



Full wwPDB EM Validation Report ⓘ

Jul 22, 2025 – 11:07 am BST

PDB ID : 9S1L / pdb_00009s1l
EMDB ID : EMD-54455
Title : Cryo-EM structure of Posidonia oceanica PSI-LHCI supercomplex
Deposited on : 2025-07-18
Resolution : 2.83 Å(reported)
Based on initial model : 5ZJI

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

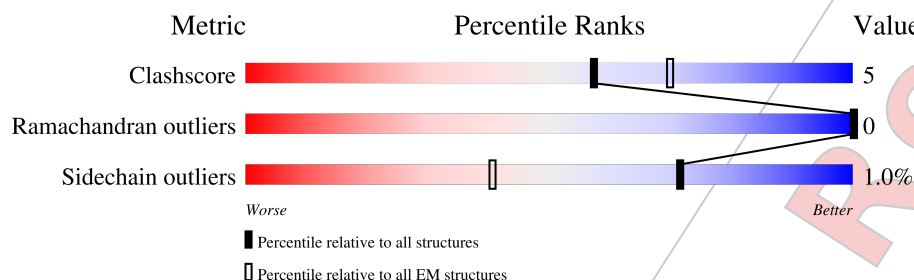
EMDB validation analysis	: 0.0.1.dev118
Mogul	: 1.8.4, CSD as541be (2020)
MolProbity	: 4-5-2 with Phenix2.0rc1
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: 1.9.13
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)

1 Overall quality at a glance

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

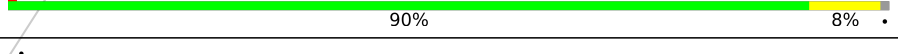
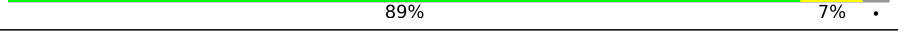
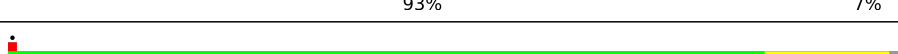
The reported resolution of this entry is 2.83 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	200	
2	2	211	
3	3	232	
4	4	200	
5	A	750	
6	B	734	
7	C	81	

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Validation Pipeline (wwPDB-VP) : 2.44

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Mol	Chain	Length	Quality of chain
8	D	155	
9	E	93	
10	F	159	
11	G	100	
12	H	95	
13	I	36	
14	J	42	
15	K	84	
16	L	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CHL	1	601	X	-	-	-
17	CHL	1	606	X	-	-	-
17	CHL	2	601	X	-	-	-
17	CHL	2	605	X	-	-	-
17	CHL	2	606	X	-	-	-
17	CHL	2	607	X	-	-	-
17	CHL	2	614	X	-	-	-
17	CHL	3	616	X	-	-	-
17	CHL	4	605	X	-	-	-
17	CHL	4	606	X	-	-	-
17	CHL	4	607	X	-	-	-
17	CHL	4	615	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	1	613	X	-	-	-
18	CLA	1	614	X	-	-	-
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	605	X	-	-	-
18	CLA	3	606	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	3	613	X	-	-	-
18	CLA	3	617	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	801	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	F	304	X	-	-	-
18	CLA	G	202	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	G	204	X	-	-	-
18	CLA	H	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	J	102	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	202	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 35475 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 Chlorophyll a-b binding protein 6, chloroplastic (Lhca1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1504	981	252	266	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2 (Lhca2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1579	1031	257	285	6		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	213	Total	C	N	O	S	0	0
			1638	1074	263	295	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4 (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1 (PsaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	724	Total	C	N	O	S	0	0
			5684	3726	968	972	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 (PsaB).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3847	996	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center (PsaC).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			614	380	106	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-1 (PsaD).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1103	708	190	201	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A (PsaE1).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	63	Total	C	N	O	S	0	0
			519	333	92	94			

- Molecule 10 is a protein called Photosystem I reaction center subunit III (PsaF).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1224	794	209	217	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit V (PsaG).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			768	500	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1 (PsaH1).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	94	Total	C	N	O	S	0	0
			736	483	114	139			

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII (PsaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	32	Total	C	N	O	S	0	0
			246	167	39	39	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX (PsaJ).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	40	Total	C	N	O	0	0
			319	216	49	54		

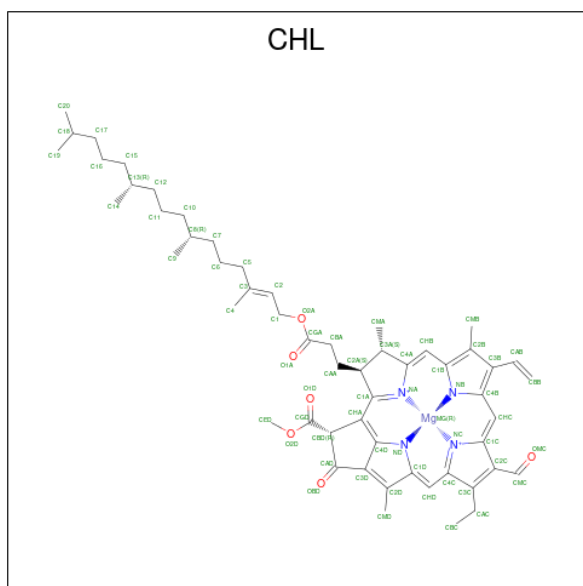
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK (PsaK).

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	55	Total	C	N	O	S	0
			386	251	62	69	4	

- Molecule 16 is a protein called Photosystem I reaction center subunit XI (PsaL).

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	152	Total	C	N	O	S	0
			1141	755	179	204	3	

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



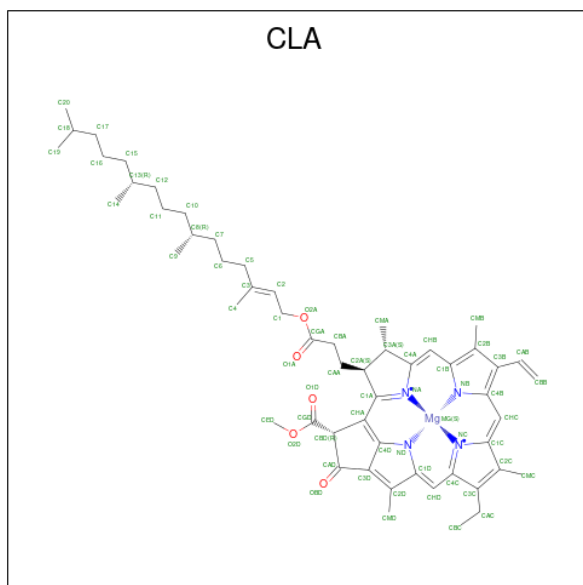
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	Total 65	55	1	4	5	0
18	A	1	Total 50	40	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 41	33	1	4	3	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 52	42	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 55	45	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 54	44	1	4	5	0
18	B	1	Total 43	35	1	4	3	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 65	55	1	4	5	0
18	B	1	Total 55	45	1	4	5	0
18	B	1	Total 55	45	1	4	5	0
18	B	1	Total 59	49	1	4	5	0
18	B	1	Total 60	50	1	4	5	0
18	B	1	Total 55	45	1	4	5	0
18	B	1	Total 50	40	1	4	5	0

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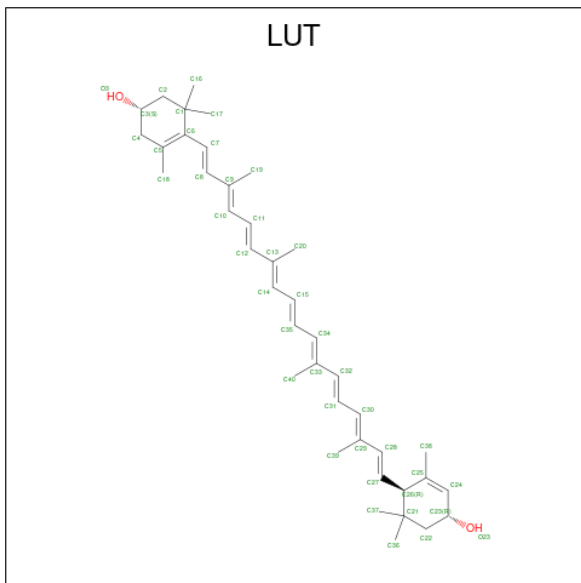
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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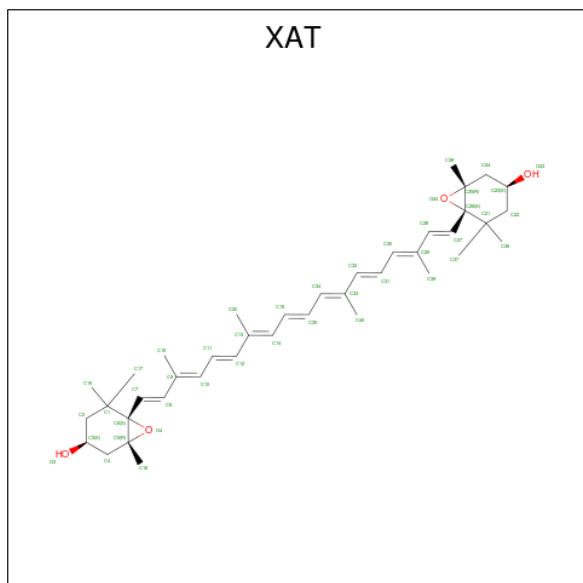
Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



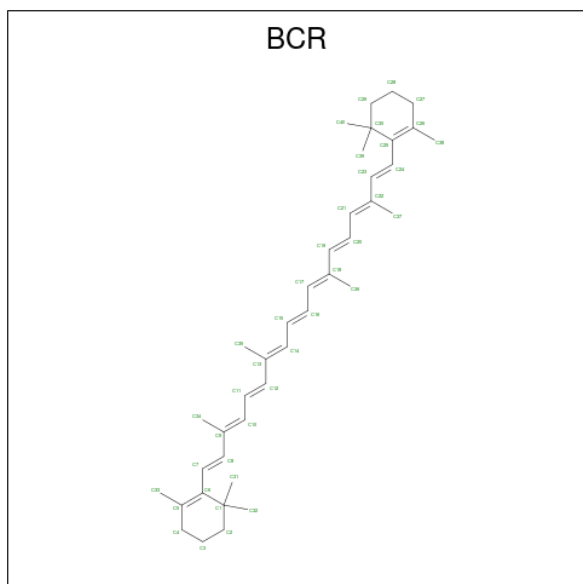
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			42	40	2	
19	1	1	Total	C	O	0
			42	40	2	
19	2	1	Total	C	O	0
			42	40	2	
19	3	1	Total	C	O	0
			42	40	2	
19	4	1	Total	C	O	0
			42	40	2	

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



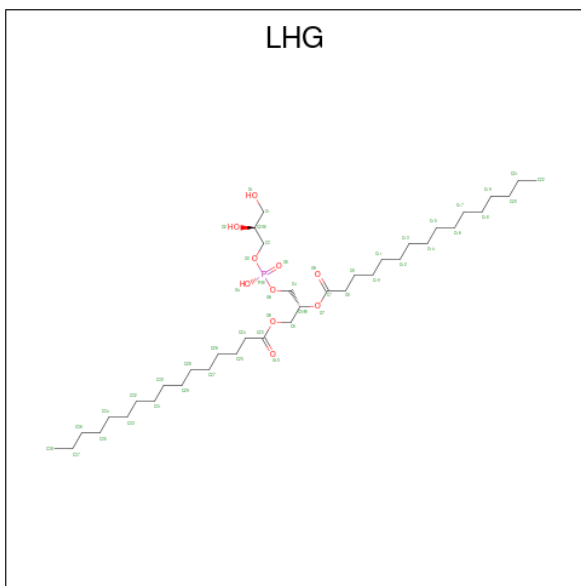
Mol	Chain	Residues	Atoms	AltConf
21	1	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



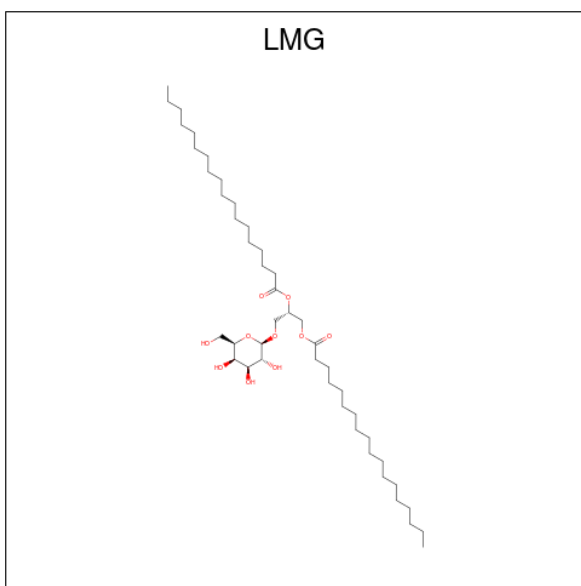
Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 38 27 10 1	0
22	2	1	Total C O P 37 26 10 1	0
22	A	1	Total C O P 49 38 10 1	0

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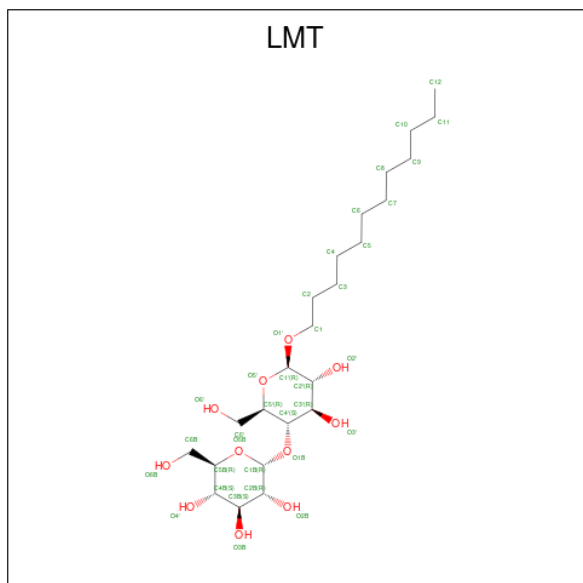
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	A	1	30	19	10	1	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



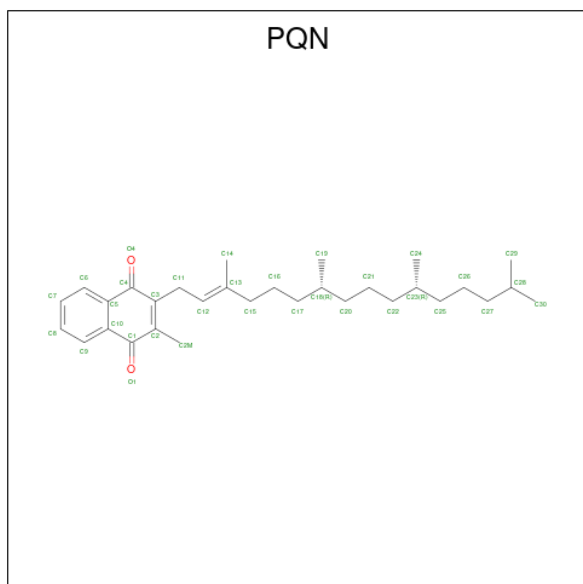
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
23	1	1	53	43	10		0
23	1	1	50	40	10		0
23	4	1	36	26	10		0
23	4	1	49	39	10		0
23	B	1	52	42	10		0
23	F	1	47	37	10		0
23	F	1	30	20	10		0

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



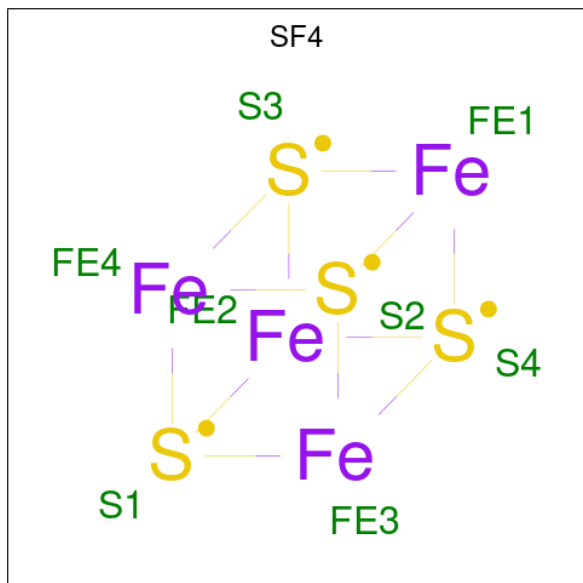
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total 35	C 24	O 11	0
24	A	1	Total 35	C 24	O 11	0
24	A	1	Total 35	C 24	O 11	0
24	G	1	Total 35	C 24	O 11	0

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



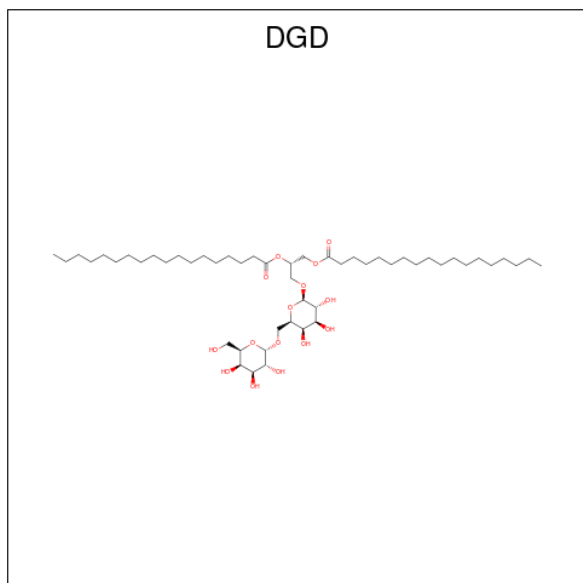
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).

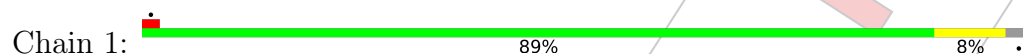


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	61	46	15	0

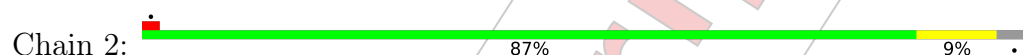
3 Residue-property plots

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

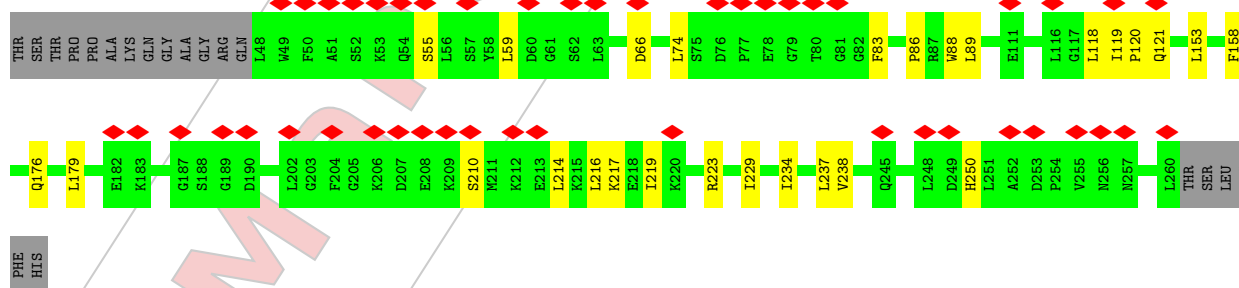
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic (Lhca1)



- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2 (Lhca2)



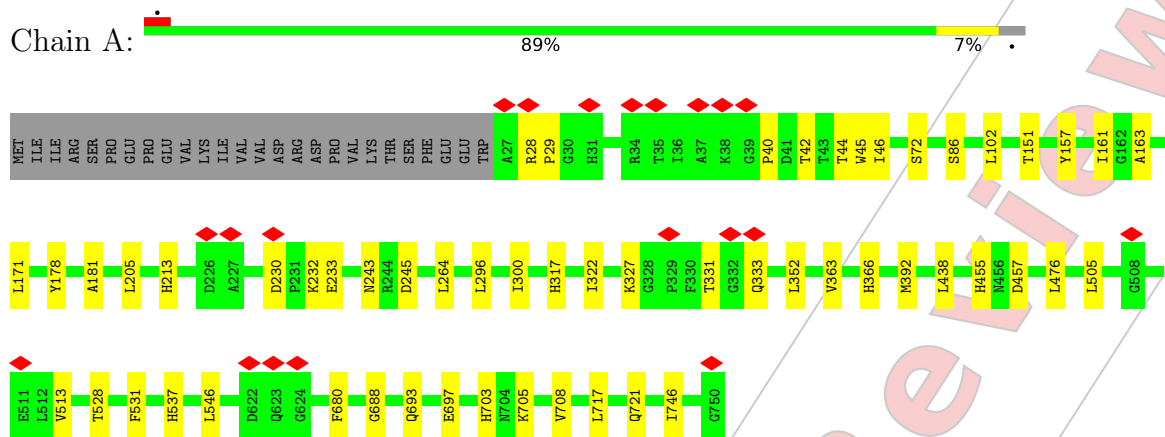
- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3)



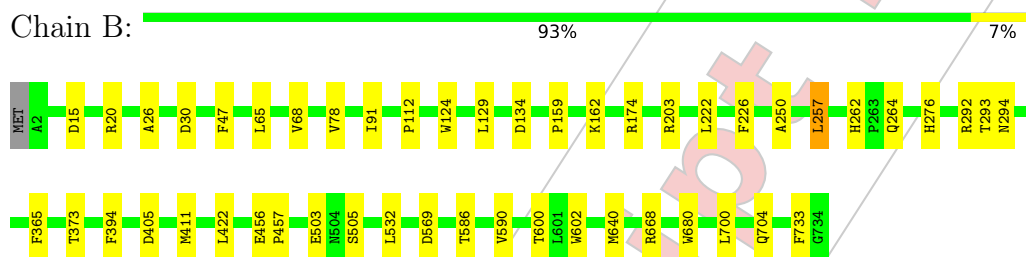
- Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)



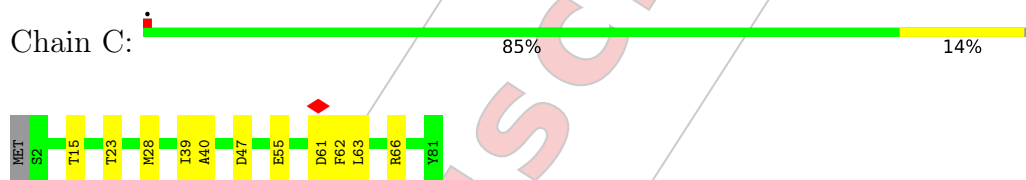
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1 (PsaA)



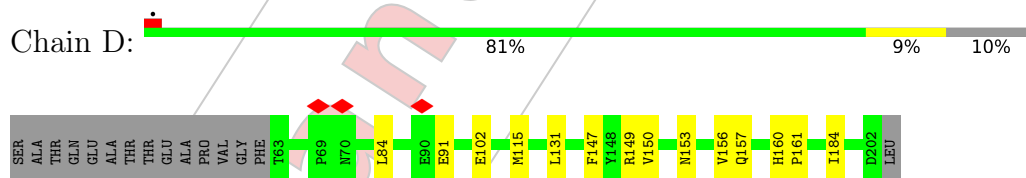
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 (PsaB)



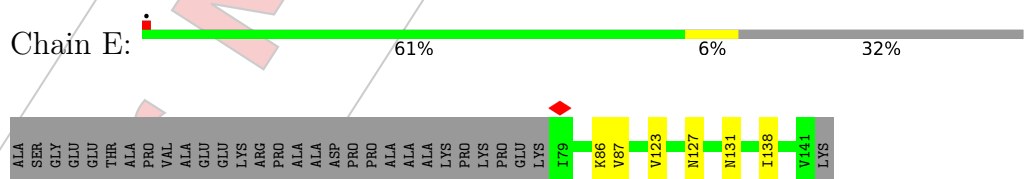
- Molecule 7: Photosystem I iron-sulfur center (PsaC)



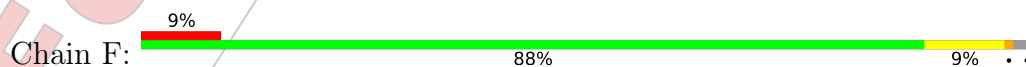
- Molecule 8: Photosystem I reaction center subunit II-1 (PsaD)



- Molecule 9: Photosystem I reaction center subunit IV A (PsaE1)



- Molecule 10: Photosystem I reaction center subunit III (PsaF)





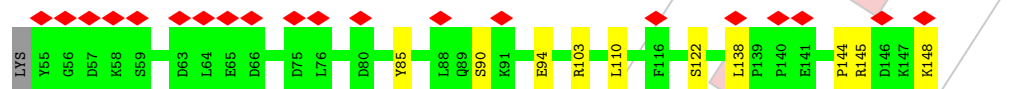
- Molecule 11: Photosystem I reaction center subunit V (PsaG)

Chain G: 96%



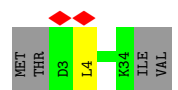
- Molecule 12: Photosystem I reaction center subunit VI-1 (PsaH1)

Chain H: 21% 88% 11%



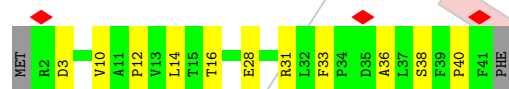
- Molecule 13: Photosystem I reaction center subunit VIII (PsaI)

Chain I: 6% 86% 11%



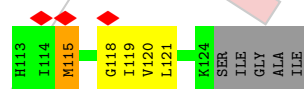
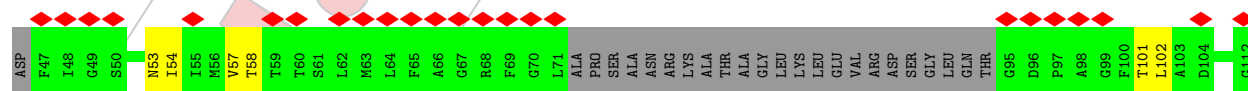
- Molecule 14: Photosystem I reaction center subunit IX (PsaJ)

Chain J: 7% 69% 26% 5%



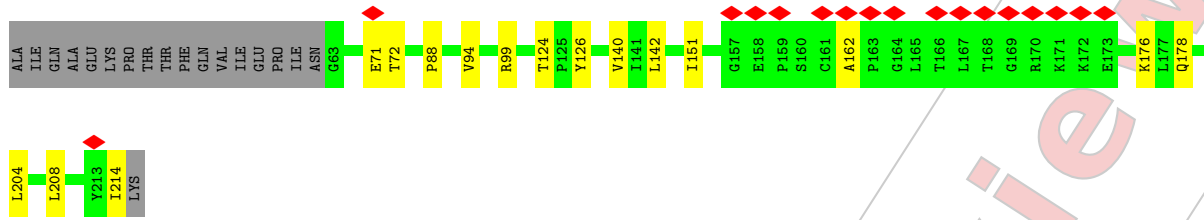
- Molecule 15: Photosystem I reaction center subunit psaK (PsaK)

Chain K: 32% 52% 12% 35%



- Molecule 16: Photosystem I reaction center subunit XI (PsaL)

Chain L: 10% 80% 9% 11%



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	40.986	Depositor
Minimum map value	-19.686	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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: XAT, PQN, LMT, LMG, SF4, DGD, CHL, BCR, LHG, CLA, LUT

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	1	0.15	0/1553	0.29	0/2119
2	2	0.15	0/1634	0.29	0/2236
3	3	0.14	0/1690	0.31	0/2292
4	4	0.15	0/1606	0.30	0/2191
5	A	0.17	0/5878	0.32	0/8020
6	B	0.18	0/6070	0.33	0/8291
7	C	0.17	0/626	0.40	0/849
8	D	0.14	0/1131	0.38	0/1530
9	E	0.14	0/531	0.29	0/721
10	F	0.17	0/1253	0.36	0/1691
11	G	0.12	0/788	0.27	0/1069
12	H	0.11	0/759	0.28	0/1030
13	I	0.14	0/252	0.30	0/343
14	J	0.15	0/328	0.34	0/448
15	K	0.11	0/390	0.25	0/525
16	L	0.11	0/1176	0.27	0/1608
All	All	0.16	0/25665	0.32	0/34963

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	1	1504	0	1491	12	0
2	2	1579	0	1524	12	0
3	3	1638	0	1602	20	0
4	4	1557	0	1519	12	0
5	A	5684	0	5539	39	0
6	B	5858	0	5635	32	0
7	C	614	0	593	8	0
8	D	1103	0	1114	10	0
9	E	519	0	512	5	0
10	F	1224	0	1257	13	0
11	G	768	0	748	2	0
12	H	736	0	723	8	0
13	I	246	0	265	1	0
14	J	319	0	330	11	0
15	K	386	0	404	8	0
16	L	1141	0	1143	11	0
17	1	96	0	68	1	0
17	2	226	0	150	5	0
17	3	47	0	31	1	0
17	4	194	0	138	5	0
18	1	628	0	553	8	0
18	2	458	0	400	5	0
18	3	601	0	463	7	0
18	4	548	0	451	3	0
18	A	2510	0	2449	37	0
18	B	2282	0	2215	36	0
18	F	140	0	113	1	0
18	G	132	0	97	1	0
18	H	51	0	41	3	0
18	J	42	0	31	1	0
18	K	128	0	91	4	0
18	L	150	0	125	3	0
19	1	84	0	112	8	0
19	2	42	0	56	1	0
19	3	42	0	56	4	0
19	4	42	0	56	5	0
20	1	44	0	56	0	0
20	2	44	0	56	1	0
20	3	44	0	56	3	0
20	4	44	0	56	0	0
21	1	40	0	56	1	0
21	2	40	0	56	5	0
21	3	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	4	40	0	56	0	0
21	A	240	0	336	15	0
21	B	240	0	336	9	0
21	F	80	0	112	2	0
21	G	40	0	56	1	0
21	I	40	0	56	0	0
21	J	80	0	112	8	0
21	K	80	0	112	3	0
21	L	160	0	224	7	0
22	1	136	0	194	4	0
22	2	37	0	44	3	0
22	A	79	0	104	3	0
23	1	103	0	149	2	0
23	4	85	0	113	0	0
23	B	52	0	77	2	0
23	F	77	0	97	2	0
24	4	35	0	46	0	0
24	A	70	0	92	1	0
24	G	35	0	46	0	0
25	A	33	0	46	0	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	61	0	83	2	0
All	All	35475	0	35024	324	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.

All (324) 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)
16:L:124:THR:HG22	16:L:126:TYR:H	1.43	0.82
6:B:262:HIS:HD2	6:B:264:GLN:H	1.30	0.81
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.67	0.76
19:3:614:LUT:H171	19:3:614:LUT:H8	1.68	0.75
6:B:411:MET:HE2	21:B:845:BCR:H292	1.68	0.74
8:D:149:ARG:HD2	8:D:157:GLN:HE21	1.53	0.74
5:A:327:LYS:HD3	5:A:333:GLN:HG2	1.70	0.73
4:4:108:VAL:HG11	19:4:616:LUT:H12	1.71	0.72
6:B:159:PRO:HA	6:B:162:LYS:HE2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:617:LHG:HC81	21:3:601:BCR:HC42	1.73	0.69
7:C:66:ARG:HD3	8:D:184:ILE:HD11	1.73	0.69
12:H:103:ARG:HD3	16:L:151:ILE:HG12	1.72	0.69
8:D:160:HIS:HB3	8:D:161:PRO:HD3	1.76	0.67
5:A:537:HIS:HB3	18:A:837:CLA:HBB1	1.77	0.66
10:F:107:LEU:HB2	10:F:120:ILE:HG21	1.78	0.66
4:4:122:ILE:HG13	4:4:123:ILE:HG23	1.78	0.65
17:4:605:CHL:HBB2	17:4:606:CHL:HBB1	1.77	0.65
1:1:186:LEU:HG	1:1:190:LYS:HE2	1.78	0.64
5:A:327:LYS:H	18:A:854:CLA:HBC3	1.63	0.64
4:4:244:HIS:HA	4:4:249:GLN:HE22	1.63	0.64
6:B:257:LEU:HD13	18:B:816:CLA:HMB3	1.79	0.64
18:3:602:CLA:H62	20:3:615:XAT:H28	1.80	0.62
16:L:162:ALA:HB2	16:L:178:GLN:HG3	1.80	0.62
12:H:145:ARG:HH21	12:H:148:LYS:HG2	1.65	0.62
3:3:229:ILE:HG21	20:3:615:XAT:H12	1.80	0.61
18:A:808:CLA:H12	18:A:810:CLA:H2	1.84	0.60
15:K:53:ASN:O	15:K:57:VAL:HG23	2.01	0.60
6:B:30:ASP:HB3	18:B:828:CLA:HAA2	1.83	0.60
18:B:811:CLA:HAC2	18:B:812:CLA:HAB	1.84	0.59
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	1.85	0.59
18:B:807:CLA:H43	18:B:826:CLA:H11	1.83	0.58
6:B:276:HIS:HB2	18:B:816:CLA:C1B	2.33	0.58
14:J:38:SER:O	21:J:101:BCR:H10C	2.03	0.58
5:A:680:PHE:HA	18:A:802:CLA:HAB	1.85	0.58
21:K:204:BCR:H382	21:K:204:BCR:H23C	1.85	0.58
3:3:210:SER:O	3:3:214:LEU:HD12	2.03	0.58
3:3:74:LEU:HD21	18:A:812:CLA:H42	1.85	0.58
5:A:42:THR:HG22	5:A:44:THR:H	1.68	0.58
7:C:15:THR:HA	7:C:28:MET:HE3	1.86	0.58
21:A:850:BCR:H352	21:A:850:BCR:H10C	1.85	0.58
6:B:317:ARG:HG3	6:B:405:ASP:HB3	1.86	0.58
1:1:100:VAL:HG11	19:1:615:LUT:H12	1.86	0.57
10:F:201:VAL:HG21	23:F:307:LMG:H112	1.87	0.57
10:F:115:ALA:HA	10:F:118:LEU:HD12	1.86	0.56
12:H:122:SER:HA	21:L:301:BCR:H322	1.88	0.56
6:B:292:ARG:HD3	11:G:105:PRO:HD3	1.87	0.56
5:A:40:PRO:O	10:F:193:THR:HG21	2.06	0.56
17:2:601:CHL:HHC	17:2:601:CHL:HBB1	1.88	0.55
1:1:209:VAL:HG13	19:1:619:LUT:H162	1.88	0.55
10:F:120:ILE:O	10:F:124:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:809:CLA:HBA2	18:B:809:CLA:HBD	1.87	0.55
5:A:243:ASN:ND2	5:A:245:ASP:H	2.04	0.55
5:A:708:VAL:HG12	10:F:180:ARG:HG3	1.89	0.55
18:A:843:CLA:H2	21:A:849:BCR:H362	1.87	0.55
2:2:207:ILE:O	2:2:211:ARG:HG3	2.06	0.54
18:A:828:CLA:H171	21:J:103:BCR:H17C	1.90	0.54
6:B:293:THR:HG22	6:B:294:ASN:H	1.72	0.54
23:1:623:LMG:H121	11:G:154:VAL:HG22	1.90	0.54
18:B:825:CLA:H143	21:B:846:BCR:H17C	1.89	0.54
17:2:606:CHL:HHC	17:2:606:CHL:HBB1	1.90	0.54
5:A:230:ASP:HB3	5:A:233:GLU:HG2	1.89	0.54
12:H:90:SER:O	12:H:94:GLU:HG3	2.09	0.53
6:B:203:ARG:HG3	6:B:250:ALA:HB1	1.90	0.53
19:1:619:LUT:C8	19:1:619:LUT:H181	2.39	0.53
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.74	0.53
5:A:72:SER:OG	5:A:178:TYR:HB2	2.09	0.53
6:B:302:LYS:O	6:B:306:GLU:HG2	2.08	0.53
18:B:839:CLA:HBC3	21:B:847:BCR:H21C	1.91	0.53
1:1:51:MET:HE3	1:1:54:GLN:HG3	1.92	0.52
1:1:234:ASN:HB2	18:1:613:CLA:HED1	1.92	0.52
5:A:102:LEU:HD11	5:A:151:THR:HA	1.91	0.52
3:3:216:LEU:O	3:3:219:ILE:HG13	2.10	0.52
3:3:234:ILE:HG21	18:3:611:CLA:HAC2	1.92	0.52
17:3:616:CHL:HHC	17:3:616:CHL:HBB1	1.92	0.52
18:B:829:CLA:HBB1	18:B:840:CLA:H13	1.92	0.51
7:C:61:ASP:HB3	9:E:131:ASN:ND2	2.26	0.51
14:J:40:PRO:HG2	21:J:101:BCR:H321	1.92	0.51
18:H:201:CLA:H2A	18:H:201:CLA:HED2	1.92	0.51
18:A:809:CLA:HAB	21:J:103:BCR:H352	1.93	0.51
19:1:619:LUT:H181	19:1:619:LUT:H8	1.93	0.51
3:3:250:HIS:CD2	18:3:611:CLA:HAA2	2.46	0.51
2:2:180:LYS:NZ	2:2:180:LYS:HB3	2.26	0.50
5:A:363:VAL:HG11	18:A:819:CLA:H191	1.94	0.50
12:H:85:TYR:HE2	16:L:94:VAL:HG11	1.77	0.50
8:D:150:VAL:HG22	8:D:156:VAL:HG12	1.92	0.50
14:J:38:SER:O	14:J:40:PRO:HD3	2.12	0.50
2:2:206:LYS:O	2:2:209:GLU:HG3	2.11	0.50
5:A:531:PHE:CZ	21:A:850:BCR:H322	2.47	0.50
18:A:854:CLA:HMA1	22:A:855:LHG:HC82	1.93	0.50
18:A:810:CLA:HAA1	18:A:810:CLA:HBD	1.94	0.49
21:L:305:BCR:H392	21:L:305:BCR:H23C	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:821:CLA:HBC3	18:A:827:CLA:H193	1.92	0.49
7:C:61:ASP:HB3	9:E:131:ASN:HD21	1.77	0.49
1:1:90:LEU:HD12	1:1:168:LYS:HG2	1.95	0.49
22:1:618:LHG:H211	22:1:618:LHG:H382	1.94	0.49
4:4:83:LEU:HD13	18:4:602:CLA:H42	1.94	0.49
6:B:129:LEU:HD23	6:B:134:ASP:HB3	1.93	0.49
2:2:135:GLU:OE2	2:2:135:GLU:HA	2.13	0.49
5:A:86:SER:HB2	5:A:163:ALA:HB3	1.95	0.49
3:3:234:ILE:O	3:3:238:VAL:HG22	2.12	0.49
18:A:803:CLA:H203	21:B:847:BCR:H321	1.95	0.49
18:A:817:CLA:H61	18:A:817:CLA:H41	1.57	0.49
2:2:229:TRP:O	2:2:233:ILE:HG22	2.12	0.49
6:B:373:THR:HG22	18:B:826:CLA:HAB	1.94	0.49
18:B:809:CLA:H62	21:L:301:BCR:HC7	1.95	0.48
19:2:615:LUT:C8	19:2:615:LUT:H181	2.43	0.48
18:B:821:CLA:HBB1	18:B:840:CLA:HED2	1.95	0.48
7:C:62:PHE:HD2	8:D:184:ILE:HG21	1.78	0.48
18:2:612:CLA:H92	18:2:612:CLA:H61	1.71	0.48
17:2:614:CHL:HHC	17:2:614:CHL:HBB1	1.95	0.48
5:A:264:LEU:HD13	15:K:120:VAL:HG11	1.95	0.48
22:A:855:LHG:H252	22:A:855:LHG:H101	1.94	0.48
2:2:209:GLU:OE1	2:2:213:LYS:HE2	2.14	0.47
5:A:205:LEU:HB3	21:A:846:BCR:H19C	1.96	0.47
18:A:841:CLA:H41	18:A:841:CLA:H61	1.61	0.47
2:2:189:PRO:HB3	17:2:607:CHL:HBC2	1.96	0.47
18:A:807:CLA:H112	18:A:807:CLA:H151	1.56	0.47
18:B:812:CLA:HBA1	18:B:812:CLA:H3A	1.48	0.47
18:B:817:CLA:H41	18:B:817:CLA:H62	1.63	0.47
19:1:615:LUT:C8	19:1:615:LUT:H181	2.45	0.47
15:K:54:ILE:O	15:K:58:THR:HG22	2.15	0.47
10:F:137:GLN:OE1	14:J:40:PRO:HG3	2.15	0.47
8:D:149:ARG:HD2	8:D:157:GLN:NE2	2.27	0.47
6:B:174:ARG:HB2	18:B:812:CLA:HBC2	1.96	0.46
7:C:55:GLU:HB3	7:C:63:LEU:HD13	1.96	0.46
23:F:306:LMG:H112	23:F:306:LMG:HC8	1.67	0.46
16:L:71:GLU:CD	16:L:71:GLU:H	2.23	0.46
8:D:147:PHE:CZ	8:D:160:HIS:HB2	2.50	0.46
18:A:817:CLA:H51	15:K:121:LEU:HD13	1.96	0.46
6:B:680:TRP:HD1	8:D:84:LEU:HD11	1.80	0.46
3:3:214:LEU:HA	3:3:217:LYS:HE2	1.98	0.46
18:B:826:CLA:H3A	18:B:826:CLA:HBA2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:31:ARG:HB3	18:J:102:CLA:HED3	1.98	0.46
1:1:74:ARG:HA	1:1:74:ARG:HD3	1.64	0.46
4:4:83:LEU:HD21	10:F:213:ILE:HD13	1.98	0.46
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.80	0.46
2:2:59:LEU:H	3:3:176:GLN:HE22	1.64	0.46
18:A:825:CLA:H193	18:A:825:CLA:H162	1.81	0.46
22:1:622:LHG:H311	18:B:840:CLA:H93	1.98	0.46
4:4:91:LYS:O	4:4:95:GLN:HG2	2.15	0.46
19:4:616:LUT:C8	19:4:616:LUT:H181	2.46	0.46
5:A:45:TRP:CE3	5:A:46:ILE:HG13	2.51	0.46
18:A:834:CLA:HBC2	18:B:809:CLA:HBC1	1.98	0.46
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.98	0.45
17:2:607:CHL:HMB2	21:2:618:BCR:H402	1.97	0.45
18:A:804:CLA:H62	18:A:804:CLA:H41	1.59	0.45
18:A:832:CLA:H8	21:L:306:BCR:H271	1.97	0.45
6:B:222:LEU:HD23	6:B:222:LEU:HA	1.82	0.45
18:3:611:CLA:C1B	19:3:614:LUT:H183	2.46	0.45
5:A:157:TYR:O	5:A:161:ILE:HG12	2.16	0.45
15:K:118:GLY:HA3	18:K:202:CLA:HBC2	1.97	0.45
23:1:620:LMG:H262	18:4:614:CLA:H2	1.98	0.45
5:A:746:ILE:HD12	5:A:746:ILE:HA	1.83	0.45
18:A:842:CLA:H193	18:A:842:CLA:H161	1.84	0.45
6:B:503:GLU:HG3	6:B:505:SER:H	1.80	0.45
9:E:123:VAL:HB	9:E:127:ASN:HA	1.98	0.45
5:A:476:LEU:HB2	5:A:528:THR:HG23	1.98	0.45
8:D:102:GLU:HA	8:D:115:MET:O	2.17	0.45
18:L:302:CLA:H3A	18:L:302:CLA:HBA2	1.66	0.45
2:2:150:LEU:HD23	2:2:150:LEU:HA	1.84	0.45
3:3:88:TRP:HE1	18:3:603:CLA:HED1	1.81	0.45
18:K:203:CLA:HBA1	18:K:203:CLA:H3A	1.49	0.45
17:4:607:CHL:H3A	17:4:607:CHL:HBA2	1.48	0.45
18:A:807:CLA:H2	18:A:807:CLA:HED2	1.98	0.45
21:A:847:BCR:H20C	21:A:847:BCR:H361	1.86	0.45
12:H:110:LEU:HD22	16:L:140:VAL:HG13	1.99	0.45
14:J:28:GLU:HA	14:J:28:GLU:OE2	2.17	0.45
17:1:606:CHL:HHC	17:1:606:CHL:HBB1	1.99	0.45
16:L:88:PRO:O	16:L:99:ARG:HD2	2.17	0.45
10:F:94:LYS:O	10:F:98:GLN:HG2	2.16	0.44
10:F:161:PHE:CE1	21:J:101:BCR:H372	2.52	0.44
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.99	0.44
6:B:704:GLN:HG3	27:B:848:DGD:HA31	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:733:PHE:CD2	12:H:144:PRO:HG2	2.52	0.44
18:B:839:CLA:HBC3	21:B:847:BCR:C21	2.48	0.44
14:J:12:PRO:O	14:J:16:THR:HG22	2.17	0.44
5:A:705:LYS:HB3	5:A:705:LYS:HE3	1.79	0.44
21:A:849:BCR:H361	21:A:849:BCR:H20C	1.84	0.44
1:1:235:ILE:HB	18:1:612:CLA:H12	1.98	0.44
17:4:605:CHL:HHC	17:4:605:CHL:HBB1	2.00	0.44
5:A:331:THR:HG21	22:A:855:LHG:O1	2.18	0.44
18:A:802:CLA:H92	18:A:802:CLA:H62	1.76	0.44
16:L:204:LEU:HD23	16:L:208:LEU:HD12	1.99	0.44
2:2:173:ASP:HB3	2:2:176:PHE:O	2.18	0.44
2:2:109:GLY:HA2	20:2:616:XAT:H181	2.00	0.44
3:3:229:ILE:HD13	3:3:229:ILE:HA	1.91	0.44
19:3:614:LUT:H181	19:3:614:LUT:H7	1.73	0.44
6:B:15:ASP:OD1	6:B:20:ARG:HB2	2.17	0.44
22:1:621:LHG:HC62	22:1:621:LHG:H241	1.40	0.44
21:A:847:BCR:H24C	21:A:847:BCR:H371	1.83	0.43
21:B:842:BCR:H24C	21:B:842:BCR:H371	1.89	0.43
18:B:807:CLA:H102	18:B:807:CLA:H61	1.86	0.43
18:B:809:CLA:H152	18:B:809:CLA:H112	1.59	0.43
21:F:302:BCR:H24C	21:F:302:BCR:H371	1.85	0.43
18:1:603:CLA:H92	18:1:603:CLA:H62	1.81	0.43
18:A:817:CLA:H2	18:K:202:CLA:HED1	2.01	0.43
4:4:220:PHE:HE1	19:4:616:LUT:H41	1.84	0.43
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.99	0.43
21:G:205:BCR:H24C	21:G:205:BCR:H371	1.80	0.43
14:J:33:PHE:CD1	21:J:101:BCR:H312	2.54	0.43
1:1:114:TRP:H	1:1:114:TRP:CD1	2.37	0.43
18:F:301:CLA:H61	18:F:301:CLA:H41	1.77	0.43
21:J:101:BCR:H393	21:J:101:BCR:H24C	1.71	0.43
22:2:617:LHG:H291	22:2:617:LHG:HC91	2.01	0.43
5:A:213:HIS:CD2	5:A:213:HIS:C	2.97	0.43
18:B:804:CLA:HBA1	18:B:804:CLA:H3A	1.76	0.43
10:F:125:GLU:HA	10:F:125:GLU:OE2	2.19	0.43
6:B:91:ILE:HB	6:B:112:PRO:HB2	2.01	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.54	0.43
18:B:838:CLA:H92	18:B:838:CLA:H61	1.84	0.43
4:4:194:LEU:HD12	19:4:616:LUT:H222	2.01	0.43
18:H:201:CLA:HBC1	21:L:306:BCR:H352	2.01	0.43
21:1:617:BCR:H24C	21:1:617:BCR:H371	1.90	0.43
19:3:614:LUT:H35	19:3:614:LUT:H401	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:617:CLA:HED1	5:A:181:ALA:HB1	2.00	0.43
5:A:703:HIS:HB3	5:A:708:VAL:O	2.19	0.43
21:A:850:BCR:H24C	21:A:850:BCR:H371	1.79	0.43
5:A:693:GLN:O	5:A:697:GLU:HG3	2.18	0.42
6:B:411:MET:HE1	18:B:829:CLA:C3C	2.48	0.42
22:1:621:LHG:HC5	22:1:621:LHG:HC81	1.38	0.42
4:4:113:LEU:HB3	4:4:114:PRO:HD3	2.00	0.42
4:4:237:GLN:HE21	4:4:237:GLN:HB2	1.65	0.42
18:A:807:CLA:H3A	18:A:830:CLA:HAB	2.01	0.42
6:B:586:THR:O	6:B:590:VAL:HG13	2.19	0.42
18:B:838:CLA:HBB2	25:B:841:PQN:H141	2.00	0.42
18:B:839:CLA:HBC2	25:B:841:PQN:H201	2.00	0.42
3:3:55:SER:O	3:3:59:LEU:HD12	2.19	0.42
4:4:225:ASN:OD1	4:4:225:ASN:C	2.61	0.42
5:A:296:LEU:O	5:A:300:ILE:HG12	2.18	0.42
5:A:505:LEU:HD11	5:A:513:VAL:HG23	2.00	0.42
1:1:164:PRO:HA	1:1:167:LYS:HD2	2.01	0.42
18:A:830:CLA:H62	18:A:830:CLA:H41	1.82	0.42
5:A:708:VAL:CG1	10:F:180:ARG:HG3	2.49	0.42
16:L:176:LYS:HD3	16:L:176:LYS:HA	1.70	0.42
19:4:616:LUT:H31	19:4:616:LUT:H391	1.95	0.42
24:A:856:LMT:H3'	24:A:856:LMT:H1B	1.76	0.42
14:J:36:ALA:HB1	21:J:101:BCR:C10	2.48	0.42
21:2:618:BCR:H23C	21:2:618:BCR:H383	2.02	0.42
18:A:829:CLA:H92	18:A:829:CLA:H61	1.94	0.42
21:A:845:BCR:H371	21:A:845:BCR:H24C	1.87	0.42
18:B:816:CLA:H3A	18:B:816:CLA:HBA2	1.84	0.42
23:B:849:LMG:H111	23:B:849:LMG:HC8	1.35	0.42
1:1:97:MET:SD	18:1:609:CLA:HBB1	2.59	0.42
21:2:618:BCR:H373	21:2:618:BCR:H19C	2.02	0.42
17:4:605:CHL:HBB2	17:4:606:CHL:CBB	2.47	0.42
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.74	0.42
21:K:204:BCR:H392	21:K:204:BCR:H24C	1.69	0.42
18:2:609:CLA:H61	18:2:609:CLA:H41	1.86	0.42
23:B:849:LMG:HC92	23:B:849:LMG:H291	1.55	0.42
8:D:153:ASN:OD1	8:D:153:ASN:C	2.63	0.42
18:1:614:CLA:HBA1	19:1:619:LUT:H41	2.02	0.42
18:A:831:CLA:HMA2	16:L:72:THR:HG21	2.01	0.42
5:A:28:ARG:HA	5:A:29:PRO:HD3	1.91	0.41
21:B:842:BCR:H20C	21:B:842:BCR:H361	1.90	0.41
7:C:39:ILE:HG12	7:C:40:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:171:LEU:HD12	5:A:171:LEU:HA	1.95	0.41
5:A:531:PHE:HZ	21:A:850:BCR:H322	1.83	0.41
6:B:26:ALA:HB2	27:B:848:DGD:HA41	2.01	0.41
6:B:668:ARG:HD2	6:B:700:LEU:O	2.19	0.41
9:E:87:VAL:HG11	9:E:138:ILE:HD11	2.02	0.41
18:K:202:CLA:HBA1	18:K:202:CLA:HBD	2.02	0.41
6:B:456:GLU:HA	6:B:457:PRO:HD3	1.94	0.41
10:F:199:ILE:HD11	14:J:14:LEU:HD23	2.02	0.41
18:1:608:CLA:H2	18:1:608:CLA:H62	1.96	0.41
19:1:615:LUT:H15	19:1:615:LUT:H201	1.95	0.41
5:A:688:GLY:HA3	6:B:569:ASP:HB2	2.02	0.41
18:B:813:CLA:H141	18:B:813:CLA:H162	1.89	0.41
7:C:23:THR:HG21	7:C:47:ASP:O	2.21	0.41
9:E:86:LYS:HA	9:E:86:LYS:HD3	1.80	0.41
18:2:604:CLA:HBA2	18:2:604:CLA:H122	2.03	0.41
3:3:86:PRO:HA	3:3:89:LEU:HD12	2.01	0.41
3:3:219:ILE:O	3:3:223:ARG:HG3	2.20	0.41
18:4:601:CLA:HBB2	18:4:602:CLA:HBC2	2.02	0.41
21:A:845:BCR:H23C	21:A:845:BCR:H403	2.02	0.41
6:B:226:PHE:CE1	18:G:203:CLA:HBC1	2.56	0.41
16:L:142:LEU:HD22	21:L:305:BCR:H401	2.02	0.41
18:1:612:CLA:HAA1	18:1:612:CLA:HBD	2.01	0.41
18:A:809:CLA:H41	18:A:809:CLA:H62	1.86	0.41
18:2:610:CLA:HBC3	22:2:617:LHG:HC62	2.03	0.41
3:3:83:PHE:HD2	18:3:603:CLA:H52	1.84	0.41
3:3:119:ILE:HG13	3:3:120:PRO:HD2	2.01	0.41
3:3:153:LEU:HD12	3:3:153:LEU:HA	1.86	0.41
21:3:601:BCR:H24C	21:3:601:BCR:H371	1.90	0.41
5:A:205:LEU:HD13	21:A:846:BCR:H20C	2.02	0.41
18:B:816:CLA:HBB1	18:B:816:CLA:HHC	2.03	0.41
18:H:201:CLA:HAC2	18:L:302:CLA:HAA2	2.03	0.41
19:1:619:LUT:H15	19:1:619:LUT:H201	1.86	0.41
3:3:179:LEU:HD23	3:3:179:LEU:HA	1.86	0.41
21:A:845:BCR:H383	21:K:204:BCR:H10C	2.01	0.41
21:2:618:BCR:H24C	21:2:618:BCR:H403	1.79	0.41
3:3:229:ILE:HG21	20:3:615:XAT:H14	2.03	0.41
5:A:455:HIS:CD2	5:A:455:HIS:C	2.98	0.41
18:A:802:CLA:H91	18:A:802:CLA:H111	1.86	0.41
18:B:801:CLA:H8	18:B:801:CLA:H51	1.75	0.41
18:B:815:CLA:HHC	18:B:815:CLA:HBB1	2.03	0.41
21:B:843:BCR:H20C	21:B:843:BCR:H361	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:4:LEU:HD23	13:I:4:LEU:HA	1.85	0.41
21:L:307:BCR:H24C	21:L:307:BCR:H371	1.87	0.41
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	2.02	0.41
21:F:305:BCR:H20C	21:F:305:BCR:H361	1.90	0.41
15:K:115:MET:HE2	15:K:119:ILE:HD11	2.02	0.41
18:2:609:CLA:H92	18:2:609:CLA:H62	1.83	0.40
18:A:818:CLA:H92	18:A:818:CLA:H62	1.95	0.40
6:B:422:LEU:HD13	6:B:532:LEU:HA	2.03	0.40
15:K:101:THR:HG22	15:K:102:LEU:H	1.86	0.40
18:1:609:CLA:H62	18:1:609:CLA:H41	1.88	0.40
3:3:66:ASP:OD1	3:3:66:ASP:N	2.52	0.40
4:4:171:ASP:HB3	4:4:174:PHE:O	2.21	0.40
5:A:232:LYS:HA	5:A:232:LYS:HD3	1.58	0.40
6:B:65:LEU:HD11	21:B:844:BCR:H281	2.02	0.40
18:B:823:CLA:H111	18:B:823:CLA:H72	1.97	0.40
12:H:138:LEU:HD23	12:H:138:LEU:HA	1.91	0.40
17:4:605:CHL:H41	17:4:605:CHL:H62	1.78	0.40
18:A:825:CLA:HBD	18:A:825:CLA:HAA2	2.02	0.40
18:A:843:CLA:H162	18:A:843:CLA:H203	1.79	0.40
18:B:813:CLA:HBB2	18:B:827:CLA:H143	2.02	0.40
21:2:618:BCR:HC7	21:2:618:BCR:H10C	1.87	0.40
18:A:817:CLA:H11	15:K:121:LEU:HD22	2.03	0.40
18:B:817:CLA:HBA2	18:B:817:CLA:H3A	1.67	0.40
18:B:823:CLA:HBD	18:B:823:CLA:HAA2	2.04	0.40
1:1:168:LYS:HE2	1:1:168:LYS:HB2	1.71	0.40
2:2:59:LEU:HD11	2:2:66:PRO:HD3	2.03	0.40
21:A:850:BCR:H20C	21:A:850:BCR:H361	1.86	0.40
18:L:302:CLA:HAA1	18:L:302:CLA:HBD	2.03	0.40

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	1	192/200 (96%)	190 (99%)	2 (1%)	0	100	100
2	2	201/211 (95%)	196 (98%)	5 (2%)	0	100	100
3	3	211/232 (91%)	207 (98%)	4 (2%)	0	100	100
4	4	196/200 (98%)	189 (96%)	7 (4%)	0	100	100
5	A	722/750 (96%)	706 (98%)	16 (2%)	0	100	100
6	B	731/734 (100%)	712 (97%)	19 (3%)	0	100	100
7	C	78/81 (96%)	70 (90%)	8 (10%)	0	100	100
8	D	138/155 (89%)	128 (93%)	10 (7%)	0	100	100
9	E	61/93 (66%)	59 (97%)	2 (3%)	0	100	100
10	F	153/159 (96%)	147 (96%)	6 (4%)	0	100	100
11	G	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
12	H	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
13	I	30/36 (83%)	30 (100%)	0	0	100	100
14	J	38/42 (90%)	36 (95%)	2 (5%)	0	100	100
15	K	51/84 (61%)	51 (100%)	0	0	100	100
16	L	150/170 (88%)	145 (97%)	5 (3%)	0	100	100
All	All	3140/3342 (94%)	3048 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	1	155/160 (97%)	154 (99%)	1 (1%)	84	92
2	2	164/169 (97%)	161 (98%)	3 (2%)	54	76
3	3	166/181 (92%)	162 (98%)	4 (2%)	44	69
4	4	166/167 (99%)	165 (99%)	1 (1%)	84	92
5	A	582/608 (96%)	578 (99%)	4 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	597/598 (100%)	591 (99%)	6 (1%)	73	87
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	119/130 (92%)	117 (98%)	2 (2%)	56	78
9	E	58/79 (73%)	58 (100%)	0	100	100
10	F	128/132 (97%)	127 (99%)	1 (1%)	79	90
11	G	82/83 (99%)	82 (100%)	0	100	100
12	H	79/80 (99%)	79 (100%)	0	100	100
13	I	28/32 (88%)	28 (100%)	0	100	100
14	J	35/37 (95%)	34 (97%)	1 (3%)	37	62
15	K	41/62 (66%)	40 (98%)	1 (2%)	44	69
16	L	118/134 (88%)	117 (99%)	1 (1%)	79	90
All	All	2588/2723 (95%)	2563 (99%)	25 (1%)	71	87

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	77	GLU
2	2	56	GLU
2	2	77	ASP
2	2	185	ASP
3	3	118	LEU
3	3	121	GLN
3	3	158	PHE
3	3	237	LEU
4	4	127	GLU
5	A	352	LEU
5	A	366	HIS
5	A	392	MET
5	A	457	ASP
6	B	47	PHE
6	B	78	VAL
6	B	257	LEU
6	B	394	PHE
6	B	600	THR
6	B	640	MET
8	D	91	GLU
8	D	131	LEU
10	F	213	ILE

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Mol	Chain	Res	Type
14	J	3	ASP
15	K	115	MET
16	L	214	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	156	GLN
1	1	222	ASN
1	1	232	HIS
1	1	234	ASN
2	2	97	GLN
2	2	231	GLN
3	3	200	ASN
3	3	221	ASN
3	3	235	GLN
4	4	69	ASN
4	4	209	ASN
4	4	237	GLN
4	4	245	ASN
4	4	249	GLN
5	A	113	GLN
5	A	213	HIS
5	A	216	HIS
5	A	243	ASN
5	A	249	GLN
5	A	293	HIS
5	A	307	HIS
5	A	542	HIS
5	A	693	GLN
6	B	10	GLN
6	B	53	GLN
6	B	89	HIS
6	B	114	ASN
6	B	170	ASN
6	B	196	HIS
6	B	210	ASN
6	B	248	GLN
6	B	262	HIS
6	B	299	HIS
6	B	319	HIS
6	B	439	HIS

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Mol	Chain	Res	Type
6	B	467	HIS
6	B	482	ASN
6	B	627	ASN
8	D	157	GLN
8	D	171	ASN
9	E	132	ASN
11	G	130	ASN
12	H	86	ASN
12	H	89	GLN
13	I	29	HIS
15	K	53	ASN
15	K	113	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

215 ligands are modelled in this entry.

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	$\# Z > 2$
18	CLA	2	608	2	45,53,73	1.58	7 (15%)	52,89,113	1.86	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	828	6	56,64,73	1.45	7 (12%)	65,102,113	1.82	9 (13%)
18	CLA	B	834	-	42,50,73	1.59	7 (16%)	48,85,113	2.02	6 (12%)
23	LMG	1	620	-	53,53,55	0.18	0	61,61,63	0.16	0
18	CLA	A	805	5	45,53,73	1.57	7 (15%)	52,89,113	2.02	7 (13%)
18	CLA	B	808	6	55,63,73	1.47	7 (12%)	64,101,113	1.81	8 (12%)
18	CLA	B	816	-	59,67,73	1.40	7 (11%)	68,105,113	1.78	9 (13%)
18	CLA	1	604	-	49,57,73	1.51	7 (14%)	55,93,113	1.94	6 (10%)
18	CLA	B	823	-	65,73,73	1.33	7 (10%)	76,113,113	1.78	13 (17%)
18	CLA	J	102	-	42,50,73	1.58	7 (16%)	48,85,113	1.99	8 (16%)
20	XAT	2	616	-	39,47,47	0.11	0	54,74,74	0.83	4 (7%)
24	LMT	4	620	-	36,36,36	0.11	0	47,47,47	0.16	0
18	CLA	3	617	5	55,63,73	1.47	7 (12%)	64,101,113	1.83	10 (15%)
22	LHG	A	855	18	29,29,48	0.37	0	32,35,54	0.35	0
18	CLA	B	809	-	65,73,73	1.34	7 (10%)	76,113,113	1.65	9 (11%)
18	CLA	A	804	5	55,63,73	1.46	7 (12%)	64,101,113	1.92	11 (17%)
21	BCR	I	101	-	41,41,41	0.13	0	56,56,56	0.25	0
18	CLA	1	607	-	43,52,73	1.60	7 (16%)	49,88,113	1.86	6 (12%)
21	BCR	2	618	-	41,41,41	0.27	0	56,56,56	0.59	1 (1%)
23	LMG	4	619	-	36,36,55	0.20	0	44,44,63	0.17	0
18	CLA	3	611	3	43,52,73	1.59	7 (16%)	49,88,113	1.84	6 (12%)
18	CLA	3	604	-	45,53,73	1.58	7 (15%)	52,89,113	1.88	8 (15%)
18	CLA	4	603	4	45,53,73	1.56	7 (15%)	52,89,113	1.99	8 (15%)
18	CLA	A	828	5	65,73,73	1.33	7 (10%)	76,113,113	1.76	9 (11%)
18	CLA	A	816	-	45,53,73	1.56	7 (15%)	52,89,113	2.00	5 (9%)
18	CLA	B	818	-	55,63,73	1.47	7 (12%)	64,101,113	1.81	10 (15%)
18	CLA	4	608	4	45,53,73	1.56	7 (15%)	52,89,113	2.00	6 (11%)
18	CLA	B	806	6	52,60,73	1.50	7 (13%)	60,97,113	1.89	10 (16%)
18	CLA	B	826	6	60,68,73	1.38	7 (11%)	70,107,113	1.81	12 (17%)
18	CLA	A	823	5	41,49,73	1.63	8 (19%)	47,84,113	2.02	9 (19%)
18	CLA	2	613	2	43,51,73	1.57	7 (16%)	49,86,113	1.97	8 (16%)
18	CLA	B	836	6	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
18	CLA	A	817	5	60,68,73	1.40	7 (11%)	70,107,113	1.75	10 (14%)
18	CLA	K	203	15	46,54,73	1.55	7 (15%)	53,90,113	1.98	8 (15%)
21	BCR	B	845	-	41,41,41	0.12	0	56,56,56	0.35	0
21	BCR	J	101	-	41,41,41	0.28	0	56,56,56	0.65	1 (1%)
22	LHG	2	617	-	36,36,48	0.34	0	39,42,54	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	822	6	60,68,73	1.39	8 (13%)	70,107,113	1.67	13 (18%)
18	CLA	A	832	5	56,64,73	1.45	7 (12%)	65,102,113	1.79	9 (13%)
18	CLA	2	603	2	43,52,73	1.59	7 (16%)	49,88,113	1.89	7 (14%)
18	CLA	4	613	4	45,53,73	1.57	7 (15%)	52,89,113	1.92	7 (13%)
18	CLA	L	304	-	45,53,73	1.59	7 (15%)	52,89,113	2.01	8 (15%)
18	CLA	A	835	5	45,53,73	1.55	7 (15%)	52,89,113	1.90	8 (15%)
18	CLA	1	608	1	65,73,73	1.33	7 (10%)	76,113,113	1.72	10 (13%)
18	CLA	A	843	-	65,73,73	1.34	7 (10%)	76,113,113	1.76	11 (14%)
17	CHL	1	601	1	54,63,74	1.60	10 (18%)	58,101,114	1.95	10 (17%)
18	CLA	A	838	5	55,63,73	1.46	7 (12%)	64,101,113	1.83	7 (10%)
18	CLA	A	818	5	59,67,73	1.41	7 (11%)	68,105,113	1.80	9 (13%)
18	CLA	A	826	-	65,73,73	1.36	7 (10%)	76,113,113	1.71	12 (15%)
18	CLA	B	820	6	55,63,73	1.45	7 (12%)	64,101,113	1.80	11 (17%)
21	BCR	A	845	-	41,41,41	0.14	0	56,56,56	0.25	0
17	CHL	3	616	-	47,55,74	1.67	9 (19%)	50,91,114	2.23	11 (22%)
18	CLA	B	827	6	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
18	CLA	2	609	2	55,63,73	1.44	7 (12%)	64,101,113	1.84	7 (10%)
18	CLA	1	610	22	55,63,73	1.46	7 (12%)	64,101,113	1.84	9 (14%)
18	CLA	B	832	6	45,53,73	1.55	6 (13%)	52,89,113	1.91	8 (15%)
18	CLA	A	819	5	65,73,73	1.35	7 (10%)	76,113,113	1.72	13 (17%)
21	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.54	1 (1%)
18	CLA	2	611	2	45,53,73	1.56	7 (15%)	52,89,113	1.99	9 (17%)
18	CLA	B	805	6	65,73,73	1.33	7 (10%)	76,113,113	1.82	8 (10%)
18	CLA	B	821	6	55,63,73	1.47	7 (12%)	64,101,113	1.81	9 (14%)
18	CLA	A	825	-	65,73,73	1.34	7 (10%)	76,113,113	1.70	12 (15%)
18	CLA	A	820	5	45,53,73	1.56	7 (15%)	52,89,113	1.99	7 (13%)
18	CLA	1	613	1	45,53,73	1.57	7 (15%)	52,89,113	1.98	9 (17%)
18	CLA	A	839	5	50,58,73	1.53	7 (14%)	58,95,113	1.92	9 (15%)
20	XAT	4	617	-	39,47,47	0.13	0	54,74,74	0.90	3 (5%)
17	CHL	4	605	-	56,64,74	1.62	10 (17%)	61,102,114	2.02	10 (16%)
18	CLA	A	811	5	65,73,73	1.34	7 (10%)	76,113,113	1.77	12 (15%)
18	CLA	2	612	-	55,63,73	1.46	7 (12%)	64,101,113	1.93	11 (17%)
18	CLA	B	835	-	50,58,73	1.53	7 (14%)	58,95,113	1.96	9 (15%)
18	CLA	4	602	4	60,68,73	1.39	7 (11%)	70,107,113	1.76	12 (17%)
18	CLA	L	303	16	60,68,73	1.40	7 (11%)	70,107,113	1.79	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	A	851	5,6	0,12,12	-	-	-		
18	CLA	4	612	4	57,65,73	1.42	7 (12%)	66,103,113	1.80	9 (13%)
18	CLA	3	605	-	47,55,73	1.53	7 (14%)	54,91,113	1.98	9 (16%)
22	LHG	1	622	18	37,37,48	0.33	0	40,43,54	0.31	0
18	CLA	4	601	4	46,54,73	1.53	7 (15%)	53,90,113	1.92	9 (16%)
18	CLA	B	838	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
25	PQN	A	844	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
18	CLA	A	830	5	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
18	CLA	2	602	2	65,73,73	1.35	7 (10%)	76,113,113	1.69	11 (14%)
18	CLA	A	803	-	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
18	CLA	A	815	5	42,50,73	1.58	7 (16%)	48,85,113	1.93	6 (12%)
18	CLA	B	811	6	43,51,73	1.53	7 (16%)	49,86,113	1.94	8 (16%)
19	LUT	1	619	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	11 (21%)
22	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.30	0
18	CLA	1	603	1	55,63,73	1.44	7 (12%)	64,101,113	1.93	9 (14%)
18	CLA	B	817	6	60,68,73	1.39	7 (11%)	70,107,113	1.82	13 (18%)
21	BCR	F	305	-	41,41,41	0.12	0	56,56,56	0.31	0
18	CLA	B	825	6	62,70,73	1.39	7 (11%)	72,109,113	1.80	12 (16%)
20	XAT	1	616	-	39,47,47	0.11	0	54,74,74	0.81	3 (5%)
18	CLA	1	602	1	61,69,73	1.41	7 (11%)	71,108,113	1.77	11 (15%)
17	CHL	2	601	2	47,55,74	1.67	9 (19%)	50,91,114	2.19	10 (20%)
18	CLA	B	804	6	65,73,73	1.34	7 (10%)	76,113,113	1.83	14 (18%)
17	CHL	2	605	-	42,50,74	1.69	8 (19%)	45,85,114	2.15	8 (17%)
18	CLA	A	829	5	65,73,73	1.34	7 (10%)	76,113,113	1.75	10 (13%)
18	CLA	B	814	6	55,63,73	1.46	7 (12%)	64,101,113	1.89	9 (14%)
21	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.28	0
18	CLA	3	603	3	55,63,73	1.46	7 (12%)	64,101,113	1.87	9 (14%)
18	CLA	A	854	22	50,58,73	1.55	7 (14%)	58,95,113	1.83	9 (15%)
18	CLA	A	801	5	65,73,73	1.33	7 (10%)	76,113,113	1.76	10 (13%)
18	CLA	A	808	5	50,58,73	1.54	7 (14%)	58,95,113	1.92	11 (18%)
18	CLA	4	609	4	54,62,73	1.47	7 (12%)	62,99,113	1.86	10 (16%)
18	CLA	3	612	-	39,48,73	1.67	8 (20%)	44,83,113	1.85	8 (18%)
18	CLA	3	610	3	43,51,73	1.58	7 (16%)	49,86,113	1.95	8 (16%)
18	CLA	A	833	5	65,73,73	1.34	7 (10%)	76,113,113	1.76	9 (11%)
21	BCR	B	847	-	41,41,41	0.13	0	56,56,56	0.32	0
18	CLA	G	202	-	45,53,73	1.58	7 (15%)	52,89,113	1.95	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	1	609	1	59,67,73	1.41	7 (11%)	69,106,113	1.77	9 (13%)
21	BCR	J	103	-	41,41,41	0.14	0	56,56,56	0.26	0
19	LUT	2	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.52	10 (19%)
18	CLA	A	814	5	45,53,73	1.58	7 (15%)	52,89,113	1.95	8 (15%)
18	CLA	B	803	6	41,49,73	1.62	7 (17%)	47,84,113	1.94	8 (17%)
18	CLA	H	201	12	51,59,73	1.50	8 (15%)	59,96,113	1.88	11 (18%)
18	CLA	4	614	4	50,58,73	1.52	7 (14%)	58,95,113	1.87	10 (17%)
21	BCR	L	306	-	41,41,41	0.11	0	56,56,56	0.26	0
18	CLA	1	612	1	65,73,73	1.34	7 (10%)	76,113,113	1.72	10 (13%)
21	BCR	L	301	-	41,41,41	0.13	0	56,56,56	0.26	0
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.45	0
19	LUT	1	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.53	9 (17%)
23	LMG	4	621	-	49,49,55	0.19	0	57,57,63	0.14	0
18	CLA	B	812	6	65,73,73	1.35	7 (10%)	76,113,113	1.83	12 (15%)
18	CLA	B	810	6	54,62,73	1.42	6 (11%)	67,100,113	2.02	10 (14%)
21	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.35	0
22	LHG	1	618	18	48,48,48	0.29	0	51,54,54	0.30	0
18	CLA	1	614	1	45,53,73	1.56	7 (15%)	52,89,113	1.92	8 (15%)
21	BCR	L	305	-	41,41,41	0.19	0	56,56,56	0.34	0
22	LHG	1	621	-	48,48,48	0.30	0	51,54,54	0.31	0
18	CLA	3	613	3	39,48,73	1.65	7 (17%)	44,83,113	1.97	7 (15%)
18	CLA	2	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.73	11 (14%)
18	CLA	B	815	6	55,63,73	1.45	7 (12%)	64,101,113	1.86	9 (14%)
21	BCR	K	205	-	41,41,41	0.11	0	56,56,56	0.21	0
18	CLA	3	608	3	45,53,73	1.58	7 (15%)	52,89,113	1.92	6 (11%)
19	LUT	3	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	K	202	-	45,53,73	1.57	7 (15%)	52,89,113	1.84	6 (11%)
18	CLA	A	812	5	54,62,73	1.47	7 (12%)	62,99,113	1.89	11 (17%)
18	CLA	1	611	1	45,53,73	1.58	7 (15%)	52,89,113	2.00	6 (11%)
18	CLA	B	824	-	50,58,73	1.51	7 (14%)	58,95,113	1.82	10 (17%)
21	BCR	K	204	-	41,41,41	0.25	0	56,56,56	0.46	0
23	LMG	B	849	-	52,52,55	0.20	0	60,60,63	0.15	0
24	LMT	A	853	-	36,36,36	0.11	0	47,47,47	0.24	0
21	BCR	A	846	-	41,41,41	0.15	0	56,56,56	0.60	2 (3%)
18	CLA	B	829	6	43,51,73	1.57	7 (16%)	49,86,113	1.99	7 (14%)
17	CHL	2	607	-	51,59,74	1.66	10 (19%)	55,96,114	2.14	13 (23%)
26	SF4	C	102	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	801	6	65,73,73	1.33	7 (10%)	76,113,113	1.70	10 (13%)
18	CLA	B	831	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	11 (14%)
18	CLA	A	834	5	65,73,73	1.35	7 (10%)	76,113,113	1.79	8 (10%)
18	CLA	A	836	5	45,53,73	1.54	7 (15%)	52,89,113	1.99	9 (17%)
18	CLA	F	303	-	42,50,73	1.59	7 (16%)	48,85,113	1.99	7 (14%)
24	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.18	0
18	CLA	A	807	5	65,73,73	1.34	7 (10%)	76,113,113	1.79	11 (14%)
17	CHL	1	606	1	40,49,74	1.71	8 (20%)	41,84,114	2.33	9 (21%)
21	BCR	L	307	-	41,41,41	0.12	0	56,56,56	0.25	0
23	LMG	F	306	-	47,47,55	0.21	0	55,55,63	0.21	0
18	CLA	B	807	-	65,73,73	1.33	7 (10%)	76,113,113	1.76	10 (13%)
18	CLA	A	809	5	55,63,73	1.45	7 (12%)	64,101,113	1.84	10 (15%)
24	LMT	A	856	-	36,36,36	0.13	0	47,47,47	0.52	0
17	CHL	2	614	2	43,51,74	1.65	7 (16%)	45,86,114	2.21	9 (20%)
18	CLA	B	837	6	47,55,73	1.52	7 (14%)	54,91,113	2.01	9 (16%)
18	CLA	3	602	3	60,68,73	1.41	7 (11%)	70,107,113	1.78	11 (15%)
18	CLA	A	810	5	50,58,73	1.53	7 (14%)	58,95,113	1.83	11 (18%)
18	CLA	A	842	-	65,73,73	1.35	7 (10%)	76,113,113	1.75	8 (10%)
18	CLA	K	201	15	38,45,73	1.71	8 (21%)	43,78,113	1.96	8 (18%)
20	XAT	3	615	-	39,47,47	0.09	0	54,74,74	0.79	3 (5%)
18	CLA	F	304	10	41,49,73	1.62	8 (19%)	47,84,113	2.10	10 (21%)
21	BCR	B	842	-	41,41,41	0.14	0	56,56,56	0.29	0
27	DGD	B	848	-	62,62,67	0.16	0	76,76,81	0.16	0
21	BCR	4	618	-	41,41,41	0.13	0	56,56,56	0.33	0
18	CLA	2	610	-	41,49,73	1.63	7 (17%)	47,84,113	1.95	7 (14%)
18	CLA	G	204	11	45,53,73	1.57	7 (15%)	52,89,113	1.91	6 (11%)
18	CLA	G	203	11	42,50,73	1.57	7 (16%)	48,85,113	2.01	5 (10%)
18	CLA	B	839	6	65,73,73	1.33	7 (10%)	76,113,113	1.78	10 (13%)
23	LMG	1	623	-	50,50,55	0.19	0	58,58,63	0.17	0
18	CLA	L	302	16	45,53,73	1.57	7 (15%)	52,89,113	1.93	7 (13%)
21	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.66	1 (1%)
18	CLA	4	611	4	40,49,73	1.62	7 (17%)	45,84,113	1.97	4 (8%)
18	CLA	A	841	5	65,73,73	1.35	7 (10%)	76,113,113	1.74	10 (13%)
18	CLA	3	607	3	45,53,73	1.56	7 (15%)	52,89,113	1.95	8 (15%)
21	BCR	3	601	-	41,41,41	0.11	0	56,56,56	0.27	0
21	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.32	0
18	CLA	B	819	6	50,58,73	1.52	7 (14%)	58,95,113	1.93	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	802	-	65,73,73	1.35	7 (10%)	76,113,113	1.88	12 (15%)
18	CLA	4	610	-	60,68,73	1.40	7 (11%)	70,107,113	1.75	10 (14%)
17	CHL	2	606	-	43,51,74	1.68	9 (20%)	45,86,114	2.07	9 (20%)
18	CLA	B	840	22	65,73,73	1.35	7 (10%)	76,113,113	1.73	12 (15%)
19	LUT	4	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.55	9 (17%)
21	BCR	B	843	-	41,41,41	0.20	0	56,56,56	0.45	0
18	CLA	F	301	-	57,65,73	1.42	7 (12%)	66,103,113	1.79	9 (13%)
18	CLA	A	806	5	65,73,73	1.34	7 (10%)	76,113,113	1.80	8 (10%)
18	CLA	1	605	-	39,48,73	1.60	7 (17%)	45,82,113	2.02	6 (13%)
23	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.15	0
18	CLA	A	821	-	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
17	CHL	4	606	-	46,54,74	1.73	10 (21%)	49,90,114	2.05	7 (14%)
18	CLA	A	837	5	51,59,73	1.48	7 (13%)	59,96,113	2.08	10 (16%)
18	CLA	B	813	6	65,73,73	1.34	7 (10%)	76,113,113	1.75	10 (13%)
18	CLA	B	830	6	43,51,73	1.56	7 (16%)	49,86,113	1.94	6 (12%)
21	BCR	F	302	-	41,41,41	0.16	0	56,56,56	0.36	0
26	SF4	C	101	7	0,12,12	-	-	-	-	-
21	BCR	1	617	-	41,41,41	0.12	0	56,56,56	0.29	0
25	PQN	B	841	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
18	CLA	3	609	3	41,49,73	1.61	7 (17%)	47,84,113	1.93	8 (17%)
17	CHL	4	607	-	51,59,74	1.67	10 (19%)	55,96,114	2.14	13 (23%)
18	CLA	4	604	-	45,53,73	1.58	7 (15%)	52,89,113	1.90	8 (15%)
18	CLA	A	802	-	65,73,73	1.34	8 (12%)	76,113,113	1.80	11 (14%)
18	CLA	A	822	5	42,50,73	1.58	7 (16%)	48,85,113	1.88	8 (16%)
21	BCR	G	205	-	41,41,41	0.11	0	56,56,56	0.34	0
18	CLA	A	840	5	65,73,73	1.32	7 (10%)	76,113,113	1.77	12 (15%)
18	CLA	B	833	6	60,68,73	1.39	7 (11%)	70,107,113	1.77	9 (12%)
18	CLA	A	813	5	65,73,73	1.33	7 (10%)	76,113,113	1.84	11 (14%)
18	CLA	3	606	-	40,49,73	1.62	7 (17%)	45,84,113	1.93	4 (8%)
18	CLA	A	827	5	65,73,73	1.34	7 (10%)	76,113,113	1.83	10 (13%)
18	CLA	A	824	5	55,63,73	1.45	7 (12%)	64,101,113	1.76	10 (15%)
18	CLA	A	831	5	50,58,73	1.55	7 (14%)	58,95,113	1.96	8 (13%)
17	CHL	4	615	4	40,49,74	1.69	7 (17%)	45,84,114	2.34	11 (24%)

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
18	CLA	2	608	2	1/1/11/20	4/13/91/115	-
18	CLA	B	828	6	1/1/13/20	9/27/105/115	-
18	CLA	B	834	-	1/1/10/20	1/10/88/115	-
23	LMG	1	620	-	-	11/48/68/70	0/1/1/1
18	CLA	A	805	5	1/1/11/20	5/13/91/115	-
18	CLA	B	808	6	1/1/13/20	8/25/103/115	-
18	CLA	B	816	-	1/1/13/20	16/30/108/115	-
18	CLA	1	604	-	1/1/11/20	3/18/96/115	-
18	CLA	B	823	-	1/1/15/20	11/37/115/115	-
18	CLA	J	102	-	1/1/10/20	6/10/88/115	-
20	XAT	2	616	-	-	0/31/93/93	0/4/4/4
24	LMT	4	620	-	-	3/21/61/61	0/2/2/2
18	CLA	3	617	5	1/1/13/20	10/25/103/115	-
22	LHG	A	855	18	-	6/34/34/53	-
18	CLA	B	809	-	1/1/15/20	18/37/115/115	-
18	CLA	A	804	5	1/1/13/20	14/25/103/115	-
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	1	607	-	1/1/11/20	0/11/89/115	-
21	BCR	2	618	-	-	14/29/63/63	0/2/2/2
23	LMG	4	619	-	-	5/31/51/70	0/1/1/1
18	CLA	3	611	3	1/1/11/20	4/11/89/115	-
18	CLA	3	604	-	1/1/11/20	4/13/91/115	-
18	CLA	4	603	4	1/1/11/20	6/13/91/115	-
18	CLA	A	828	5	1/1/15/20	14/37/115/115	-
18	CLA	A	816	-	1/1/11/20	4/13/91/115	-
18	CLA	B	818	-	1/1/13/20	5/25/103/115	-
18	CLA	4	608	4	1/1/11/20	3/13/91/115	-
18	CLA	B	806	6	1/1/12/20	1/22/100/115	-
18	CLA	B	826	6	1/1/14/20	12/31/109/115	-
18	CLA	A	823	5	1/1/10/20	3/8/86/115	-
18	CLA	2	613	2	1/1/10/20	4/11/89/115	-
18	CLA	B	836	6	1/1/15/20	10/37/115/115	-
18	CLA	A	817	5	1/1/14/20	16/31/109/115	-
18	CLA	K	203	15	1/1/11/20	7/15/93/115	-
21	BCR	B	845	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	101	-	-	6/29/63/63	0/2/2/2
22	LHG	2	617	-	-	6/41/41/53	-
18	CLA	B	822	6	1/1/14/20	22/31/109/115	-
18	CLA	A	832	5	1/1/13/20	3/27/105/115	-
18	CLA	2	603	2	1/1/11/20	5/11/89/115	-
18	CLA	4	613	4	1/1/11/20	4/13/91/115	-
18	CLA	L	304	-	1/1/11/20	9/13/91/115	-
18	CLA	A	835	5	1/1/11/20	3/13/91/115	-
18	CLA	1	608	1	1/1/15/20	18/37/115/115	-
18	CLA	A	843	-	1/1/15/20	13/37/115/115	-
17	CHL	1	601	1	3/3/18/26	10/25/123/137	-
18	CLA	A	838	5	1/1/13/20	6/25/103/115	-
18	CLA	A	818	5	1/1/13/20	9/30/108/115	-
18	CLA	A	826	-	1/1/15/20	11/37/115/115	-
18	CLA	B	820	6	1/1/13/20	11/25/103/115	-
21	BCR	A	845	-	-	4/29/63/63	0/2/2/2
17	CHL	3	616	-	3/3/16/26	6/17/115/137	-
18	CLA	B	827	6	1/1/15/20	17/37/115/115	-
18	CLA	2	609	2	1/1/13/20	3/25/103/115	-
18	CLA	1	610	22	1/1/13/20	4/25/103/115	-
18	CLA	B	832	6	1/1/11/20	5/13/91/115	-
18	CLA	A	819	5	1/1/15/20	20/37/115/115	-
21	BCR	A	847	-	-	3/29/63/63	0/2/2/2
18	CLA	2	611	2	1/1/11/20	4/13/91/115	-
18	CLA	B	805	6	1/1/15/20	21/37/115/115	-
18	CLA	B	821	6	1/1/13/20	8/25/103/115	-
18	CLA	A	825	-	1/1/15/20	18/37/115/115	-
18	CLA	A	820	5	1/1/11/20	1/13/91/115	-
18	CLA	1	613	1	1/1/11/20	6/13/91/115	-
18	CLA	A	839	5	1/1/12/20	10/19/97/115	-
20	XAT	4	617	-	-	0/31/93/93	0/4/4/4
17	CHL	4	605	-	3/3/18/26	3/27/125/137	-
18	CLA	A	811	5	1/1/15/20	11/37/115/115	-
18	CLA	2	612	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	835	-	1/1/12/20	5/19/97/115	-
18	CLA	4	602	4	1/1/14/20	8/31/109/115	-
18	CLA	L	303	16	1/1/14/20	14/31/109/115	-
26	SF4	A	851	5,6	-	-	0/6/5/5
18	CLA	4	612	4	1/1/13/20	17/28/106/115	-
18	CLA	3	605	-	1/1/11/20	6/16/94/115	-
22	LHG	1	622	18	-	5/42/42/53	-
18	CLA	4	601	4	1/1/11/20	6/15/93/115	-
18	CLA	B	838	-	1/1/15/20	12/37/115/115	-
25	PQN	A	844	-	-	7/23/43/43	0/2/2/2
18	CLA	A	830	5	1/1/15/20	13/37/115/115	-
18	CLA	2	602	2	1/1/15/20	11/37/115/115	-
18	CLA	A	803	-	1/1/15/20	8/37/115/115	-
18	CLA	A	815	5	1/1/10/20	5/10/88/115	-
18	CLA	B	811	6	1/1/10/20	2/11/89/115	-
19	LUT	1	619	-	-	2/29/67/67	0/2/2/2
22	LHG	A	852	-	-	11/53/53/53	-
18	CLA	1	603	1	1/1/13/20	6/25/103/115	-
18	CLA	B	817	6	1/1/14/20	16/31/109/115	-
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
18	CLA	B	825	6	1/1/14/20	12/34/112/115	-
20	XAT	1	616	-	-	0/31/93/93	0/4/4/4
18	CLA	1	602	1	1/1/14/20	13/33/111/115	-
17	CHL	2	601	2	3/3/16/26	4/17/115/137	-
18	CLA	B	804	6	1/1/15/20	15/37/115/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	A	829	5	1/1/15/20	16/37/115/115	-
18	CLA	B	814	6	1/1/13/20	10/25/103/115	-
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
18	CLA	3	603	3	1/1/13/20	8/25/103/115	-
18	CLA	A	854	22	1/1/12/20	4/19/97/115	-
18	CLA	A	801	5	1/1/15/20	11/37/115/115	-
18	CLA	A	808	5	1/1/12/20	7/19/97/115	-
18	CLA	4	609	4	1/1/12/20	4/24/102/115	-
18	CLA	3	612	-	1/1/10/20	0/6/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	610	3	1/1/10/20	6/11/89/115	-
18	CLA	A	833	5	1/1/15/20	17/37/115/115	-
21	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	CLA	G	202	-	1/1/11/20	7/13/91/115	-
18	CLA	1	609	1	1/1/14/20	7/29/107/115	-
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
19	LUT	2	615	-	-	1/29/67/67	0/2/2/2
18	CLA	A	814	5	1/1/11/20	3/13/91/115	-
18	CLA	B	803	6	1/1/10/20	0/8/86/115	-
18	CLA	H	201	12	1/1/12/20	12/21/99/115	-
18	CLA	4	614	4	1/1/12/20	8/19/97/115	-
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	1	612	1	1/1/15/20	16/37/115/115	-
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
21	BCR	A	849	-	-	4/29/63/63	0/2/2/2
19	LUT	1	615	-	-	1/29/67/67	0/2/2/2
23	LMG	4	621	-	-	9/44/64/70	0/1/1/1
18	CLA	B	812	6	1/1/15/20	17/37/115/115	-
18	CLA	B	810	6	1/1/13/20	6/25/101/115	-
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
22	LHG	1	618	18	-	11/53/53/53	-
18	CLA	1	614	1	1/1/11/20	7/13/91/115	-
21	BCR	L	305	-	-	3/29/63/63	0/2/2/2
22	LHG	1	621	-	-	13/53/53/53	-
18	CLA	3	613	3	1/1/10/20	0/6/84/115	-
18	CLA	2	604	-	1/1/15/20	18/37/115/115	-
18	CLA	B	815	6	1/1/13/20	5/25/103/115	-
21	BCR	K	205	-	-	4/29/63/63	0/2/2/2
18	CLA	3	608	3	1/1/11/20	2/13/91/115	-
19	LUT	3	614	-	-	2/29/67/67	0/2/2/2
18	CLA	K	202	-	1/1/11/20	6/13/91/115	-
18	CLA	A	812	5	1/1/12/20	9/24/102/115	-
18	CLA	1	611	1	1/1/11/20	5/13/91/115	-
18	CLA	B	824	-	1/1/12/20	3/19/97/115	-
21	BCR	K	204	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	B	849	-	-	13/47/67/70	0/1/1/1
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
21	BCR	A	846	-	-	5/29/63/63	0/2/2/2
18	CLA	B	829	6	1/1/10/20	4/11/89/115	-
17	CHL	2	607	-	3/3/17/26	7/21/119/137	-
26	SF4	C	102	7	-	-	0/6/5/5
18	CLA	B	801	6	1/1/15/20	19/37/115/115	-
18	CLA	B	831	-	1/1/15/20	16/37/115/115	-
18	CLA	A	834	5	1/1/15/20	15/37/115/115	-
18	CLA	A	836	5	1/1/11/20	6/13/91/115	-
18	CLA	F	303	-	1/1/10/20	1/10/88/115	-
24	LMT	G	201	-	-	2/21/61/61	0/2/2/2
18	CLA	A	807	5	1/1/15/20	16/37/115/115	-
17	CHL	1	606	1	3/3/15/26	3/8/106/137	-
21	BCR	L	307	-	-	4/29/63/63	0/2/2/2
23	LMG	F	306	-	-	10/42/62/70	0/1/1/1
18	CLA	B	807	-	1/1/15/20	14/37/115/115	-
18	CLA	A	809	5	1/1/13/20	8/25/103/115	-
24	LMT	A	856	-	-	5/21/61/61	0/2/2/2
17	CHL	2	614	2	3/3/15/26	5/12/110/137	-
18	CLA	B	837	6	1/1/11/20	6/16/94/115	-
18	CLA	3	602	3	1/1/14/20	14/31/109/115	-
18	CLA	A	810	5	1/1/12/20	6/19/97/115	-
18	CLA	A	842	-	1/1/15/20	17/37/115/115	-
18	CLA	K	201	15	1/1/8/20	0/2/76/115	-
20	XAT	3	615	-	-	0/31/93/93	0/4/4/4
18	CLA	F	304	10	1/1/10/20	2/8/86/115	-
21	BCR	B	842	-	-	0/29/63/63	0/2/2/2
27	DGD	B	848	-	-	7/50/90/95	0/2/2/2
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
18	CLA	2	610	-	1/1/10/20	1/8/86/115	-
18	CLA	G	204	11	1/1/11/20	5/13/91/115	-
18	CLA	G	203	11	1/1/10/20	1/10/88/115	-
18	CLA	B	839	6	1/1/15/20	15/37/115/115	-
23	LMG	1	623	-	-	10/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	302	16	1/1/11/20	6/13/91/115	-
21	BCR	A	850	-	-	7/29/63/63	0/2/2/2
18	CLA	4	611	4	1/1/10/20	2/8/86/115	-
18	CLA	A	841	5	1/1/15/20	13/37/115/115	-
18	CLA	3	607	3	1/1/11/20	6/13/91/115	-
21	BCR	3	601	-	-	0/29/63/63	0/2/2/2
21	BCR	B	846	-	-	3/29/63/63	0/2/2/2
18	CLA	B	819	6	1/1/12/20	7/19/97/115	-
18	CLA	B	802	-	1/1/15/20	17/37/115/115	-
18	CLA	4	610	-	1/1/14/20	11/31/109/115	-
17	CHL	2	606	-	3/3/15/26	4/12/110/137	-
18	CLA	B	840	22	1/1/15/20	25/37/115/115	-
19	LUT	4	616	-	-	1/29/67/67	0/2/2/2
21	BCR	B	843	-	-	3/29/63/63	0/2/2/2
18	CLA	F	301	-	1/1/13/20	11/28/106/115	-
18	CLA	A	806	5	1/1/15/20	20/37/115/115	-
18	CLA	1	605	-	1/1/9/20	2/8/82/115	-
23	LMG	F	307	-	-	0/25/45/70	0/1/1/1
18	CLA	A	821	-	1/1/15/20	14/37/115/115	-
17	CHL	4	606	-	3/3/16/26	6/15/113/137	-
18	CLA	A	837	5	1/1/12/20	8/21/99/115	-
18	CLA	B	813	6	1/1/15/20	16/37/115/115	-
18	CLA	B	830	6	1/1/10/20	3/11/89/115	-
21	BCR	F	302	-	-	0/29/63/63	0/2/2/2
26	SF4	C	101	7	-	-	0/6/5/5
21	BCR	1	617	-	-	2/29/63/63	0/2/2/2
25	PQN	B	841	-	-	7/23/43/43	0/2/2/2
18	CLA	3	609	3	1/1/10/20	4/8/86/115	-
17	CHL	4	607	-	3/3/17/26	8/21/119/137	-
18	CLA	4	604	-	1/1/11/20	5/13/91/115	-
18	CLA	A	802	-	1/1/15/20	11/37/115/115	-
18	CLA	A	822	5	1/1/10/20	4/10/88/115	-
21	BCR	G	205	-	-	0/29/63/63	0/2/2/2
18	CLA	A	840	5	1/1/15/20	16/37/115/115	-
18	CLA	B	833	6	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	813	5	1/1/15/20	15/37/115/115	-
18	CLA	3	606	-	1/1/10/20	3/8/86/115	-
18	CLA	A	827	5	1/1/15/20	11/37/115/115	-
18	CLA	A	824	5	1/1/13/20	12/25/103/115	-
18	CLA	A	831	5	1/1/12/20	11/19/97/115	-
17	CHL	4	615	4	3/3/15/26	2/10/106/137	-

