure of rabbit RyR1 complexed with FKBP12.6, calmodulin, ADP, 4-chloro-m-cresol, caffeine, and Mg²⁺
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.37 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:

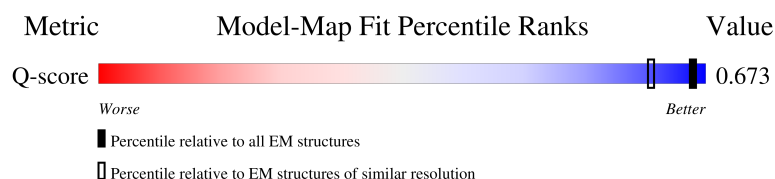
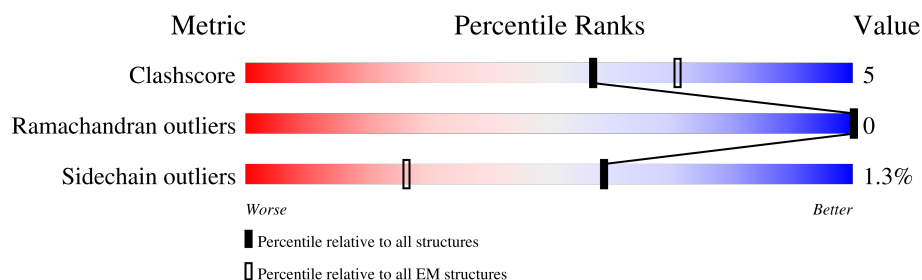
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.37 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	4742 (1.87 - 2.87)

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	107	78% 22%
1	F	107	79% 21%
1	G	107	78% 22%
1	H	107	78% 22%

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Mol	Chain	Length	Quality of chain
2	I	148	35% 93% 7%
2	J	148	35% 92% 8%
2	K	148	36% 89% 11%
2	L	148	35% 90% 10%
3	A	5037	7% 73% 11% 16%
3	B	5037	7% 73% 11% 16%
3	C	5037	7% 73% 11% 16%
3	D	5037	6% 73% 11% 16%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 148682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	J	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	K	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	L	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		

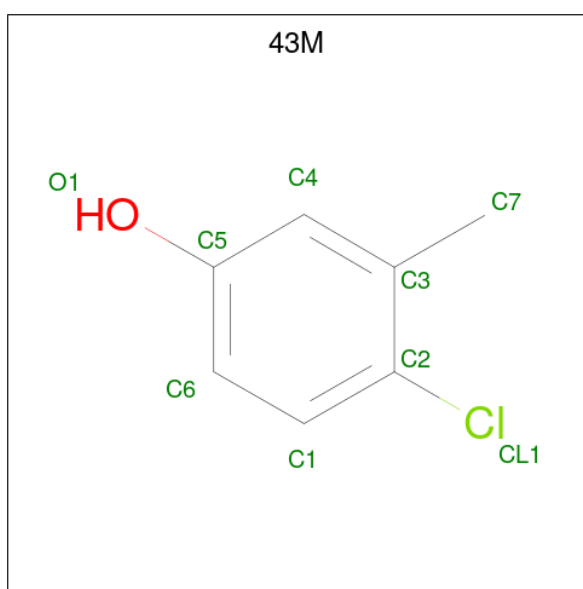
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23
L	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4249	Total	C	N	O	S	2	0
			33891	21593	5830	6234	234		
3	B	4249	Total	C	N	O	S	2	0
			33891	21593	5830	6234	234		
3	C	4249	Total	C	N	O	S	2	0
			33891	21593	5830	6234	234		
3	D	4249	Total	C	N	O	S	2	0
			33891	21593	5830	6234	234		

- Molecule 4 is 4-CHLORO-3-METHYLPHENOL (CCD ID: 43M) (formula: C₇H₇ClO) (labeled as "Ligand of Interest" by depositor).



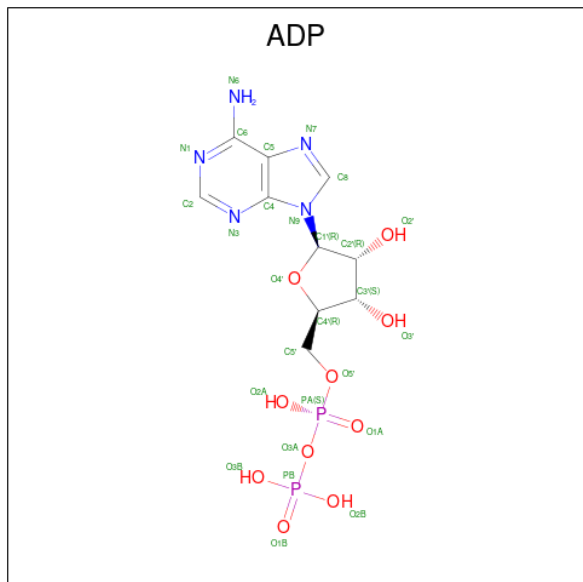
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	

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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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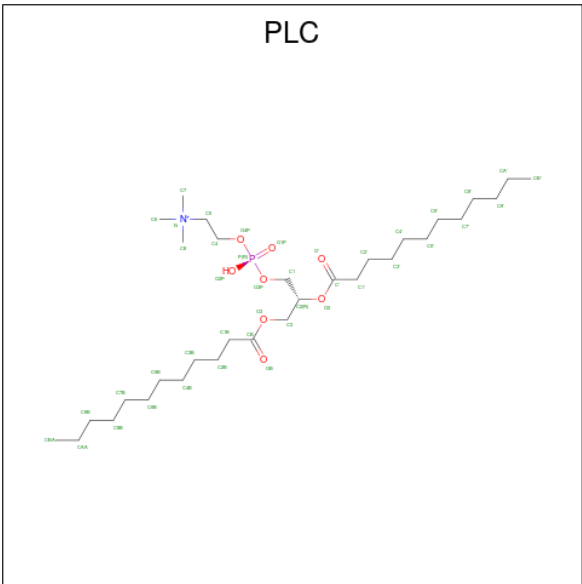
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Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

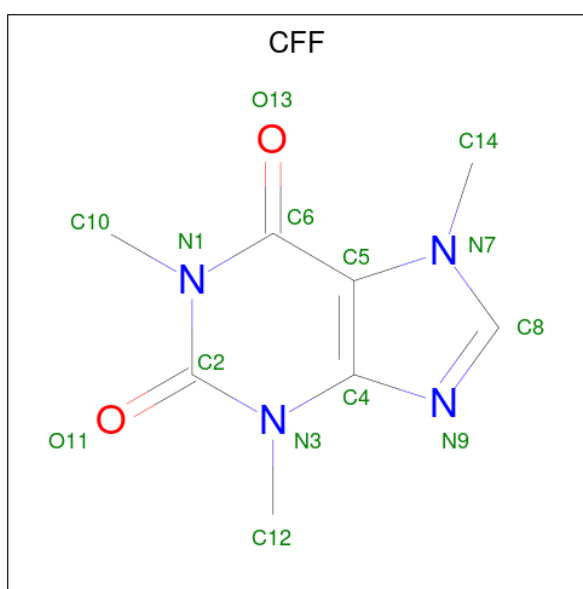
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	

- Molecule 7 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
7	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
7	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
7	D	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 8 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total 1	Mg 1	0
9	C	1	Total 1	Mg 1	0
9	D	1	Total 1	Mg 1	0

- Molecule 10 is water.

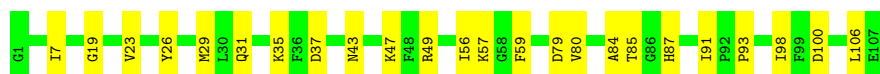
Mol	Chain	Residues	Atoms		AltConf
10	E	25	Total 25	O 25	0
10	I	62	Total 62	O 62	0
10	J	71	Total 71	O 71	0
10	K	64	Total 64	O 64	0
10	L	72	Total 72	O 72	0
10	F	24	Total 24	O 24	0
10	G	24	Total 24	O 24	0
10	H	24	Total 24	O 24	0
10	A	1182	Total 1182	O 1182	0
10	B	1192	Total 1192	O 1192	0
10	C	1183	Total 1183	O 1183	0
10	D	1187	Total 1187	O 1187	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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:  78% 22%



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:  79% 21%



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:  78% 22%

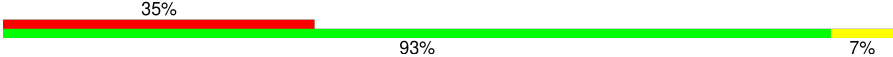


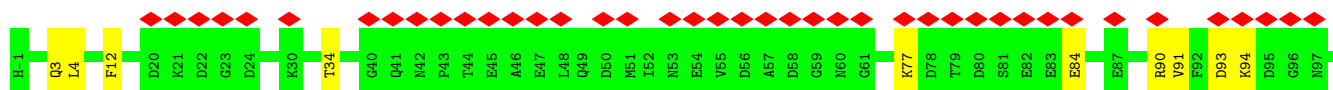
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

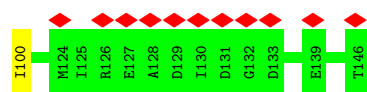
Chain H:  78% 22%



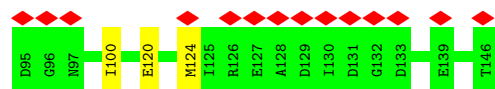
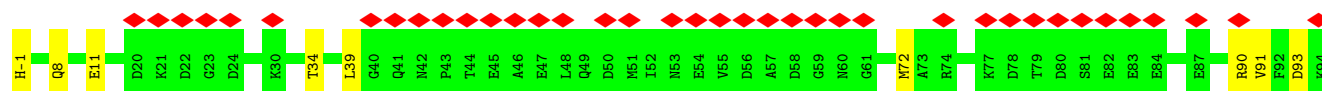
- Molecule 2: Calmodulin-1

Chain I:  35% 93% 7%

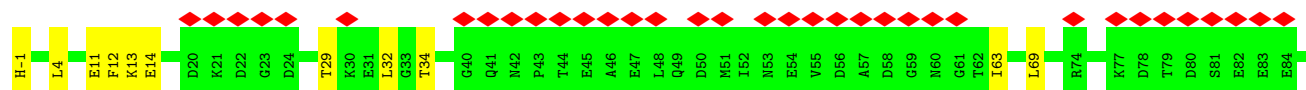
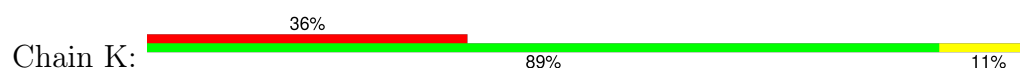




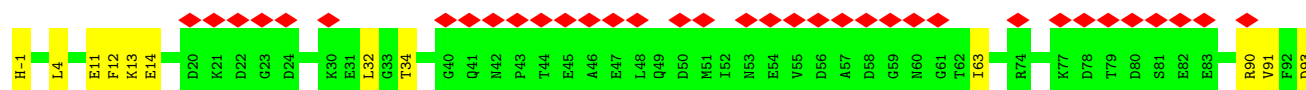
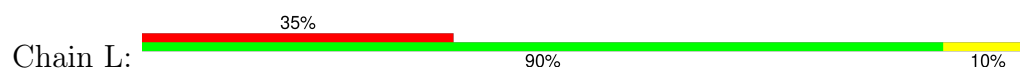
• Molecule 2: Calmodulin-1



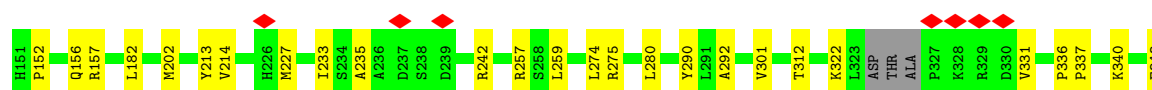
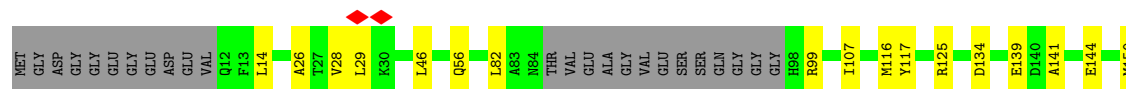
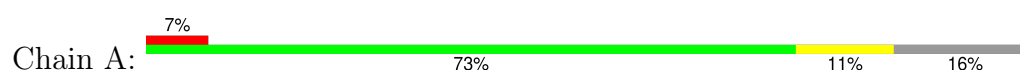
• Molecule 2: Calmodulin-1

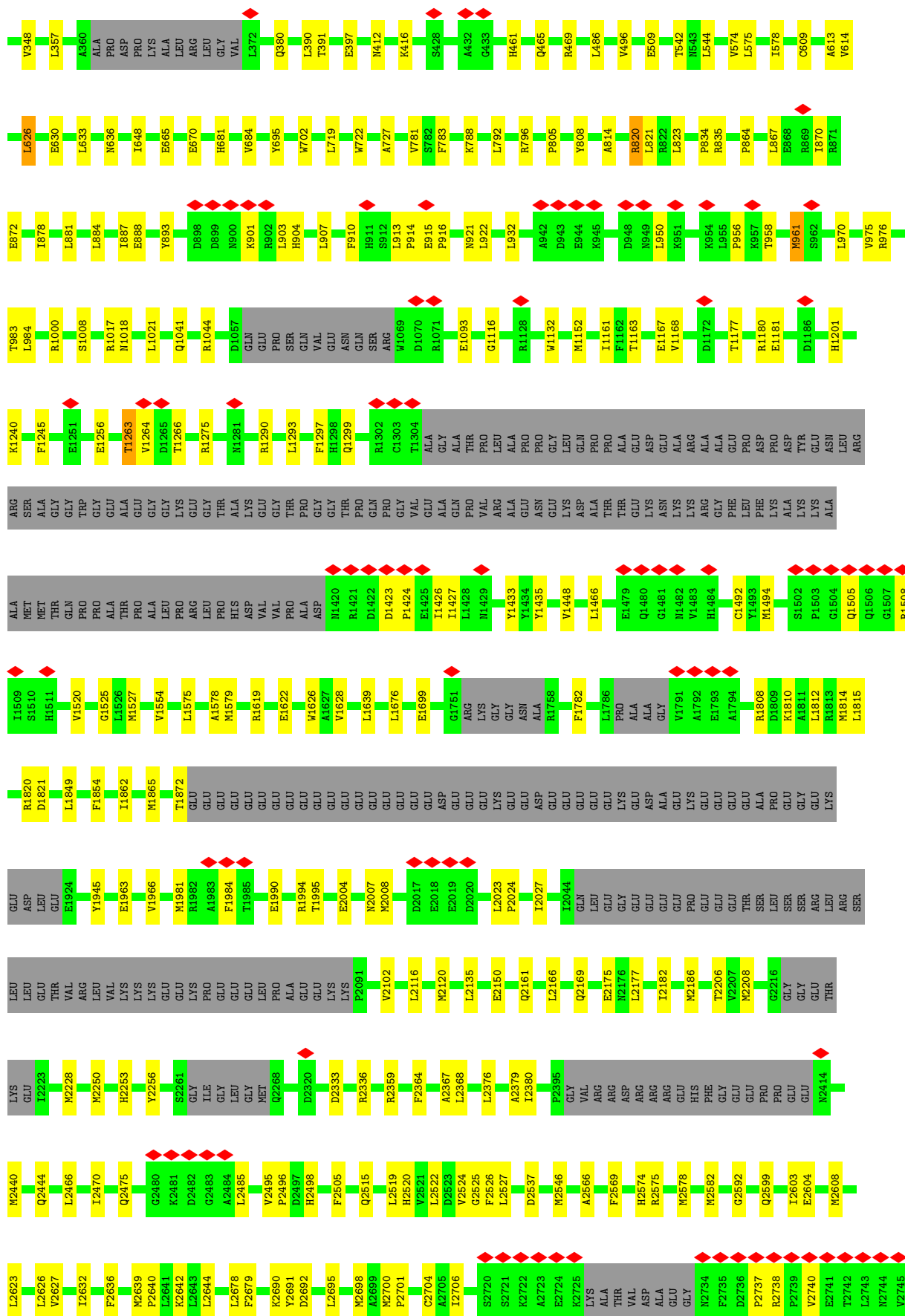


• Molecule 2: Calmodulin-1



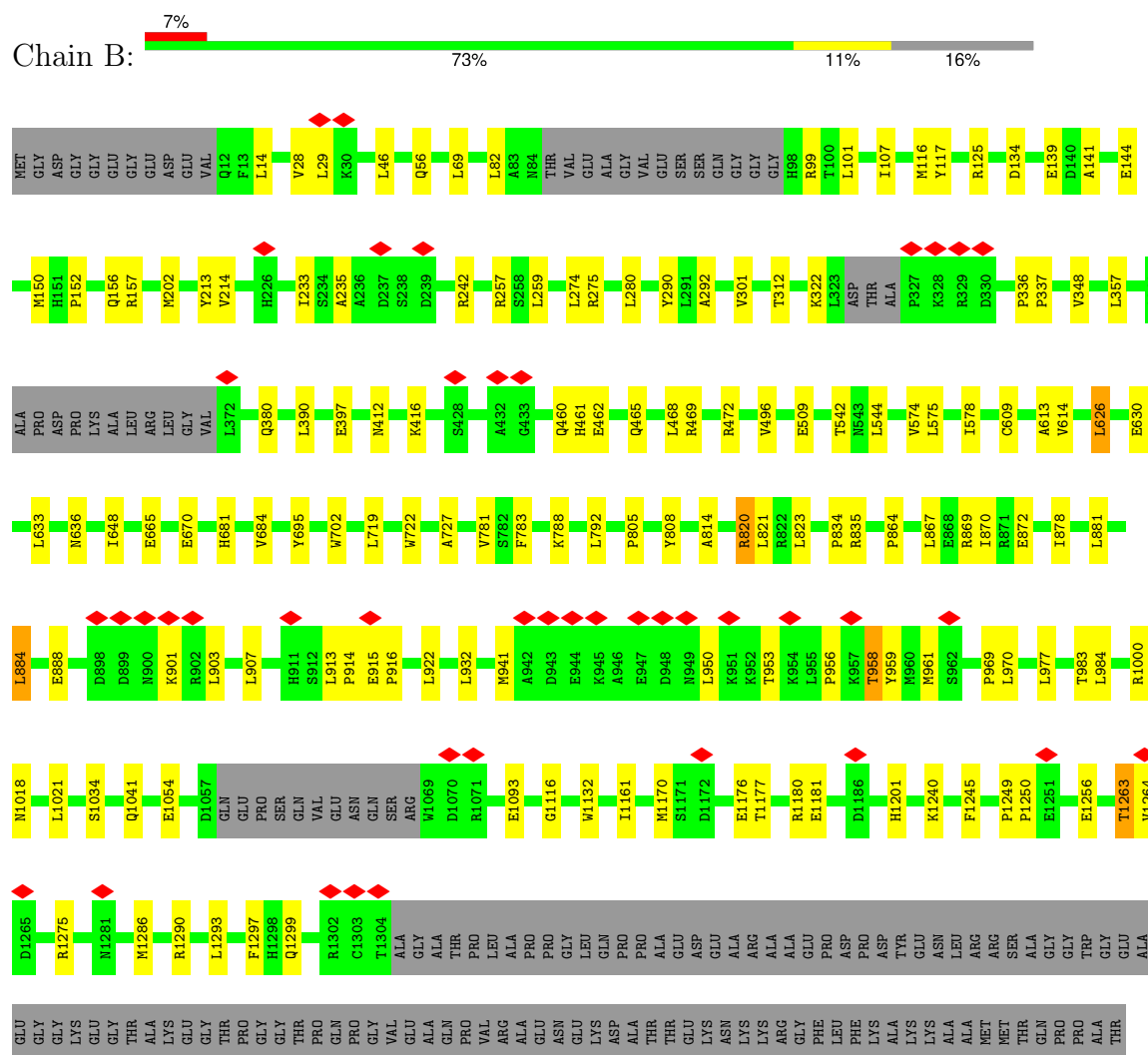
• Molecule 3: Ryanodine receptor 1





LEU	ALA	E4206	T3969	E3712	ASP	L3365	R3248	I3070	L2926	T2966	R2806	12746
ARG	ARG	Q4209	Q3970	E3712	ALA	R3369	D3252	M3081	L2927	L2867	W2807	12747
LEU	LEU	V4210	G3971	Y3720	D3587	R3368	G3253	M3081	K2928	S2868	P2808	12748
TRP	ALA	P3972	P3972	M3723	P3589	K3371	G3254	K3089	F2929	R2869	I2809	12749
GLY	ALA	F4217	L3980	M3723	V3593	E3377	G3255	L3092	L2930	E2870	L2809	12750
ALA	ALA	I4218	F3996	I3728	V3593	Q3378	L3256	L3092	Q2931	L2871	E2811	12751
LEU	ALA	V4221	F3996	I3728	A3601	L3379	A3257	L3092	M2932	Q2872	S2812	12752
ALA	ARG	V4221	F3996	I3728	V3602	R3380	E3258	K3105	G2935	A2874	L2813	12753
GLY	LEU	E4224	M4000	L3735	V3602	L3380	M3266	M3106	A2936	F2754	K2814	12754
GLY	ARG	G4225	G4225	L3735	Y3604	L3381	I3270	V3107	V2937	I2755	A2815	12755
LEU	GLY	G4226	Q4005	GLY	E3607	L3382	I3270	E3108	Q2937	I2756	M2816	12756
VAL	LEU	S4007	D4006	GLY	Q3608	A3383	I3274	E3108	V2937	K2757	M2816	12757
GLU	SER	I4241	S4007	GLU	Q3608	K3384	L3274	G3113	V2937	F2758	A2818	12758
ALA	ALA	I4242	S4007	GLU	Q3608	A3384	L3281	LYS	R2938	A2759	W2819	12759
LEU	ALA	M4245	I4010	GLU	H3611	A3385	L3281	VAL	R2938	E2760	E2820	12760
LEU	LEU	E4253	K4014	GLU	P3612	A3386	P3289	ALA	G2940	E2761	TRP	12761
VAL	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2762	TRP	12762
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2763	TRP	12763
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2764	TRP	12764
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2765	TRP	12765
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2766	TRP	12766
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2767	TRP	12767
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2768	TRP	12768
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2769	TRP	12769
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2770	TRP	12770
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2771	TRP	12771
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2772	TRP	12772
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2773	TRP	12773
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THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2782	TRP	12782
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2783	TRP	12783
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2784	TRP	12784
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2785	TRP	12785
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THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2788	TRP	12788
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2789	TRP	12789
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2790	TRP	12790
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2791	TRP	12791
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2792	TRP	12792
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2793	TRP	12793
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2794	TRP	12794
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2795	TRP	12795
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2796	TRP	12796
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2797	TRP	12797
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2798	TRP	12798
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2799	TRP	12799
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2800	TRP	12800
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2801	TRP	12801
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2802	TRP	12802
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2803	TRP	12803
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2804	TRP	12804
THR	ARG	E4253	M4047	GLU	P3612	A3387	P3289	ALA	G2940	E2805	TRP	12805

