



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 03:27 PM EDT

PDB ID : 9ZN9 / pdb_00009zn9
EMDB ID : EMD-74439
Title : Structure of rabbit RyR1 complexed with FKBP12.6, calmodulin, ATP, 4-chloro-m-cresol, and caffeine
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.77 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

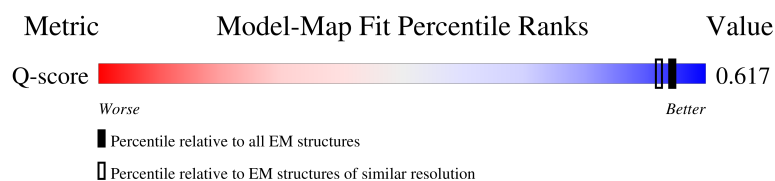
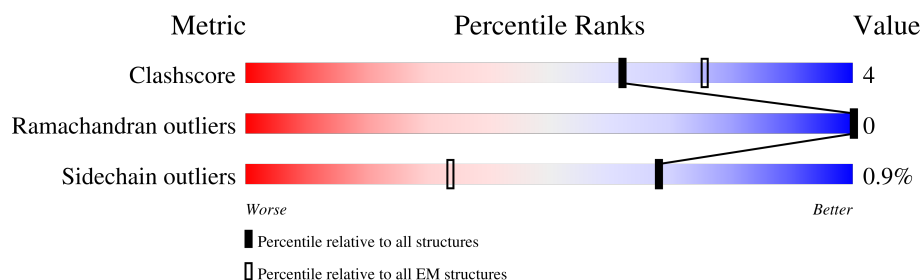
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	148	35% 85% 15%
2	J	148	36% 84% 16%
2	K	148	32% 84% 16%
2	L	148	34% 86% 14%
3	A	5037	7% 75% 9% 16%
3	B	5037	7% 75% 9% 16%
3	C	5037	7% 75% 9% 16%
3	D	5037	7% 75% 10% 16%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 146239 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		

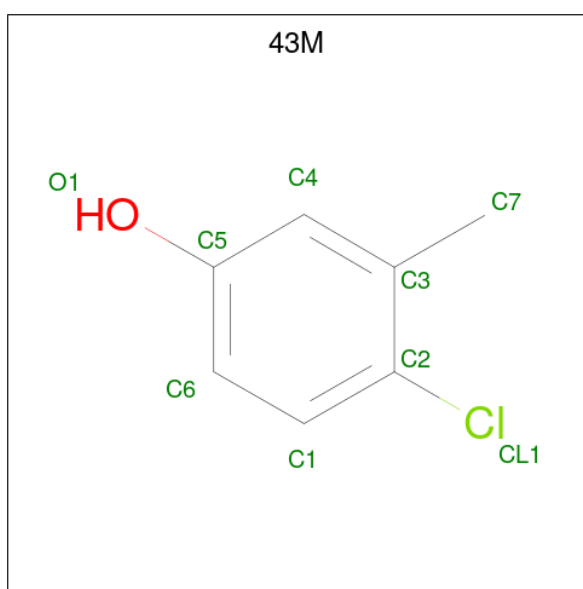
There are 4 discrepancies between the modelled and reference sequences:

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	1	0
			33879	21584	5829	6232	234		
3	C	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	D	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	B	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		

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



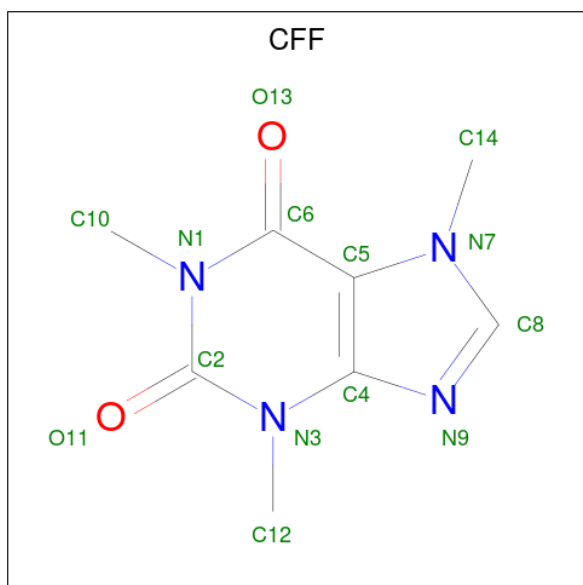
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	

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

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

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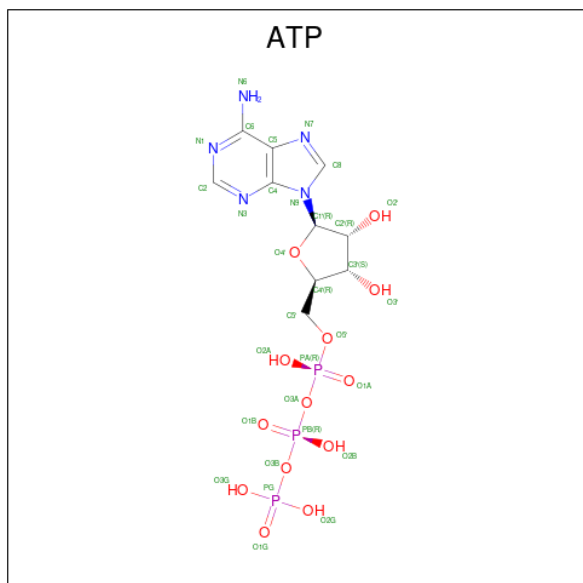
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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	4	2	
5	B	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
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	

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Mol	Chain	Residues	Atoms					AltConf
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	
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	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	

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	E	14	Total	O	0
			14	14	
9	F	15	Total	O	0
			15	15	
9	G	15	Total	O	0
			15	15	
9	H	15	Total	O	0
			15	15	
9	I	30	Total	O	0
			30	30	
9	J	30	Total	O	0
			30	30	
9	K	30	Total	O	0
			30	30	

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Mol	Chain	Residues	Atoms		AltConf
9	L	33	Total 33	O 33	0
9	A	704	Total 704	O 704	0
9	C	673	Total 673	O 673	0
9	D	692	Total 692	O 692	0
9	B	672	Total 672	O 672	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: 



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

Chain F: 



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

Chain G: 



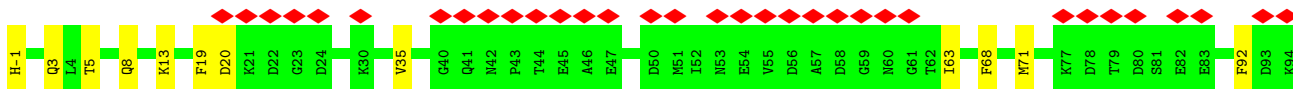
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

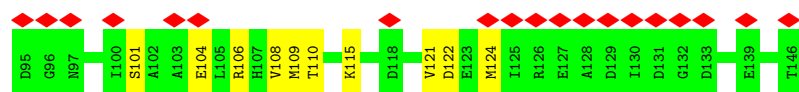
Chain H: 



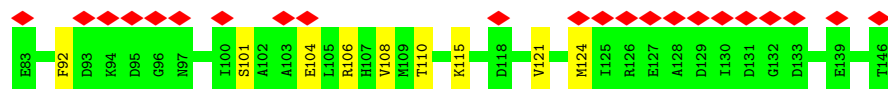
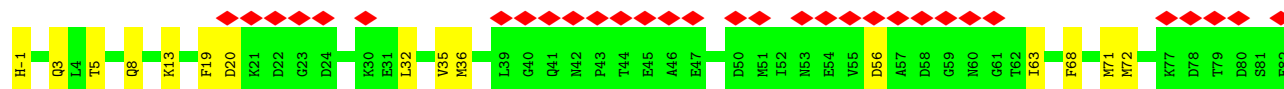
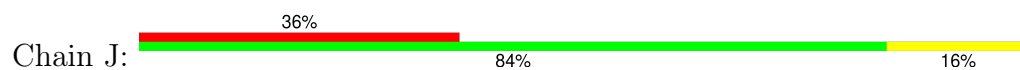
- Molecule 2: Calmodulin-1

Chain I: 

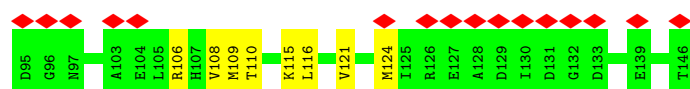
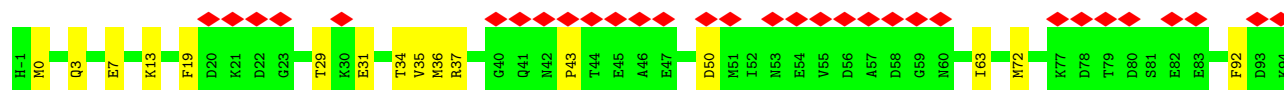
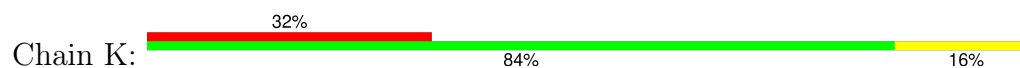




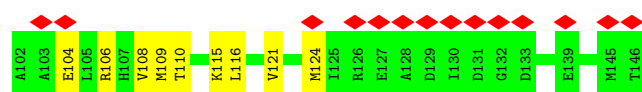
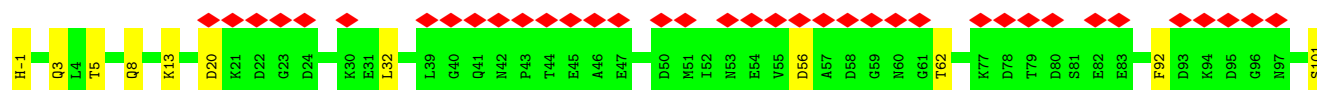
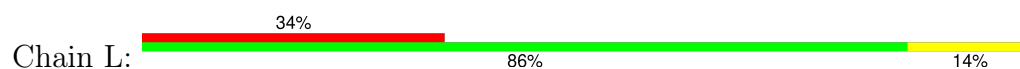
• Molecule 2: Calmodulin-1



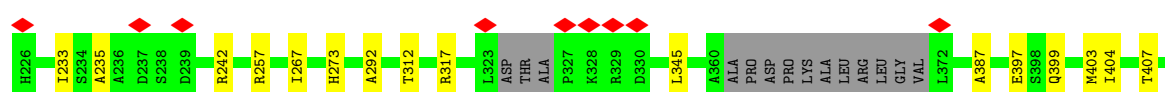
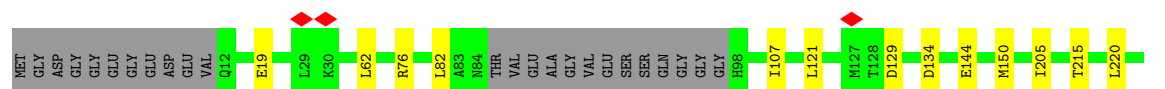
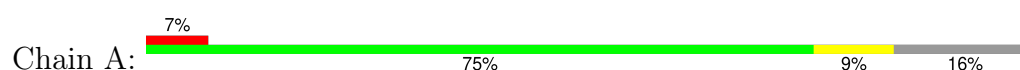
• Molecule 2: Calmodulin-1

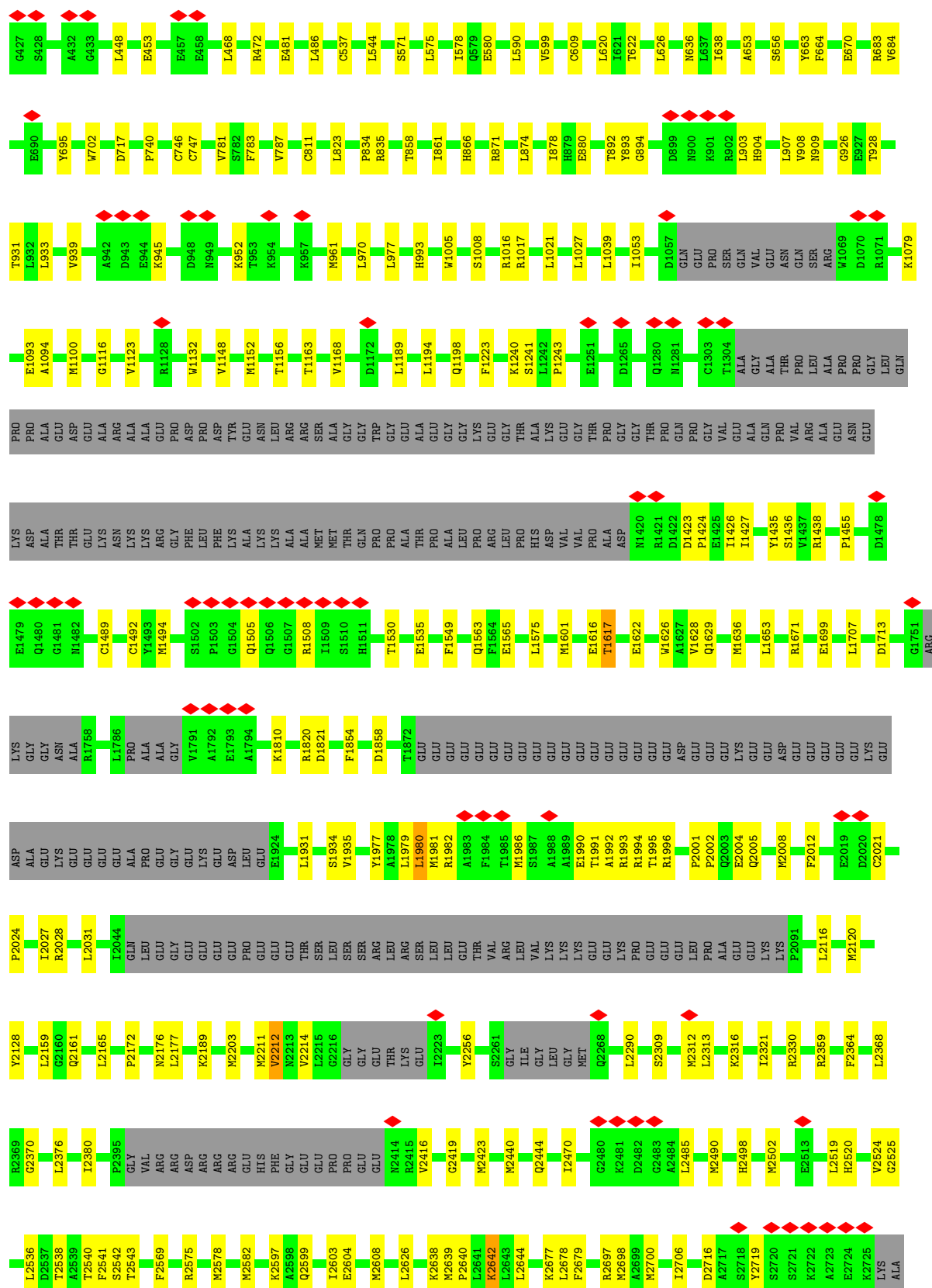


• Molecule 2: Calmodulin-1



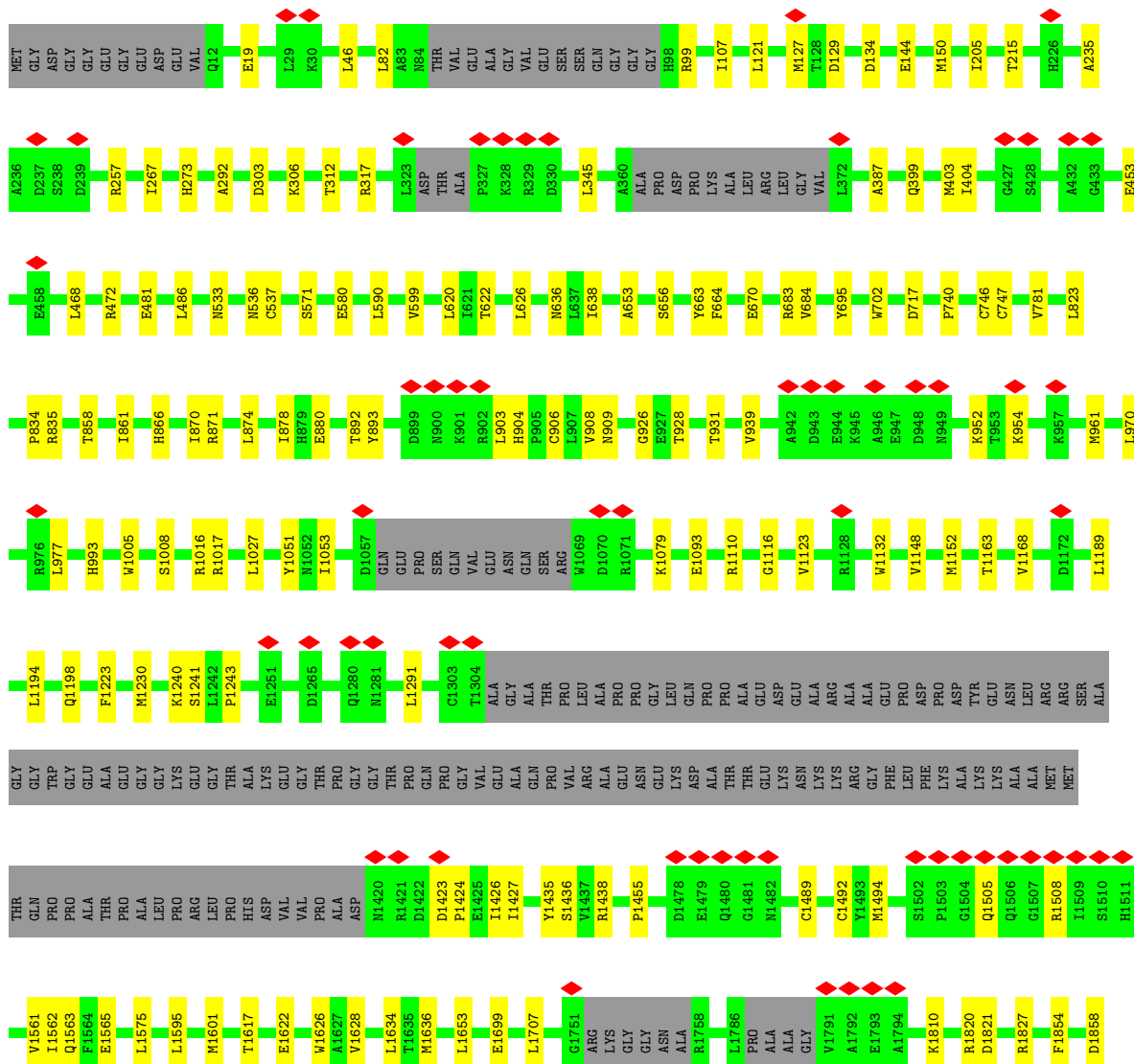
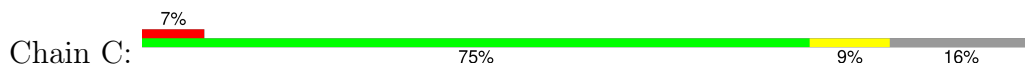
• Molecule 3: Ryanodine receptor 1