All (1154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	CMC-C2C	5.45	1.56	1.45
17	2	605	CHL	CMC-C2C	5.40	1.56	1.45
17	3	616	CHL	CMC-C2C	5.36	1.56	1.45
17	1	606	CHL	CMC-C2C	5.35	1.56	1.45
17	4	605	CHL	CMC-C2C	5.34	1.56	1.45
17	2	601	CHL	CMC-C2C	5.33	1.56	1.45
17	4	606	CHL	CMC-C2C	5.32	1.56	1.45
17	2	614	CHL	CMC-C2C	5.30	1.56	1.45
17	1	601	CHL	CMC-C2C	5.29	1.56	1.45
17	2	607	CHL	CMC-C2C	5.28	1.56	1.45
17	4	615	CHL	CMC-C2C	5.27	1.56	1.45
17	4	607	CHL	CMC-C2C	5.22	1.56	1.45
18	B	831	CLA	MG-NA	5.06	2.18	2.06
18	3	612	CLA	MG-NA	5.04	2.18	2.06
18	3	610	CLA	MG-NA	5.03	2.18	2.06
18	B	812	CLA	MG-NA	5.03	2.18	2.06
18	A	839	CLA	MG-NA	5.03	2.18	2.06
18	B	834	CLA	MG-NA	5.02	2.18	2.06
18	4	603	CLA	MG-NA	5.02	2.18	2.06
18	J	102	CLA	MG-NA	5.02	2.18	2.06
18	L	304	CLA	MG-NA	5.02	2.18	2.06
18	B	838	CLA	MG-NA	5.01	2.18	2.06
18	3	603	CLA	MG-NA	5.01	2.18	2.06
18	F	303	CLA	MG-NA	5.01	2.18	2.06
18	G	204	CLA	MG-NA	5.00	2.18	2.06
18	A	825	CLA	MG-NA	5.00	2.18	2.06
18	2	611	CLA	MG-NA	5.00	2.18	2.06
18	3	604	CLA	MG-NA	4.99	2.18	2.06
18	G	202	CLA	MG-NA	4.99	2.18	2.06
18	A	808	CLA	MG-NA	4.98	2.18	2.06
18	B	815	CLA	MG-NA	4.98	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	MG-NA	4.98	2.18	2.06
18	A	823	CLA	MG-NA	4.98	2.18	2.06
18	3	606	CLA	MG-NA	4.98	2.18	2.06
18	1	605	CLA	MG-NA	4.98	2.18	2.06
18	K	203	CLA	MG-NA	4.98	2.18	2.06
18	A	854	CLA	MG-NA	4.97	2.18	2.06
18	B	835	CLA	MG-NA	4.97	2.18	2.06
18	3	602	CLA	MG-NA	4.97	2.18	2.06
18	3	605	CLA	MG-NA	4.97	2.18	2.06
18	K	201	CLA	MG-NA	4.97	2.18	2.06
18	F	304	CLA	MG-NA	4.97	2.18	2.06
18	4	613	CLA	MG-NA	4.96	2.18	2.06
18	A	841	CLA	MG-NA	4.96	2.18	2.06
18	4	611	CLA	MG-NA	4.96	2.18	2.06
18	4	604	CLA	MG-NA	4.96	2.18	2.06
18	4	614	CLA	MG-NA	4.96	2.18	2.06
18	3	607	CLA	MG-NA	4.96	2.18	2.06
18	L	302	CLA	MG-NA	4.96	2.18	2.06
18	1	612	CLA	MG-NA	4.96	2.18	2.06
18	A	811	CLA	MG-NA	4.96	2.18	2.06
18	A	815	CLA	MG-NA	4.96	2.18	2.06
18	B	804	CLA	MG-NA	4.95	2.18	2.06
18	K	202	CLA	MG-NA	4.95	2.18	2.06
18	B	805	CLA	MG-NA	4.95	2.18	2.06
18	B	814	CLA	MG-NA	4.95	2.18	2.06
18	1	613	CLA	MG-NA	4.95	2.18	2.06
18	B	828	CLA	MG-NA	4.95	2.18	2.06
18	4	612	CLA	MG-NA	4.95	2.18	2.06
18	3	611	CLA	MG-NA	4.95	2.18	2.06
18	2	610	CLA	MG-NA	4.94	2.18	2.06
18	2	613	CLA	MG-NA	4.94	2.18	2.06
18	A	817	CLA	MG-NA	4.94	2.18	2.06
18	A	814	CLA	MG-NA	4.94	2.18	2.06
18	B	829	CLA	MG-NA	4.94	2.18	2.06
18	1	610	CLA	MG-NA	4.94	2.18	2.06
18	A	830	CLA	MG-NA	4.93	2.18	2.06
18	1	602	CLA	MG-NA	4.93	2.18	2.06
18	B	819	CLA	MG-NA	4.93	2.18	2.06
18	2	602	CLA	MG-NA	4.93	2.18	2.06
18	A	843	CLA	MG-NA	4.93	2.18	2.06
18	A	822	CLA	MG-NA	4.93	2.18	2.06
18	A	833	CLA	MG-NA	4.93	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	611	CLA	MG-NA	4.93	2.18	2.06
18	A	804	CLA	MG-NA	4.93	2.18	2.06
18	A	831	CLA	MG-NA	4.92	2.18	2.06
18	4	610	CLA	MG-NA	4.92	2.18	2.06
18	A	842	CLA	MG-NA	4.92	2.18	2.06
18	2	604	CLA	MG-NA	4.92	2.18	2.06
18	B	823	CLA	MG-NA	4.92	2.18	2.06
18	3	613	CLA	MG-NA	4.92	2.17	2.06
18	A	816	CLA	MG-NA	4.92	2.17	2.06
18	2	612	CLA	MG-NA	4.92	2.17	2.06
18	3	617	CLA	MG-NA	4.92	2.17	2.06
18	1	607	CLA	MG-NA	4.91	2.17	2.06
18	A	813	CLA	MG-NA	4.91	2.17	2.06
18	A	806	CLA	MG-NA	4.91	2.17	2.06
18	A	838	CLA	MG-NA	4.91	2.17	2.06
18	B	837	CLA	MG-NA	4.91	2.17	2.06
18	1	604	CLA	MG-NA	4.90	2.17	2.06
18	A	820	CLA	MG-NA	4.90	2.17	2.06
18	B	810	CLA	MG-NA	4.90	2.17	2.06
18	A	824	CLA	MG-NA	4.90	2.17	2.06
18	A	835	CLA	MG-NA	4.90	2.17	2.06
18	1	614	CLA	MG-NA	4.89	2.17	2.06
18	B	827	CLA	MG-NA	4.89	2.17	2.06
18	A	837	CLA	MG-NA	4.89	2.17	2.06
18	A	805	CLA	MG-NA	4.89	2.17	2.06
18	3	609	CLA	MG-NA	4.89	2.17	2.06
18	B	818	CLA	MG-NA	4.89	2.17	2.06
18	A	801	CLA	MG-NA	4.89	2.17	2.06
18	4	602	CLA	MG-NA	4.89	2.17	2.06
18	A	807	CLA	MG-NA	4.88	2.17	2.06
18	B	833	CLA	MG-NA	4.88	2.17	2.06
18	F	301	CLA	MG-NA	4.88	2.17	2.06
18	2	603	CLA	MG-NA	4.88	2.17	2.06
18	B	840	CLA	MG-NA	4.88	2.17	2.06
18	B	806	CLA	MG-NA	4.88	2.17	2.06
18	4	601	CLA	MG-NA	4.88	2.17	2.06
18	A	828	CLA	MG-NA	4.87	2.17	2.06
18	A	809	CLA	MG-NA	4.87	2.17	2.06
18	A	812	CLA	MG-NA	4.87	2.17	2.06
18	B	821	CLA	MG-NA	4.87	2.17	2.06
18	2	608	CLA	MG-NA	4.87	2.17	2.06
18	2	609	CLA	MG-NA	4.87	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	829	CLA	MG-NA	4.87	2.17	2.06
18	B	836	CLA	MG-NA	4.87	2.17	2.06
18	3	608	CLA	MG-NA	4.87	2.17	2.06
18	A	821	CLA	MG-NA	4.87	2.17	2.06
18	G	203	CLA	MG-NA	4.86	2.17	2.06
18	B	839	CLA	MG-NA	4.86	2.17	2.06
18	B	826	CLA	MG-NA	4.86	2.17	2.06
18	B	807	CLA	MG-NA	4.86	2.17	2.06
18	1	603	CLA	MG-NA	4.86	2.17	2.06
18	A	836	CLA	MG-NA	4.86	2.17	2.06
18	B	801	CLA	MG-NA	4.85	2.17	2.06
18	B	809	CLA	MG-NA	4.85	2.17	2.06
18	B	830	CLA	MG-NA	4.85	2.17	2.06
18	1	609	CLA	MG-NA	4.85	2.17	2.06
18	A	810	CLA	MG-NA	4.84	2.17	2.06
18	4	608	CLA	MG-NA	4.84	2.17	2.06
18	A	826	CLA	MG-NA	4.84	2.17	2.06
18	H	201	CLA	MG-NA	4.84	2.17	2.06
18	A	834	CLA	MG-NA	4.84	2.17	2.06
18	A	840	CLA	MG-NA	4.84	2.17	2.06
18	A	827	CLA	MG-NA	4.84	2.17	2.06
18	B	820	CLA	MG-NA	4.83	2.17	2.06
18	A	818	CLA	MG-NA	4.83	2.17	2.06
18	B	813	CLA	MG-NA	4.83	2.17	2.06
18	4	609	CLA	MG-NA	4.82	2.17	2.06
18	A	819	CLA	MG-NA	4.81	2.17	2.06
18	B	817	CLA	MG-NA	4.81	2.17	2.06
18	B	825	CLA	MG-NA	4.81	2.17	2.06
18	1	608	CLA	MG-NA	4.80	2.17	2.06
18	L	303	CLA	MG-NA	4.80	2.17	2.06
18	B	803	CLA	MG-NA	4.79	2.17	2.06
18	A	832	CLA	MG-NA	4.79	2.17	2.06
18	A	803	CLA	MG-NA	4.79	2.17	2.06
18	B	822	CLA	MG-NA	4.79	2.17	2.06
18	B	811	CLA	MG-NA	4.78	2.17	2.06
18	B	824	CLA	MG-NA	4.78	2.17	2.06
18	B	816	CLA	MG-NA	4.78	2.17	2.06
18	B	802	CLA	MG-NA	4.77	2.17	2.06
18	A	802	CLA	MG-NA	4.76	2.17	2.06
18	B	832	CLA	MG-NA	4.72	2.17	2.06
18	3	612	CLA	C4B-NB	4.24	1.39	1.35
18	3	610	CLA	C4B-NB	4.24	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	C4B-NB	4.24	1.39	1.35
18	F	303	CLA	C4B-NB	4.22	1.39	1.35
18	A	823	CLA	C4B-NB	4.22	1.39	1.35
18	2	610	CLA	C4B-NB	4.20	1.39	1.35
18	K	201	CLA	C4B-NB	4.19	1.38	1.35
18	A	803	CLA	C4B-NB	4.17	1.38	1.35
18	4	604	CLA	C4B-NB	4.15	1.38	1.35
18	K	202	CLA	C4B-NB	4.14	1.38	1.35
18	A	854	CLA	C4B-NB	4.14	1.38	1.35
18	1	602	CLA	C4B-NB	4.13	1.38	1.35
18	2	604	CLA	C4B-NB	4.13	1.38	1.35
18	4	609	CLA	C4B-NB	4.13	1.38	1.35
19	1	615	LUT	C34-C33	4.13	1.41	1.35
18	2	608	CLA	C4B-NB	4.12	1.38	1.35
18	3	606	CLA	C4B-NB	4.12	1.38	1.35
18	A	819	CLA	C4B-NB	4.11	1.38	1.35
18	3	605	CLA	C4B-NB	4.11	1.38	1.35
19	3	614	LUT	C30-C29	4.10	1.41	1.35
18	3	608	CLA	C4B-NB	4.10	1.38	1.35
18	1	611	CLA	C4B-NB	4.09	1.38	1.35
18	3	603	CLA	C4B-NB	4.08	1.38	1.35
18	3	604	CLA	C4B-NB	4.08	1.38	1.35
18	B	831	CLA	C4B-NB	4.08	1.38	1.35
18	J	102	CLA	C4B-NB	4.06	1.38	1.35
18	K	203	CLA	C4B-NB	4.05	1.38	1.35
18	4	611	CLA	C4B-NB	4.05	1.38	1.35
18	A	832	CLA	C4B-NB	4.05	1.38	1.35
18	A	842	CLA	C4B-NB	4.05	1.38	1.35
19	2	615	LUT	C34-C33	4.04	1.41	1.35
19	3	614	LUT	C10-C9	4.04	1.41	1.35
18	1	605	CLA	C4B-NB	4.04	1.38	1.35
18	G	204	CLA	C4B-NB	4.04	1.38	1.35
18	2	612	CLA	C4B-NB	4.03	1.38	1.35
18	B	827	CLA	C4B-NB	4.03	1.38	1.35
18	B	821	CLA	C4B-NB	4.03	1.38	1.35
18	3	611	CLA	C4B-NB	4.03	1.38	1.35
18	3	613	CLA	C4B-NB	4.03	1.38	1.35
18	A	826	CLA	C4B-NB	4.03	1.38	1.35
18	L	302	CLA	C4B-NB	4.02	1.38	1.35
19	2	615	LUT	C14-C13	4.02	1.41	1.35
19	4	616	LUT	C34-C33	4.02	1.41	1.35
18	4	610	CLA	C4B-NB	4.01	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	613	CLA	C4B-NB	4.01	1.38	1.35
18	B	836	CLA	C4B-NB	4.01	1.38	1.35
18	A	811	CLA	C4B-NB	4.01	1.38	1.35
18	B	823	CLA	C4B-NB	4.01	1.38	1.35
18	1	610	CLA	C4B-NB	4.01	1.38	1.35
18	2	602	CLA	C4B-NB	4.01	1.38	1.35
18	L	304	CLA	C4B-NB	4.00	1.38	1.35
18	1	613	CLA	C4B-NB	4.00	1.38	1.35
18	A	808	CLA	C4B-NB	4.00	1.38	1.35
18	3	617	CLA	C4B-NB	4.00	1.38	1.35
18	B	803	CLA	C4B-NB	4.00	1.38	1.35
18	B	830	CLA	C4B-NB	4.00	1.38	1.35
19	4	616	LUT	C14-C13	4.00	1.41	1.35
18	G	202	CLA	C4B-NB	4.00	1.38	1.35
18	G	203	CLA	C4B-NB	3.99	1.38	1.35
18	A	838	CLA	C4B-NB	3.99	1.38	1.35
18	B	806	CLA	C4B-NB	3.99	1.38	1.35
18	H	201	CLA	C4B-NB	3.99	1.38	1.35
18	4	608	CLA	C4B-NB	3.99	1.38	1.35
18	B	802	CLA	C4B-NB	3.99	1.38	1.35
18	A	825	CLA	C4B-NB	3.99	1.38	1.35
18	B	840	CLA	C4B-NB	3.99	1.38	1.35
19	3	614	LUT	C14-C13	3.99	1.41	1.35
19	1	615	LUT	C30-C29	3.98	1.41	1.35
18	3	602	CLA	C4B-NB	3.98	1.38	1.35
18	B	817	CLA	C4B-NB	3.98	1.38	1.35
18	1	604	CLA	C4B-NB	3.98	1.38	1.35
18	A	821	CLA	C4B-NB	3.98	1.38	1.35
18	B	837	CLA	C4B-NB	3.98	1.38	1.35
18	A	804	CLA	C4B-NB	3.97	1.38	1.35
18	B	810	CLA	C4B-NB	3.97	1.38	1.35
18	2	613	CLA	C4B-NB	3.97	1.38	1.35
19	2	615	LUT	C30-C29	3.97	1.41	1.35
19	2	615	LUT	C10-C9	3.96	1.41	1.35
18	1	609	CLA	C4B-NB	3.96	1.38	1.35
18	3	609	CLA	C4B-NB	3.96	1.38	1.35
19	1	615	LUT	C10-C9	3.96	1.41	1.35
18	B	834	CLA	C4B-NB	3.95	1.38	1.35
19	1	619	LUT	C10-C9	3.95	1.41	1.35
19	3	614	LUT	C34-C33	3.95	1.41	1.35
18	A	801	CLA	C4B-NB	3.94	1.38	1.35
18	A	831	CLA	C4B-NB	3.94	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	619	LUT	C34-C33	3.94	1.41	1.35
18	2	611	CLA	C4B-NB	3.94	1.38	1.35
18	3	607	CLA	C4B-NB	3.94	1.38	1.35
18	L	303	CLA	C4B-NB	3.94	1.38	1.35
18	1	607	CLA	C4B-NB	3.93	1.38	1.35
19	1	615	LUT	C14-C13	3.93	1.41	1.35
18	B	812	CLA	C4B-NB	3.92	1.38	1.35
18	A	839	CLA	C4B-NB	3.92	1.38	1.35
18	4	603	CLA	C4B-NB	3.90	1.38	1.35
18	B	814	CLA	C4B-NB	3.90	1.38	1.35
18	A	828	CLA	C4B-NB	3.90	1.38	1.35
18	B	829	CLA	C4B-NB	3.90	1.38	1.35
19	4	616	LUT	C30-C29	3.90	1.41	1.35
19	4	616	LUT	C10-C9	3.90	1.40	1.35
18	A	818	CLA	C4B-NB	3.89	1.38	1.35
18	B	815	CLA	C4B-NB	3.89	1.38	1.35
18	A	822	CLA	C4B-NB	3.89	1.38	1.35
18	B	801	CLA	C4B-NB	3.89	1.38	1.35
18	B	818	CLA	C4B-NB	3.88	1.38	1.35
18	F	301	CLA	C4B-NB	3.88	1.38	1.35
18	A	814	CLA	C4B-NB	3.88	1.38	1.35
18	A	824	CLA	C4B-NB	3.88	1.38	1.35
18	B	808	CLA	C4B-NB	3.88	1.38	1.35
18	B	826	CLA	C4B-NB	3.88	1.38	1.35
18	1	608	CLA	C4B-NB	3.87	1.38	1.35
18	4	602	CLA	C4B-NB	3.87	1.38	1.35
18	A	816	CLA	C4B-NB	3.87	1.38	1.35
18	A	805	CLA	C4B-NB	3.87	1.38	1.35
18	A	820	CLA	C4B-NB	3.87	1.38	1.35
18	A	836	CLA	C4B-NB	3.87	1.38	1.35
18	A	830	CLA	C4B-NB	3.87	1.38	1.35
17	4	607	CHL	C4B-NB	3.87	1.38	1.35
18	2	603	CLA	C4B-NB	3.86	1.38	1.35
18	2	609	CLA	C4B-NB	3.86	1.38	1.35
18	B	825	CLA	C4B-NB	3.86	1.38	1.35
18	F	304	CLA	C4B-NB	3.86	1.38	1.35
18	A	812	CLA	C4B-NB	3.86	1.38	1.35
18	B	819	CLA	C4B-NB	3.85	1.38	1.35
18	A	815	CLA	C4B-NB	3.85	1.38	1.35
18	4	612	CLA	C4B-NB	3.85	1.38	1.35
18	1	603	CLA	C4B-NB	3.84	1.38	1.35
19	1	619	LUT	C14-C13	3.84	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	834	CLA	C4B-NB	3.84	1.38	1.35
18	4	601	CLA	C4B-NB	3.84	1.38	1.35
18	B	835	CLA	C4B-NB	3.83	1.38	1.35
18	B	807	CLA	C4B-NB	3.83	1.38	1.35
18	A	829	CLA	C4B-NB	3.83	1.38	1.35
18	B	828	CLA	C4B-NB	3.83	1.38	1.35
18	A	813	CLA	C4B-NB	3.83	1.38	1.35
18	1	612	CLA	C4B-NB	3.82	1.38	1.35
18	A	841	CLA	C4B-NB	3.82	1.38	1.35
17	2	605	CHL	C4B-NB	3.82	1.38	1.35
19	1	619	LUT	C30-C29	3.80	1.40	1.35
18	4	614	CLA	C4B-NB	3.80	1.38	1.35
18	A	833	CLA	C4B-NB	3.80	1.38	1.35
17	4	615	CHL	CAB-C3B	-3.80	1.43	1.51
18	A	827	CLA	C4B-NB	3.79	1.38	1.35
18	B	809	CLA	C4B-NB	3.79	1.38	1.35
18	1	614	CLA	C4B-NB	3.79	1.38	1.35
18	A	817	CLA	C4B-NB	3.78	1.38	1.35
17	2	606	CHL	C4B-NB	3.78	1.38	1.35
18	B	805	CLA	C4B-NB	3.78	1.38	1.35
17	2	601	CHL	C4B-NB	3.77	1.38	1.35
17	4	606	CHL	C4B-NB	3.77	1.38	1.35
18	B	813	CLA	C4B-NB	3.77	1.38	1.35
18	B	824	CLA	C4B-NB	3.76	1.38	1.35
17	2	614	CHL	C4B-NB	3.75	1.38	1.35
18	B	804	CLA	C4B-NB	3.75	1.38	1.35
17	4	605	CHL	C4B-NB	3.75	1.38	1.35
18	A	809	CLA	C4B-NB	3.75	1.38	1.35
18	A	807	CLA	C4B-NB	3.75	1.38	1.35
18	B	833	CLA	C4B-NB	3.73	1.38	1.35
18	B	820	CLA	C4B-NB	3.73	1.38	1.35
18	B	838	CLA	C4B-NB	3.73	1.38	1.35
18	A	810	CLA	C4B-NB	3.72	1.38	1.35
17	1	606	CHL	C4B-NB	3.72	1.38	1.35
18	B	822	CLA	C4B-NB	3.72	1.38	1.35
18	A	835	CLA	C4B-NB	3.71	1.38	1.35
18	A	840	CLA	C4B-NB	3.70	1.38	1.35
18	B	816	CLA	C4B-NB	3.69	1.38	1.35
17	3	616	CHL	C4B-NB	3.69	1.38	1.35
18	A	837	CLA	C4B-NB	3.68	1.38	1.35
17	2	607	CHL	C4B-NB	3.68	1.38	1.35
18	B	832	CLA	C4B-NB	3.67	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	839	CLA	C4B-NB	3.67	1.38	1.35
18	A	806	CLA	C4B-NB	3.66	1.38	1.35
17	4	605	CHL	C3B-C2B	-3.63	1.35	1.40
17	4	615	CHL	C4B-NB	3.59	1.38	1.35
18	B	811	CLA	C4B-NB	3.58	1.38	1.35
17	4	606	CHL	C3B-C2B	-3.58	1.35	1.40
17	4	607	CHL	C3B-C2B	-3.58	1.35	1.40
18	A	802	CLA	C4B-NB	3.57	1.38	1.35
17	2	606	CHL	C3B-C2B	-3.53	1.35	1.40
17	2	607	CHL	C3B-C2B	-3.53	1.35	1.40
17	1	601	CHL	C3B-C2B	-3.52	1.35	1.40
17	1	601	CHL	C4B-NB	3.50	1.38	1.35
17	2	601	CHL	C3B-C2B	-3.49	1.35	1.40
17	2	614	CHL	O2D-CGD	3.47	1.41	1.33
17	2	605	CHL	C3B-C2B	-3.46	1.35	1.40
17	2	605	CHL	O2D-CGD	3.45	1.41	1.33
17	1	606	CHL	C3B-C2B	-3.43	1.35	1.40
17	2	606	CHL	O2D-CGD	3.42	1.41	1.33
17	3	616	CHL	C3B-C2B	-3.42	1.35	1.40
18	4	609	CLA	CHC-C1C	3.42	1.43	1.35
18	A	826	CLA	CHC-C1C	3.40	1.43	1.35
17	1	606	CHL	O2D-CGD	3.39	1.41	1.30
17	4	606	CHL	O2D-CGD	3.38	1.41	1.33
18	B	802	CLA	CHC-C1C	3.38	1.43	1.35
18	B	808	CLA	C3B-C2B	-3.37	1.35	1.40
18	B	820	CLA	CHC-C1C	3.37	1.43	1.35
17	4	615	CHL	O2D-CGD	3.37	1.41	1.30
18	B	832	CLA	CHC-C1C	3.37	1.43	1.35
17	4	606	CHL	O2A-CGA	3.36	1.42	1.30
17	4	605	CHL	O2D-CGD	3.36	1.41	1.33
17	3	616	CHL	O2D-CGD	3.36	1.41	1.33
18	A	834	CLA	C3B-C2B	-3.36	1.35	1.40
18	A	814	CLA	C3B-C2B	-3.35	1.35	1.40
18	1	602	CLA	CHC-C1C	3.35	1.43	1.35
18	A	819	CLA	CHC-C1C	3.35	1.43	1.35
18	A	831	CLA	CHC-C1C	3.34	1.43	1.35
18	B	822	CLA	CHC-C1C	3.34	1.43	1.35
18	B	821	CLA	CHC-C1C	3.34	1.43	1.35
18	B	825	CLA	CHC-C1C	3.34	1.43	1.35
18	3	617	CLA	CHC-C1C	3.33	1.43	1.35
18	B	806	CLA	CHC-C1C	3.33	1.43	1.35
17	2	607	CHL	O2D-CGD	3.32	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	608	CLA	CHC-C1C	3.32	1.43	1.35
18	A	802	CLA	CHC-C1C	3.32	1.43	1.35
18	B	836	CLA	CHC-C1C	3.32	1.43	1.35
18	B	827	CLA	CHC-C1C	3.31	1.43	1.35
18	3	609	CLA	CHC-C1C	3.31	1.43	1.35
18	A	822	CLA	CHC-C1C	3.31	1.43	1.35
18	A	830	CLA	CHC-C1C	3.31	1.43	1.35
18	A	840	CLA	CHC-C1C	3.31	1.43	1.35
18	B	824	CLA	CHC-C1C	3.31	1.43	1.35
18	B	821	CLA	C3B-C2B	-3.30	1.35	1.40
18	1	614	CLA	CHC-C1C	3.30	1.43	1.35
18	2	602	CLA	CHC-C1C	3.30	1.43	1.35
18	B	829	CLA	CHC-C1C	3.30	1.43	1.35
18	1	609	CLA	CHC-C1C	3.30	1.43	1.35
18	A	829	CLA	CHC-C1C	3.30	1.43	1.35
18	B	804	CLA	CHC-C1C	3.29	1.43	1.35
18	A	808	CLA	CHC-C1C	3.29	1.43	1.35
18	B	828	CLA	CHC-C1C	3.29	1.43	1.35
18	4	608	CLA	CHC-C1C	3.29	1.43	1.35
17	2	614	CHL	C3B-C2B	-3.29	1.35	1.40
18	A	831	CLA	C3B-C2B	-3.28	1.35	1.40
18	B	811	CLA	CHC-C1C	3.28	1.43	1.35
18	A	815	CLA	CHC-C1C	3.28	1.43	1.35
18	K	201	CLA	CHC-C1C	3.28	1.43	1.35
18	A	838	CLA	CHC-C1C	3.28	1.43	1.35
18	B	803	CLA	CHC-C1C	3.28	1.43	1.35
18	A	832	CLA	CHC-C1C	3.28	1.43	1.35
18	A	807	CLA	CHC-C1C	3.27	1.43	1.35
18	A	854	CLA	CHC-C1C	3.27	1.43	1.35
18	1	611	CLA	CHC-C1C	3.27	1.43	1.35
18	B	828	CLA	C3B-C2B	-3.27	1.35	1.40
18	2	604	CLA	CHC-C1C	3.27	1.43	1.35
18	B	831	CLA	C3B-C2B	-3.27	1.35	1.40
17	1	601	CHL	O2D-CGD	3.27	1.41	1.30
18	2	610	CLA	CHC-C1C	3.27	1.43	1.35
18	B	830	CLA	CHC-C1C	3.26	1.43	1.35
18	F	301	CLA	CHC-C1C	3.26	1.43	1.35
17	4	607	CHL	O2D-CGD	3.26	1.41	1.33
18	A	814	CLA	CHC-C1C	3.26	1.43	1.35
18	A	824	CLA	CHC-C1C	3.26	1.43	1.35
18	4	602	CLA	CHC-C1C	3.26	1.43	1.35
18	A	827	CLA	CHC-C1C	3.26	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	604	CLA	CHC-C1C	3.26	1.43	1.35
18	B	810	CLA	CHC-C1C	3.26	1.43	1.35
18	B	809	CLA	CHC-C1C	3.26	1.43	1.35
18	3	602	CLA	CHC-C1C	3.26	1.43	1.35
18	A	809	CLA	CHC-C1C	3.26	1.43	1.35
18	A	805	CLA	CHC-C1C	3.26	1.43	1.35
18	B	834	CLA	C3B-C2B	-3.25	1.35	1.40
18	F	303	CLA	CHC-C1C	3.25	1.43	1.35
18	2	613	CLA	CHC-C1C	3.25	1.43	1.35
18	H	201	CLA	CHC-C1C	3.25	1.43	1.35
18	3	606	CLA	CHC-C1C	3.25	1.43	1.35
18	A	803	CLA	C3B-C2B	-3.25	1.35	1.40
18	A	810	CLA	CHC-C1C	3.25	1.43	1.35
18	B	817	CLA	CHC-C1C	3.25	1.43	1.35
18	A	806	CLA	CHC-C1C	3.24	1.43	1.35
18	4	611	CLA	CHC-C1C	3.24	1.43	1.35
18	L	304	CLA	CHC-C1C	3.24	1.43	1.35
18	B	812	CLA	CHC-C1C	3.24	1.43	1.35
18	B	813	CLA	CHC-C1C	3.24	1.43	1.35
18	K	203	CLA	CHC-C1C	3.24	1.43	1.35
18	1	613	CLA	CHC-C1C	3.24	1.43	1.35
18	B	814	CLA	C3B-C2B	-3.24	1.35	1.40
18	2	609	CLA	CHC-C1C	3.24	1.43	1.35
18	A	834	CLA	CHC-C1C	3.24	1.43	1.35
18	2	612	CLA	C3B-C2B	-3.24	1.35	1.40
18	G	203	CLA	CHC-C1C	3.24	1.43	1.35
18	L	303	CLA	CHC-C1C	3.24	1.43	1.35
18	A	815	CLA	C3B-C2B	-3.24	1.35	1.40
18	B	818	CLA	CHC-C1C	3.24	1.43	1.35
18	K	202	CLA	CHC-C1C	3.24	1.43	1.35
18	A	801	CLA	CHC-C1C	3.24	1.43	1.35
18	A	812	CLA	CHC-C1C	3.24	1.43	1.35
18	A	818	CLA	CHC-C1C	3.24	1.43	1.35
17	2	601	CHL	O2D-CGD	3.24	1.41	1.33
18	3	610	CLA	CHC-C1C	3.23	1.43	1.35
18	A	821	CLA	CHC-C1C	3.23	1.43	1.35
18	A	823	CLA	CHC-C1C	3.23	1.43	1.35
18	1	610	CLA	CHC-C1C	3.23	1.43	1.35
18	A	829	CLA	C3B-C2B	-3.23	1.35	1.40
18	B	835	CLA	CHC-C1C	3.23	1.43	1.35
18	F	304	CLA	CHC-C1C	3.23	1.43	1.35
18	L	304	CLA	C3B-C2B	-3.23	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	617	CLA	C3B-C2B	-3.23	1.35	1.40
18	B	838	CLA	C3B-C2B	-3.23	1.35	1.40
18	3	604	CLA	C3B-C2B	-3.22	1.35	1.40
18	A	828	CLA	CHC-C1C	3.22	1.43	1.35
18	A	811	CLA	CHC-C1C	3.22	1.43	1.35
18	B	833	CLA	CHC-C1C	3.22	1.43	1.35
18	B	840	CLA	CHC-C1C	3.22	1.43	1.35
18	B	815	CLA	CHC-C1C	3.22	1.43	1.35
18	A	817	CLA	CHC-C1C	3.22	1.43	1.35
18	3	608	CLA	C3B-C2B	-3.22	1.35	1.40
18	4	603	CLA	C3B-C2B	-3.22	1.35	1.40
18	2	603	CLA	CHC-C1C	3.22	1.43	1.35
18	3	612	CLA	CHC-C1C	3.22	1.43	1.35
18	A	816	CLA	CHC-C1C	3.21	1.43	1.35
18	B	805	CLA	CHC-C1C	3.21	1.43	1.35
18	1	612	CLA	C3B-C2B	-3.21	1.35	1.40
18	A	835	CLA	CHC-C1C	3.21	1.43	1.35
18	1	603	CLA	C3B-C2B	-3.21	1.35	1.40
18	A	813	CLA	CHC-C1C	3.21	1.43	1.35
18	B	831	CLA	CHC-C1C	3.21	1.43	1.35
18	G	202	CLA	CHC-C1C	3.21	1.43	1.35
18	A	841	CLA	CHC-C1C	3.21	1.43	1.35
18	G	204	CLA	CHC-C1C	3.21	1.43	1.35
18	B	808	CLA	CHC-C1C	3.21	1.43	1.35
18	A	803	CLA	CHC-C1C	3.21	1.43	1.35
18	A	820	CLA	CHC-C1C	3.21	1.43	1.35
18	A	819	CLA	C3B-C2B	-3.21	1.35	1.40
18	A	809	CLA	C3B-C2B	-3.21	1.35	1.40
18	3	613	CLA	CHC-C1C	3.20	1.43	1.35
18	1	611	CLA	C3B-C2B	-3.20	1.35	1.40
18	B	801	CLA	CHC-C1C	3.20	1.43	1.35
18	J	102	CLA	CHC-C1C	3.20	1.43	1.35
18	1	608	CLA	CHC-C1C	3.20	1.43	1.35
18	2	612	CLA	CHC-C1C	3.20	1.43	1.35
18	A	821	CLA	C3B-C2B	-3.20	1.35	1.40
18	1	612	CLA	CHC-C1C	3.20	1.43	1.35
18	2	608	CLA	C3B-C2B	-3.20	1.35	1.40
18	3	605	CLA	CHC-C1C	3.20	1.43	1.35
18	1	604	CLA	CHC-C1C	3.19	1.43	1.35
18	1	603	CLA	CHC-C1C	3.19	1.43	1.35
18	4	613	CLA	CHC-C1C	3.19	1.43	1.35
18	B	823	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	814	CLA	CHC-C1C	3.19	1.43	1.35
18	B	829	CLA	C3B-C2B	-3.19	1.35	1.40
18	3	604	CLA	CHC-C1C	3.18	1.43	1.35
18	B	805	CLA	C3B-C2B	-3.18	1.36	1.40
18	B	832	CLA	C3B-C2B	-3.18	1.36	1.40
18	B	838	CLA	CHC-C1C	3.18	1.43	1.35
18	1	607	CLA	C3B-C2B	-3.18	1.36	1.40
18	1	602	CLA	C3B-C2B	-3.18	1.36	1.40
18	2	603	CLA	C3B-C2B	-3.18	1.36	1.40
18	B	835	CLA	C3B-C2B	-3.18	1.36	1.40
18	2	611	CLA	CHC-C1C	3.18	1.43	1.35
18	1	609	CLA	C3B-C2B	-3.18	1.36	1.40
18	A	841	CLA	C3B-C2B	-3.18	1.36	1.40
18	A	825	CLA	CHC-C1C	3.18	1.43	1.35
18	B	819	CLA	CHC-C1C	3.18	1.43	1.35
18	B	834	CLA	CHC-C1C	3.18	1.43	1.35
18	1	605	CLA	CHC-C1C	3.17	1.43	1.35
18	A	838	CLA	C3B-C2B	-3.17	1.36	1.40
18	1	607	CLA	CHC-C1C	3.17	1.43	1.35
18	3	608	CLA	CHC-C1C	3.17	1.43	1.35
18	4	610	CLA	CHC-C1C	3.17	1.43	1.35
18	A	839	CLA	CHC-C1C	3.17	1.43	1.35
18	A	843	CLA	CHC-C1C	3.17	1.43	1.35
18	2	602	CLA	C3B-C2B	-3.17	1.36	1.40
18	4	614	CLA	CHC-C1C	3.17	1.43	1.35
18	A	833	CLA	C3B-C2B	-3.17	1.36	1.40
18	1	605	CLA	C3B-C2B	-3.17	1.36	1.40
18	4	601	CLA	CHC-C1C	3.17	1.43	1.35
18	L	302	CLA	CHC-C1C	3.17	1.43	1.35
18	A	837	CLA	CHC-C1C	3.16	1.43	1.35
18	B	837	CLA	CHC-C1C	3.16	1.43	1.35
18	3	607	CLA	CHC-C1C	3.16	1.43	1.35
18	3	611	CLA	CHC-C1C	3.16	1.43	1.35
18	4	612	CLA	C3B-C2B	-3.16	1.36	1.40
18	3	603	CLA	C3B-C2B	-3.16	1.36	1.40
18	B	826	CLA	CHC-C1C	3.16	1.43	1.35
18	A	816	CLA	C3B-C2B	-3.16	1.36	1.40
18	A	804	CLA	CHC-C1C	3.15	1.43	1.35
18	B	818	CLA	C3B-C2B	-3.15	1.36	1.40
18	B	827	CLA	C3B-C2B	-3.15	1.36	1.40
18	A	807	CLA	C3B-C2B	-3.15	1.36	1.40
18	2	609	CLA	C3B-C2B	-3.15	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	842	CLA	CHC-C1C	3.15	1.43	1.35
18	A	836	CLA	CHC-C1C	3.15	1.43	1.35
18	1	608	CLA	C3B-C2B	-3.15	1.36	1.40
18	3	603	CLA	CHC-C1C	3.14	1.43	1.35
18	2	611	CLA	C3B-C2B	-3.14	1.36	1.40
18	B	816	CLA	CHC-C1C	3.14	1.43	1.35
18	4	602	CLA	C3B-C2B	-3.14	1.36	1.40
18	4	611	CLA	C3B-C2B	-3.14	1.36	1.40
18	4	608	CLA	C3B-C2B	-3.14	1.36	1.40
18	B	825	CLA	C3B-C2B	-3.14	1.36	1.40
18	4	612	CLA	CHC-C1C	3.14	1.43	1.35
18	A	818	CLA	C3B-C2B	-3.13	1.36	1.40
18	4	610	CLA	C3B-C2B	-3.13	1.36	1.40
18	A	842	CLA	C3B-C2B	-3.13	1.36	1.40
18	1	610	CLA	C3B-C2B	-3.13	1.36	1.40
18	L	303	CLA	C3B-C2B	-3.13	1.36	1.40
18	B	840	CLA	C3B-C2B	-3.13	1.36	1.40
18	A	828	CLA	C3B-C2B	-3.13	1.36	1.40
18	B	803	CLA	C3B-C2B	-3.13	1.36	1.40
18	2	604	CLA	C3B-C2B	-3.13	1.36	1.40
18	A	817	CLA	C3B-C2B	-3.12	1.36	1.40
18	3	602	CLA	C3B-C2B	-3.12	1.36	1.40
18	A	839	CLA	C3B-C2B	-3.12	1.36	1.40
18	B	807	CLA	C3B-C2B	-3.12	1.36	1.40
18	G	204	CLA	C3B-C2B	-3.12	1.36	1.40
18	A	826	CLA	C3B-C2B	-3.12	1.36	1.40
18	A	804	CLA	C3B-C2B	-3.12	1.36	1.40
18	3	609	CLA	C3B-C2B	-3.11	1.36	1.40
18	B	820	CLA	C3B-C2B	-3.11	1.36	1.40
18	4	604	CLA	C3B-C2B	-3.11	1.36	1.40
18	L	302	CLA	C3B-C2B	-3.11	1.36	1.40
18	B	836	CLA	C3B-C2B	-3.11	1.36	1.40
18	A	836	CLA	C3B-C2B	-3.11	1.36	1.40
18	F	304	CLA	C3B-C2B	-3.11	1.36	1.40
18	A	832	CLA	C3B-C2B	-3.11	1.36	1.40
18	G	202	CLA	C3B-C2B	-3.10	1.36	1.40
18	B	807	CLA	CHC-C1C	3.10	1.42	1.35
18	B	802	CLA	C3B-C2B	-3.10	1.36	1.40
18	4	614	CLA	C3B-C2B	-3.10	1.36	1.40
18	A	806	CLA	C3B-C2B	-3.10	1.36	1.40
18	4	609	CLA	C3B-C2B	-3.10	1.36	1.40
18	A	823	CLA	C3B-C2B	-3.10	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	839	CLA	CHC-C1C	3.10	1.42	1.35
18	B	804	CLA	C3B-C2B	-3.09	1.36	1.40
18	3	613	CLA	C3B-C2B	-3.09	1.36	1.40
18	A	808	CLA	C3B-C2B	-3.09	1.36	1.40
18	J	102	CLA	C3B-C2B	-3.09	1.36	1.40
18	A	801	CLA	C3B-C2B	-3.08	1.36	1.40
18	3	611	CLA	C3B-C2B	-3.08	1.36	1.40
18	B	817	CLA	C3B-C2B	-3.08	1.36	1.40
18	3	607	CLA	C3B-C2B	-3.08	1.36	1.40
18	A	830	CLA	C3B-C2B	-3.08	1.36	1.40
18	B	806	CLA	C3B-C2B	-3.08	1.36	1.40
18	B	830	CLA	C3B-C2B	-3.08	1.36	1.40
18	1	613	CLA	C3B-C2B	-3.07	1.36	1.40
18	B	809	CLA	C3B-C2B	-3.07	1.36	1.40
18	2	613	CLA	C3B-C2B	-3.07	1.36	1.40
18	B	839	CLA	C3B-C2B	-3.07	1.36	1.40
18	A	811	CLA	C3B-C2B	-3.07	1.36	1.40
18	B	819	CLA	C3B-C2B	-3.06	1.36	1.40
18	B	801	CLA	C3B-C2B	-3.06	1.36	1.40
18	A	833	CLA	CHC-C1C	3.06	1.42	1.35
18	A	812	CLA	C3B-C2B	-3.05	1.36	1.40
18	3	606	CLA	C3B-C2B	-3.05	1.36	1.40
18	4	613	CLA	C3B-C2B	-3.05	1.36	1.40
18	2	610	CLA	C3B-C2B	-3.05	1.36	1.40
18	4	603	CLA	CHC-C1C	3.05	1.42	1.35
17	2	606	CHL	MG-NA	3.04	2.13	2.06
18	F	303	CLA	C3B-C2B	-3.04	1.36	1.40
18	1	614	CLA	C3B-C2B	-3.04	1.36	1.40
18	A	824	CLA	C3B-C2B	-3.04	1.36	1.40
18	A	854	CLA	C3B-C2B	-3.04	1.36	1.40
18	B	816	CLA	C3B-C2B	-3.03	1.36	1.40
18	B	815	CLA	C3B-C2B	-3.03	1.36	1.40
18	A	802	CLA	C3B-C2B	-3.03	1.36	1.40
17	4	606	CHL	MG-NA	3.03	2.13	2.06
18	4	601	CLA	C3B-C2B	-3.02	1.36	1.40
18	B	822	CLA	C3B-C2B	-3.02	1.36	1.40
17	4	605	CHL	MG-NA	3.02	2.13	2.06
18	B	833	CLA	C3B-C2B	-3.02	1.36	1.40
18	A	822	CLA	C3B-C2B	-3.02	1.36	1.40
18	A	825	CLA	C3B-C2B	-3.02	1.36	1.40
18	1	604	CLA	C3B-C2B	-3.01	1.36	1.40
18	A	805	CLA	C3B-C2B	-3.01	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	607	CHL	MG-NA	3.01	2.13	2.06
18	K	202	CLA	C3B-C2B	-3.01	1.36	1.40
18	3	612	CLA	C3B-C2B	-3.01	1.36	1.40
17	2	605	CHL	MG-NA	3.01	2.13	2.06
18	3	610	CLA	C3B-C2B	-3.01	1.36	1.40
18	3	605	CLA	C3B-C2B	-3.00	1.36	1.40
18	A	810	CLA	C3B-C2B	-3.00	1.36	1.40
18	A	835	CLA	C3B-C2B	-3.00	1.36	1.40
18	B	837	CLA	C3B-C2B	-3.00	1.36	1.40
18	A	827	CLA	C3B-C2B	-2.99	1.36	1.40
18	K	201	CLA	C3B-C2B	-2.99	1.36	1.40
17	2	607	CHL	O2A-CGA	2.98	1.42	1.33
18	A	810	CLA	C1D-ND	-2.98	1.34	1.37
18	B	811	CLA	C3B-C2B	-2.98	1.36	1.40
17	4	605	CHL	O2A-CGA	2.97	1.42	1.33
17	1	606	CHL	MG-NA	2.97	2.13	2.06
17	2	607	CHL	MG-NA	2.96	2.13	2.06
17	2	614	CHL	MG-NA	2.96	2.13	2.06
18	A	802	CLA	C1D-ND	-2.96	1.34	1.37
18	G	203	CLA	C3B-C2B	-2.96	1.36	1.40
18	A	820	CLA	C3B-C2B	-2.96	1.36	1.40
18	B	812	CLA	C3B-C2B	-2.95	1.36	1.40
17	2	601	CHL	MG-NA	2.94	2.13	2.06
17	4	607	CHL	O2A-CGA	2.94	1.41	1.33
18	F	301	CLA	C3B-C2B	-2.94	1.36	1.40
18	B	813	CLA	C3B-C2B	-2.94	1.36	1.40
18	B	802	CLA	C1D-ND	-2.93	1.34	1.37
18	A	813	CLA	C3B-C2B	-2.91	1.36	1.40
18	K	203	CLA	C3B-C2B	-2.90	1.36	1.40
18	A	837	CLA	C3B-C2B	-2.90	1.36	1.40
18	B	826	CLA	C3B-C2B	-2.89	1.36	1.40
18	B	823	CLA	C3B-C2B	-2.89	1.36	1.40
17	1	601	CHL	O2A-CGA	2.89	1.41	1.33
18	A	843	CLA	C3B-C2B	-2.88	1.36	1.40
17	4	615	CHL	MG-NA	2.87	2.13	2.06
18	A	826	CLA	C1D-ND	-2.87	1.34	1.37
18	A	806	CLA	C1D-ND	-2.86	1.34	1.37
17	3	616	CHL	O2A-CGA	2.86	1.42	1.33
18	B	825	CLA	C1D-ND	-2.86	1.34	1.37
18	A	812	CLA	C1D-ND	-2.84	1.34	1.37
18	B	820	CLA	C1D-ND	-2.83	1.34	1.37
18	B	836	CLA	C1D-ND	-2.83	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	601	CHL	O2A-CGA	2.83	1.42	1.33
18	B	824	CLA	C1D-ND	-2.83	1.34	1.37
17	3	616	CHL	MG-NA	2.83	2.13	2.06
17	1	601	CHL	MG-NA	2.83	2.13	2.06
18	B	839	CLA	C1D-ND	-2.82	1.34	1.37
18	H	201	CLA	C3B-C2B	-2.82	1.36	1.40
18	B	833	CLA	C1D-ND	-2.82	1.34	1.37
18	1	614	CLA	C1D-ND	-2.81	1.34	1.37
18	F	304	CLA	C1D-ND	-2.81	1.34	1.37
19	1	619	LUT	C8-C9	-2.81	1.39	1.45
18	A	805	CLA	C1D-ND	-2.81	1.34	1.37
19	4	616	LUT	C8-C9	-2.80	1.39	1.45
18	A	834	CLA	C1D-ND	-2.80	1.34	1.37
18	B	804	CLA	C1D-ND	-2.80	1.34	1.37
18	A	813	CLA	C1D-ND	-2.80	1.34	1.37
18	A	840	CLA	C1D-ND	-2.80	1.34	1.37
18	A	827	CLA	C1D-ND	-2.80	1.34	1.37
18	A	841	CLA	C1D-ND	-2.79	1.34	1.37
18	4	608	CLA	C1D-ND	-2.79	1.34	1.37
18	3	608	CLA	C1D-ND	-2.78	1.34	1.37
18	3	602	CLA	C1D-ND	-2.78	1.34	1.37
18	B	813	CLA	C1D-ND	-2.78	1.34	1.37
18	A	840	CLA	C3B-C2B	-2.78	1.36	1.40
18	2	608	CLA	C1D-ND	-2.78	1.34	1.37
18	B	822	CLA	C1D-ND	-2.78	1.34	1.37
18	A	843	CLA	C1D-ND	-2.78	1.34	1.37
19	2	615	LUT	C8-C9	-2.78	1.40	1.45
18	2	609	CLA	C1D-ND	-2.77	1.34	1.37
18	A	807	CLA	C1D-ND	-2.77	1.34	1.37
18	B	809	CLA	C1D-ND	-2.77	1.34	1.37
18	B	829	CLA	C1D-ND	-2.77	1.34	1.37
18	A	814	CLA	C1D-ND	-2.77	1.34	1.37
18	G	203	CLA	C1D-ND	-2.77	1.34	1.37
18	B	821	CLA	C1D-ND	-2.76	1.34	1.37
18	B	818	CLA	C1D-ND	-2.76	1.34	1.37
18	A	830	CLA	C1D-ND	-2.76	1.34	1.37
18	B	816	CLA	C1D-ND	-2.76	1.34	1.37
18	B	828	CLA	C1D-ND	-2.76	1.34	1.37
18	A	822	CLA	C1D-ND	-2.75	1.34	1.37
18	4	601	CLA	C1D-ND	-2.75	1.34	1.37
18	B	832	CLA	C1D-ND	-2.75	1.34	1.37
18	A	831	CLA	C1D-ND	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	835	CLA	C1D-ND	-2.74	1.34	1.37
18	B	815	CLA	C1D-ND	-2.74	1.34	1.37
18	A	803	CLA	C1D-ND	-2.74	1.34	1.37
18	B	811	CLA	C1D-ND	-2.74	1.34	1.37
18	A	818	CLA	C1D-ND	-2.74	1.34	1.37
18	A	837	CLA	C1D-ND	-2.74	1.34	1.37
18	B	812	CLA	C1D-ND	-2.74	1.34	1.37
18	A	821	CLA	C1D-ND	-2.74	1.34	1.37
18	F	301	CLA	C1D-ND	-2.73	1.34	1.37
18	A	804	CLA	C1D-ND	-2.73	1.34	1.37
18	A	829	CLA	C1D-ND	-2.73	1.34	1.37
18	B	807	CLA	C1D-ND	-2.73	1.34	1.37
18	A	828	CLA	C1D-ND	-2.72	1.34	1.37
18	B	819	CLA	C1D-ND	-2.72	1.34	1.37
19	3	614	LUT	C8-C9	-2.72	1.40	1.45
19	1	615	LUT	C8-C9	-2.72	1.40	1.45
18	B	831	CLA	C1D-ND	-2.72	1.34	1.37
18	B	806	CLA	C1D-ND	-2.72	1.34	1.37
18	B	838	CLA	C1D-ND	-2.71	1.34	1.37
18	B	840	CLA	C1D-ND	-2.71	1.34	1.37
18	1	610	CLA	C1D-ND	-2.71	1.34	1.37
18	1	604	CLA	C1D-ND	-2.71	1.34	1.37
18	4	614	CLA	C1D-ND	-2.71	1.34	1.37
18	2	613	CLA	C1D-ND	-2.70	1.34	1.37
18	1	608	CLA	C1D-ND	-2.70	1.34	1.37
18	3	607	CLA	C1D-ND	-2.70	1.34	1.37
18	A	832	CLA	C1D-ND	-2.70	1.34	1.37
18	4	613	CLA	C1D-ND	-2.70	1.34	1.37
18	1	607	CLA	C1D-ND	-2.70	1.34	1.37
18	4	609	CLA	C1D-ND	-2.70	1.34	1.37
18	A	815	CLA	C1D-ND	-2.70	1.34	1.37
18	A	808	CLA	C1D-ND	-2.70	1.34	1.37
18	G	202	CLA	C1D-ND	-2.70	1.34	1.37
18	B	835	CLA	C1D-ND	-2.69	1.34	1.37
18	1	602	CLA	C1D-ND	-2.69	1.34	1.37
18	1	611	CLA	C1D-ND	-2.69	1.34	1.37
18	L	303	CLA	C1D-ND	-2.69	1.34	1.37
18	B	823	CLA	C1D-ND	-2.69	1.34	1.37
18	B	803	CLA	C1D-ND	-2.69	1.34	1.37
18	4	602	CLA	C1D-ND	-2.68	1.34	1.37
18	3	606	CLA	C1D-ND	-2.68	1.34	1.37
18	A	833	CLA	C1D-ND	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	838	CLA	C1D-ND	-2.68	1.34	1.37
18	A	809	CLA	C1D-ND	-2.68	1.34	1.37
18	B	808	CLA	C1D-ND	-2.68	1.34	1.37
18	B	827	CLA	C1D-ND	-2.68	1.34	1.37
18	A	839	CLA	C1D-ND	-2.67	1.34	1.37
18	4	612	CLA	C1D-ND	-2.67	1.34	1.37
18	1	612	CLA	C1D-ND	-2.67	1.34	1.37
18	B	837	CLA	C1D-ND	-2.67	1.34	1.37
18	L	304	CLA	C1D-ND	-2.67	1.34	1.37
18	1	603	CLA	C1D-ND	-2.67	1.34	1.37
18	B	810	CLA	C1D-ND	-2.67	1.34	1.37
18	4	604	CLA	C1D-ND	-2.67	1.34	1.37
18	B	814	CLA	C1D-ND	-2.67	1.34	1.37
18	A	817	CLA	C1D-ND	-2.66	1.34	1.37
18	B	830	CLA	C1D-ND	-2.66	1.34	1.37
18	1	605	CLA	C1D-ND	-2.66	1.34	1.37
18	3	617	CLA	C1D-ND	-2.66	1.34	1.37
18	A	824	CLA	C1D-ND	-2.66	1.34	1.37
18	A	811	CLA	C1D-ND	-2.65	1.34	1.37
18	B	826	CLA	C1D-ND	-2.65	1.34	1.37
18	B	824	CLA	C3B-C2B	-2.65	1.36	1.40
18	A	842	CLA	C1D-ND	-2.65	1.34	1.37
18	4	611	CLA	C1D-ND	-2.65	1.34	1.37
18	2	604	CLA	C1D-ND	-2.65	1.34	1.37
18	2	602	CLA	C1D-ND	-2.64	1.34	1.37
18	2	610	CLA	C1D-ND	-2.63	1.34	1.37
18	1	609	CLA	C1D-ND	-2.63	1.34	1.37
18	A	801	CLA	C1D-ND	-2.62	1.34	1.37
18	A	825	CLA	C1D-ND	-2.62	1.34	1.37
18	1	613	CLA	C1D-ND	-2.62	1.34	1.37
18	B	801	CLA	C1D-ND	-2.61	1.34	1.37
18	B	817	CLA	C1D-ND	-2.61	1.34	1.37
18	B	834	CLA	C1D-ND	-2.60	1.34	1.37
18	2	603	CLA	C1D-ND	-2.60	1.34	1.37
18	B	805	CLA	C1D-ND	-2.60	1.34	1.37
18	4	610	CLA	C1D-ND	-2.60	1.34	1.37
18	L	302	CLA	C1D-ND	-2.60	1.34	1.37
18	3	609	CLA	C1D-ND	-2.59	1.34	1.37
18	3	605	CLA	C1D-ND	-2.59	1.34	1.37
18	A	820	CLA	C1D-ND	-2.59	1.34	1.37
18	A	836	CLA	C1D-ND	-2.58	1.34	1.37
18	A	816	CLA	C1D-ND	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	C1D-ND	-2.58	1.34	1.37
18	3	613	CLA	C1D-ND	-2.58	1.34	1.37
18	4	603	CLA	C1D-ND	-2.57	1.34	1.37
18	A	823	CLA	C1D-ND	-2.57	1.34	1.37
18	3	604	CLA	C1D-ND	-2.56	1.34	1.37
18	A	819	CLA	C1D-ND	-2.56	1.34	1.37
18	K	203	CLA	C1D-ND	-2.56	1.34	1.37
18	F	303	CLA	C1D-ND	-2.55	1.34	1.37
18	H	201	CLA	C1D-ND	-2.55	1.34	1.37
17	4	605	CHL	C2-C3	2.54	1.39	1.33
18	2	611	CLA	C1D-ND	-2.53	1.34	1.37
18	3	611	CLA	C1D-ND	-2.52	1.34	1.37
18	J	102	CLA	C1D-ND	-2.51	1.34	1.37
18	3	603	CLA	C1D-ND	-2.51	1.34	1.37
18	A	854	CLA	C1D-ND	-2.50	1.34	1.37
18	A	829	CLA	C1B-CHB	-2.50	1.34	1.41
18	G	204	CLA	C1D-ND	-2.50	1.34	1.37
18	3	612	CLA	C1D-ND	-2.49	1.34	1.37
17	1	601	CHL	C2-C3	2.49	1.39	1.33
18	K	202	CLA	C1D-ND	-2.48	1.34	1.37
18	2	611	CLA	C1B-CHB	-2.47	1.34	1.41
18	3	610	CLA	C1D-ND	-2.47	1.34	1.37
18	K	201	CLA	C1D-ND	-2.47	1.34	1.37
18	A	808	CLA	C1B-CHB	-2.47	1.34	1.41
18	4	603	CLA	C1B-CHB	-2.47	1.34	1.41
17	4	607	CHL	CHC-C1C	2.47	1.41	1.35
18	B	814	CLA	C1B-CHB	-2.47	1.34	1.41
18	A	820	CLA	C1B-CHB	-2.46	1.34	1.41
18	1	611	CLA	C1B-CHB	-2.46	1.34	1.41
17	2	601	CHL	CHC-C1C	2.46	1.41	1.35
18	B	830	CLA	C1B-CHB	-2.46	1.34	1.41
18	B	805	CLA	C1B-CHB	-2.45	1.34	1.41
18	A	814	CLA	C1B-CHB	-2.45	1.34	1.41
18	A	816	CLA	C1B-CHB	-2.45	1.34	1.41
18	3	603	CLA	C1B-CHB	-2.45	1.34	1.41
17	1	606	CHL	CHC-C1C	2.45	1.41	1.35
18	B	835	CLA	C1B-CHB	-2.45	1.34	1.41
18	3	610	CLA	C1B-CHB	-2.45	1.34	1.41
17	4	606	CHL	CHC-C1C	2.44	1.41	1.35
18	B	817	CLA	C1B-CHB	-2.44	1.34	1.41
18	B	831	CLA	C1B-CHB	-2.44	1.34	1.41
18	1	603	CLA	C1B-CHB	-2.44	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	815	CLA	C1B-CHB	-2.44	1.34	1.41
18	B	827	CLA	C1B-CHB	-2.43	1.34	1.41
18	L	304	CLA	C1B-CHB	-2.43	1.34	1.41
18	3	604	CLA	C1B-CHB	-2.43	1.34	1.41
18	B	806	CLA	C1B-CHB	-2.43	1.34	1.41
18	A	824	CLA	C1B-CHB	-2.43	1.34	1.41
18	1	612	CLA	C1B-CHB	-2.43	1.34	1.41
18	4	610	CLA	C1B-CHB	-2.43	1.34	1.41
18	3	617	CLA	C1B-CHB	-2.43	1.34	1.41
18	A	831	CLA	C1B-CHB	-2.43	1.34	1.41
18	A	838	CLA	C1B-CHB	-2.43	1.34	1.41
17	1	601	CHL	CHC-C1C	2.42	1.41	1.35
18	A	823	CLA	C1B-CHB	-2.42	1.34	1.41
18	G	202	CLA	C1B-CHB	-2.42	1.34	1.41
18	A	834	CLA	C1B-CHB	-2.42	1.34	1.41
18	A	819	CLA	C1B-CHB	-2.42	1.34	1.41
18	2	603	CLA	C1B-CHB	-2.42	1.34	1.41
18	4	614	CLA	C1B-CHB	-2.42	1.34	1.41
18	G	204	CLA	C1B-CHB	-2.42	1.34	1.41
18	3	606	CLA	C1B-CHB	-2.42	1.34	1.41
18	3	612	CLA	C1B-CHB	-2.42	1.34	1.41
18	2	608	CLA	C1B-CHB	-2.42	1.34	1.41
18	4	604	CLA	C1B-CHB	-2.41	1.34	1.41
18	A	821	CLA	C1B-CHB	-2.41	1.34	1.41
18	3	605	CLA	C1B-CHB	-2.41	1.34	1.41
18	A	817	CLA	C1B-CHB	-2.41	1.34	1.41
18	A	825	CLA	C1B-CHB	-2.41	1.34	1.41
18	F	304	CLA	C1B-CHB	-2.41	1.34	1.41
18	4	611	CLA	C1B-CHB	-2.41	1.34	1.41
18	B	840	CLA	C1B-CHB	-2.41	1.34	1.41
18	2	610	CLA	C1B-CHB	-2.41	1.34	1.41
18	A	811	CLA	C1B-CHB	-2.41	1.34	1.41
18	B	823	CLA	C1B-CHB	-2.41	1.34	1.41
18	F	303	CLA	C1B-CHB	-2.41	1.34	1.41
18	2	604	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	833	CLA	C1B-CHB	-2.40	1.34	1.41
18	J	102	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	812	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	806	CLA	C1B-CHB	-2.40	1.34	1.41
18	L	302	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	805	CLA	C1B-CHB	-2.40	1.34	1.41
18	B	804	CLA	C1B-CHB	-2.40	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	609	CLA	C1B-CHB	-2.40	1.34	1.41
17	2	605	CHL	CHC-C1C	2.40	1.41	1.35
18	B	829	CLA	C1B-CHB	-2.40	1.34	1.41
18	1	613	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	826	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	828	CLA	C1B-CHB	-2.40	1.34	1.41
18	A	841	CLA	C1B-CHB	-2.40	1.34	1.41
18	B	836	CLA	C1B-CHB	-2.39	1.34	1.41
18	B	811	CLA	C1B-CHB	-2.39	1.34	1.41
18	2	613	CLA	C1B-CHB	-2.39	1.34	1.41
18	A	810	CLA	C1B-CHB	-2.39	1.34	1.41
18	B	828	CLA	C1B-CHB	-2.39	1.34	1.41
17	4	615	CHL	CHC-C1C	2.39	1.41	1.35
18	B	834	CLA	C1B-CHB	-2.39	1.34	1.41
18	A	809	CLA	C1B-CHB	-2.39	1.34	1.41
18	A	807	CLA	C1B-CHB	-2.39	1.34	1.41
17	2	614	CHL	CHC-C1C	2.39	1.41	1.35
18	A	822	CLA	C1B-CHB	-2.39	1.34	1.41
19	4	616	LUT	C32-C33	-2.39	1.40	1.45
18	4	602	CLA	C1B-CHB	-2.39	1.34	1.41
18	A	842	CLA	C1B-CHB	-2.39	1.34	1.41
18	A	839	CLA	C1B-CHB	-2.39	1.34	1.41
18	B	838	CLA	C1B-CHB	-2.39	1.34	1.41
18	4	601	CLA	C1B-CHB	-2.39	1.34	1.41
18	B	839	CLA	C1B-CHB	-2.39	1.34	1.41
18	2	602	CLA	C1B-CHB	-2.38	1.34	1.41
18	1	605	CLA	C1B-CHB	-2.38	1.34	1.41
18	3	611	CLA	C1B-CHB	-2.38	1.34	1.41
18	B	833	CLA	C1B-CHB	-2.38	1.34	1.41
18	4	613	CLA	C1B-CHB	-2.38	1.34	1.41
18	3	609	CLA	C1B-CHB	-2.38	1.34	1.41
18	A	827	CLA	C1B-CHB	-2.38	1.34	1.41
18	A	804	CLA	C1B-CHB	-2.38	1.34	1.41
18	K	203	CLA	C1B-CHB	-2.38	1.34	1.41
18	B	810	CLA	C1B-CHB	-2.38	1.34	1.41
18	A	854	CLA	C1B-CHB	-2.38	1.34	1.41
18	H	201	CLA	C1B-CHB	-2.38	1.34	1.41
17	2	606	CHL	CHC-C1C	2.38	1.41	1.35
18	1	602	CLA	C1B-CHB	-2.38	1.34	1.41
18	1	607	CLA	C1B-CHB	-2.37	1.34	1.41
18	1	604	CLA	C1B-CHB	-2.37	1.34	1.41
18	B	818	CLA	C1B-CHB	-2.37	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	816	CLA	C1B-CHB	-2.37	1.34	1.41
19	1	619	LUT	C32-C33	-2.37	1.40	1.45
18	B	803	CLA	C1B-CHB	-2.37	1.34	1.41
18	B	821	CLA	C1B-CHB	-2.37	1.34	1.41
18	1	608	CLA	C1B-CHB	-2.37	1.34	1.41
18	B	820	CLA	C1B-CHB	-2.37	1.34	1.41
18	B	826	CLA	C1B-CHB	-2.37	1.34	1.41
18	3	613	CLA	C1B-CHB	-2.37	1.34	1.41
18	B	808	CLA	C1B-CHB	-2.36	1.34	1.41
18	A	813	CLA	C1B-CHB	-2.36	1.34	1.41
18	B	801	CLA	C1B-CHB	-2.36	1.34	1.41
17	4	606	CHL	CBA-CGA	2.36	1.56	1.50
18	B	815	CLA	C1B-CHB	-2.36	1.34	1.41
18	K	201	CLA	C1B-CHB	-2.36	1.34	1.41
18	4	608	CLA	C1B-CHB	-2.35	1.34	1.41
18	B	822	CLA	C1B-CHB	-2.35	1.34	1.41
18	4	609	CLA	C1B-CHB	-2.35	1.34	1.41
18	4	612	CLA	C1B-CHB	-2.35	1.34	1.41
18	A	837	CLA	C1B-CHB	-2.35	1.34	1.41
18	3	608	CLA	C1B-CHB	-2.34	1.34	1.41
18	A	840	CLA	C1B-CHB	-2.34	1.34	1.41
18	B	807	CLA	C1B-CHB	-2.34	1.34	1.41
17	4	607	CHL	C2-C3	2.34	1.39	1.32
18	1	614	CLA	C1B-CHB	-2.34	1.34	1.41
18	A	832	CLA	C1B-CHB	-2.34	1.34	1.41
18	B	812	CLA	C1B-CHB	-2.34	1.34	1.41
19	4	616	LUT	C12-C13	-2.34	1.40	1.45
18	B	824	CLA	C1B-CHB	-2.34	1.34	1.41
18	K	202	CLA	C1B-CHB	-2.34	1.34	1.41
18	3	607	CLA	C1B-CHB	-2.34	1.34	1.41
18	A	803	CLA	C1B-CHB	-2.34	1.34	1.41
19	1	619	LUT	C12-C13	-2.34	1.40	1.45
18	B	809	CLA	C1B-CHB	-2.33	1.34	1.41
18	1	610	CLA	C1B-CHB	-2.33	1.34	1.41
17	2	607	CHL	CHC-C1C	2.33	1.40	1.35
17	4	605	CHL	CHC-C1C	2.33	1.40	1.35
19	1	615	LUT	C12-C13	-2.33	1.40	1.45
19	2	615	LUT	C32-C33	-2.33	1.40	1.45
18	2	612	CLA	C1B-CHB	-2.33	1.34	1.41
18	B	813	CLA	C1B-CHB	-2.33	1.34	1.41
18	A	830	CLA	C1B-CHB	-2.33	1.34	1.41
18	F	301	CLA	C1B-CHB	-2.33	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	203	CLA	C1B-CHB	-2.33	1.34	1.41
18	L	303	CLA	C1B-CHB	-2.33	1.34	1.41
18	A	835	CLA	C1B-CHB	-2.32	1.34	1.41
18	A	818	CLA	C1B-CHB	-2.32	1.34	1.41
18	3	602	CLA	C1B-CHB	-2.32	1.34	1.41
18	B	832	CLA	C1B-CHB	-2.32	1.34	1.41
18	2	609	CLA	C1B-CHB	-2.32	1.34	1.41
19	2	615	LUT	C28-C29	-2.32	1.41	1.45
19	1	615	LUT	C32-C33	-2.32	1.41	1.45
18	B	825	CLA	C1B-CHB	-2.31	1.34	1.41
19	1	615	LUT	C28-C29	-2.31	1.41	1.45
18	B	837	CLA	C1B-CHB	-2.31	1.34	1.41
18	B	819	CLA	C1B-CHB	-2.31	1.34	1.41
19	4	616	LUT	C28-C29	-2.31	1.41	1.45
18	A	802	CLA	C1B-CHB	-2.30	1.34	1.41
17	3	616	CHL	CHC-C1C	2.30	1.40	1.35
18	A	836	CLA	C1B-CHB	-2.30	1.34	1.41
19	2	615	LUT	C12-C13	-2.30	1.41	1.45
17	2	607	CHL	C2-C3	2.29	1.38	1.32
18	B	834	CLA	MG-NC	2.29	2.11	2.06
19	1	619	LUT	C28-C29	-2.28	1.41	1.45
18	A	843	CLA	C1B-CHB	-2.27	1.34	1.41
18	A	801	CLA	C1B-CHB	-2.27	1.34	1.41
17	4	615	CHL	MG-NC	2.27	2.11	2.06
17	2	614	CHL	MG-NC	2.26	2.11	2.06
18	B	802	CLA	C1B-CHB	-2.26	1.34	1.41
18	3	610	CLA	MG-NC	2.24	2.11	2.06
18	H	201	CLA	CAA-C2A	2.24	1.58	1.54
18	3	612	CLA	MG-NC	2.24	2.11	2.06
18	A	825	CLA	MG-NC	2.24	2.11	2.06
17	2	606	CHL	MG-NC	2.23	2.11	2.06
18	B	812	CLA	MG-NC	2.23	2.11	2.06
18	K	202	CLA	MG-NC	2.23	2.11	2.06
18	3	603	CLA	MG-NC	2.23	2.11	2.06
17	1	601	CHL	MG-NC	2.23	2.11	2.06
18	A	823	CLA	MG-NC	2.22	2.11	2.06
19	3	614	LUT	C12-C13	-2.22	1.41	1.45
17	1	606	CHL	MG-NC	2.22	2.11	2.06
18	B	831	CLA	MG-NC	2.21	2.11	2.06
18	B	838	CLA	MG-NC	2.21	2.11	2.06
18	A	843	CLA	MG-NC	2.21	2.11	2.06
18	K	201	CLA	MG-NC	2.20	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	614	CLA	MG-NC	2.20	2.11	2.06
18	4	610	CLA	MG-NC	2.20	2.11	2.06
19	3	614	LUT	C32-C33	-2.20	1.41	1.45
18	3	607	CLA	MG-NC	2.19	2.11	2.06
18	J	102	CLA	MG-NC	2.19	2.11	2.06
18	A	854	CLA	MG-NC	2.19	2.11	2.06
19	3	614	LUT	C28-C29	-2.19	1.41	1.45
18	G	204	CLA	MG-NC	2.19	2.11	2.06
18	3	604	CLA	MG-NC	2.19	2.11	2.06
18	F	303	CLA	MG-NC	2.19	2.11	2.06
18	4	603	CLA	MG-NC	2.19	2.11	2.06
18	A	839	CLA	MG-NC	2.19	2.11	2.06
17	2	605	CHL	MG-NC	2.19	2.11	2.06
18	4	611	CLA	MG-NC	2.18	2.11	2.06
18	2	610	CLA	MG-NC	2.18	2.11	2.06
18	G	202	CLA	MG-NC	2.18	2.11	2.06
18	B	807	CLA	MG-NC	2.17	2.11	2.06
18	B	837	CLA	MG-NC	2.17	2.11	2.06
18	A	816	CLA	MG-NC	2.17	2.11	2.06
18	3	606	CLA	MG-NC	2.17	2.11	2.06
18	2	611	CLA	MG-NC	2.17	2.11	2.06
18	L	302	CLA	MG-NC	2.17	2.11	2.06
18	L	304	CLA	MG-NC	2.17	2.11	2.06
18	A	842	CLA	MG-NC	2.17	2.11	2.06
18	B	808	CLA	MG-NC	2.16	2.11	2.06
18	1	613	CLA	MG-NC	2.16	2.11	2.06
18	4	613	CLA	MG-NC	2.16	2.11	2.06
18	B	818	CLA	MG-NC	2.16	2.11	2.06
17	4	606	CHL	MG-NC	2.16	2.11	2.06
18	3	602	CLA	MG-NC	2.16	2.11	2.06
18	1	602	CLA	MG-NC	2.16	2.11	2.06
18	B	819	CLA	MG-NC	2.16	2.11	2.06
18	4	604	CLA	MG-NC	2.16	2.11	2.06
18	H	201	CLA	MG-NC	2.16	2.11	2.06
17	2	607	CHL	MG-NC	2.15	2.11	2.06
18	2	613	CLA	MG-NC	2.15	2.11	2.06
18	B	815	CLA	MG-NC	2.15	2.11	2.06
17	4	607	CHL	MG-NC	2.15	2.11	2.06
18	1	605	CLA	MG-NC	2.15	2.11	2.06
18	4	602	CLA	MG-NC	2.15	2.11	2.06
18	3	613	CLA	MG-NC	2.15	2.11	2.06
18	F	304	CLA	MG-NC	2.15	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	MG-NC	2.15	2.11	2.06
18	3	611	CLA	MG-NC	2.15	2.11	2.06
18	A	833	CLA	MG-NC	2.15	2.11	2.06
18	1	604	CLA	MG-NC	2.15	2.11	2.06
17	2	601	CHL	MG-NC	2.15	2.11	2.06
18	A	828	CLA	MG-NC	2.14	2.11	2.06
18	B	826	CLA	MG-NC	2.14	2.11	2.06
18	3	605	CLA	MG-NC	2.14	2.11	2.06
18	B	827	CLA	MG-NC	2.14	2.11	2.06
18	1	610	CLA	MG-NC	2.14	2.11	2.06
18	A	817	CLA	MG-NC	2.14	2.11	2.06
18	K	203	CLA	MG-NC	2.14	2.11	2.06
18	B	805	CLA	MG-NC	2.14	2.11	2.06
18	A	820	CLA	MG-NC	2.13	2.11	2.06
18	A	837	CLA	MG-NC	2.13	2.11	2.06
18	1	607	CLA	MG-NC	2.13	2.11	2.06
18	B	835	CLA	MG-NC	2.13	2.11	2.06
18	A	803	CLA	MG-NC	2.13	2.11	2.06
18	A	830	CLA	MG-NC	2.13	2.11	2.06
18	B	823	CLA	MG-NC	2.13	2.11	2.06
18	B	839	CLA	MG-NC	2.13	2.11	2.06
18	A	804	CLA	MG-NC	2.13	2.11	2.06
18	F	301	CLA	MG-NC	2.13	2.11	2.06
18	2	604	CLA	MG-NC	2.13	2.11	2.06
18	A	807	CLA	MG-NC	2.13	2.11	2.06
18	A	821	CLA	MG-NC	2.13	2.11	2.06
18	A	827	CLA	MG-NC	2.13	2.11	2.06
18	1	608	CLA	MG-NC	2.13	2.11	2.06
18	1	611	CLA	MG-NC	2.13	2.11	2.06
17	4	605	CHL	MG-NC	2.13	2.11	2.06
18	A	808	CLA	MG-NC	2.13	2.11	2.06
18	B	825	CLA	MG-NC	2.13	2.11	2.06
18	B	813	CLA	MG-NC	2.13	2.11	2.06
18	B	830	CLA	MG-NC	2.12	2.11	2.06
18	A	801	CLA	MG-NC	2.12	2.11	2.06
18	A	841	CLA	MG-NC	2.12	2.11	2.06
18	A	822	CLA	MG-NC	2.12	2.11	2.06
18	A	838	CLA	MG-NC	2.11	2.11	2.06
18	2	602	CLA	MG-NC	2.11	2.11	2.06
18	A	836	CLA	MG-NC	2.11	2.11	2.06
18	A	813	CLA	MG-NC	2.11	2.11	2.06
17	2	607	CHL	C3B-CAB	-2.11	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	840	CLA	MG-NC	2.11	2.11	2.06
17	4	605	CHL	C3B-CAB	-2.11	1.43	1.47
18	A	824	CLA	MG-NC	2.11	2.11	2.06
18	B	814	CLA	MG-NC	2.11	2.11	2.06
18	3	609	CLA	MG-NC	2.11	2.11	2.06
18	A	811	CLA	MG-NC	2.11	2.11	2.06
18	B	829	CLA	MG-NC	2.11	2.11	2.06
18	G	203	CLA	MG-NC	2.11	2.11	2.06
17	3	616	CHL	MG-NC	2.11	2.11	2.06
18	A	809	CLA	MG-NC	2.11	2.11	2.06
18	1	612	CLA	MG-NC	2.11	2.11	2.06
18	B	809	CLA	MG-NC	2.11	2.11	2.06
18	4	601	CLA	MG-NC	2.11	2.11	2.06
18	A	829	CLA	MG-NC	2.11	2.11	2.06
18	A	805	CLA	MG-NC	2.11	2.11	2.06
18	3	608	CLA	MG-NC	2.10	2.11	2.06
18	A	826	CLA	MG-NC	2.10	2.11	2.06
18	A	814	CLA	MG-NC	2.10	2.11	2.06
18	A	832	CLA	MG-NC	2.10	2.11	2.06
18	B	804	CLA	MG-NC	2.10	2.11	2.06
18	3	617	CLA	MG-NC	2.10	2.11	2.06
18	1	614	CLA	MG-NC	2.10	2.11	2.06
18	4	612	CLA	MG-NC	2.10	2.11	2.06
18	A	835	CLA	MG-NC	2.10	2.11	2.06
18	A	812	CLA	MG-NC	2.10	2.11	2.06
17	4	607	CHL	C3B-CAB	-2.10	1.43	1.47
18	2	603	CLA	MG-NC	2.10	2.11	2.06
18	2	608	CLA	MG-NC	2.10	2.11	2.06
18	A	819	CLA	MG-NC	2.09	2.11	2.06
18	B	801	CLA	MG-NC	2.09	2.11	2.06
18	A	831	CLA	MG-NC	2.09	2.11	2.06
18	A	806	CLA	MG-NC	2.09	2.11	2.06
18	1	609	CLA	MG-NC	2.08	2.11	2.06
18	A	815	CLA	MG-NC	2.08	2.11	2.06
17	4	606	CHL	C3B-CAB	-2.08	1.43	1.47
18	B	817	CLA	MG-NC	2.08	2.11	2.06
17	2	605	CHL	C3B-CAB	-2.08	1.43	1.47
18	B	824	CLA	MG-NC	2.08	2.11	2.06
18	4	608	CLA	MG-NC	2.07	2.11	2.06
18	B	810	CLA	MG-NC	2.07	2.11	2.06
18	A	840	CLA	MG-NC	2.07	2.11	2.06
18	L	303	CLA	MG-NC	2.07	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	834	CLA	MG-NC	2.07	2.11	2.06
18	B	806	CLA	MG-NC	2.07	2.11	2.06
18	A	818	CLA	MG-NC	2.07	2.11	2.06
18	B	833	CLA	MG-NC	2.07	2.11	2.06
18	B	816	CLA	MG-NC	2.07	2.11	2.06
18	B	821	CLA	MG-NC	2.07	2.11	2.06
18	B	811	CLA	MG-NC	2.06	2.11	2.06
17	1	601	CHL	C3B-CAB	-2.06	1.43	1.47
17	1	606	CHL	C3B-CAB	-2.06	1.43	1.47
18	B	802	CLA	MG-NC	2.06	2.11	2.06
18	B	820	CLA	MG-NC	2.06	2.11	2.06
18	B	822	CLA	MG-NC	2.05	2.11	2.06
18	K	201	CLA	CAA-C2A	2.05	1.57	1.53
18	3	612	CLA	CAA-C2A	2.05	1.57	1.53
18	A	802	CLA	C3D-C4D	-2.05	1.39	1.44
17	2	601	CHL	C3B-CAB	-2.05	1.43	1.47
18	B	828	CLA	MG-NC	2.04	2.11	2.06
17	2	606	CHL	C3B-CAB	-2.04	1.43	1.47
18	1	603	CLA	MG-NC	2.04	2.11	2.06
18	B	803	CLA	MG-NC	2.04	2.11	2.06
18	A	810	CLA	MG-NC	2.04	2.11	2.06
18	B	831	CLA	CAA-C2A	2.04	1.57	1.54
18	F	304	CLA	CAA-C2A	2.04	1.57	1.53
18	2	609	CLA	MG-NC	2.03	2.11	2.06
18	A	802	CLA	MG-NC	2.03	2.11	2.06
18	A	823	CLA	CAA-C2A	2.03	1.57	1.53
18	B	822	CLA	CHD-C1D	2.02	1.42	1.38
18	B	836	CLA	MG-NC	2.02	2.11	2.06
18	4	609	CLA	MG-NC	2.02	2.11	2.06
17	2	606	CHL	O1D-CGD	2.01	1.26	1.21
17	3	616	CHL	C3B-CAB	-2.01	1.43	1.47

All (1486) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	802	CLA	C4A-NA-C1A	11.39	111.83	106.71
17	3	616	CHL	C4A-NA-C1A	11.27	111.77	106.71
18	A	837	CLA	C4A-NA-C1A	11.20	111.74	106.71
18	B	805	CLA	C4A-NA-C1A	11.11	111.70	106.71
18	2	612	CLA	C4A-NA-C1A	11.08	111.69	106.71
18	A	813	CLA	C4A-NA-C1A	11.06	111.68	106.71
17	4	615	CHL	C4A-NA-C1A	11.05	111.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	827	CLA	C4A-NA-C1A	11.03	111.67	106.71
17	2	607	CHL	C4A-NA-C1A	10.98	111.64	106.71
18	B	804	CLA	C4A-NA-C1A	10.90	111.61	106.71
18	B	831	CLA	C4A-NA-C1A	10.86	111.59	106.71
18	A	807	CLA	C4A-NA-C1A	10.83	111.58	106.71
18	B	812	CLA	C4A-NA-C1A	10.75	111.54	106.71
18	1	603	CLA	C4A-NA-C1A	10.71	111.52	106.71
18	K	203	CLA	C4A-NA-C1A	10.71	111.52	106.71
18	A	806	CLA	C4A-NA-C1A	10.70	111.52	106.71
17	2	601	CHL	C4A-NA-C1A	10.69	111.51	106.71
17	4	607	CHL	C4A-NA-C1A	10.65	111.49	106.71
18	F	304	CLA	C4A-NA-C1A	10.64	111.49	106.71
18	4	611	CLA	C4A-NA-C1A	10.63	111.49	106.71
17	1	606	CHL	C4A-NA-C1A	10.60	111.47	106.71
18	L	304	CLA	C4A-NA-C1A	10.60	111.47	106.71
18	B	837	CLA	C4A-NA-C1A	10.60	111.47	106.71
18	1	611	CLA	C4A-NA-C1A	10.57	111.46	106.71
18	A	802	CLA	C4A-NA-C1A	10.57	111.46	106.71
18	B	807	CLA	C4A-NA-C1A	10.56	111.45	106.71
18	A	834	CLA	C4A-NA-C1A	10.56	111.45	106.71
18	4	608	CLA	C4A-NA-C1A	10.55	111.45	106.71
18	B	814	CLA	C4A-NA-C1A	10.55	111.45	106.71
18	A	805	CLA	C4A-NA-C1A	10.54	111.45	106.71
18	B	834	CLA	C4A-NA-C1A	10.53	111.44	106.71
18	A	804	CLA	C4A-NA-C1A	10.53	111.44	106.71
18	A	816	CLA	C4A-NA-C1A	10.51	111.43	106.71
18	B	839	CLA	C4A-NA-C1A	10.51	111.43	106.71
18	2	611	CLA	C4A-NA-C1A	10.51	111.43	106.71
18	A	836	CLA	C4A-NA-C1A	10.50	111.42	106.71
18	A	833	CLA	C4A-NA-C1A	10.48	111.42	106.71
18	A	801	CLA	C4A-NA-C1A	10.47	111.42	106.71
18	B	835	CLA	C4A-NA-C1A	10.42	111.39	106.71
18	A	842	CLA	C4A-NA-C1A	10.40	111.38	106.71
17	4	605	CHL	C4A-NA-C1A	10.40	111.38	106.71
18	1	604	CLA	C4A-NA-C1A	10.38	111.37	106.71
18	A	840	CLA	C4A-NA-C1A	10.35	111.36	106.71
18	B	819	CLA	C4A-NA-C1A	10.33	111.35	106.71
18	3	603	CLA	C4A-NA-C1A	10.32	111.34	106.71
18	A	820	CLA	C4A-NA-C1A	10.30	111.33	106.71
18	3	606	CLA	C4A-NA-C1A	10.29	111.33	106.71
18	3	605	CLA	C4A-NA-C1A	10.29	111.33	106.71
17	1	601	CHL	C4A-NA-C1A	10.28	111.33	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	614	CHL	C4A-NA-C1A	10.27	111.33	106.71
18	G	203	CLA	C4A-NA-C1A	10.27	111.32	106.71
18	4	603	CLA	C4A-NA-C1A	10.27	111.32	106.71
18	3	607	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	A	828	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	B	810	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	B	829	CLA	C4A-NA-C1A	10.25	111.31	106.71
18	1	612	CLA	C4A-NA-C1A	10.25	111.31	106.71
18	A	811	CLA	C4A-NA-C1A	10.23	111.31	106.71
18	L	302	CLA	C4A-NA-C1A	10.21	111.30	106.71
18	A	841	CLA	C4A-NA-C1A	10.21	111.30	106.71
18	B	815	CLA	C4A-NA-C1A	10.20	111.29	106.71
18	G	202	CLA	C4A-NA-C1A	10.20	111.29	106.71
18	3	610	CLA	C4A-NA-C1A	10.19	111.29	106.71
18	1	613	CLA	C4A-NA-C1A	10.19	111.28	106.71
18	B	817	CLA	C4A-NA-C1A	10.18	111.28	106.71
18	B	813	CLA	C4A-NA-C1A	10.16	111.27	106.71
18	A	808	CLA	C4A-NA-C1A	10.13	111.26	106.71
18	B	826	CLA	C4A-NA-C1A	10.12	111.26	106.71
18	A	809	CLA	C4A-NA-C1A	10.11	111.25	106.71
18	2	609	CLA	C4A-NA-C1A	10.11	111.25	106.71
18	A	814	CLA	C4A-NA-C1A	10.10	111.25	106.71
18	1	607	CLA	C4A-NA-C1A	10.07	111.23	106.71
18	1	610	CLA	C4A-NA-C1A	10.06	111.23	106.71
18	A	812	CLA	C4A-NA-C1A	10.05	111.22	106.71
18	2	613	CLA	C4A-NA-C1A	10.04	111.22	106.71
18	1	614	CLA	C4A-NA-C1A	10.04	111.22	106.71
18	4	612	CLA	C4A-NA-C1A	10.03	111.21	106.71
18	4	613	CLA	C4A-NA-C1A	10.02	111.21	106.71
18	3	617	CLA	C4A-NA-C1A	10.00	111.20	106.71
18	A	829	CLA	C4A-NA-C1A	10.00	111.20	106.71
18	A	839	CLA	C4A-NA-C1A	9.99	111.20	106.71
18	2	603	CLA	C4A-NA-C1A	9.97	111.19	106.71
18	F	303	CLA	C4A-NA-C1A	9.97	111.19	106.71
18	1	605	CLA	C4A-NA-C1A	9.96	111.19	106.71
18	B	828	CLA	C4A-NA-C1A	9.95	111.18	106.71
18	2	604	CLA	C4A-NA-C1A	9.94	111.18	106.71
18	3	613	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	J	102	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	3	602	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	3	611	CLA	C4A-NA-C1A	9.93	111.17	106.71
18	B	823	CLA	C4A-NA-C1A	9.92	111.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	601	CLA	C4A-NA-C1A	9.91	111.16	106.71
18	A	843	CLA	C4A-NA-C1A	9.91	111.16	106.71
17	2	605	CHL	C4A-NA-C1A	9.90	111.16	106.71
18	B	840	CLA	C4A-NA-C1A	9.90	111.16	106.71
18	3	608	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	B	838	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	B	827	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	A	838	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	A	831	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	A	835	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	K	201	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	A	823	CLA	C4A-NA-C1A	9.86	111.14	106.71
18	4	604	CLA	C4A-NA-C1A	9.83	111.13	106.71
18	B	811	CLA	C4A-NA-C1A	9.82	111.12	106.71
18	G	204	CLA	C4A-NA-C1A	9.82	111.12	106.71
18	1	602	CLA	C4A-NA-C1A	9.81	111.12	106.71
18	A	830	CLA	C4A-NA-C1A	9.77	111.10	106.71
18	B	833	CLA	C4A-NA-C1A	9.76	111.09	106.71
18	A	803	CLA	C4A-NA-C1A	9.76	111.09	106.71
18	1	608	CLA	C4A-NA-C1A	9.76	111.09	106.71
18	4	609	CLA	C4A-NA-C1A	9.74	111.09	106.71
18	B	825	CLA	C4A-NA-C1A	9.74	111.08	106.71
18	B	830	CLA	C4A-NA-C1A	9.73	111.08	106.71
18	A	832	CLA	C4A-NA-C1A	9.73	111.08	106.71
18	L	303	CLA	C4A-NA-C1A	9.71	111.07	106.71
18	4	614	CLA	C4A-NA-C1A	9.71	111.07	106.71
18	3	604	CLA	C4A-NA-C1A	9.70	111.07	106.71
18	A	821	CLA	C4A-NA-C1A	9.70	111.07	106.71
18	B	836	CLA	C4A-NA-C1A	9.64	111.04	106.71
18	A	826	CLA	C4A-NA-C1A	9.62	111.03	106.71
18	1	609	CLA	C4A-NA-C1A	9.60	111.02	106.71
18	A	819	CLA	C4A-NA-C1A	9.60	111.02	106.71
18	B	818	CLA	C4A-NA-C1A	9.59	111.02	106.71
17	4	606	CHL	C4A-NA-C1A	9.58	111.01	106.71
18	A	818	CLA	C4A-NA-C1A	9.58	111.01	106.71
18	4	602	CLA	C4A-NA-C1A	9.54	111.00	106.71
18	B	801	CLA	C4A-NA-C1A	9.52	110.98	106.71
18	B	806	CLA	C4A-NA-C1A	9.52	110.98	106.71
18	B	808	CLA	C4A-NA-C1A	9.51	110.98	106.71
18	B	821	CLA	C4A-NA-C1A	9.50	110.97	106.71
18	A	815	CLA	C4A-NA-C1A	9.49	110.97	106.71
18	2	610	CLA	C4A-NA-C1A	9.48	110.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	817	CLA	C4A-NA-C1A	9.48	110.97	106.71
18	F	301	CLA	C4A-NA-C1A	9.46	110.96	106.71
18	4	610	CLA	C4A-NA-C1A	9.44	110.95	106.71
18	H	201	CLA	C4A-NA-C1A	9.44	110.95	106.71
18	2	602	CLA	C4A-NA-C1A	9.40	110.93	106.71
18	2	608	CLA	C4A-NA-C1A	9.37	110.92	106.71
18	A	825	CLA	C4A-NA-C1A	9.28	110.88	106.71
18	B	803	CLA	C4A-NA-C1A	9.27	110.87	106.71
18	B	820	CLA	C4A-NA-C1A	9.25	110.86	106.71
18	K	202	CLA	C4A-NA-C1A	9.25	110.86	106.71
17	2	606	CHL	C4A-NA-C1A	9.20	110.84	106.71
18	A	822	CLA	C4A-NA-C1A	9.19	110.84	106.71
18	B	832	CLA	C4A-NA-C1A	9.18	110.83	106.71
18	B	809	CLA	C4A-NA-C1A	9.14	110.81	106.71
18	3	609	CLA	C4A-NA-C1A	9.09	110.79	106.71
18	A	824	CLA	C4A-NA-C1A	9.03	110.77	106.71
18	3	612	CLA	C4A-NA-C1A	9.01	110.76	106.71
18	A	810	CLA	C4A-NA-C1A	9.00	110.75	106.71
18	B	824	CLA	C4A-NA-C1A	8.97	110.74	106.71
18	B	816	CLA	C4A-NA-C1A	8.75	110.64	106.71
18	A	854	CLA	C4A-NA-C1A	8.71	110.62	106.71
18	B	822	CLA	C4A-NA-C1A	8.19	110.39	106.71
18	B	810	CLA	CAB-C3B-C4B	5.79	137.37	128.46
19	3	614	LUT	C15-C35-C34	5.38	134.50	123.47
17	1	606	CHL	CAA-C2A-C3A	-5.36	103.58	116.10
18	B	806	CLA	O2D-CGD-CBD	4.75	119.71	111.27
18	A	831	CLA	O2D-CGD-CBD	4.64	119.52	111.27
18	B	807	CLA	O2D-CGD-CBD	4.59	119.43	111.27
18	B	837	CLA	O2D-CGD-CBD	4.59	119.42	111.27
18	A	816	CLA	O2D-CGD-CBD	4.56	119.37	111.27
18	B	812	CLA	O2D-CGD-CBD	4.52	119.30	111.27
18	B	832	CLA	O2D-CGD-CBD	4.48	119.23	111.27
18	B	816	CLA	O2D-CGD-CBD	4.46	119.19	111.27
18	B	819	CLA	O2D-CGD-CBD	4.46	119.19	111.27
19	3	614	LUT	C39-C29-C30	-4.44	116.71	122.92
18	B	809	CLA	O2D-CGD-CBD	4.38	119.05	111.27
18	B	804	CLA	O2D-CGD-CBD	4.38	119.05	111.27
18	B	821	CLA	O2D-CGD-CBD	4.38	119.05	111.27
18	B	810	CLA	CAB-C3B-C2B	-4.37	116.12	124.69
18	B	835	CLA	O2D-CGD-CBD	4.36	119.01	111.27
18	B	827	CLA	O2D-CGD-CBD	4.36	119.01	111.27
18	A	827	CLA	O2D-CGD-CBD	4.34	118.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	805	CLA	O2D-CGD-CBD	4.33	118.96	111.27
18	B	839	CLA	O2D-CGD-CBD	4.31	118.93	111.27
18	1	613	CLA	O2D-CGD-CBD	4.31	118.92	111.27
18	A	804	CLA	O2D-CGD-CBD	4.30	118.91	111.27
18	A	839	CLA	O2D-CGD-CBD	4.30	118.91	111.27
18	A	806	CLA	O2D-CGD-CBD	4.29	118.89	111.27
18	A	854	CLA	O2D-CGD-CBD	4.29	118.89	111.27
18	B	801	CLA	O2D-CGD-CBD	4.29	118.89	111.27
18	A	803	CLA	O2D-CGD-CBD	4.28	118.88	111.27
18	A	837	CLA	O2D-CGD-CBD	4.28	118.87	111.27
17	2	614	CHL	CAA-C2A-C3A	-4.28	103.58	114.26
18	A	820	CLA	O2D-CGD-CBD	4.28	118.86	111.27
18	B	815	CLA	O2D-CGD-CBD	4.27	118.85	111.27
18	4	610	CLA	O2D-CGD-CBD	4.27	118.85	111.27
18	A	818	CLA	O2D-CGD-CBD	4.26	118.84	111.27
17	4	615	CHL	CAB-C3B-C4B	4.25	135.00	128.46
18	B	826	CLA	O2D-CGD-CBD	4.22	118.76	111.27
18	A	813	CLA	O2D-CGD-CBD	4.22	118.76	111.27
18	B	830	CLA	O2D-CGD-CBD	4.22	118.76	111.27
18	B	840	CLA	O2D-CGD-CBD	4.21	118.75	111.27
18	B	823	CLA	O2D-CGD-CBD	4.20	118.74	111.27
18	B	808	CLA	O2D-CGD-CBD	4.20	118.73	111.27
18	A	825	CLA	O2D-CGD-CBD	4.19	118.72	111.27
18	B	814	CLA	O2D-CGD-CBD	4.18	118.70	111.27
18	A	838	CLA	O2D-CGD-CBD	4.18	118.70	111.27
17	4	615	CHL	CAA-C2A-C3A	-4.18	103.81	114.26
18	A	815	CLA	O2D-CGD-CBD	4.18	118.69	111.27
18	1	608	CLA	O2D-CGD-CBD	4.18	118.69	111.27
19	4	616	LUT	C15-C35-C34	4.18	132.03	123.47
17	4	606	CHL	O2D-CGD-CBD	4.17	118.69	111.27
19	1	619	LUT	C35-C15-C14	4.17	132.02	123.47
18	A	829	CLA	O2D-CGD-CBD	4.17	118.68	111.27
18	A	841	CLA	O2D-CGD-CBD	4.16	118.67	111.27
18	4	609	CLA	O2D-CGD-CBD	4.16	118.67	111.27
17	4	605	CHL	O2D-CGD-CBD	4.16	118.66	111.27
18	A	826	CLA	O2D-CGD-CBD	4.15	118.65	111.27
17	2	605	CHL	CAA-C2A-C3A	-4.15	103.89	114.26
18	B	828	CLA	O2D-CGD-CBD	4.15	118.64	111.27
18	A	809	CLA	O2D-CGD-CBD	4.13	118.61	111.27
17	4	607	CHL	O2D-CGD-CBD	4.13	118.61	111.27
18	A	823	CLA	O2D-CGD-CBD	4.12	118.60	111.27
18	G	202	CLA	O2D-CGD-CBD	4.12	118.59	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	830	CLA	O2D-CGD-CBD	4.12	118.59	111.27
18	4	601	CLA	O2D-CGD-CBD	4.12	118.59	111.27
18	A	833	CLA	O2D-CGD-CBD	4.11	118.58	111.27
18	1	609	CLA	O2D-CGD-CBD	4.11	118.58	111.27
18	B	825	CLA	O2D-CGD-CBD	4.11	118.57	111.27
18	F	301	CLA	O2D-CGD-CBD	4.11	118.57	111.27
17	2	606	CHL	CAA-C2A-C3A	-4.10	104.00	114.26
18	B	833	CLA	O2D-CGD-CBD	4.10	118.56	111.27
18	3	605	CLA	O2D-CGD-CBD	4.10	118.55	111.27
17	2	601	CHL	O2D-CGD-CBD	4.08	118.53	111.27
19	1	619	LUT	C19-C9-C10	-4.08	117.20	122.92
18	A	819	CLA	O2D-CGD-CBD	4.08	118.52	111.27
18	1	604	CLA	O2D-CGD-CBD	4.08	118.51	111.27
18	B	803	CLA	O2D-CGD-CBD	4.07	118.51	111.27
18	B	811	CLA	O2D-CGD-CBD	4.07	118.51	111.27
18	3	608	CLA	O2D-CGD-CBD	4.07	118.50	111.27
18	L	303	CLA	O2D-CGD-CBD	4.07	118.49	111.27
18	4	612	CLA	O2D-CGD-CBD	4.06	118.48	111.27
18	1	605	CLA	O2D-CGD-CBD	4.05	118.47	111.27
18	G	204	CLA	O2D-CGD-CBD	4.05	118.47	111.27
18	4	608	CLA	O2D-CGD-CBD	4.05	118.46	111.27
18	3	602	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	J	102	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	3	617	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	2	610	CLA	O2D-CGD-CBD	4.02	118.42	111.27
18	A	843	CLA	O2D-CGD-CBD	4.02	118.40	111.27
18	4	602	CLA	O2D-CGD-CBD	4.01	118.39	111.27
18	A	802	CLA	O2D-CGD-CBD	4.01	118.39	111.27
18	A	832	CLA	O2D-CGD-CBD	4.00	118.38	111.27
18	2	608	CLA	O2D-CGD-CBD	3.99	118.36	111.27
18	G	203	CLA	O2D-CGD-CBD	3.99	118.36	111.27
18	A	842	CLA	O2D-CGD-CBD	3.99	118.35	111.27
18	B	802	CLA	O2D-CGD-CBD	3.98	118.35	111.27
19	1	615	LUT	C15-C35-C34	3.98	131.63	123.47
19	1	615	LUT	C19-C9-C10	-3.98	117.35	122.92
18	1	603	CLA	O2D-CGD-CBD	3.98	118.34	111.27
18	L	302	CLA	O2D-CGD-CBD	3.97	118.33	111.27
18	A	812	CLA	O2D-CGD-CBD	3.97	118.32	111.27
18	A	821	CLA	O2D-CGD-CBD	3.97	118.32	111.27
18	2	613	CLA	O2D-CGD-CBD	3.96	118.30	111.27
18	2	609	CLA	O2D-CGD-CBD	3.96	118.30	111.27
18	A	836	CLA	O2D-CGD-CBD	3.95	118.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	828	CLA	O2D-CGD-CBD	3.95	118.28	111.27
18	A	808	CLA	O2D-CGD-CBD	3.94	118.28	111.27
17	2	607	CHL	O2D-CGD-CBD	3.93	118.26	111.27
18	A	817	CLA	O2D-CGD-CBD	3.93	118.26	111.27
18	B	810	CLA	O2D-CGD-CBD	3.93	118.25	111.27
19	2	615	LUT	C19-C9-C10	-3.93	117.42	122.92
20	4	617	XAT	C7-C8-C9	3.93	131.62	125.53
18	B	831	CLA	O2D-CGD-CBD	3.92	118.24	111.27
18	B	838	CLA	O2D-CGD-CBD	3.92	118.23	111.27
18	A	834	CLA	O2D-CGD-CBD	3.92	118.23	111.27
19	3	614	LUT	C19-C9-C10	-3.91	117.45	122.92
17	3	616	CHL	O2D-CGD-CBD	3.91	118.21	111.27
18	3	604	CLA	O2D-CGD-CBD	3.90	118.19	111.27
18	A	811	CLA	O2D-CGD-CBD	3.89	118.18	111.27
18	3	610	CLA	O2D-CGD-CBD	3.89	118.18	111.27
18	L	304	CLA	O2D-CGD-CBD	3.89	118.17	111.27
18	K	202	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	4	613	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	B	829	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	B	836	CLA	O2D-CGD-CBD	3.88	118.16	111.27
18	A	810	CLA	O2D-CGD-CBD	3.87	118.15	111.27
18	B	820	CLA	O2D-CGD-CBD	3.87	118.15	111.27
18	1	614	CLA	O2D-CGD-CBD	3.87	118.14	111.27
18	1	610	CLA	O2D-CGD-CBD	3.86	118.13	111.27
18	A	807	CLA	O2D-CGD-CBD	3.86	118.12	111.27
18	B	818	CLA	O2D-CGD-CBD	3.86	118.12	111.27
19	3	614	LUT	C40-C33-C34	-3.86	117.52	122.92
19	3	614	LUT	C32-C33-C34	3.85	124.85	118.94
19	4	616	LUT	C19-C9-C10	-3.84	117.54	122.92
18	A	840	CLA	O2D-CGD-CBD	3.84	118.09	111.27
19	1	619	LUT	C39-C29-C30	-3.83	117.55	122.92
18	2	612	CLA	O2D-CGD-CBD	3.83	118.08	111.27
19	4	616	LUT	C39-C29-C30	-3.83	117.56	122.92
18	1	611	CLA	O2D-CGD-CBD	3.83	118.07	111.27
19	1	615	LUT	C39-C29-C30	-3.82	117.57	122.92
18	B	824	CLA	O2D-CGD-CBD	3.82	118.05	111.27
19	3	614	LUT	C28-C29-C30	3.79	124.76	118.94
18	2	602	CLA	O2D-CGD-CBD	3.79	118.00	111.27
17	2	614	CHL	O2D-CGD-CBD	3.78	117.99	111.27
18	1	602	CLA	O2D-CGD-CBD	3.78	117.98	111.27
18	B	834	CLA	O2D-CGD-CBD	3.77	117.97	111.27
18	B	805	CLA	O2D-CGD-CBD	3.77	117.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	609	CLA	O2D-CGD-CBD	3.77	117.96	111.27
18	A	801	CLA	O2D-CGD-CBD	3.76	117.96	111.27
18	A	835	CLA	O2D-CGD-CBD	3.76	117.96	111.27
18	1	612	CLA	O2D-CGD-CBD	3.76	117.95	111.27
18	2	604	CLA	O2D-CGD-CBD	3.76	117.94	111.27
18	B	817	CLA	O2D-CGD-CBD	3.76	117.94	111.27
18	4	614	CLA	O2D-CGD-CBD	3.75	117.93	111.27
18	3	603	CLA	O2D-CGD-CBD	3.74	117.91	111.27
18	B	816	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
19	2	615	LUT	C39-C29-C30	-3.72	117.72	122.92
17	2	605	CHL	O2D-CGD-CBD	3.70	117.84	111.27
17	2	606	CHL	O2D-CGD-CBD	3.69	117.82	111.27
18	B	813	CLA	O2D-CGD-CBD	3.68	117.81	111.27
18	B	824	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
18	A	822	CLA	O2D-CGD-CBD	3.67	117.79	111.27
19	2	615	LUT	C15-C35-C34	3.66	130.98	123.47
18	F	303	CLA	O2D-CGD-CBD	3.64	117.73	111.27
18	2	611	CLA	O2D-CGD-CBD	3.63	117.72	111.27
18	3	607	CLA	O2D-CGD-CBD	3.63	117.72	111.27
18	K	203	CLA	O2D-CGD-CBD	3.63	117.71	111.27
18	4	603	CLA	O2D-CGD-CBD	3.62	117.69	111.27
17	4	606	CHL	CAA-C2A-C3A	-3.60	102.91	112.78
18	A	837	CLA	C4-C3-C5	-3.60	111.86	115.98
18	A	814	CLA	O2D-CGD-CBD	3.56	117.59	111.27
17	4	615	CHL	CAB-C3B-C2B	-3.54	117.75	124.69
18	F	304	CLA	O2D-CGD-CBD	3.52	117.53	111.27
18	3	605	CLA	CHD-C1D-ND	-3.48	121.25	124.45
18	B	822	CLA	O2D-CGD-CBD	3.48	117.45	111.27
18	A	803	CLA	CHD-C1D-ND	-3.46	121.27	124.45
17	4	605	CHL	CAA-C2A-C3A	-3.46	103.30	112.78
18	B	823	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
18	4	604	CLA	O2D-CGD-CBD	3.45	117.40	111.27
18	A	843	CLA	O2A-CGA-CBA	3.42	122.63	111.91
20	4	617	XAT	O24-C25-C24	-3.42	110.82	113.38
17	1	601	CHL	C1-C2-C3	3.41	131.95	126.04
19	1	619	LUT	C20-C13-C14	-3.41	118.15	122.92
18	A	831	CLA	O2A-CGA-CBA	3.39	122.56	111.91
18	B	817	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
20	3	615	XAT	O24-C25-C24	-3.38	110.84	113.38
18	A	843	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
18	B	807	CLA	O2A-CGA-CBA	3.36	122.46	111.91
18	A	813	CLA	CMB-C2B-C1B	-3.36	123.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	201	CLA	O2D-CGD-CBD	3.35	117.23	111.27
18	4	614	CLA	O2A-CGA-CBA	3.35	122.43	111.91
18	A	824	CLA	O2D-CGD-CBD	3.35	117.22	111.27
18	A	810	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
18	A	837	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
18	B	812	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
21	J	101	BCR	C23-C24-C25	3.31	136.51	127.20
18	A	840	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	A	825	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	B	802	CLA	C1-C2-C3	3.30	131.75	126.04
20	2	616	XAT	O4-C5-C4	-3.29	110.91	113.38
20	1	616	XAT	C7-C8-C9	3.28	130.62	125.53
18	B	826	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
18	A	820	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
18	H	201	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
18	B	832	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	B	816	CLA	C12-C11-C10	-3.27	102.05	113.62
18	A	805	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
17	4	605	CHL	C1-C2-C3	3.23	131.63	126.04
18	A	827	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
18	B	830	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
18	3	603	CLA	O2A-CGA-CBA	3.22	122.02	111.91
18	2	613	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
18	A	821	CLA	CHD-C1D-ND	-3.21	121.50	124.45
19	4	616	LUT	C40-C33-C34	-3.21	118.42	122.92
18	4	609	CLA	O2A-CGA-CBA	3.21	121.97	111.91
18	A	826	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
18	B	802	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	4	609	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
17	2	601	CHL	CHD-C1D-ND	-3.20	121.52	124.45
18	A	819	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
17	2	607	CHL	CAA-C2A-C3A	-3.19	104.03	112.78
18	B	808	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
18	A	834	CLA	O2A-CGA-CBA	3.19	121.92	111.91
18	1	610	CLA	O2A-CGA-CBA	3.19	121.92	111.91
18	A	833	CLA	O2A-CGA-CBA	3.19	121.91	111.91
17	2	601	CHL	CAA-C2A-C3A	-3.18	104.06	112.78
18	A	811	CLA	O2A-CGA-CBA	3.18	121.89	111.91
18	A	801	CLA	O2A-CGA-CBA	3.18	121.88	111.91
18	A	802	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
17	4	607	CHL	C1-C2-C3	3.17	131.88	126.75
18	A	825	CLA	O2A-CGA-CBA	3.17	121.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	821	CLA	O2A-CGA-CBA	3.17	121.85	111.91
18	1	609	CLA	O2A-CGA-CBA	3.17	121.85	111.91
18	B	838	CLA	O2A-CGA-CBA	3.16	121.83	111.91
18	2	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	4	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	B	821	CLA	O2A-CGA-CBA	3.16	121.81	111.91
18	B	806	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
18	4	614	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
18	3	612	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
18	B	836	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
18	B	827	CLA	O2A-CGA-CBA	3.15	121.80	111.91
18	F	303	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
18	A	813	CLA	O2A-CGA-CBA	3.15	121.79	111.91
17	1	601	CHL	O2A-CGA-CBA	3.15	121.79	111.91
18	A	823	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
18	A	821	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
18	A	830	CLA	O2A-CGA-CBA	3.14	121.77	111.91
18	A	854	CLA	O2A-CGA-CBA	3.14	121.77	111.91
18	B	836	CLA	O2A-CGA-CBA	3.14	121.76	111.91
18	A	817	CLA	O2A-CGA-CBA	3.14	121.76	111.91
18	A	830	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	1	615	LUT	C40-C33-C34	-3.14	118.53	122.92
18	1	604	CLA	O2A-CGA-CBA	3.13	121.74	111.91
18	A	803	CLA	O2A-CGA-CBA	3.13	121.74	111.91
18	2	602	CLA	O2A-CGA-CBA	3.13	121.74	111.91
18	4	602	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
18	1	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	B	840	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
18	A	838	CLA	O2A-CGA-CBA	3.13	121.73	111.91
18	B	825	CLA	O2A-CGA-CBA	3.13	121.72	111.91
18	B	814	CLA	O2A-CGA-CBA	3.12	121.70	111.91
18	A	831	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	B	831	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	A	826	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	A	808	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
18	2	612	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	A	837	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	B	840	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	B	827	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
18	A	812	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
18	A	811	CLA	CHD-C1D-ND	-3.11	121.60	124.45
18	A	811	CLA	CMB-C2B-C1B	-3.11	123.68	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	824	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
18	4	608	CLA	CHD-C1D-ND	-3.11	121.60	124.45
18	B	822	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
18	B	836	CLA	C1-C2-C3	3.10	131.41	126.04
18	3	610	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
18	A	843	CLA	CHD-C1D-ND	-3.10	121.60	124.45
18	3	606	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
18	1	614	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
18	A	826	CLA	O2A-CGA-CBA	3.10	121.63	111.91
18	2	609	CLA	O2A-CGA-CBA	3.10	121.62	111.91
18	A	824	CLA	O2A-CGA-CBA	3.09	121.61	111.91
18	4	604	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
18	A	828	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
18	B	825	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
18	A	829	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
18	B	818	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
18	K	203	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
18	B	810	CLA	CHD-C1D-ND	-3.08	121.62	124.45
18	B	813	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	2	615	LUT	C40-C33-C34	-3.08	118.61	122.92
18	2	608	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
18	4	601	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
18	A	806	CLA	O2A-CGA-CBA	3.07	121.55	111.91
18	B	805	CLA	O2A-CGA-CBA	3.07	121.54	111.91
18	3	604	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
18	B	829	CLA	CHD-C1D-ND	-3.07	121.63	124.45
18	B	828	CLA	O2A-CGA-CBA	3.07	121.54	111.91
18	B	821	CLA	CHD-C1D-ND	-3.07	121.64	124.45
18	A	808	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	808	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	815	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	817	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	810	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
18	B	812	CLA	O2A-CGA-CBA	3.06	121.52	111.91
18	A	818	CLA	O2A-CGA-CBA	3.06	121.52	111.91
18	A	810	CLA	O2A-CGA-CBA	3.06	121.51	111.91
18	A	834	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
18	H	201	CLA	C4-C3-C5	-3.06	112.49	115.98
18	B	819	CLA	O2A-CGA-CBA	3.05	121.49	111.91
18	B	822	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	F	304	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
18	2	610	CLA	CMB-C2B-C1B	-3.05	123.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	609	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
19	1	619	LUT	C12-C13-C14	3.05	123.62	118.94
18	A	835	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
18	B	811	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
18	1	611	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	4	612	CLA	O2A-CGA-CBA	3.05	121.47	111.91
18	3	608	CLA	CHD-C1D-ND	-3.04	121.66	124.45
18	1	604	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
18	2	603	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
18	2	604	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
18	1	602	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
18	4	610	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
18	A	815	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
18	B	820	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	2	615	LUT	C35-C15-C14	3.03	129.69	123.47
18	K	201	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
18	B	806	CLA	O2A-CGA-CBA	3.03	121.41	111.91
18	3	613	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
18	A	802	CLA	CHD-C1D-ND	-3.03	121.67	124.45
18	2	611	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
17	1	601	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
18	A	831	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
18	B	839	CLA	O2A-CGA-CBA	3.02	121.38	111.91
18	A	812	CLA	O2A-CGA-CBA	3.02	121.37	111.91
18	B	815	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	1	610	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	3	614	LUT	C20-C13-C14	-3.01	118.70	122.92
18	1	613	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
18	F	303	CLA	CHD-C1D-ND	-3.01	121.69	124.45
18	A	822	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
18	B	835	CLA	O2A-CGA-CBA	3.01	121.35	111.91
19	1	619	LUT	C40-C33-C34	-3.01	118.71	122.92
18	A	842	CLA	O2A-CGA-CBA	3.01	121.35	111.91
18	B	839	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
18	1	612	CLA	O2A-CGA-CBA	3.00	121.34	111.91
18	A	808	CLA	CHD-C1D-ND	-3.00	121.69	124.45
18	A	824	CLA	CHD-C1D-ND	-3.00	121.69	124.45
18	4	613	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
18	B	805	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
18	B	833	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
18	1	611	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
18	B	819	CLA	CMB-C2B-C1B	-3.00	123.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	615	LUT	C20-C13-C14	-3.00	118.72	122.92
18	3	602	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
18	B	810	CLA	O2A-CGA-CBA	3.00	121.31	111.91
18	B	823	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	A	839	CLA	O2A-CGA-CBA	2.99	121.30	111.91
18	A	818	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	B	836	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	A	842	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	A	807	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	2	604	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	B	815	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	F	301	CLA	O2A-CGA-CBA	2.99	121.28	111.91
18	4	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	4	608	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	B	804	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	A	841	CLA	O2A-CGA-CBA	2.98	121.28	111.91
18	1	603	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
18	B	837	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
18	G	202	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
18	A	833	CLA	CHD-C1D-ND	-2.98	121.72	124.45
18	2	602	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
18	3	607	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
18	G	204	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
18	B	824	CLA	O2A-CGA-CBA	2.98	121.25	111.91
17	3	616	CHL	CAA-C2A-C3A	-2.97	104.63	112.78
18	3	605	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
18	A	806	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
18	A	834	CLA	CHD-C1D-ND	-2.97	121.72	124.45
18	A	818	CLA	C12-C11-C10	-2.97	103.12	113.62
18	B	814	CLA	CHD-C1D-ND	-2.97	121.73	124.45
18	B	833	CLA	O2A-CGA-CBA	2.97	121.22	111.91
18	G	203	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
18	2	604	CLA	O2A-CGA-CBA	2.97	121.21	111.91
18	A	827	CLA	O2A-CGA-CBA	2.96	121.21	111.91
18	B	801	CLA	CHD-C1D-ND	-2.96	121.73	124.45
18	1	608	CLA	CHD-C1D-ND	-2.96	121.73	124.45
18	B	809	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
18	A	803	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
18	2	602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
18	B	816	CLA	O2A-CGA-CBA	2.96	121.19	111.91
18	3	617	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
18	3	613	CLA	CHD-C1D-ND	-2.96	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	854	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
18	B	823	CLA	O2A-CGA-CBA	2.95	121.17	111.91
18	A	840	CLA	CHD-C1D-ND	-2.95	121.74	124.45
19	1	615	LUT	C20-C13-C14	-2.95	118.79	122.92
18	1	602	CLA	C1-C2-C3	2.95	131.15	126.04
18	L	304	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
18	B	835	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
18	A	817	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
18	K	202	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
25	B	841	PQN	C11-C3-C4	-2.94	115.35	118.50
18	F	301	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
18	B	822	CLA	O2A-CGA-CBA	2.94	121.13	111.91
18	A	816	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
18	1	602	CLA	O2A-CGA-CBA	2.94	121.13	111.91
18	B	813	CLA	CHD-C1D-ND	-2.94	121.75	124.45
18	B	809	CLA	O2A-CGA-CBA	2.94	121.13	111.91
17	4	607	CHL	O2A-CGA-CBA	2.94	121.13	111.91
17	1	606	CHL	CMA-C3A-C2A	-2.93	109.25	116.10
18	3	611	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
18	4	610	CLA	O2A-CGA-CBA	2.93	121.11	111.91
18	A	807	CLA	O2A-CGA-CBA	2.93	121.11	111.91
18	A	827	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	L	303	CLA	O2A-CGA-CBA	2.93	121.10	111.91
18	A	838	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
18	1	608	CLA	O2A-CGA-CBA	2.93	121.10	111.91
18	B	832	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
18	B	821	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
18	3	605	CLA	O2A-CGA-CBA	2.92	121.08	111.91
18	4	611	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
18	B	825	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	A	819	CLA	CHD-C1D-ND	-2.92	121.77	124.45
17	1	606	CHL	C2A-C3A-C4A	2.92	105.51	101.78
18	A	828	CLA	O2A-CGA-CBA	2.92	121.07	111.91
18	2	609	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
18	A	801	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	4	603	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
18	A	806	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	B	802	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
18	3	602	CLA	O2A-CGA-CBA	2.91	121.05	111.91
18	1	602	CLA	CHD-C1D-ND	-2.91	121.78	124.45
18	L	302	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
18	2	611	CLA	CHD-C1D-ND	-2.91	121.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	303	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
18	B	817	CLA	CHD-C1D-ND	-2.90	121.78	124.45
18	A	836	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	A	837	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	2	603	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	B	831	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
18	B	820	CLA	O2A-CGA-CBA	2.90	121.00	111.91
18	1	605	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	4	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
17	2	605	CHL	CHD-C1D-ND	-2.89	121.80	124.45
18	1	607	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	A	839	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	3	609	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	B	807	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	3	617	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	F	301	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	B	838	CLA	C1-C2-C3	2.89	131.03	126.04
18	B	804	CLA	CHD-C1D-ND	-2.88	121.81	124.45
18	1	608	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
18	B	801	CLA	O2A-CGA-CBA	2.88	120.94	111.91
18	1	603	CLA	O2A-CGA-CBA	2.88	120.93	111.91
18	A	833	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
18	A	819	CLA	O2A-CGA-CBA	2.87	120.93	111.91
18	A	838	CLA	CHD-C1D-ND	-2.87	121.81	124.45
17	2	607	CHL	C1-C2-C3	2.87	131.40	126.75
18	J	102	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
18	J	102	CLA	CHD-C1D-ND	-2.87	121.81	124.45
18	B	803	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
18	A	842	CLA	CHD-C1D-ND	-2.87	121.82	124.45
18	B	824	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	A	844	PQN	C11-C3-C4	-2.87	115.43	118.50
18	H	201	CLA	O2A-CGA-CBA	2.86	120.90	111.91
18	A	817	CLA	C1-C2-C3	2.86	131.00	126.04
18	A	829	CLA	O2A-CGA-CBA	2.86	120.89	111.91
18	3	603	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
18	B	803	CLA	CHD-C1D-ND	-2.86	121.82	124.45
18	A	810	CLA	CHD-C1D-ND	-2.86	121.83	124.45
18	A	830	CLA	C1-C2-C3	2.86	130.99	126.04
18	A	802	CLA	O2A-CGA-CBA	2.86	120.88	111.91
18	A	841	CLA	CHD-C1D-ND	-2.86	121.83	124.45
18	A	804	CLA	O2A-CGA-CBA	2.86	120.88	111.91
18	A	825	CLA	CHD-C1D-ND	-2.86	121.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	809	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	2	616	XAT	C7-C8-C9	2.86	129.96	125.53
18	B	806	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	B	840	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	A	840	CLA	O2A-CGA-CBA	2.85	120.85	111.91
18	B	820	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	A	804	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
18	G	203	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	L	303	CLA	C1-C2-C3	2.85	130.97	126.04
18	A	828	CLA	C1-C2-C3	2.85	130.97	126.04
18	B	829	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
18	B	838	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
18	4	601	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	B	833	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	B	835	CLA	CHD-C1D-ND	-2.84	121.84	124.45
19	1	619	LUT	C15-C35-C34	2.84	129.29	123.47
18	A	809	CLA	O2A-CGA-CBA	2.84	120.82	111.91
17	4	607	CHL	CAA-C2A-C3A	-2.84	105.01	112.78
18	A	805	CLA	CHD-C1D-ND	-2.84	121.85	124.45
18	B	828	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	3	614	LUT	C30-C31-C32	2.84	132.07	123.22
18	A	801	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
18	B	818	CLA	C1-C2-C3	2.83	130.94	126.04
17	4	607	CHL	CHD-C1D-ND	-2.83	121.85	124.45
18	A	813	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	3	612	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	823	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	829	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	841	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
18	B	827	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	836	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
18	B	834	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	4	616	LUT	C20-C13-C14	-2.82	118.97	122.92
18	4	611	CLA	CHD-C1D-ND	-2.82	121.86	124.45
18	A	830	CLA	CHD-C1D-ND	-2.82	121.87	124.45
18	A	828	CLA	CHD-C1D-ND	-2.82	121.87	124.45
18	B	823	CLA	C1-C2-C3	2.81	130.90	126.04
17	4	605	CHL	CHD-C1D-ND	-2.81	121.87	124.45
18	3	609	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	A	818	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	3	608	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
18	B	828	CLA	CHD-C1D-ND	-2.80	121.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	304	CLA	CHD-C1D-ND	-2.80	121.88	124.45
18	2	608	CLA	CHD-C1D-ND	-2.80	121.88	124.45
18	A	809	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
18	A	811	CLA	C1-C2-C3	2.80	130.88	126.04
18	B	839	CLA	CHD-C1D-ND	-2.79	121.89	124.45
18	A	832	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
19	1	615	LUT	C35-C15-C14	2.79	129.19	123.47
17	3	616	CHL	CHD-C1D-ND	-2.79	121.89	124.45
18	A	814	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
18	B	837	CLA	O2A-CGA-CBA	2.79	120.65	111.91
18	1	612	CLA	CHD-C1D-ND	-2.79	121.89	124.45
18	B	826	CLA	O2A-CGA-CBA	2.79	120.65	111.91
18	3	602	CLA	CHD-C1D-ND	-2.78	121.89	124.45
17	1	601	CHL	CHD-C1D-ND	-2.78	121.90	124.45
18	L	303	CLA	CHD-C1D-ND	-2.78	121.90	124.45
18	B	801	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
17	2	607	CHL	O2A-CGA-CBA	2.78	120.63	111.91
18	B	831	CLA	O2A-CGA-CBA	2.78	120.63	111.91
18	B	825	CLA	C4-C3-C5	-2.77	110.60	115.27
18	1	610	CLA	CHD-C1D-ND	-2.77	121.90	124.45
18	4	602	CLA	O2A-CGA-CBA	2.77	120.61	111.91
18	2	610	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	A	814	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	A	812	CLA	C1-C2-C3	2.77	130.84	126.04
18	K	203	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	H	201	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	F	304	CLA	CHD-C1D-ND	-2.77	121.91	124.45
17	4	606	CHL	CHD-C1D-ND	-2.76	121.91	124.45
18	2	613	CLA	CHD-C1D-ND	-2.76	121.91	124.45
18	B	813	CLA	C1-C2-C3	2.76	130.82	126.04
18	1	613	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	2	602	CLA	C1-C2-C3	2.76	130.82	126.04
18	B	813	CLA	O2A-CGA-CBA	2.76	120.57	111.91
18	B	834	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
18	A	832	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	812	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	814	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
18	A	854	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	818	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	804	CLA	O2A-CGA-CBA	2.76	120.56	111.91
19	4	616	LUT	C32-C33-C34	2.76	123.17	118.94
18	A	839	CLA	CHD-C1D-ND	-2.76	121.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	801	CLA	C1-C2-C3	2.75	130.81	126.04
18	A	822	CLA	CHD-C1D-ND	-2.75	121.92	124.45
18	4	602	CLA	CHD-C1D-ND	-2.75	121.93	124.45
18	B	808	CLA	CHD-C1D-ND	-2.75	121.93	124.45
18	3	603	CLA	CHD-C1D-ND	-2.75	121.93	124.45
18	1	607	CLA	CHD-C1D-ND	-2.74	121.93	124.45
17	2	614	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
18	A	809	CLA	CHD-C1D-ND	-2.74	121.94	124.45
18	1	612	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
18	1	604	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	K	202	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	A	804	CLA	C1-C2-C3	2.73	130.76	126.04
18	B	816	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	3	617	CLA	O2A-CGA-CBA	2.73	120.47	111.91
18	A	823	CLA	CMA-C3A-C2A	-2.73	109.73	116.10
18	3	607	CLA	CHD-C1D-ND	-2.73	121.95	124.45
18	B	830	CLA	CHD-C1D-ND	-2.73	121.95	124.45
18	A	817	CLA	CHD-C1D-ND	-2.73	121.95	124.45
18	A	815	CLA	CHD-C1D-ND	-2.72	121.95	124.45
18	3	610	CLA	CHD-C1D-ND	-2.72	121.95	124.45
18	B	802	CLA	O2A-CGA-CBA	2.72	120.44	111.91
18	1	605	CLA	CHD-C1D-ND	-2.71	121.96	124.45
18	3	606	CLA	CHD-C1D-ND	-2.71	121.96	124.45
18	A	812	CLA	CHD-C1D-ND	-2.71	121.97	124.45
18	1	610	CLA	C1-C2-C3	2.71	130.72	126.04
18	A	832	CLA	O2A-CGA-CBA	2.71	120.40	111.91
18	4	612	CLA	CMB-C2B-C1B	-2.71	124.31	128.46
18	G	204	CLA	CHD-C1D-ND	-2.70	121.97	124.45
17	1	606	CHL	CHD-C1D-ND	-2.70	121.97	124.45
18	G	202	CLA	CHD-C1D-ND	-2.70	121.97	124.45
17	2	606	CHL	CHD-C1D-ND	-2.69	121.98	124.45
18	A	804	CLA	CHD-C1D-ND	-2.69	121.98	124.45
18	B	804	CLA	C1-C2-C3	2.69	130.70	126.04
18	F	304	CLA	CMA-C3A-C2A	-2.69	109.82	116.10
19	1	619	LUT	C39-C29-C28	2.69	122.31	118.08
18	2	612	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
17	2	607	CHL	CHD-C1D-ND	-2.68	121.99	124.45
18	B	805	CLA	CHD-C1D-ND	-2.68	121.99	124.45
18	2	612	CLA	CHD-C1D-ND	-2.68	121.99	124.45
18	4	604	CLA	CHD-C1D-ND	-2.68	121.99	124.45
20	1	616	XAT	O4-C5-C4	-2.68	111.37	113.38
18	3	613	CLA	CMA-C3A-C2A	-2.68	109.85	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	820	CLA	C1-C2-C3	2.68	130.67	126.04
18	B	837	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	1	615	LUT	C32-C33-C34	2.67	123.04	118.94
18	A	854	CLA	C1-C2-C3	2.67	131.07	126.75
17	4	605	CHL	O2A-CGA-CBA	2.66	120.27	111.91
17	4	615	CHL	CHD-C1D-ND	-2.66	122.01	124.45
18	3	609	CLA	CMA-C3A-C2A	-2.65	109.91	116.10
18	K	201	CLA	CHD-C1D-ND	-2.65	122.02	124.45
18	B	821	CLA	C1-C2-C3	2.65	130.63	126.04
18	3	612	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
18	1	609	CLA	CHD-C1D-ND	-2.65	122.02	124.45
18	4	602	CLA	C1-C2-C3	2.65	130.62	126.04
18	B	803	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
17	1	606	CHL	CMB-C2B-C1B	-2.64	124.40	128.46
18	B	811	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	A	820	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	3	611	CLA	CHD-C1D-ND	-2.64	122.03	124.45
17	2	614	CHL	CHD-C1D-ND	-2.63	122.04	124.45
18	4	614	CLA	CHD-C1D-ND	-2.63	122.04	124.45
21	A	847	BCR	C7-C8-C9	2.63	130.21	126.23
18	A	835	CLA	CHD-C1D-ND	-2.62	122.04	124.45
18	4	613	CLA	CHD-C1D-ND	-2.62	122.05	124.45
18	4	612	CLA	CHD-C1D-ND	-2.61	122.06	124.45
18	L	302	CLA	CHD-C1D-ND	-2.60	122.06	124.45
18	B	827	CLA	C1-C2-C3	2.60	130.54	126.04
18	B	838	CLA	CHD-C1D-ND	-2.60	122.06	124.45
17	2	605	CHL	CMB-C2B-C1B	-2.60	124.47	128.46
18	A	807	CLA	CHD-C1D-ND	-2.60	122.07	124.45
18	B	833	CLA	C1-C2-C3	2.59	130.53	126.04
18	A	801	CLA	C1-C2-C3	2.59	130.53	126.04
17	4	607	CHL	CMB-C2B-C1B	-2.59	124.48	128.46
17	2	601	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
18	4	603	CLA	O2A-CGA-CBA	2.58	122.33	114.03
18	F	301	CLA	C1-C2-C3	2.58	130.50	126.04
18	B	818	CLA	O2A-CGA-CBA	2.58	119.99	111.91
18	1	609	CLA	C1-C2-C3	2.58	130.50	126.04
18	2	604	CLA	C1-C2-C3	2.57	130.49	126.04
18	2	610	CLA	CMA-C3A-C2A	-2.57	110.10	116.10
18	2	609	CLA	C1-C2-C3	2.57	130.49	126.04
20	1	616	XAT	O24-C25-C24	-2.57	111.45	113.38
17	4	606	CHL	CMB-C2B-C1B	-2.57	124.52	128.46
18	3	604	CLA	CHD-C1D-ND	-2.56	122.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	603	CLA	C1-C2-C3	2.56	130.47	126.04
18	A	813	CLA	C1-C2-C3	2.56	130.46	126.04
18	1	603	CLA	C1-C2-C3	2.55	130.46	126.04
18	B	819	CLA	CHD-C1D-ND	-2.55	122.11	124.45
18	B	826	CLA	C1-C2-C3	2.55	130.45	126.04
17	2	601	CHL	CMB-C2B-C1B	-2.54	124.55	128.46
18	B	824	CLA	CMB-C2B-C3B	2.54	129.44	124.68
18	A	843	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
19	4	616	LUT	C35-C15-C14	2.54	128.68	123.47
17	4	607	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
18	2	602	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
18	A	809	CLA	C1-C2-C3	2.53	130.42	126.04
18	B	806	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
18	A	834	CLA	C1-C2-C3	2.53	130.42	126.04
18	4	609	CLA	C1-C2-C3	2.53	130.42	126.04
19	2	615	LUT	C39-C29-C28	2.53	122.06	118.08
18	A	829	CLA	C1-C2-C3	2.53	130.41	126.04
18	A	840	CLA	C1-C2-C3	2.53	130.41	126.04
18	A	818	CLA	C1-C2-C3	2.52	130.40	126.04
18	B	807	CLA	CHD-C1D-ND	-2.52	122.14	124.45
18	K	201	CLA	CMA-C3A-C2A	-2.52	110.22	116.10
18	B	826	CLA	CHD-C1D-ND	-2.51	122.14	124.45
18	A	838	CLA	C1-C2-C3	2.51	130.39	126.04
18	A	805	CLA	O2A-CGA-CBA	2.51	122.10	114.03
17	2	606	CHL	CMB-C2B-C1B	-2.51	124.60	128.46
18	B	839	CLA	C1-C2-C3	2.50	130.37	126.04
18	A	821	CLA	C1-C2-C3	2.50	130.37	126.04
19	2	615	LUT	C32-C33-C34	2.50	122.78	118.94
17	4	615	CHL	CMB-C2B-C1B	-2.50	124.62	128.46
18	B	831	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
17	3	616	CHL	C2C-C3C-C4C	2.50	108.27	106.49
18	A	806	CLA	C1-C2-C3	2.49	130.36	126.04
18	B	825	CLA	C1-C2-C3	2.49	130.36	126.04
18	H	201	CLA	C1-C2-C3	2.49	130.36	126.04
18	1	614	CLA	CHD-C1D-ND	-2.49	122.17	124.45
18	A	830	CLA	C12-C11-C10	-2.49	101.81	113.24
18	A	829	CLA	C12-C11-C10	-2.49	101.81	113.24
18	A	839	CLA	C1-C2-C3	2.49	130.78	126.75
18	A	803	CLA	C1-C2-C3	2.49	130.34	126.04
18	A	802	CLA	C12-C11-C10	-2.48	101.82	113.24
18	B	812	CLA	C1-C2-C3	2.48	130.33	126.04
18	B	816	CLA	CMB-C2B-C3B	2.47	129.31	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	842	CLA	C1-C2-C3	2.47	130.32	126.04
19	4	616	LUT	C39-C29-C28	2.47	121.97	118.08
18	B	805	CLA	C5-C3-C2	2.47	126.12	121.12
17	3	616	CHL	CMB-C2B-C1B	-2.47	124.67	128.46
18	1	608	CLA	C1-C2-C3	2.47	130.31	126.04
18	B	831	CLA	C1-C2-C3	2.47	130.31	126.04
18	A	802	CLA	C1-C2-C3	2.46	130.31	126.04
18	B	832	CLA	C3C-C4C-NC	-2.46	107.81	110.57
18	B	824	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
18	A	816	CLA	CHD-C1D-ND	-2.46	122.19	124.45
18	4	601	CLA	O2A-CGA-CBA	2.46	121.94	112.23
18	B	810	CLA	C1-C2-C3	2.46	130.29	126.04
20	2	616	XAT	C27-C28-C29	2.45	129.33	125.53
18	A	814	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
18	1	611	CLA	O2A-CGA-CBA	2.45	121.89	114.03
18	4	602	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
17	2	607	CHL	CMB-C2B-C1B	-2.44	124.71	128.46
20	3	615	XAT	C7-C8-C9	2.44	129.32	125.53
18	A	828	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
17	4	607	CHL	C2C-C3C-C4C	2.44	108.23	106.49
17	2	606	CHL	C2A-C3A-C4A	2.44	105.81	101.87
17	1	601	CHL	C2A-C3A-C4A	2.44	105.81	101.87
18	3	603	CLA	C4-C3-C5	-2.44	111.17	115.27
18	A	810	CLA	C3C-C4C-NC	-2.44	107.84	110.57
18	A	843	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
18	B	833	CLA	C12-C11-C10	-2.43	102.06	113.24
18	B	820	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
18	B	808	CLA	C1-C2-C3	2.43	130.24	126.04
18	A	802	CLA	C3C-C4C-NC	-2.43	107.85	110.57
18	B	828	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
18	L	303	CLA	C3C-C4C-NC	-2.42	107.85	110.57
18	4	602	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
18	4	604	CLA	O2A-CGA-CBA	2.42	121.81	114.03
18	A	826	CLA	C1-C2-C3	2.42	130.22	126.04
18	B	835	CLA	C1-C2-C3	2.41	130.66	126.75
18	A	811	CLA	C12-C11-C10	-2.41	102.16	113.24
18	A	836	CLA	O2A-CGA-CBA	2.41	121.78	114.03
18	4	614	CLA	C1-C2-C3	2.41	130.65	126.75
18	2	602	CLA	C12-C11-C10	-2.41	102.16	113.24
18	A	827	CLA	C4-C3-C5	-2.41	111.22	115.27
18	3	602	CLA	C12-C11-C10	-2.41	102.17	113.24
18	3	609	CLA	CAA-C2A-C3A	-2.41	110.48	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	825	CLA	C12-C11-C10	-2.40	102.19	113.24
18	L	302	CLA	O2A-CGA-CBA	2.40	121.75	114.03
18	A	833	CLA	C12-C11-C10	-2.40	102.19	113.24
18	A	806	CLA	C12-C11-C10	-2.40	102.20	113.24
18	A	826	CLA	C12-C11-C10	-2.40	102.20	113.24
17	2	614	CHL	C2A-C1A-CHA	2.40	128.06	123.86
18	2	611	CLA	O2A-CGA-CBA	2.40	121.74	114.03
18	B	817	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
18	B	816	CLA	C1-C2-C3	2.40	130.19	126.04
18	4	602	CLA	C12-C11-C10	-2.40	102.22	113.24
21	A	850	BCR	C7-C8-C9	-2.39	122.62	126.23
18	4	603	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
18	2	613	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
18	B	819	CLA	C1-C2-C3	2.39	130.62	126.75
18	B	822	CLA	C3C-C4C-NC	-2.39	107.89	110.57
18	1	608	CLA	C12-C11-C10	-2.39	102.28	113.24
17	4	607	CHL	C2A-C3A-C4A	2.38	105.72	101.87
18	4	614	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	B	837	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	A	825	CLA	C1-C2-C3	2.38	130.16	126.04
18	B	815	CLA	C1-C2-C3	2.38	130.16	126.04
18	B	823	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	A	841	CLA	C1-C2-C3	2.38	130.16	126.04
18	1	608	CLA	C4-C3-C5	-2.38	111.27	115.27
18	A	821	CLA	C12-C11-C10	-2.38	102.32	113.24
18	4	614	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
18	A	842	CLA	C12-C11-C10	-2.37	102.33	113.24
18	A	824	CLA	C1-C2-C3	2.37	130.15	126.04
18	B	823	CLA	C12-C11-C10	-2.37	102.34	113.24
19	1	619	LUT	C32-C33-C34	2.37	122.58	118.94
18	A	829	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
17	1	601	CHL	CMB-C2B-C1B	-2.37	124.82	128.46
18	B	838	CLA	C12-C11-C10	-2.37	102.36	113.24
21	A	846	BCR	C21-C20-C19	2.36	130.60	123.22
18	3	602	CLA	C1-C2-C3	2.36	130.13	126.04
18	3	611	CLA	O2A-CGA-CBA	2.36	121.63	114.03
18	A	804	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
18	B	833	CLA	C3C-C4C-NC	-2.36	107.92	110.57
18	B	806	CLA	C1-C2-C3	2.36	130.13	126.04
18	B	813	CLA	C4-C3-C5	-2.36	111.30	115.27
18	B	816	CLA	C3C-C4C-NC	-2.36	107.92	110.57
18	L	303	CLA	C12-C11-C10	-2.36	102.40	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	C1-C2-C3	2.36	130.12	126.04
18	K	203	CLA	O2A-CGA-CBA	2.36	121.54	112.23
18	3	602	CLA	C4-C3-C5	-2.35	111.31	115.27
18	A	834	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
17	2	601	CHL	C4D-CHA-C1A	2.35	124.11	121.25
18	A	834	CLA	C12-C11-C10	-2.35	102.45	113.24
18	B	818	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
18	B	809	CLA	C3C-C4C-NC	-2.35	107.94	110.57
17	2	605	CHL	C2A-C3A-C4A	2.35	105.66	101.87
18	B	820	CLA	C4-C3-C5	-2.34	111.33	115.27
18	K	202	CLA	O2A-CGA-CBA	2.34	121.56	114.03
18	B	824	CLA	C1-C2-C3	2.34	130.54	126.75
19	1	615	LUT	C39-C29-C28	2.34	121.77	118.08
18	B	832	CLA	O2A-CGA-CBA	2.34	121.55	114.03
18	F	304	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
18	G	204	CLA	O2A-CGA-CBA	2.34	121.55	114.03
18	A	812	CLA	C4-C3-C5	-2.34	111.34	115.27
18	A	840	CLA	C12-C11-C10	-2.34	102.49	113.24
18	A	824	CLA	C3C-C4C-NC	-2.34	107.95	110.57
18	A	843	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
18	A	819	CLA	C12-C11-C10	-2.34	102.50	113.24
18	A	843	CLA	C1-C2-C3	2.34	130.08	126.04
18	3	607	CLA	O2A-CGA-CBA	2.33	121.52	114.03
18	3	609	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
18	A	817	CLA	C12-C11-C10	-2.33	102.53	113.24
19	1	619	LUT	C8-C9-C10	2.33	122.52	118.94
18	K	201	CLA	OBD-CAD-CBD	-2.33	121.21	125.97
18	4	610	CLA	C12-C11-C10	-2.33	102.54	113.24
18	2	603	CLA	O2A-CGA-CBA	2.33	121.50	114.03
18	2	603	CLA	C3C-C4C-NC	-2.32	107.97	110.57
18	1	612	CLA	C1-C2-C3	2.32	130.06	126.04
18	A	808	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	B	822	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
18	B	839	CLA	C12-C11-C10	-2.32	102.58	113.24
19	2	615	LUT	C12-C13-C14	2.32	122.50	118.94
19	3	614	LUT	C12-C13-C14	2.32	122.50	118.94
18	1	609	CLA	C12-C11-C10	-2.32	102.59	113.24
18	3	604	CLA	O2A-CGA-CBA	2.32	121.48	114.03
18	B	812	CLA	C4-C3-C5	-2.32	111.38	115.27
18	4	613	CLA	O2A-CGA-CBA	2.32	121.47	114.03
18	B	817	CLA	C3C-C4C-NC	-2.31	107.97	110.57
18	A	824	CLA	O1D-CGD-CBD	-2.31	119.75	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	823	CLA	C4-C3-C5	-2.31	111.38	115.27
17	3	616	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
18	B	807	CLA	C4-C3-C5	-2.31	111.38	115.27
18	B	830	CLA	C3C-C4C-NC	-2.31	107.98	110.57
18	B	822	CLA	C1-C2-C3	2.31	130.04	126.04
17	3	616	CHL	CBC-CAC-C3C	-2.31	106.06	112.43
17	4	615	CHL	C2A-C3A-C4A	2.31	105.60	101.87
18	A	841	CLA	C12-C11-C10	-2.31	102.63	113.24
18	A	840	CLA	CMB-C2B-C3B	2.31	129.00	124.68
18	A	843	CLA	C12-C11-C10	-2.31	102.64	113.24
18	A	840	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
20	2	616	XAT	O24-C25-C24	-2.30	111.65	113.38
18	B	818	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
18	4	612	CLA	C4-C3-C5	-2.30	111.40	115.27
18	A	819	CLA	C4-C3-C5	-2.30	111.40	115.27
18	1	613	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
18	3	608	CLA	O2A-CGA-CBA	2.30	121.43	114.03
18	B	809	CLA	C1-C2-C3	2.30	130.02	126.04
18	A	806	CLA	C3C-C4C-NC	-2.30	107.99	110.57
18	A	831	CLA	C1-C2-C3	2.30	130.47	126.75
18	A	820	CLA	O2A-CGA-CBA	2.30	121.42	114.03
18	A	813	CLA	C4-C3-C5	-2.30	111.41	115.27
17	3	616	CHL	C2A-C3A-C4A	2.30	105.58	101.87
18	A	824	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
18	B	829	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
19	4	616	LUT	C19-C9-C8	2.30	121.69	118.08
18	B	826	CLA	C12-C11-C10	-2.29	102.69	113.24
17	4	615	CHL	C2A-C1A-CHA	2.29	127.87	123.86
18	1	603	CLA	C3C-C4C-NC	-2.29	108.00	110.57
18	L	303	CLA	C4-C3-C5	-2.29	111.41	115.27
18	4	608	CLA	O2A-CGA-CBA	2.29	121.40	114.03
18	B	805	CLA	C12-C11-C10	-2.29	102.71	113.24
18	K	203	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
18	1	612	CLA	C4-C3-C5	-2.29	111.42	115.27
18	B	837	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
18	A	813	CLA	CMB-C2B-C3B	2.29	128.96	124.68
18	B	831	CLA	C12-C11-C10	-2.29	102.73	113.24
17	2	614	CHL	C2C-C3C-C4C	2.28	108.12	106.49
18	A	810	CLA	CMB-C2B-C3B	2.28	128.95	124.68
18	B	823	CLA	CMB-C2B-C3B	2.28	128.95	124.68
18	A	832	CLA	C3C-C4C-NC	-2.28	108.01	110.57
18	1	613	CLA	O2A-CGA-CBA	2.28	121.36	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	808	CLA	C1-C2-C3	2.28	130.43	126.75
18	A	817	CLA	C3C-C4C-NC	-2.27	108.02	110.57
18	B	820	CLA	C3C-C4C-NC	-2.27	108.02	110.57
17	4	605	CHL	O2A-CGA-O1A	-2.27	117.86	123.59
18	A	827	CLA	C12-C11-C10	-2.27	102.80	113.24
18	2	604	CLA	C12-C11-C10	-2.27	102.80	113.24
18	B	802	CLA	C4-C3-C5	-2.27	111.45	115.27
18	B	802	CLA	C2C-C1C-NC	-2.27	107.84	109.97
18	A	818	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	B	804	CLA	C12-C11-C10	-2.27	102.81	113.24
18	B	817	CLA	CMB-C2B-C3B	2.27	128.92	124.68
18	A	819	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
18	4	610	CLA	C1-C2-C3	2.27	129.97	126.04
18	A	819	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	A	835	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	A	803	CLA	C12-C11-C10	-2.27	102.83	113.24
18	B	838	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
17	4	605	CHL	C2A-C3A-C4A	2.26	105.53	101.87
18	4	602	CLA	C3C-C4C-NC	-2.26	108.03	110.57
17	4	605	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
20	3	615	XAT	C27-C28-C29	2.26	129.04	125.53
17	2	601	CHL	C2A-C3A-C4A	2.26	105.52	101.87
18	A	837	CLA	C1-C2-C3	2.26	129.95	126.04
17	2	606	CHL	C2C-C3C-C4C	2.26	108.10	106.49
18	B	840	CLA	C3C-C4C-NC	-2.26	108.04	110.57
18	2	602	CLA	C3C-C4C-NC	-2.26	108.04	110.57
18	B	827	CLA	C12-C11-C10	-2.26	102.86	113.24
17	2	607	CHL	C2A-C3A-C4A	2.26	105.51	101.87
18	1	612	CLA	C12-C11-C10	-2.26	102.88	113.24
18	4	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
18	B	817	CLA	C12-C11-C10	-2.25	102.88	113.24
17	4	615	CHL	C2C-C3C-C4C	2.25	108.10	106.49
18	H	201	CLA	C3C-C4C-NC	-2.25	108.04	110.57
18	4	603	CLA	C2D-C1D-ND	2.25	111.76	110.10
18	A	820	CLA	CMB-C2B-C3B	2.25	128.89	124.68
18	H	201	CLA	CMB-C2B-C3B	2.25	128.89	124.68
18	A	808	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	A	821	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	B	822	CLA	C12-C11-C10	-2.25	102.90	113.24
18	B	836	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	B	813	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	1	607	CLA	O2A-CGA-CBA	2.25	121.25	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	607	CHL	O2A-CGA-O1A	-2.25	117.92	123.59
18	A	804	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
18	A	838	CLA	C3C-C4C-NC	-2.24	108.05	110.57
18	B	803	CLA	C3C-C4C-NC	-2.24	108.06	110.57
18	B	811	CLA	C3C-C4C-NC	-2.24	108.06	110.57
18	A	810	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
18	B	804	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
17	1	601	CHL	C2C-C3C-C4C	2.24	108.08	106.49
18	A	810	CLA	C1-C2-C3	2.24	130.37	126.75
18	A	830	CLA	C3C-C4C-NC	-2.24	108.06	110.57
17	2	601	CHL	C2C-C3C-C4C	2.24	108.08	106.49
19	3	614	LUT	C1-C6-C7	2.24	122.11	115.78
18	B	801	CLA	C12-C11-C10	-2.24	102.96	113.24
18	A	837	CLA	CMB-C2B-C3B	2.24	128.86	124.68
18	B	836	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
18	2	612	CLA	O1D-CGD-CBD	-2.23	119.91	124.48
18	B	809	CLA	C12-C11-C10	-2.23	102.97	113.24
18	A	825	CLA	CMB-C2B-C3B	2.23	128.86	124.68
18	1	602	CLA	C12-C11-C10	-2.23	102.99	113.24
18	B	812	CLA	CMB-C2B-C3B	2.23	128.85	124.68
18	A	814	CLA	O2A-CGA-CBA	2.23	121.19	114.03
18	B	836	CLA	C12-C11-C10	-2.23	103.00	113.24
18	B	824	CLA	C3C-C4C-NC	-2.23	108.08	110.57
17	4	605	CHL	C4D-CHA-C1A	2.22	123.96	121.25
18	F	301	CLA	C12-C11-C10	-2.22	102.55	113.29
18	1	609	CLA	C3C-C4C-NC	-2.22	108.14	110.57
18	B	837	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
18	B	812	CLA	C11-C12-C13	2.22	123.10	115.92
18	B	840	CLA	C1-C2-C3	2.22	129.89	126.04
18	B	802	CLA	C12-C11-C10	-2.22	103.03	113.24
18	A	807	CLA	C12-C11-C10	-2.22	103.04	113.24
18	1	614	CLA	O2A-CGA-CBA	2.22	121.16	114.03
18	A	822	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	B	829	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	A	814	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
18	2	612	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	B	807	CLA	C12-C11-C10	-2.22	103.06	113.24
18	2	608	CLA	O2A-CGA-CBA	2.21	121.14	114.03
21	2	618	BCR	C10-C11-C12	2.21	130.12	123.22
18	B	801	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	A	812	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	A	804	CLA	O2D-CGD-O1D	-2.21	119.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	612	CLA	C1-C2-C3	2.21	129.86	126.04
18	B	828	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	B	810	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	G	203	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	B	805	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	3	613	CLA	CAA-C2A-C3A	-2.20	110.96	116.10
17	4	607	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
18	1	602	CLA	C3C-C4C-NC	-2.20	108.10	110.57
18	B	832	CLA	CMD-C2D-C1D	2.20	128.59	124.71
18	3	602	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
18	B	804	CLA	C3C-C4C-NC	-2.20	108.10	110.57
18	B	839	CLA	C3C-C4C-NC	-2.20	108.10	110.57
18	2	611	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
18	A	813	CLA	C12-C11-C10	-2.20	103.14	113.24
17	2	601	CHL	O2A-CGA-CBA	2.20	120.91	112.23
18	A	826	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
18	B	808	CLA	C3C-C4C-NC	-2.19	108.11	110.57
18	2	612	CLA	C4-C3-C5	-2.19	111.58	115.27
19	1	615	LUT	C12-C13-C14	2.19	122.31	118.94
18	A	826	CLA	C3C-C4C-NC	-2.19	108.11	110.57
18	B	817	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	3	607	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
18	B	828	CLA	C1-C2-C3	2.19	129.83	126.04
18	A	807	CLA	C5-C3-C2	2.19	125.55	121.12
18	1	613	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
18	B	813	CLA	C12-C11-C10	-2.19	103.19	113.24
18	A	803	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
18	A	835	CLA	O2A-CGA-CBA	2.19	121.05	114.03
18	B	829	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
18	A	835	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
18	A	819	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
18	1	605	CLA	C2A-C1A-CHA	2.18	126.10	122.71
18	B	831	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	A	841	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	3	610	CLA	C2D-C1D-ND	2.18	111.71	110.10
18	B	817	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	A	807	CLA	C3C-C4C-NC	-2.18	108.13	110.57
18	A	831	CLA	C3C-C4C-NC	-2.18	108.13	110.57
18	B	823	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	2	604	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
18	B	811	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	B	826	CLA	CMB-C2B-C3B	2.17	128.75	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	304	CLA	CED-O2D-CGD	2.17	120.85	115.94
18	1	603	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	A	828	CLA	C12-C11-C10	-2.17	103.26	113.24
18	B	832	CLA	C2C-C1C-NC	-2.17	107.94	109.97
18	A	843	CLA	CMB-C2B-C3B	2.17	128.74	124.68
18	B	822	CLA	CED-O2D-CGD	2.17	120.85	115.94
18	B	823	CLA	C2D-C1D-ND	2.17	111.70	110.10
18	B	838	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	3	602	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
18	B	802	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	A	836	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	A	827	CLA	CMB-C2B-C3B	2.17	128.74	124.68
18	2	610	CLA	CAA-C2A-C3A	-2.17	111.04	116.10
18	G	202	CLA	O2A-CGA-CBA	2.17	121.00	114.03
17	4	606	CHL	C4D-CHA-C1A	2.17	123.89	121.25
18	A	811	CLA	C2D-C1D-ND	2.17	111.70	110.10
17	4	615	CHL	C4D-CHA-C1A	2.17	123.89	121.25
18	A	833	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	B	820	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
18	B	819	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
18	A	840	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	1	603	CLA	CMD-C2D-C1D	2.16	128.53	124.71
18	F	303	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	A	812	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
18	K	203	CLA	C3C-C4C-NC	-2.16	108.15	110.57
18	4	601	CLA	C3C-C4C-NC	-2.16	108.15	110.57
18	1	604	CLA	C3C-C4C-NC	-2.16	108.15	110.57
18	A	812	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
18	3	603	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
18	4	612	CLA	C1-C2-C3	2.15	129.77	126.04
18	A	825	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	B	806	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	B	814	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	3	611	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	1	608	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	3	612	CLA	CAA-C2A-C3A	-2.15	111.07	116.10
18	B	830	CLA	CMB-C2B-C3B	2.15	128.70	124.68
18	3	608	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	A	811	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
17	4	607	CHL	OMC-CMC-C2C	-2.15	120.83	125.69
18	3	617	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	H	201	CLA	O1D-CGD-CBD	-2.15	120.09	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	840	CLA	C4-C3-C5	-2.15	111.66	115.27
18	A	820	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	B	823	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	1	602	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	A	805	CLA	CMB-C2B-C3B	2.15	128.69	124.68
18	A	841	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
18	A	817	CLA	C5-C3-C2	2.14	125.46	121.12
17	1	606	CHL	C2A-C1A-CHA	2.14	127.60	123.85
18	A	804	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	841	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	4	614	CLA	CMB-C2B-C3B	2.14	128.69	124.68
18	B	814	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
18	A	839	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	819	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
18	A	814	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	B	827	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	B	824	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	B	826	CLA	C4-C3-C5	-2.14	111.67	115.27
18	A	815	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	B	806	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	2	610	CLA	C2D-C1D-ND	2.14	111.68	110.10
18	A	830	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
18	B	822	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	2	612	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
18	2	604	CLA	C4-C3-C5	-2.14	111.68	115.27
18	2	613	CLA	CMB-C2B-C3B	2.13	128.67	124.68
18	1	607	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	3	613	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	3	603	CLA	CMD-C2D-C1D	2.13	128.47	124.71
18	A	802	CLA	CMB-C2B-C3B	2.13	128.66	124.68
18	A	829	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	B	827	CLA	C4-C3-C5	-2.13	111.69	115.27
18	B	831	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
18	G	202	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	B	834	CLA	CMD-C2D-C1D	2.13	128.46	124.71
17	2	605	CHL	C4D-CHA-C1A	2.13	123.84	121.25
18	B	825	CLA	C3C-C4C-NC	-2.13	108.19	110.57
18	L	304	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
18	2	602	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
18	B	826	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
18	B	827	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
18	A	833	CLA	C4-C3-C5	-2.12	111.70	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	609	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	B	815	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	2	603	CLA	CMD-C2D-C1D	2.12	128.45	124.71
18	2	613	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
18	L	304	CLA	O2A-CGA-CBA	2.12	120.84	114.03
18	J	102	CLA	CED-O2D-CGD	2.12	120.73	115.94
18	4	604	CLA	C3C-C4C-NC	-2.12	108.20	110.57
18	B	818	CLA	C3C-C4C-NC	-2.12	108.20	110.57
18	B	812	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
18	K	201	CLA	CAA-C2A-C3A	-2.12	111.16	116.10
18	2	604	CLA	C3C-C4C-NC	-2.12	108.20	110.57
18	A	808	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
18	3	617	CLA	C1-C2-C3	2.12	129.70	126.04
18	3	612	CLA	CMB-C2B-C3B	2.11	128.63	124.68
18	B	819	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	1	612	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	A	805	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	A	818	CLA	CMD-C2D-C1D	2.11	128.44	124.71
18	A	816	CLA	O2A-CGA-CBA	2.11	120.81	114.03
18	A	825	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	B	814	CLA	C3C-C4C-NC	-2.11	108.20	110.57
17	1	606	CHL	C2C-C3C-C4C	2.11	107.99	106.49
17	4	606	CHL	O2A-CGA-O1A	-2.11	118.04	123.30
18	4	612	CLA	C12-C11-C10	-2.11	103.10	113.29
18	B	838	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
17	3	616	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
18	A	807	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
18	A	854	CLA	CAC-C3C-C2C	2.11	131.14	127.53
18	A	802	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	A	854	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	4	609	CLA	C3C-C4C-NC	-2.11	108.21	110.57
18	B	826	CLA	C3C-C4C-NC	-2.11	108.21	110.57
17	4	615	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
18	A	810	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
18	L	302	CLA	C3C-C4C-NC	-2.11	108.21	110.57
18	A	822	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
18	A	809	CLA	C3C-C4C-NC	-2.11	108.21	110.57
18	A	832	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
18	K	202	CLA	C3C-C4C-NC	-2.10	108.21	110.57
18	A	836	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
18	B	802	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
18	4	612	CLA	C3C-C4C-NC	-2.10	108.21	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	822	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
18	B	825	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	A	804	CLA	C4-C3-C5	-2.10	111.74	115.27
18	3	604	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	1	610	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
17	4	607	CHL	CBC-CAC-C3C	-2.10	106.65	112.43
18	F	303	CLA	CMB-C2B-C3B	2.10	128.60	124.68
18	F	303	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	A	821	CLA	CED-O2D-CGD	2.10	120.68	115.94
18	4	601	CLA	CMB-C2B-C3B	2.10	128.60	124.68
18	B	804	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
17	2	607	CHL	C2C-C3C-C4C	2.10	107.98	106.49
18	B	825	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
18	1	613	CLA	C3C-C4C-NC	-2.10	108.22	110.57
18	1	614	CLA	CMB-C2B-C3B	2.10	128.60	124.68
18	B	811	CLA	CMB-C2B-C3B	2.09	128.60	124.68
18	B	801	CLA	C4-C3-C5	-2.09	111.75	115.27
18	A	826	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	1	619	LUT	C31-C30-C29	2.09	130.30	127.31
18	B	808	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
18	A	839	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	4	602	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	2	612	CLA	CMD-C2D-C1D	2.09	128.40	124.71
18	A	823	CLA	CAA-C2A-C3A	-2.09	111.22	116.10
18	B	828	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
18	3	611	CLA	CMD-C2D-C1D	2.09	128.40	124.71
18	A	823	CLA	CMB-C2B-C3B	2.09	128.59	124.68
18	A	829	CLA	CMB-C2B-C3B	2.09	128.59	124.68
18	2	604	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	B	802	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	1	613	CLA	CMD-C2D-C1D	2.09	128.39	124.71
18	4	614	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	3	605	CLA	CED-O2D-CGD	2.09	120.66	115.94
18	A	811	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	B	821	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	3	610	CLA	CMB-C2B-C3B	2.09	128.58	124.68
18	A	824	CLA	CMB-C2B-C3B	2.09	128.58	124.68
18	A	808	CLA	CMB-C2B-C3B	2.09	128.58	124.68
18	A	831	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
18	4	609	CLA	CMB-C2B-C3B	2.08	128.58	124.68
18	3	605	CLA	C3C-C4C-NC	-2.08	108.23	110.57
18	A	825	CLA	O2D-CGD-O1D	-2.08	119.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	813	CLA	CMB-C2B-C3B	2.08	128.57	124.68
18	2	611	CLA	C2D-C1D-ND	2.08	111.64	110.10
18	A	801	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	J	102	CLA	CMD-C2D-C1D	2.08	128.38	124.71
18	2	609	CLA	C3C-C4C-NC	-2.08	108.24	110.57
20	4	617	XAT	O4-C5-C4	-2.08	111.82	113.38
18	A	803	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
18	4	610	CLA	CMB-C2B-C3B	2.08	128.57	124.68
17	3	616	CHL	O2A-CGA-CBA	2.08	120.45	112.23
18	A	832	CLA	C5-C3-C2	2.08	125.32	121.12
18	4	609	CLA	C2C-C1C-NC	-2.08	108.03	109.97
18	A	833	CLA	C1-C2-C3	2.08	129.63	126.04
18	2	608	CLA	C3C-C4C-NC	-2.07	108.24	110.57
18	A	801	CLA	C12-C11-C10	-2.07	103.71	113.24
18	B	806	CLA	CMB-C2B-C3B	2.07	128.56	124.68
18	B	818	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	B	811	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
18	3	607	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	A	811	CLA	CMB-C2B-C3B	2.07	128.56	124.68
18	B	822	CLA	CMB-C2B-C3B	2.07	128.56	124.68
18	A	812	CLA	CMB-C2B-C3B	2.07	128.55	124.68
18	A	826	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	A	811	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
18	L	303	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	1	611	CLA	C2D-C1D-ND	2.07	111.63	110.10
18	3	604	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	A	826	CLA	C2C-C1C-NC	-2.07	108.03	109.97
18	B	807	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	3	617	CLA	C4-C3-C5	-2.07	111.79	115.27
18	2	613	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	G	204	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	2	602	CLA	CMD-C2D-C1D	2.07	128.35	124.71
18	B	812	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	3	605	CLA	C2D-C1D-ND	2.06	111.62	110.10
18	4	602	CLA	CMB-C2B-C3B	2.06	128.54	124.68
18	A	803	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	4	601	CLA	CMD-C2D-C1D	2.06	128.35	124.71
18	A	802	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
18	H	201	CLA	CMD-C2D-C1D	2.06	128.34	124.71
18	3	617	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	3	602	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	810	CLA	CMD-C2D-C1D	2.06	128.34	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	606	CLA	CMB-C2B-C3B	2.06	128.53	124.68
18	A	801	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	835	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	812	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
18	L	304	CLA	C3C-C4C-NC	-2.06	108.27	110.57
17	2	607	CHL	OMC-CMC-C2C	-2.06	121.04	125.69
21	A	846	BCR	C20-C19-C18	2.06	132.19	126.42
18	A	817	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
18	A	801	CLA	C2D-C1D-ND	2.05	111.62	110.10
18	A	837	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	B	834	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
18	B	803	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
18	A	821	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	B	804	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
18	A	832	CLA	C1-C2-C3	2.05	129.59	126.04
18	A	828	CLA	CMB-C2B-C3B	2.05	128.52	124.68
18	K	203	CLA	CMB-C2B-C3B	2.05	128.52	124.68
18	4	608	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	4	603	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	A	807	CLA	CED-O2D-CGD	2.05	120.58	115.94
18	B	840	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	B	807	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
18	A	842	CLA	C3C-C4C-NC	-2.05	108.28	110.57
18	B	831	CLA	C3C-C4C-NC	-2.05	108.28	110.57
17	1	606	CHL	C4D-CHA-C1A	2.05	123.74	121.25
18	A	823	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
18	A	808	CLA	CMD-C2D-C1D	2.05	128.32	124.71
18	B	807	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
18	A	822	CLA	CED-O2D-CGD	2.04	120.56	115.94
18	B	839	CLA	C4D-CHA-C1A	2.04	123.74	121.25
18	B	835	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	1	610	CLA	C2D-C1D-ND	2.04	111.61	110.10
18	1	612	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
18	A	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
18	A	827	CLA	C3C-C4C-NC	-2.04	108.28	110.57
18	B	817	CLA	CMD-C2D-C1D	2.04	128.31	124.71
18	A	836	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	B	821	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	L	303	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	J	102	CLA	C3C-C4C-NC	-2.04	108.28	110.57
18	B	803	CLA	CAA-C2A-C3A	-2.04	111.33	116.10
18	4	604	CLA	CED-O2D-CGD	2.04	120.55	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	605	CLA	CMD-C2D-C1D	2.04	128.31	124.71
18	A	840	CLA	C4-C3-C5	-2.04	111.84	115.27
18	J	102	CLA	C2D-C1D-ND	2.04	111.61	110.10
18	3	612	CLA	CMD-C2D-C1D	2.04	128.31	124.71
17	1	601	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
18	1	607	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	A	827	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
18	3	612	CLA	C3C-C4C-NC	-2.04	108.29	110.57
18	4	604	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
18	B	835	CLA	CED-O2D-CGD	2.04	120.54	115.94
18	4	601	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
19	2	615	LUT	C31-C30-C29	2.04	130.22	127.31
18	F	301	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	B	837	CLA	CMD-C2D-C1D	2.03	128.30	124.71
18	4	613	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
18	A	813	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	B	819	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	A	807	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	2	614	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
18	3	610	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	B	804	CLA	CMB-C2B-C3B	2.03	128.48	124.68
18	B	840	CLA	CMB-C2B-C3B	2.03	128.48	124.68
18	A	819	CLA	CMD-C2D-C1D	2.03	128.29	124.71
17	1	601	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	840	CLA	C12-C11-C10	-2.03	103.91	113.24
17	2	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
18	B	825	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	1	614	CLA	C3C-C4C-NC	-2.03	108.30	110.57
17	2	607	CHL	C2A-C1A-CHA	2.03	127.41	123.86
18	3	610	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	A	839	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	A	815	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	A	823	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	3	613	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	3	617	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	B	820	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	F	304	CLA	CMB-C2B-C3B	2.03	128.47	124.68
18	A	822	CLA	CMB-C2B-C3B	2.02	128.47	124.68
18	B	804	CLA	CMD-C2D-C1D	2.02	128.28	124.71
18	A	830	CLA	CMB-C2B-C3B	2.02	128.46	124.68
18	F	304	CLA	C3C-C4C-NC	-2.02	108.30	110.57
18	L	303	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	817	CLA	C1-C2-C3	2.02	129.54	126.04
18	2	603	CLA	CMB-C2B-C3B	2.02	128.46	124.68
18	2	611	CLA	CMB-C2B-C3B	2.02	128.46	124.68
18	B	815	CLA	C4-C3-C5	-2.02	111.87	115.27
18	A	825	CLA	CMD-C2D-C1D	2.02	128.27	124.71
18	B	825	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
18	4	610	CLA	C2D-C1D-ND	2.02	111.59	110.10
18	B	839	CLA	C4-C3-C5	-2.02	111.88	115.27
18	A	810	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	B	833	CLA	CMB-C2B-C3B	2.02	128.45	124.68
18	4	613	CLA	C3C-C4C-NC	-2.02	108.31	110.57
17	2	614	CHL	C2A-C3A-C4A	2.02	105.13	101.87
18	A	840	CLA	CED-O2D-CGD	2.02	120.50	115.94
18	A	835	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
18	B	836	CLA	CMB-C2B-C3B	2.02	128.45	124.68
18	A	819	CLA	CMB-C2B-C3B	2.02	128.45	124.68
18	4	611	CLA	C3C-C4C-NC	-2.02	108.31	110.57
18	L	302	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
18	1	608	CLA	O2D-CGD-O1D	-2.02	119.90	123.84
19	3	614	LUT	C35-C15-C14	2.02	127.60	123.47
18	B	804	CLA	C2D-C1D-ND	2.02	111.59	110.10
17	2	606	CHL	C4D-CHA-C1A	2.01	123.70	121.25
18	B	809	CLA	CMD-C2D-C1D	2.01	128.26	124.71
18	3	607	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
18	B	840	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
18	F	304	CLA	CED-O2D-CGD	2.01	120.49	115.94
18	4	609	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	F	304	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	A	813	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	1	602	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	1	610	CLA	C3C-C4C-NC	-2.01	108.32	110.57
18	B	821	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	1	602	CLA	CMD-C2D-C1D	2.01	128.25	124.71
18	F	301	CLA	C2D-C1D-ND	2.01	111.58	110.10
17	2	605	CHL	C2A-C1A-CHA	2.01	127.37	123.86
18	A	809	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
17	2	606	CHL	C2A-C1A-CHA	2.01	127.37	123.86
18	1	605	CLA	CBD-CHA-C1A	2.01	130.87	128.50
18	K	201	CLA	CMB-C2B-C3B	2.01	128.43	124.68
18	B	801	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
18	B	815	CLA	CMB-C2B-C3B	2.01	128.43	124.68
18	K	201	CLA	C3C-C4C-NC	-2.00	108.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	826	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
18	1	614	CLA	C2D-C1D-ND	2.00	111.58	110.10
18	A	854	CLA	CMD-C2D-C1D	2.00	128.25	124.71
18	A	836	CLA	CMD-C2D-C1D	2.00	128.24	124.71
18	2	611	CLA	C3C-C4C-NC	-2.00	108.33	110.57
18	1	609	CLA	CMB-C2B-C3B	2.00	128.42	124.68
18	A	837	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
18	A	809	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
18	3	604	CLA	CMD-C2D-C1D	2.00	128.24	124.71