- Molecule 3: Ryanodine receptor 1

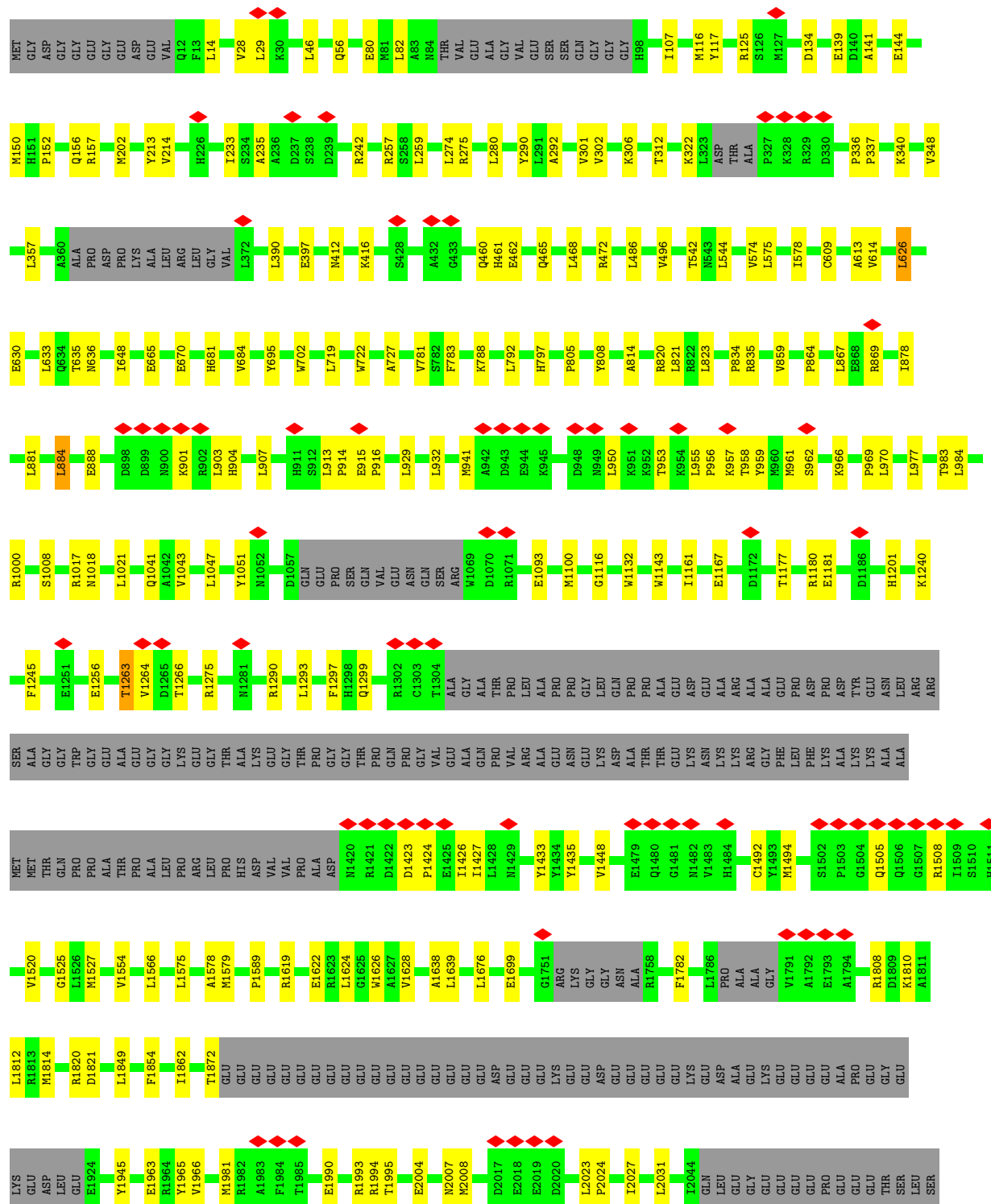




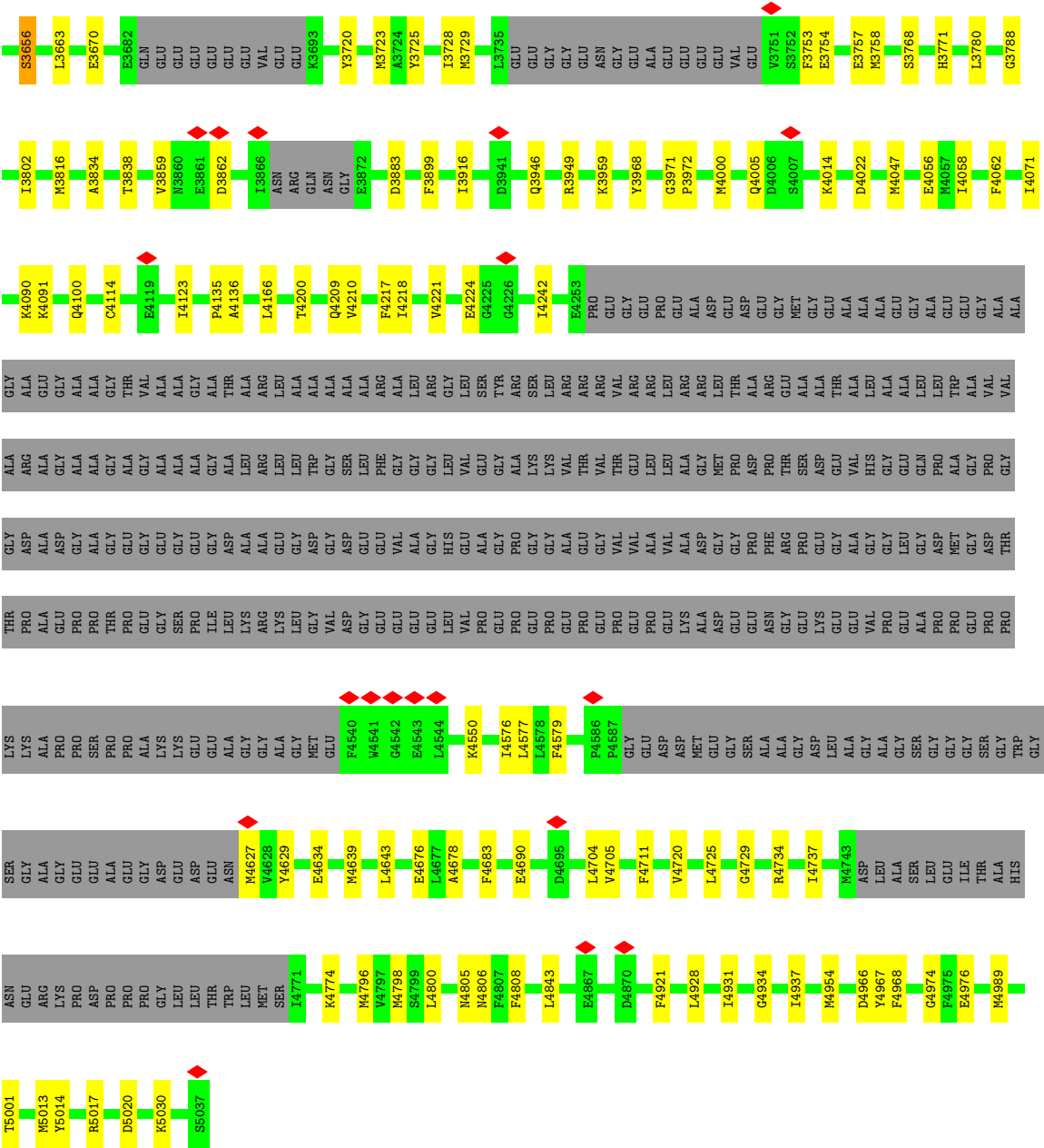




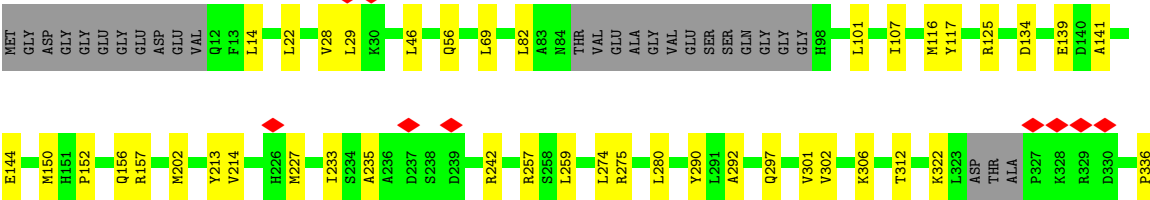
• Molecule 3: Ryanodine receptor 1



Y3540	F3435	L3316	V3125	F2973	K2887	LYS	Y2777	F2526	L2380	R2199	SER
K3543	R3436	L3327	T3132	V2980	G2888	THR	G2778	L2527	P2395	T2206	ARG
L3553	M3437	G3328	L3136	V2981	G2889	ARG	E2779	D2537	GLY	V2207	LEU
Q3554	R3453	I3329	L3137	S2982	G2900	LYS	N2780	M2546	VAL	M2208	SER
L3557	E3463	A3332	D3155	S2983	T2901	ILE	V2781	A2566	ARG	E2209	LEU
K3562	E3464	T3333	D3160	G2984	H2902	SER	D2782	A2566	ASP	V2210	GLU
V3563	M3465	M3334	D3160	G2985	P2903	GLN	E2783	F2569	ARG	G2216	THR
E3564	M3466	M3335	T3168	V2986	L2904	ALA	E2784	H2574	ARG	GLY	VAL
S3568	S3467	A3342	L3175	E2987	V2906	THR	L2785	R2575	ARG	GLY	ARG
K3571	T3471	F3341	L3175	K2988	P2907	ASP	T2787	M2578	GLY	THR	LYS
Q3572	ALA	I2986	L3190	V2908	T2908	PRO	H2788	M2582	GLY	LYS	LYS
K3572	ASP	L3003	V3203	D2909	T2910	ARG	P2789	L2583	GLU	I2223	LYS
M3573	S3347	P3004	L3210	L2911	L2912	GLY	M2790	H2584	PRO	M2228	GLU
R3577	LYS	K3023	L3214	Q3209	T2912	LYS	L2791	R2588	GLU	R2244	PRO
R3582	ALA	V3024	R3225	A2913	A2913	THR	R2792	G2592	GLY	S2249	GLU
GLU	E3035	K3034	R3225	K2914	E2915	THR	P2793	K2597	M2423	H2253	LEU
ASP	E3036	K3036	R3225	K2916	K2916	THR	Y2794	A2598	M2440	Y2256	ALA
ALA	E3037	M3038	R3225	R2918	A2917	THR	P2796	Q2599	Q2444	S2261	GLY
D3587	GLN	I3039	L3246	D2919	R2918	THR	S2798	I2603	L2466	ILE	LYS
P3588	GLY	R3053	R3247	R2920	E2921	THR	E2799	E2604	L2470	GLY	LYS
P3589	GLY	R3056	R3248	E2922	E2922	THR	K2800	M2608	Q2475	LEU	P2091
L3603	GLY	L3056	R3248	K2922	E2922	THR	D2801	L2626	Q2475	GLY	V2102
Y3604	SER	L3056	E3265	K2922	E2922	THR	D2802	L2627	Q2475	GLY	L2116
E3607	ASP	N3066	E3265	A2923	E2923	THR	E2803	L2632	L2273	GLY	M2120
Q3608	GLU	I3070	I3270	Q2924	Q2924	THR	L2804	F2636	C2310	L2135	L2135
R3611	THR	M3081	L3274	E2925	E2925	THR	Y2805	M2639	L2313	E2150	E2150
P3612	LYS	K3089	L3277	L2927	L2927	THR	R2806	L2641	Q2161	Q2161	Q2161
TTR	LYS	K3089	L3277	K2928	K2928	THR	W2807	L2642	L2165	L2165	L2165
LYS	ARG	K3089	L3281	F2929	F2929	THR	P2808	L2644	L2166	L2166	L2166
LYS	ARG	L3092	L3281	L2930	L2930	THR	K2809	L2678	Q2169	Q2169	Q2169
LYS	GLY	I3103	P3289	L2930	Q2931	THR	K2810	R2336	E2175	E2175	E2175
LYS	ASP	E3104	P3289	Q2931	Q2931	THR	E2811	R2336	E2176	E2176	E2176
ALA	ARG	K3106	P3289	M2933	M2933	THR	S2812	R2336	L2177	L2177	L2177
VAL	ARG	R3107	P3289	G2934	G2934	THR	L2813	R2336	M2178	M2178	M2178
LEU	LEU	V3107	P3289	Y2935	Y2935	THR	K2814	R2336	L2182	L2182	L2182
PRO	PRO	L3112	P3289	A2936	A2936	THR	A2815	R2336	E2175	E2175	E2175
ALA	ALA	G3113	P3289	V2937	V2937	THR	M2816	R2336	E2176	E2176	E2176
ALA	GLY	LYS	P3289	T2938	T2938	THR	L2817	R2336	L2182	L2182	L2182
ALA	ALA	VAL	P3289	R2939	R2939	THR	A2818	R2336	E2176	E2176	E2176
P3301	P3301	SER	P3289	G2940	G2940	THR	W2819	R2336	A2367	A2367	A2367
T3308	T3308	GLN	P3289	L2941	L2941	THR	E2820	R2336	L2368	L2368	L2368
L3412	L3412	ALA	P3289	L2941	L2941	THR	THR	R2336	L2376	L2376	L2376
L3413	L3413	ALA	P3289	K2942	K2942	THR	ILE	R2336	A2367	A2367	A2367
L3414	L3414	ARG	P3289	D2943	D2943	THR	GLU	R2336	L2368	L2368	L2368
Y3415	Y3415	THR	P3289	M2944	M2944	THR	E2765	R2336	L2376	L2376	L2376
V3416	V3416	GLN	P3289	E2945	E2945	THR	K2765	R2336	A2367	A2367	A2367
R3420	R3420	VAL	P3289	E2945	E2945	THR	W2766	R2336	L2368	L2368	L2368
L3434	L3434	K3123	P3289	L2946	L2946	THR	T2762	R2336	L2368	L2368	L2368
		G3124	P3289	D2947	D2947	THR	H2763	R2336	L2368	L2368	L2368
			P3289	T2948	T2948	THR	E2764	R2336	L2368	L2368	L2368
			P3289	S2949	S2949	THR	K2765	R2336	L2368	L2368	L2368
			P3289	K2953	K2953	THR	W2766	R2336	L2368	L2368	L2368
			P3289	F2957	F2957	THR	T2771	R2336	L2368	L2368	L2368
			P3289	S2970	S2970	LYS	Q2772	R2336	L2368	L2368	L2368
			P3289			LYS	N2773	R2336	L2368	L2368	L2368
			P3289			LYS	W2774	R2336	L2368	L2368	L2368
			P3289			LYS	W2775	R2336	L2368	L2368	L2368
			P3289			LYS	S2776	R2336	L2368	L2368	L2368



● Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	294178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.049	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLC, CFF, 43M, MG, ADP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.19	0/835	0.34	0/1123
1	F	0.19	0/835	0.34	0/1123
1	G	0.19	0/835	0.34	0/1123
1	H	0.19	0/835	0.34	0/1123
2	I	0.13	0/1026	0.30	0/1386
2	J	0.13	0/1026	0.27	0/1386
2	K	0.13	0/1026	0.29	0/1386
2	L	0.13	0/1026	0.30	0/1386
3	A	0.19	0/34653	0.33	3/46920 (0.0%)
3	B	0.19	0/34653	0.33	2/46920 (0.0%)
3	C	0.20	0/34653	0.36	6/46920 (0.0%)
3	D	0.19	0/34653	0.32	0/46920
All	All	0.19	0/146056	0.33	11/197716 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
3	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4690	GLU	CG-CD-OE2	-18.53	75.78	118.40
3	C	4690	GLU	CG-CD-OE1	17.23	158.03	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4690	GLU	OE1-CD-OE2	-15.40	85.95	122.90
3	C	3608	GLN	CB-CG-CD	-7.65	99.59	112.60
3	A	3607	GLU	CA-C-N	-7.03	109.62	120.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3608	GLN	Sidechain
3	B	3608	GLN	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	E	819	0	824	13	0
1	F	819	0	824	11	0
1	G	819	0	824	13	0
1	H	819	0	824	13	0
2	I	1017	0	841	7	0
2	J	1017	0	841	7	0
2	K	1017	0	841	11	0
2	L	1017	0	841	9	0
3	A	33891	0	33518	324	0
3	B	33891	0	33518	332	0
3	C	33891	0	33518	338	0
3	D	33891	0	33518	324	0
4	A	27	0	18	2	0
4	B	27	0	18	1	0
4	C	27	0	18	2	0
4	D	27	0	18	1	0
5	A	81	0	36	0	0
5	B	81	0	36	0	0
5	C	81	0	36	0	0
5	D	81	0	36	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	42	0	64	2	0
7	B	42	0	64	1	0
7	C	42	0	64	3	0
7	D	42	0	64	1	0
8	A	14	0	8	0	0
8	B	14	0	8	0	0
8	C	14	0	8	1	0
8	D	14	0	8	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1182	0	0	2	0
10	B	1192	0	0	1	0
10	C	1183	0	0	1	0
10	D	1187	0	0	2	0
10	E	25	0	0	0	0
10	F	24	0	0	0	0
10	G	24	0	0	0	0
10	H	24	0	0	0	0
10	I	62	0	0	0	0
10	J	71	0	0	0	0
10	K	64	0	0	0	0
10	L	72	0	0	0	0
All	All	148682	0	141236	1368	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 5.

The worst 5 of 1368 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)
3:B:2782:ASP:HB3	3:B:2785:LEU:HD22	1.40	1.03
3:A:2782:ASP:HB3	3:A:2785:LEU:HD22	1.40	1.00
3:B:907:LEU:HB3	3:B:961:MET:HE1	1.52	0.92
3:D:907:LEU:HB3	3:D:961:MET:HE1	1.56	0.88
3:A:4091:LYS:H	3:A:4091:LYS:HE2	1.39	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	G	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	I	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
2	J	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
2	K	146/148 (99%)	140 (96%)	6 (4%)	0	100	100
2	L	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
3	A	4199/5037 (83%)	4119 (98%)	80 (2%)	0	100	100
3	B	4199/5037 (83%)	4120 (98%)	79 (2%)	0	100	100
3	C	4199/5037 (83%)	4120 (98%)	79 (2%)	0	100	100
3	D	4199/5037 (83%)	4121 (98%)	78 (2%)	0	100	100
All	All	17800/21168 (84%)	17453 (98%)	347 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/88 (100%)	85 (97%)	3 (3%)	32	51
1	F	88/88 (100%)	84 (96%)	4 (4%)	24	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	88/88 (100%)	85 (97%)	3 (3%)	32	51
1	H	88/88 (100%)	85 (97%)	3 (3%)	32	51
2	I	82/127 (65%)	80 (98%)	2 (2%)	43	63
2	J	82/127 (65%)	80 (98%)	2 (2%)	43	63
2	K	82/127 (65%)	79 (96%)	3 (4%)	30	47
2	L	82/127 (65%)	80 (98%)	2 (2%)	43	63
3	A	3697/4276 (86%)	3652 (99%)	45 (1%)	63	79
3	B	3697/4276 (86%)	3653 (99%)	44 (1%)	63	79
3	C	3697/4276 (86%)	3656 (99%)	41 (1%)	65	81
3	D	3697/4276 (86%)	3650 (99%)	47 (1%)	61	78
All	All	15468/17964 (86%)	15269 (99%)	199 (1%)	59	78

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	859	VAL
3	C	3528	THR
3	C	983	THR
3	C	2816	MET
3	C	4966	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	797	HIS
3	D	4947	GLN
3	D	1506	GLN
3	D	2931	GLN
3	B	1133	HIS

5.3.3 RNA ⓘ

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 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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$
5	ADP	D	5106	9	28,29,29	1.39	4 (14%)	43,45,45	1.83	8 (18%)
4	43M	B	5103	-	9,9,9	0.39	0	12,12,12	0.49	0
5	ADP	A	5107	9	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
5	ADP	B	5106	9	28,29,29	1.39	5 (17%)	43,45,45	1.84	8 (18%)
8	CFF	A	5109	-	15,15,15	0.61	0	23,23,23	0.80	2 (8%)
4	43M	A	5103	-	9,9,9	0.39	0	12,12,12	0.49	0
4	43M	D	5101	-	9,9,9	0.40	0	12,12,12	0.50	0
5	ADP	B	5107	9	28,29,29	1.39	4 (14%)	43,45,45	1.80	8 (18%)
8	CFF	D	5109	-	15,15,15	0.62	0	23,23,23	0.79	1 (4%)
7	PLC	D	5108	-	41,41,41	0.52	0	47,49,49	0.53	0
4	43M	B	5102	-	9,9,9	0.42	0	12,12,12	0.48	0
5	ADP	D	5104	-	28,29,29	1.36	3 (10%)	43,45,45	1.94	9 (20%)
5	ADP	C	5106	9	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)
4	43M	A	5102	-	9,9,9	0.42	0	12,12,12	0.49	0
4	43M	A	5101	-	9,9,9	0.39	0	12,12,12	0.49	0
8	CFF	C	5109	-	15,15,15	0.62	0	23,23,23	0.78	1 (4%)
4	43M	C	5101	-	9,9,9	0.41	0	12,12,12	0.50	0
5	ADP	C	5104	-	28,29,29	1.35	3 (10%)	43,45,45	1.94	9 (20%)
7	PLC	A	5108	-	41,41,41	0.52	0	47,49,49	0.54	0
5	ADP	A	5104	-	28,29,29	1.36	3 (10%)	43,45,45	1.94	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	43M	C	5103	-	9,9,9	0.42	0	12,12,12	0.49	0
7	PLC	B	5108	-	41,41,41	0.52	0	47,49,49	0.53	0
4	43M	B	5101	-	9,9,9	0.41	0	12,12,12	0.49	0
5	ADP	B	5104	-	28,29,29	1.36	3 (10%)	43,45,45	1.94	9 (20%)
5	ADP	D	5107	9	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
4	43M	D	5103	-	9,9,9	0.39	0	12,12,12	0.50	0
5	ADP	C	5107	9	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
8	CFF	B	5109	-	15,15,15	0.62	0	23,23,23	0.78	1 (4%)
4	43M	D	5102	-	9,9,9	0.44	0	12,12,12	0.49	0
7	PLC	C	5108	-	41,41,41	0.51	0	47,49,49	0.53	0
4	43M	C	5102	-	9,9,9	0.43	0	12,12,12	0.50	0
5	ADP	A	5106	9	28,29,29	1.39	5 (17%)	43,45,45	1.84	8 (18%)