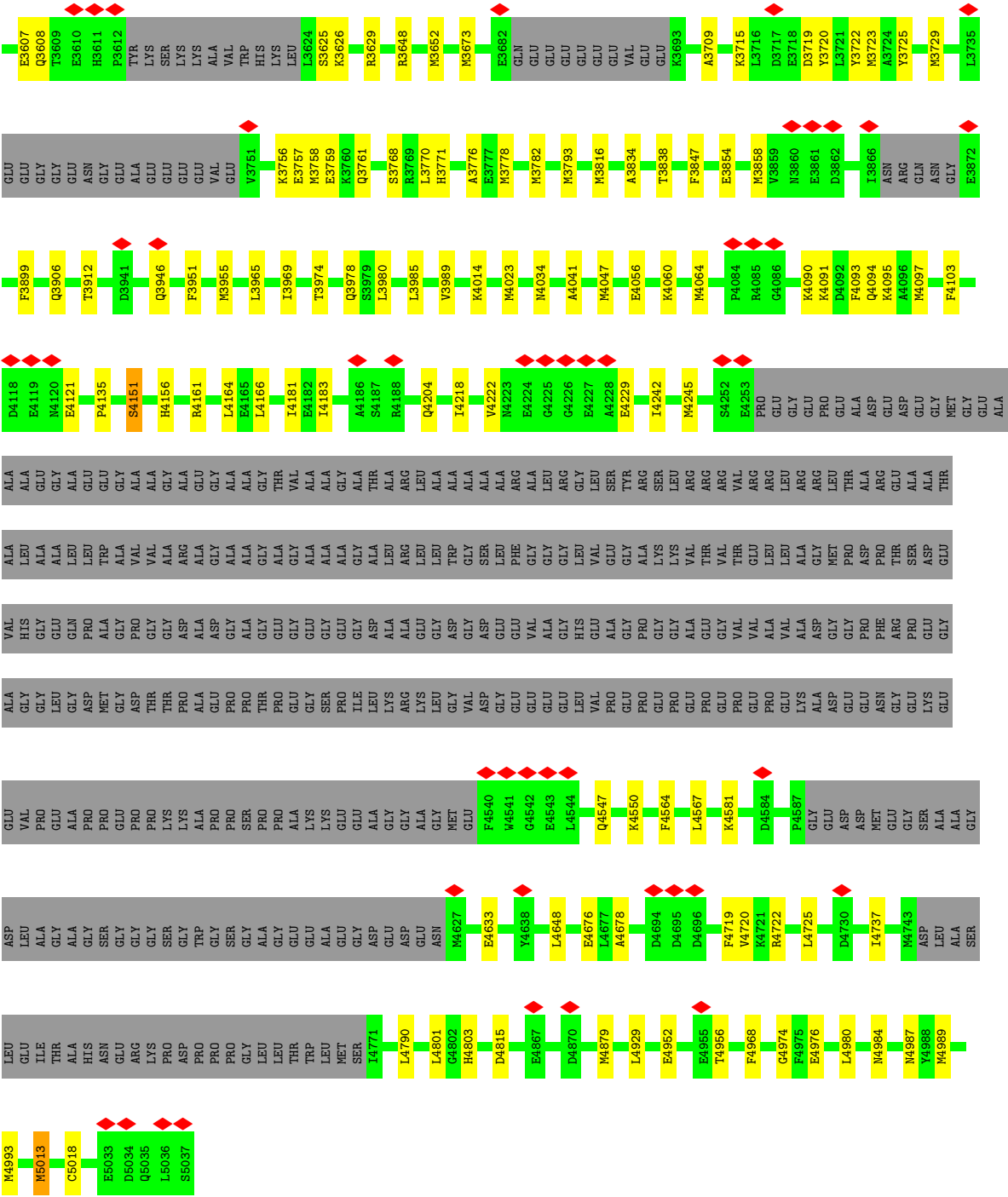




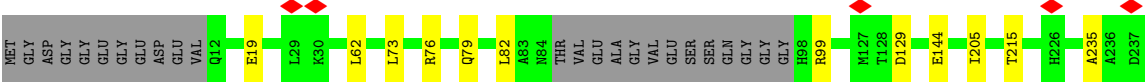
- Molecule 3: Ryanodine receptor 1

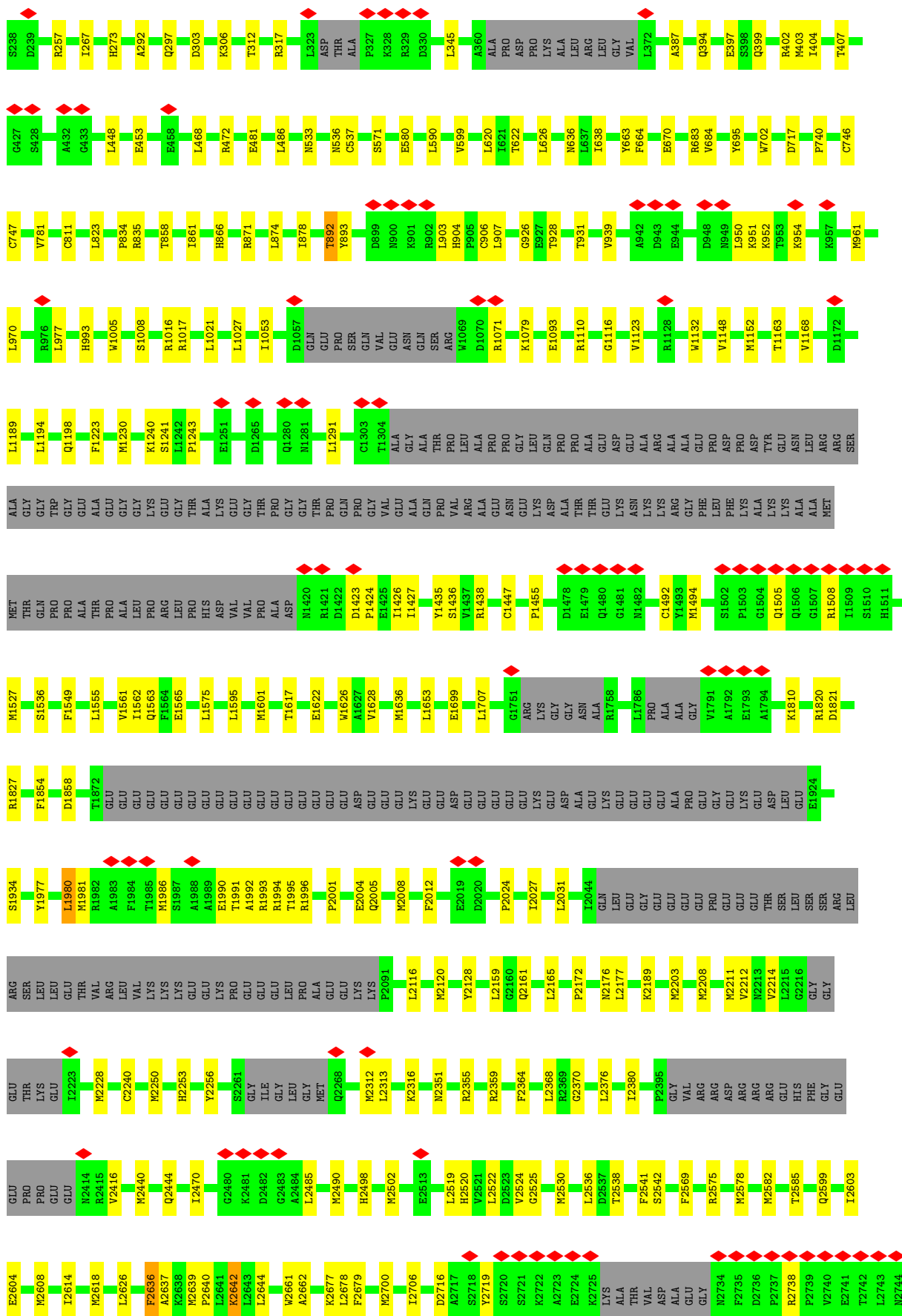


ASP	ARG	Y3503	Y3506	T3528	D3531	K3534	L3535	A3536	Y3540	Y3543	D3544	T3545	D3546	F3547	E3548	Y3549	E3550	F3552	L3553	L3557	H3558	L3559	K3562	V3563	E3564	G3565	S3566	P3567	S3568	L3569	R3570	V3571	Q3572	K3573	G3581	R3582	GLU	ASP	ALA	D3587	P3588	P3589	T3592	V3593	R3594	Y3604												
A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	L3405	L3408	Y3409	R3414	K3420	M3437	H3449	R3453	E3463	I3464	N3465	N3466	M3467	T3471	ASP	ASP	SER	LYS	SER	LYS	LYS	MET	ALA	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	LYS	ARG	GLY							
C3170	S3171	L3175	G3176	T3177	T3178	K3179	Y3182	V3183	E3184	R3187	L3194	S3223	P3224	R3225	M3250	P3292	PRO	ALA	LEU	ALA	GLY	ALA	P3301	L3312	L3312	G3327	G3328	I3329	D3330	E3331	A3332	A3339	Q3343	R3348	T3361	I3362	E3377	Q3378	L3379	R3380	L3381	E3382																
T2948	R2965	I2969	S2970	F2973	I2974	A2979	V2980	V2981	S2982	G2983	G2984	A2985	V2986	E2987	L3003	P3004	K3023	K3034	E3035	M3038	L3056	K3082	E3104	K3105	M3106	V3107	L3112	G3113	LYS	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	T3132	L3136	R3167	L3168	L3169																
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	A2916	A2917	S2918	D2919	R2920	E2921	K2922	A2923	Q2924	Y2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	Y2935	A2936	V2937	T2938	R2939	G2940	L2941	K2942	D2943	M2944	E2945	L2946	D2947
F2769	R2697	M2700	I2706	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	F2364	L2368	R2369	G2370	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	K2597	A2598	Q2599	I2603	E2604	M2608	I2614	M2618	L2626	M2639	P2640	L2641	K2642	L2643	L2644	I2470	I2476	G2480	K2481	D2482													
G2483	A2484	L2485	H2498	M2502	E2513	H2514	Q2515	L2519	H2520	V2524	G2525	M2530	L2536	D2537	T2538	F2541	S2542	R2575	M2578	T2585	P2585	K2597	A2598	Q2599	I2603	E2604	M2608	I2614	M2618	L2626	M2639	P2640	L2641	K2642	L2643	L2644	I2470	I2476	G2480	K2481	D2482																	
GLY	THR	VAL	LEU	VAL	LYS	LYS	GLU	LYS	PRO	GLU	LEU	PRO	ALA	GLU	LYS	P2091	L2116	M2120	Y2128	L2159	G2160	Q2161	L2165	P2172	N2176	L2177	K2189	M2203	G2216	GLY	GLY	THR	LYS	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU																
M1981	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992	R1993	R1994	T1995	R1996	E1997	P2001	Q2004	Q2005	M2008	F2012	E2019	D2020	P2024	I2027	L2031	I2044	GLN	LEU	GLU	GLY	GLU	GLU	PRO	GLU	PRO	GLU	LYS	ARG	LEU	ARG	SER	LEU															
T1872	GLU	ARG	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	LYS	GLU	LYS	GLU	ASP	ALA	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLY	GLY	LYS	GLU	ASP	LEU	SER	SER	ARG	LEU														



● 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	259362	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 ($e^-/\text{\AA}^2$)	71.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.289	Depositor
Minimum map value	0.000	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 43M, CA, ZN, CFF, 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	0.12	0/835	0.28	0/1123
1	F	0.11	0/835	0.27	0/1123
1	G	0.11	0/835	0.27	0/1123
1	H	0.11	0/835	0.28	0/1123
2	I	0.10	0/1026	0.29	0/1386
2	J	0.10	0/1026	0.30	0/1386
2	K	0.11	0/1026	0.32	0/1386
2	L	0.10	0/1026	0.30	0/1386
3	A	0.12	0/34640	0.29	0/46902
3	B	0.12	0/34640	0.28	0/46902
3	C	0.12	0/34640	0.29	0/46902
3	D	0.12	0/34640	0.29	0/46902
All	All	0.12	0/146004	0.29	0/197644

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	819	0	824	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	819	0	824	6	0
1	G	819	0	824	8	0
1	H	819	0	824	9	0
2	I	1017	0	841	12	0
2	J	1017	0	841	15	0
2	K	1017	0	841	16	0
2	L	1017	0	841	12	0
3	A	33879	0	33511	277	0
3	B	33879	0	33511	283	0
3	C	33879	0	33511	287	0
3	D	33879	0	33511	294	0
4	A	36	0	24	0	0
4	B	36	0	24	0	0
4	C	36	0	24	0	0
4	D	36	0	24	0	0
5	A	14	0	10	0	0
5	B	14	0	10	0	0
5	C	14	0	10	0	0
5	D	14	0	10	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	62	0	24	0	0
7	B	62	0	24	0	0
7	C	62	0	24	0	0
7	D	62	0	24	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	704	0	0	1	0
9	B	672	0	0	0	0
9	C	673	0	0	1	0
9	D	692	0	0	1	0
9	E	14	0	0	0	0
9	F	15	0	0	0	0
9	G	15	0	0	0	0
9	H	15	0	0	0	0
9	I	30	0	0	0	0
9	J	30	0	0	0	0
9	K	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	33	0	0	0	0
All	All	146239	0	140936	1215	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 4.

The worst 5 of 1215 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:D:4090:LYS:HG3	3:D:4121:GLU:HB3	1.64	0.80
3:B:2801:ASP:HA	3:B:2804:ILE:HG12	1.66	0.78
3:D:2801:ASP:HA	3:D:2804:ILE:HG12	1.66	0.77
3:D:2208:MET:HE2	3:D:2250:MET:HE1	1.68	0.76
3:C:2801:ASP:HA	3:C:2804:ILE:HG12	1.66	0.76

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	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
1	F	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
1	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	H	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	I	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	J	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	K	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	L	146/148 (99%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	4198/5037 (83%)	4124 (98%)	74 (2%)	0	100	100
3	B	4198/5037 (83%)	4118 (98%)	80 (2%)	0	100	100
3	C	4198/5037 (83%)	4119 (98%)	79 (2%)	0	100	100
3	D	4198/5037 (83%)	4120 (98%)	78 (2%)	0	100	100
All	All	17796/21168 (84%)	17455 (98%)	341 (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	65
1	F	88/88 (100%)	88 (100%)	0	100	100
1	G	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	87 (99%)	1 (1%)	65	85
2	I	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	J	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	K	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	L	82/127 (65%)	80 (98%)	2 (2%)	43	74
3	A	3696/4276 (86%)	3658 (99%)	38 (1%)	68	86
3	B	3696/4276 (86%)	3668 (99%)	28 (1%)	73	89
3	C	3696/4276 (86%)	3668 (99%)	28 (1%)	73	89
3	D	3696/4276 (86%)	3664 (99%)	32 (1%)	70	87
All	All	15464/17964 (86%)	15323 (99%)	141 (1%)	68	87

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	297	GLN

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Mol	Chain	Res	Type
3	B	977	LEU
3	B	2893	GLU
3	A	3790	THR
3	A	3608	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	4558	ASN
3	B	3882	GLN
3	B	489	ASN
3	B	2253	HIS
3	B	5015	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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
4	43M	C	5101	-	9,9,9	0.39	0	12,12,12	0.52	0
4	43M	C	5102	-	9,9,9	0.40	0	12,12,12	0.53	0
4	43M	B	5101	-	9,9,9	0.40	0	12,12,12	0.53	0
4	43M	A	5101	-	9,9,9	0.39	0	12,12,12	0.54	0
4	43M	A	5102	-	9,9,9	0.38	0	12,12,12	0.52	0
4	43M	D	5105	-	9,9,9	0.37	0	12,12,12	0.56	0
5	CFF	A	5103	-	15,15,15	0.59	0	23,23,23	0.72	1 (4%)
4	43M	D	5102	-	9,9,9	0.38	0	12,12,12	0.53	0
4	43M	A	5107	-	9,9,9	0.38	0	12,12,12	0.53	0
4	43M	D	5107	-	9,9,9	0.37	0	12,12,12	0.52	0
7	ATP	B	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
7	ATP	A	5106	-	32,33,33	0.28	0	48,52,52	0.36	0
7	ATP	C	5108	-	32,33,33	0.28	0	48,52,52	0.38	0
7	ATP	C	5106	-	32,33,33	0.28	0	48,52,52	0.36	0
7	ATP	D	5106	-	32,33,33	0.29	0	48,52,52	0.36	0
4	43M	B	5105	-	9,9,9	0.38	0	12,12,12	0.55	0
4	43M	C	5105	-	9,9,9	0.36	0	12,12,12	0.55	0
7	ATP	D	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
5	CFF	C	5103	-	15,15,15	0.58	0	23,23,23	0.74	1 (4%)
4	43M	D	5101	-	9,9,9	0.39	0	12,12,12	0.54	0
7	ATP	A	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
4	43M	B	5102	-	9,9,9	0.38	0	12,12,12	0.53	0
5	CFF	B	5103	-	15,15,15	0.59	0	23,23,23	0.73	1 (4%)
4	43M	A	5105	-	9,9,9	0.35	0	12,12,12	0.55	0
5	CFF	D	5103	-	15,15,15	0.59	0	23,23,23	0.73	1 (4%)
4	43M	C	5107	-	9,9,9	0.39	0	12,12,12	0.53	0
4	43M	B	5107	-	9,9,9	0.38	0	12,12,12	0.52	0
7	ATP	B	5106	-	32,33,33	0.28	0	48,52,52	0.36	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
4	43M	C	5101	-	-	-	0/1/1/1
4	43M	C	5102	-	-	-	0/1/1/1
4	43M	A	5101	-	-	-	0/1/1/1
4	43M	B	5101	-	-	-	0/1/1/1
4	43M	A	5102	-	-	-	0/1/1/1
4	43M	D	5105	-	-	-	0/1/1/1
5	CFF	A	5103	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	43M	D	5102	-	-	-	0/1/1/1
4	43M	A	5107	-	-	-	0/1/1/1
4	43M	D	5107	-	-	-	0/1/1/1
7	ATP	B	5108	-	-	5/22/38/38	0/3/3/3
7	ATP	A	5106	-	-	7/22/38/38	0/3/3/3
7	ATP	C	5108	-	-	5/22/38/38	0/3/3/3
7	ATP	C	5106	-	-	5/22/38/38	0/3/3/3
7	ATP	D	5106	-	-	5/22/38/38	0/3/3/3
4	43M	B	5105	-	-	-	0/1/1/1
4	43M	C	5105	-	-	-	0/1/1/1
7	ATP	D	5108	-	-	6/22/38/38	0/3/3/3
5	CFF	C	5103	-	-	-	0/2/2/2
4	43M	D	5101	-	-	-	0/1/1/1
7	ATP	A	5108	-	-	7/22/38/38	0/3/3/3
4	43M	B	5102	-	-	-	0/1/1/1
5	CFF	B	5103	-	-	-	0/2/2/2
4	43M	A	5105	-	-	-	0/1/1/1
5	CFF	D	5103	-	-	-	0/2/2/2
4	43M	C	5107	-	-	-	0/1/1/1
4	43M	B	5107	-	-	-	0/1/1/1
7	ATP	B	5106	-	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	CFF	C12-N3-C2	2.39	121.50	117.33
5	D	5103	CFF	C12-N3-C2	2.39	121.50	117.33
5	B	5103	CFF	C12-N3-C2	2.37	121.46	117.33
5	A	5103	CFF	C12-N3-C2	2.34	121.41	117.33

There are no chirality outliers.

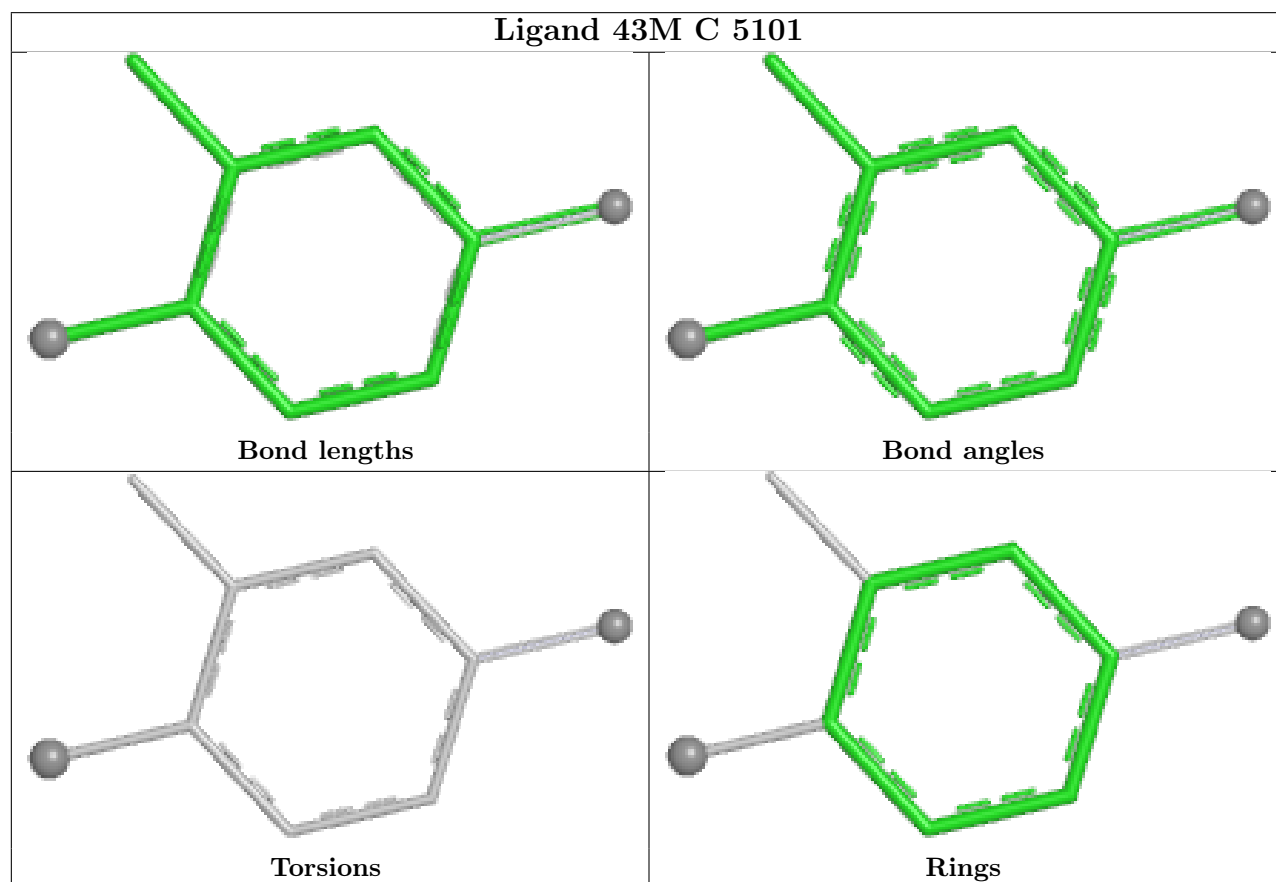
5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5106	ATP	C5'-O5'-PA-O2A
7	A	5106	ATP	C5'-O5'-PA-O3A
7	A	5108	ATP	PB-O3B-PG-O2G
7	C	5106	ATP	C5'-O5'-PA-O2A
7	C	5106	ATP	C5'-O5'-PA-O3A