All (179) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	601	CHL	NC
17	1	601	CHL	ND
17	1	601	CHL	NA
17	1	606	CHL	NC
17	1	606	CHL	ND
17	1	606	CHL	NA
17	2	601	CHL	NC
17	2	601	CHL	ND
17	2	601	CHL	NA
17	2	605	CHL	NC
17	2	605	CHL	ND
17	2	605	CHL	NA
17	2	606	CHL	NC
17	2	606	CHL	ND
17	2	606	CHL	NA
17	2	607	CHL	NC
17	2	607	CHL	ND
17	2	607	CHL	NA
17	2	614	CHL	NC
17	2	614	CHL	ND
17	2	614	CHL	NA
17	3	616	CHL	NC
17	3	616	CHL	ND
17	3	616	CHL	NA
17	4	605	CHL	NC
17	4	605	CHL	ND
17	4	605	CHL	NA
17	4	606	CHL	NC
17	4	606	CHL	ND

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Mol	Chain	Res	Type	Atom
17	4	606	CHL	NA
17	4	607	CHL	NC
17	4	607	CHL	ND
17	4	607	CHL	NA
17	4	615	CHL	NC
17	4	615	CHL	ND
17	4	615	CHL	NA
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	605	CLA	ND
18	1	607	CLA	ND
18	1	608	CLA	ND
18	1	609	CLA	ND
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	1	614	CLA	ND
18	2	602	CLA	ND
18	2	603	CLA	ND
18	2	604	CLA	ND
18	2	608	CLA	ND
18	2	609	CLA	ND
18	2	610	CLA	ND
18	2	611	CLA	ND
18	2	612	CLA	ND
18	2	613	CLA	ND
18	3	602	CLA	ND
18	3	603	CLA	ND
18	3	604	CLA	ND
18	3	605	CLA	ND
18	3	606	CLA	ND
18	3	607	CLA	ND
18	3	608	CLA	ND
18	3	609	CLA	ND
18	3	610	CLA	ND
18	3	611	CLA	ND
18	3	612	CLA	ND
18	3	613	CLA	ND
18	3	617	CLA	ND
18	4	601	CLA	ND

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Mol	Chain	Res	Type	Atom
18	4	602	CLA	ND
18	4	603	CLA	ND
18	4	604	CLA	ND
18	4	608	CLA	ND
18	4	609	CLA	ND
18	4	610	CLA	ND
18	4	611	CLA	ND
18	4	612	CLA	ND
18	4	613	CLA	ND
18	4	614	CLA	ND
18	A	801	CLA	ND
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND
18	A	806	CLA	ND
18	A	807	CLA	ND
18	A	808	CLA	ND
18	A	809	CLA	ND
18	A	810	CLA	ND
18	A	811	CLA	ND
18	A	812	CLA	ND
18	A	813	CLA	ND
18	A	814	CLA	ND
18	A	815	CLA	ND
18	A	816	CLA	ND
18	A	817	CLA	ND
18	A	818	CLA	ND
18	A	819	CLA	ND
18	A	820	CLA	ND
18	A	821	CLA	ND
18	A	822	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	825	CLA	ND
18	A	826	CLA	ND
18	A	827	CLA	ND
18	A	828	CLA	ND
18	A	829	CLA	ND
18	A	830	CLA	ND
18	A	831	CLA	ND
18	A	832	CLA	ND

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Mol	Chain	Res	Type	Atom
18	A	833	CLA	ND
18	A	834	CLA	ND
18	A	835	CLA	ND
18	A	836	CLA	ND
18	A	837	CLA	ND
18	A	838	CLA	ND
18	A	839	CLA	ND
18	A	840	CLA	ND
18	A	841	CLA	ND
18	A	842	CLA	ND
18	A	843	CLA	ND
18	A	854	CLA	ND
18	B	801	CLA	ND
18	B	802	CLA	ND
18	B	803	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND
18	B	806	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	812	CLA	ND
18	B	813	CLA	ND
18	B	814	CLA	ND
18	B	815	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	818	CLA	ND
18	B	819	CLA	ND
18	B	820	CLA	ND
18	B	821	CLA	ND
18	B	822	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	826	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	829	CLA	ND
18	B	830	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	831	CLA	ND
18	B	832	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	838	CLA	ND
18	B	839	CLA	ND
18	B	840	CLA	ND
18	F	301	CLA	ND
18	F	303	CLA	ND
18	F	304	CLA	ND
18	G	202	CLA	ND
18	G	203	CLA	ND
18	G	204	CLA	ND
18	H	201	CLA	ND
18	J	102	CLA	ND
18	K	201	CLA	ND
18	K	202	CLA	ND
18	K	203	CLA	ND
18	L	302	CLA	ND
18	L	303	CLA	ND
18	L	304	CLA	ND

All (1565) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	601	CHL	CBA-CGA-O2A-C1
17	2	605	CHL	CHA-CBD-CGD-O2D
17	2	606	CHL	C3A-C2A-CAA-CBA
17	2	607	CHL	C3C-C2C-CMC-OMC
17	2	607	CHL	CHA-CBD-CGD-O1D
17	2	614	CHL	C1A-C2A-CAA-CBA
17	2	614	CHL	CBD-CGD-O2D-CED
17	3	616	CHL	CBA-CGA-O2A-C1
17	4	605	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	C2-C3-C5-C6
17	4	607	CHL	C1A-C2A-CAA-CBA
17	4	607	CHL	C3A-C2A-CAA-CBA
17	4	607	CHL	CHA-CBD-CGD-O1D
17	4	607	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	4	607	CHL	O2A-C1-C2-C3
17	4	607	CHL	C1-C2-C3-C5
17	4	615	CHL	C1A-C2A-CAA-CBA
18	1	603	CLA	CHA-CBD-CGD-O1D
18	1	608	CLA	C11-C12-C13-C14
18	1	609	CLA	C11-C10-C8-C9
18	1	611	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	C1-C2-C3-C4
18	1	613	CLA	C1A-C2A-CAA-CBA
18	1	613	CLA	C3A-C2A-CAA-CBA
18	2	602	CLA	CBD-CGD-O2D-CED
18	2	603	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	C1-C2-C3-C4
18	2	604	CLA	C1-C2-C3-C5
18	2	608	CLA	C1A-C2A-CAA-CBA
18	2	608	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	CBD-CGD-O2D-CED
18	2	611	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	C1-C2-C3-C5
18	3	602	CLA	CHA-CBD-CGD-O2D
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	C1A-C2A-CAA-CBA
18	3	607	CLA	C3A-C2A-CAA-CBA
18	3	610	CLA	CHA-CBD-CGD-O2D
18	3	610	CLA	CBD-CGD-O2D-CED
18	3	617	CLA	C4-C3-C5-C6
18	4	601	CLA	CHA-CBD-CGD-O1D
18	4	602	CLA	CHA-CBD-CGD-O1D
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C4-C3-C5-C6
18	4	610	CLA	C1A-C2A-CAA-CBA
18	4	610	CLA	CHA-CBD-CGD-O2D
18	4	611	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C3A-C2A-CAA-CBA
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	C1-C2-C3-C4
18	4	612	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	801	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	O2A-C1-C2-C3
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C2-C3-C5-C6
18	A	817	CLA	C4-C3-C5-C6
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	C1-C2-C3-C5
18	A	821	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	C2-C3-C5-C6
18	A	825	CLA	O1A-CGA-O2A-C1
18	A	827	CLA	C14-C13-C15-C16
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	C11-C10-C8-C7
18	A	829	CLA	C11-C12-C13-C14
18	A	830	CLA	C2-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C3A-C2A-CAA-CBA
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	837	CLA	C4-C3-C5-C6
18	A	839	CLA	C1A-C2A-CAA-CBA
18	A	839	CLA	CAD-CBD-CGD-O2D
18	A	839	CLA	C1-C2-C3-C4
18	A	839	CLA	C1-C2-C3-C5
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	840	CLA	C1-C2-C3-C4
18	A	841	CLA	C2-C3-C5-C6
18	A	841	CLA	C4-C3-C5-C6
18	B	801	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C1-C2-C3-C5
18	B	802	CLA	C14-C13-C15-C16
18	B	804	CLA	C3A-C2A-CAA-CBA
18	B	807	CLA	C11-C12-C13-C14
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C1-C2-C3-C4
18	B	810	CLA	C1-C2-C3-C4
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	C1-C2-C3-C4
18	B	816	CLA	C1-C2-C3-C5
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	817	CLA	C4-C3-C5-C6
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	C1-C2-C3-C4
18	B	821	CLA	C2-C3-C5-C6
18	B	821	CLA	C4-C3-C5-C6
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	C1-C2-C3-C4
18	B	822	CLA	C1-C2-C3-C5
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	831	CLA	C1A-C2A-CAA-CBA
18	B	831	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	C2A-CAA-CBA-CGA
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CHA-CBD-CGD-O1D
18	B	840	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	CAD-CBD-CGD-O1D
18	B	840	CLA	CAD-CBD-CGD-O2D
18	B	840	CLA	C6-C7-C8-C9
18	F	301	CLA	C3A-C2A-CAA-CBA
18	G	204	CLA	CBD-CGD-O2D-CED
18	G	204	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CBD-CGD-O2D-CED
18	J	102	CLA	C1A-C2A-CAA-CBA
18	J	102	CLA	C3A-C2A-CAA-CBA
18	J	102	CLA	CAD-CBD-CGD-O1D
18	J	102	CLA	CAD-CBD-CGD-O2D
18	K	202	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C3A-C2A-CAA-CBA
18	L	302	CLA	C1A-C2A-CAA-CBA
18	L	302	CLA	C3A-C2A-CAA-CBA
18	L	302	CLA	CHA-CBD-CGD-O1D
18	L	302	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	C1-C2-C3-C4
18	L	303	CLA	C1-C2-C3-C5
18	L	304	CLA	C1A-C2A-CAA-CBA
19	3	614	LUT	C27-C28-C29-C30
19	3	614	LUT	C27-C28-C29-C39
21	2	618	BCR	C7-C8-C9-C10
21	2	618	BCR	C11-C12-C13-C14
21	2	618	BCR	C11-C12-C13-C35
21	2	618	BCR	C17-C18-C19-C20
21	2	618	BCR	C36-C18-C19-C20
21	A	845	BCR	C23-C24-C25-C26
21	A	845	BCR	C23-C24-C25-C30
21	A	846	BCR	C36-C18-C19-C20
21	A	846	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
21	A	848	BCR	C21-C22-C23-C24
21	A	848	BCR	C37-C22-C23-C24
21	A	850	BCR	C11-C12-C13-C35
21	B	843	BCR	C7-C8-C9-C34
21	J	101	BCR	C22-C23-C24-C25
21	J	101	BCR	C23-C24-C25-C26
21	K	204	BCR	C23-C24-C25-C26
21	K	204	BCR	C23-C24-C25-C30
21	L	301	BCR	C1-C6-C7-C8
21	L	301	BCR	C21-C22-C23-C24
21	L	301	BCR	C37-C22-C23-C24
21	L	306	BCR	C23-C24-C25-C26
22	1	618	LHG	C4-O6-P-O5
22	1	621	LHG	O9-C7-O7-C5
22	1	621	LHG	C8-C7-O7-C5
22	1	621	LHG	O10-C23-O8-C6
22	1	621	LHG	C24-C23-O8-C6
22	1	622	LHG	C3-O3-P-O4
22	1	622	LHG	C3-O3-P-O5
22	2	617	LHG	C4-O6-P-O4
22	A	855	LHG	C3-O3-P-O4
22	A	855	LHG	C4-O6-P-O4
23	1	623	LMG	O6-C1-O1-C7
23	1	623	LMG	O10-C28-O8-C9
23	1	623	LMG	C29-C28-O8-C9
23	B	849	LMG	O9-C10-O7-C8
23	B	849	LMG	C11-C10-O7-C8
23	B	849	LMG	O10-C28-O8-C9
23	B	849	LMG	C29-C28-O8-C9
23	F	306	LMG	C2-C1-O1-C7
23	F	306	LMG	O6-C1-O1-C7
23	F	306	LMG	O9-C10-O7-C8
23	F	306	LMG	C11-C10-O7-C8
23	F	306	LMG	O10-C28-O8-C9
23	F	306	LMG	C29-C28-O8-C9
24	4	620	LMT	C2-C1-O1'-C1'
24	A	853	LMT	C2'-C1'-O1'-C1
24	A	853	LMT	O5'-C1'-O1'-C1
24	A	853	LMT	C2-C1-O1'-C1'
24	A	856	LMT	O5'-C1'-O1'-C1
24	G	201	LMT	C2'-C1'-O1'-C1
24	G	201	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
27	B	848	DGD	C2B-C1B-O2G-C2G
27	B	848	DGD	O1B-C1B-O2G-C2G
17	2	614	CHL	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	O1D-CGD-O2D-CED
18	B	812	CLA	C10-C11-C12-C13
24	A	856	LMT	C3'-C4'-O1B-C1B
18	1	605	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	3	610	CLA	O1D-CGD-O2D-CED
18	L	304	CLA	O1D-CGD-O2D-CED
17	2	605	CHL	CBD-CGD-O2D-CED
17	2	606	CHL	CBD-CGD-O2D-CED
17	4	606	CHL	CBD-CGD-O2D-CED
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	CBD-CGD-O2D-CED
18	3	609	CLA	CBD-CGD-O2D-CED
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	CBD-CGD-O2D-CED
18	A	833	CLA	CBD-CGD-O2D-CED
18	B	801	CLA	CBD-CGD-O2D-CED
18	F	304	CLA	CBD-CGD-O2D-CED
18	J	102	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	O1A-CGA-O2A-C1
17	3	616	CHL	O1A-CGA-O2A-C1
18	A	822	CLA	O1D-CGD-O2D-CED
18	J	102	CLA	O1D-CGD-O2D-CED
24	A	853	LMT	O5B-C1B-O1B-C4'
17	2	606	CHL	O1D-CGD-O2D-CED
18	3	605	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	1	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	3	617	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	805	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	O1A-CGA-O2A-C1
18	A	817	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	O1A-CGA-O2A-C1
18	A	842	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	840	CLA	O1A-CGA-O2A-C1
18	H	201	CLA	O1A-CGA-O2A-C1
18	3	605	CLA	C2-C1-O2A-CGA
18	F	301	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C3-C5-C6-C7
18	2	604	CLA	C3-C5-C6-C7
18	A	840	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	818	CLA	C3-C5-C6-C7
18	B	839	CLA	C3-C5-C6-C7
18	F	301	CLA	C3-C5-C6-C7
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	833	CLA	CBA-CGA-O2A-C1
18	B	812	CLA	CBA-CGA-O2A-C1
18	B	840	CLA	CBA-CGA-O2A-C1
18	H	201	CLA	CBA-CGA-O2A-C1
18	A	823	CLA	O1D-CGD-O2D-CED
18	A	854	CLA	C2C-C3C-CAC-CBC
18	B	817	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	C4-C3-C5-C6
18	4	609	CLA	C2-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	F	301	CLA	C2-C3-C5-C6
18	L	303	CLA	CBD-CGD-O2D-CED
17	4	607	CHL	C2A-CAA-CBA-CGA
18	1	612	CLA	C2A-CAA-CBA-CGA
18	3	611	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	A	816	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2A-CAA-CBA-CGA
18	A	837	CLA	C2A-CAA-CBA-CGA
18	A	839	CLA	C2A-CAA-CBA-CGA
18	B	819	CLA	C2A-CAA-CBA-CGA
18	B	823	CLA	C2A-CAA-CBA-CGA
18	L	304	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	B	833	CLA	C3-C5-C6-C7
18	3	610	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	CBA-CGA-O2A-C1
18	A	817	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C1-C2-C3-C5
18	B	820	CLA	C1-C2-C3-C5
17	4	606	CHL	O1D-CGD-O2D-CED
18	A	814	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED
18	3	617	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	832	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	O1A-CGA-O2A-C1
18	1	614	CLA	O1D-CGD-O2D-CED
21	2	618	BCR	C9-C10-C11-C12
18	A	854	CLA	C4C-C3C-CAC-CBC
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	B	809	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	O1A-CGA-O2A-C1
18	K	203	CLA	CBA-CGA-O2A-C1
18	3	608	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	O1A-CGA-O2A-C1
18	B	807	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	3	605	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	C5-C6-C7-C8
18	A	824	CLA	C4-C3-C5-C6
18	B	817	CLA	C2-C3-C5-C6
18	1	614	CLA	C2A-CAA-CBA-CGA
18	3	605	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C2A-CAA-CBA-CGA
18	L	302	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C1-C2-C3-C5
18	A	833	CLA	C1-C2-C3-C5
18	A	834	CLA	O1D-CGD-O2D-CED
18	B	801	CLA	O1D-CGD-O2D-CED
18	B	801	CLA	C5-C6-C7-C8
18	2	602	CLA	O1D-CGD-O2D-CED
18	3	605	CLA	CBA-CGA-O2A-C1
18	3	617	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	CBA-CGA-O2A-C1
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	832	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	A	817	CLA	C10-C11-C12-C13
17	1	601	CHL	C5-C6-C7-C8
18	1	608	CLA	C10-C11-C12-C13
18	A	819	CLA	C5-C6-C7-C8
18	A	833	CLA	C8-C10-C11-C12
18	B	807	CLA	C15-C16-C17-C18
18	B	831	CLA	C15-C16-C17-C18
18	B	840	CLA	C8-C10-C11-C12
24	A	856	LMT	C2'-C1'-O1'-C1
18	A	818	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	C2-C3-C5-C6
18	1	608	CLA	C14-C13-C15-C16
18	1	612	CLA	C11-C10-C8-C9
18	4	612	CLA	C6-C7-C8-C9
18	A	802	CLA	C14-C13-C15-C16
18	A	807	CLA	C14-C13-C15-C16
18	A	817	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
18	A	825	CLA	C11-C12-C13-C14
18	A	826	CLA	C6-C7-C8-C9
18	A	826	CLA	C14-C13-C15-C16
18	A	828	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C12-C13-C14
18	A	834	CLA	C11-C10-C8-C9
18	A	840	CLA	C11-C12-C13-C14
18	A	841	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C12-C13-C14
18	B	801	CLA	C11-C12-C13-C14
18	B	802	CLA	C6-C7-C8-C9
18	B	809	CLA	C6-C7-C8-C9
18	B	813	CLA	C14-C13-C15-C16
18	B	816	CLA	C11-C10-C8-C9
18	B	825	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	B	831	CLA	C14-C13-C15-C16
18	B	839	CLA	C11-C10-C8-C9
18	B	840	CLA	C14-C13-C15-C16
18	L	303	CLA	C11-C10-C8-C9
25	A	844	PQN	C19-C18-C20-C21
25	A	844	PQN	C24-C23-C25-C26
25	B	841	PQN	C19-C18-C20-C21
18	A	833	CLA	O1D-CGD-O2D-CED
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	C13-C15-C16-C17
18	B	815	CLA	C5-C6-C7-C8
18	A	803	CLA	C2A-CAA-CBA-CGA
18	B	838	CLA	C2A-CAA-CBA-CGA
21	2	618	BCR	C7-C8-C9-C34
21	B	843	BCR	C7-C8-C9-C10
23	1	620	LMG	C28-C29-C30-C31
17	2	607	CHL	O1A-CGA-O2A-C1
18	B	804	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C10-C11-C12-C13
18	A	806	CLA	C10-C11-C12-C13
18	A	826	CLA	C15-C16-C17-C18
18	B	805	CLA	C10-C11-C12-C13
18	L	303	CLA	C10-C11-C12-C13
18	4	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	A	804	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	CBA-CGA-O2A-C1
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	829	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C10-C11-C12-C13
18	A	807	CLA	C10-C11-C12-C13
18	A	821	CLA	C15-C16-C17-C18
18	A	826	CLA	C5-C6-C7-C8
18	A	828	CLA	C5-C6-C7-C8
18	A	843	CLA	C8-C10-C11-C12
18	B	802	CLA	C8-C10-C11-C12
18	B	804	CLA	C10-C11-C12-C13
18	B	840	CLA	C5-C6-C7-C8
18	1	609	CLA	C10-C11-C12-C13
18	2	602	CLA	C10-C11-C12-C13
18	4	610	CLA	C10-C11-C12-C13
18	4	612	CLA	C5-C6-C7-C8
18	A	806	CLA	C15-C16-C17-C18
18	A	811	CLA	C15-C16-C17-C18
18	B	802	CLA	C10-C11-C12-C13
18	B	817	CLA	C5-C6-C7-C8
18	B	822	CLA	C5-C6-C7-C8
18	B	838	CLA	C13-C15-C16-C17
18	A	830	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1A-CGA-O2A-C1
17	2	605	CHL	O1D-CGD-O2D-CED
18	A	802	CLA	C10-C11-C12-C13
18	A	828	CLA	C15-C16-C17-C18
18	B	838	CLA	C15-C16-C17-C18
24	4	620	LMT	C5'-C4'-O1B-C1B
18	A	841	CLA	C15-C16-C17-C18
18	3	602	CLA	C5-C6-C7-C8
18	A	827	CLA	C10-C11-C12-C13
18	A	834	CLA	C5-C6-C7-C8
18	A	842	CLA	C10-C11-C12-C13
18	1	602	CLA	C11-C10-C8-C7
18	A	806	CLA	C12-C13-C15-C16
18	A	807	CLA	C11-C12-C13-C15
18	A	811	CLA	C11-C12-C13-C15
18	A	833	CLA	C12-C13-C15-C16
18	A	842	CLA	C12-C13-C15-C16
18	A	843	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	B	809	CLA	C11-C12-C13-C15
18	B	831	CLA	C11-C12-C13-C15
25	B	841	PQN	C16-C17-C18-C20
25	B	841	PQN	C21-C22-C23-C25
18	A	826	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1A-CGA-O2A-C1
18	3	607	CLA	C2A-CAA-CBA-CGA
18	G	202	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	C5-C6-C7-C8
18	1	610	CLA	C5-C6-C7-C8
18	1	612	CLA	C15-C16-C17-C18
18	A	830	CLA	C10-C11-C12-C13
18	A	842	CLA	C5-C6-C7-C8
18	A	807	CLA	O1A-CGA-O2A-C1
18	1	608	CLA	C5-C6-C7-C8
18	B	814	CLA	C5-C6-C7-C8
18	A	812	CLA	C5-C6-C7-C8
18	A	802	CLA	C8-C10-C11-C12
18	A	828	CLA	C10-C11-C12-C13
18	B	807	CLA	C5-C6-C7-C8
18	B	813	CLA	C13-C15-C16-C17
18	A	841	CLA	O1D-CGD-O2D-CED
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	C5-C6-C7-C8
18	A	819	CLA	C13-C15-C16-C17
18	A	838	CLA	C5-C6-C7-C8
18	B	823	CLA	C13-C15-C16-C17
18	B	825	CLA	C10-C11-C12-C13
18	A	843	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	C5-C6-C7-C8
18	B	822	CLA	C8-C10-C11-C12
18	B	828	CLA	C5-C6-C7-C8
18	3	617	CLA	C1-C2-C3-C5
22	1	622	LHG	C3-O3-P-O6
22	2	617	LHG	C4-O6-P-O3
22	A	852	LHG	C3-O3-P-O6
22	A	855	LHG	C3-O3-P-O6
22	A	855	LHG	C4-O6-P-O3
18	4	609	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C8-C10-C11-C12
18	A	825	CLA	C15-C16-C17-C18
18	A	830	CLA	C5-C6-C7-C8
18	B	839	CLA	C15-C16-C17-C18
18	4	613	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C4-C3-C5-C6
18	4	610	CLA	C5-C6-C7-C8
18	A	840	CLA	C5-C6-C7-C8
18	B	801	CLA	C10-C11-C12-C13
18	B	804	CLA	C13-C15-C16-C17
18	B	823	CLA	C5-C6-C7-C8
18	B	826	CLA	C10-C11-C12-C13
18	3	603	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	G	204	CLA	C2A-CAA-CBA-CGA
18	A	807	CLA	C16-C17-C18-C20
18	2	612	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1
18	A	843	CLA	C5-C6-C7-C8
18	B	817	CLA	C10-C11-C12-C13
18	B	805	CLA	C5-C6-C7-C8
18	3	602	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
18	A	824	CLA	O1D-CGD-O2D-CED
18	3	617	CLA	C6-C7-C8-C10
18	A	824	CLA	C6-C7-C8-C9
18	A	833	CLA	C16-C17-C18-C20
18	B	807	CLA	C16-C17-C18-C20
18	A	826	CLA	CBA-CGA-O2A-C1
17	4	607	CHL	C1-C2-C3-C4
18	A	808	CLA	C1-C2-C3-C5
18	A	831	CLA	C1-C2-C3-C5
18	B	824	CLA	C1-C2-C3-C5
18	B	835	CLA	C1-C2-C3-C5
18	A	834	CLA	C2C-C3C-CAC-CBC
18	A	833	CLA	C15-C16-C17-C18
18	B	813	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	B	848	DGD	C4A-C5A-C6A-C7A
18	B	833	CLA	O1D-CGD-O2D-CED
23	1	620	LMG	C2-C1-O1-C7
18	B	822	CLA	CBA-CGA-O2A-C1
17	2	601	CHL	O1A-CGA-O2A-C1
18	A	813	CLA	C10-C11-C12-C13
18	B	820	CLA	C6-C7-C8-C9
18	L	303	CLA	C11-C12-C13-C15
18	B	822	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	C4-C3-C5-C6
22	A	855	LHG	C9-C10-C11-C12
18	4	612	CLA	C2-C3-C5-C6
18	4	602	CLA	C11-C10-C8-C9
18	A	801	CLA	C11-C12-C13-C14
18	A	811	CLA	C11-C10-C8-C9
18	A	817	CLA	C6-C7-C8-C9
18	A	830	CLA	C11-C12-C13-C14
18	B	802	CLA	C11-C10-C8-C9
25	B	841	PQN	C21-C22-C23-C24
23	4	619	LMG	C31-C32-C33-C34
18	1	613	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	A	831	CLA	C2A-CAA-CBA-CGA
18	B	821	CLA	O1A-CGA-O2A-C1
21	A	850	BCR	C11-C12-C13-C14
23	4	619	LMG	C28-C29-C30-C31
24	4	620	LMT	C3'-C4'-O1B-C1B
18	3	617	CLA	C6-C7-C8-C9
18	A	806	CLA	C16-C17-C18-C20
18	A	807	CLA	C16-C17-C18-C19
18	A	833	CLA	C16-C17-C18-C19
18	B	836	CLA	C16-C17-C18-C20
18	3	603	CLA	C5-C6-C7-C8
18	B	805	CLA	C8-C10-C11-C12
18	3	609	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	C5-C6-C7-C8
23	1	623	LMG	C36-C37-C38-C39
18	4	601	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBD-CGD-O2D-CED
27	B	848	DGD	C1B-C2B-C3B-C4B
18	A	842	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	A	840	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	CBA-CGA-O2A-C1
18	A	801	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	K	203	CLA	O1D-CGD-O2D-CED
17	4	606	CHL	C3A-C2A-CAA-CBA
18	4	603	CLA	C3A-C2A-CAA-CBA
18	4	610	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	B	808	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
23	B	849	LMG	C14-C15-C16-C17
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	C16-C17-C18-C19
22	A	852	LHG	C4-C5-C6-O8
23	1	623	LMG	C7-C8-C9-O8
18	1	603	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	O2A-C1-C2-C3
18	1	608	CLA	C3-C5-C6-C7
18	B	807	CLA	C13-C15-C16-C17
18	A	825	CLA	C4-C3-C5-C6
18	A	842	CLA	C4-C3-C5-C6
18	A	806	CLA	C2-C3-C5-C6
18	A	807	CLA	C2-C3-C5-C6
18	A	825	CLA	C2-C3-C5-C6
18	B	828	CLA	C2-C3-C5-C6
18	B	840	CLA	C2-C3-C5-C6
18	B	840	CLA	C1-C2-C3-C5
18	B	805	CLA	C2A-CAA-CBA-CGA
23	1	620	LMG	C22-C23-C24-C25
18	B	820	CLA	C6-C7-C8-C10
18	B	827	CLA	C16-C17-C18-C20
18	A	811	CLA	CBA-CGA-O2A-C1
18	B	801	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	834	CLA	CBD-CGD-O2D-CED
23	1	623	LMG	O6-C5-C6-O5
18	B	822	CLA	C2-C1-O2A-CGA
18	B	828	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	C3-C5-C6-C7
18	A	838	CLA	C3-C5-C6-C7
18	B	838	CLA	C3-C5-C6-C7
19	1	619	LUT	C1-C6-C7-C8
19	1	619	LUT	C5-C6-C7-C8
21	2	618	BCR	C1-C6-C7-C8
21	2	618	BCR	C5-C6-C7-C8
21	2	618	BCR	C23-C24-C25-C26
21	2	618	BCR	C23-C24-C25-C30
21	4	618	BCR	C23-C24-C25-C26
21	4	618	BCR	C23-C24-C25-C30
21	A	845	BCR	C1-C6-C7-C8
21	A	846	BCR	C23-C24-C25-C26
21	A	850	BCR	C5-C6-C7-C8
21	J	101	BCR	C23-C24-C25-C30
21	K	205	BCR	C23-C24-C25-C26
21	K	205	BCR	C23-C24-C25-C30
21	L	301	BCR	C5-C6-C7-C8
21	L	305	BCR	C23-C24-C25-C26
21	L	305	BCR	C23-C24-C25-C30
21	L	306	BCR	C23-C24-C25-C30
21	L	307	BCR	C1-C6-C7-C8
21	L	307	BCR	C5-C6-C7-C8
18	B	811	CLA	C2A-CAA-CBA-CGA
18	B	831	CLA	CBA-CGA-O2A-C1
18	1	602	CLA	C10-C11-C12-C13
18	2	602	CLA	C15-C16-C17-C18
18	A	804	CLA	C5-C6-C7-C8
18	A	842	CLA	C15-C16-C17-C18
18	B	809	CLA	C15-C16-C17-C18
18	B	836	CLA	C15-C16-C17-C18
18	1	602	CLA	C14-C13-C15-C16
18	A	810	CLA	O1D-CGD-O2D-CED
18	G	202	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	C2-C3-C5-C6
18	4	602	CLA	C11-C10-C8-C7
18	4	612	CLA	C6-C7-C8-C10
18	A	801	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	A	801	CLA	C12-C13-C15-C16
18	A	811	CLA	C11-C10-C8-C7
18	A	817	CLA	C6-C7-C8-C10
18	A	828	CLA	C11-C10-C8-C7
18	A	828	CLA	C11-C12-C13-C15
18	A	830	CLA	C11-C12-C13-C15
18	A	842	CLA	C2-C3-C5-C6
18	B	801	CLA	C2-C3-C5-C6
18	B	802	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	804	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C10-C8-C7
18	B	805	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C12-C13-C15
18	B	833	CLA	C2-C3-C5-C6
18	B	839	CLA	C11-C10-C8-C7
25	A	844	PQN	C17-C18-C20-C21
25	B	841	PQN	C17-C18-C20-C21
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	O1A-CGA-O2A-C1
18	2	604	CLA	C15-C16-C17-C18
18	A	817	CLA	C11-C12-C13-C14
18	A	824	CLA	C6-C7-C8-C10
18	B	817	CLA	C11-C12-C13-C14
18	K	203	CLA	O1A-CGA-O2A-C1
18	4	614	CLA	CBA-CGA-O2A-C1
18	A	807	CLA	CBA-CGA-O2A-C1
18	B	804	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
17	3	616	CHL	C2A-CAA-CBA-CGA
18	A	828	CLA	C2A-CAA-CBA-CGA
18	K	203	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	821	CLA	C16-C17-C18-C20
23	1	620	LMG	O6-C1-O1-C7
18	A	843	CLA	C15-C16-C17-C18
18	B	833	CLA	C5-C6-C7-C8
18	B	816	CLA	C10-C11-C12-C13
18	B	839	CLA	C10-C11-C12-C13
18	4	614	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	4	610	CLA	C3-C5-C6-C7
23	4	621	LMG	C2-C1-O1-C7
22	1	618	LHG	O7-C5-C6-O8
23	F	306	LMG	O1-C7-C8-O7
18	1	608	CLA	C8-C10-C11-C12
18	1	612	CLA	C5-C6-C7-C8
18	B	801	CLA	C4-C3-C5-C6
18	B	805	CLA	C4-C3-C5-C6
18	B	816	CLA	C2-C3-C5-C6
18	1	602	CLA	C11-C12-C13-C14
18	1	608	CLA	C11-C10-C8-C9
18	1	612	CLA	C14-C13-C15-C16
18	A	806	CLA	C14-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C14
18	A	813	CLA	C11-C10-C8-C9
18	A	819	CLA	C14-C13-C15-C16
18	A	825	CLA	C11-C10-C8-C9
18	A	833	CLA	C14-C13-C15-C16
18	B	804	CLA	C11-C12-C13-C14
18	B	812	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	B	831	CLA	C11-C12-C13-C14
25	B	841	PQN	C16-C17-C18-C19
18	1	610	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	C2A-CAA-CBA-CGA
18	B	826	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	CBA-CGA-O2A-C1
18	A	832	CLA	O1D-CGD-O2D-CED
18	B	838	CLA	C8-C10-C11-C12
18	A	812	CLA	O1A-CGA-O2A-C1
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	607	CHL	C1A-C2A-CAA-CBA
17	4	606	CHL	C1A-C2A-CAA-CBA
18	2	613	CLA	C1A-C2A-CAA-CBA
18	4	603	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	835	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	804	CLA	C1A-C2A-CAA-CBA
18	B	808	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C1A-C2A-CAA-CBA
18	L	303	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C16-C17-C18-C19
18	B	827	CLA	C16-C17-C18-C19
18	L	303	CLA	C11-C12-C13-C14
18	B	838	CLA	C10-C11-C12-C13
22	1	621	LHG	C4-O6-P-O3
23	B	849	LMG	O6-C5-C6-O5
24	A	856	LMT	O5B-C5B-C6B-O6B
18	B	820	CLA	C3-C5-C6-C7
18	A	818	CLA	C10-C11-C12-C13
18	A	811	CLA	C10-C11-C12-C13
18	A	813	CLA	C8-C10-C11-C12
18	L	302	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C16-C17-C18-C19
18	B	822	CLA	C10-C11-C12-C13
18	B	805	CLA	O1D-CGD-O2D-CED
17	2	614	CHL	C3A-C2A-CAA-CBA
17	4	615	CHL	C3A-C2A-CAA-CBA
18	1	608	CLA	C15-C16-C17-C18
18	A	813	CLA	C15-C16-C17-C18
18	4	614	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C6-C7-C8-C9
18	B	839	CLA	C16-C17-C18-C19
18	A	825	CLA	C3-C5-C6-C7
22	1	621	LHG	C4-C5-C6-O8
23	4	621	LMG	C7-C8-C9-O8
23	1	620	LMG	C8-C7-O1-C1
18	A	840	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C5-C6-C7-C8
18	3	608	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	C11-C12-C13-C14
18	4	602	CLA	CBD-CGD-O2D-CED
24	A	856	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
18	A	826	CLA	C10-C11-C12-C13
18	A	834	CLA	C4-C3-C5-C6
18	B	815	CLA	C4-C3-C5-C6
18	G	202	CLA	CBD-CGD-O2D-CED
18	2	604	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	4	614	CLA	C1-C2-C3-C5
18	3	607	CLA	O1D-CGD-O2D-CED
18	B	825	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	C4C-C3C-CAC-CBC
18	1	602	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C15-C16-C17-C18
23	B	849	LMG	C21-C22-C23-C24
18	1	610	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	CBA-CGA-O2A-C1
18	B	833	CLA	CBA-CGA-O2A-C1
18	2	612	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C6-C7-C8-C10
18	B	839	CLA	C16-C17-C18-C20
18	B	831	CLA	C10-C11-C12-C13
18	4	610	CLA	CAA-CBA-CGA-O2A
23	B	849	LMG	O1-C7-C8-O7
18	A	813	CLA	C1-C2-C3-C5
18	B	827	CLA	C10-C11-C12-C13
18	3	602	CLA	O1A-CGA-O2A-C1
18	A	813	CLA	C4-C3-C5-C6
18	1	602	CLA	C11-C12-C13-C15
18	1	608	CLA	C11-C12-C13-C15
18	1	612	CLA	C12-C13-C15-C16
18	4	610	CLA	C6-C7-C8-C10
18	A	803	CLA	C6-C7-C8-C10
18	A	813	CLA	C11-C10-C8-C7
18	A	813	CLA	C12-C13-C15-C16
18	A	819	CLA	C12-C13-C15-C16
18	A	825	CLA	C11-C10-C8-C7
18	A	842	CLA	C11-C12-C13-C15
18	A	843	CLA	C11-C12-C13-C15
18	B	801	CLA	C11-C12-C13-C15
18	B	805	CLA	C2-C3-C5-C6
18	B	805	CLA	C11-C12-C13-C15
18	B	807	CLA	C11-C12-C13-C15
18	B	812	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B	823	CLA	C11-C10-C8-C7
18	B	823	CLA	C11-C12-C13-C15
18	B	823	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C7
18	B	826	CLA	C11-C10-C8-C7
18	B	828	CLA	C6-C7-C8-C10
18	B	839	CLA	C11-C12-C13-C15
18	B	839	CLA	C12-C13-C15-C16
18	B	840	CLA	C11-C10-C8-C7
18	B	840	CLA	C12-C13-C15-C16
18	A	801	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	C3-C5-C6-C7
18	3	602	CLA	C6-C7-C8-C9
18	4	610	CLA	C6-C7-C8-C9
18	A	802	CLA	C11-C10-C8-C9
18	A	807	CLA	C11-C12-C13-C14
18	A	819	CLA	C11-C12-C13-C14
18	A	840	CLA	C11-C10-C8-C9
18	A	842	CLA	C11-C10-C8-C9
18	A	842	CLA	C14-C13-C15-C16
18	A	843	CLA	C11-C12-C13-C14
18	B	801	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C10-C8-C9
18	B	823	CLA	C6-C7-C8-C9
18	B	826	CLA	C11-C10-C8-C9
18	B	840	CLA	C11-C12-C13-C14
18	F	301	CLA	C6-C7-C8-C9
18	A	813	CLA	CBA-CGA-O2A-C1
18	B	838	CLA	CBA-CGA-O2A-C1
18	2	610	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	C8-C10-C11-C12
18	4	601	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	828	CLA	C8-C10-C11-C12
18	B	809	CLA	C5-C6-C7-C8
18	B	830	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C16-C17-C18-C19
18	B	813	CLA	C8-C10-C11-C12
18	A	817	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
18	B	840	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	A	834	CLA	C2-C3-C5-C6
18	B	807	CLA	C2-C3-C5-C6
18	B	826	CLA	C2-C3-C5-C6
18	B	817	CLA	C8-C10-C11-C12
18	1	603	CLA	CBA-CGA-O2A-C1
18	B	801	CLA	CBA-CGA-O2A-C1
18	3	617	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C3A-C2A-CAA-CBA
18	A	837	CLA	C3A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA
18	B	839	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3-C5-C6-C7
18	B	805	CLA	C16-C17-C18-C19
18	B	835	CLA	CBA-CGA-O2A-C1
22	1	618	LHG	C4-C5-C6-O8
23	B	849	LMG	O1-C7-C8-C9
23	F	306	LMG	O1-C7-C8-C9
18	A	812	CLA	O2A-C1-C2-C3
18	A	831	CLA	O2A-C1-C2-C3
18	B	831	CLA	O2A-C1-C2-C3
18	A	842	CLA	C3-C5-C6-C7
18	A	819	CLA	C2-C3-C5-C6
18	4	613	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	C2A-CAA-CBA-CGA
18	A	825	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	CBA-CGA-O2A-C1
17	1	601	CHL	C6-C7-C8-C9
18	1	609	CLA	C5-C6-C7-C8
18	1	602	CLA	O1A-CGA-O2A-C1
18	1	610	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
23	1	623	LMG	C2-C1-O1-C7
27	B	848	DGD	O2G-C2G-C3G-O3G
18	B	805	CLA	C16-C17-C18-C20
18	B	817	CLA	C11-C12-C13-C15
18	B	824	CLA	C2-C1-O2A-CGA
18	A	818	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2	604	CLA	C11-C10-C8-C9
18	A	803	CLA	C6-C7-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	B	817	CLA	C11-C10-C8-C9
18	B	822	CLA	C6-C7-C8-C9
18	B	823	CLA	C14-C13-C15-C16
18	B	825	CLA	C14-C13-C15-C16
18	B	838	CLA	C14-C13-C15-C16
18	B	839	CLA	C11-C12-C13-C14
18	B	840	CLA	C11-C10-C8-C9
18	A	819	CLA	C10-C11-C12-C13
18	3	603	CLA	C6-C7-C8-C9
18	B	812	CLA	C16-C17-C18-C19
19	2	615	LUT	C1-C6-C7-C8
21	A	845	BCR	C5-C6-C7-C8
21	A	850	BCR	C1-C6-C7-C8
21	J	103	BCR	C23-C24-C25-C26
21	J	103	BCR	C23-C24-C25-C30
21	K	205	BCR	C1-C6-C7-C8
21	K	205	BCR	C5-C6-C7-C8
18	A	830	CLA	C13-C15-C16-C17
18	2	613	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	O1A-CGA-O2A-C1
18	A	813	CLA	C13-C15-C16-C17
18	A	817	CLA	C11-C12-C13-C15
18	B	828	CLA	C11-C10-C8-C9
18	B	809	CLA	C10-C11-C12-C13
18	B	814	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	C15-C16-C17-C18
18	B	804	CLA	C15-C16-C17-C18
22	1	618	LHG	O6-C4-C5-C6
18	1	609	CLA	C11-C10-C8-C7
18	2	604	CLA	C11-C10-C8-C7
18	3	602	CLA	C6-C7-C8-C10
18	A	806	CLA	C11-C10-C8-C7
18	A	819	CLA	C11-C12-C13-C15
18	A	825	CLA	C11-C12-C13-C15
18	A	826	CLA	C6-C7-C8-C10
18	A	827	CLA	C12-C13-C15-C16
18	A	829	CLA	C11-C12-C13-C15
18	A	840	CLA	C11-C10-C8-C7
18	A	842	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
18	B	801	CLA	C11-C10-C8-C7
18	B	809	CLA	C12-C13-C15-C16
18	B	813	CLA	C11-C10-C8-C7
18	B	816	CLA	C6-C7-C8-C10
18	B	816	CLA	C11-C10-C8-C7
18	B	817	CLA	C11-C10-C8-C7
18	B	823	CLA	C6-C7-C8-C10
18	B	827	CLA	C12-C13-C15-C16
18	B	838	CLA	C12-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C10
18	B	840	CLA	C11-C12-C13-C15
18	F	301	CLA	C6-C7-C8-C10
21	2	618	BCR	C19-C20-C21-C22
18	3	603	CLA	C6-C7-C8-C10
18	A	829	CLA	C15-C16-C17-C18
18	4	608	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C16-C17-C18-C20
23	1	620	LMG	C33-C34-C35-C36
17	3	616	CHL	CBD-CGD-O2D-CED
18	1	613	CLA	CAD-CBD-CGD-O2D
18	2	602	CLA	CAD-CBD-CGD-O2D
18	2	613	CLA	CAD-CBD-CGD-O2D
18	3	609	CLA	CAD-CBD-CGD-O2D
18	3	617	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	604	CLA	CAD-CBD-CGD-O2D
18	A	808	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	830	CLA	CAD-CBD-CGD-O2D
18	B	809	CLA	CAD-CBD-CGD-O2D
18	B	819	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	CAD-CBD-CGD-O2D
18	F	303	CLA	CAD-CBD-CGD-O2D
18	G	202	CLA	CAD-CBD-CGD-O2D
22	A	852	LHG	C32-C33-C34-C35
18	A	802	CLA	C13-C15-C16-C17
21	A	847	BCR	C6-C7-C8-C9
18	A	828	CLA	CBA-CGA-O2A-C1
22	1	621	LHG	C2-C3-O3-P
18	A	801	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	1	618	LHG	O6-C4-C5-O7
18	2	604	CLA	C8-C10-C11-C12
18	A	824	CLA	C5-C6-C7-C8
18	4	602	CLA	C11-C12-C13-C15
18	A	829	CLA	C16-C17-C18-C20
18	B	831	CLA	O1D-CGD-O2D-CED
17	2	605	CHL	CHA-CBD-CGD-O1D
17	2	607	CHL	CHA-CBD-CGD-O2D
17	4	605	CHL	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	3	602	CLA	CHA-CBD-CGD-O1D
18	3	610	CLA	CHA-CBD-CGD-O1D
18	4	603	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	805	CLA	CHA-CBD-CGD-O1D
18	A	805	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O1D
18	A	819	CLA	CHA-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	O1A-CGA-O2A-C1
23	B	849	LMG	C2-C1-O1-C7
23	B	849	LMG	C16-C17-C18-C19
23	4	621	LMG	O1-C7-C8-O7
23	4	621	LMG	O7-C8-C9-O8
18	A	825	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	L	303	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1D-CGD-O2D-CED
22	1	618	LHG	C23-C24-C25-C26
25	A	844	PQN	C16-C17-C18-C19
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	CBD-CGD-O2D-CED
21	A	847	BCR	C7-C8-C9-C34
21	A	846	BCR	C17-C18-C19-C20
21	L	305	BCR	C21-C22-C23-C24
18	2	604	CLA	C1A-C2A-CAA-CBA
18	A	837	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
18	B	839	CLA	C1A-C2A-CAA-CBA
18	2	602	CLA	C16-C17-C18-C20
18	A	827	CLA	C1-C2-C3-C5
22	1	618	LHG	C4-O6-P-O3
22	A	852	LHG	C4-O6-P-O3
22	1	618	LHG	C5-C4-O6-P
22	A	852	LHG	C3-O3-P-O5
22	A	855	LHG	C4-O6-P-O5
18	3	602	CLA	C11-C12-C13-C15
18	A	804	CLA	C6-C7-C8-C10
18	A	809	CLA	C6-C7-C8-C10
23	B	849	LMG	O6-C1-O1-C7
18	A	831	CLA	CBD-CGD-O2D-CED
17	3	616	CHL	CAD-CBD-CGD-O1D
18	4	601	CLA	CAD-CBD-CGD-O1D
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	813	CLA	CAD-CBD-CGD-O1D
18	A	824	CLA	CAD-CBD-CGD-O1D
18	A	827	CLA	CAD-CBD-CGD-O1D
18	A	833	CLA	CAD-CBD-CGD-O1D
18	B	804	CLA	CAD-CBD-CGD-O1D
18	B	812	CLA	CAD-CBD-CGD-O1D
18	B	828	CLA	CAD-CBD-CGD-O1D
18	H	201	CLA	C2-C3-C5-C6
18	B	805	CLA	C15-C16-C17-C18
18	A	819	CLA	C16-C17-C18-C19
18	B	826	CLA	C11-C12-C13-C14
17	1	601	CHL	CAD-CBD-CGD-O2D
18	1	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	1	612	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C12-C13-C15
18	A	819	CLA	C6-C7-C8-C10
18	A	826	CLA	C11-C12-C13-C15
18	A	834	CLA	C11-C10-C8-C7
18	A	840	CLA	C6-C7-C8-C10
18	B	802	CLA	C12-C13-C15-C16
18	B	812	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C12-C13-C15
18	B	813	CLA	C12-C13-C15-C16
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C6-C7-C8-C10
18	B	836	CLA	C12-C13-C15-C16
25	A	844	PQN	C22-C23-C25-C26
18	B	801	CLA	CAA-CBA-CGA-O2A
17	2	607	CHL	C1C-C2C-CMC-OMC
23	4	621	LMG	O1-C7-C8-C9
22	1	621	LHG	O7-C5-C6-O8
22	A	852	LHG	O7-C5-C6-O8
23	1	623	LMG	O7-C8-C9-O8
18	B	816	CLA	O2A-C1-C2-C3
18	A	810	CLA	CBA-CGA-O2A-C1
18	B	815	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C6-C7-C8-C9
18	A	826	CLA	C11-C12-C13-C14
18	A	828	CLA	C14-C13-C15-C16
18	A	829	CLA	C11-C10-C8-C9
18	A	843	CLA	C11-C10-C8-C9
18	A	843	CLA	C14-C13-C15-C16
18	B	801	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C9
18	2	604	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	O1D-CGD-O2D-CED
18	A	809	CLA	C6-C7-C8-C9
18	3	602	CLA	C2A-CAA-CBA-CGA
21	2	618	BCR	C10-C11-C12-C13
21	A	846	BCR	C18-C19-C20-C21
21	A	850	BCR	C10-C11-C12-C13
18	A	833	CLA	C3-C5-C6-C7
18	4	601	CLA	CAA-CBA-CGA-O2A
18	B	833	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	836	CLA	C5-C6-C7-C8
18	B	840	CLA	C16-C17-C18-C19
18	3	617	CLA	C5-C6-C7-C8
18	A	810	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	C2A-CAA-CBA-CGA
18	B	815	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C1-C2-C3-C5
18	B	813	CLA	C1-C2-C3-C5
18	A	804	CLA	C2-C1-O2A-CGA
18	A	806	CLA	C2-C1-O2A-CGA
18	A	812	CLA	C2-C1-O2A-CGA
18	A	804	CLA	C6-C7-C8-C9
23	1	620	LMG	C17-C18-C19-C20
22	A	852	LHG	C25-C26-C27-C28
18	B	813	CLA	C4-C3-C5-C6
21	1	617	BCR	C23-C24-C25-C30
18	4	610	CLA	C8-C10-C11-C12
17	1	606	CHL	C2C-C3C-CAC-CBC
18	A	837	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	CBD-CGD-O2D-CED
18	1	608	CLA	C1-C2-C3-C5
22	2	617	LHG	C3-O3-P-O6
18	A	807	CLA	C12-C13-C15-C16
18	B	801	CLA	C6-C7-C8-C10
18	B	831	CLA	C3-C5-C6-C7
18	1	602	CLA	C11-C10-C8-C9
18	A	813	CLA	C14-C13-C15-C16
18	A	819	CLA	C6-C7-C8-C9
18	A	840	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C12-C13-C14
18	B	812	CLA	C11-C12-C13-C14
18	B	813	CLA	C11-C12-C13-C14
18	3	602	CLA	C11-C12-C13-C14
18	A	801	CLA	C15-C16-C17-C18
18	A	829	CLA	CBD-CGD-O2D-CED
18	B	801	CLA	C8-C10-C11-C12
18	B	827	CLA	C13-C15-C16-C17
18	1	602	CLA	C12-C13-C15-C16
18	B	828	CLA	C11-C10-C8-C7
23	1	623	LMG	C33-C34-C35-C36
18	A	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	826	CLA	C11-C12-C13-C15
18	B	819	CLA	CBA-CGA-O2A-C1
17	2	601	CHL	CBD-CGD-O2D-CED
23	4	621	LMG	C24-C25-C26-C27
18	A	827	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	C5-C6-C7-C8
18	B	808	CLA	C5-C6-C7-C8
18	B	808	CLA	C6-C7-C8-C9
18	1	608	CLA	C4-C3-C5-C6
18	B	826	CLA	C4-C3-C5-C6
18	B	804	CLA	C5-C6-C7-C8
18	B	827	CLA	C15-C16-C17-C18
17	1	601	CHL	C2-C1-O2A-CGA
18	4	614	CLA	C2-C1-O2A-CGA
18	B	805	CLA	C2-C1-O2A-CGA
18	A	834	CLA	C8-C10-C11-C12
18	B	807	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	CBA-CGA-O2A-C1
22	2	617	LHG	C2-C3-O3-P
22	2	617	LHG	C5-C4-O6-P
18	3	604	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	839	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	K	202	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C11-C12-C13-C14
18	1	604	CLA	O2A-C1-C2-C3
18	1	612	CLA	CBD-CGD-O2D-CED
18	A	809	CLA	C4-C3-C5-C6
18	A	801	CLA	C14-C13-C15-C16
18	A	827	CLA	C6-C7-C8-C9
18	A	841	CLA	C6-C7-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	B	802	CLA	C11-C12-C13-C14
18	B	825	CLA	C6-C7-C8-C9
18	B	809	CLA	C16-C17-C18-C19
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	816	CLA	CAA-CBA-CGA-O1A
21	A	849	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
21	A	849	BCR	C16-C17-C18-C36
21	A	850	BCR	C16-C17-C18-C36
21	B	844	BCR	C11-C10-C9-C34
21	B	844	BCR	C20-C21-C22-C37
21	F	305	BCR	C35-C13-C14-C15
21	L	307	BCR	C11-C10-C9-C34
18	2	608	CLA	CAA-CBA-CGA-O2A
18	A	824	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C5-C6-C7-C8
18	B	808	CLA	C6-C7-C8-C10
25	A	844	PQN	C26-C27-C28-C30
18	B	820	CLA	O2A-C1-C2-C3
18	L	304	CLA	CAA-CBA-CGA-O1A
18	B	833	CLA	C4-C3-C5-C6
18	1	614	CLA	C1A-C2A-CAA-CBA
18	3	604	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	A	840	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C11-C12-C13-C15
18	2	604	CLA	C11-C12-C13-C15
18	4	612	CLA	C11-C10-C8-C7
18	A	840	CLA	C11-C12-C13-C15
18	A	841	CLA	C12-C13-C15-C16
18	A	843	CLA	C6-C7-C8-C10
18	B	822	CLA	C11-C10-C8-C7
18	B	816	CLA	C5-C6-C7-C8
18	A	835	CLA	CAA-CBA-CGA-O1A
18	1	614	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C2A-CAA-CBA-CGA
18	G	204	CLA	CAA-CBA-CGA-O1A
18	2	603	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	C8-C10-C11-C12
18	B	838	CLA	C5-C6-C7-C8
18	A	827	CLA	O1D-CGD-O2D-CED
21	A	849	BCR	C11-C10-C9-C8
21	A	849	BCR	C16-C17-C18-C19
21	A	850	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	B	844	BCR	C11-C10-C9-C8
21	B	844	BCR	C20-C21-C22-C23
21	F	305	BCR	C12-C13-C14-C15
21	L	307	BCR	C11-C10-C9-C8
22	1	621	LHG	C11-C12-C13-C14
18	1	608	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	C3-C5-C6-C7
18	B	823	CLA	O1A-CGA-O2A-C1
25	B	841	PQN	C13-C15-C16-C17
18	1	609	CLA	C4-C3-C5-C6
18	2	612	CLA	C4-C3-C5-C6
18	B	820	CLA	C4-C3-C5-C6
18	A	825	CLA	C2-C1-O2A-CGA
18	A	837	CLA	C2-C1-O2A-CGA
18	B	809	CLA	C2-C1-O2A-CGA
18	B	815	CLA	C2-C3-C5-C6
18	1	611	CLA	CAA-CBA-CGA-O2A
18	2	611	CLA	CAA-CBA-CGA-O2A
18	B	836	CLA	C11-C12-C13-C14
18	2	608	CLA	CAA-CBA-CGA-O1A
18	B	839	CLA	C2A-CAA-CBA-CGA
17	1	606	CHL	C4C-C3C-CAC-CBC
23	4	621	LMG	C20-C21-C22-C23
18	4	602	CLA	O1A-CGA-O2A-C1
19	4	616	LUT	C1-C6-C7-C8
21	1	617	BCR	C23-C24-C25-C26
21	B	843	BCR	C1-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C30
21	J	101	BCR	C1-C6-C7-C8
18	B	818	CLA	C4-C3-C5-C6
17	2	606	CHL	C1A-C2A-CAA-CBA
18	3	607	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	C8-C10-C11-C12
18	A	835	CLA	CAA-CBA-CGA-O2A
18	L	304	CLA	CAA-CBA-CGA-O2A
18	2	612	CLA	C6-C7-C8-C9
22	A	852	LHG	C10-C11-C12-C13
17	4	606	CHL	CAA-CBA-CGA-O2A
18	3	604	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C2A-CAA-CBA-CGA
18	F	301	CLA	C5-C6-C7-C8
18	3	607	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	A	816	CLA	CAA-CBA-CGA-O2A
18	B	801	CLA	C16-C17-C18-C19
18	1	608	CLA	C11-C10-C8-C7
22	A	852	LHG	C14-C15-C16-C17
18	A	802	CLA	C1-C2-C3-C4
18	A	818	CLA	C1-C2-C3-C4
18	A	828	CLA	C1-C2-C3-C4
18	A	840	CLA	C16-C17-C18-C19
18	G	204	CLA	CAA-CBA-CGA-O2A
23	F	306	LMG	O7-C8-C9-O8
18	1	609	CLA	O1A-CGA-O2A-C1
18	A	802	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	CAA-CBA-CGA-O2A
23	1	620	LMG	C11-C12-C13-C14
18	1	603	CLA	C4-C3-C5-C6
18	2	604	CLA	C4-C3-C5-C6
18	A	827	CLA	C4-C3-C5-C6
18	4	612	CLA	C11-C10-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	821	CLA	C6-C7-C8-C9
18	A	830	CLA	C6-C7-C8-C9
18	B	827	CLA	C6-C7-C8-C9
18	B	836	CLA	C14-C13-C15-C16
18	B	839	CLA	C14-C13-C15-C16
18	B	817	CLA	C3-C5-C6-C7
23	B	849	LMG	C17-C18-C19-C20
18	1	614	CLA	C3A-C2A-CAA-CBA
18	A	811	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	B	816	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	CAA-CBA-CGA-O2A
22	1	622	LHG	O7-C7-C8-C9
18	2	611	CLA	CAA-CBA-CGA-O1A
17	2	614	CHL	CAD-CBD-CGD-O2D
18	1	604	CLA	CAD-CBD-CGD-O2D
18	2	604	CLA	CAD-CBD-CGD-O2D
18	4	602	CLA	CAD-CBD-CGD-O2D
18	A	805	CLA	CAD-CBD-CGD-O2D
18	A	807	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	814	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	820	CLA	CAD-CBD-CGD-O2D
18	A	825	CLA	CAD-CBD-CGD-O2D
18	A	834	CLA	CAD-CBD-CGD-O2D
18	A	837	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	811	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	831	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	K	202	CLA	CAD-CBD-CGD-O2D
18	K	203	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	2	603	CLA	C2A-CAA-CBA-CGA
23	F	306	LMG	C32-C33-C34-C35
18	A	807	CLA	C2-C1-O2A-CGA
18	A	808	CLA	C1-C2-C3-C4
18	B	832	CLA	CAA-CBA-CGA-O2A
18	A	843	CLA	C4-C3-C5-C6
18	B	839	CLA	C5-C6-C7-C8
21	2	618	BCR	C21-C22-C23-C24
27	B	848	DGD	C1G-C2G-C3G-O3G
18	K	202	CLA	CAA-CBA-CGA-O1A
18	A	825	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	CAA-CBA-CGA-O2A
18	K	202	CLA	CAA-CBA-CGA-O2A
18	2	604	CLA	O2A-C1-C2-C3
18	4	614	CLA	O2A-C1-C2-C3
18	A	808	CLA	O2A-C1-C2-C3
18	A	818	CLA	O2A-C1-C2-C3
18	A	828	CLA	O2A-C1-C2-C3
18	A	854	CLA	O2A-C1-C2-C3
18	B	821	CLA	O2A-C1-C2-C3
18	2	602	CLA	C2A-CAA-CBA-CGA
18	A	842	CLA	C8-C10-C11-C12
18	1	603	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	1	613	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	3	604	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	4	604	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	824	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	834	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CHA-CBD-CGD-O1D
18	B	801	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	827	CLA	CHA-CBD-CGD-O1D
18	B	827	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	CHA-CBD-CGD-O2D
18	L	304	CLA	CHA-CBD-CGD-O1D
18	G	202	CLA	CAA-CBA-CGA-O1A
22	1	618	LHG	O7-C7-C8-C9
23	1	620	LMG	C36-C37-C38-C39
27	B	848	DGD	CBB-CCB-CDB-CEB
17	1	601	CHL	C6-C7-C8-C10
18	A	829	CLA	CAA-CBA-CGA-O2A
23	1	620	LMG	O8-C28-C29-C30
23	4	619	LMG	O7-C8-C9-O8
18	A	840	CLA	C15-C16-C17-C18
18	B	826	CLA	O1A-CGA-O2A-C1
17	3	616	CHL	CAA-CBA-CGA-O2A
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
18	B	817	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C16-C17-C18-C19
18	1	611	CLA	CAA-CBA-CGA-O1A
18	B	831	CLA	C12-C13-C15-C16
18	1	608	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	822	CLA	C11-C10-C8-C9
18	1	603	CLA	CAA-CBA-CGA-O1A
18	1	613	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	1	608	CLA	C16-C17-C18-C20
18	A	838	CLA	C6-C7-C8-C9
18	4	604	CLA	C2A-CAA-CBA-CGA
18	2	602	CLA	C4-C3-C5-C6
18	B	822	CLA	C4-C3-C5-C6
18	A	825	CLA	CAA-CBA-CGA-O1A
18	H	201	CLA	CAA-CBA-CGA-O1A
17	1	601	CHL	CHA-CBD-CGD-O2D
18	3	606	CLA	CHA-CBD-CGD-O2D
18	3	610	CLA	C1A-C2A-CAA-CBA
18	3	611	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
22	A	852	LHG	C31-C32-C33-C34
18	B	821	CLA	C6-C7-C8-C10
22	1	622	LHG	O9-C7-C8-C9
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	C6-C7-C8-C10
18	B	833	CLA	CAA-CBA-CGA-O1A
18	1	614	CLA	CAA-CBA-CGA-O1A
18	4	603	CLA	CAA-CBA-CGA-O2A
18	B	825	CLA	C3-C5-C6-C7
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	C2-C3-C5-C6
18	A	841	CLA	C16-C17-C18-C20
25	A	844	PQN	C26-C27-C28-C29
18	2	602	CLA	CAA-CBA-CGA-O1A
22	1	618	LHG	O9-C7-C8-C9
23	4	621	LMG	O7-C10-C11-C12
22	1	621	LHG	C32-C33-C34-C35
19	1	615	LUT	C1-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C26
21	J	101	BCR	C5-C6-C7-C8
18	2	604	CLA	C13-C15-C16-C17
18	2	609	CLA	CAA-CBA-CGA-O1A
23	4	619	LMG	O8-C28-C29-C30
17	4	606	CHL	CAA-CBA-CGA-O1A
18	A	802	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	A	841	CLA	C16-C17-C18-C19
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	CAA-CBA-CGA-O1A
18	2	609	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	CAA-CBA-CGA-O1A
18	B	819	CLA	CAA-CBA-CGA-O1A
23	1	623	LMG	C15-C16-C17-C18
18	2	602	CLA	CAD-CBD-CGD-O1D
18	2	612	CLA	CAD-CBD-CGD-O1D
18	2	613	CLA	CAD-CBD-CGD-O1D
18	3	609	CLA	CAD-CBD-CGD-O1D
18	4	610	CLA	CAD-CBD-CGD-O1D
18	A	831	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CAD-CBD-CGD-O1D
18	B	814	CLA	CAD-CBD-CGD-O1D
18	G	203	CLA	CAD-CBD-CGD-O1D
18	4	612	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	C10-C11-C12-C13
18	2	604	CLA	C11-C12-C13-C14
18	A	841	CLA	C14-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C9
18	B	838	CLA	C11-C12-C13-C14
18	B	829	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	C13-C15-C16-C17
18	2	602	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	CAA-CBA-CGA-O2A
22	1	621	LHG	O7-C7-C8-C9
18	B	826	CLA	CAA-CBA-CGA-O2A
18	H	201	CLA	CAA-CBA-CGA-O2A
22	2	617	LHG	O7-C7-C8-C9
23	1	620	LMG	C29-C30-C31-C32
18	A	809	CLA	C3-C5-C6-C7
18	A	821	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	823	CLA	C4-C3-C5-C6
22	1	621	LHG	C33-C34-C35-C36
17	1	601	CHL	CHA-CBD-CGD-O1D
17	1	606	CHL	CHA-CBD-CGD-O1D
18	1	608	CLA	C6-C7-C8-C10
18	1	608	CLA	C12-C13-C15-C16
18	1	609	CLA	C2-C3-C5-C6
18	2	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	3	606	CLA	C3A-C2A-CAA-CBA
18	3	606	CLA	CHA-CBD-CGD-O1D
18	3	611	CLA	CHA-CBD-CGD-O1D
18	3	611	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	C11-C10-C8-C7
18	A	821	CLA	C6-C7-C8-C10
18	A	828	CLA	C12-C13-C15-C16
18	A	830	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C12-C13-C15
18	B	809	CLA	C6-C7-C8-C10
18	B	821	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C6-C7-C8-C10
18	B	833	CLA	C6-C7-C8-C10
18	B	838	CLA	C11-C12-C13-C15
18	L	303	CLA	C11-C10-C8-C7
18	1	602	CLA	CAA-CBA-CGA-O1A
21	A	847	BCR	C7-C8-C9-C10
21	B	846	BCR	C21-C22-C23-C24
21	J	101	BCR	C21-C22-C23-C24
21	K	204	BCR	C21-C22-C23-C24
21	L	301	BCR	C11-C12-C13-C14
22	1	621	LHG	O9-C7-C8-C9
23	4	621	LMG	O9-C10-C11-C12
18	G	202	CLA	CAA-CBA-CGA-O2A
18	A	821	CLA	CAA-CBA-CGA-O2A
22	1	618	LHG	C24-C25-C26-C27
22	A	852	LHG	C27-C28-C29-C30
18	B	819	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	C15-C16-C17-C18
18	A	821	CLA	CAA-CBA-CGA-O1A
18	B	840	CLA	CAA-CBA-CGA-O1A
23	4	619	LMG	O10-C28-C29-C30
18	K	202	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	C2A-CAA-CBA-CGA
18	B	822	CLA	C11-C12-C13-C15
18	B	822	CLA	CAA-CBA-CGA-O1A
18	L	303	CLA	C4-C3-C5-C6
17	1	601	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

124 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	828	CLA	1	0
23	1	620	LMG	1	0
18	B	816	CLA	4	0
18	B	823	CLA	2	0
18	J	102	CLA	1	0
20	2	616	XAT	1	0
18	3	617	CLA	1	0
22	A	855	LHG	3	0
18	B	809	CLA	4	0
18	A	804	CLA	1	0
21	2	618	BCR	5	0
18	3	611	CLA	3	0
18	A	828	CLA	1	0
18	B	826	CLA	3	0
18	A	817	CLA	4	0
18	K	203	CLA	1	0
21	B	845	BCR	1	0
21	J	101	BCR	6	0
22	2	617	LHG	3	0
18	A	832	CLA	1	0
18	1	608	CLA	1	0
18	A	843	CLA	2	0
18	A	818	CLA	1	0
21	A	845	BCR	3	0
17	3	616	CHL	1	0
18	B	827	CLA	1	0
18	2	609	CLA	2	0
18	A	819	CLA	1	0
21	A	847	BCR	2	0
18	B	821	CLA	2	0
18	A	825	CLA	2	0
18	1	613	CLA	1	0
17	4	605	CHL	4	0
18	2	612	CLA	1	0
18	4	602	CLA	2	0
22	1	622	LHG	1	0
18	4	601	CLA	1	0
18	B	838	CLA	2	0
18	A	830	CLA	2	0
18	A	803	CLA	1	0
18	B	811	CLA	1	0
19	1	619	LUT	5	0
18	1	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	817	CLA	2	0
21	F	305	BCR	1	0
18	B	825	CLA	1	0
17	2	601	CHL	1	0
18	B	804	CLA	1	0
18	A	829	CLA	1	0
21	B	844	BCR	1	0
18	3	603	CLA	2	0
18	A	854	CLA	2	0
18	A	808	CLA	1	0
21	B	847	BCR	3	0
18	1	609	CLA	2	0
21	J	103	BCR	2	0
19	2	615	LUT	1	0
18	H	201	CLA	3	0
18	4	614	CLA	1	0
21	L	306	BCR	2	0
18	1	612	CLA	2	0
21	L	301	BCR	2	0
21	A	849	BCR	3	0
19	1	615	LUT	3	0
18	B	812	CLA	3	0
22	1	618	LHG	1	0
18	1	614	CLA	1	0
21	L	305	BCR	2	0
22	1	621	LHG	2	0
18	2	604	CLA	1	0
18	B	815	CLA	1	0
19	3	614	LUT	4	0
18	K	202	CLA	3	0
18	A	812	CLA	1	0
21	K	204	BCR	3	0
23	B	849	LMG	2	0
21	A	846	BCR	2	0
18	B	829	CLA	2	0
17	2	607	CHL	2	0
18	B	801	CLA	1	0
18	A	834	CLA	1	0
18	A	836	CLA	1	0
18	A	807	CLA	3	0
17	1	606	CHL	1	0
21	L	307	BCR	1	0

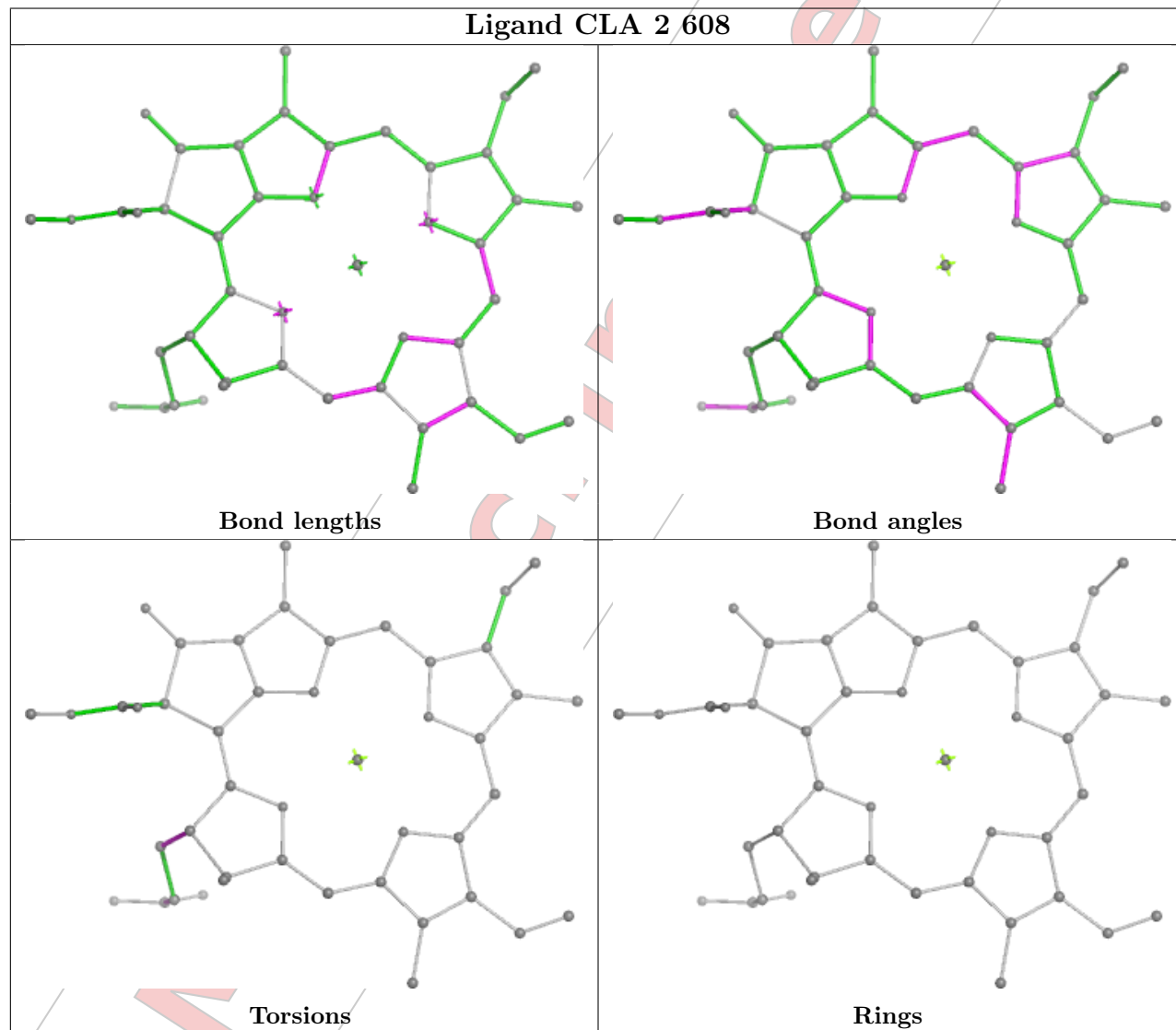
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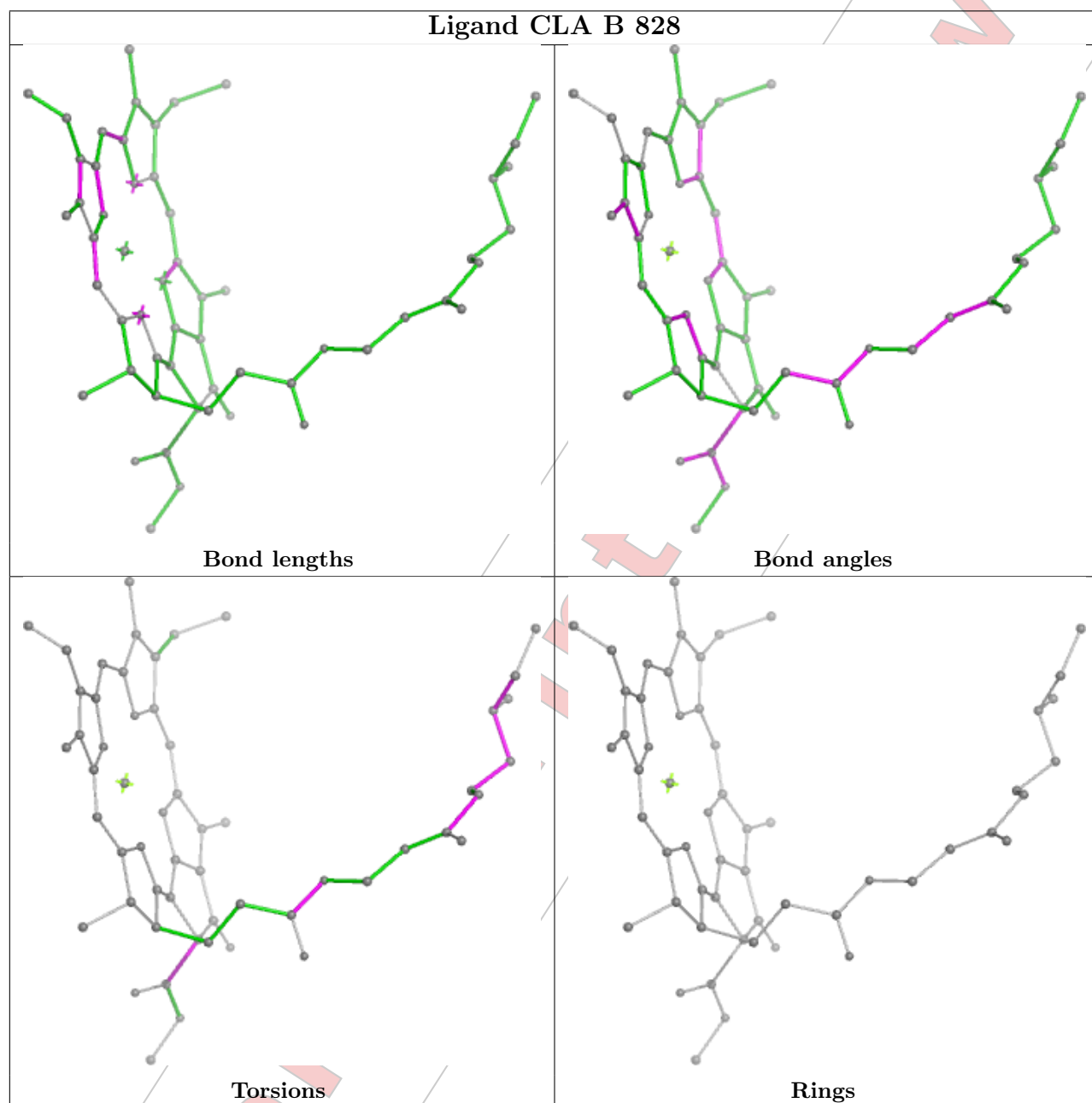
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	F	306	LMG	1	0
18	B	807	CLA	2	0
18	A	809	CLA	2	0
24	A	856	LMT	1	0
17	2	614	CHL	1	0
18	3	602	CLA	1	0
18	A	810	CLA	2	0
18	A	842	CLA	1	0
20	3	615	XAT	3	0
21	B	842	BCR	2	0
27	B	848	DGD	2	0
18	2	610	CLA	1	0
18	G	203	CLA	1	0
18	B	839	CLA	3	0
23	1	623	LMG	1	0
18	L	302	CLA	3	0
21	A	850	BCR	5	0
18	A	841	CLA	1	0
21	3	601	BCR	2	0
21	B	846	BCR	1	0
17	2	606	CHL	1	0
18	B	840	CLA	3	0
19	4	616	LUT	5	0
21	B	843	BCR	1	0
18	F	301	CLA	1	0
18	A	806	CLA	1	0
23	F	307	LMG	1	0
18	A	821	CLA	1	0
17	4	606	CHL	2	0
18	A	837	CLA	1	0
18	B	813	CLA	2	0
21	F	302	BCR	1	0
21	1	617	BCR	1	0
25	B	841	PQN	2	0
17	4	607	CHL	1	0
18	A	802	CLA	3	0
21	G	205	BCR	1	0
18	A	827	CLA	1	0
18	A	831	CLA	1	0

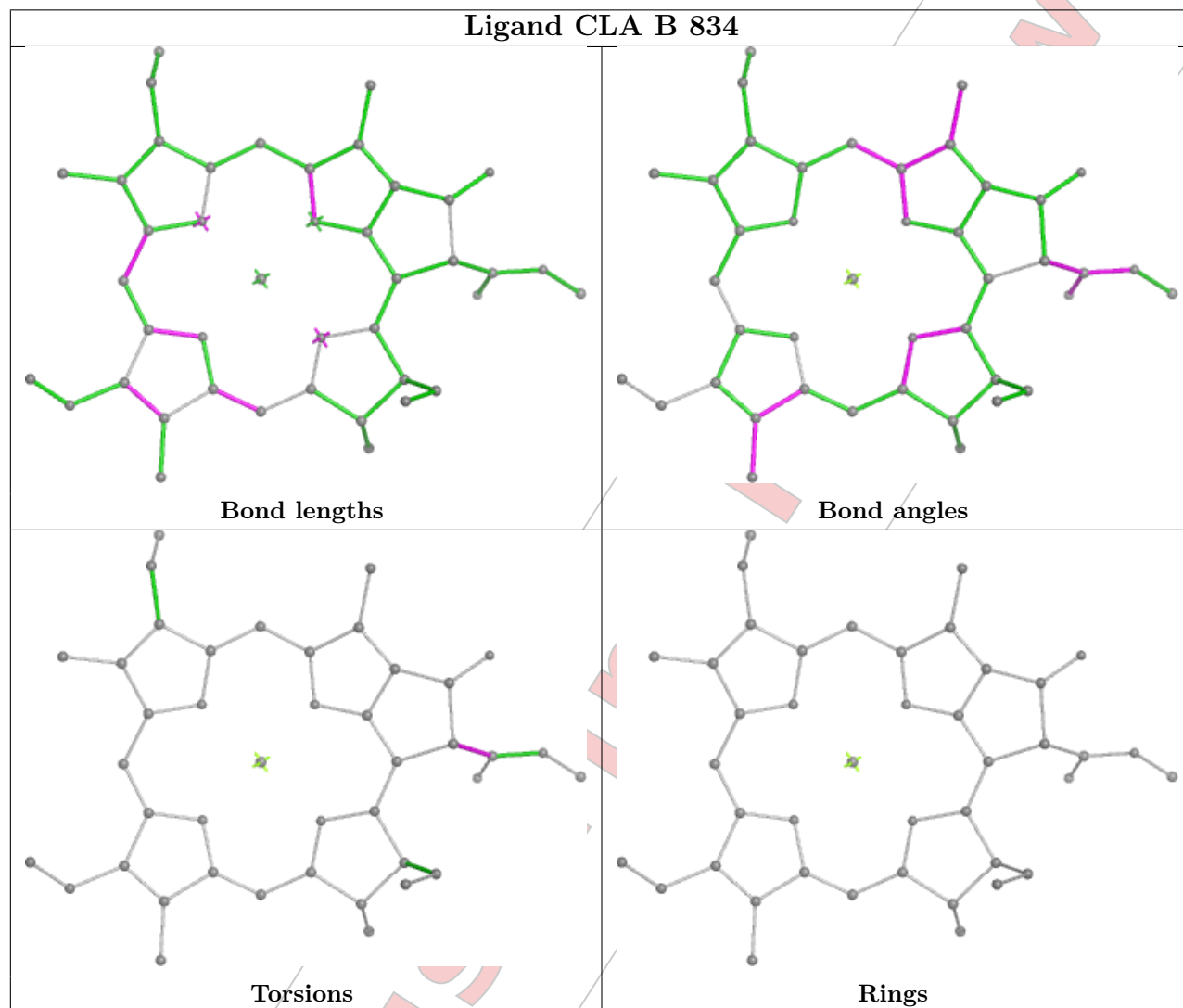
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

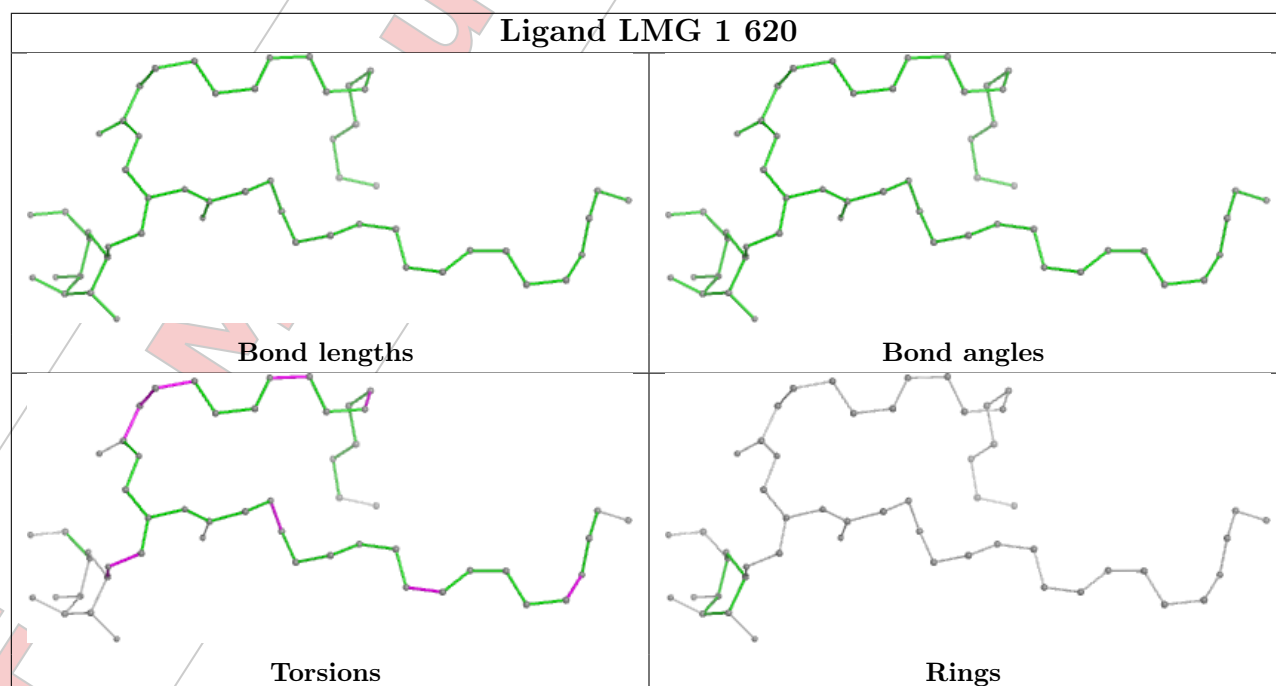




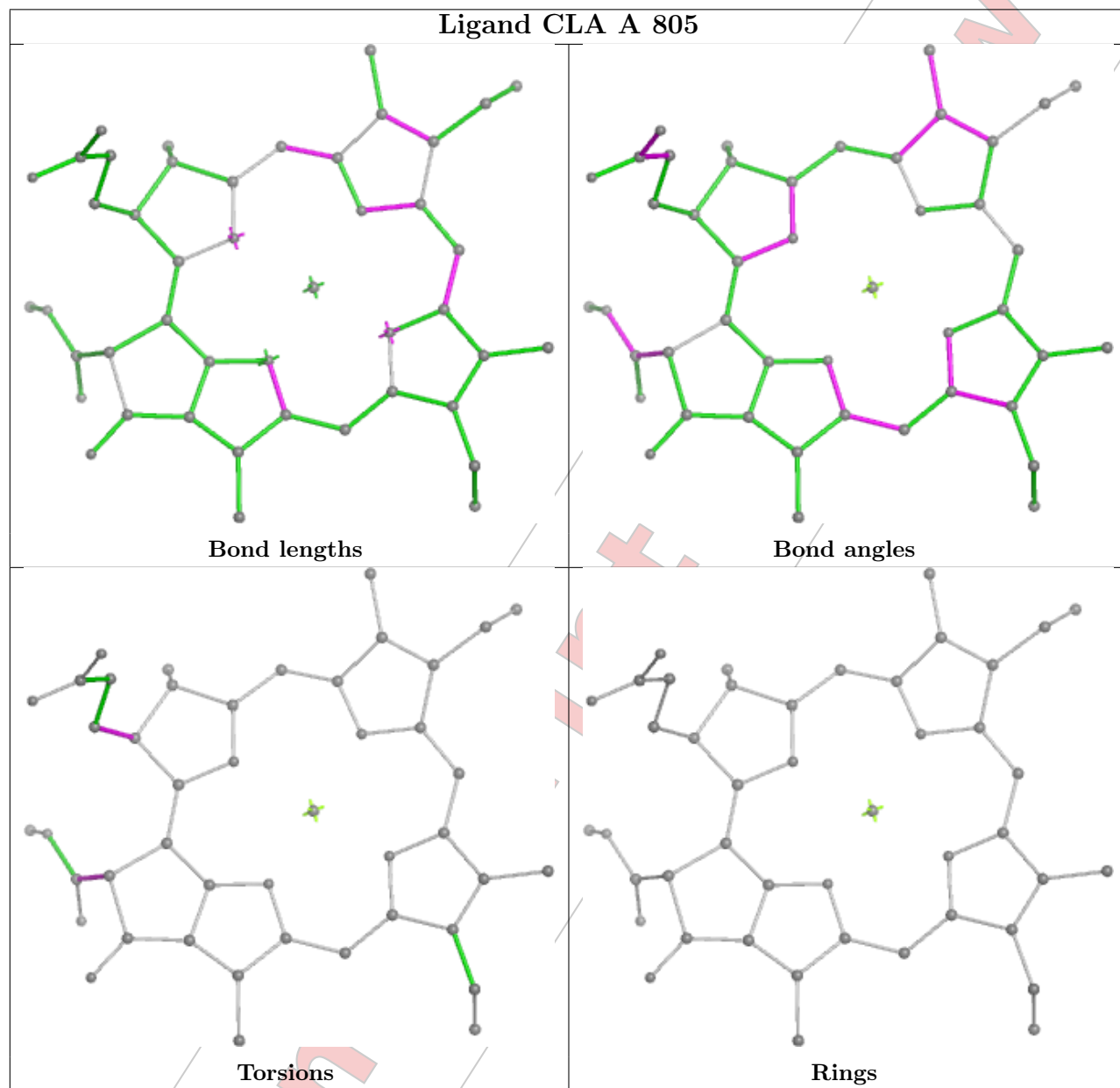
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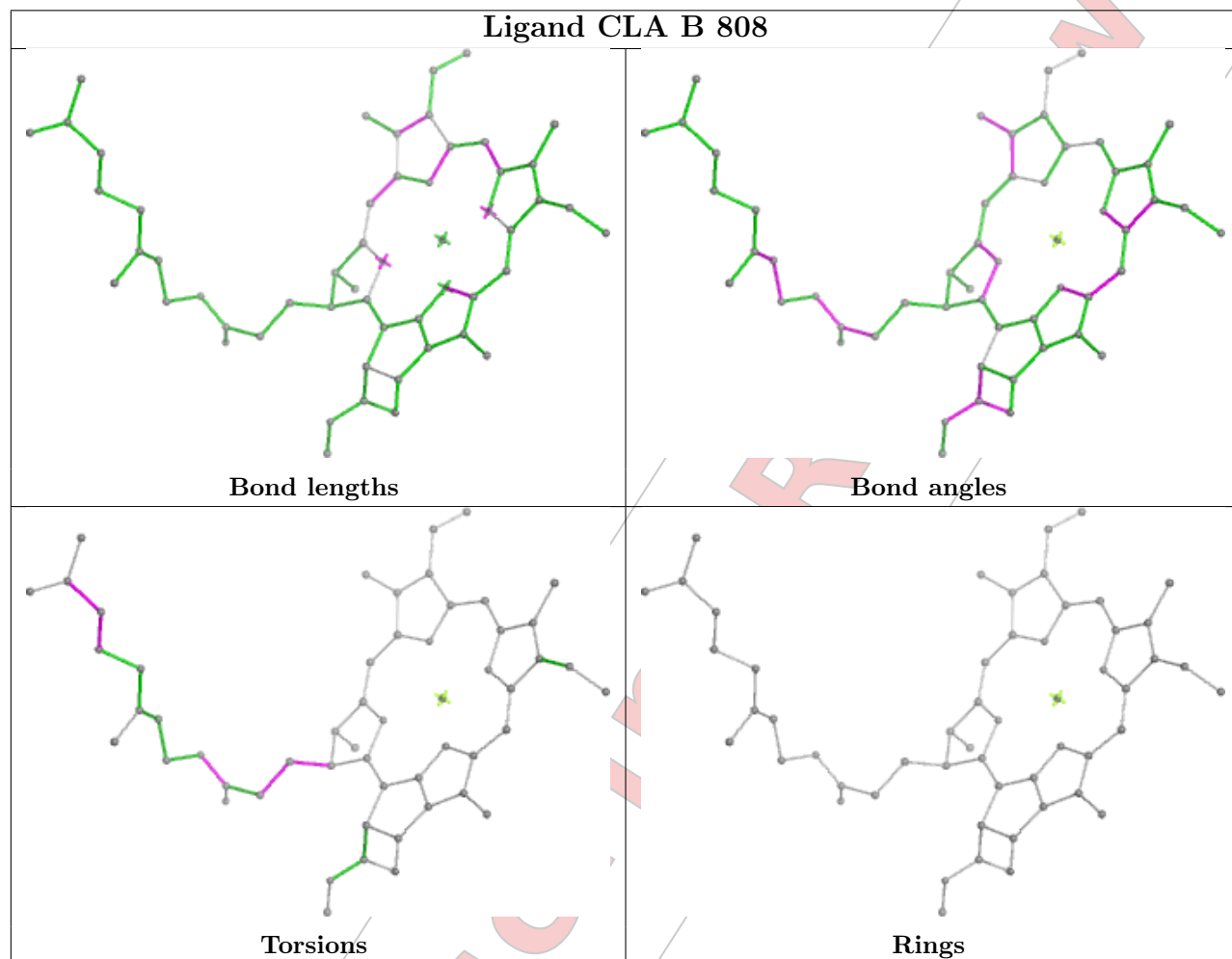


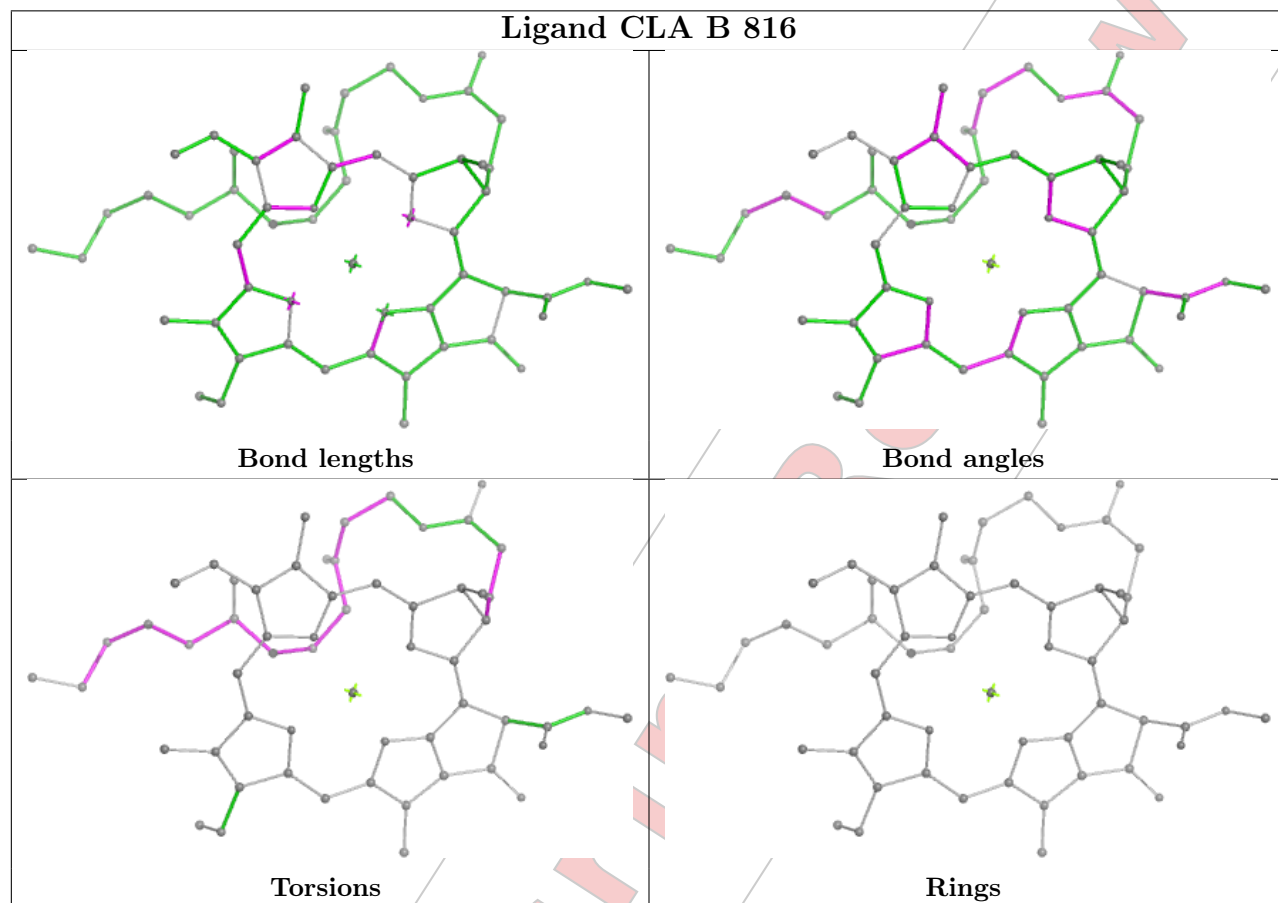
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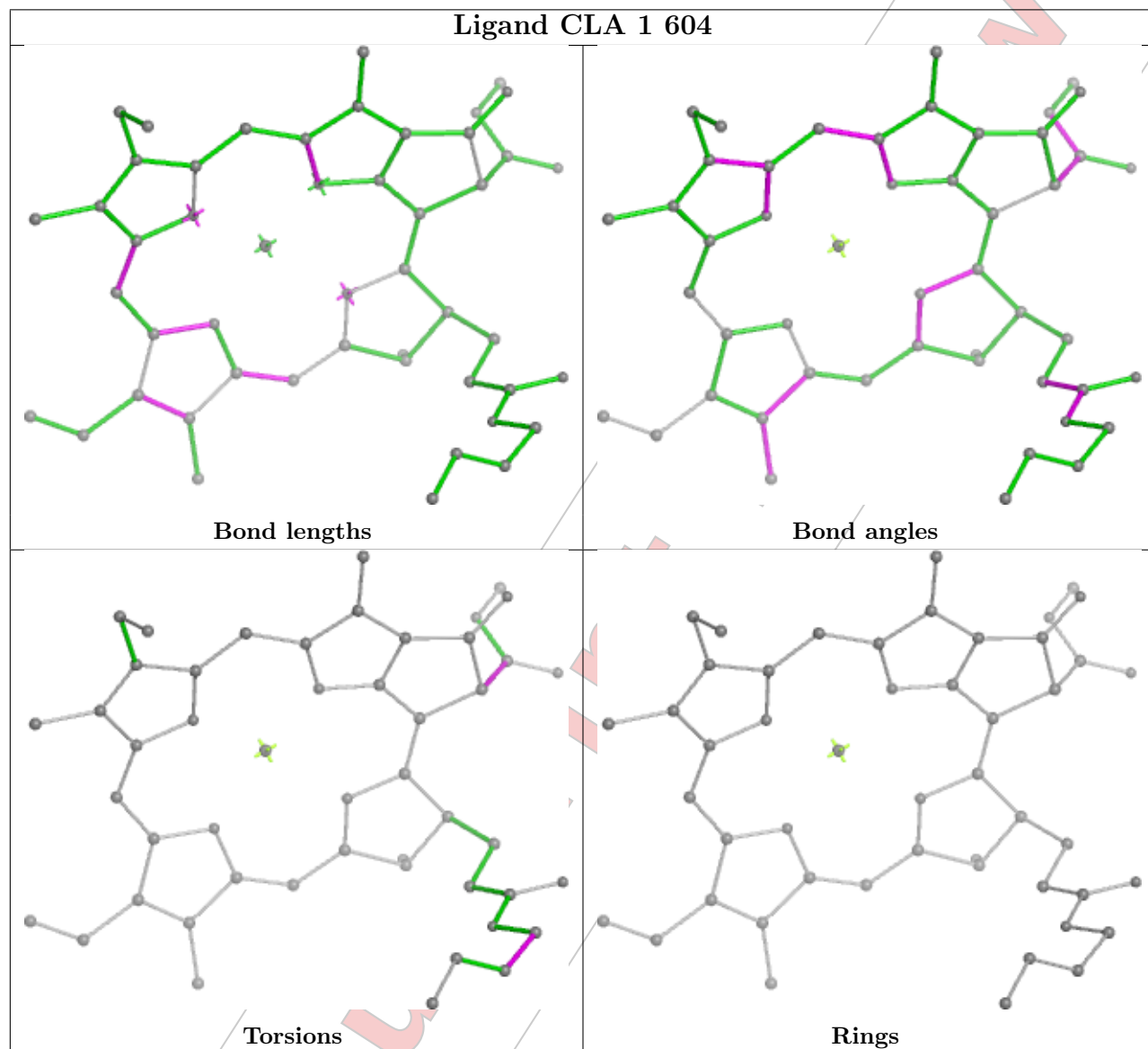
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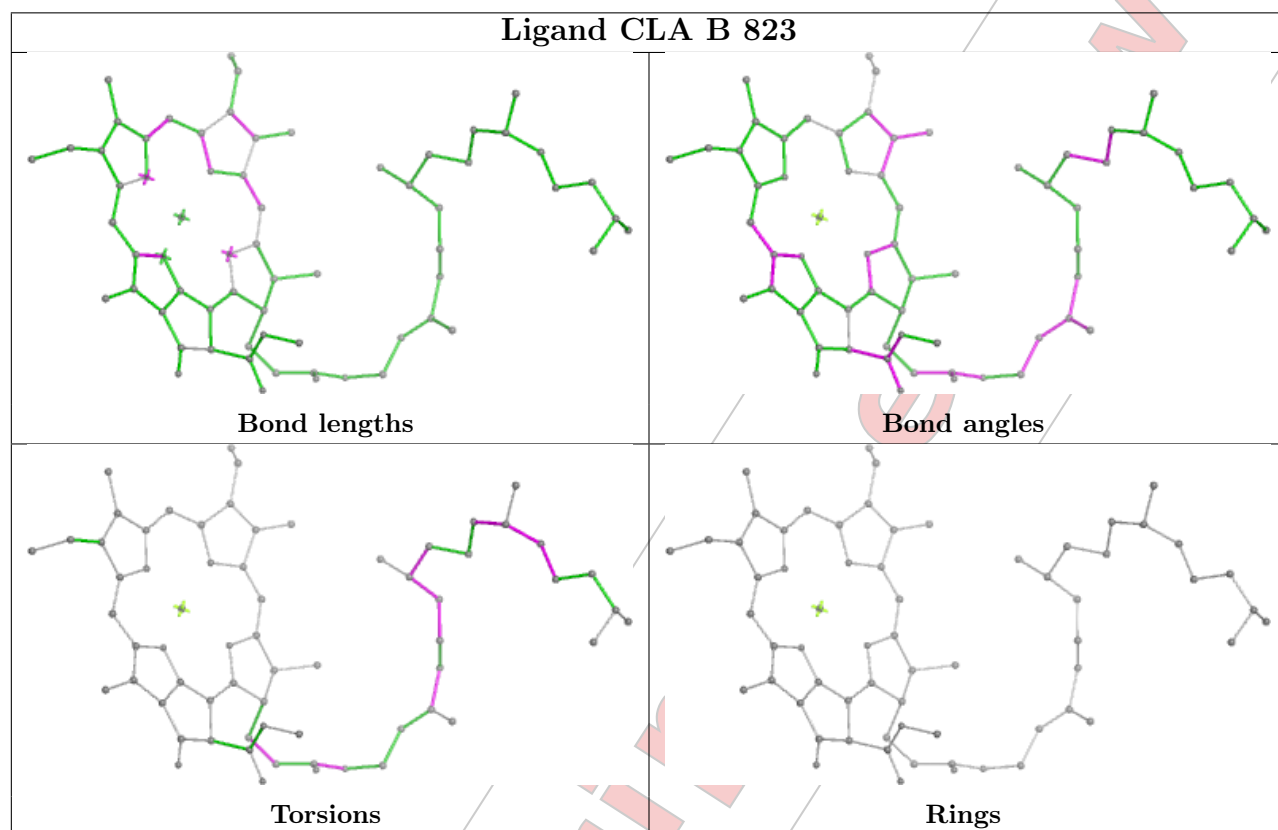




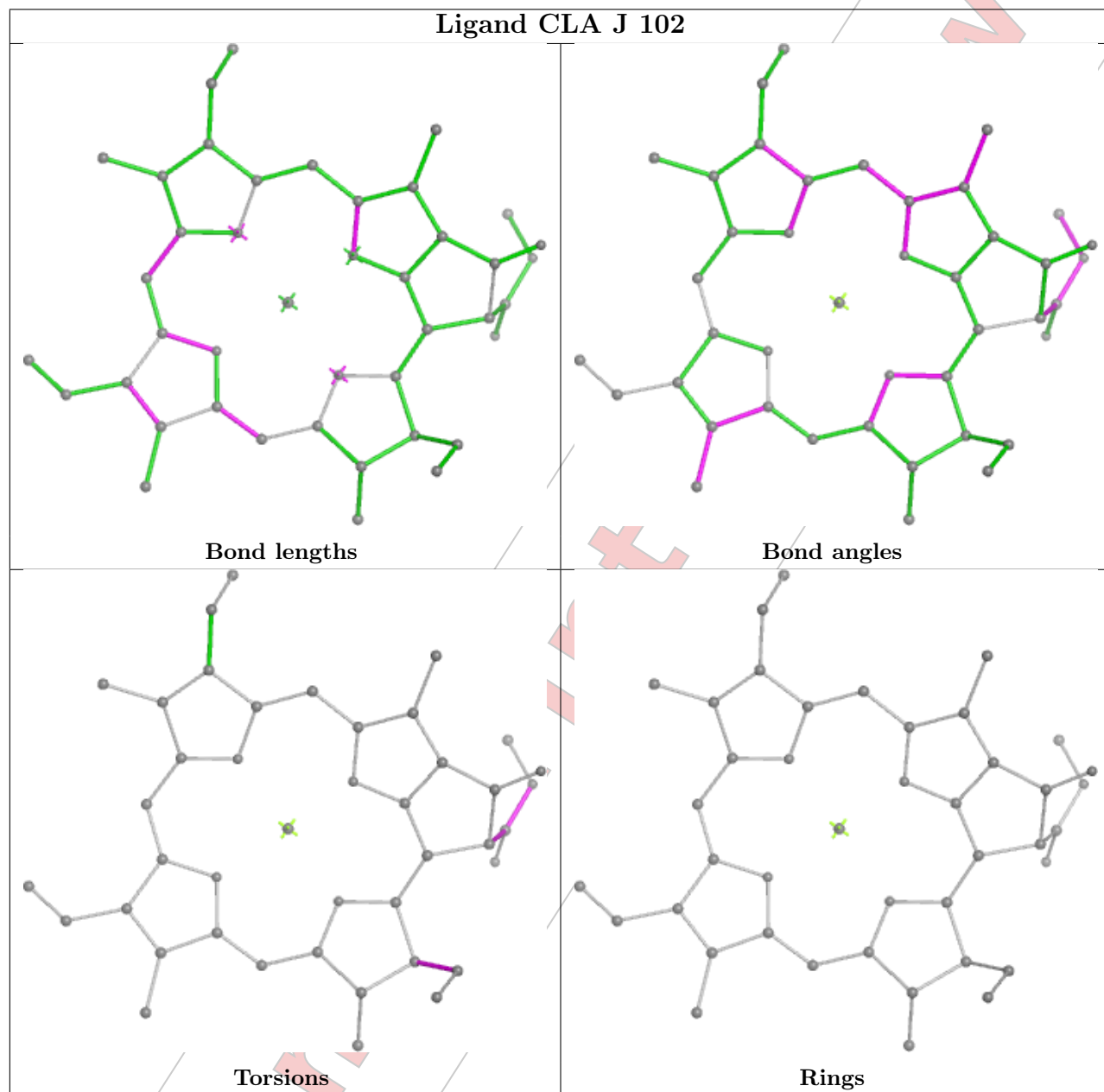


Ligand CLA 1 604

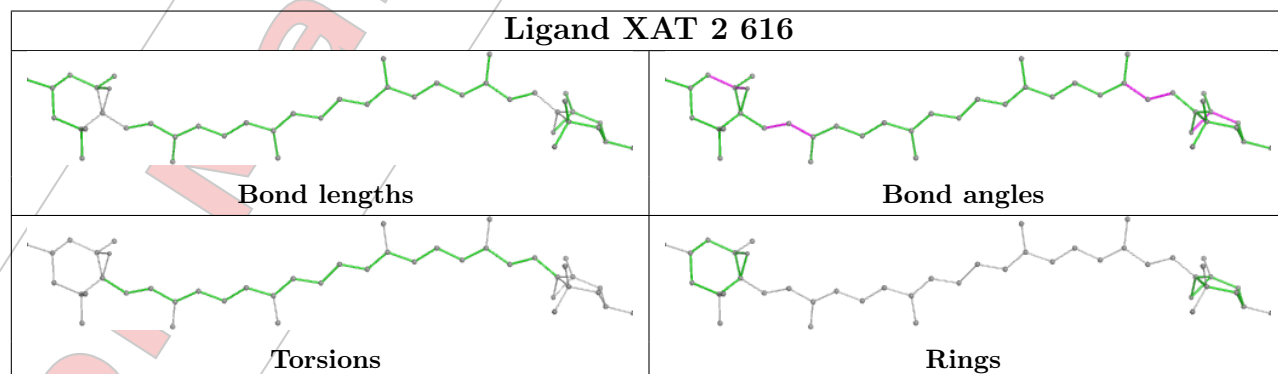


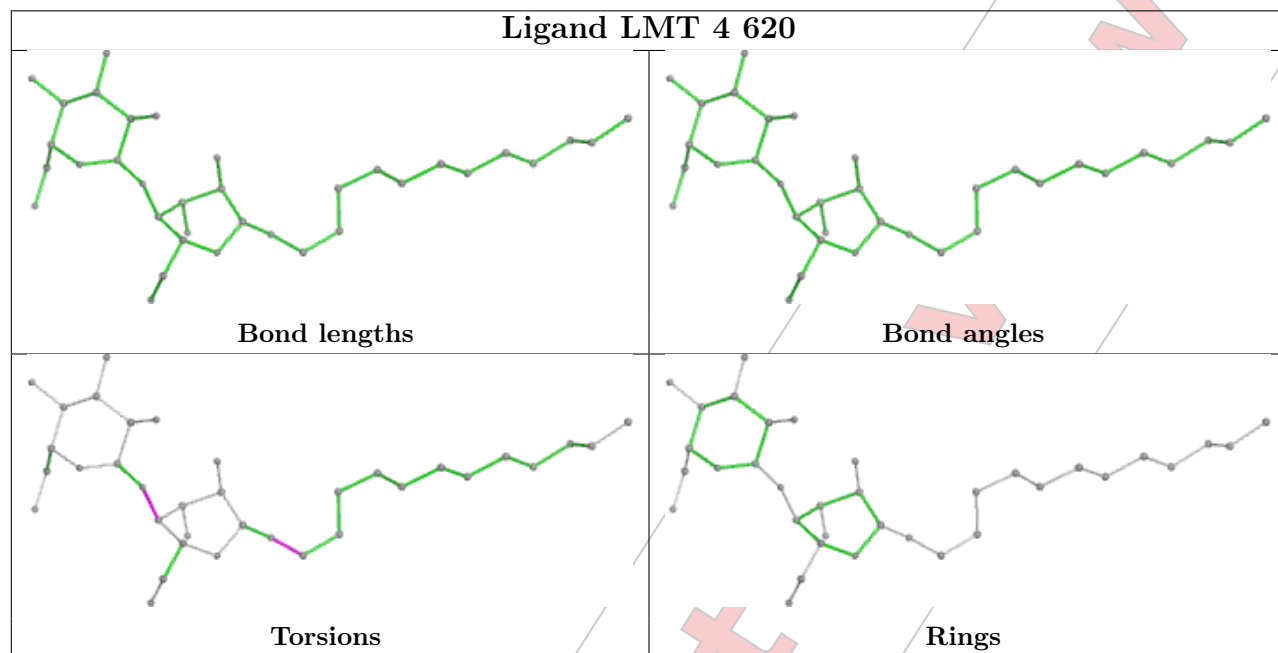


Ligand CLA J 102

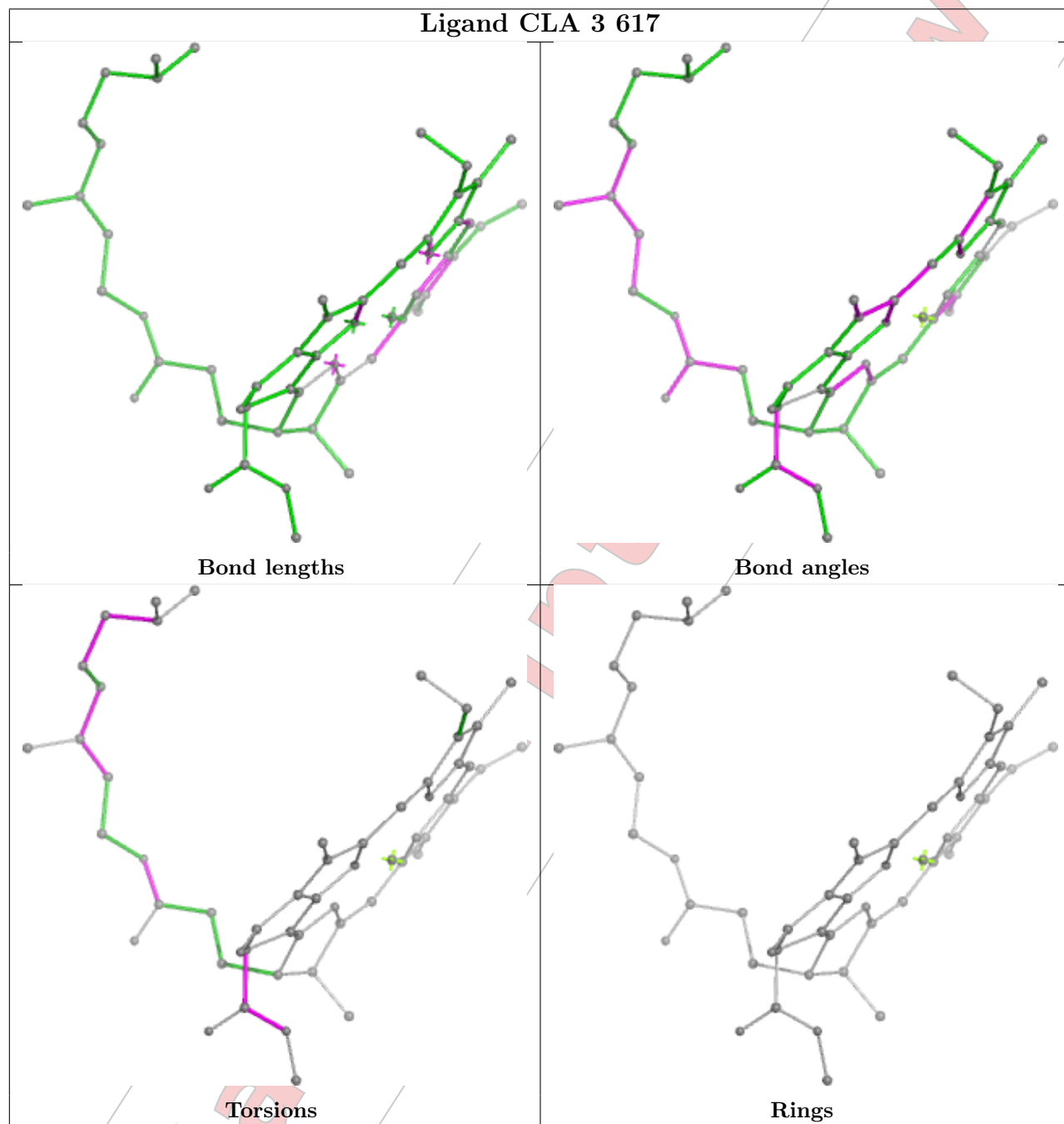


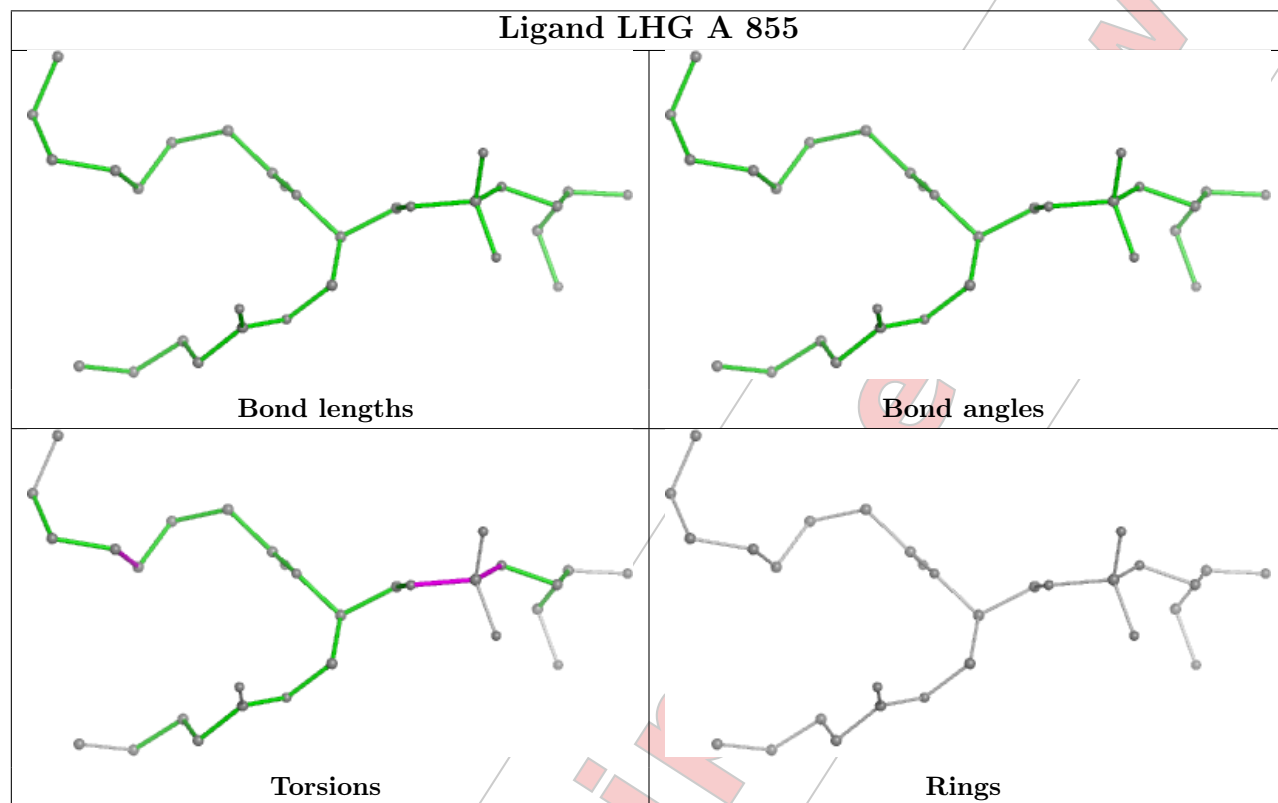
Ligand XAT 2 616

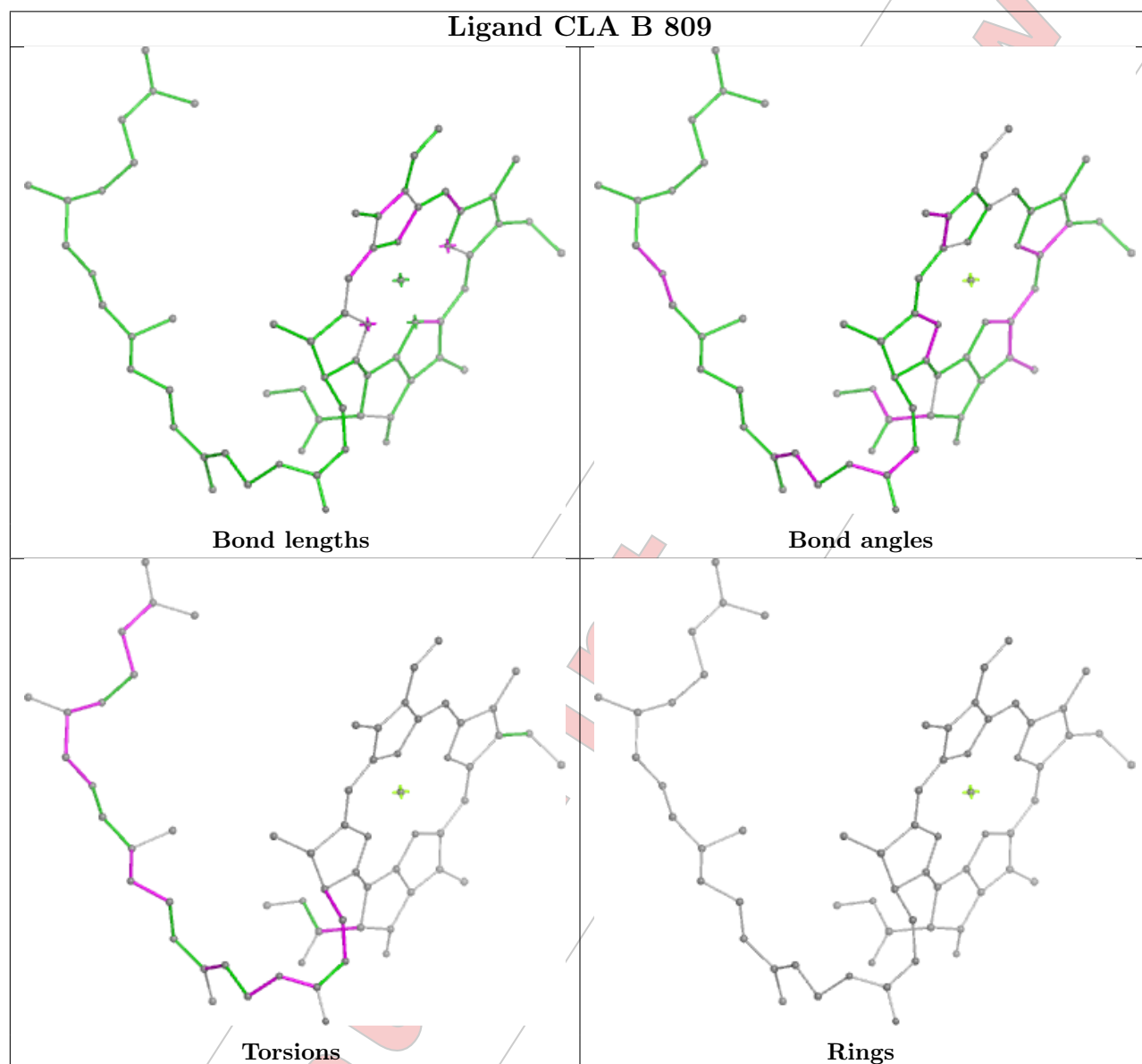




Ligand CLA 3 617

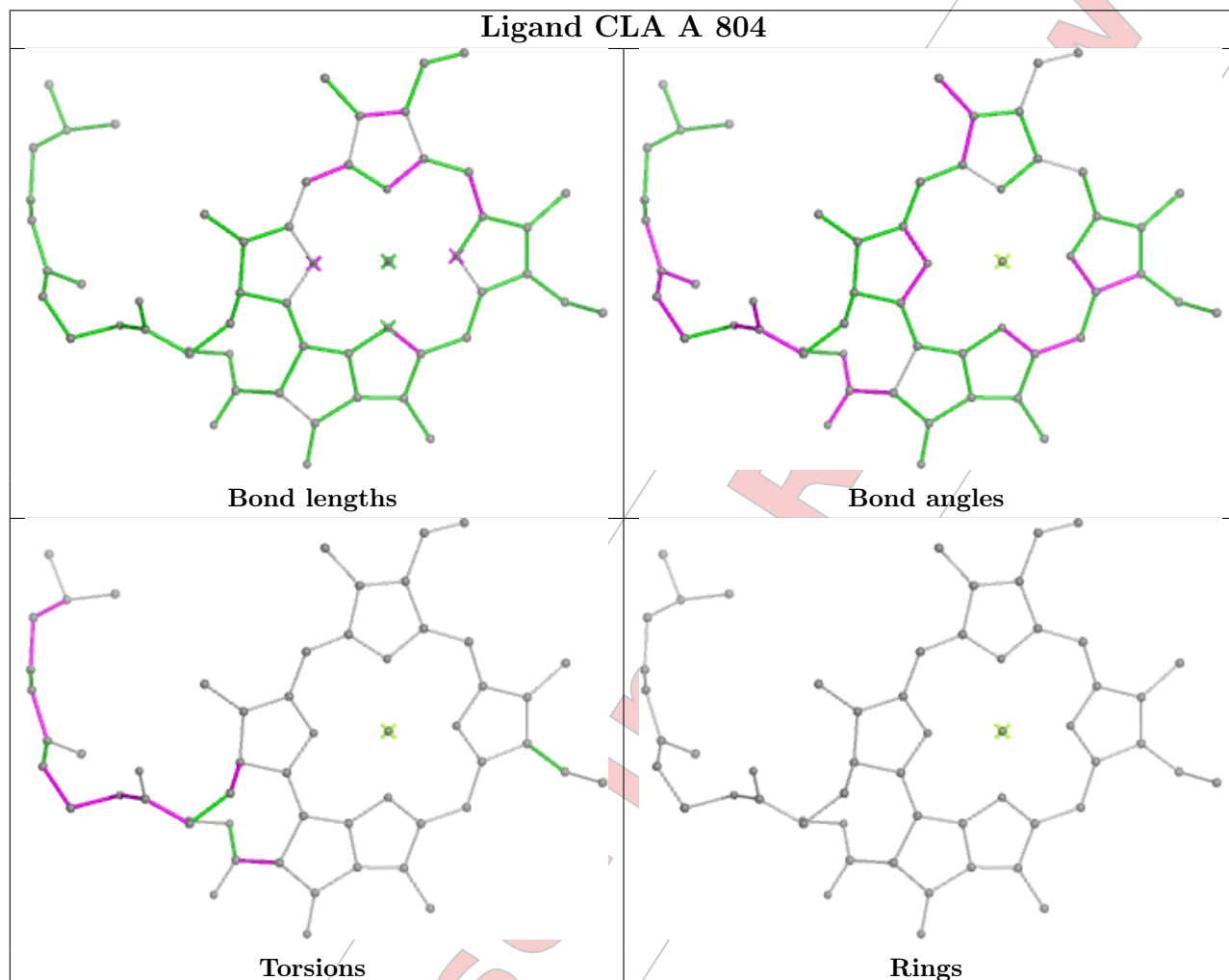




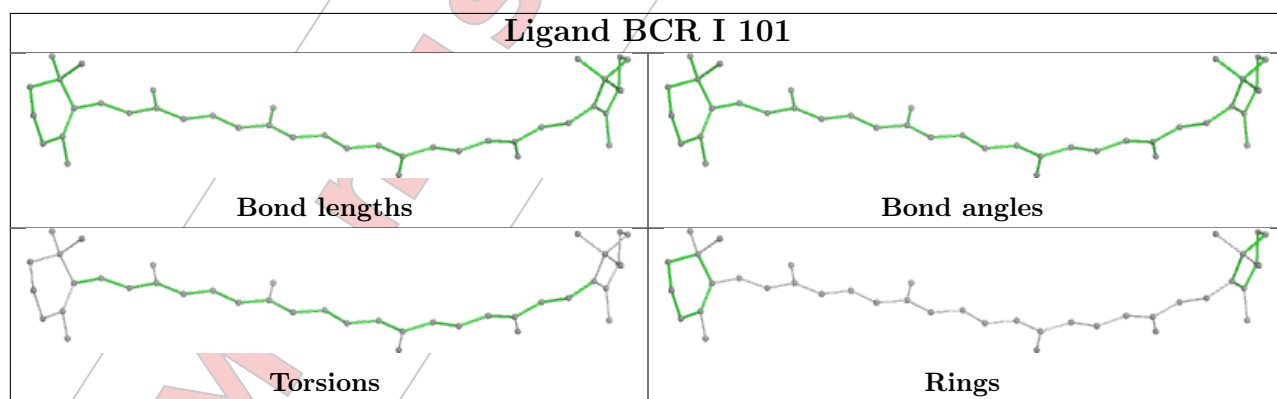


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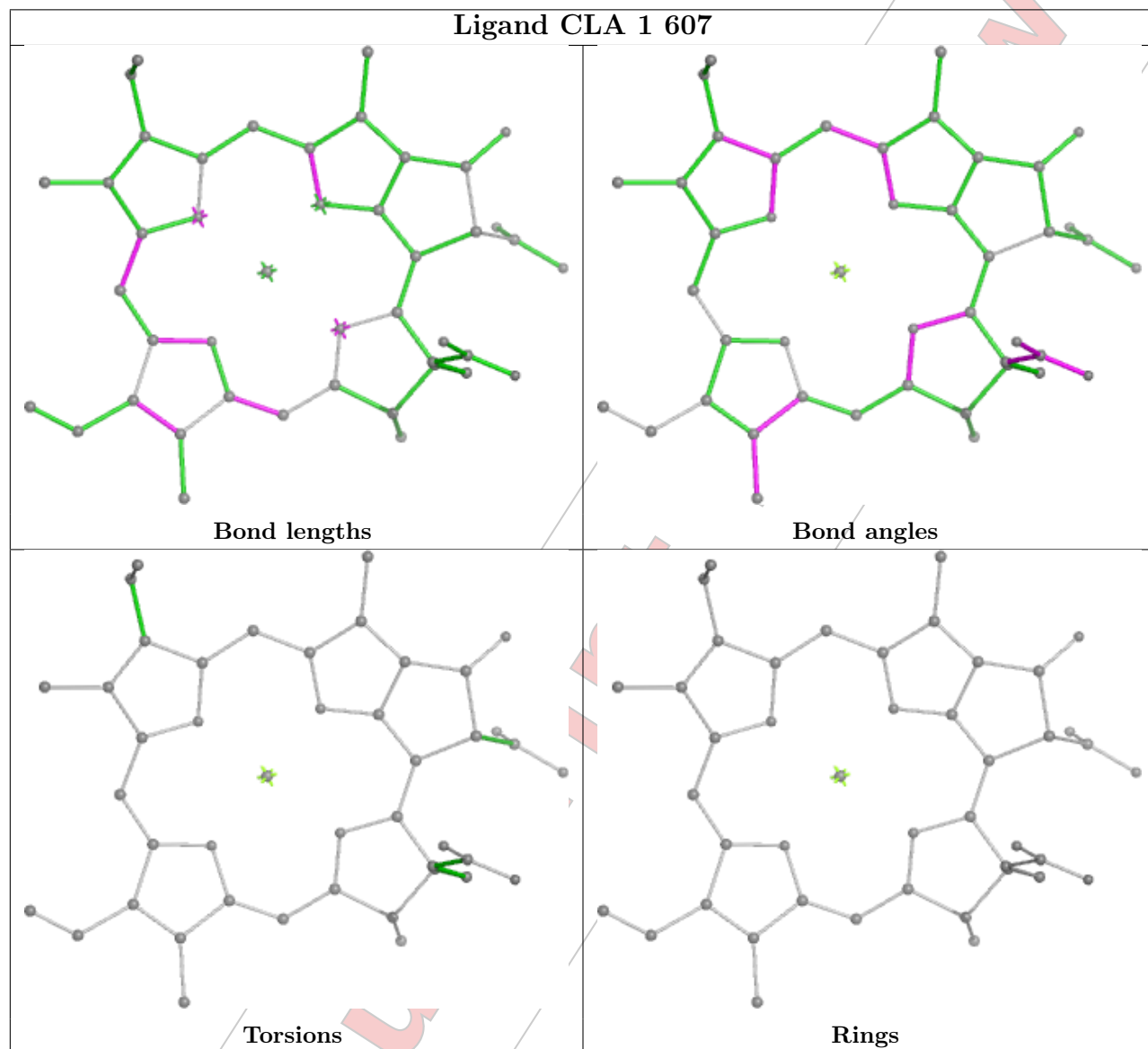
Ligand CLA A 804



