



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:23 AM EDT

PDB ID : 1JB0 / pdb_00001jb0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

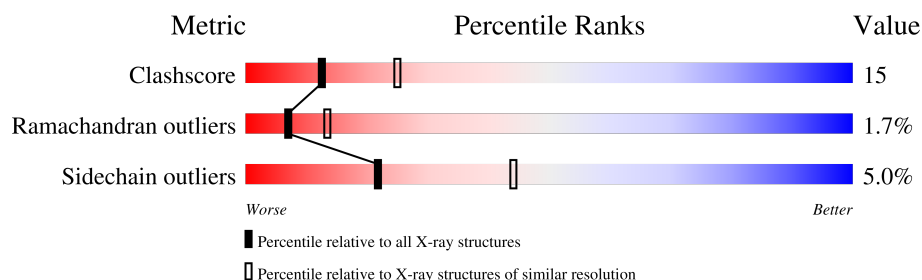
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	755	67% 26% 5% •
2	B	740	68% 27% 5% •
3	C	80	68% 28% • •
4	D	138	64% 31% • •
5	E	75	67% 21% • 8%
6	F	164	55% 27% • 14%
7	I	38	68% 26% 5%
8	J	41	54% 37% 10%

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Mol	Chain	Length	Quality of chain
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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	LHG	A	5003	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 24198 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- Molecule 3 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ARG	PRO	conflict	UNP P25902
L	144	VAL	-	SEE REMARK 999	UNP P25902
L	145	VAL	-	SEE REMARK 999	UNP P25902
L	146	ASP	-	SEE REMARK 999	UNP P25902
L	147	GLY	-	SEE REMARK 999	UNP P25902
L	148	ILE	-	SEE REMARK 999	UNP P25902
L	149	MET	-	SEE REMARK 999	UNP P25902
L	150	THR	-	SEE REMARK 999	UNP P25902
L	151	GLY	-	SEE REMARK 999	UNP P25902
L	152	LEU	-	SEE REMARK 999	UNP P25902
L	153	PHE	-	SEE REMARK 999	UNP P25902
L	154	ASN	-	SEE REMARK 999	UNP P25902

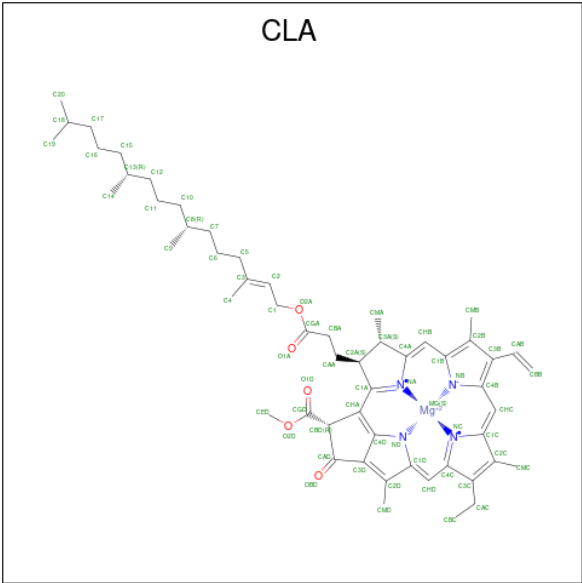
- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	M	31	241	161	36	43	1	0	0	0

- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	233	164	34	35	0	0	0

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	59	49	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	A	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
13	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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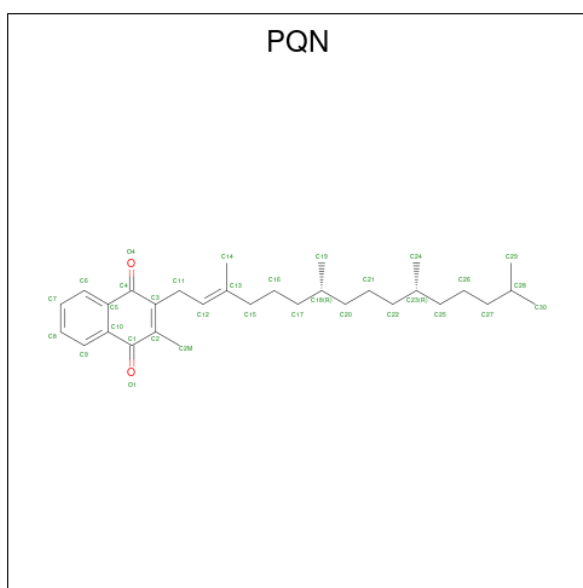
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

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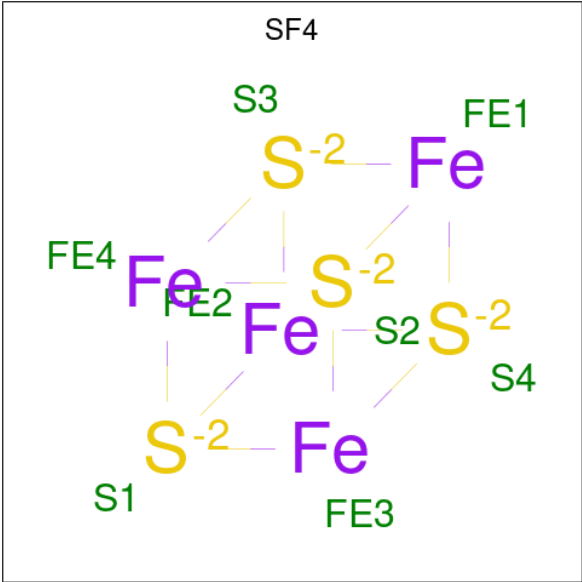
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



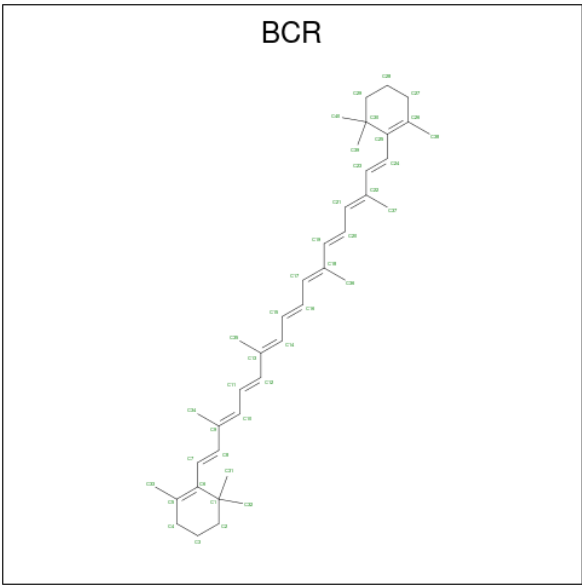
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			33	31	2		
14	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



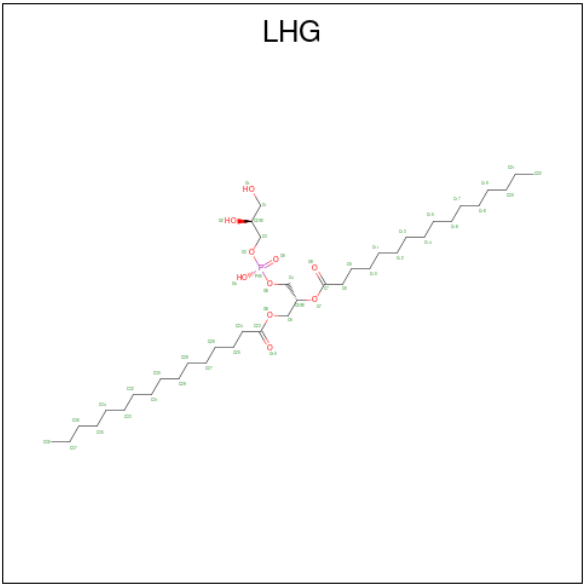
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		

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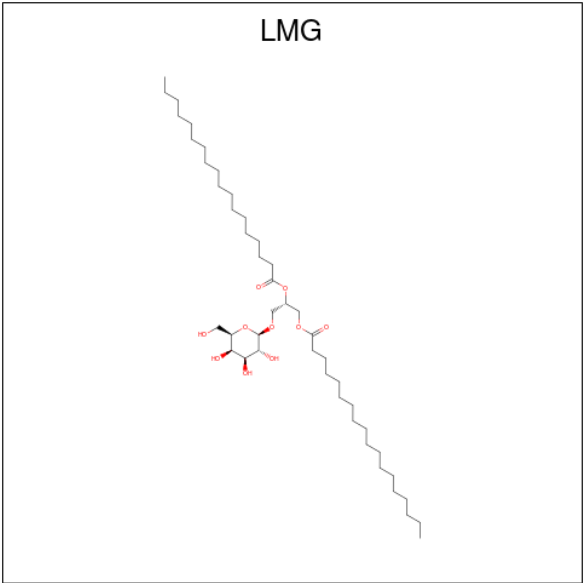
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	A	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 25 25	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	M	1	Total C 40 40	0	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			49	38	10	1		
17	A	1	Total	C	O	P	0	0
			27	16	10	1		
17	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		
20	C	21	Total	O	0	0
			21	21		
20	D	17	Total	O	0	0
			17	17		
20	E	5	Total	O	0	0
			5	5		
20	F	6	Total	O	0	0
			6	6		
20	I	3	Total	O	0	0
			3	3		
20	J	1	Total	O	0	0
			1	1		
20	L	27	Total	O	0	0
			27	27		
20	M	3	Total	O	0	0
			3	3		

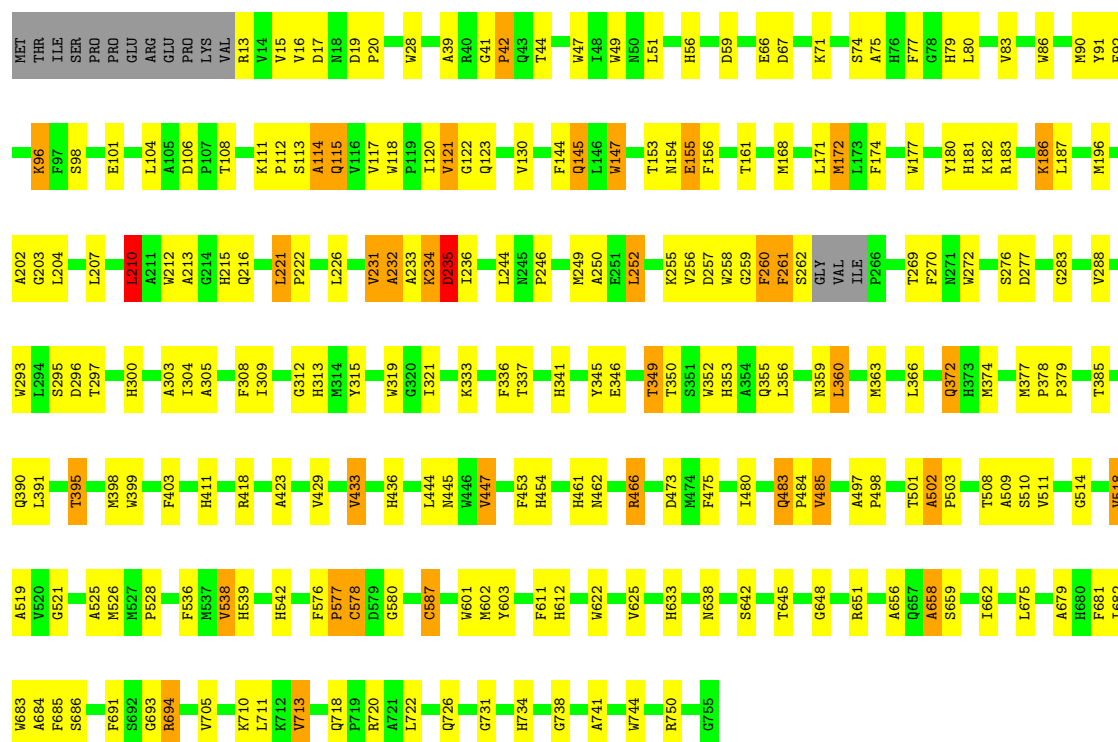
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

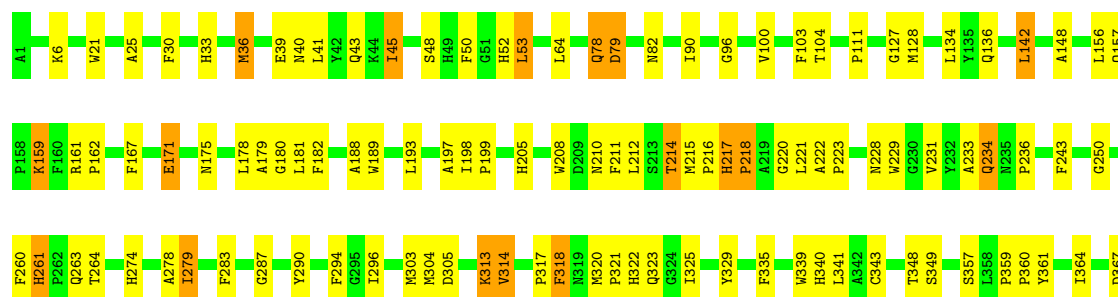
• Molecule 1: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

Chain A: 



• Molecule 2: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

Chain B: 





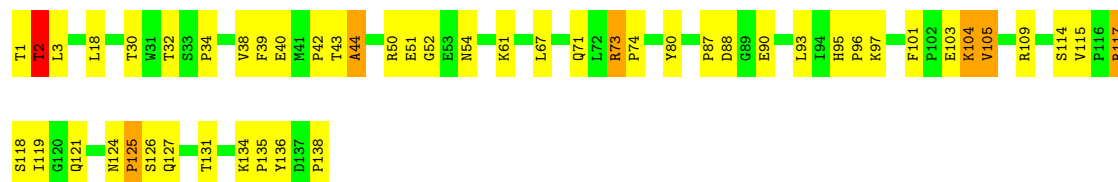
● Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 68% 28%



● Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D: 64% 31%



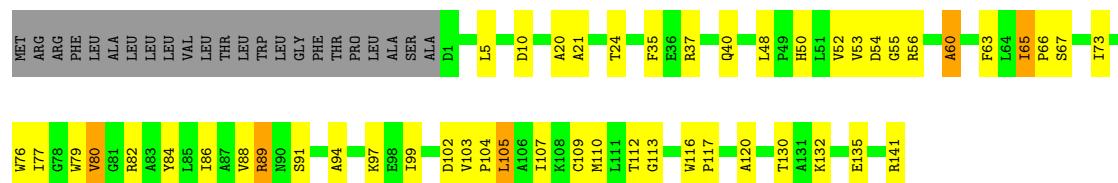
● Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E: 67% 21% 8%



● Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F: 55% 27% 14%



● Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I: 68% 26% 5%



- Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX



- Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X



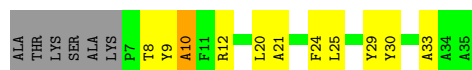
- Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI



- Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII



- Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (30.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24198	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LHG, BCR, CLA, PQN, CA, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/5983	1.04	40/8158 (0.5%)
2	B	0.66	2/6096 (0.0%)	1.02	34/8332 (0.4%)
3	C	0.91	0/608	1.30	12/824 (1.5%)
4	D	0.65	0/1101	1.19	7/1492 (0.5%)
5	E	0.64	0/551	1.26	8/750 (1.1%)
6	F	0.55	1/1087 (0.1%)	1.02	1/1476 (0.1%)
7	I	0.84	0/312	1.15	1/425 (0.2%)
8	J	0.48	0/350	1.18	4/477 (0.8%)
9	K	0.72	0/219	1.50	5/297 (1.7%)
10	L	0.77	0/1148	1.04	3/1558 (0.2%)
11	M	0.75	0/244	1.13	1/332 (0.3%)
12	X	0.52	0/242	1.09	2/332 (0.6%)
All	All	0.65	3/17941 (0.0%)	1.07	118/24453 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	589	MET	SD-CE	-8.57	1.58	1.79
2	B	36	MET	SD-CE	-7.66	1.60	1.79
6	F	65	ILE	CA-CB	5.15	1.57	1.54

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	131	THR	N-CA-C	-13.95	89.86	109.95
9	K	35	GLN	N-CA-C	10.55	125.45	109.62
11	M	30	TYR	N-CA-C	10.04	132.18	110.80
2	B	482	SER	N-CA-C	-8.83	102.52	113.38
2	B	553	MET	CA-C-N	8.38	128.50	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	219	0
2	B	5879	0	5632	239	0
3	C	598	0	580	17	0
4	D	1075	0	1077	41	0
5	E	539	0	528	10	0
6	F	1065	0	1079	45	0
7	I	301	0	306	8	0
8	J	338	0	347	23	0
9	K	222	0	110	5	0
10	L	1119	0	1125	22	0
11	M	241	0	264	13	0
12	X	233	0	231	6	0
13	A	2687	0	2675	130	0
13	B	2349	0	2304	132	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	10	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	21	0
16	B	265	0	369	15	0
16	F	40	0	56	2	0
16	I	80	0	112	4	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	0
20	A	53	0	0	5	0
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	1
20	M	3	0	0	1	0
All	All	24198	0	23804	728	1

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 15.

The worst 5 of 728 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)
8:J:31:ARG:HD3	16:J:4013:BCR:H312	1.25	1.17
2:B:622:LEU:HD12	13:B:1012:CLA:H11	1.29	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.05
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:4048:HOH:O	20:L:4048:HOH:O[2_655]	1.94	0.26

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	9	17
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	20
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	18
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	5	9
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	1
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	5	9
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	0
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	9	18
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	4
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	2	3
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	7	13

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE
2	B	234	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	563 (96%)	26 (4%)	25	50
2	B	595/597 (100%)	563 (95%)	32 (5%)	20	41
3	C	67/67 (100%)	65 (97%)	2 (3%)	36	64
4	D	115/115 (100%)	105 (91%)	10 (9%)	9	21
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	66
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	34
8	J	36/36 (100%)	34 (94%)	2 (6%)	19	39
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	25
11	M	26/26 (100%)	24 (92%)	2 (8%)	12	25
12	X	20/24 (83%)	19 (95%)	1 (5%)	22	44
All	All	1765/1811 (98%)	1676 (95%)	89 (5%)	22	44

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	698	ARG
6	F	80	VAL
3	C	65	ARG
4	D	104	LYS
8	J	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	648	ASN
4	D	95	HIS
2	B	678	GLN
4	D	54	ASN
6	F	40	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	LHG	A	5003	13	26,26,48	2.37	5 (19%)	29,32,54	1.58	5 (17%)
13	CLA	B	1226	2	69,73,73	1.30	6 (8%)	82,113,113	1.66	10 (12%)
16	BCR	A	4001	-	41,41,41	1.39	6 (14%)	56,56,56	1.93	16 (28%)
13	CLA	B	1023	-	69,73,73	1.40	9 (13%)	82,113,113	1.58	5 (6%)
13	CLA	B	1222	20	50,54,73	1.36	7 (14%)	59,90,113	1.96	9 (15%)
16	BCR	B	4014	-	41,41,41	1.25	7 (17%)	56,56,56	2.04	22 (39%)
13	CLA	B	1217	2	51,55,73	1.44	7 (13%)	60,91,113	2.09	8 (13%)
13	CLA	B	1206	2	69,73,73	1.19	4 (5%)	82,113,113	1.63	8 (9%)
13	CLA	B	1210	2	69,73,73	1.34	7 (10%)	82,113,113	1.59	7 (8%)
13	CLA	A	1104	1	69,73,73	1.37	8 (11%)	82,113,113	1.79	11 (13%)
13	CLA	A	1137	1	51,55,73	1.51	5 (9%)	60,91,113	1.83	9 (15%)
13	CLA	A	1111	1	64,68,73	1.24	6 (9%)	76,107,113	1.77	11 (14%)
13	CLA	K	1401	-	49,53,73	1.48	7 (14%)	58,89,113	1.82	5 (8%)
13	CLA	B	1219	20	59,63,73	1.42	8 (13%)	70,101,113	1.81	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1121	1	55,59,73	1.49	8 (14%)	64,96,113	1.85	9 (14%)
13	CLA	A	1011	1	69,73,73	1.29	6 (8%)	82,113,113	1.97	16 (19%)
13	CLA	B	1229	2	69,73,73	1.24	7 (10%)	82,113,113	1.67	7 (8%)
13	CLA	A	1138	1	69,73,73	1.23	9 (13%)	82,113,113	1.65	8 (9%)
13	CLA	A	1120	1	53,57,73	1.39	6 (11%)	61,93,113	1.99	10 (16%)
13	CLA	A	1122	1	63,67,73	1.25	7 (11%)	74,105,113	1.70	10 (13%)
13	CLA	A	1124	20	69,73,73	1.21	6 (8%)	82,113,113	1.63	9 (10%)
13	CLA	A	1117	1	69,73,73	1.34	10 (14%)	82,113,113	1.77	11 (13%)
16	BCR	B	4004	-	41,41,41	1.55	5 (12%)	56,56,56	2.07	19 (33%)
18	LMG	B	5002	-	55,55,55	0.89	3 (5%)	63,63,63	1.29	3 (4%)
13	CLA	A	1136	1	69,73,73	1.33	8 (11%)	82,113,113	1.56	7 (8%)
13	CLA	B	1208	2	49,53,73	1.44	7 (14%)	58,89,113	1.86	9 (15%)
15	SF4	C	3003	3	0,12,12	-	-	-	-	-
16	BCR	A	4008	-	41,41,41	1.29	8 (19%)	56,56,56	1.94	20 (35%)
13	CLA	A	1103	1	69,73,73	1.17	4 (5%)	82,113,113	1.68	11 (13%)
14	PQN	A	2001	-	34,34,34	3.62	17 (50%)	43,45,45	2.11	3 (6%)
13	CLA	B	1201	2	58,62,73	1.38	9 (15%)	68,99,113	1.89	9 (13%)
13	CLA	A	1109	1,13	69,73,73	1.25	8 (11%)	82,113,113	1.67	8 (9%)
13	CLA	A	1132	1	69,73,73	1.22	6 (8%)	82,113,113	1.65	9 (10%)
13	CLA	A	1106	1	69,73,73	1.29	7 (10%)	82,113,113	1.71	8 (9%)
13	CLA	A	1123	20	69,73,73	1.32	6 (8%)	82,113,113	1.64	11 (13%)
13	CLA	A	1128	1	69,73,73	1.42	10 (14%)	82,113,113	1.61	8 (9%)
13	CLA	B	1213	2	59,63,73	1.48	11 (18%)	70,101,113	1.74	7 (10%)
13	CLA	B	1221	2	58,62,73	1.60	12 (20%)	68,99,113	1.82	9 (13%)
16	BCR	F	4016	-	41,41,41	1.27	5 (12%)	56,56,56	1.85	16 (28%)
15	SF4	C	3002	3	0,12,12	-	-	-	-	-
13	CLA	A	1135	1	55,59,73	1.36	5 (9%)	64,96,113	1.94	9 (14%)
13	CLA	A	1110	1	58,62,73	1.35	7 (12%)	68,99,113	1.91	8 (11%)
13	CLA	A	1118	1	65,69,73	1.38	9 (13%)	77,108,113	1.86	10 (12%)
13	CLA	B	1218	2	49,53,73	1.48	8 (16%)	58,89,113	2.06	9 (15%)
16	BCR	J	4013	-	41,41,41	1.29	4 (9%)	56,56,56	1.89	19 (33%)
16	BCR	L	4019	-	41,41,41	1.46	8 (19%)	56,56,56	1.86	15 (26%)
13	CLA	A	1119	20	69,73,73	1.29	9 (13%)	82,113,113	1.71	10 (12%)
13	CLA	B	1236	2	51,55,73	1.45	7 (13%)	60,91,113	1.74	7 (11%)
16	BCR	J	4015	-	41,41,41	1.42	5 (12%)	56,56,56	1.93	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1214	2	63,67,73	1.37	8 (12%)	74,105,113	1.73	10 (13%)
13	CLA	A	1402	-	45,49,73	1.57	7 (15%)	54,83,113	1.82	5 (9%)
16	BCR	M	4021	-	41,41,41	1.37	7 (17%)	56,56,56	1.84	15 (26%)
13	CLA	J	1303	8	41,45,73	1.66	9 (21%)	50,78,113	1.99	6 (12%)
13	CLA	B	1220	2	49,53,73	1.47	5 (10%)	58,89,113	1.84	5 (8%)
13	CLA	B	1021	2	69,73,73	1.28	6 (8%)	82,113,113	1.64	9 (10%)
13	CLA	B	1211	2	69,73,73	1.27	7 (10%)	82,113,113	1.72	9 (10%)
13	CLA	L	1502	10	69,73,73	1.36	8 (11%)	82,113,113	1.66	8 (9%)
13	CLA	A	1022	20	69,73,73	1.29	11 (15%)	82,113,113	1.59	9 (10%)
13	CLA	A	1115	1	58,62,73	1.47	10 (17%)	68,99,113	1.69	7 (10%)
16	BCR	B	4010	-	41,41,41	1.27	6 (14%)	56,56,56	1.93	19 (33%)
13	CLA	B	1012	20	69,73,73	1.34	6 (8%)	82,113,113	1.66	11 (13%)
13	CLA	A	1105	1	55,59,73	1.53	8 (14%)	64,96,113	1.87	8 (12%)
13	CLA	B	1232	20	49,53,73	1.55	8 (16%)	58,89,113	1.87	10 (17%)
13	CLA	B	1225	2	69,73,73	1.44	10 (14%)	82,113,113	1.60	11 (13%)
13	CLA	B	1215	2	64,68,73	1.38	8 (12%)	76,107,113	1.81	9 (11%)
13	CLA	B	1235	2	69,73,73	1.25	9 (13%)	82,113,113	1.74	10 (12%)
13	CLA	M	1601	20	49,53,73	1.49	7 (14%)	58,89,113	2.07	8 (13%)
13	CLA	B	1223	2	69,73,73	1.33	6 (8%)	82,113,113	1.68	9 (10%)
13	CLA	A	1116	1	58,62,73	1.47	10 (17%)	68,99,113	1.79	9 (13%)
13	CLA	B	1204	2	69,73,73	1.17	6 (8%)	82,113,113	1.70	9 (10%)
13	CLA	B	1203	2	69,73,73	1.28	5 (7%)	82,113,113	1.53	6 (7%)
13	CLA	B	1216	20	69,73,73	1.27	6 (8%)	82,113,113	1.66	8 (9%)
13	CLA	A	1112	1	49,53,73	1.53	9 (18%)	58,89,113	1.89	9 (15%)
13	CLA	A	1101	1	69,73,73	1.22	6 (8%)	82,113,113	1.67	7 (8%)
13	CLA	A	1129	1	54,58,73	1.41	7 (12%)	64,95,113	1.98	12 (18%)
13	CLA	B	1230	2	62,66,73	1.40	12 (19%)	73,104,113	1.87	11 (15%)
15	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
13	CLA	B	1207	2	69,73,73	1.34	8 (11%)	82,113,113	1.71	12 (14%)
13	CLA	A	1125	1	69,73,73	1.30	6 (8%)	82,113,113	1.70	10 (12%)
13	CLA	A	1013	-	69,73,73	1.39	9 (13%)	82,113,113	1.66	11 (13%)
13	CLA	A	1113	1	49,53,73	1.42	6 (12%)	58,89,113	2.06	10 (17%)
16	BCR	B	4006	-	41,41,41	1.26	5 (12%)	56,56,56	2.06	20 (35%)
13	CLA	A	1114	20	53,57,73	1.37	8 (15%)	61,93,113	1.93	8 (13%)
13	CLA	B	1202	2	69,73,73	1.30	6 (8%)	82,113,113	1.56	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1231	2	49,53,73	1.46	9 (18%)	58,89,113	1.93	11 (18%)
16	BCR	I	4020	-	41,41,41	1.27	6 (14%)	56,56,56	1.86	19 (33%)
16	BCR	A	4007	-	41,41,41	1.36	5 (12%)	56,56,56	1.84	17 (30%)
14	PQN	B	2002	-	34,34,34	3.53	17 (50%)	43,45,45	2.03	6 (13%)
13	CLA	B	1238	20	69,73,73	1.25	6 (8%)	82,113,113	1.58	8 (9%)
16	BCR	L	4022	-	41,41,41	1.66	7 (17%)	56,56,56	1.77	13 (23%)
13	CLA	A	1134	1	49,53,73	1.42	6 (12%)	58,89,113	2.00	8 (13%)
13	CLA	B	1212	2	49,53,73	1.49	9 (18%)	58,89,113	1.91	7 (12%)
16	BCR	I	4018	-	41,41,41	1.31	7 (17%)	56,56,56	1.84	16 (28%)
13	CLA	X	1701	12	49,53,73	1.48	5 (10%)	58,89,113	1.97	8 (13%)
13	CLA	A	1102	1,13	63,67,73	1.34	6 (9%)	74,105,113	1.78	9 (12%)
13	CLA	B	1224	2	69,73,73	1.39	9 (13%)	82,113,113	1.75	12 (14%)
13	CLA	L	1501	10	69,73,73	1.38	7 (10%)	82,113,113	1.68	10 (12%)
13	CLA	B	1209	2	49,53,73	1.45	6 (12%)	58,89,113	2.01	8 (13%)
13	CLA	L	1503	20	69,73,73	1.31	6 (8%)	82,113,113	1.59	7 (8%)
16	BCR	A	4002	-	41,41,41	1.28	4 (9%)	56,56,56	1.81	18 (32%)
16	BCR	B	4017	-	41,41,41	1.29	4 (9%)	56,56,56	1.78	19 (33%)
13	CLA	A	1108	1	49,53,73	1.48	5 (10%)	58,89,113	1.83	7 (12%)
13	CLA	A	1131	1	69,73,73	1.15	4 (5%)	82,113,113	1.59	10 (12%)
17	LHG	B	5004	-	22,22,48	2.87	5 (22%)	25,28,54	1.15	2 (8%)
13	CLA	F	1301	20	49,53,73	1.50	8 (16%)	58,89,113	1.93	8 (13%)
16	BCR	A	4003	-	41,41,41	1.44	6 (14%)	56,56,56	1.98	21 (37%)
13	CLA	B	1227	2	49,53,73	1.41	7 (14%)	58,89,113	2.04	11 (18%)
13	CLA	A	1801	17	56,60,73	1.50	11 (19%)	65,97,113	2.05	9 (13%)
16	BCR	J	4012	-	41,41,41	1.32	5 (12%)	56,56,56	1.96	17 (30%)
13	CLA	A	1133	1	58,62,73	1.33	7 (12%)	68,99,113	1.90	9 (13%)
13	CLA	A	1130	1	69,73,73	1.20	7 (10%)	82,113,113	1.80	9 (10%)
13	CLA	A	1126	1	69,73,73	1.24	6 (8%)	82,113,113	1.55	8 (9%)
13	CLA	A	1127	1	69,73,73	1.29	6 (8%)	82,113,113	1.61	5 (6%)
13	CLA	A	1140	1	69,73,73	1.27	8 (11%)	82,113,113	1.72	10 (12%)
13	CLA	B	1239	2	69,73,73	1.17	8 (11%)	82,113,113	1.64	7 (8%)
13	CLA	J	1302	8	49,53,73	1.52	6 (12%)	58,89,113	2.02	7 (12%)
16	BCR	B	4005	-	41,41,41	1.57	7 (17%)	56,56,56	2.15	20 (35%)
17	LHG	A	5001	-	48,48,48	1.80	7 (14%)	51,54,54	1.30	3 (5%)
13	CLA	A	1237	20	69,73,73	1.22	8 (11%)	82,113,113	1.58	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	1139	20	55,59,73	1.44	6 (10%)	64,96,113	1.81	9 (14%)
13	CLA	B	1205	2	69,73,73	1.28	6 (8%)	82,113,113	1.62	8 (9%)
16	BCR	A	4011	-	41,41,41	1.38	6 (14%)	56,56,56	2.09	19 (33%)
13	CLA	B	1228	2	53,57,73	1.37	8 (15%)	61,93,113	1.88	6 (9%)
13	CLA	B	1234	2	64,68,73	1.42	8 (12%)	76,107,113	1.68	9 (11%)
13	CLA	B	1233	20	49,53,73	1.41	4 (8%)	58,89,113	1.96	8 (13%)
13	CLA	A	1107	1	69,73,73	1.24	7 (10%)	82,113,113	1.76	12 (14%)
16	BCR	B	4009	-	25,25,41	1.34	4 (16%)	33,33,56	1.89	10 (30%)