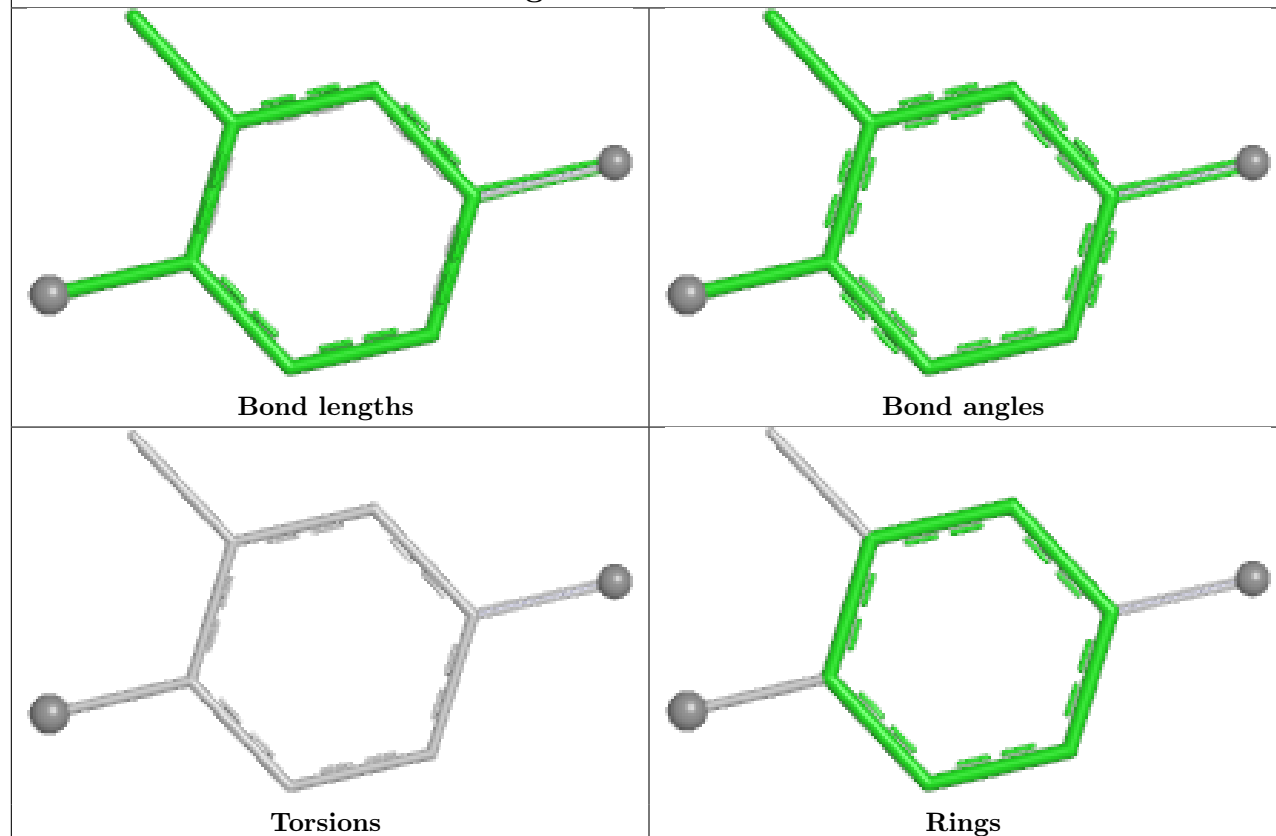
There are no ring outliers.

No monomer is involved in short contacts.

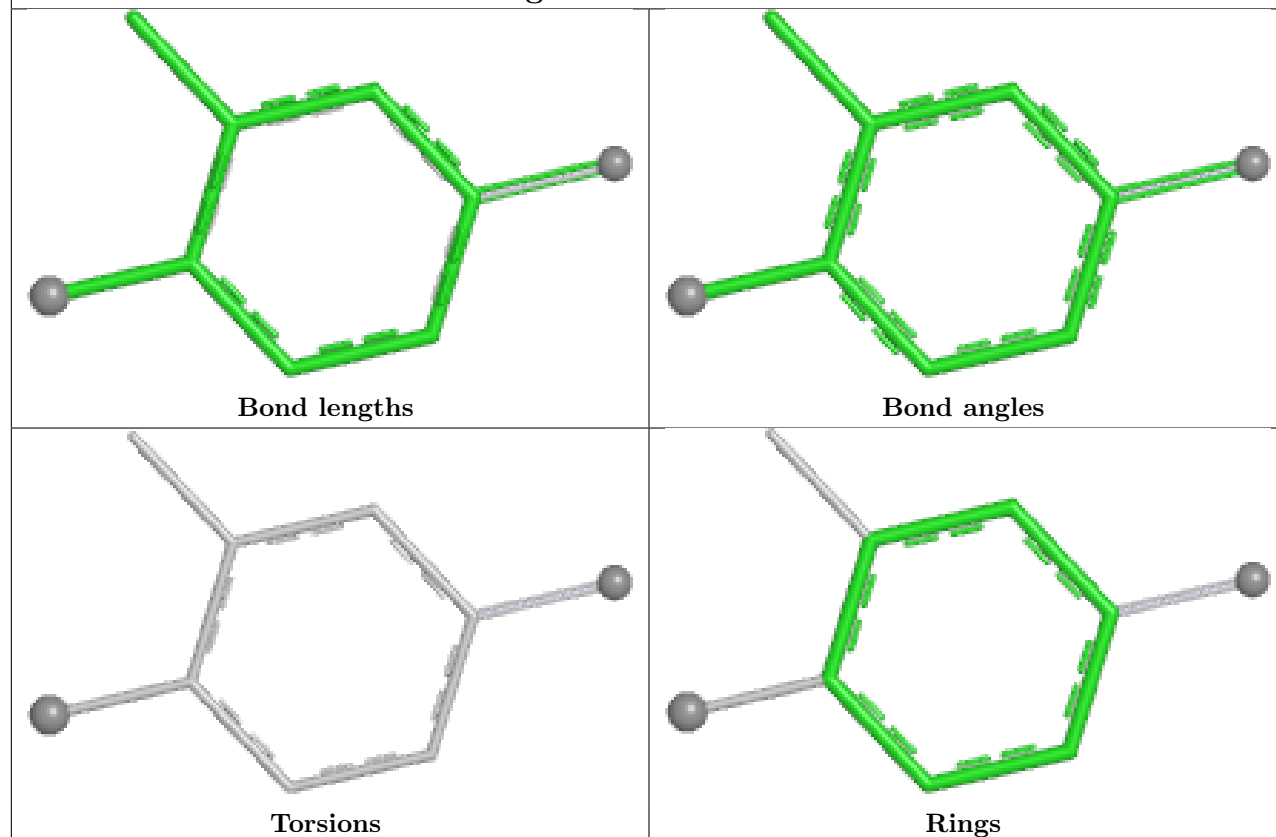
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



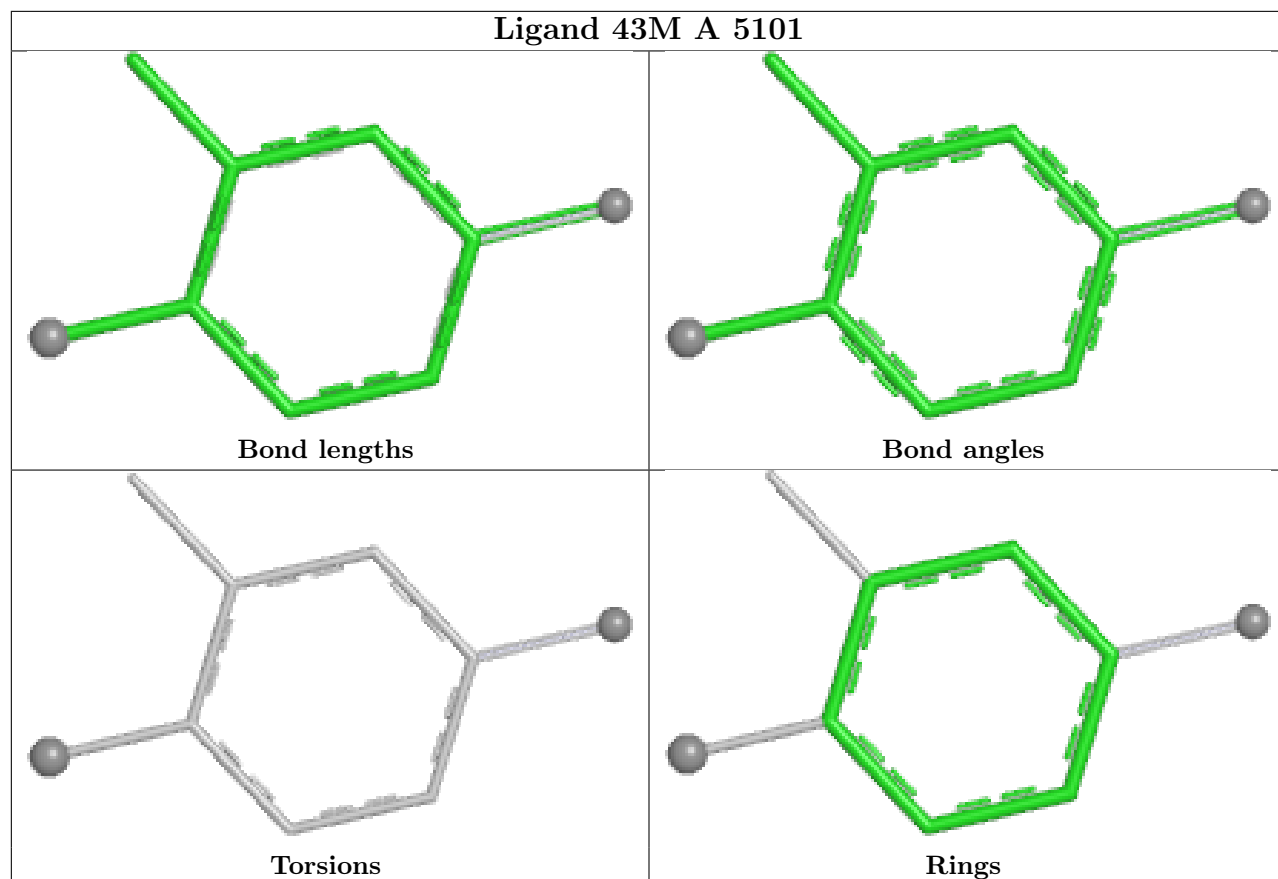
Ligand 43M C 5102



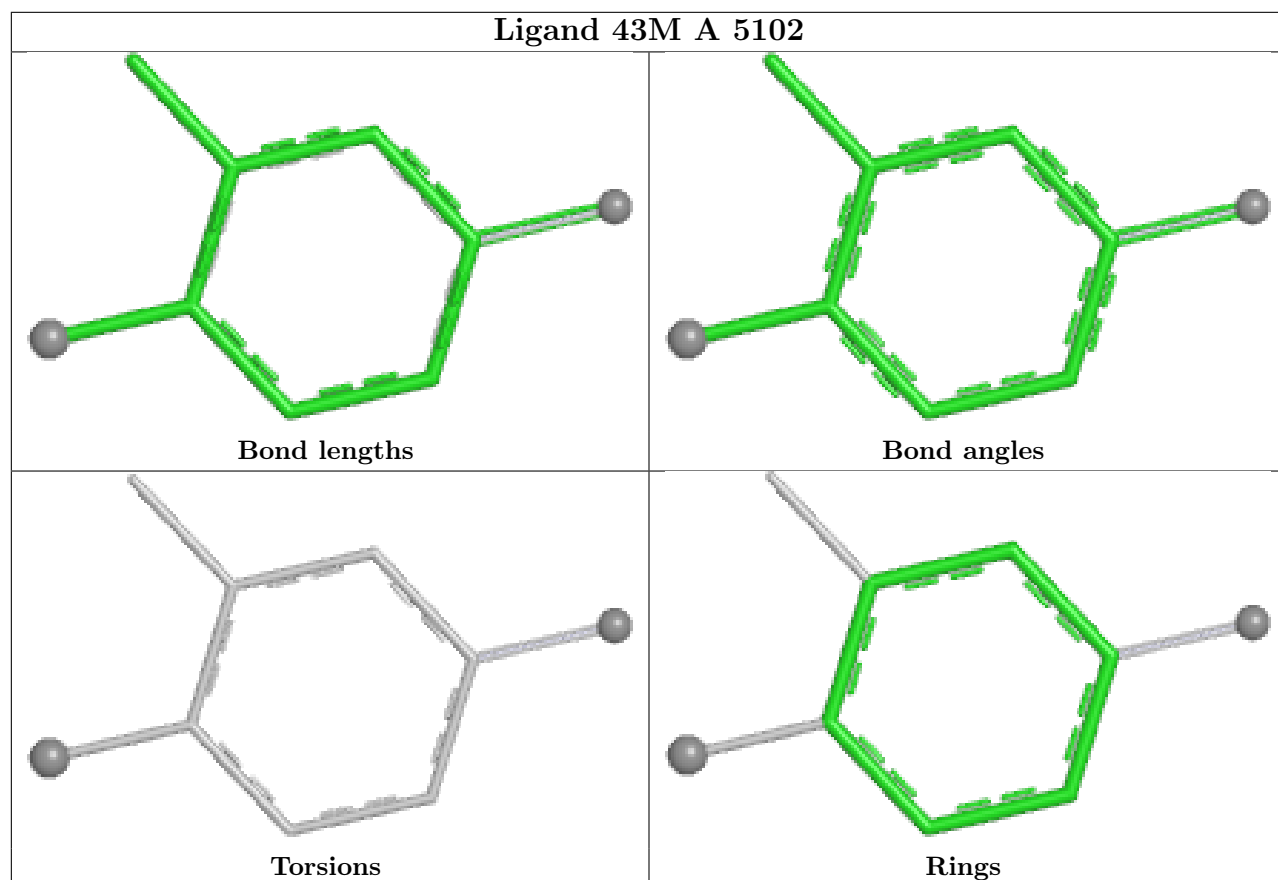
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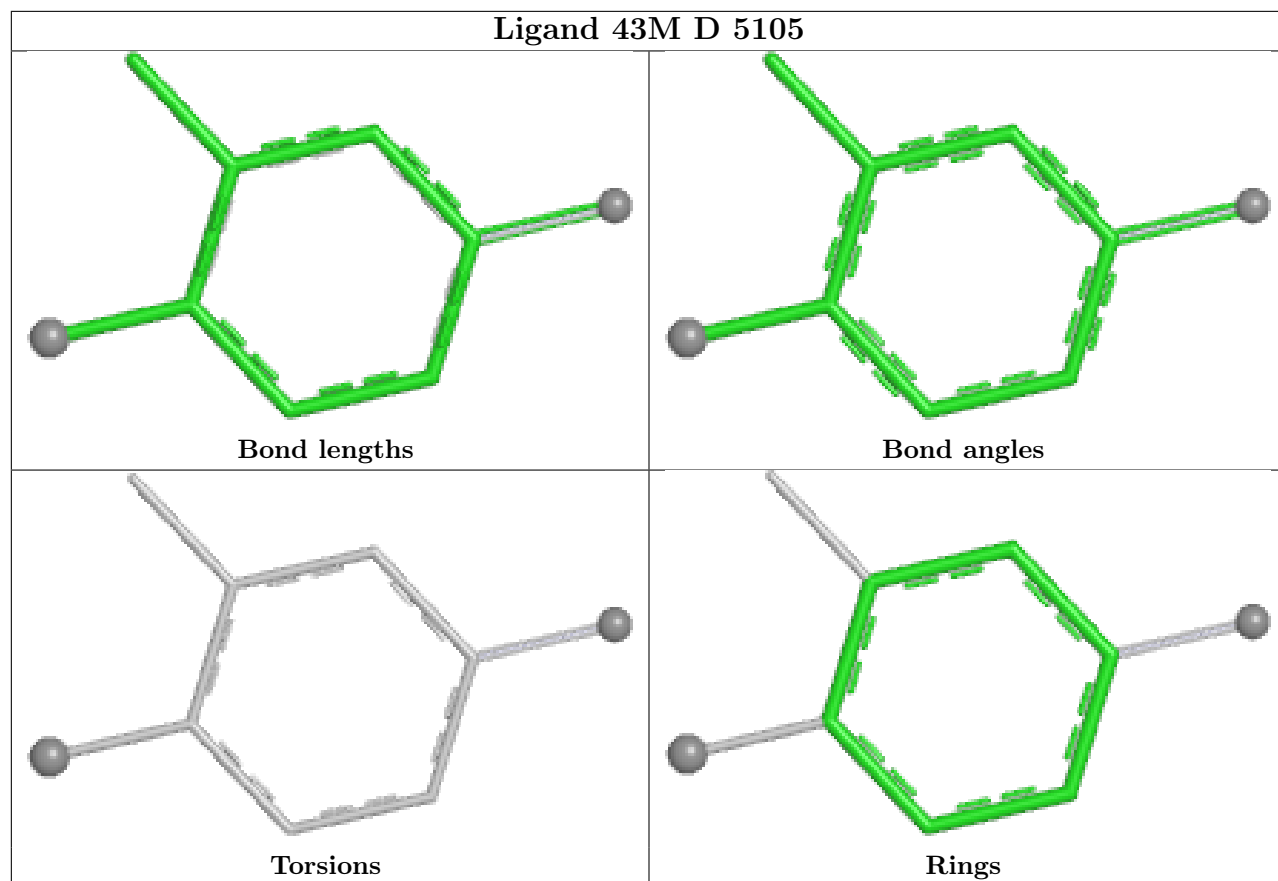