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
5	ADP	D	5106	9	-	2/16/32/32	0/3/3/3
4	43M	B	5103	-	-	-	0/1/1/1
5	ADP	A	5107	9	-	5/16/32/32	0/3/3/3
5	ADP	B	5106	9	-	2/16/32/32	0/3/3/3
8	CFF	A	5109	-	-	-	0/2/2/2
4	43M	A	5103	-	-	-	0/1/1/1
4	43M	D	5101	-	-	-	0/1/1/1
5	ADP	B	5107	9	-	5/16/32/32	0/3/3/3
8	CFF	D	5109	-	-	-	0/2/2/2
7	PLC	D	5108	-	-	16/45/45/45	-
4	43M	B	5102	-	-	-	0/1/1/1
5	ADP	D	5104	-	-	5/16/32/32	0/3/3/3
5	ADP	C	5106	9	-	1/16/32/32	0/3/3/3
4	43M	A	5102	-	-	-	0/1/1/1
4	43M	A	5101	-	-	-	0/1/1/1
8	CFF	C	5109	-	-	-	0/2/2/2
4	43M	C	5101	-	-	-	0/1/1/1
5	ADP	C	5104	-	-	5/16/32/32	0/3/3/3
7	PLC	A	5108	-	-	18/45/45/45	-
5	ADP	A	5104	-	-	5/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	43M	C	5103	-	-	-	0/1/1/1
7	PLC	B	5108	-	-	15/45/45/45	-
4	43M	B	5101	-	-	-	0/1/1/1
5	ADP	B	5104	-	-	5/16/32/32	0/3/3/3
5	ADP	D	5107	9	-	5/16/32/32	0/3/3/3
5	ADP	C	5107	9	-	5/16/32/32	0/3/3/3
4	43M	D	5103	-	-	-	0/1/1/1
8	CFF	B	5109	-	-	-	0/2/2/2
4	43M	D	5102	-	-	-	0/1/1/1
7	PLC	C	5108	-	-	16/45/45/45	-
4	43M	C	5102	-	-	-	0/1/1/1
5	ADP	A	5106	9	-	2/16/32/32	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5106	ADP	C5-C4	4.58	1.47	1.39
5	C	5107	ADP	C5-C4	4.57	1.47	1.39
5	A	5107	ADP	C5-C4	4.57	1.47	1.39
5	B	5106	ADP	C5-C4	4.55	1.47	1.39
5	B	5107	ADP	C5-C4	4.55	1.47	1.39

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5104	ADP	C5'-C4-N3	-6.25	118.11	126.72
5	C	5104	ADP	C5'-C4-N3	-6.23	118.13	126.72
5	D	5104	ADP	C5'-C4-N3	-6.22	118.15	126.72
5	B	5104	ADP	C5'-C4-N3	-6.20	118.19	126.72
5	C	5107	ADP	C5'-C4-N3	-5.88	118.63	126.72

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

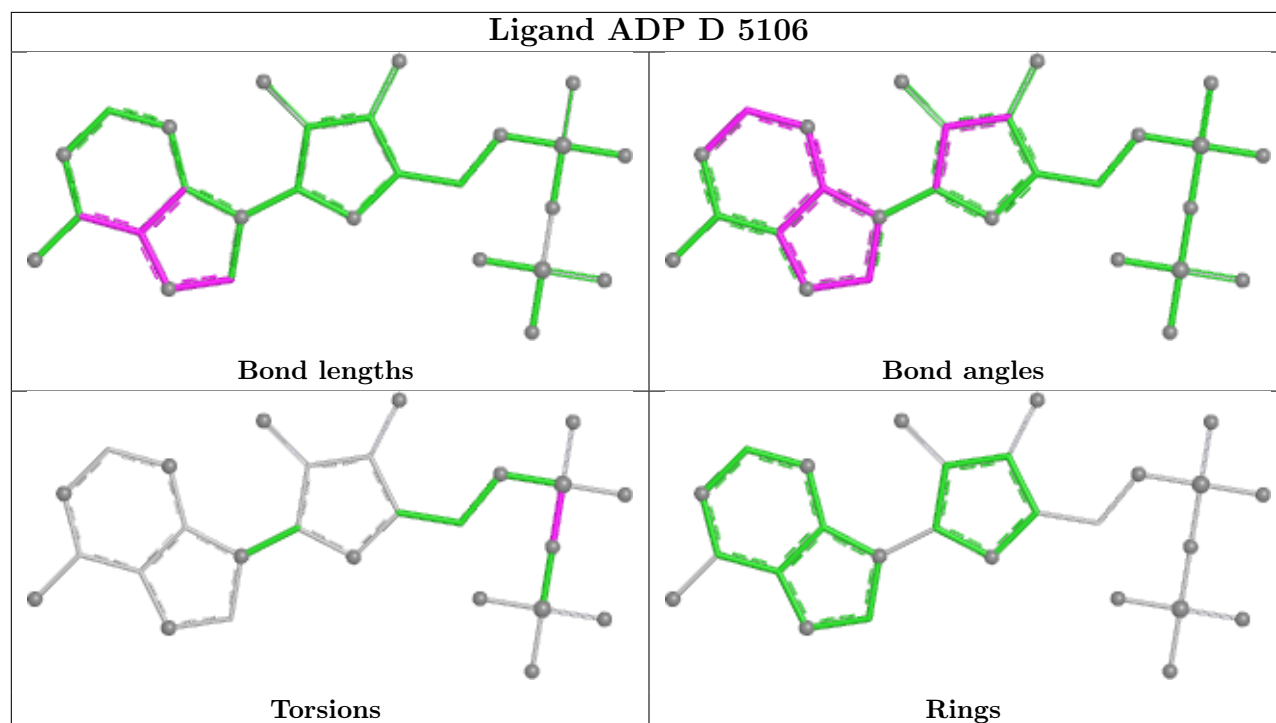
Mol	Chain	Res	Type	Atoms
5	A	5104	ADP	C5'-O5'-PA-O1A
5	A	5104	ADP	C5'-O5'-PA-O2A
5	A	5104	ADP	C5'-O5'-PA-O3A
5	A	5107	ADP	C5'-O5'-PA-O1A
5	A	5107	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

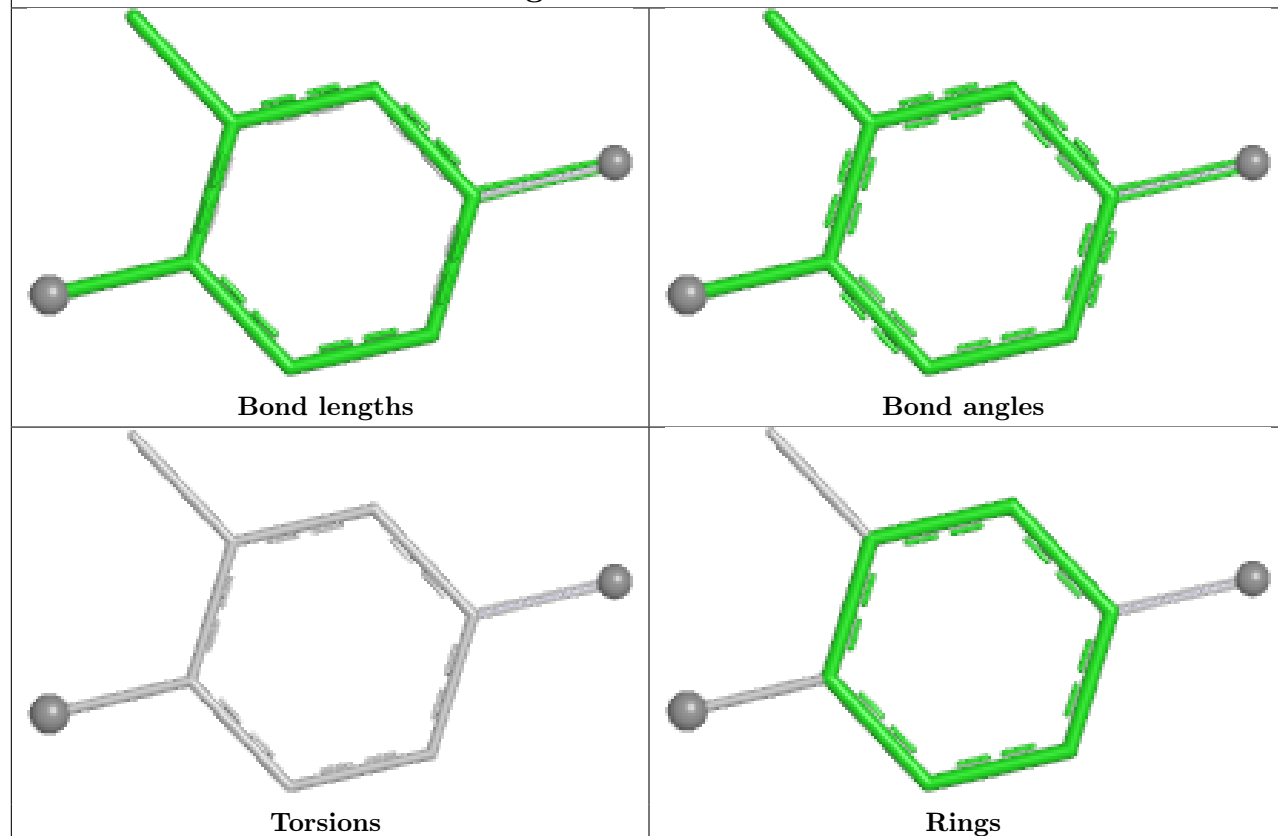
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5103	43M	1	0
4	A	5103	43M	2	0
7	D	5108	PLC	1	0
8	C	5109	CFF	1	0
7	A	5108	PLC	2	0
4	C	5103	43M	2	0
7	B	5108	PLC	1	0
4	D	5103	43M	1	0
7	C	5108	PLC	3	0

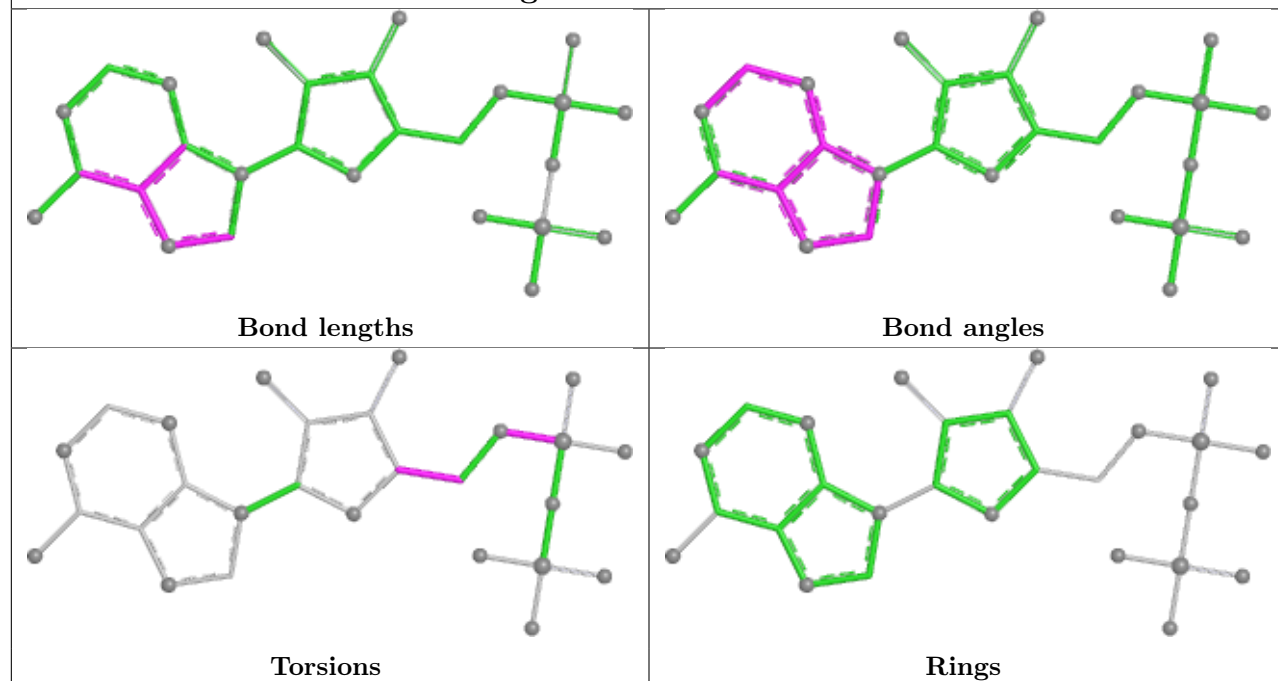
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