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
17	LHG	A	5003	13	1/1/5/5	10/31/31/53	-
13	CLA	B	1226	2	-	9/39/115/115	-
16	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1023	-	-	2/39/115/115	-
13	CLA	B	1222	20	-	8/17/93/115	-
16	BCR	B	4014	-	-	1/29/63/63	0/2/2/2
13	CLA	B	1217	2	-	6/18/94/115	-
13	CLA	B	1206	2	-	12/39/115/115	-
13	CLA	B	1210	2	-	14/39/115/115	-
13	CLA	A	1104	1	-	16/39/115/115	-
13	CLA	A	1137	1	-	5/18/94/115	-
13	CLA	A	1111	1	-	12/33/109/115	-
13	CLA	K	1401	-	-	7/15/91/115	-
13	CLA	B	1219	20	-	11/27/103/115	-
13	CLA	A	1121	1	-	10/23/99/115	-
13	CLA	A	1011	1	-	4/39/115/115	-
13	CLA	B	1229	2	-	16/39/115/115	-
13	CLA	A	1138	1	-	6/39/115/115	-
13	CLA	A	1120	1	-	11/20/96/115	-
13	CLA	A	1122	1	-	10/32/108/115	-
13	CLA	A	1124	20	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1117	1	-	11/39/115/115	-
16	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
18	LMG	B	5002	-	-	8/50/70/70	0/1/1/1
13	CLA	A	1136	1	-	7/39/115/115	-
13	CLA	B	1208	2	-	5/15/91/115	-
15	SF4	C	3003	3	-	-	0/6/5/5
16	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1103	1	-	16/39/115/115	-
14	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
13	CLA	B	1201	2	-	5/26/102/115	-
13	CLA	A	1109	1,13	-	13/39/115/115	-
13	CLA	A	1132	1	-	9/39/115/115	-
13	CLA	A	1106	1	-	17/39/115/115	-
13	CLA	A	1123	20	-	13/39/115/115	-
13	CLA	A	1128	1	-	9/39/115/115	-
13	CLA	B	1213	2	-	9/27/103/115	-
13	CLA	B	1221	2	-	9/26/102/115	-
16	BCR	F	4016	-	-	5/29/63/63	0/2/2/2
15	SF4	C	3002	3	-	-	0/6/5/5
13	CLA	A	1135	1	-	6/23/99/115	-
13	CLA	A	1110	1	-	5/26/102/115	-
13	CLA	A	1118	1	-	15/35/111/115	-
13	CLA	B	1218	2	-	6/15/91/115	-
16	BCR	J	4013	-	-	4/29/63/63	0/2/2/2
16	BCR	L	4019	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1119	20	-	6/39/115/115	-
13	CLA	B	1236	2	-	6/18/94/115	-
16	BCR	J	4015	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1214	2	-	7/32/108/115	-
13	CLA	A	1402	-	-	4/9/81/115	-
16	BCR	M	4021	-	-	4/29/63/63	0/2/2/2
13	CLA	J	1303	8	-	1/4/76/115	-
13	CLA	B	1220	2	-	4/15/91/115	-
13	CLA	B	1021	2	-	8/39/115/115	-
13	CLA	B	1211	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	L	1502	10	-	9/39/115/115	-
13	CLA	A	1022	20	-	7/39/115/115	-
13	CLA	A	1115	1	-	1/26/102/115	-
16	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1012	20	-	8/39/115/115	-
13	CLA	A	1105	1	-	7/23/99/115	-
13	CLA	B	1232	20	-	0/15/91/115	-
13	CLA	B	1225	2	-	12/39/115/115	-
13	CLA	B	1215	2	-	8/33/109/115	-
13	CLA	B	1235	2	-	3/39/115/115	-
13	CLA	M	1601	20	-	9/15/91/115	-
13	CLA	B	1223	2	-	10/39/115/115	-
13	CLA	A	1116	1	-	12/26/102/115	-
13	CLA	B	1204	2	-	0/39/115/115	-
13	CLA	B	1203	2	-	16/39/115/115	-
13	CLA	B	1216	20	-	4/39/115/115	-
13	CLA	A	1112	1	-	3/15/91/115	-
13	CLA	A	1101	1	-	6/39/115/115	-
13	CLA	A	1129	1	-	3/21/97/115	-
13	CLA	B	1230	2	-	8/31/107/115	-
15	SF4	A	3001	1,2	-	-	0/6/5/5
13	CLA	B	1207	2	-	7/39/115/115	-
13	CLA	A	1125	1	-	7/39/115/115	-
13	CLA	A	1013	-	-	12/39/115/115	-
13	CLA	A	1113	1	-	4/15/91/115	-
16	BCR	B	4006	-	-	5/29/63/63	0/2/2/2
13	CLA	A	1114	20	-	9/20/96/115	-
13	CLA	B	1202	2	-	14/39/115/115	-
13	CLA	B	1231	2	-	6/15/91/115	-
16	BCR	I	4020	-	-	4/29/63/63	0/2/2/2
16	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
14	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
13	CLA	B	1238	20	-	2/39/115/115	-
16	BCR	L	4022	-	-	1/29/63/63	0/2/2/2
13	CLA	A	1134	1	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1212	2	-	7/15/91/115	-
16	BCR	I	4018	-	-	0/29/63/63	0/2/2/2
13	CLA	X	1701	12	-	8/15/91/115	-
13	CLA	A	1102	1,13	-	13/32/108/115	-
13	CLA	B	1224	2	-	15/39/115/115	-
13	CLA	L	1501	10	-	12/39/115/115	-
13	CLA	B	1209	2	-	2/15/91/115	-
13	CLA	L	1503	20	-	10/39/115/115	-
16	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
16	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1108	1	-	9/15/91/115	-
13	CLA	A	1131	1	-	7/39/115/115	-
17	LHG	B	5004	-	-	6/26/26/53	-
13	CLA	F	1301	20	-	4/15/91/115	-
16	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
13	CLA	B	1227	2	-	9/15/91/115	-
13	CLA	A	1801	17	-	13/24/100/115	-
16	BCR	J	4012	-	-	3/29/63/63	0/2/2/2
13	CLA	A	1133	1	-	5/26/102/115	-
13	CLA	A	1130	1	-	8/39/115/115	-
13	CLA	A	1126	1	-	10/39/115/115	-
13	CLA	A	1127	1	-	9/39/115/115	-
13	CLA	A	1140	1	-	8/39/115/115	-
13	CLA	B	1239	2	-	5/39/115/115	-
13	CLA	J	1302	8	-	10/15/91/115	-
16	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
17	LHG	A	5001	-	-	17/53/53/53	-
13	CLA	A	1237	20	-	9/39/115/115	-
13	CLA	A	1139	20	-	8/23/99/115	-
13	CLA	B	1205	2	-	9/39/115/115	-
16	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	B	1228	2	-	10/20/96/115	-
13	CLA	B	1234	2	-	8/33/109/115	-
13	CLA	B	1233	20	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1107	1	-	12/39/115/115	-
16	BCR	B	4009	-	-	4/18/35/63	0/1/1/2

The worst 5 of 883 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	2001	PQN	O4-C4	9.40	1.42	1.23
14	B	2002	PQN	O4-C4	9.07	1.42	1.23
14	A	2001	PQN	O1-C1	9.05	1.42	1.23
17	B	5004	LHG	P-O5	8.83	1.81	1.50
14	A	2001	PQN	C12-C13	8.57	1.52	1.33

The worst 5 of 1247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1217	CLA	C4A-NA-C1A	12.19	112.24	106.68
13	A	1130	CLA	C4A-NA-C1A	12.12	112.21	106.68
13	M	1601	CLA	C4A-NA-C1A	12.07	112.18	106.68
13	A	1113	CLA	C4A-NA-C1A	11.89	112.10	106.68
13	A	1118	CLA	C4A-NA-C1A	11.79	112.06	106.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	5003	LHG	C2

5 of 900 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CLA	C2B-C3B-CAB-CBB
13	A	1011	CLA	C4B-C3B-CAB-CBB
13	A	1022	CLA	C4B-C3B-CAB-CBB
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1102	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

107 monomers are involved in 306 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5003	LHG	2	0
13	B	1226	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	4001	BCR	2	0
13	B	1023	CLA	4	0
13	B	1222	CLA	2	0
16	B	4014	BCR	1	0
13	B	1217	CLA	3	0
13	B	1206	CLA	2	0
13	B	1210	CLA	5	0
13	A	1104	CLA	3	0
13	A	1137	CLA	3	0
13	A	1111	CLA	1	0
13	K	1401	CLA	1	0
13	B	1219	CLA	4	0
13	A	1011	CLA	9	0
13	B	1229	CLA	4	0
13	A	1138	CLA	2	0
13	A	1120	CLA	2	0
13	A	1122	CLA	2	0
13	A	1124	CLA	6	0
13	A	1117	CLA	3	0
16	B	4004	BCR	1	0
18	B	5002	LMG	5	0
13	A	1136	CLA	5	0
16	A	4008	BCR	1	0
13	A	1103	CLA	6	0
14	A	2001	PQN	1	0
13	B	1201	CLA	1	0
13	A	1109	CLA	1	0
13	A	1132	CLA	4	0
13	A	1106	CLA	5	0
13	A	1123	CLA	4	0
13	A	1128	CLA	6	0
13	B	1213	CLA	3	0
13	B	1221	CLA	8	0
16	F	4016	BCR	2	0
13	A	1135	CLA	3	0
13	A	1118	CLA	4	0
16	J	4013	BCR	7	0
13	A	1119	CLA	2	0
13	B	1236	CLA	4	0
16	J	4015	BCR	5	0
13	B	1214	CLA	7	0
13	A	1402	CLA	1	0

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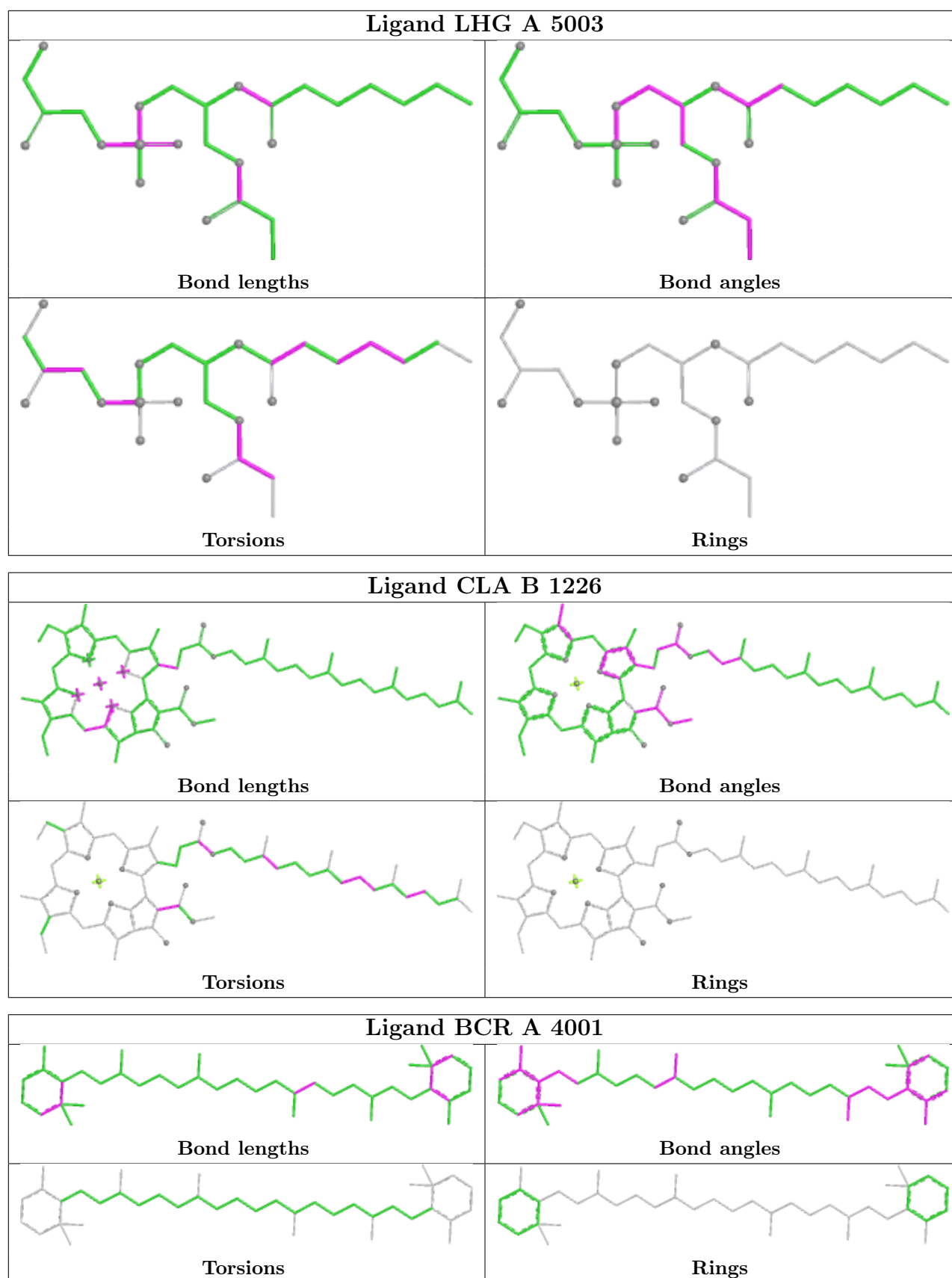
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	4021	BCR	2	0
13	B	1220	CLA	3	0
13	B	1021	CLA	7	0
13	B	1211	CLA	5	0
13	L	1502	CLA	7	0
13	A	1022	CLA	2	0
16	B	4010	BCR	2	0
13	B	1012	CLA	17	0
13	A	1105	CLA	2	0
13	B	1225	CLA	8	0
13	B	1215	CLA	5	0
13	B	1235	CLA	3	0
13	M	1601	CLA	1	0
13	B	1223	CLA	3	0
13	A	1116	CLA	4	0
13	B	1204	CLA	1	0
13	B	1203	CLA	6	0
13	B	1216	CLA	1	0
13	A	1112	CLA	4	0
13	A	1101	CLA	2	0
13	B	1230	CLA	5	0
13	B	1207	CLA	5	0
13	A	1125	CLA	2	0
13	A	1013	CLA	11	0
16	B	4006	BCR	4	0
13	A	1114	CLA	1	0
13	B	1202	CLA	4	0
16	A	4007	BCR	4	0
14	B	2002	PQN	1	0
13	B	1238	CLA	3	0
16	L	4022	BCR	1	0
13	A	1134	CLA	1	0
13	B	1212	CLA	1	0
16	I	4018	BCR	4	0
13	X	1701	CLA	1	0
13	B	1224	CLA	5	0
13	L	1501	CLA	2	0
13	L	1503	CLA	2	0
16	A	4002	BCR	2	0
16	B	4017	BCR	1	0
13	A	1108	CLA	3	0
13	A	1131	CLA	1	0

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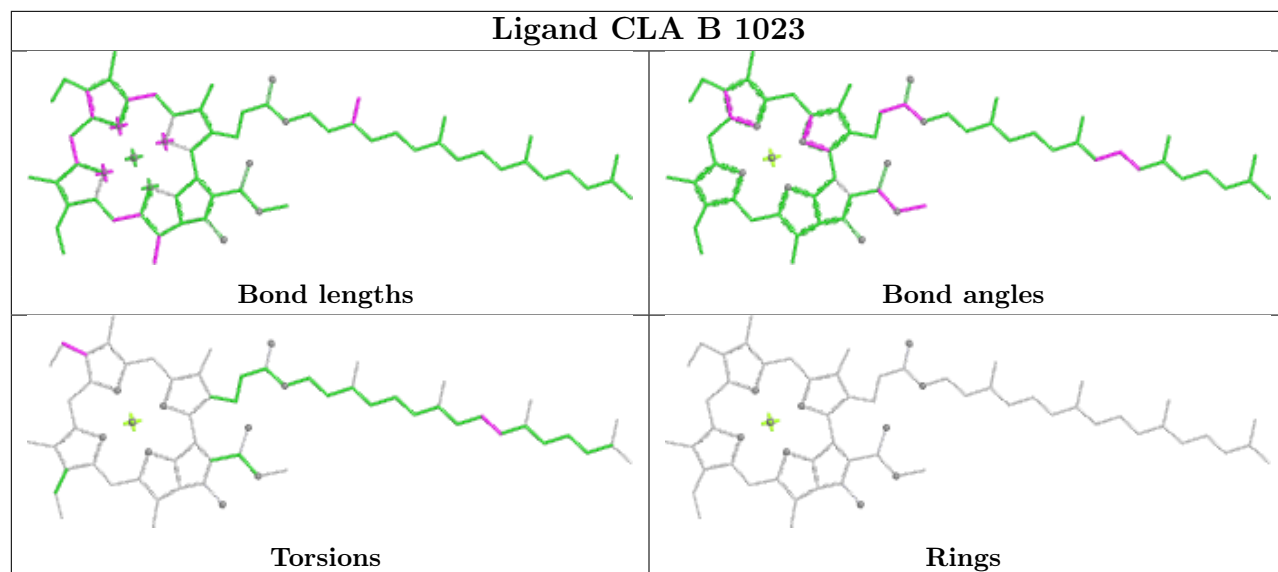
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	5004	LHG	1	0
13	F	1301	CLA	1	0
16	A	4003	BCR	1	0
13	B	1227	CLA	3	0
13	A	1801	CLA	4	0
16	J	4012	BCR	4	0
13	A	1133	CLA	2	0
13	A	1130	CLA	1	0
13	A	1126	CLA	13	0
13	A	1127	CLA	2	0
13	A	1140	CLA	9	0
13	J	1302	CLA	1	0
16	B	4005	BCR	1	0
17	A	5001	LHG	4	0
13	A	1237	CLA	4	0
13	B	1205	CLA	1	0
16	A	4011	BCR	12	0
13	B	1228	CLA	3	0
13	B	1234	CLA	2	0
13	A	1107	CLA	3	0
16	B	4009	BCR	5	0

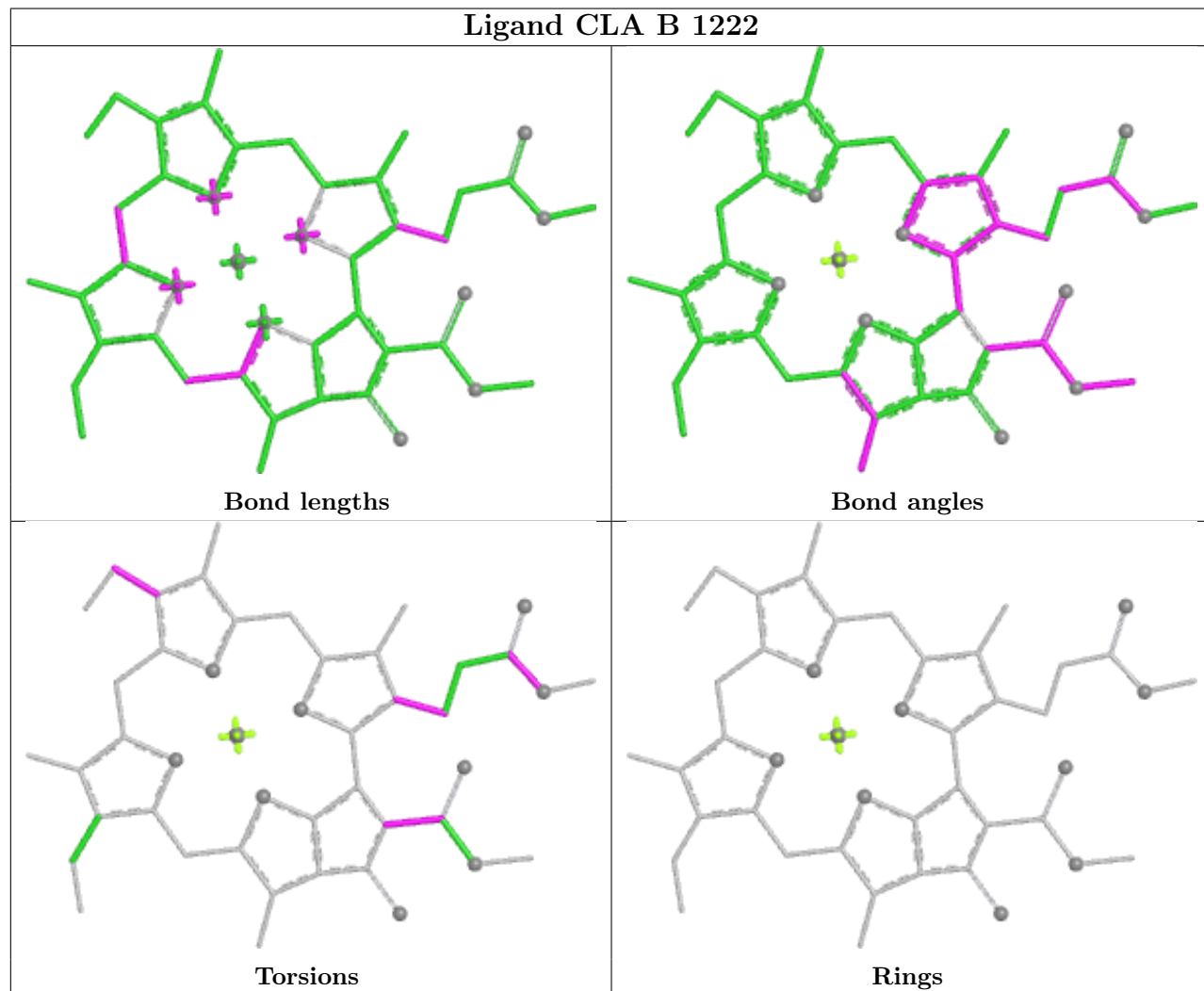
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

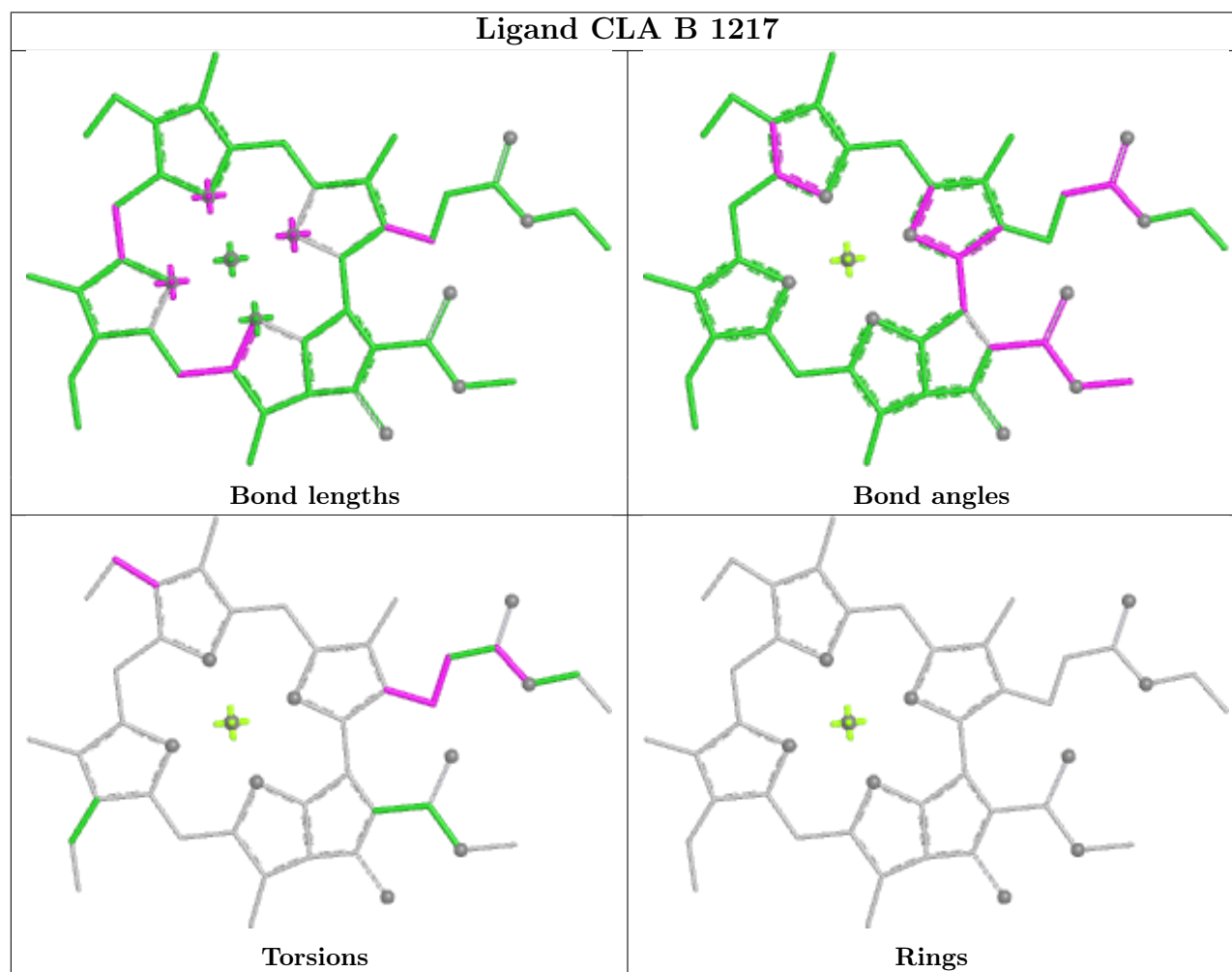
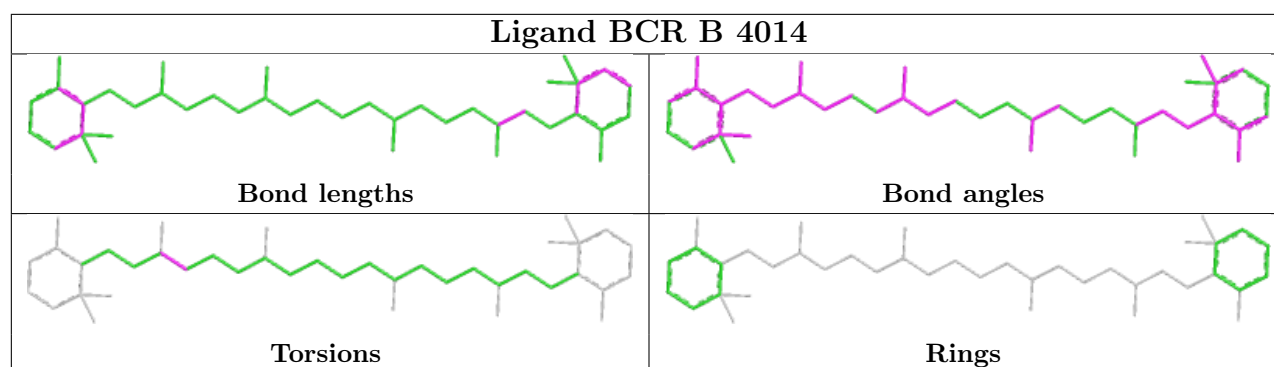


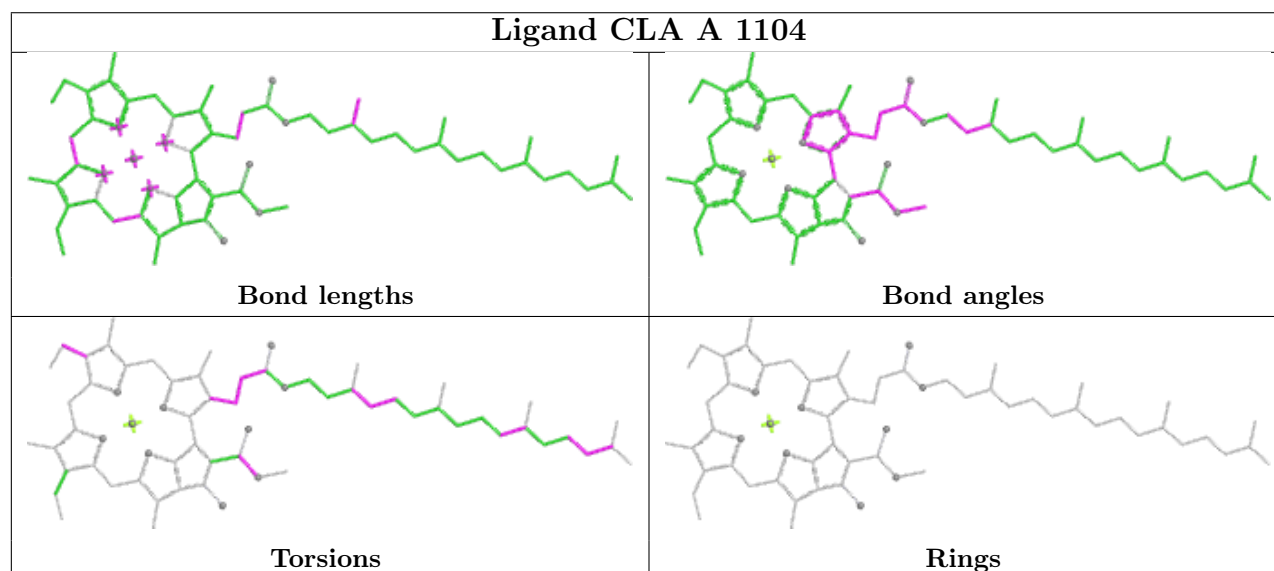
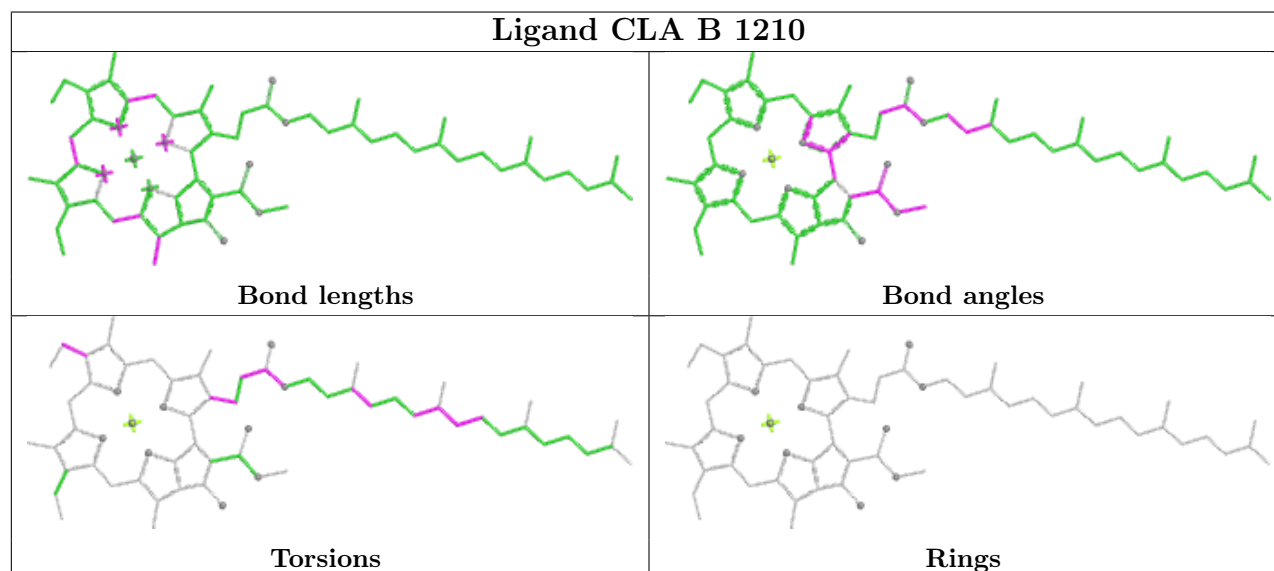
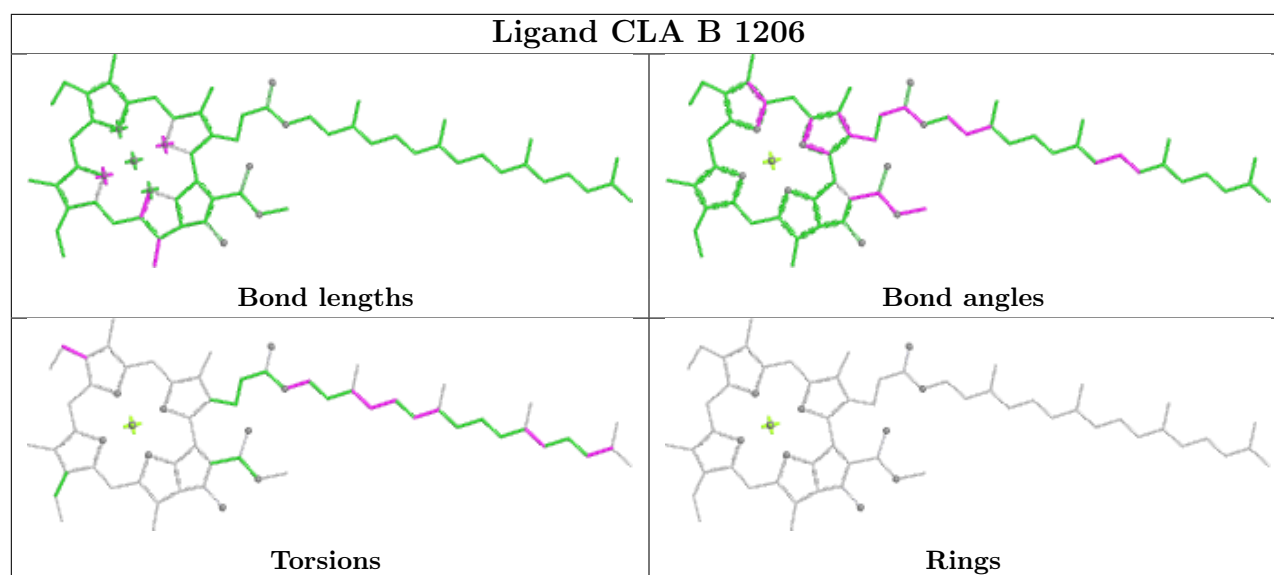
Ligand CLA B 1023



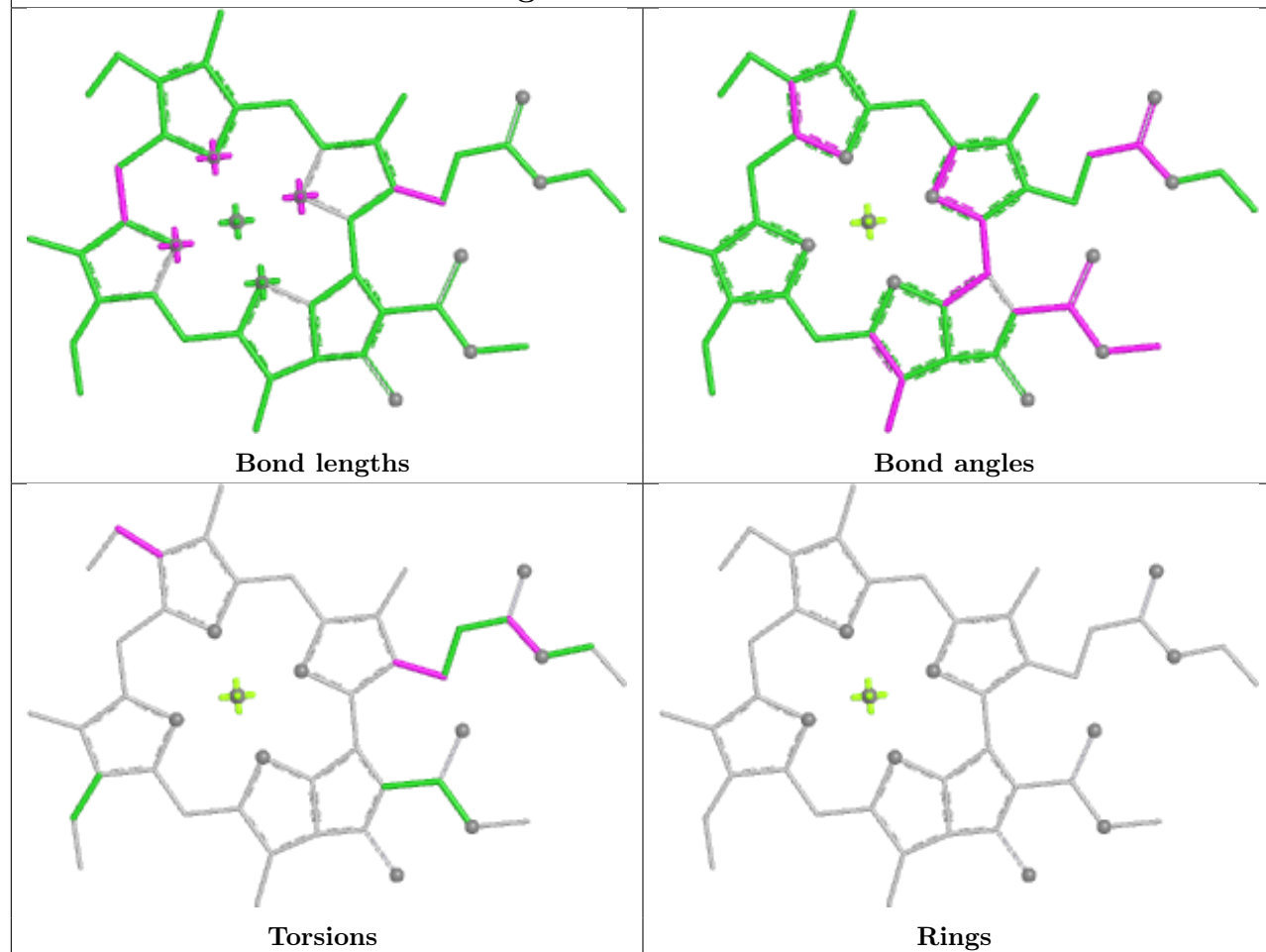
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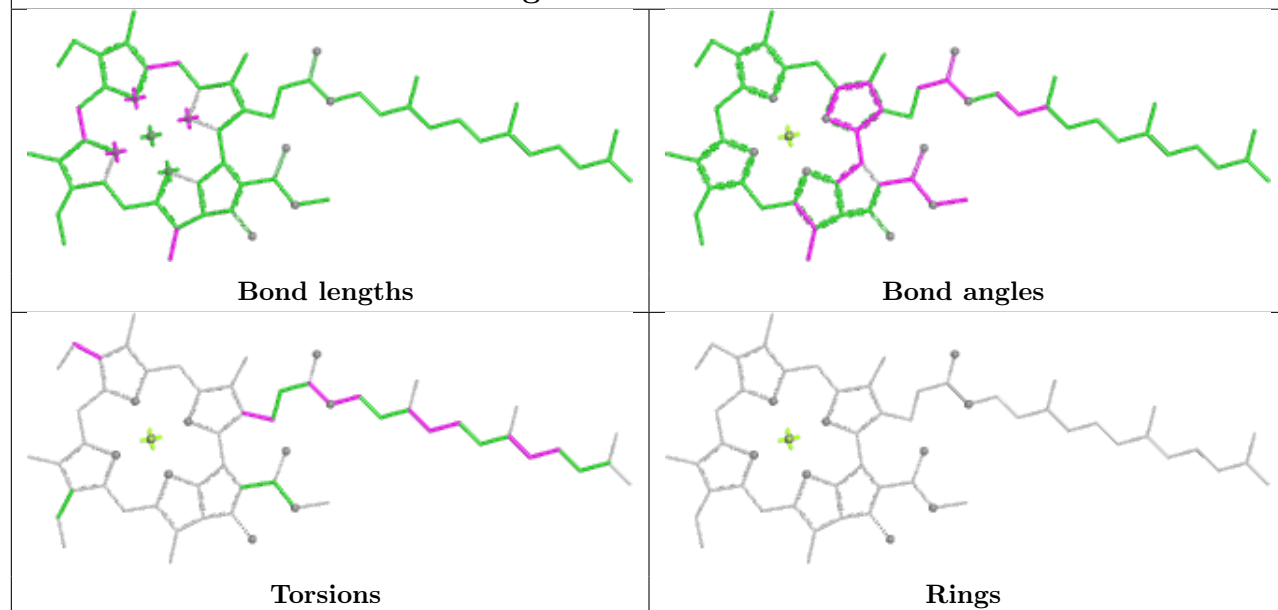