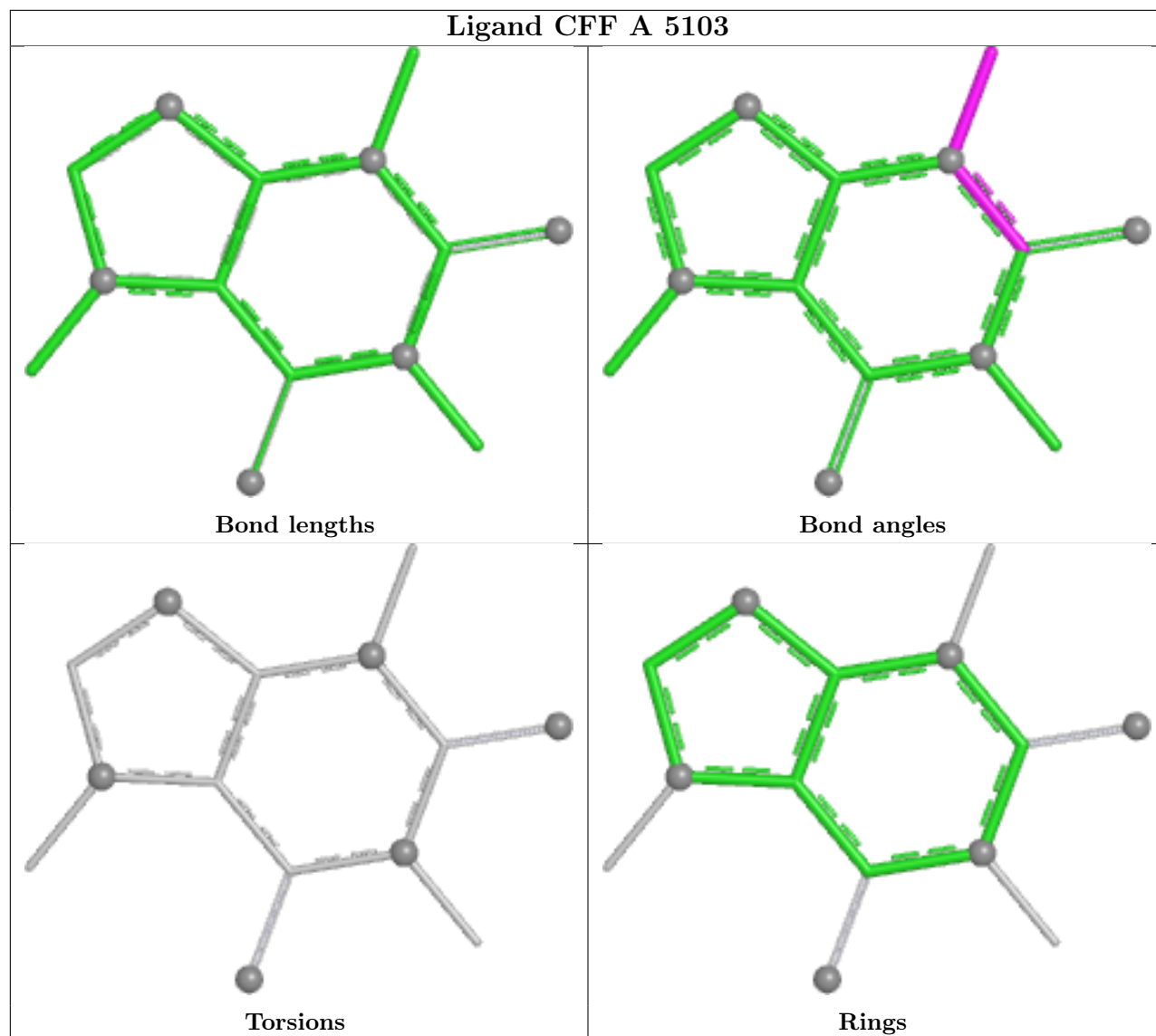
Ligand 43M A 5101



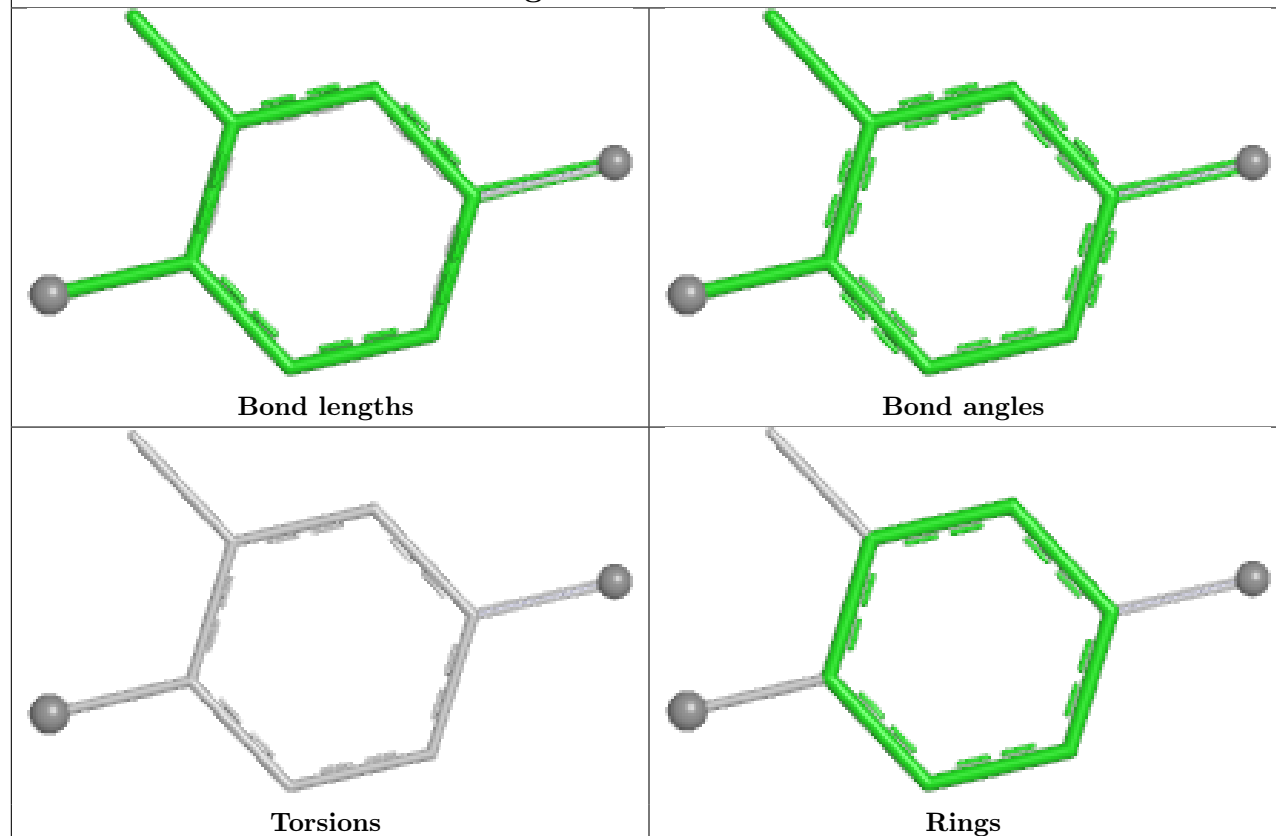
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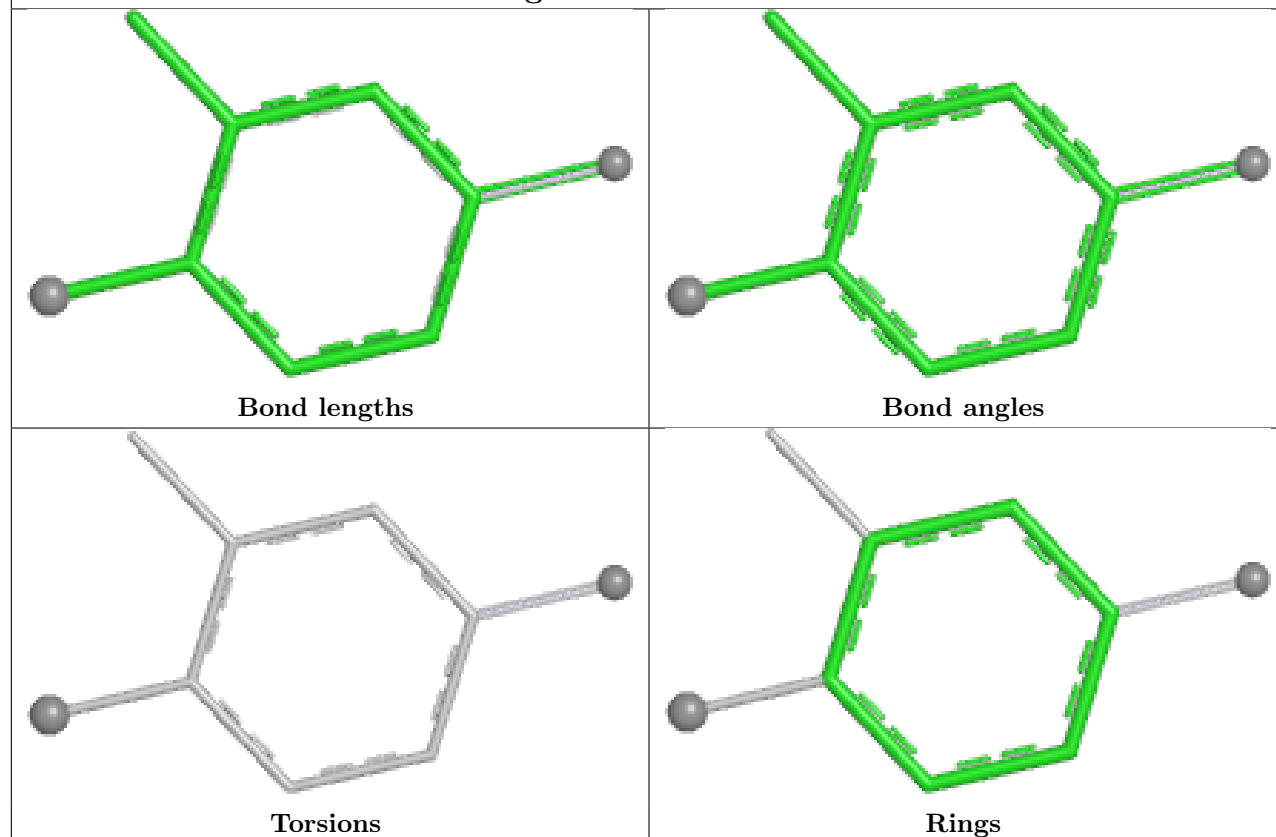


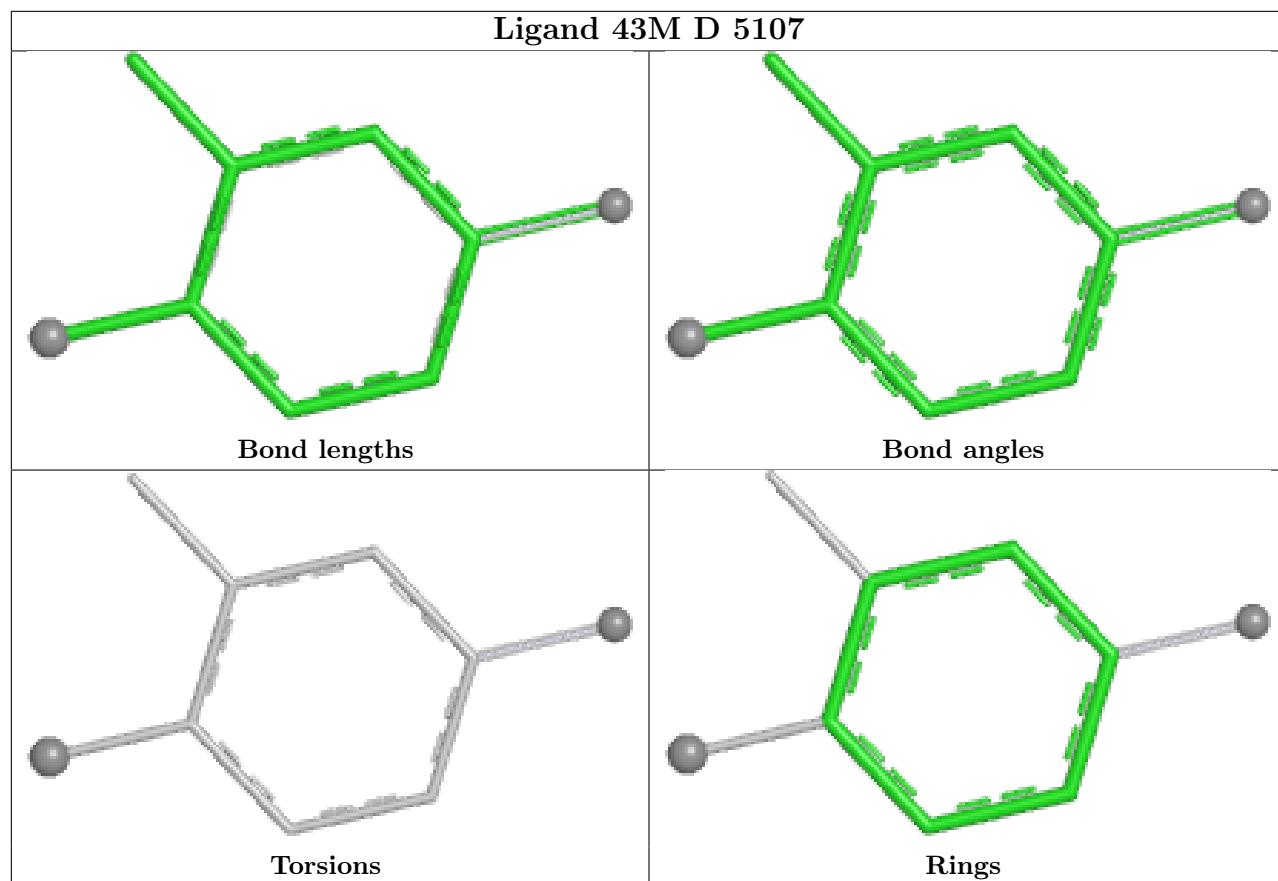


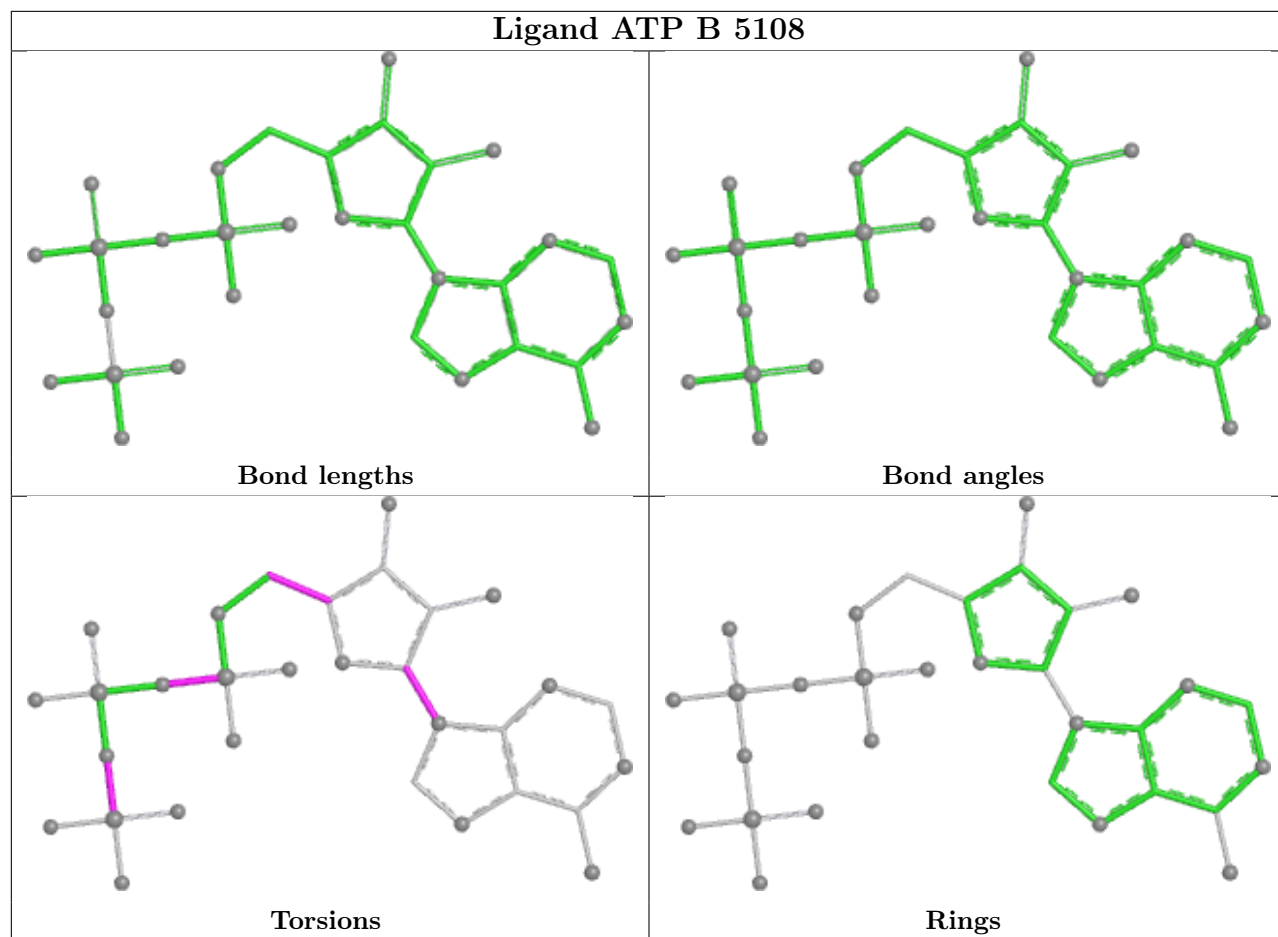
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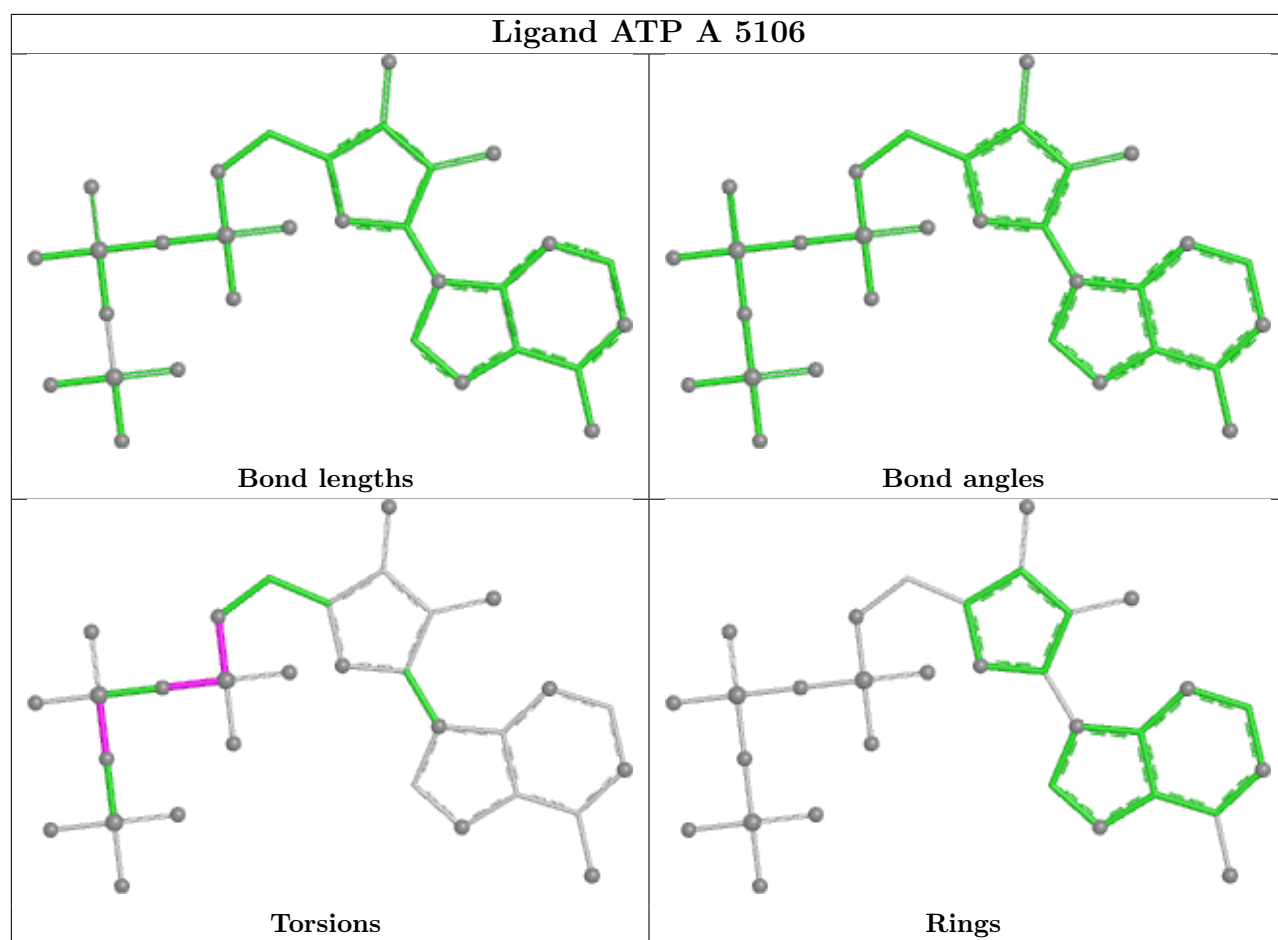