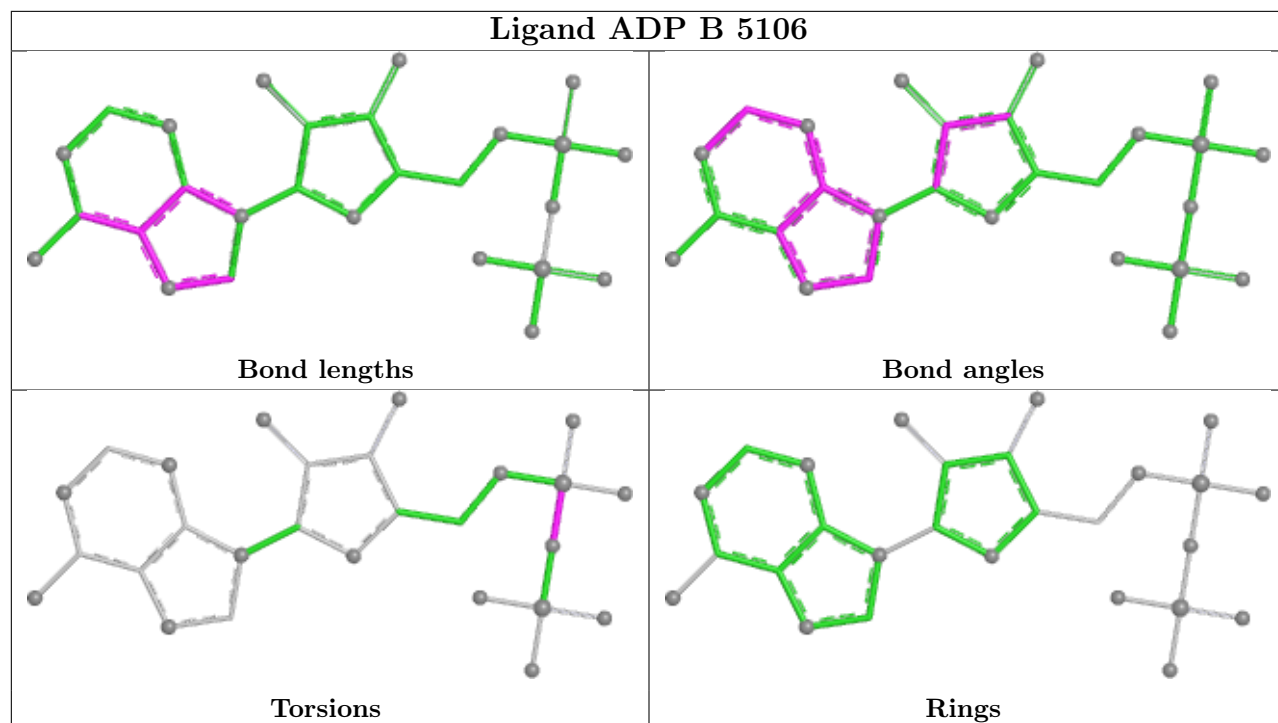


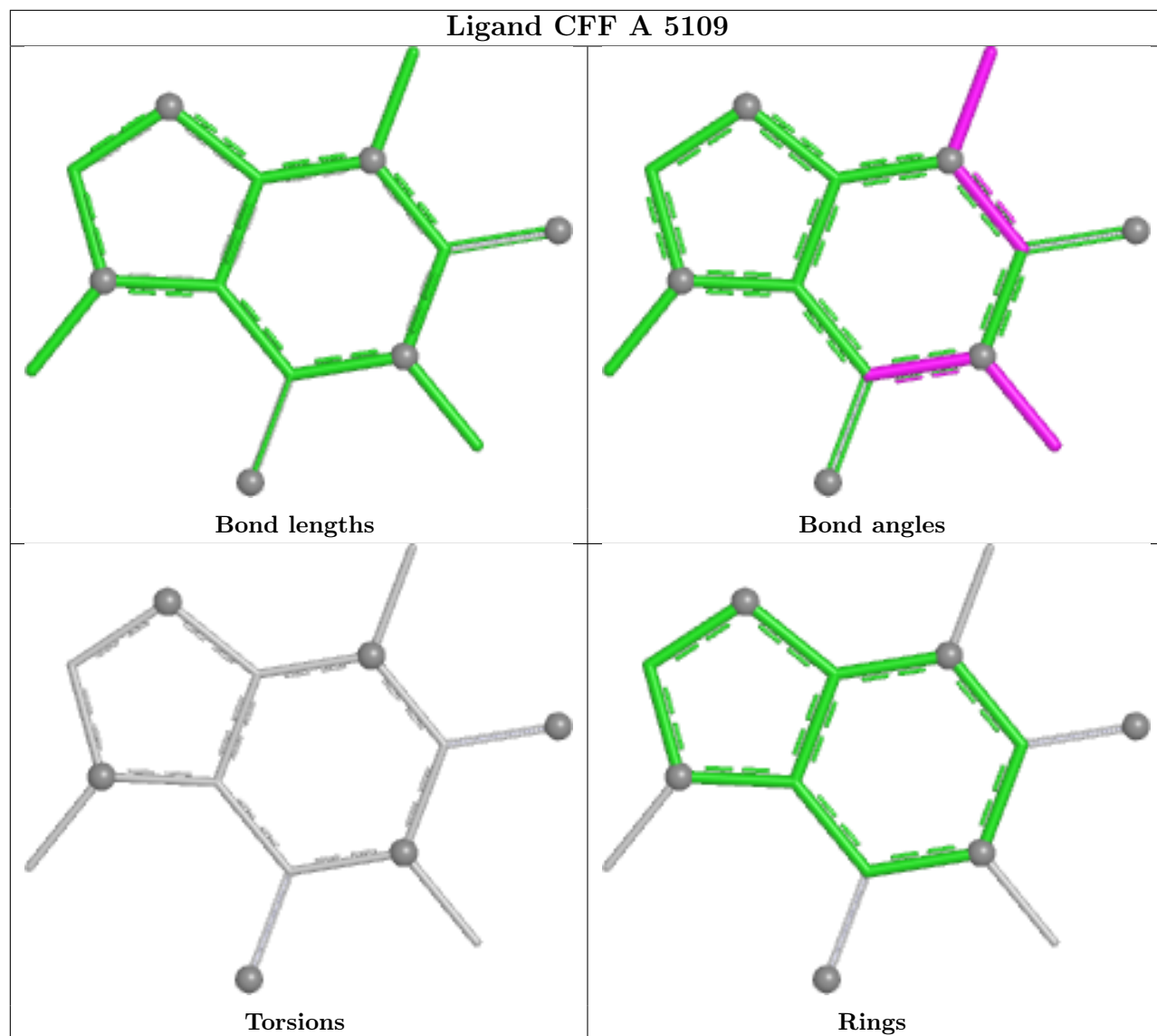
Ligand 43M B 5103



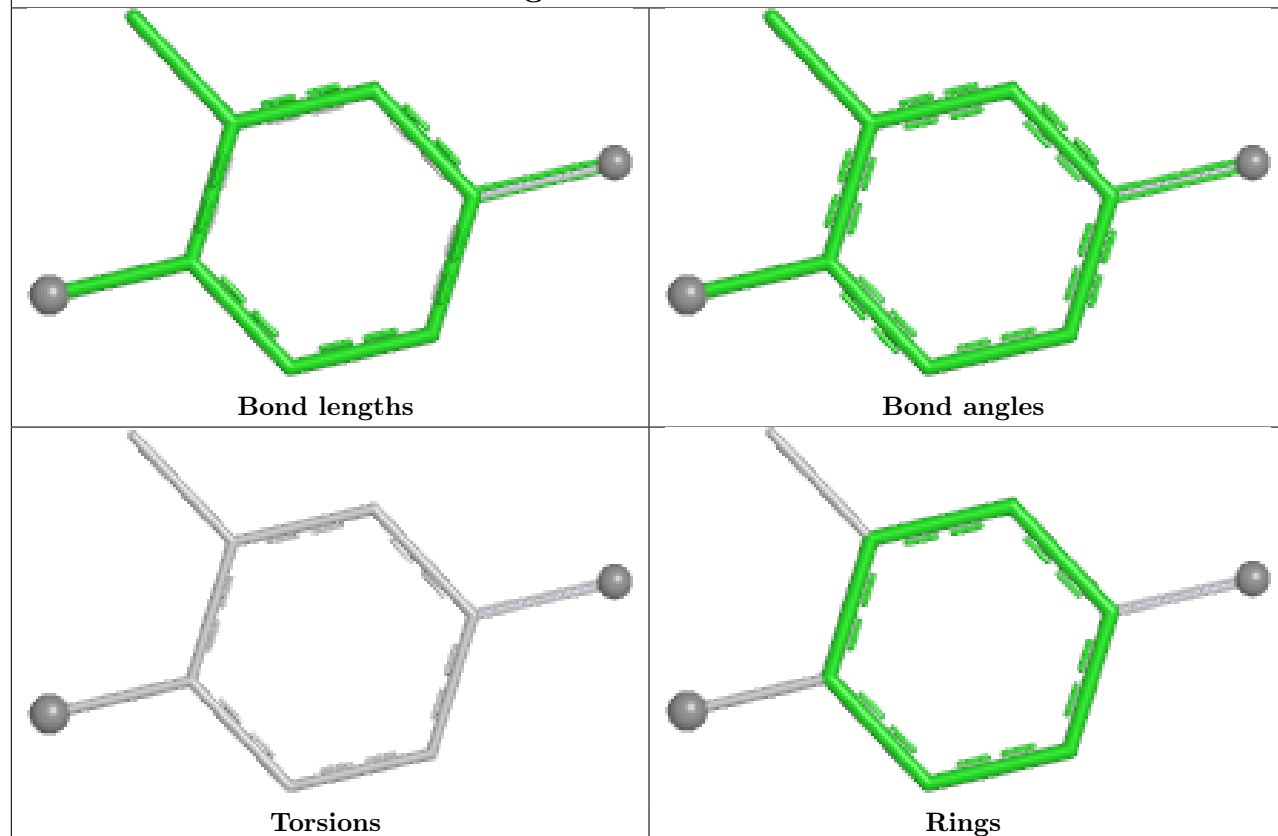
Ligand ADP A 5107



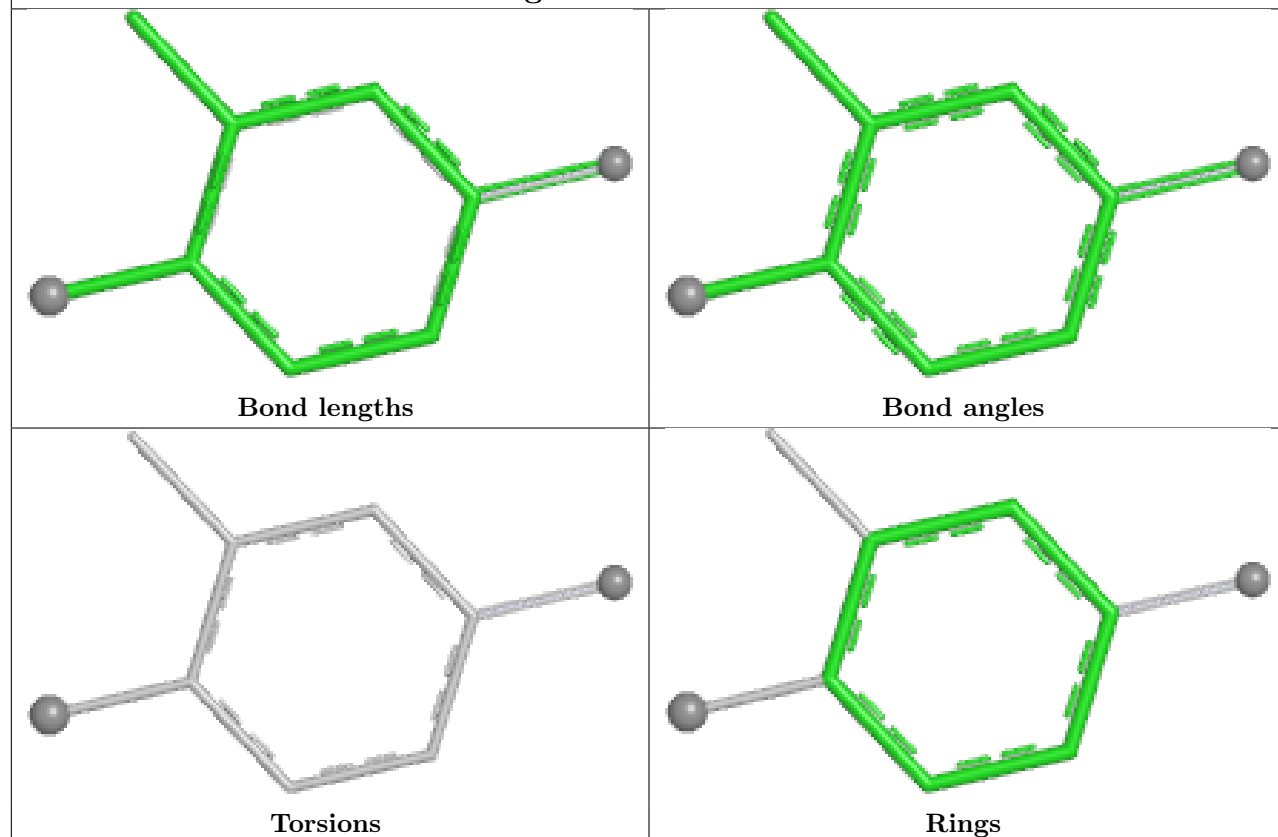


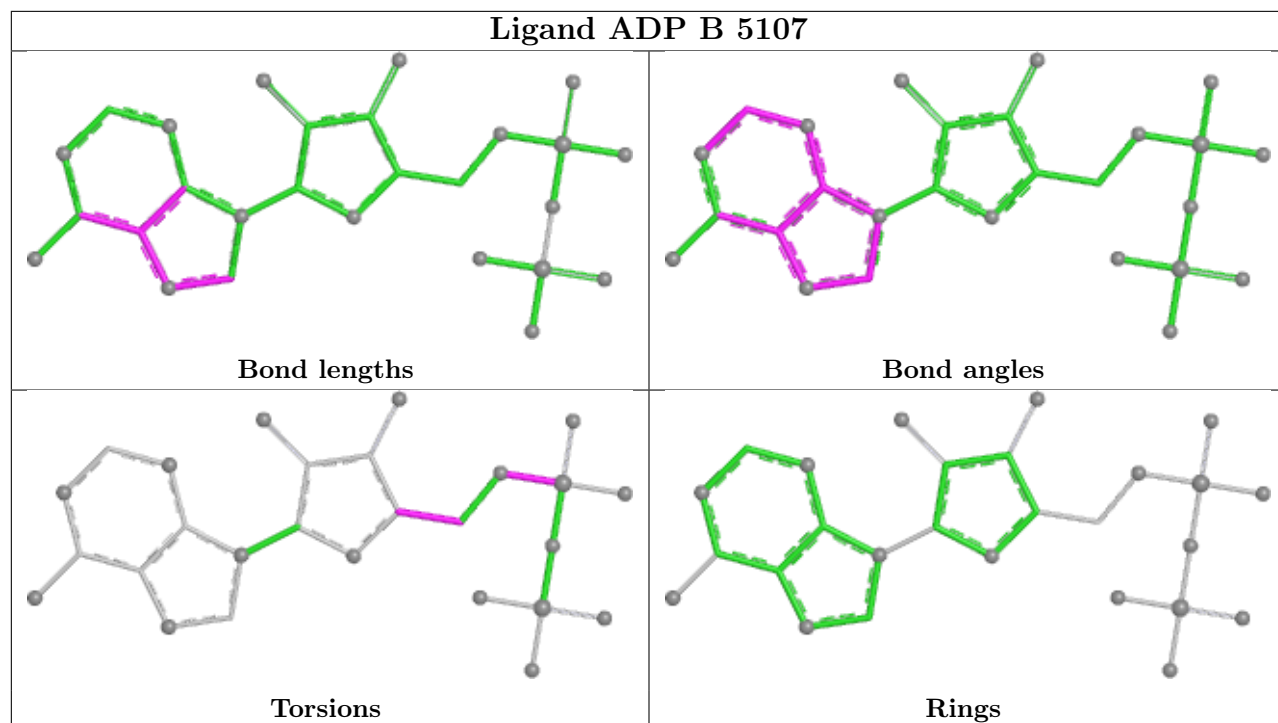


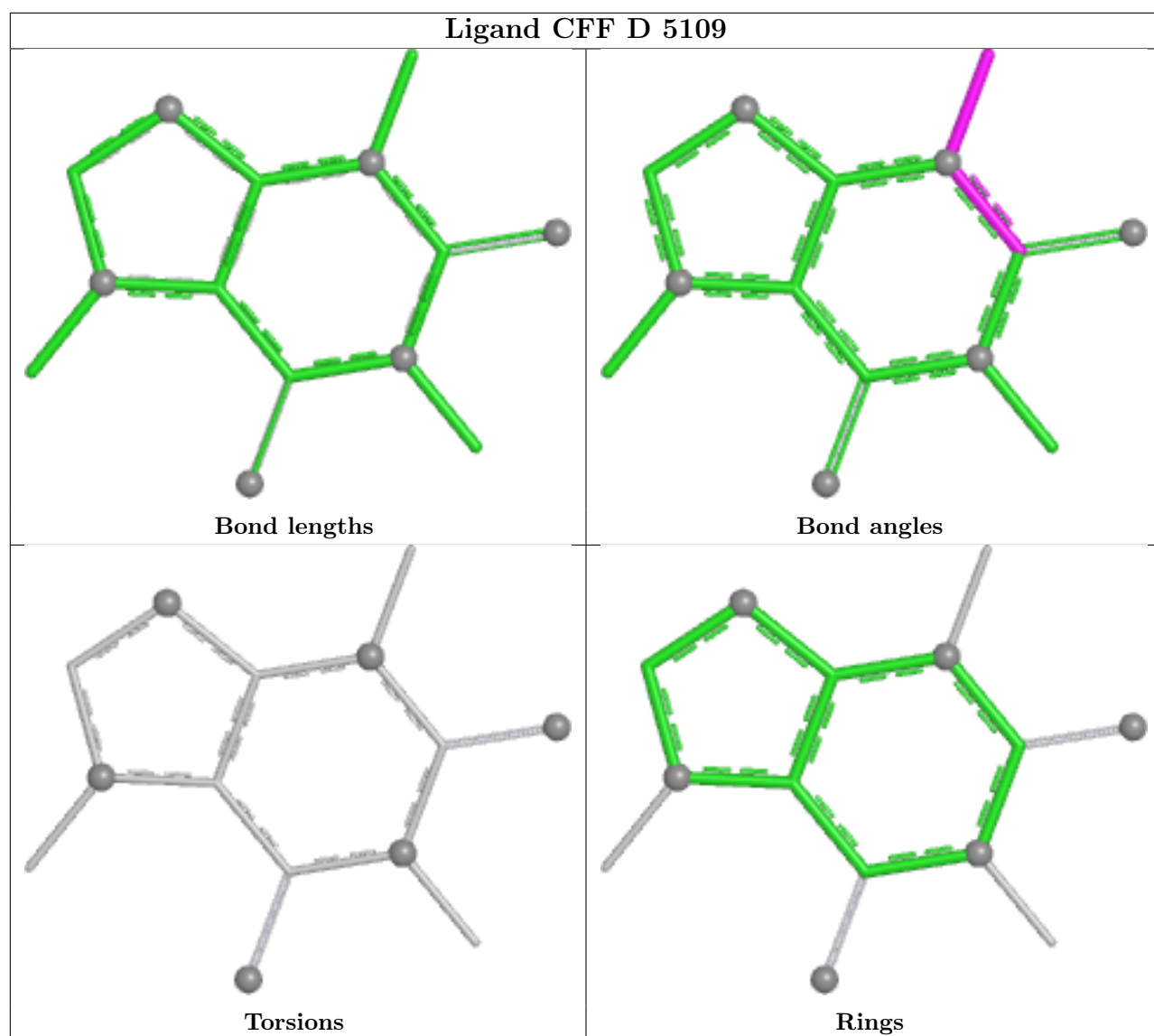
Ligand 43M A 5103

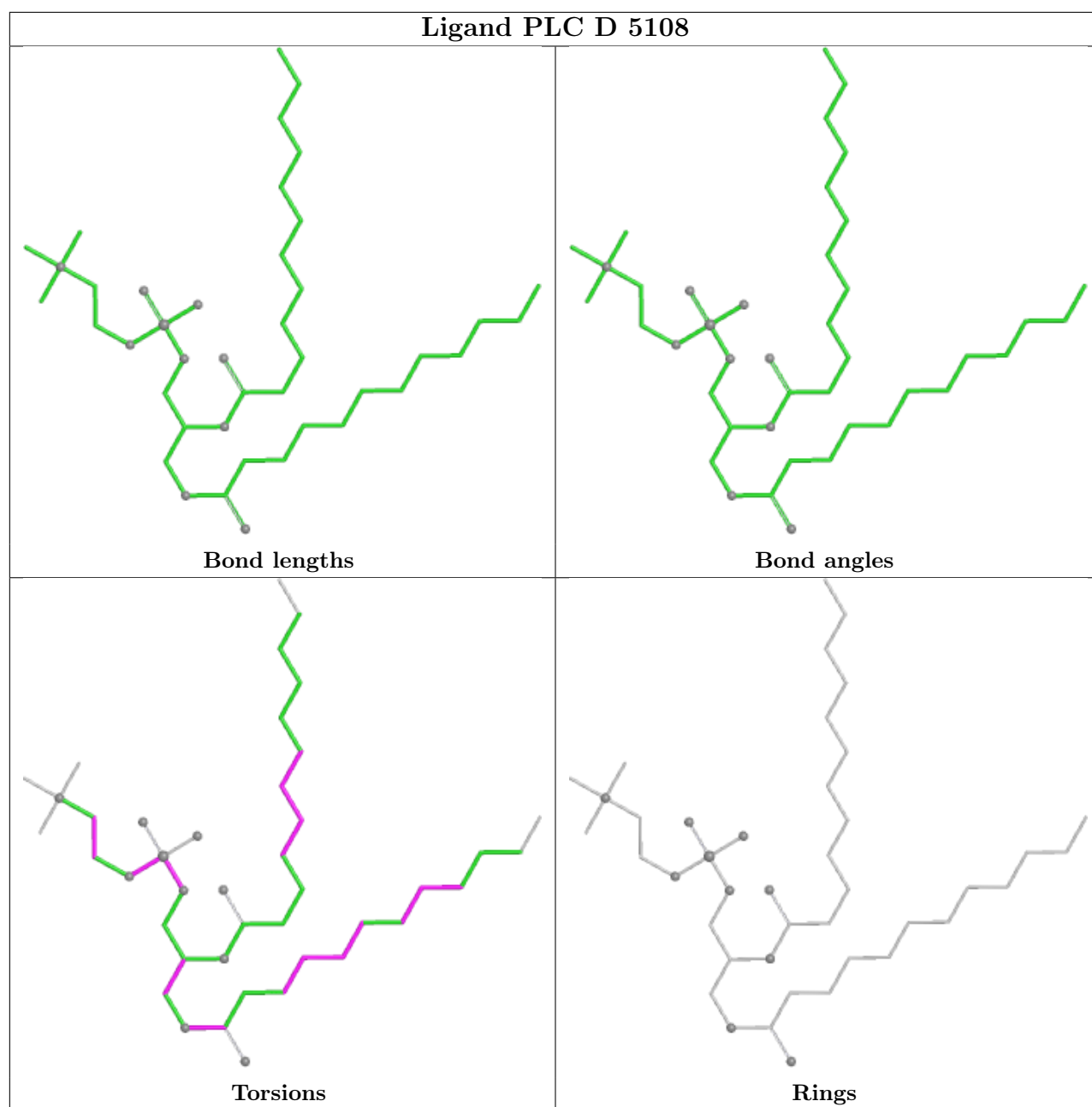


Ligand 43M D 5101