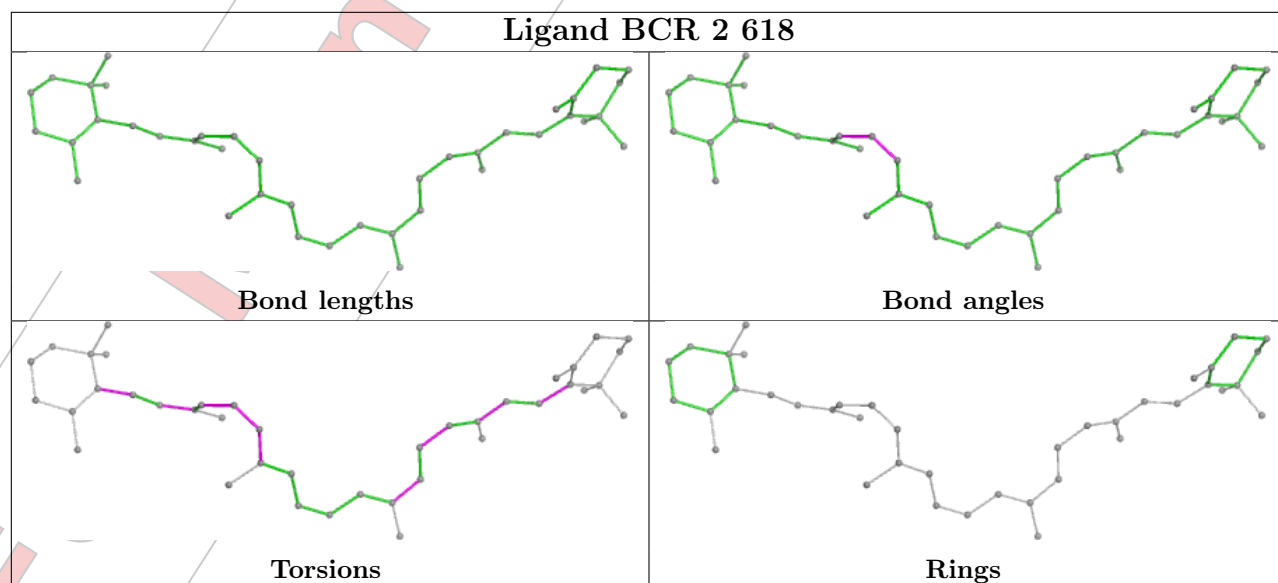
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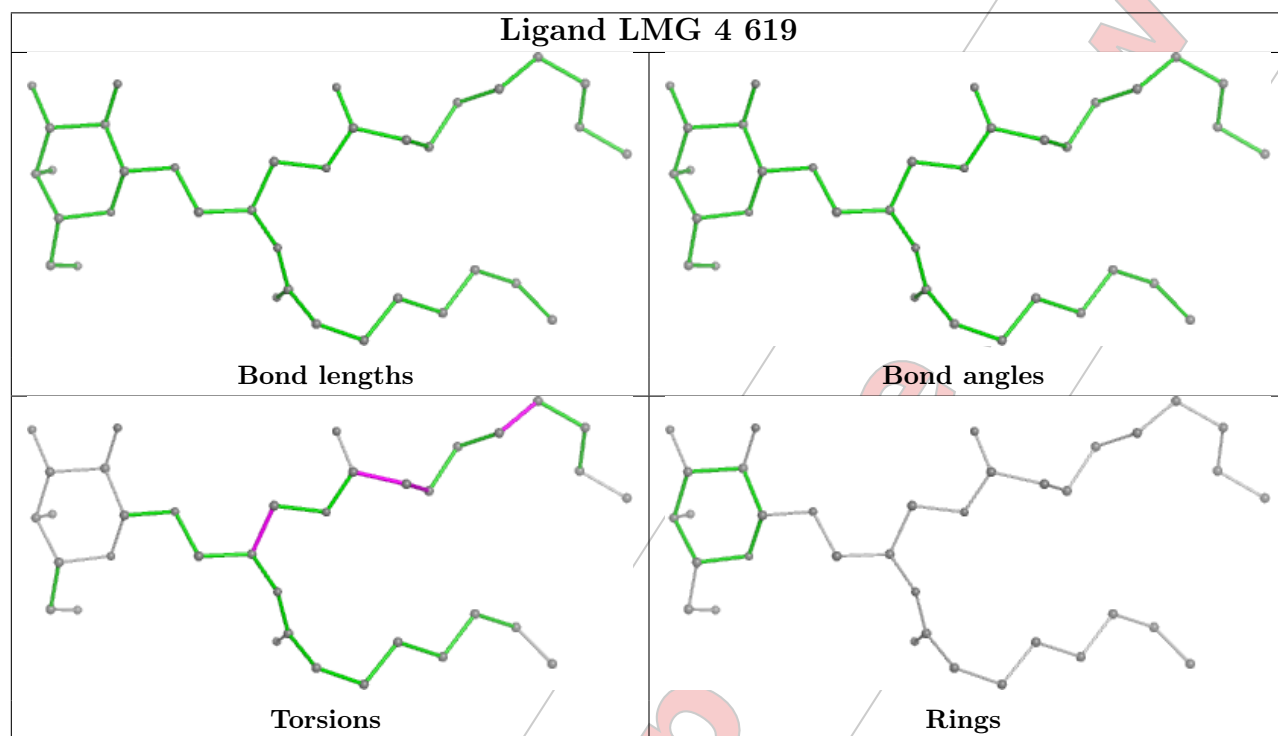


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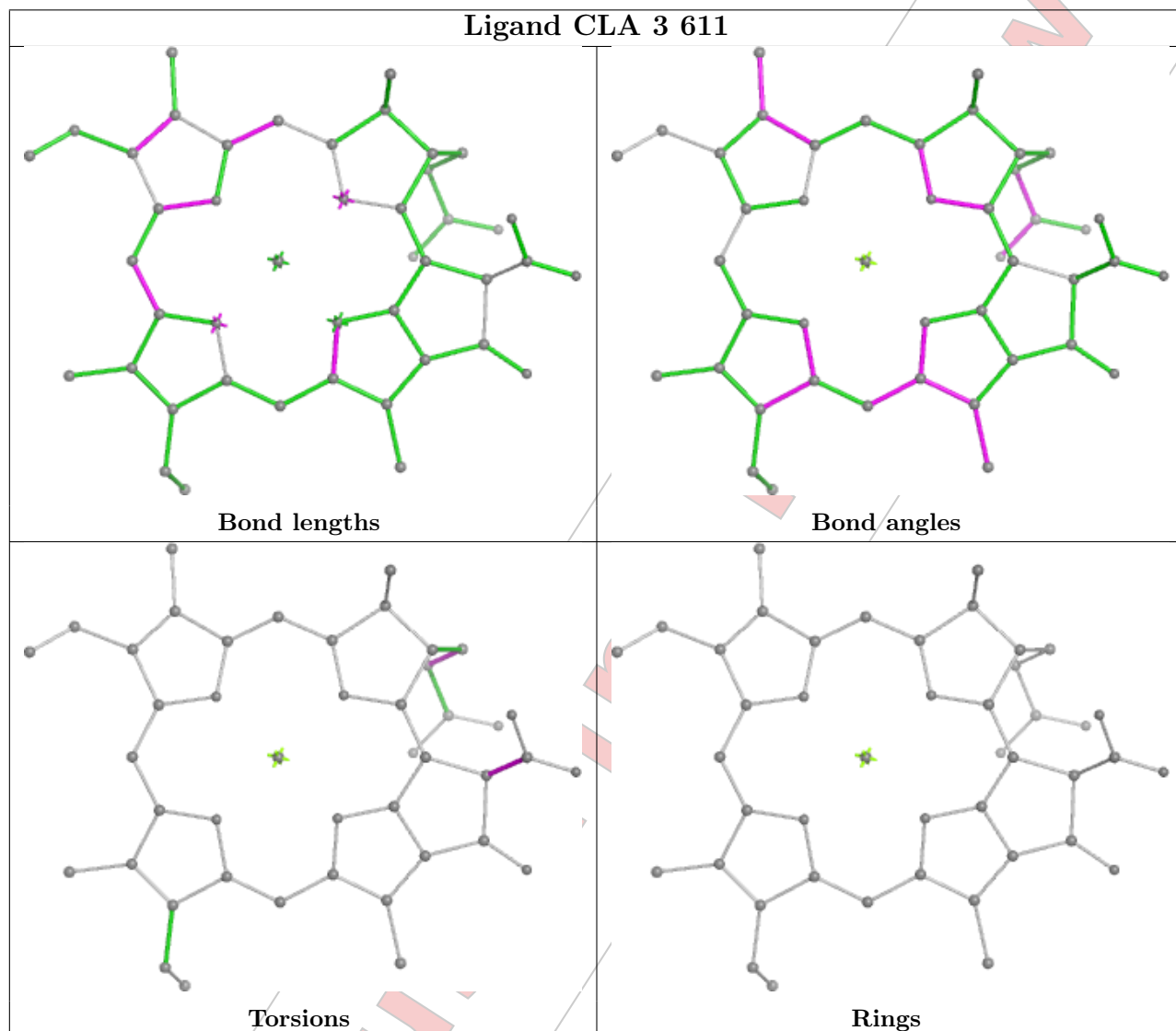


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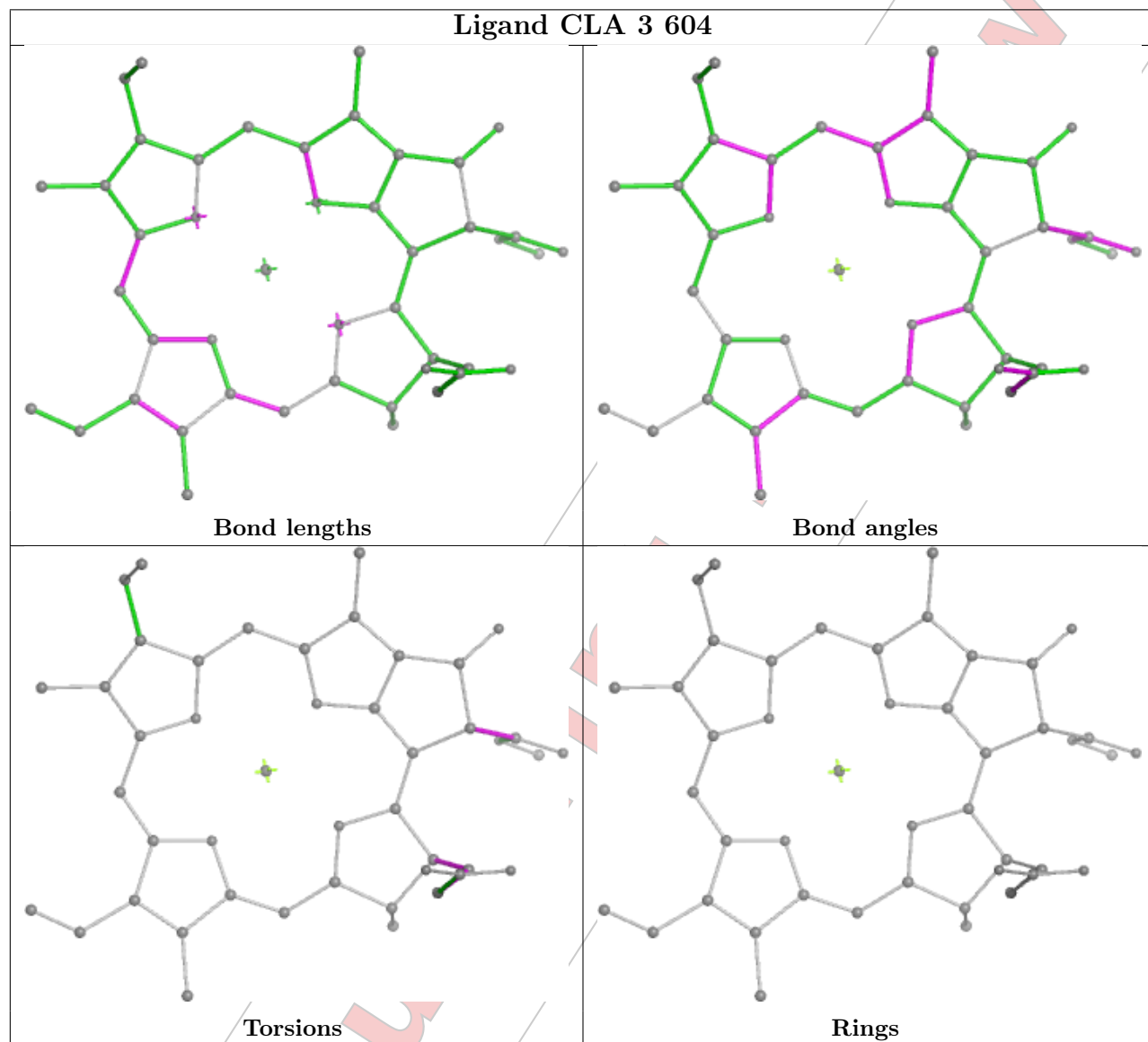




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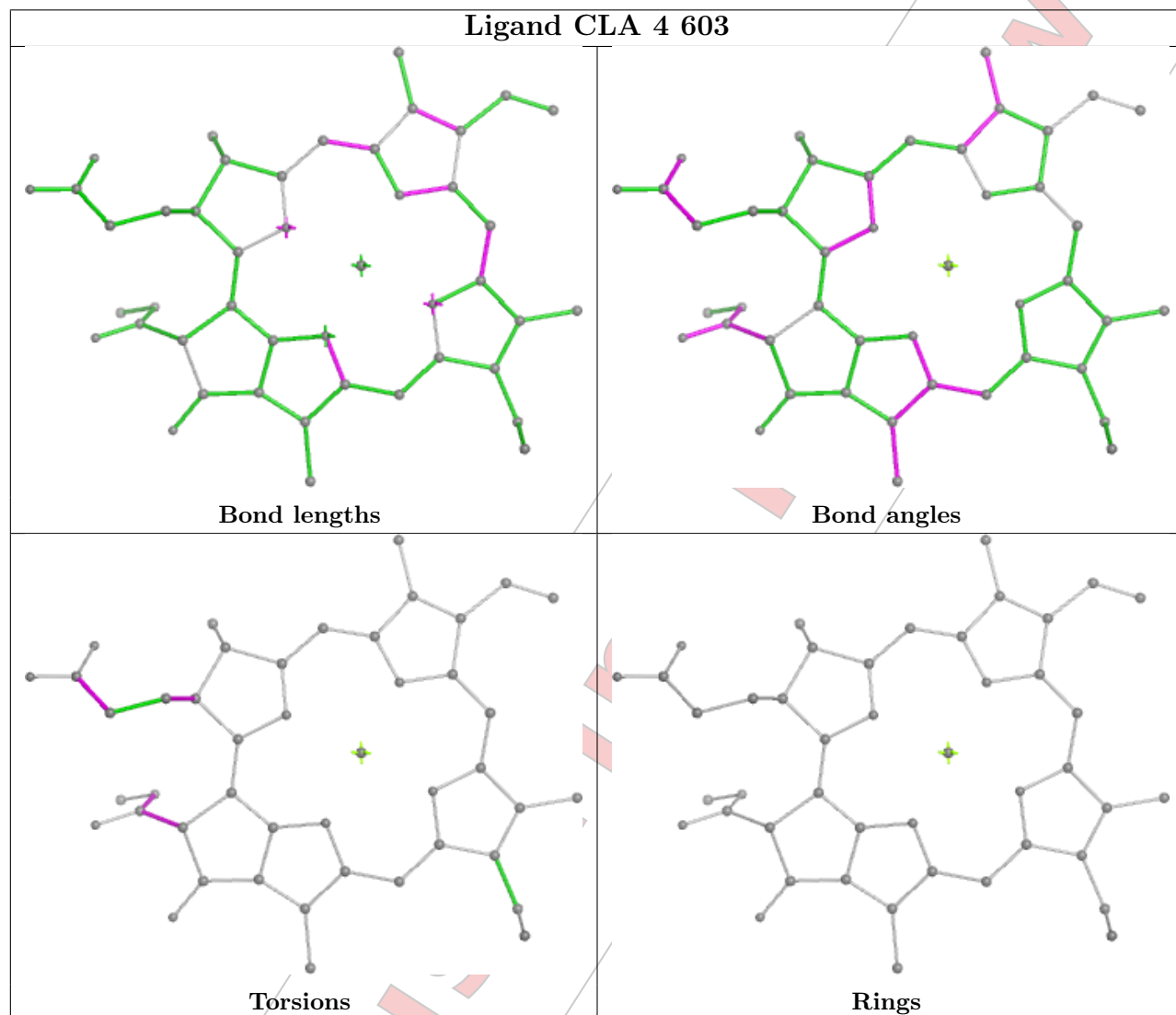


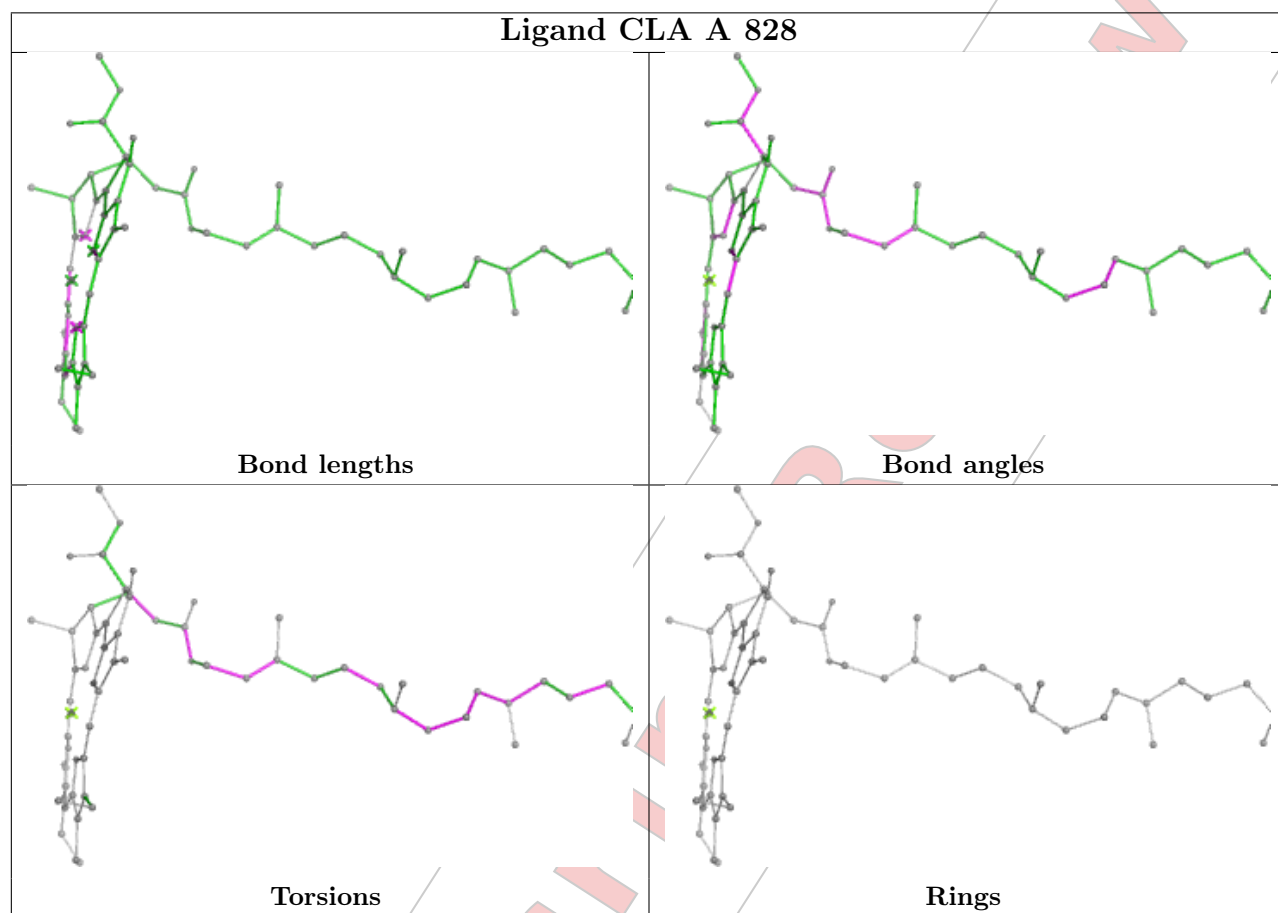
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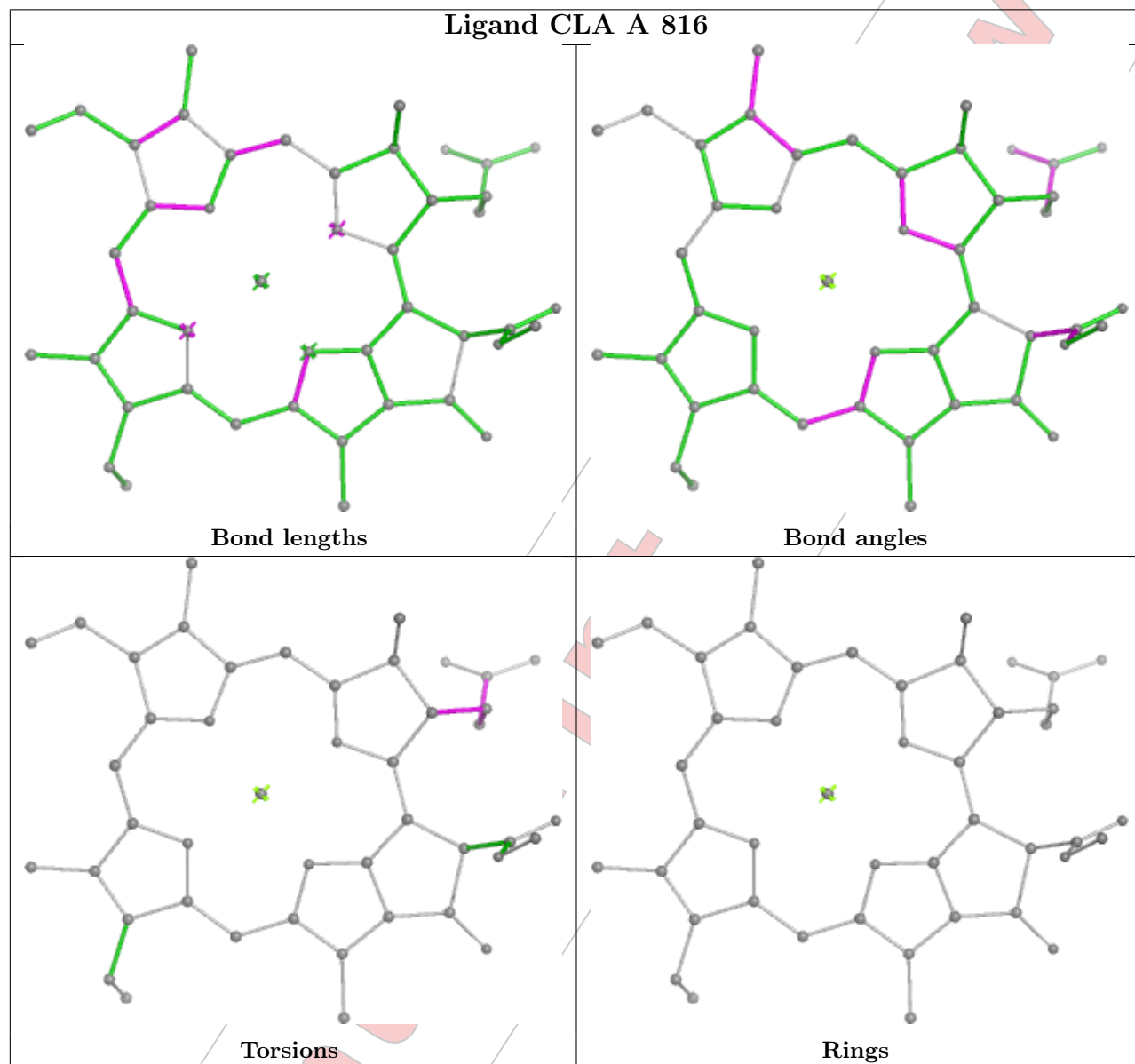
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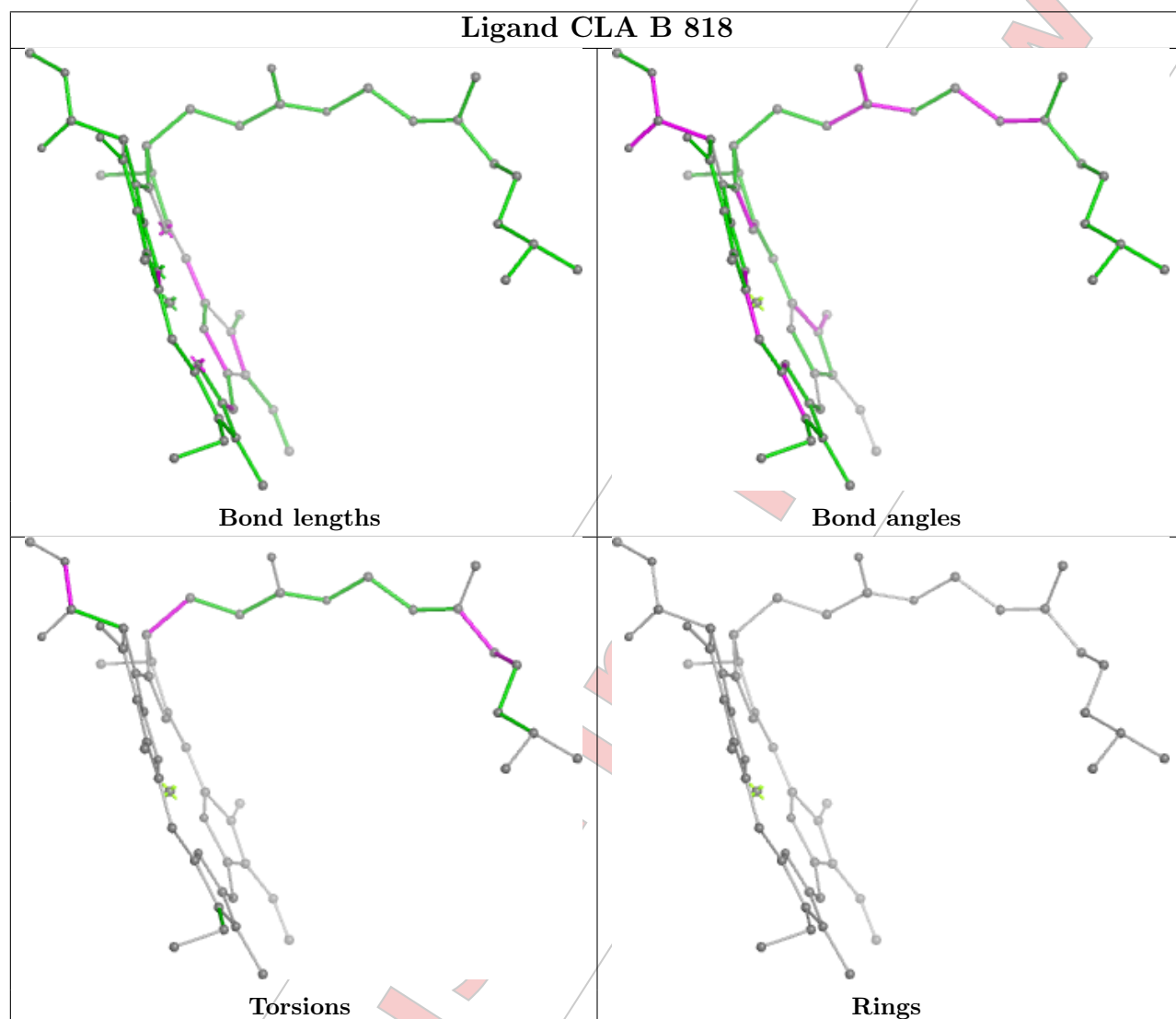
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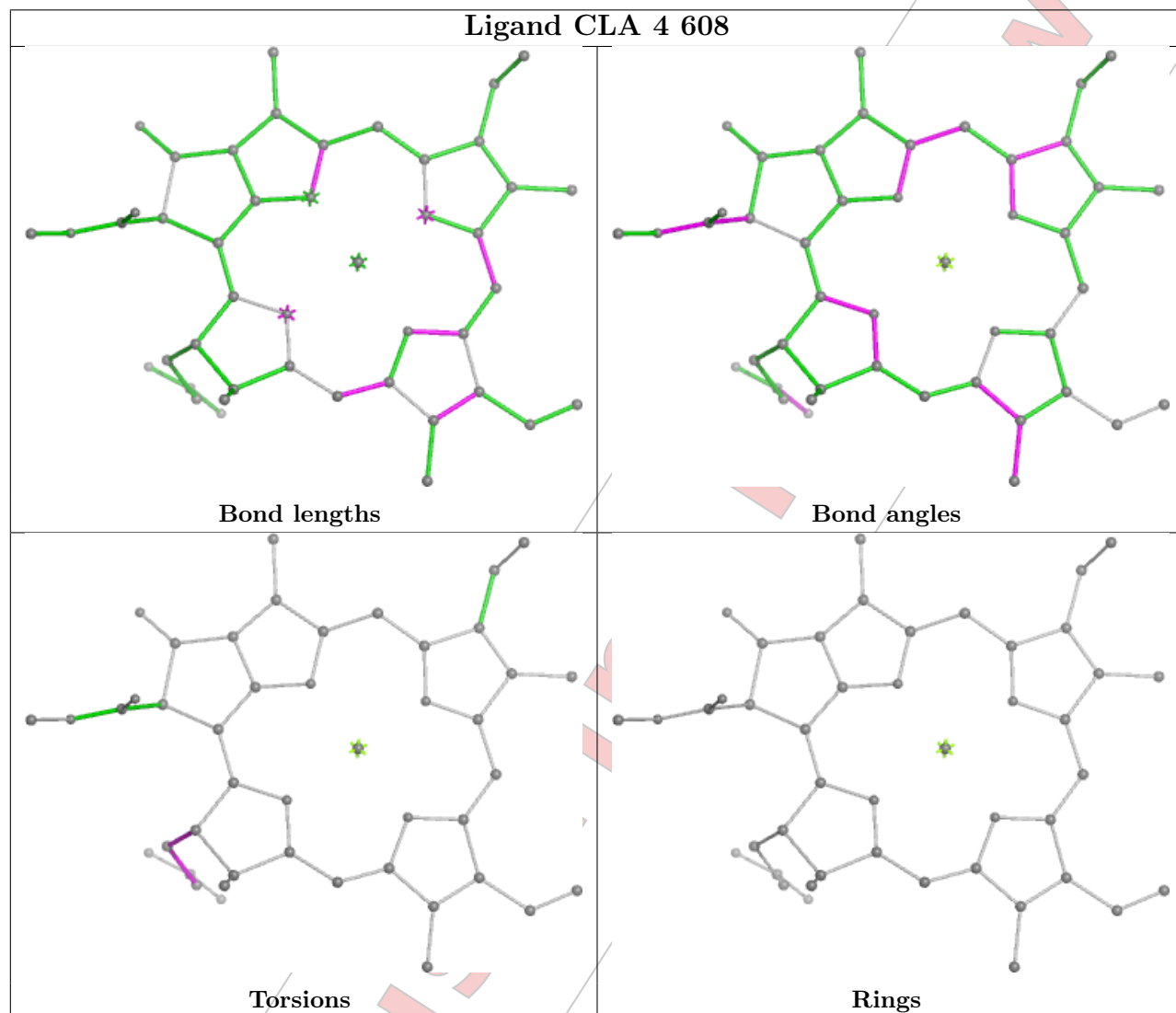




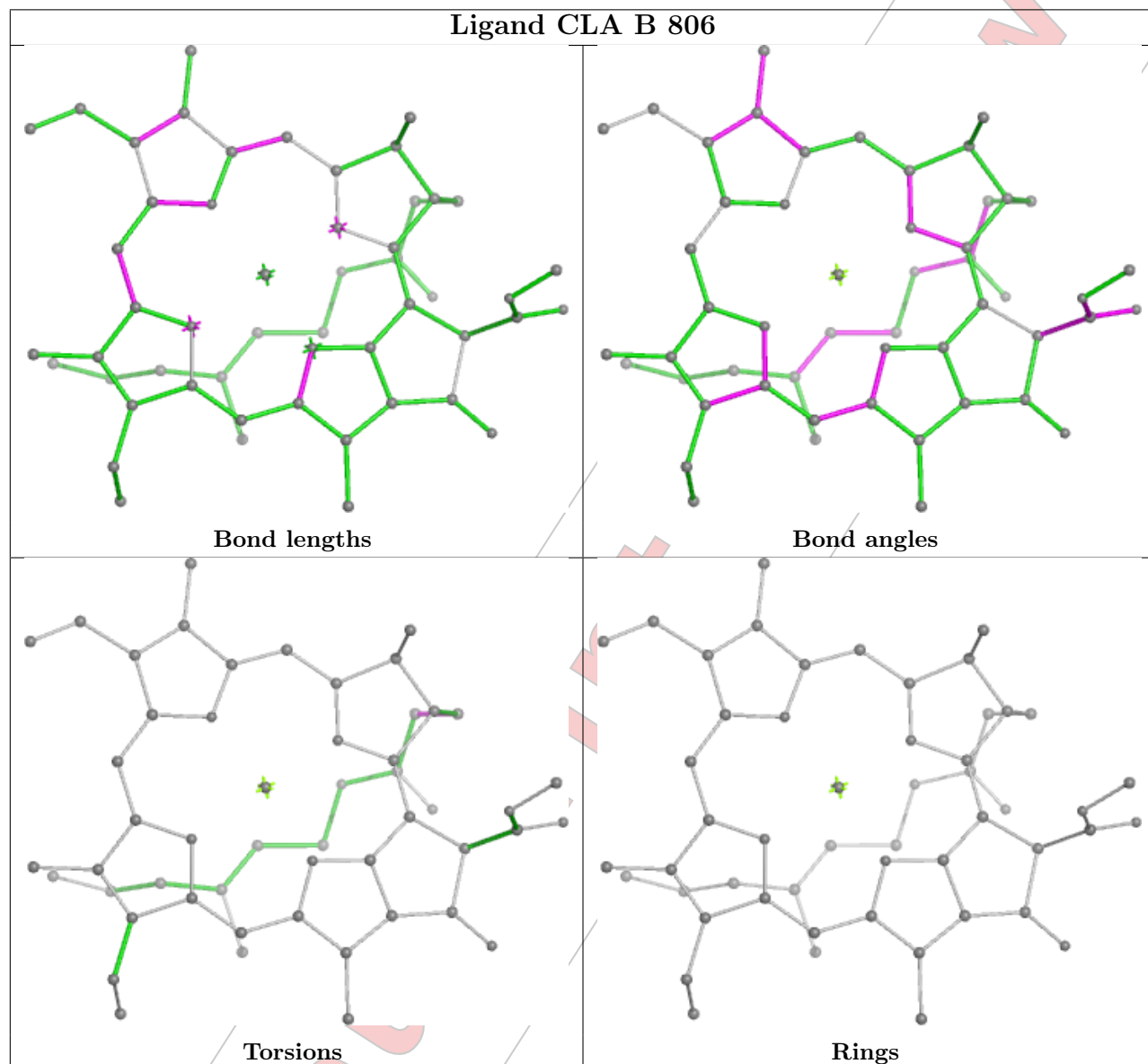
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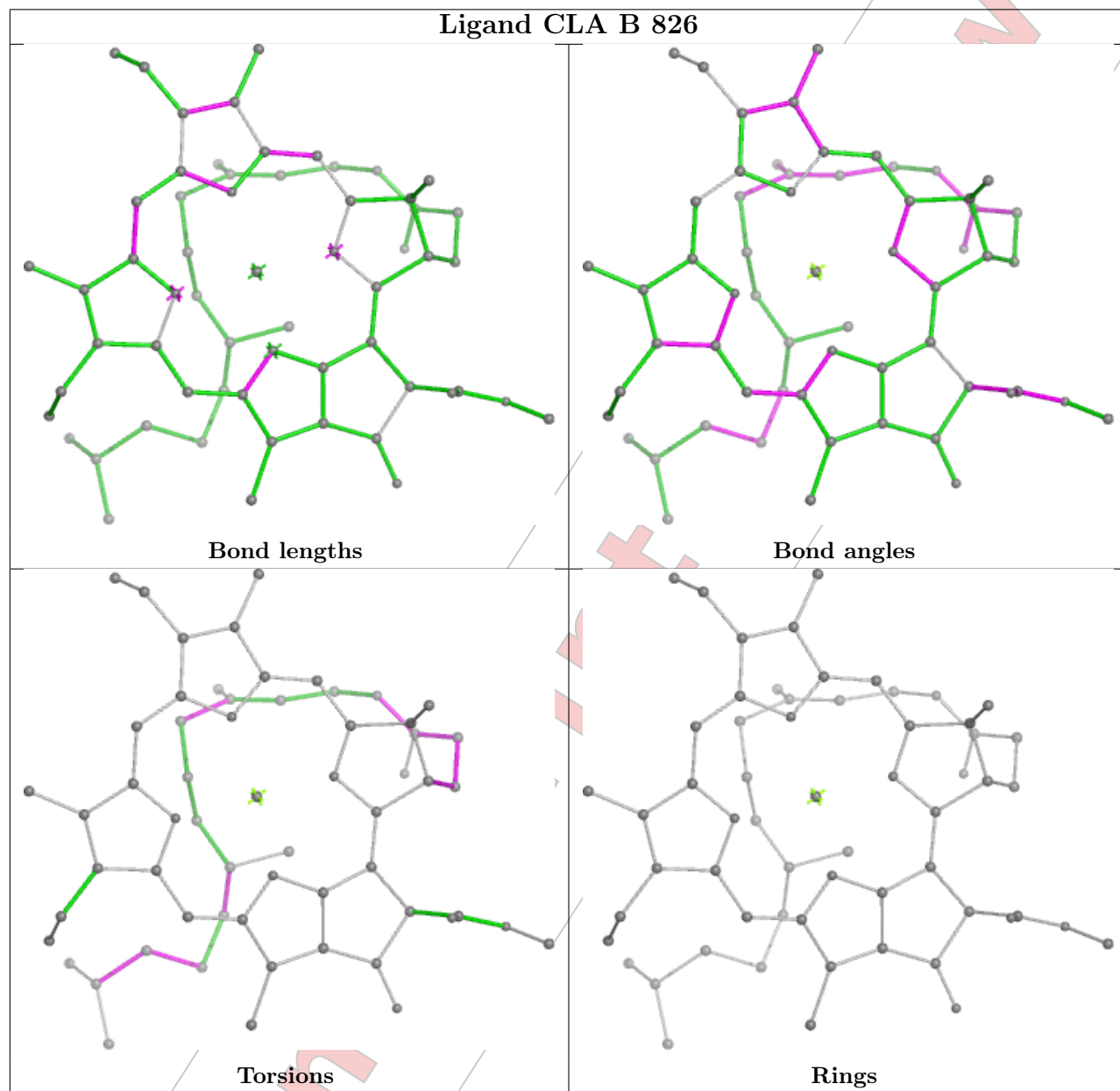




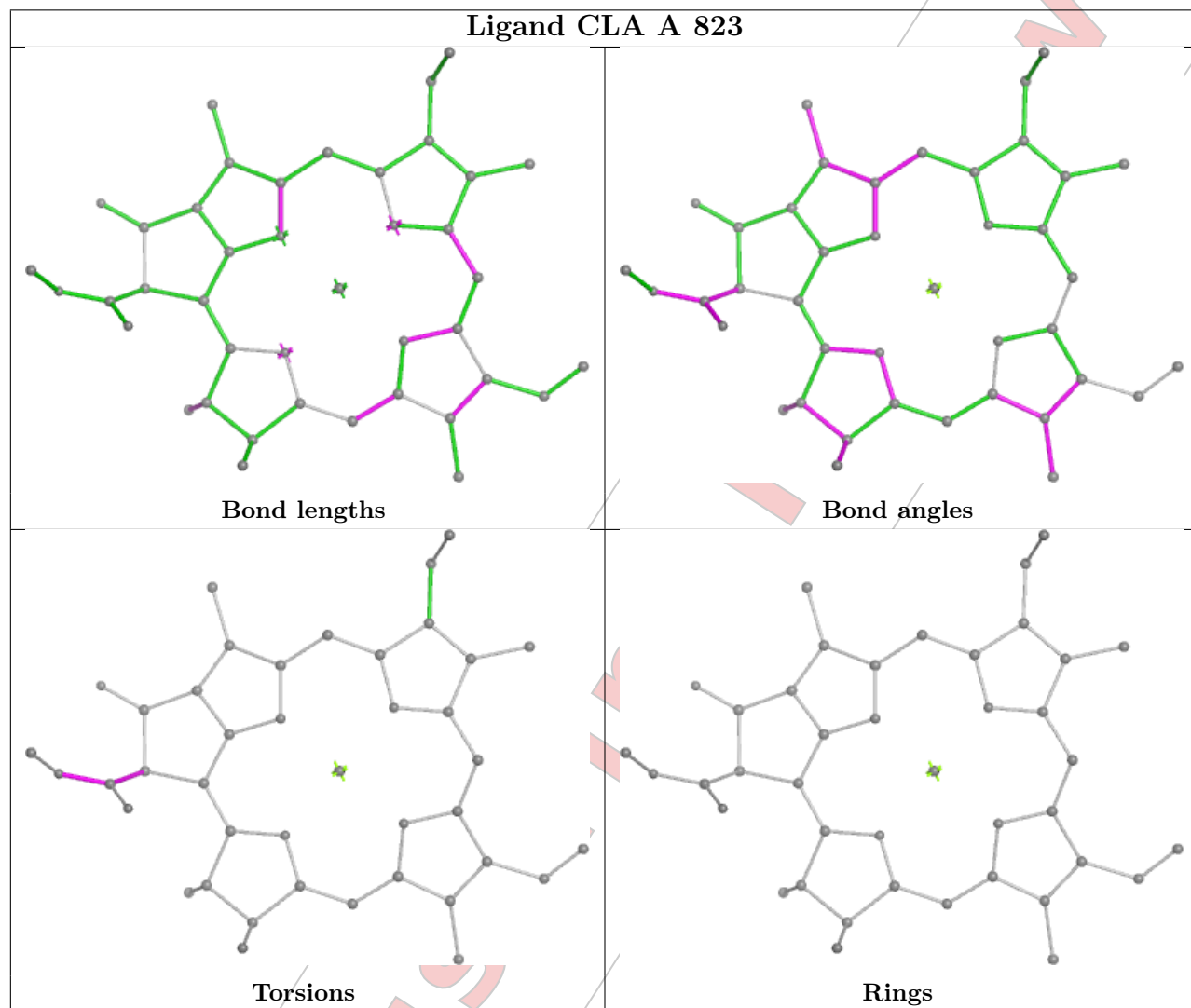
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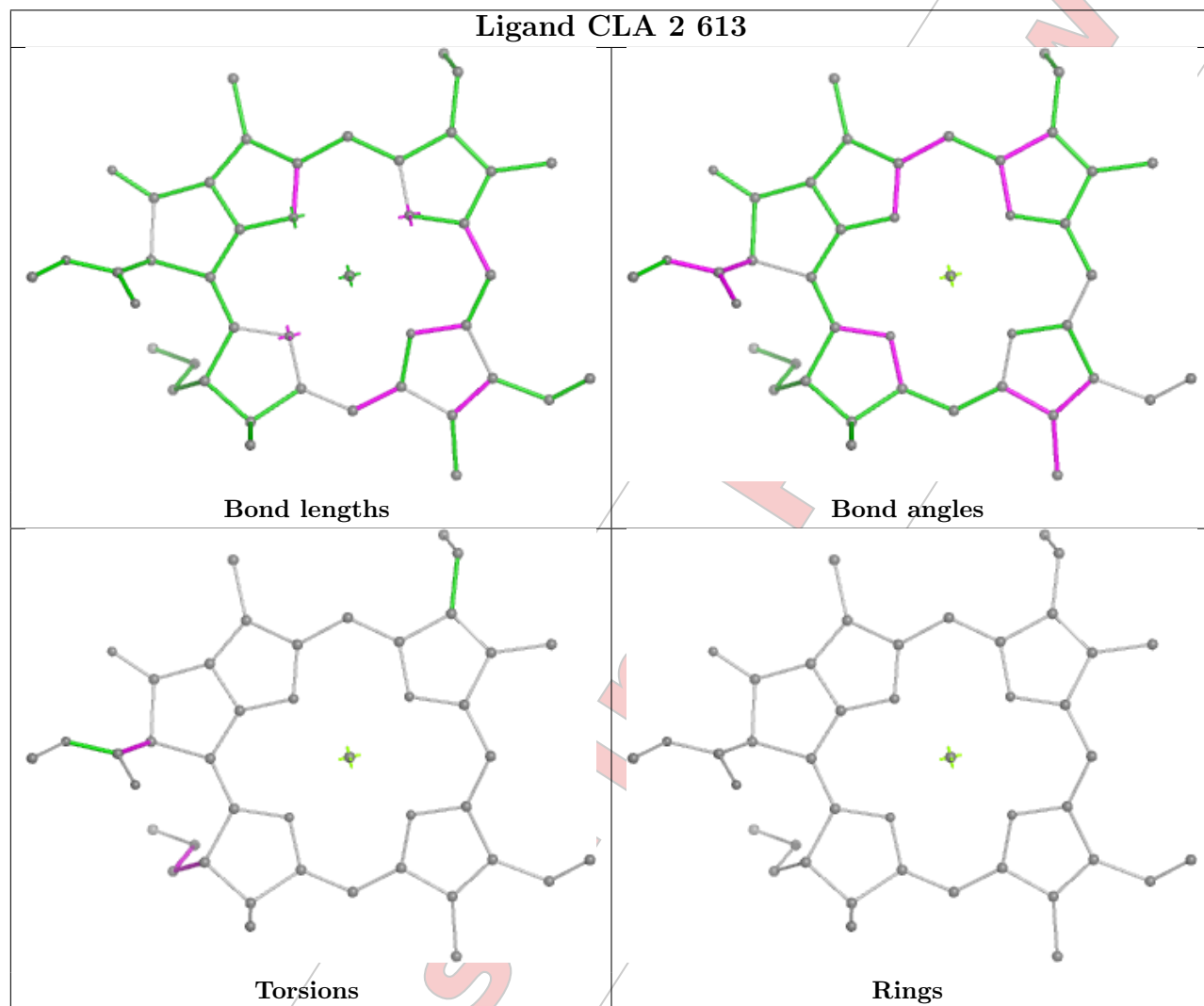
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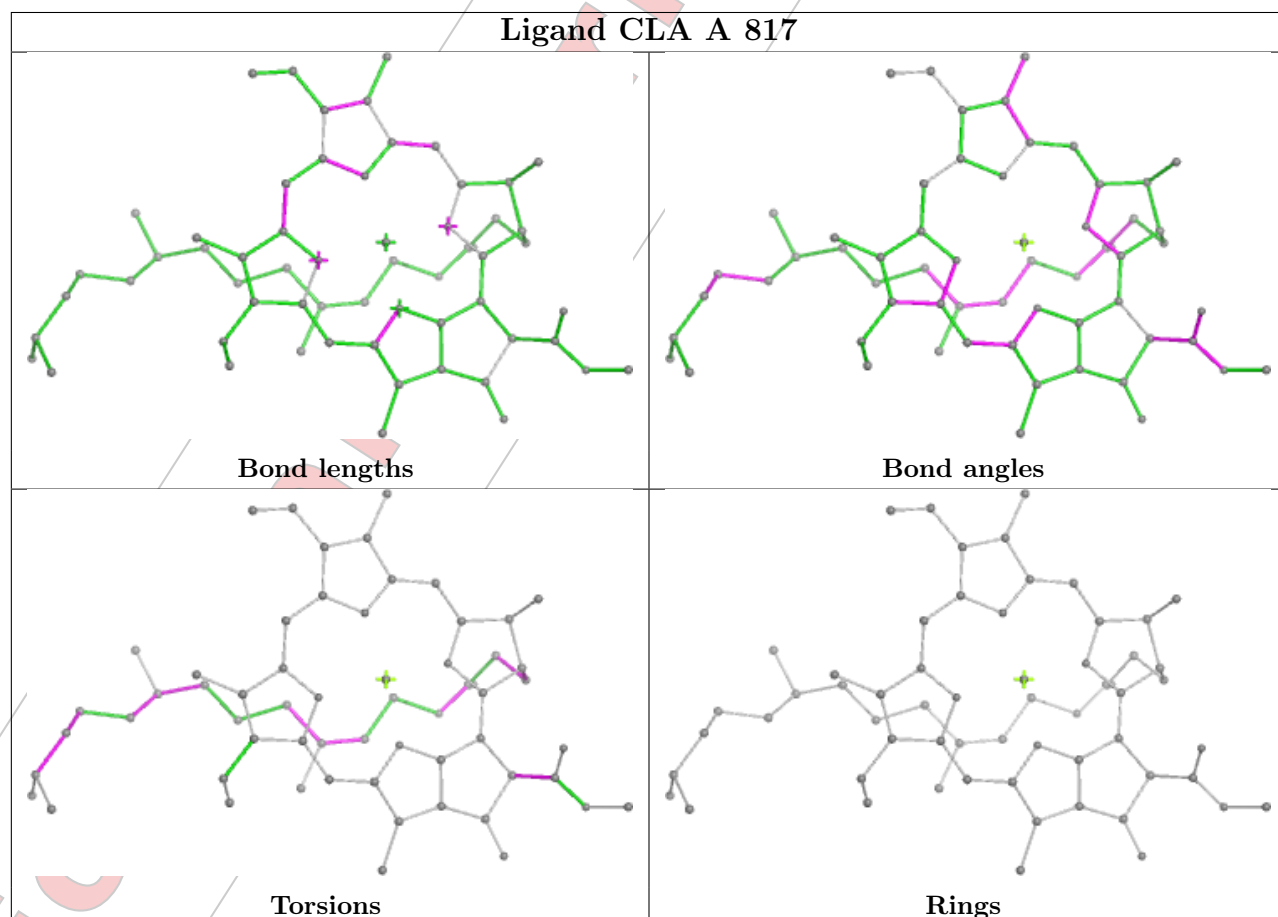
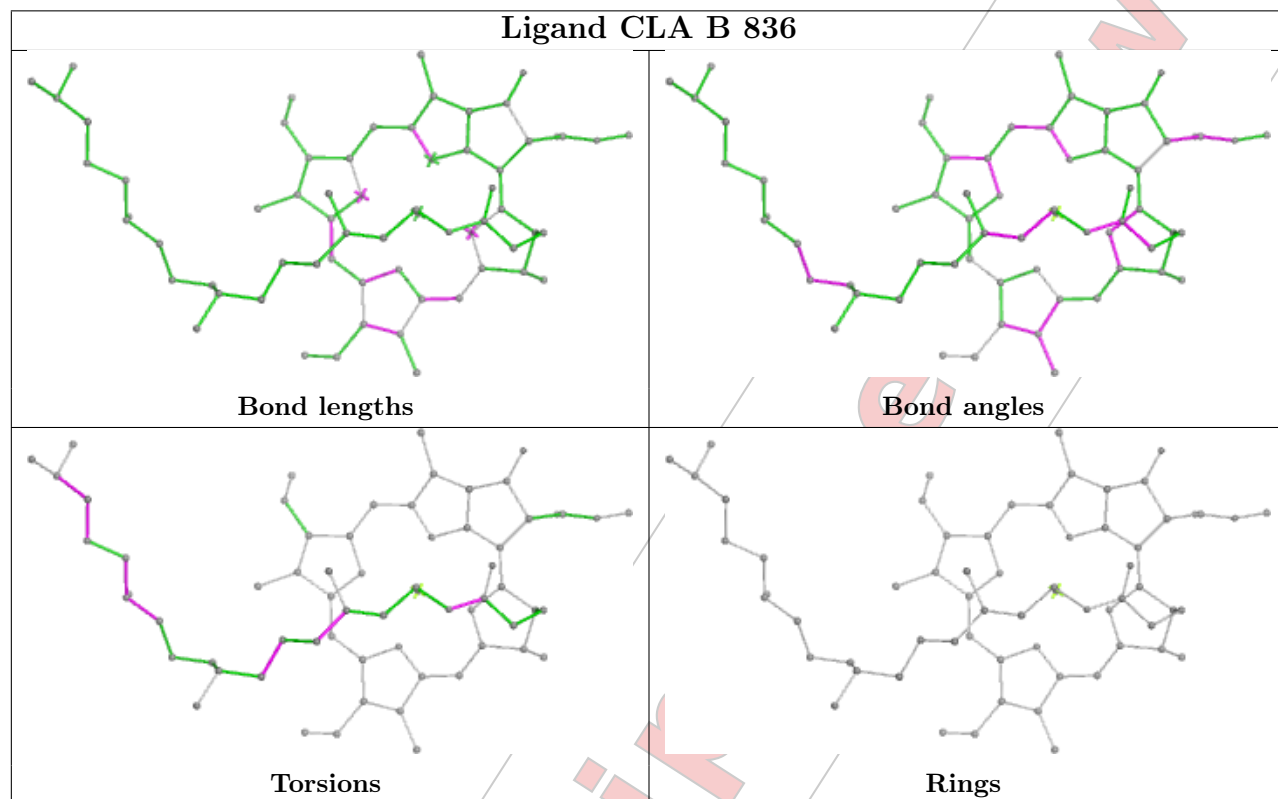


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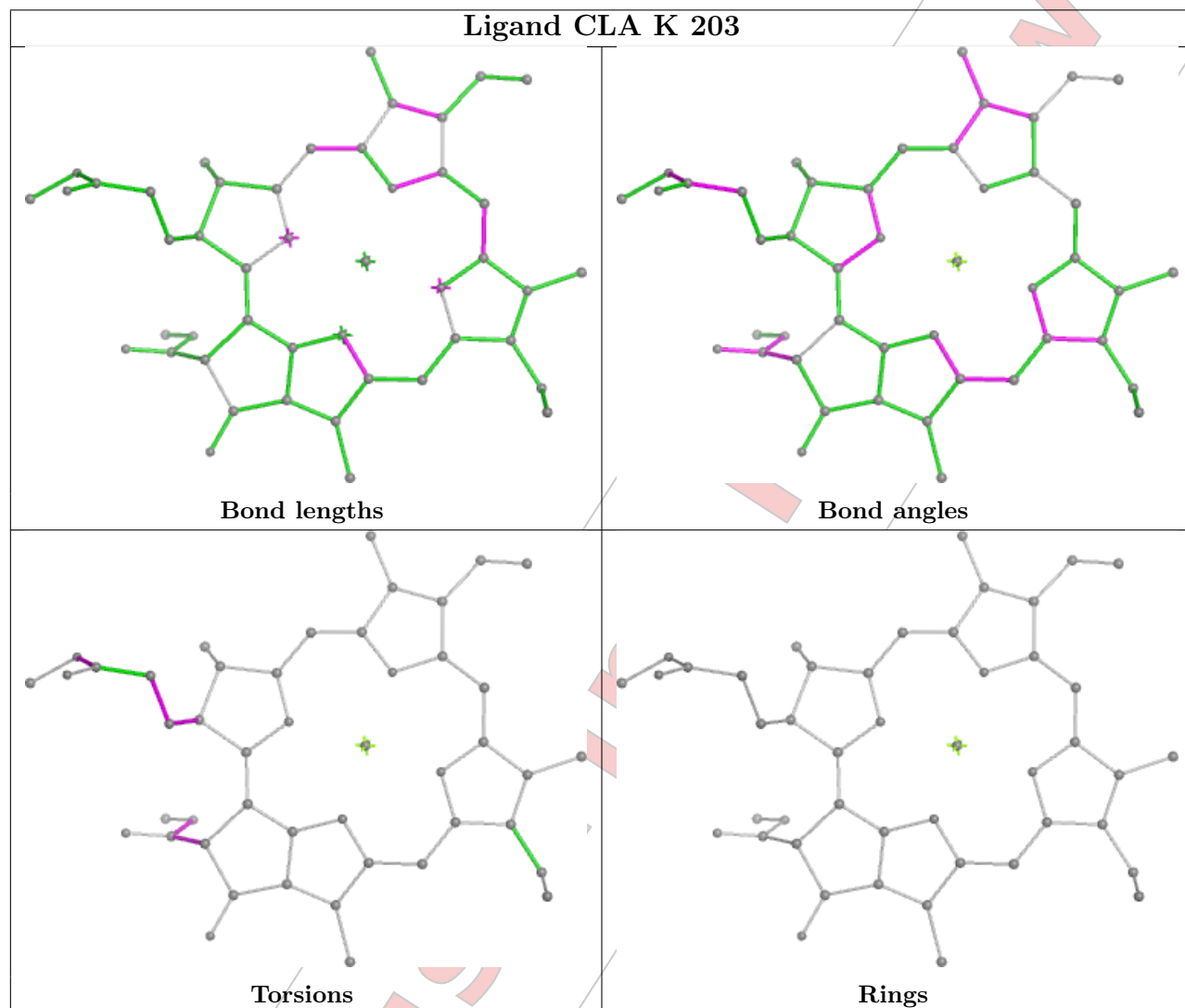


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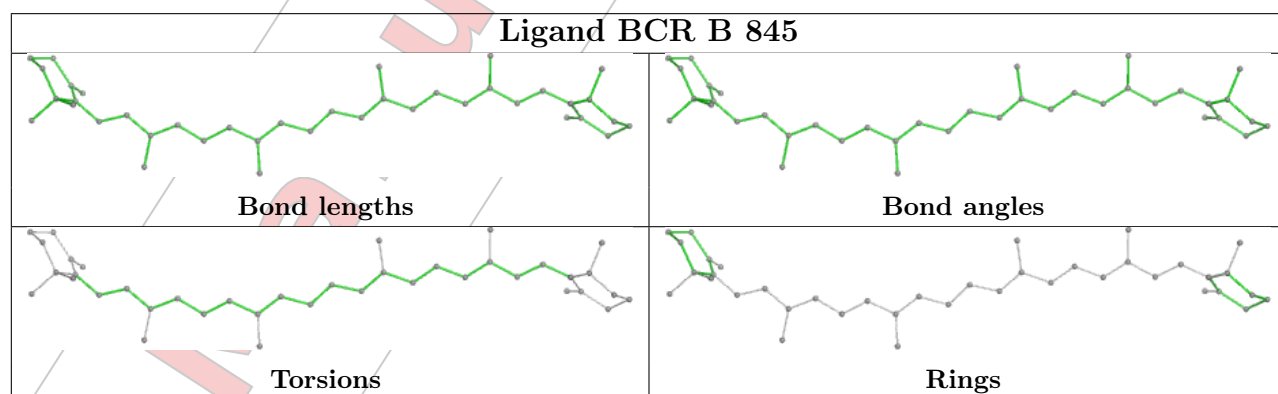


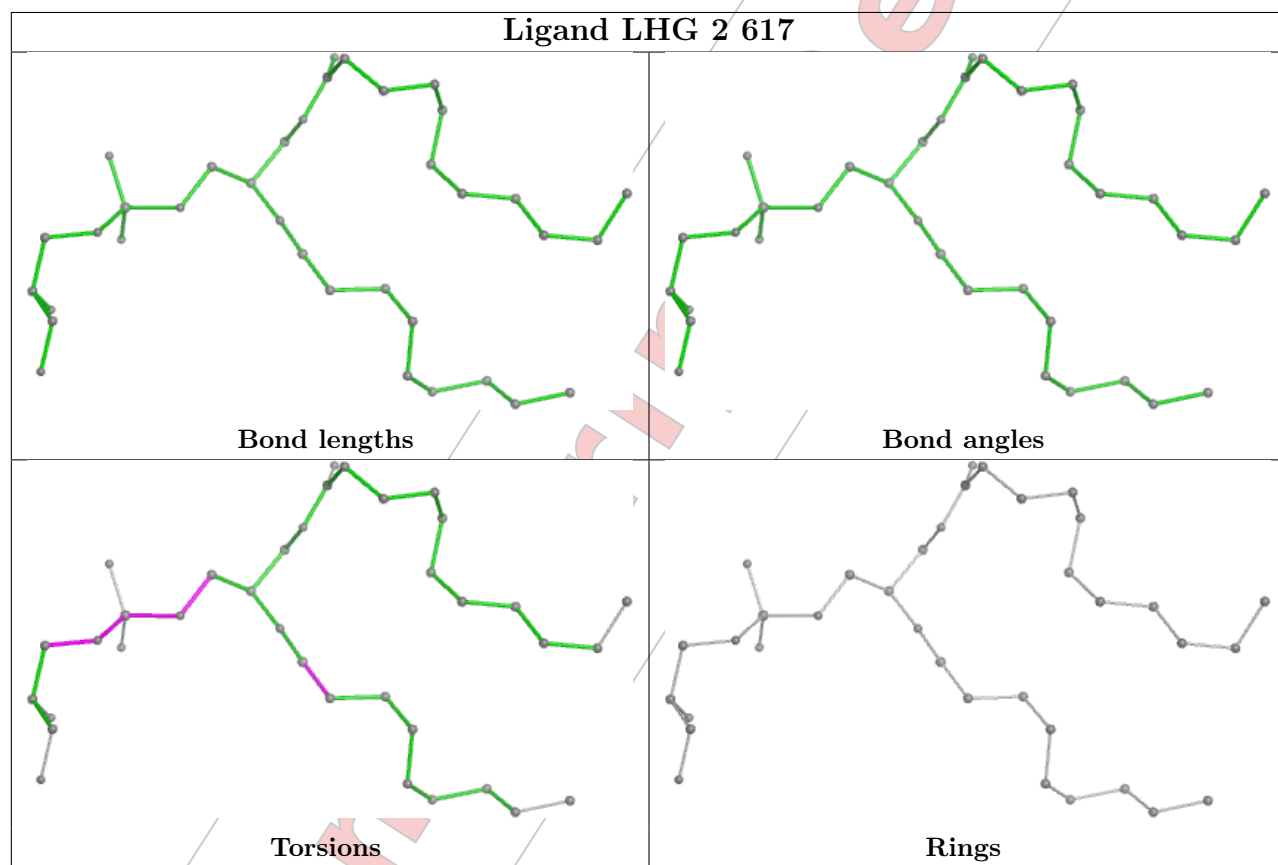
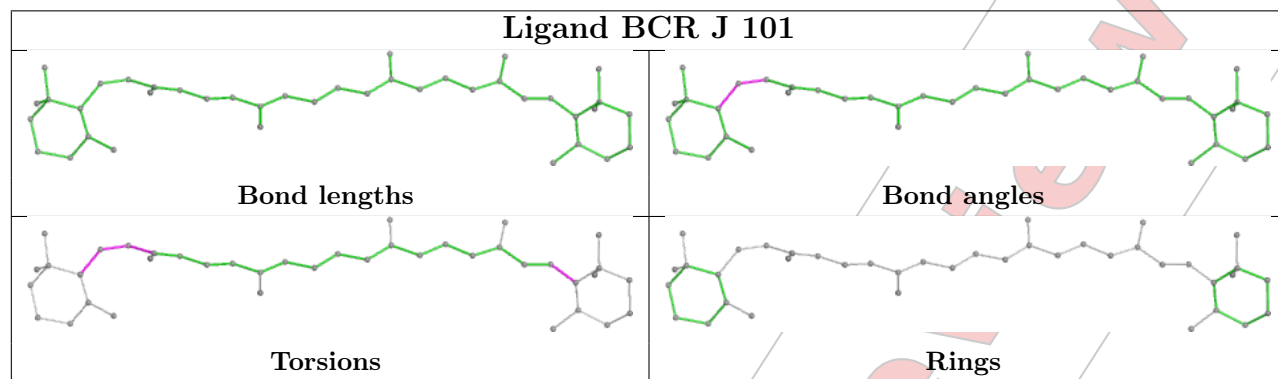


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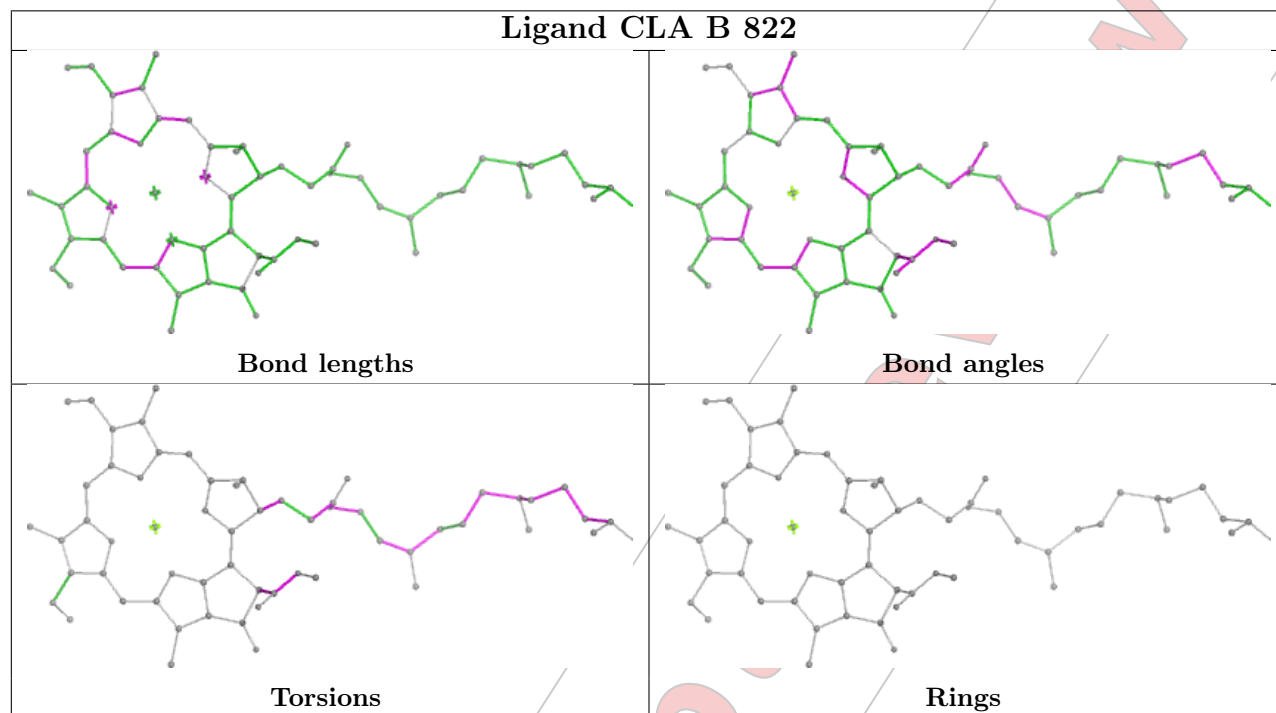


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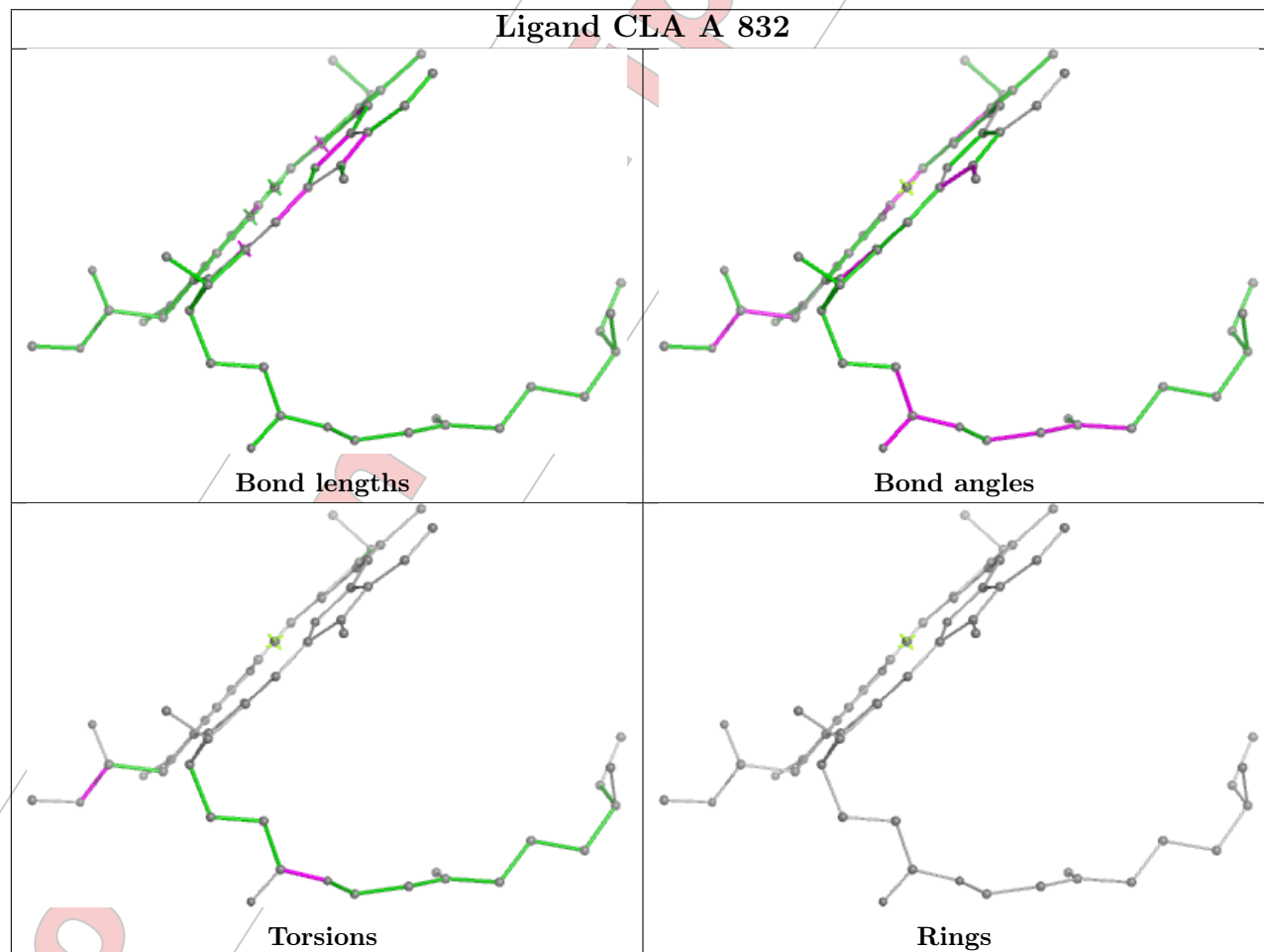


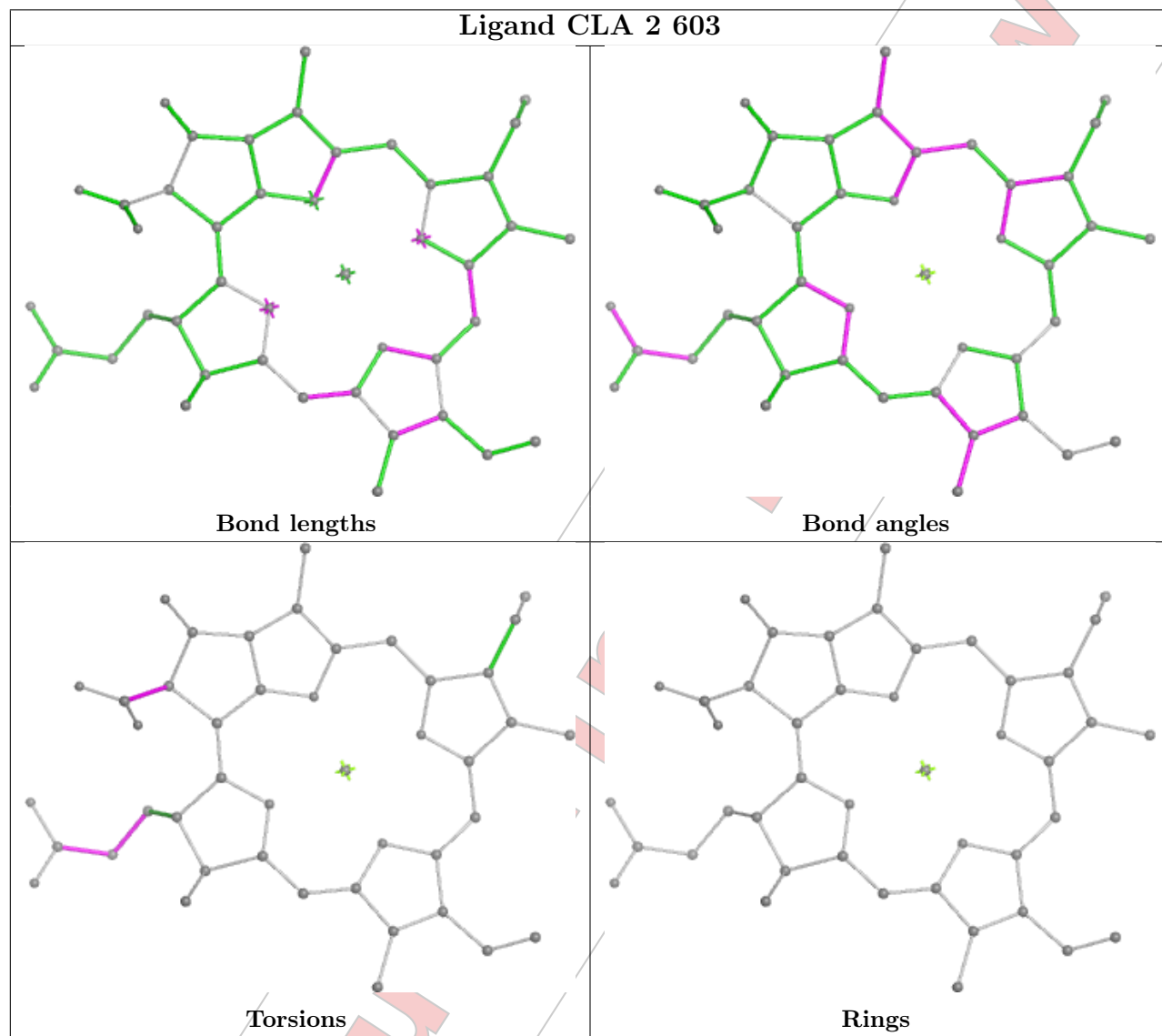


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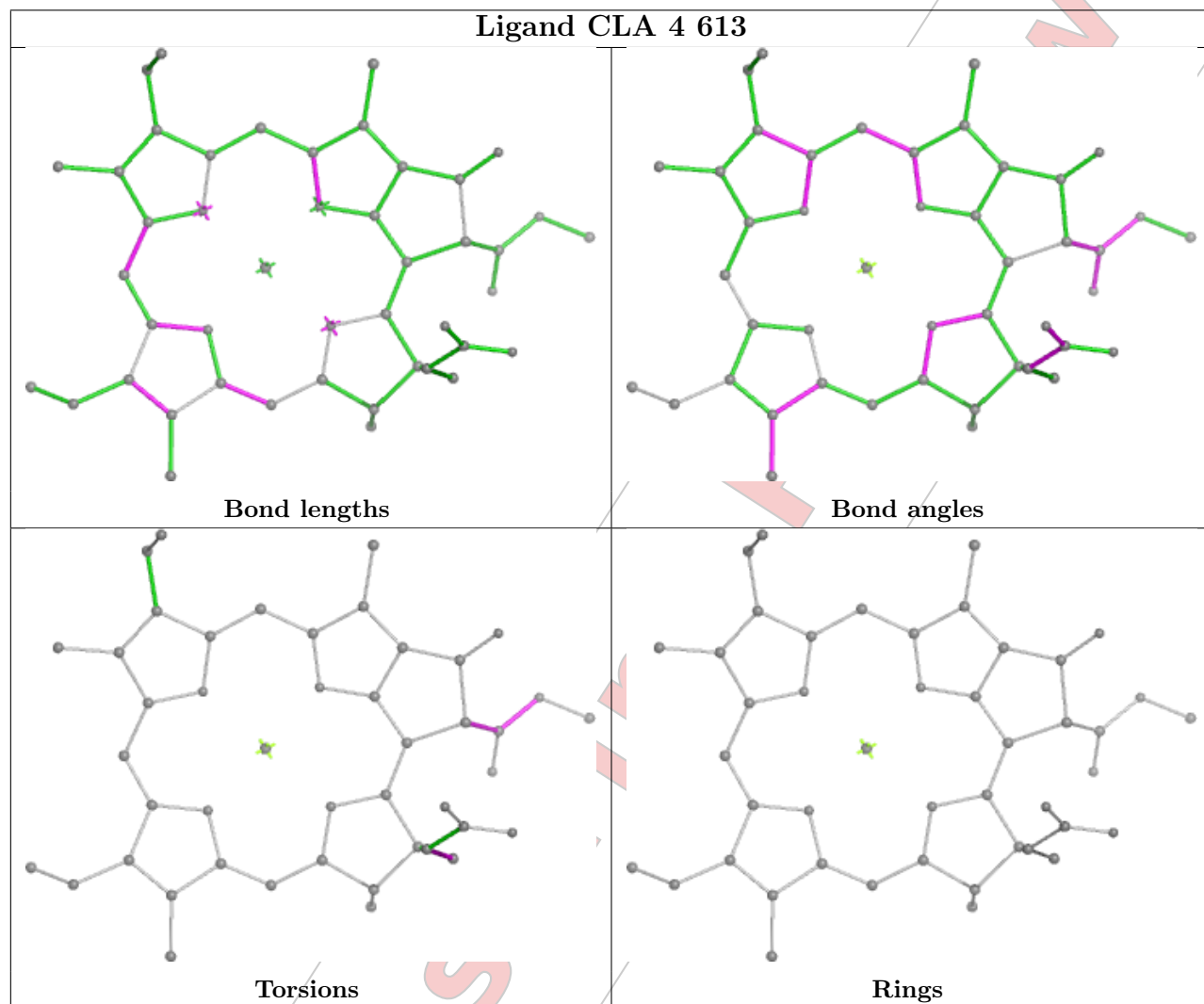


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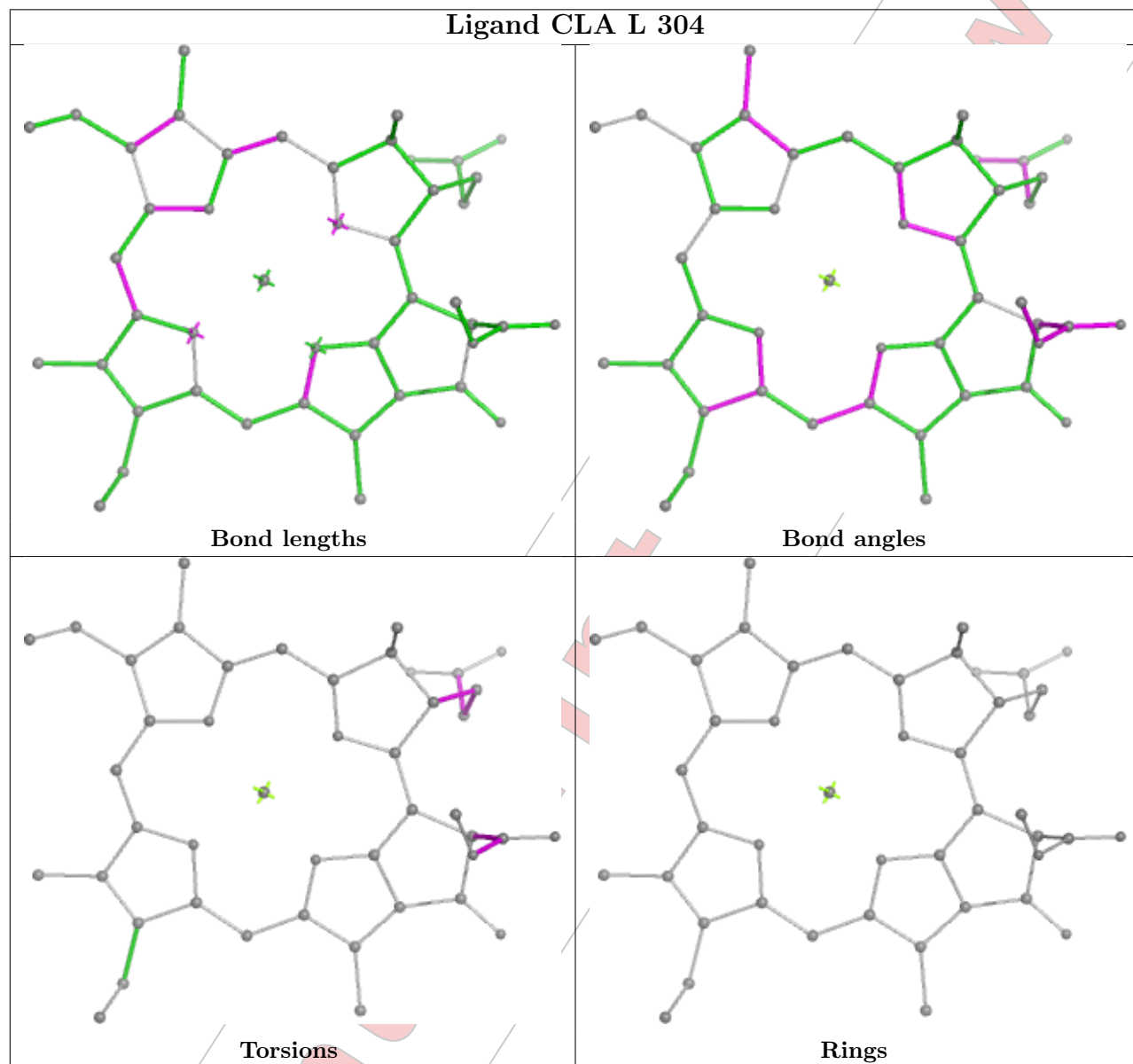




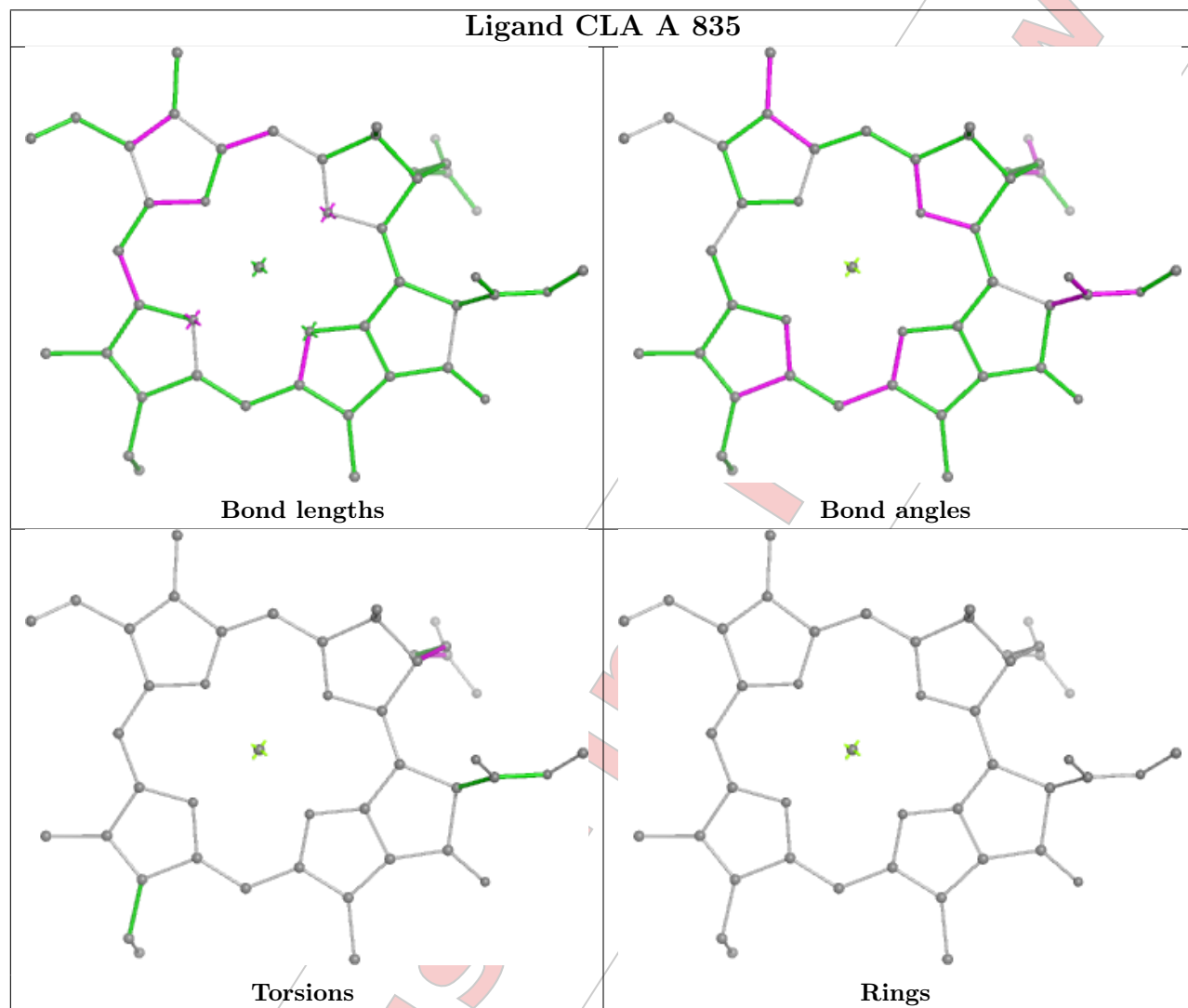
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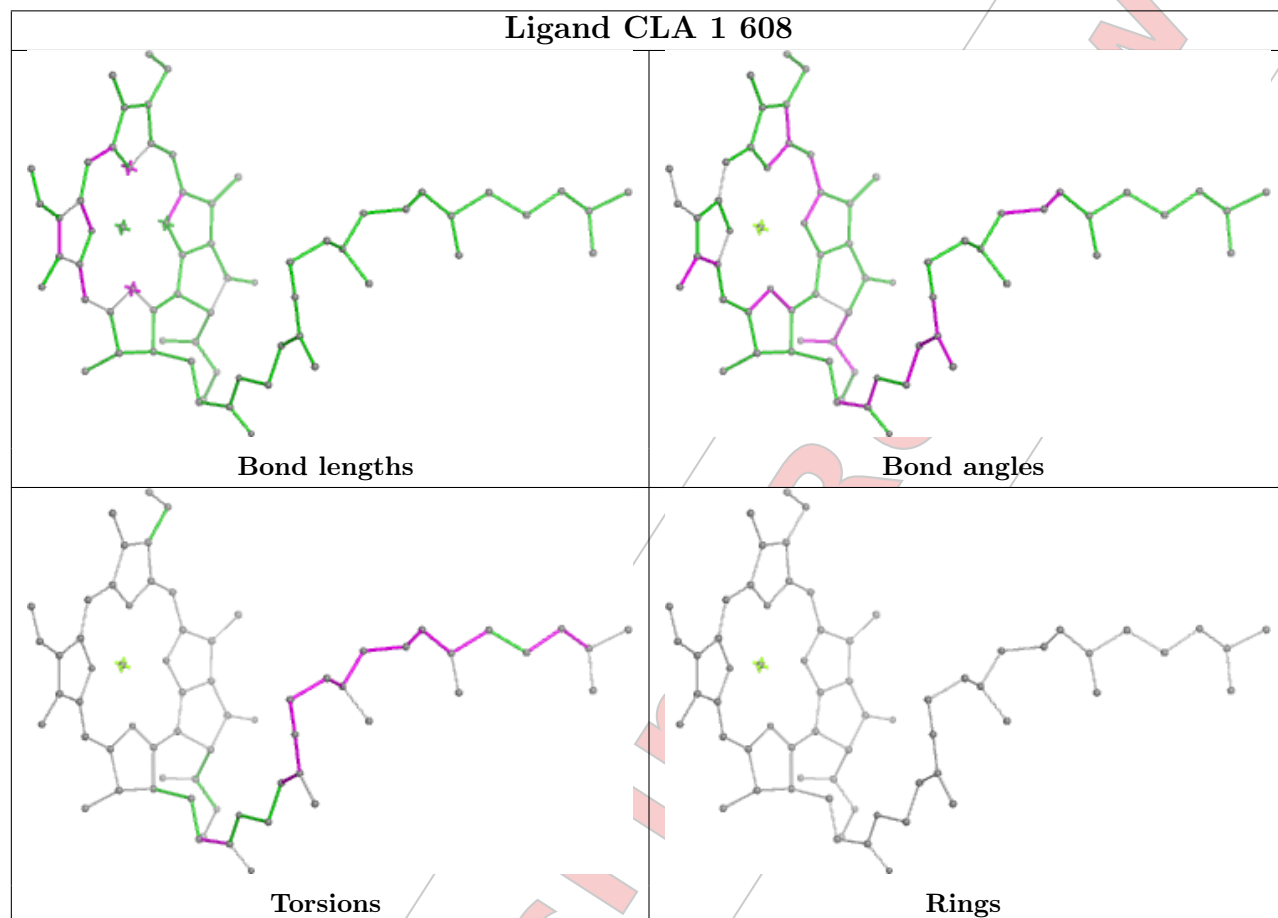
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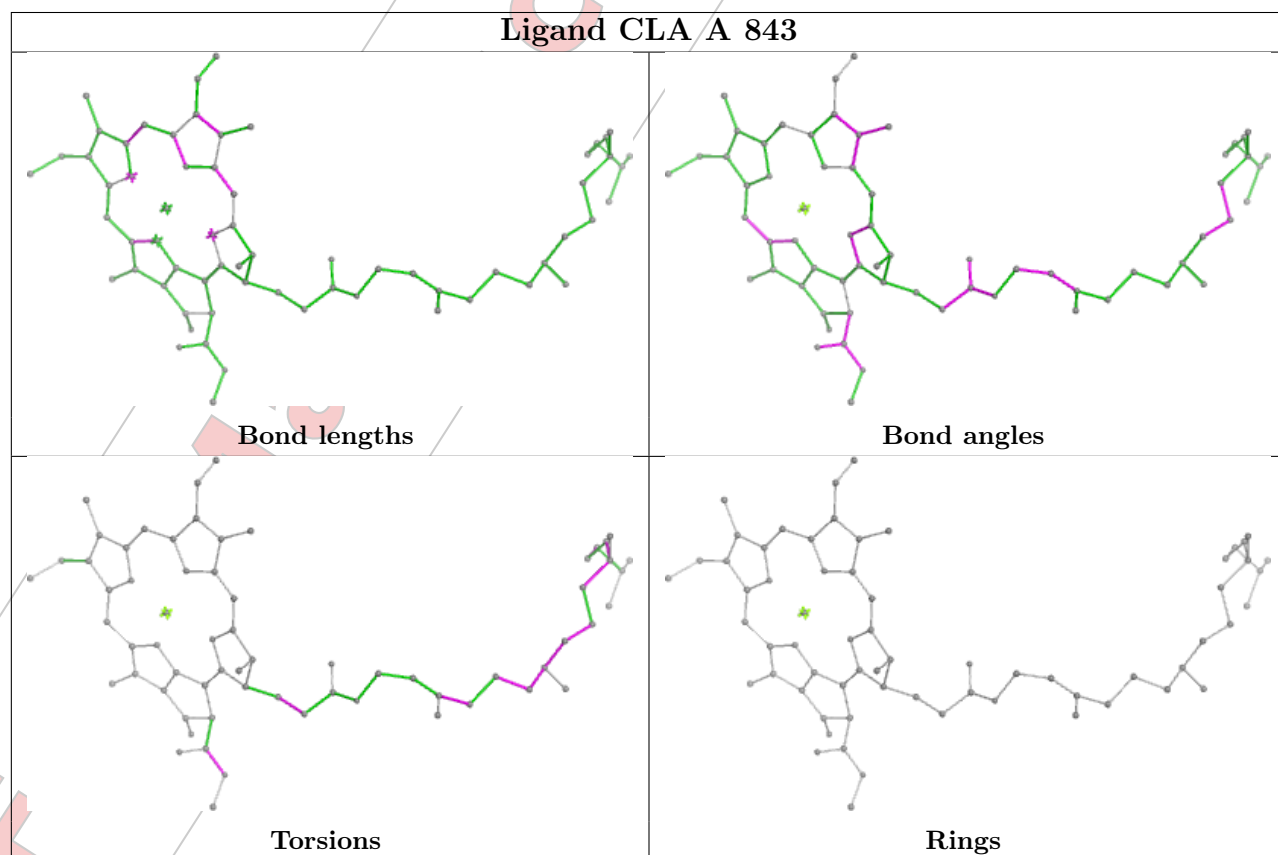
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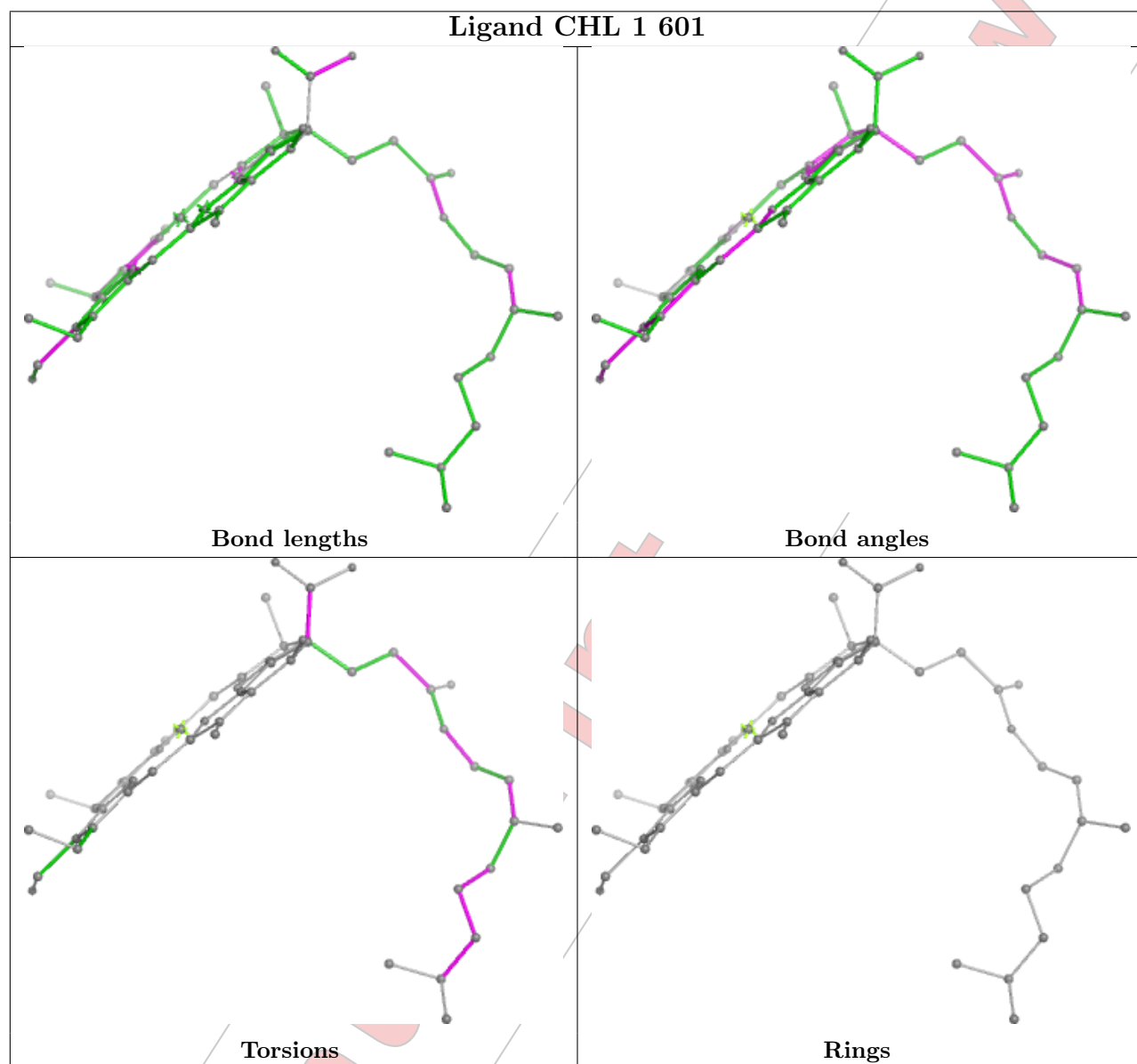


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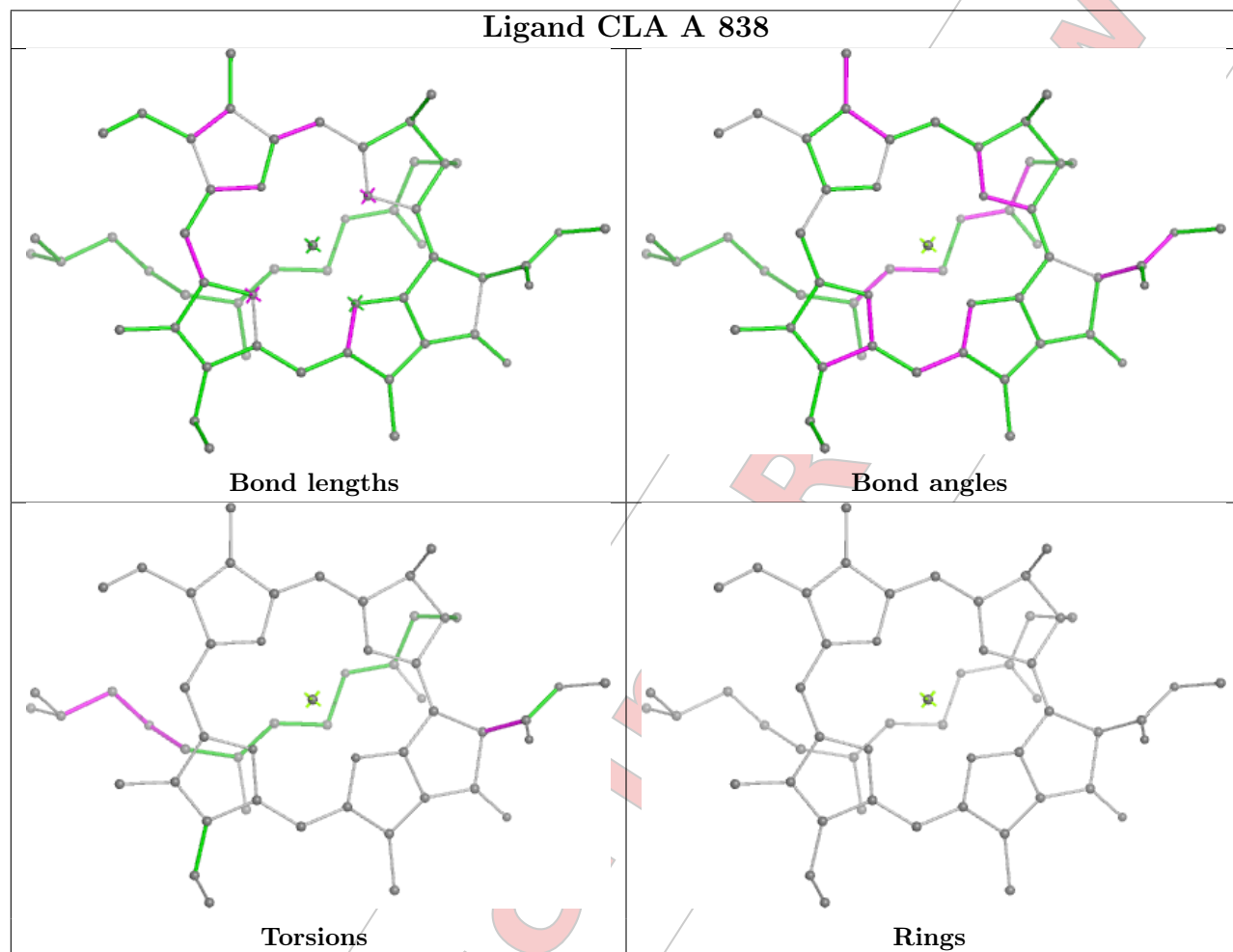


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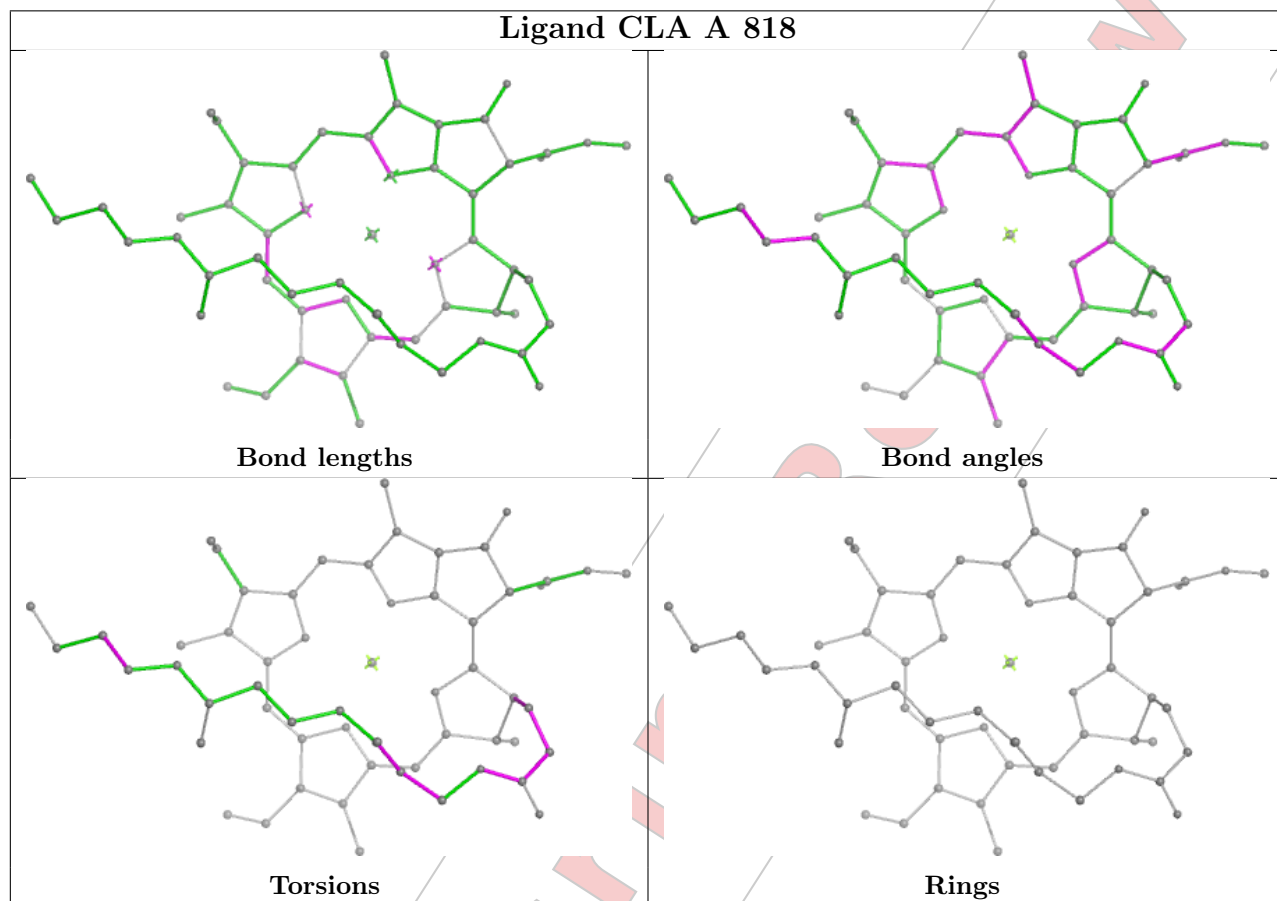


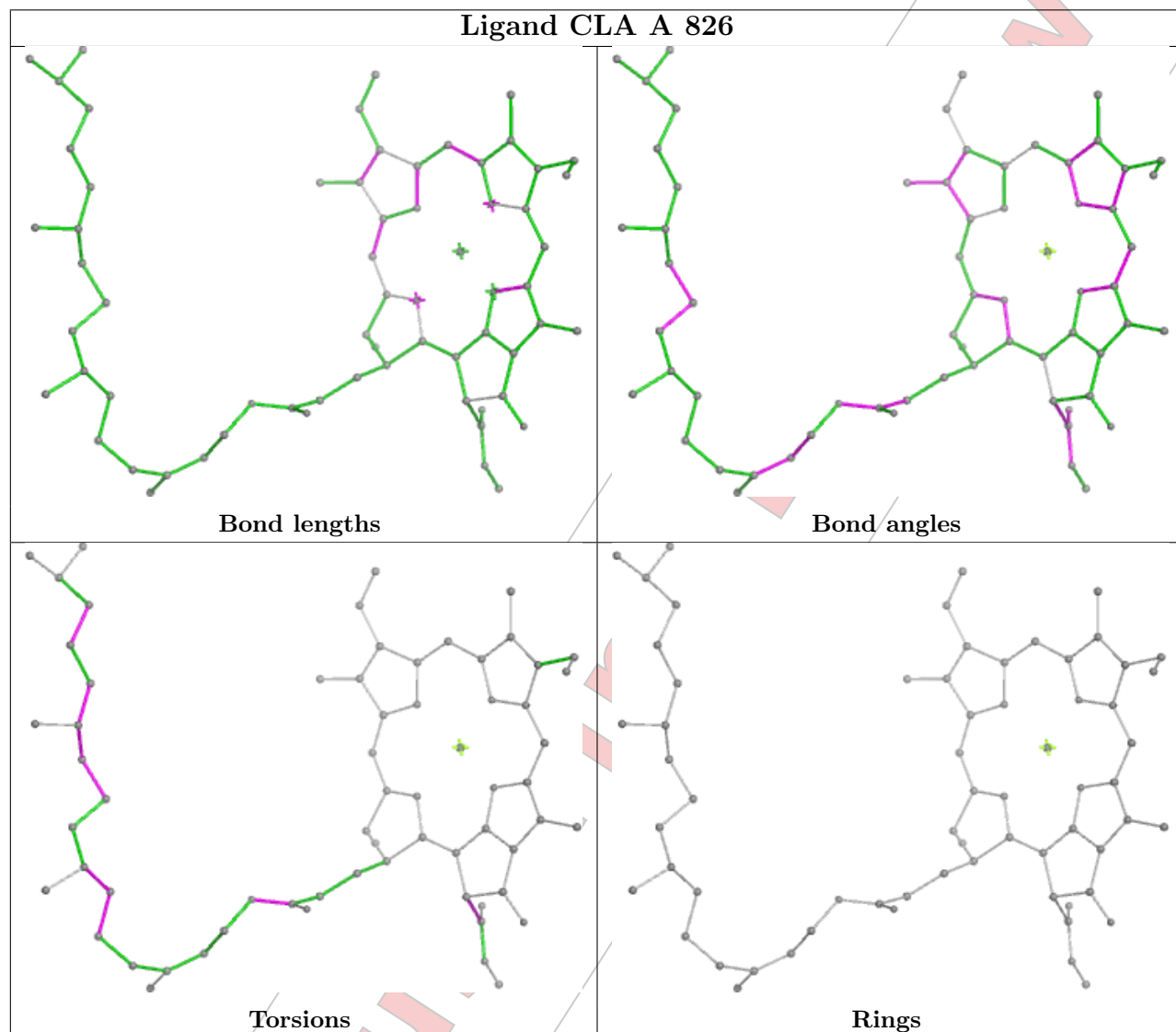


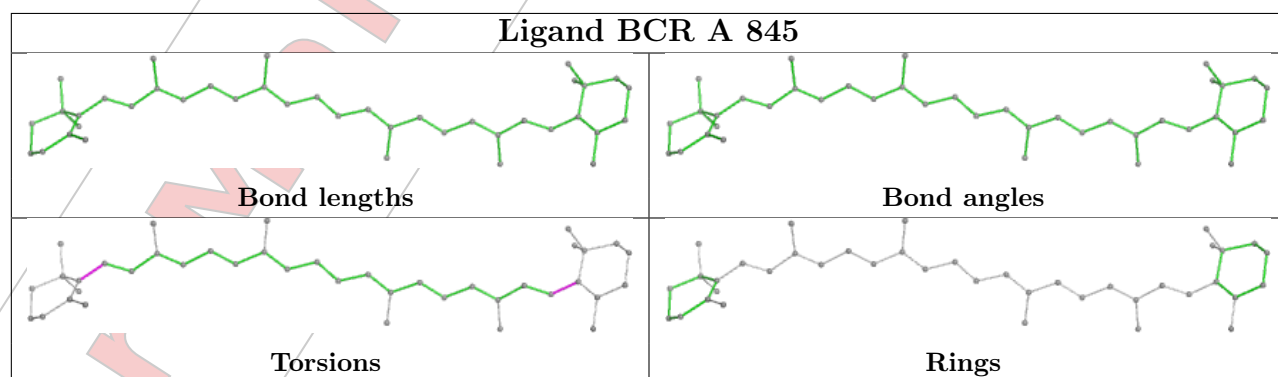
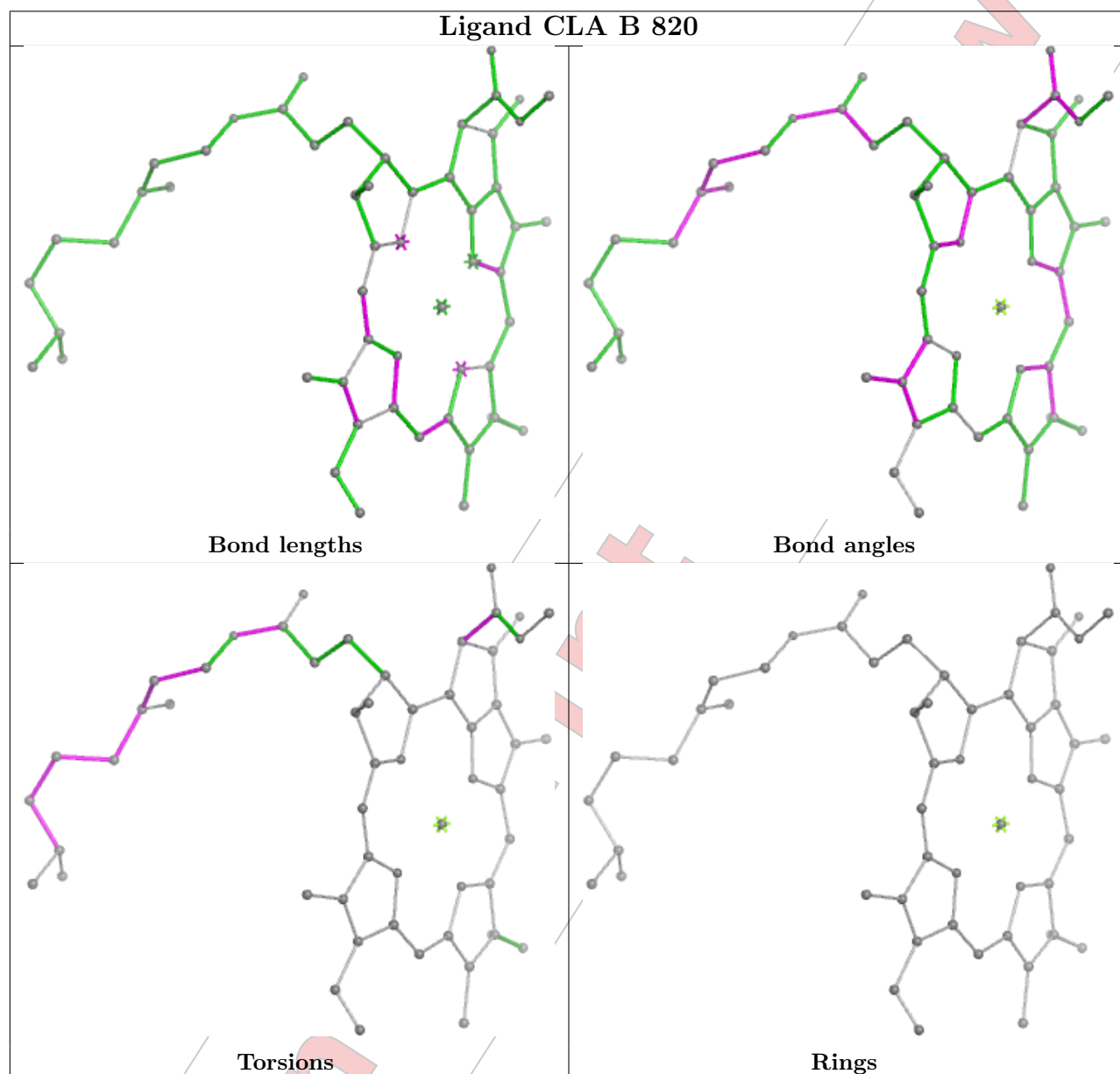
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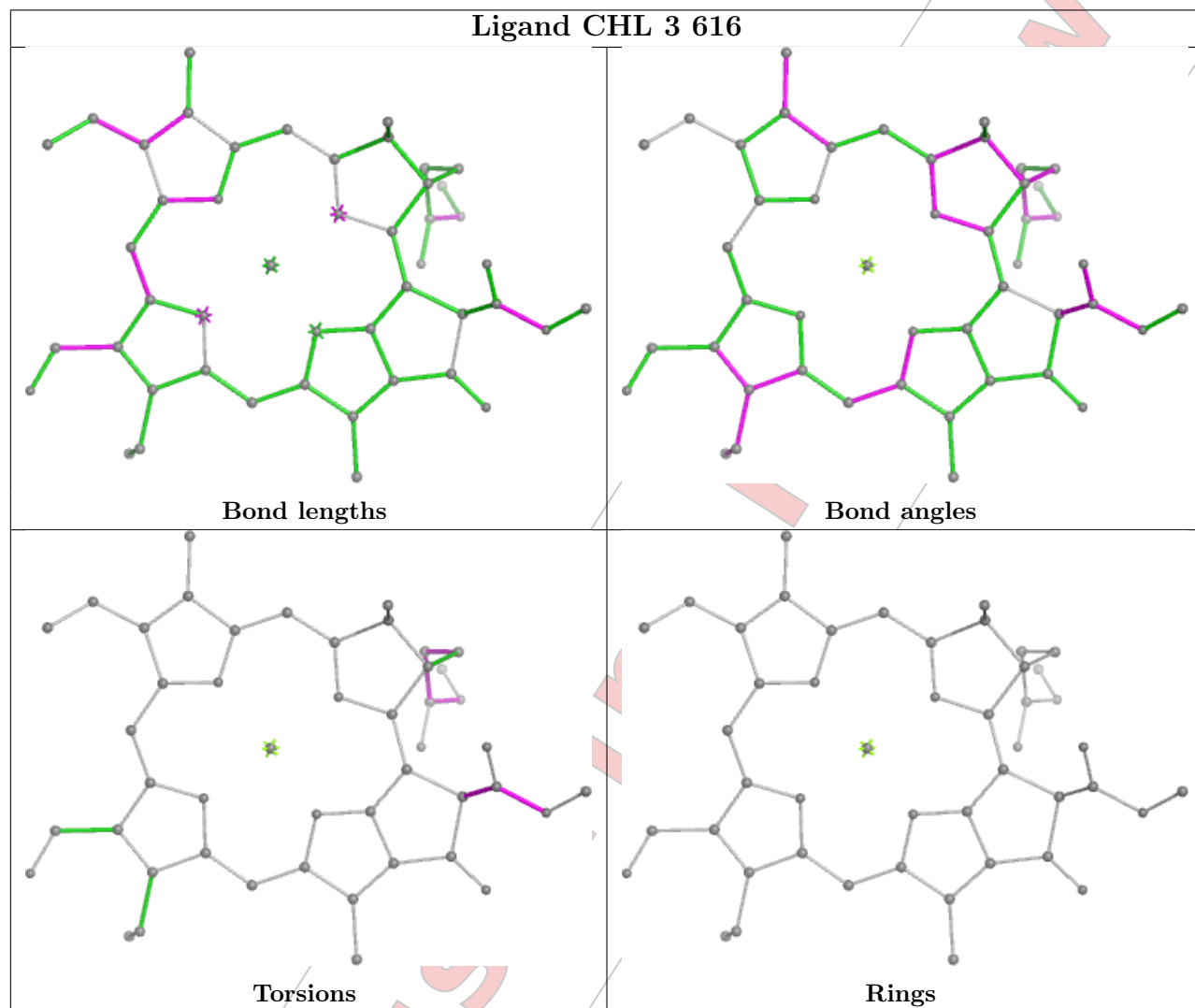
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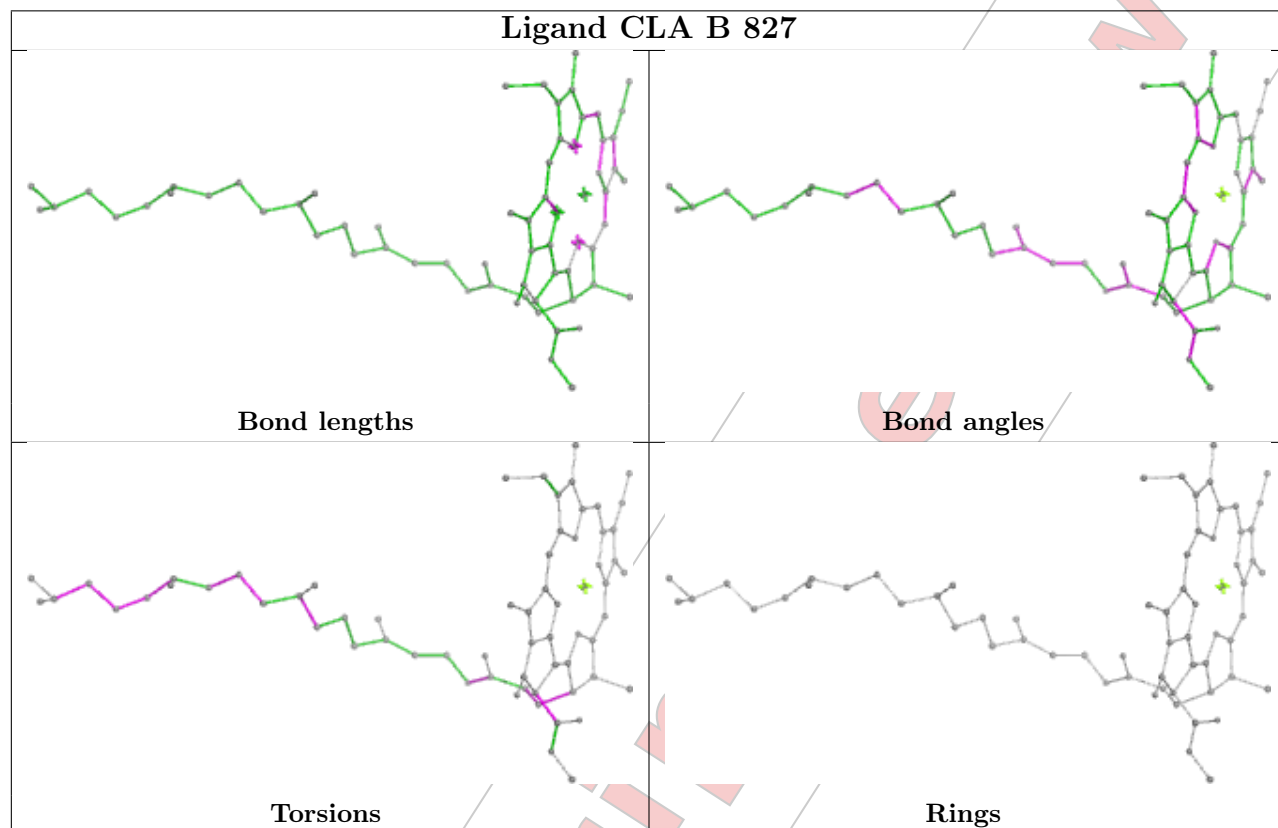


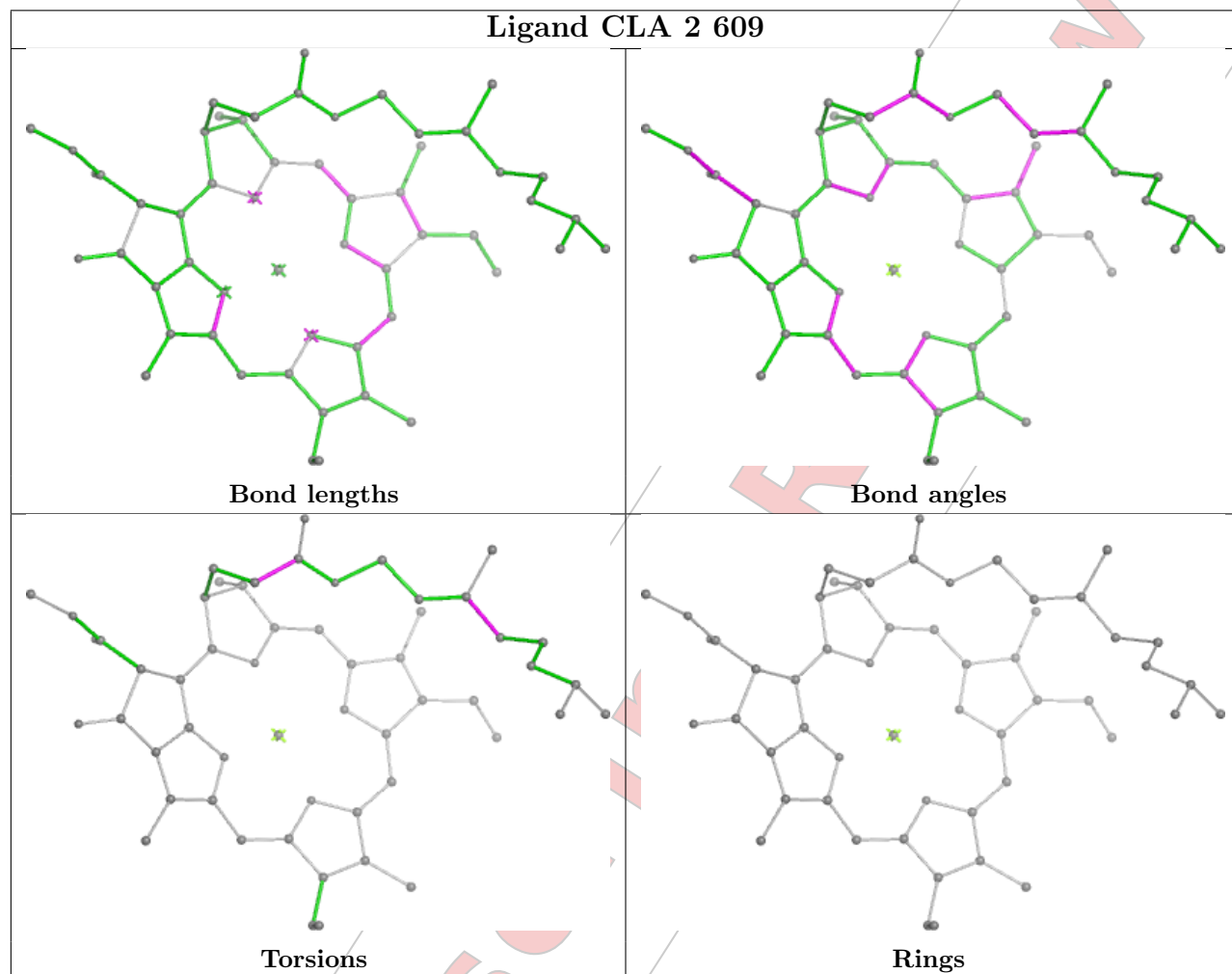




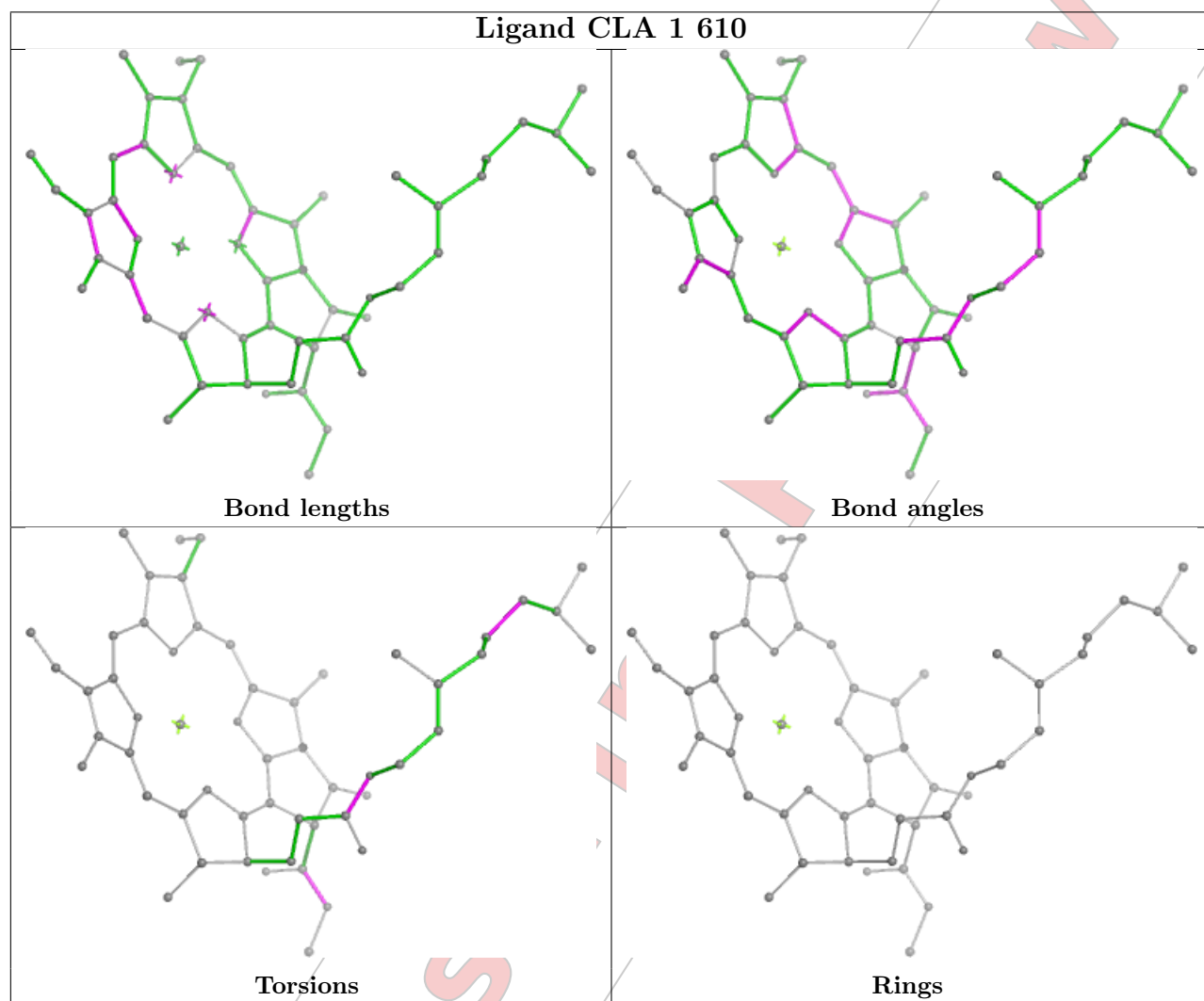
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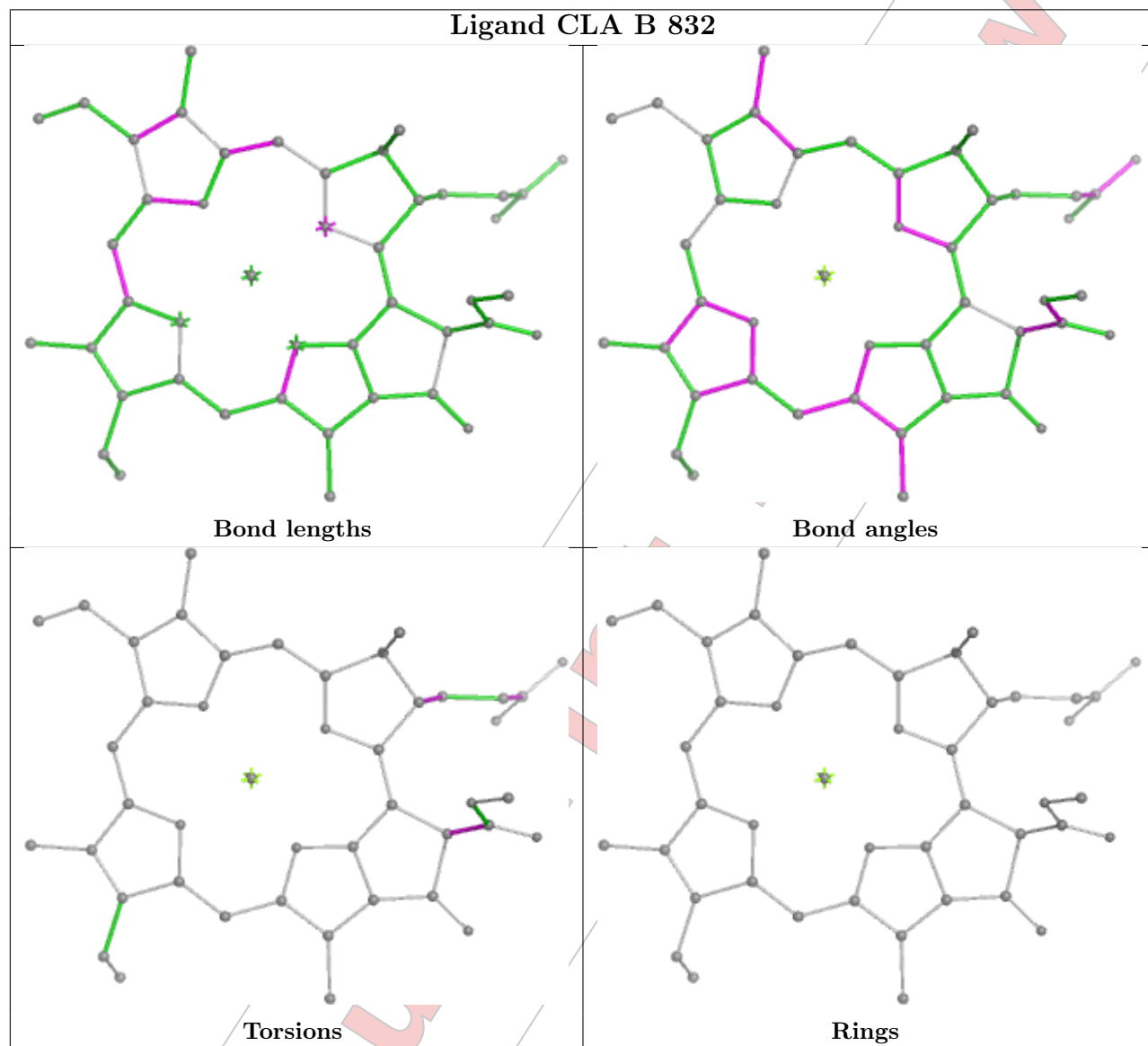