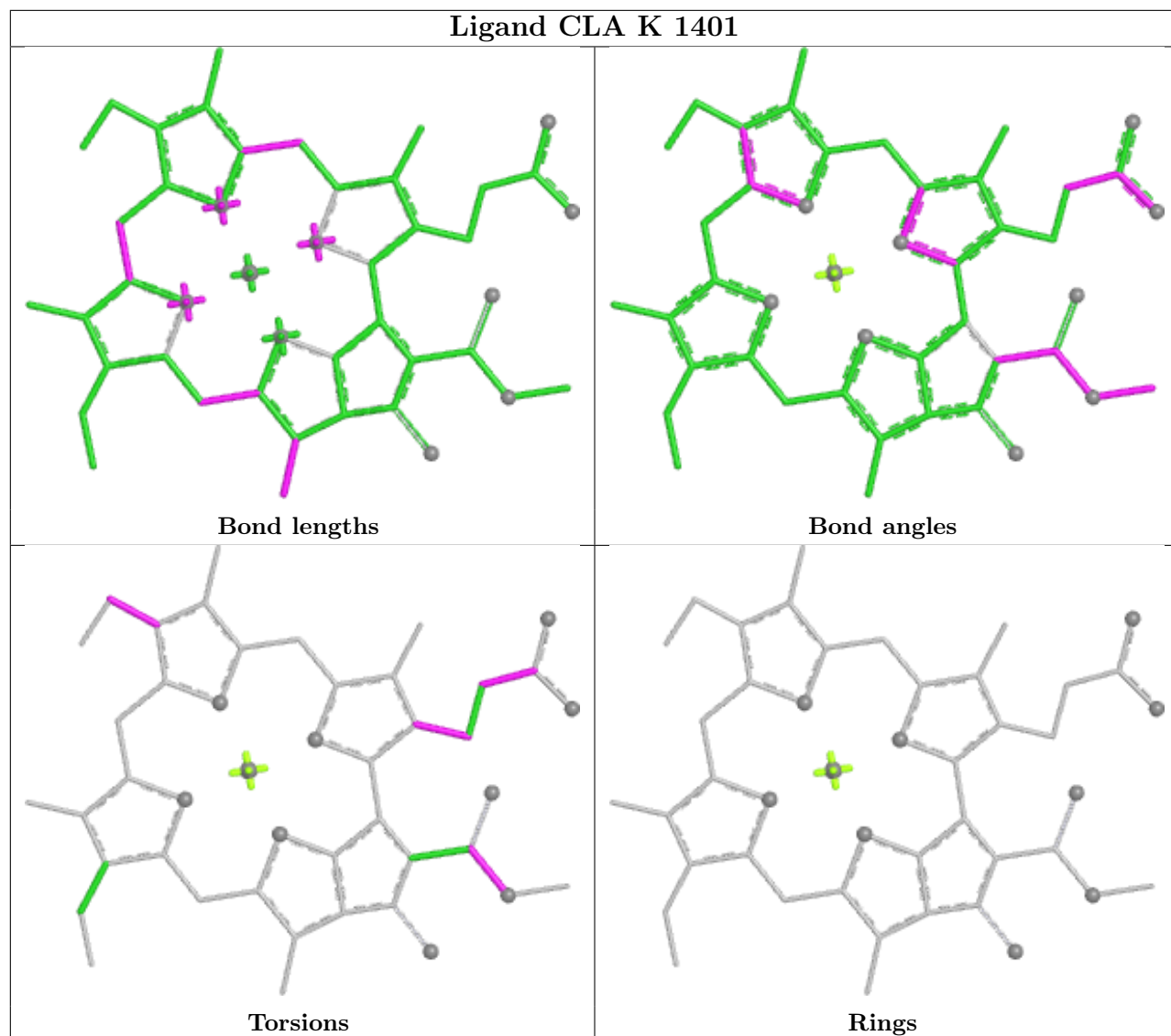
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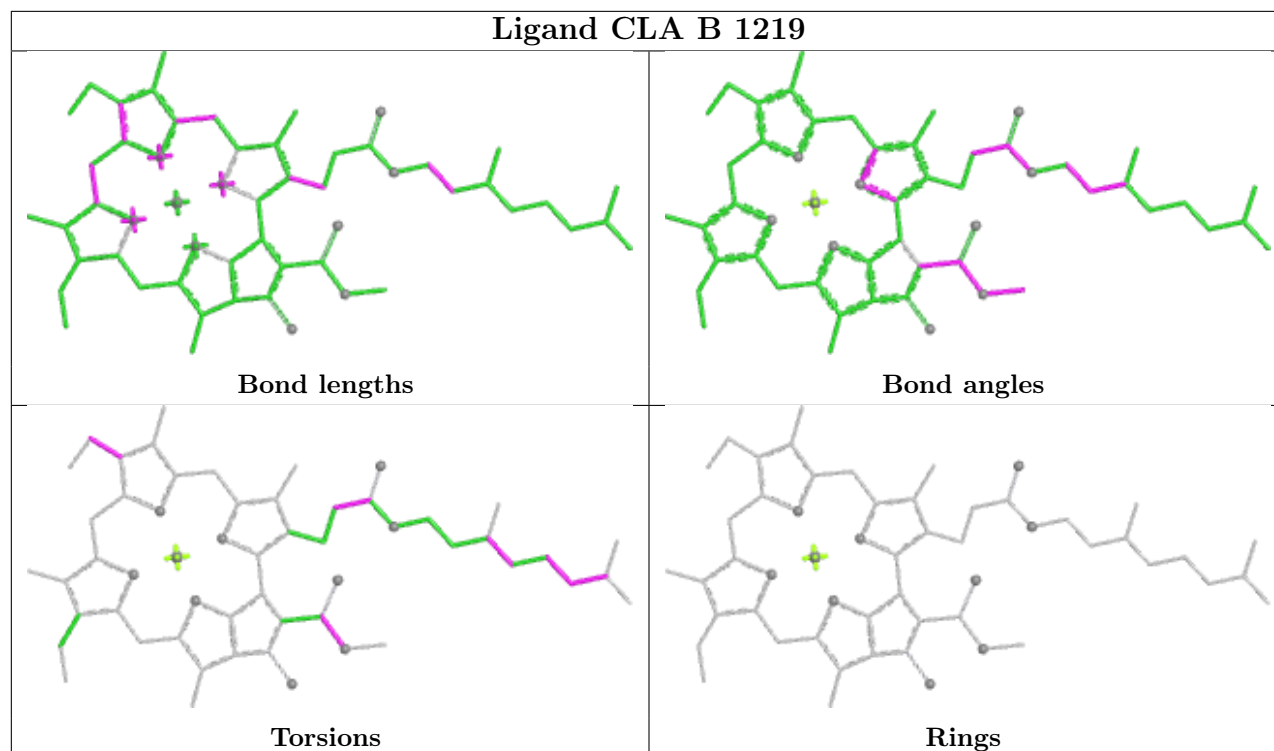
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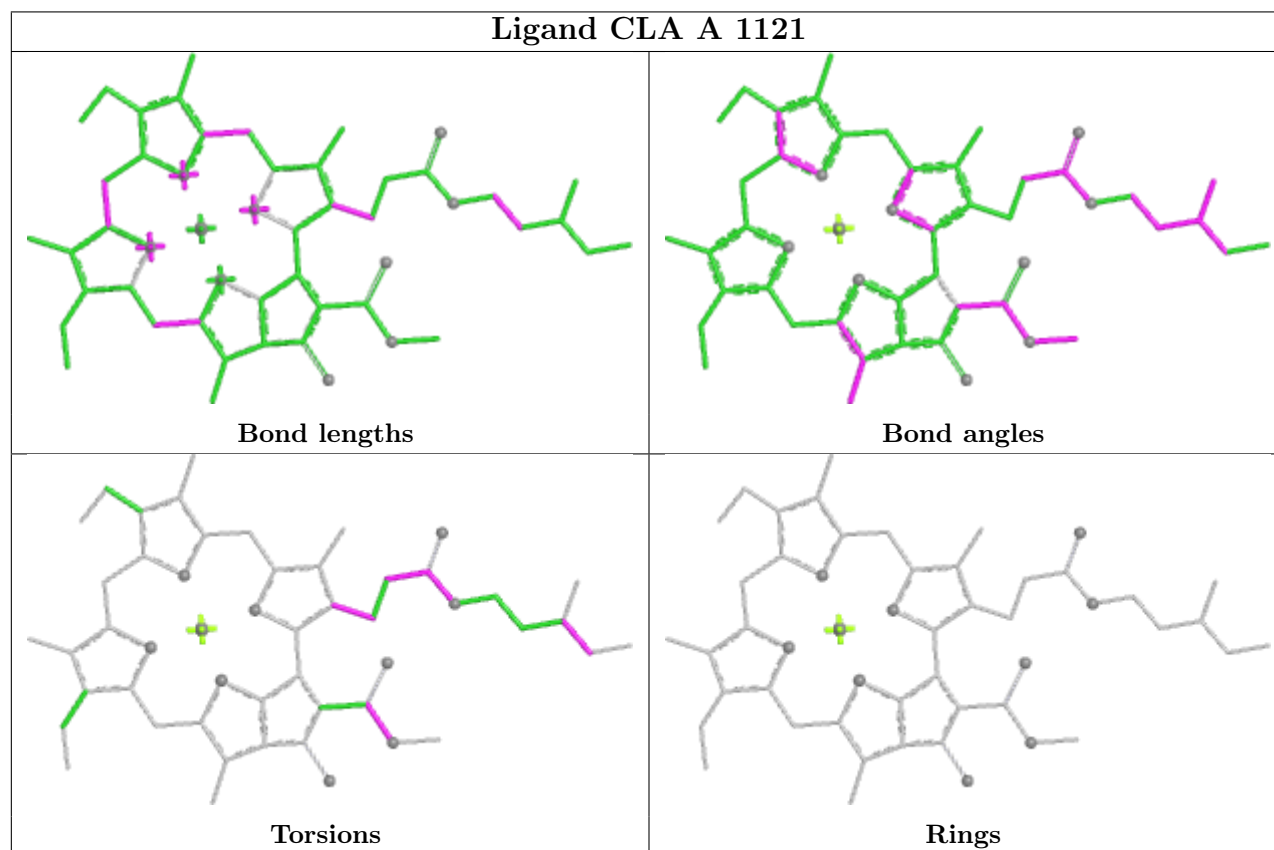
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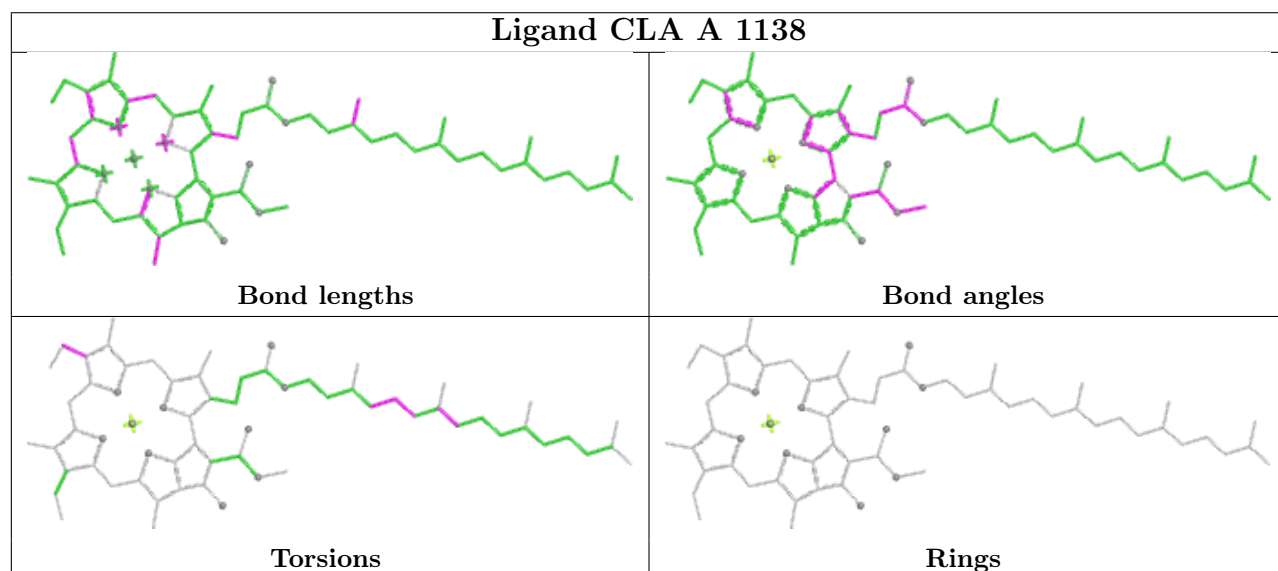
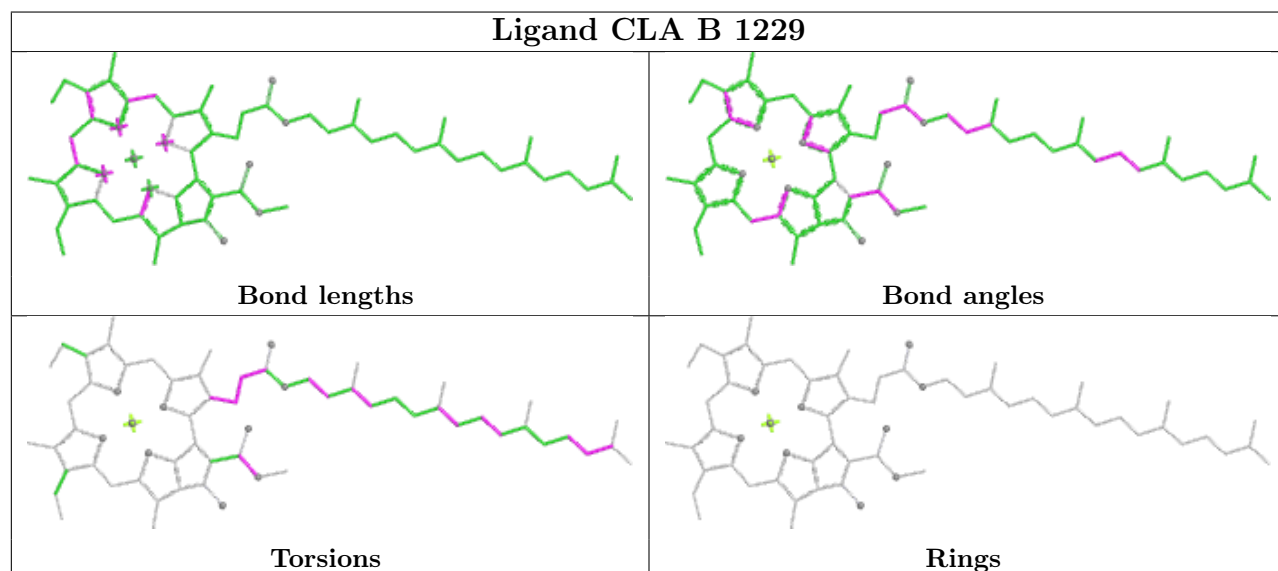
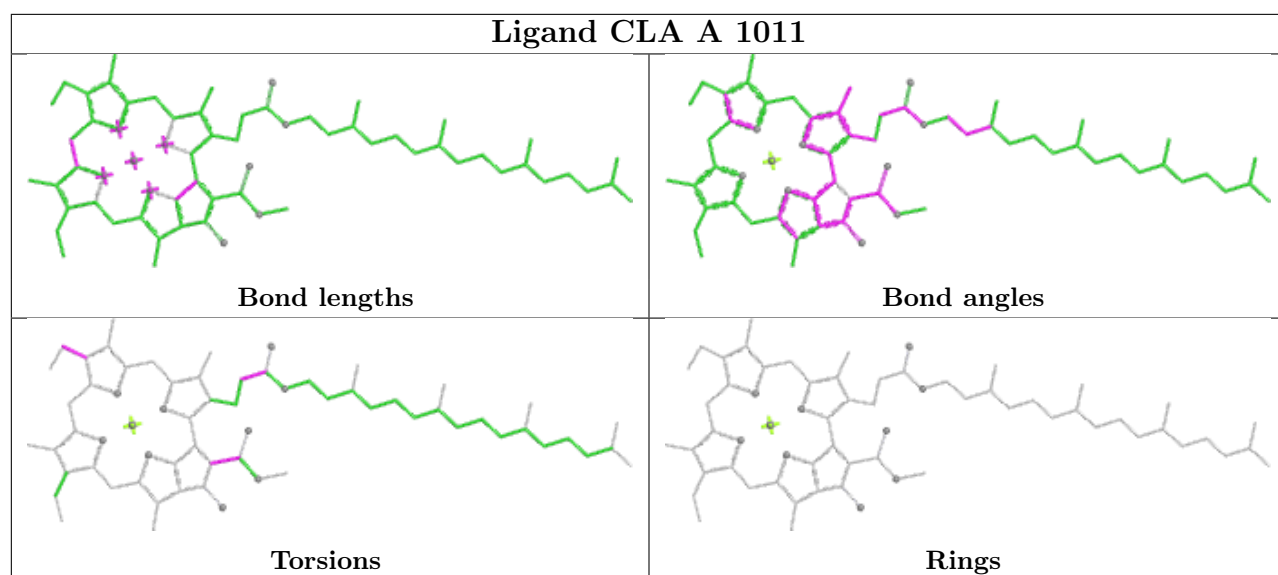


Ligand CLA B 1219

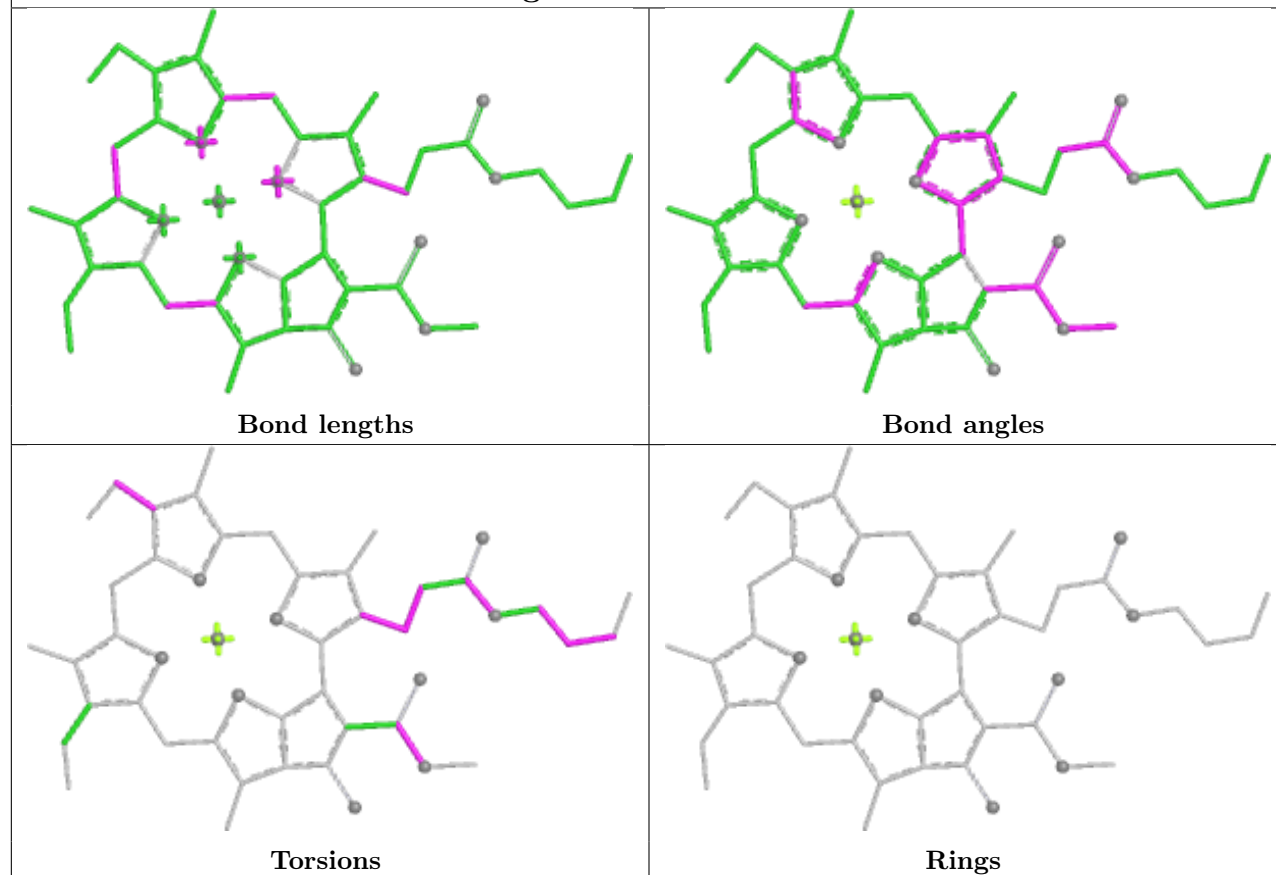


Ligand CLA A 1121

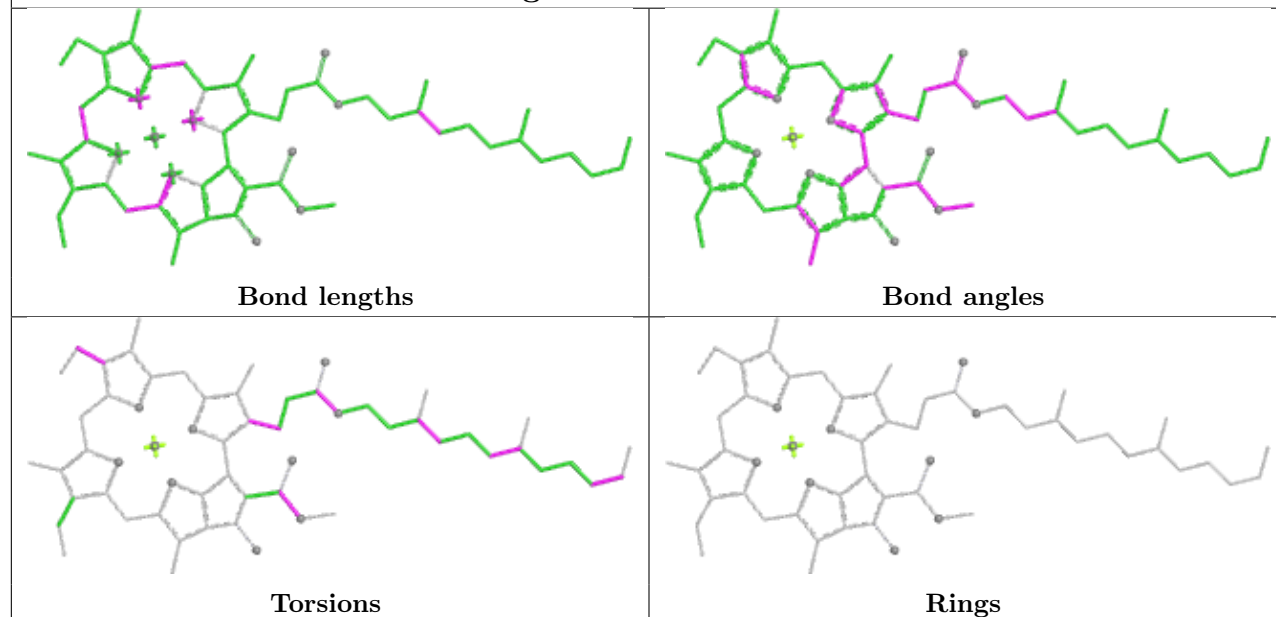


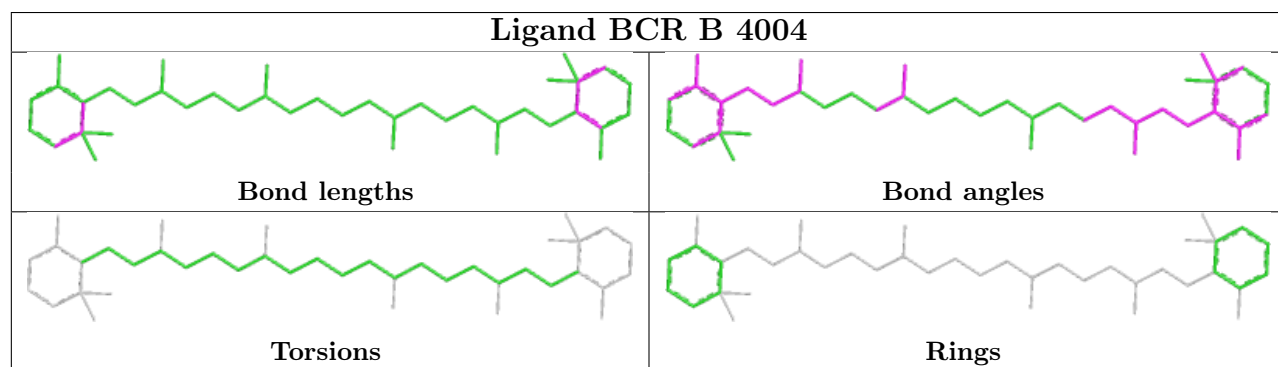
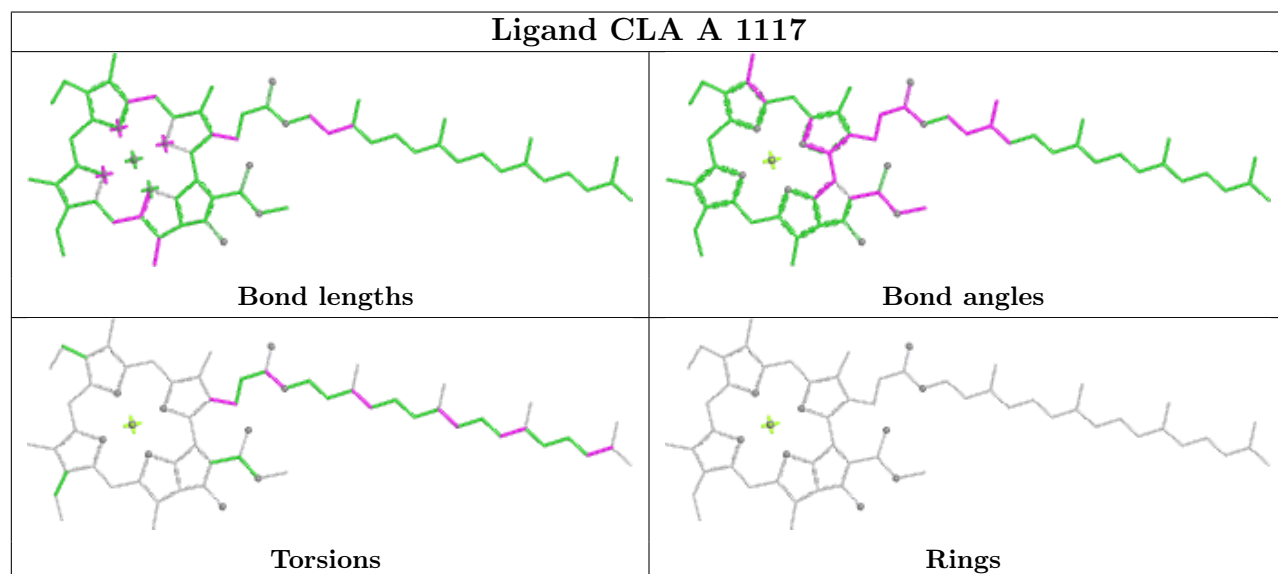
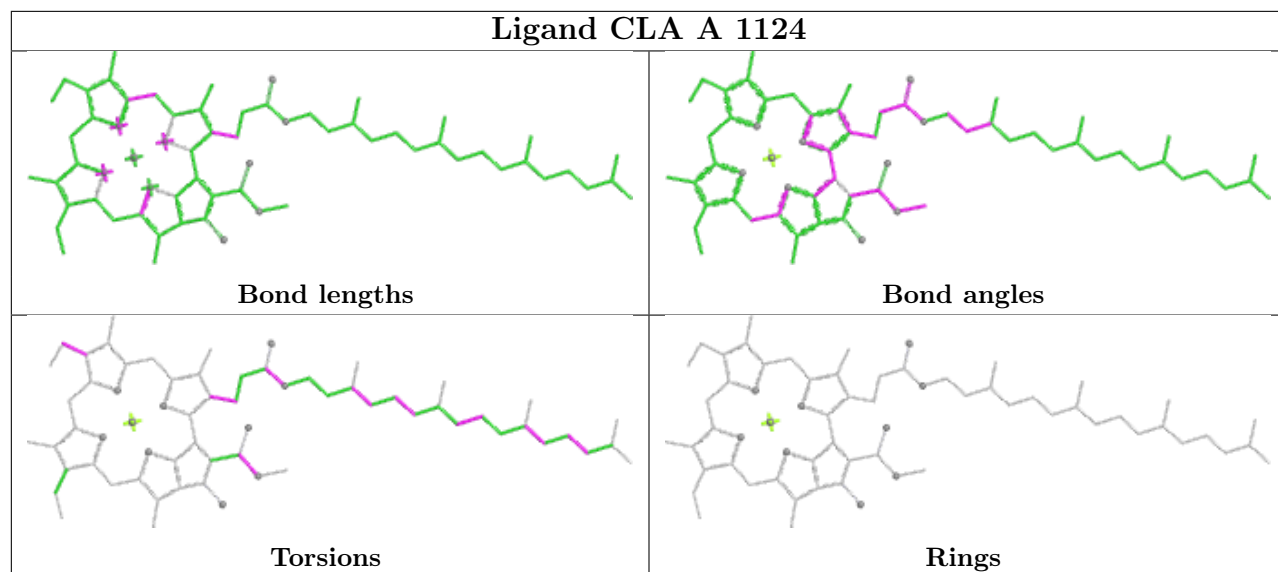