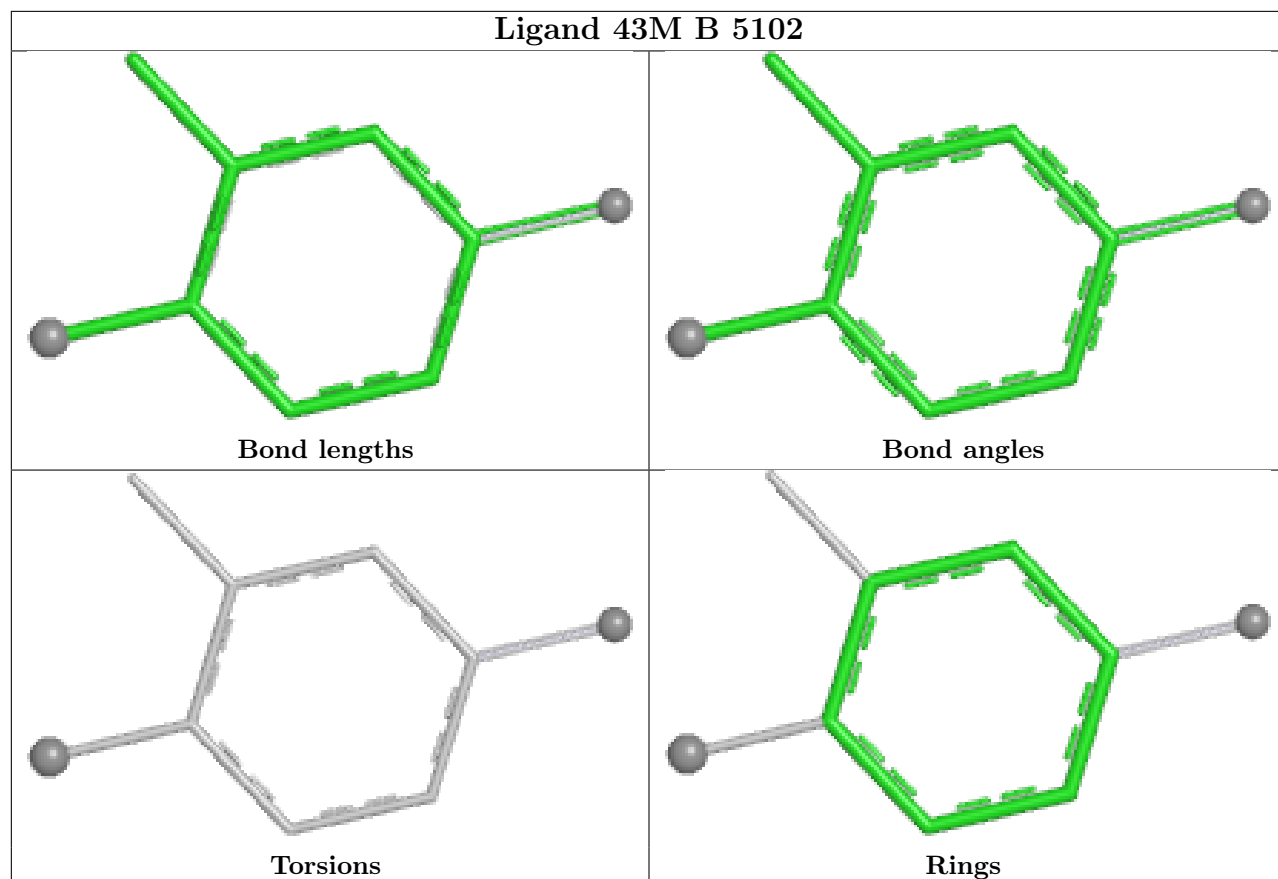




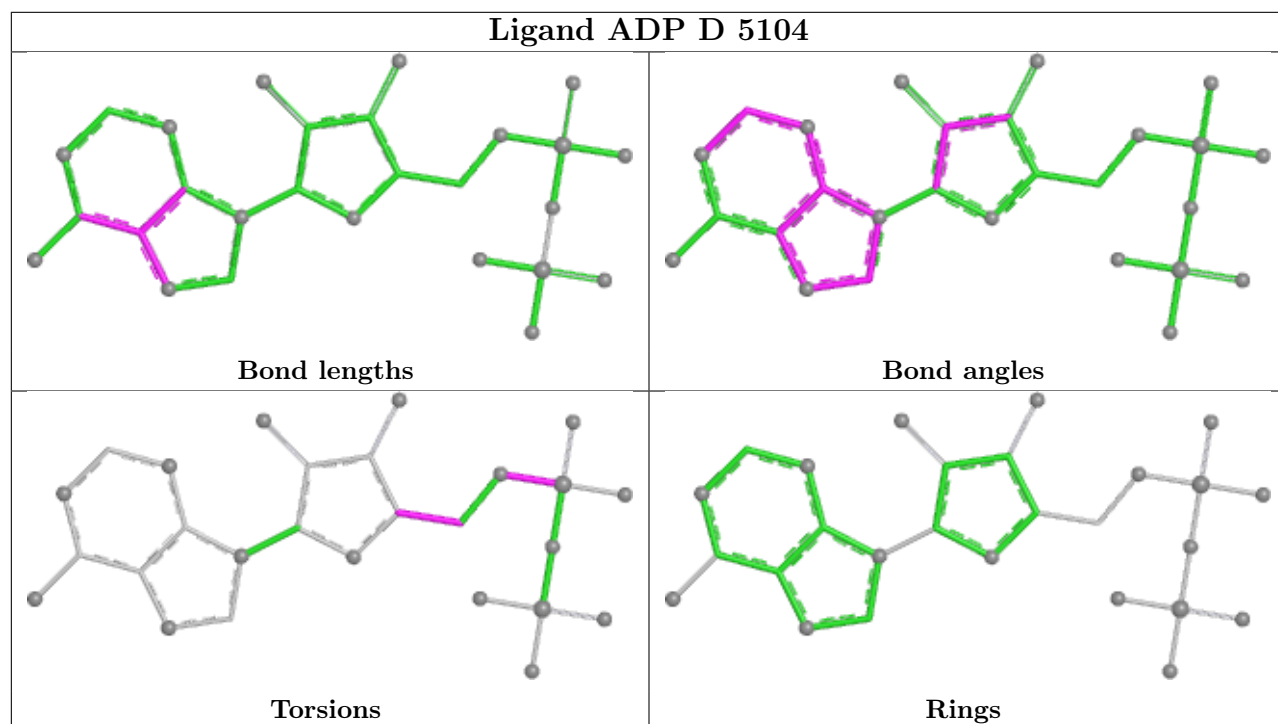


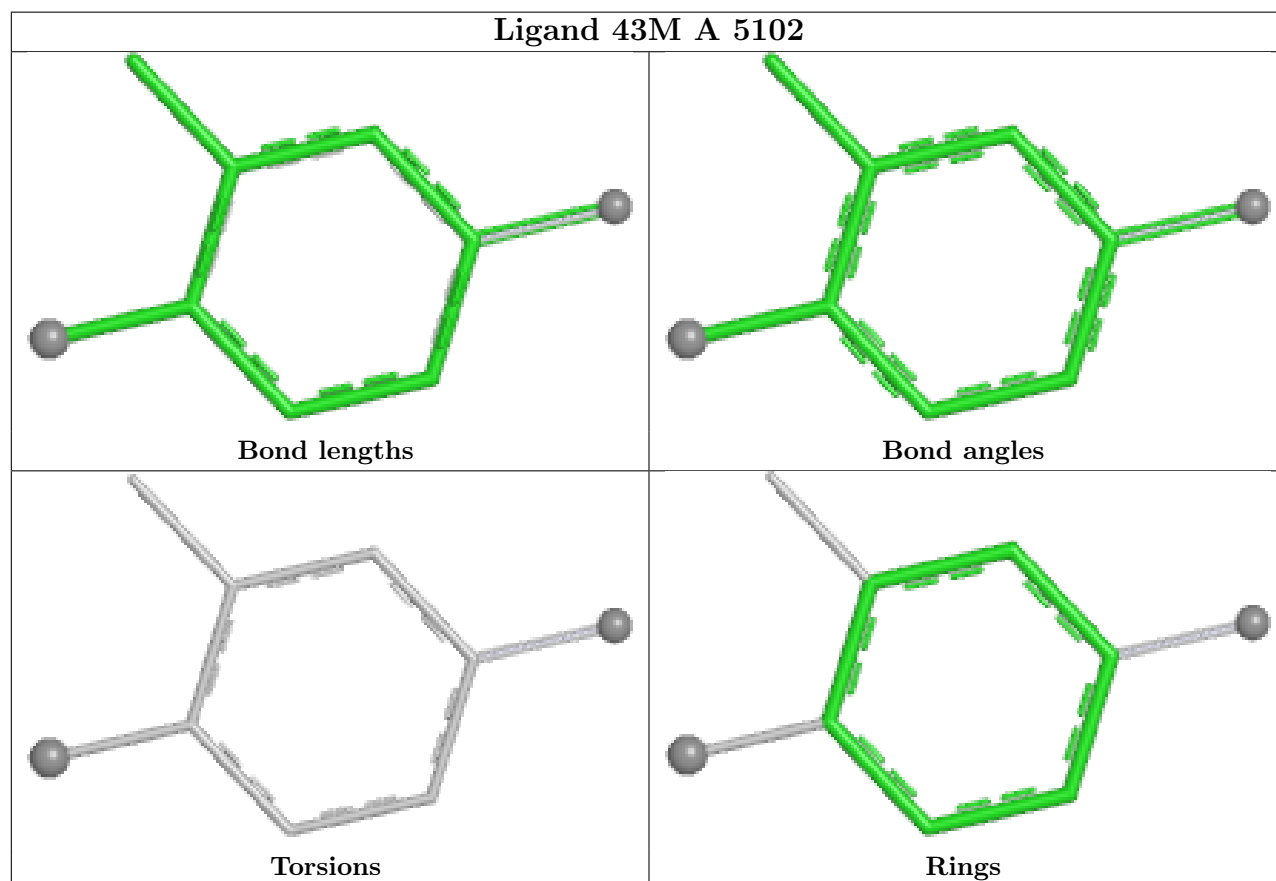
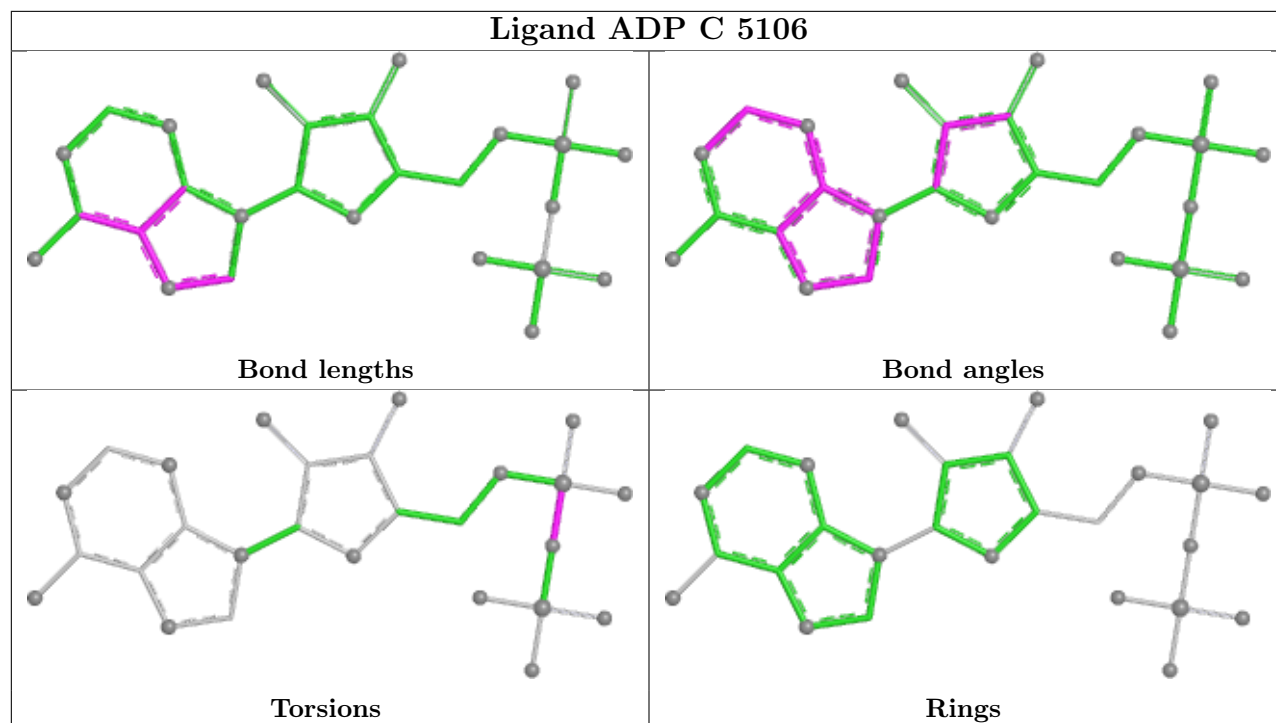


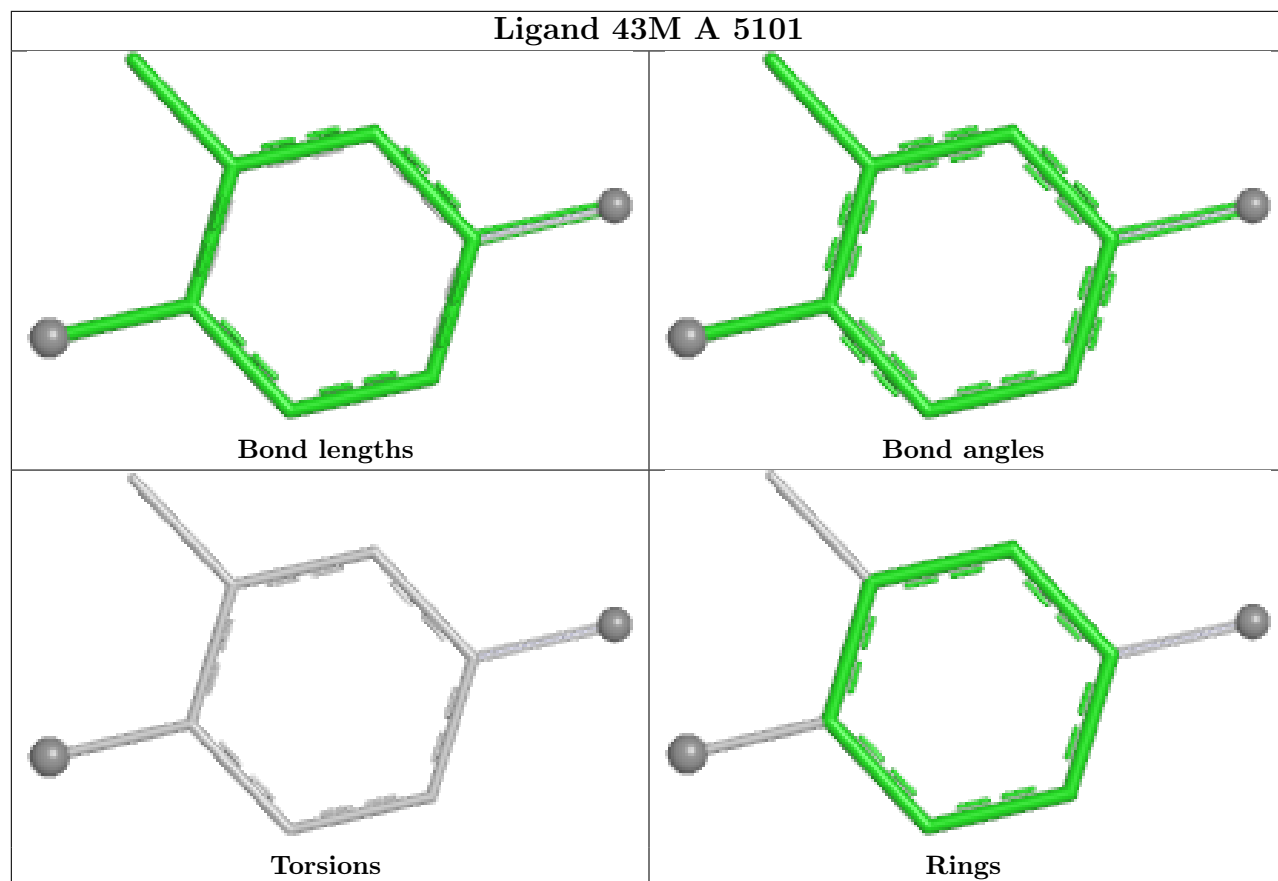
Ligand 43M B 5102

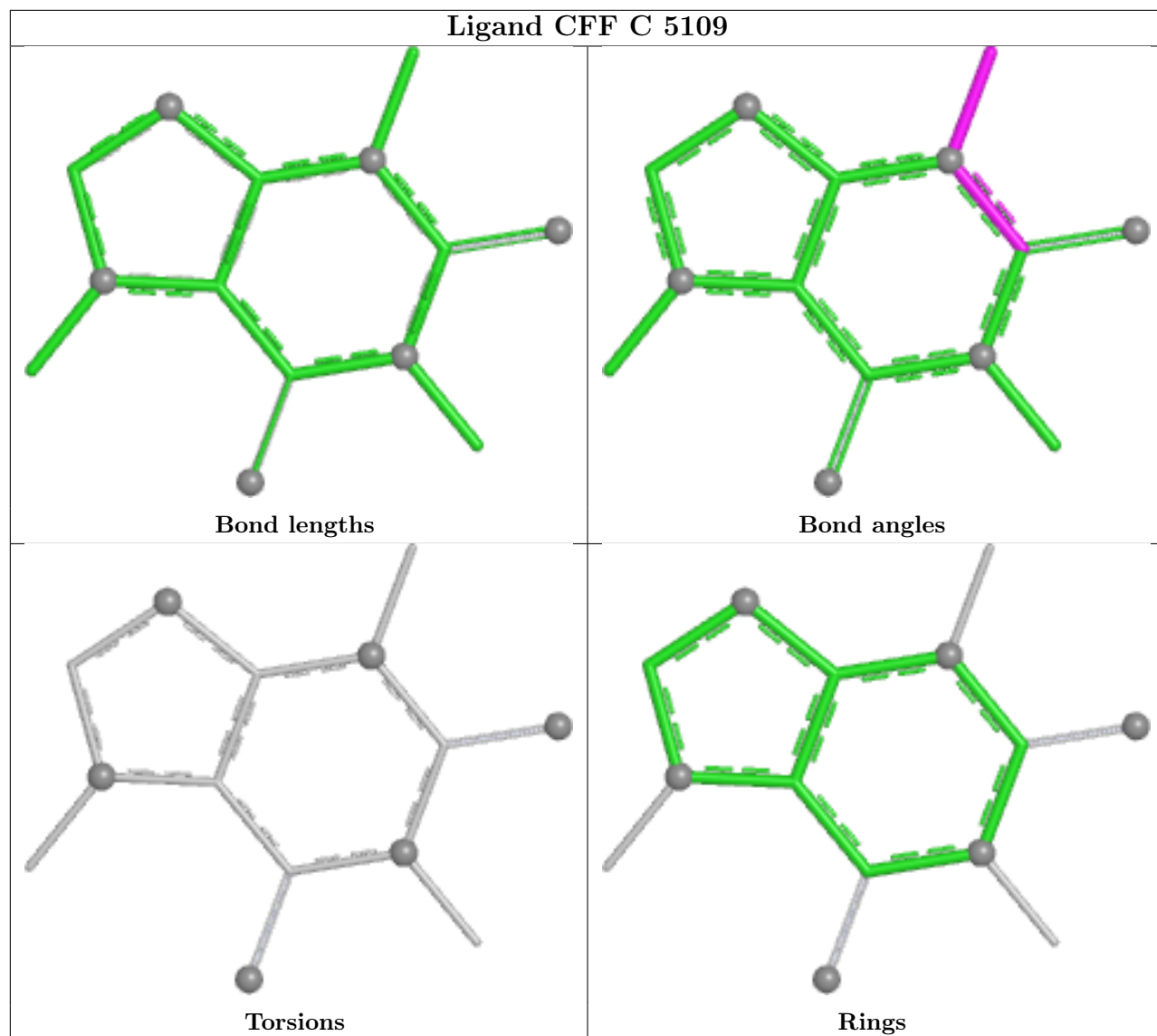


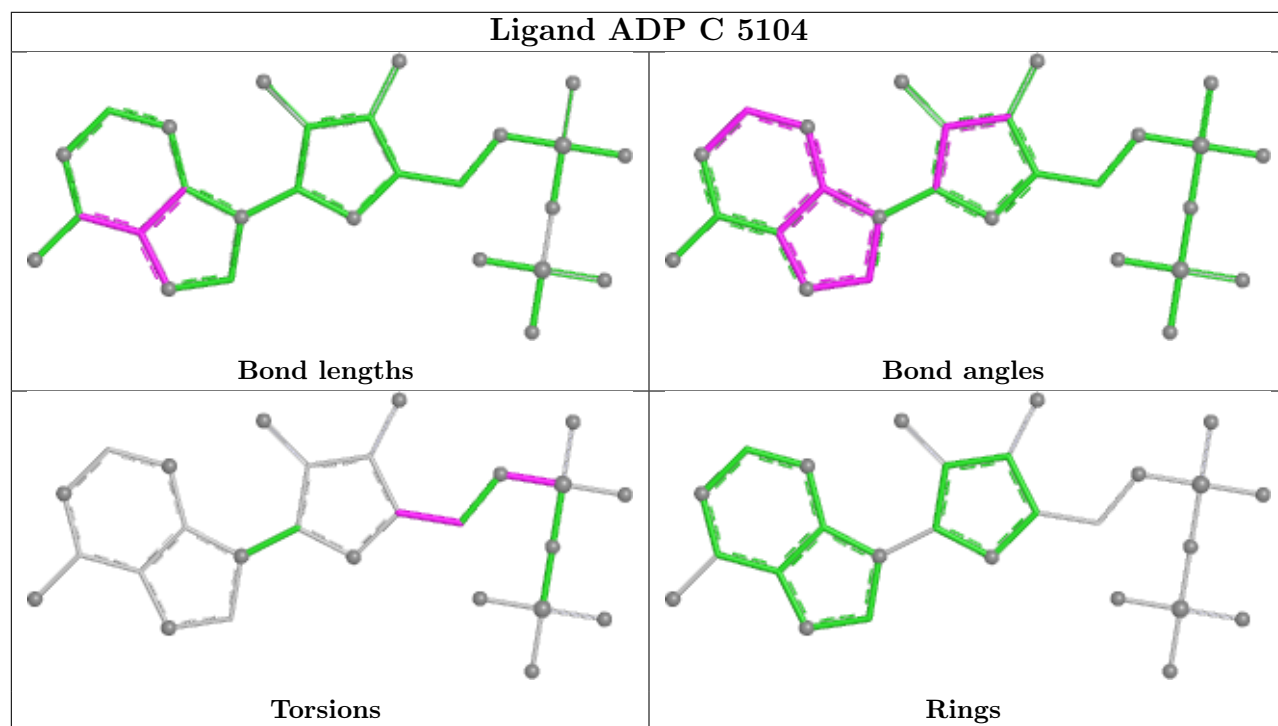
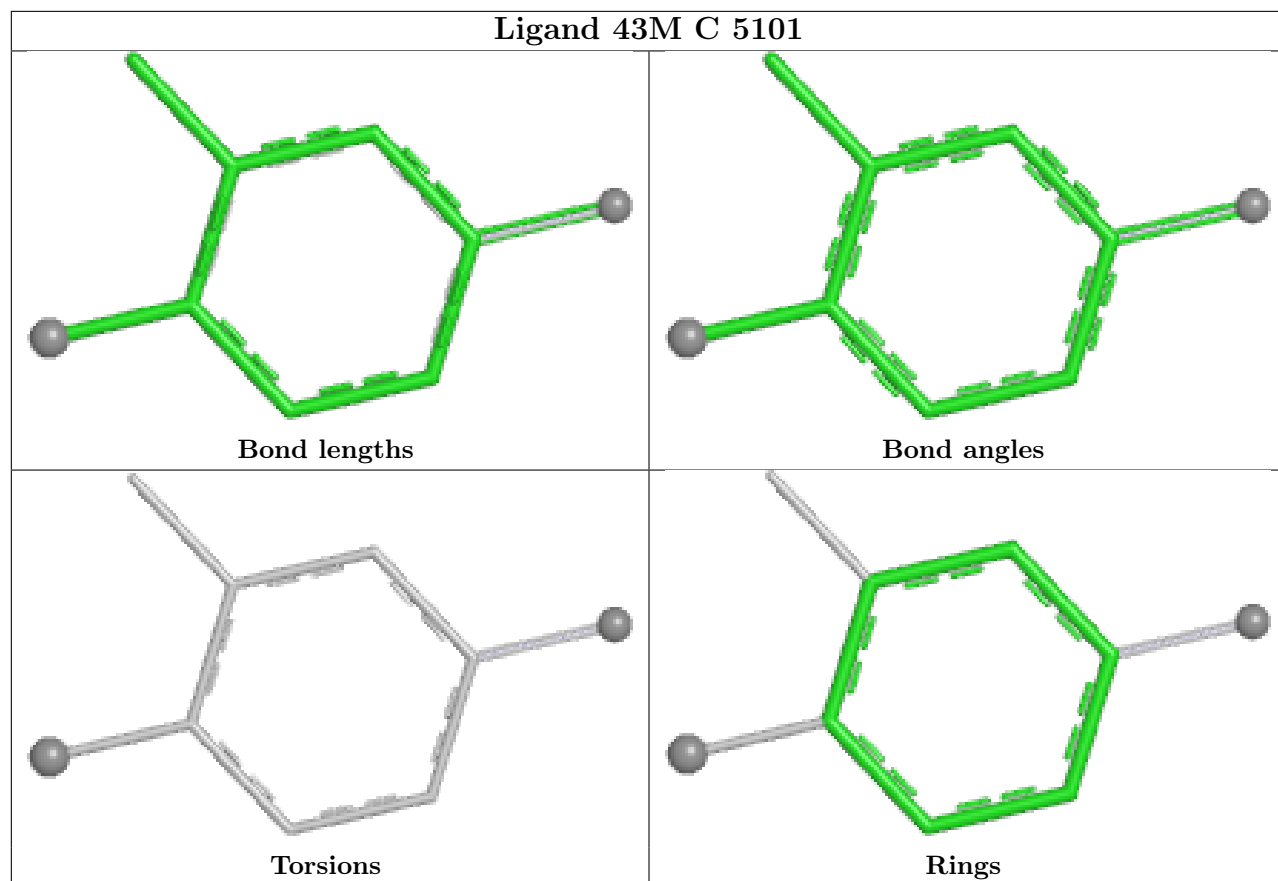
Ligand ADP D 5104