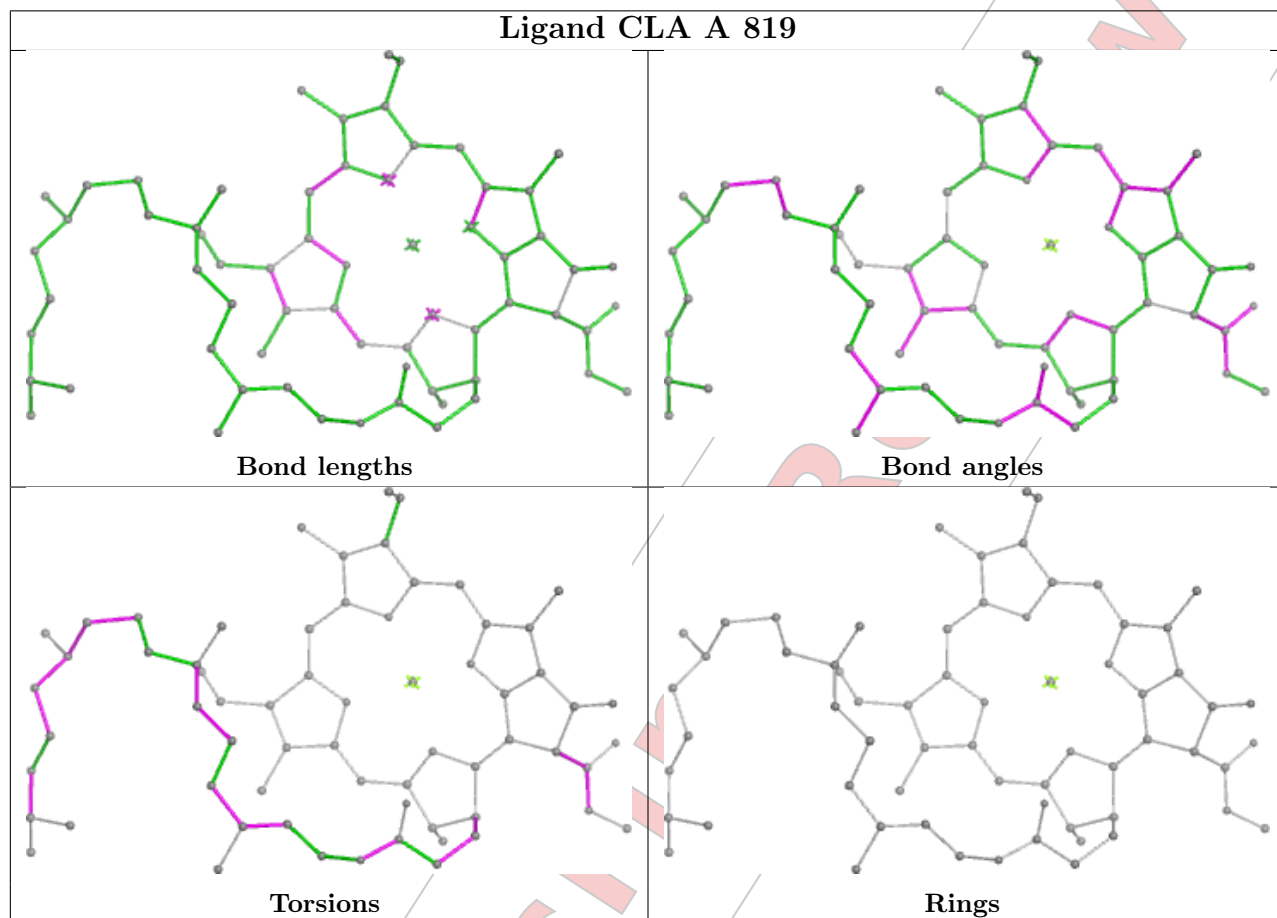
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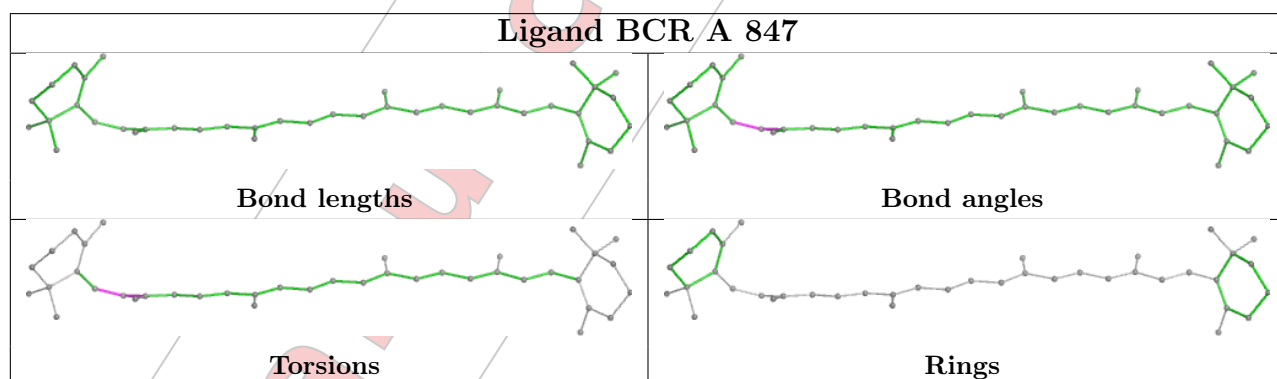
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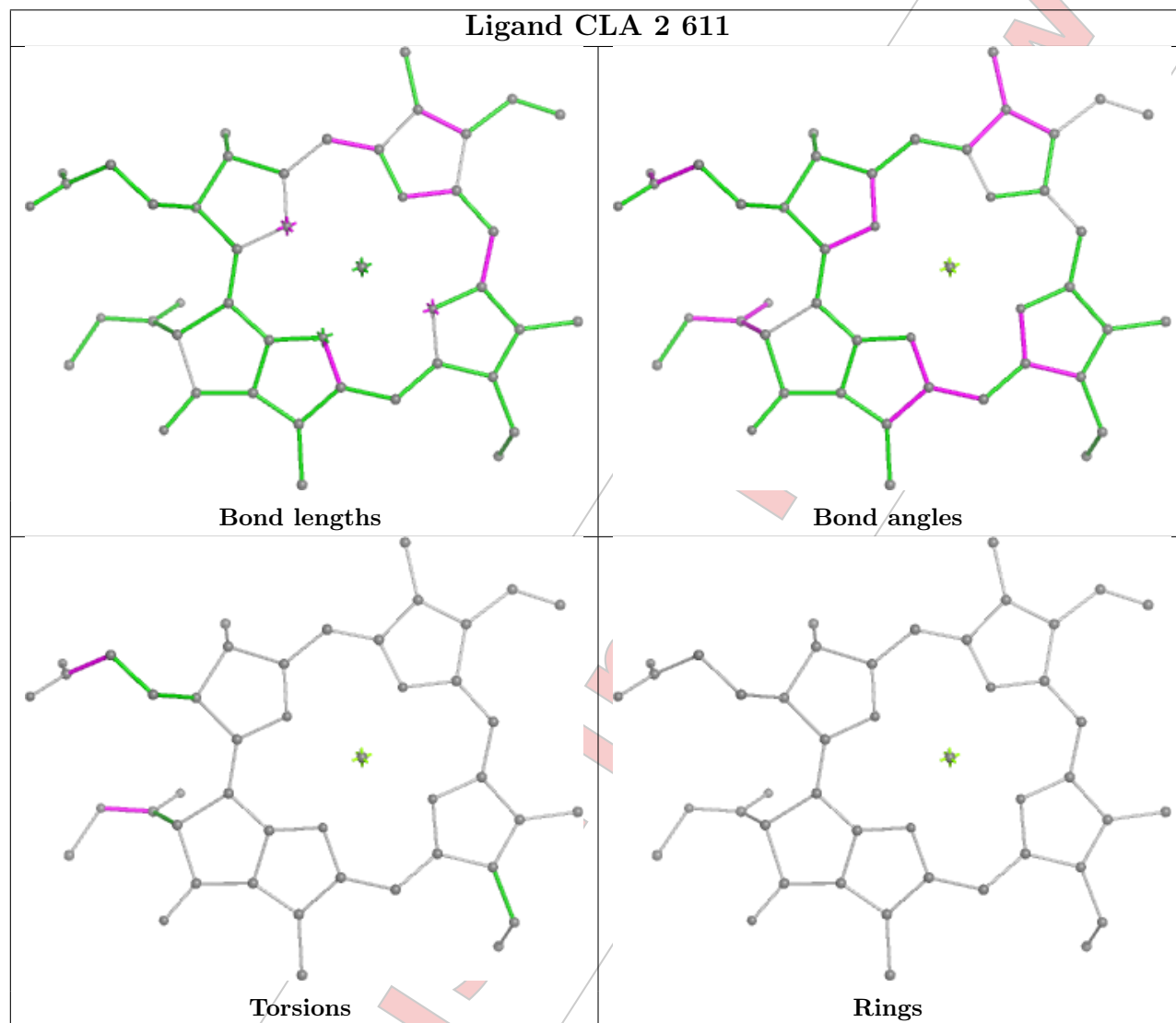


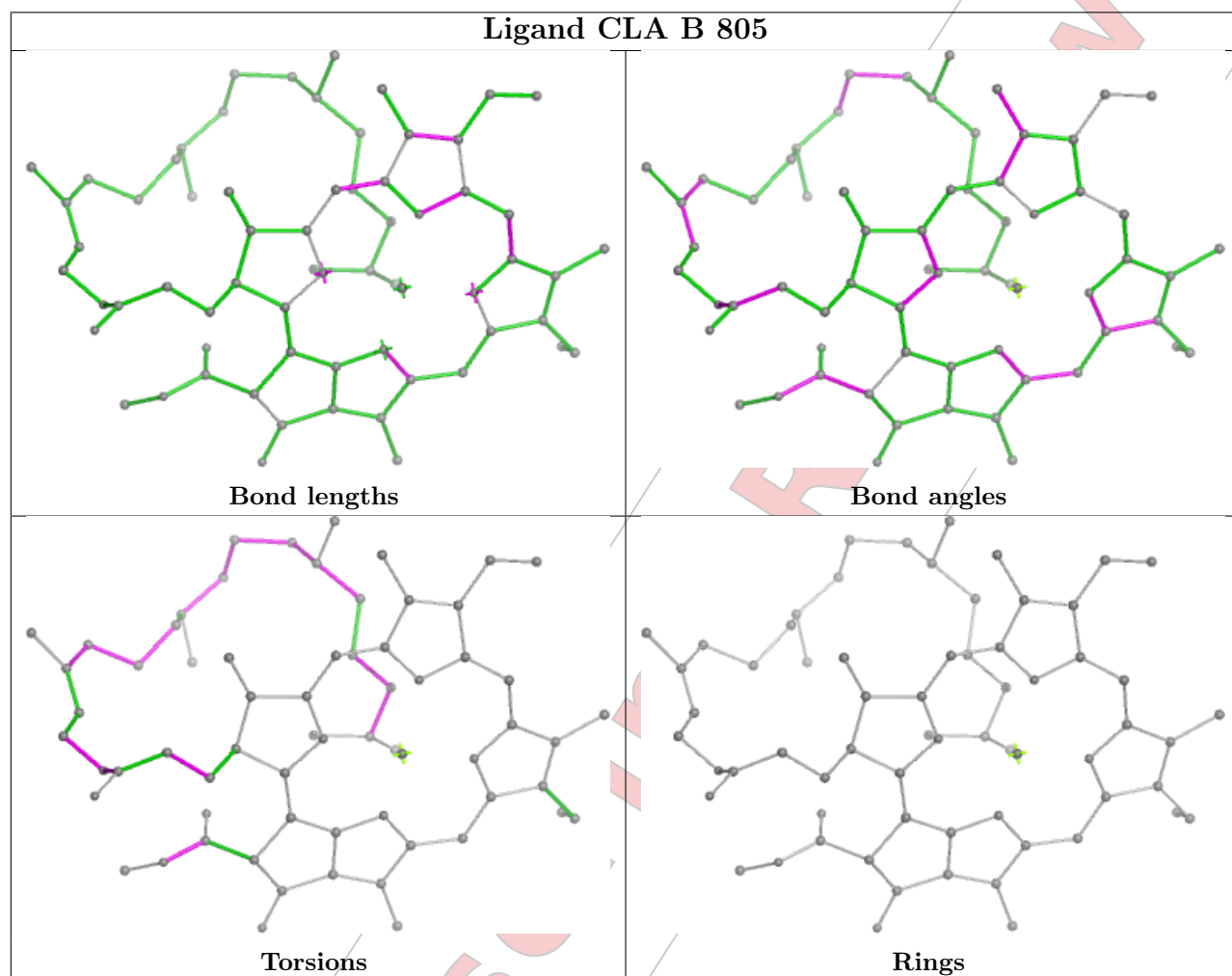
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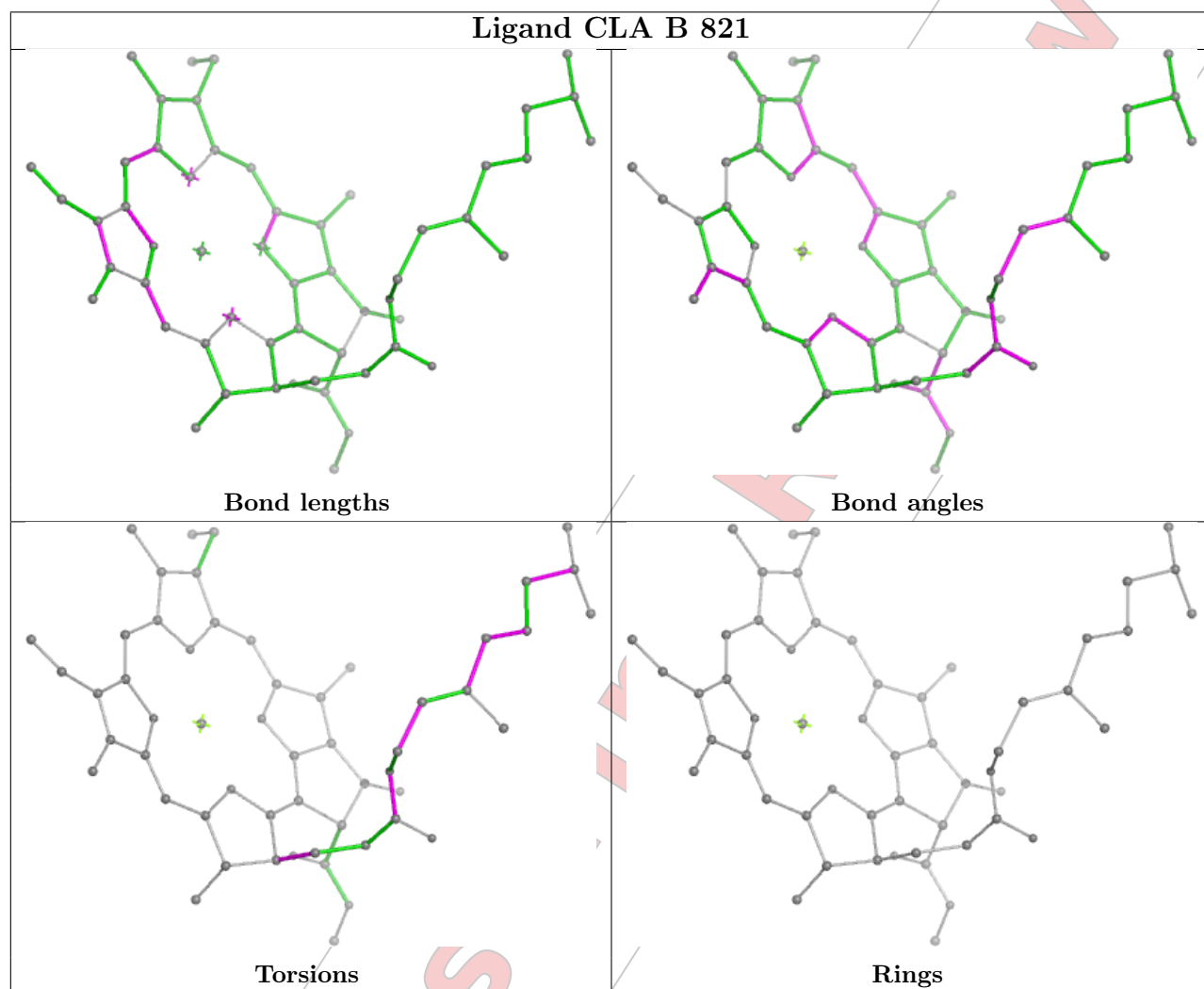


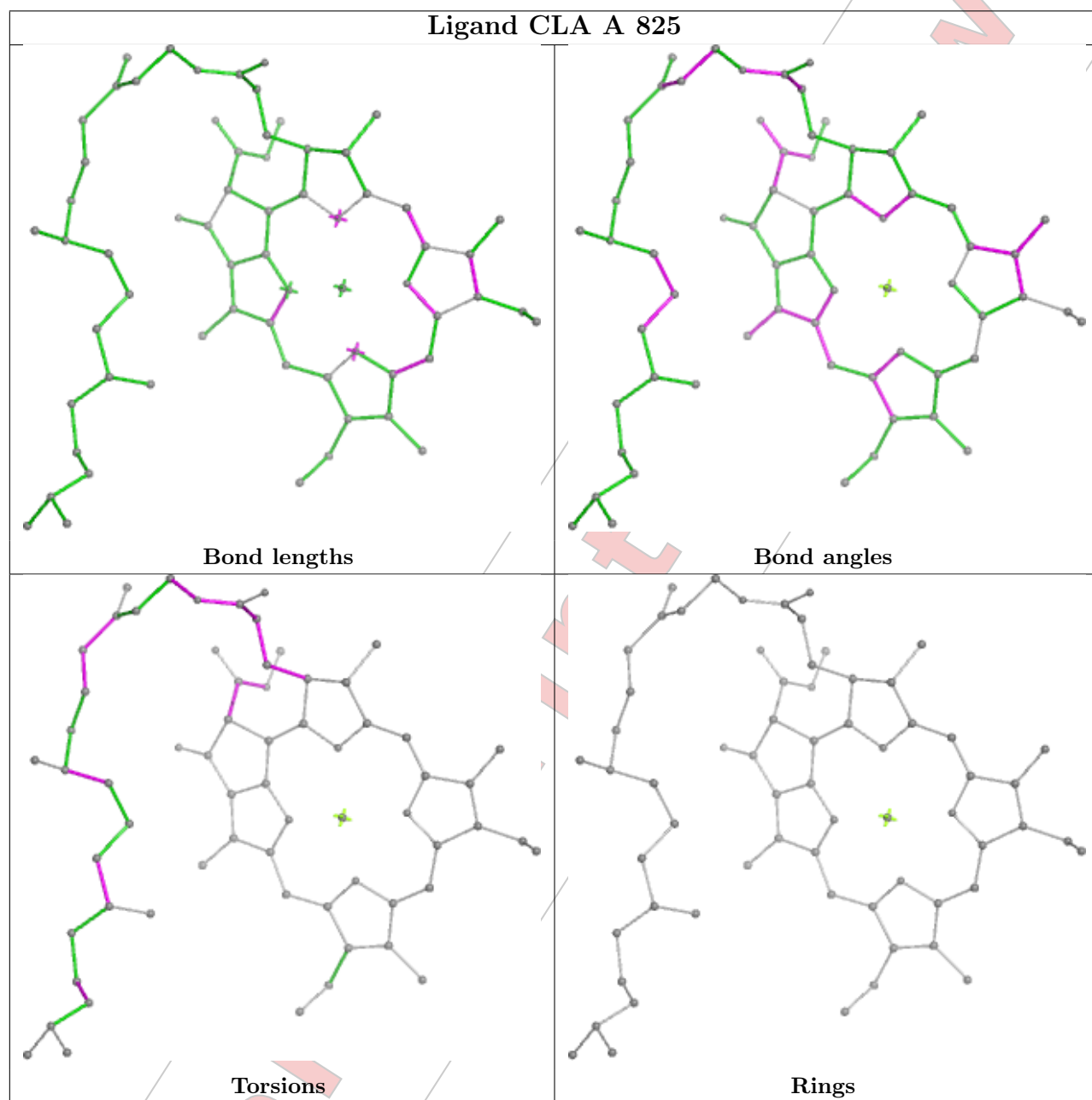
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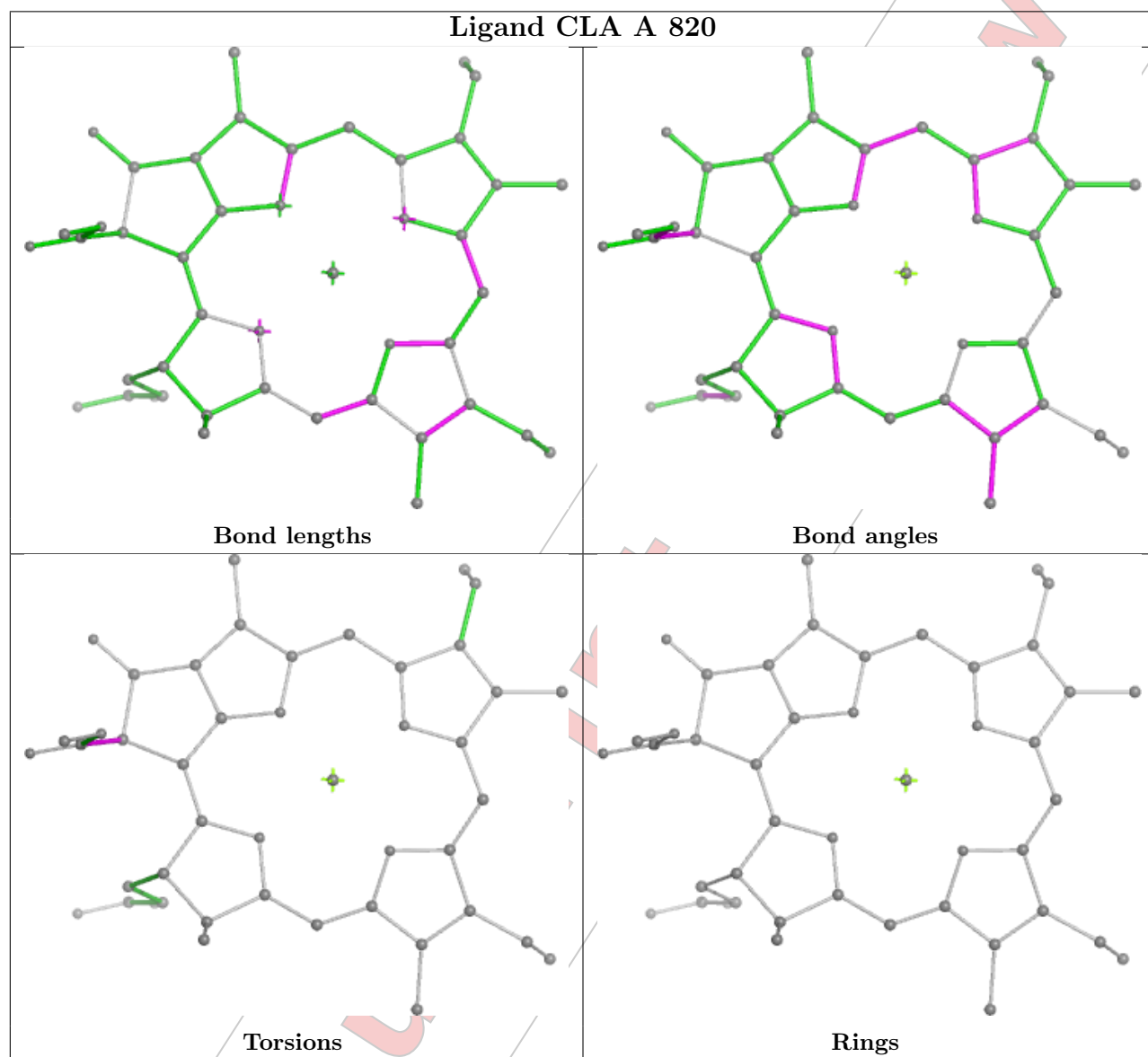




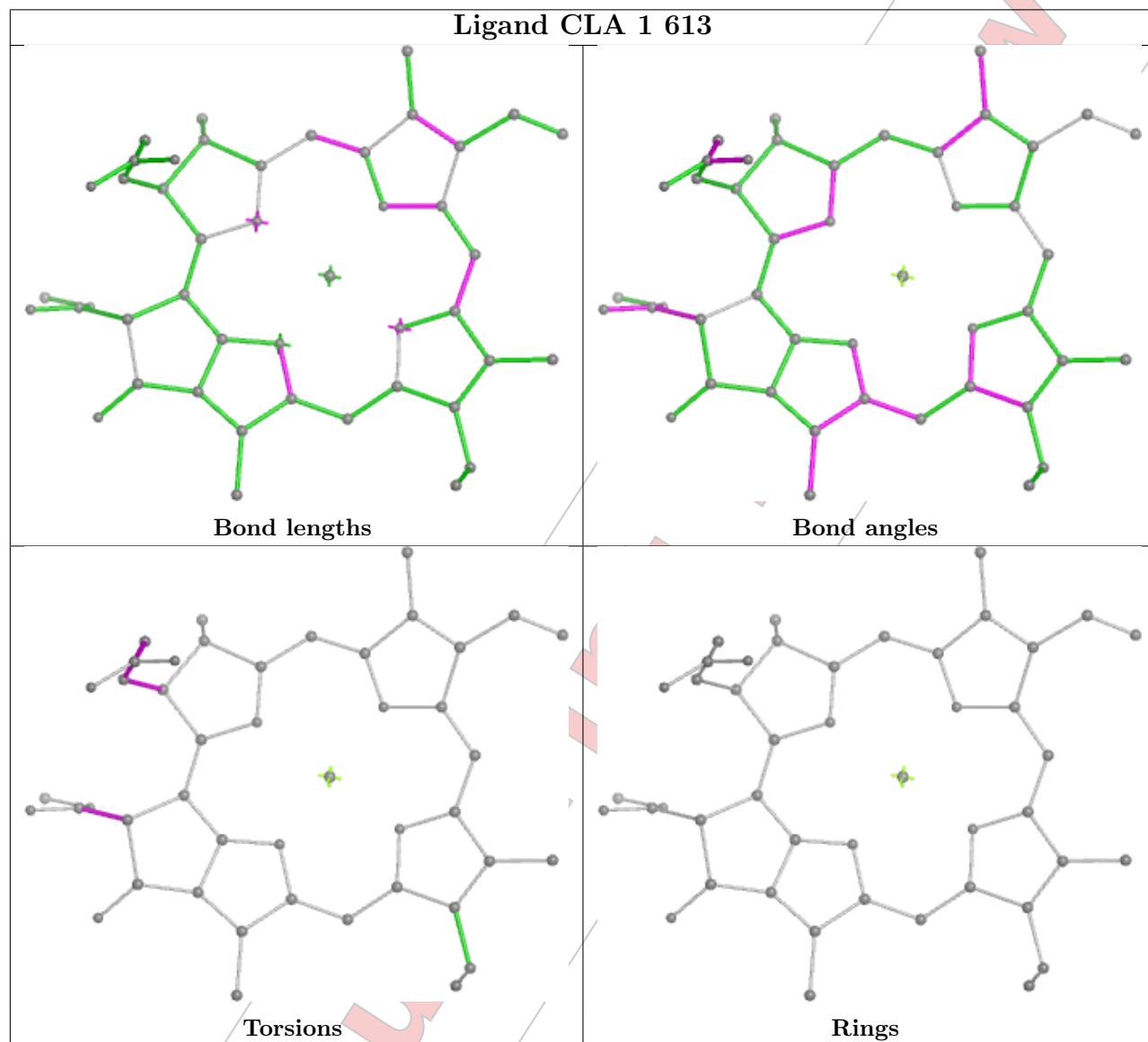




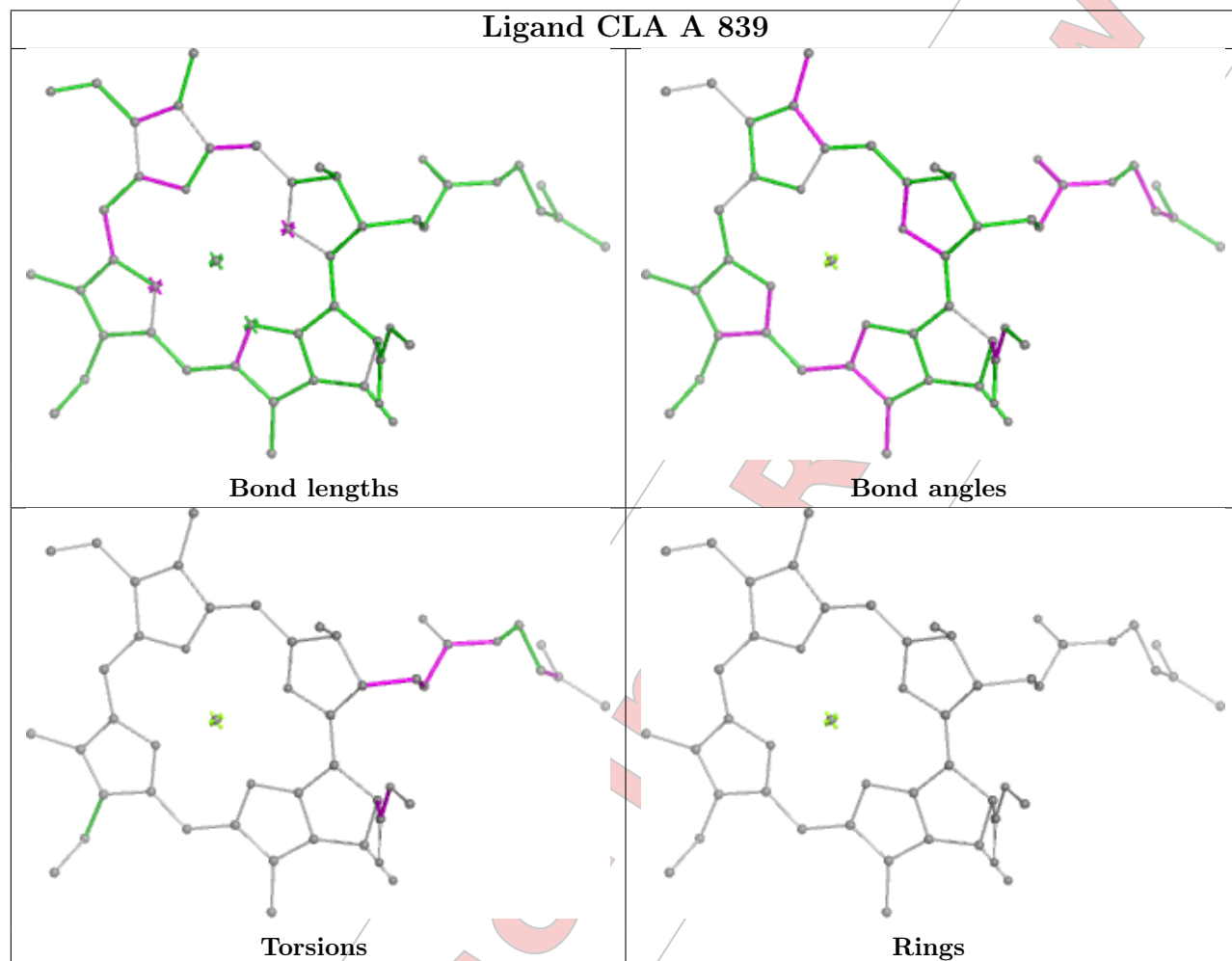
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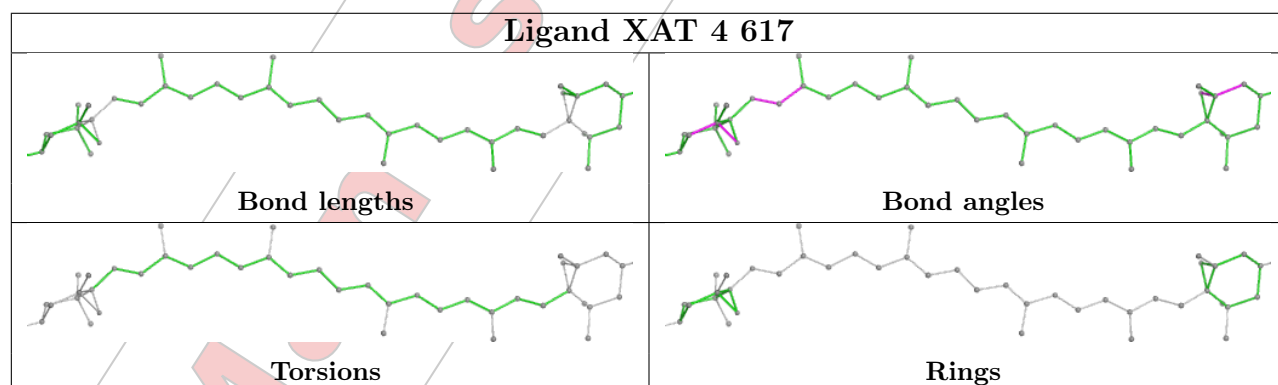
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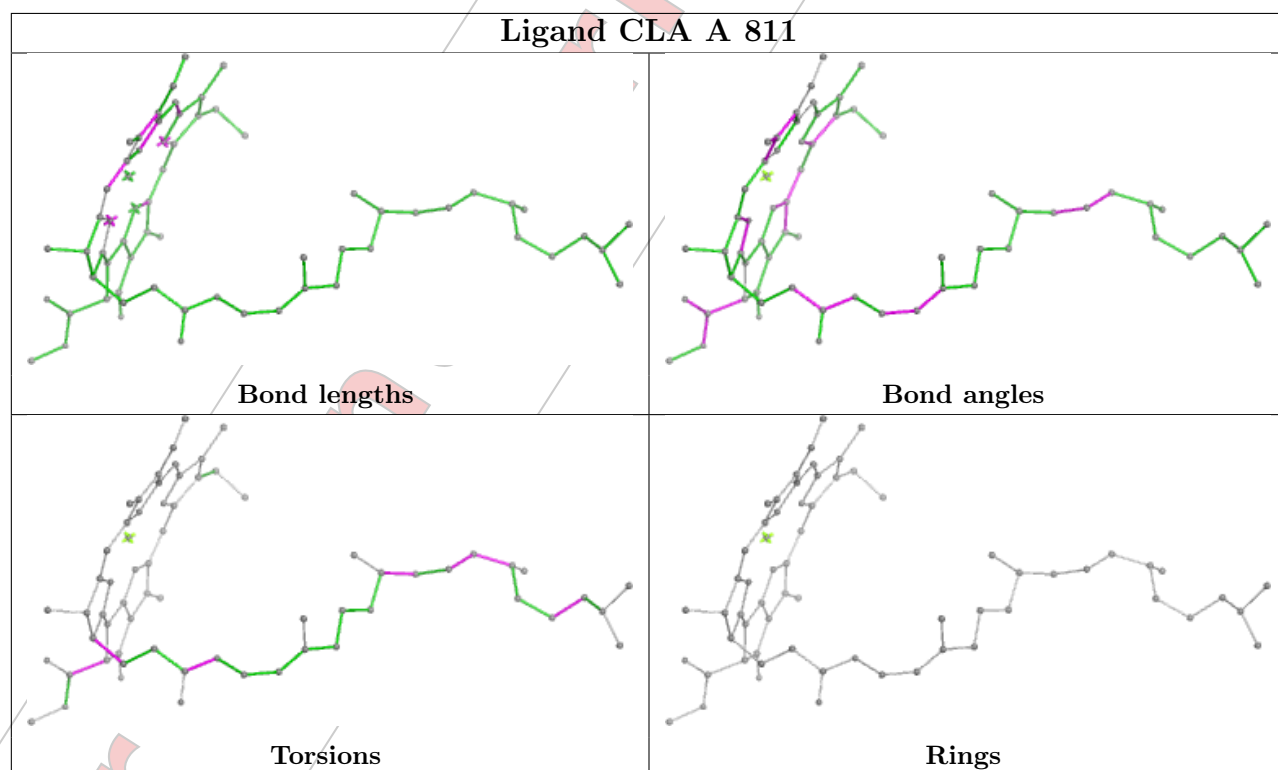
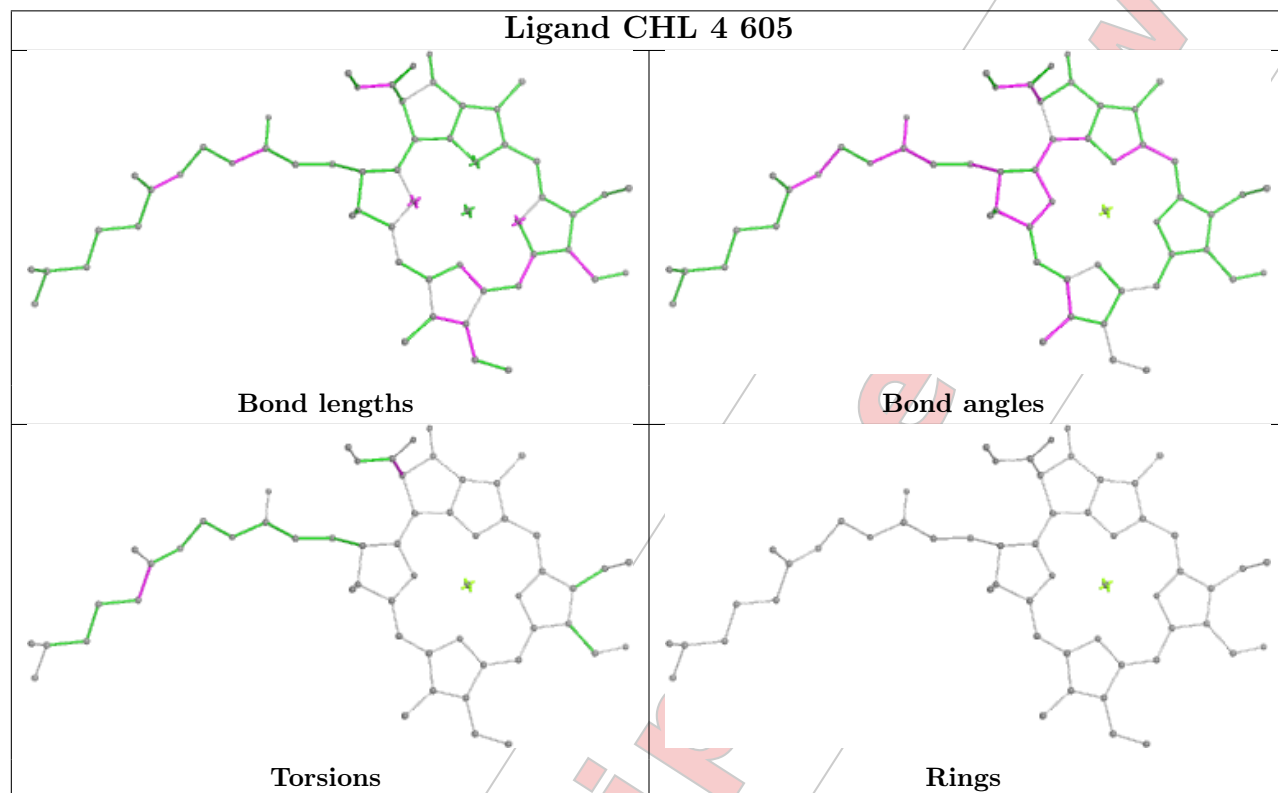


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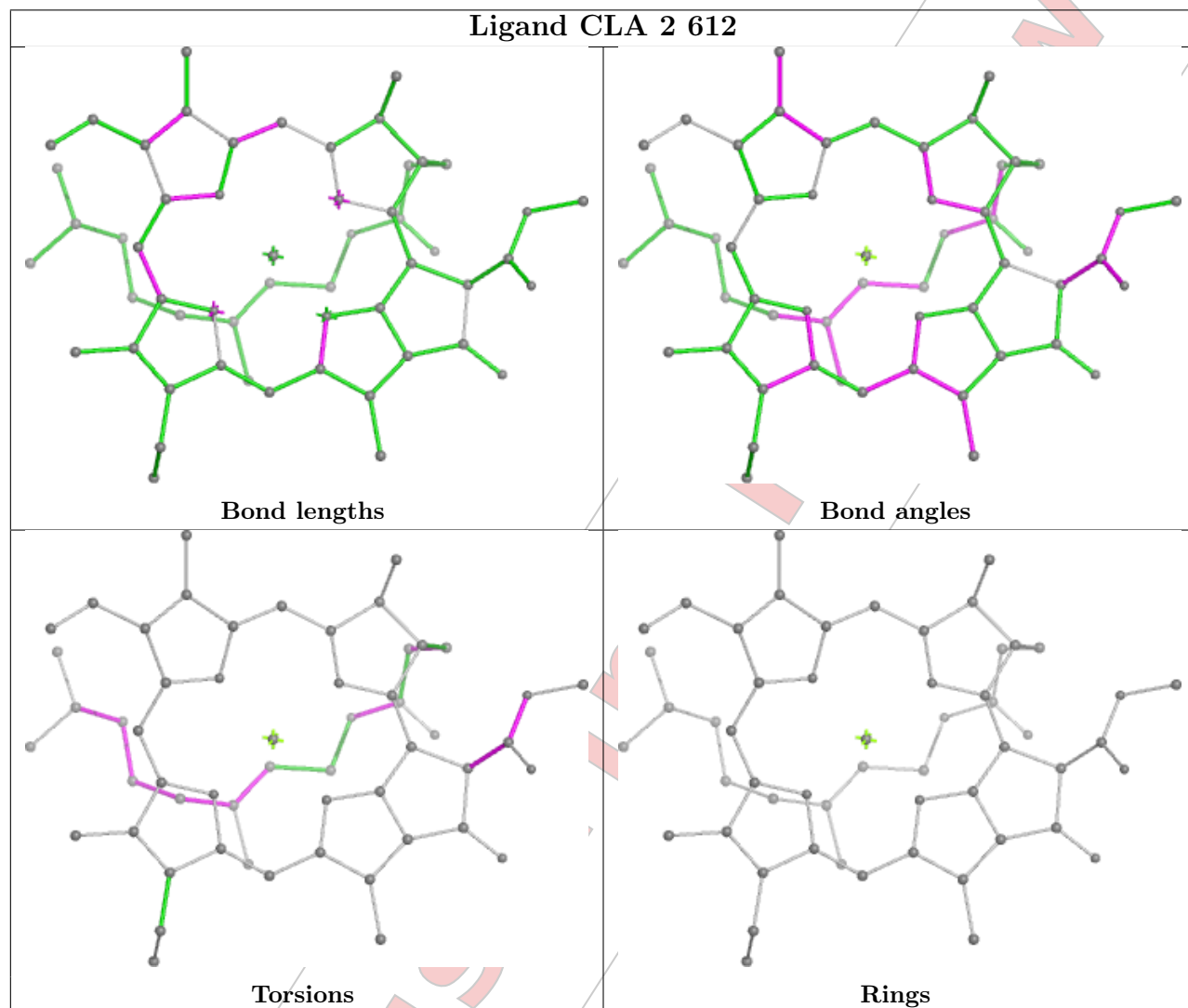


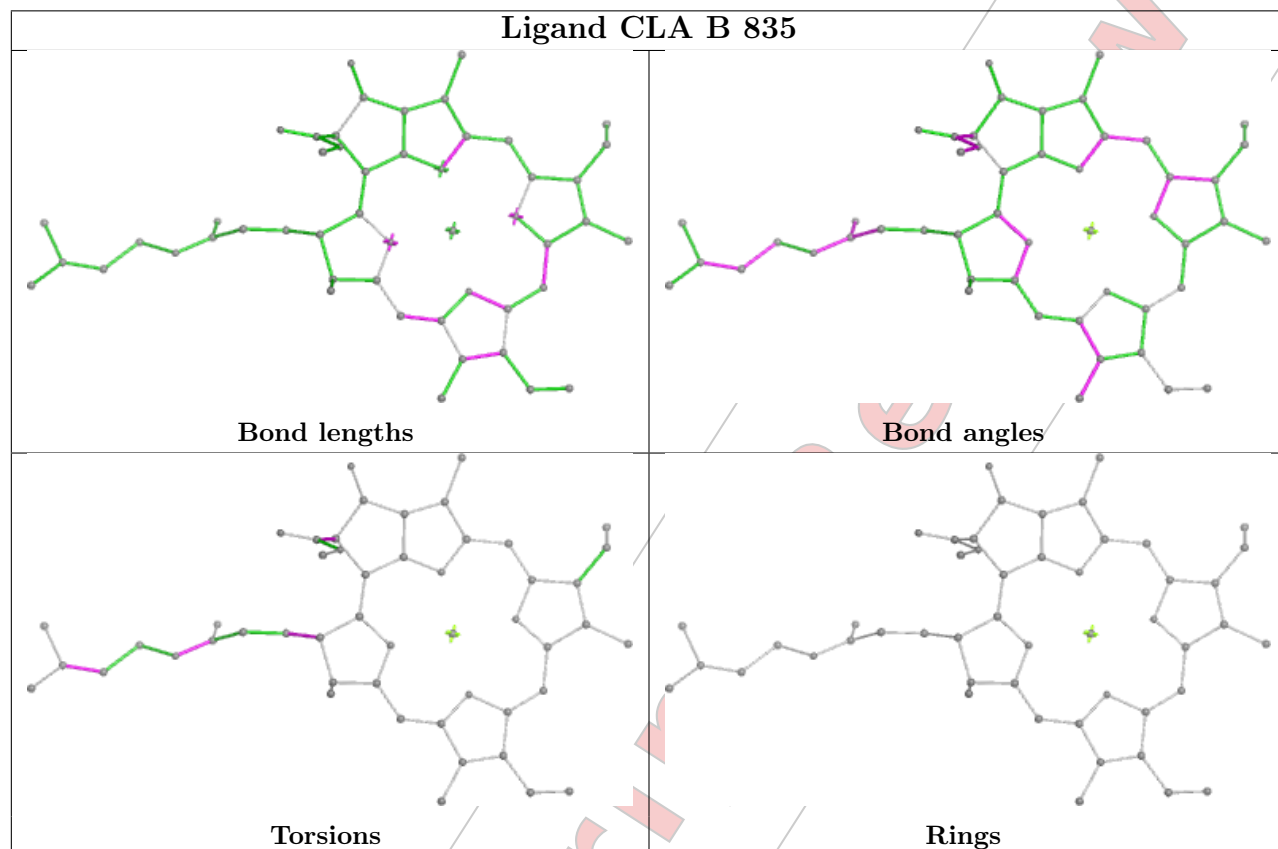
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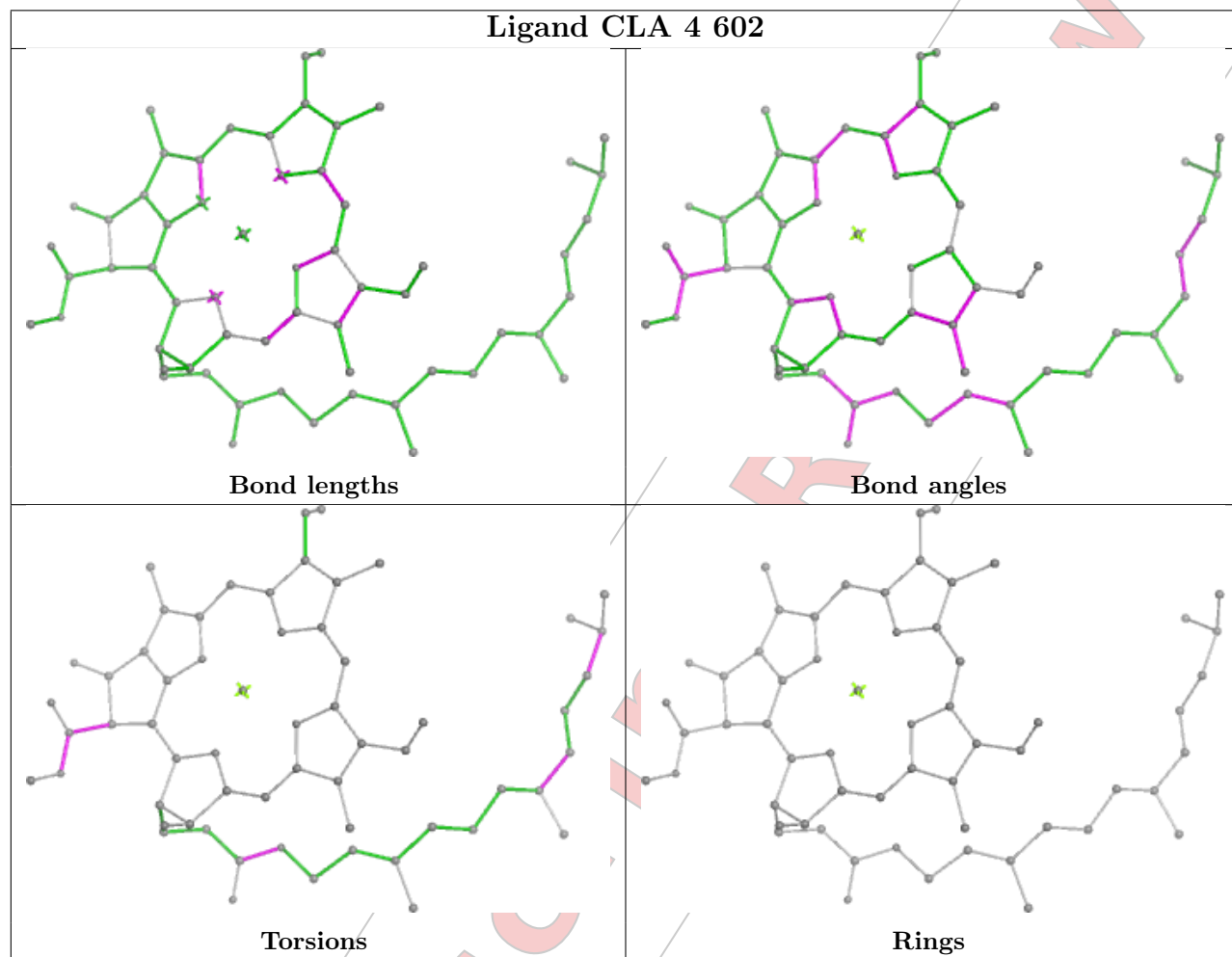


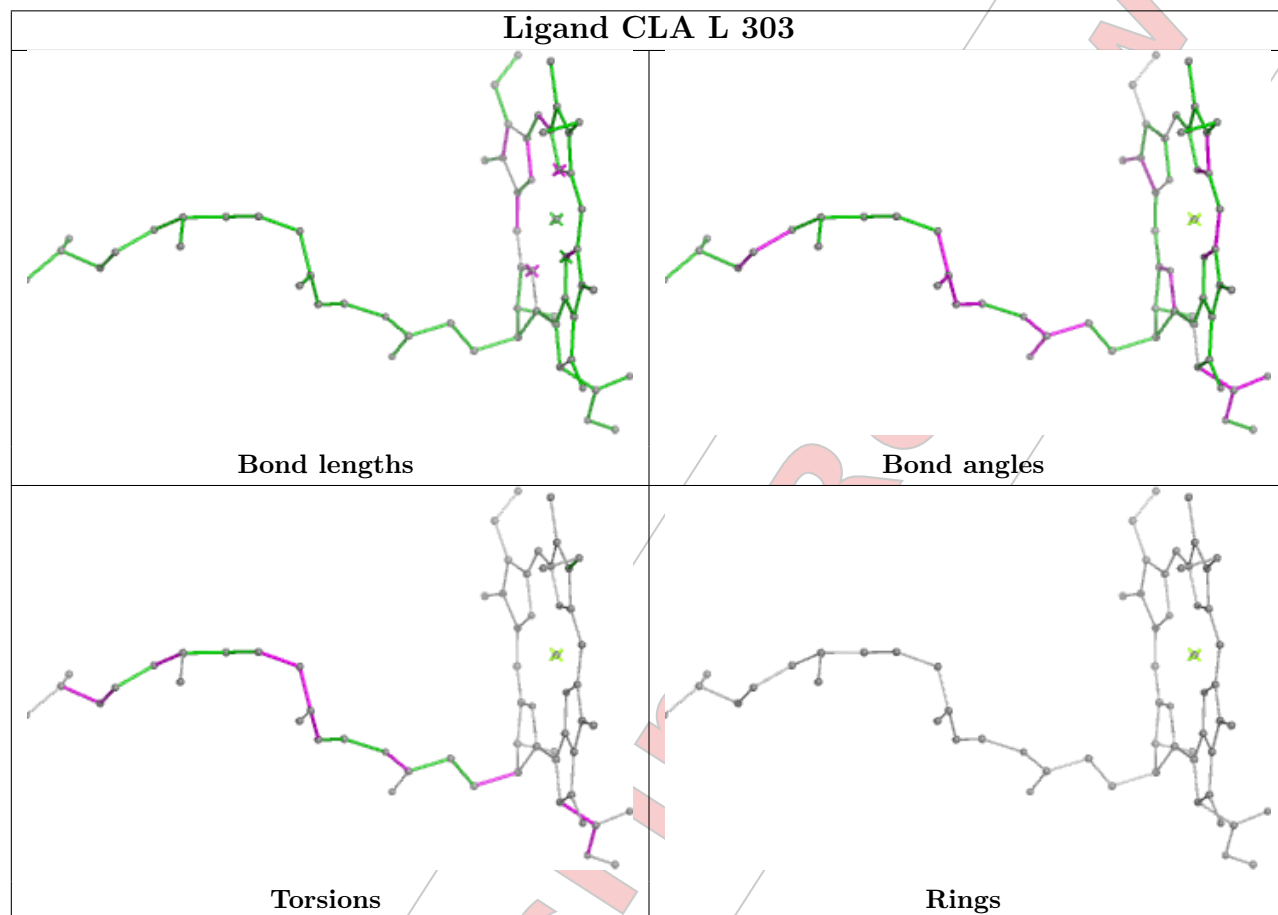


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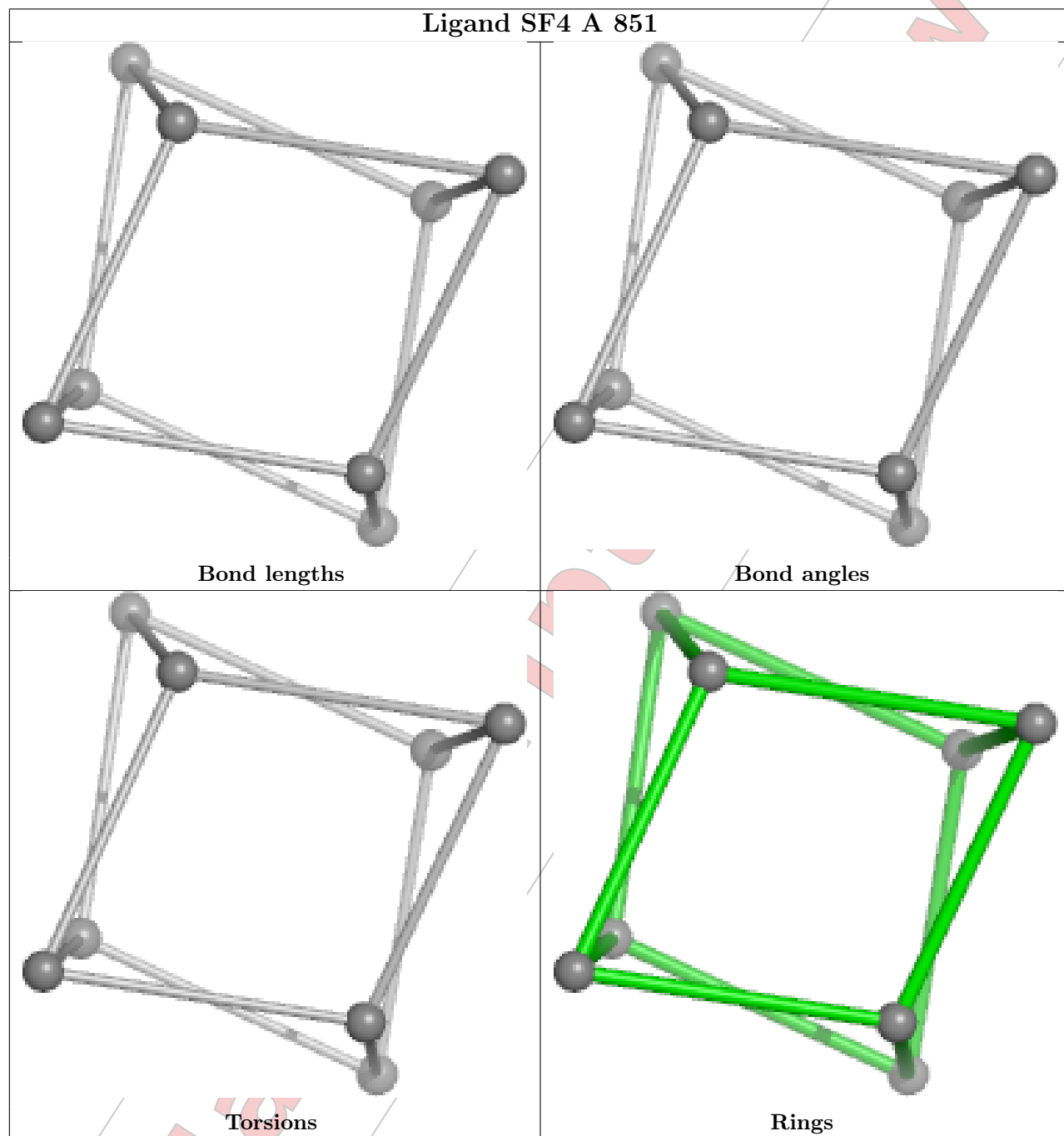




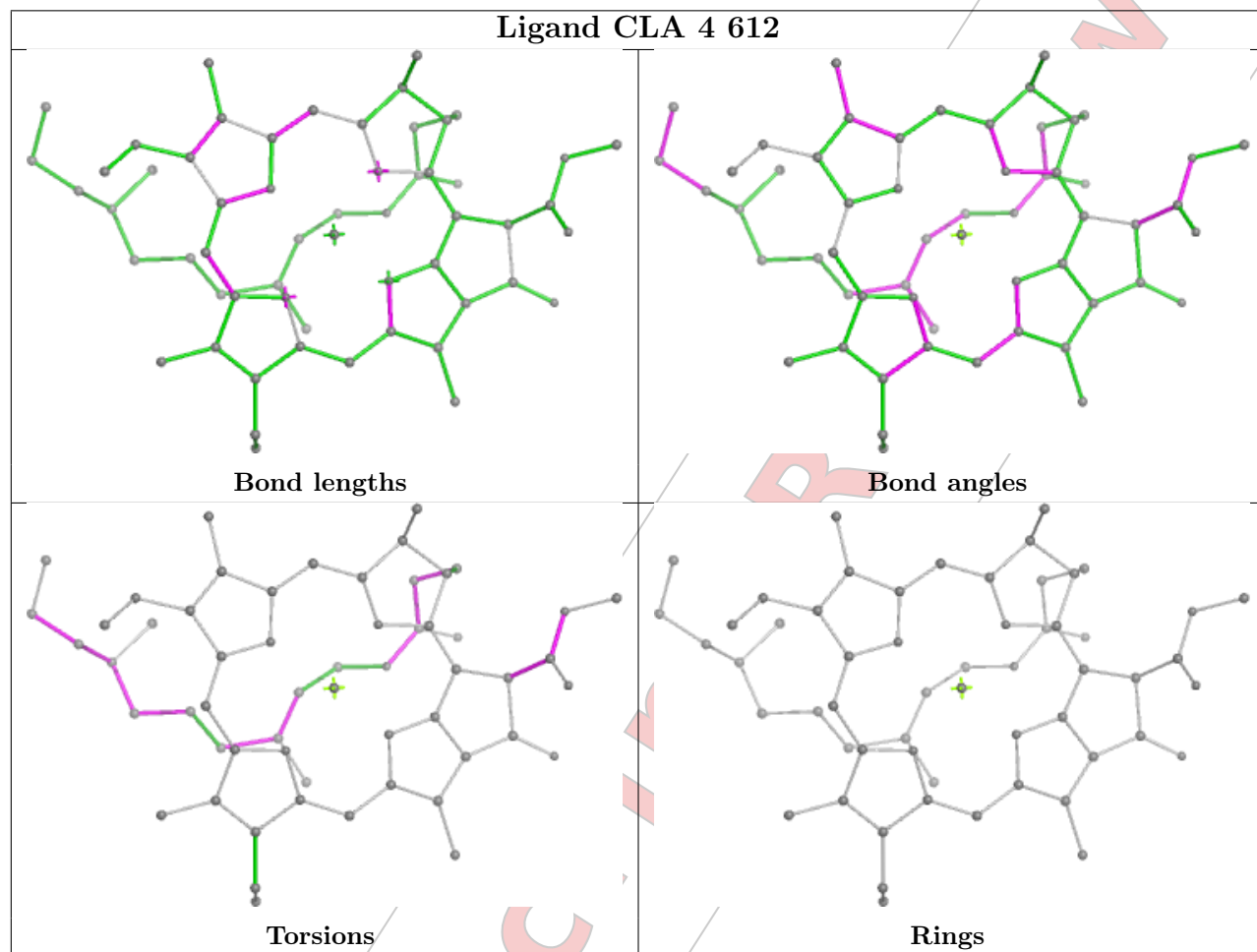




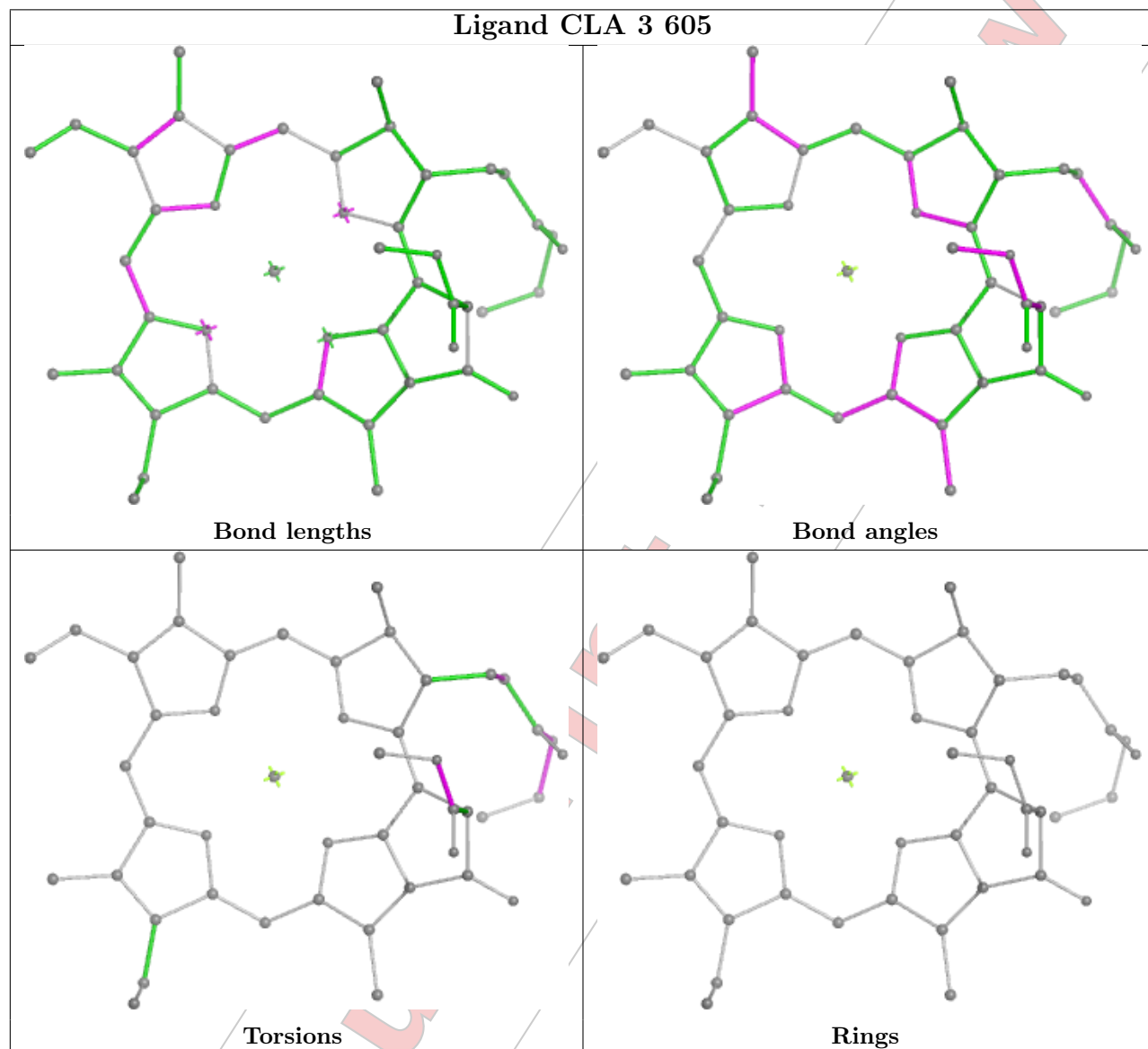
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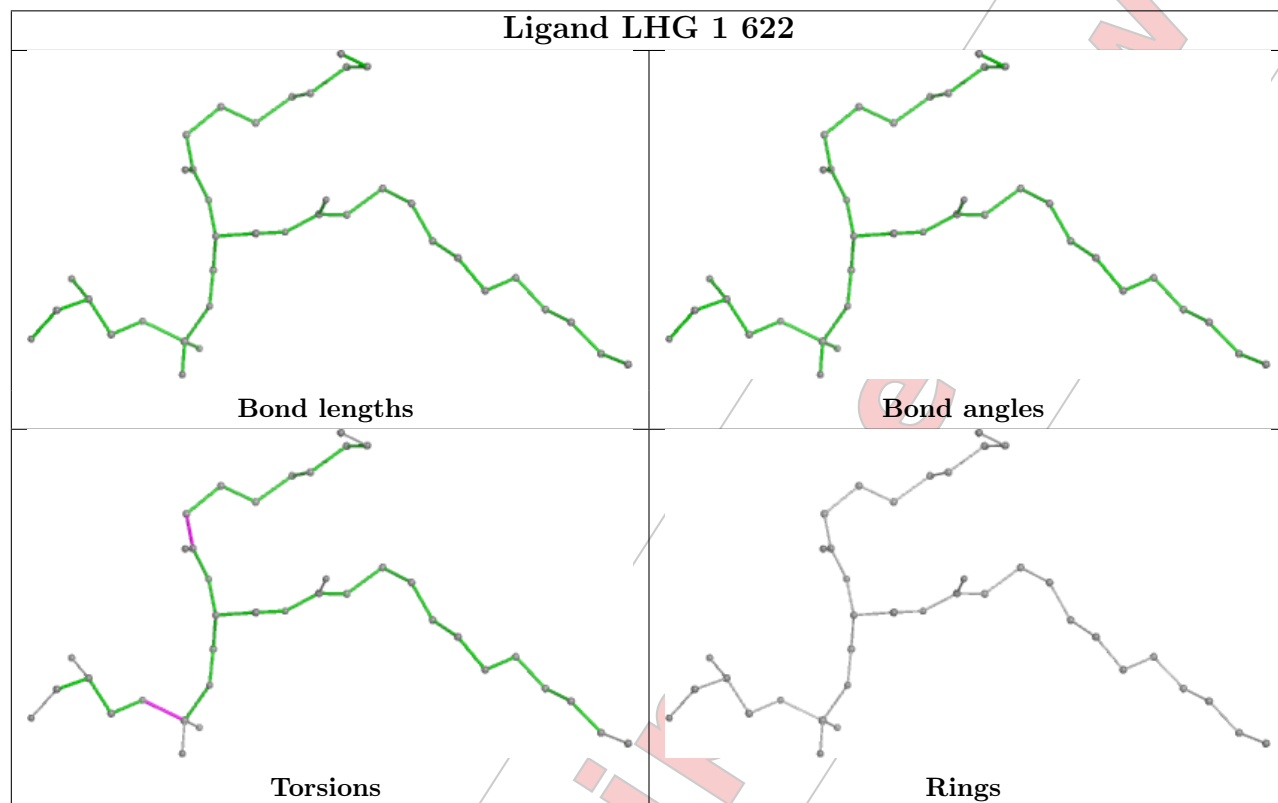


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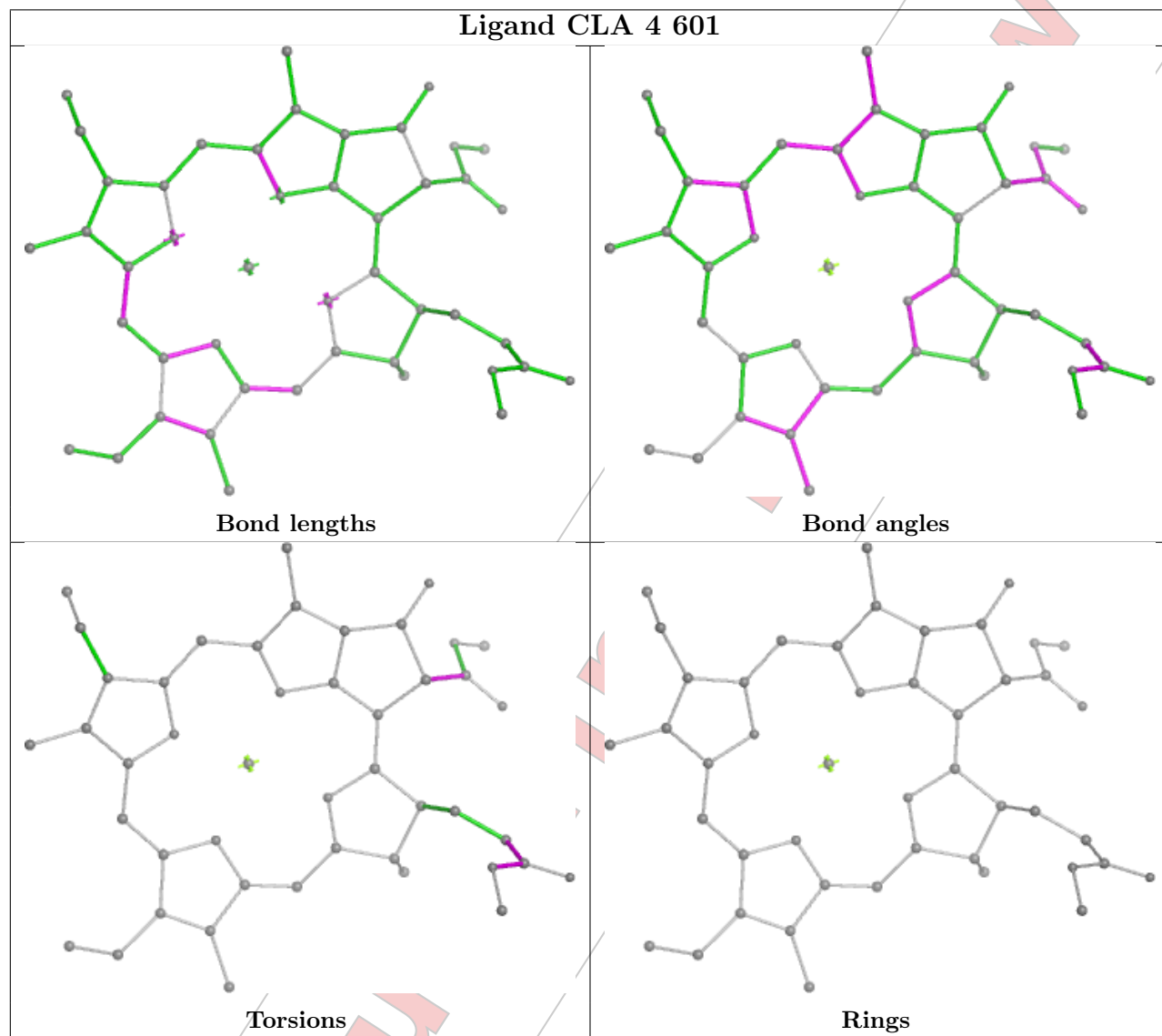


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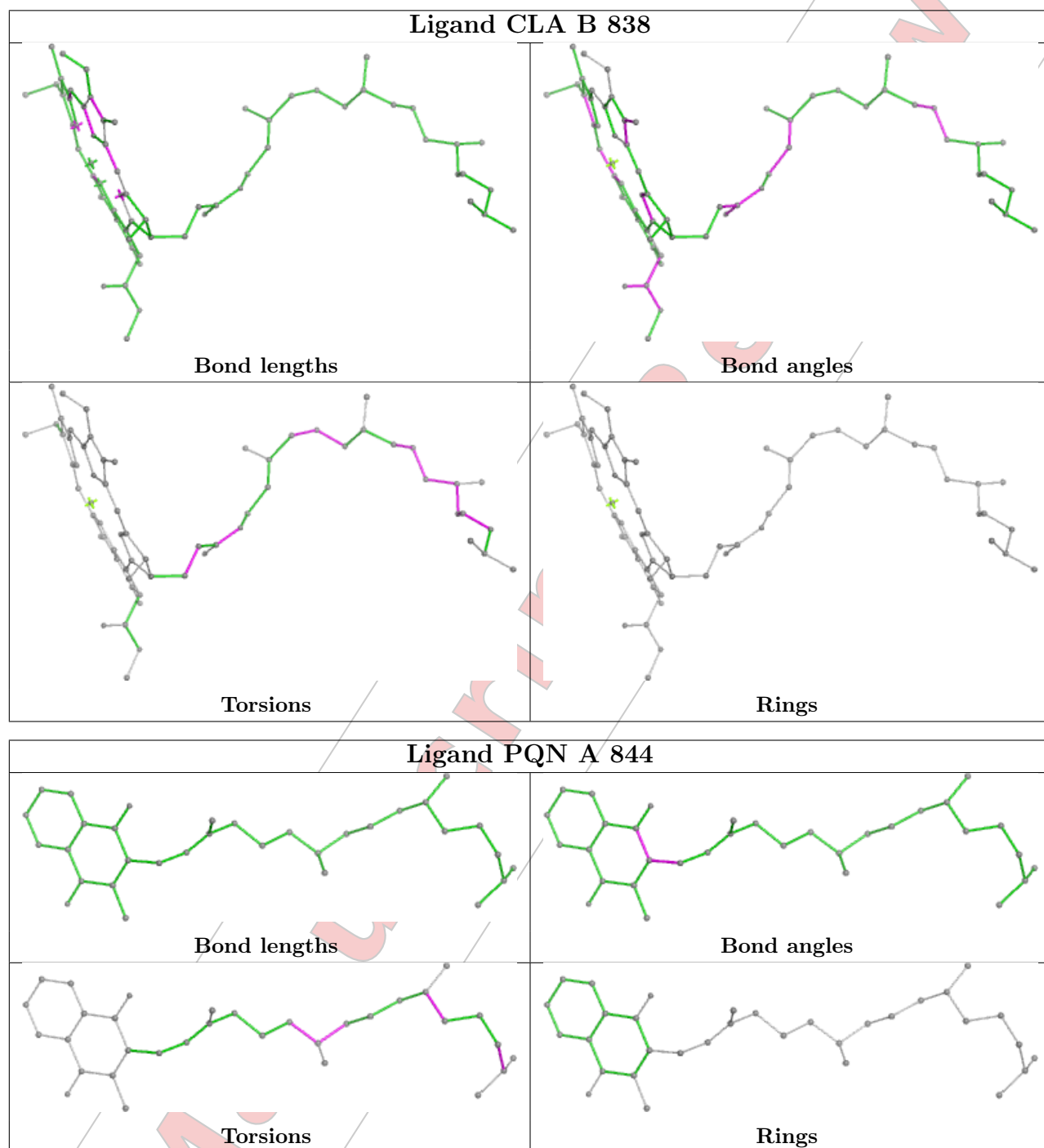




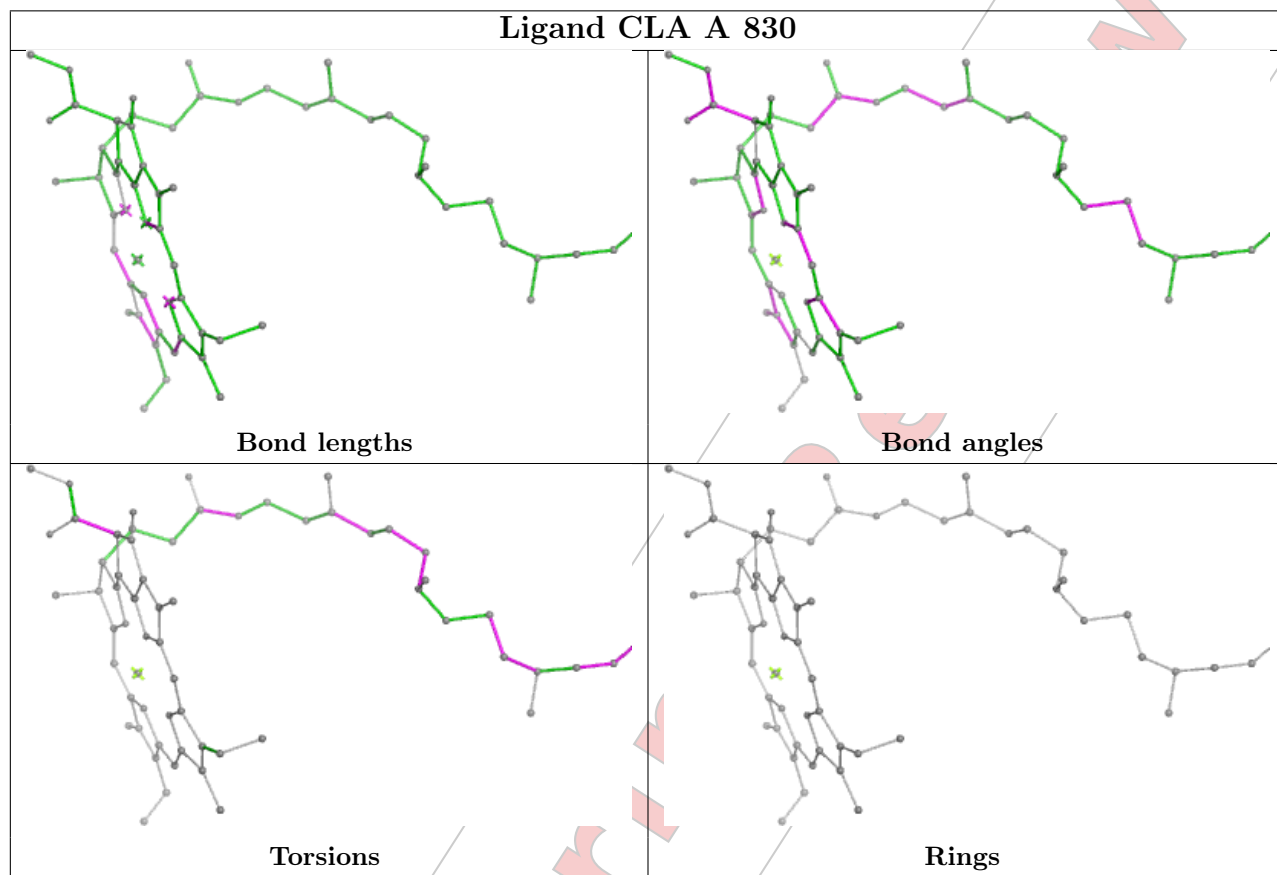
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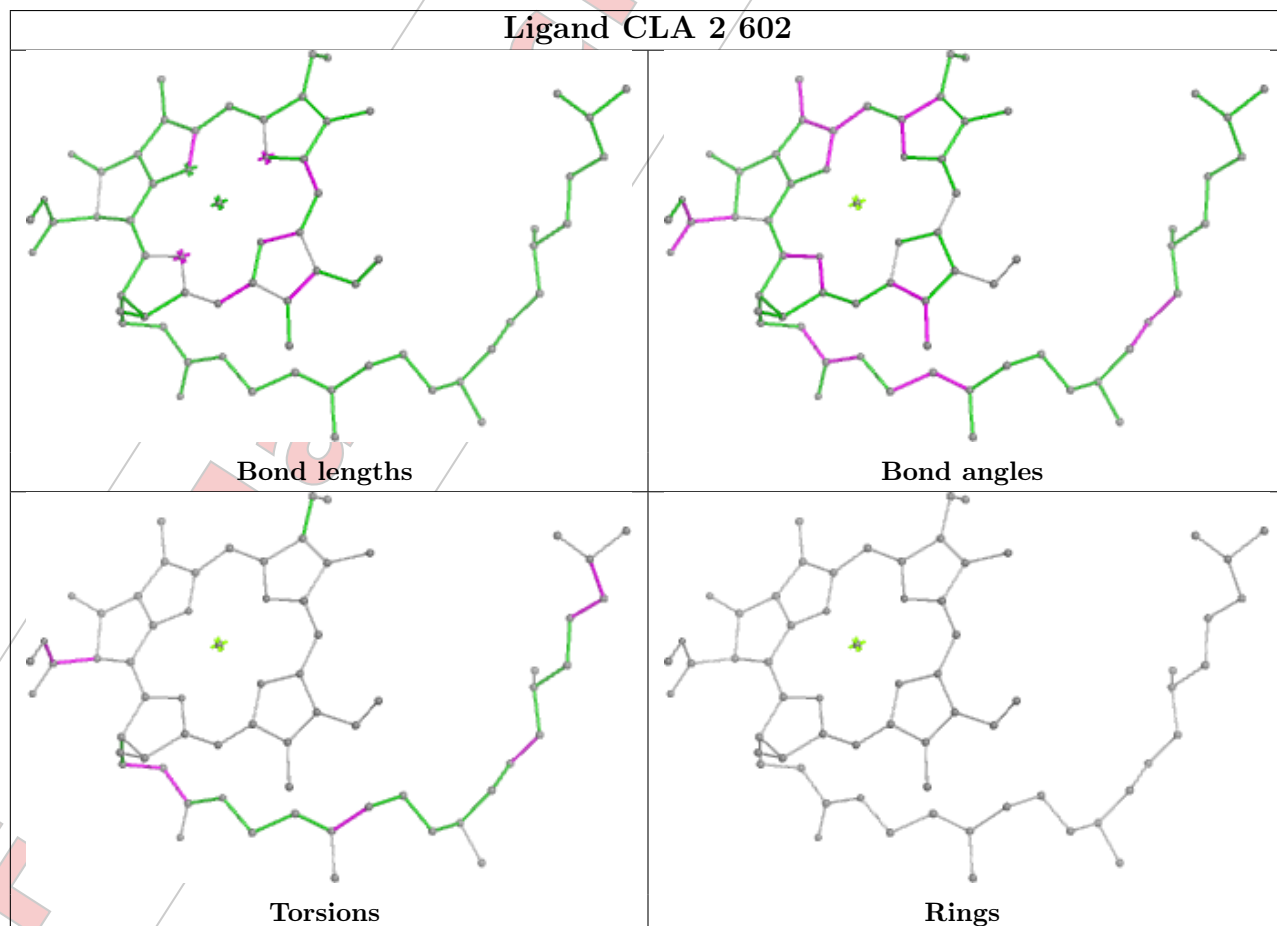
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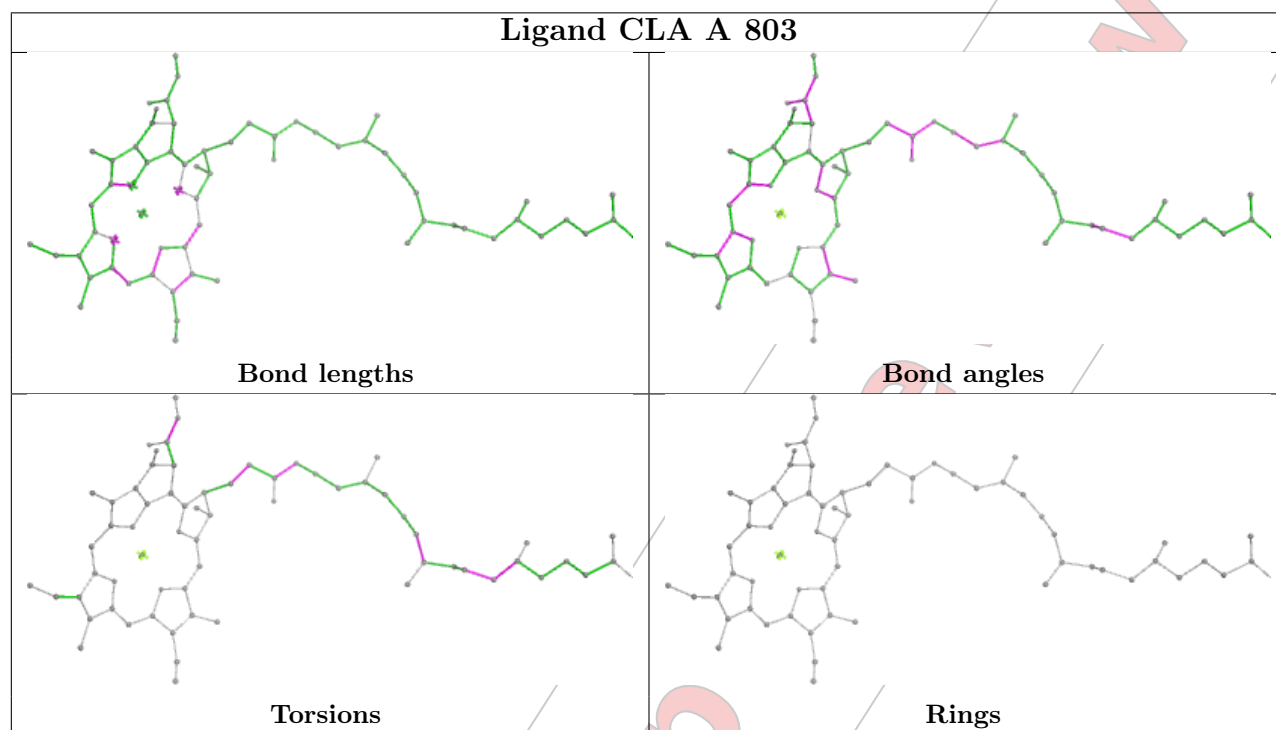


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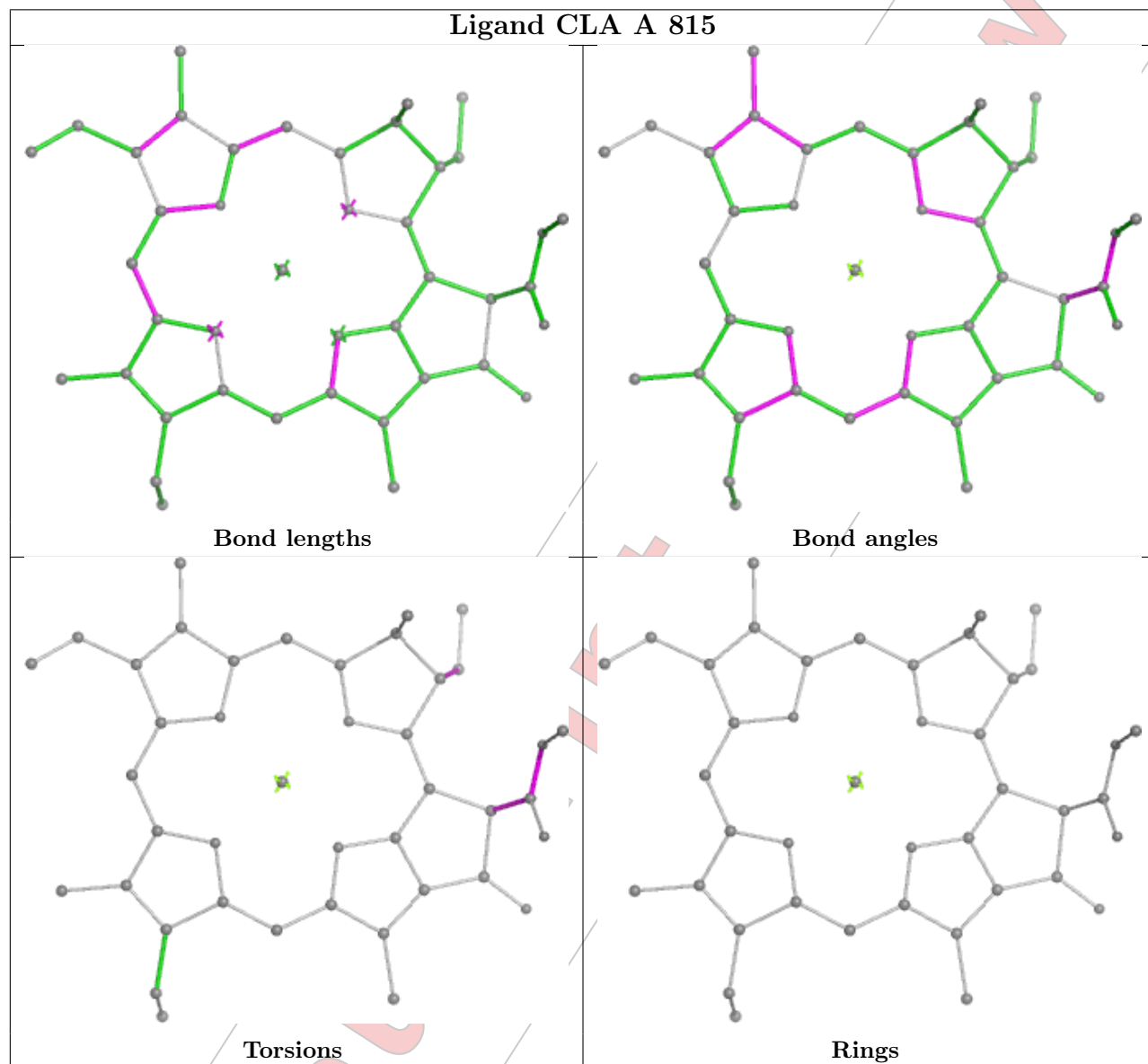


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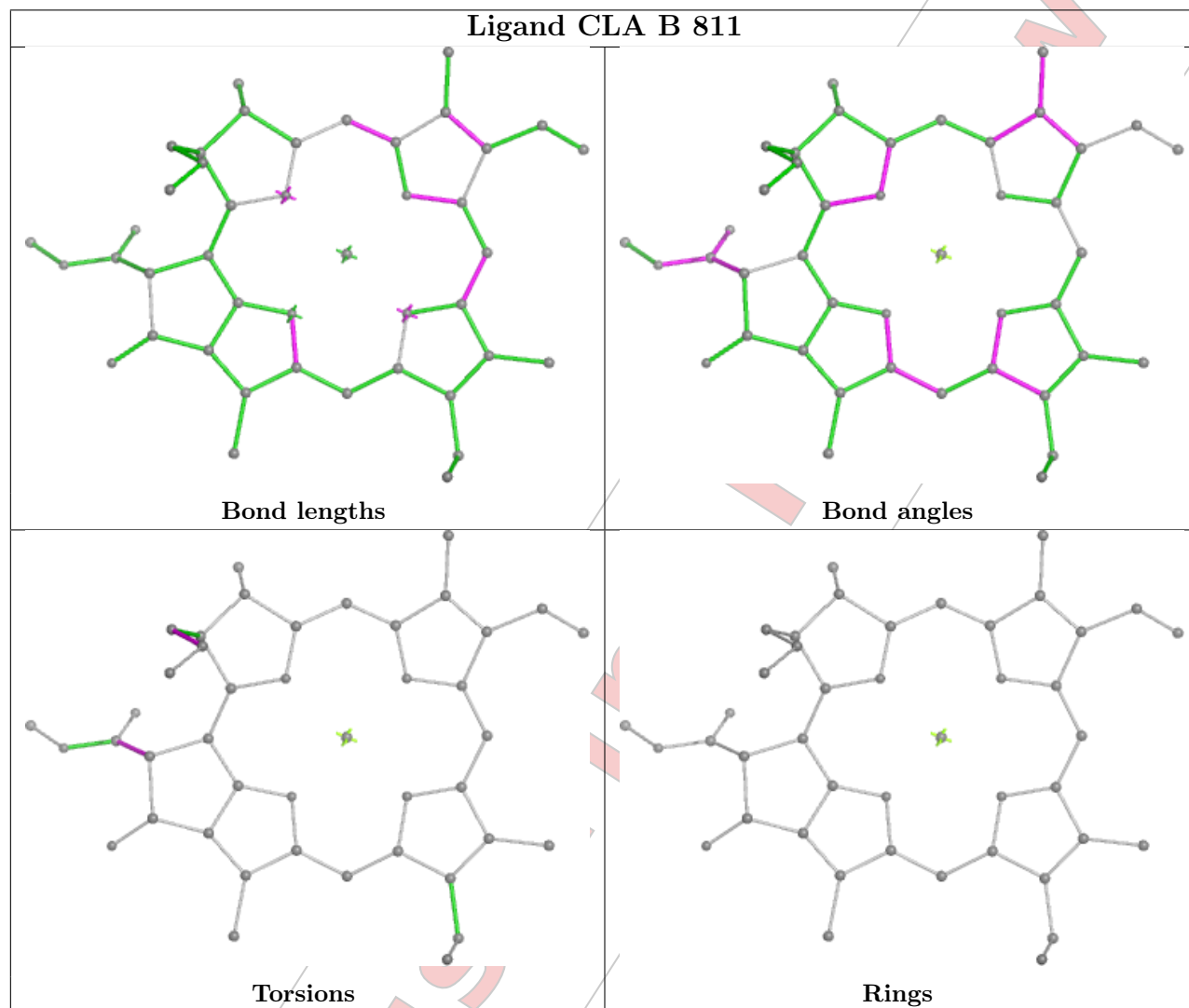




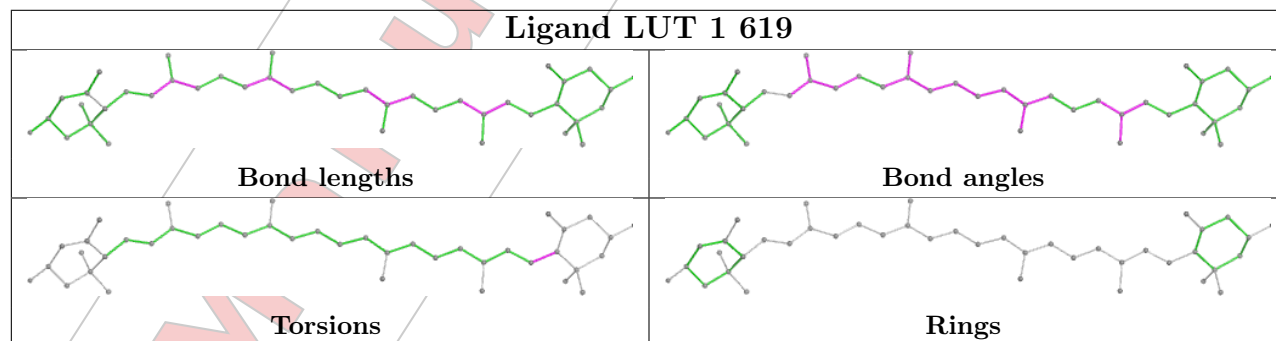
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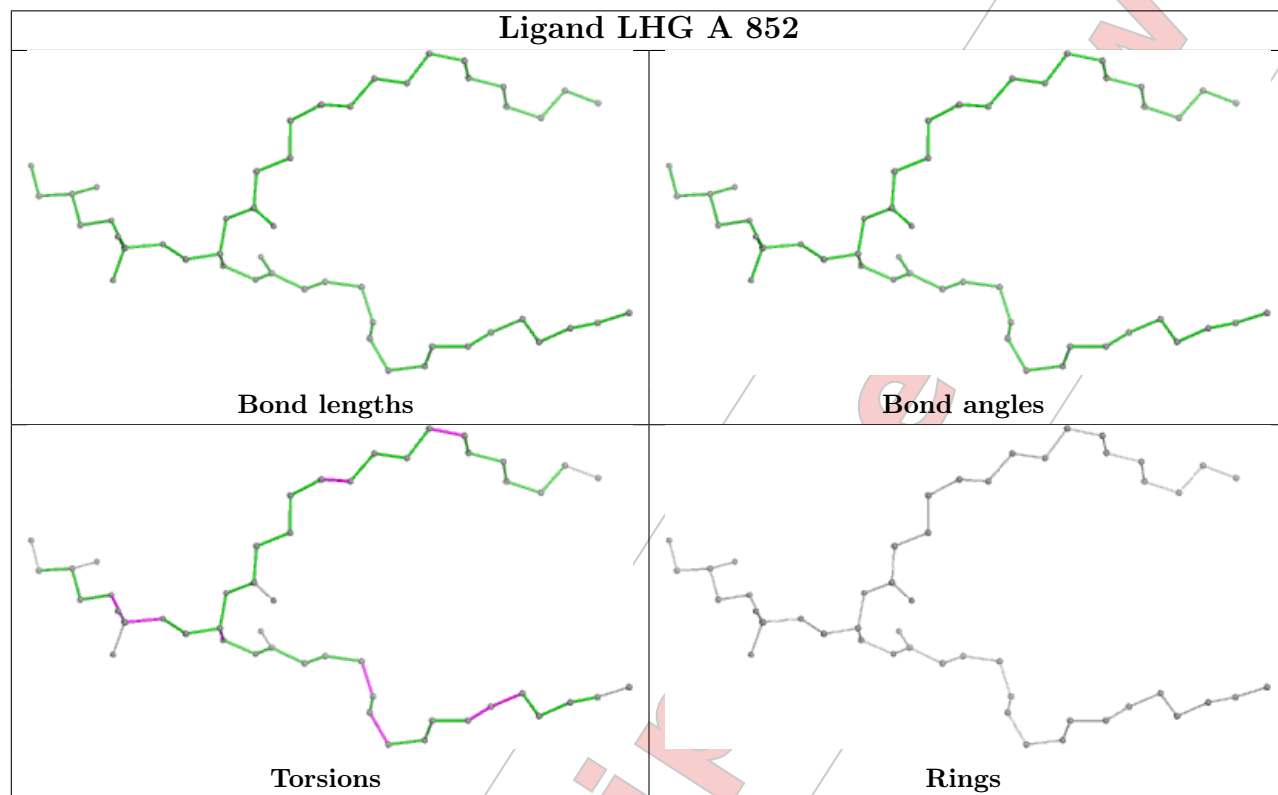


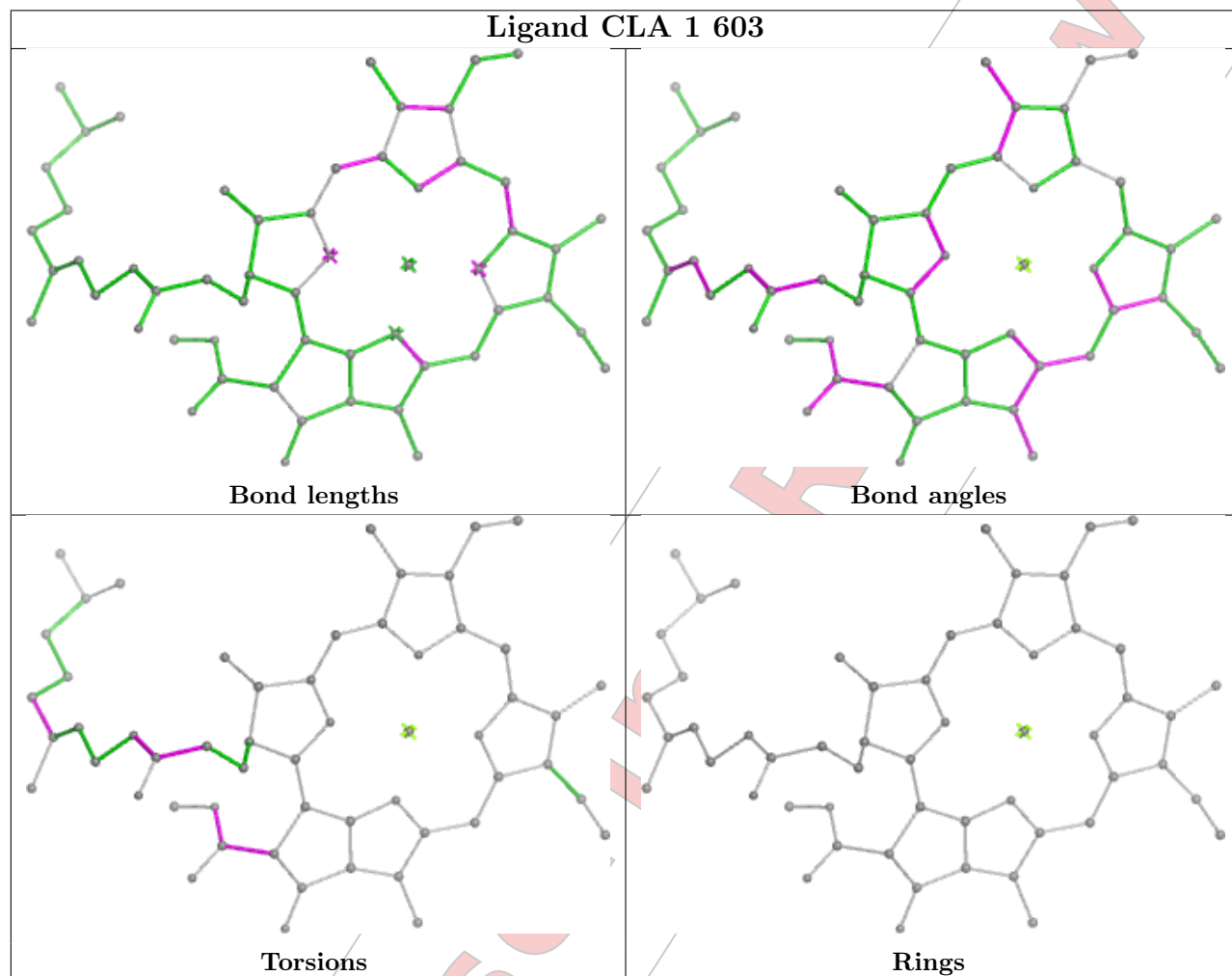
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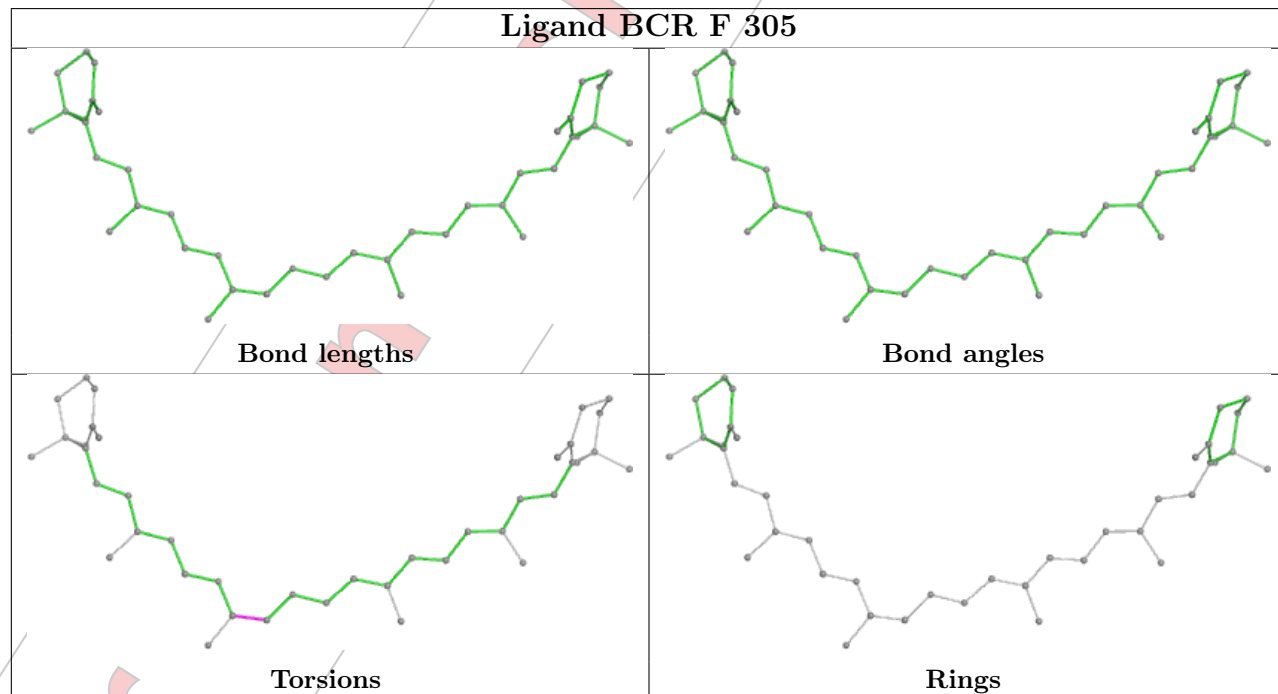
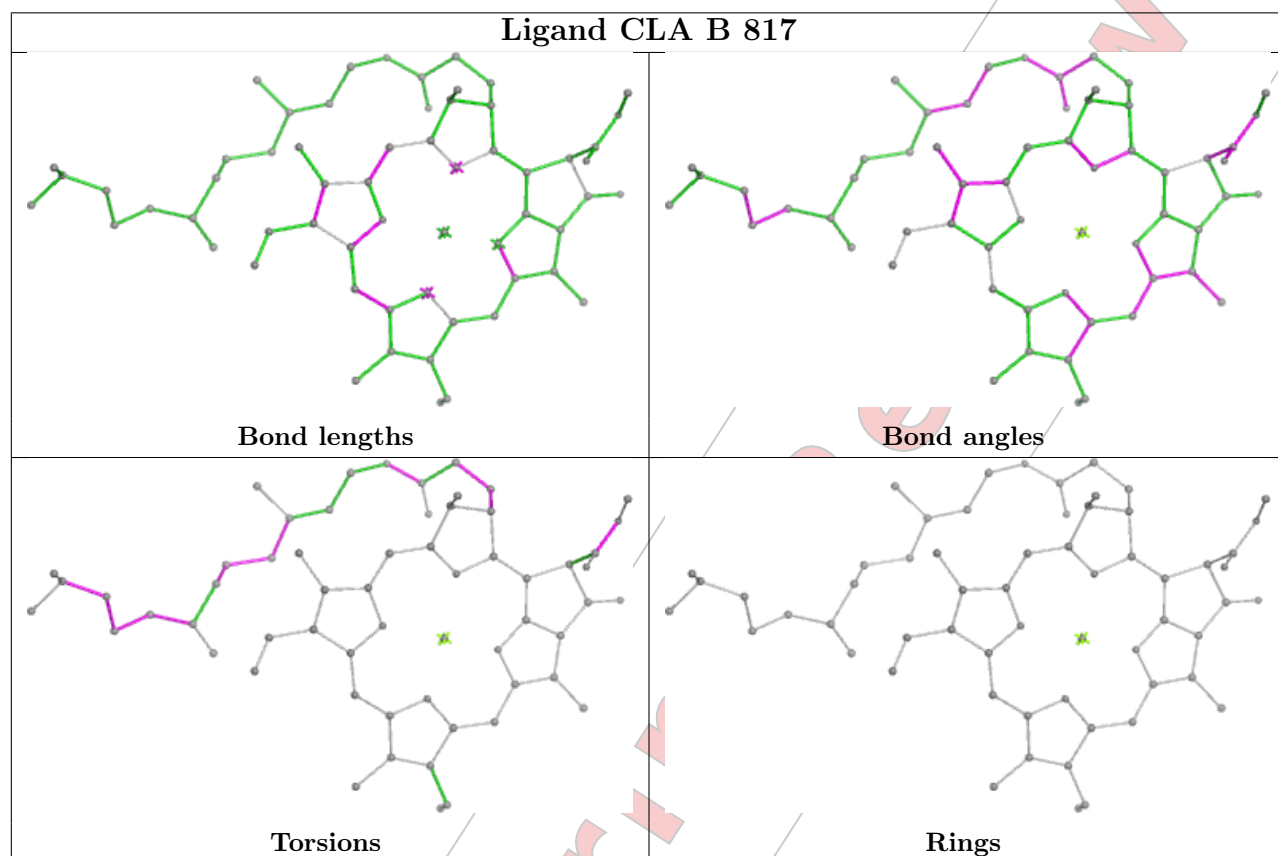


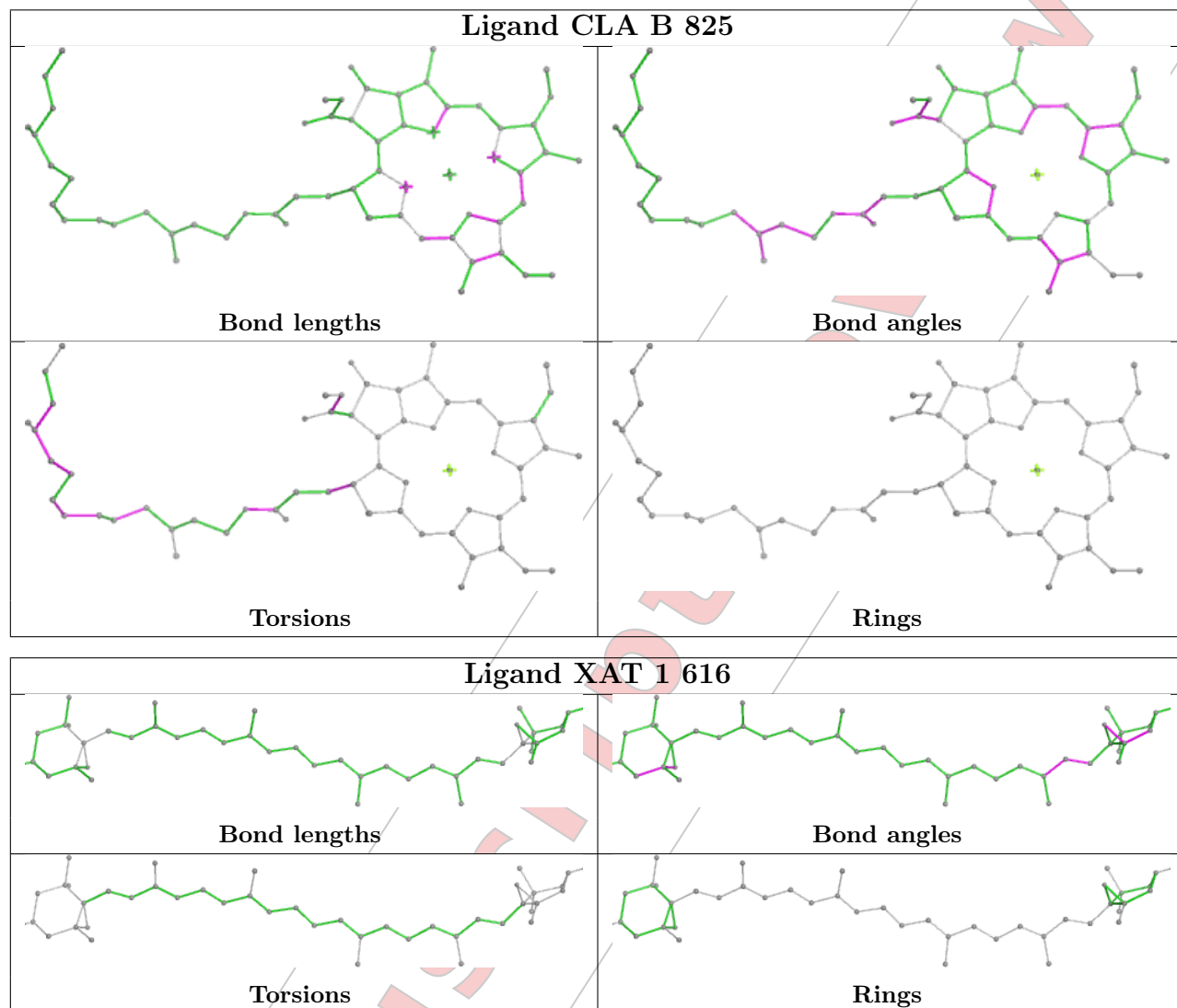
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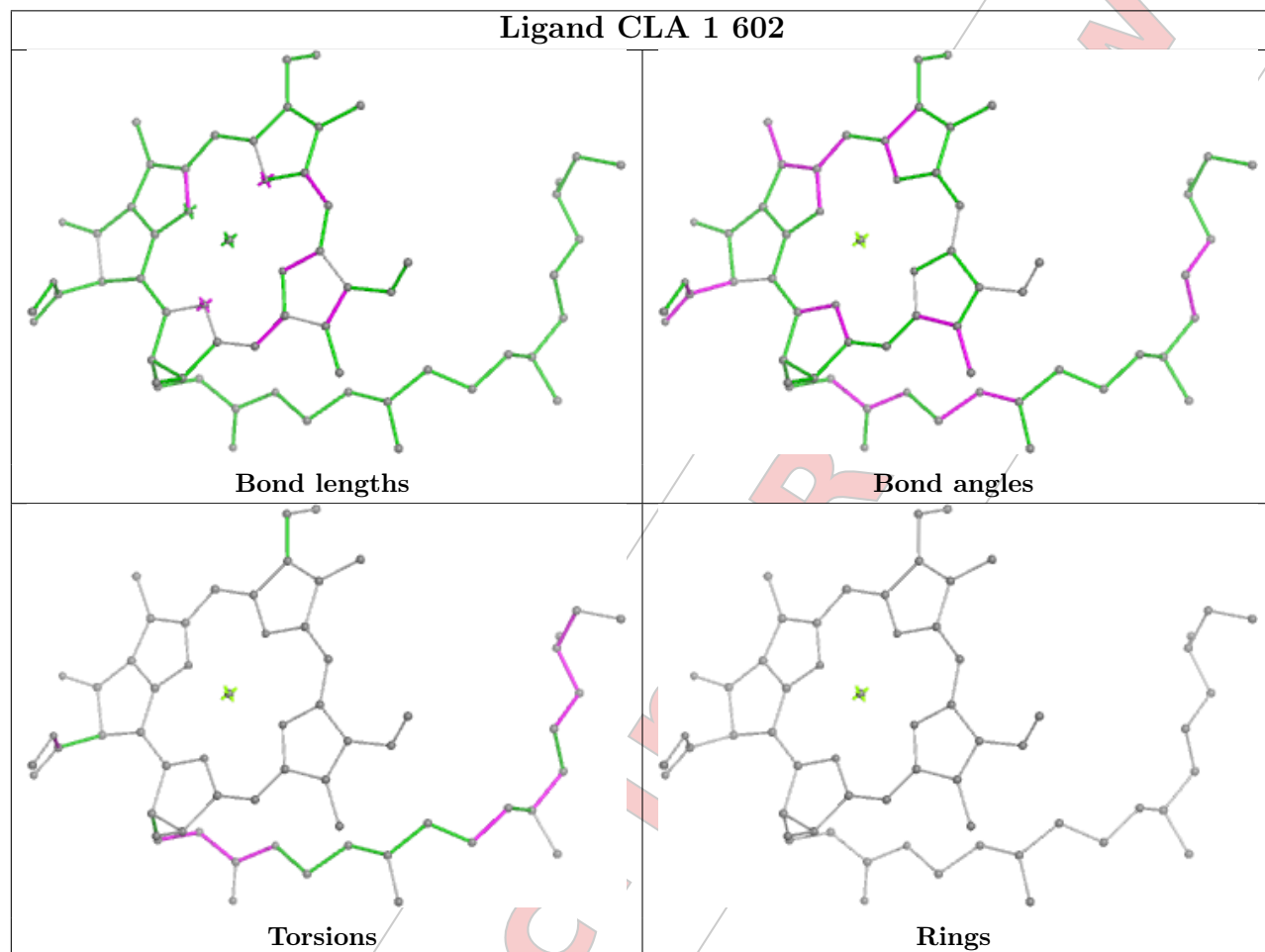




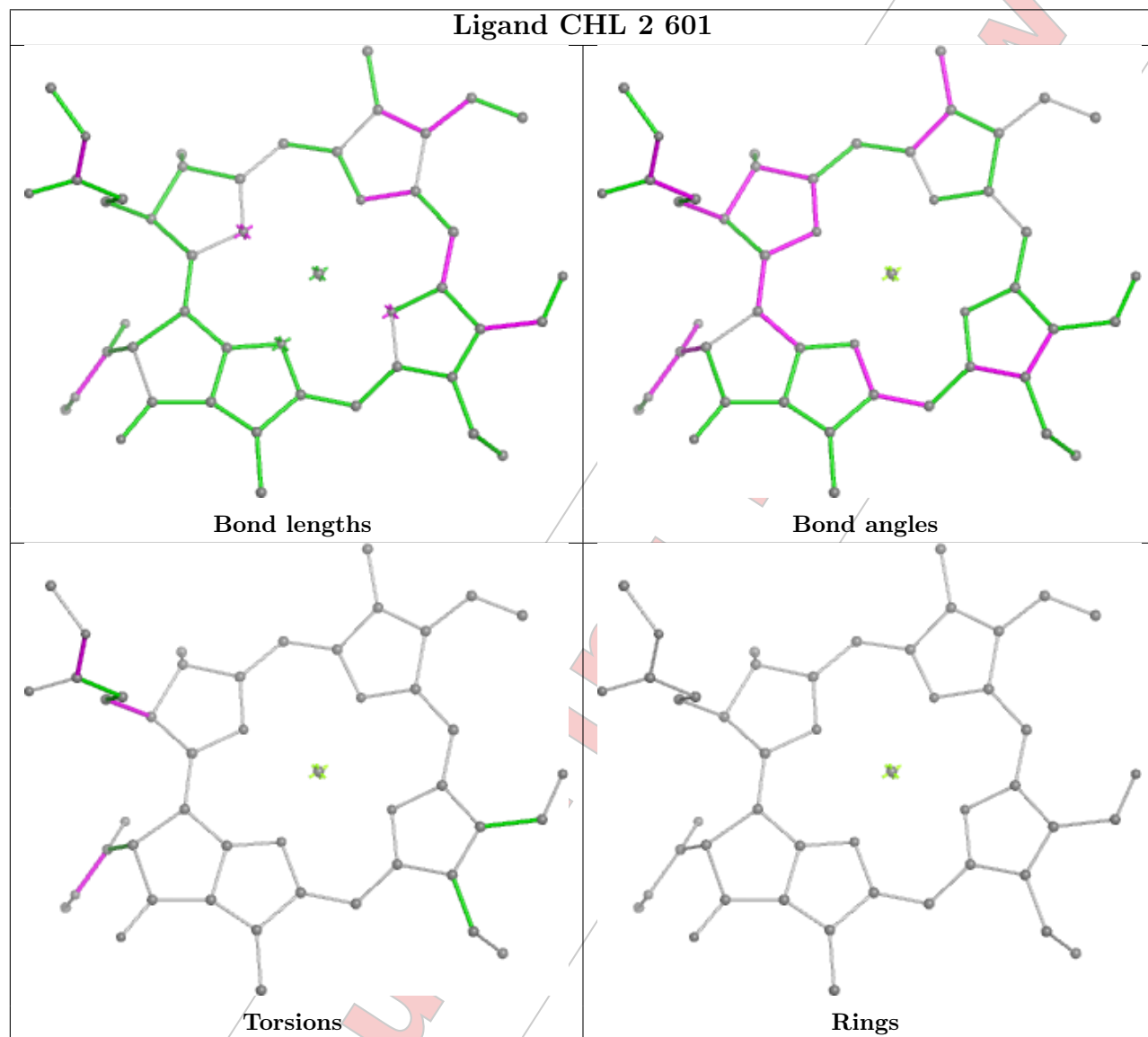




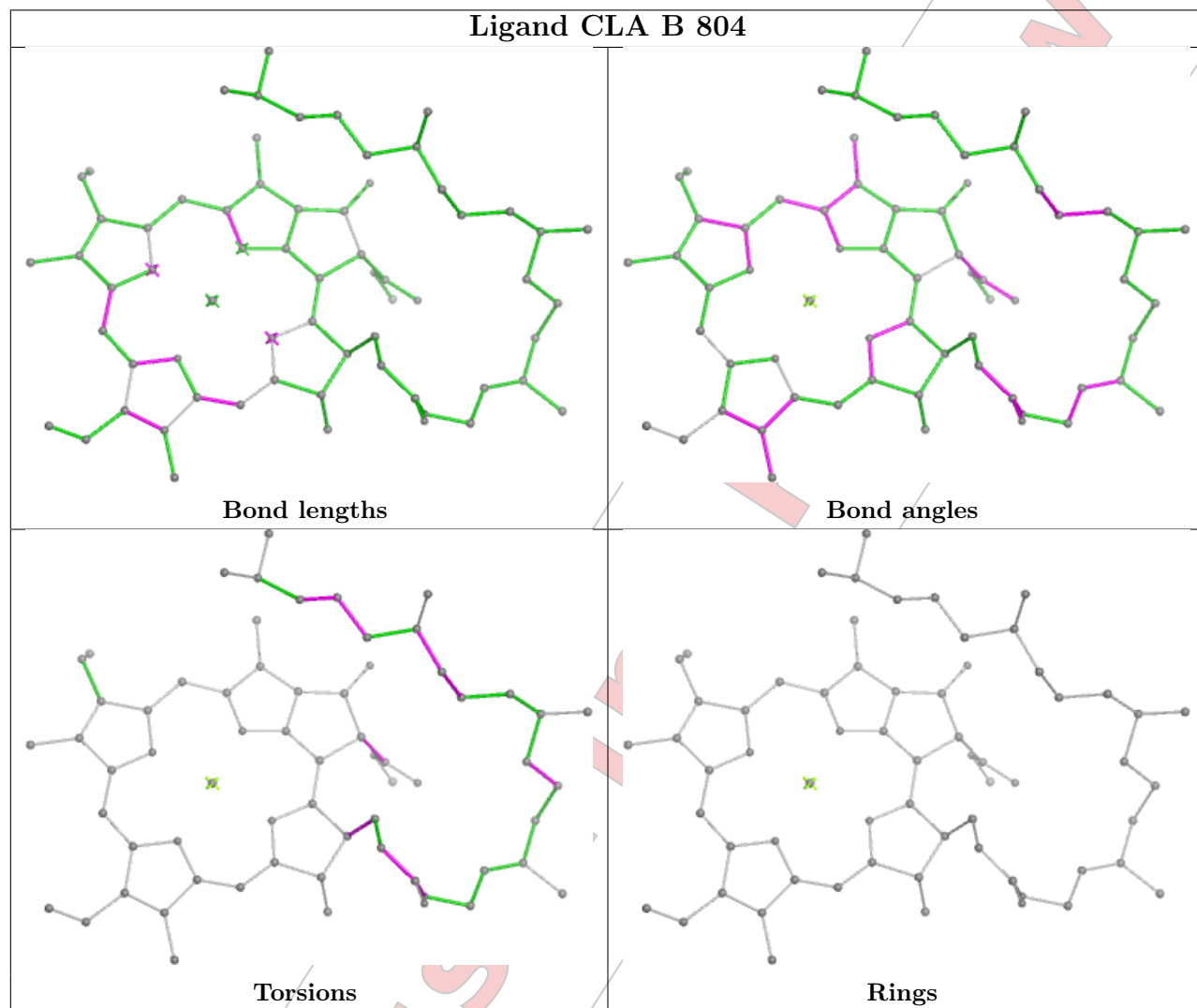
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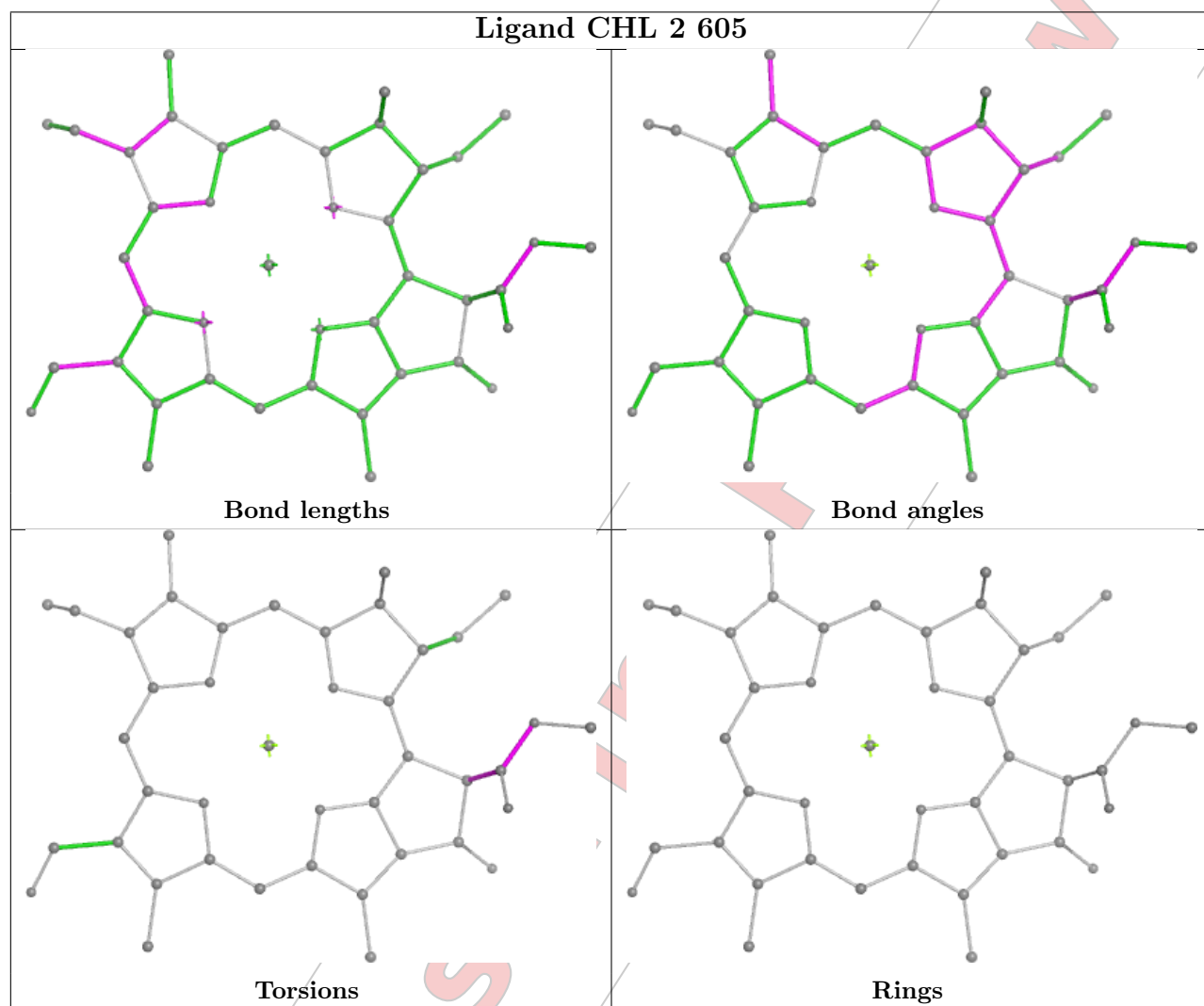