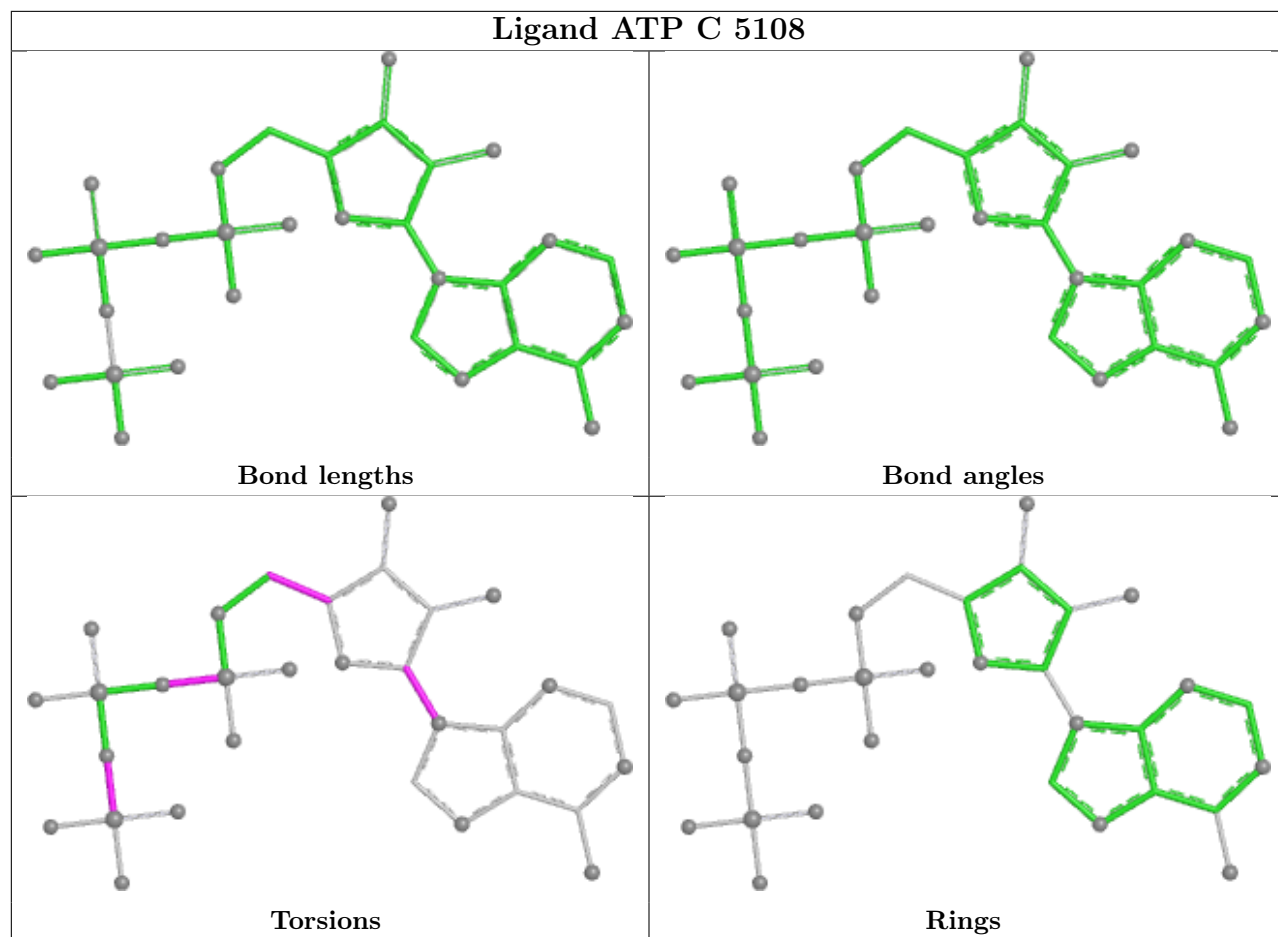
Ligand 43M A 5107

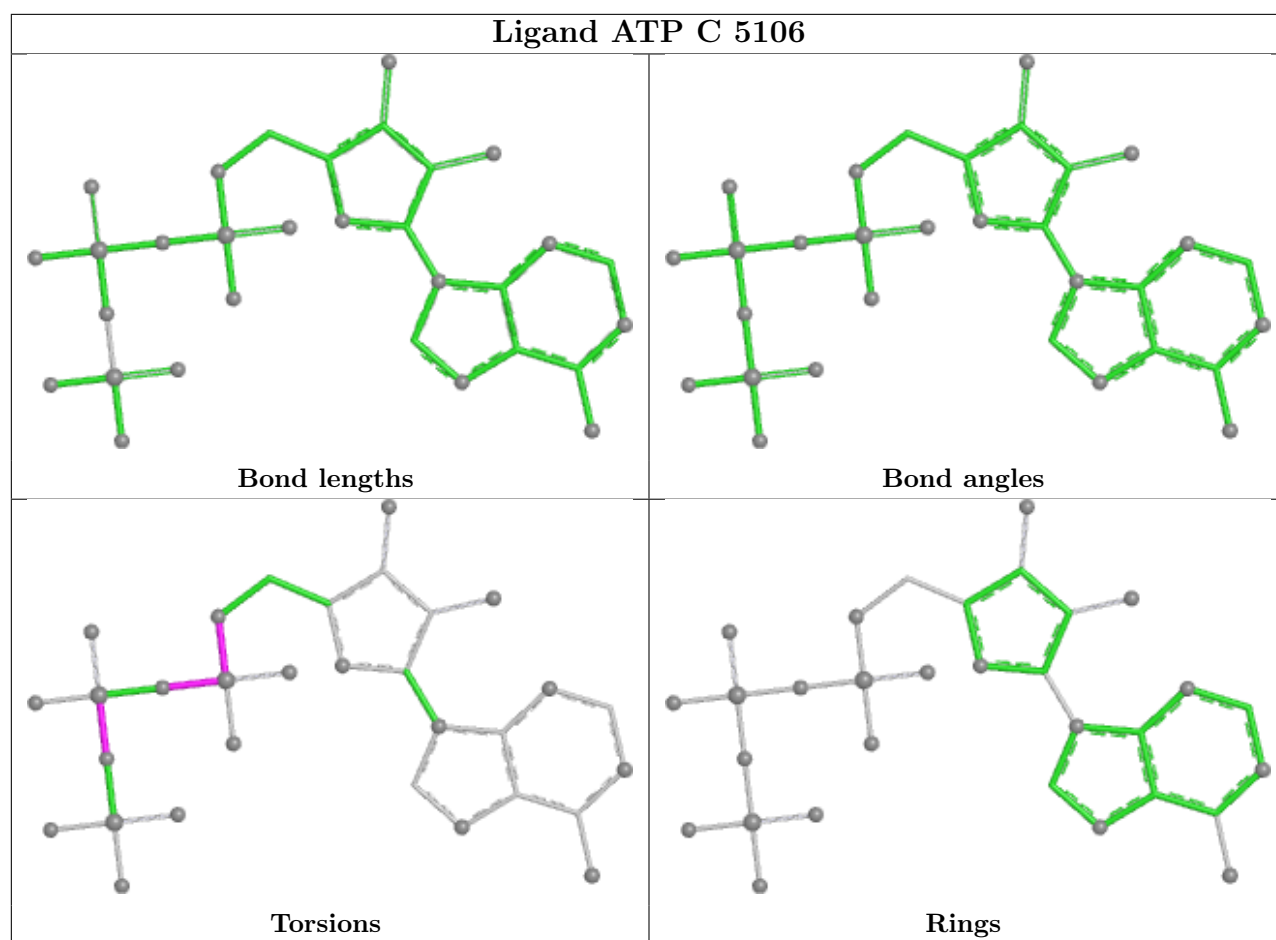


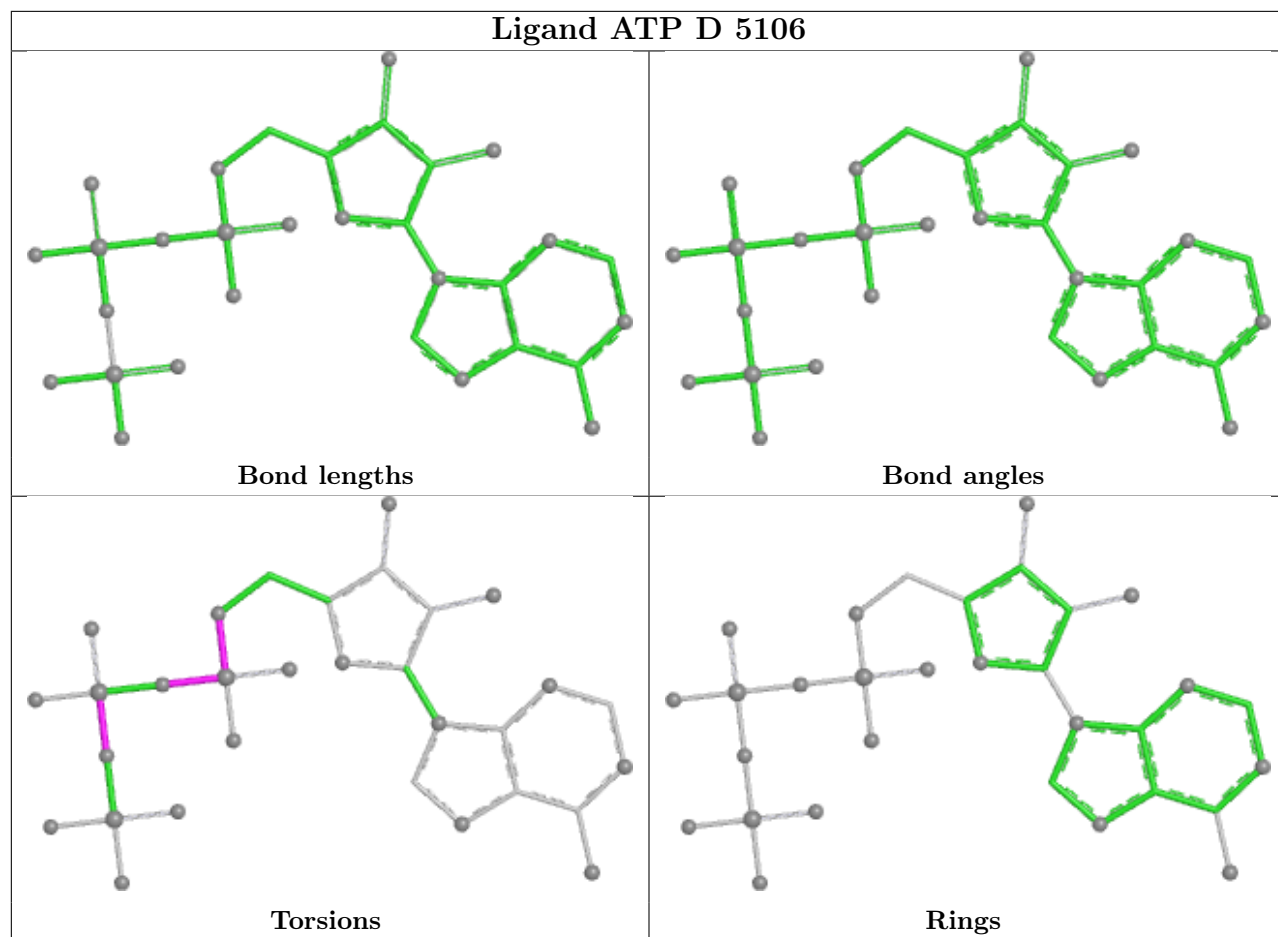




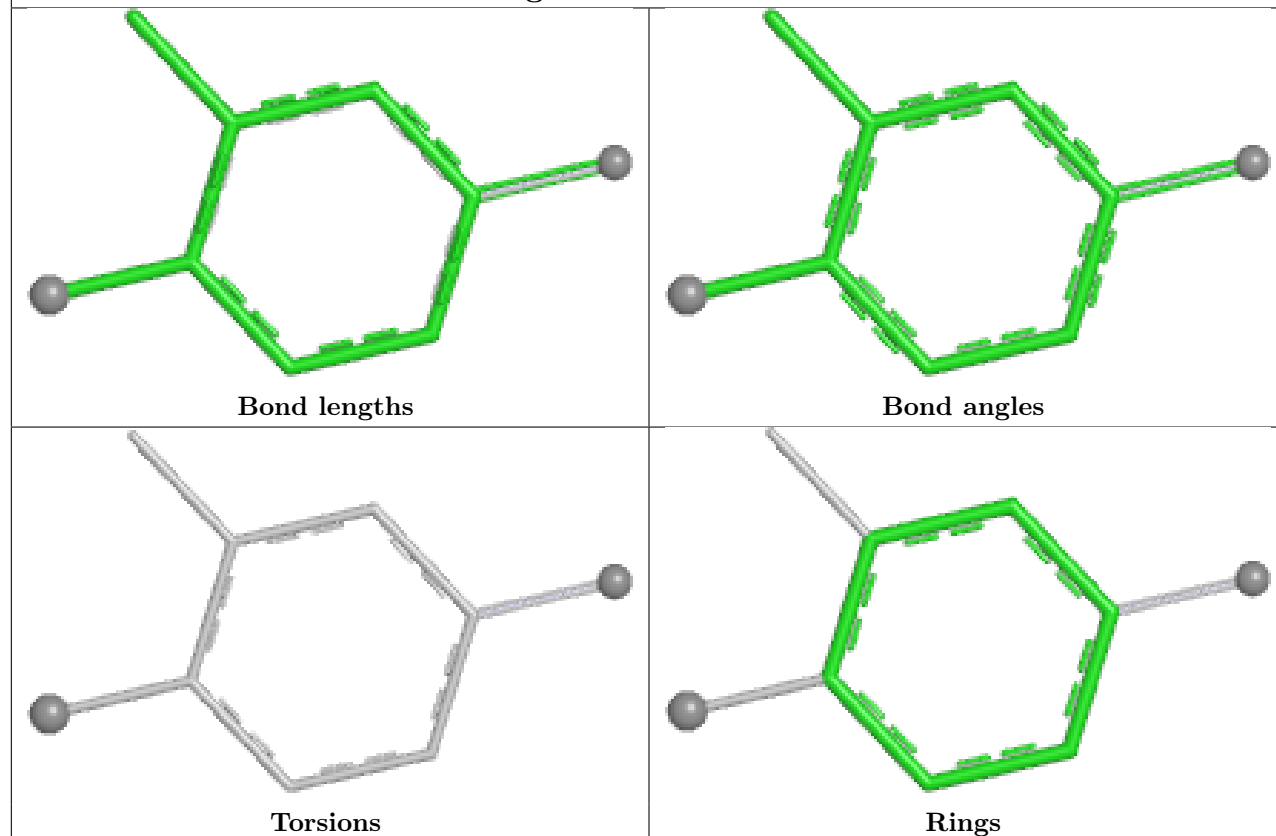




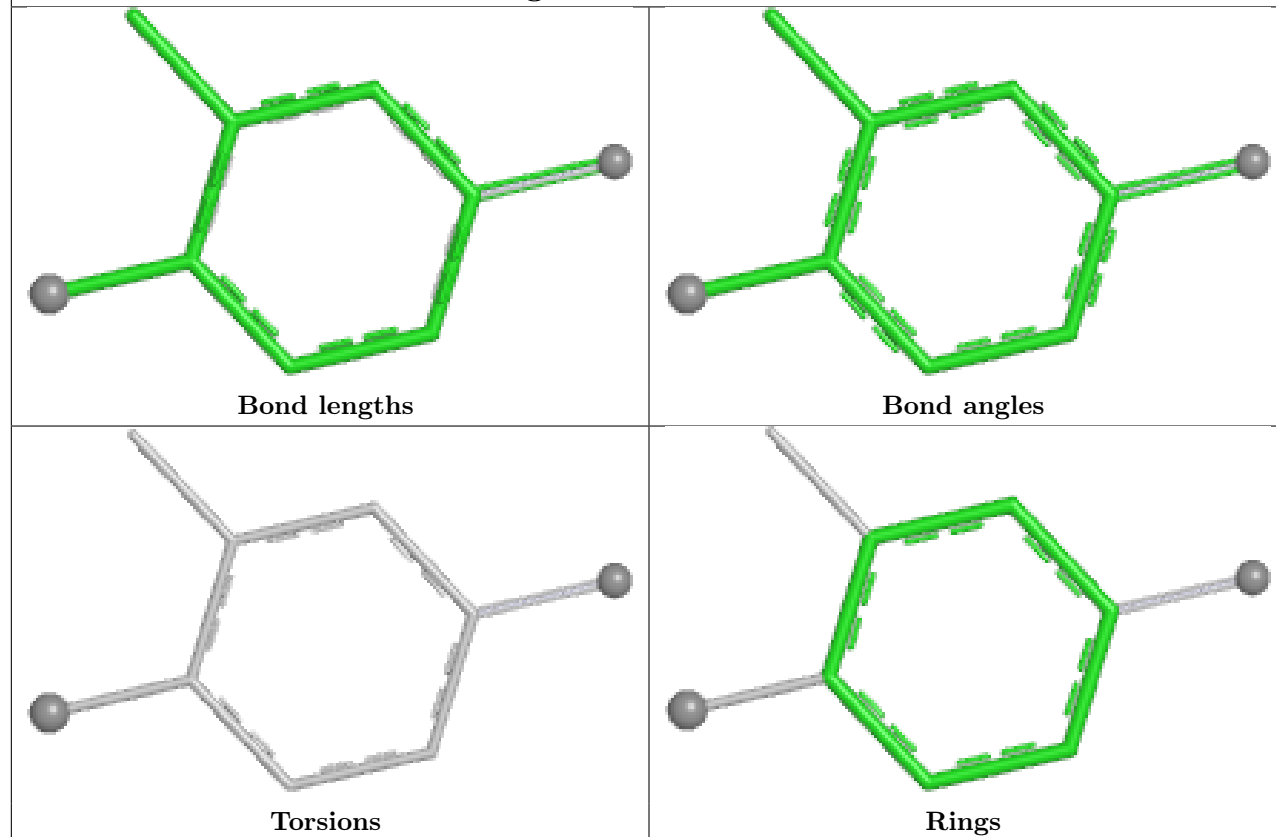


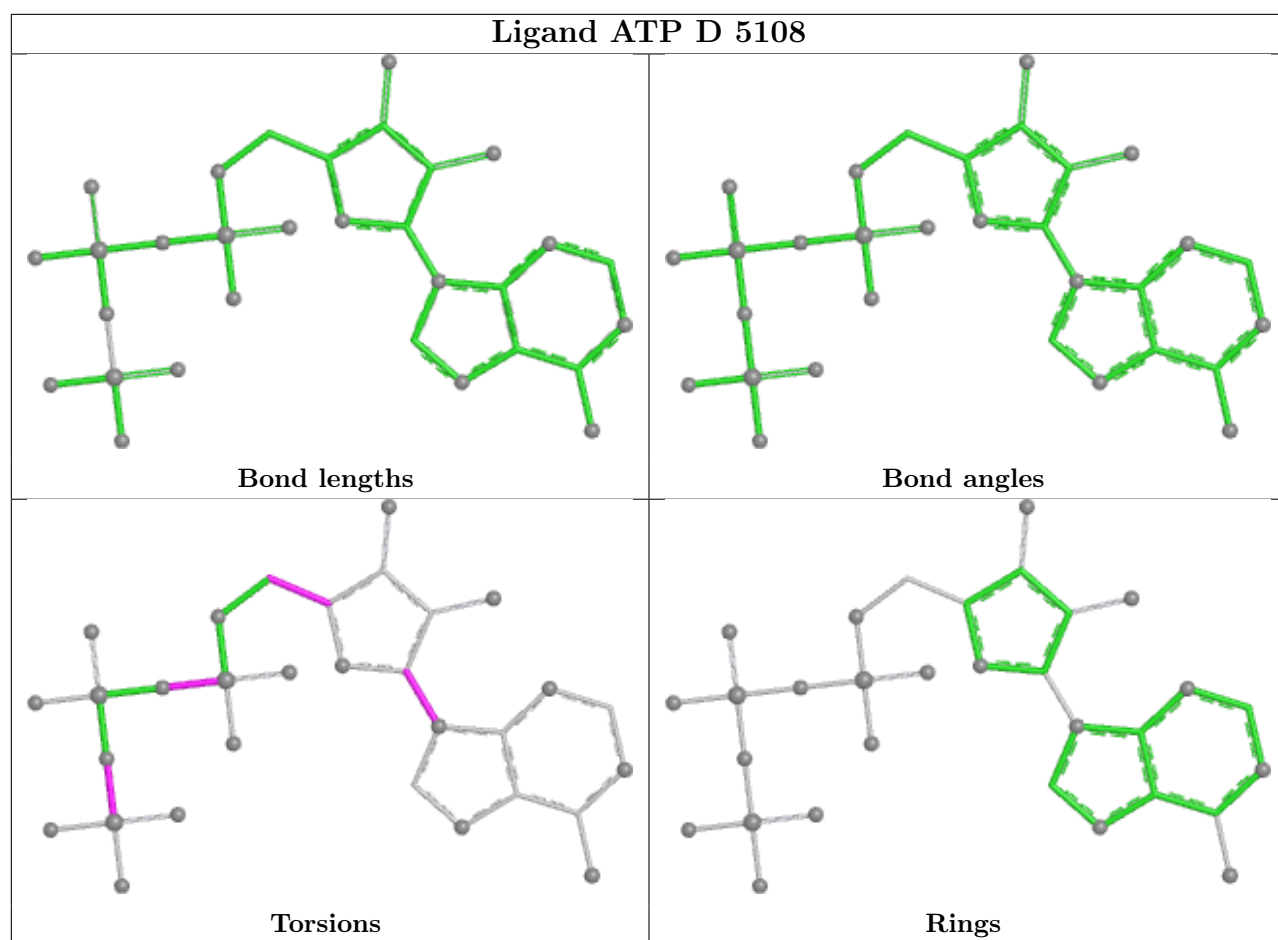


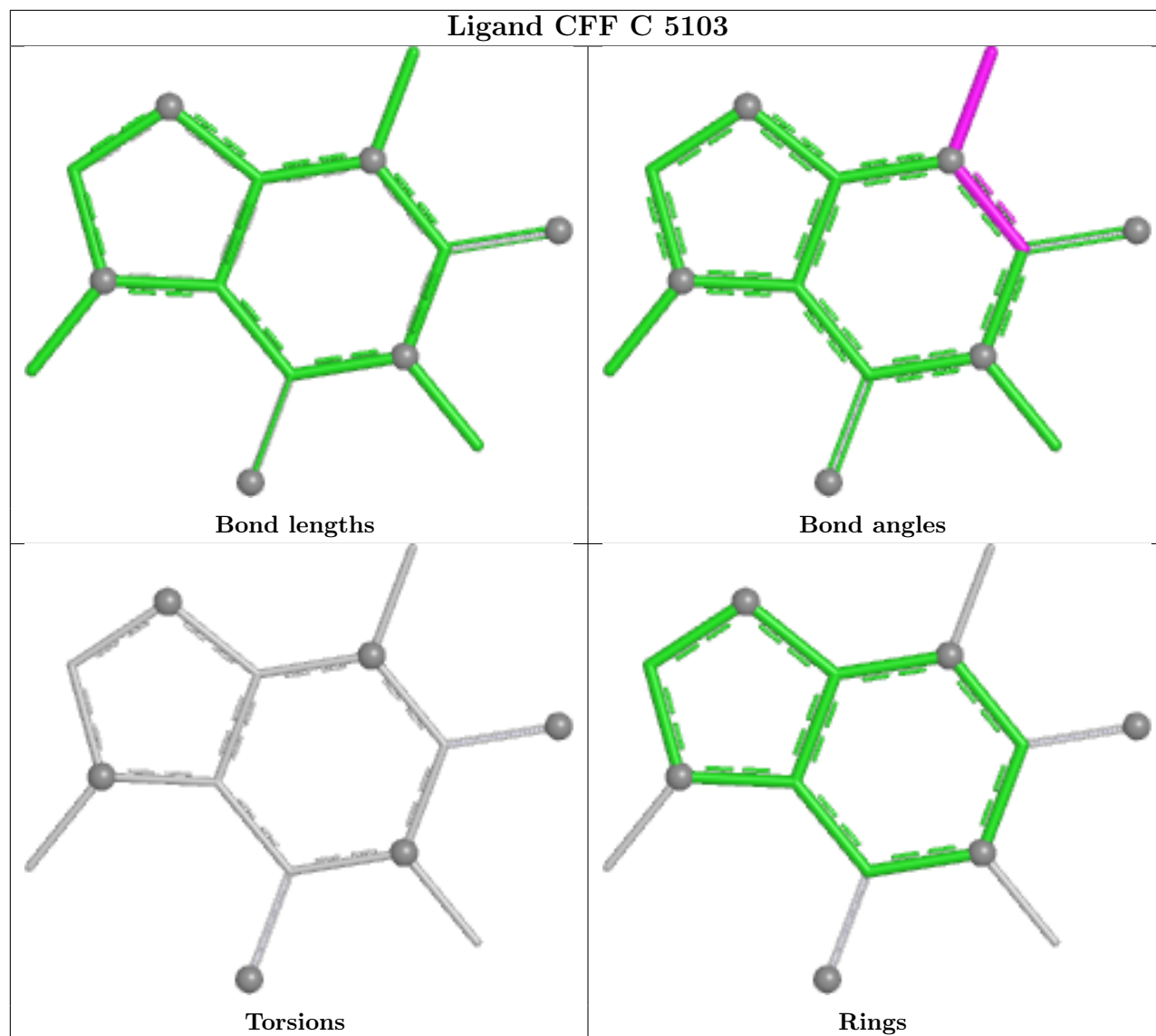
Ligand 43M B 5105

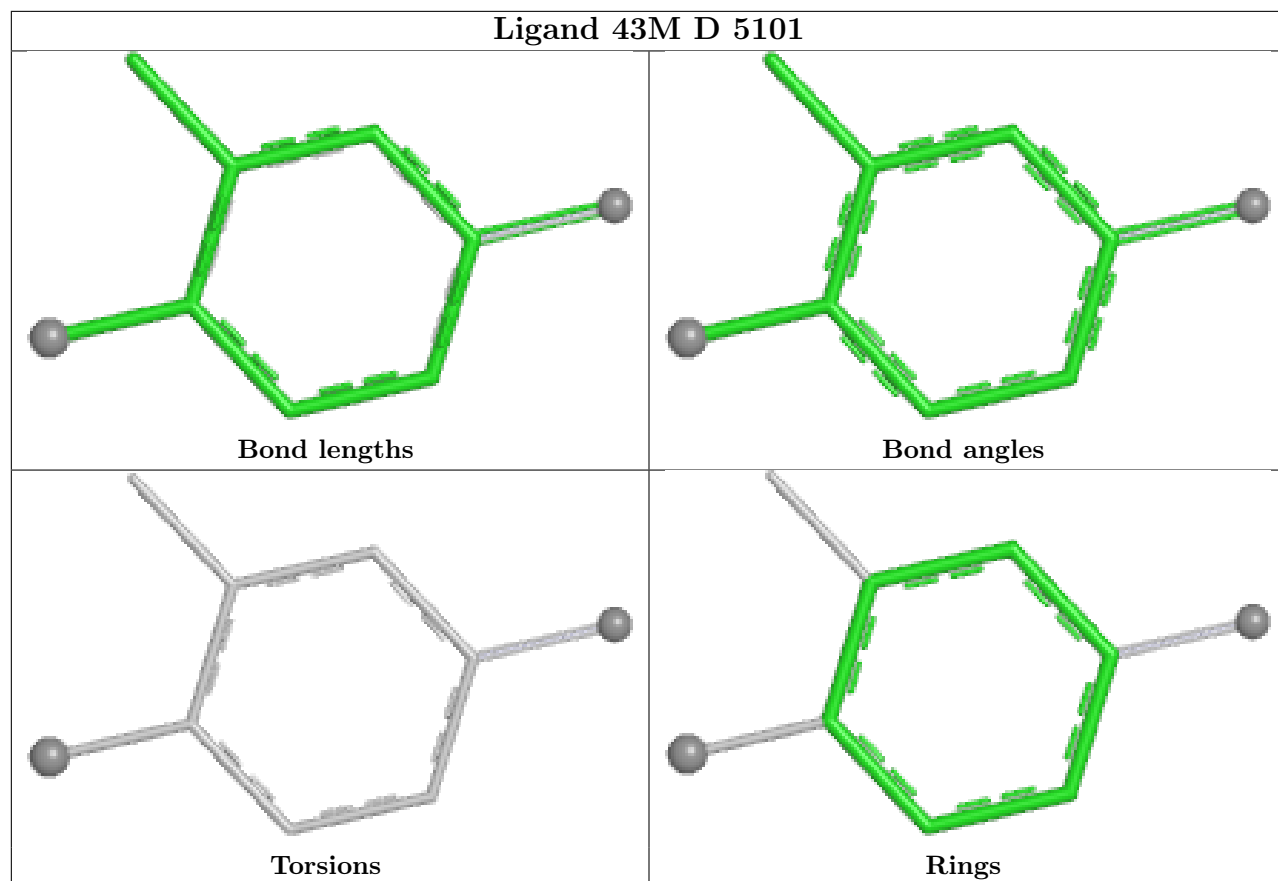


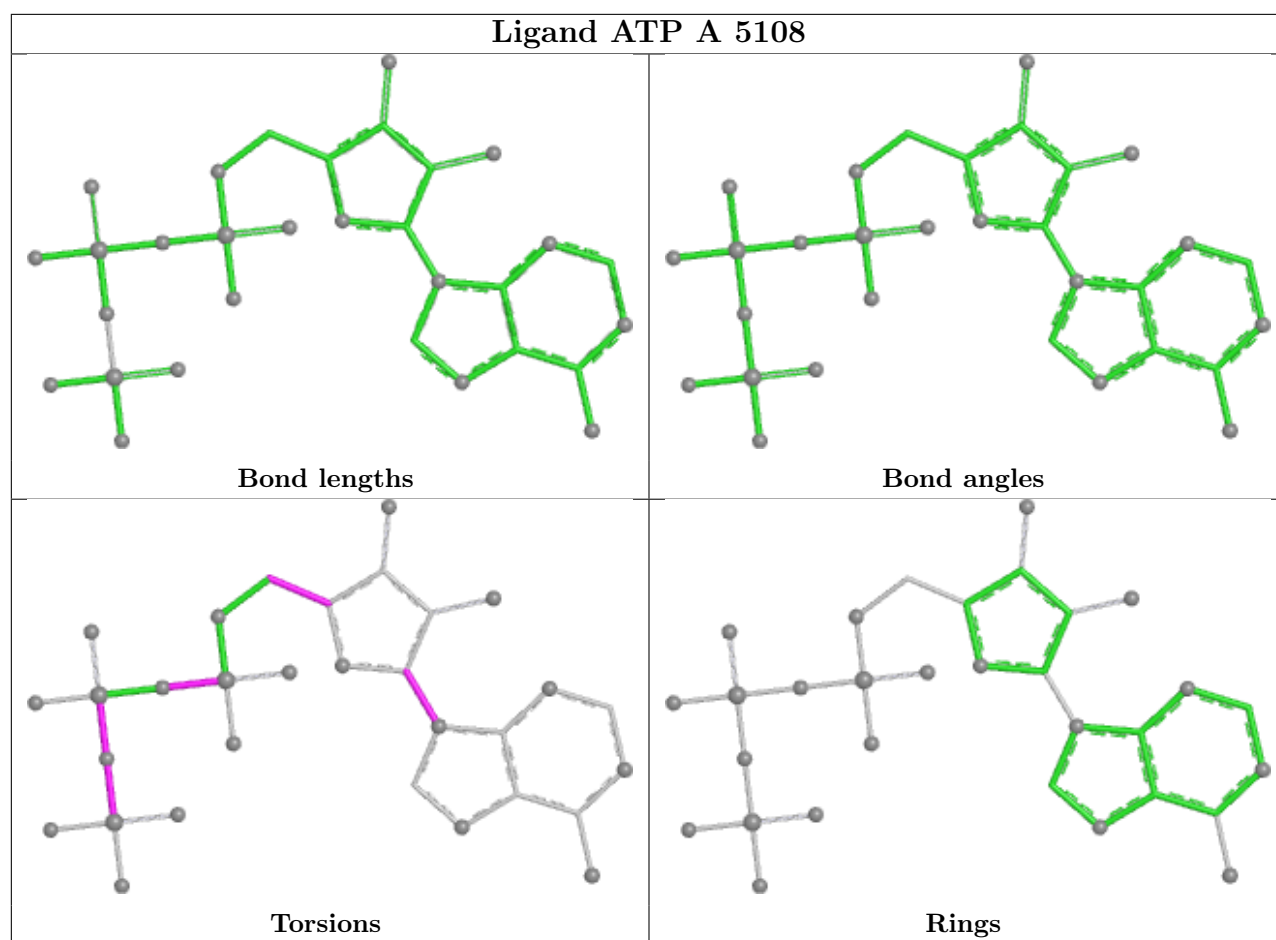
Ligand 43M C 5105

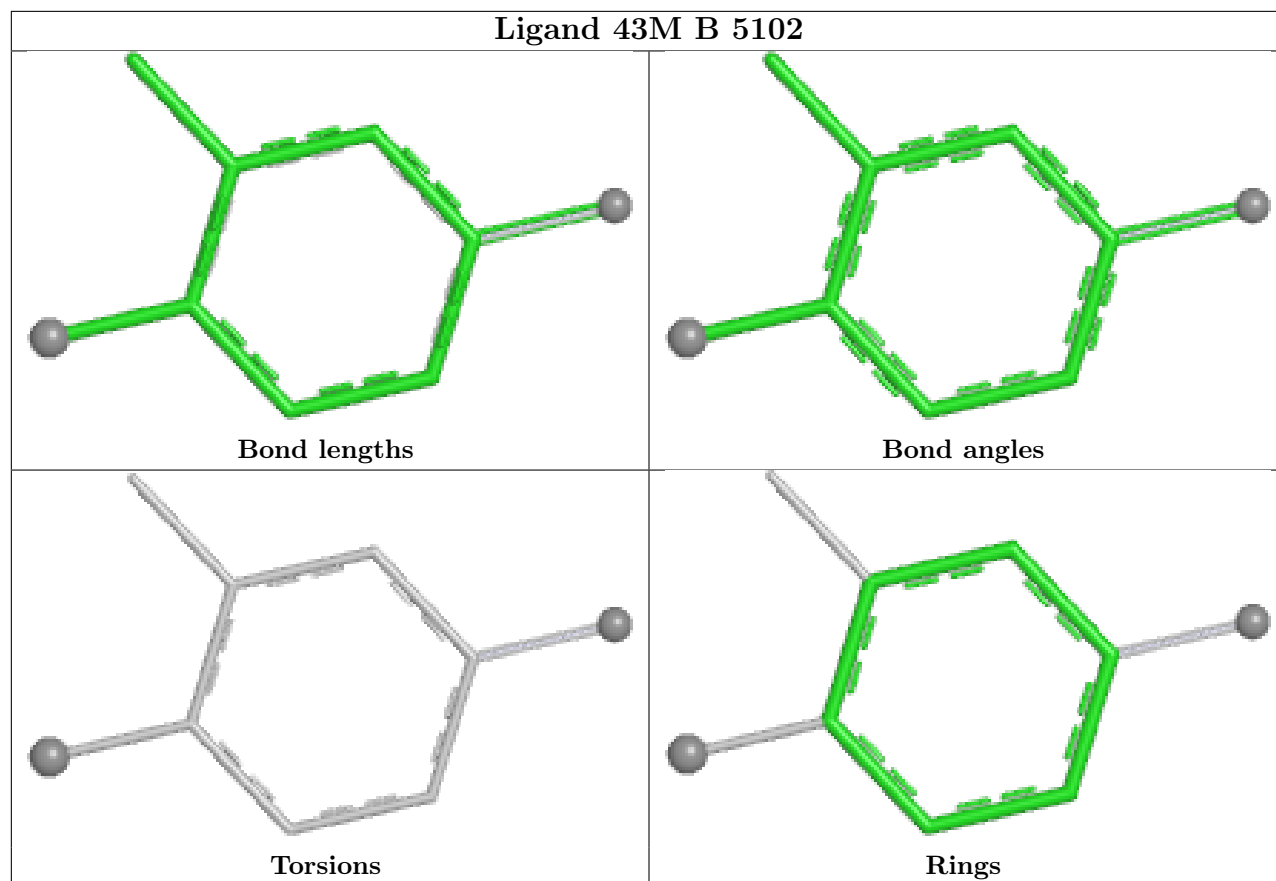


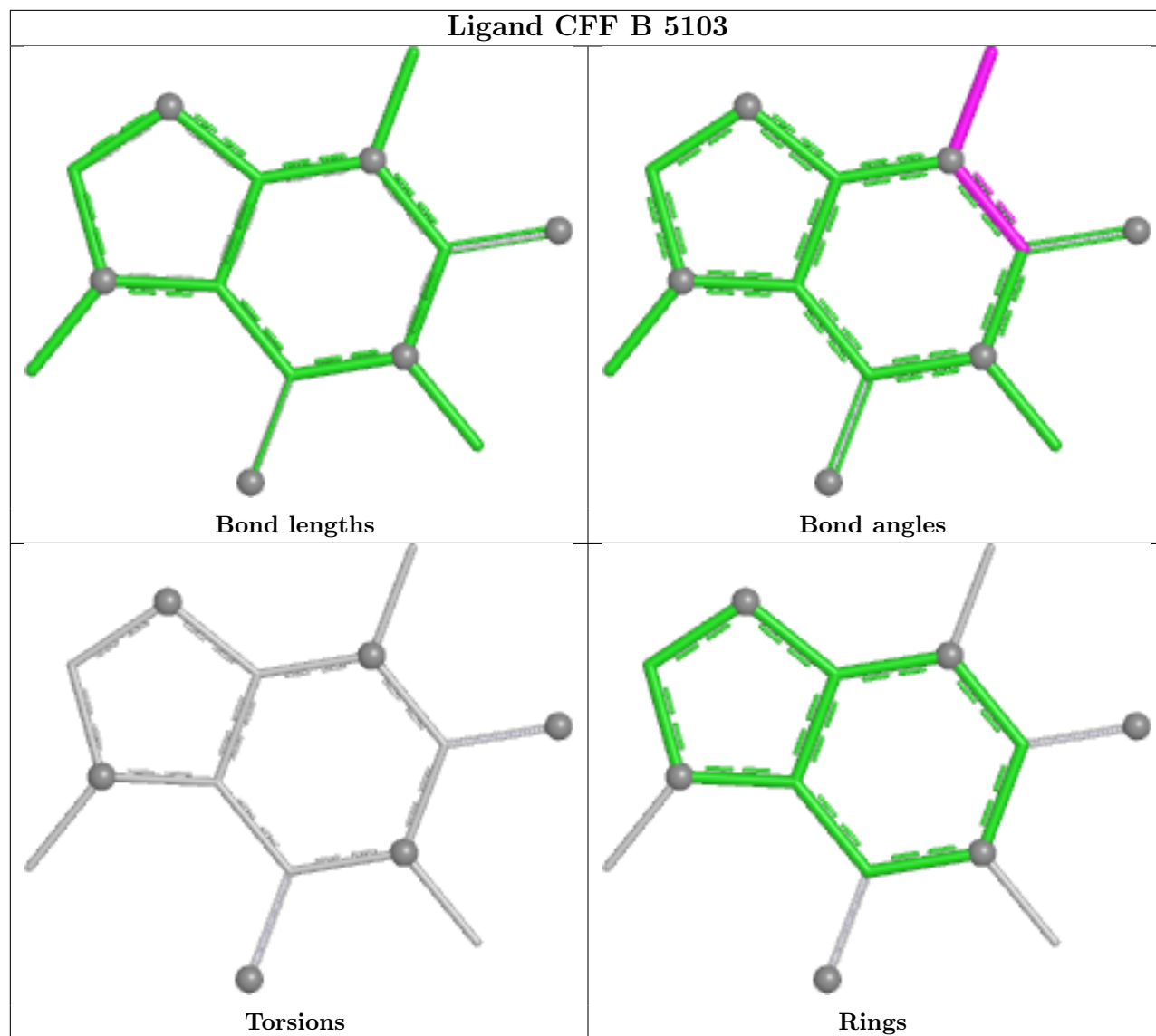


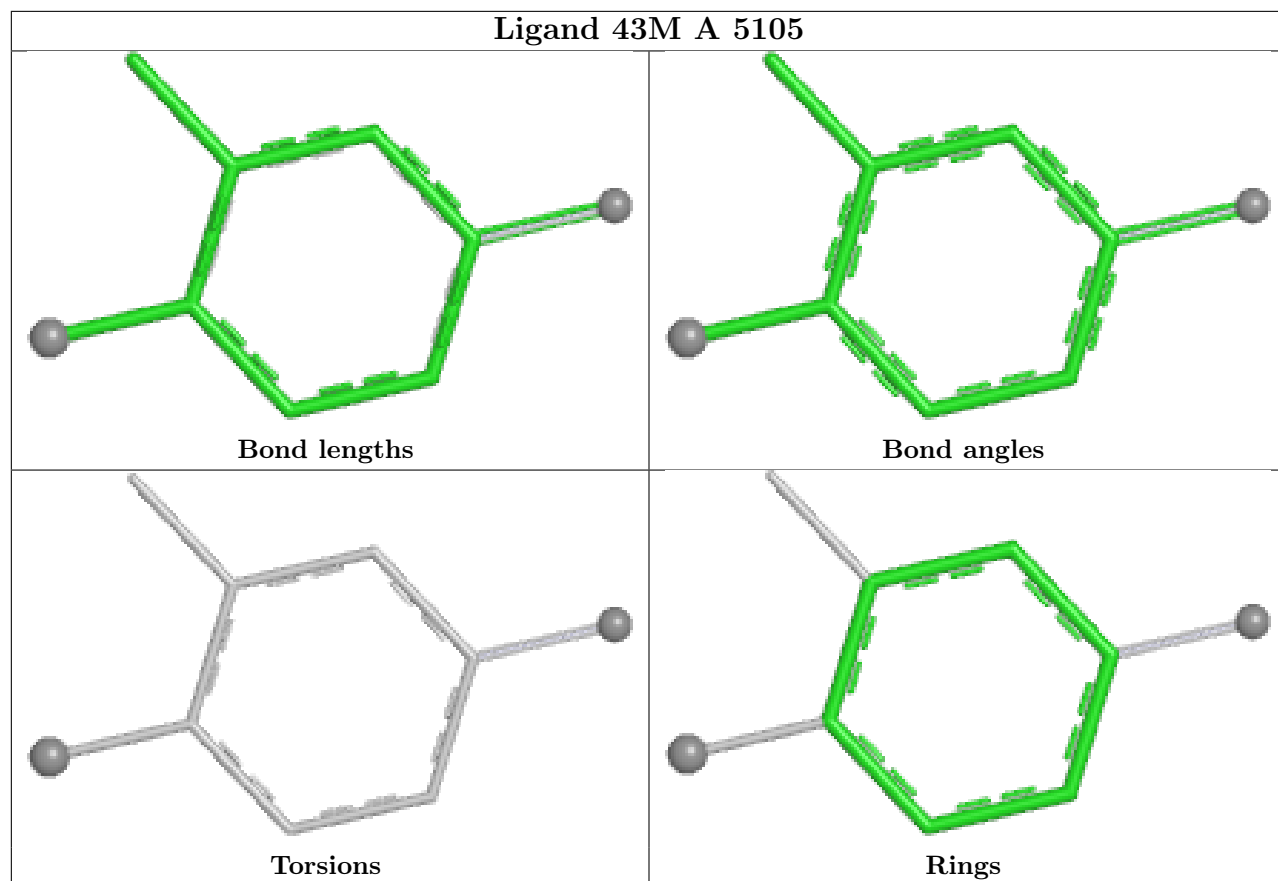


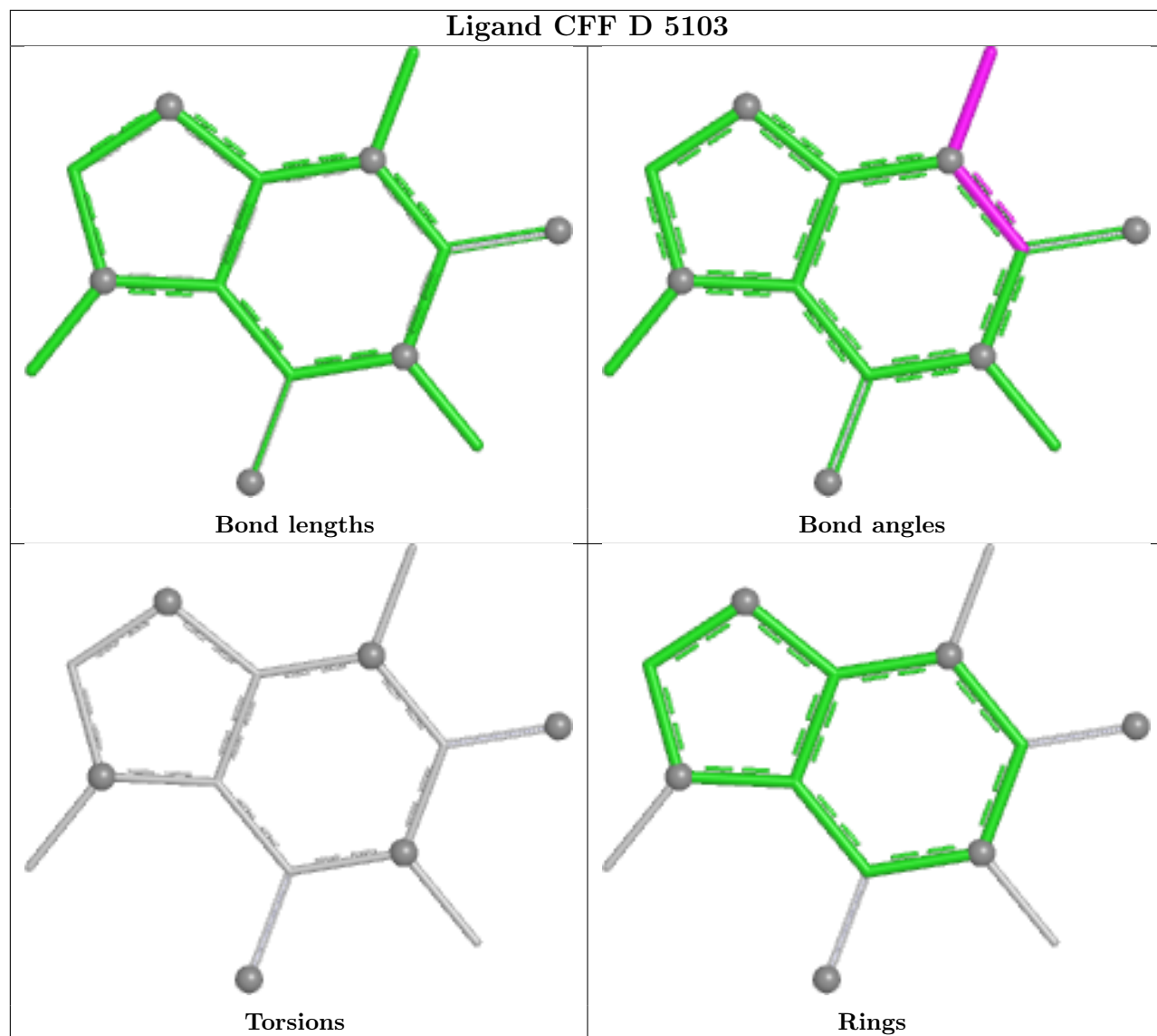