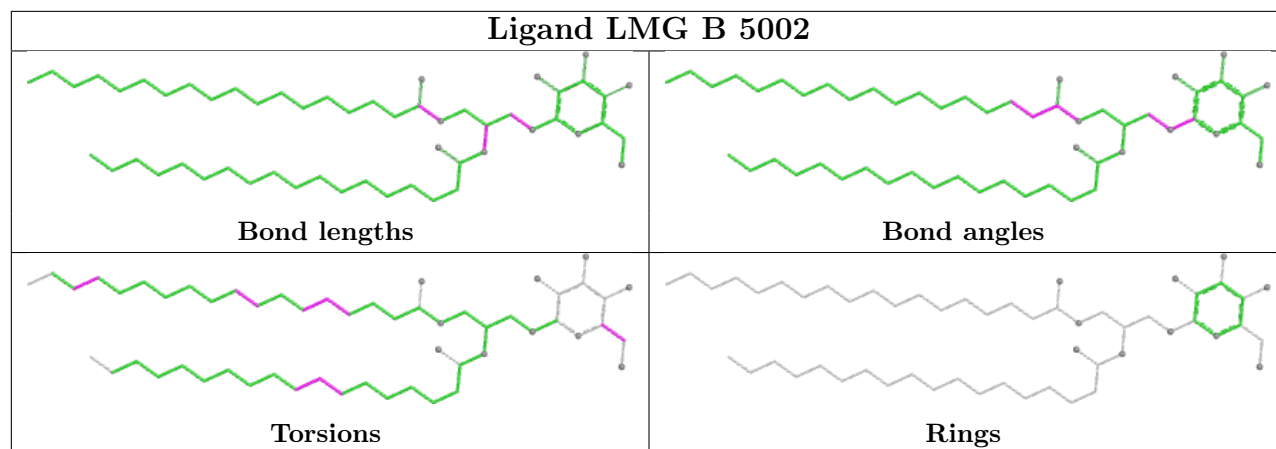
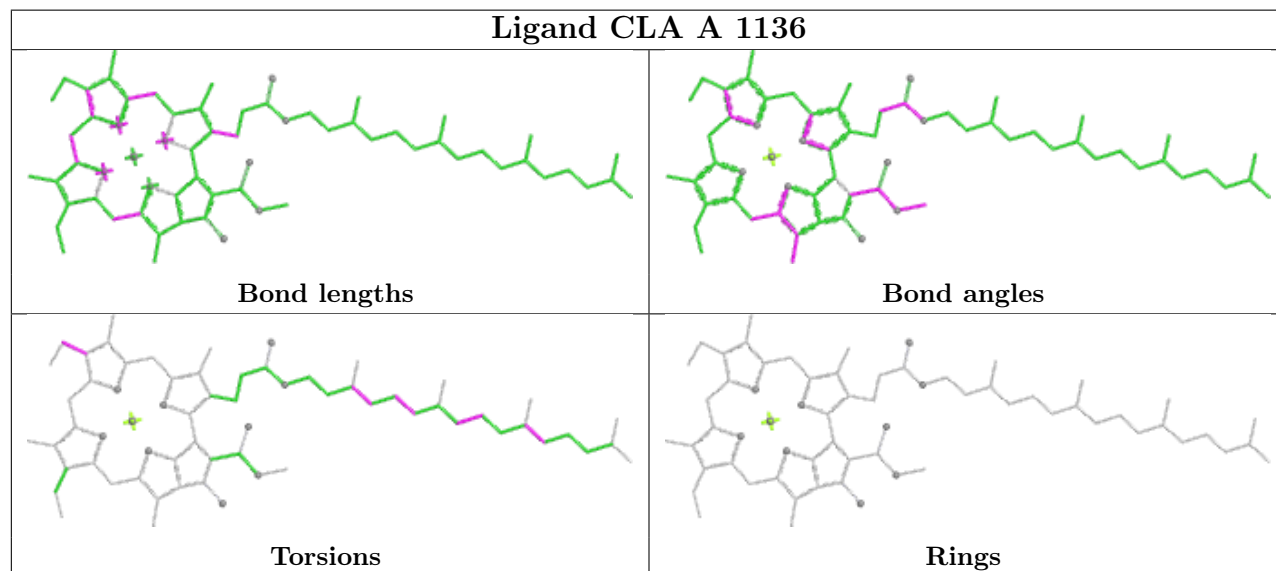
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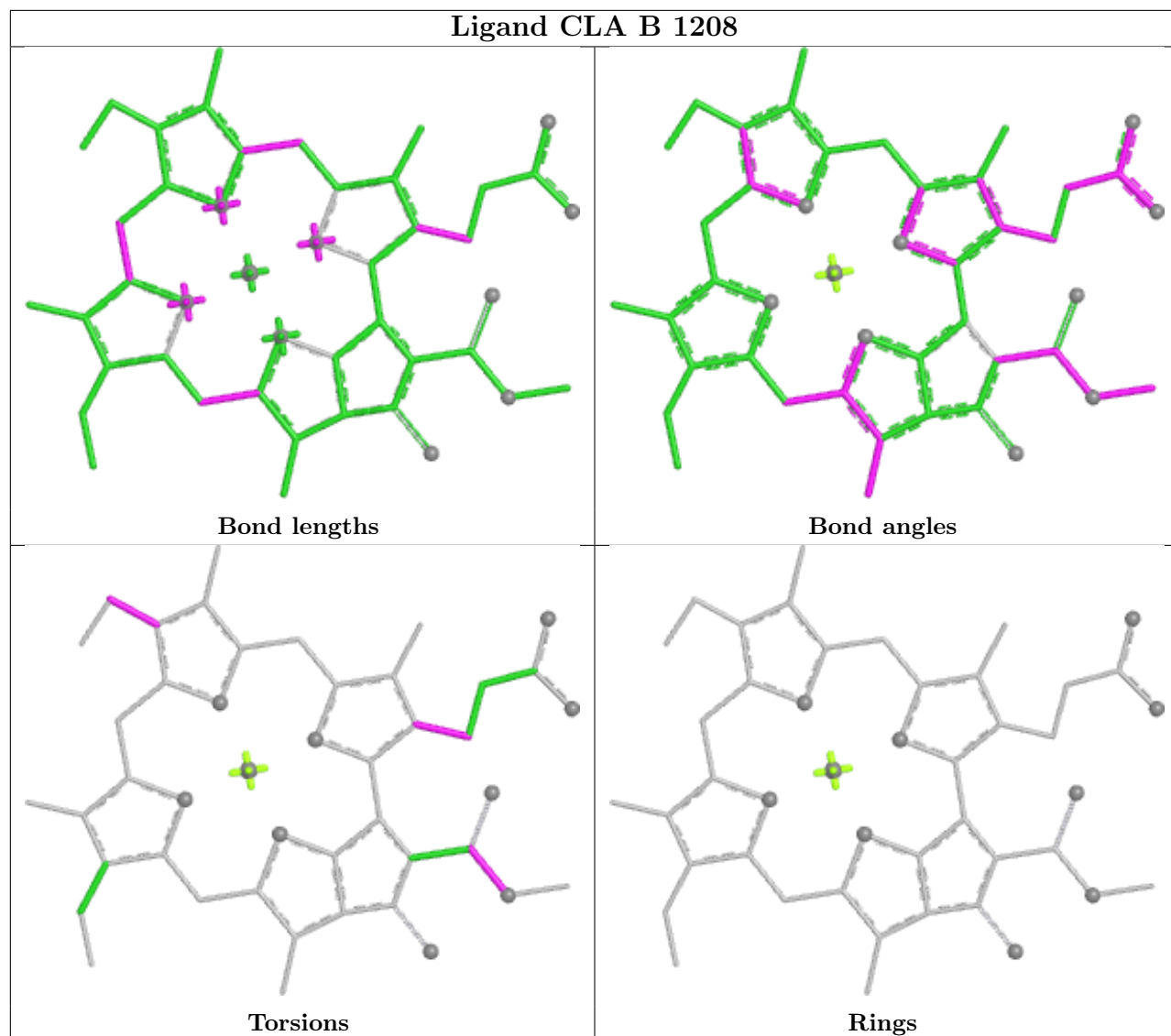
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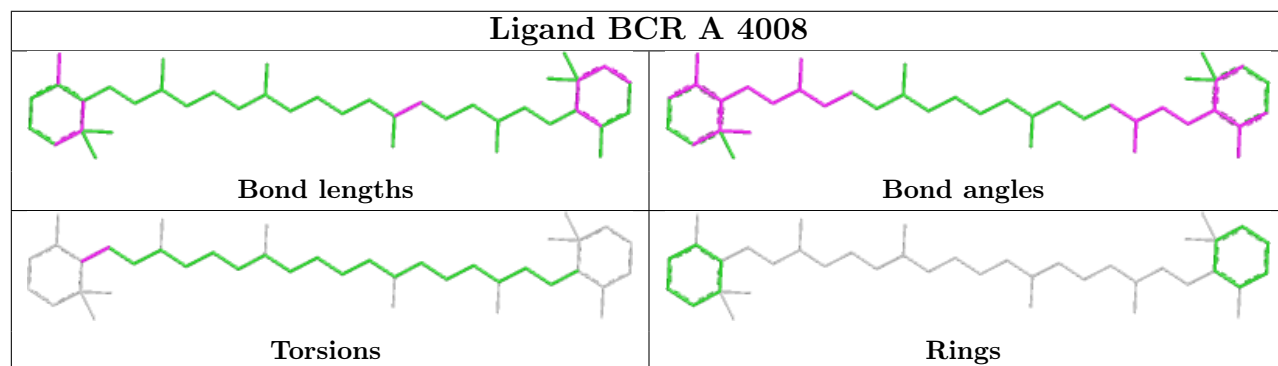


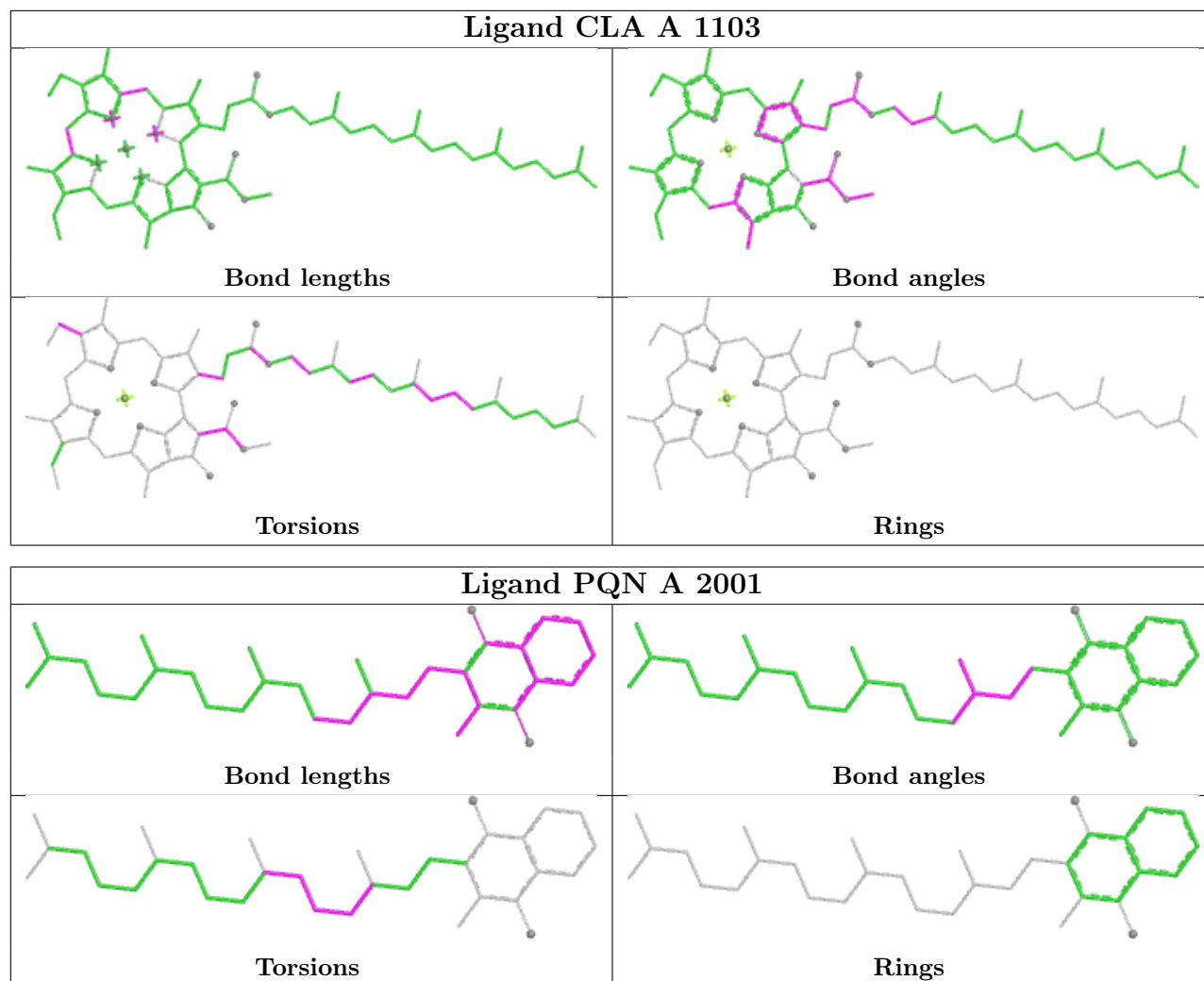
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Ligand CLA B 1208

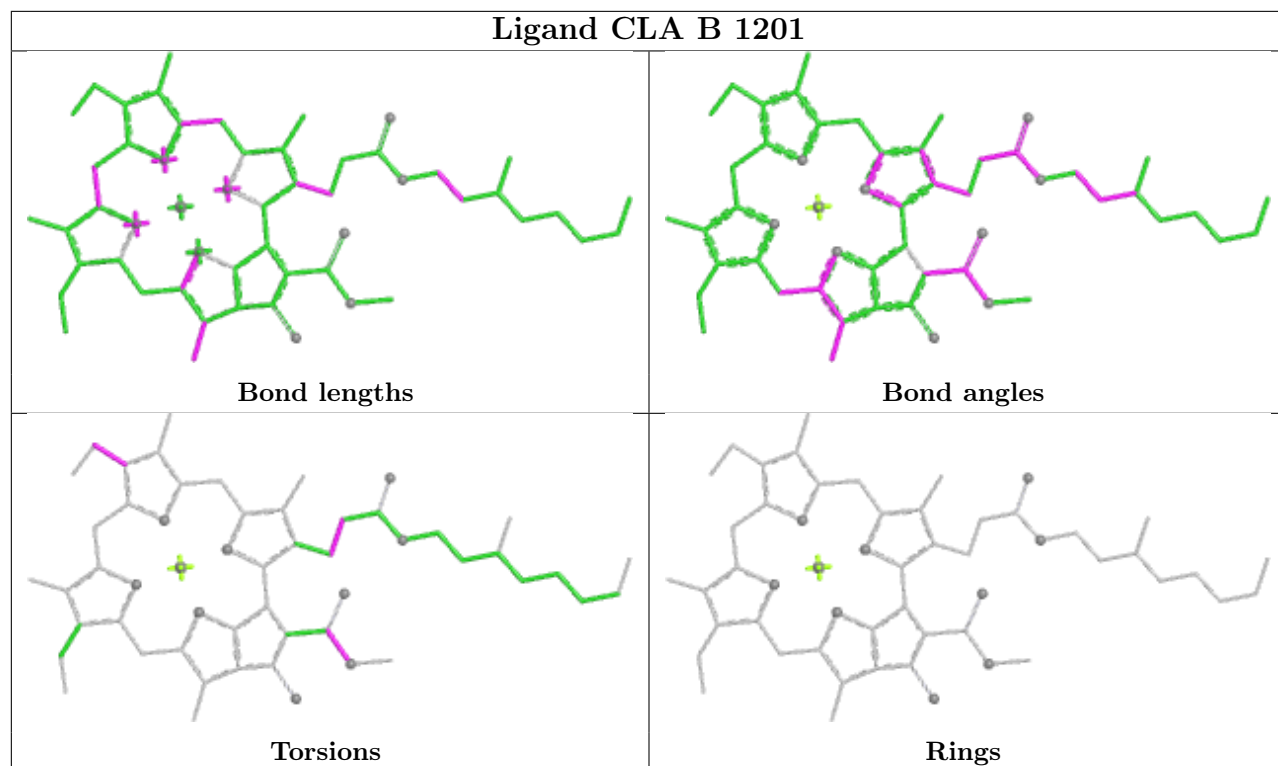


Ligand BCR A 4008

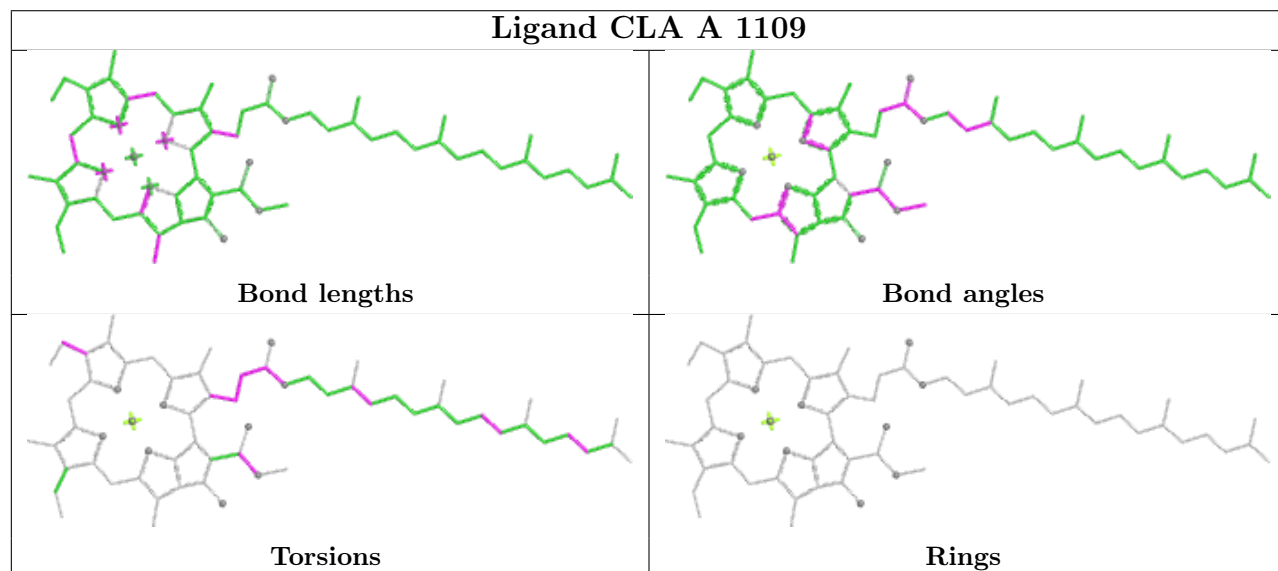


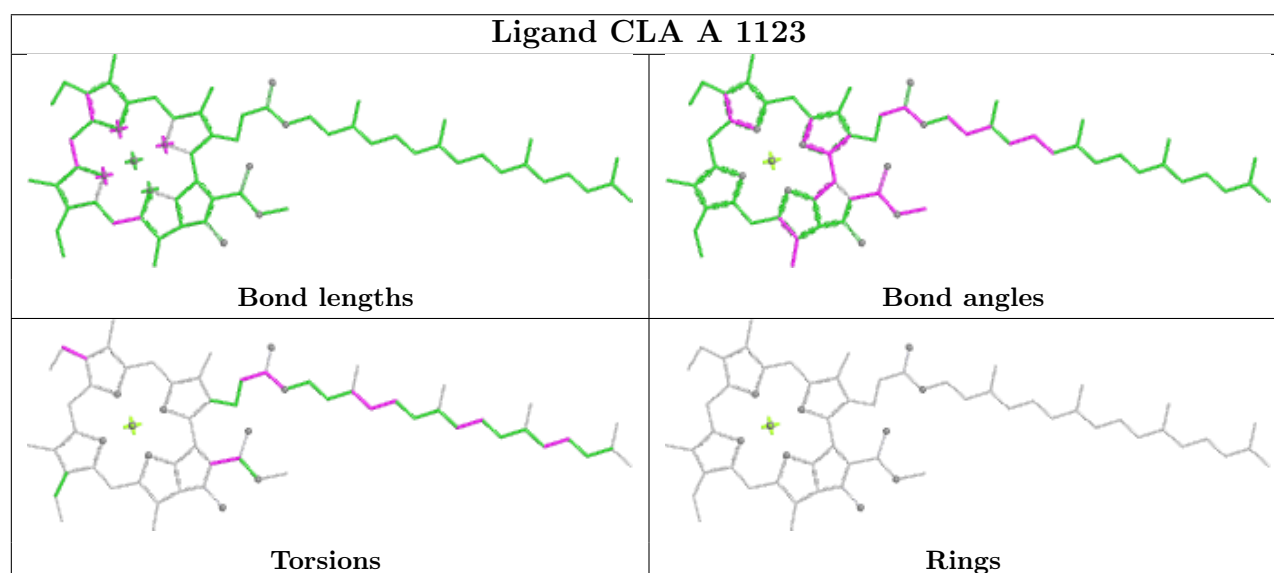
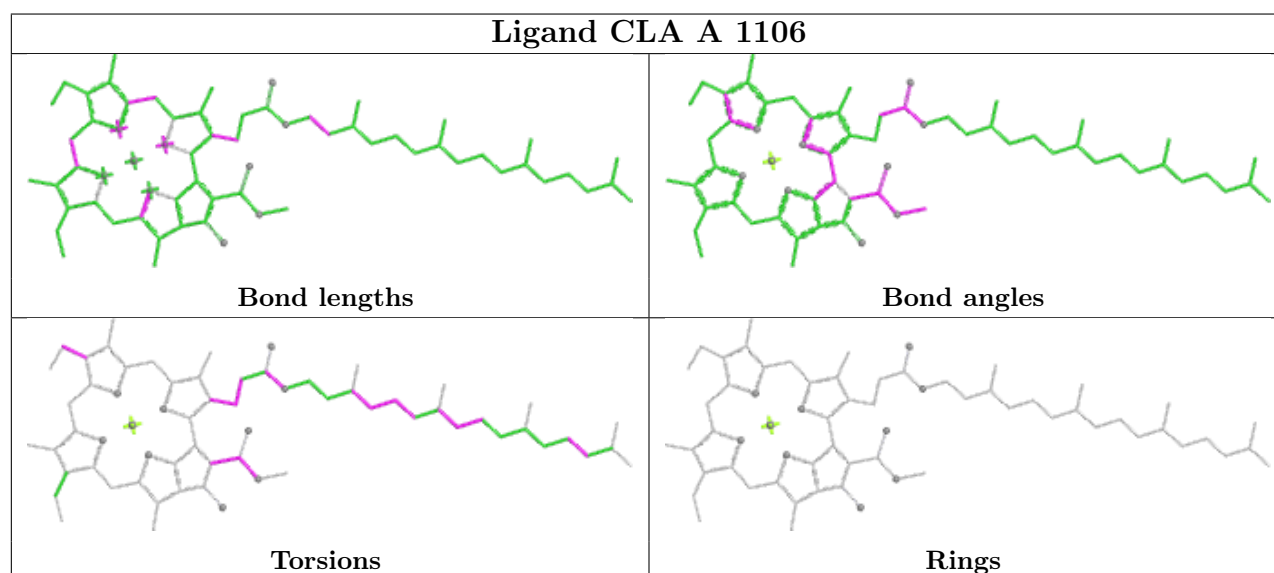
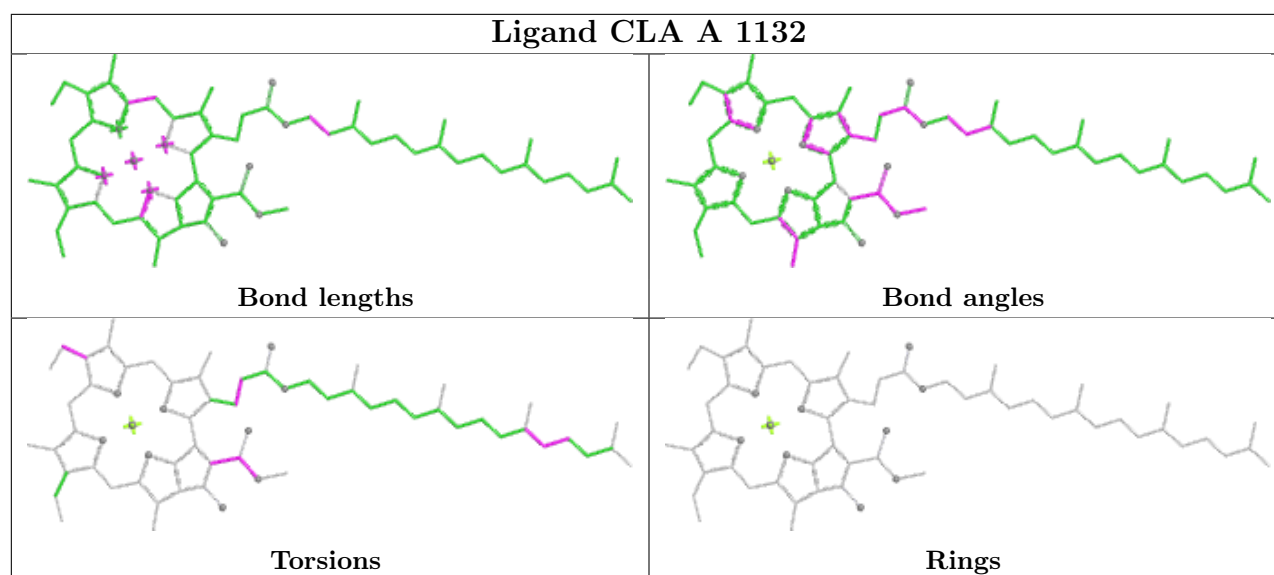


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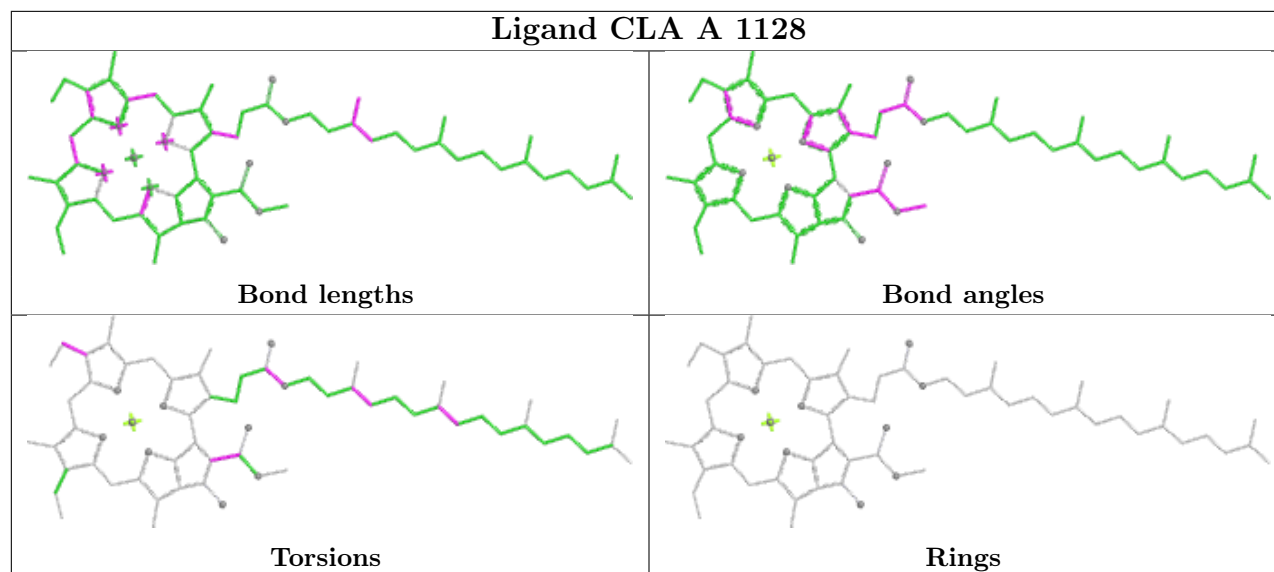


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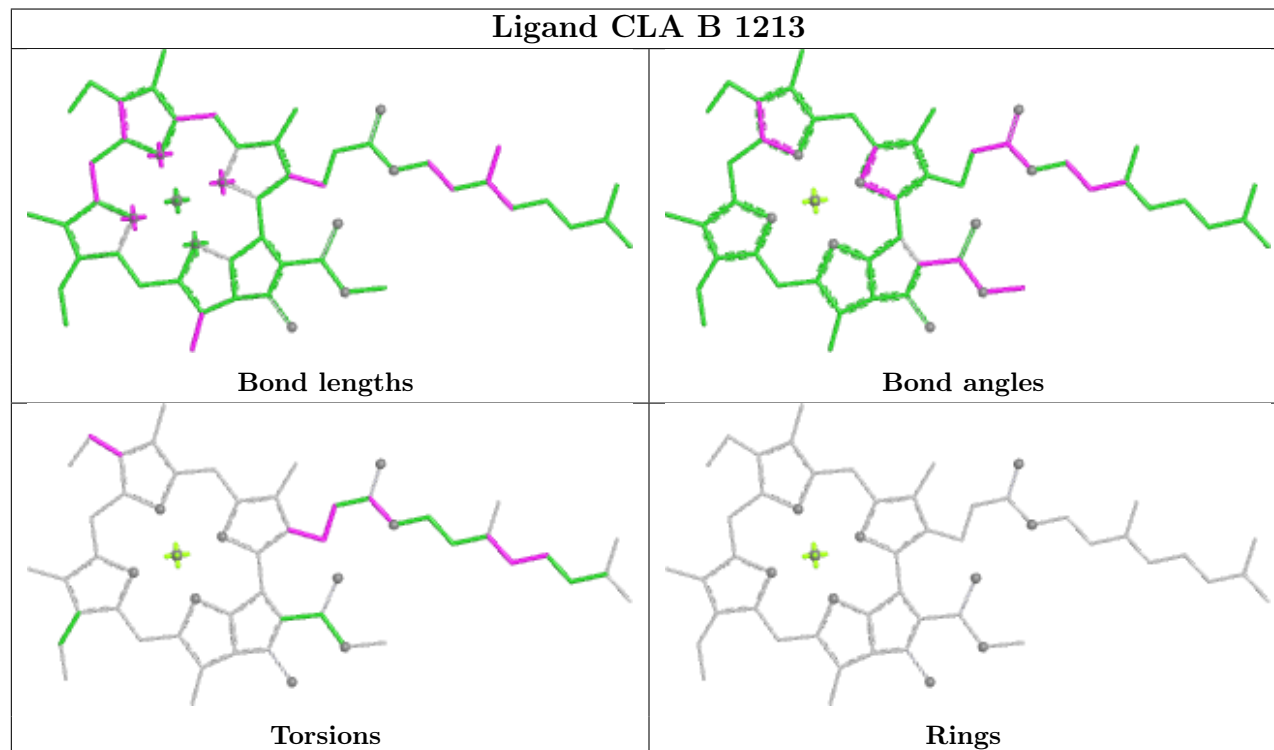


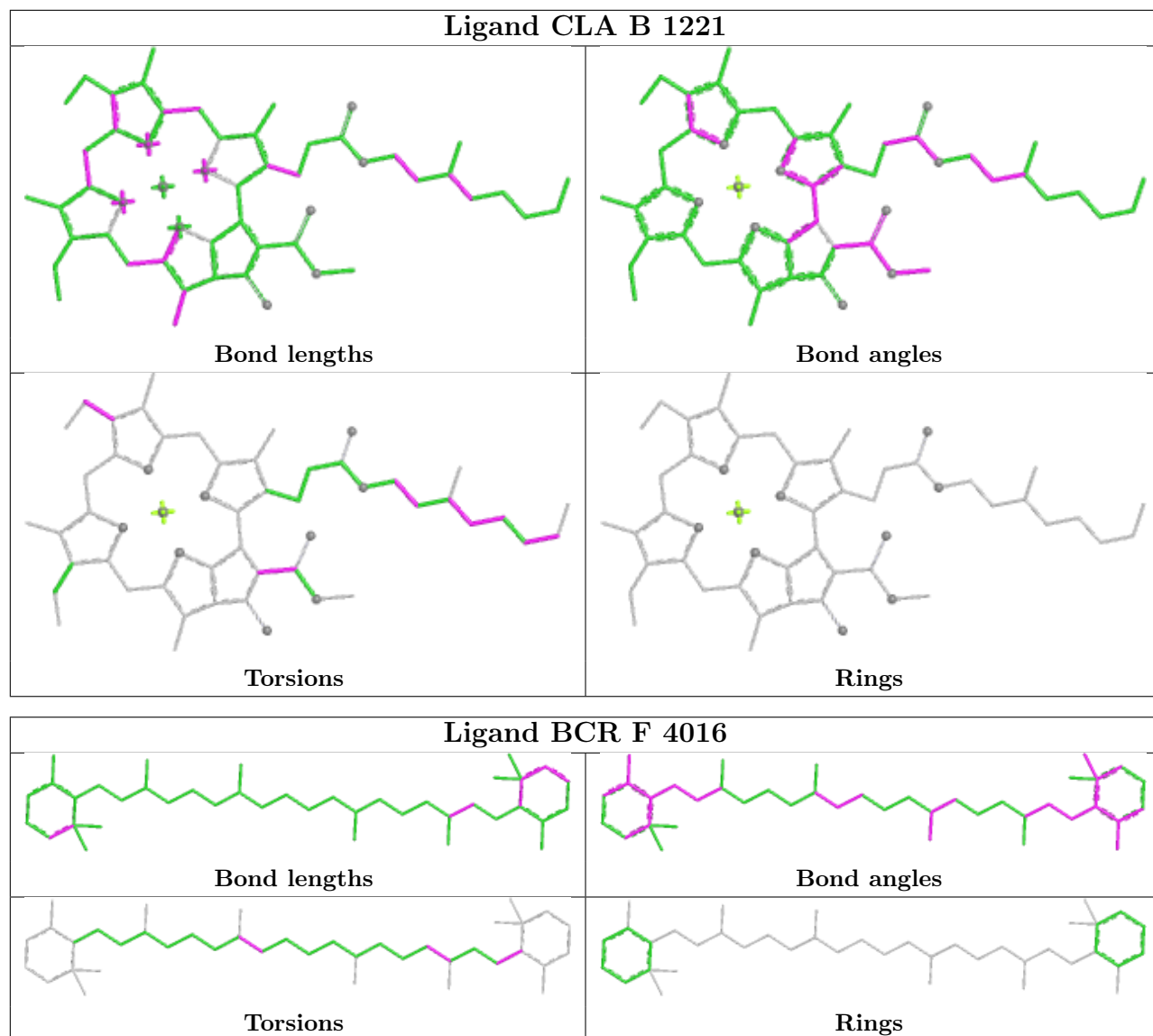


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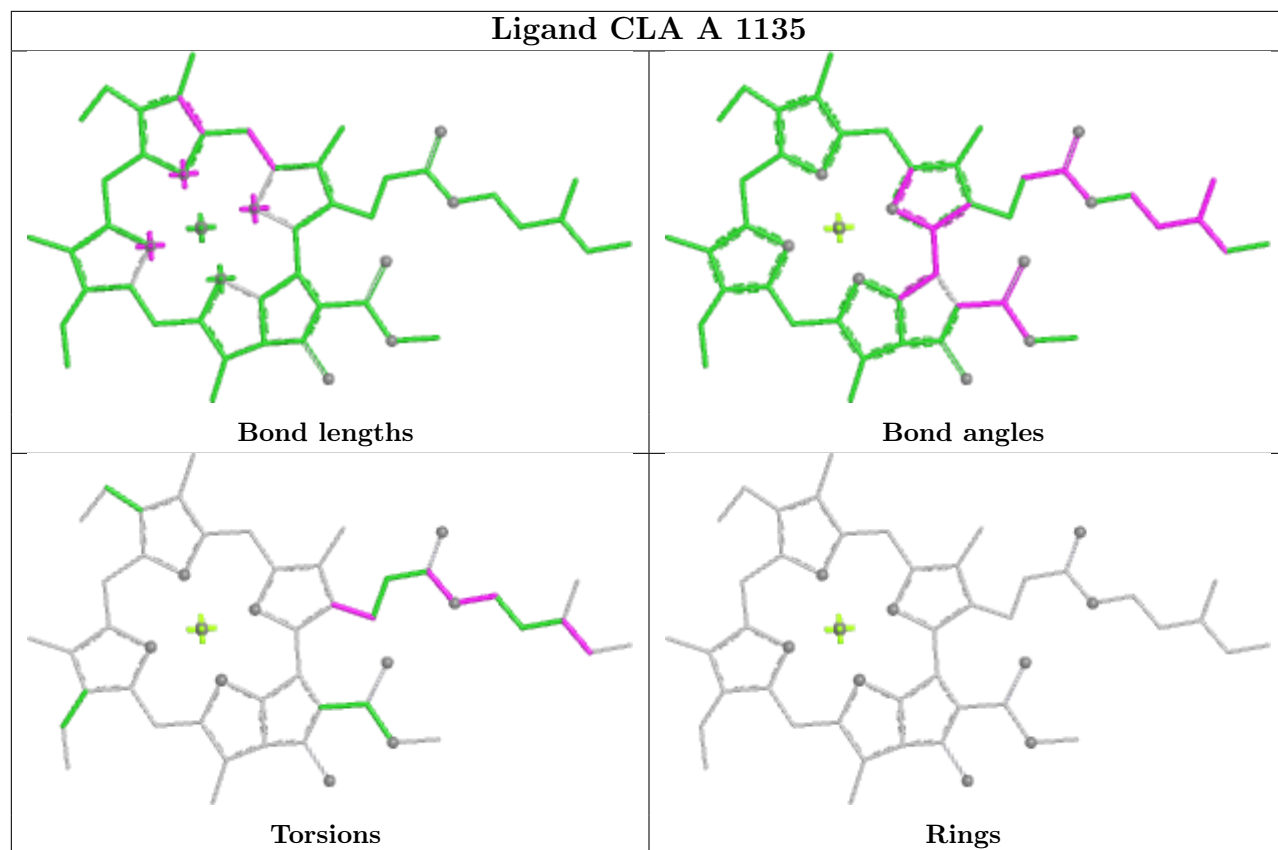