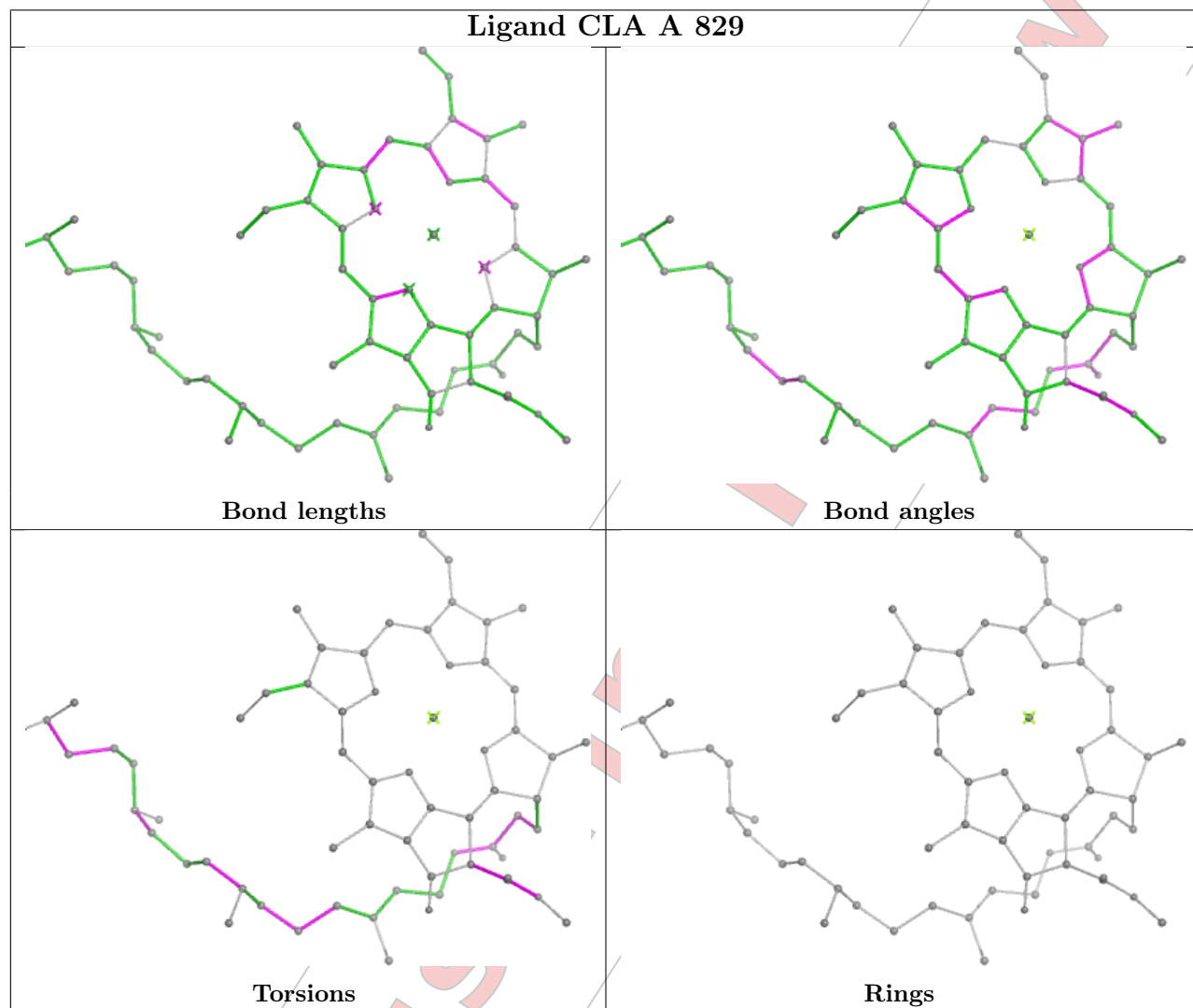
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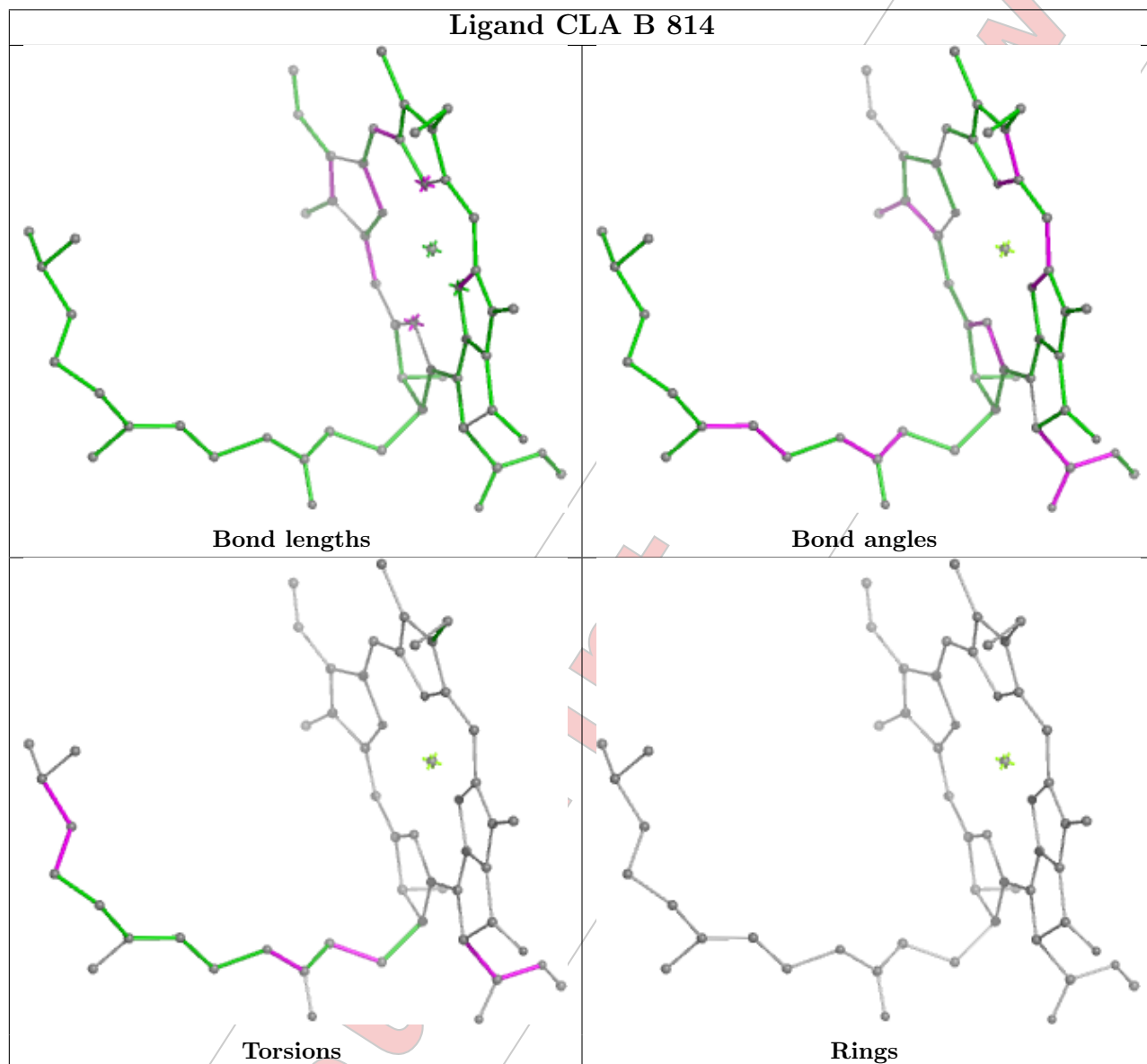




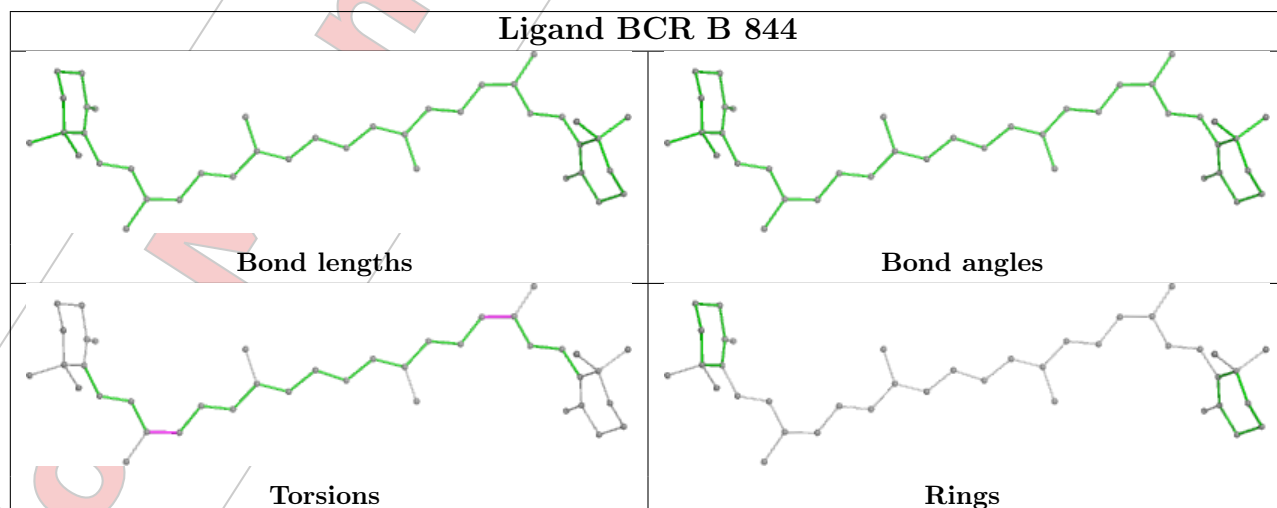


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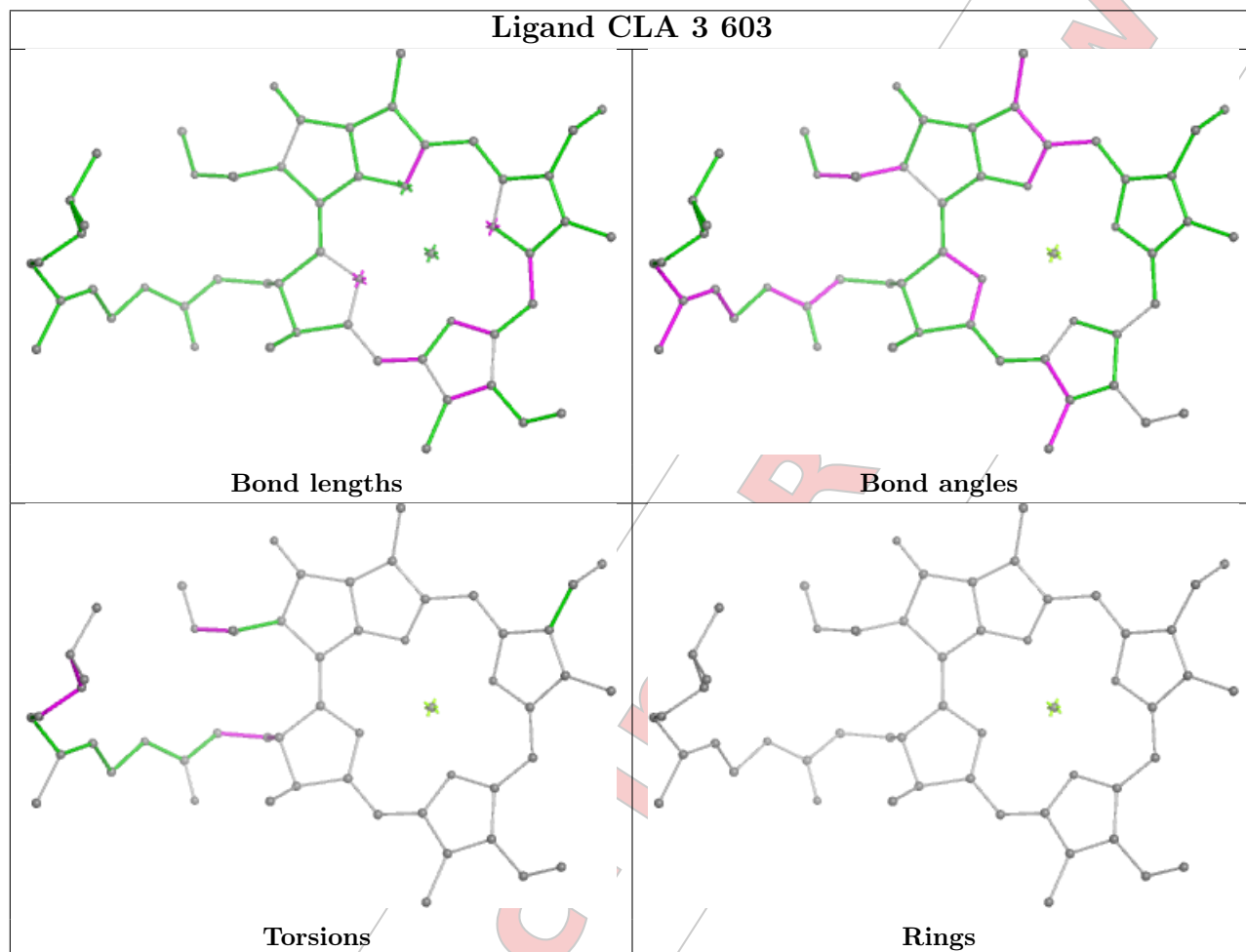
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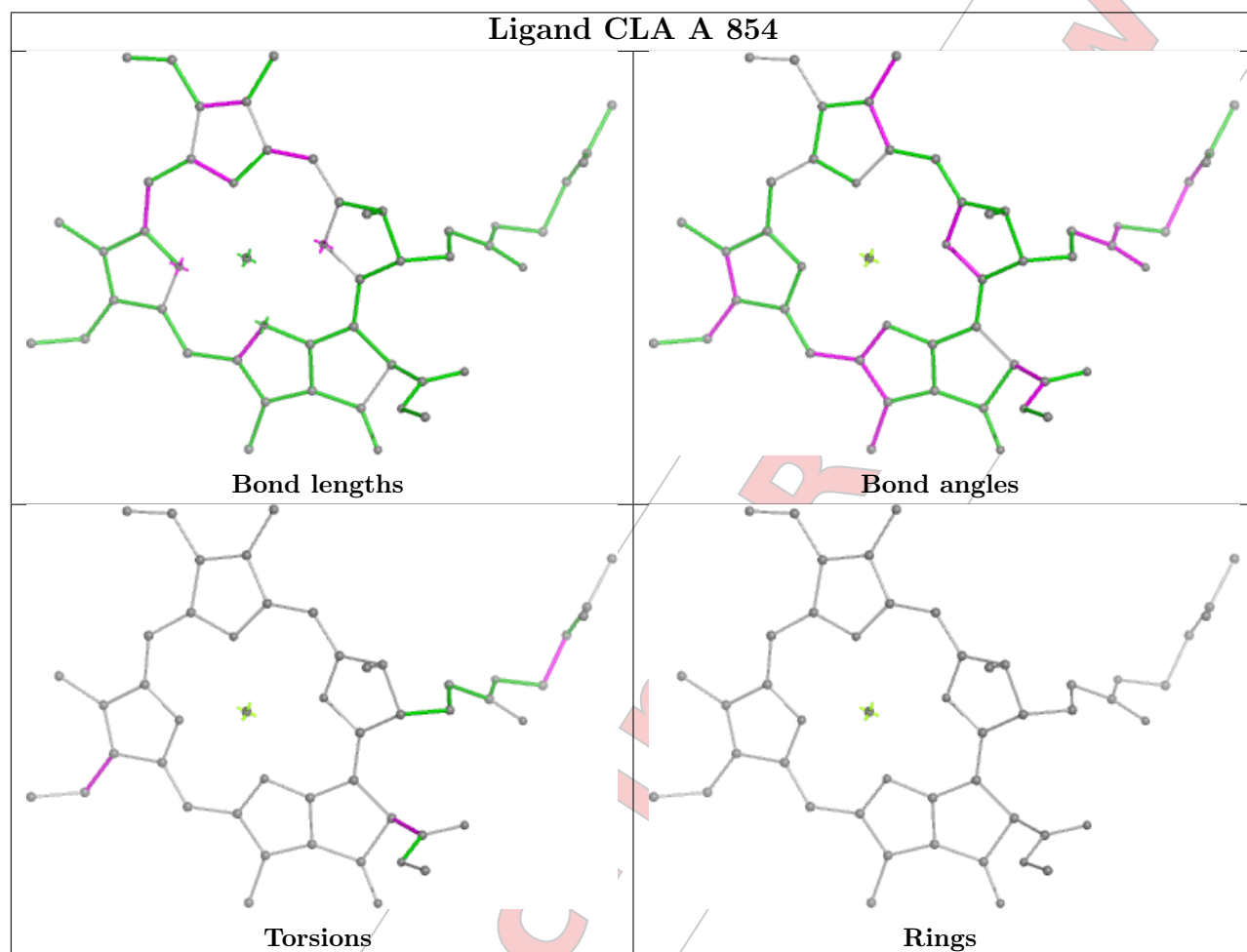


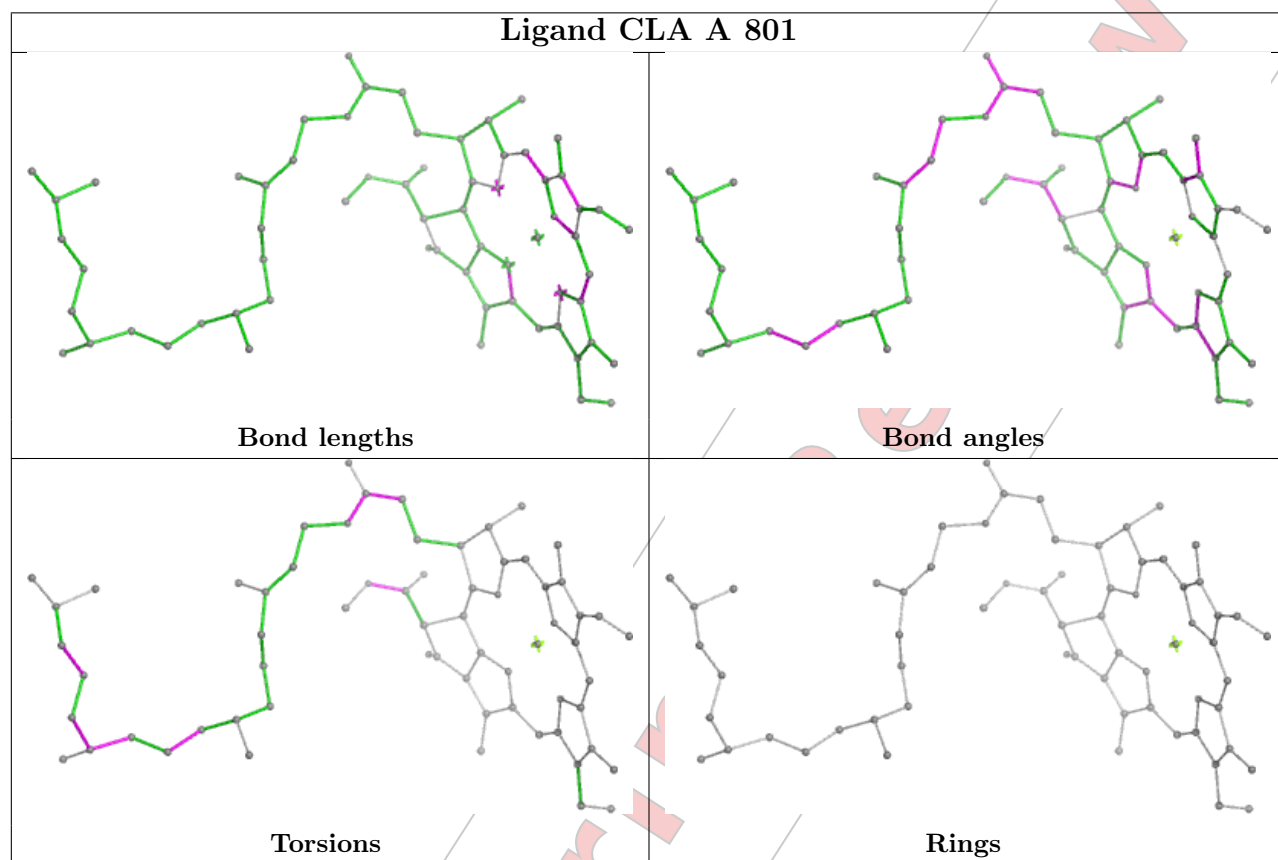
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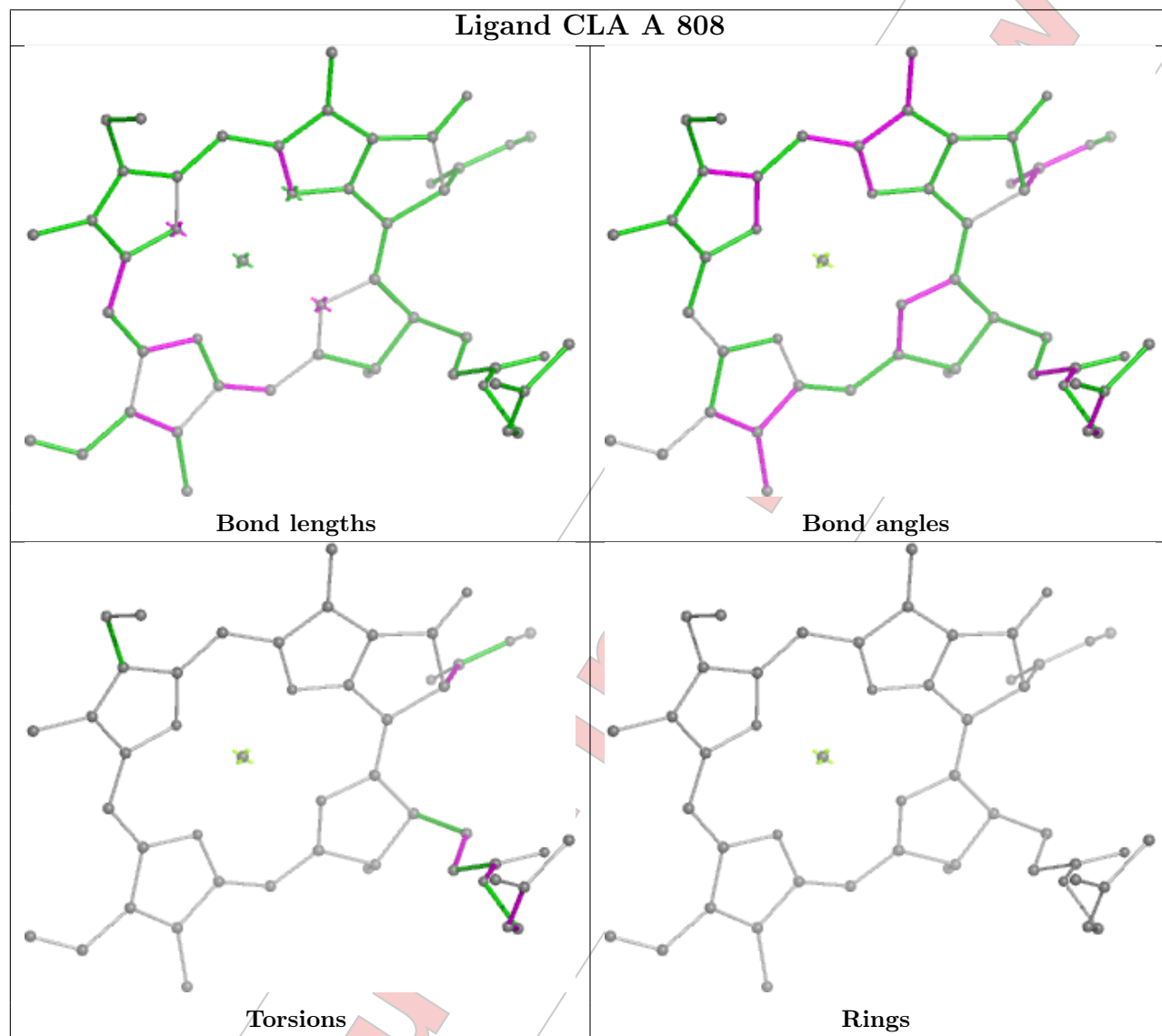


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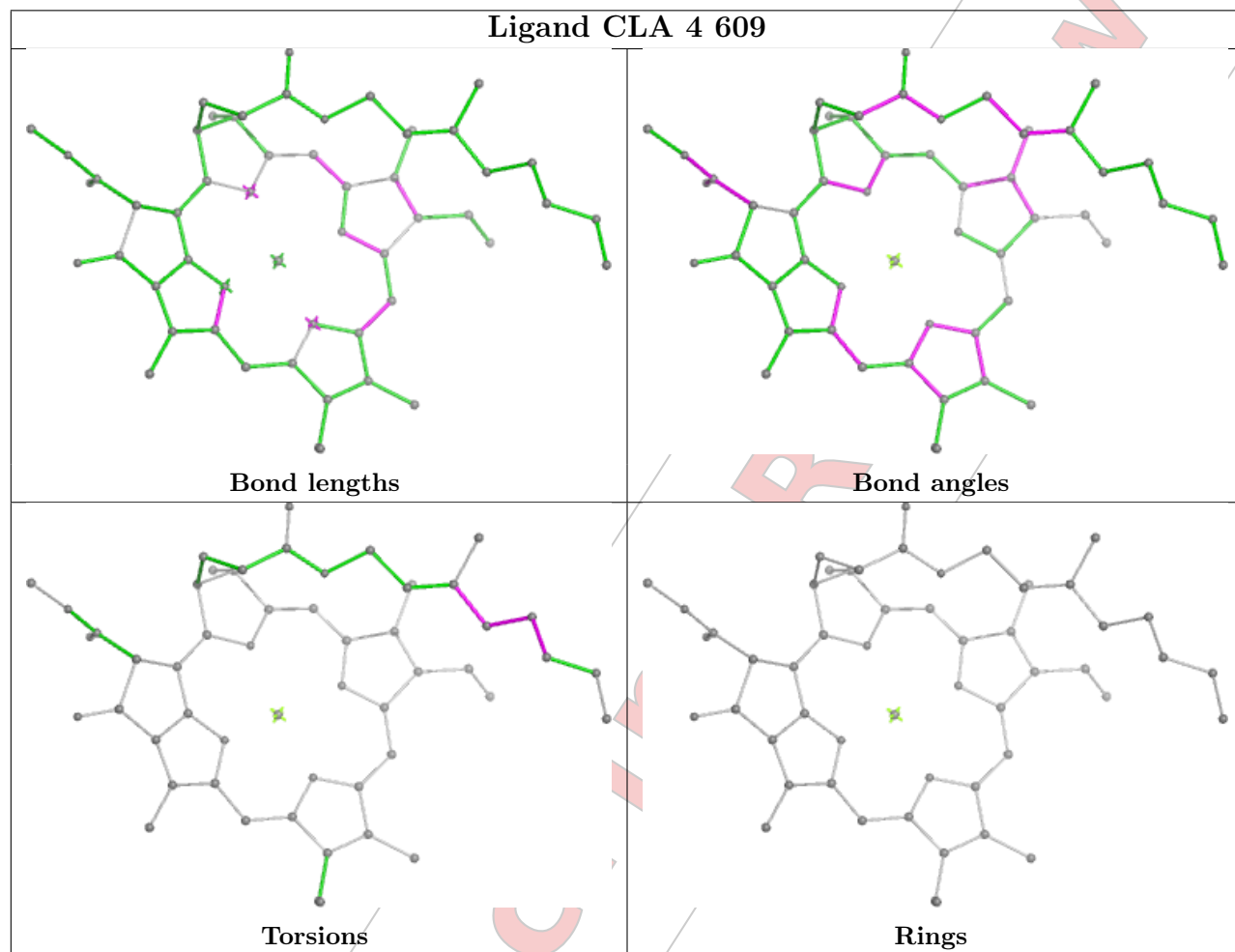


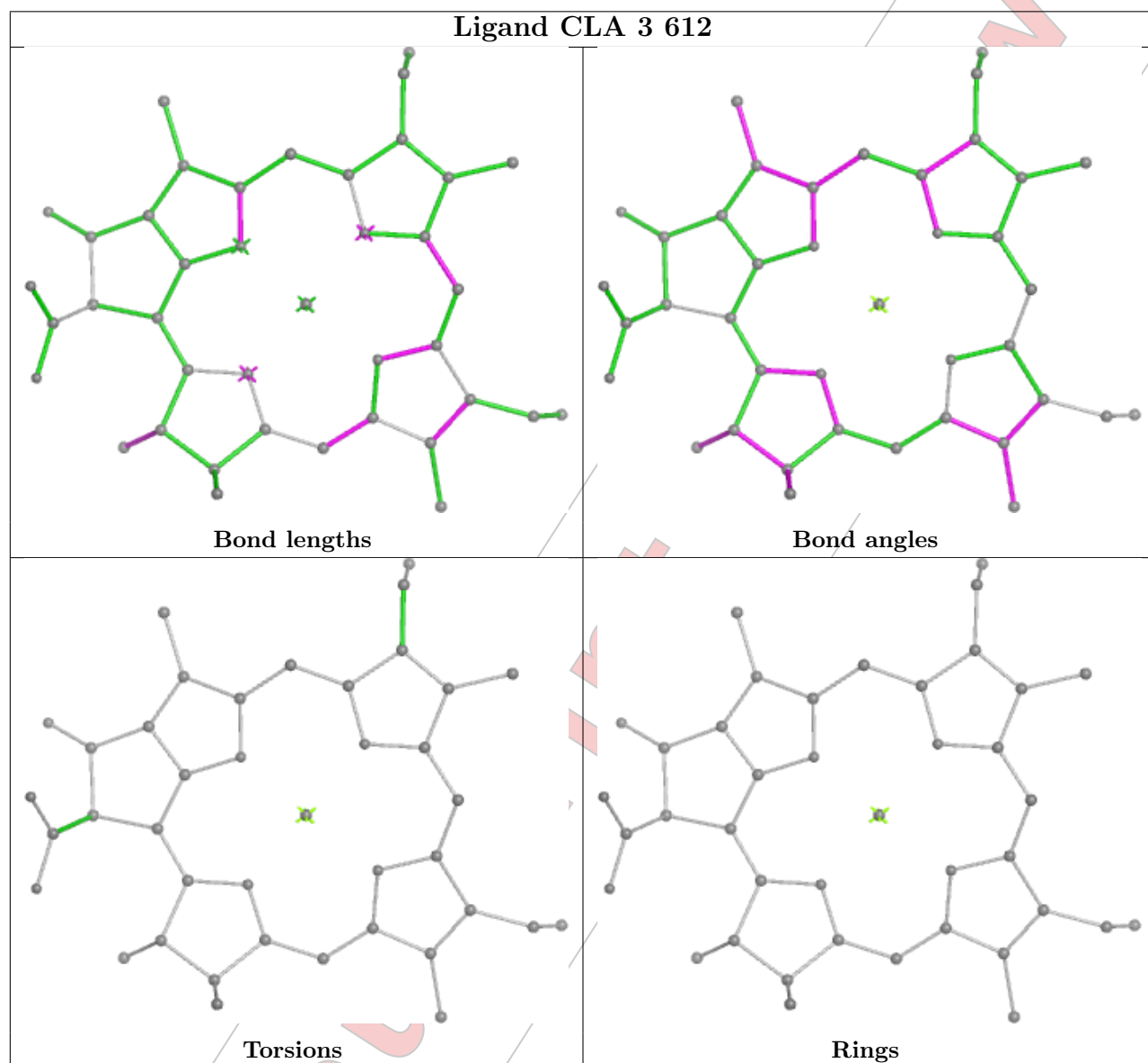




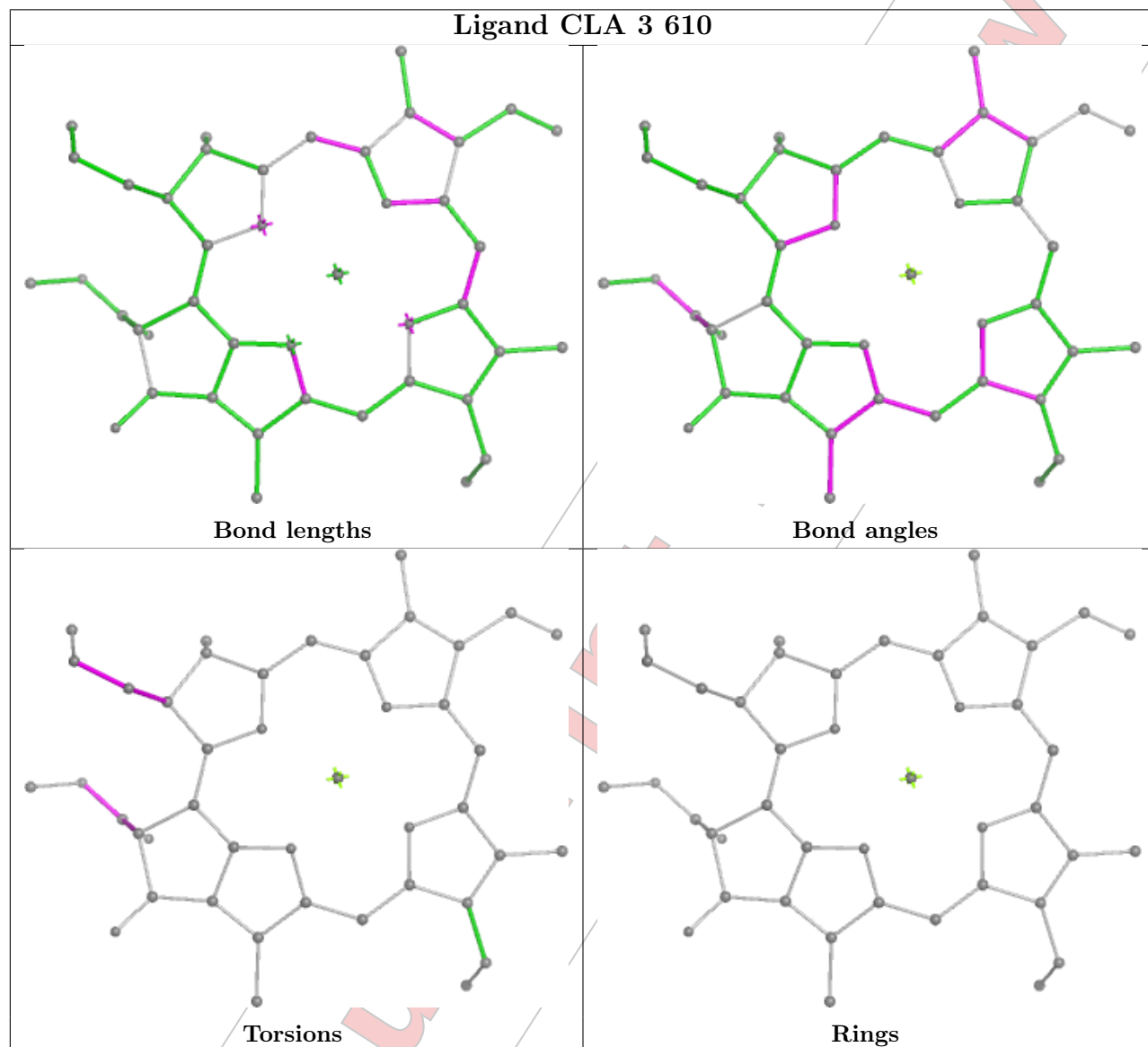


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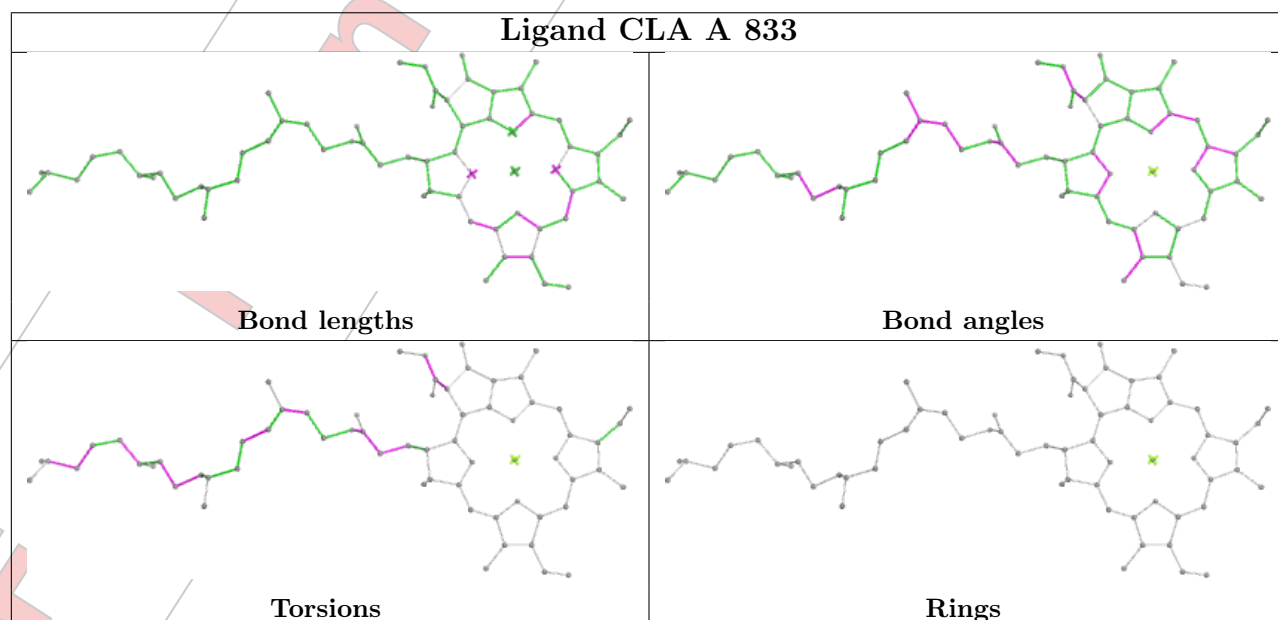


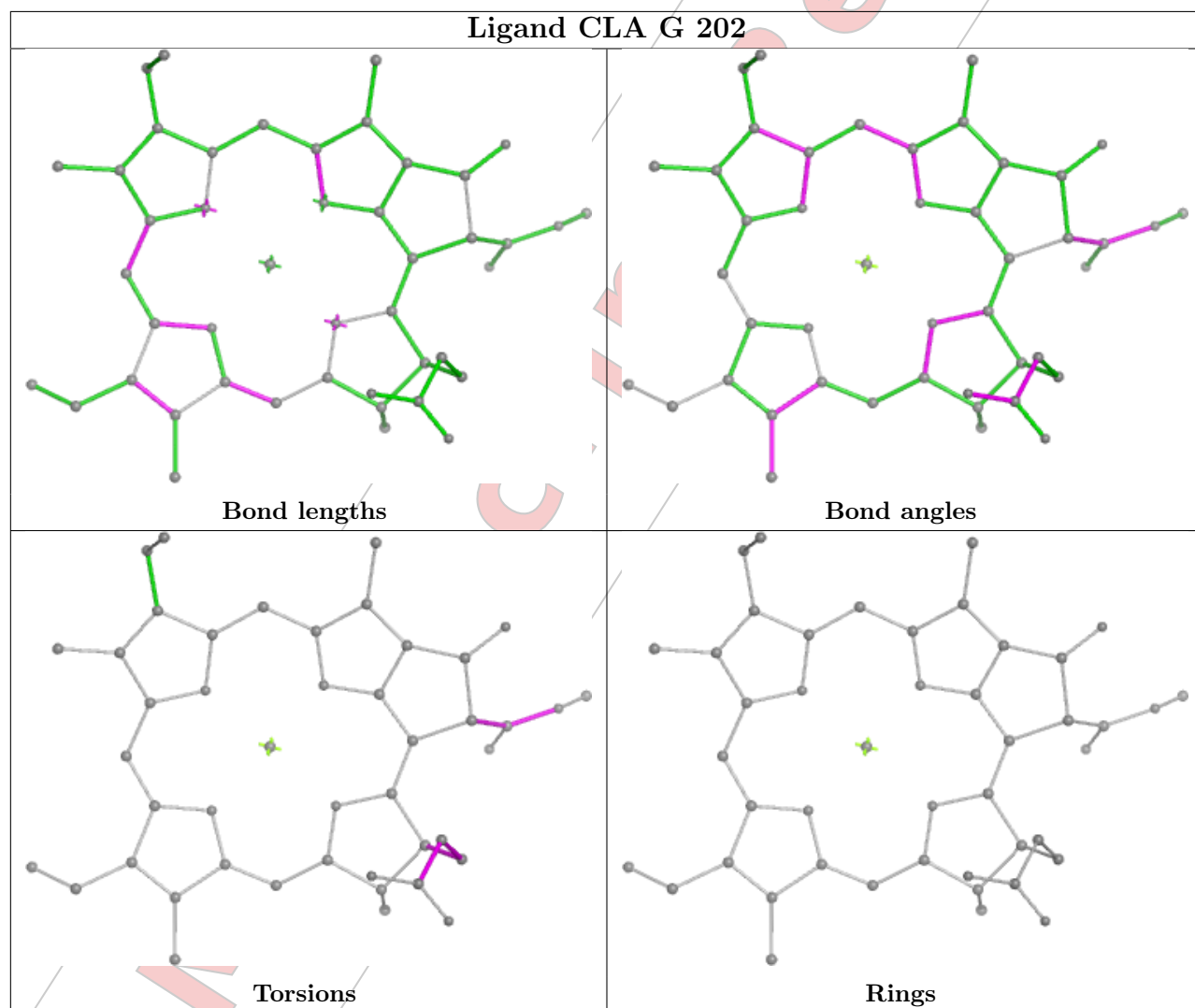
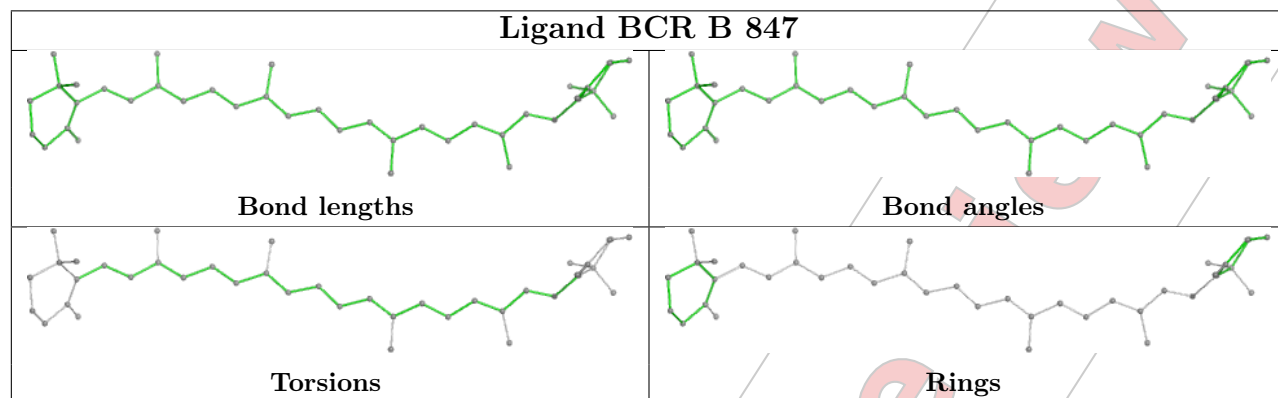


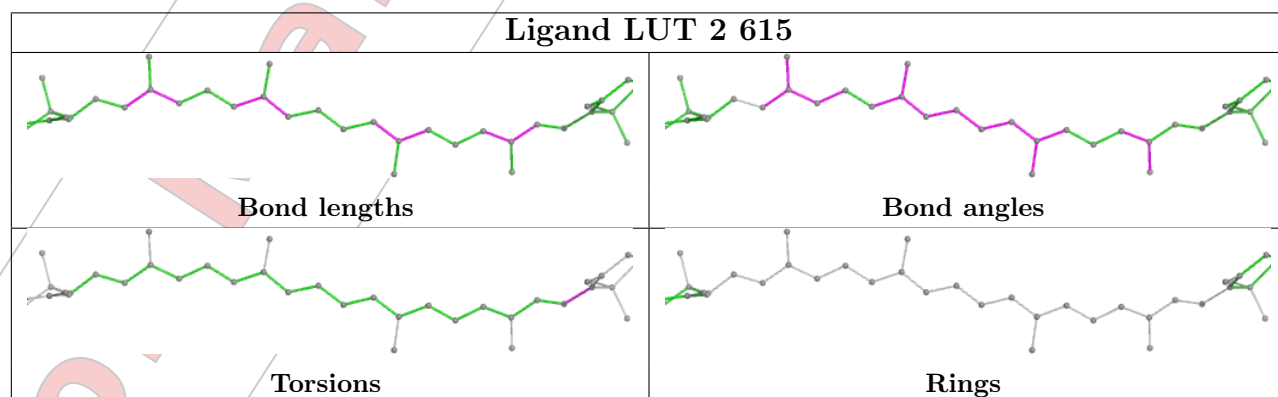
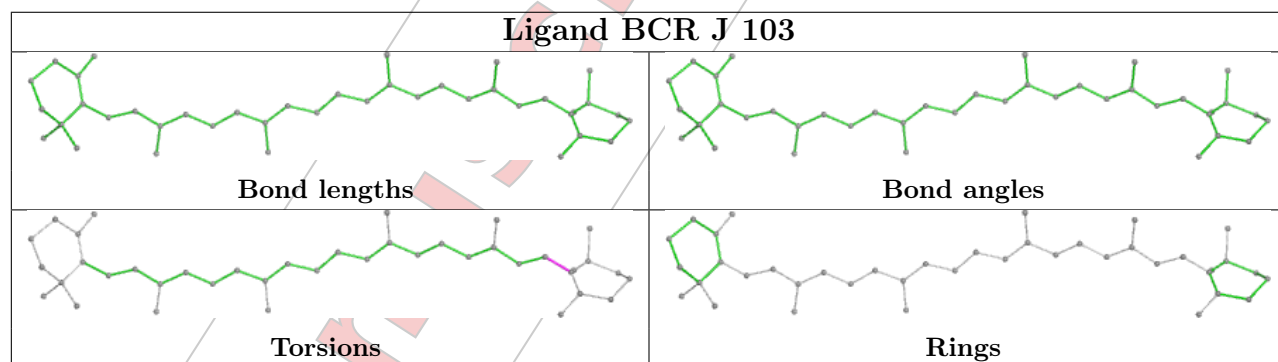
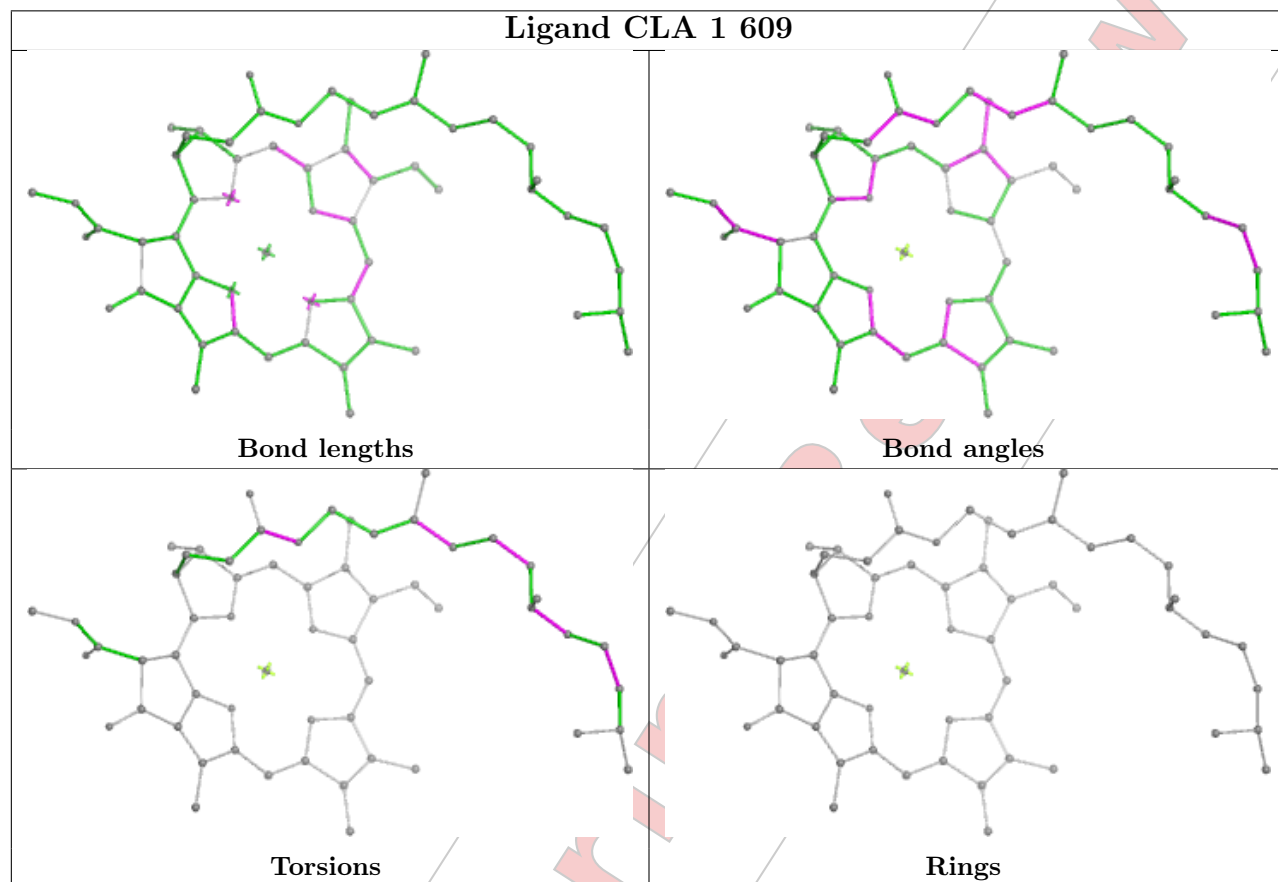
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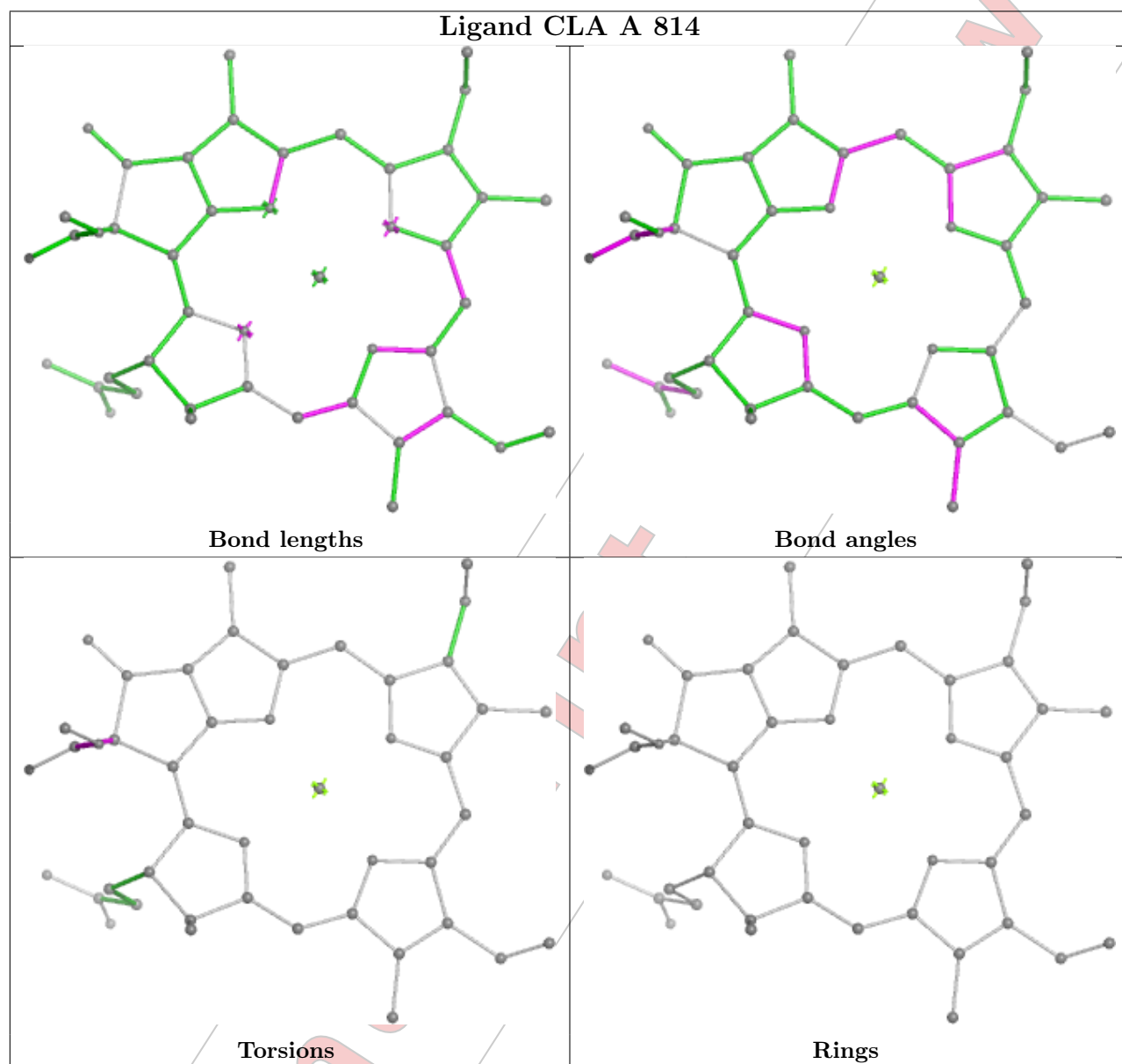


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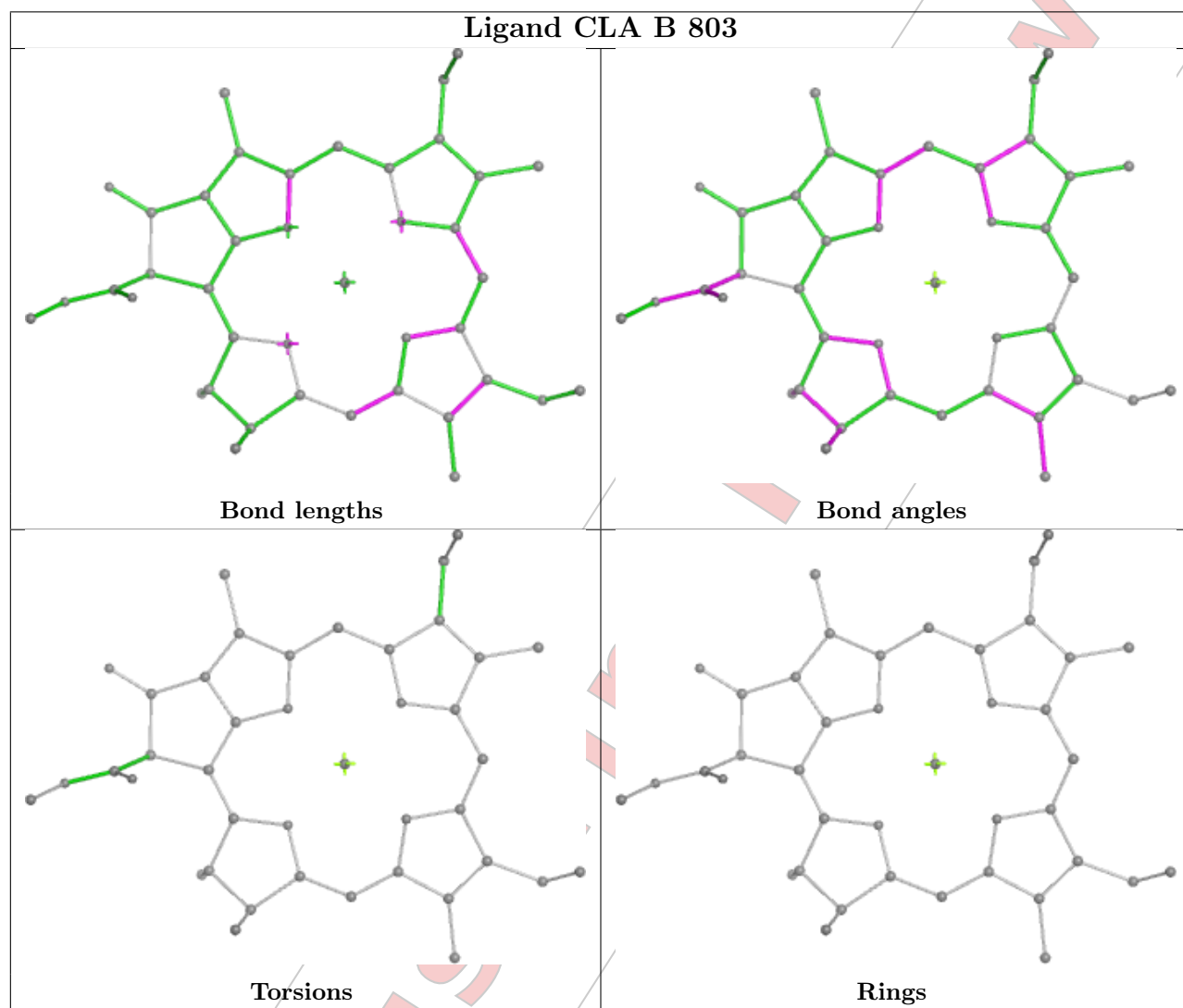




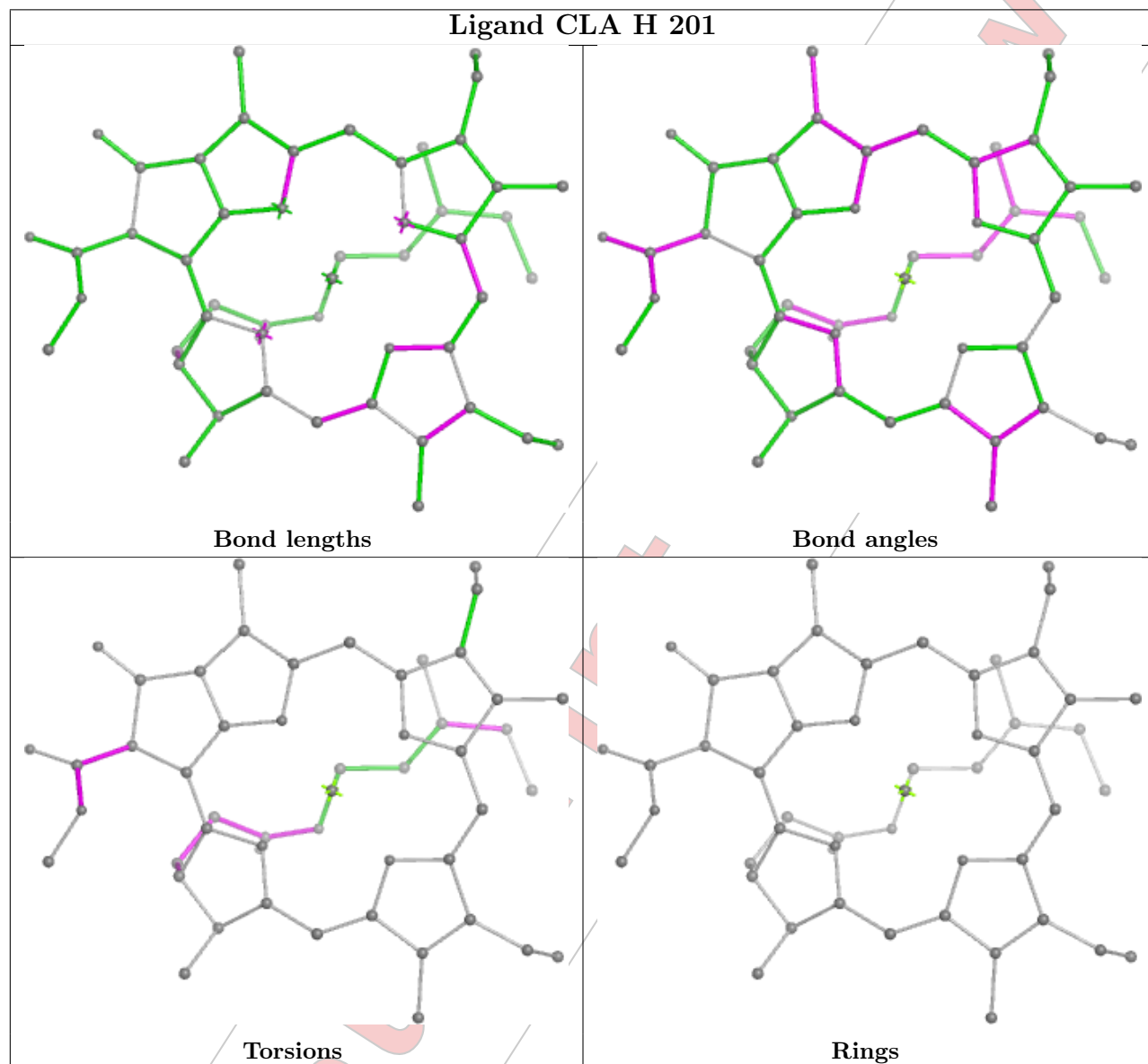




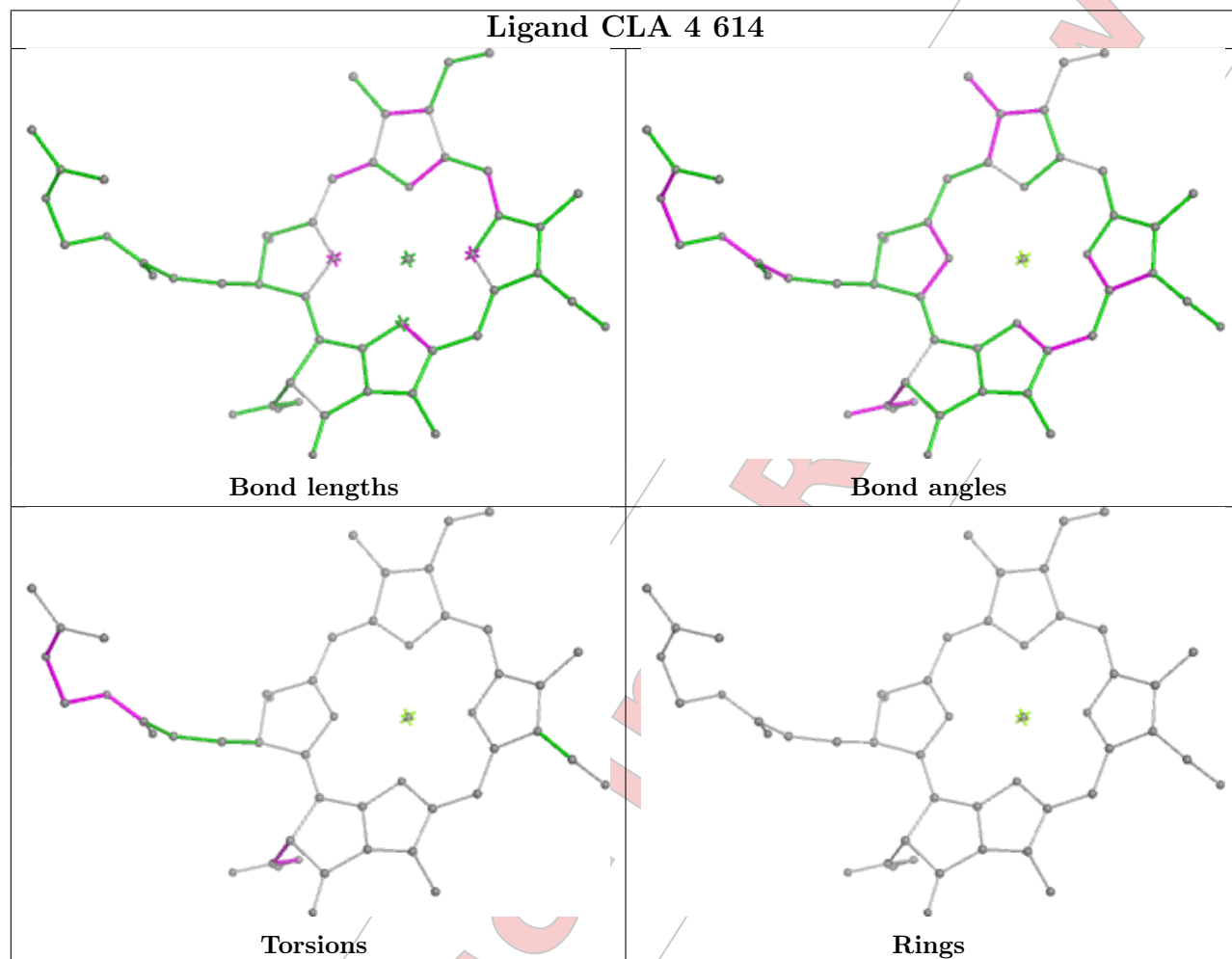
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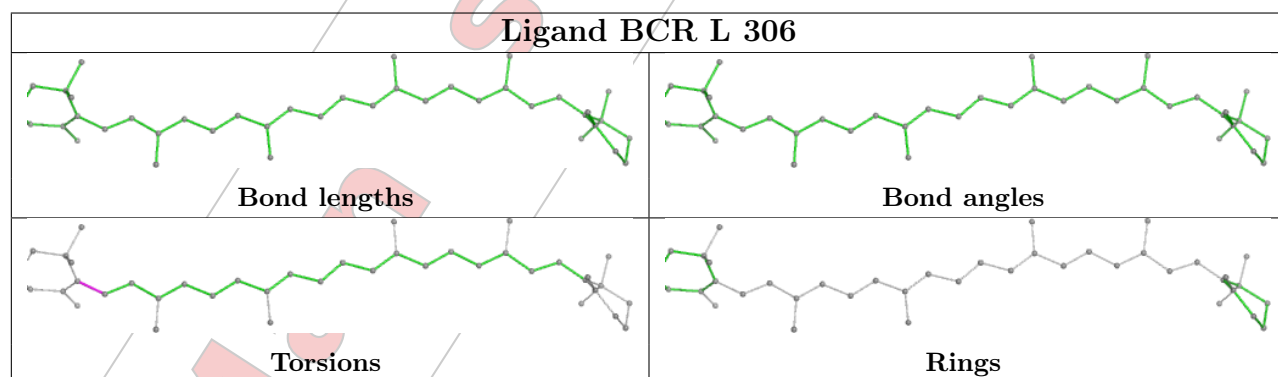
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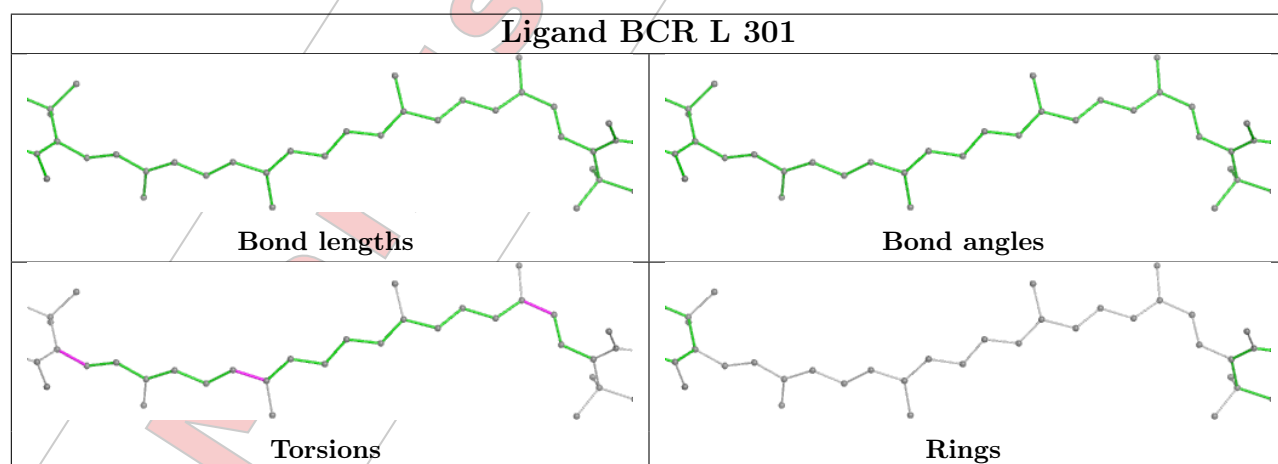
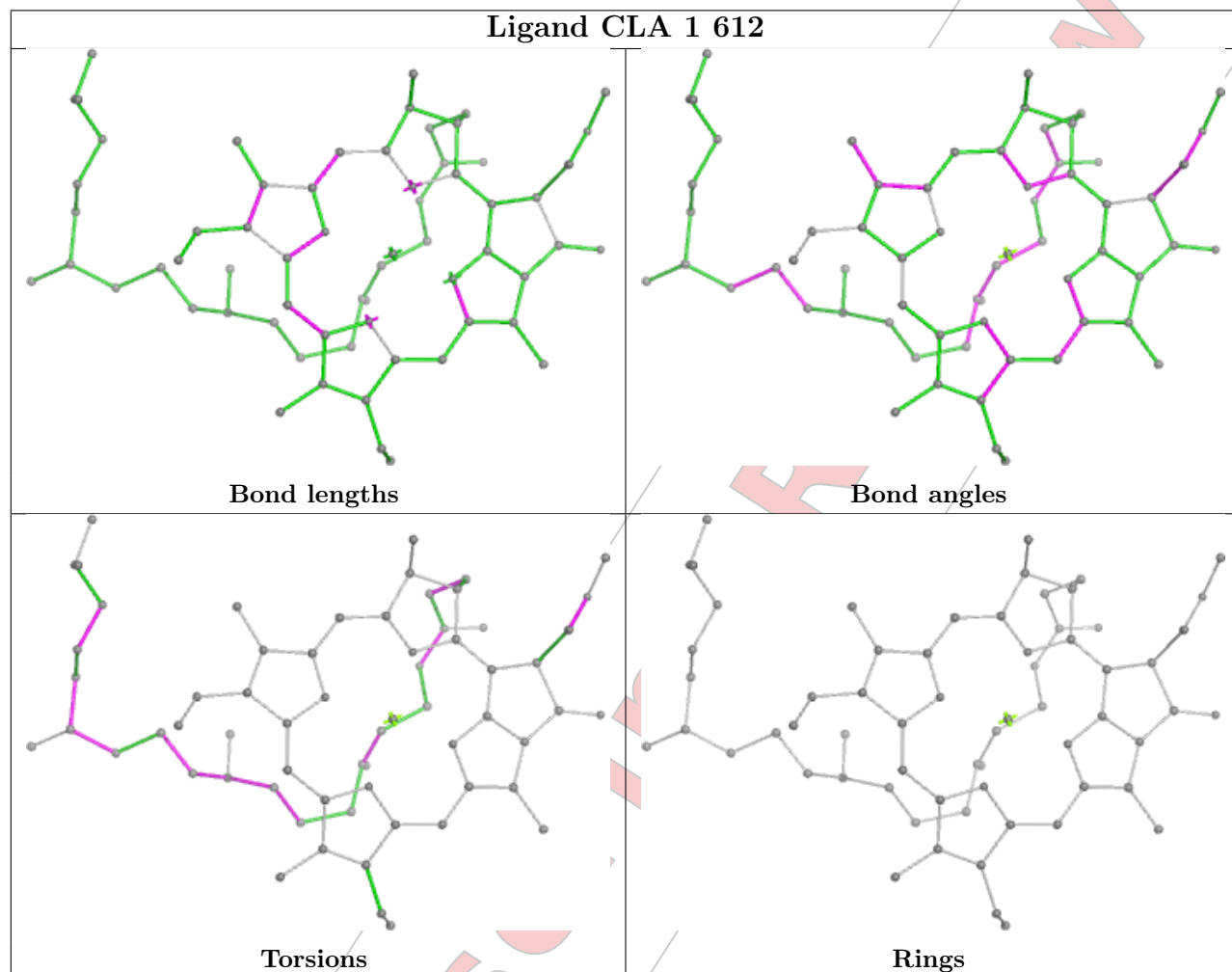


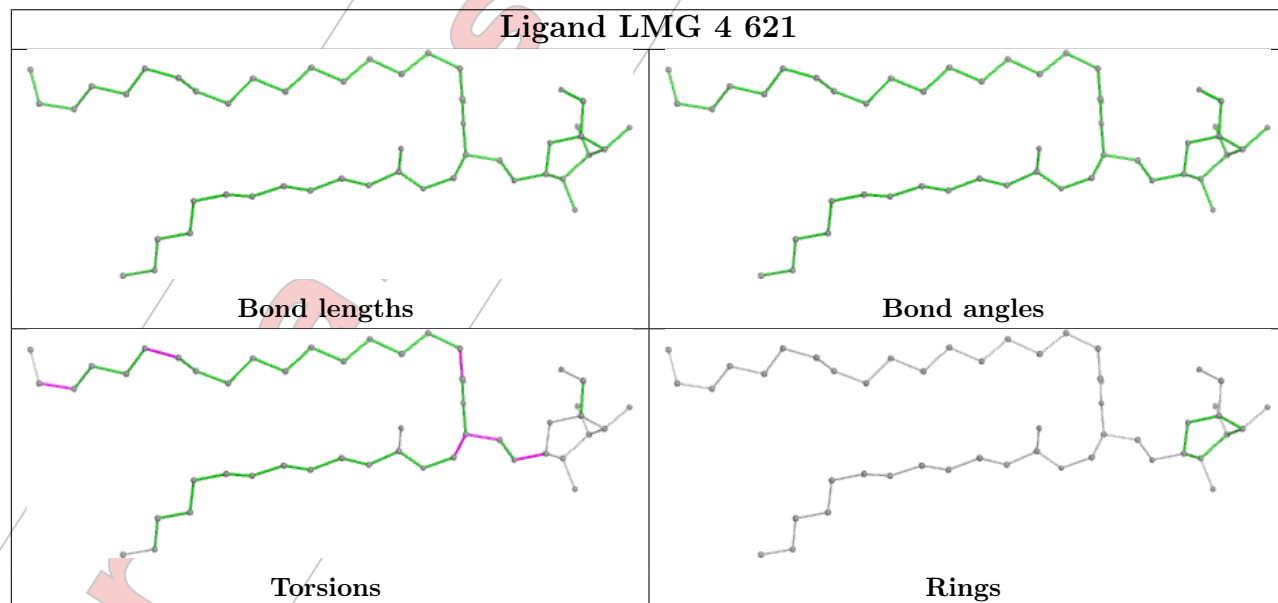
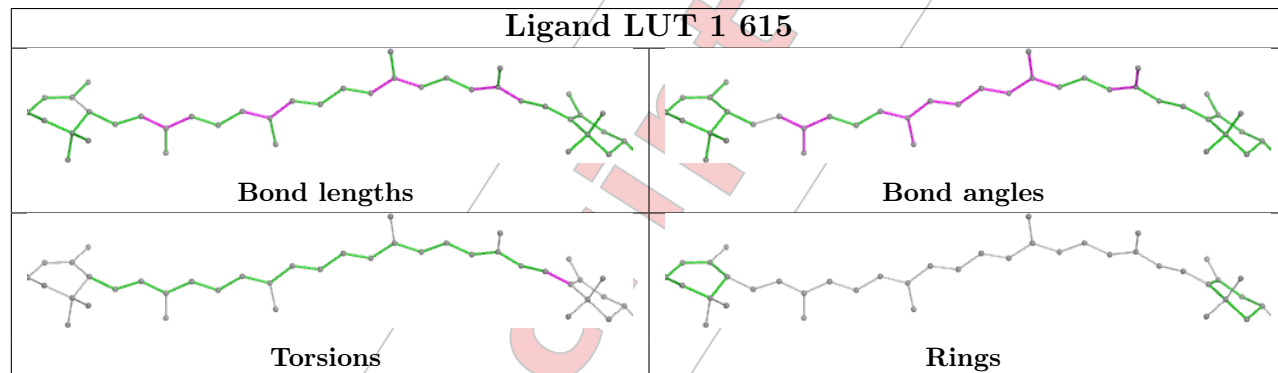
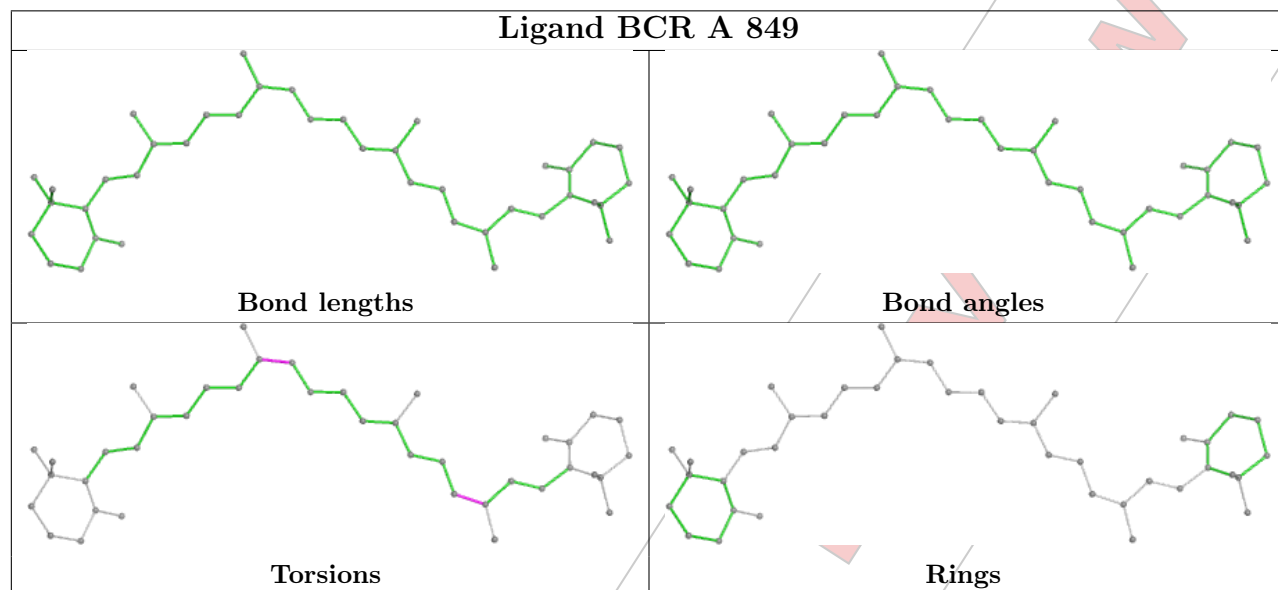
Ligand CLA 4 614

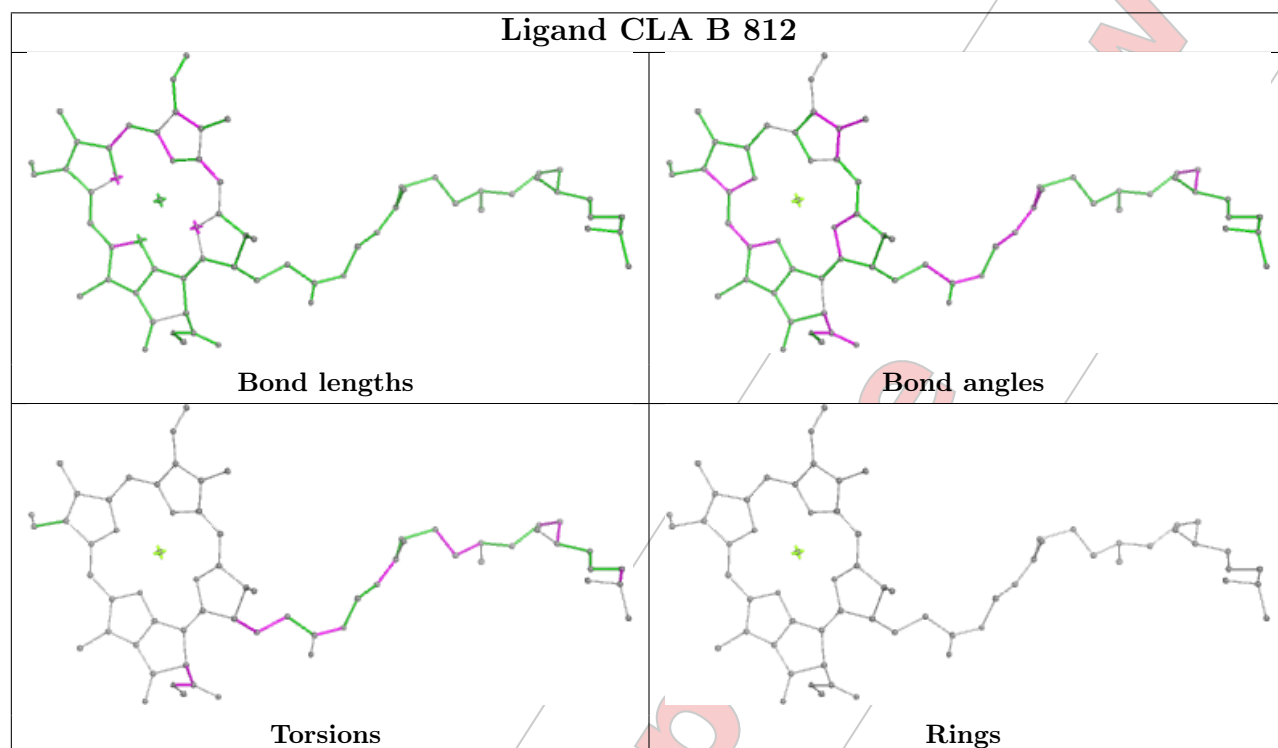


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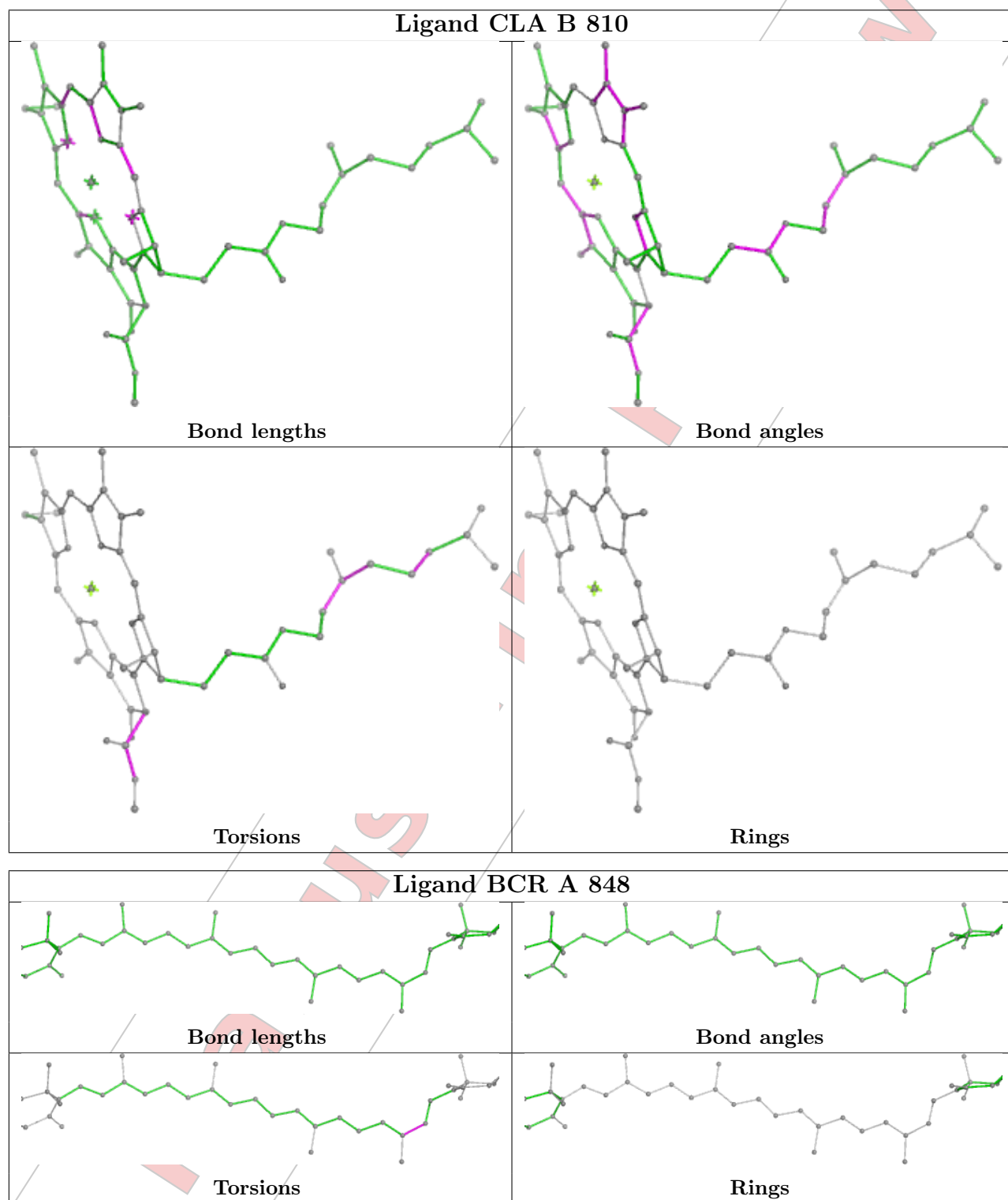


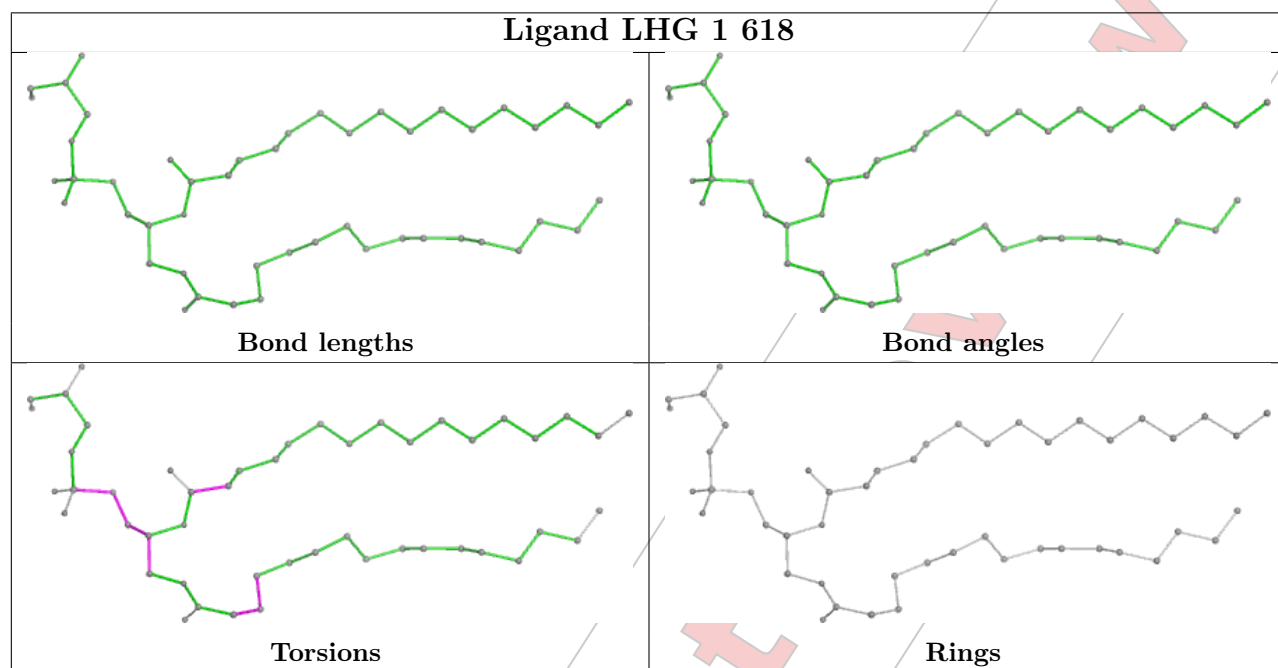




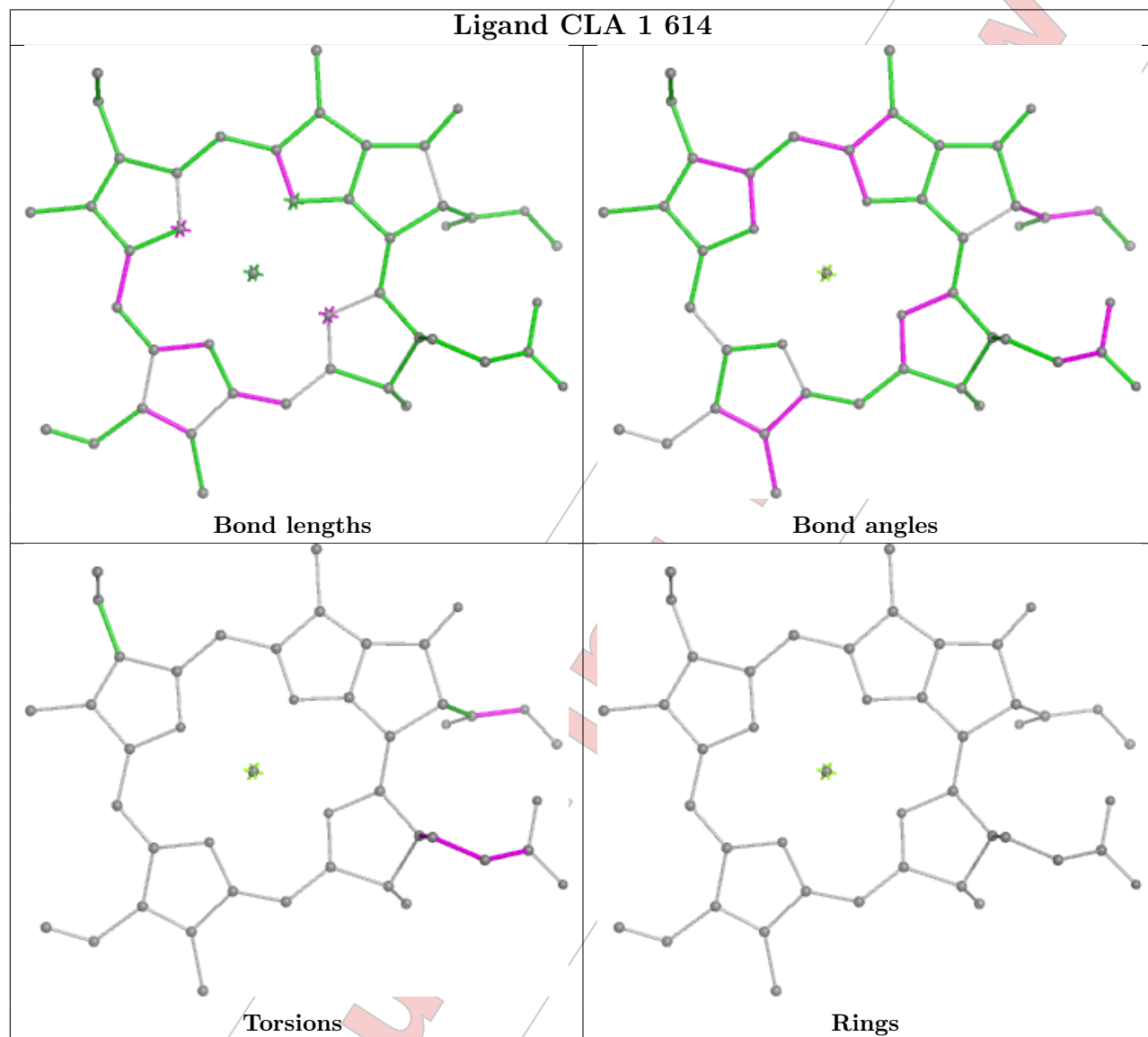


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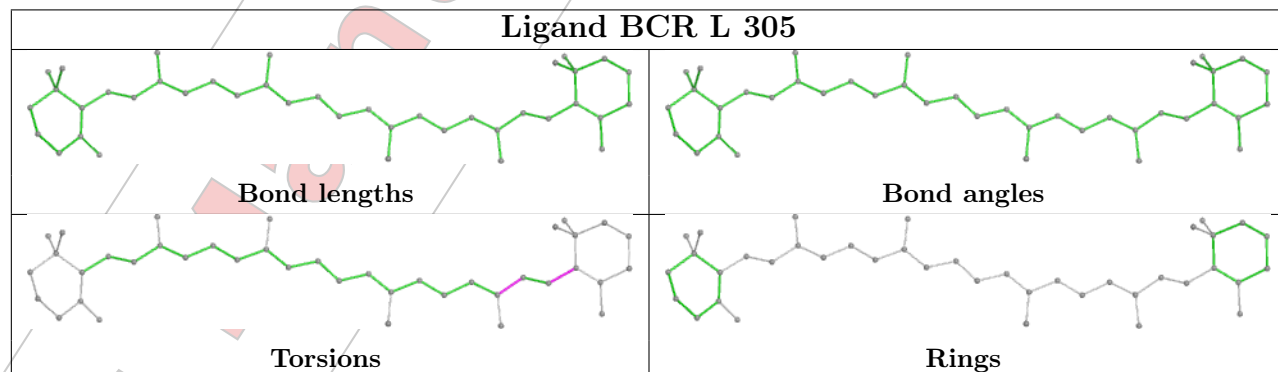


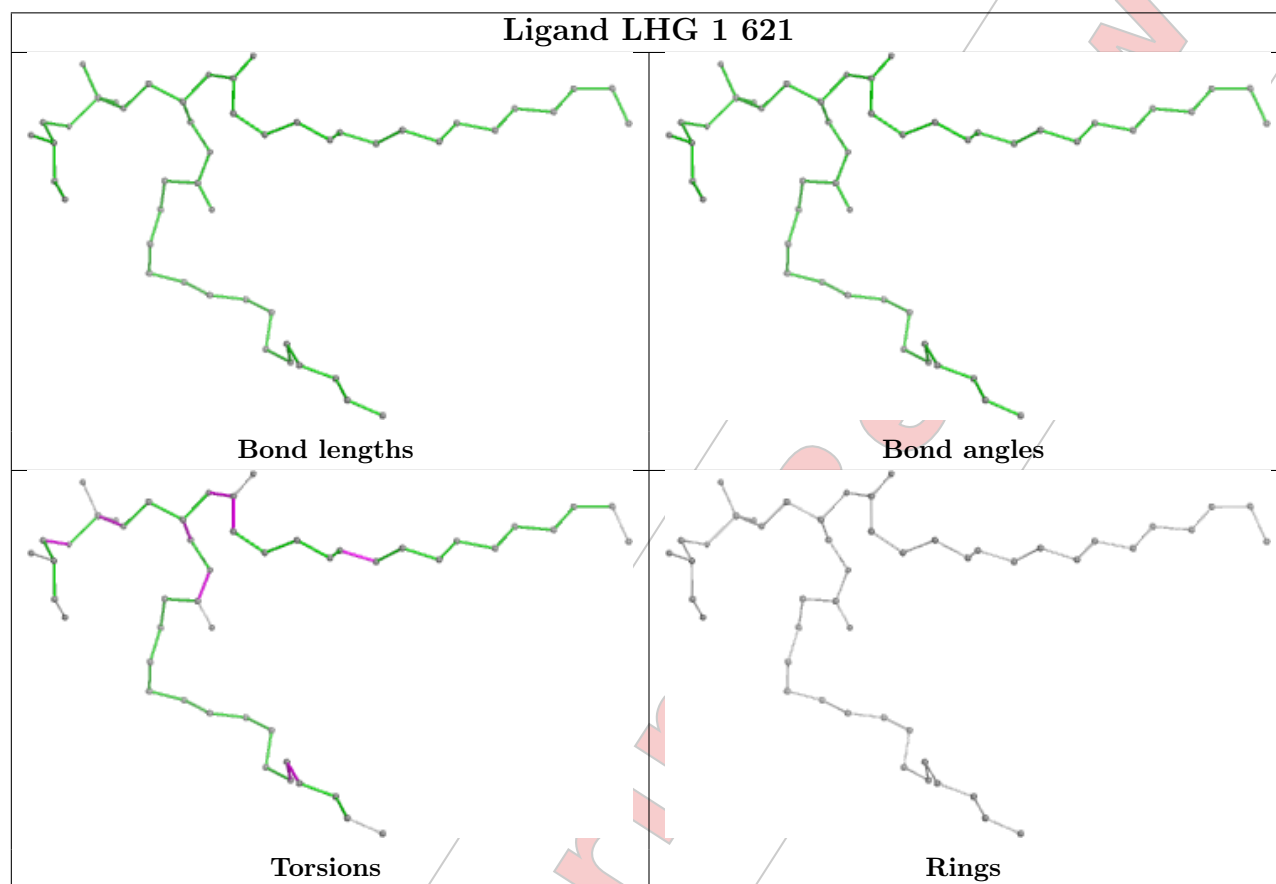


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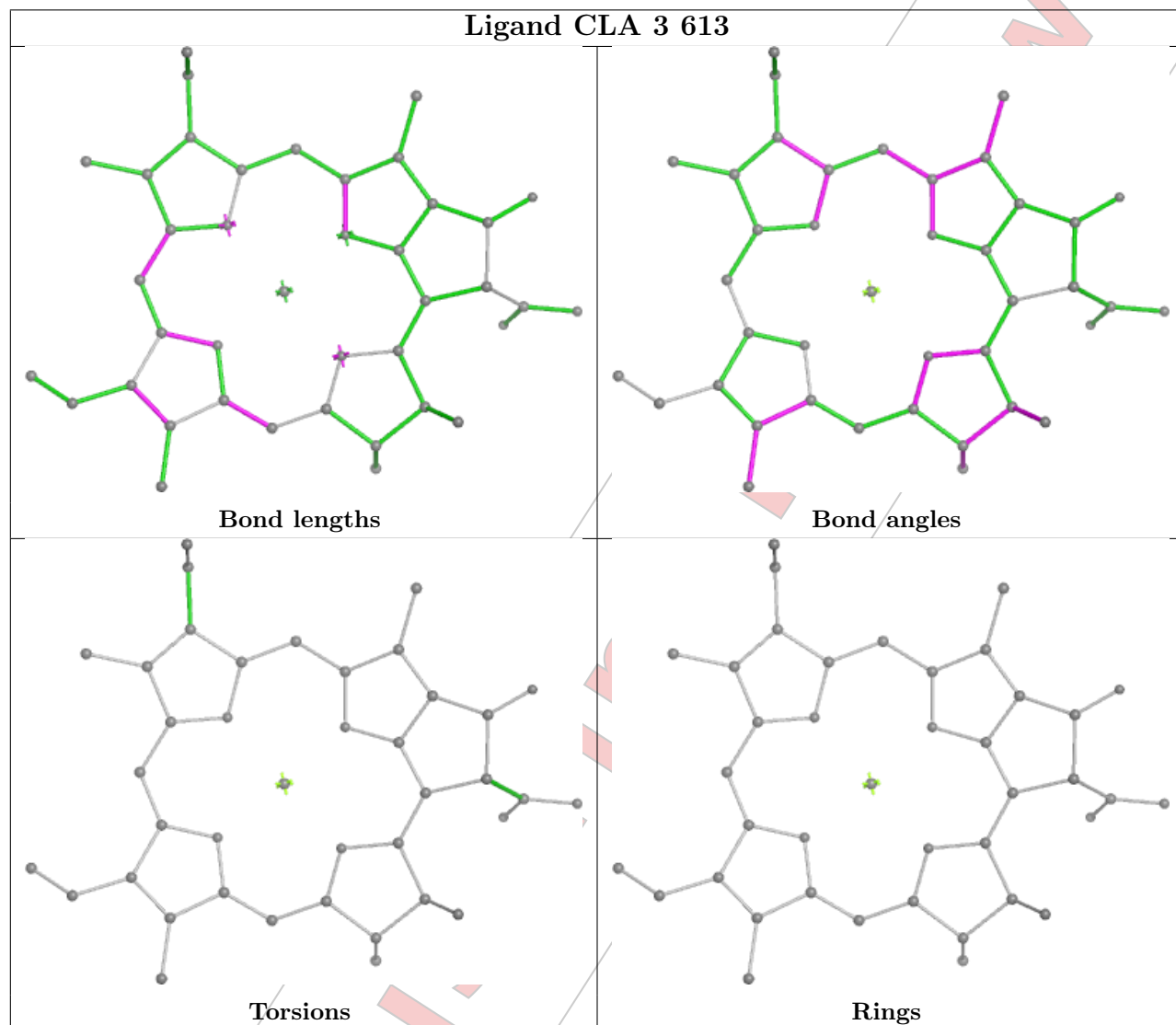


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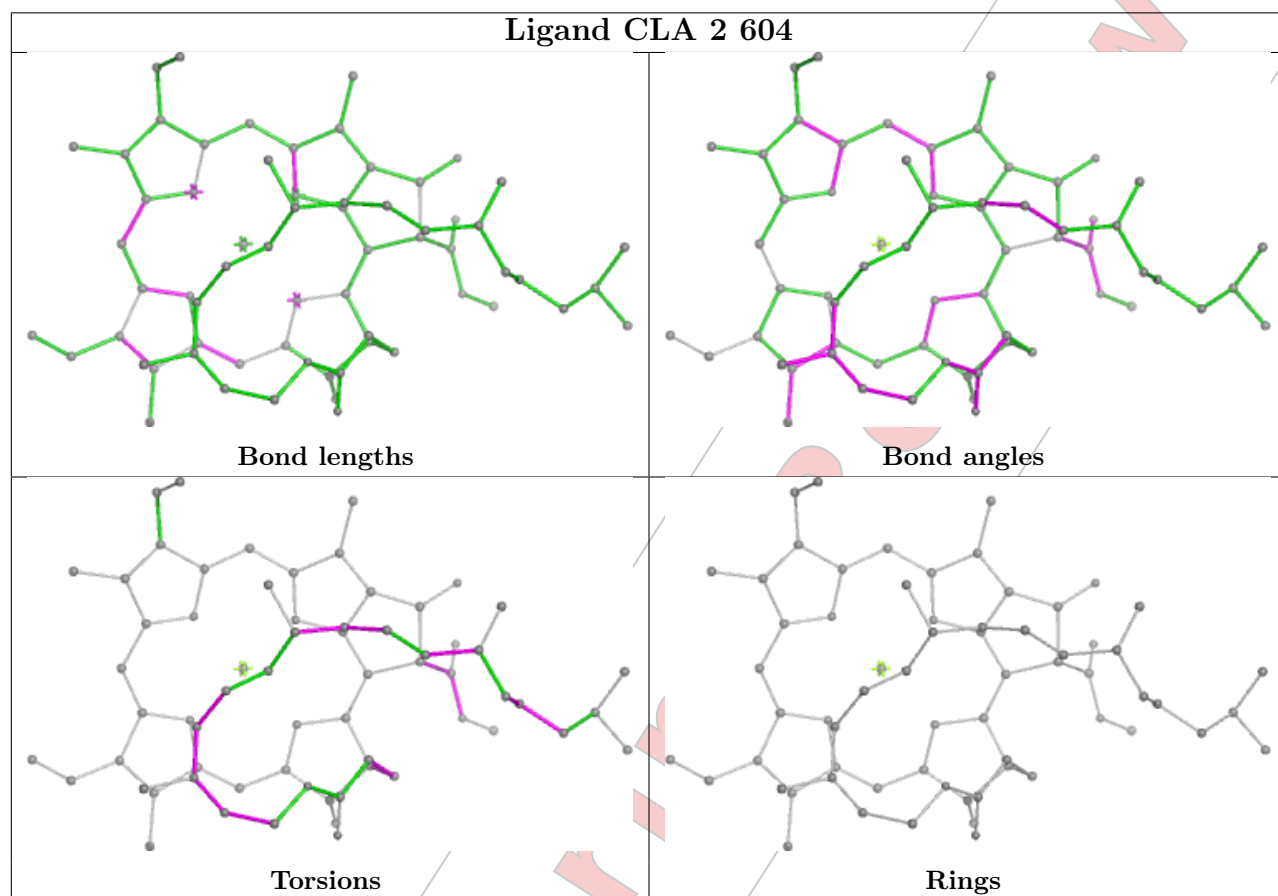




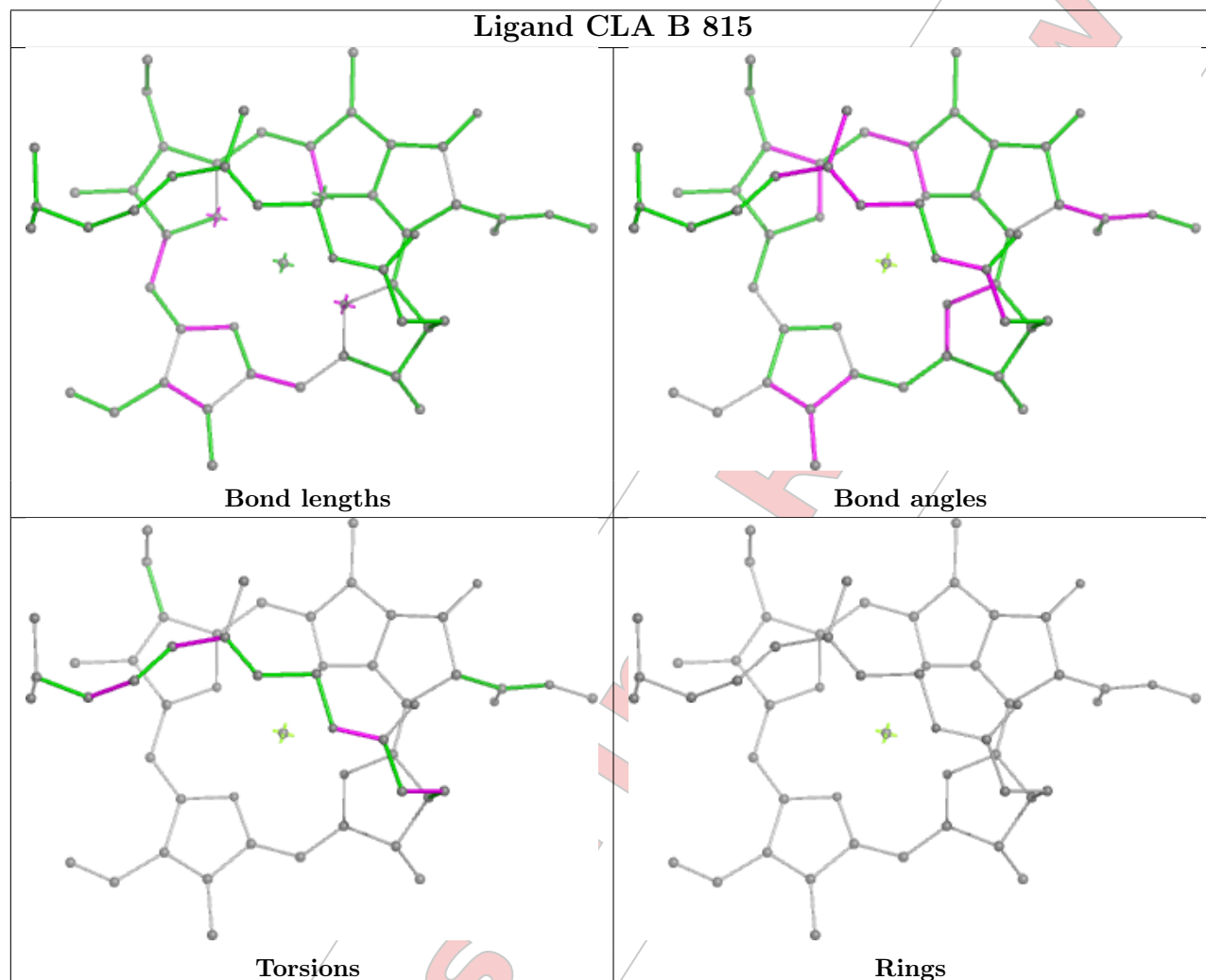
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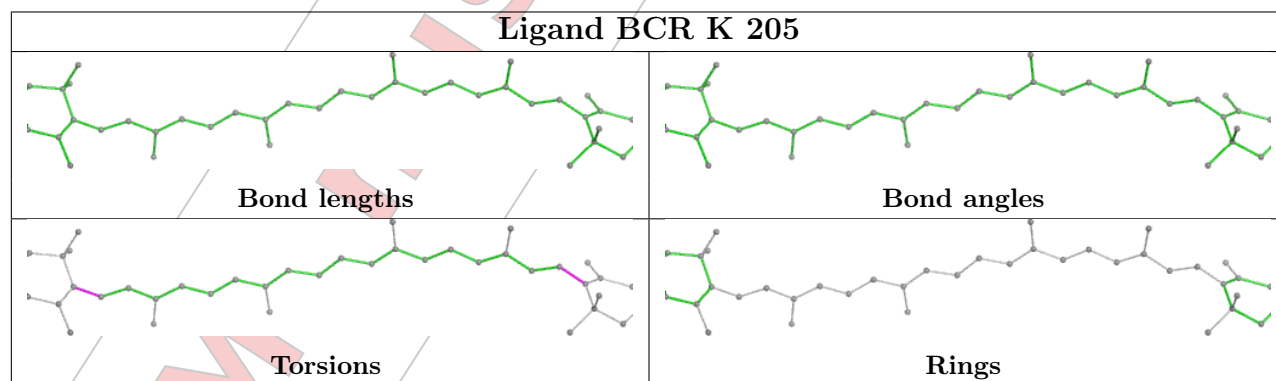
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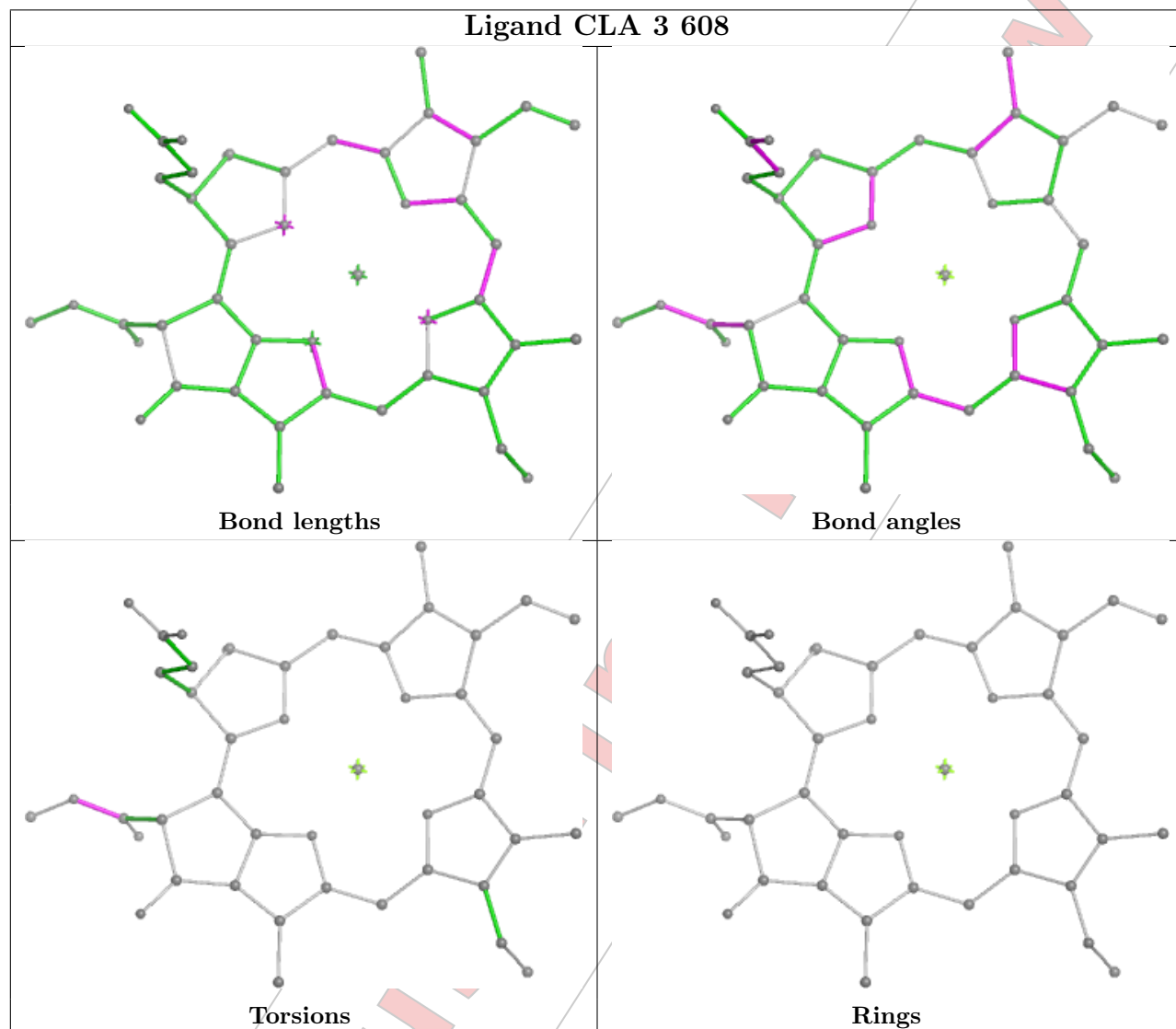
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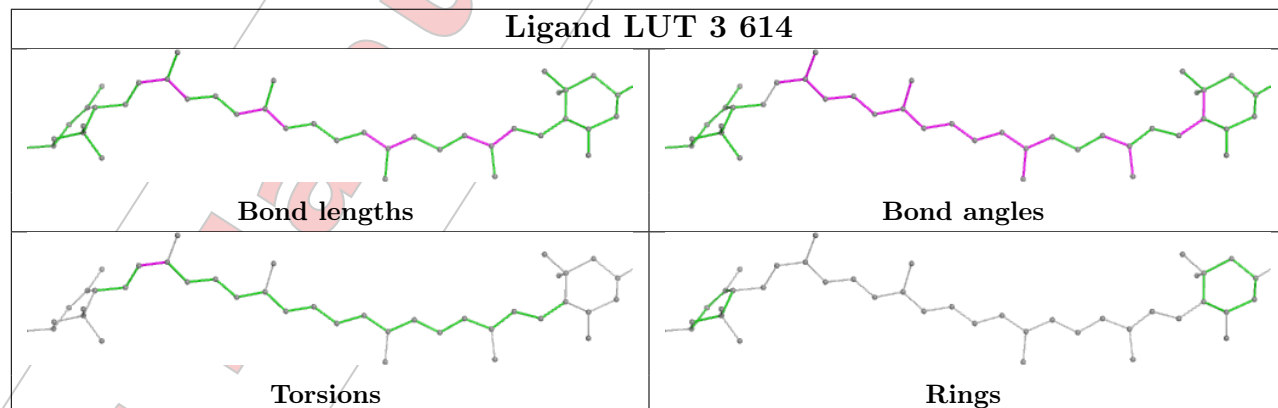
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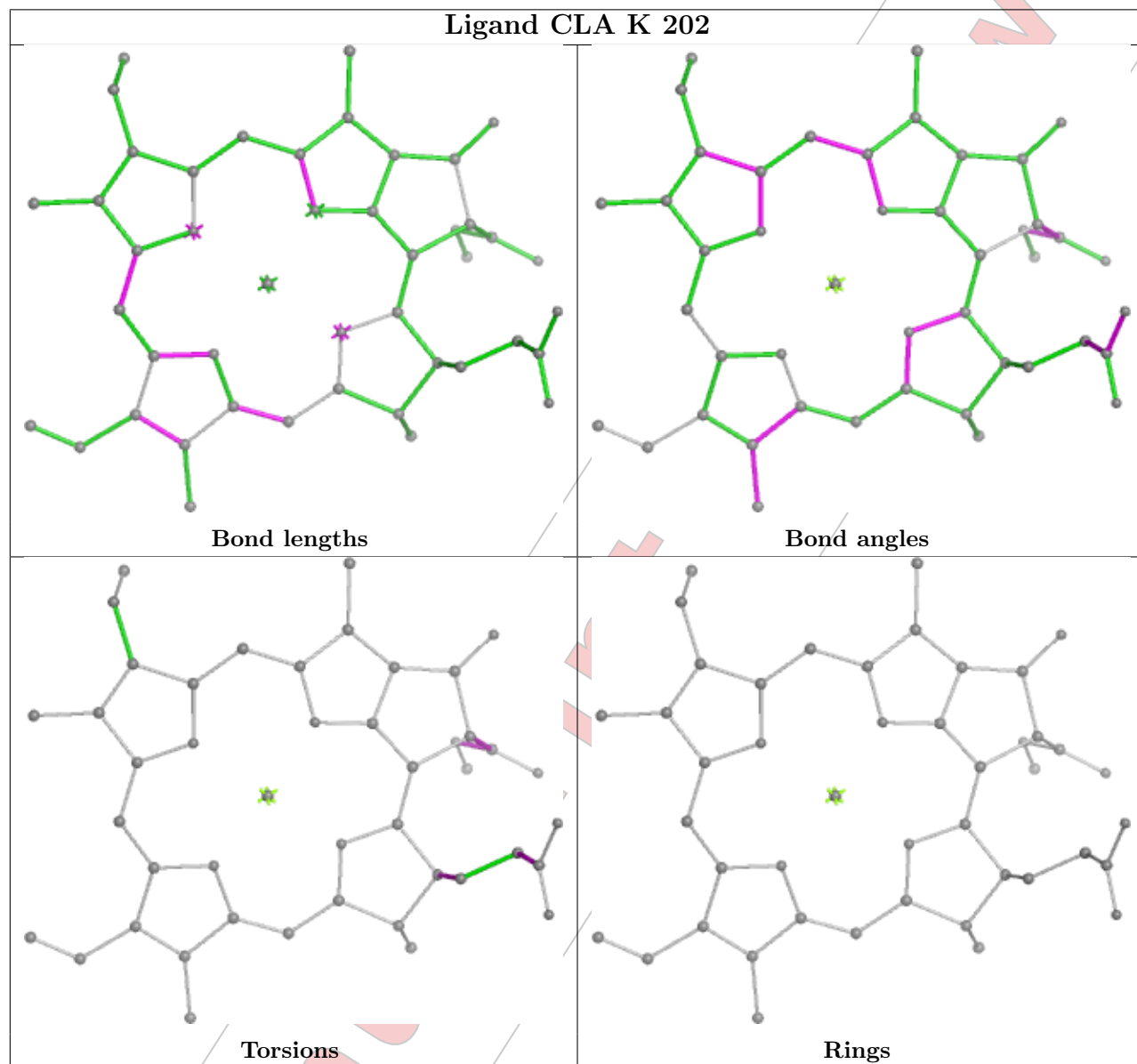
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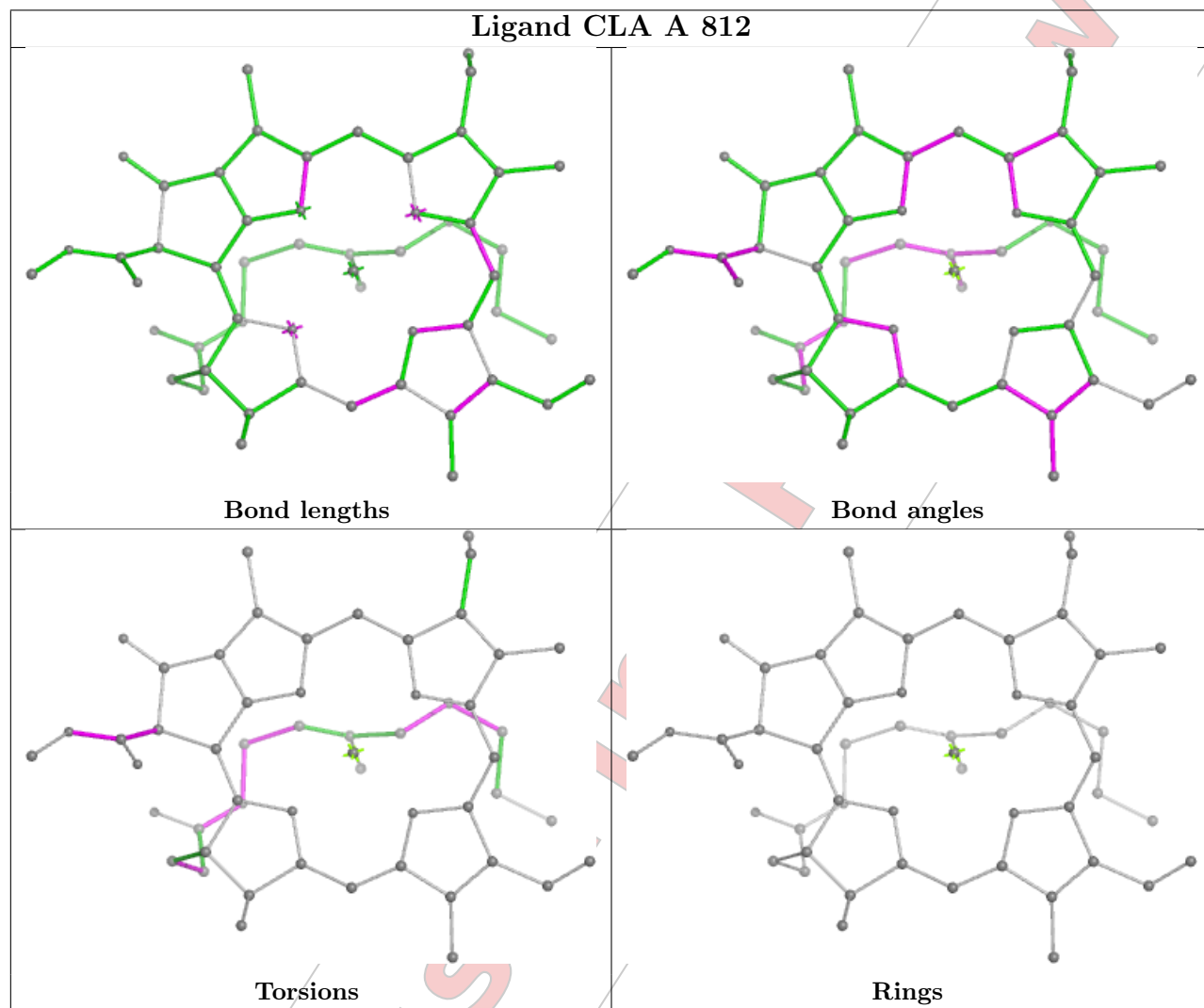


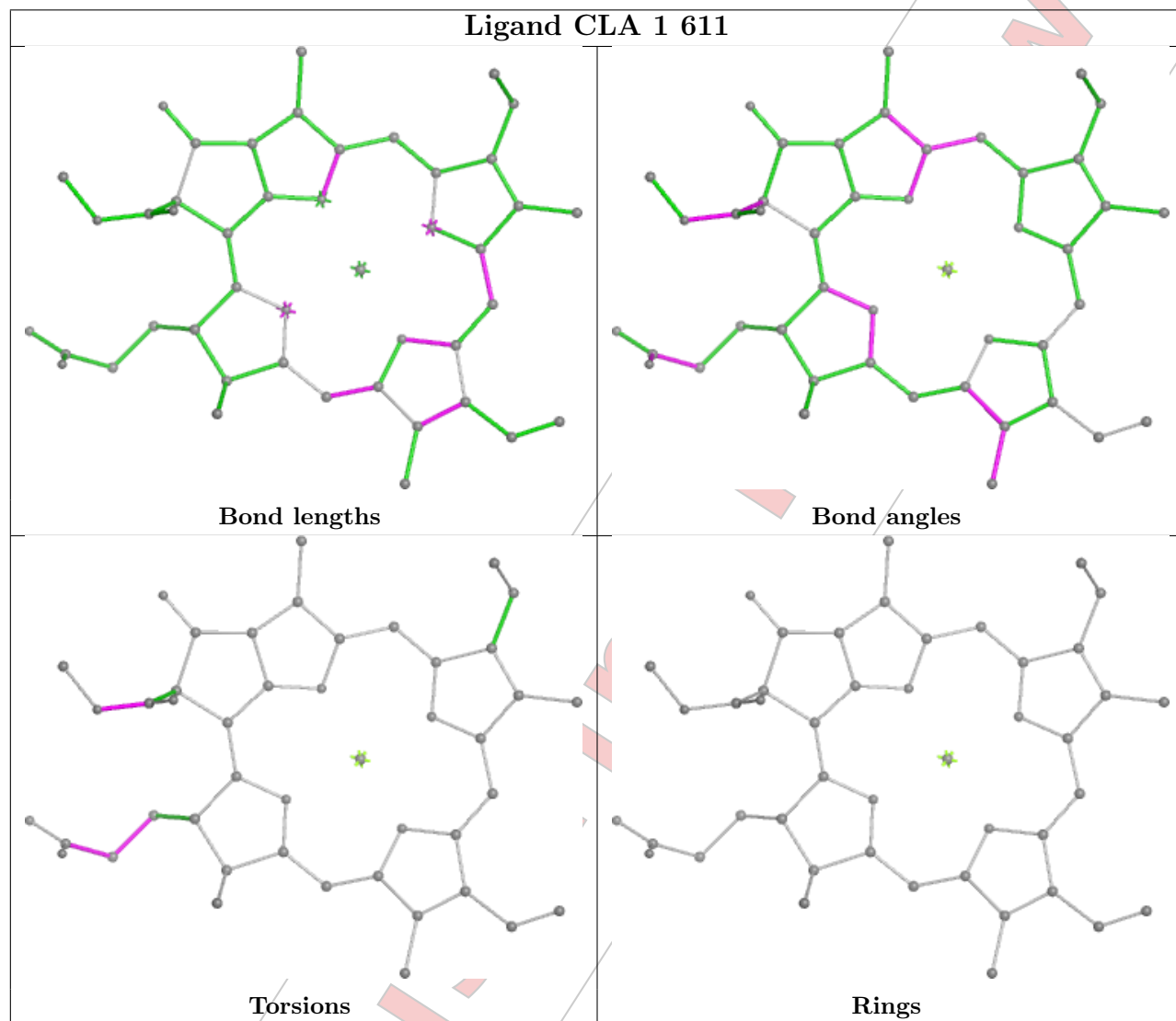
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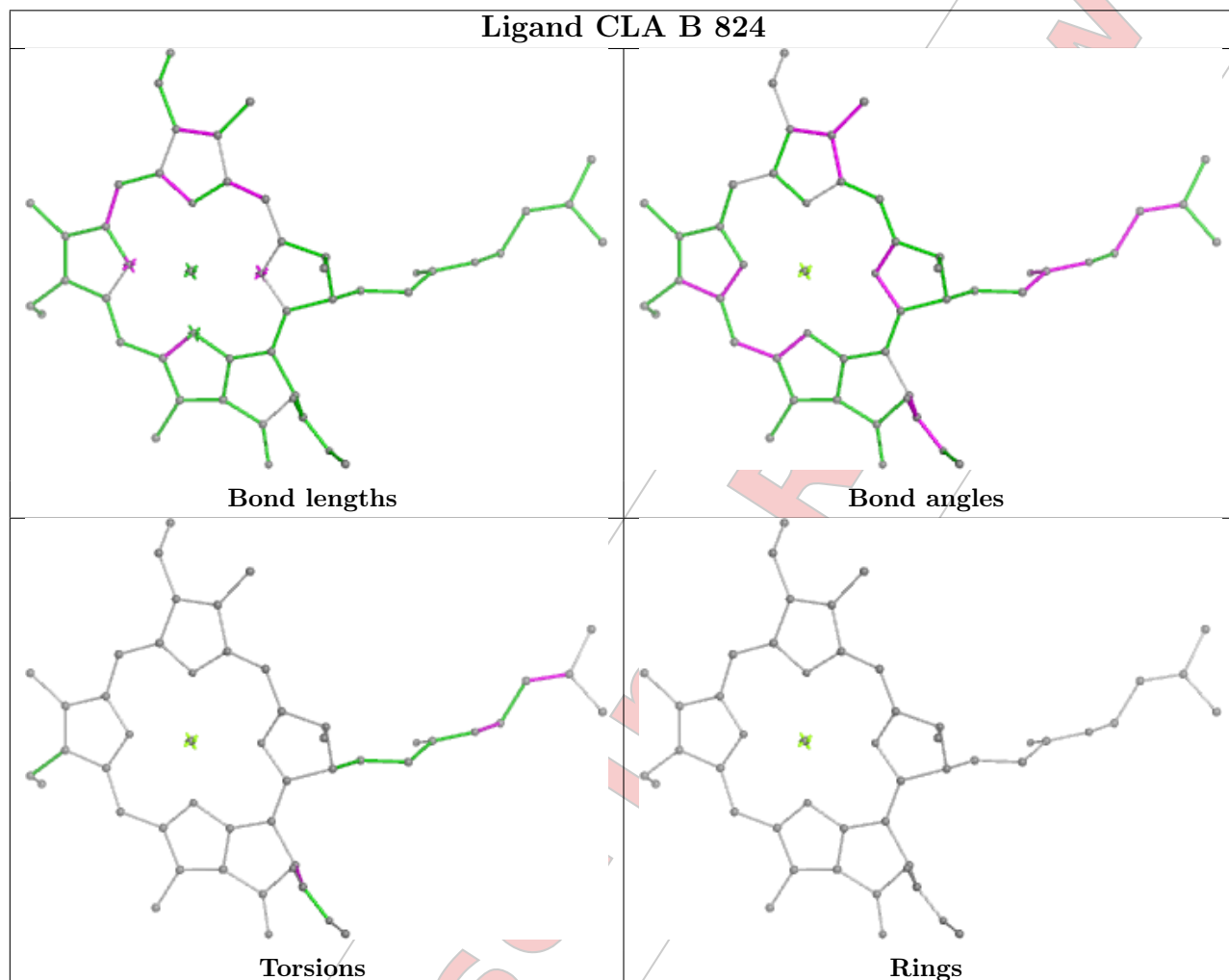
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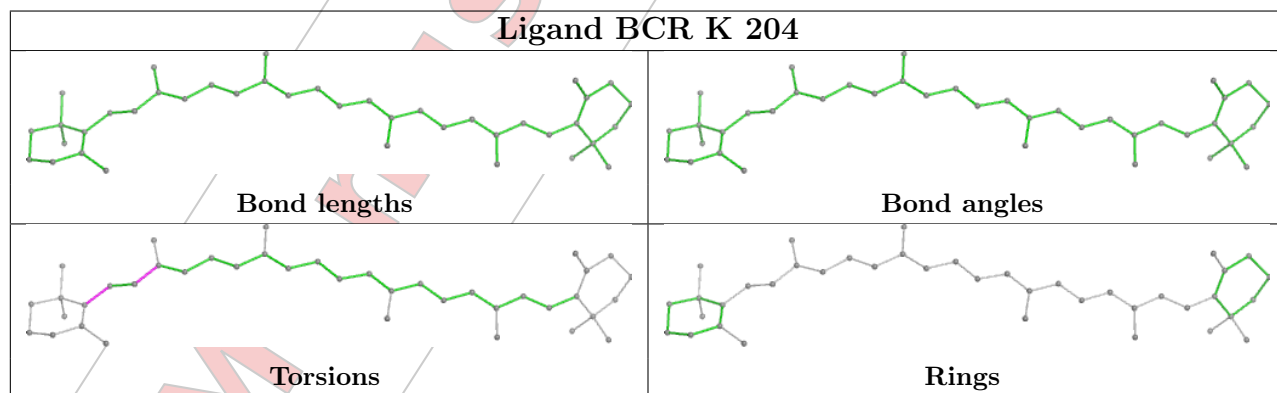


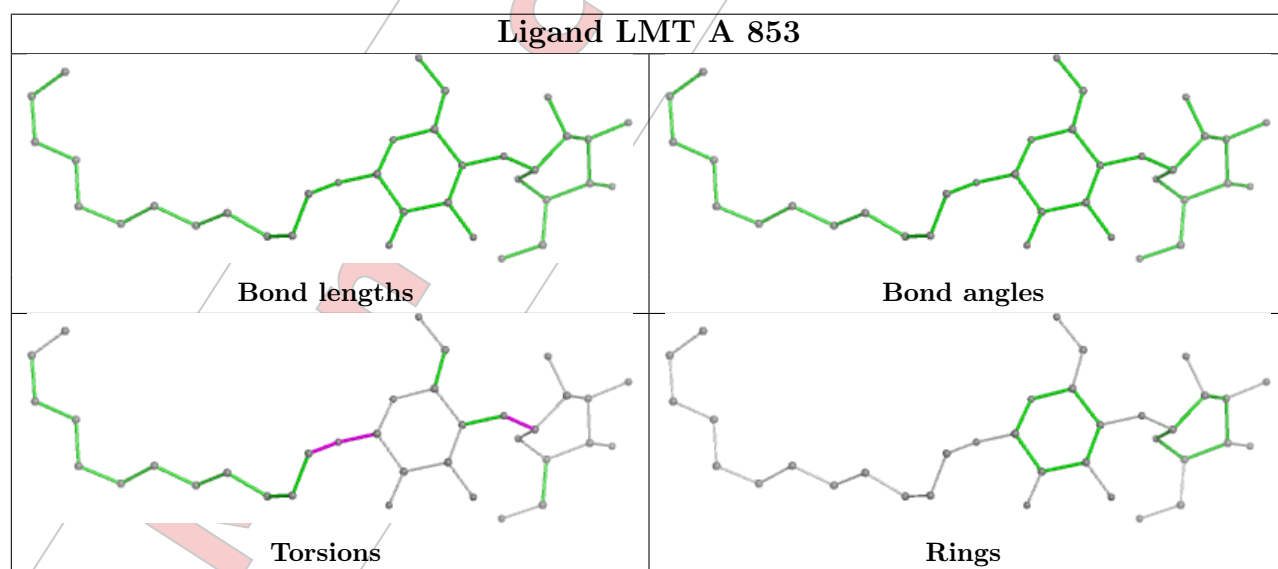
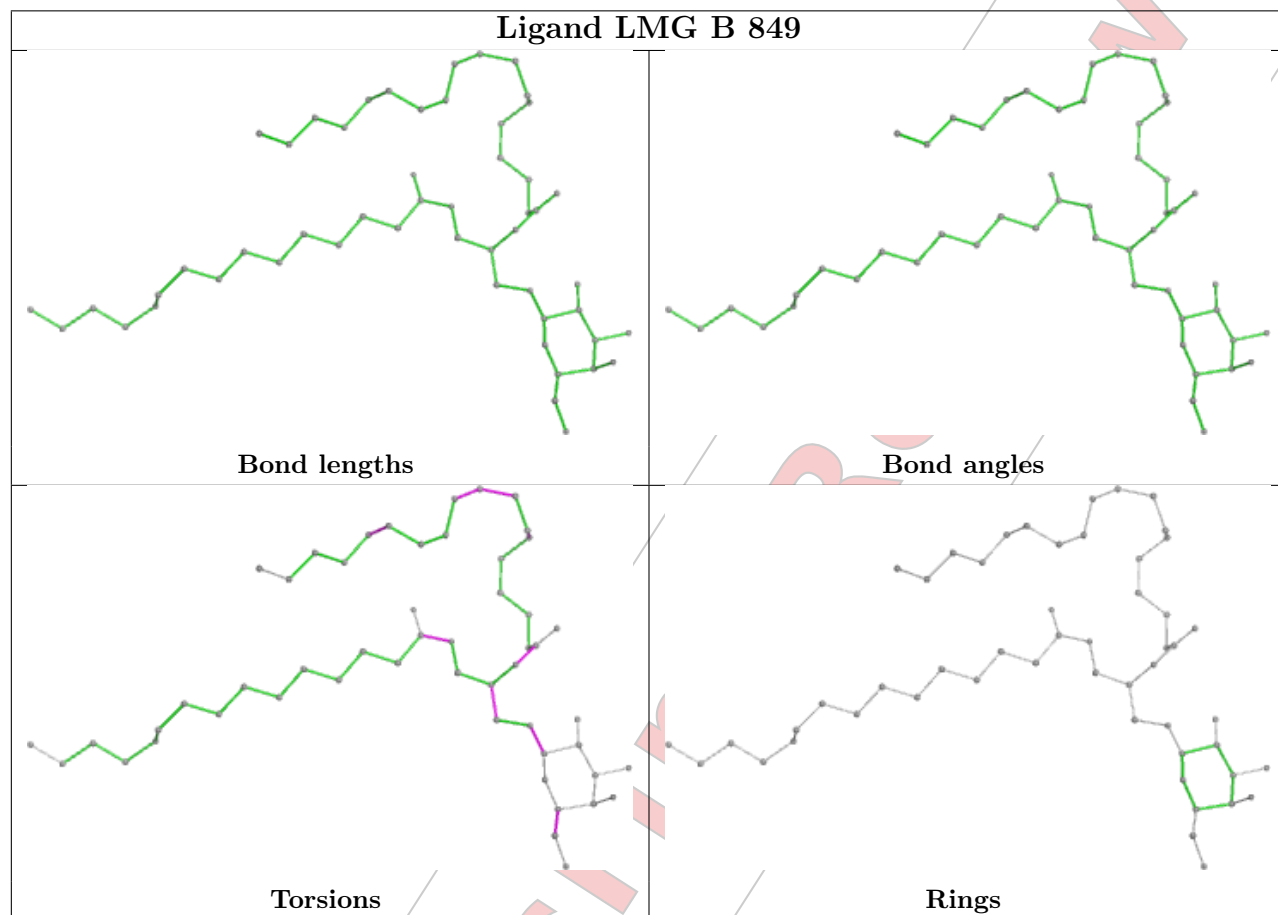