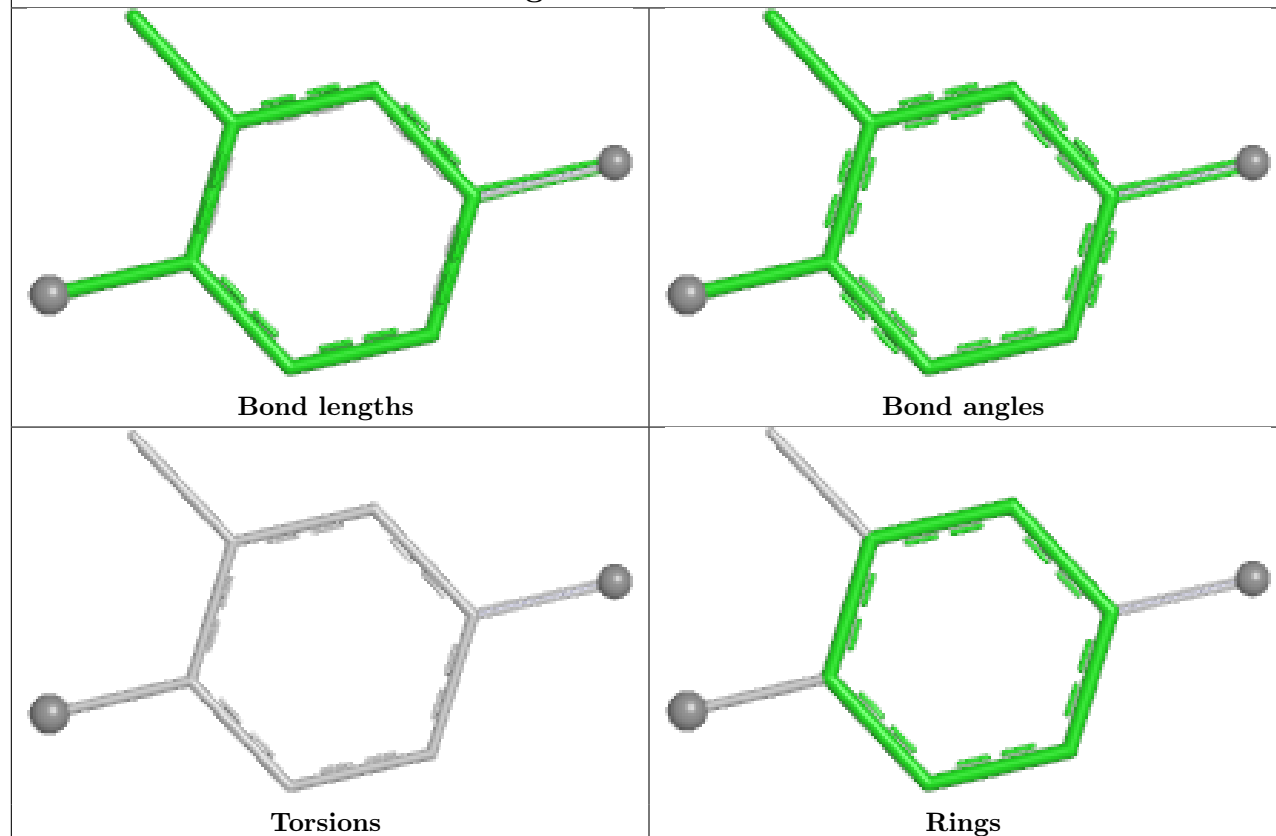




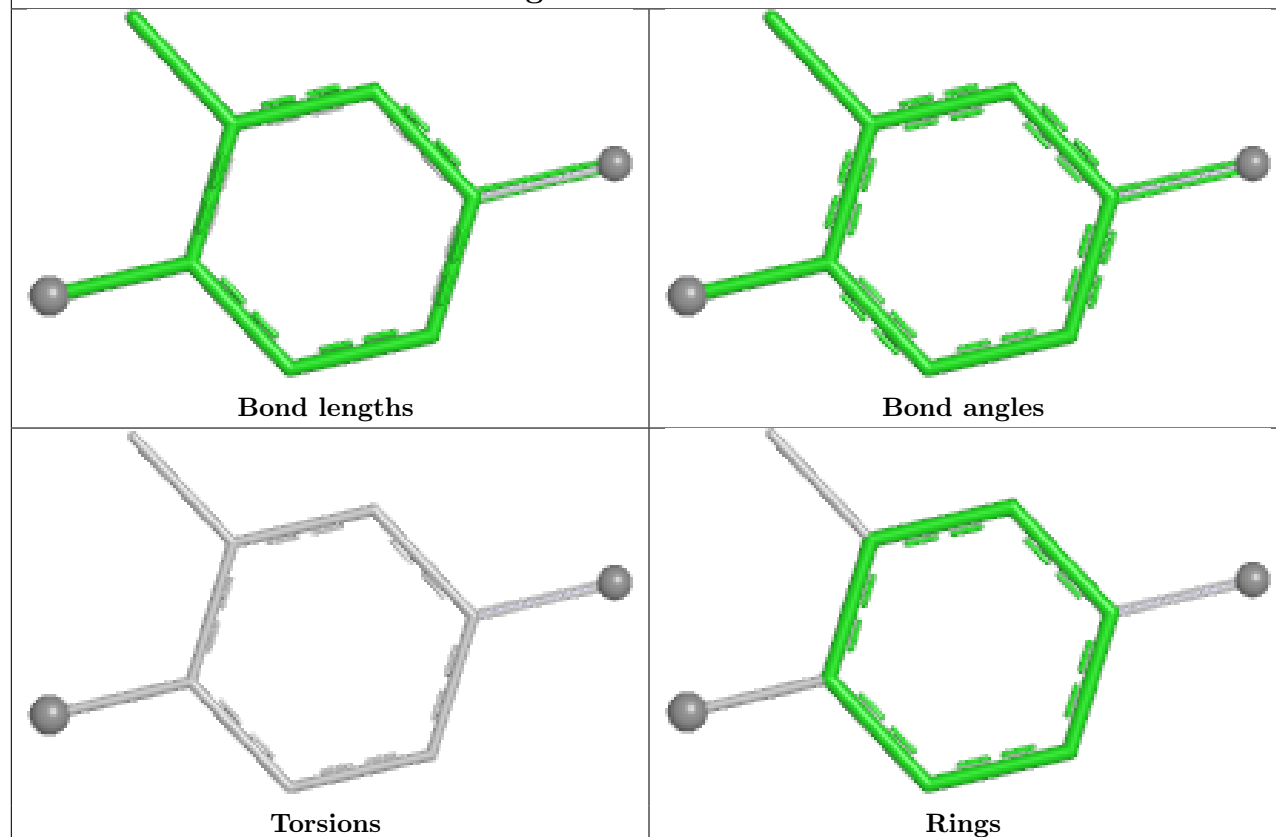


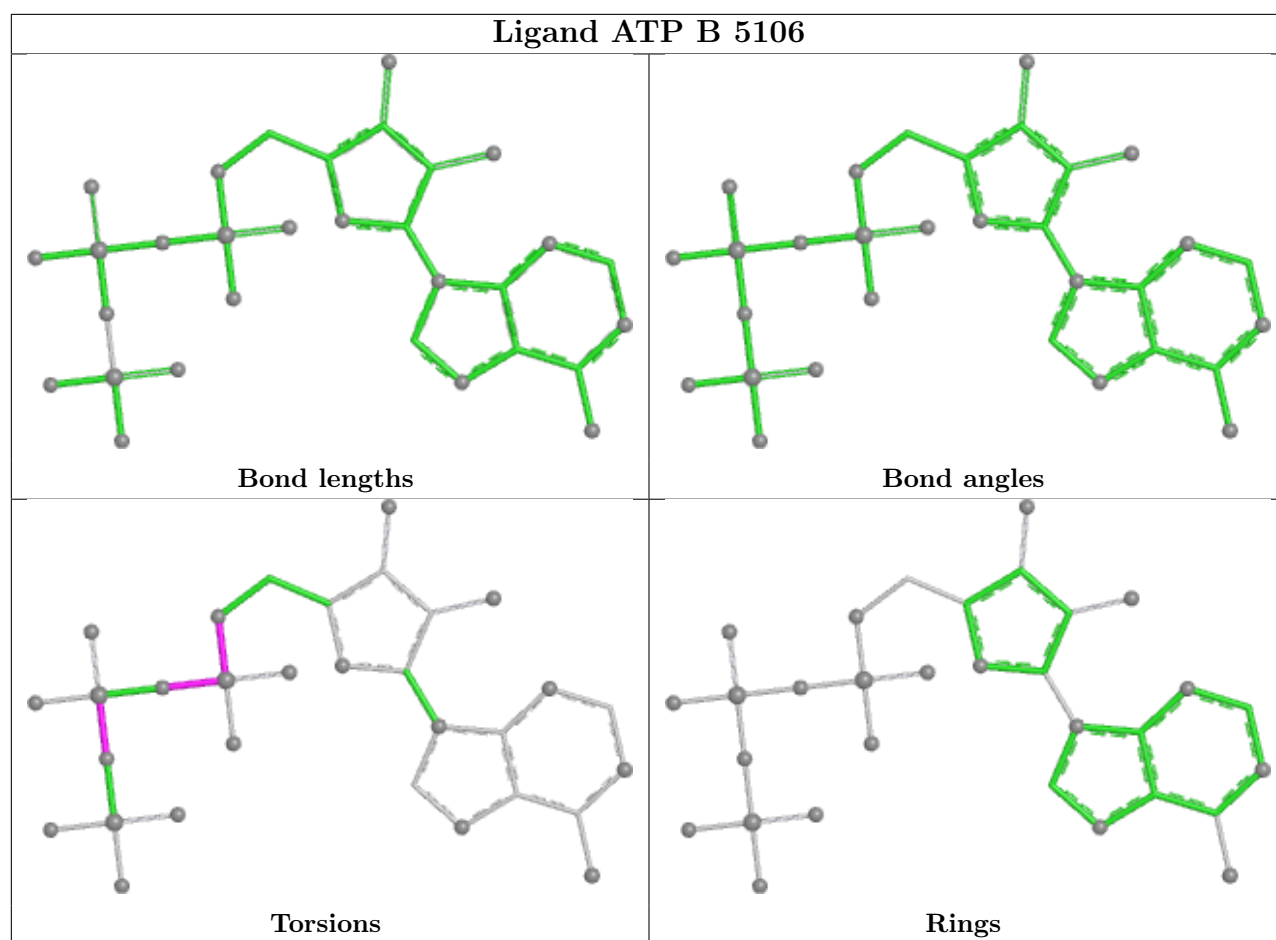


Ligand 43M C 5107



Ligand 43M B 5107





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.

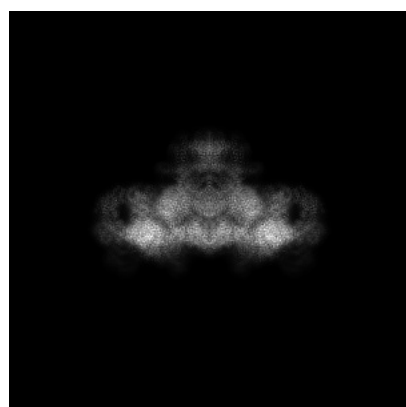
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74439. These allow visual inspection of the internal detail of the map and identification of artifacts.

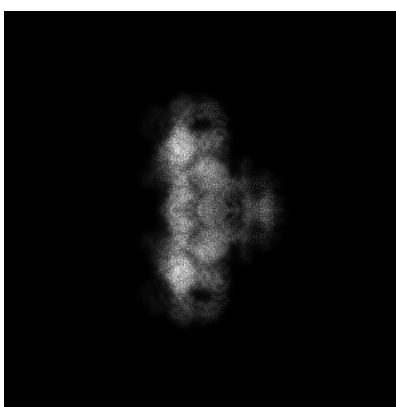
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

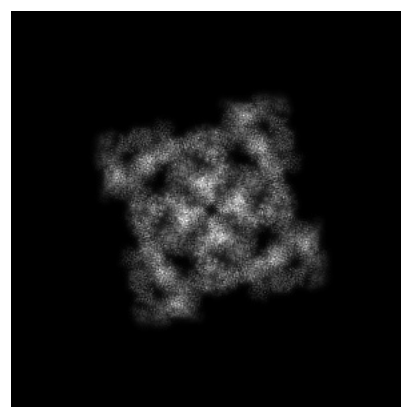
6.1.1 Primary map



X



Y

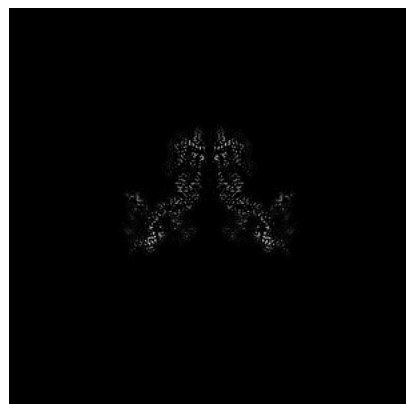