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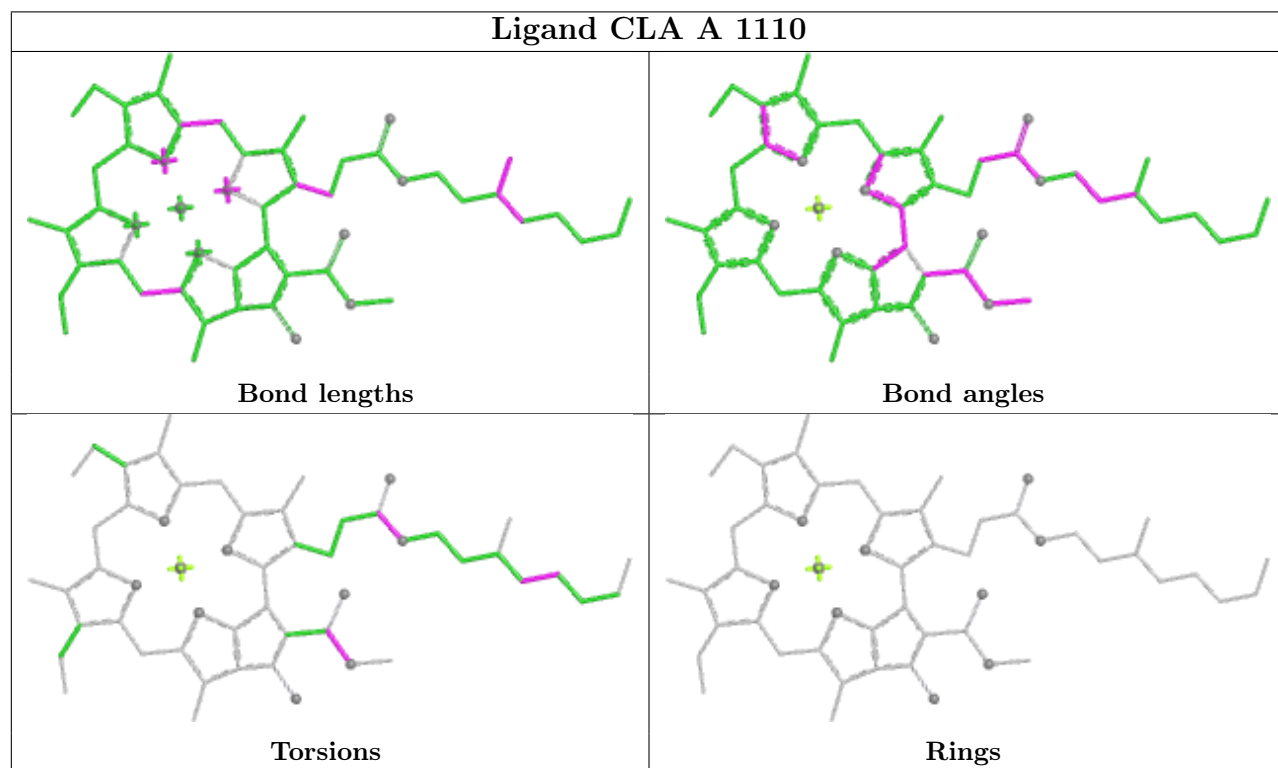




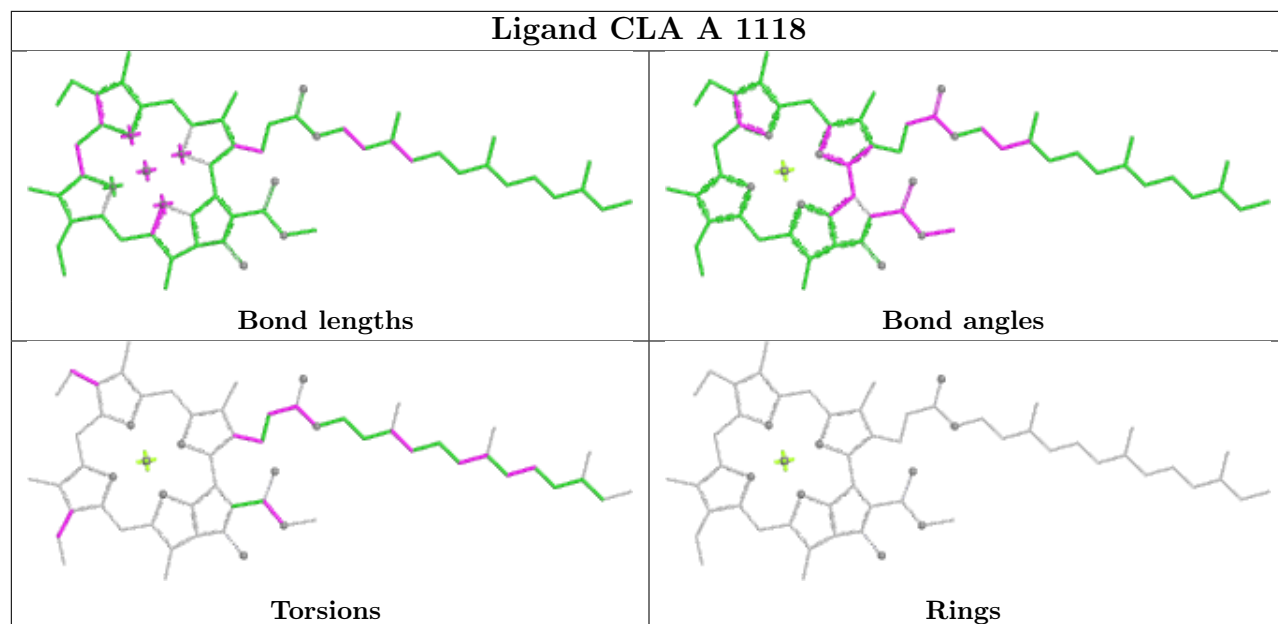
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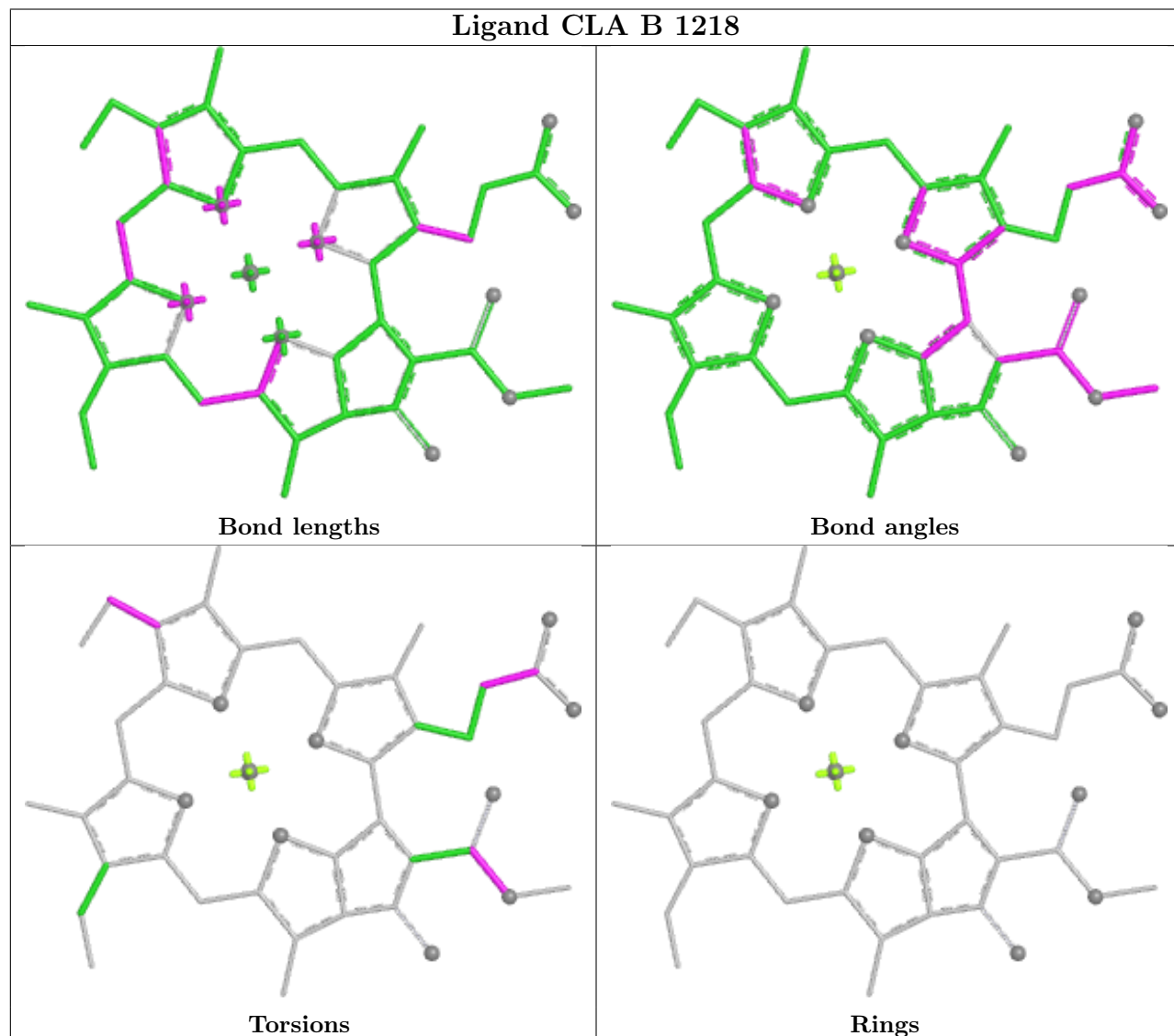
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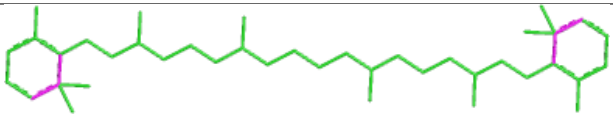
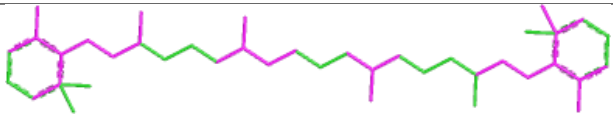
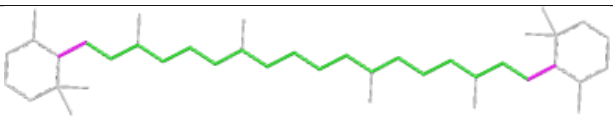
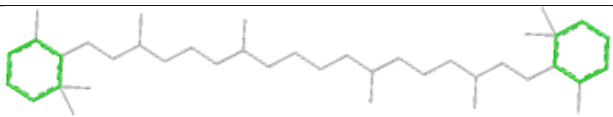


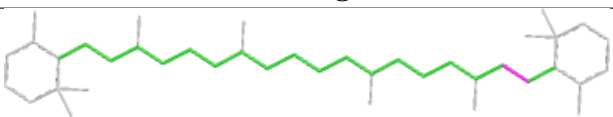
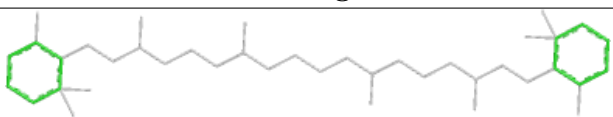
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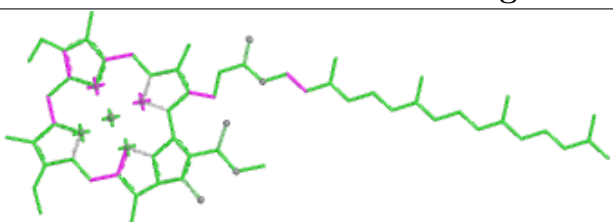
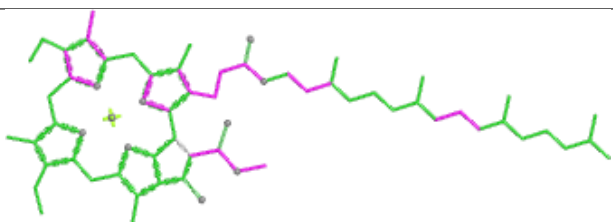
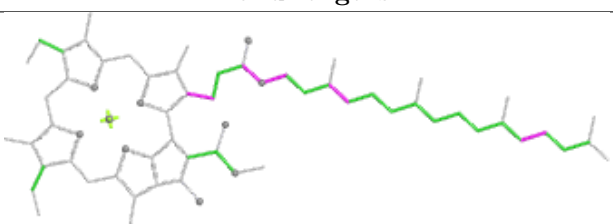
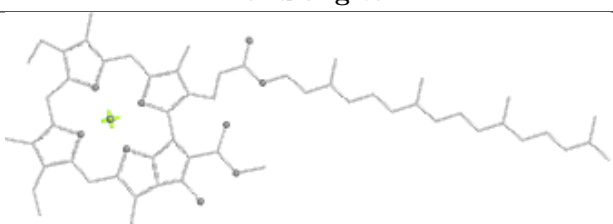


Ligand CLA B 1218

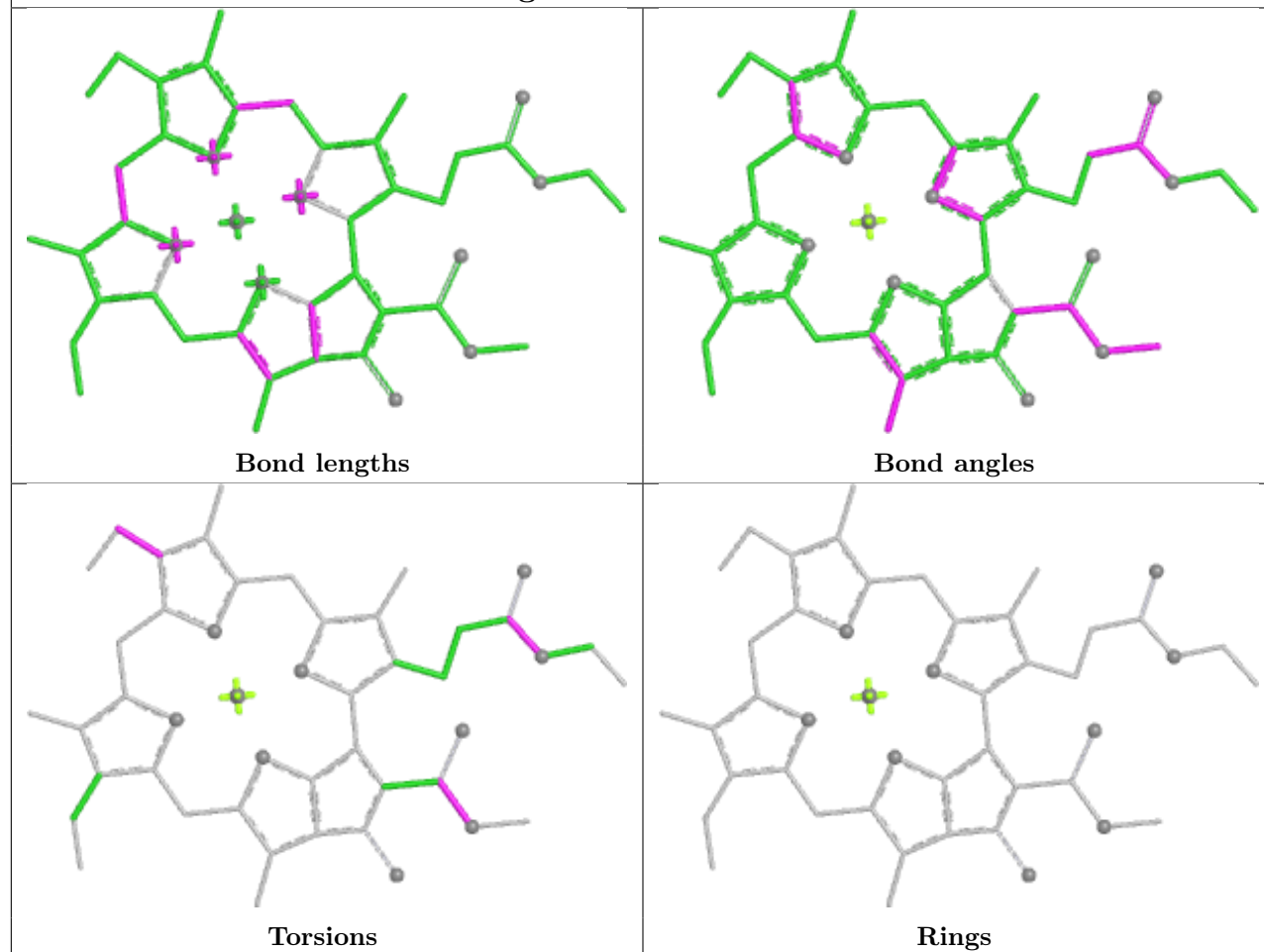


Ligand BCR J 4013	
	
Bond lengths	Bond angles
	
Torsions	Rings

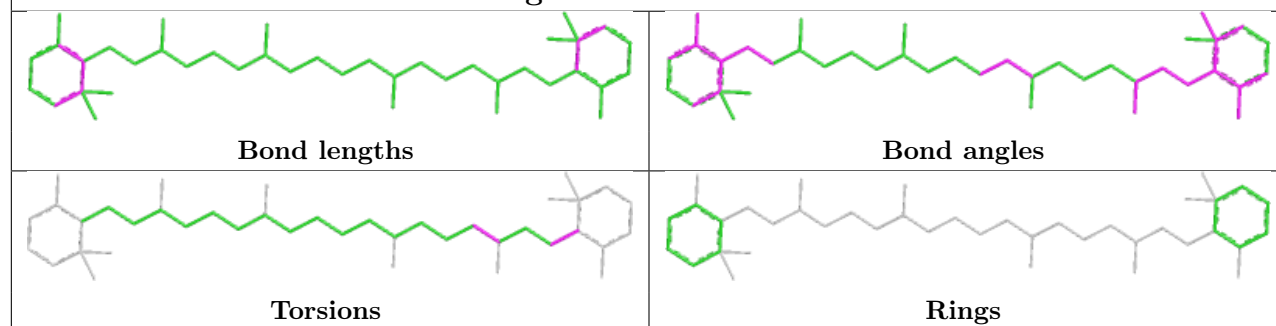
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1119	
	
Bond lengths	Bond angles
	
Torsions	Rings

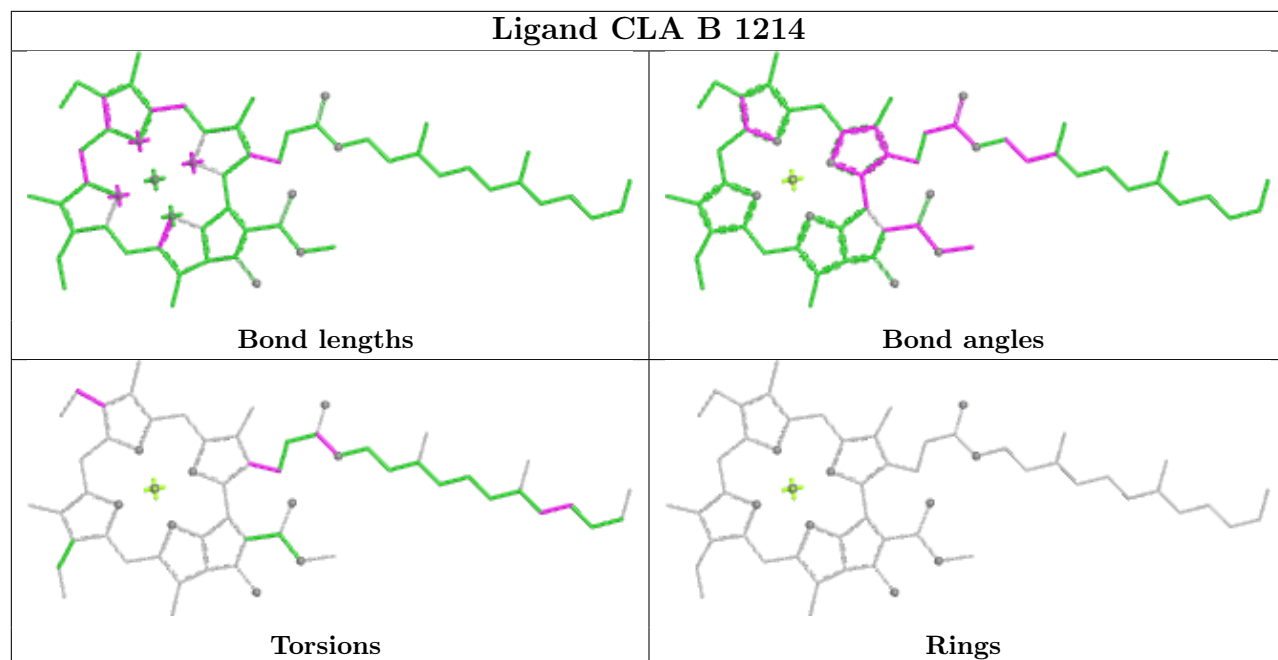
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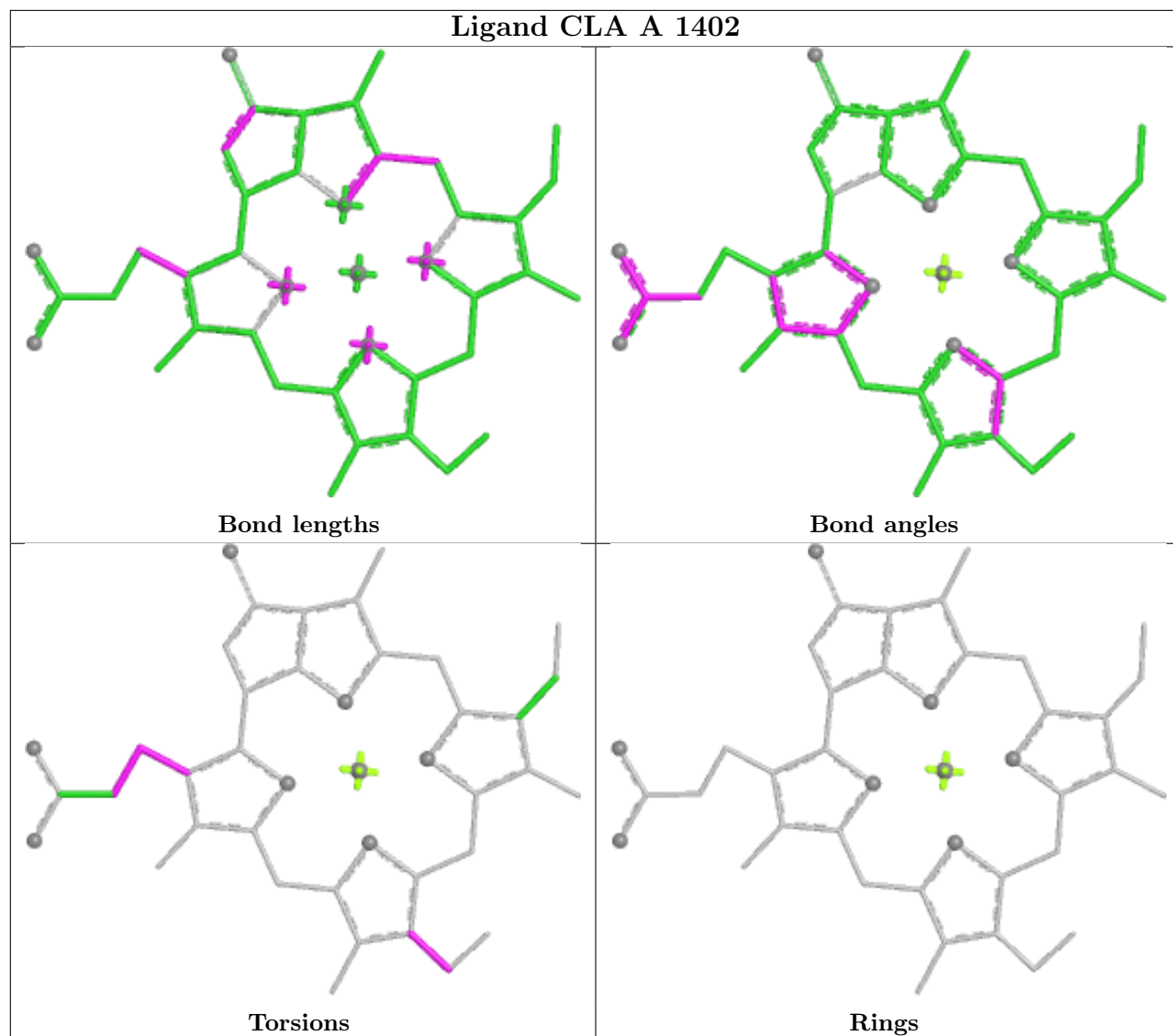
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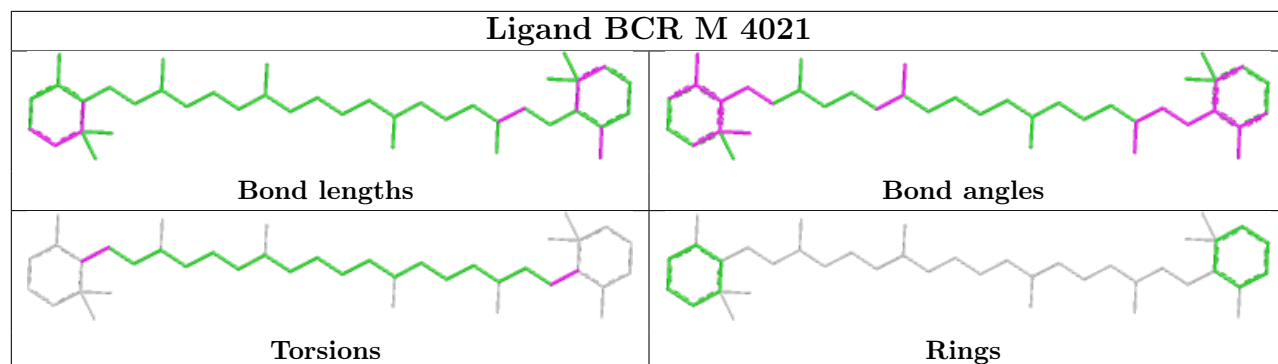
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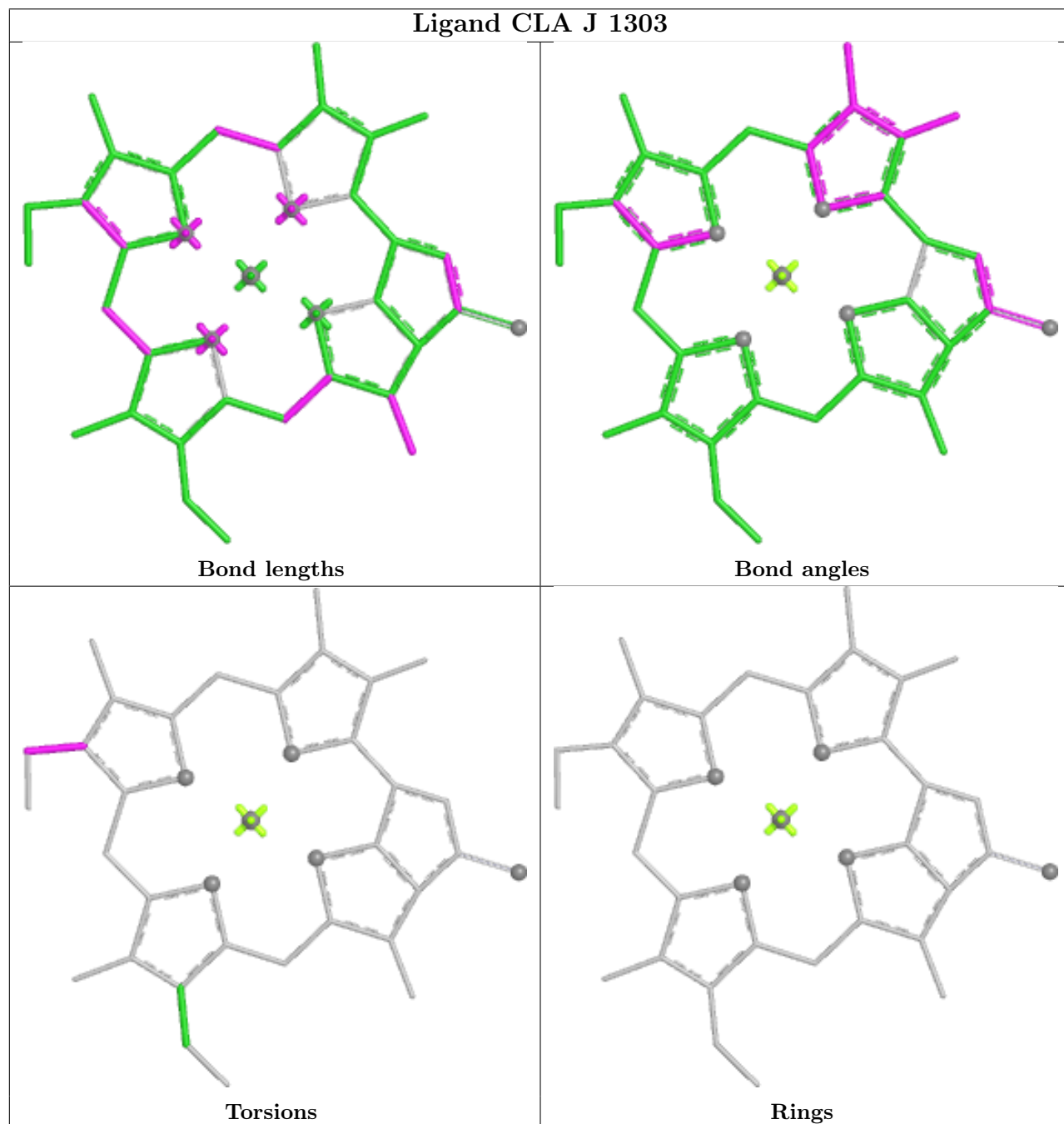
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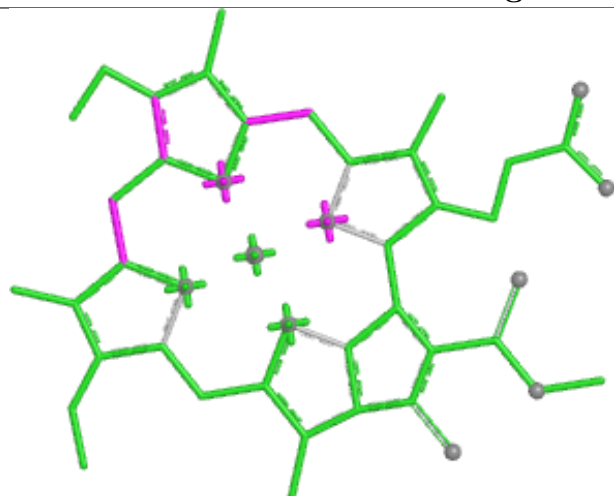
Ligand BCR M 4021



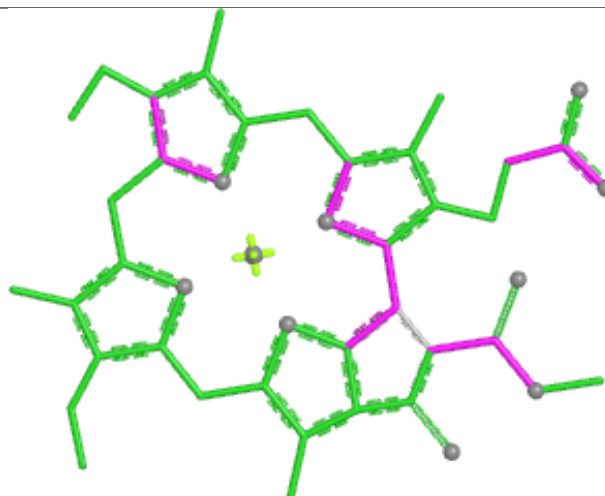
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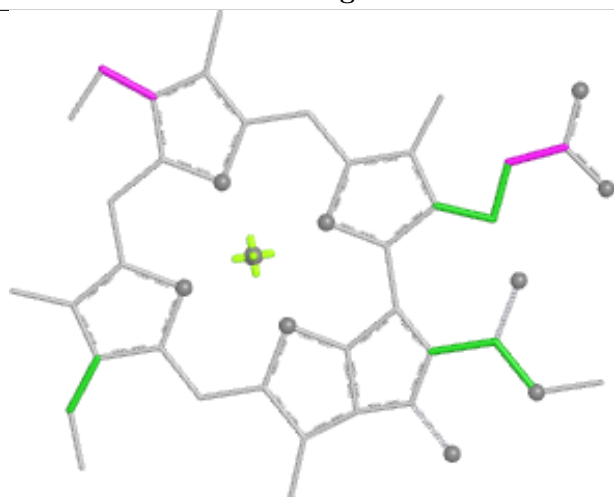
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Bond lengths



Bond angles

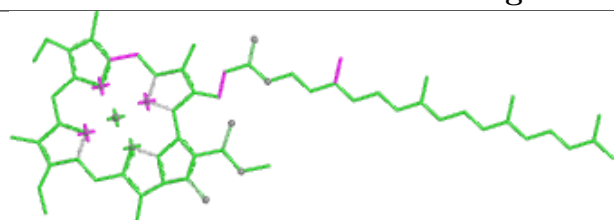


Torsions

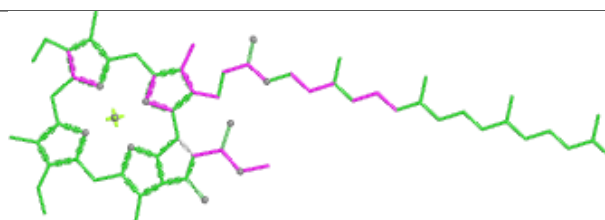


Rings

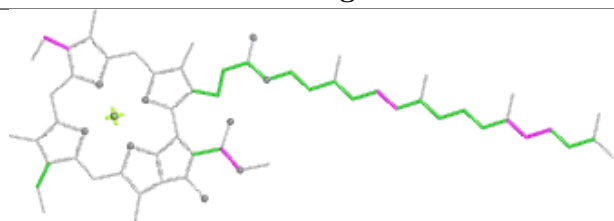
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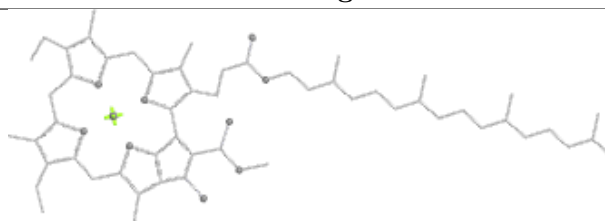
Bond lengths