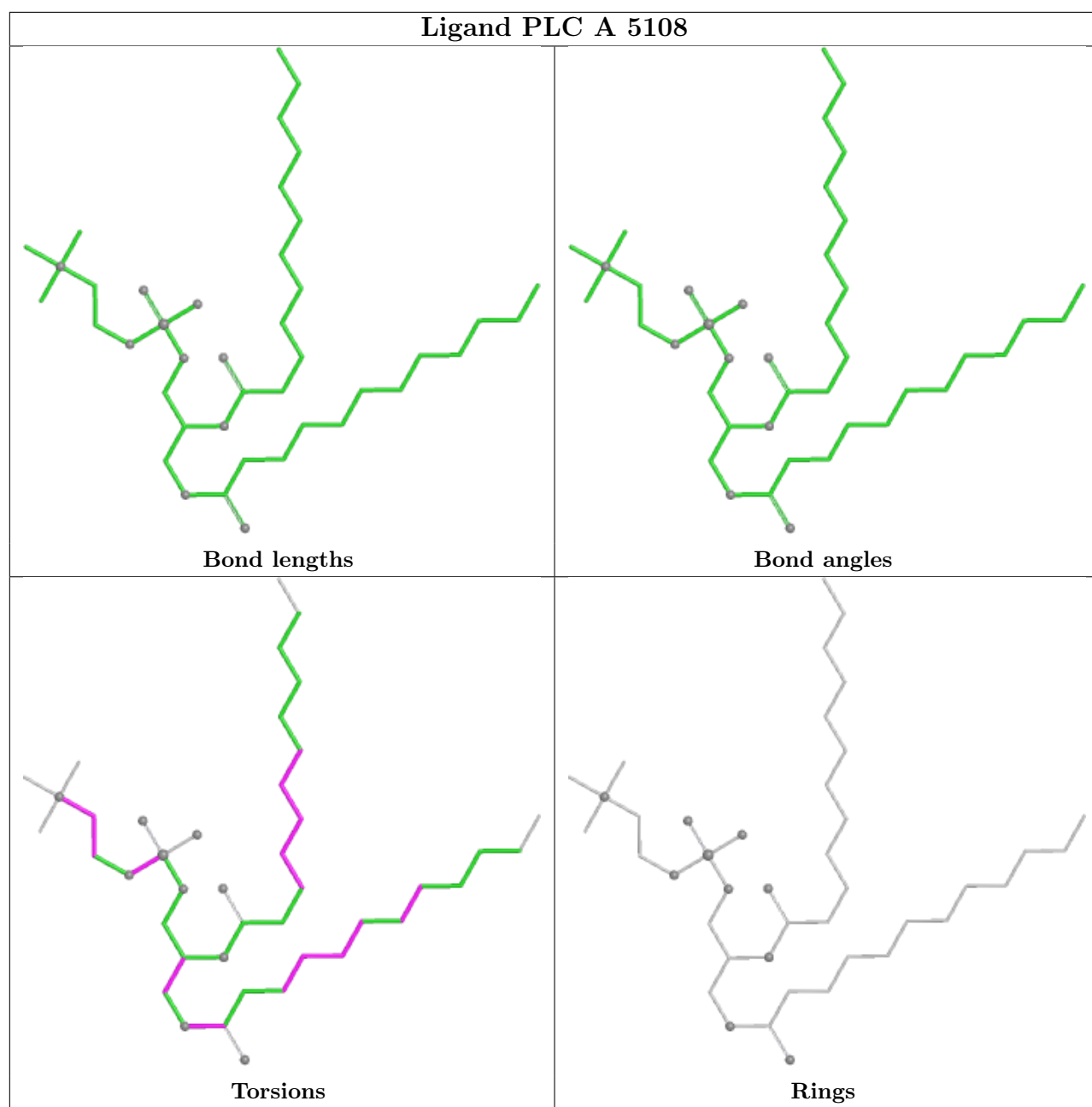




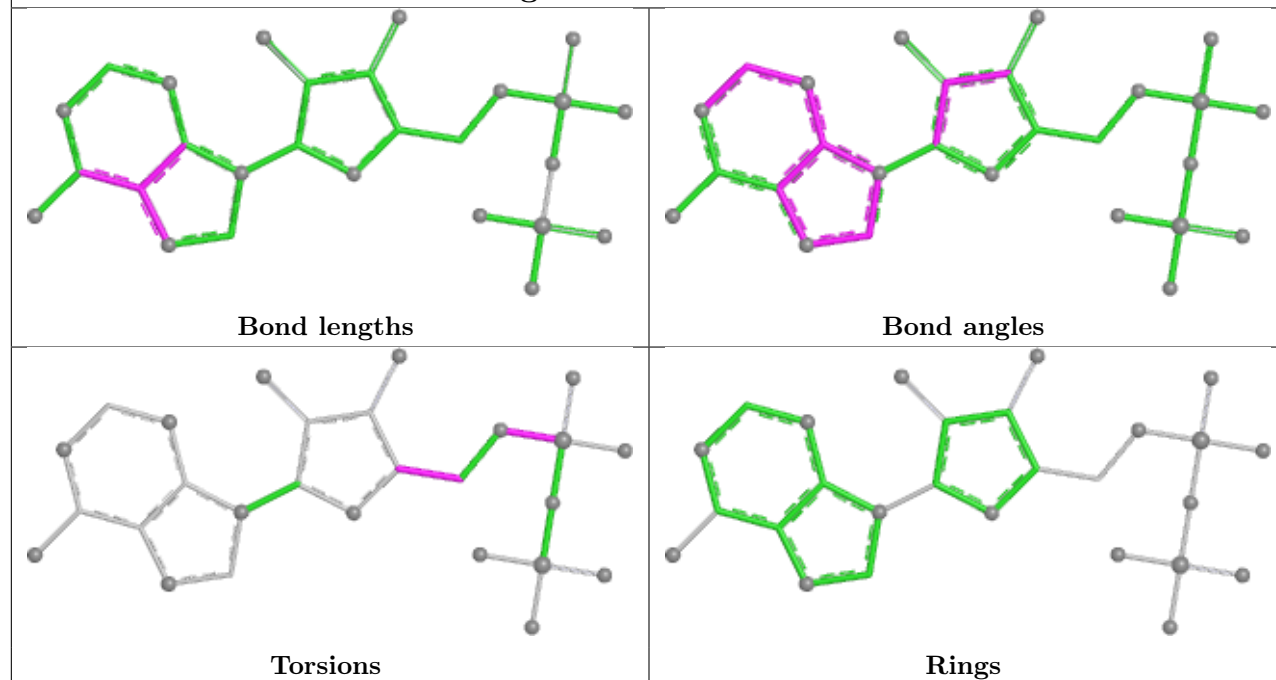




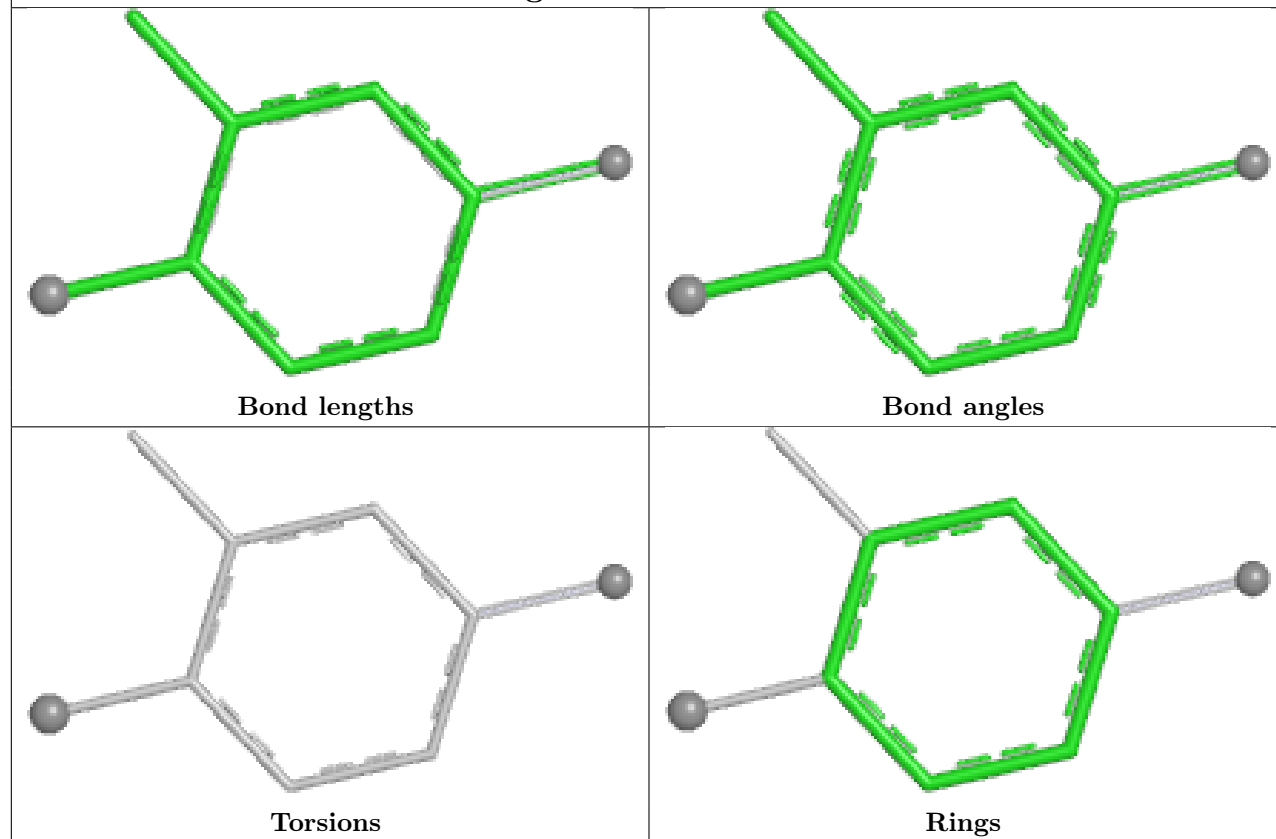


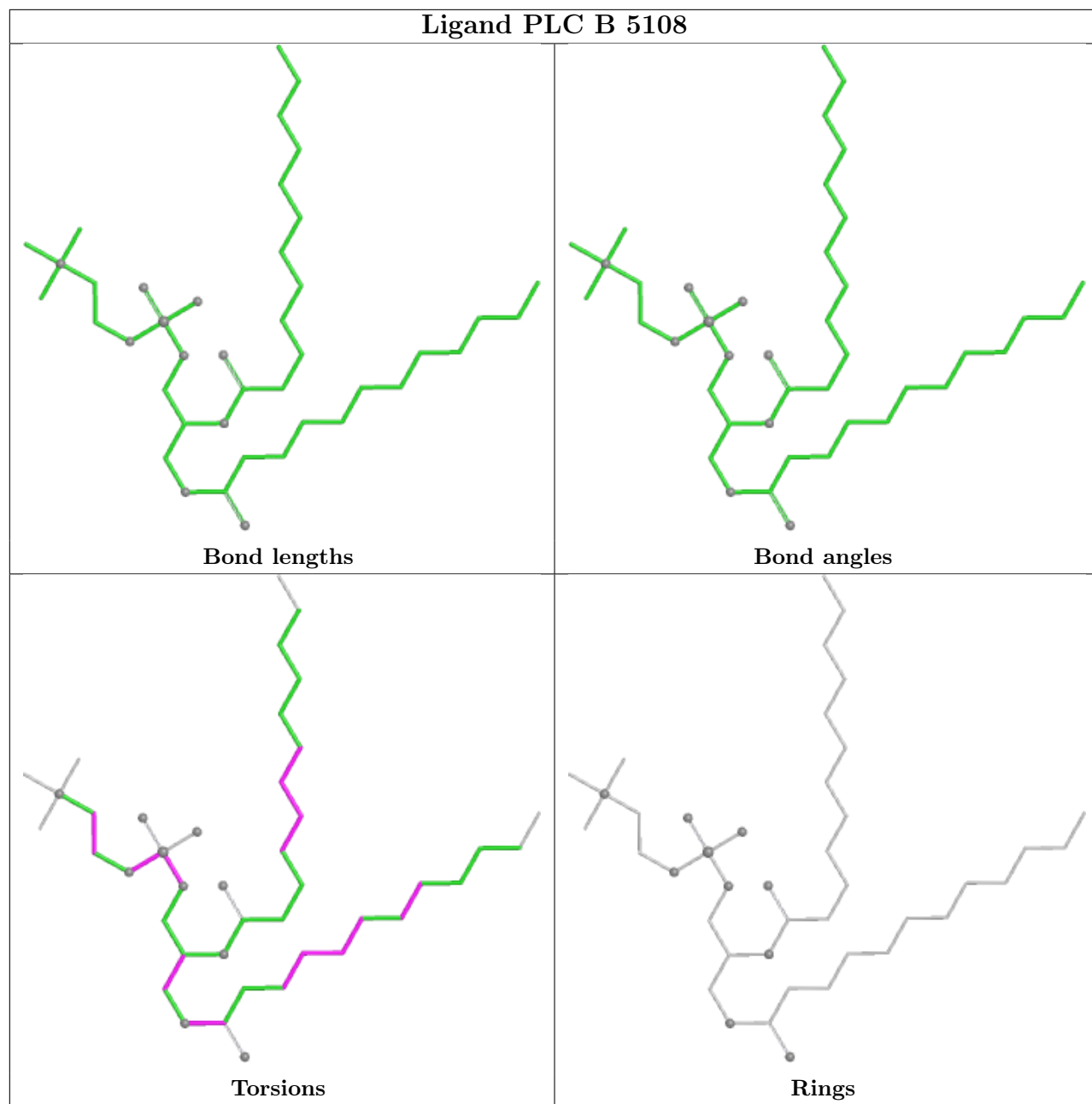


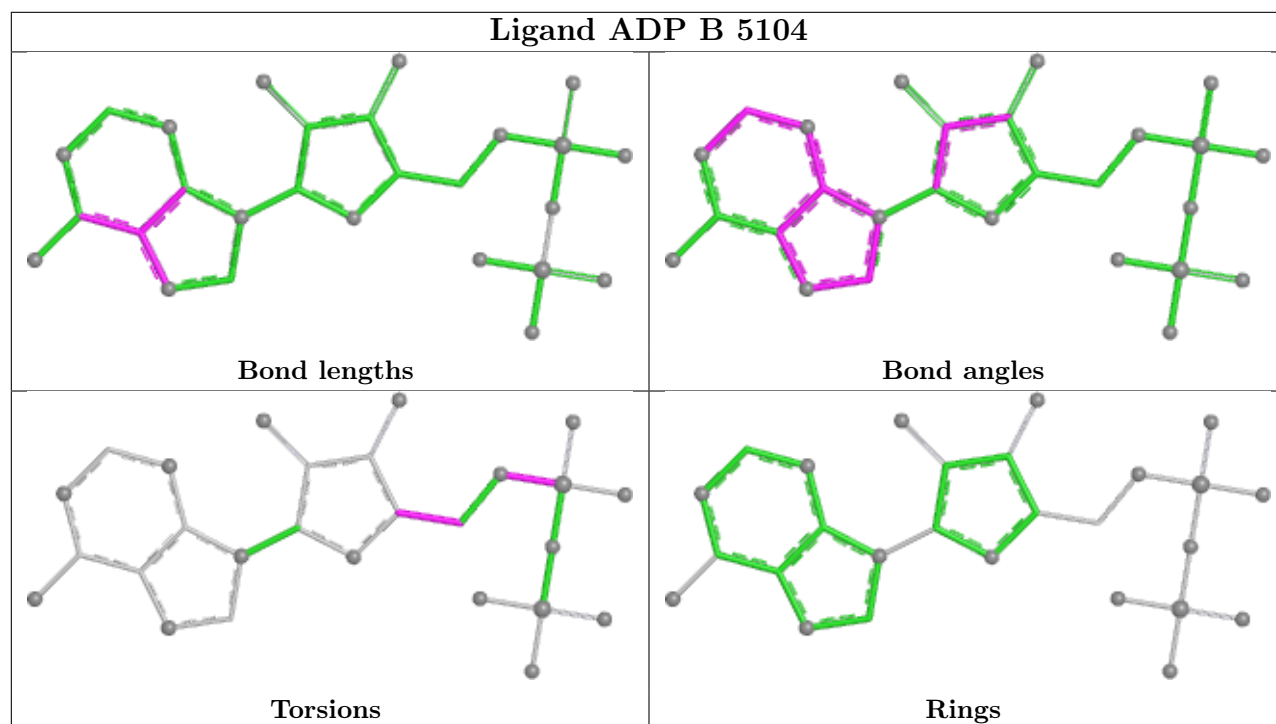
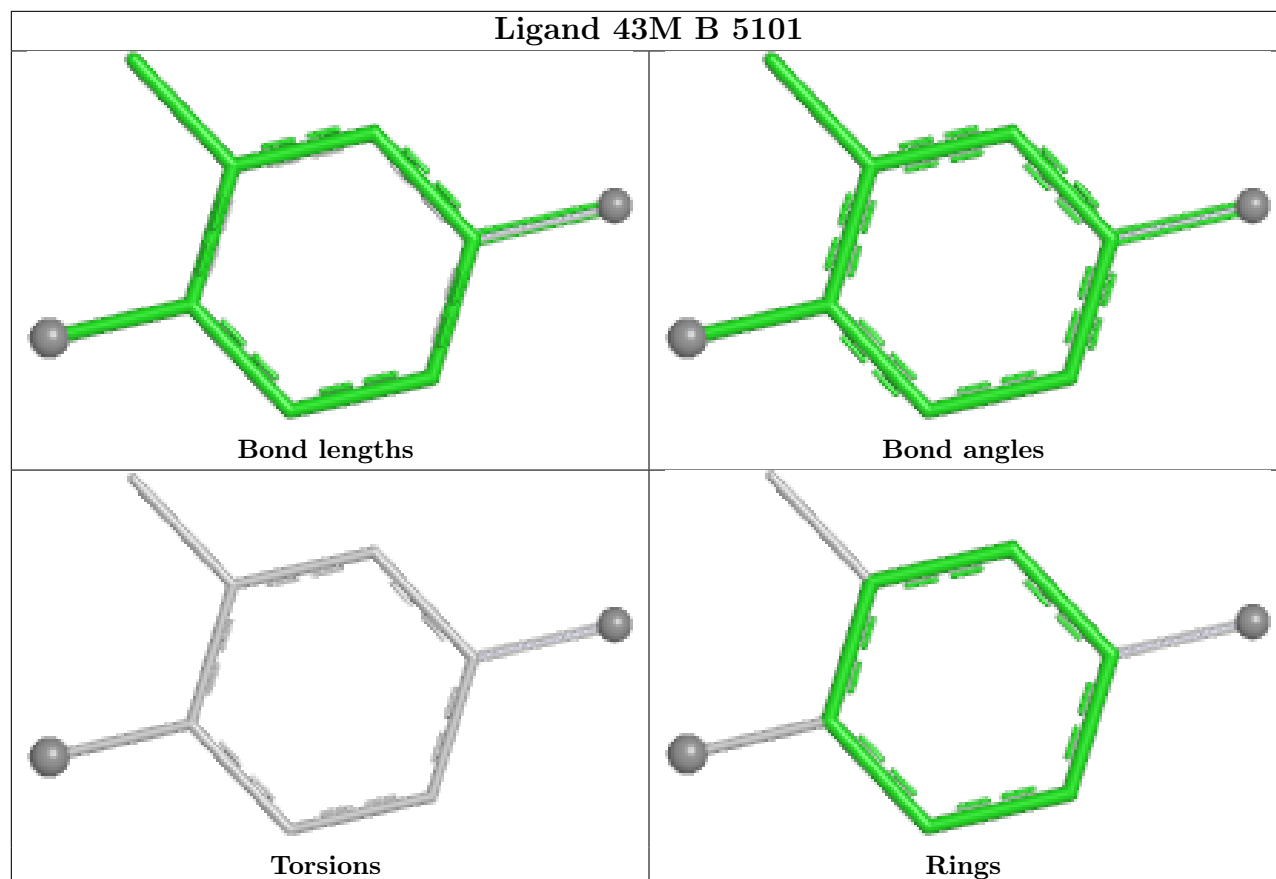
Ligand ADP A 5104

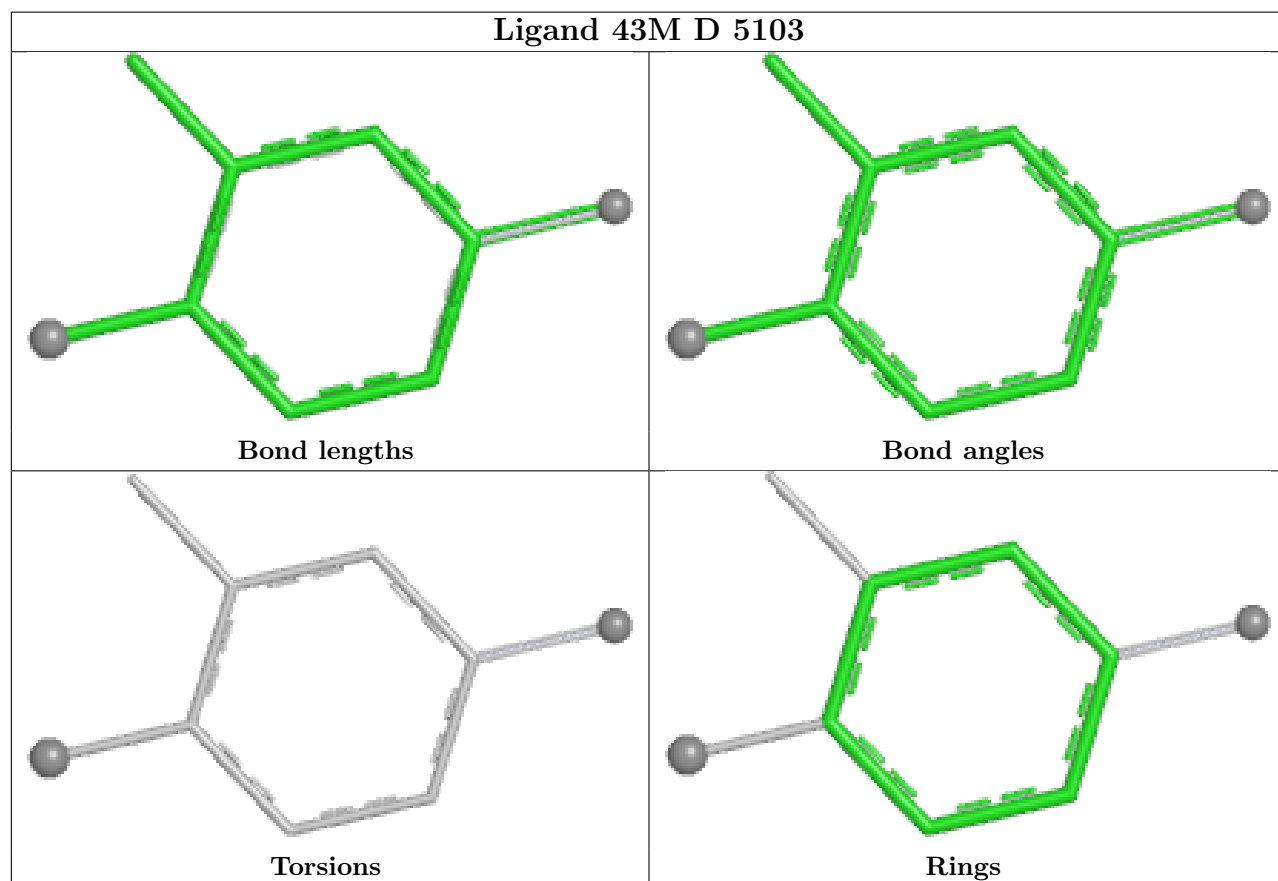
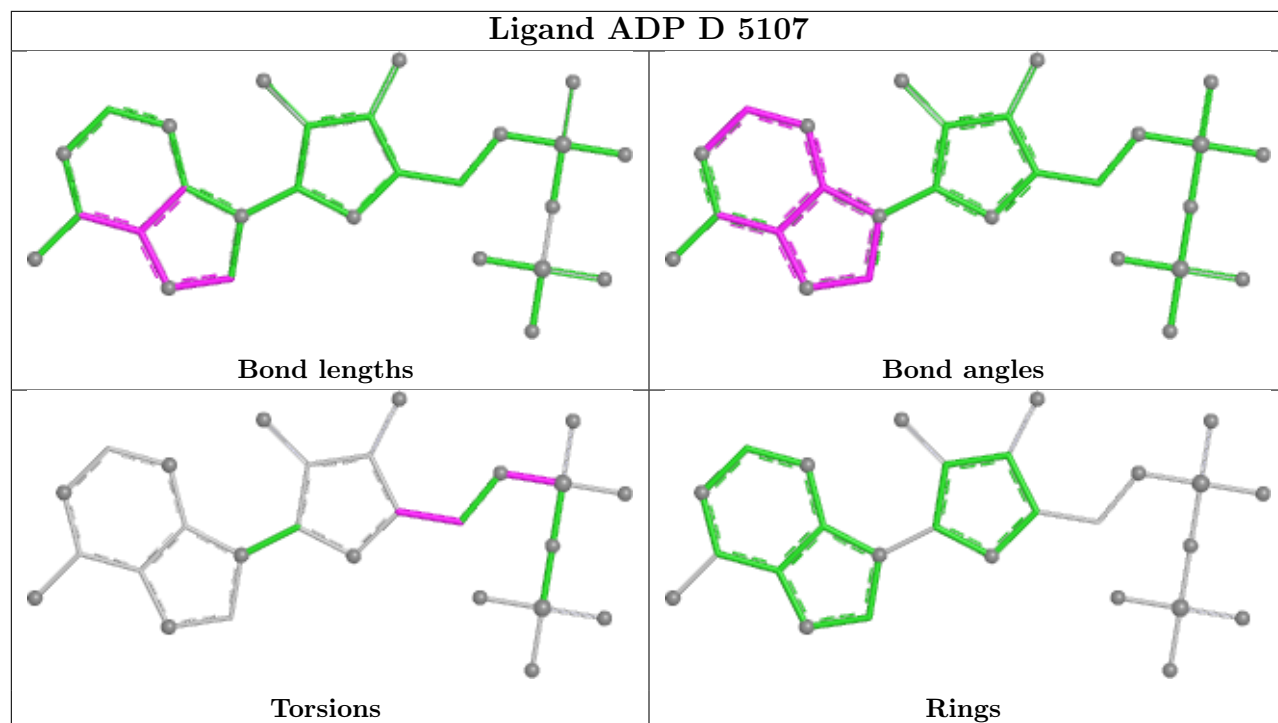