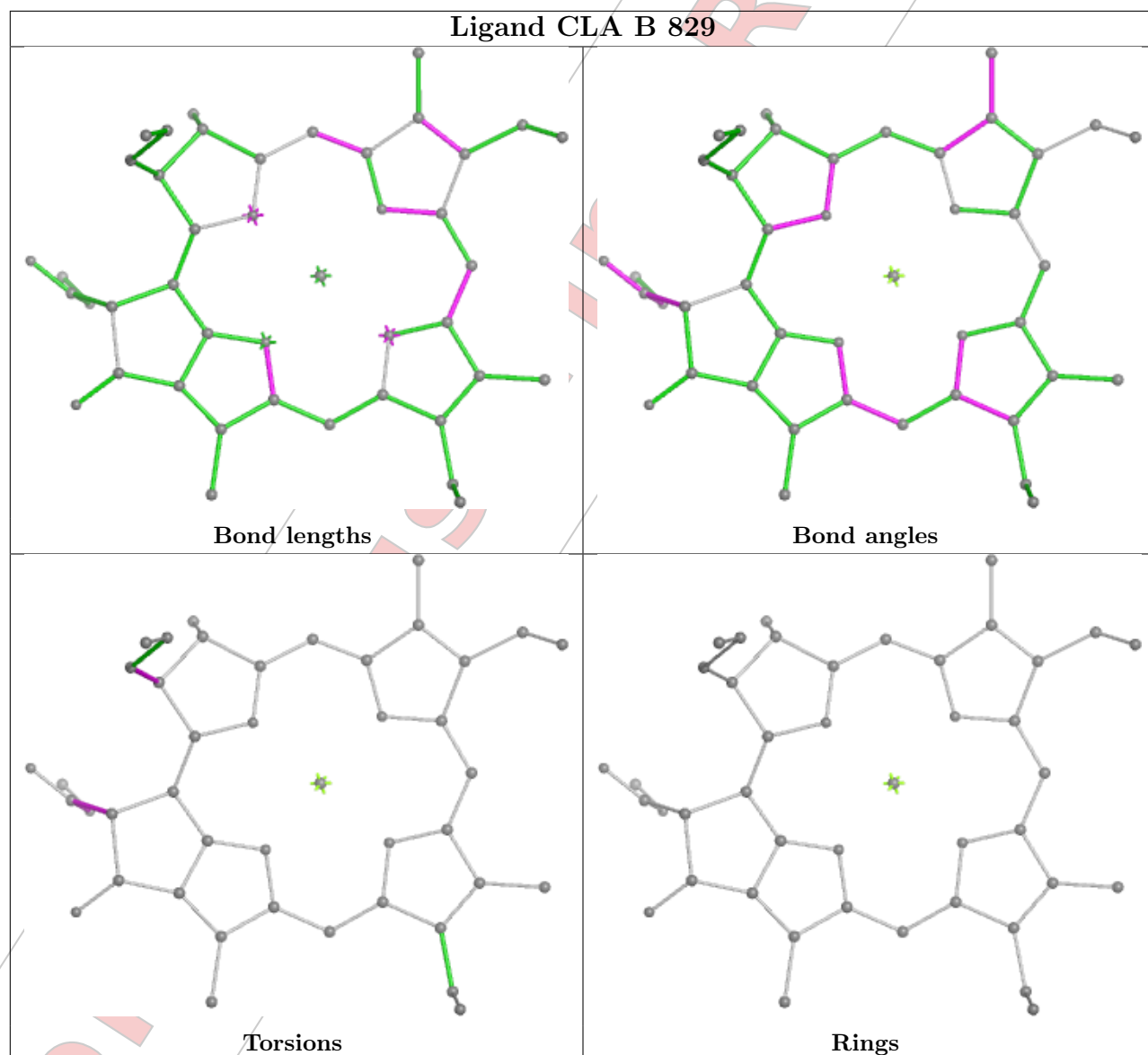
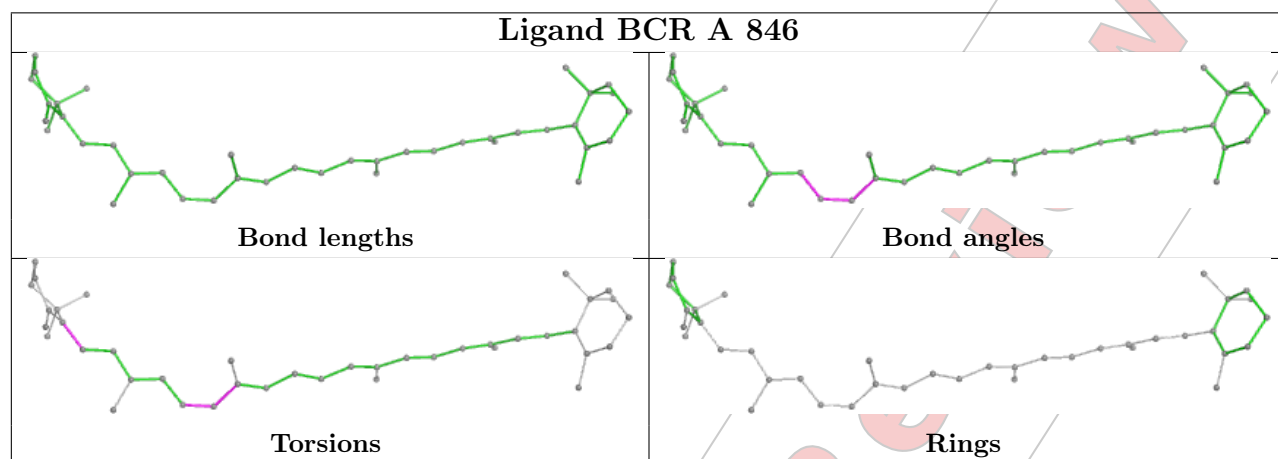
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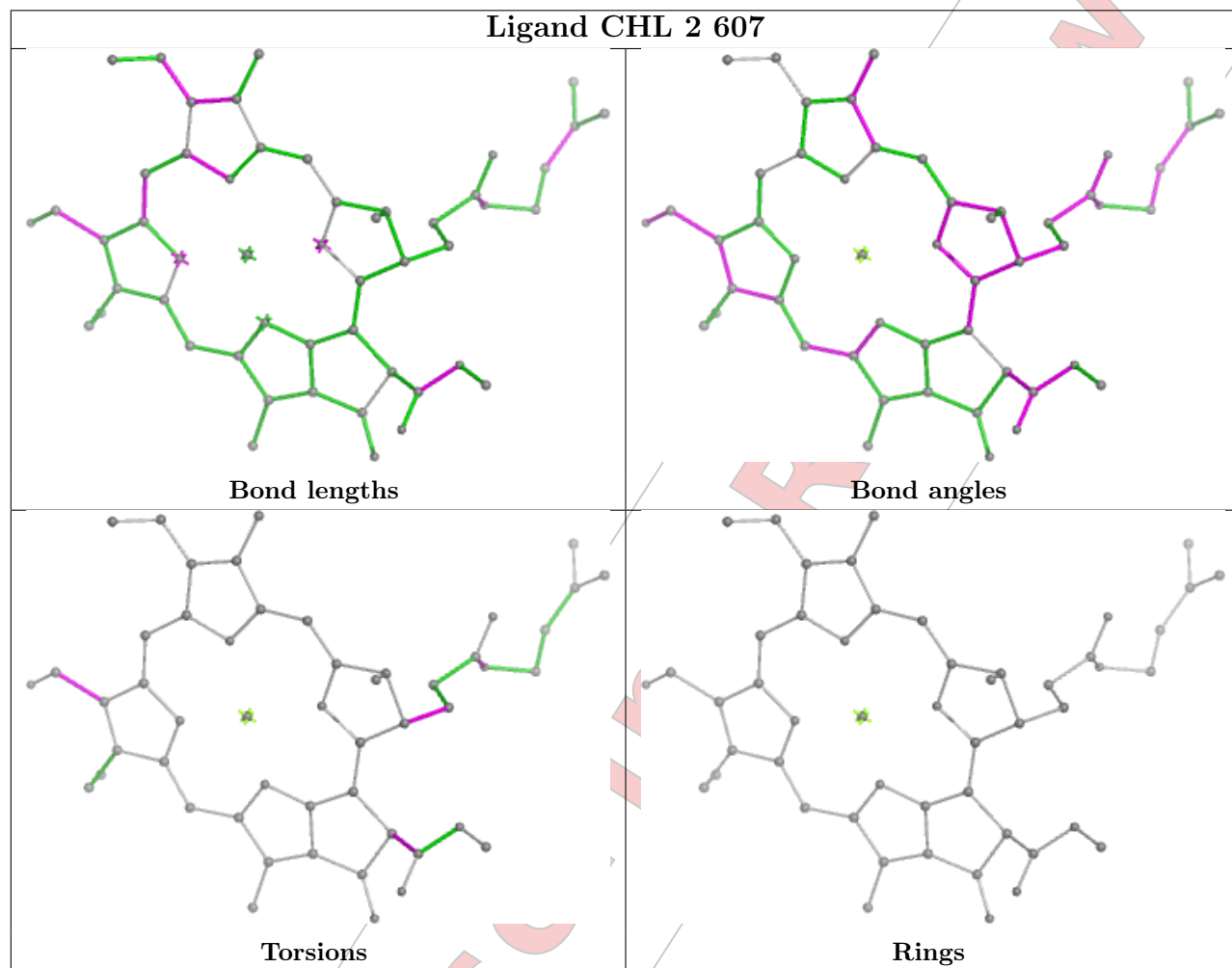


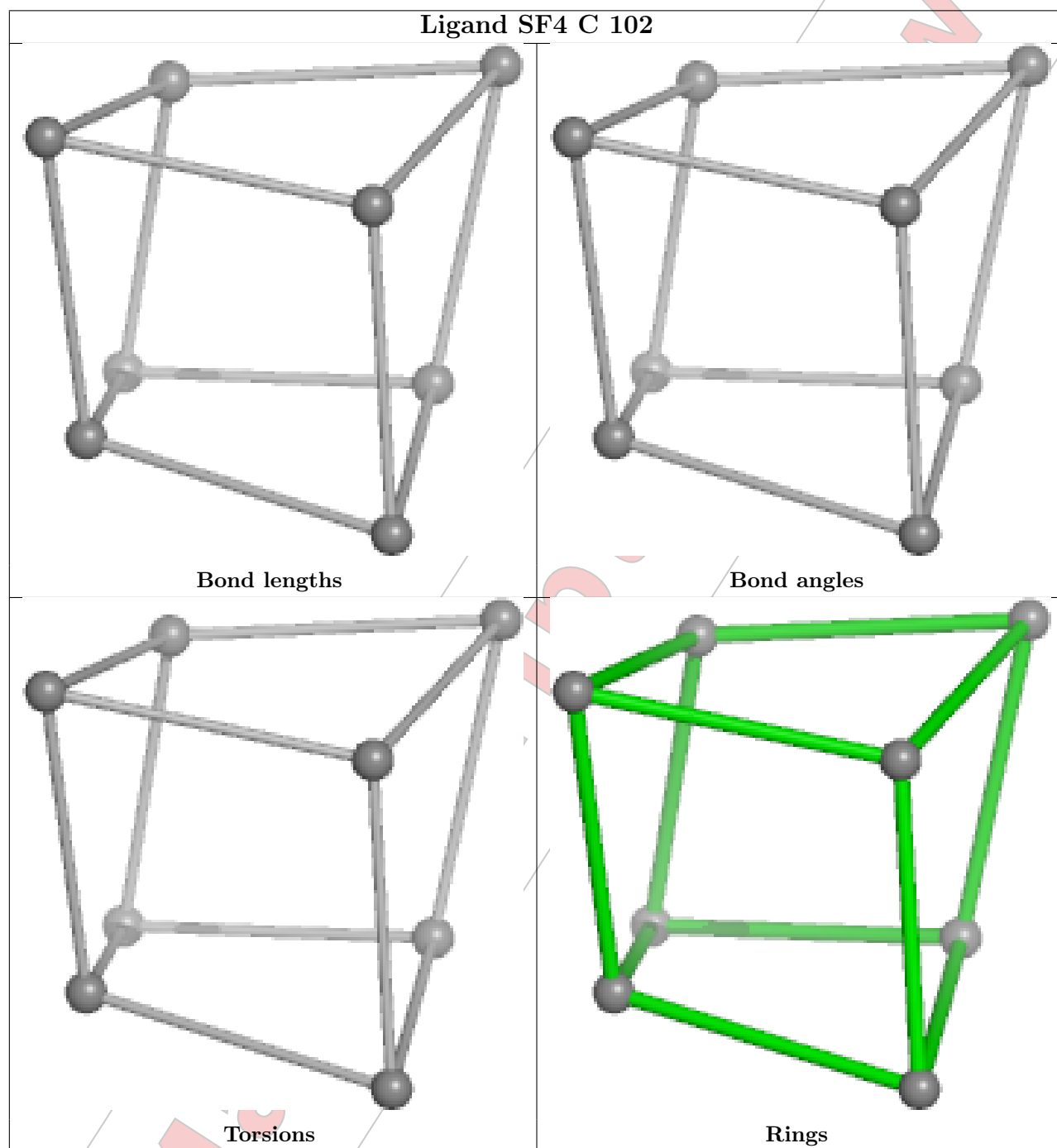
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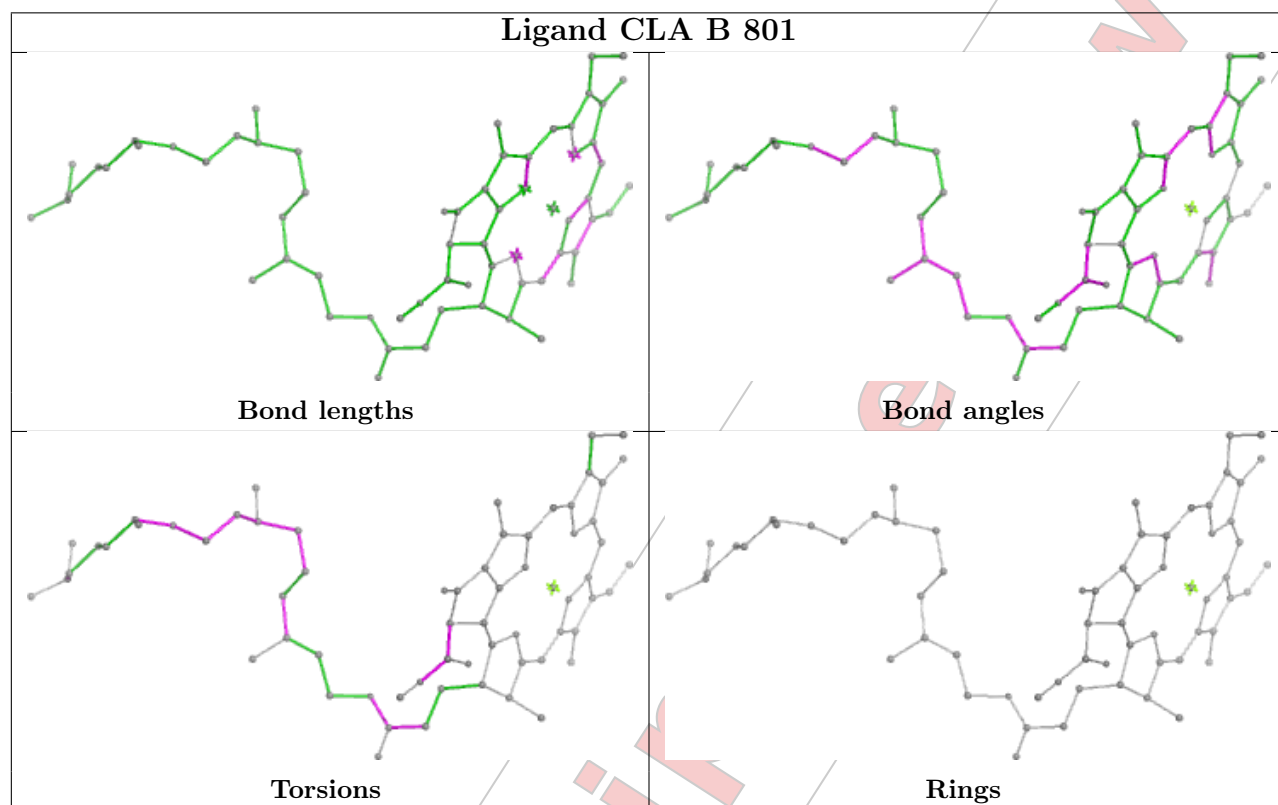


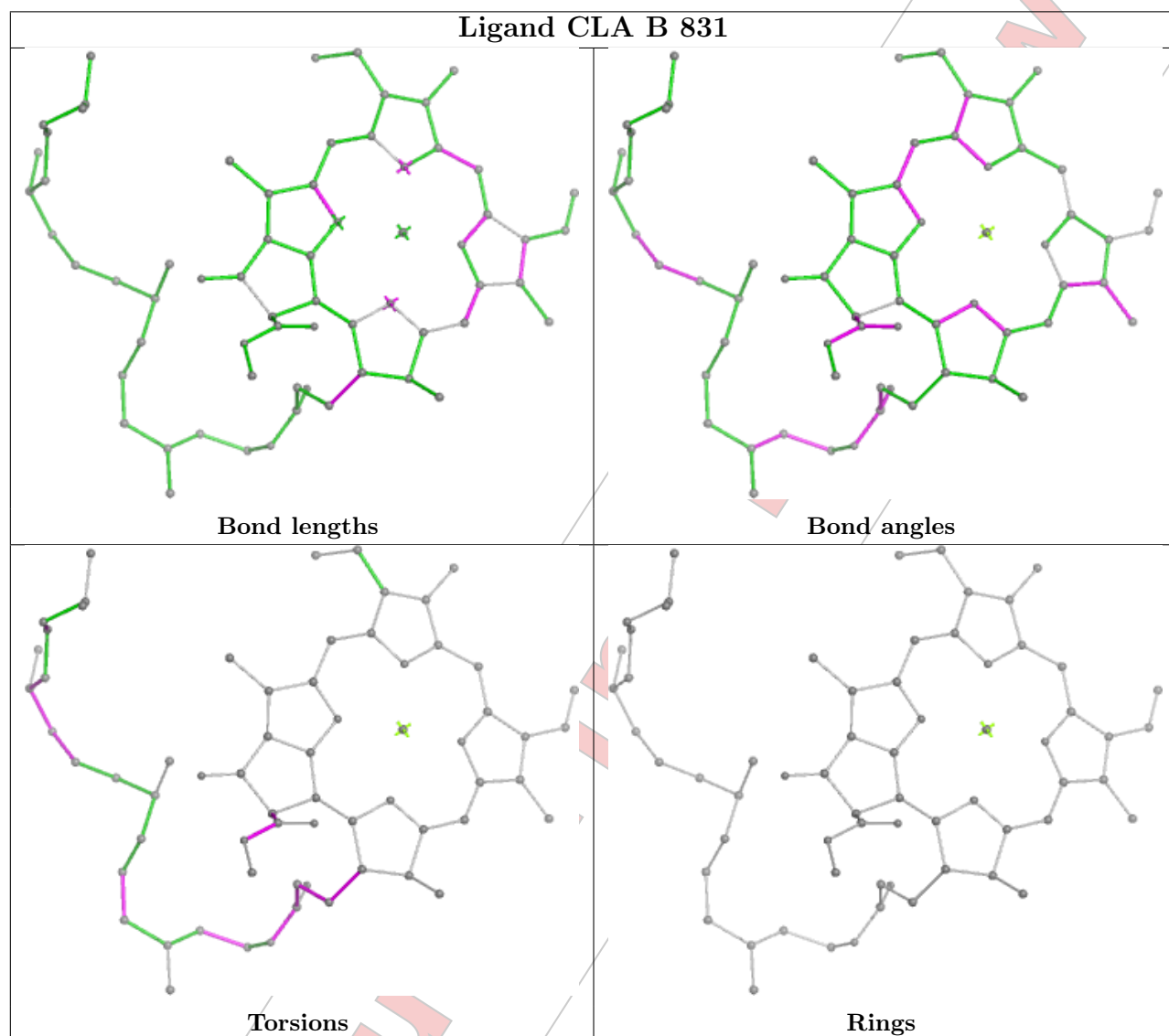




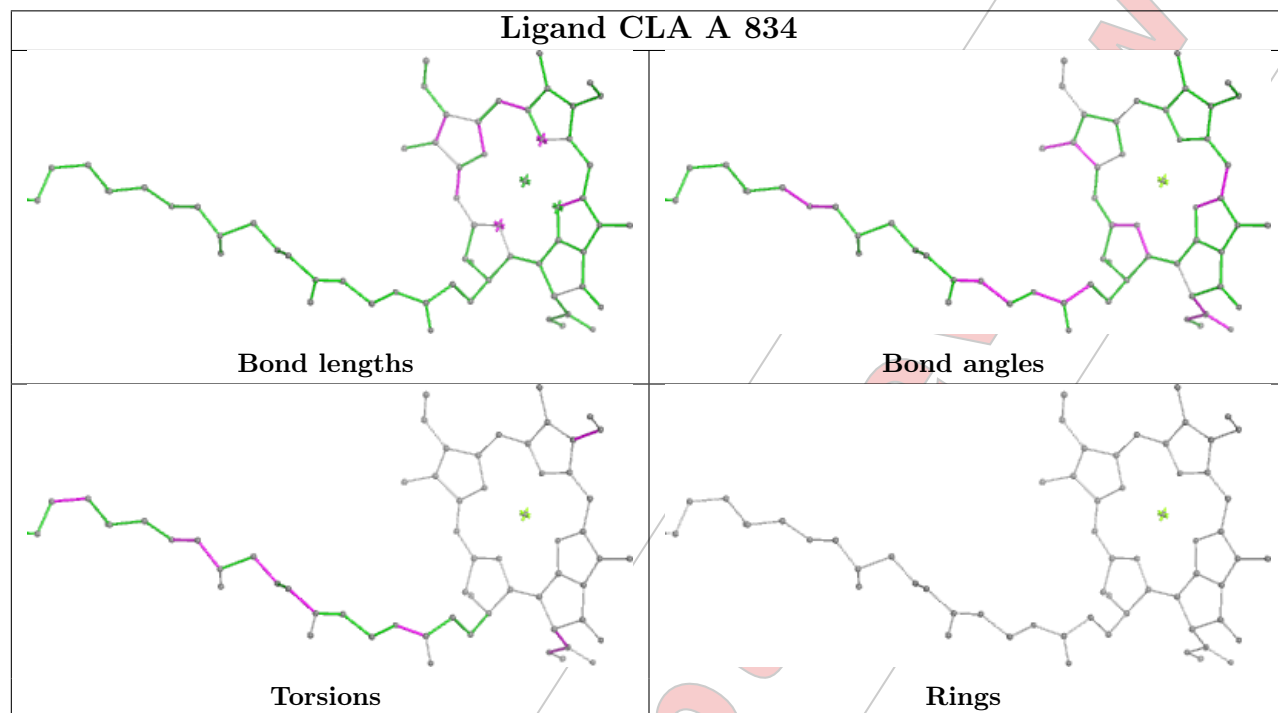




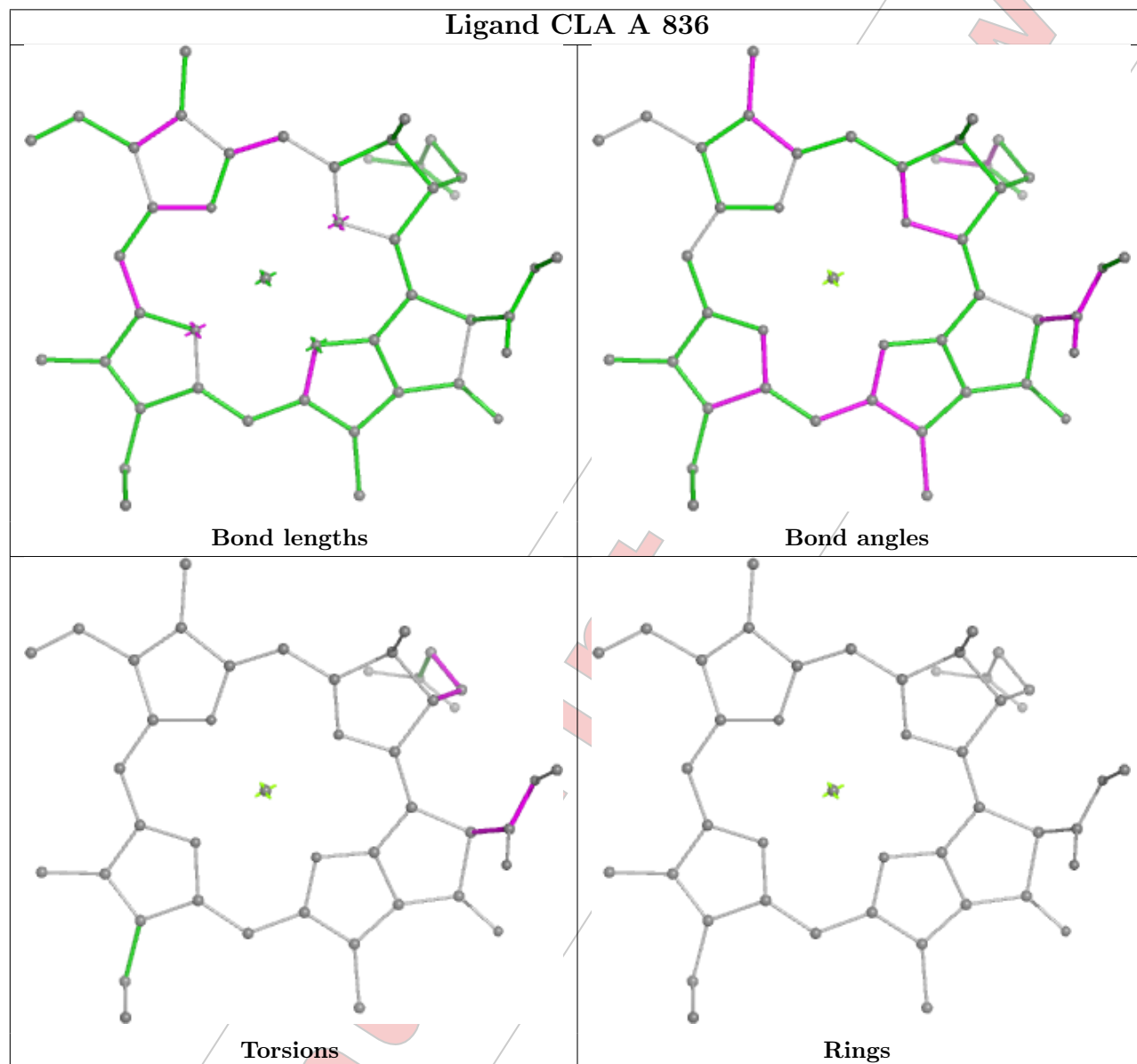




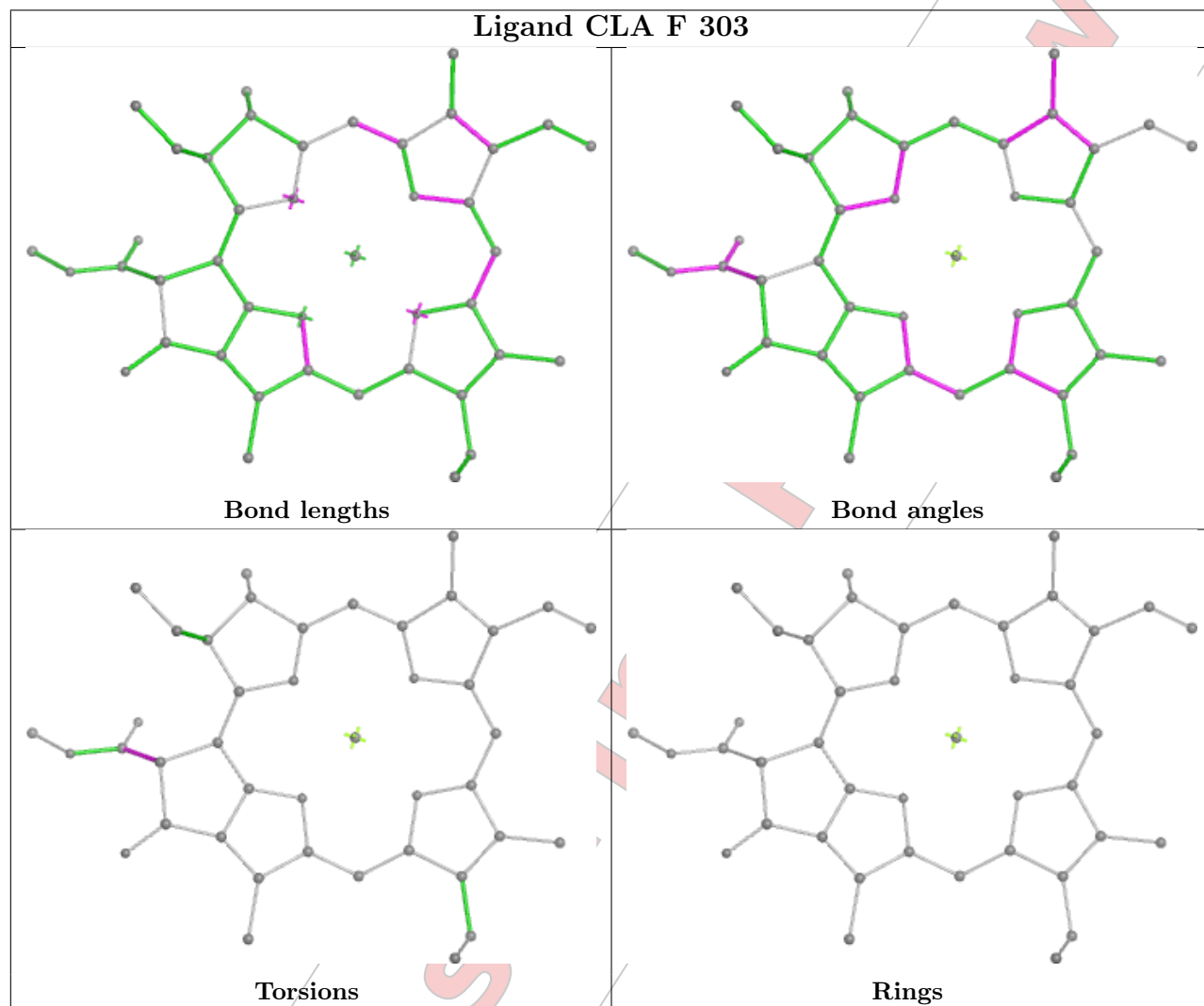
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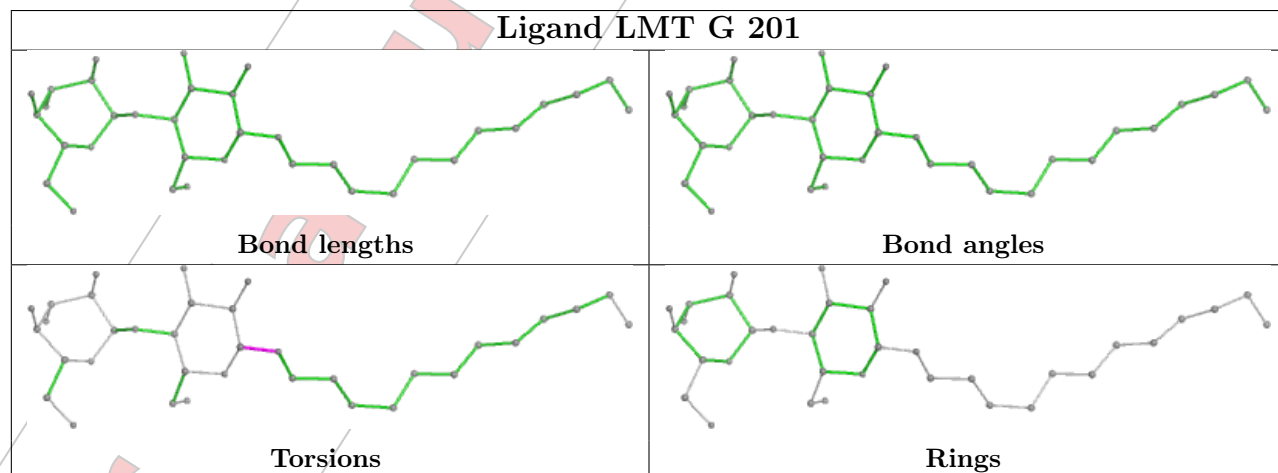
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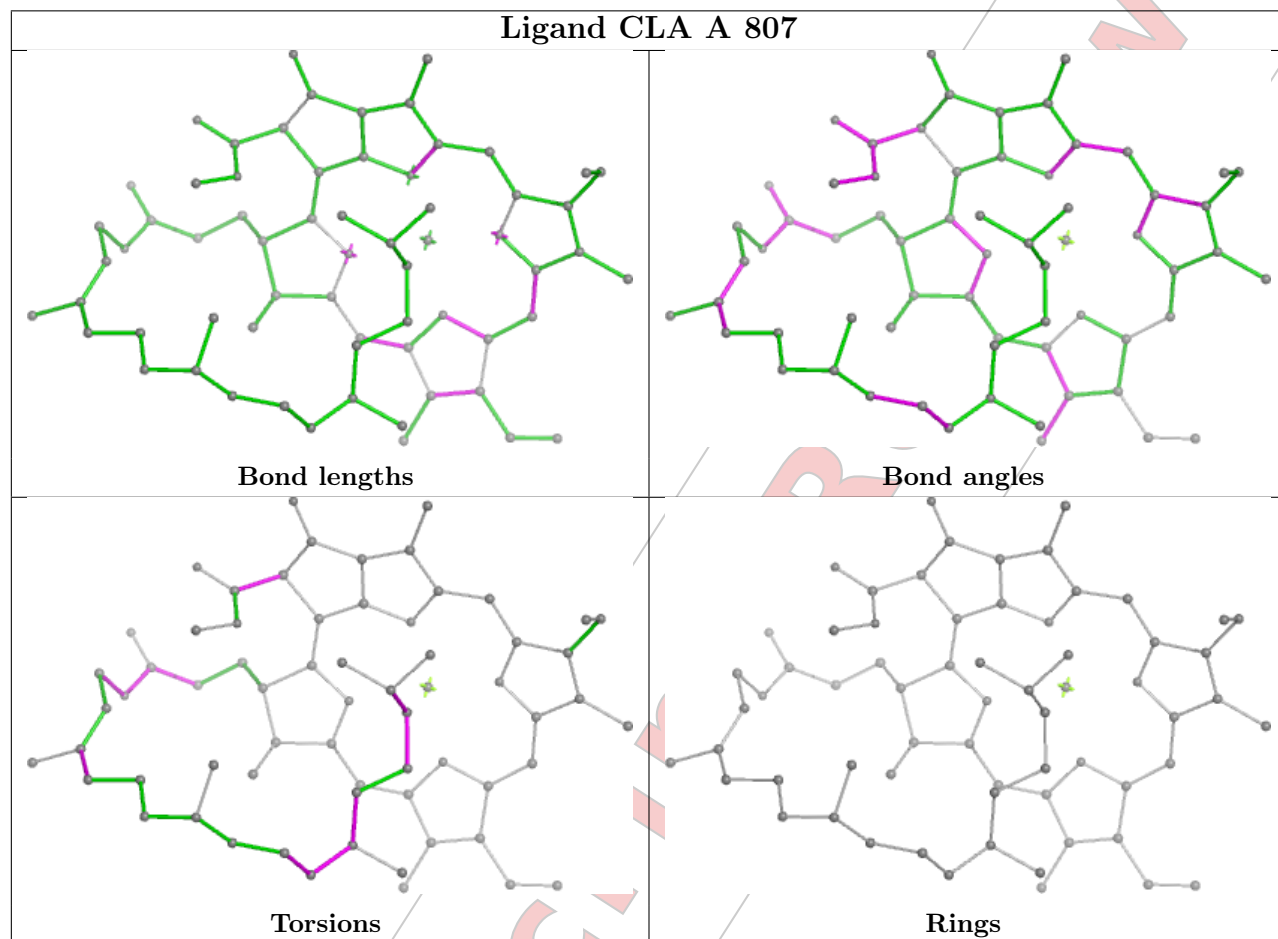
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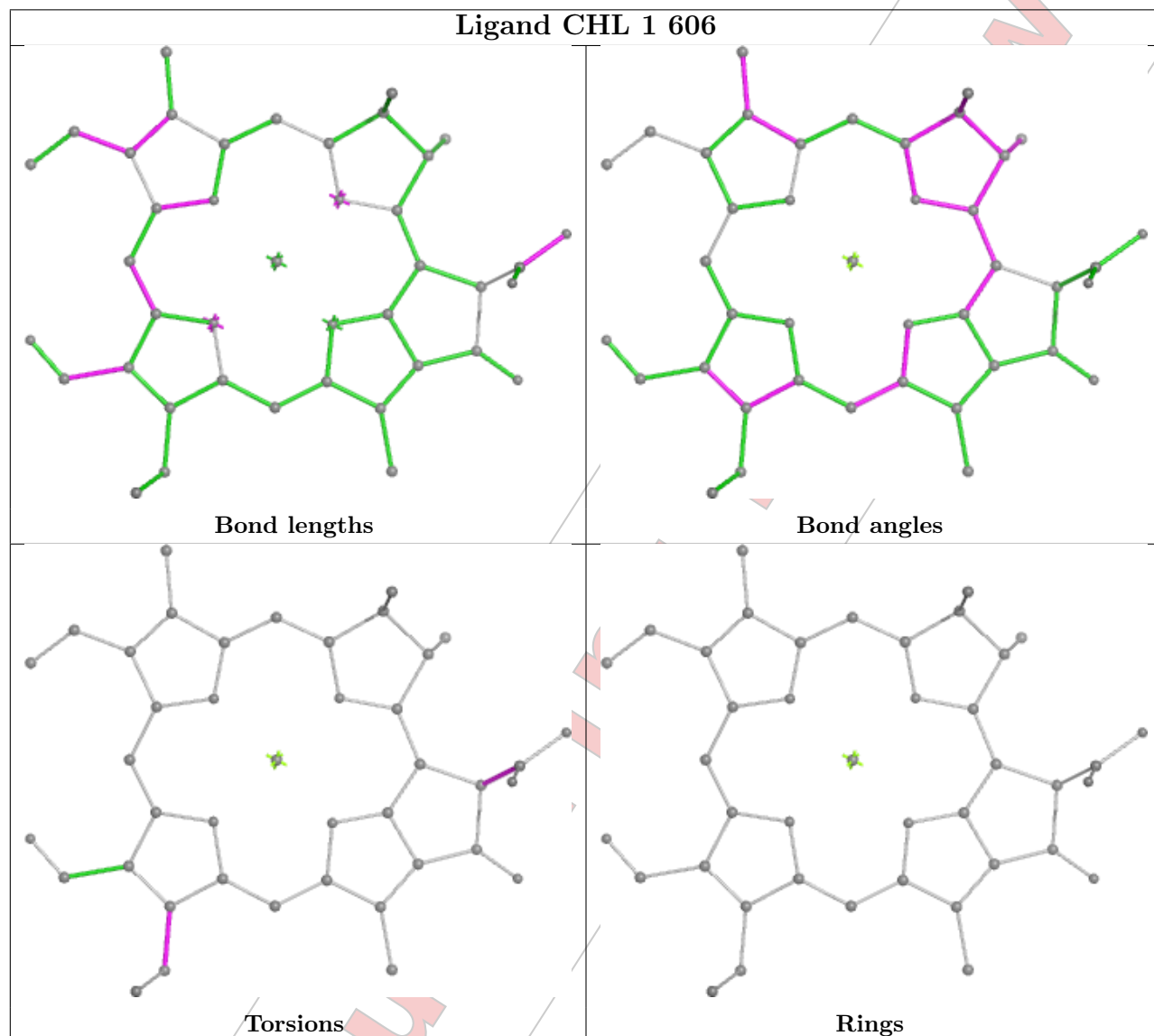
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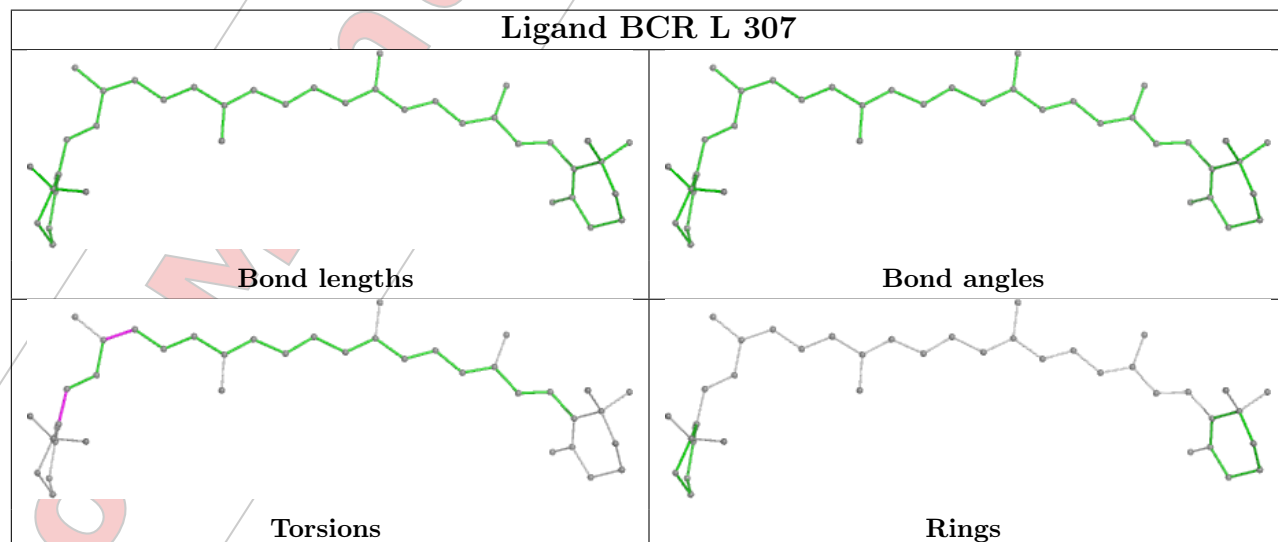
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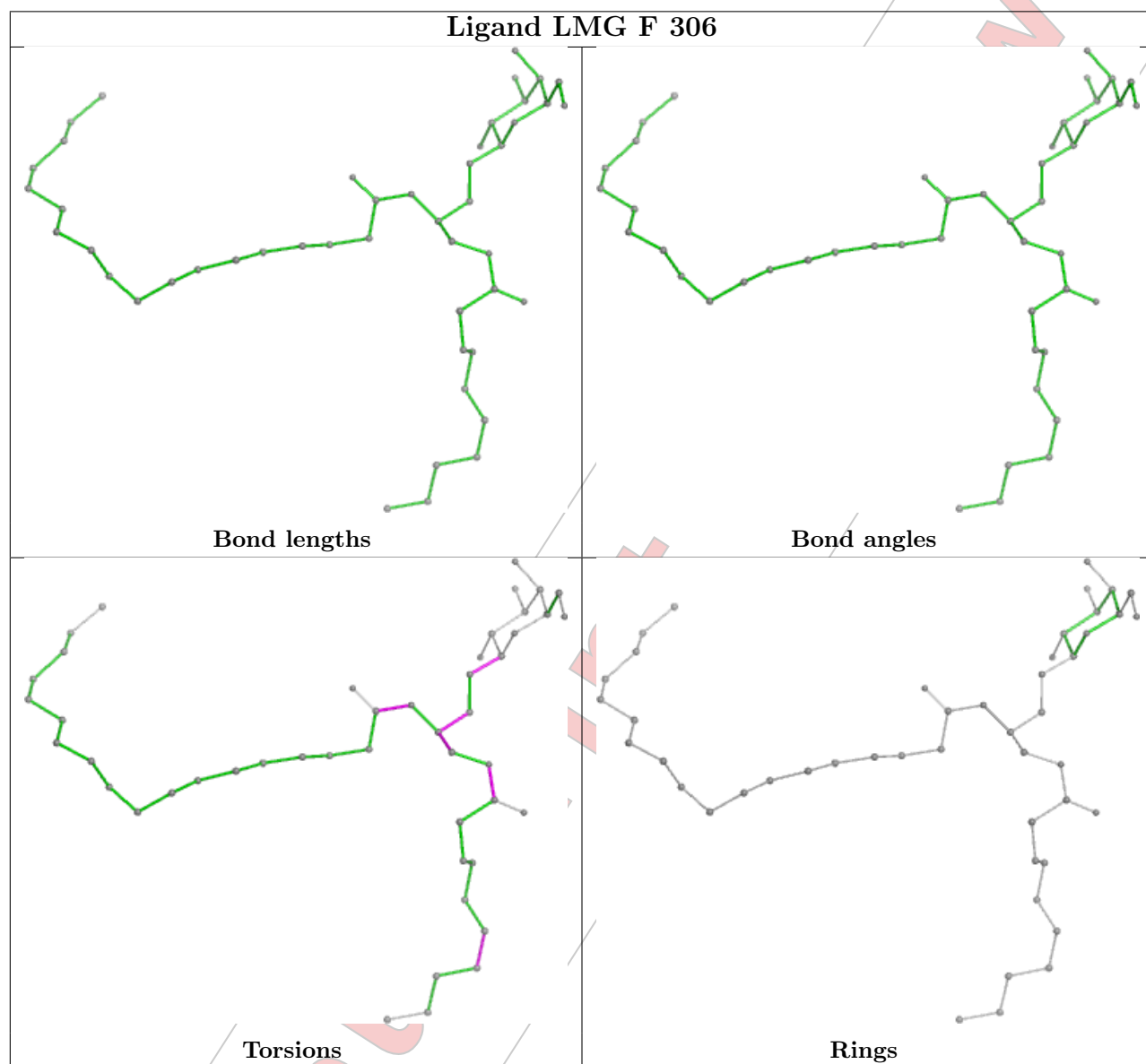


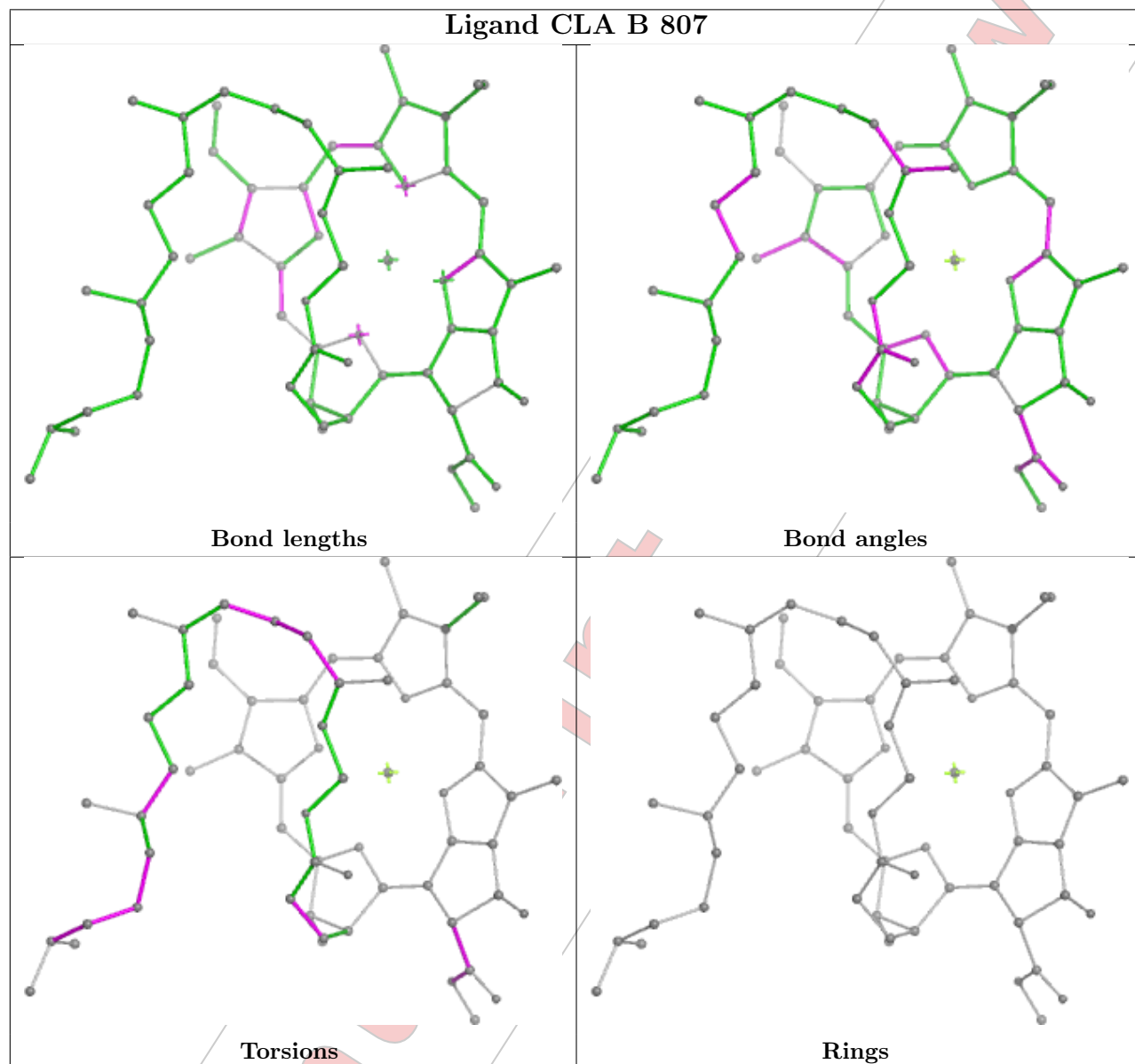
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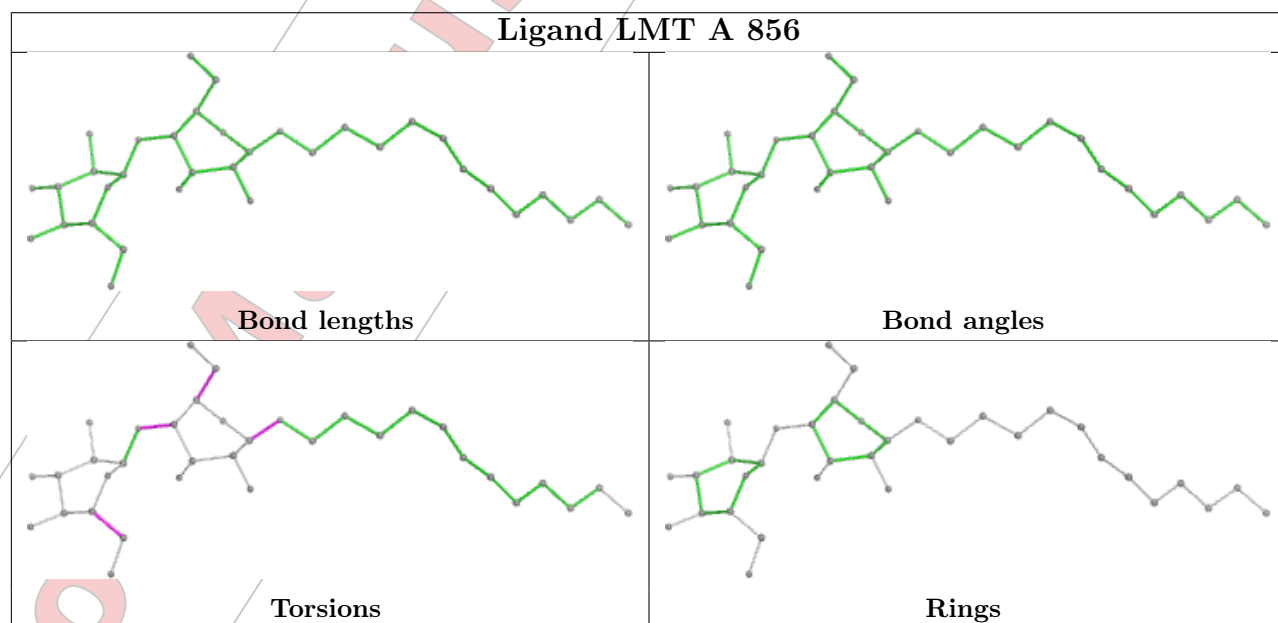
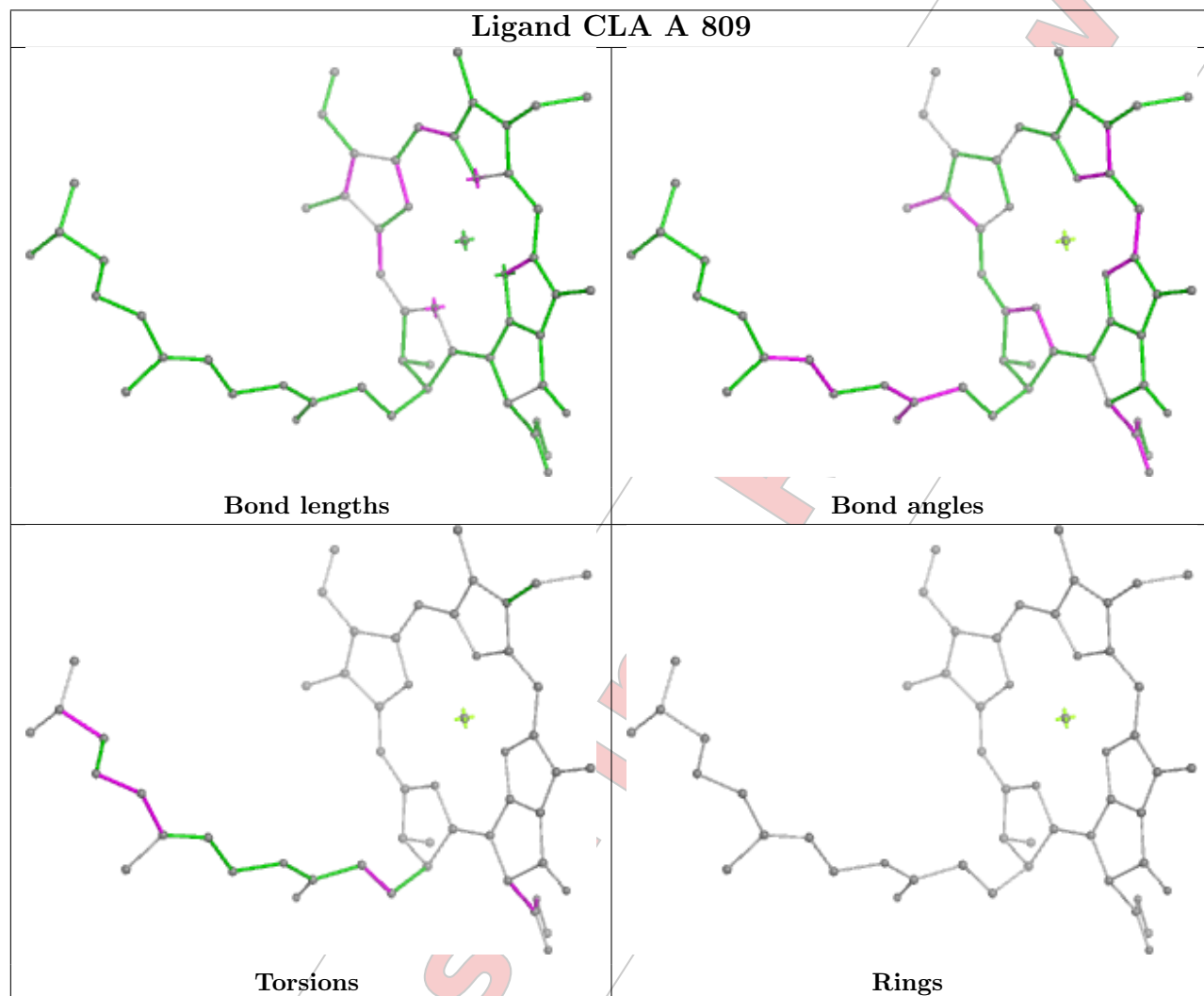


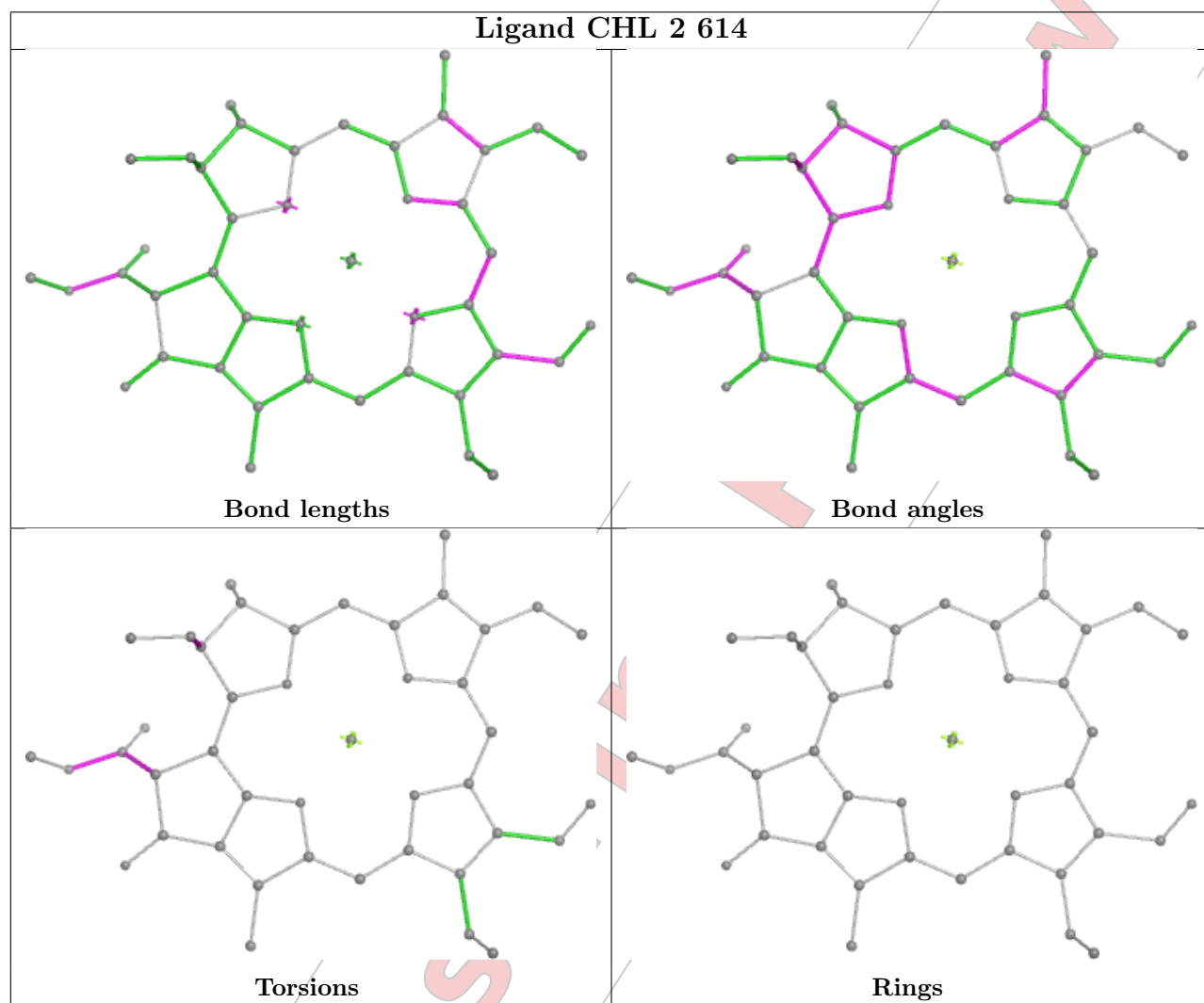
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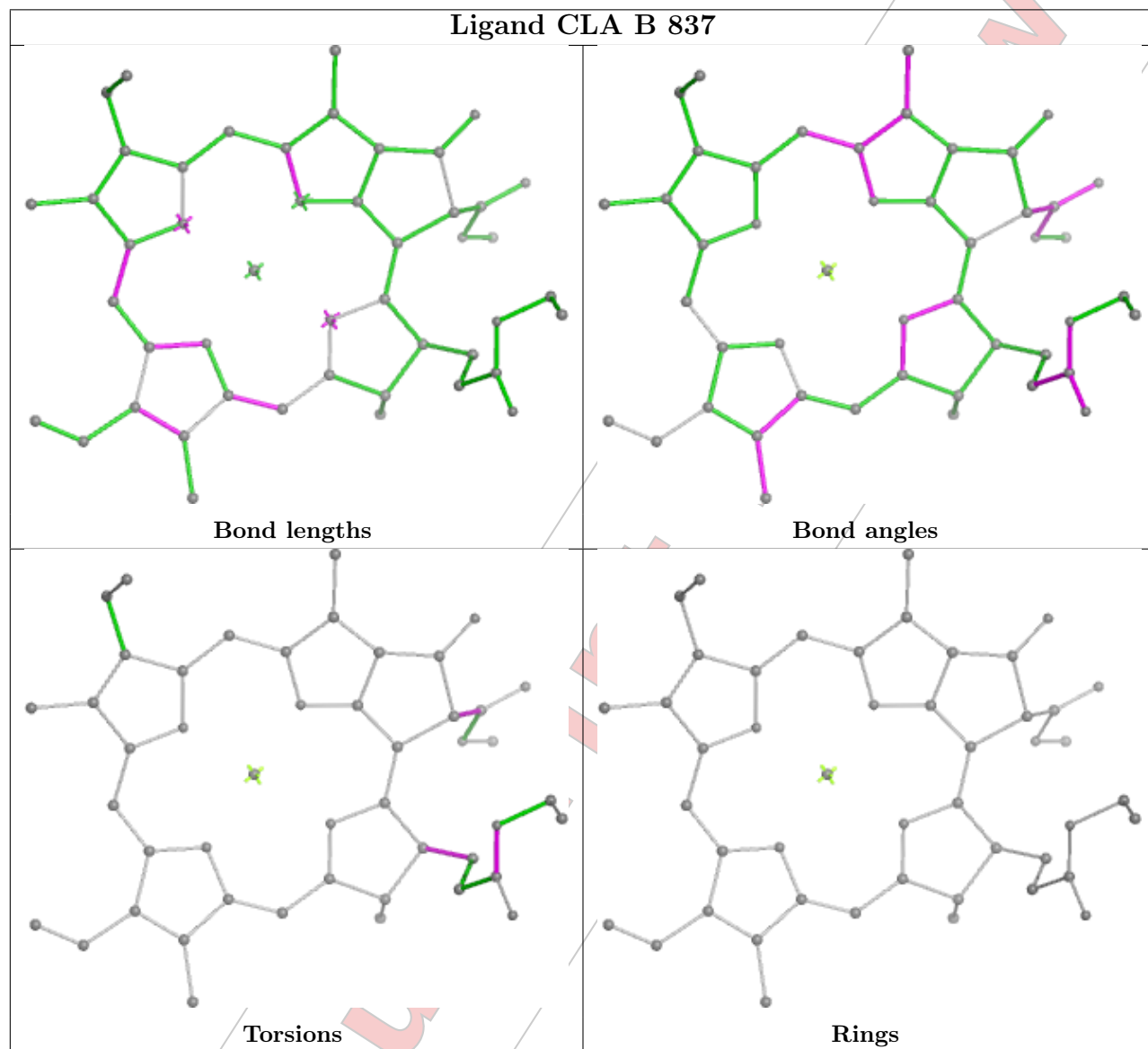


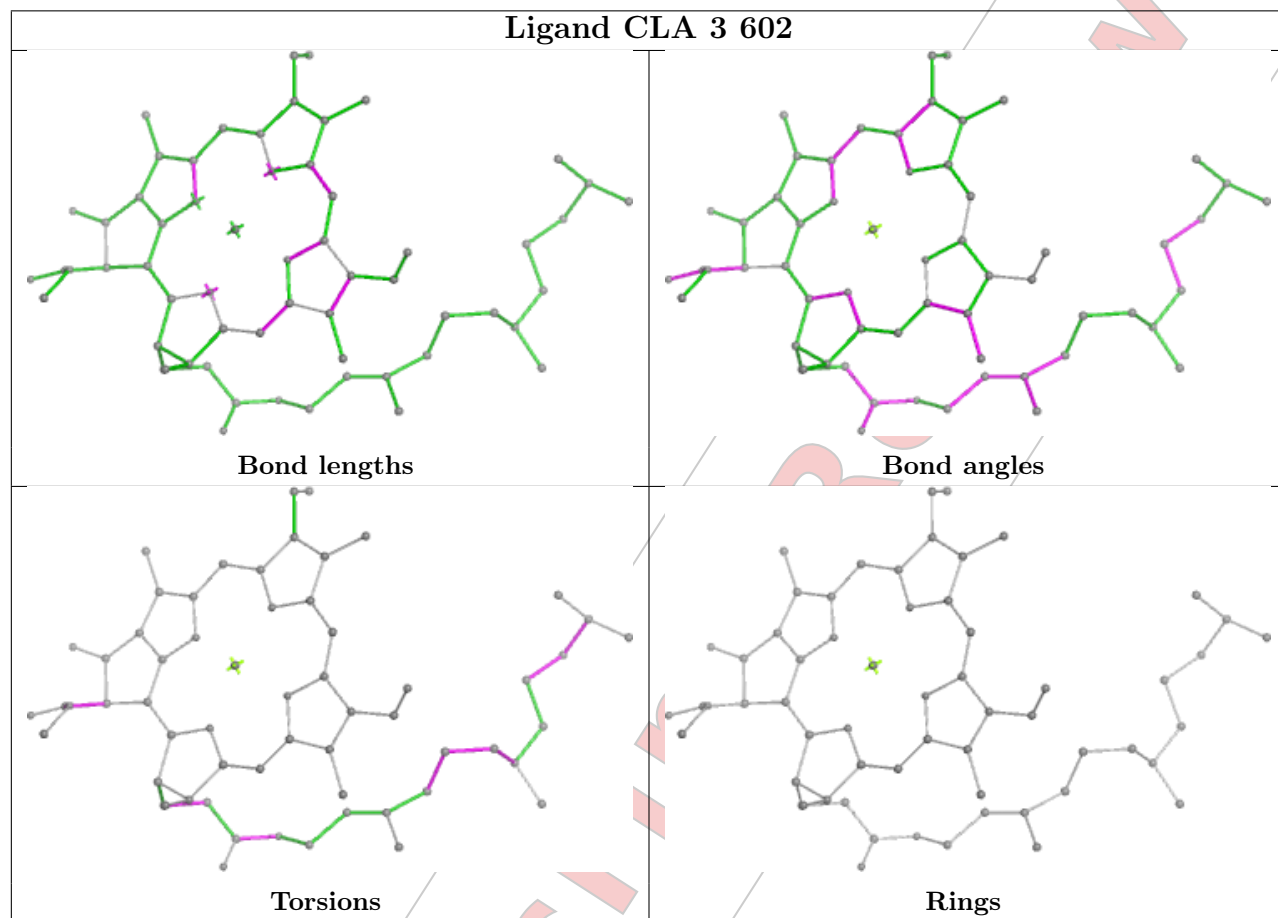


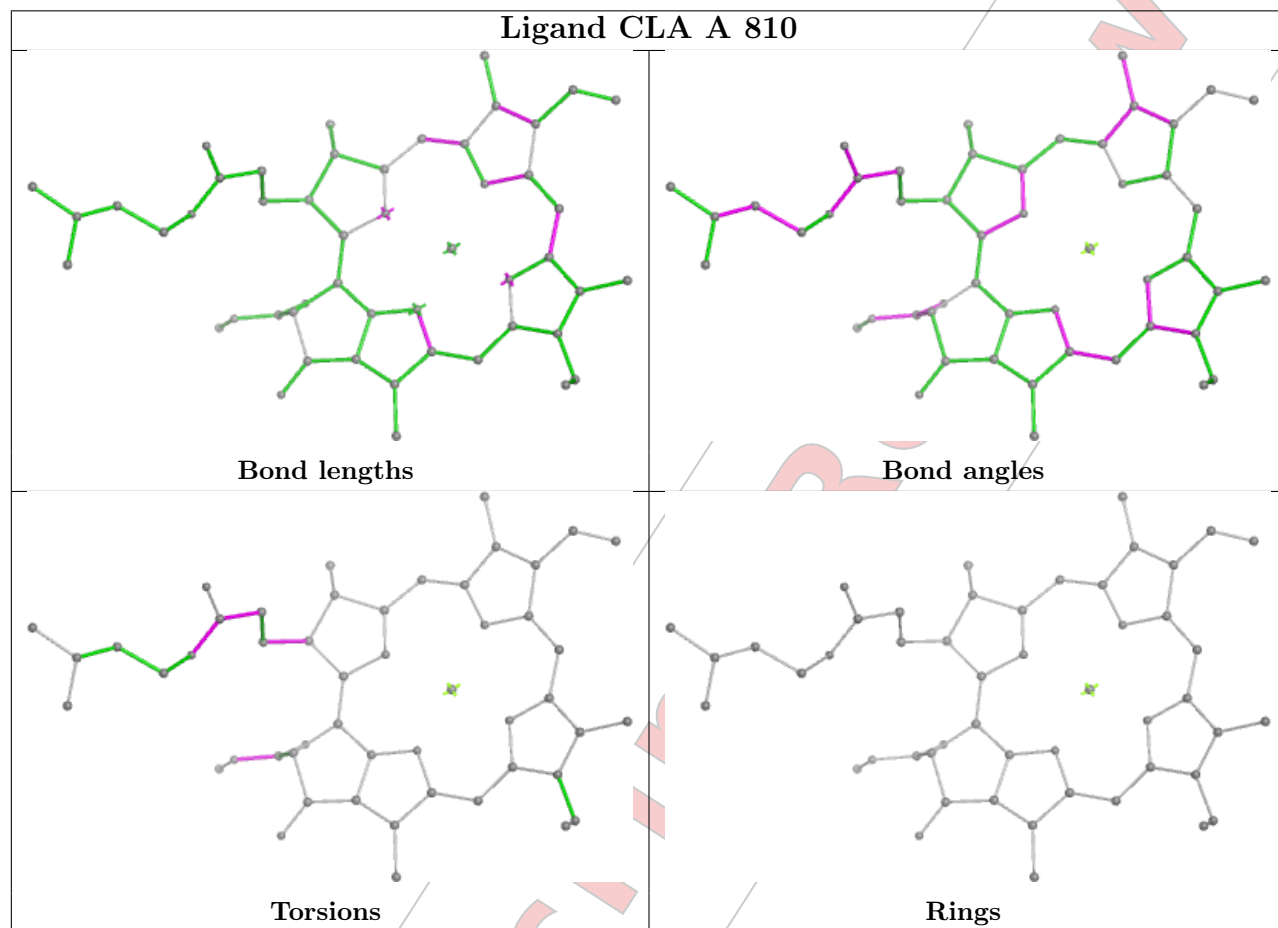


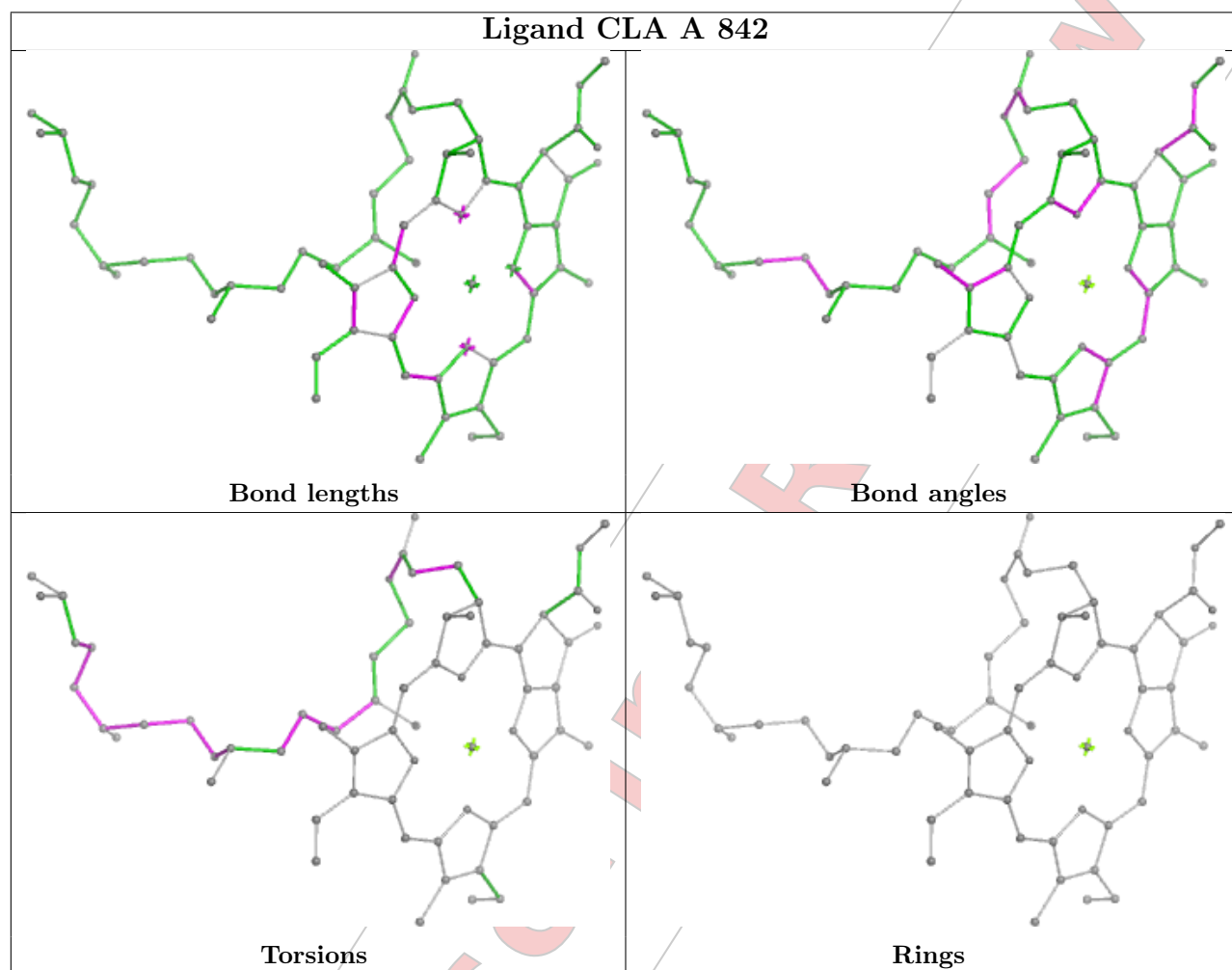


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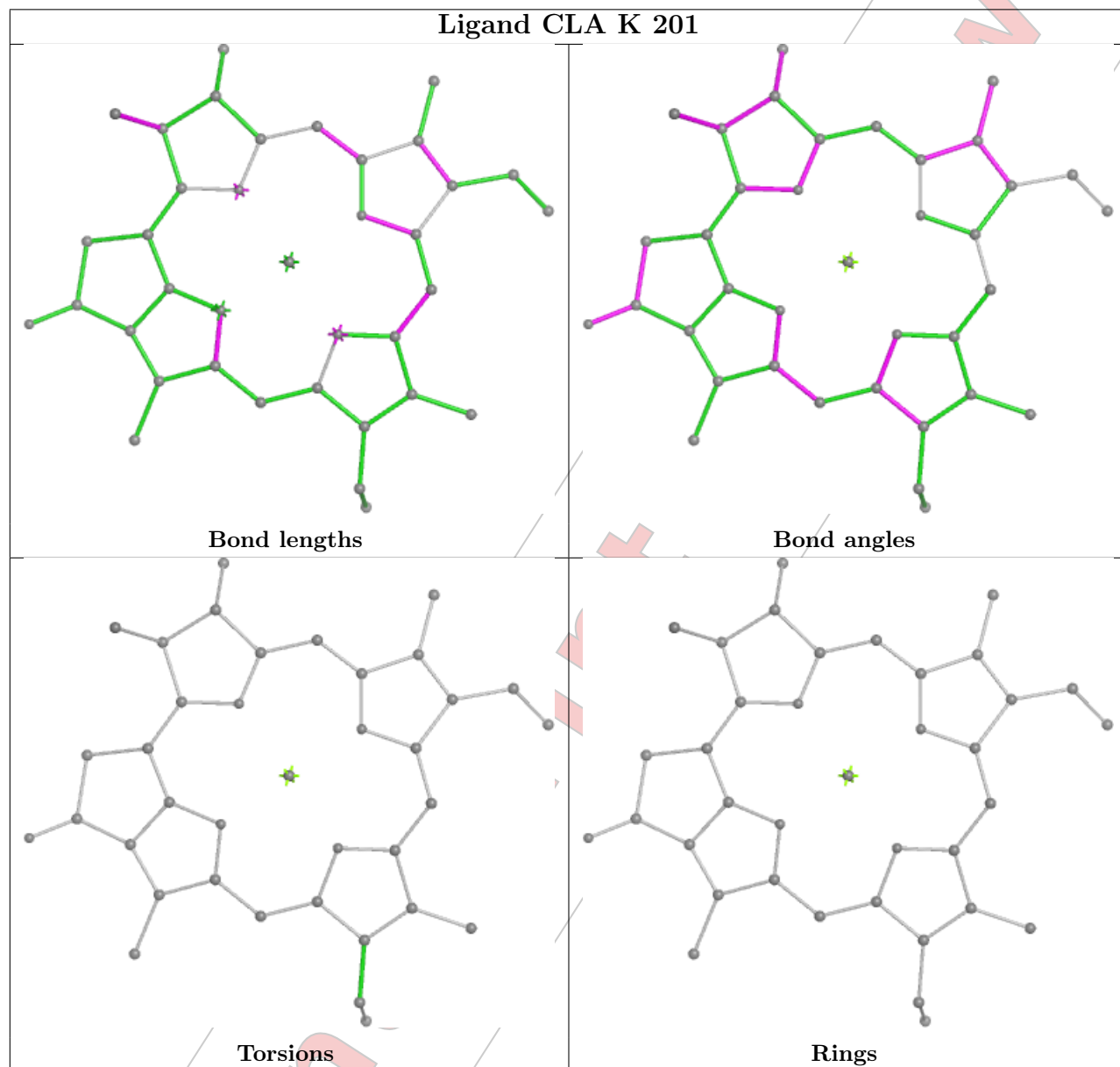




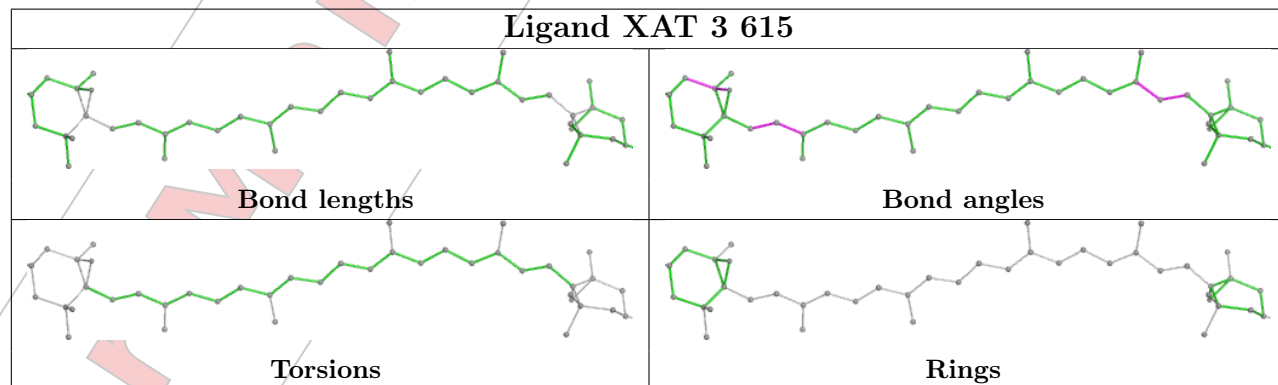




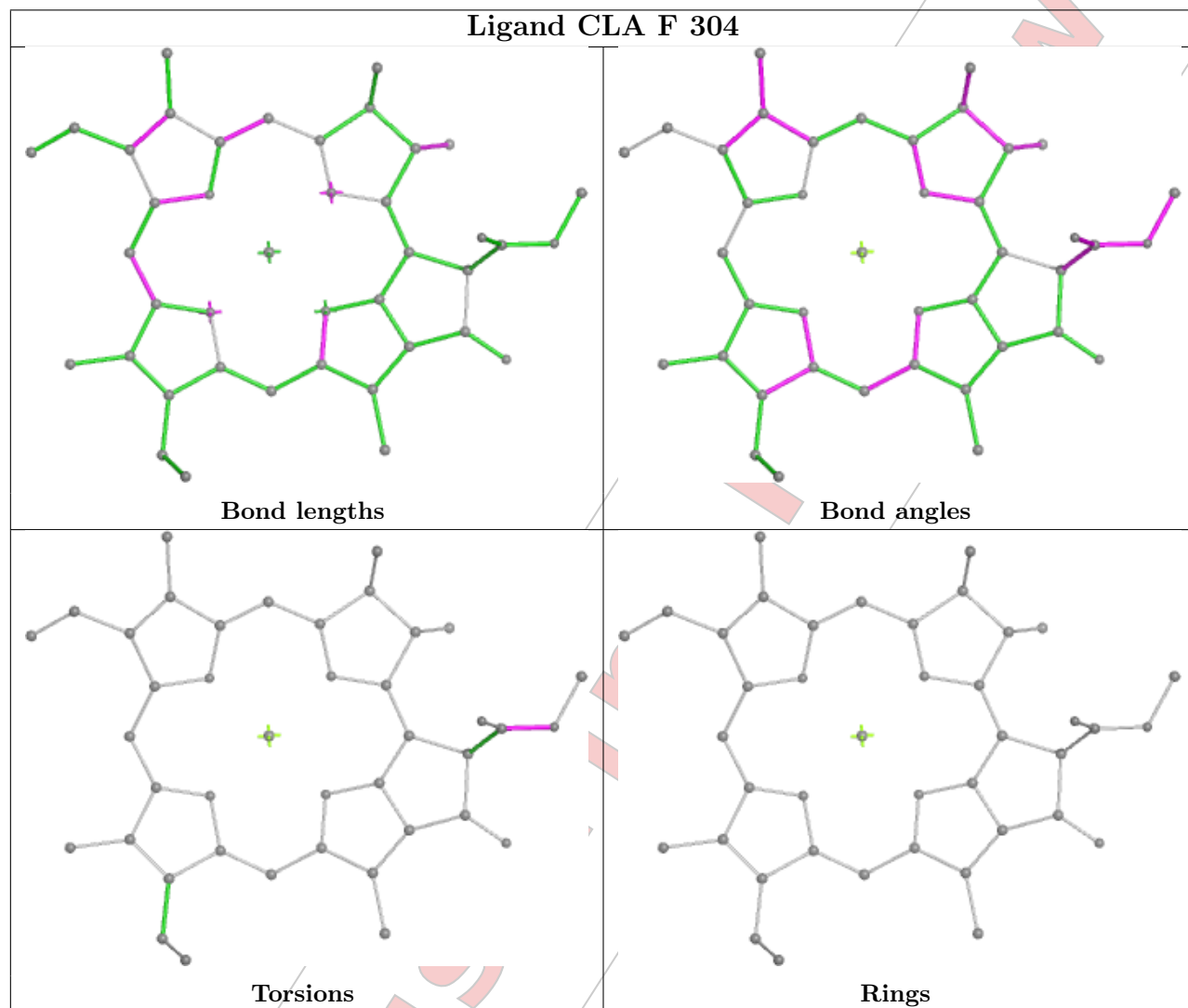
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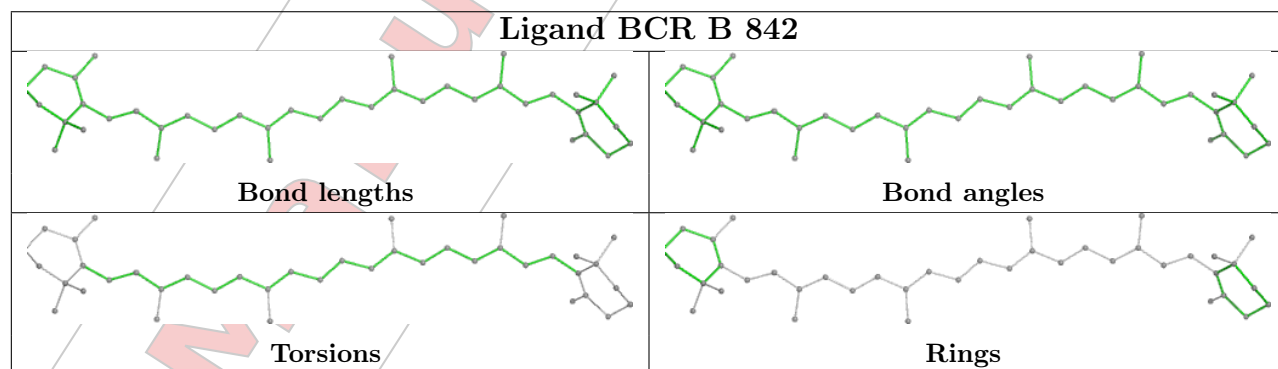
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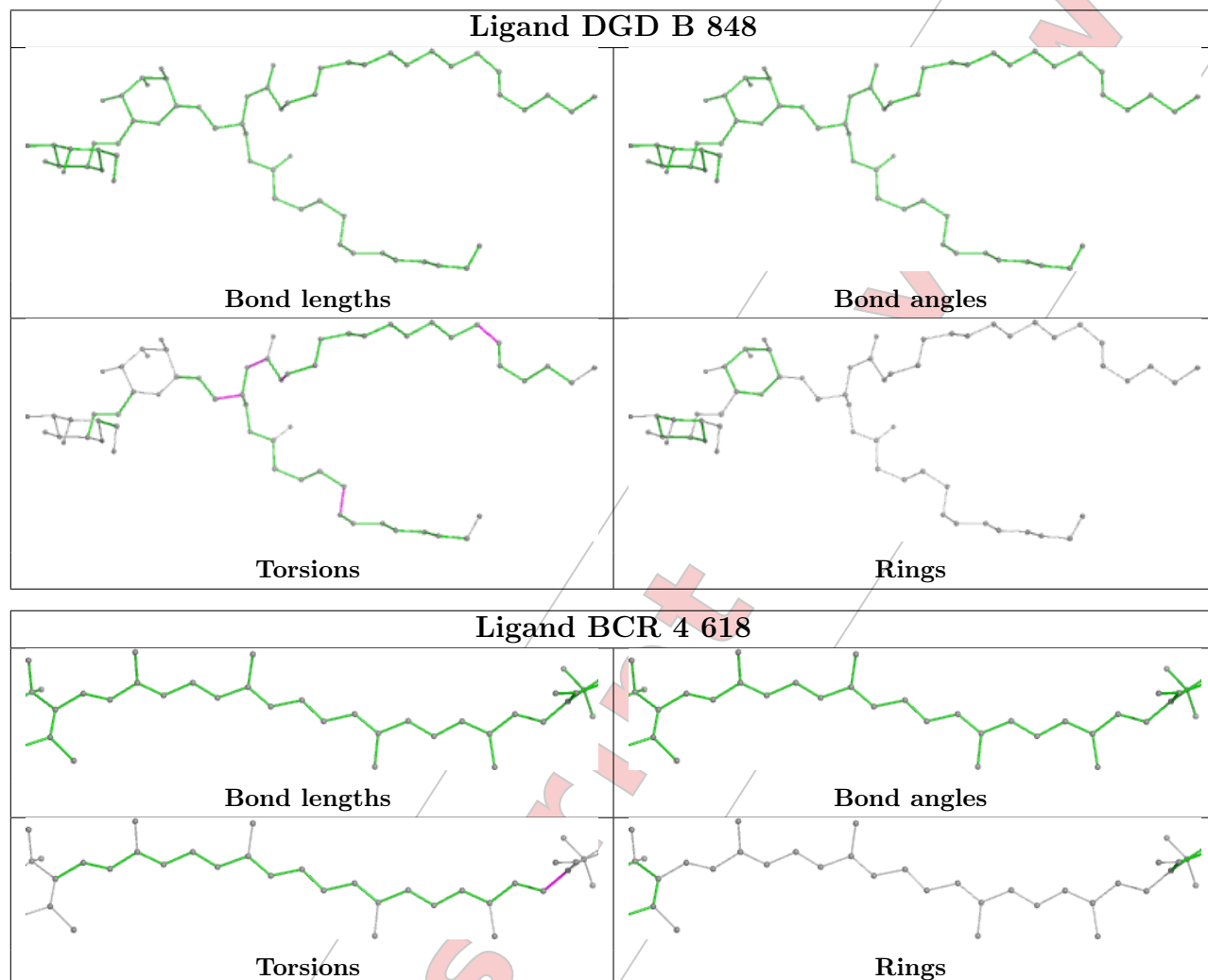


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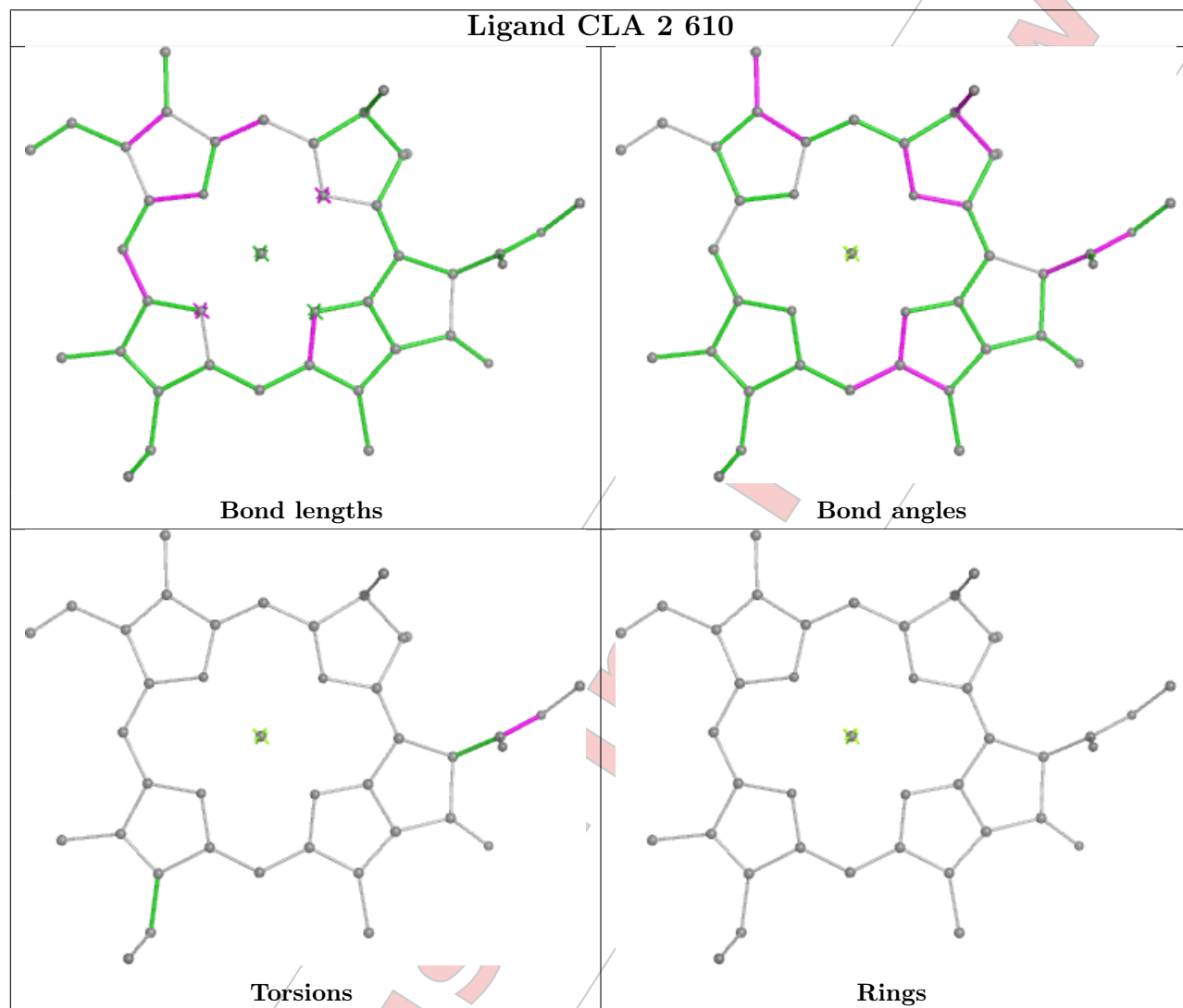


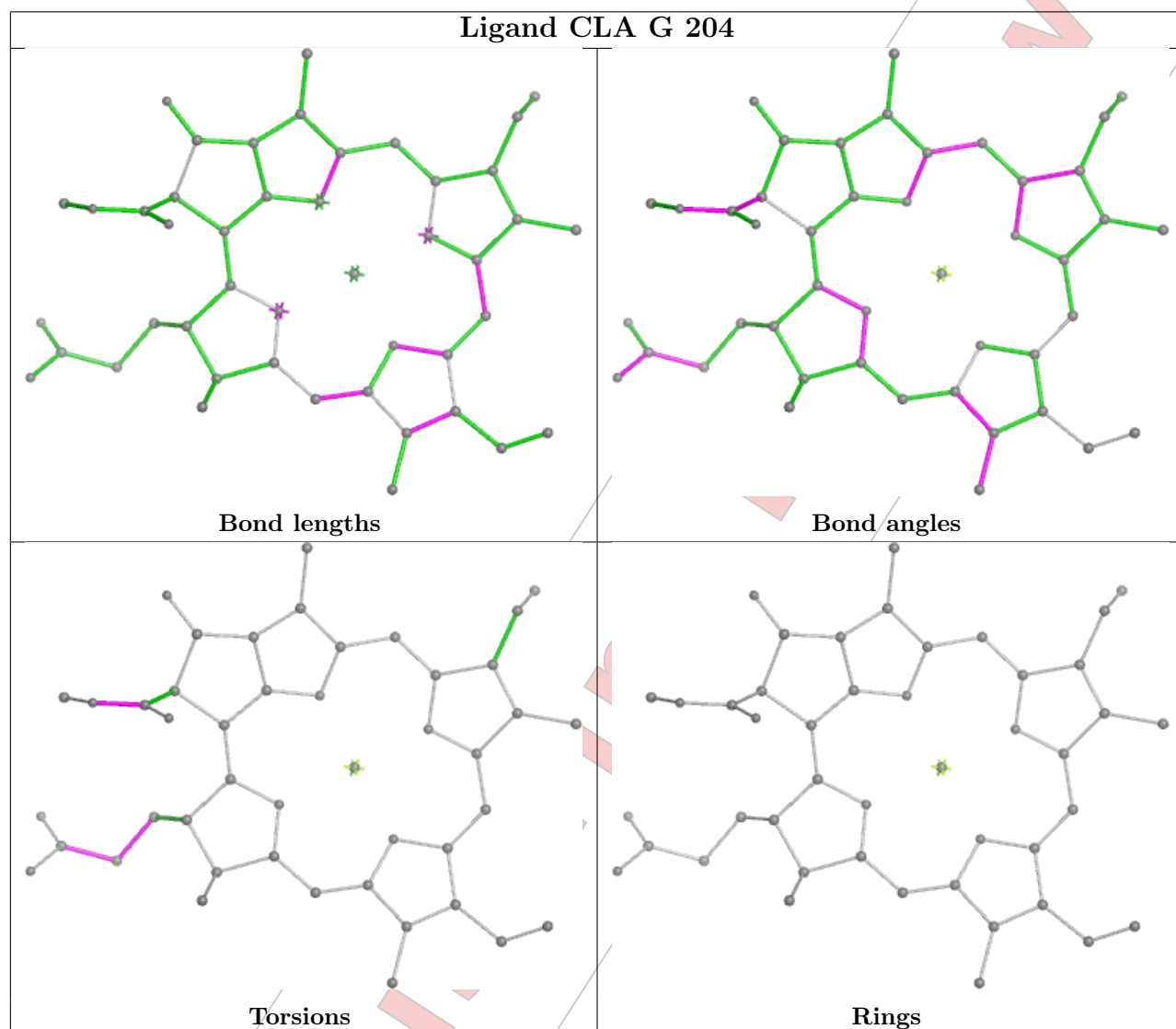
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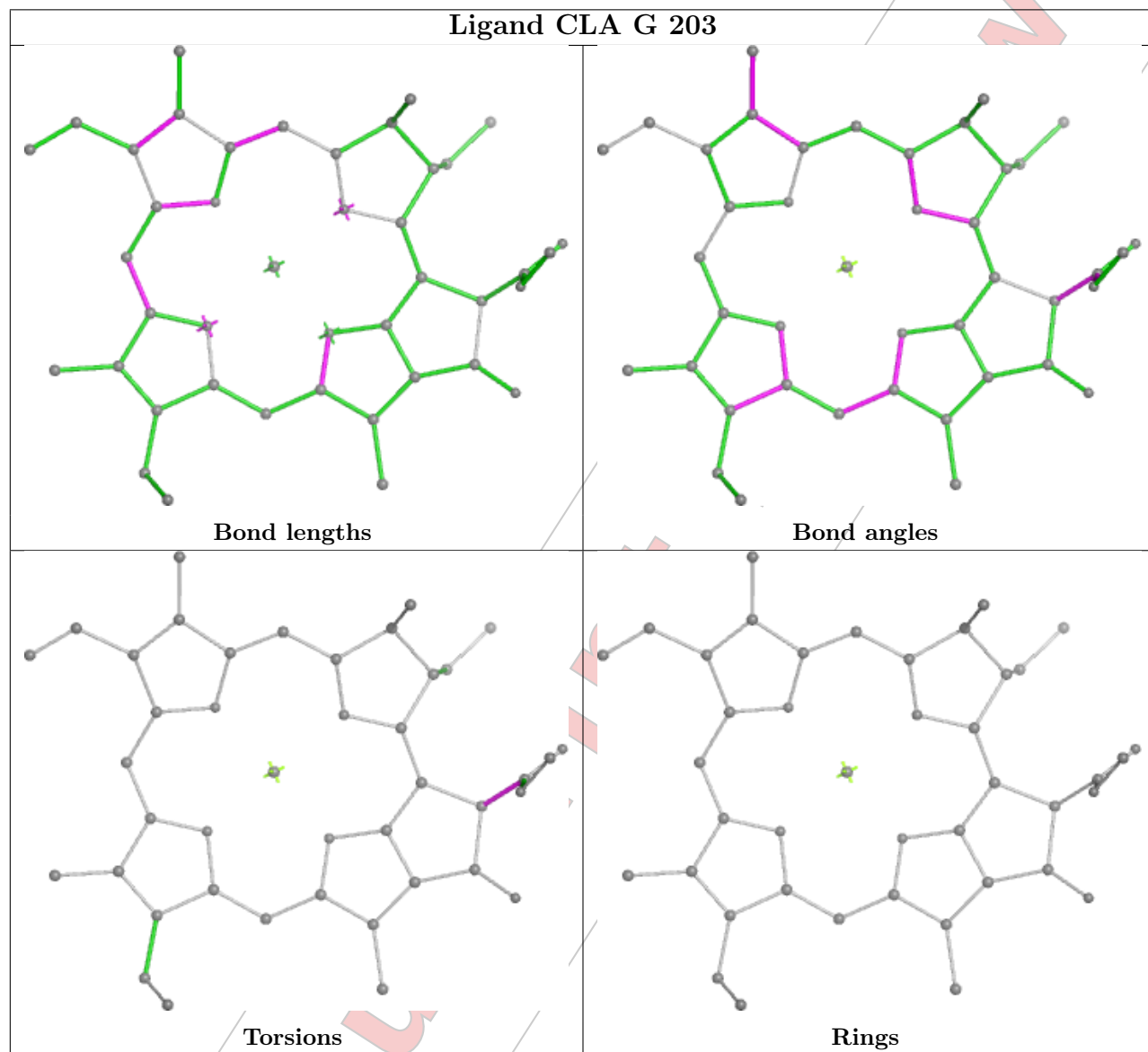


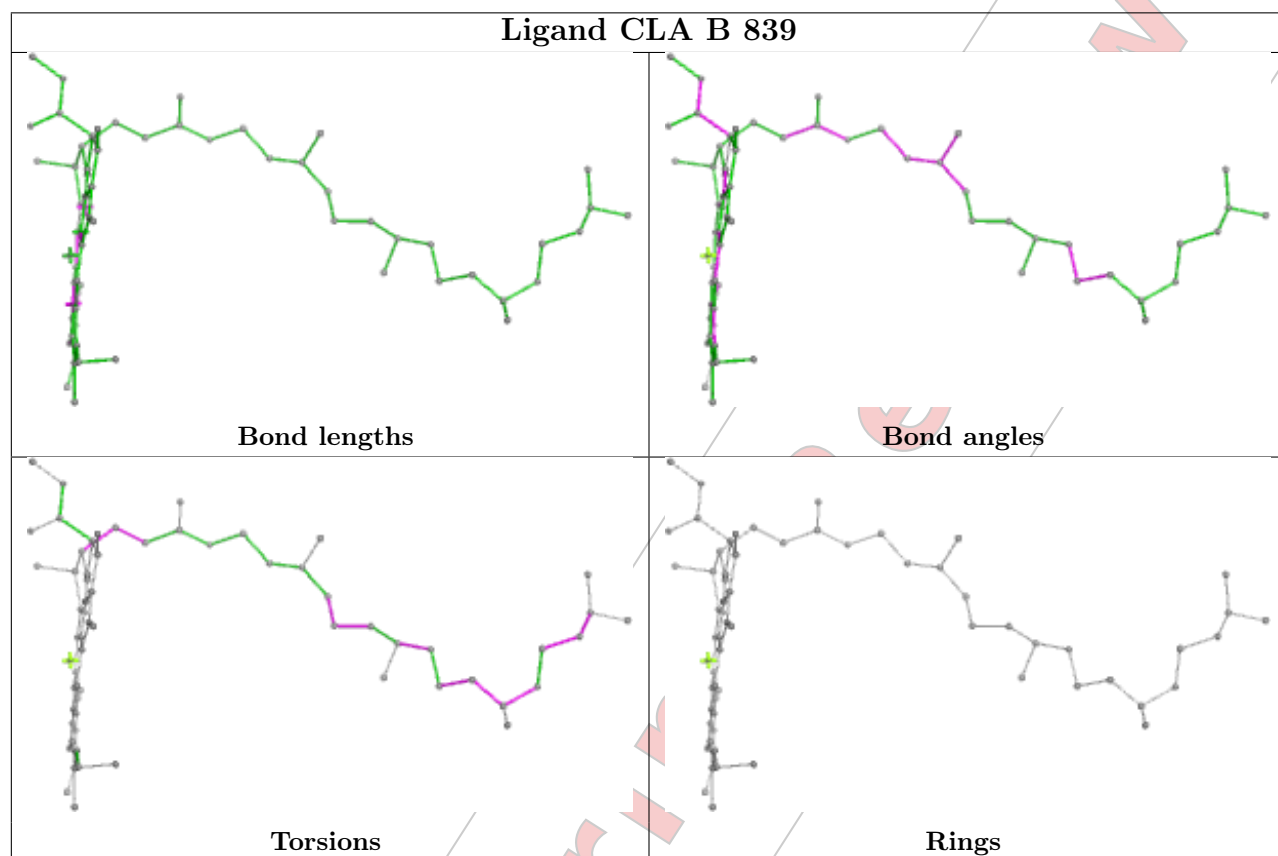
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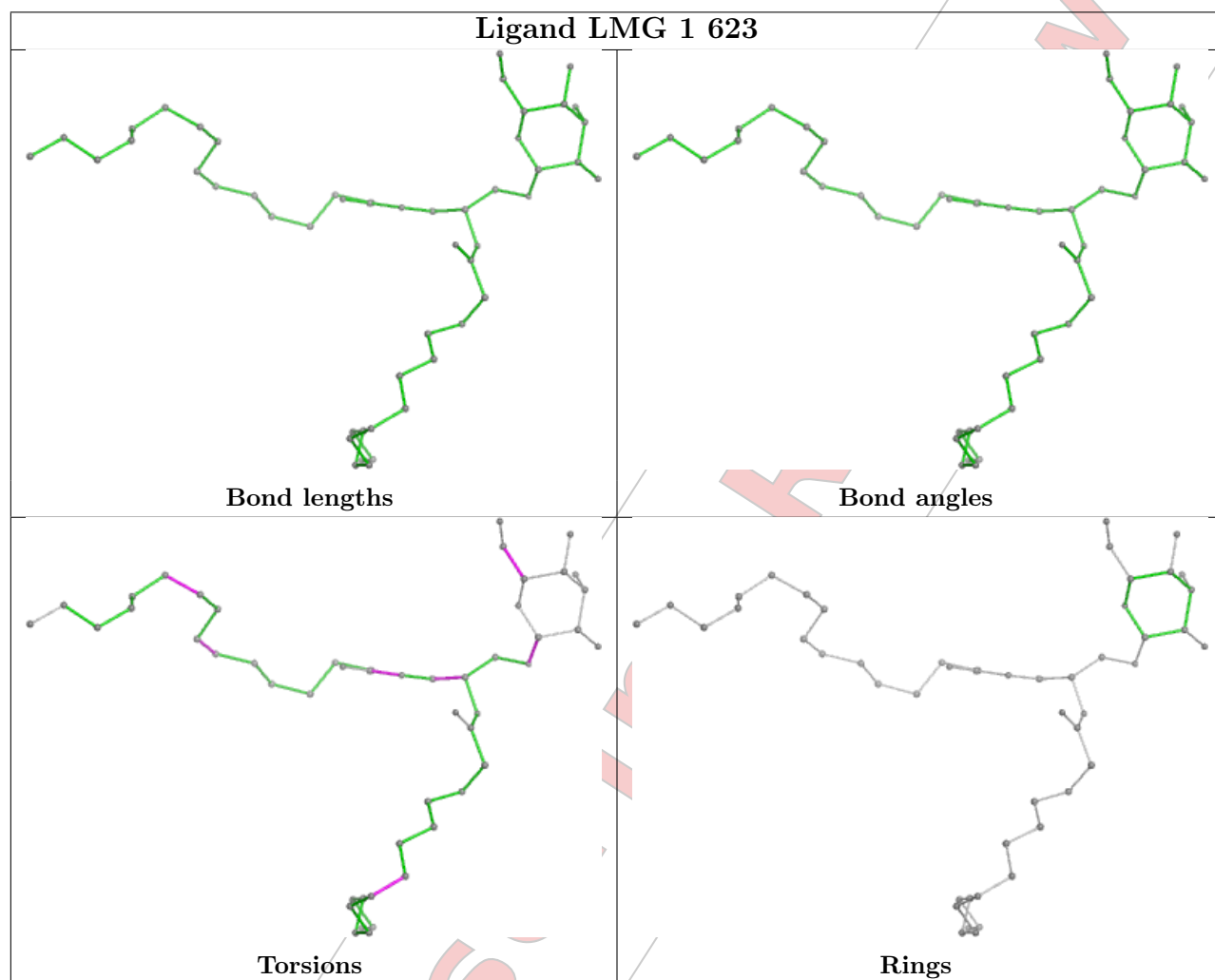




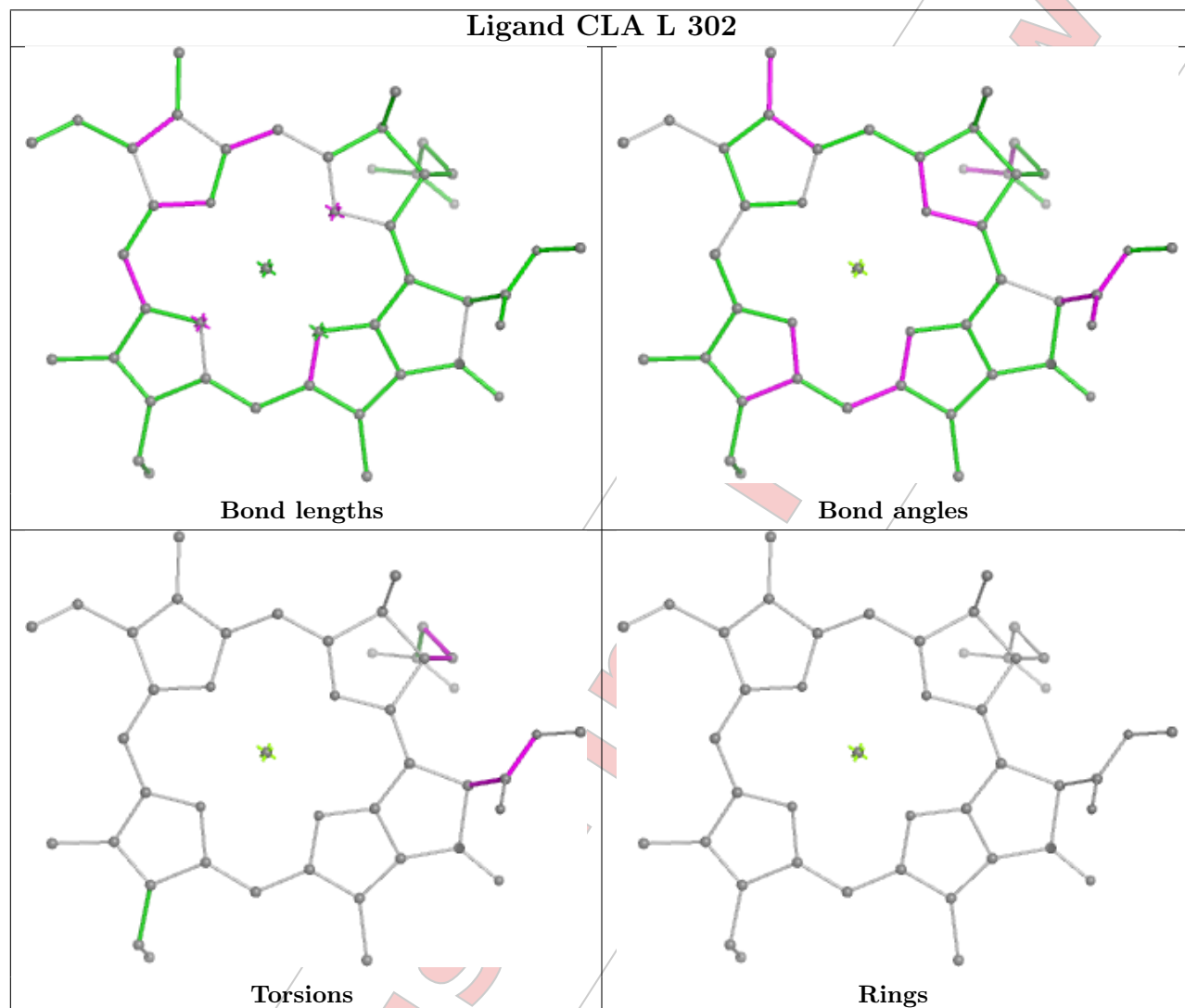
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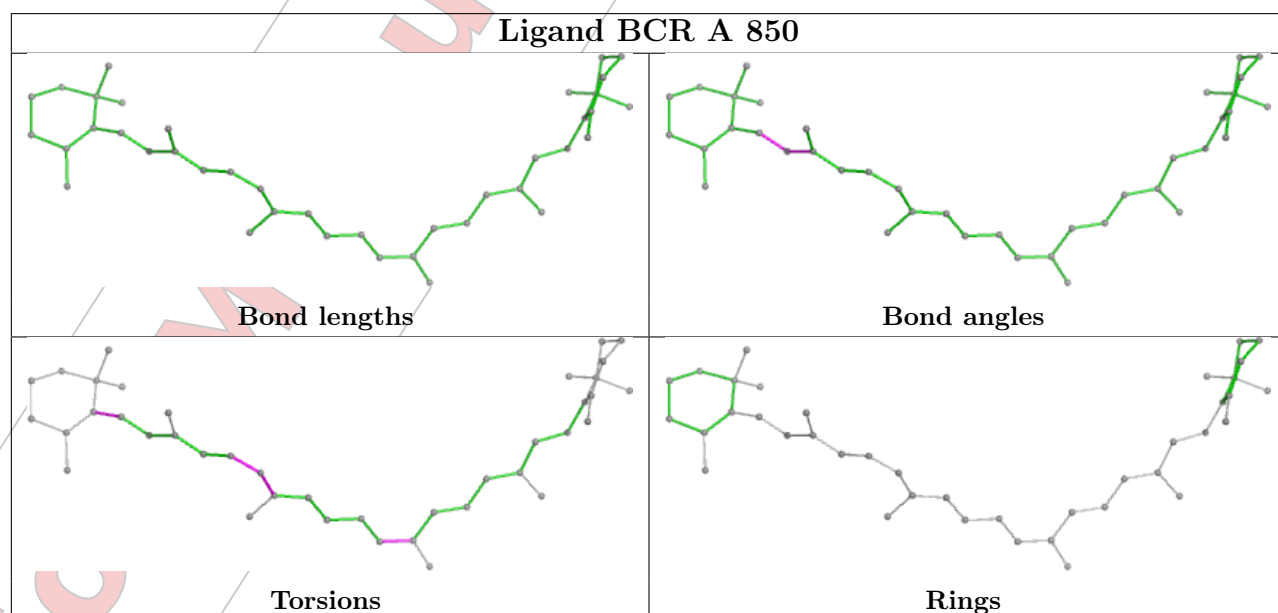


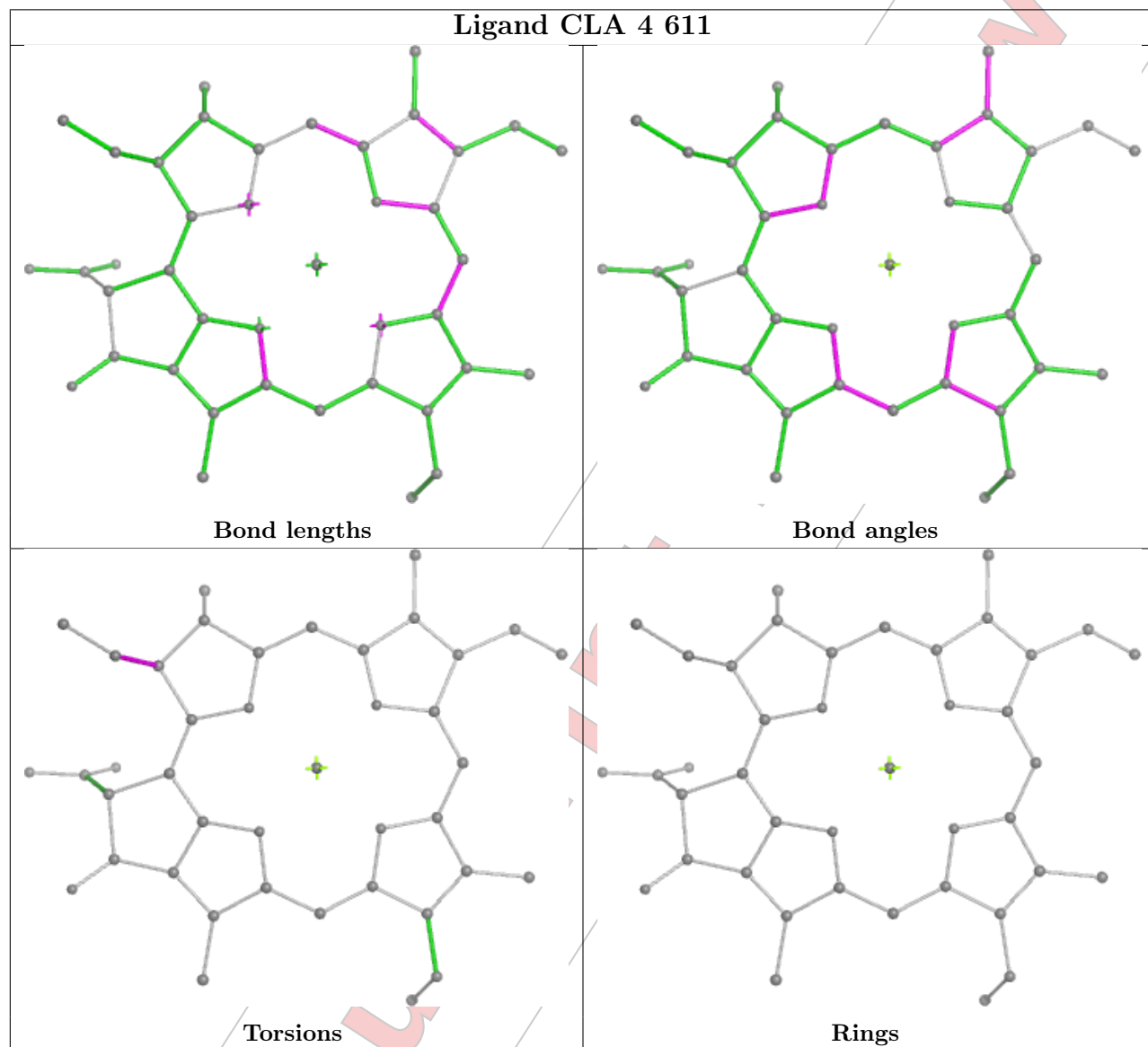


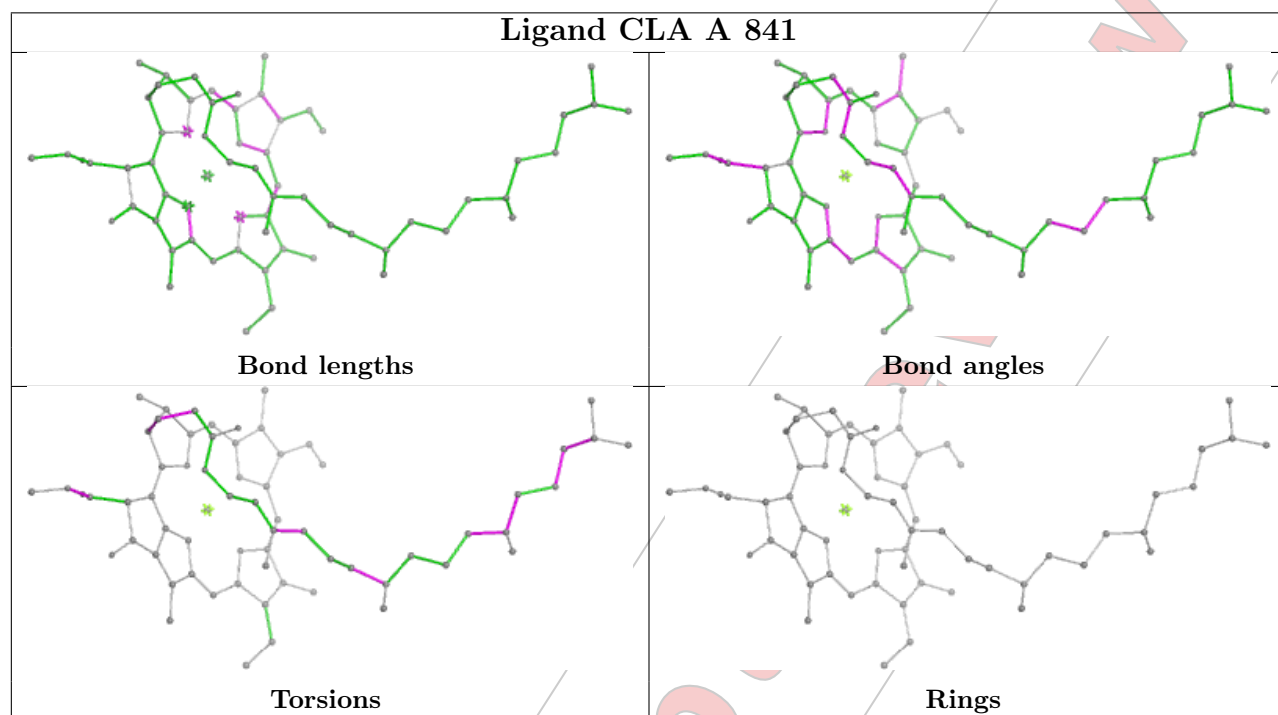
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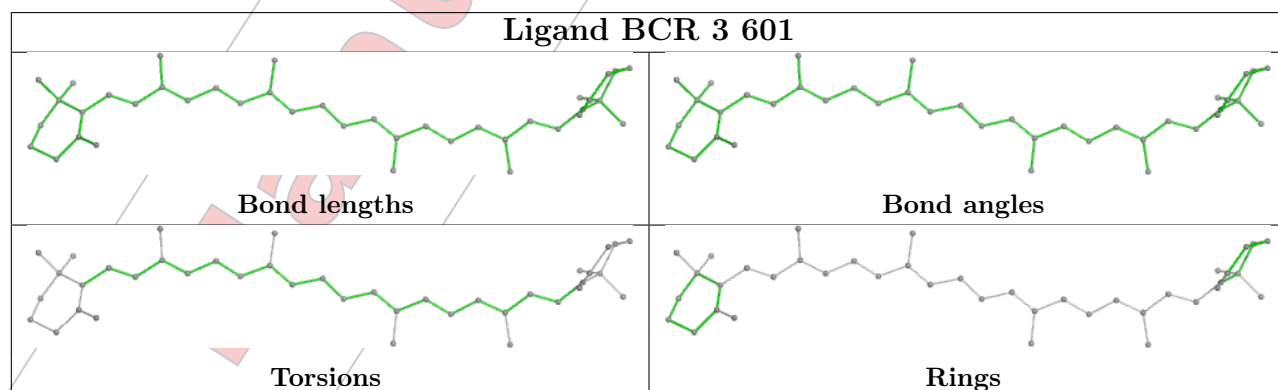
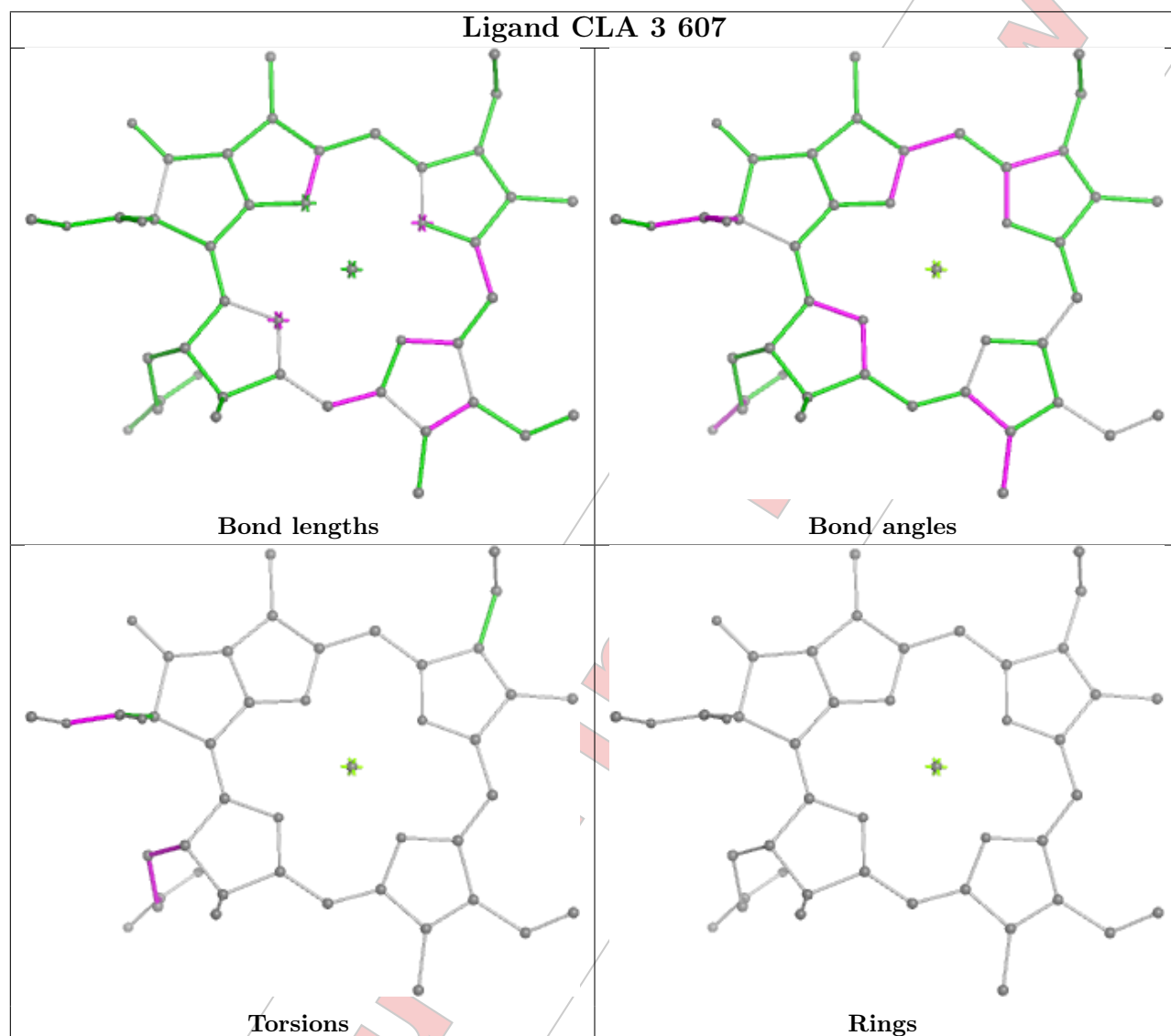