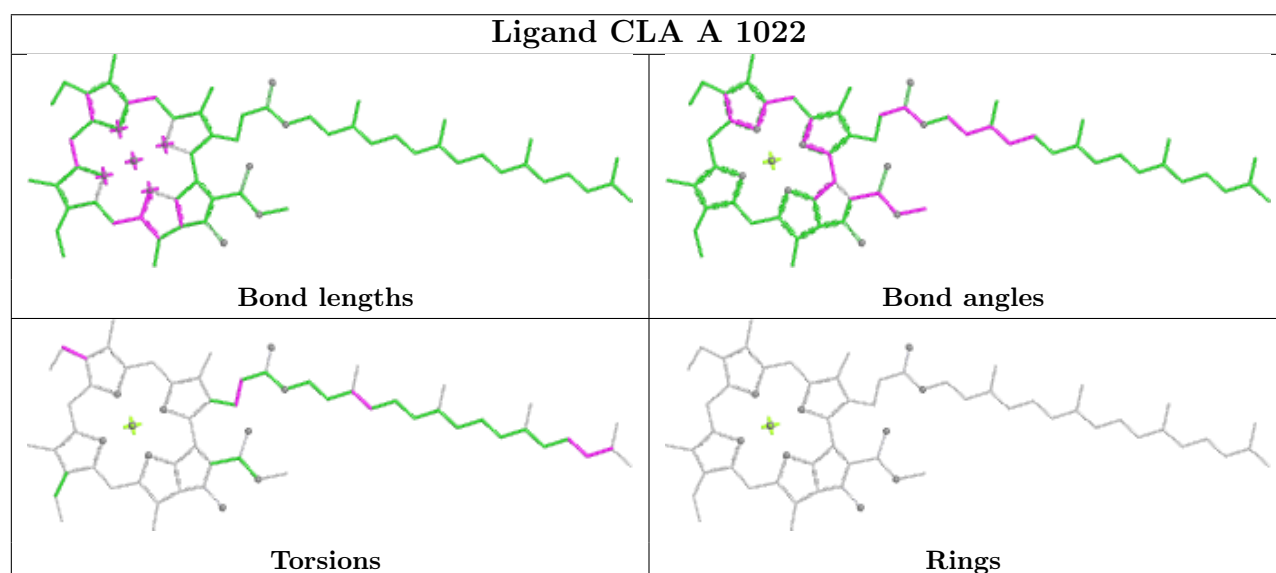
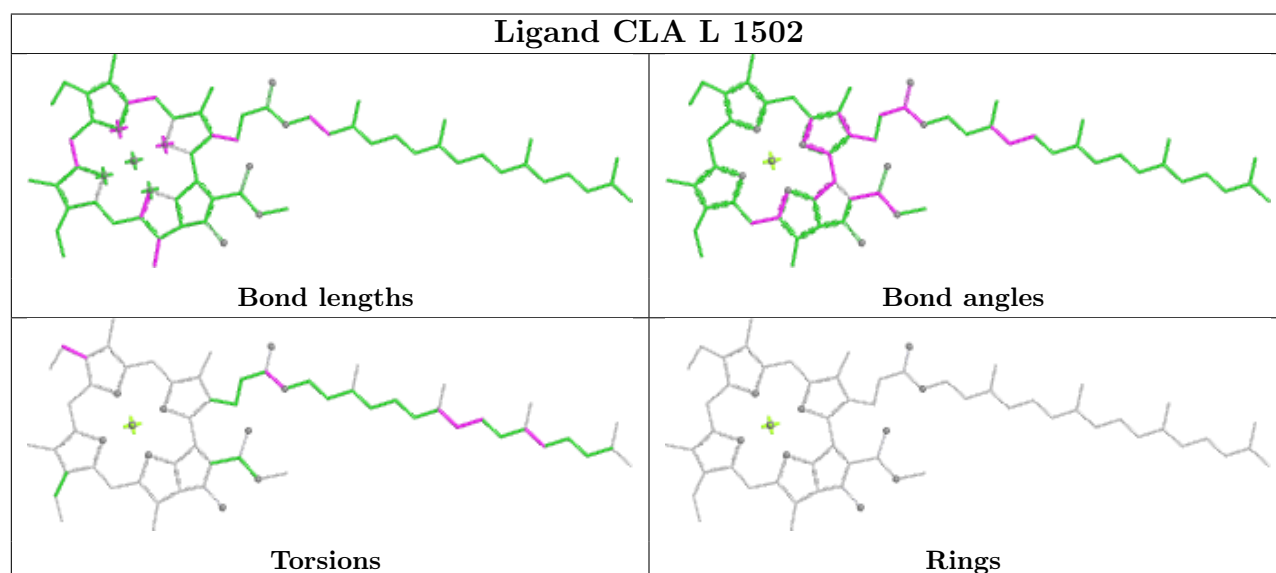
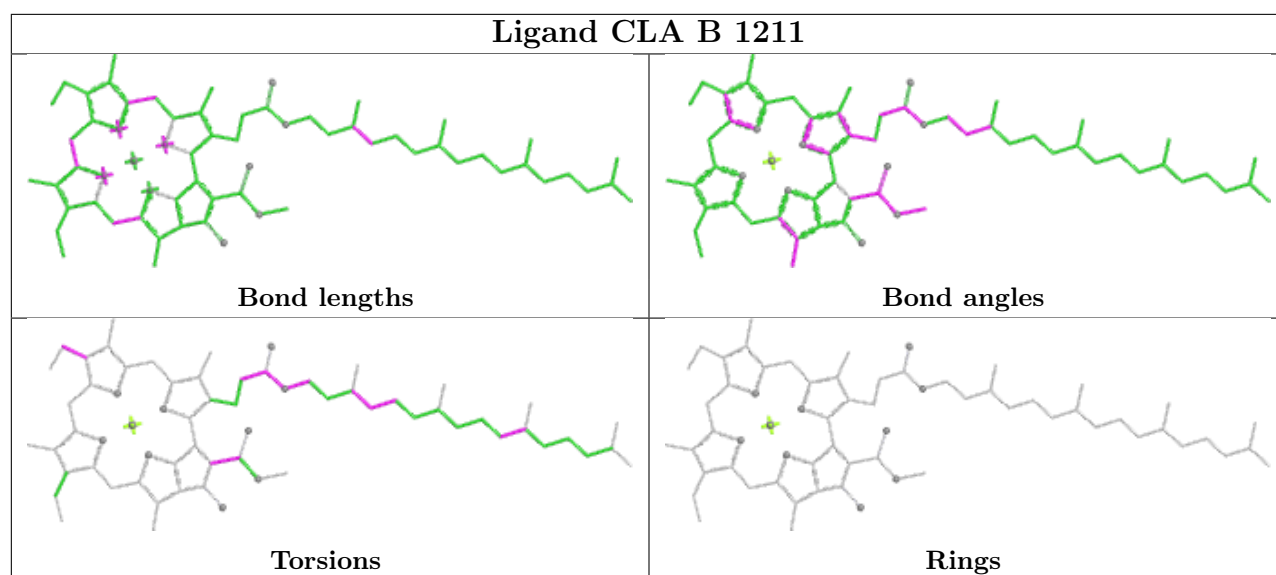
Bond angles

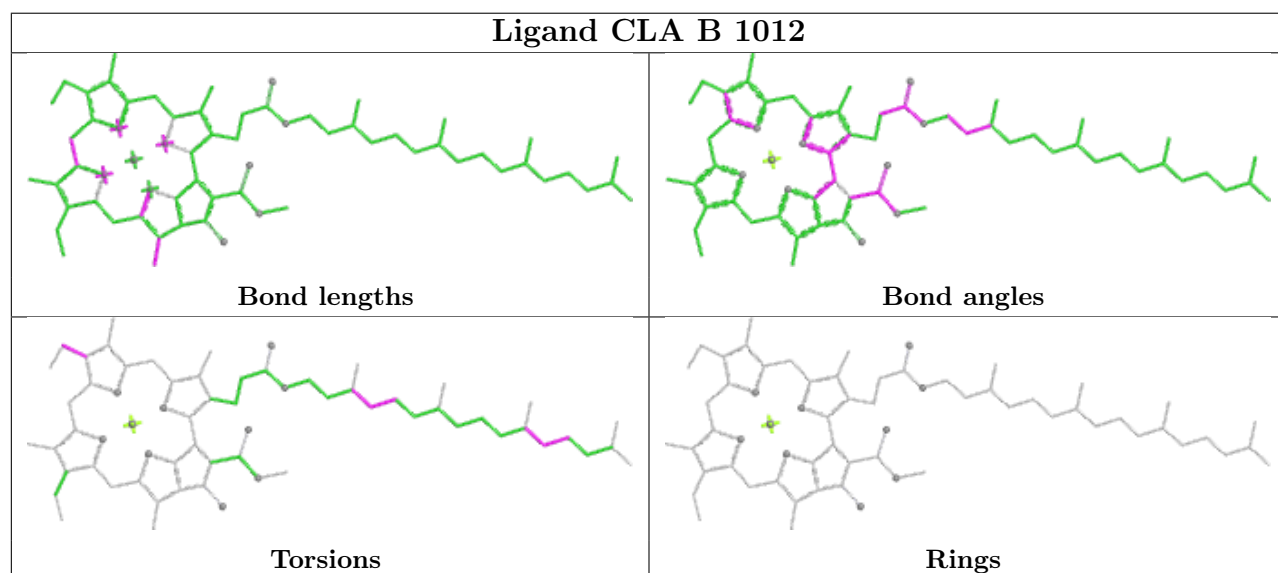
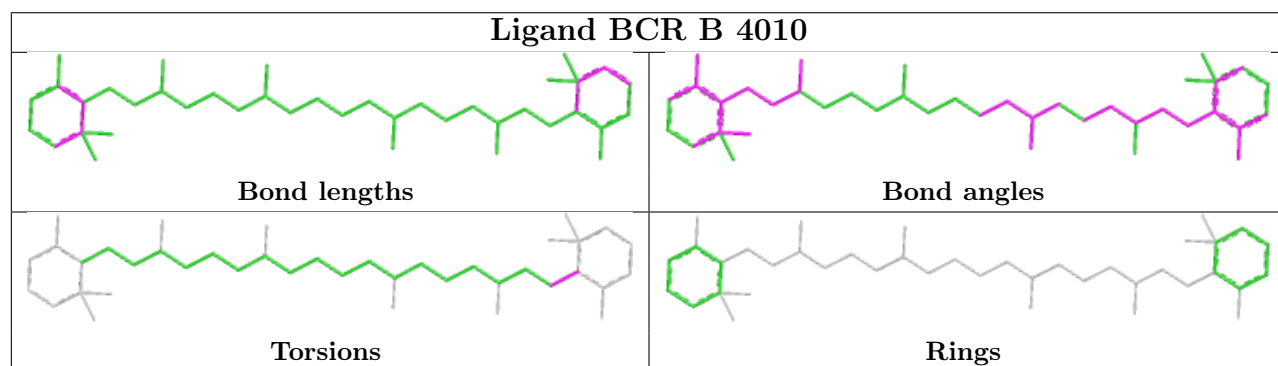
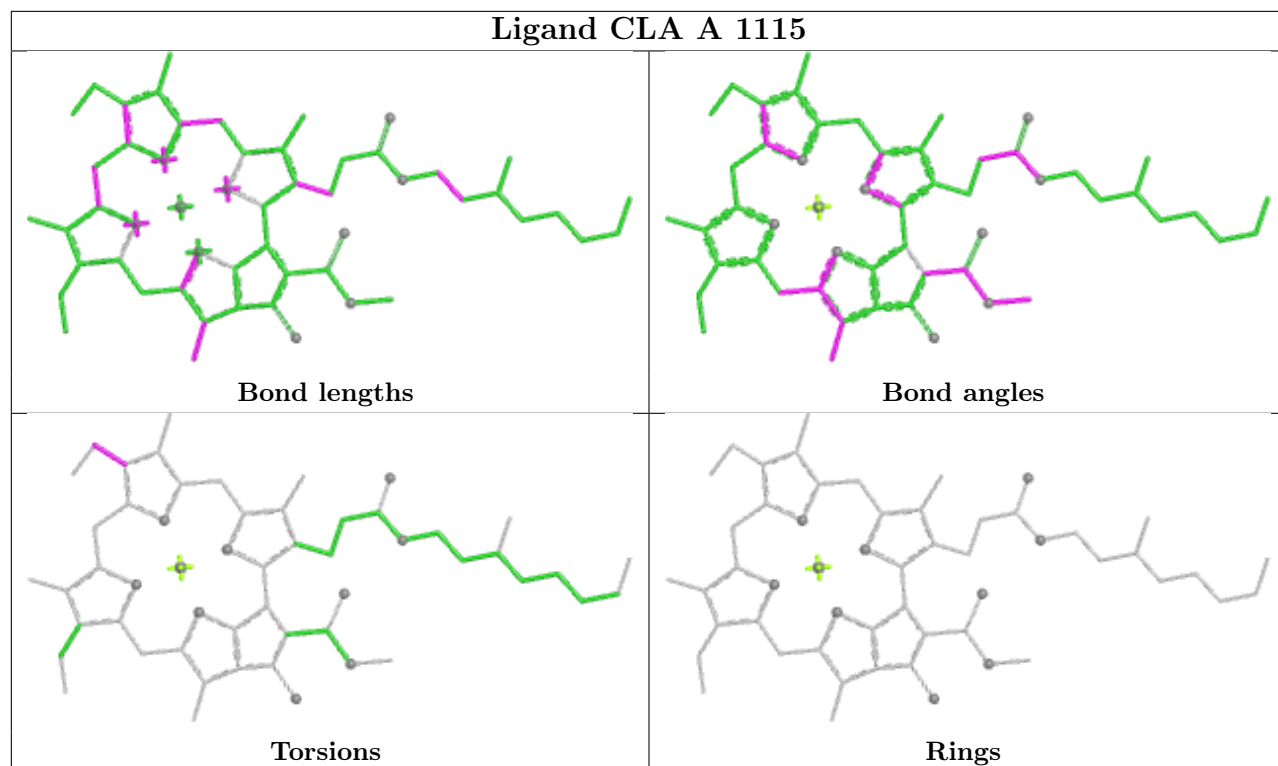


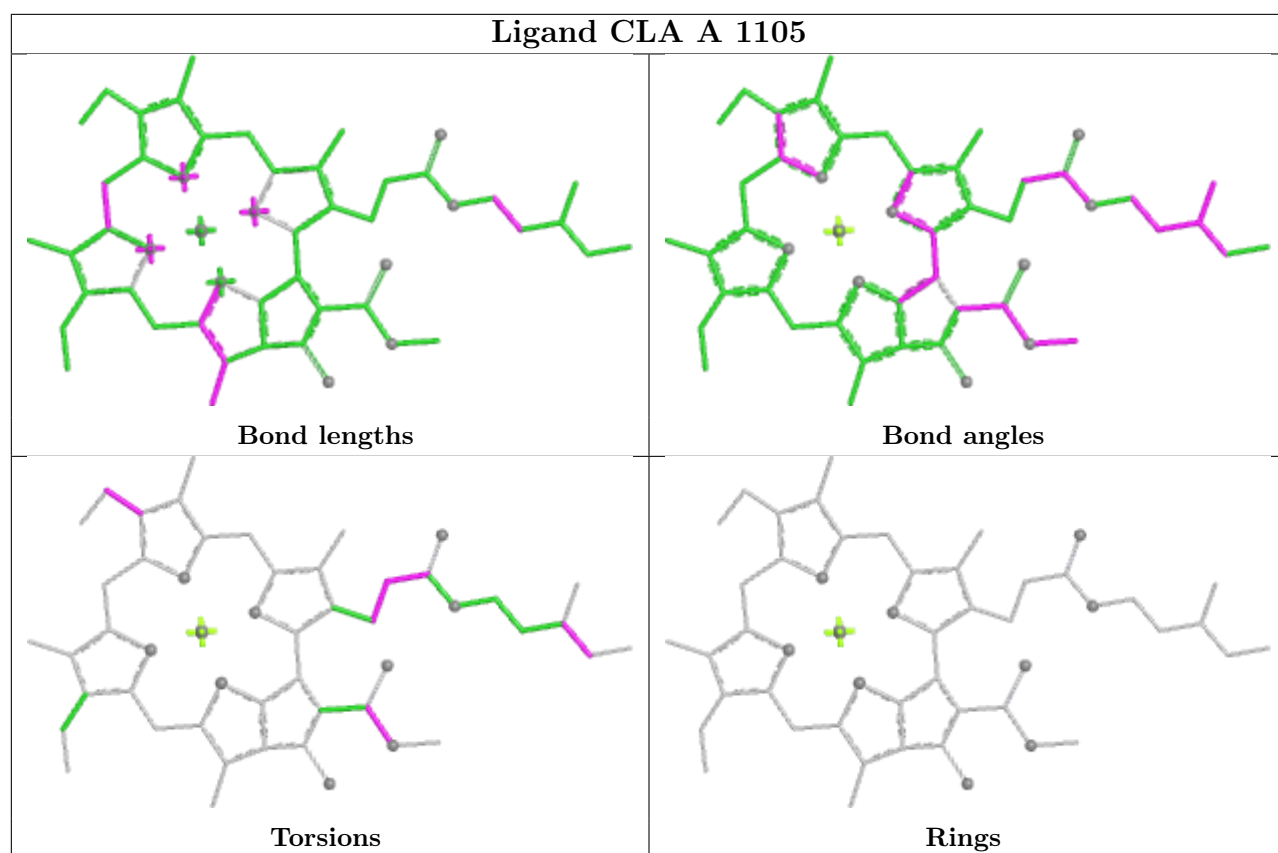
Torsions



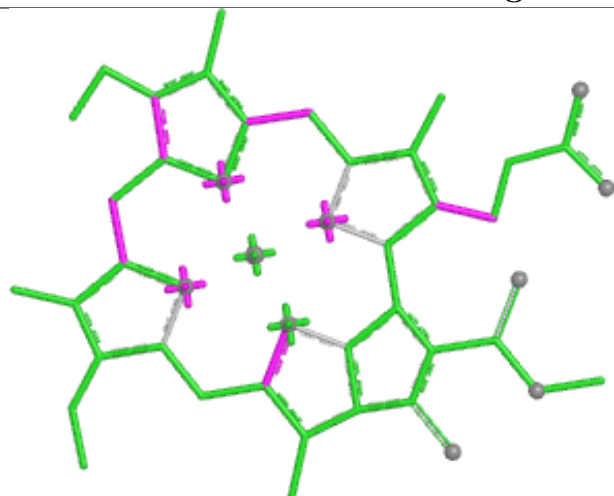
Rings



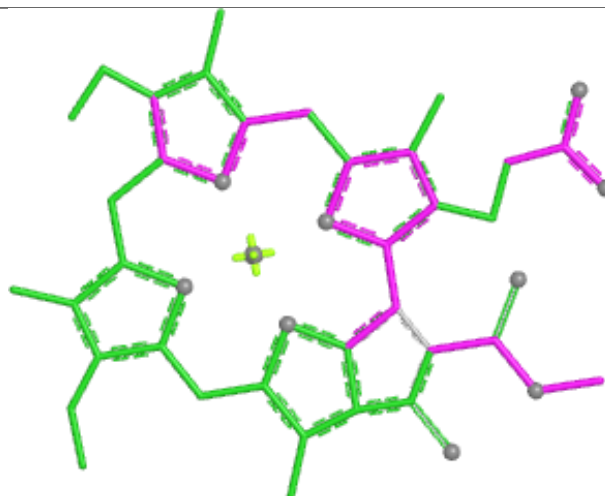




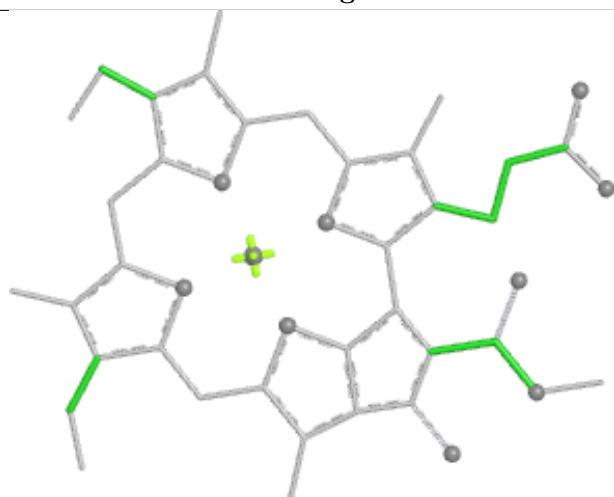
Ligand CLA B 1232



Bond lengths



Bond angles

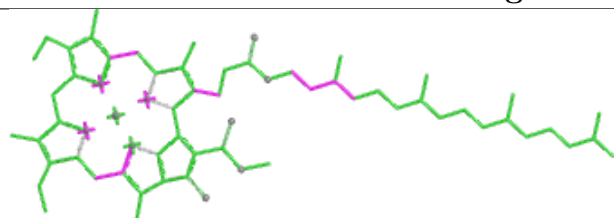


Torsions

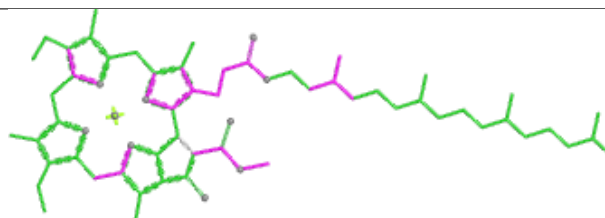


Rings

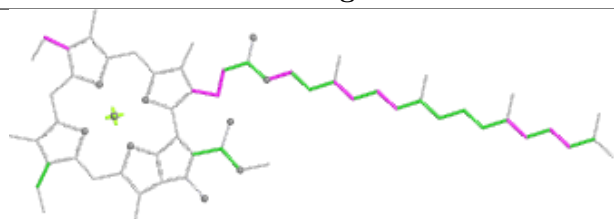
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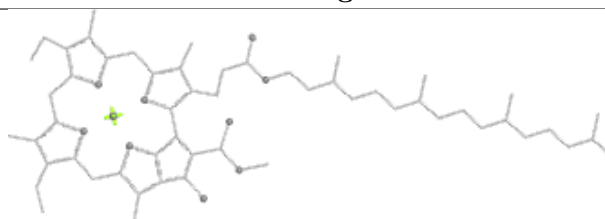
Bond lengths



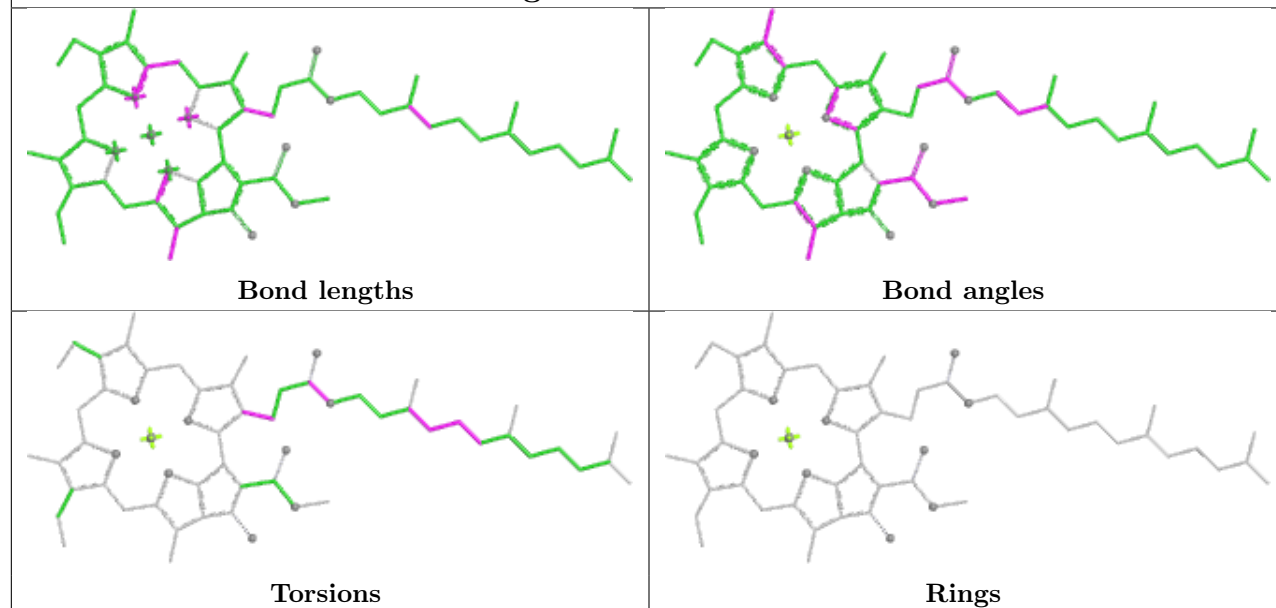
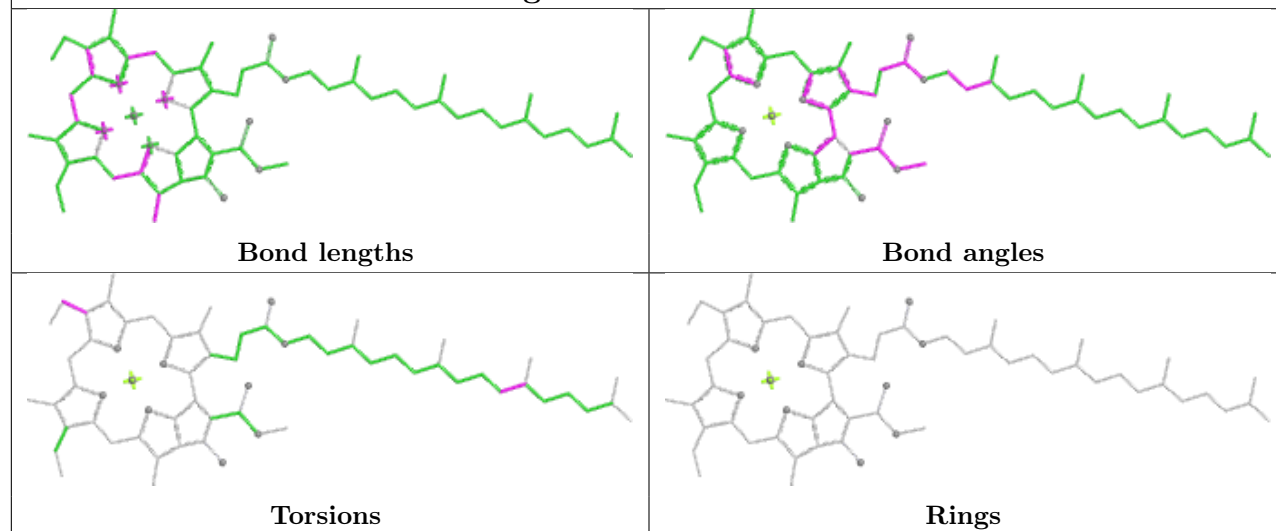
Bond angles



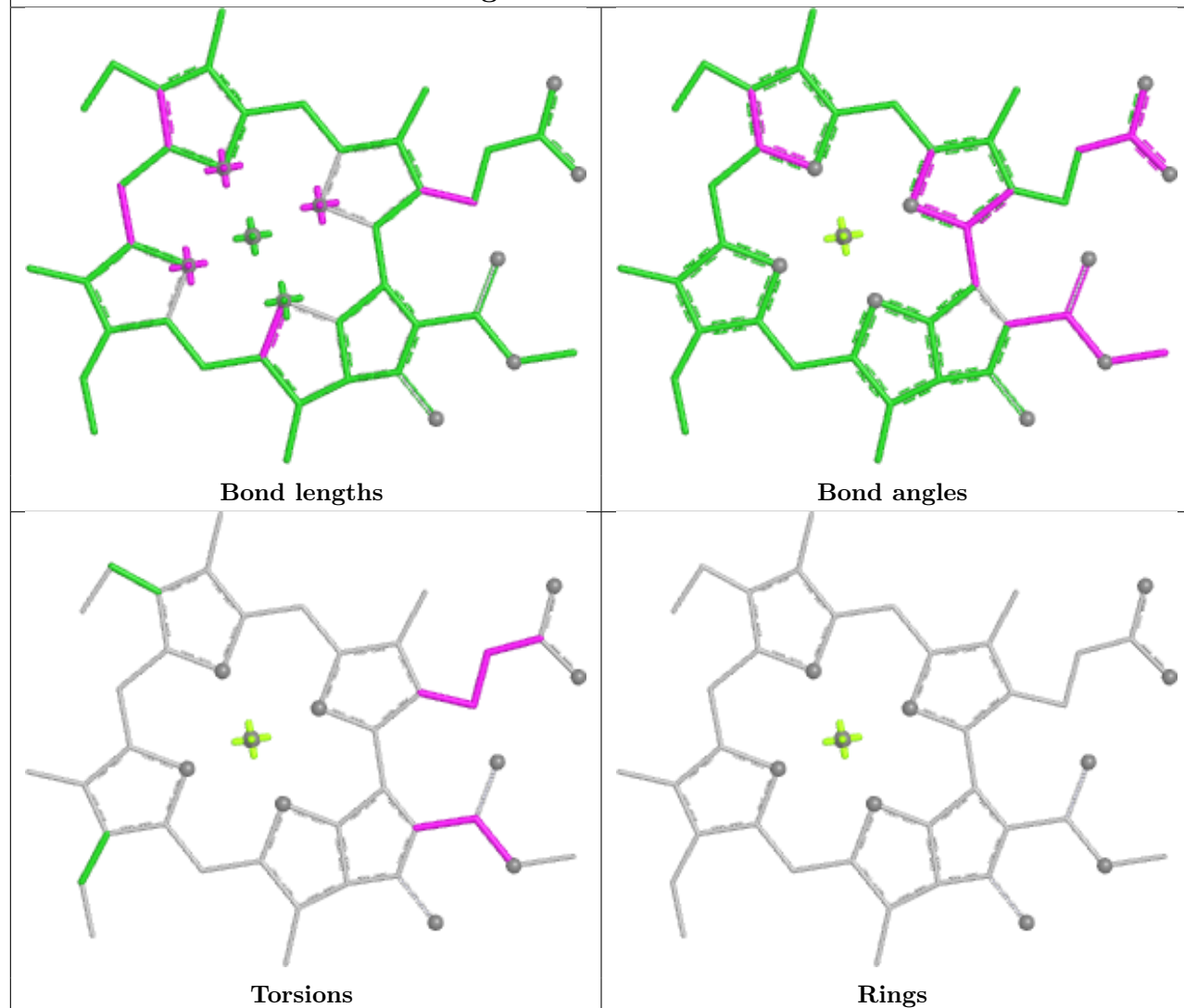
Torsions



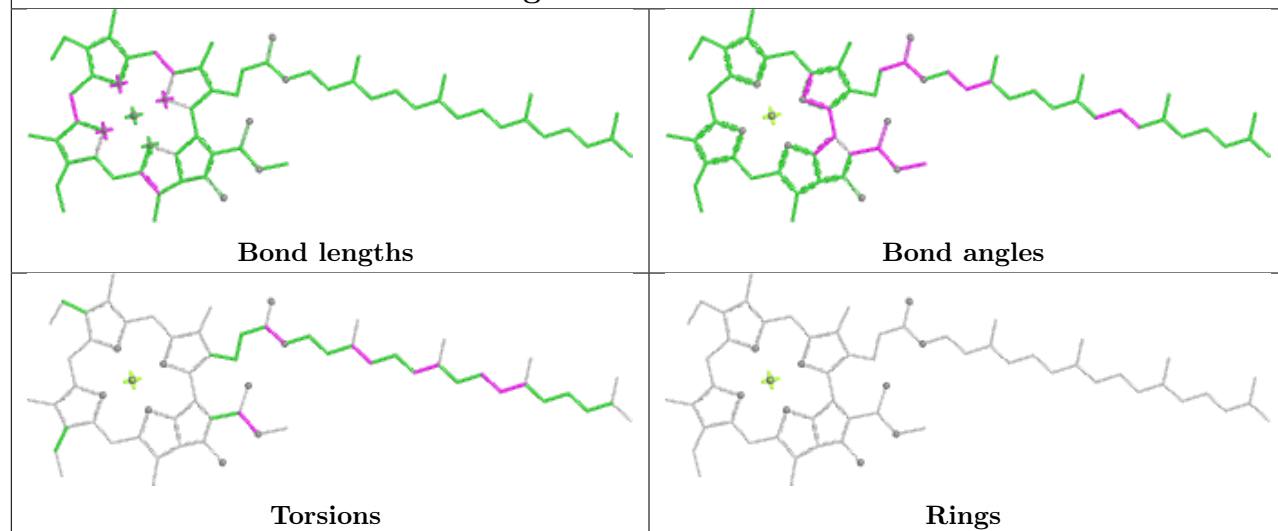
Rings

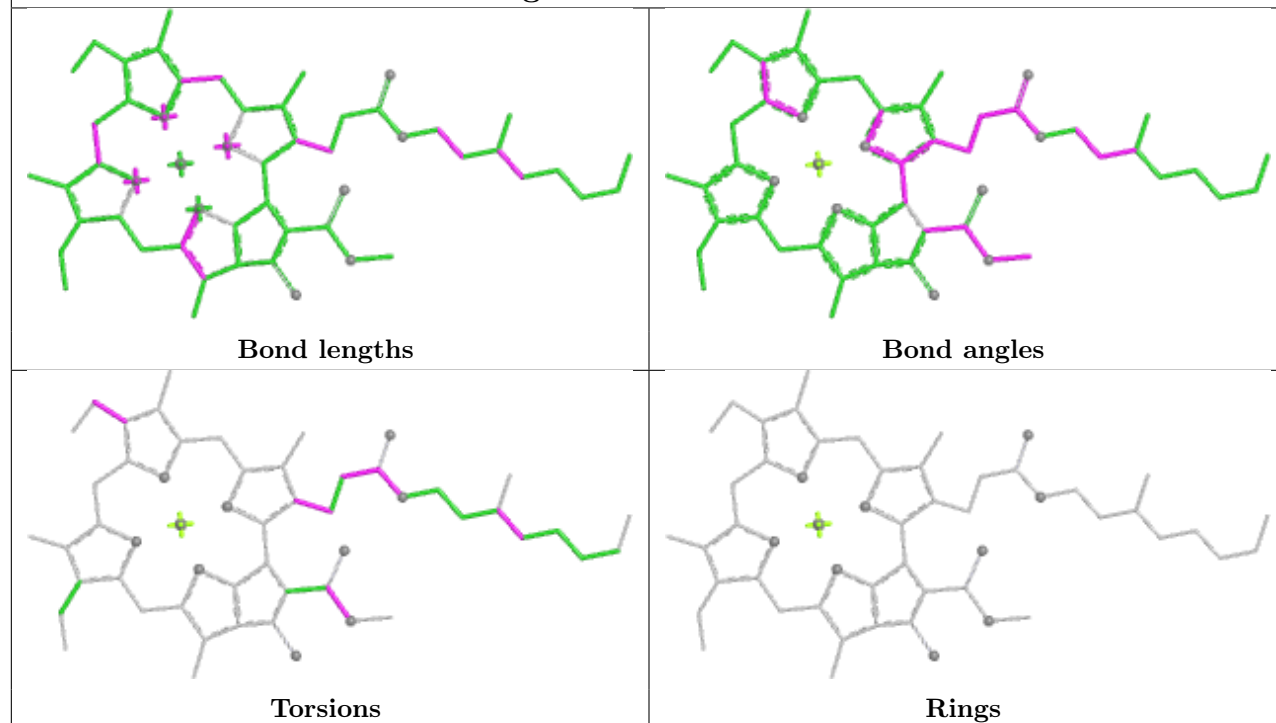
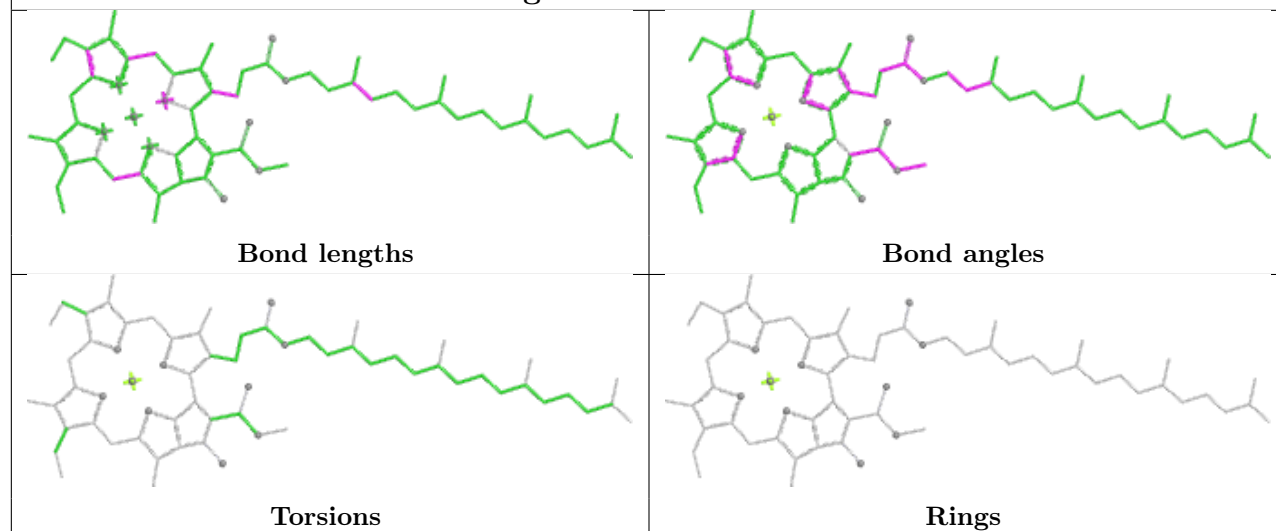
Ligand CLA B 1215**Ligand CLA B 1235**