Z

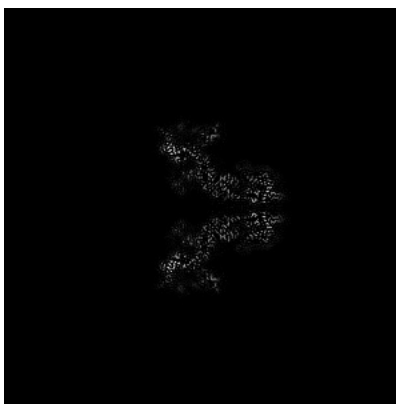
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

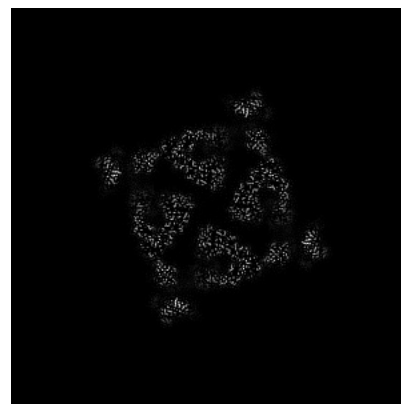
6.2.1 Primary map



X Index: 256



Y Index: 256

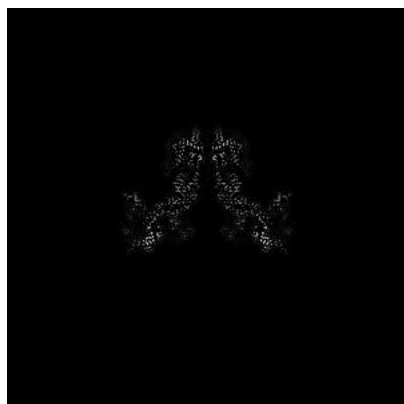


Z Index: 256

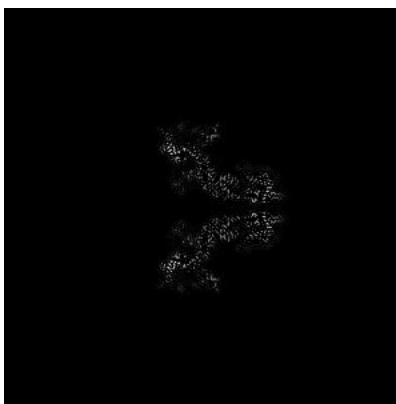
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

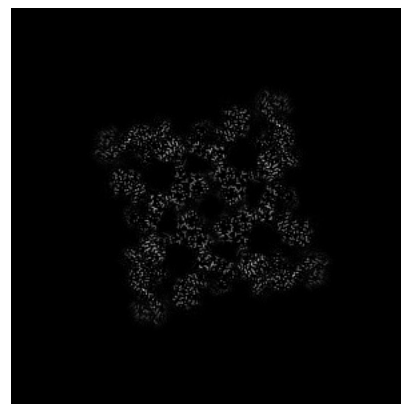
6.3.1 Primary map



X Index: 256



Y Index: 256

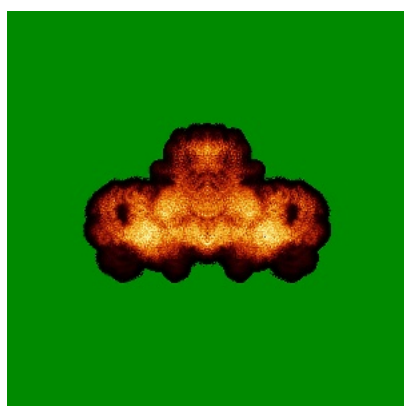


Z Index: 230

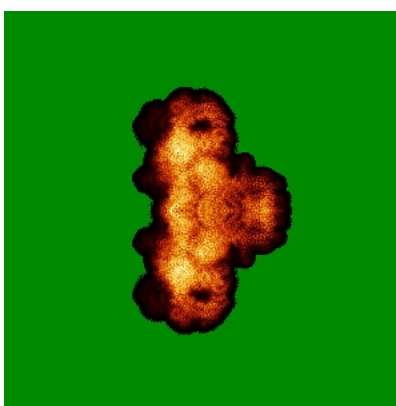
The images above show the largest variance slices of the map in three orthogonal directions.