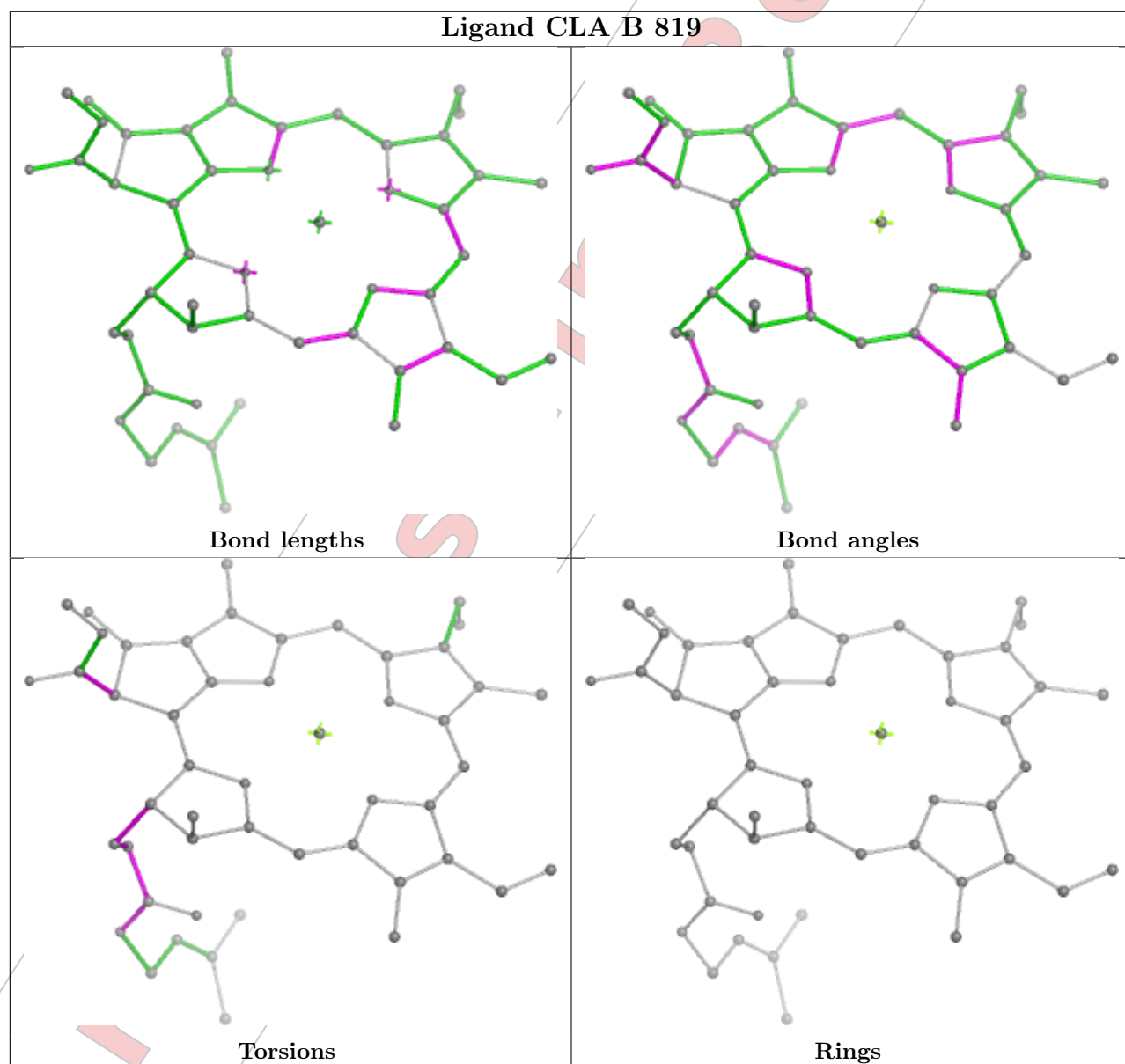
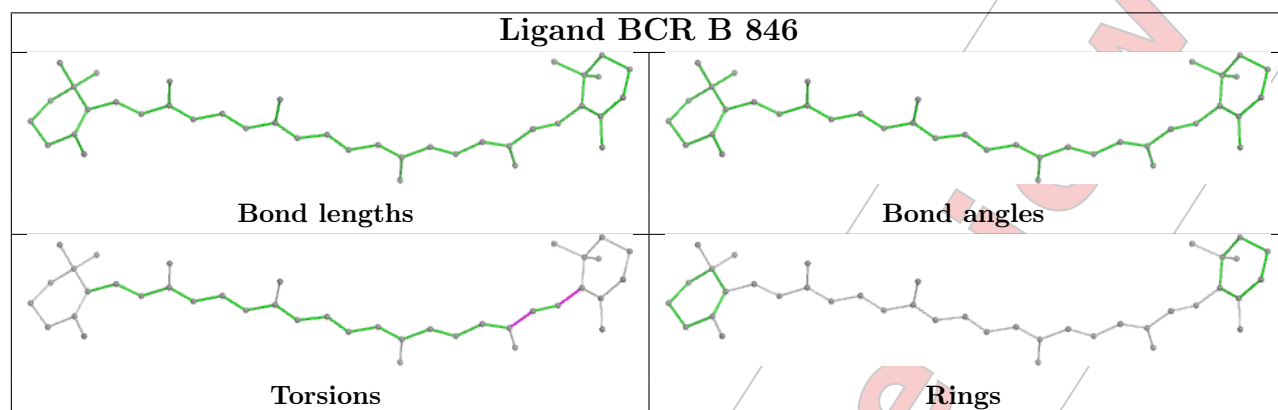
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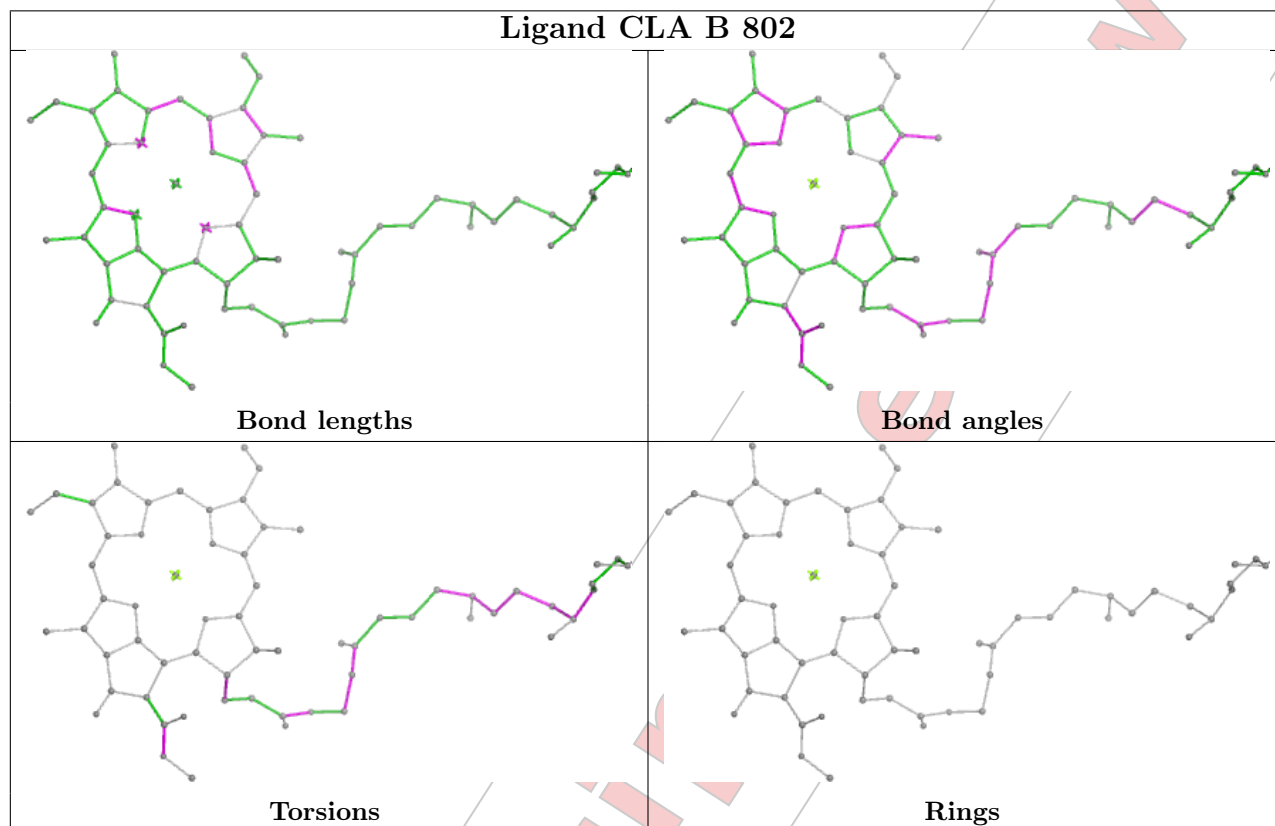




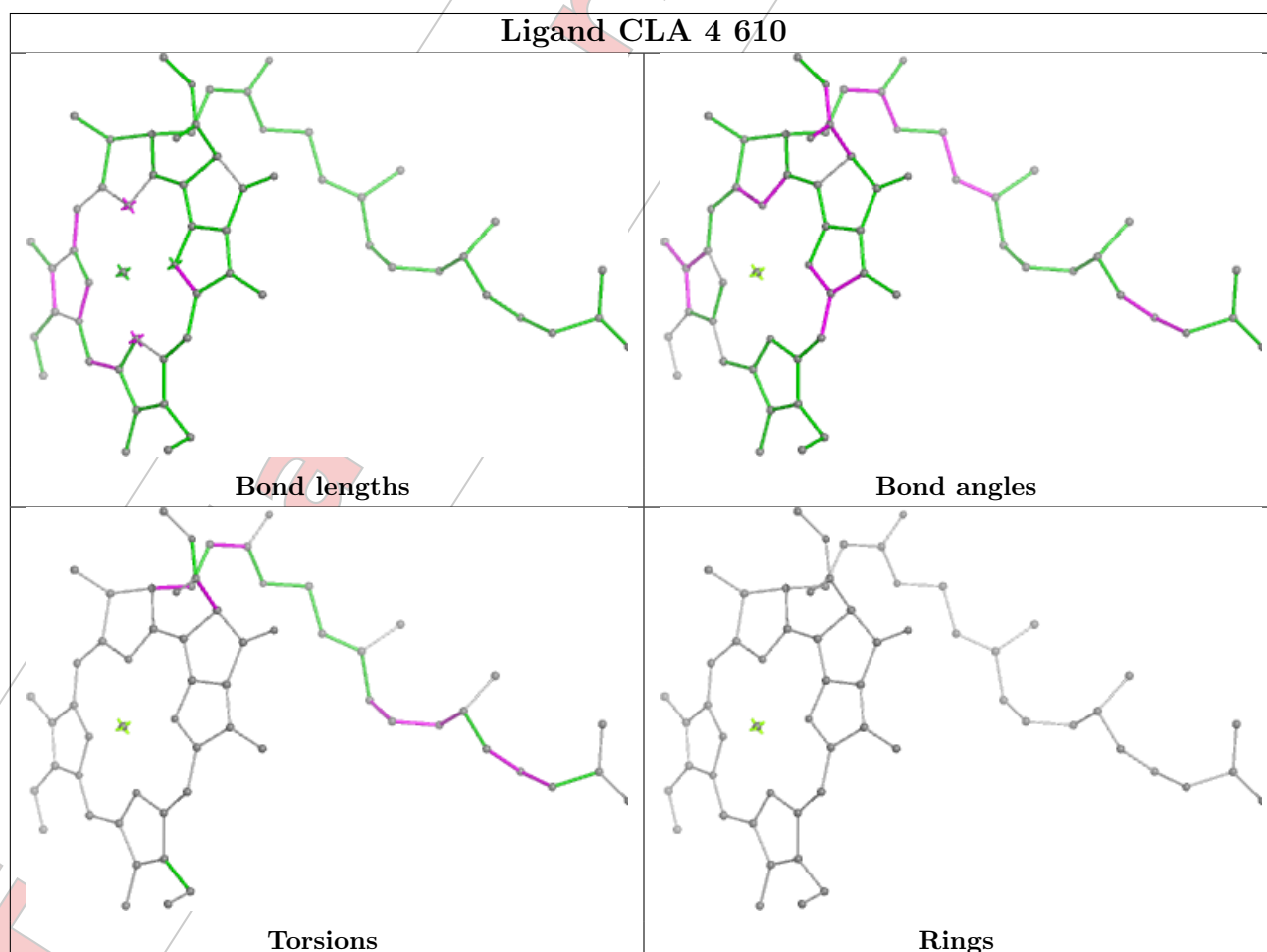




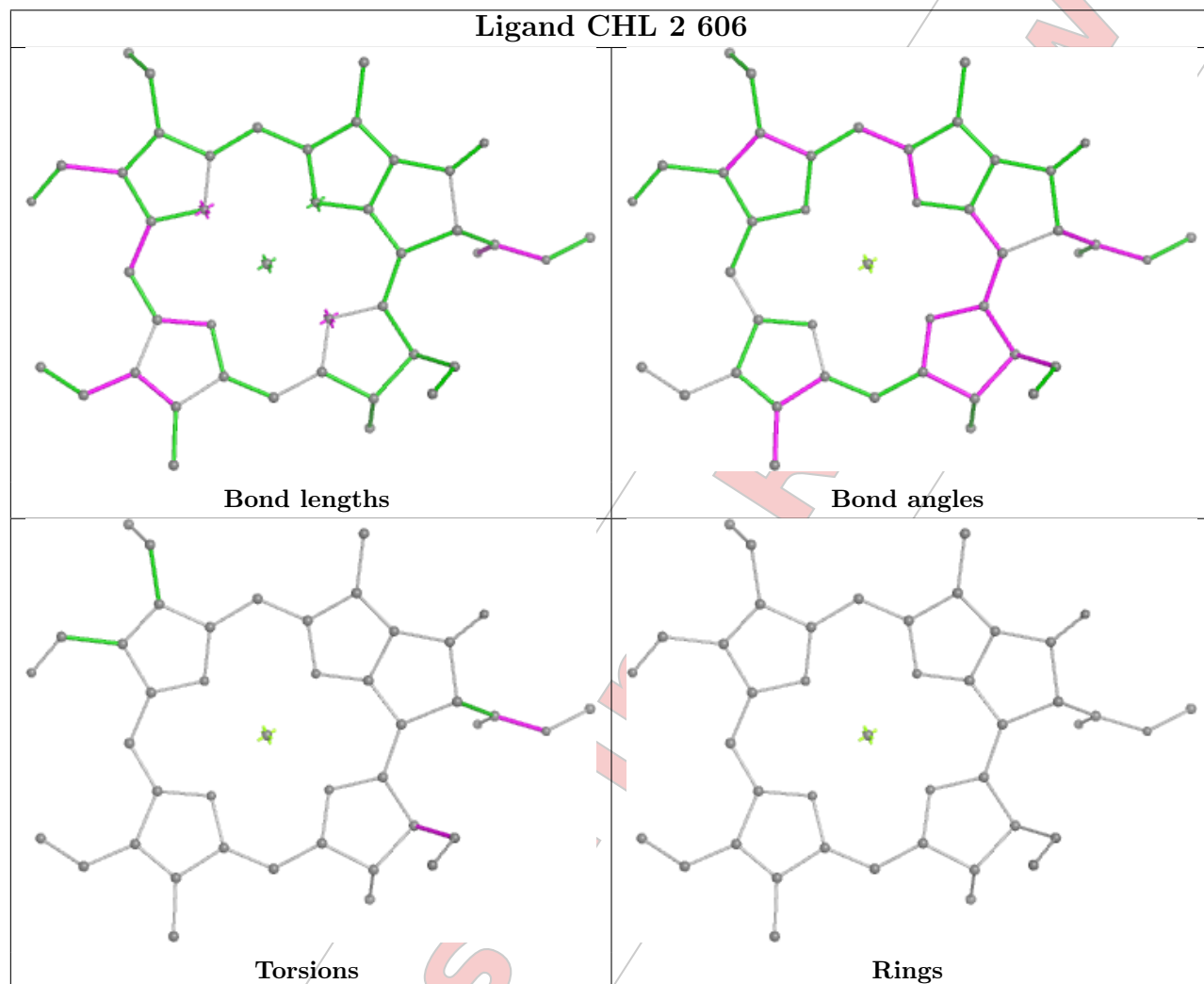
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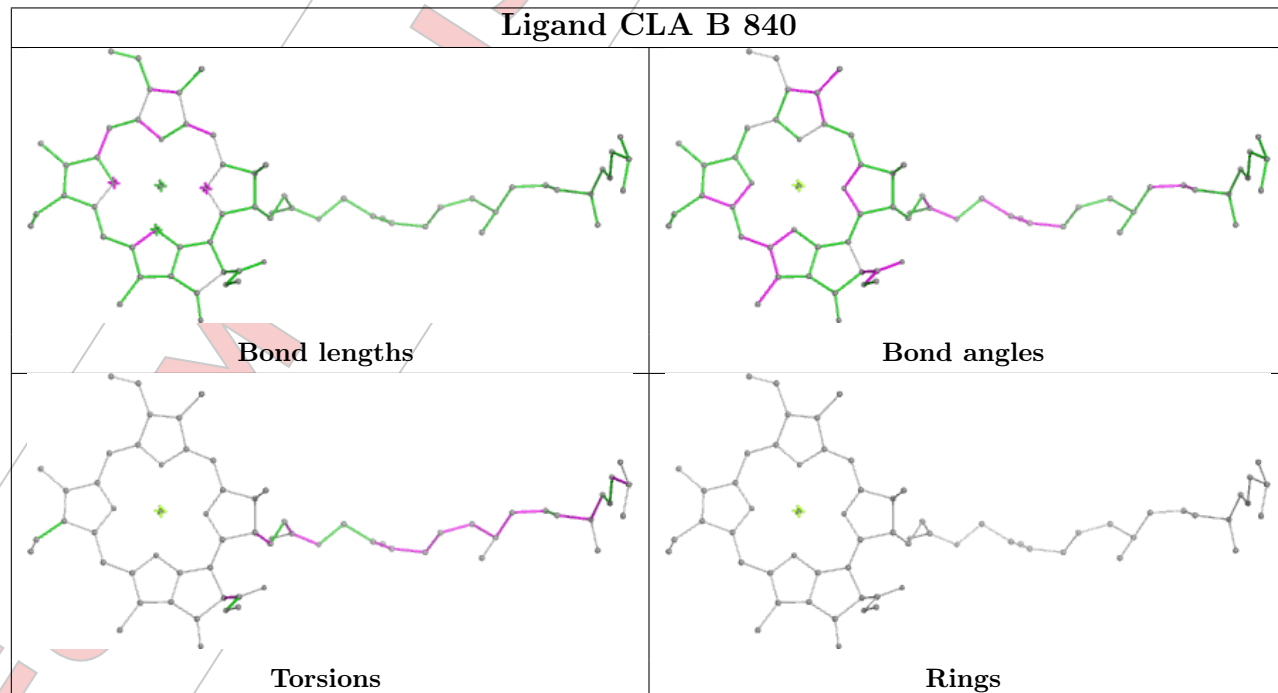
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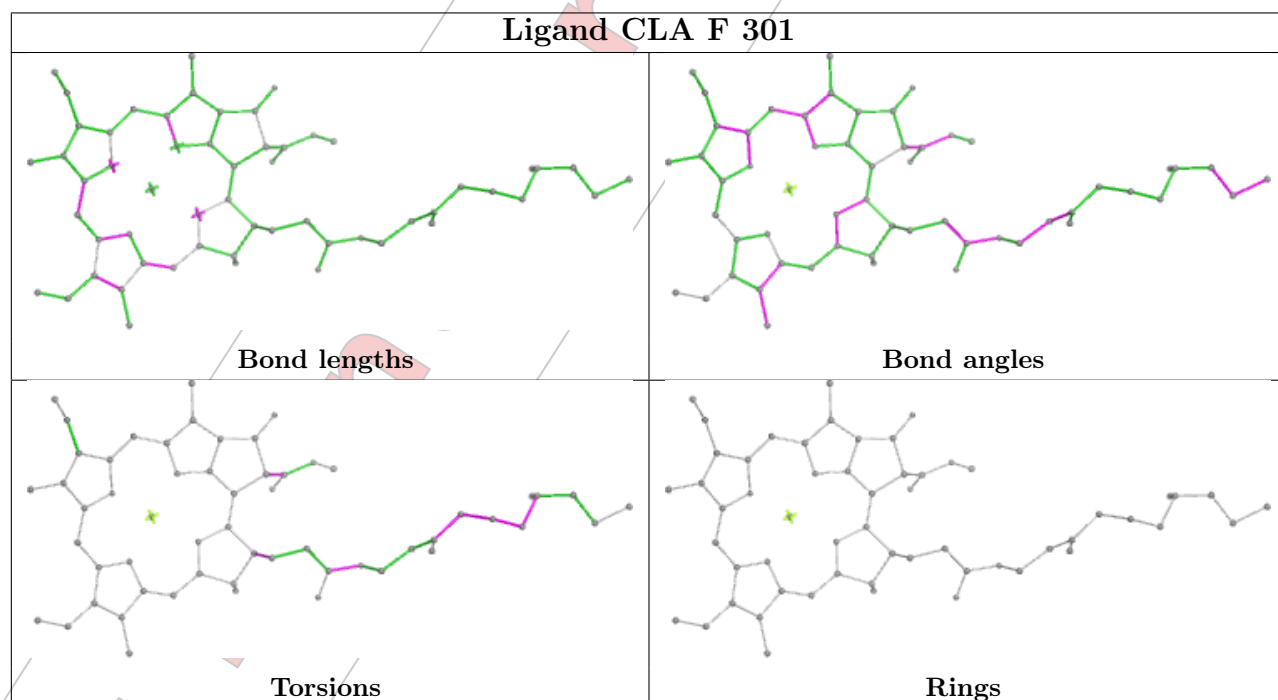
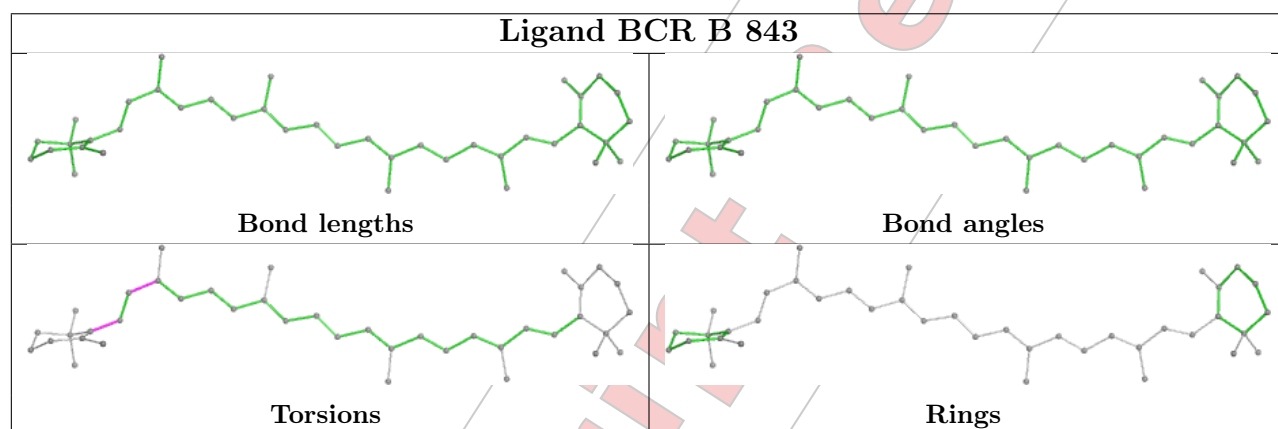
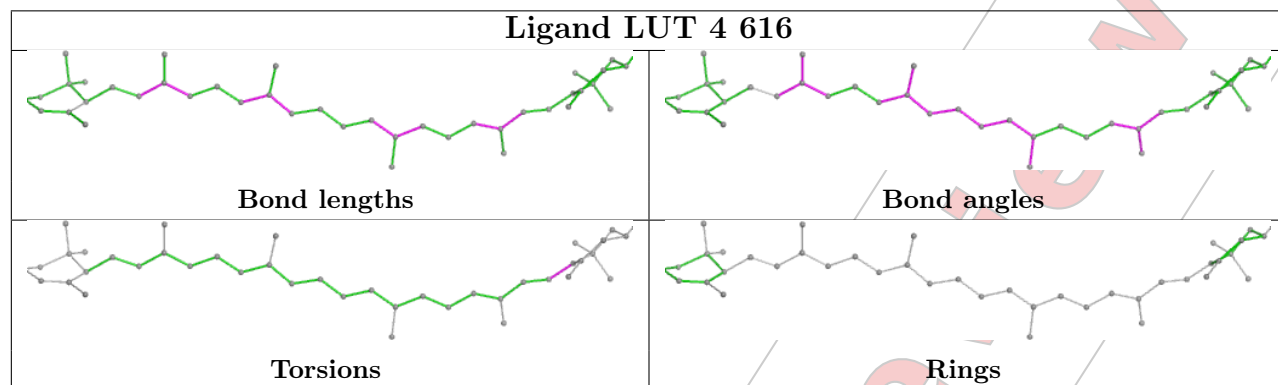


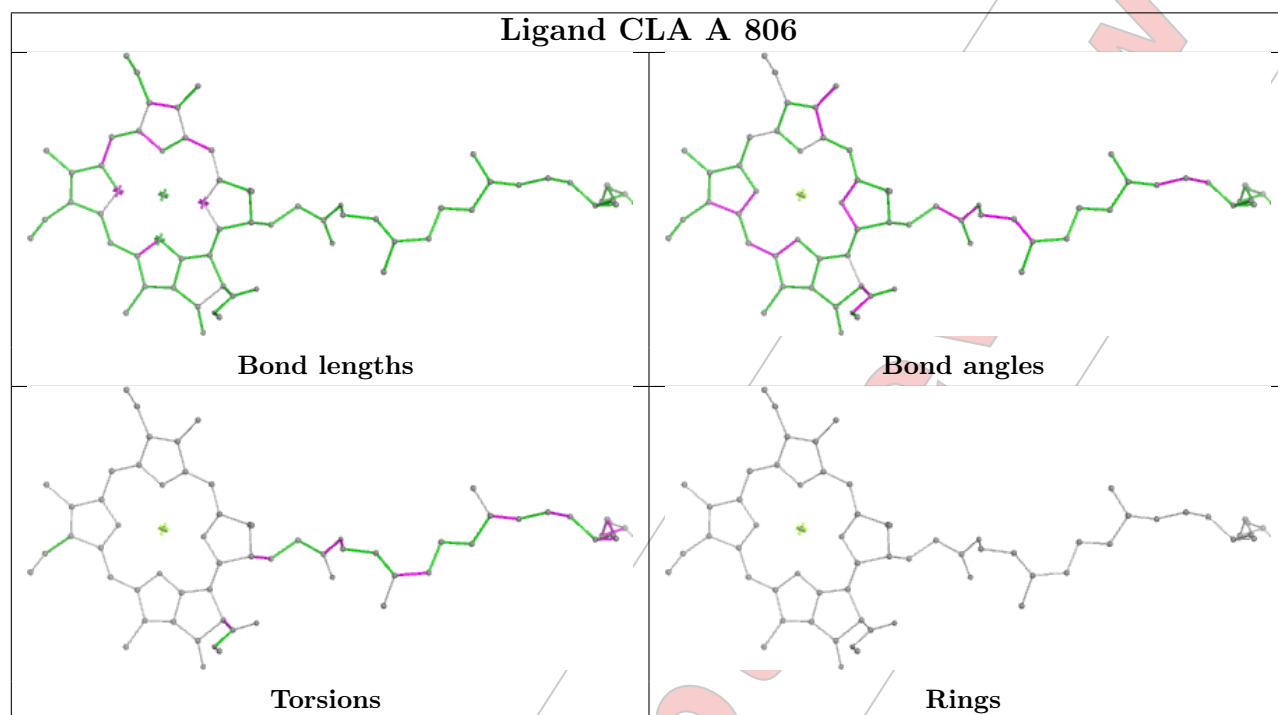
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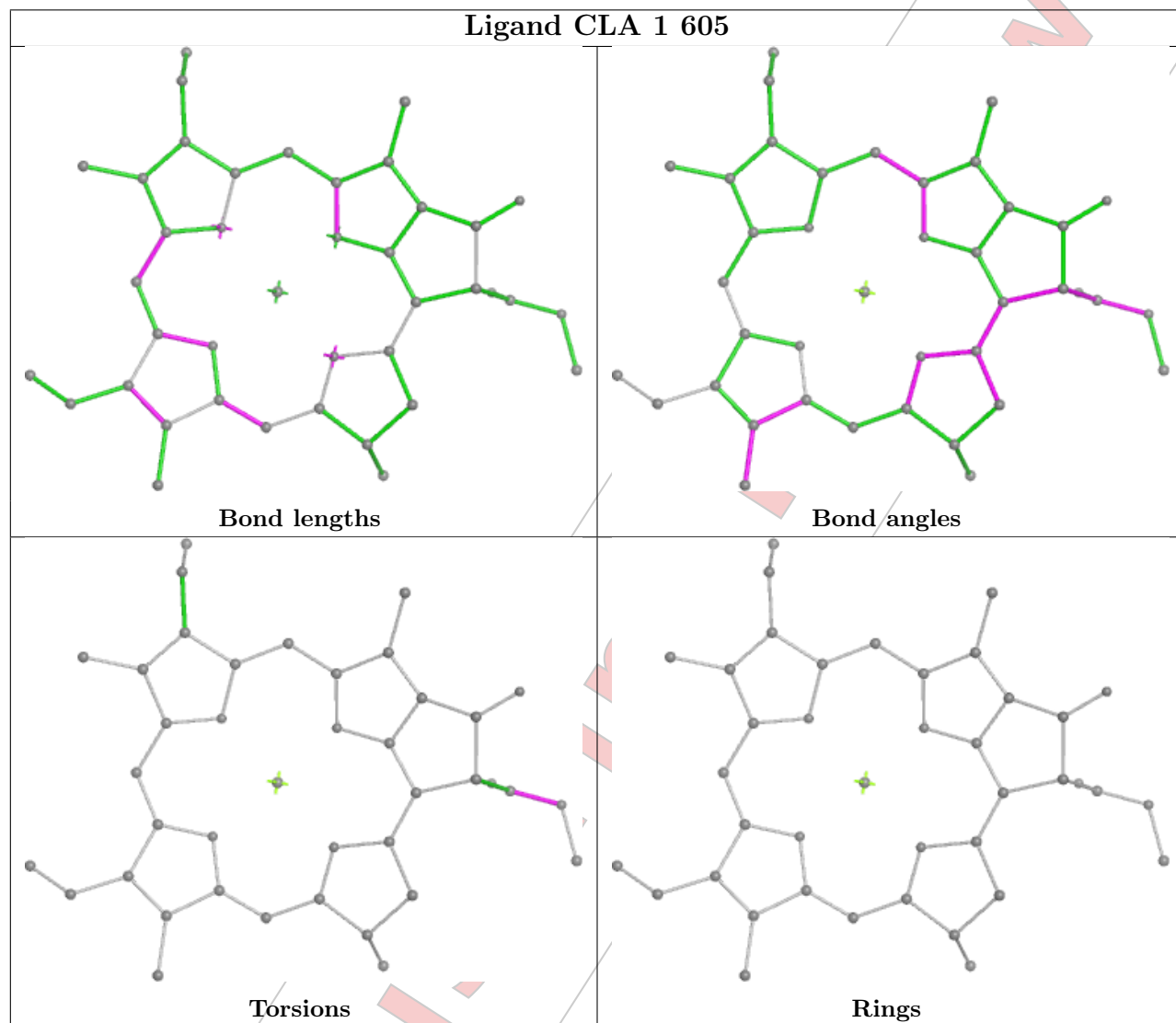
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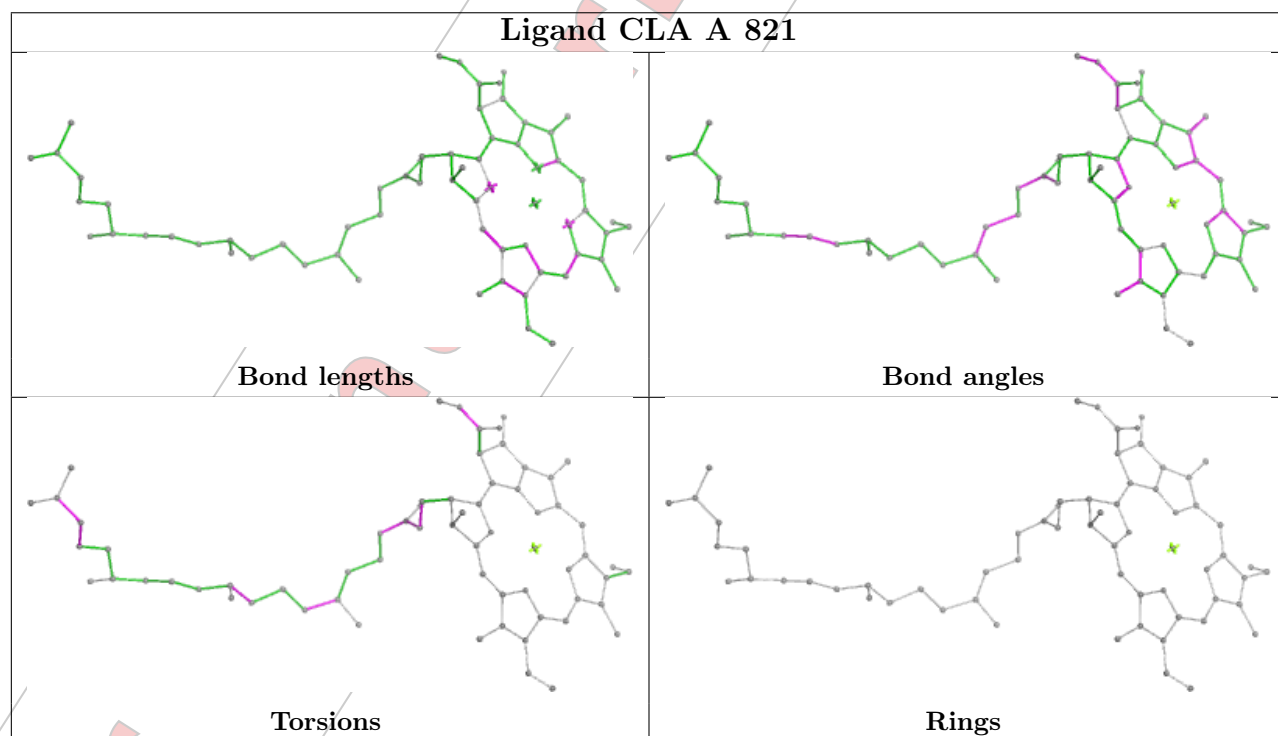
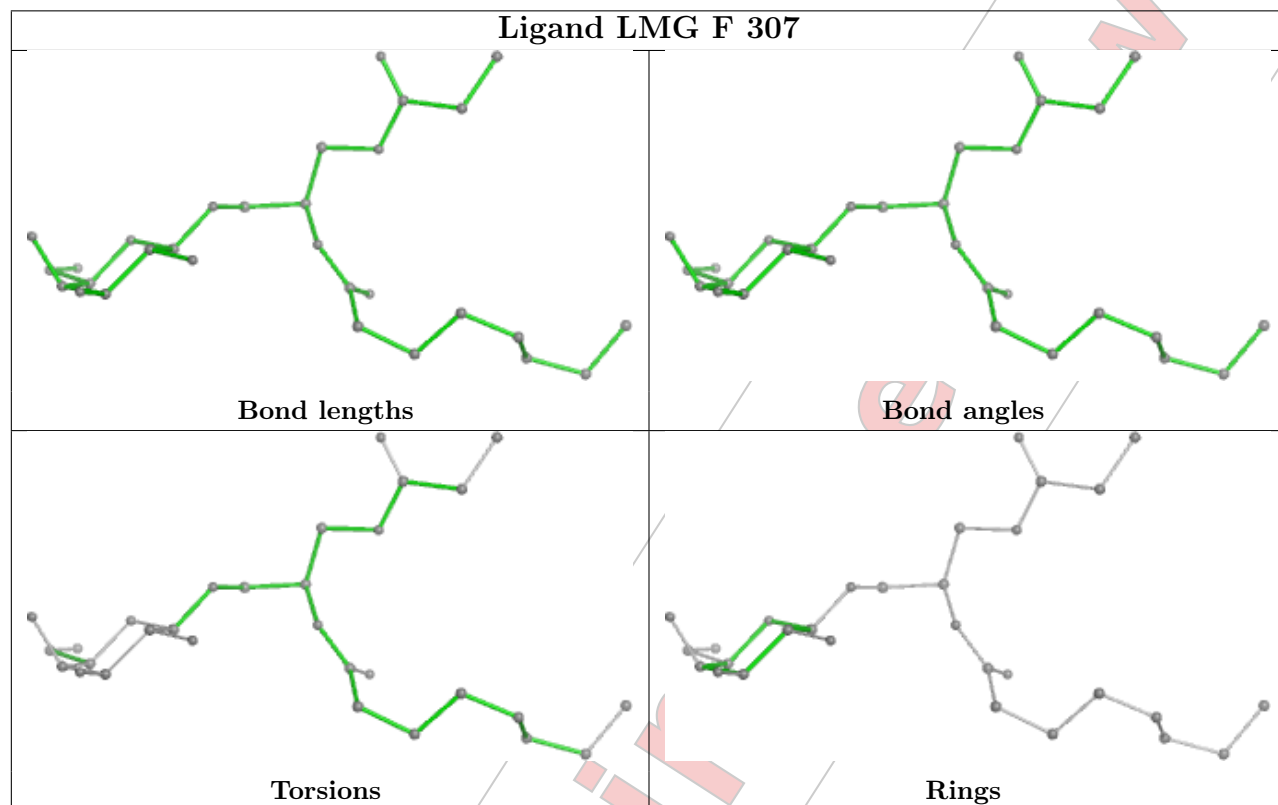




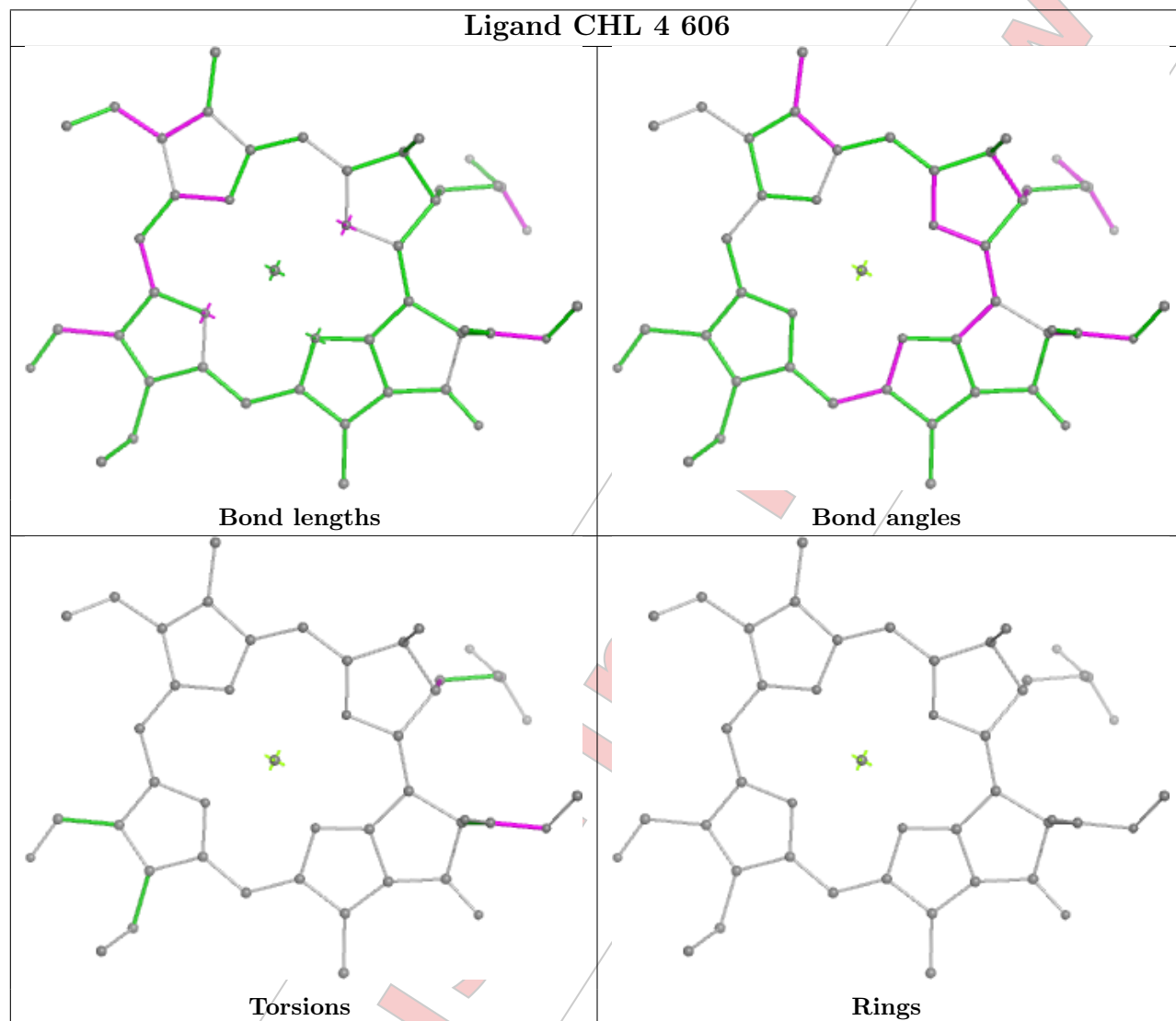
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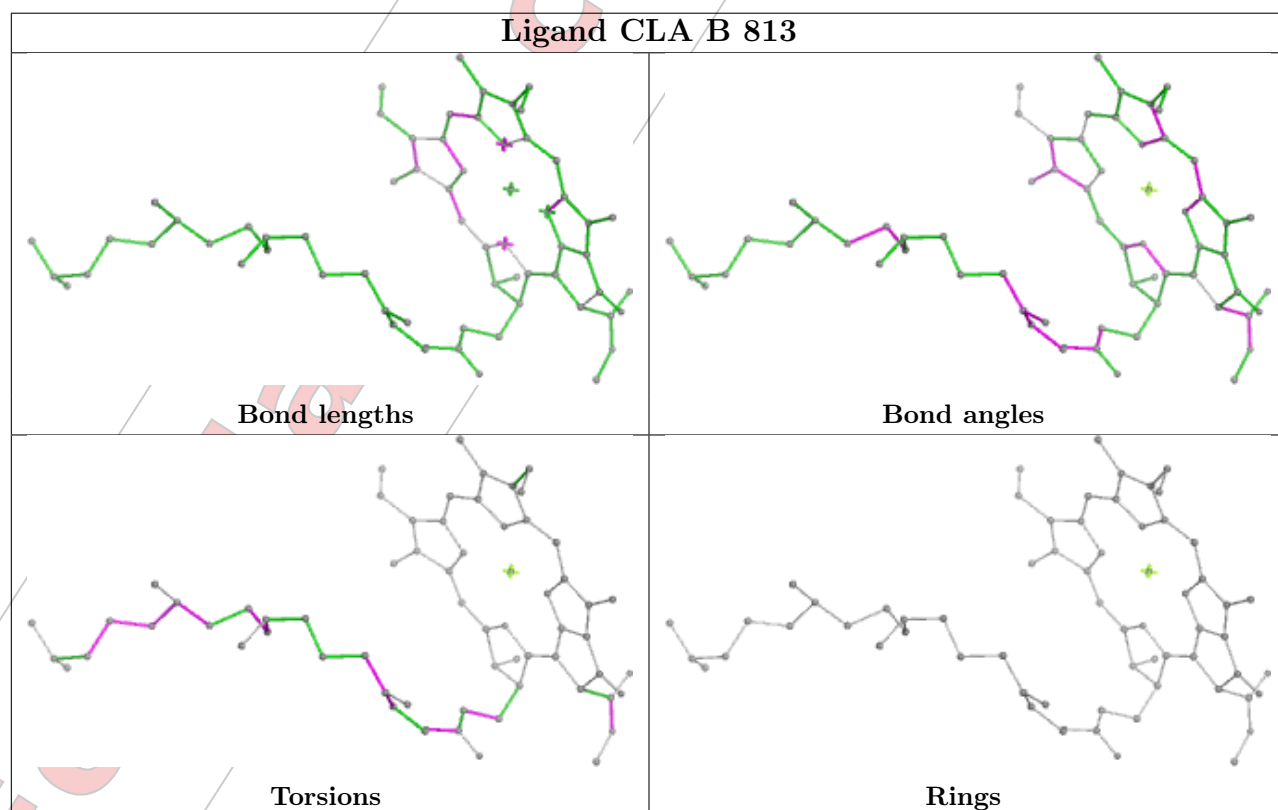
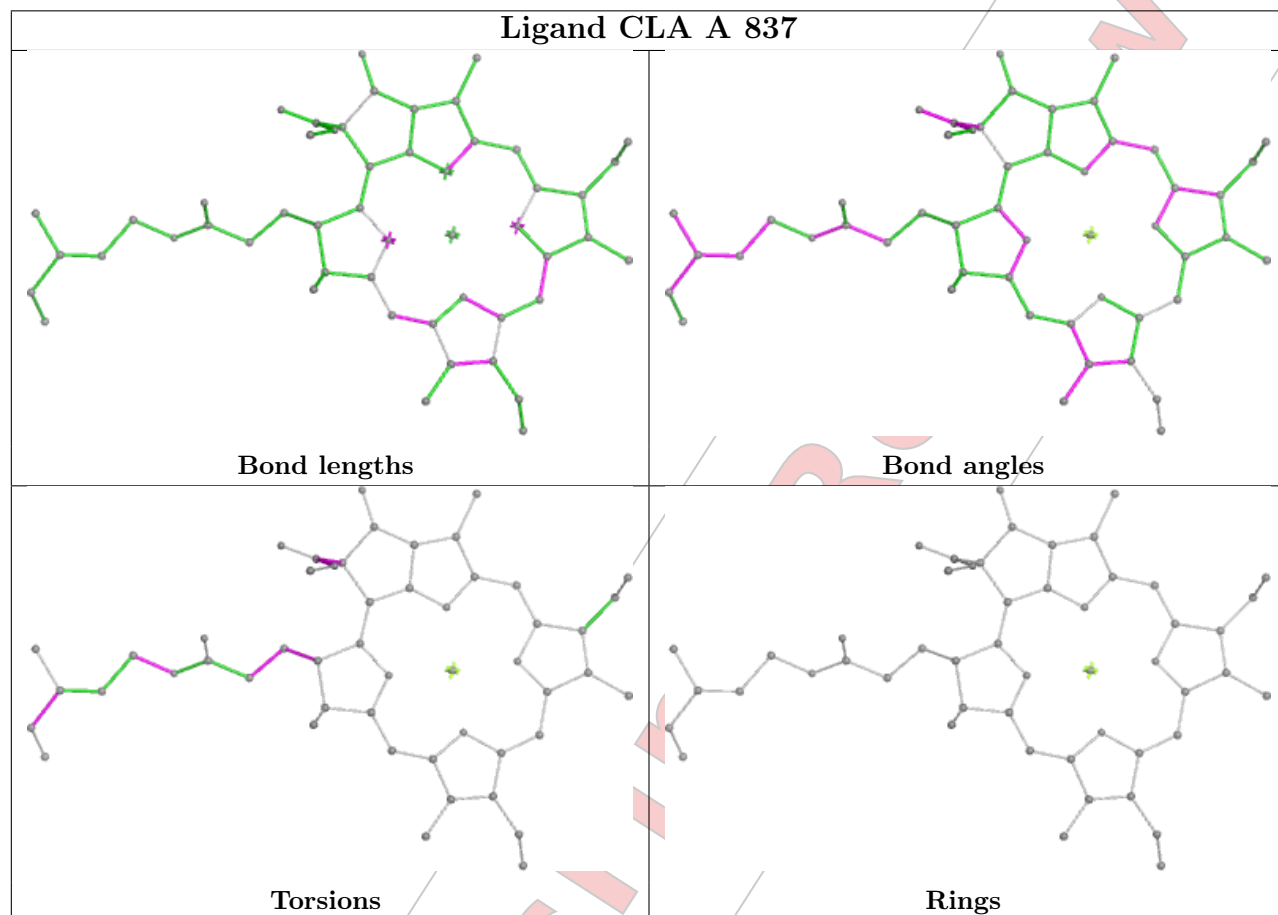


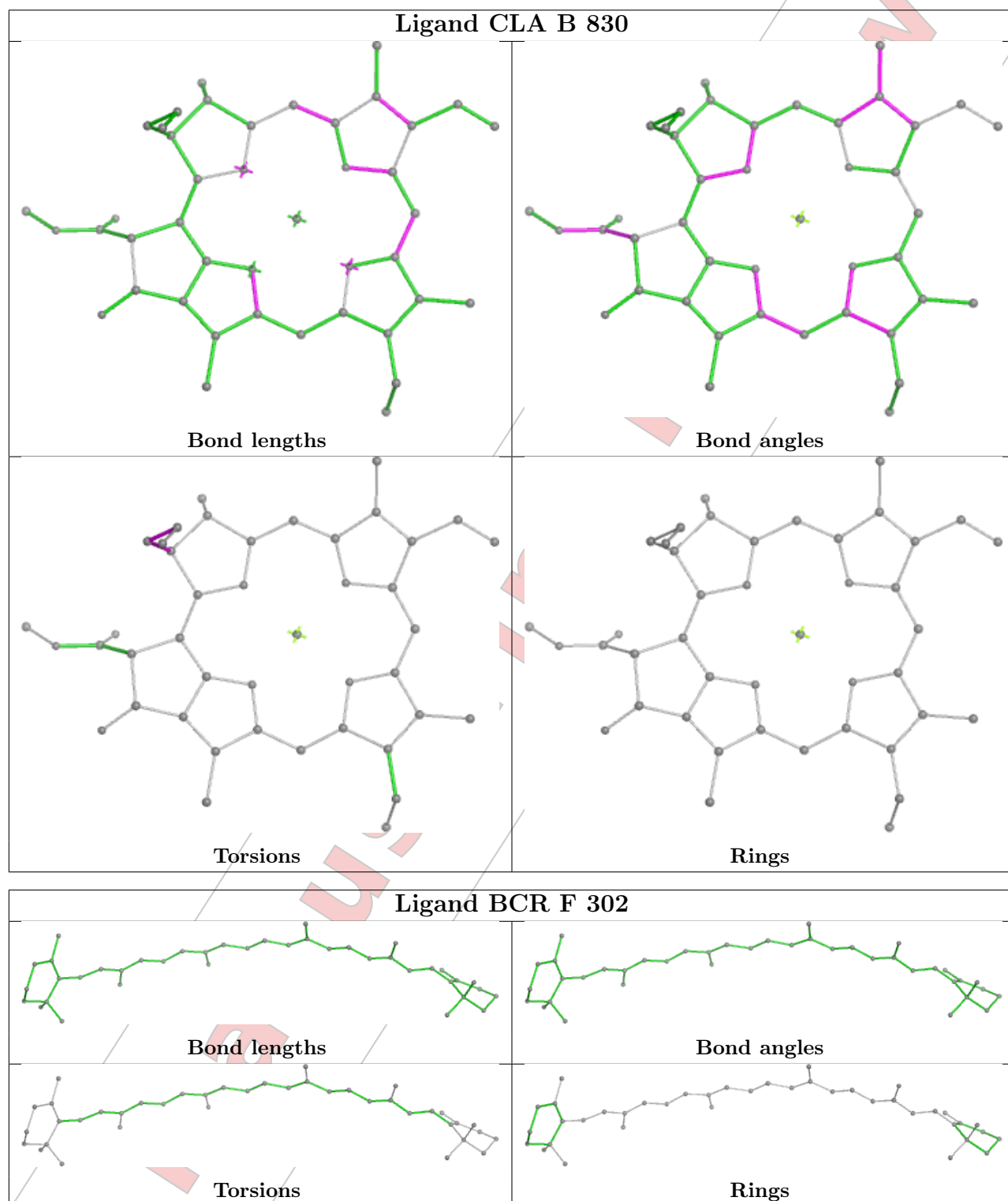
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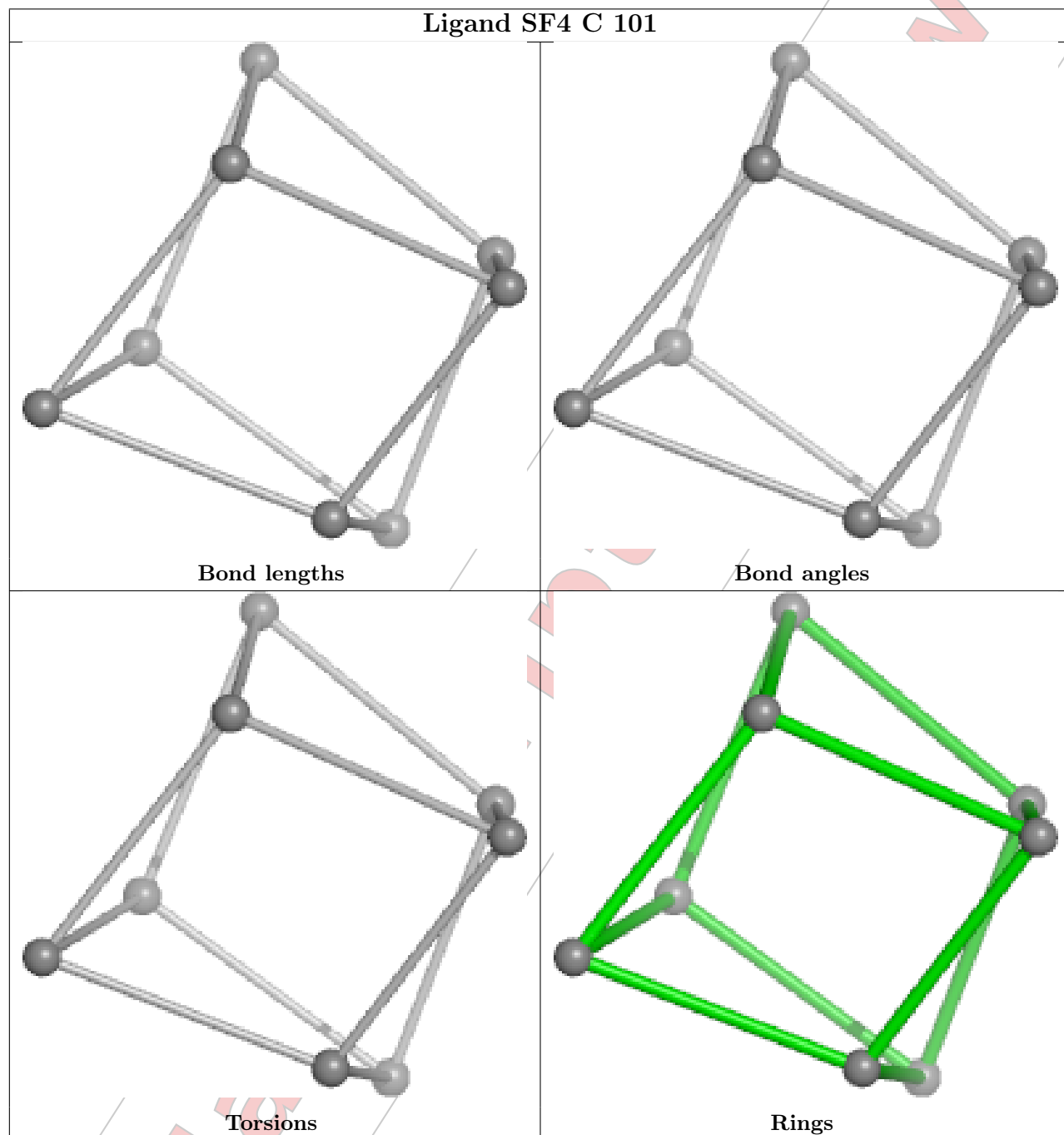
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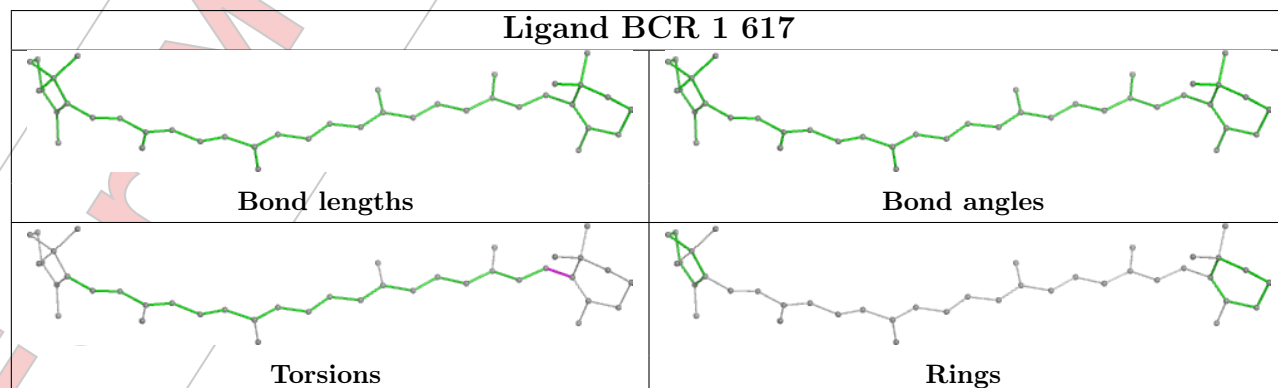


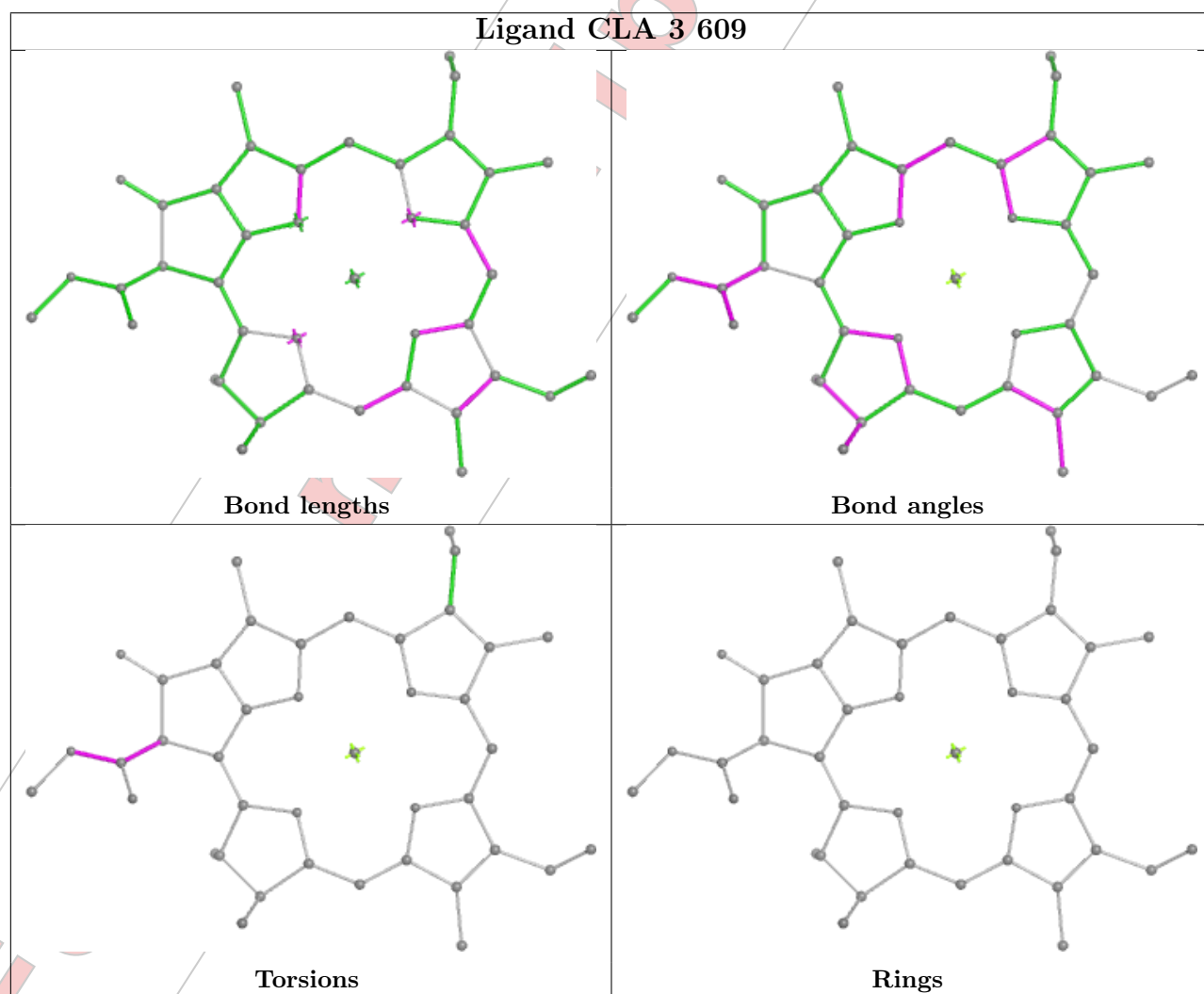
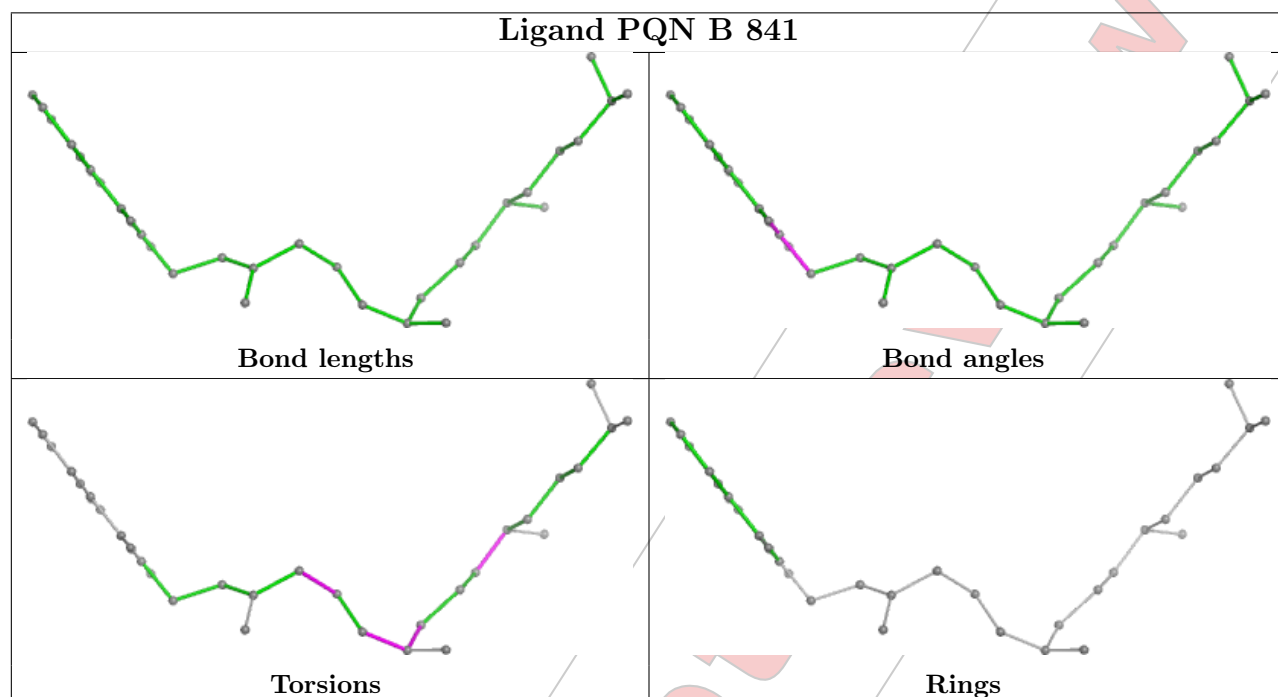


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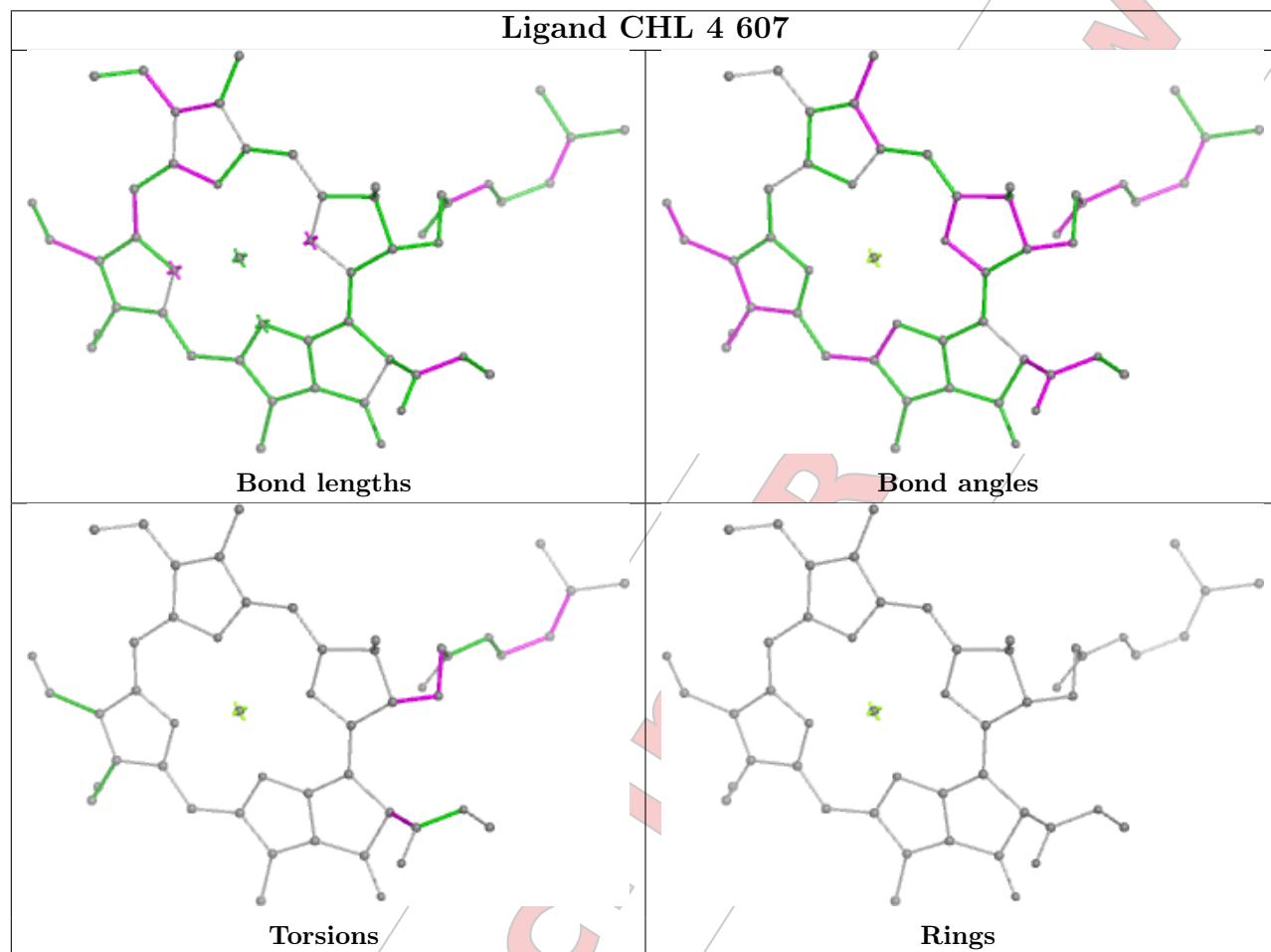


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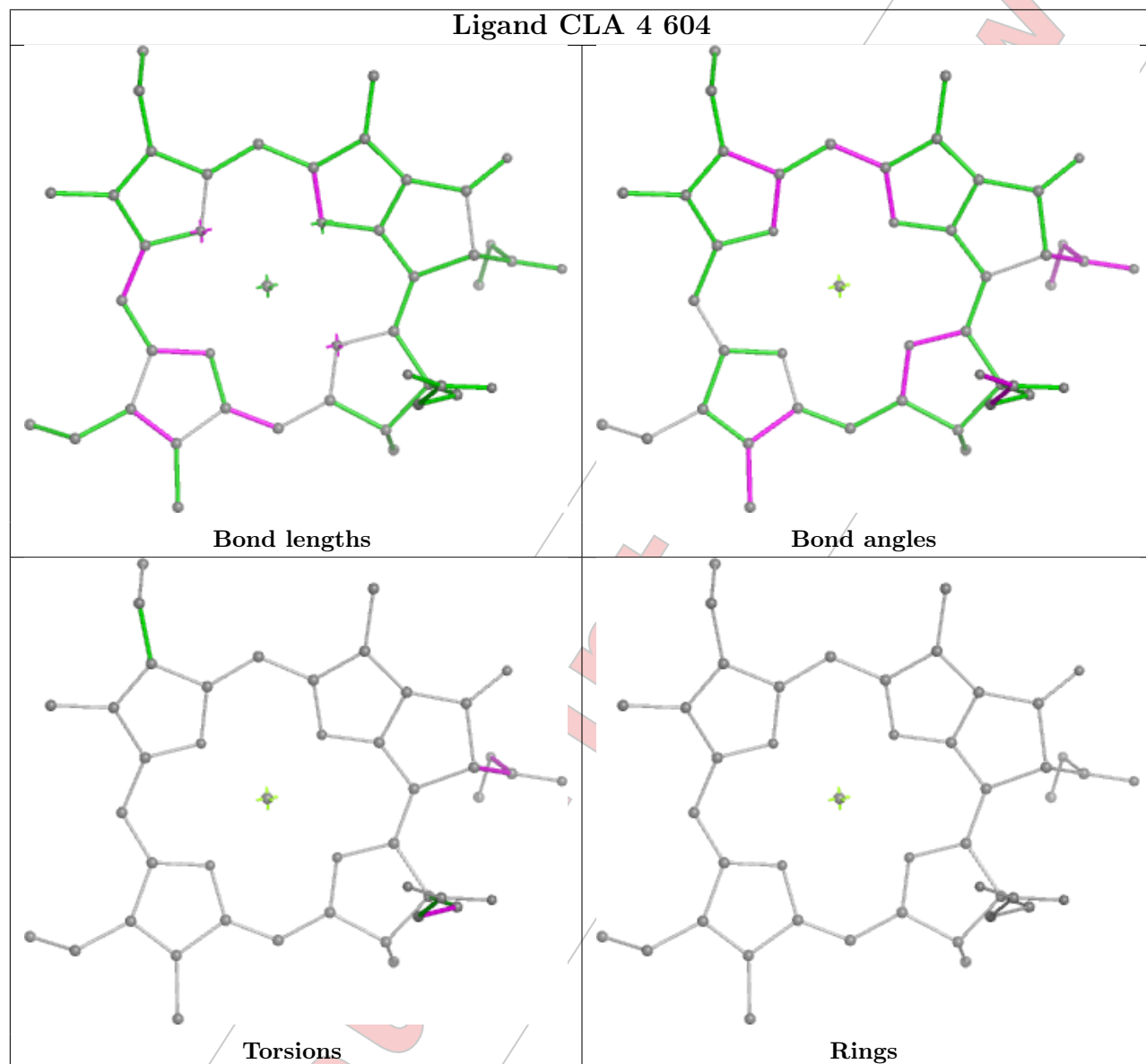


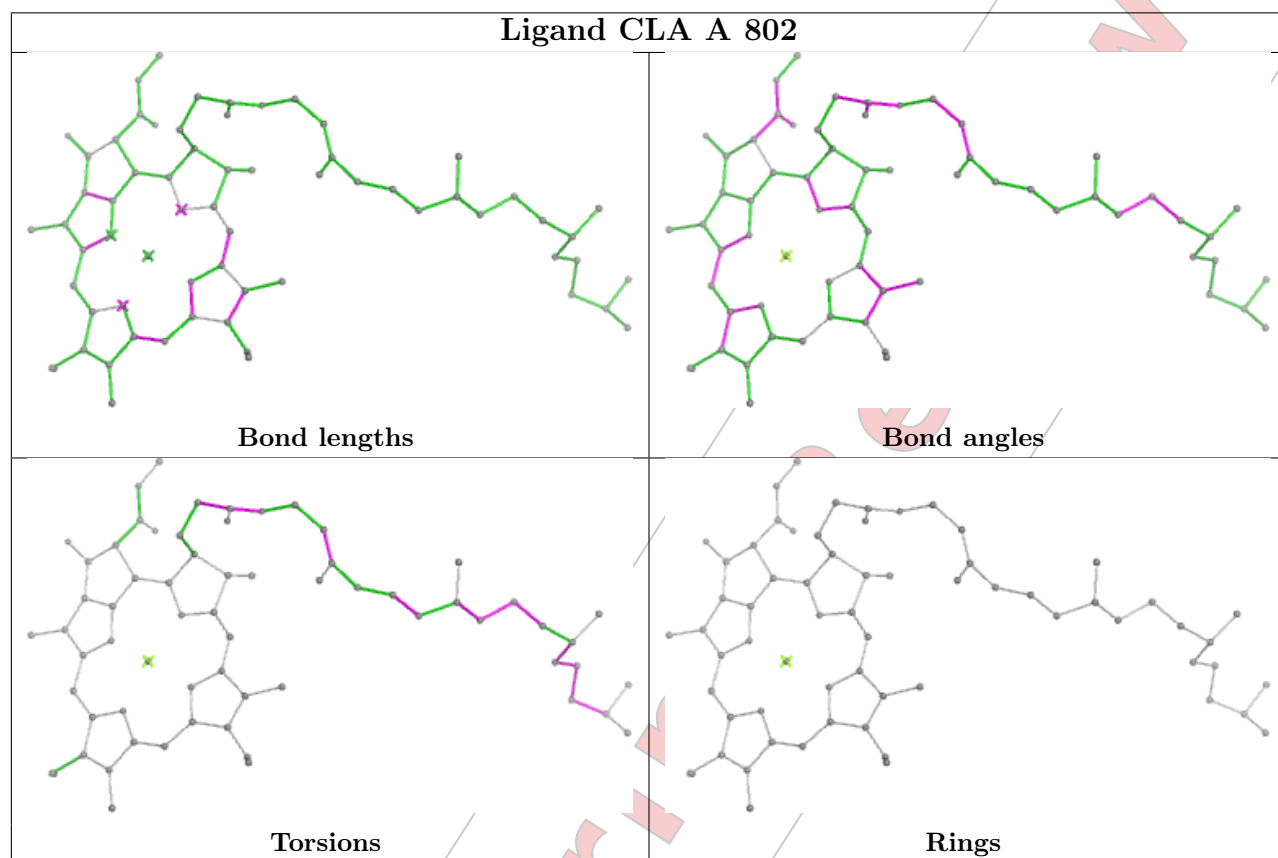


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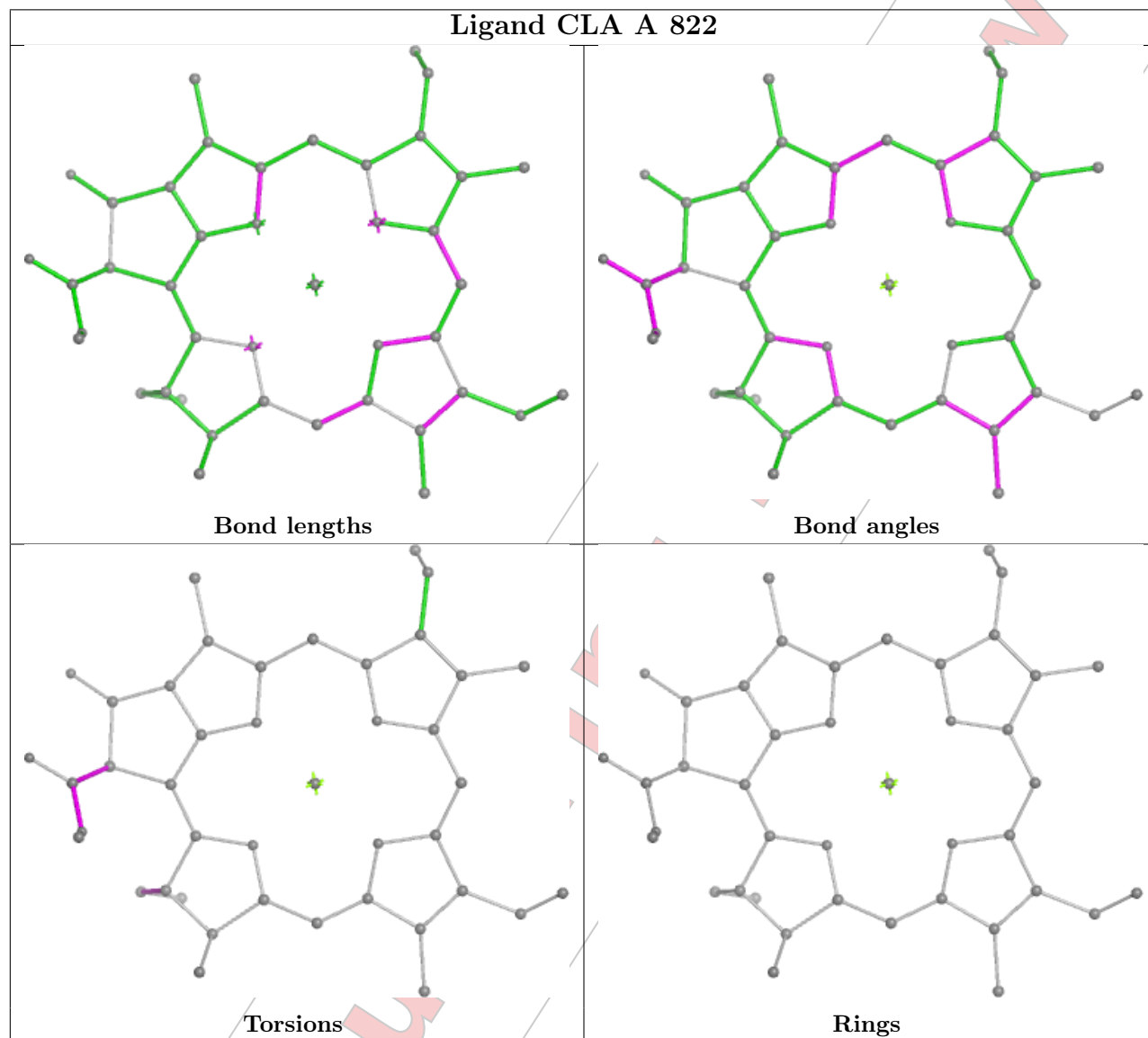


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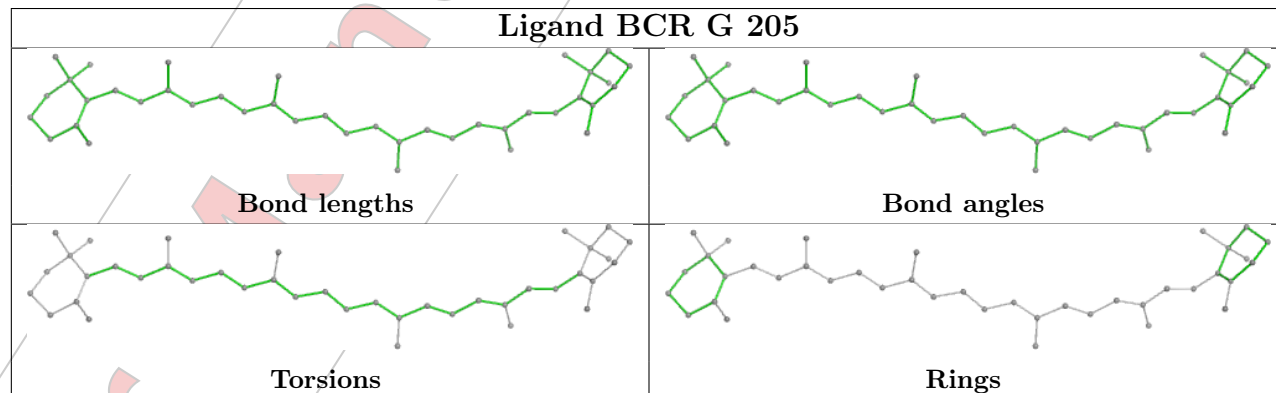


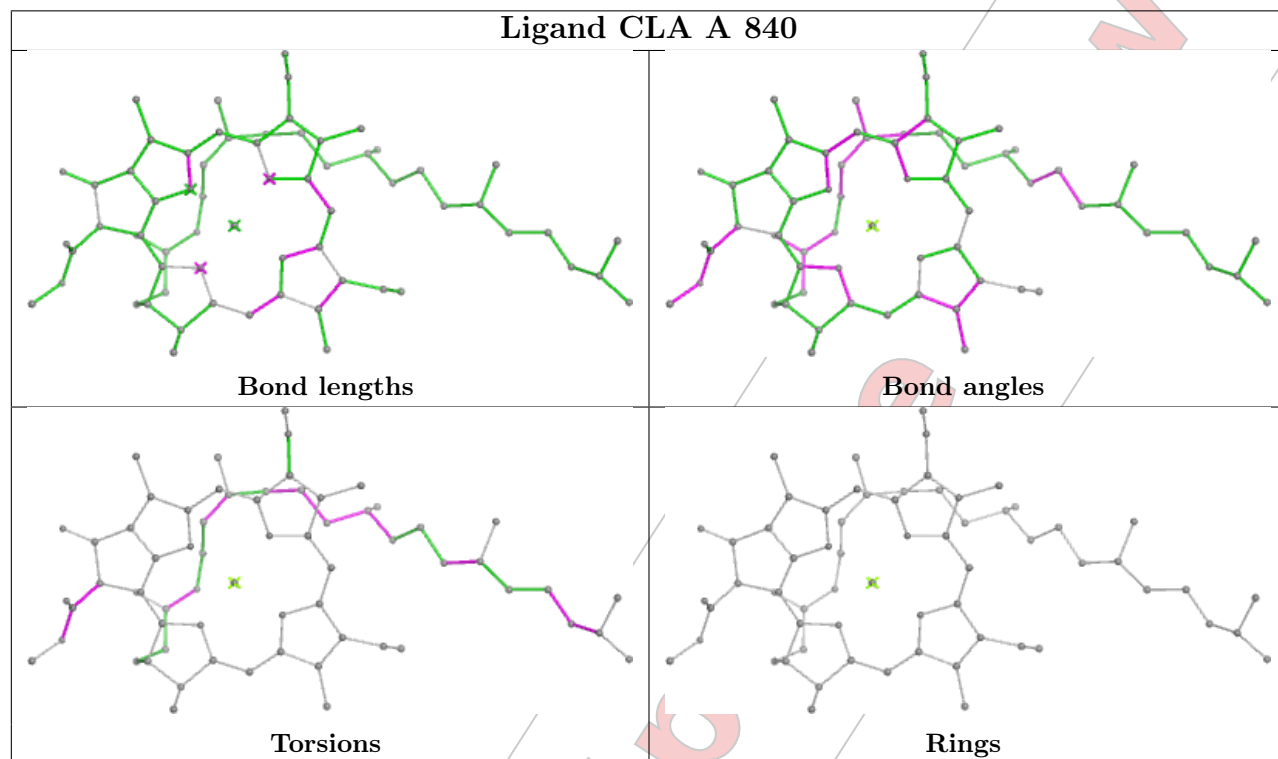


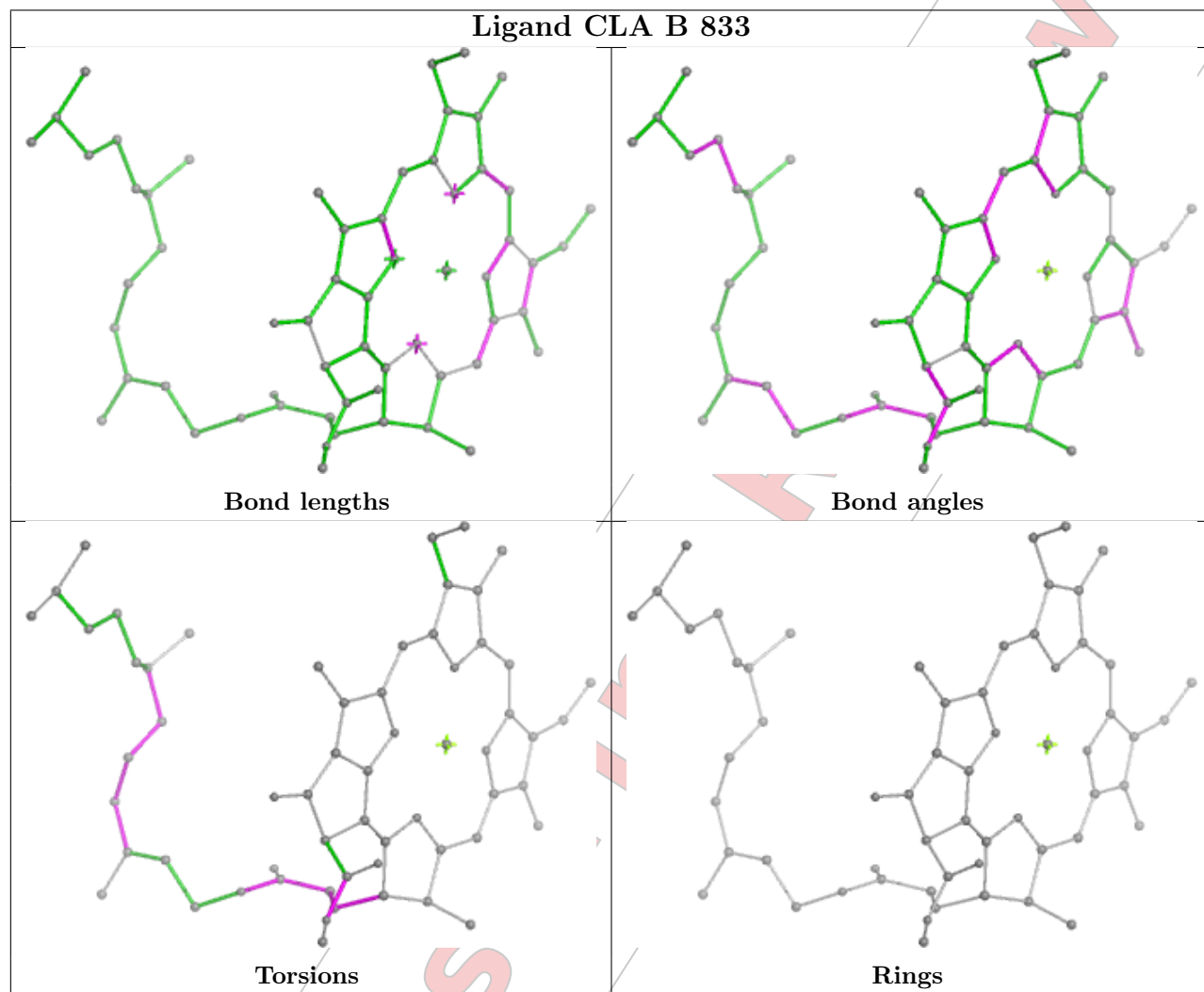
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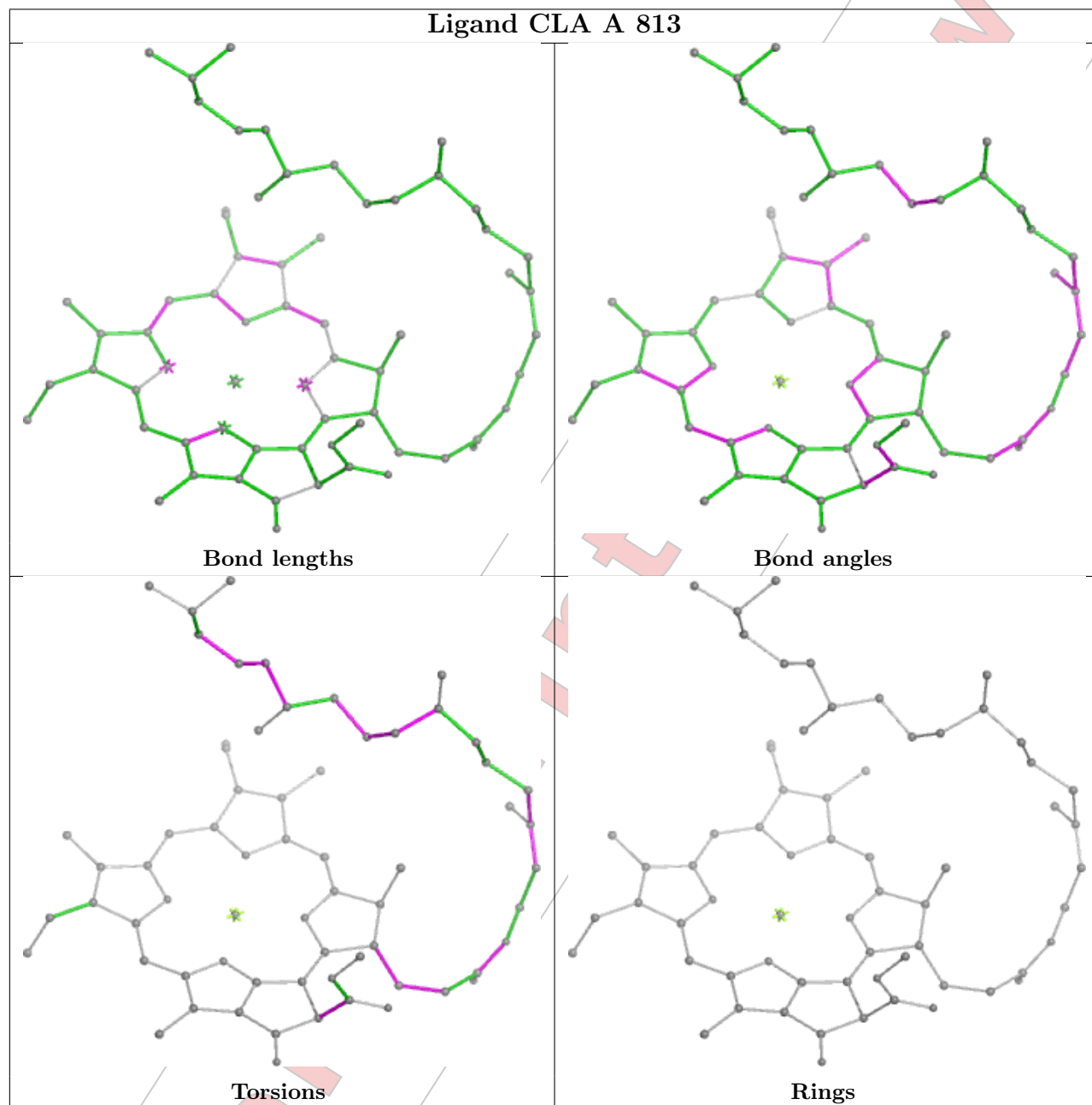




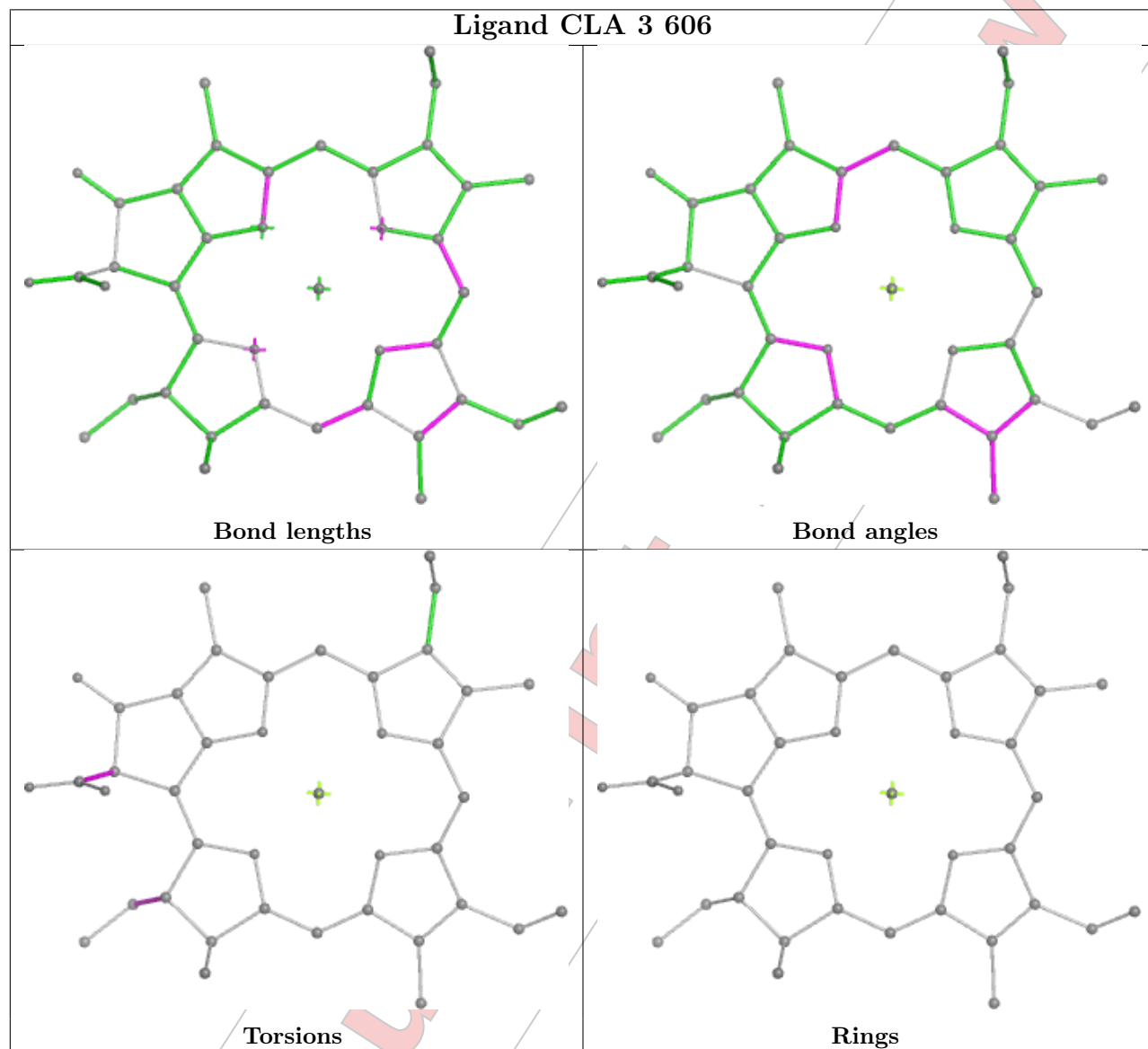


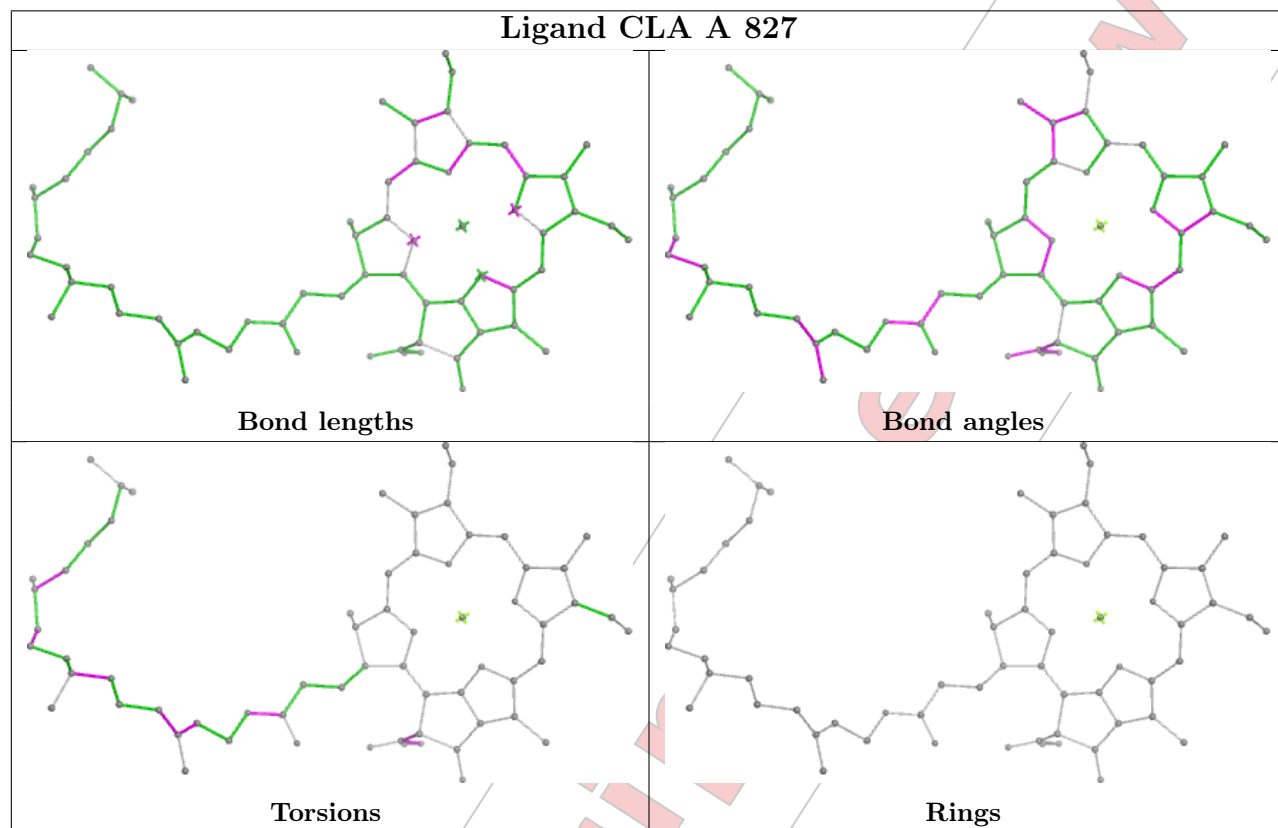
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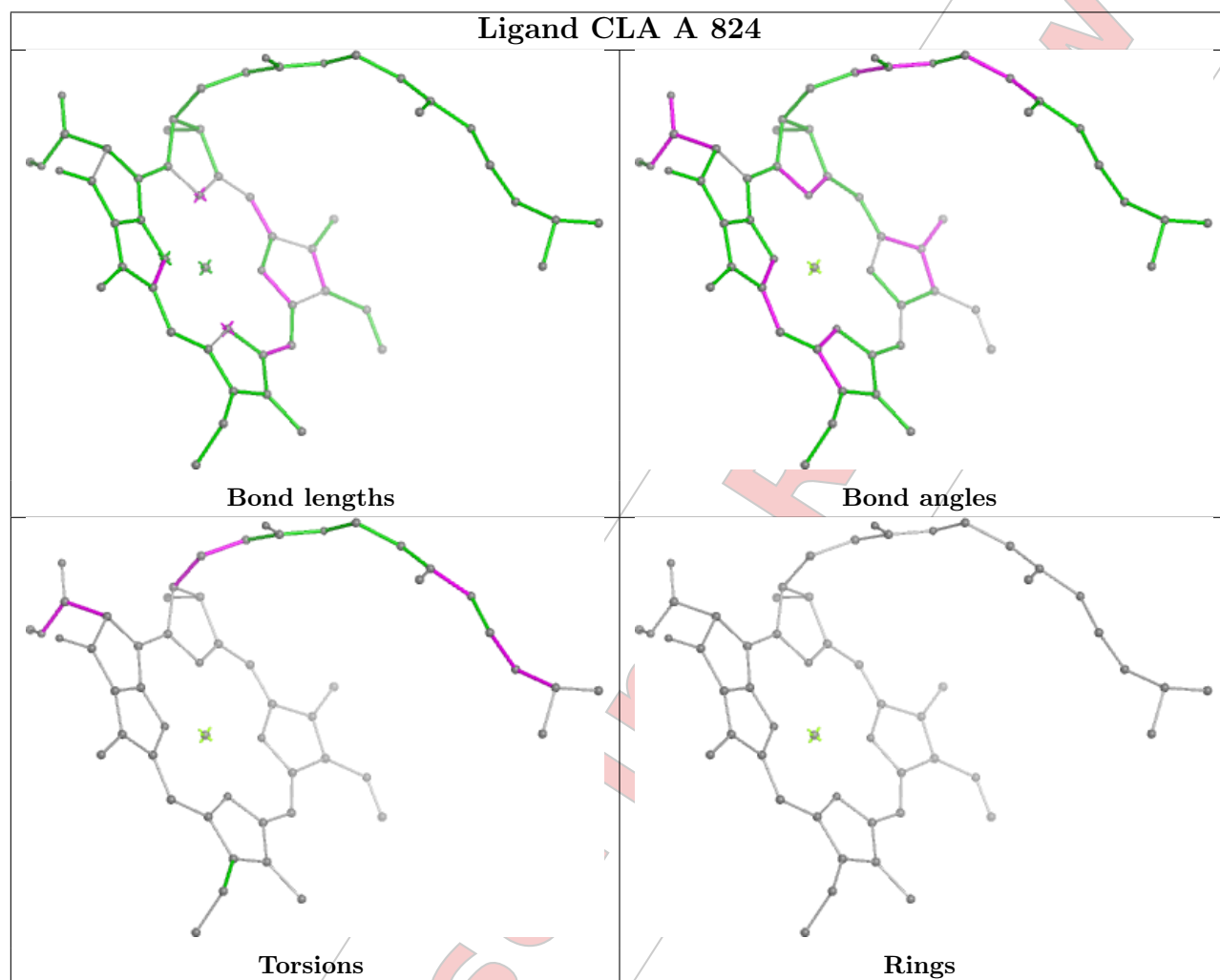
Ligand CLA A 813

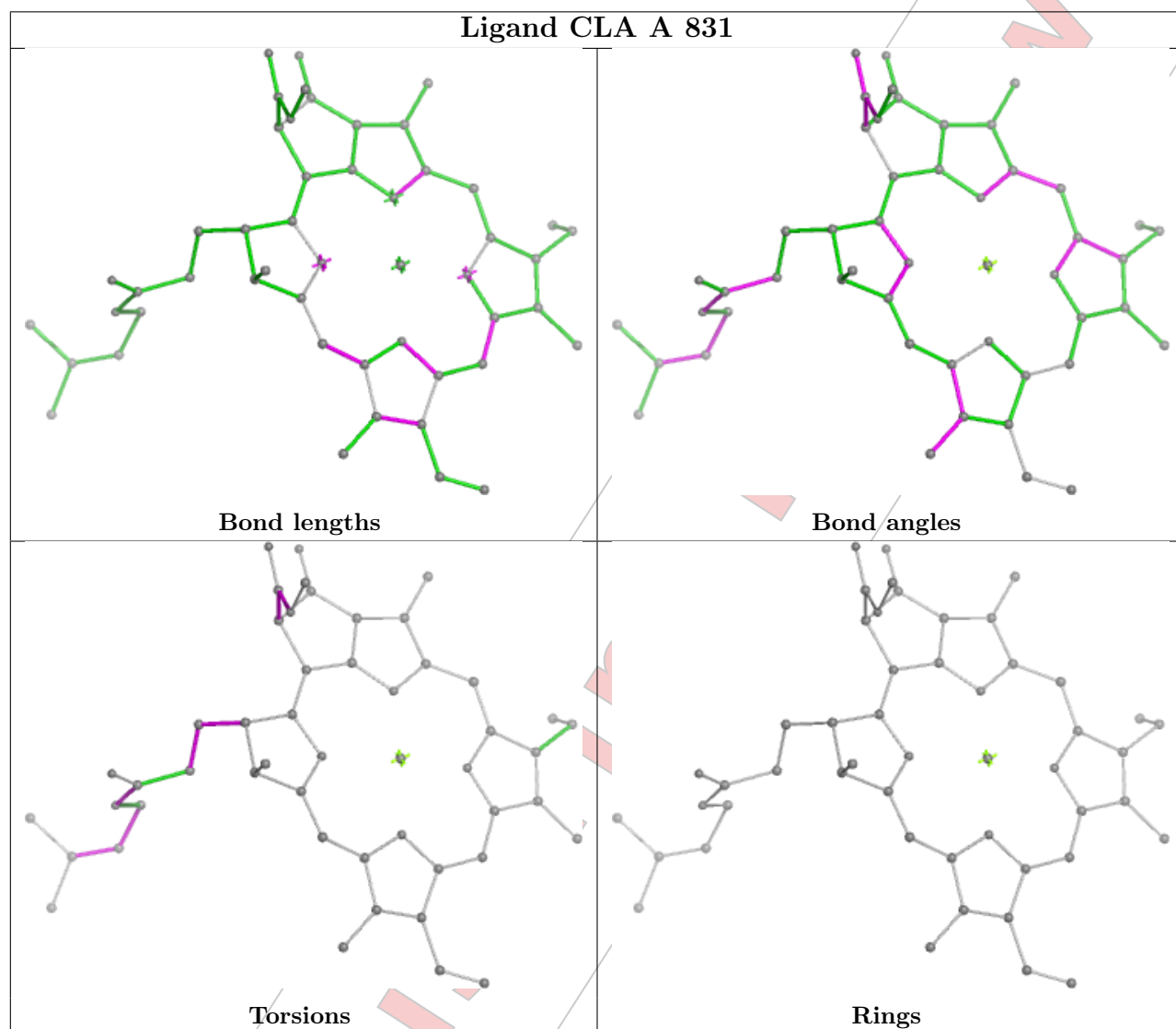


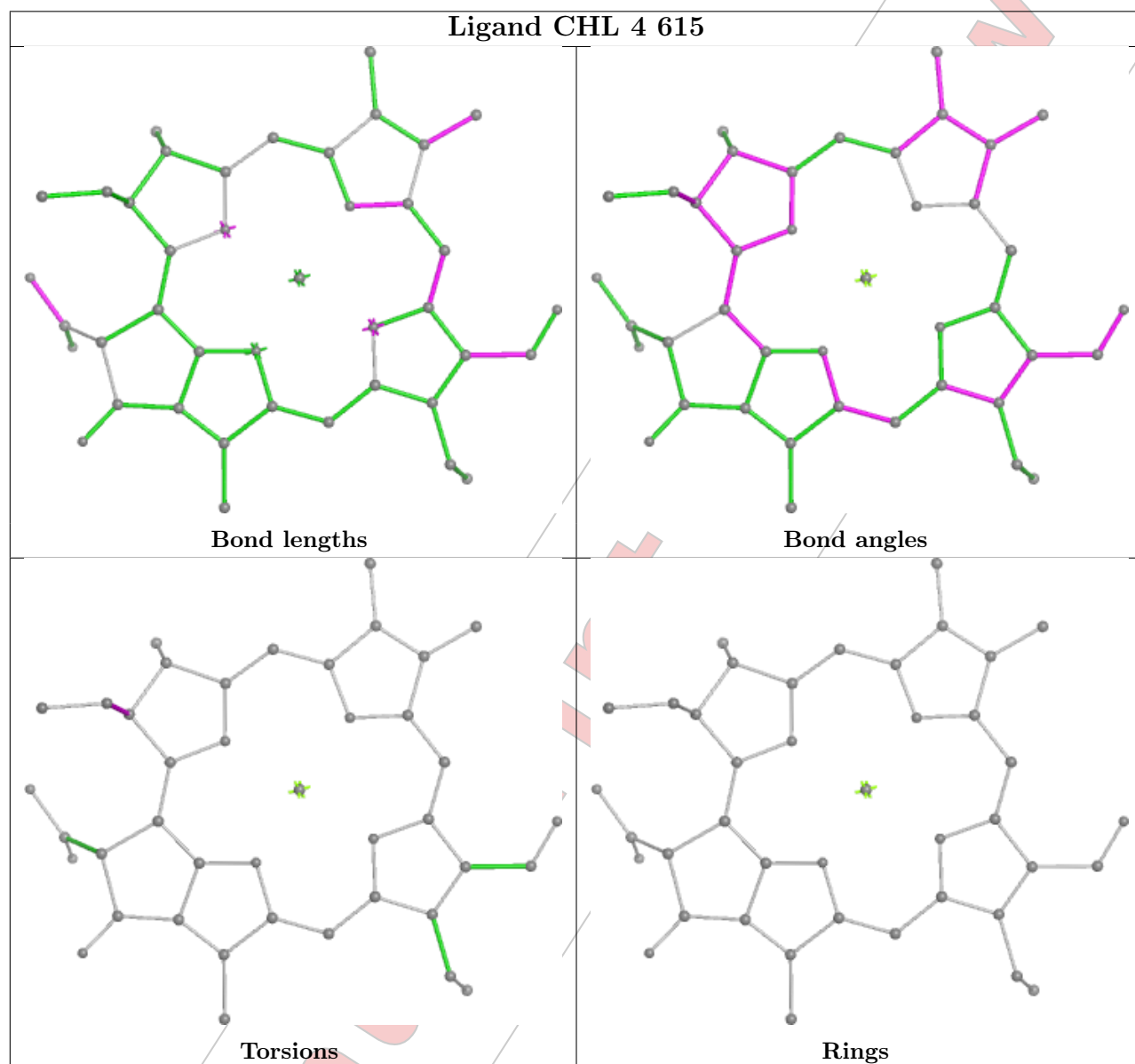
Ligand CLA 3 606











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.

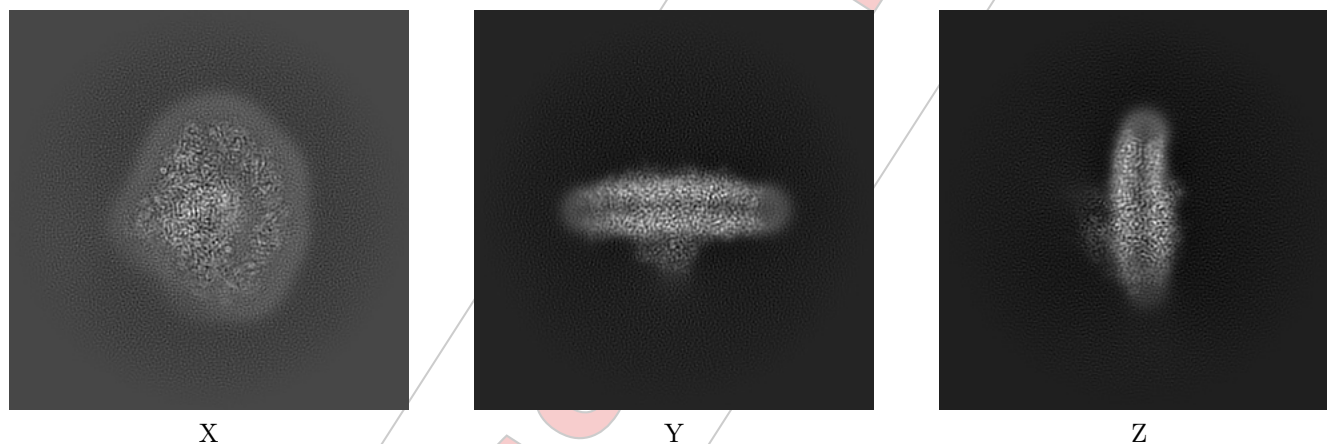
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54455. 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](#)

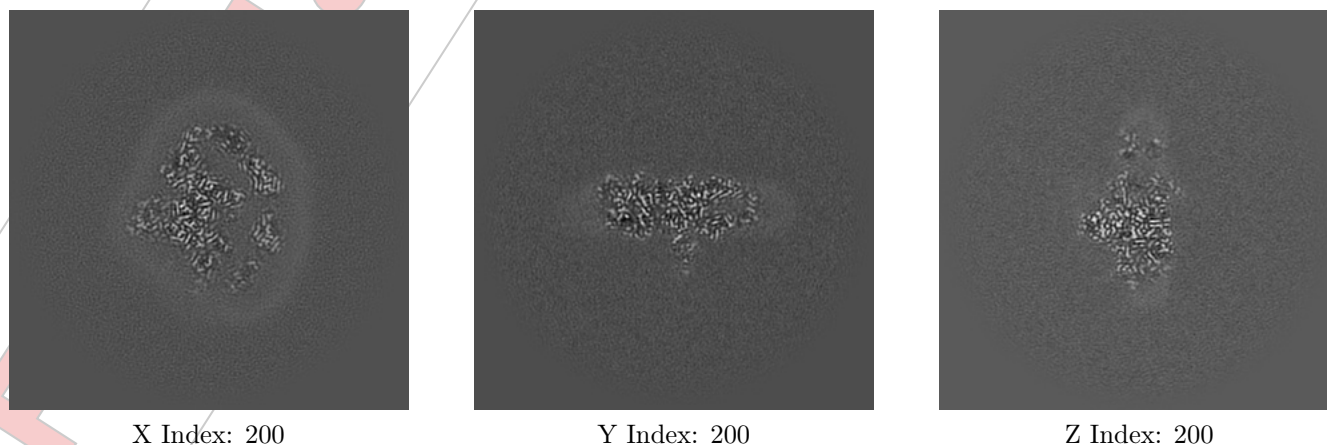
6.1.1 Primary map



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

6.2 Central slices [i](#)

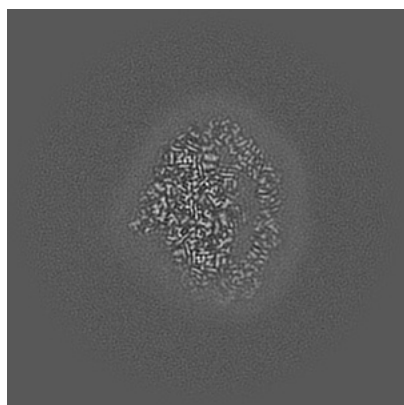
6.2.1 Primary map



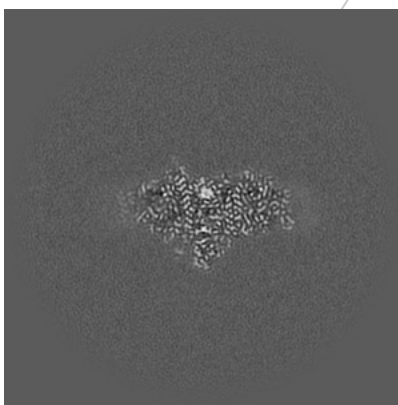
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

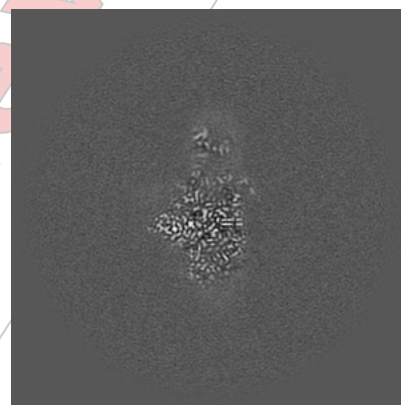
6.3.1 Primary map



X Index: 215



Y Index: 184

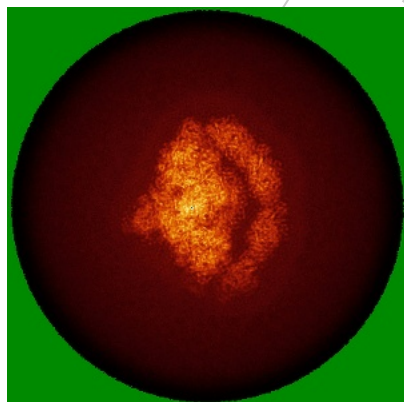


Z Index: 198

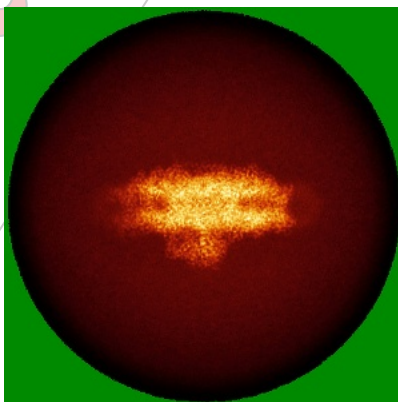
The images above show the largest variance slices of the map in three orthogonal directions.

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

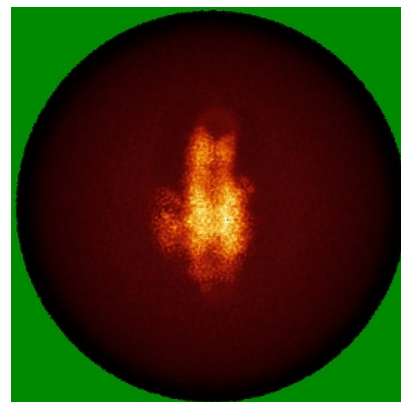
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

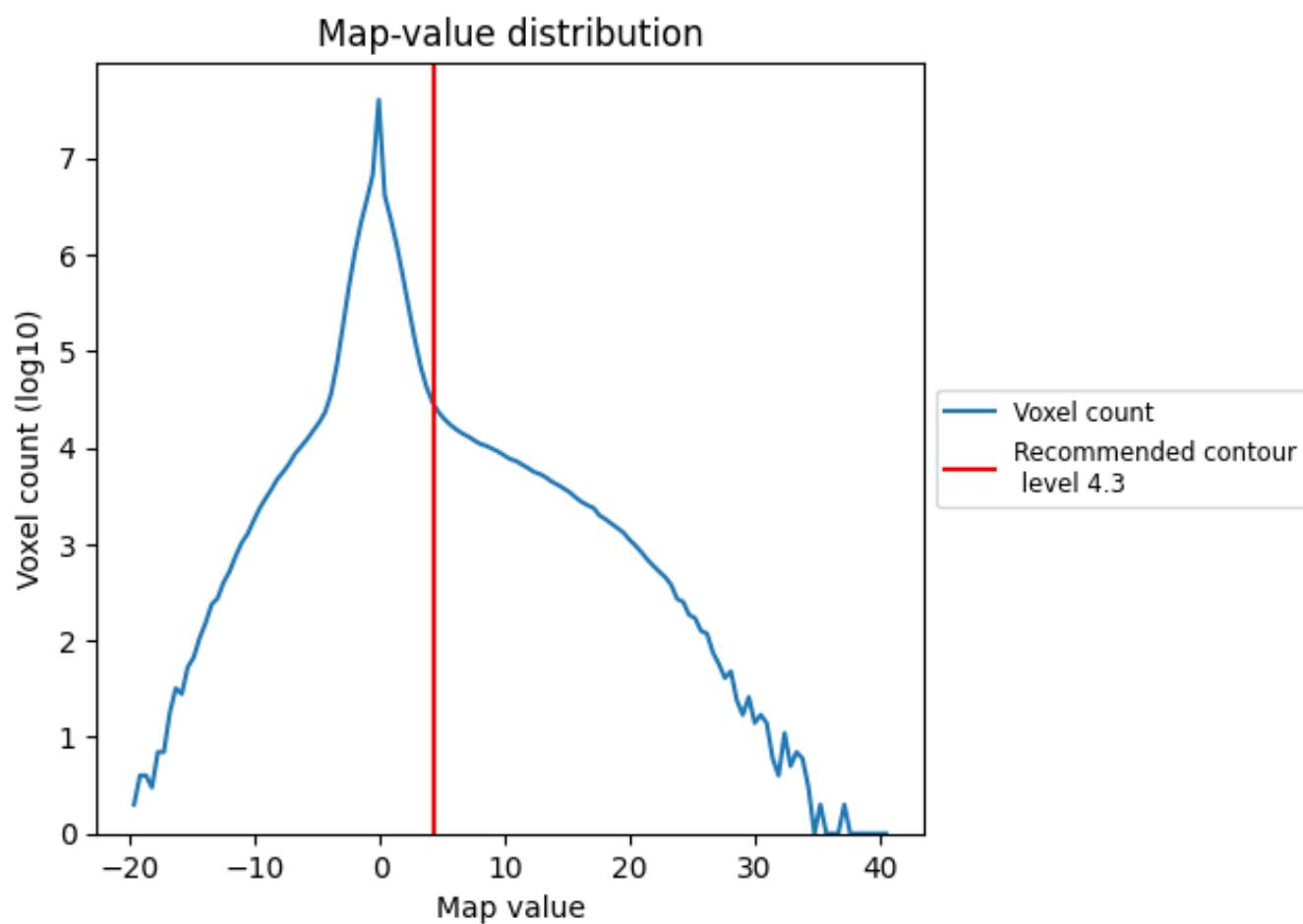
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

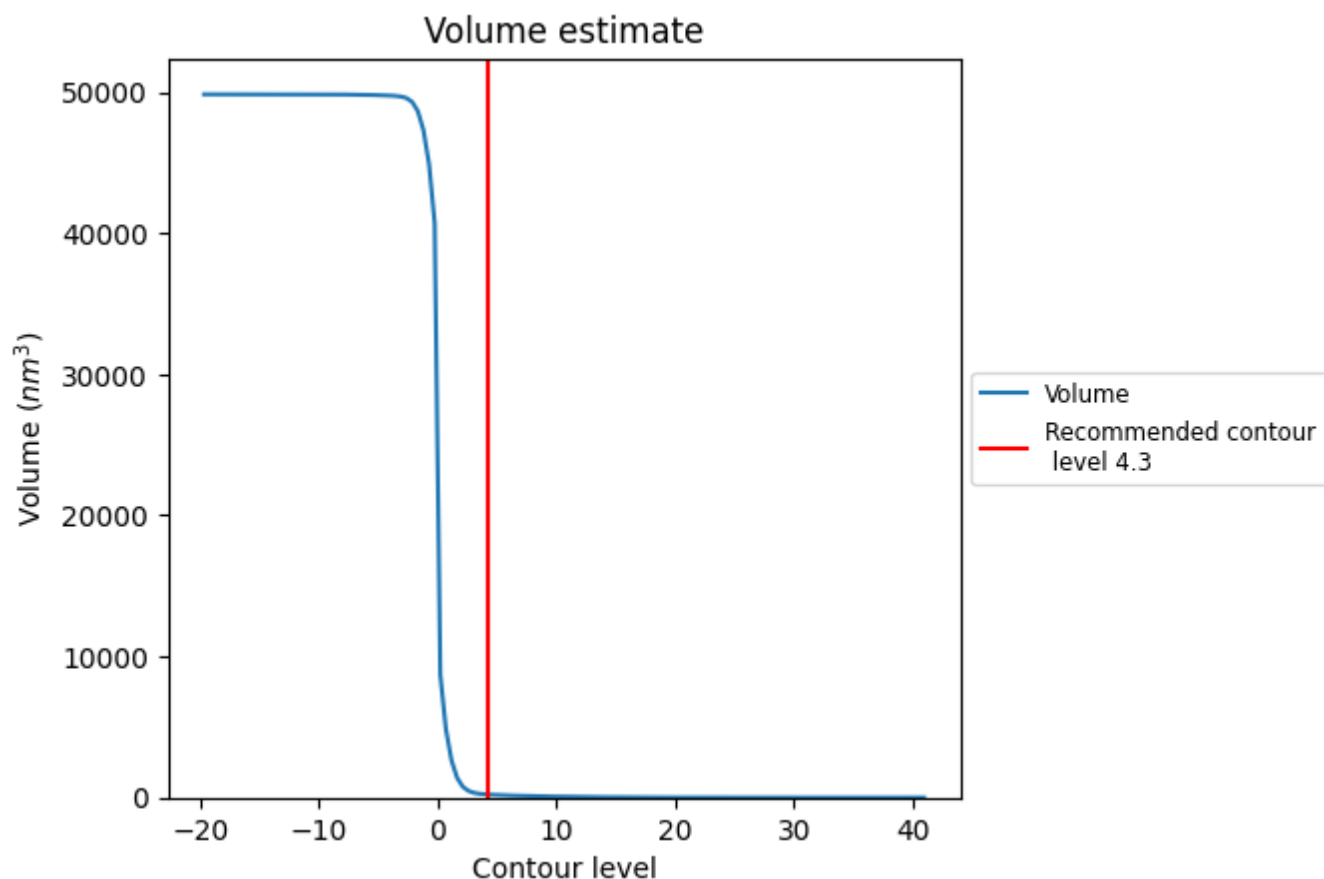
This section contains the results of statistical analysis of the map.

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.

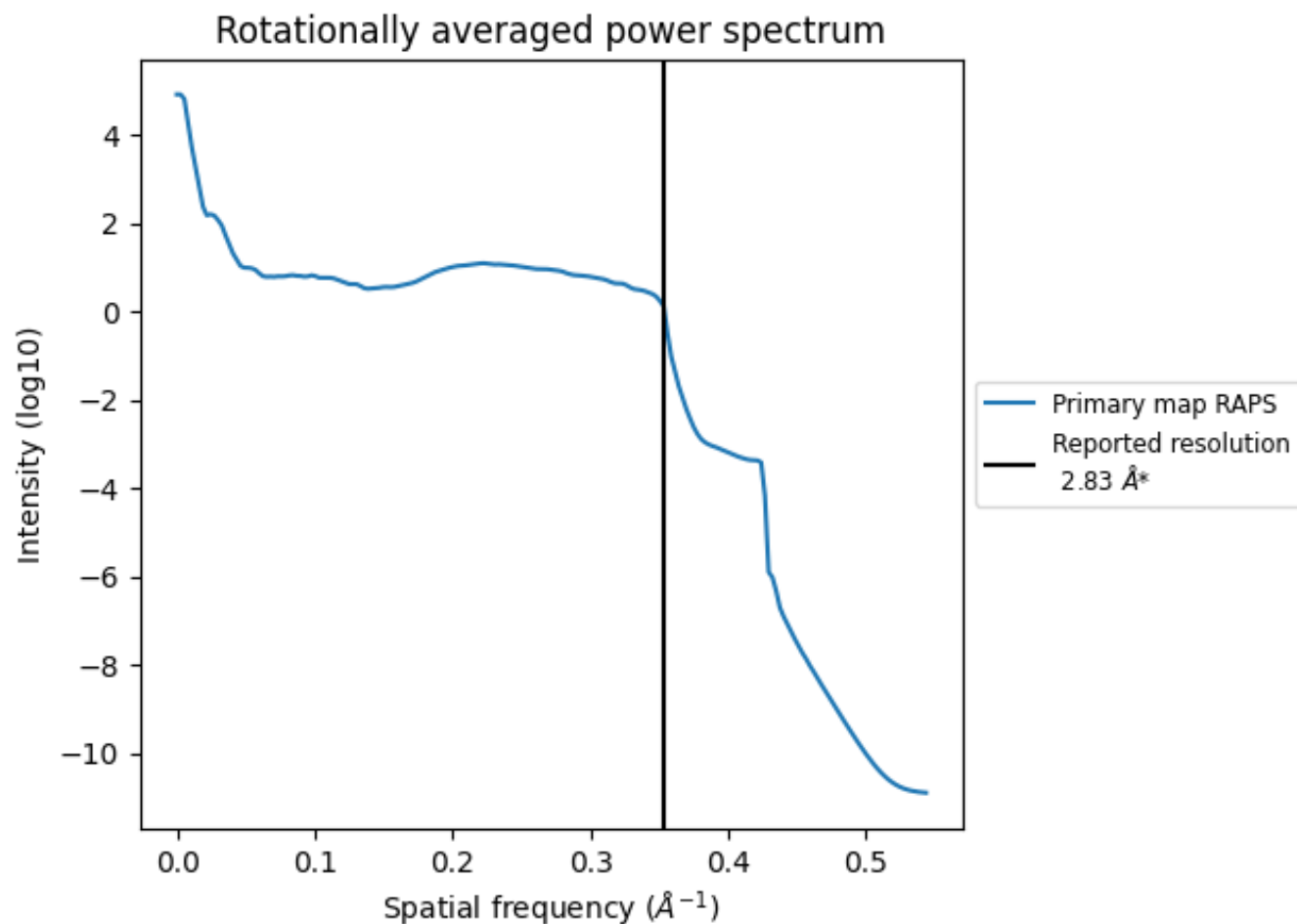
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm^3 ; this corresponds to an approximate mass of 192 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 0.353 Å⁻¹

8 Fourier-Shell correlation ⓘ

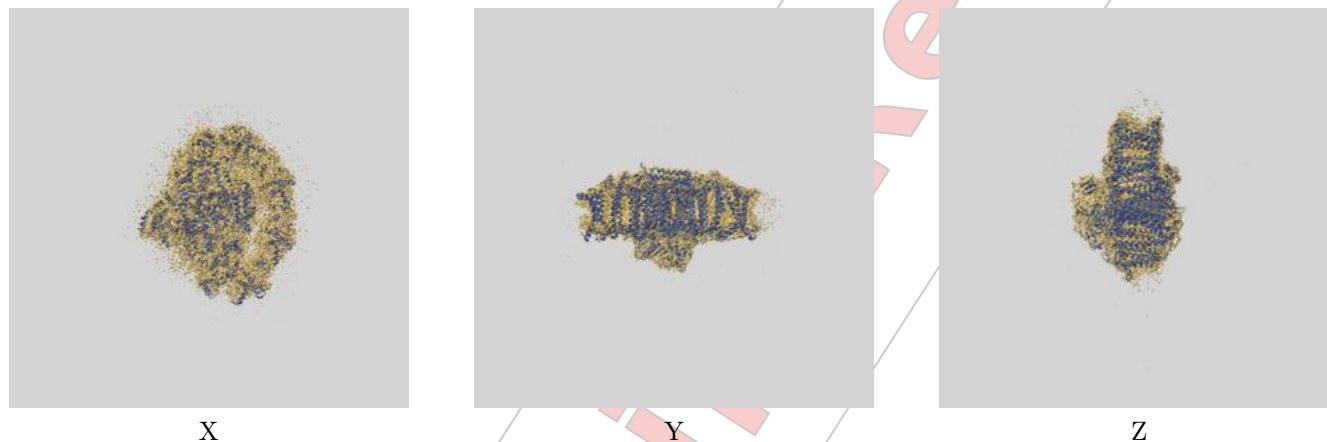
This section was not generated. No FSC curve or half-maps provided.

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9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-54455 and PDB model 9S1L. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay ⓘ



The images above show the 3D surface view of the map at the recommended contour level 4.3 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](#)



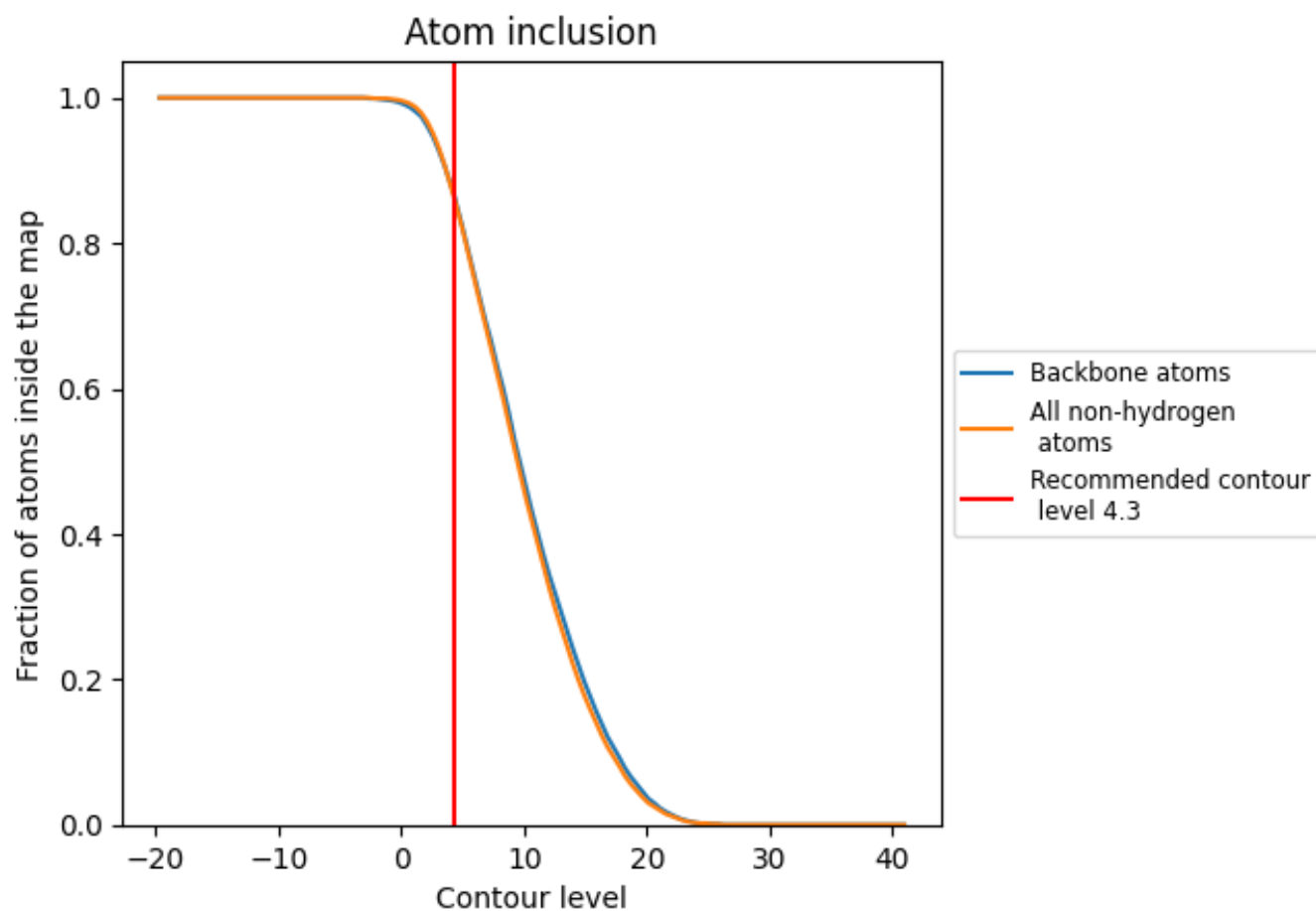
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.5940
1	 0.8810	 0.5940
2	 0.8480	 0.5650
3	 0.6900	 0.5240
4	 0.8740	 0.5890
A	 0.9050	 0.6120
B	 0.9380	 0.6240
C	 0.9280	 0.6080
D	 0.8550	 0.5960
E	 0.8450	 0.5930
F	 0.7980	 0.5730
G	 0.8770	 0.5950
H	 0.6370	 0.5330
I	 0.8880	 0.5990
J	 0.7290	 0.5240
K	 0.4710	 0.4880
L	 0.7980	 0.5810