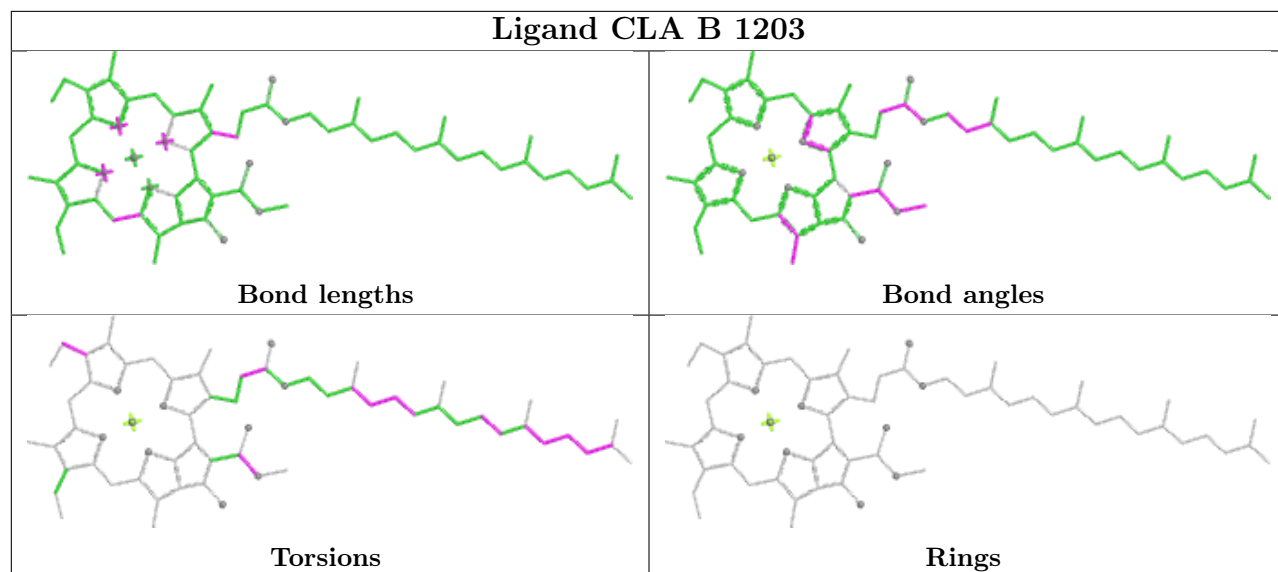
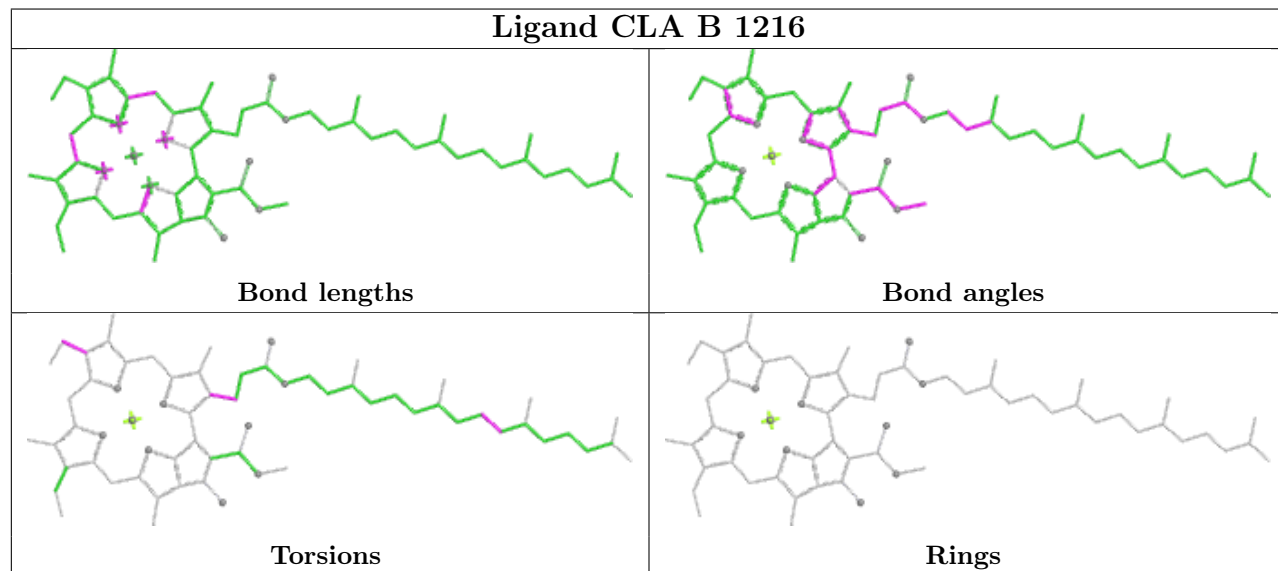
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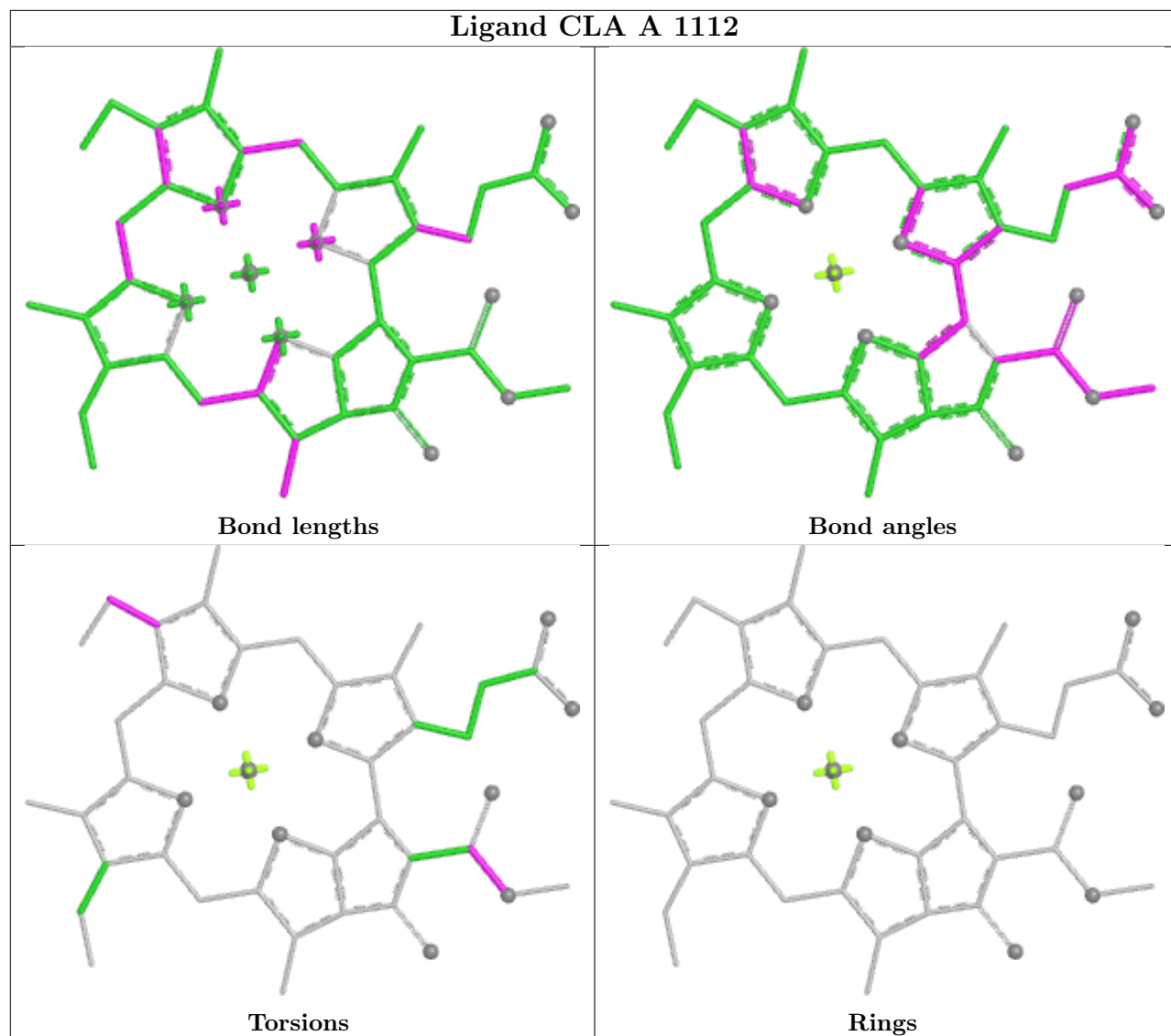
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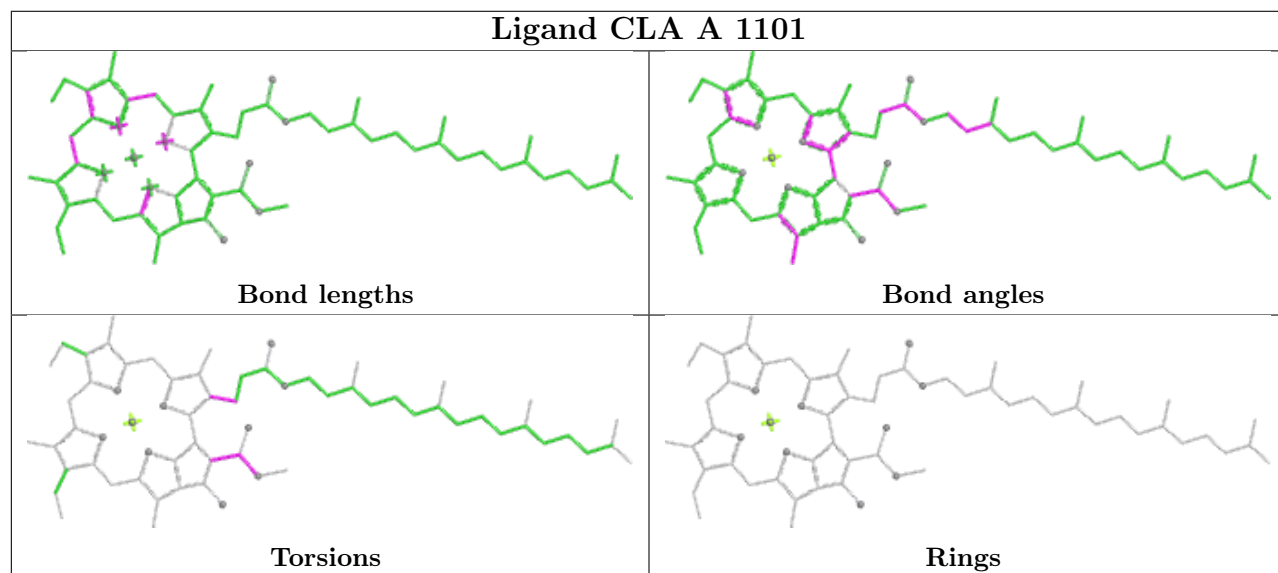
Ligand CLA A 1116**Ligand CLA B 1204**

Ligand CLA B 1203**Ligand CLA B 1216**

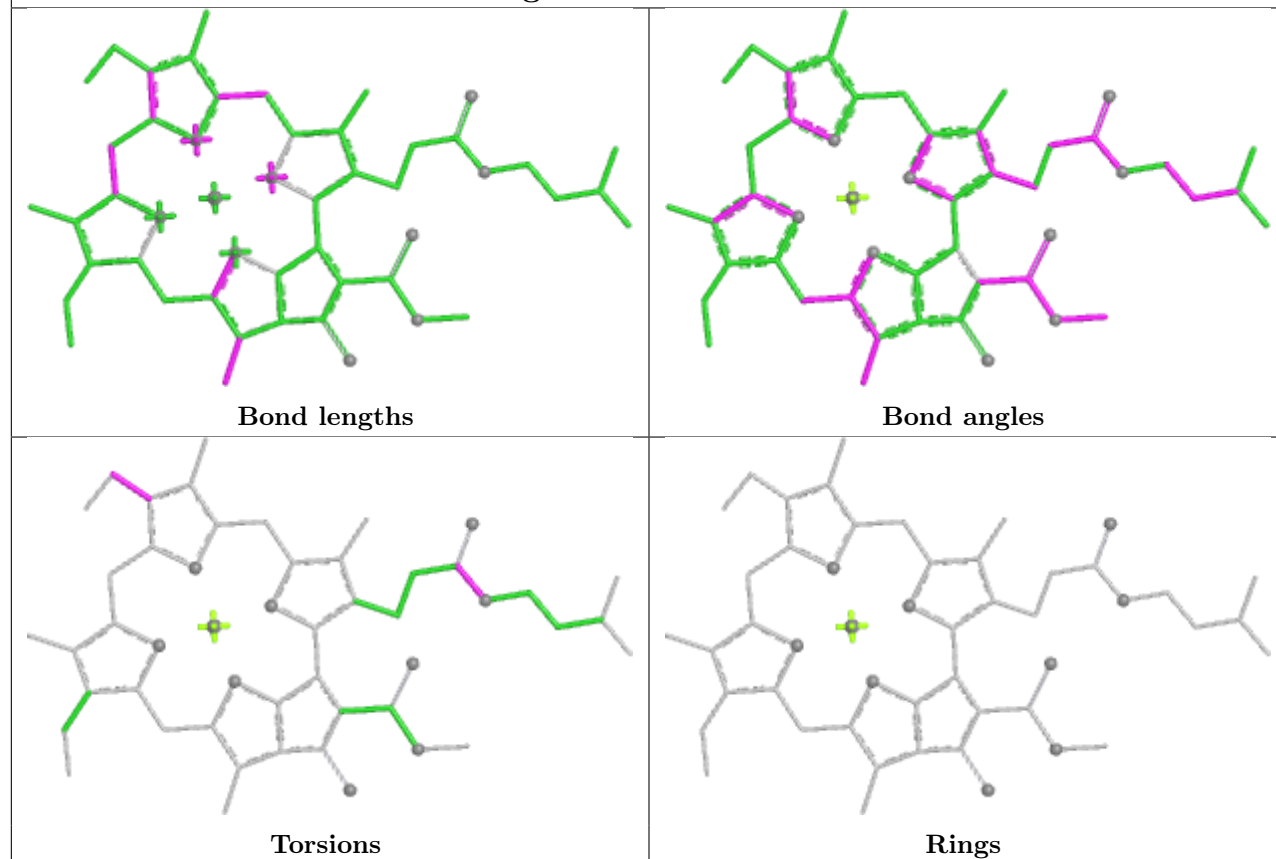
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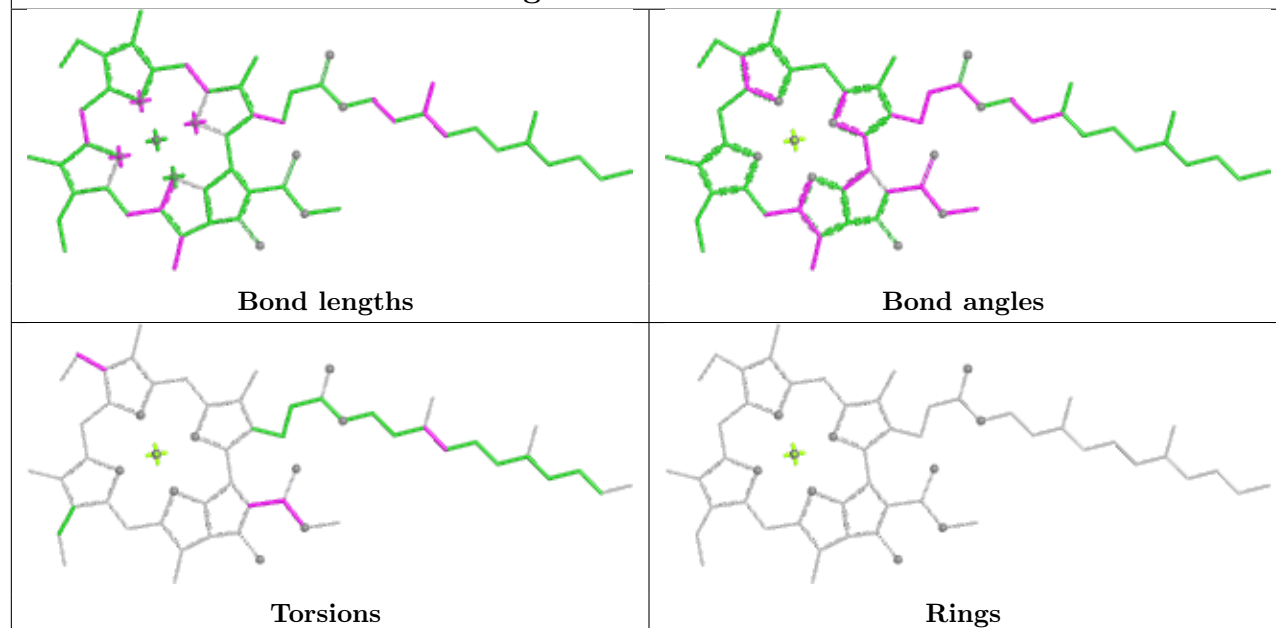
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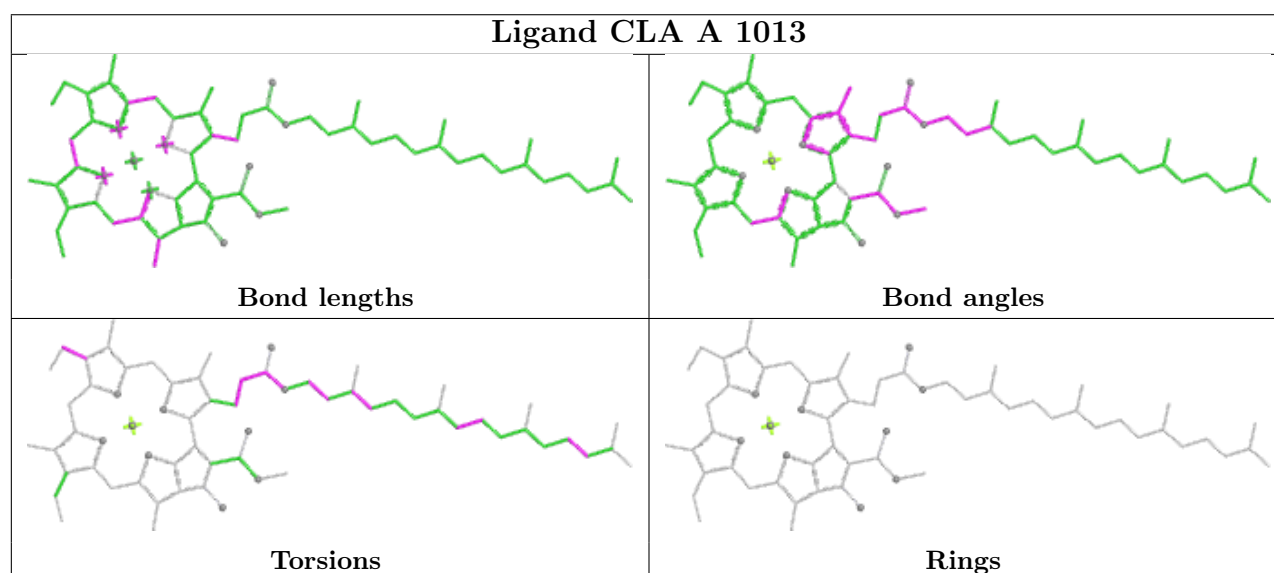
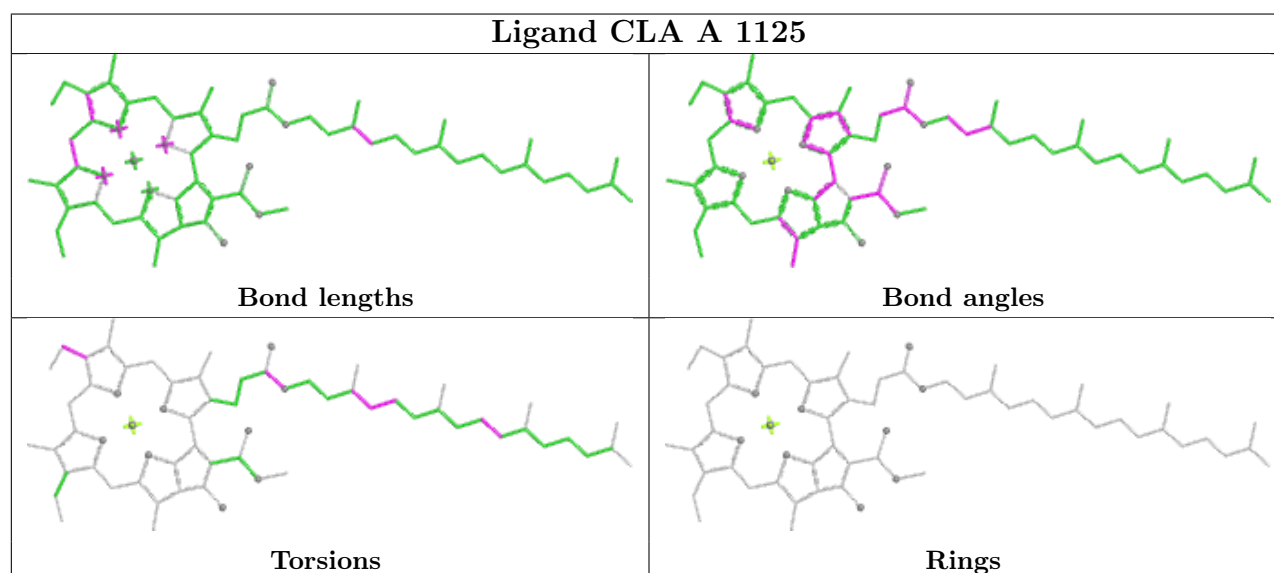
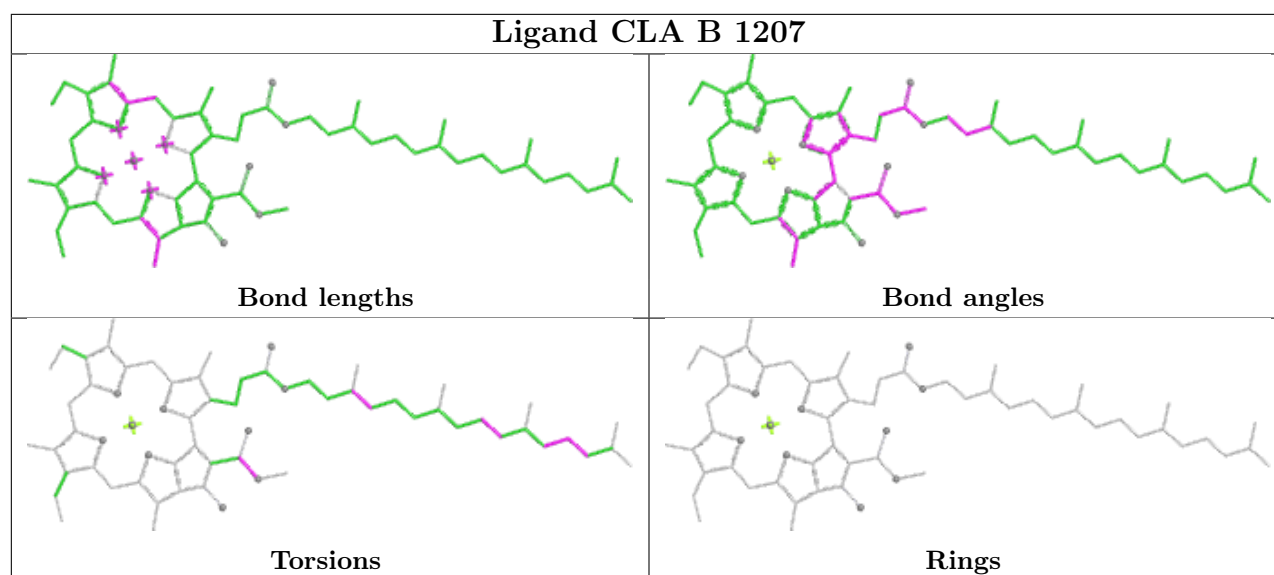