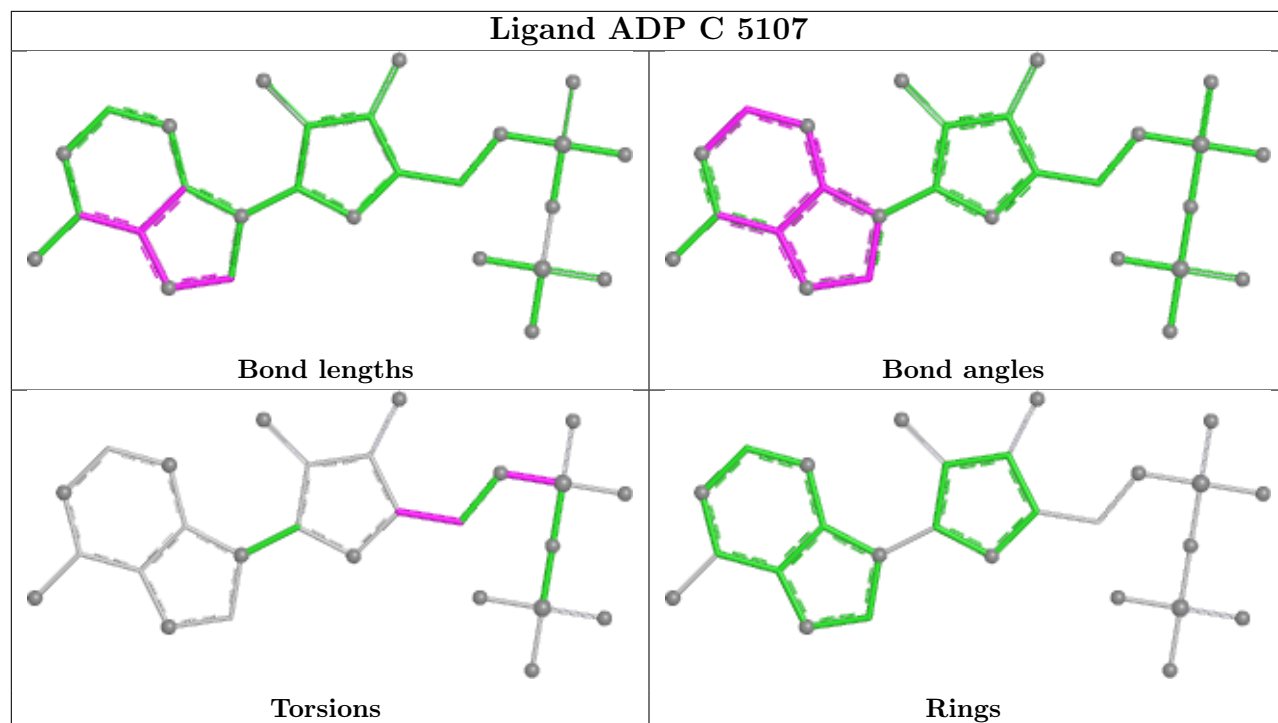
Ligand 43M C 5103

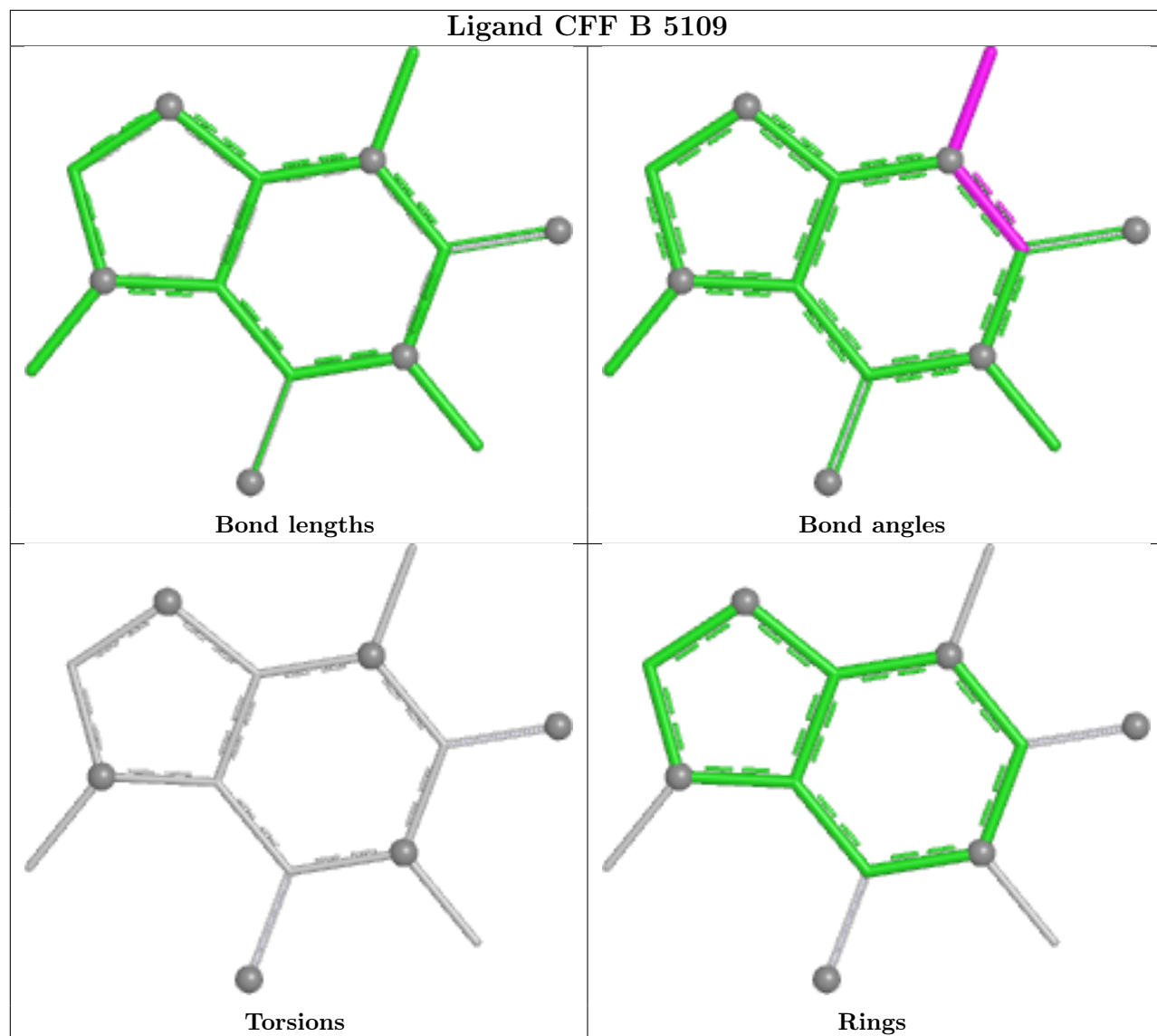


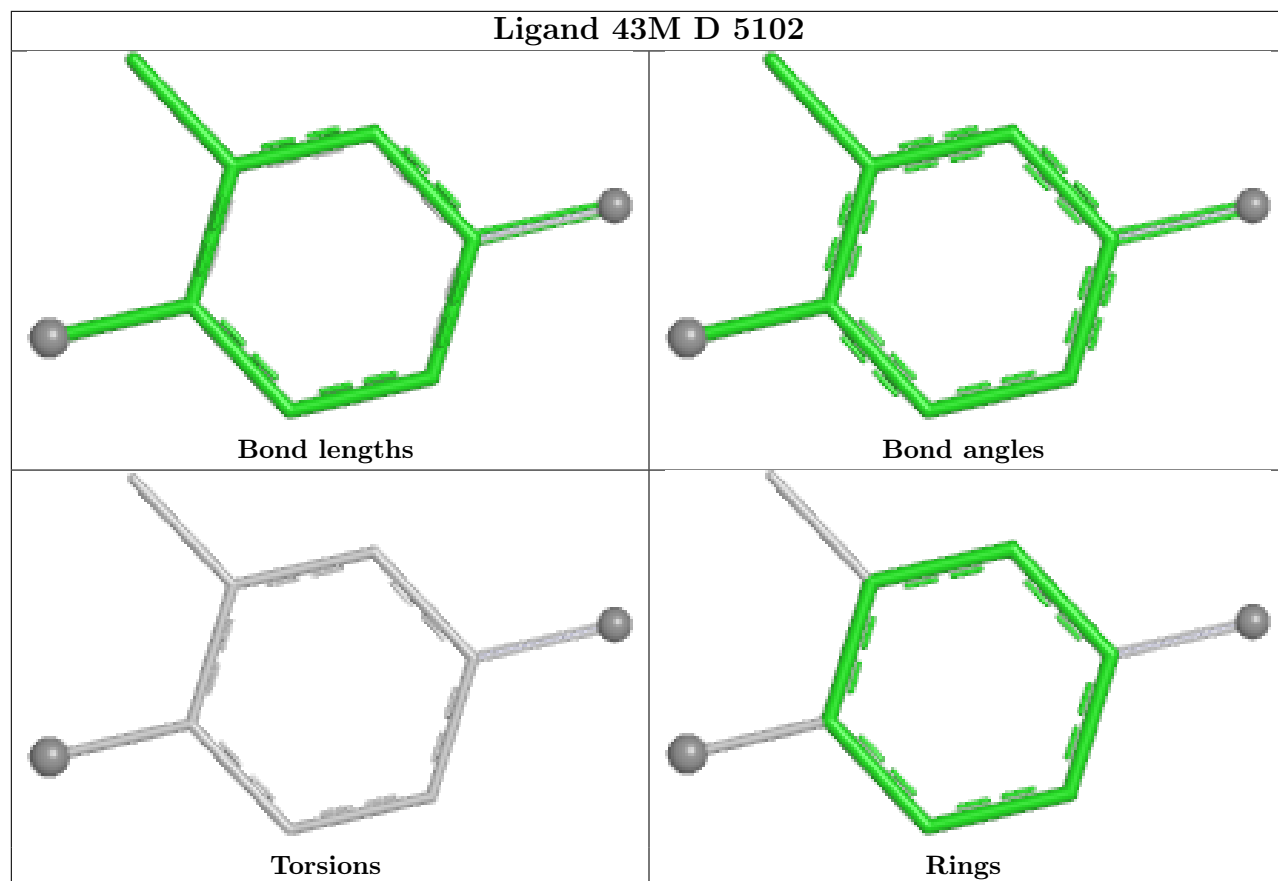


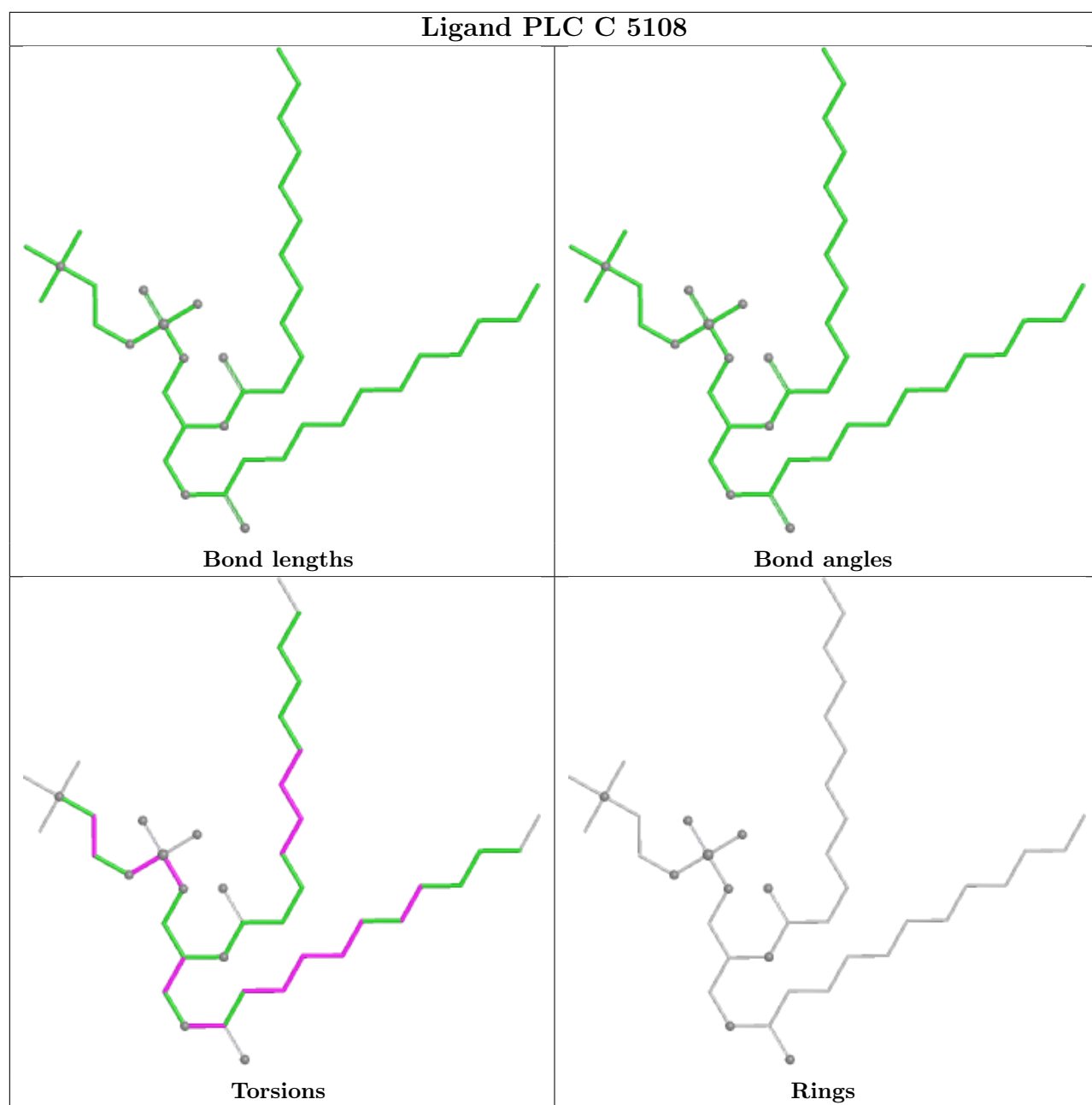


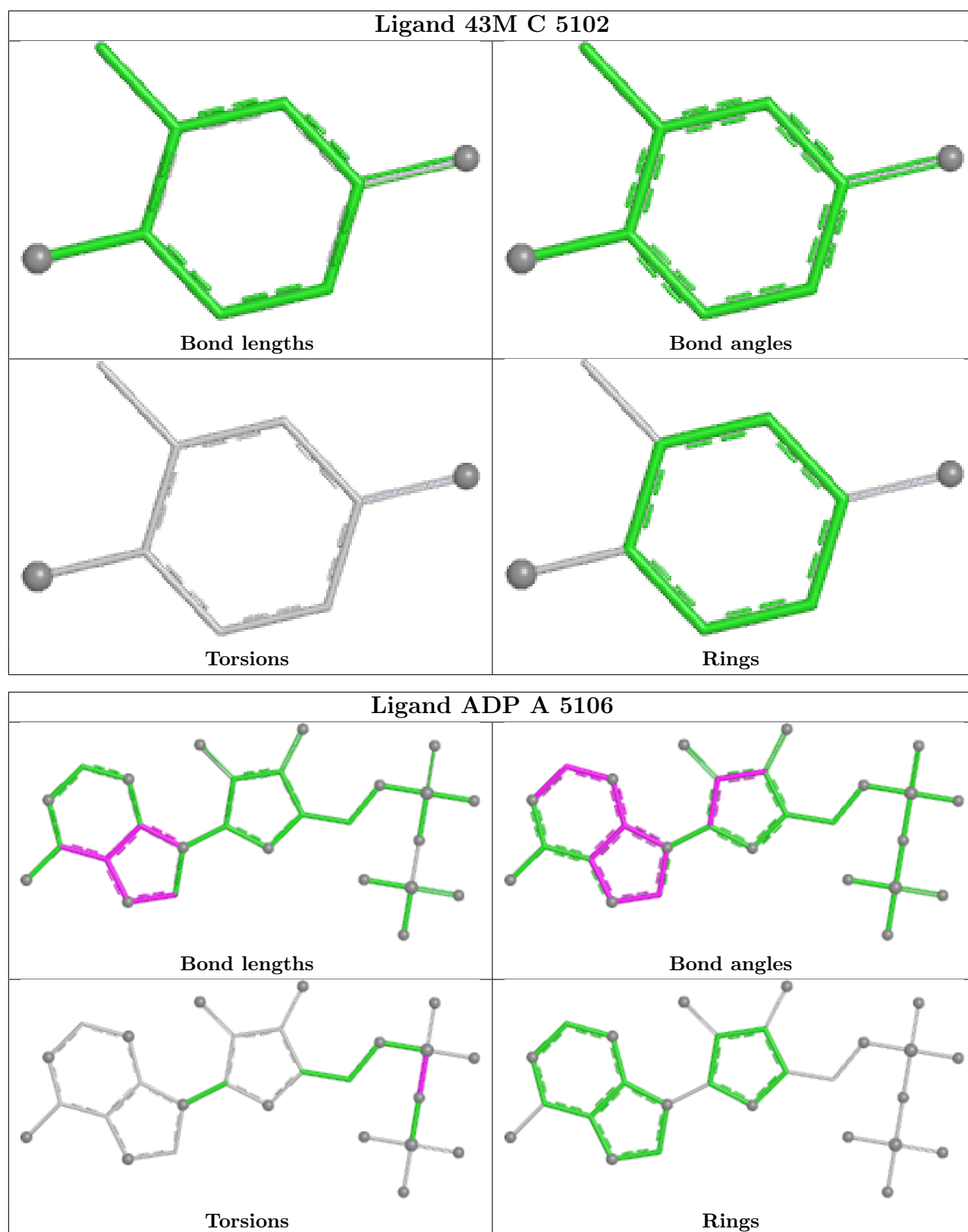












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

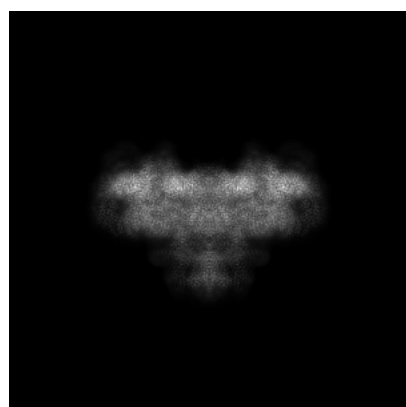
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74441. These allow visual inspection of the internal detail of the map and identification of artifacts.

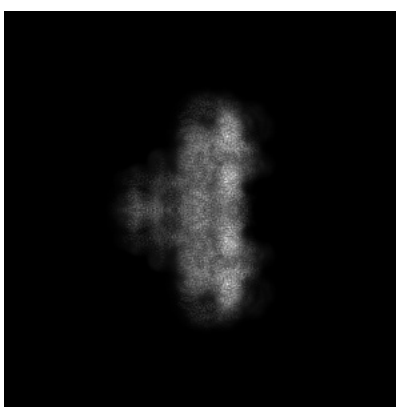
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

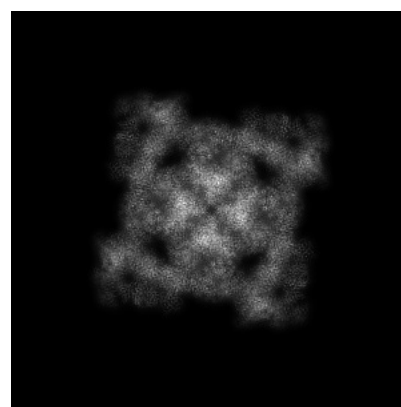
6.1.1 Primary map



X



Y

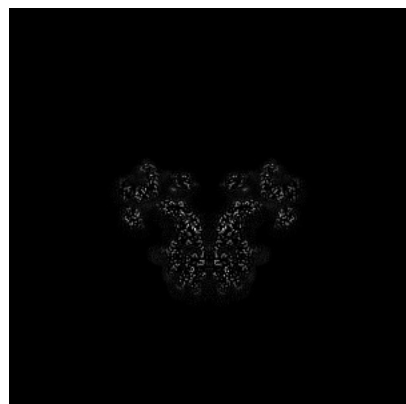


Z

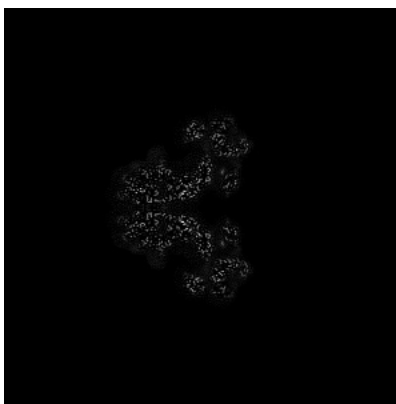
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

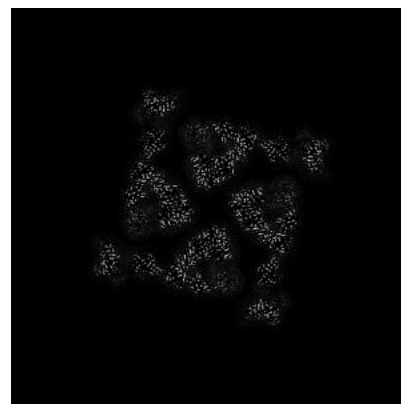
6.2.1 Primary map



X Index: 300



Y Index: 300

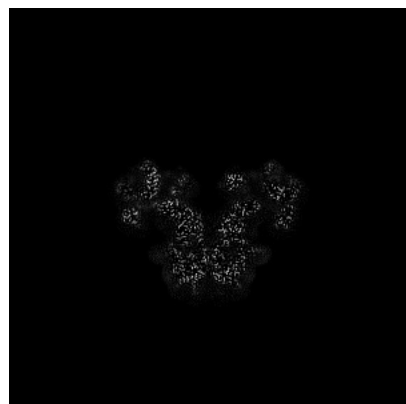


Z Index: 300

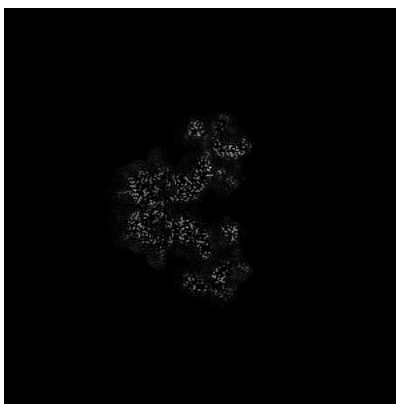
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

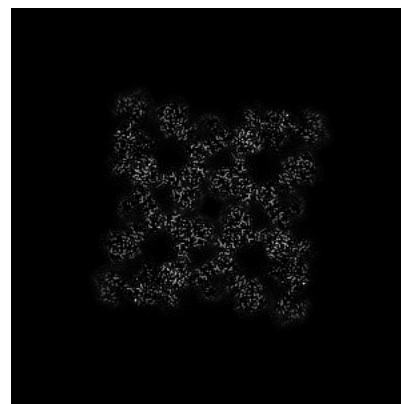
6.3.1 Primary map



X Index: 304



Y Index: 304

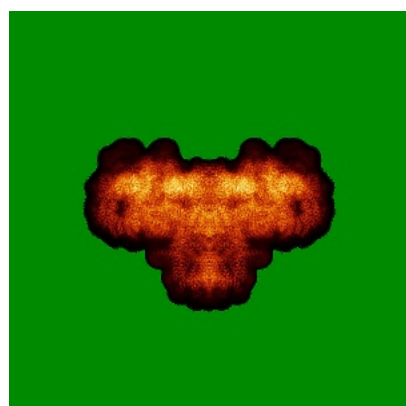


Z Index: 332

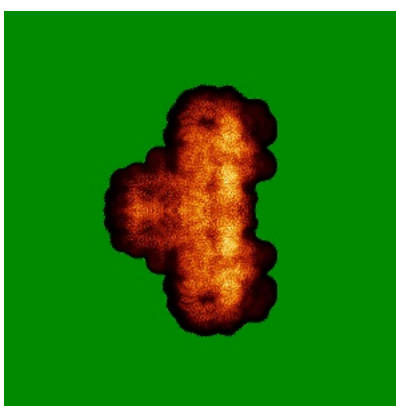
The images above show the largest variance slices of the map in three orthogonal directions.