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

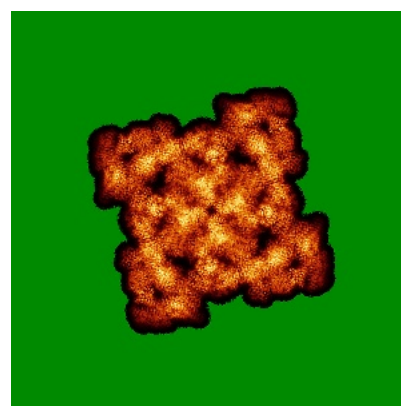
6.4.1 Primary map



X



Y

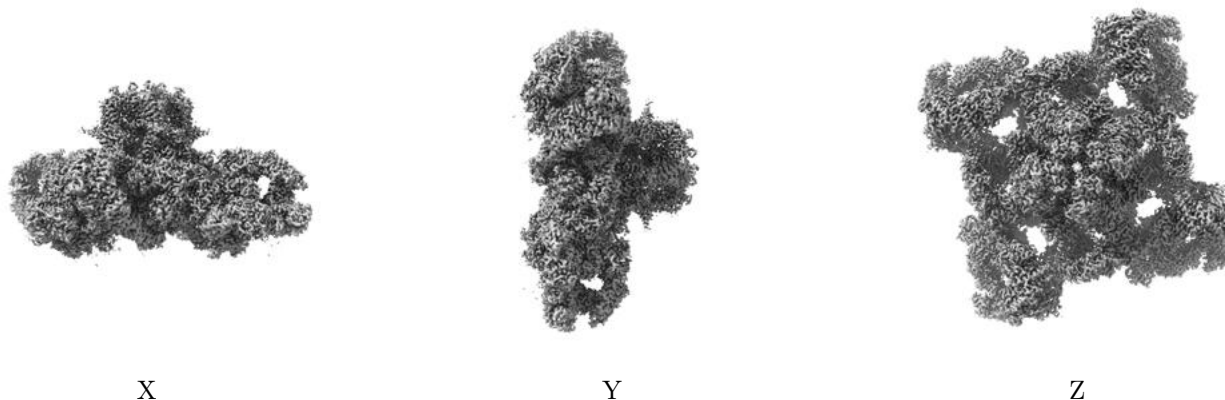


Z

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

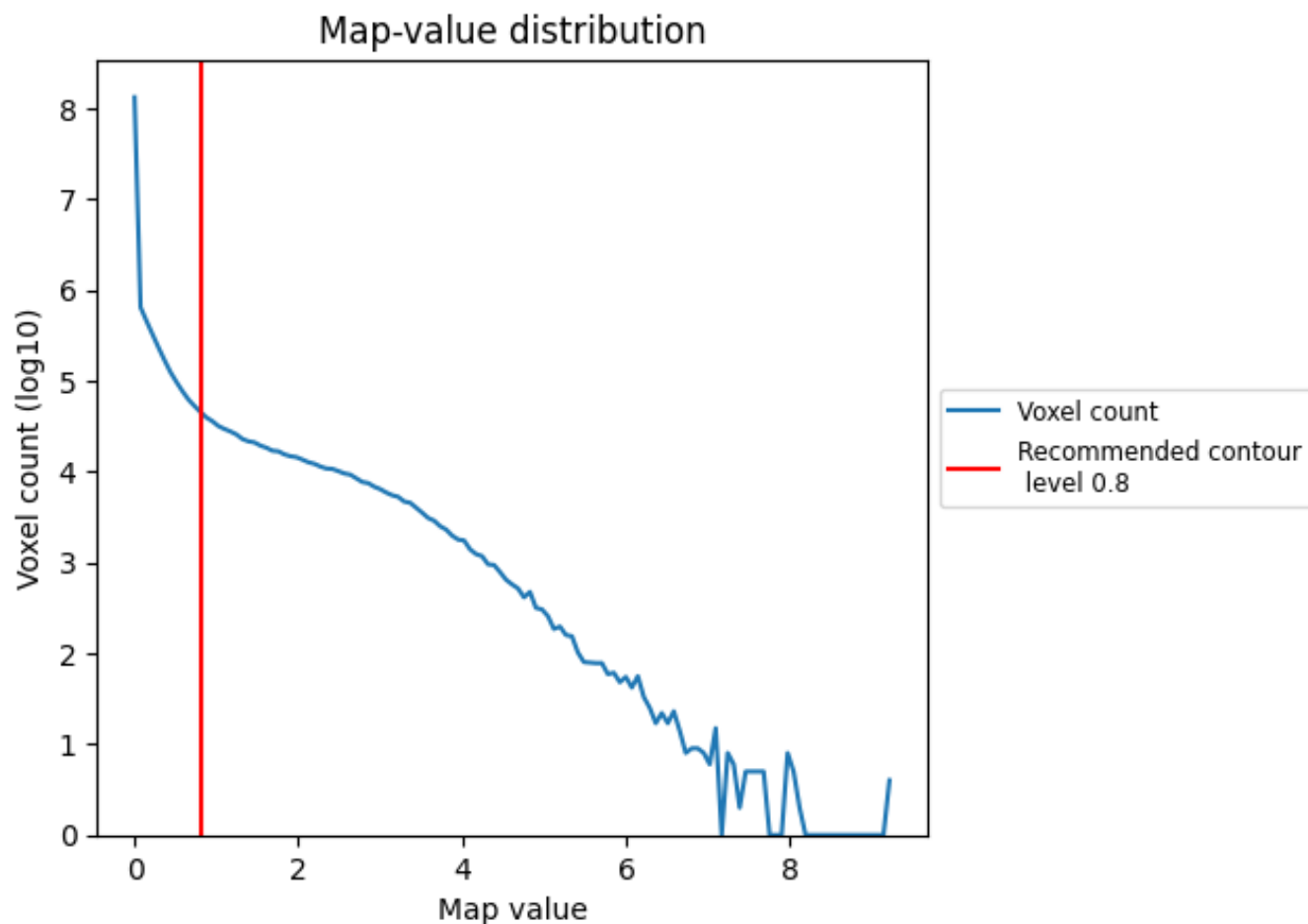
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

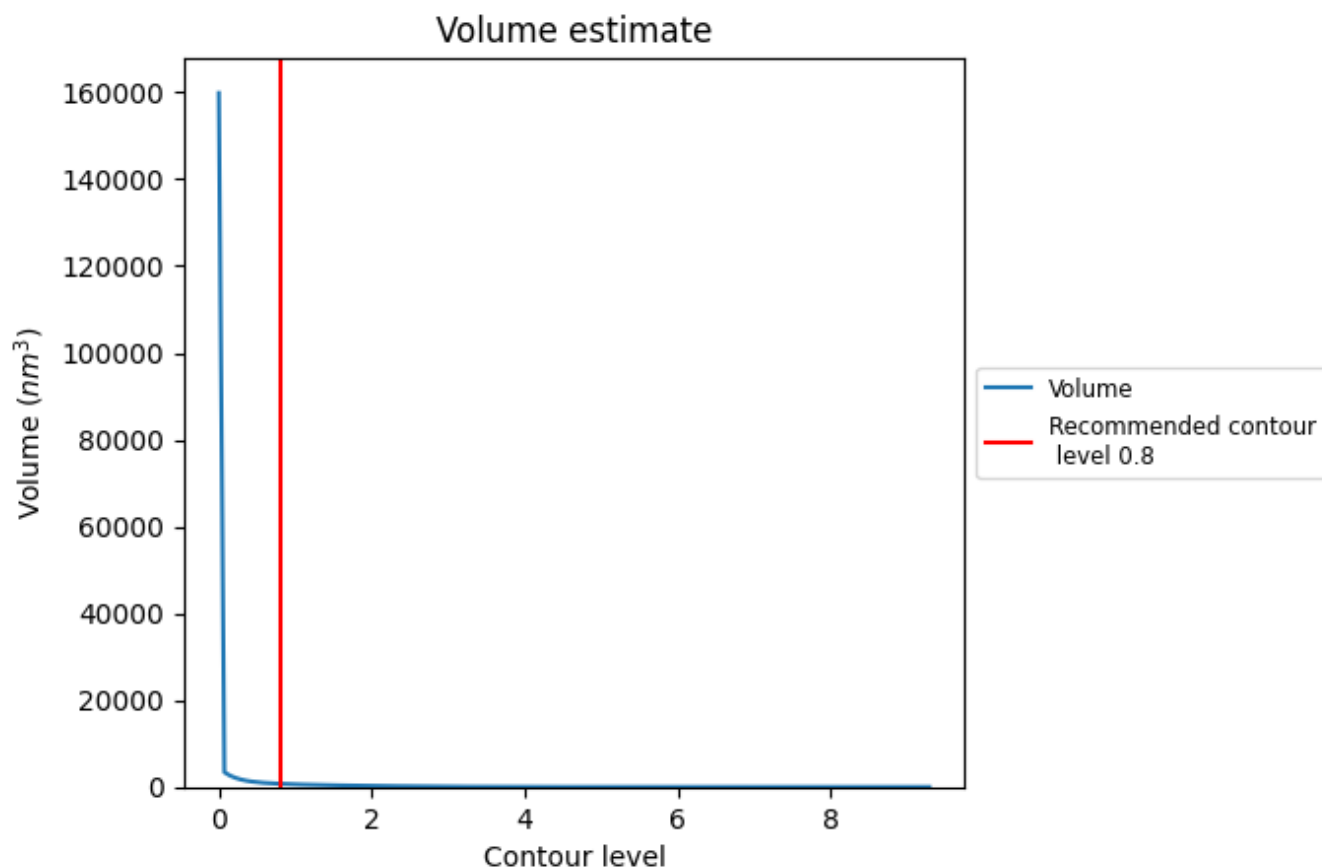
This section contains the results of statistical analysis of the map.

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.

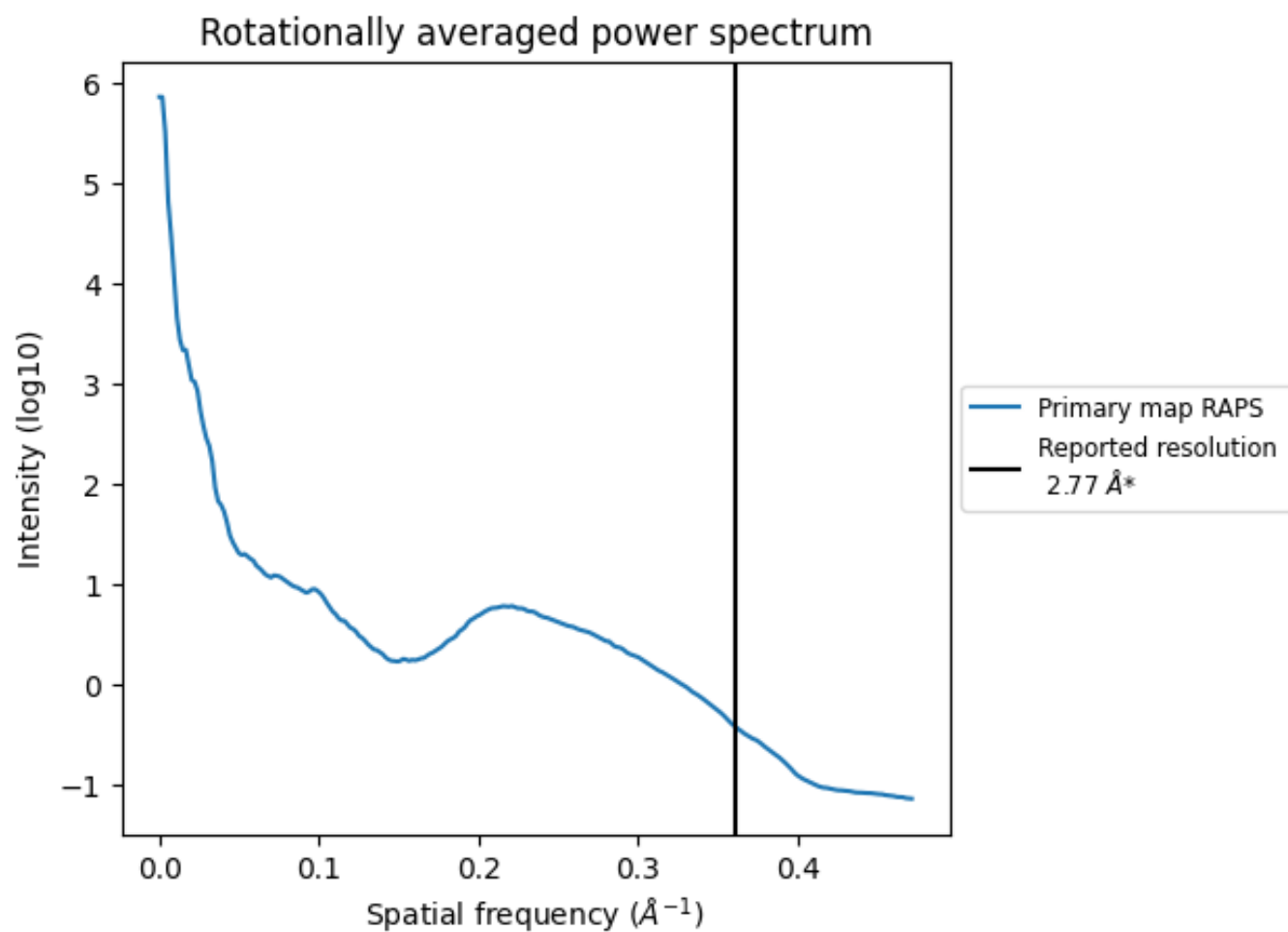
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 735 nm^3 ; this corresponds to an approximate mass of 664 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 0.361 Å⁻¹

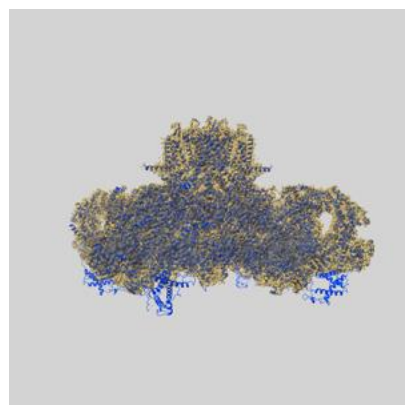
8 Fourier-Shell correlation

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

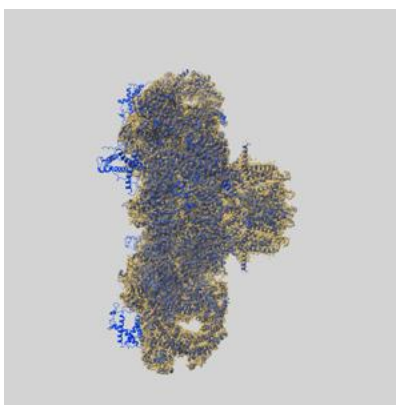
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74439 and PDB model 9ZN9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

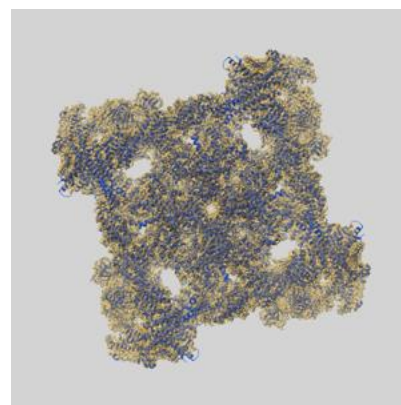
9.1 Map-model overlay [i](#)



X



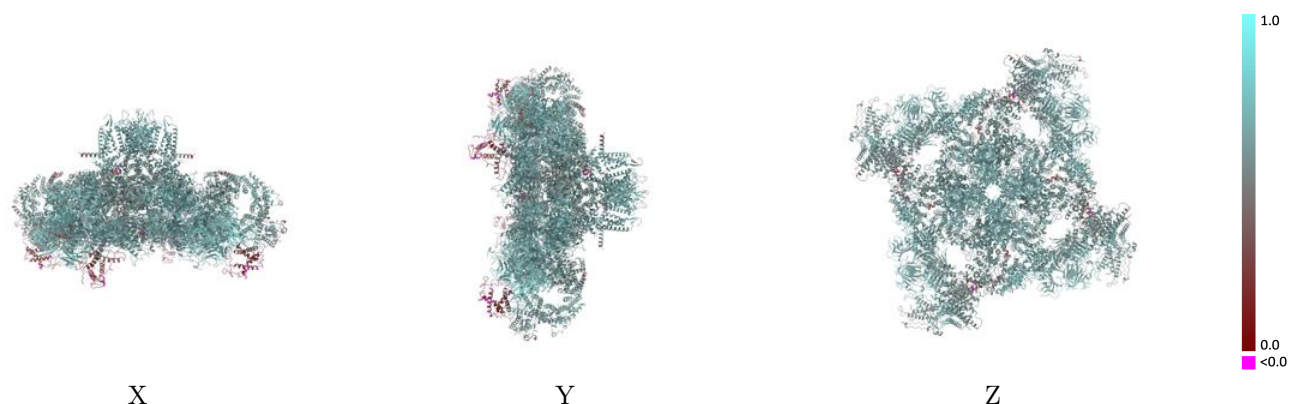
Y



Z

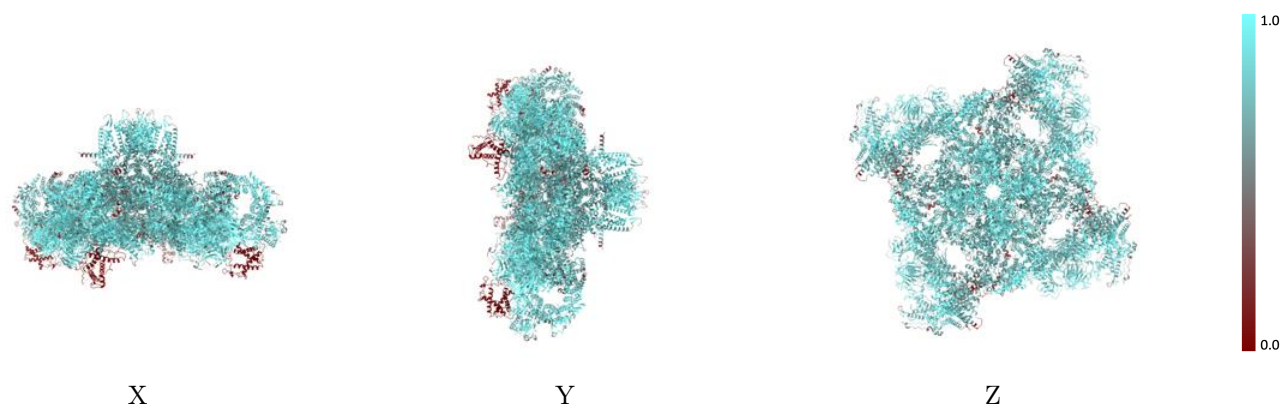
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



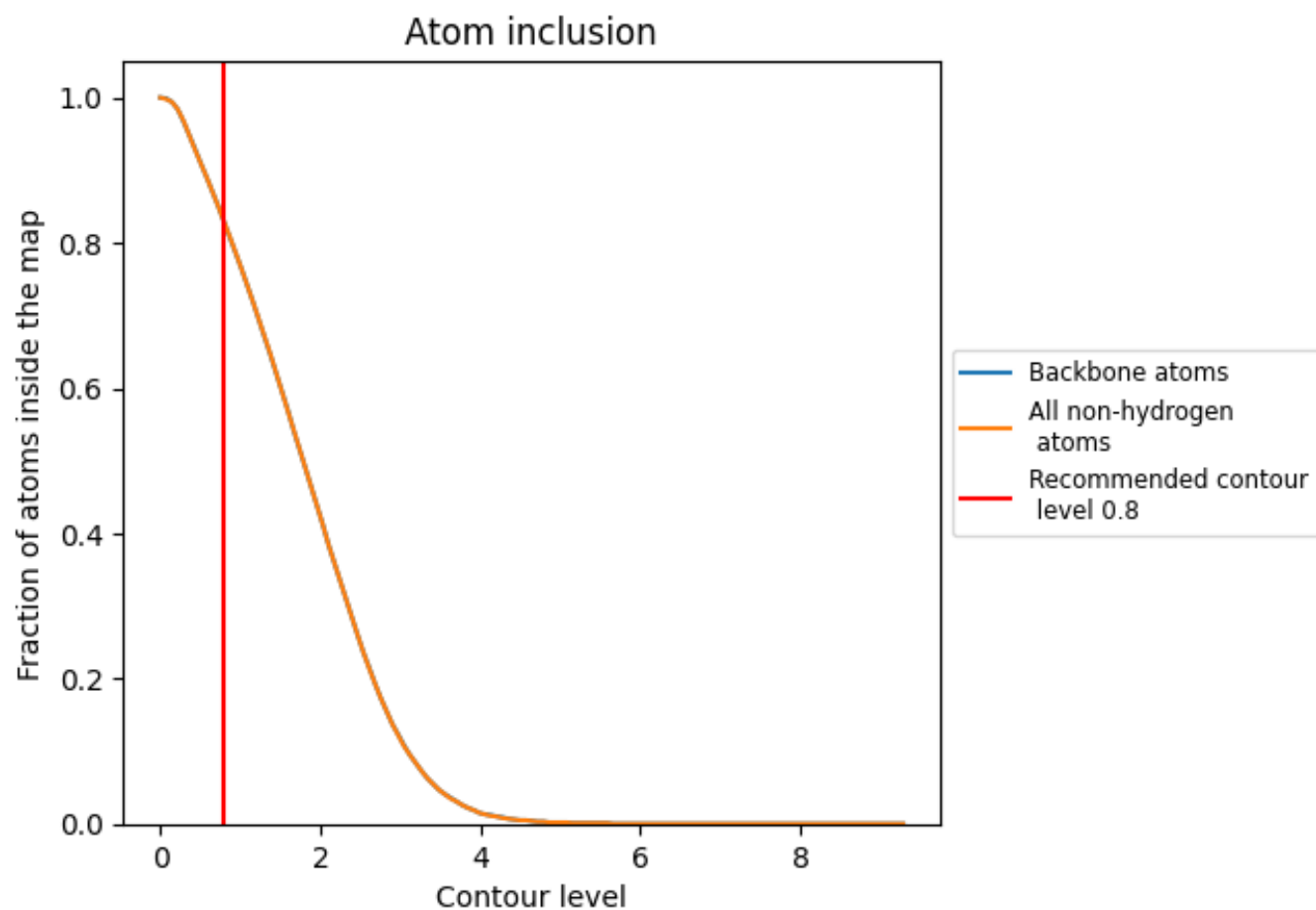
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.6170
A	0.8380	0.6200
B	0.8380	0.6190
C	0.8380	0.6190
D	0.8380	0.6190
E	0.9120	0.6580
F	0.9020	0.6550
G	0.9030	0.6560
H	0.9070	0.6560
I	0.5510	0.5010
J	0.5450	0.5020
K	0.5660	0.5100
L	0.5500	0.5020

1.0

0.0

<0.0