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

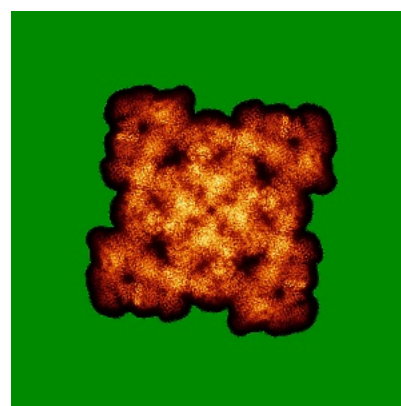
6.4.1 Primary map



X



Y

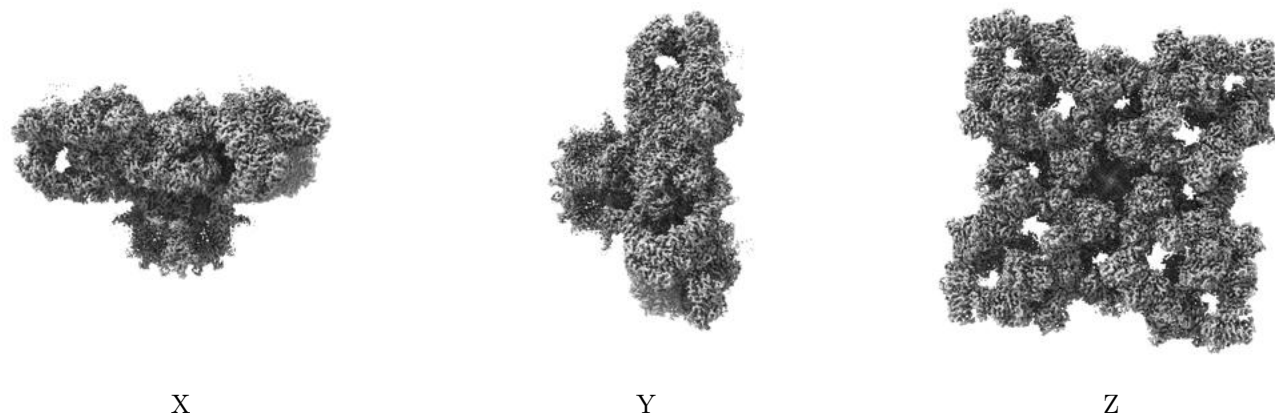


Z

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

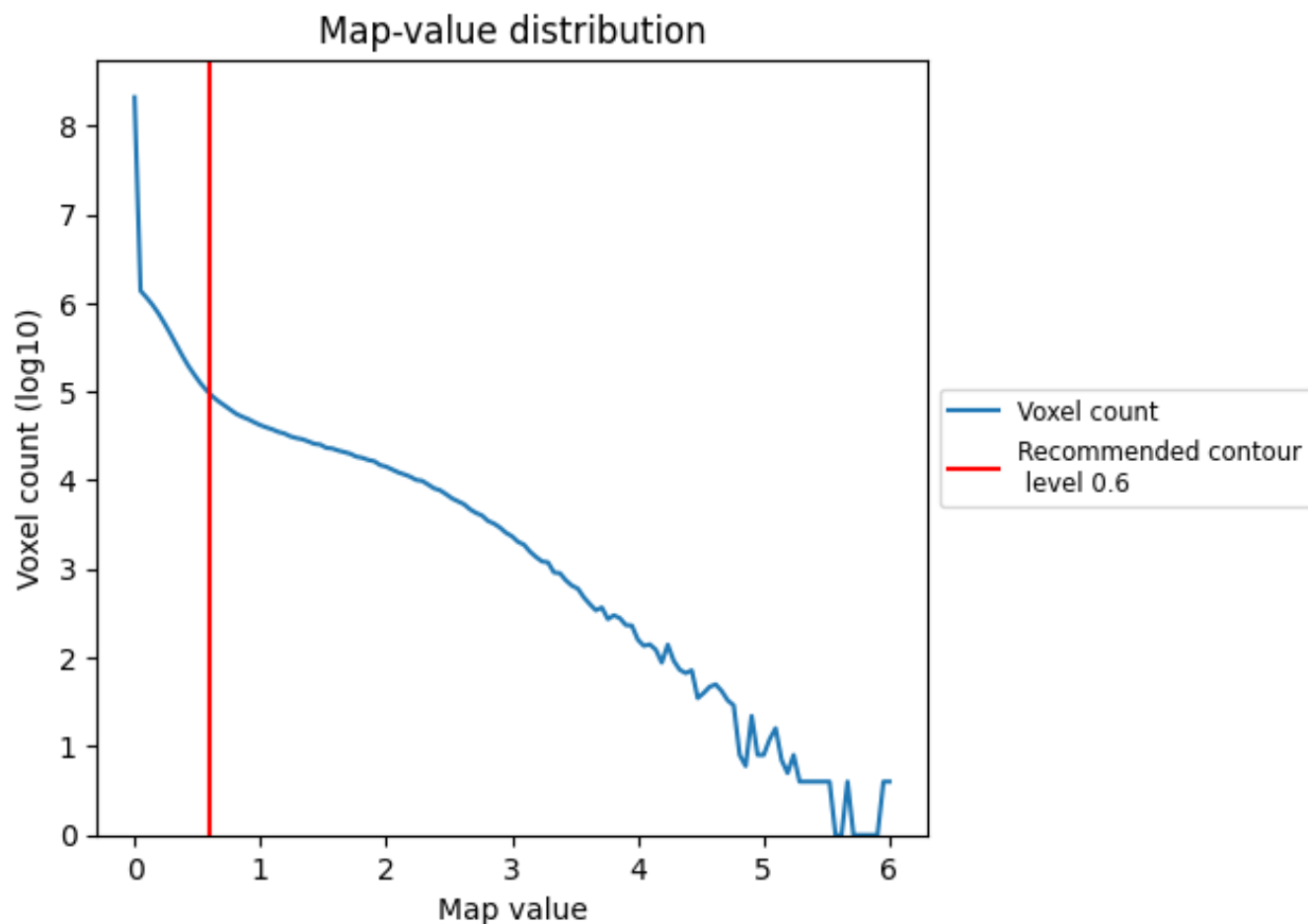
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

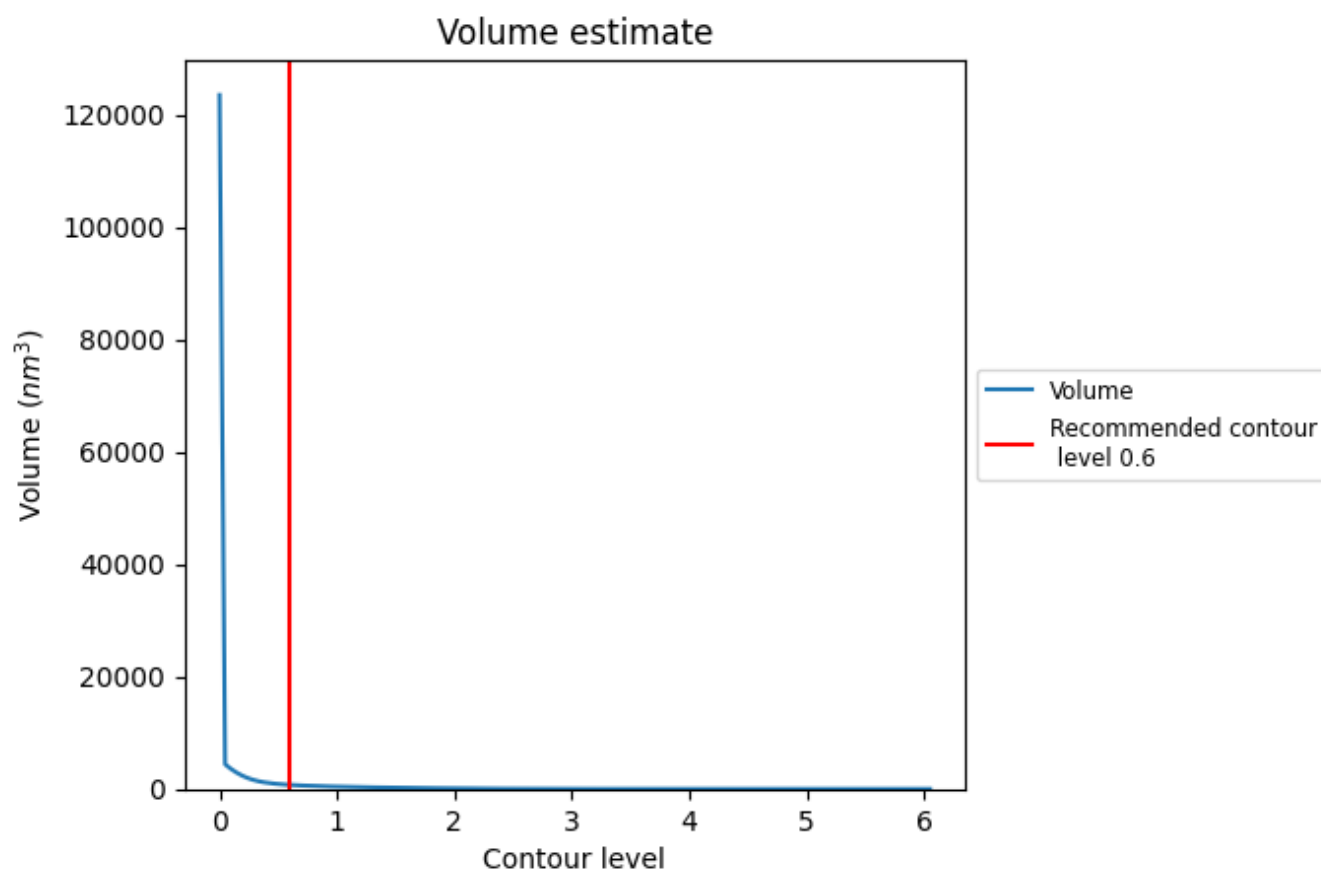
This section contains the results of statistical analysis of the map.

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.

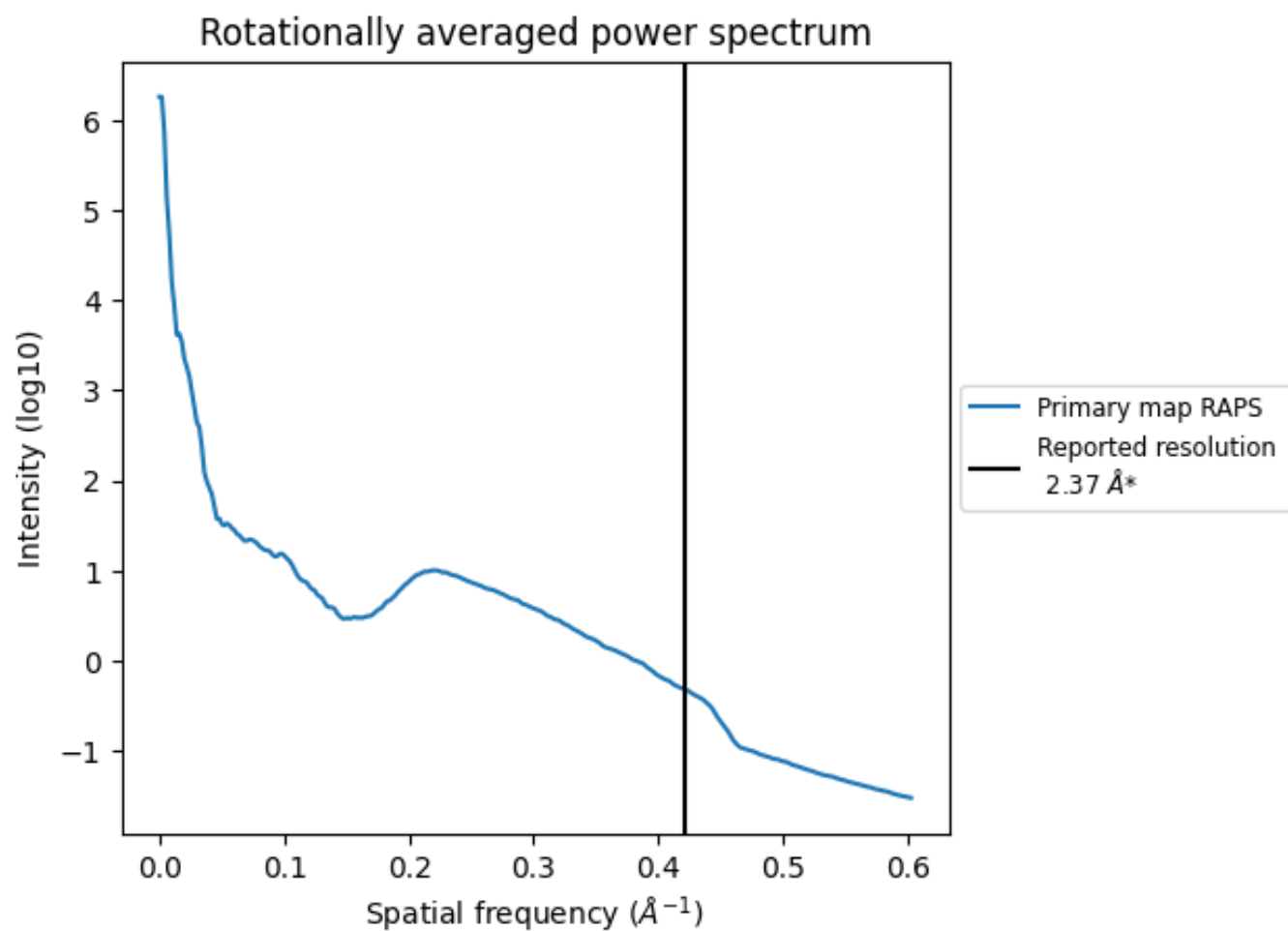
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 725 nm³; this corresponds to an approximate mass of 655 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 0.422 Å⁻¹

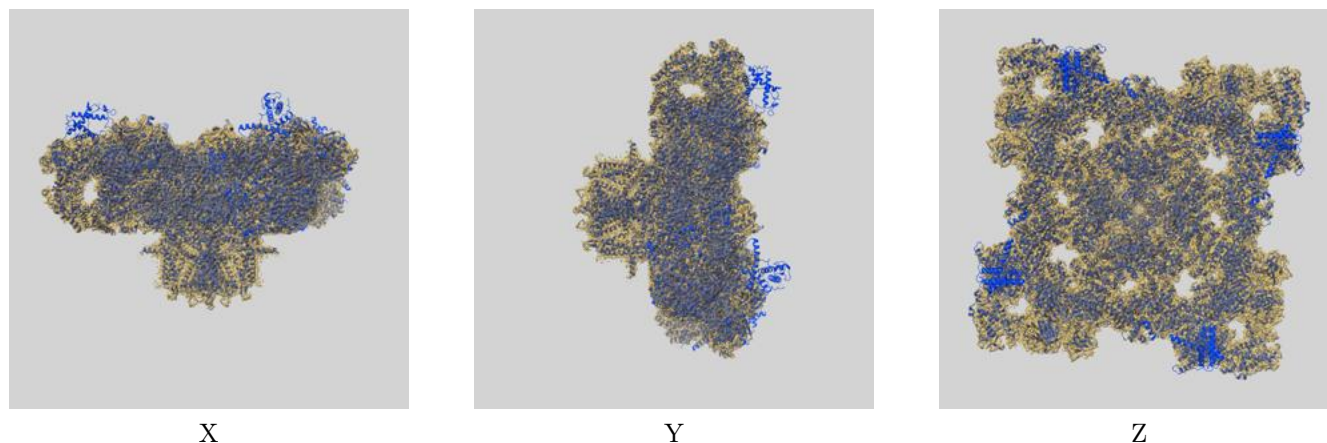
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

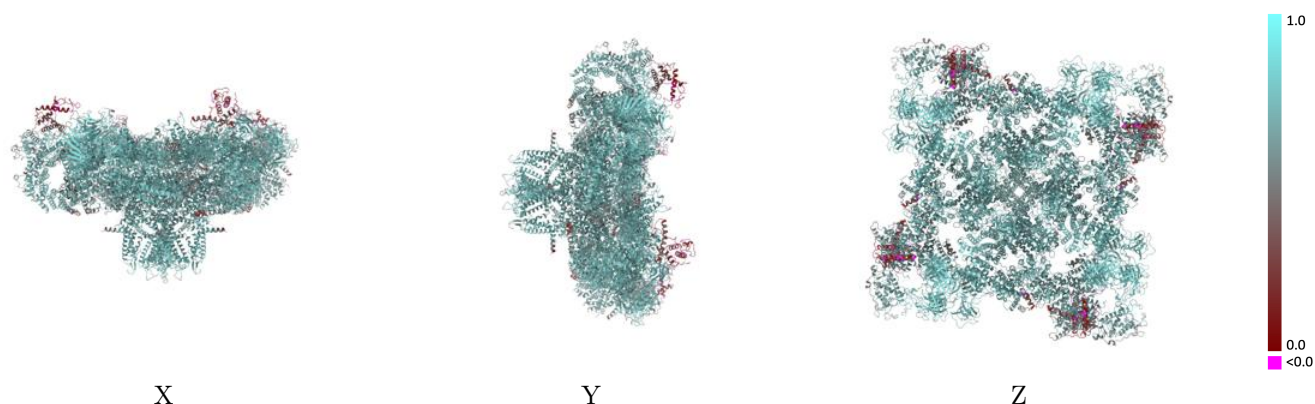
This section contains information regarding the fit between EMDB map EMD-74441 and PDB model 9ZNA. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



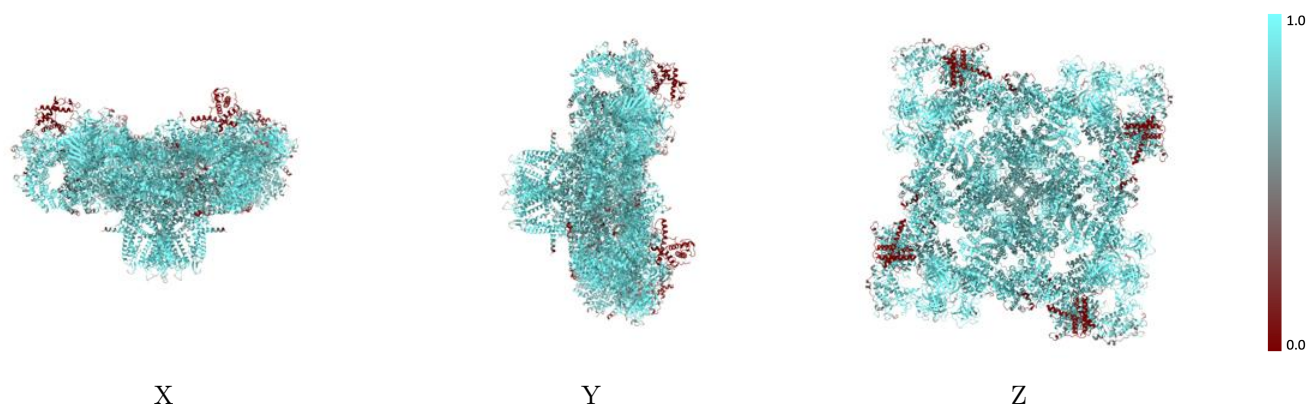
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



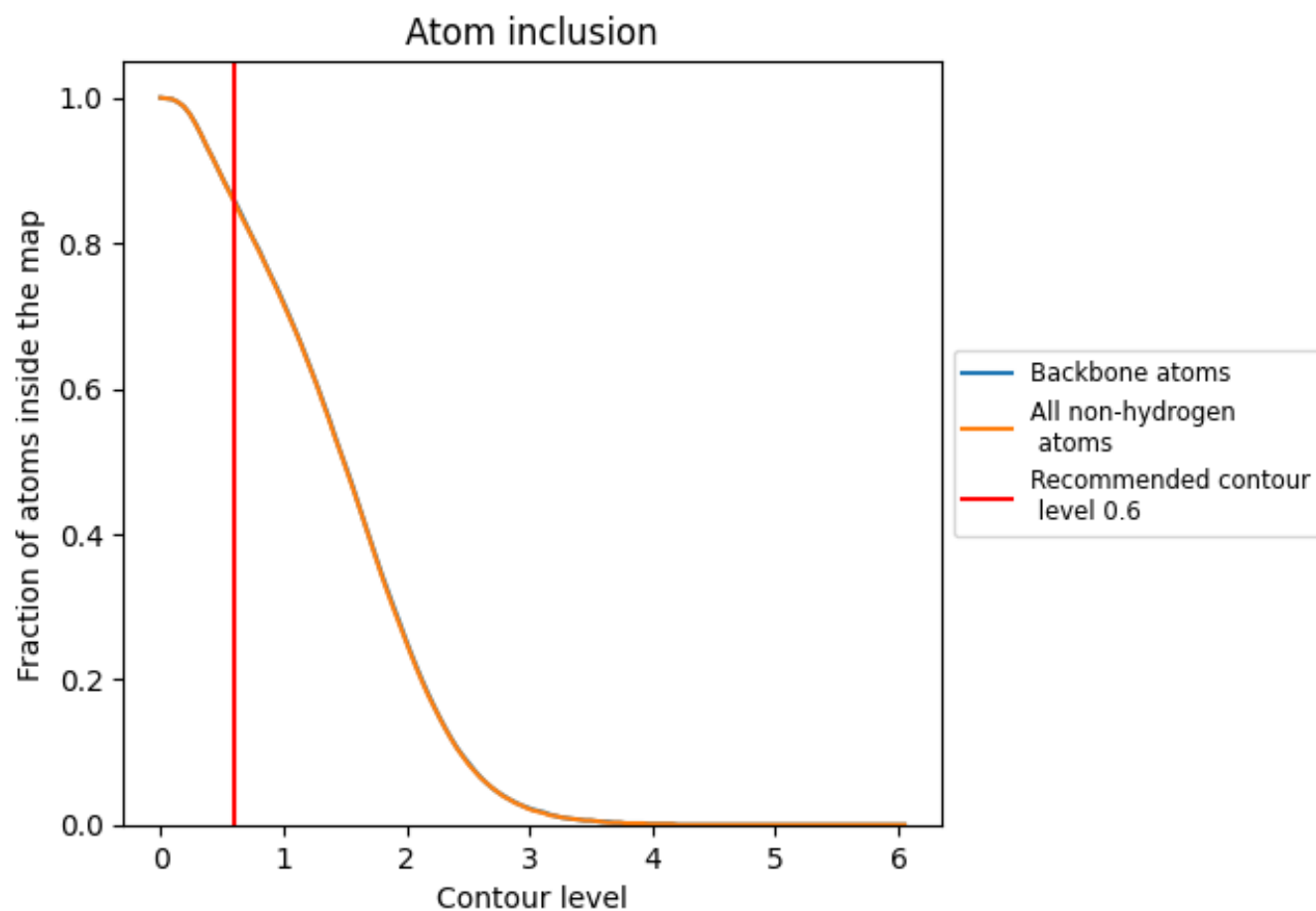
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8570	0.6730
A	0.8680	0.6780
B	0.8680	0.6770
C	0.8680	0.6770
D	0.8680	0.6780
E	0.9190	0.6950
F	0.9210	0.6950
G	0.9220	0.6960
H	0.9220	0.6960
I	0.5460	0.5150
J	0.5440	0.5130
K	0.5490	0.5190
L	0.5480	0.5190

1.0

0.0

<0.0