Ligand CLA A 1129

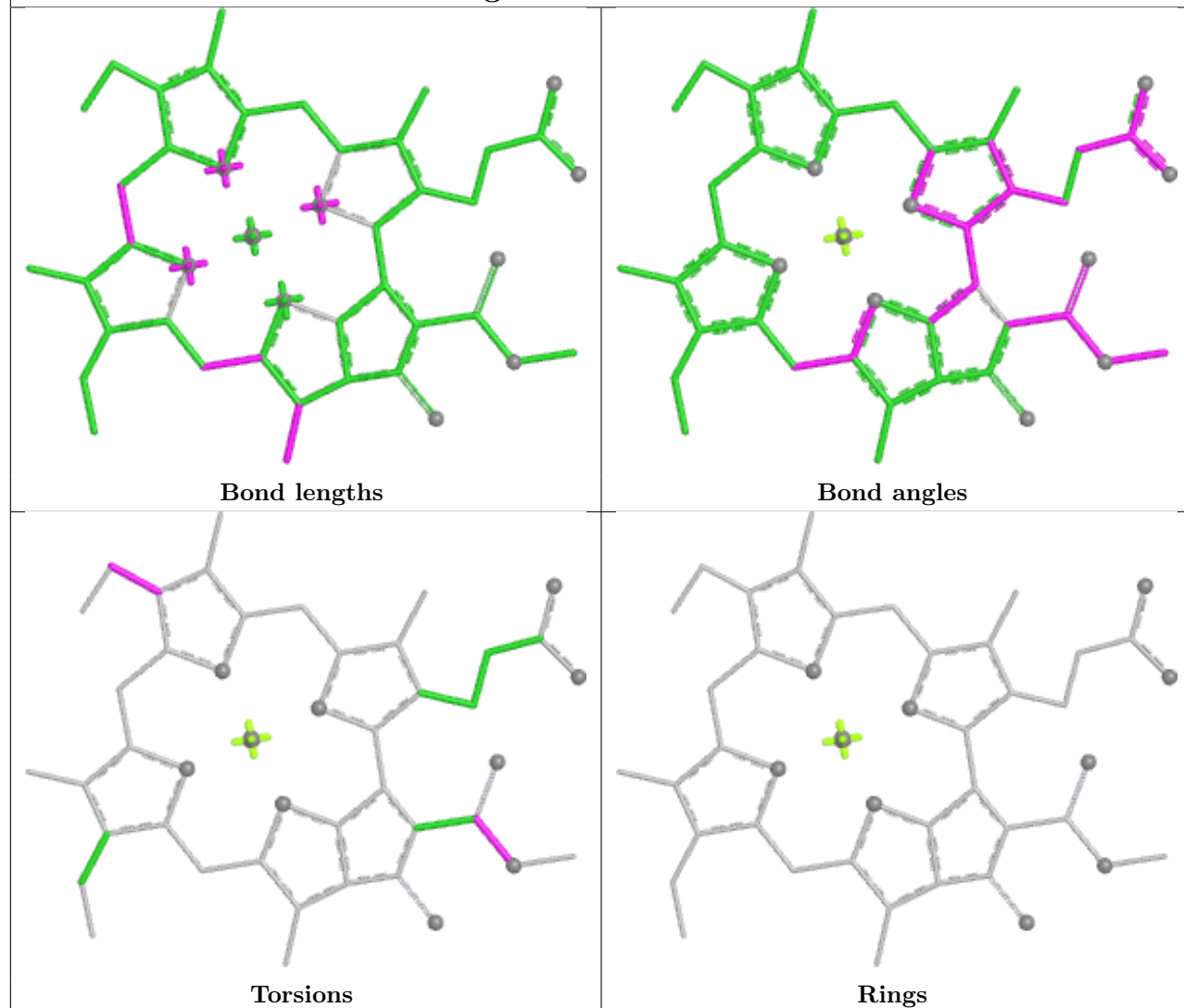


Ligand CLA B 1230

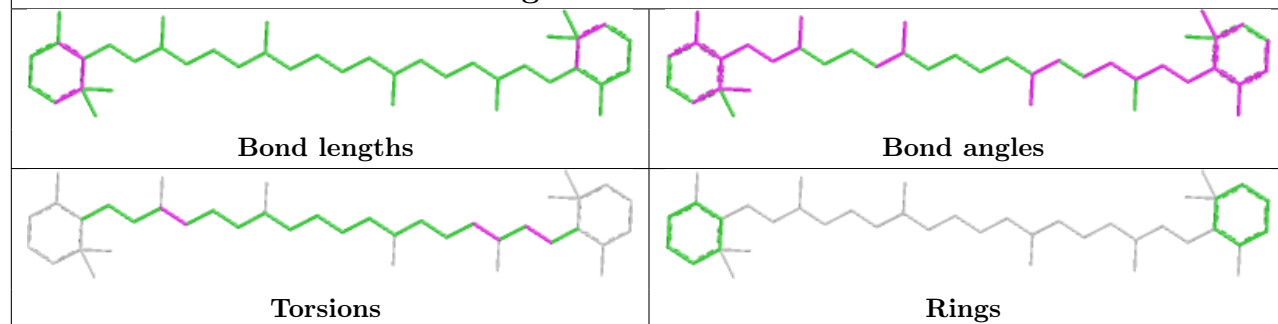




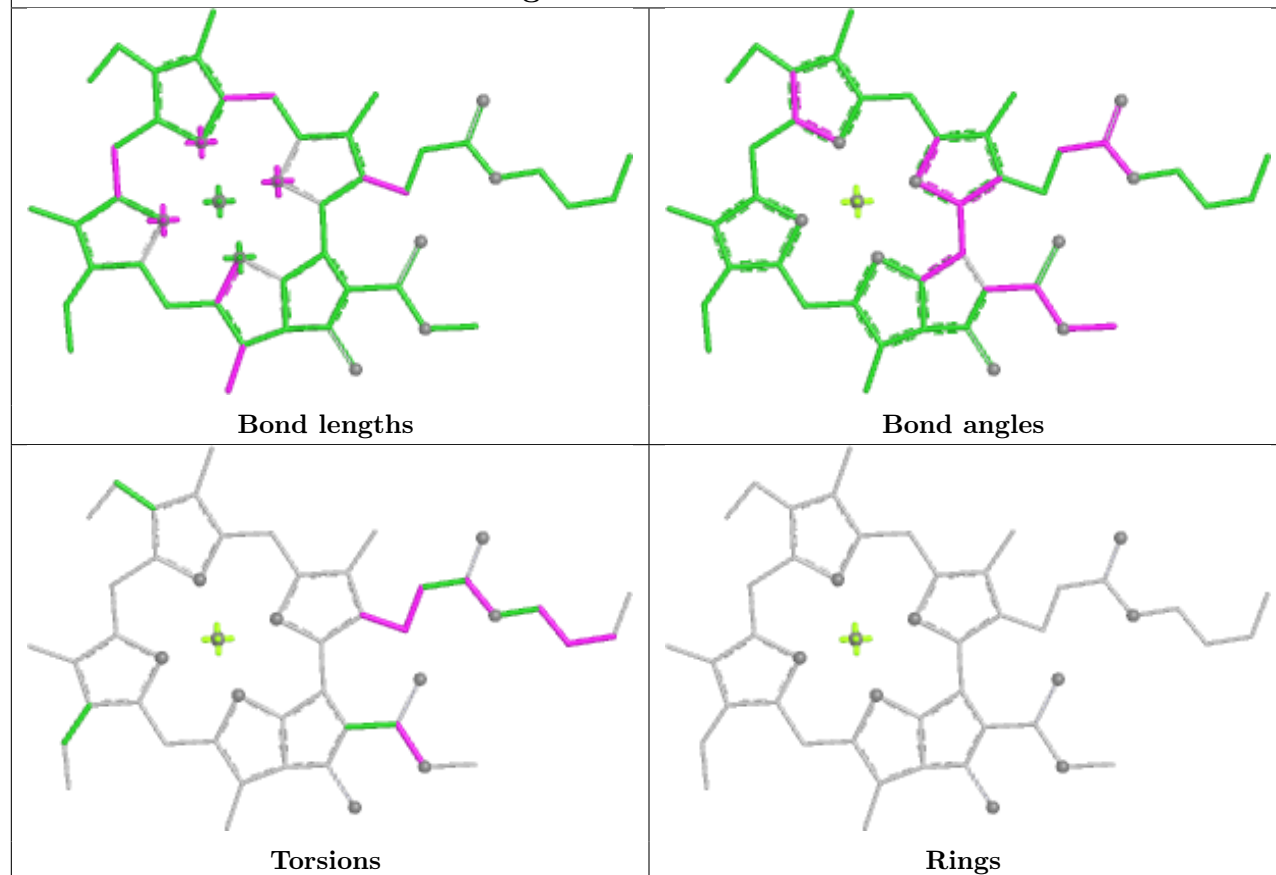
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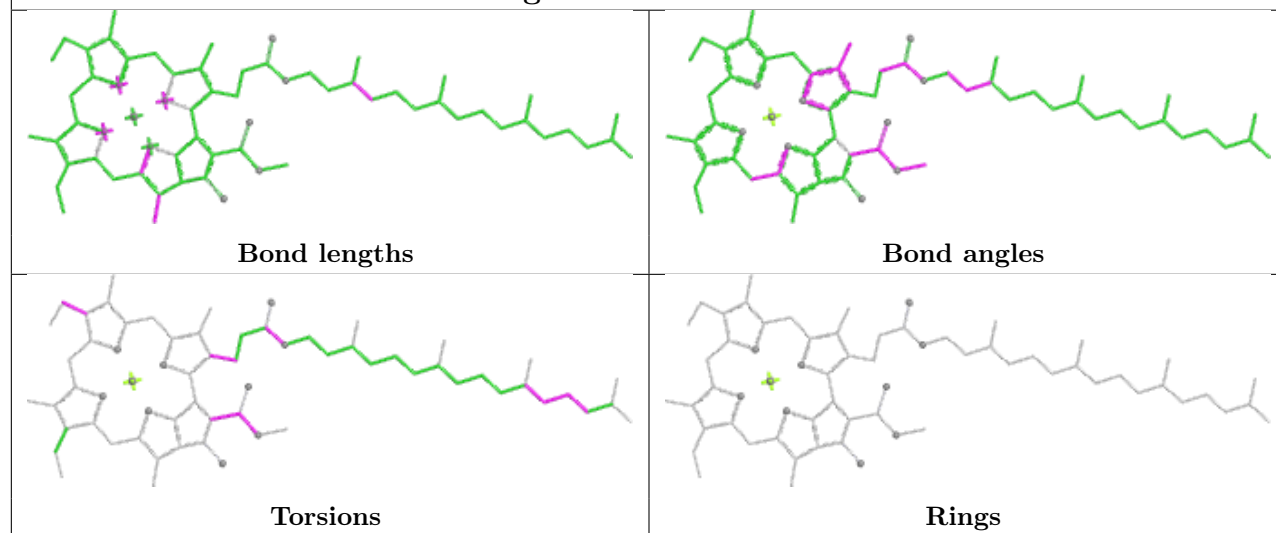
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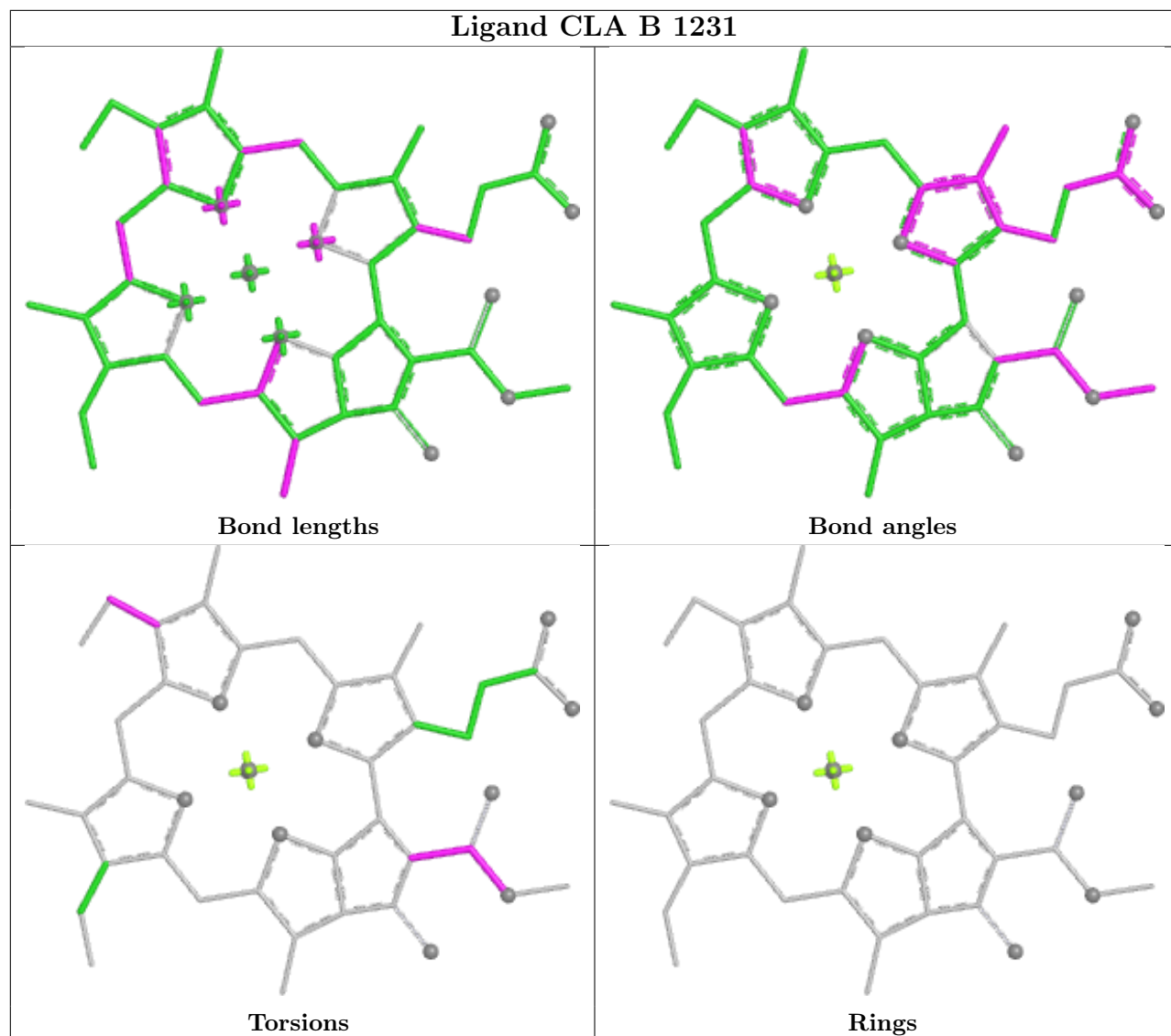
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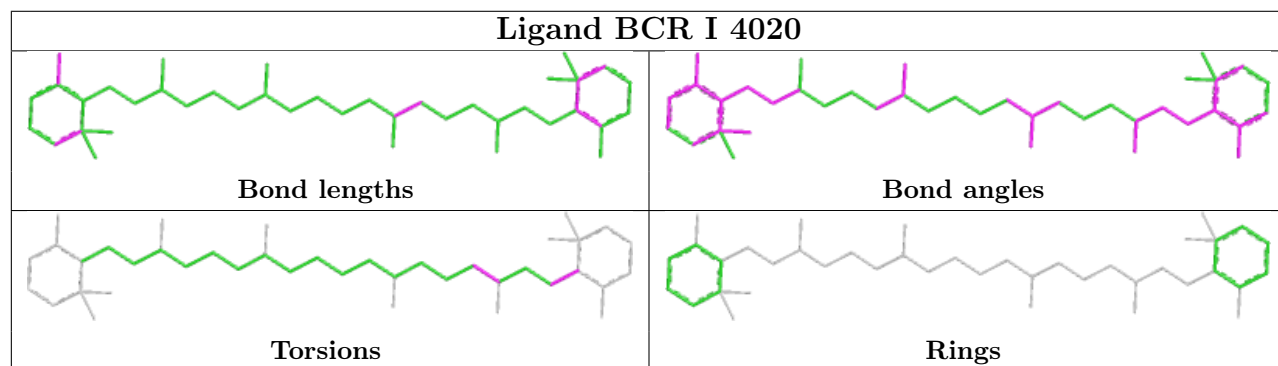
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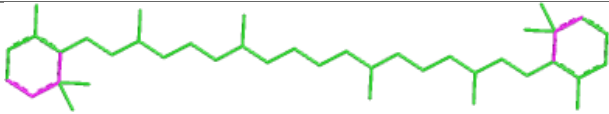
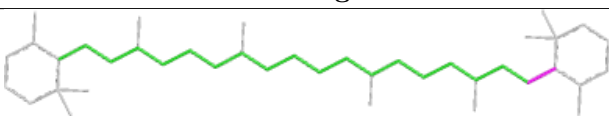
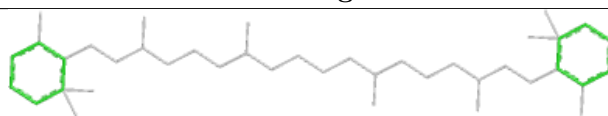


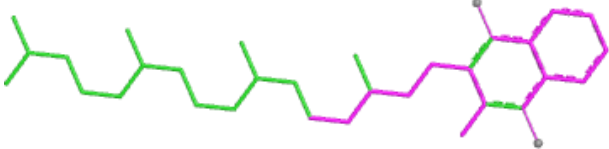
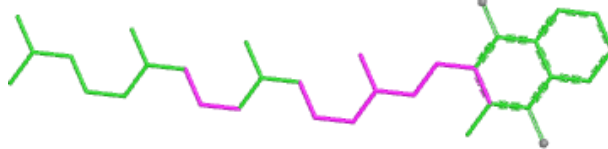
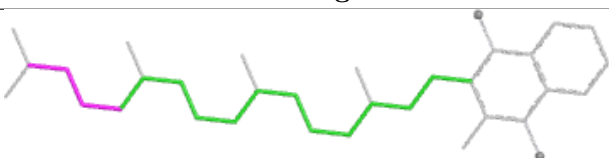
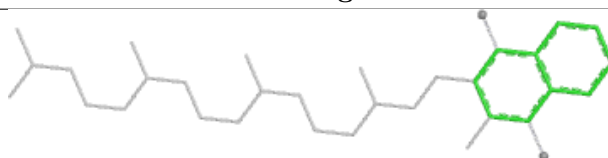
Ligand CLA B 1231

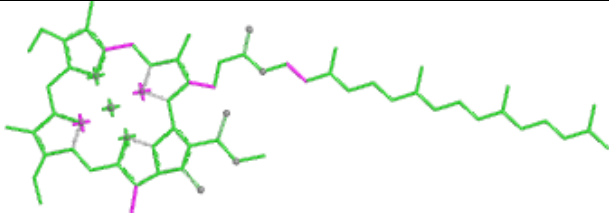
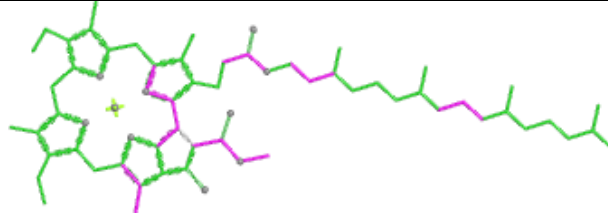
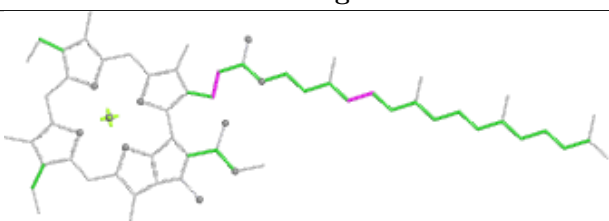
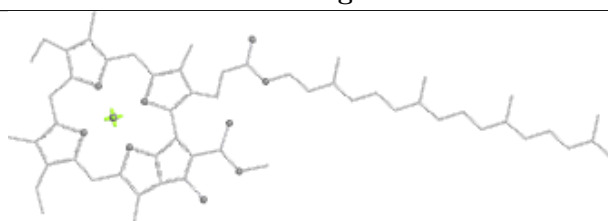


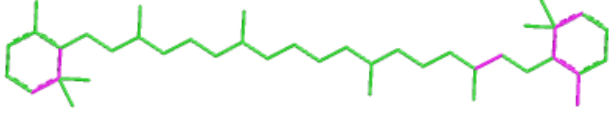
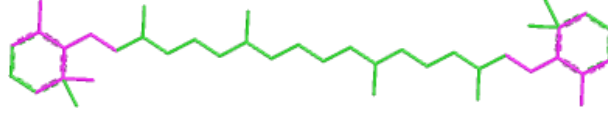
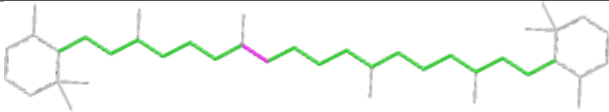
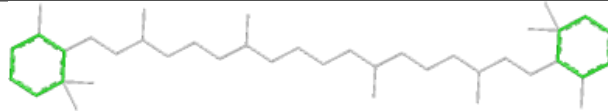
Ligand BCR I 4020



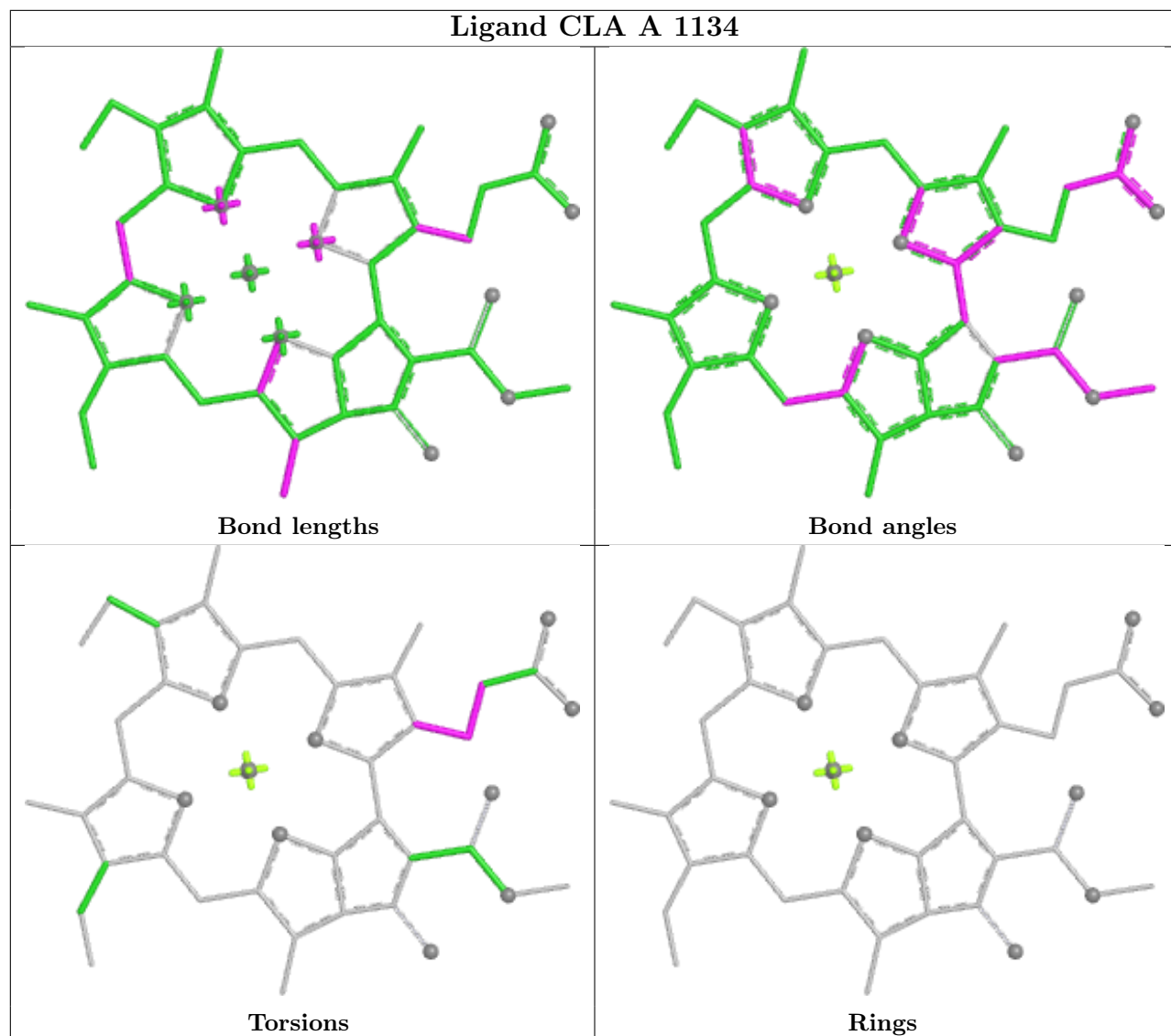
Ligand BCR A 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B 2002	
	
Bond lengths	Bond angles
	
Torsions	Rings

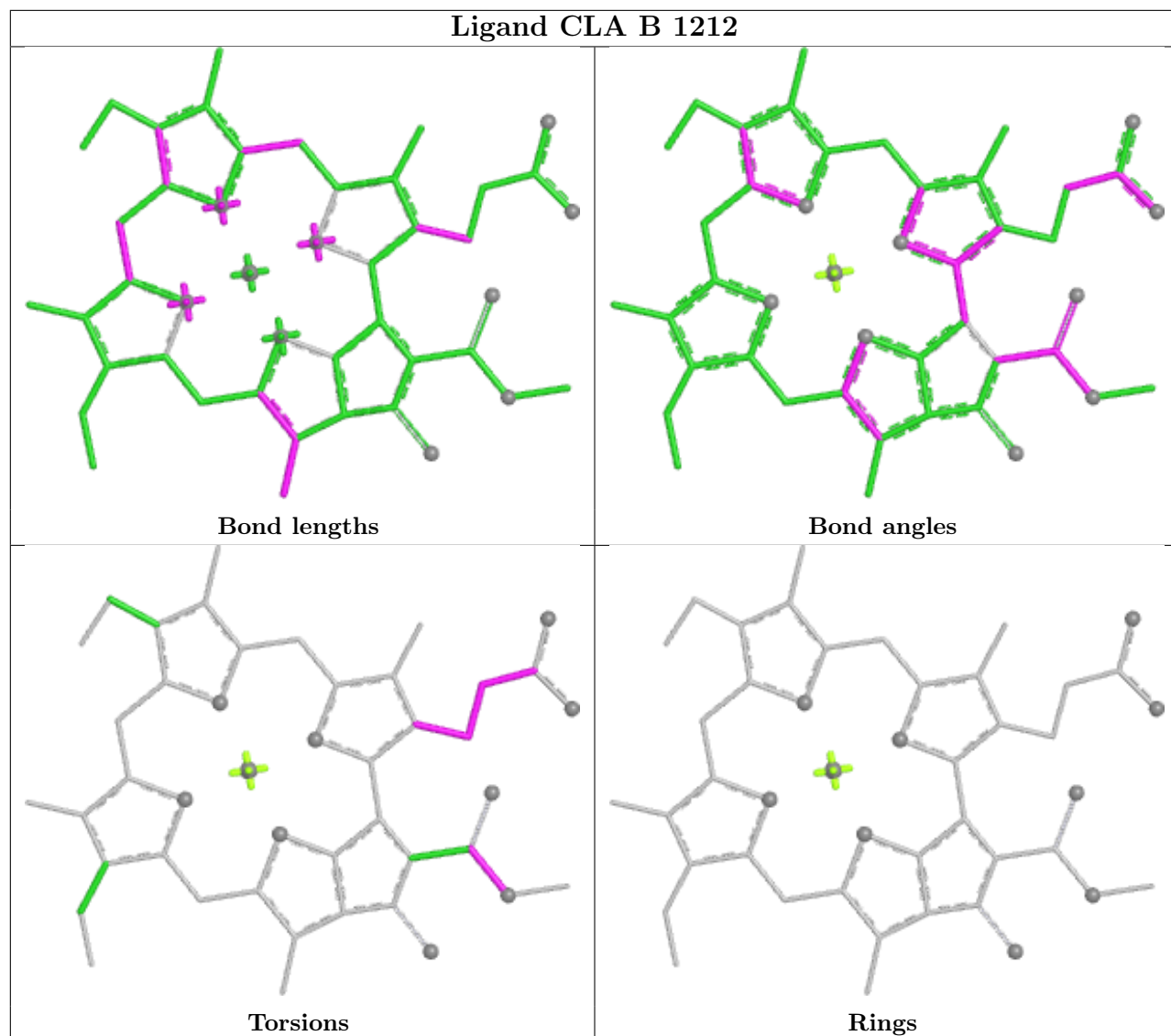
Ligand CLA B 1238	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 4022	
	
Bond lengths	Bond angles
	
Torsions	Rings

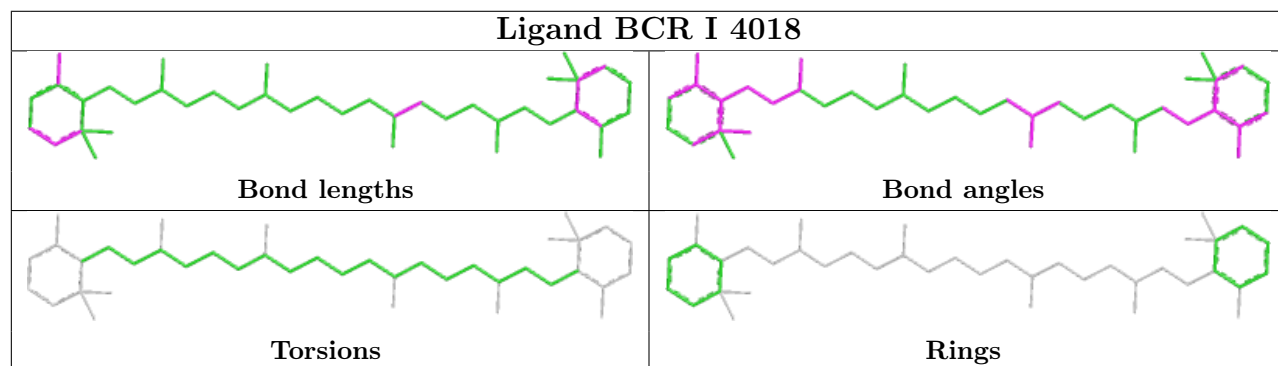
Ligand CLA A 1134



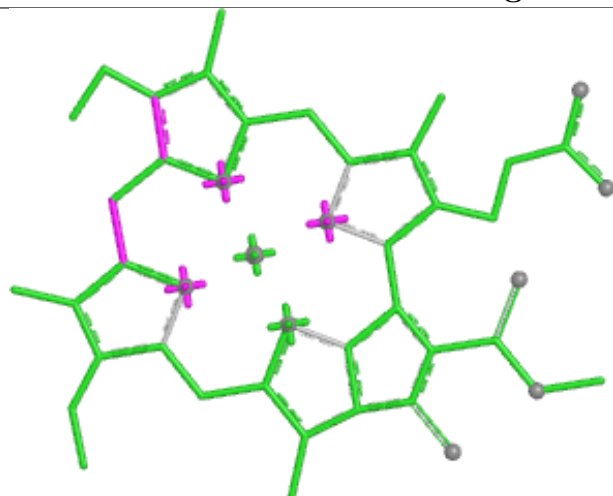
Ligand CLA B 1212



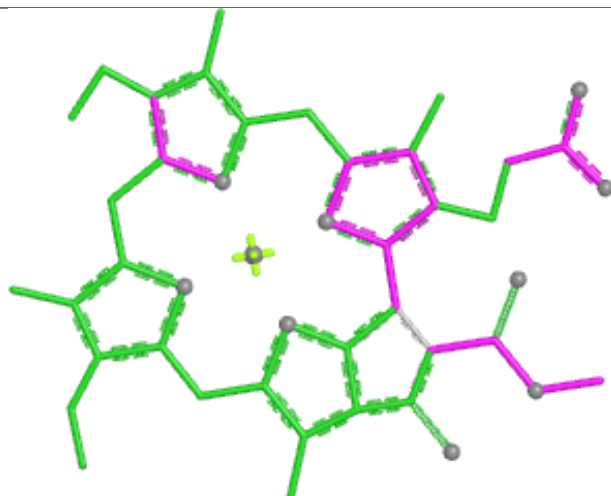
Ligand BCR I 4018



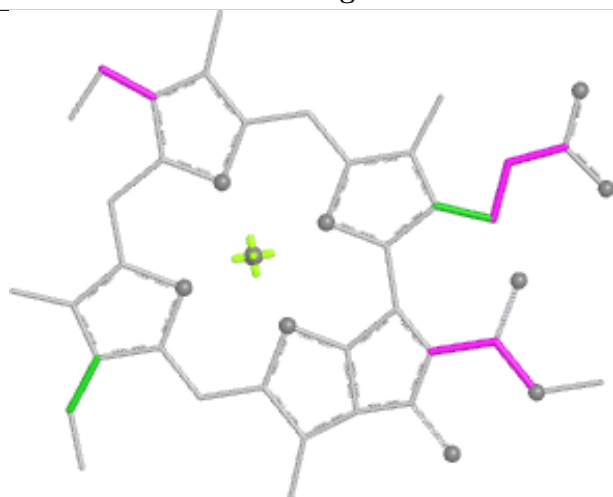
Ligand CLA X 1701



Bond lengths



Bond angles

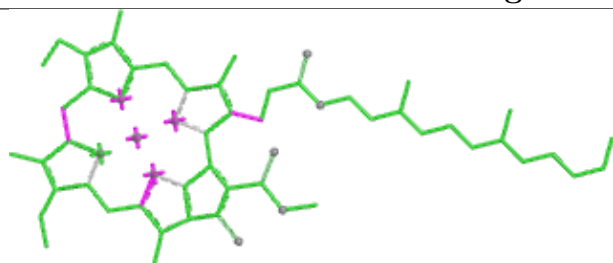


Torsions

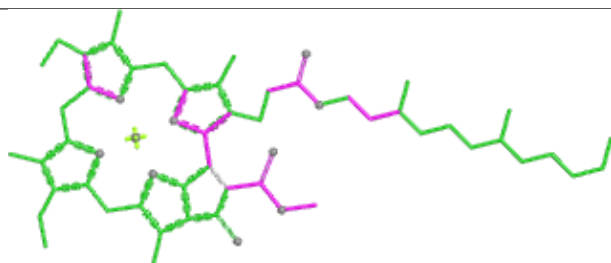


Rings

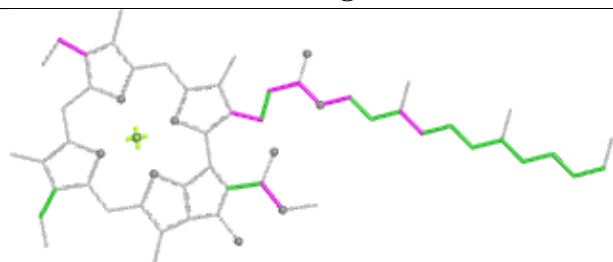
Ligand CLA A 1102



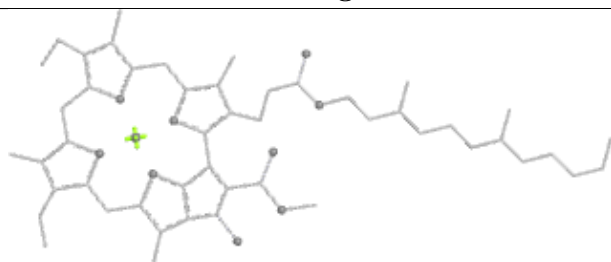
Bond lengths



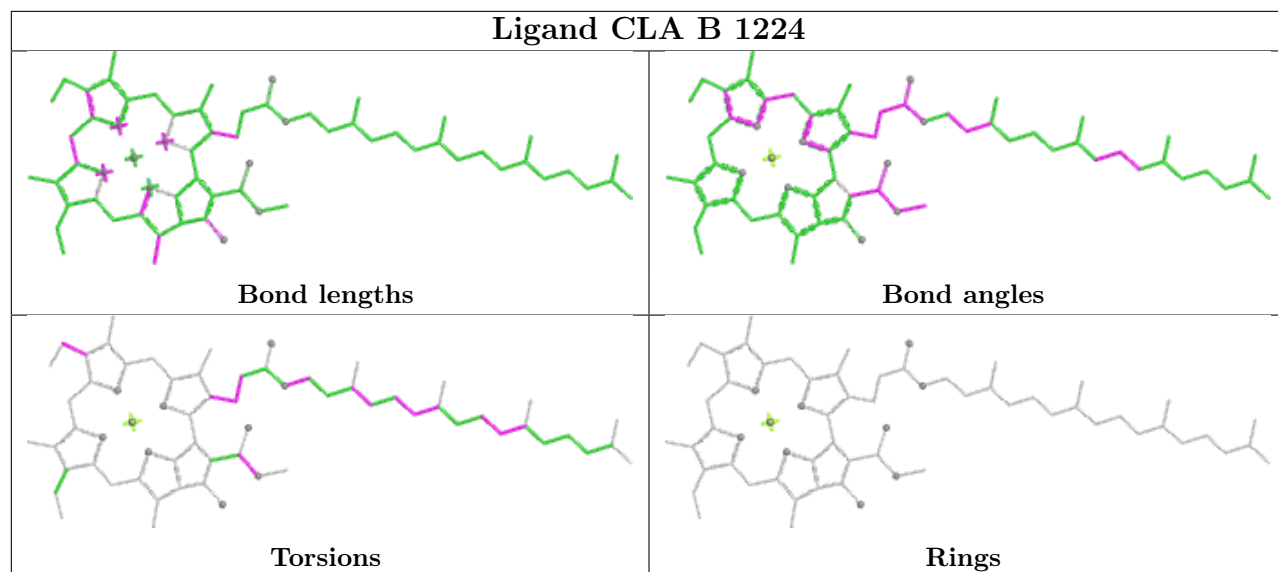
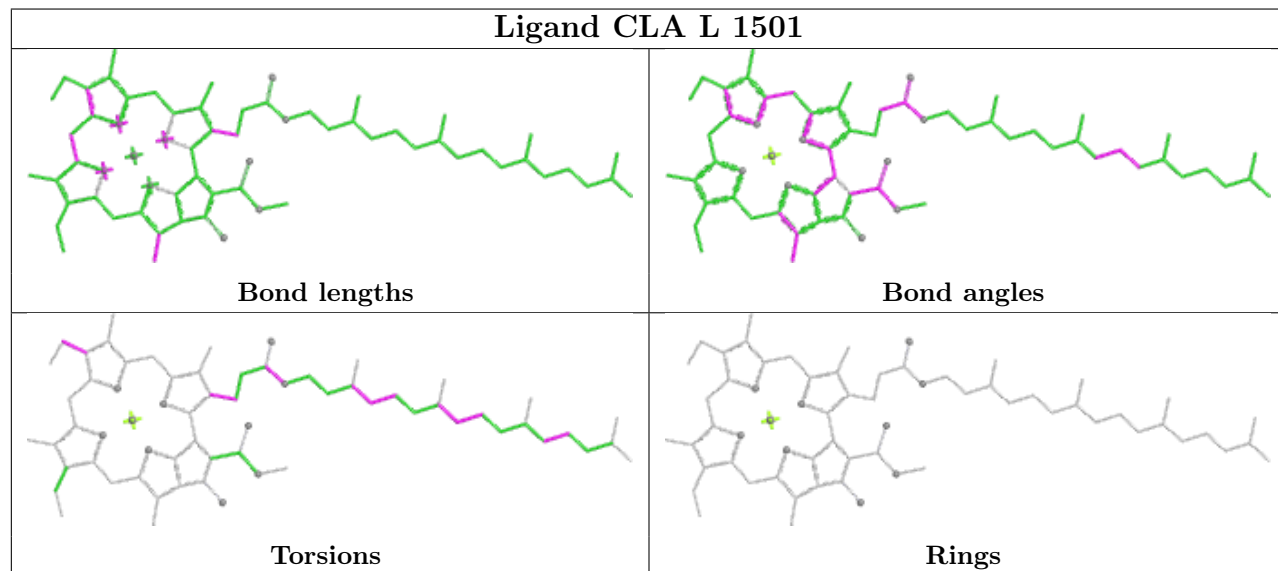
Bond angles



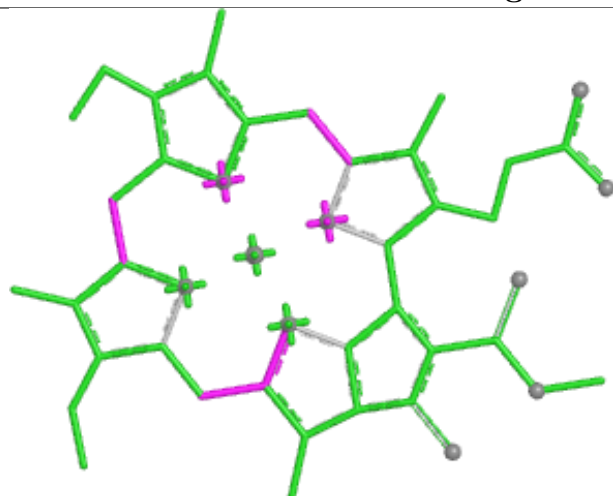
Torsions



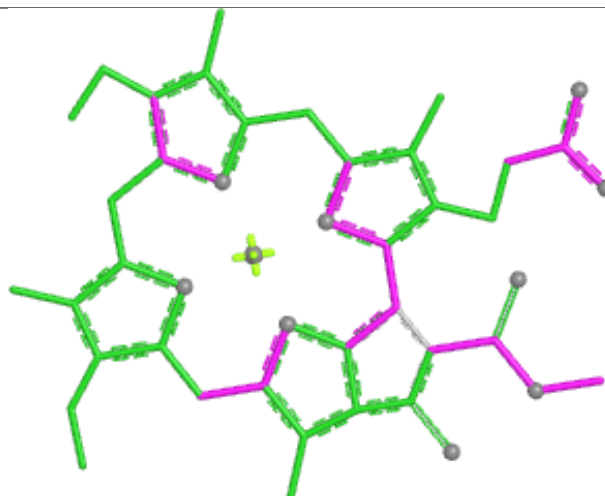
Rings

Ligand CLA B 1224**Ligand CLA L 1501**

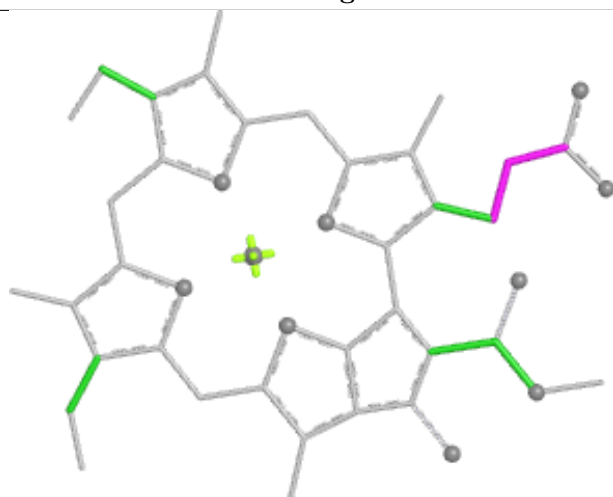
Ligand CLA B 1209



Bond lengths



Bond angles

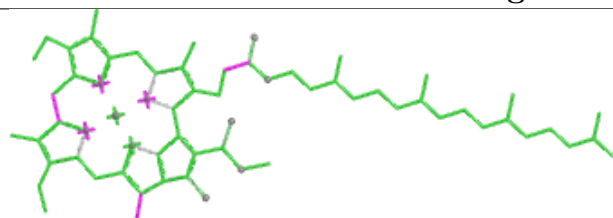


Torsions

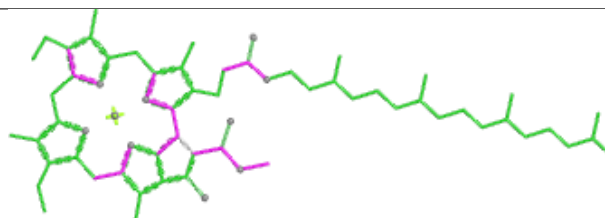


Rings

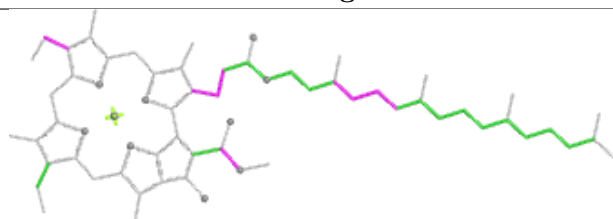
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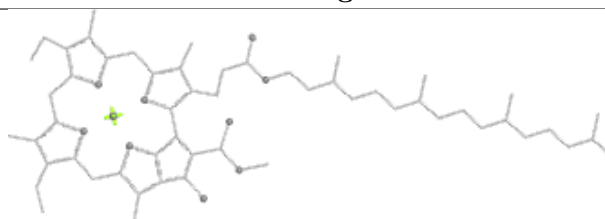
Bond lengths



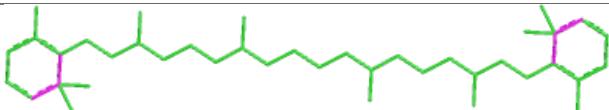
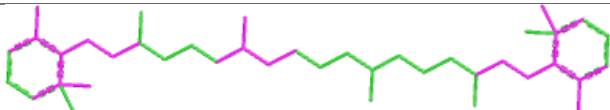
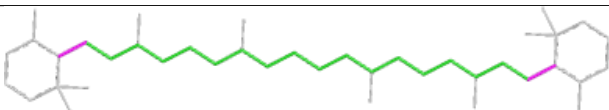
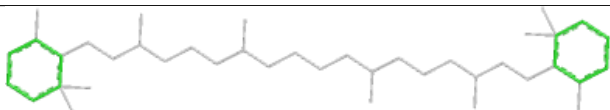
Bond angles

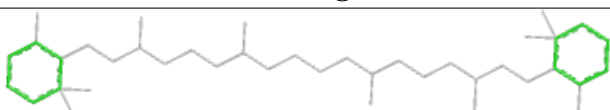


Torsions

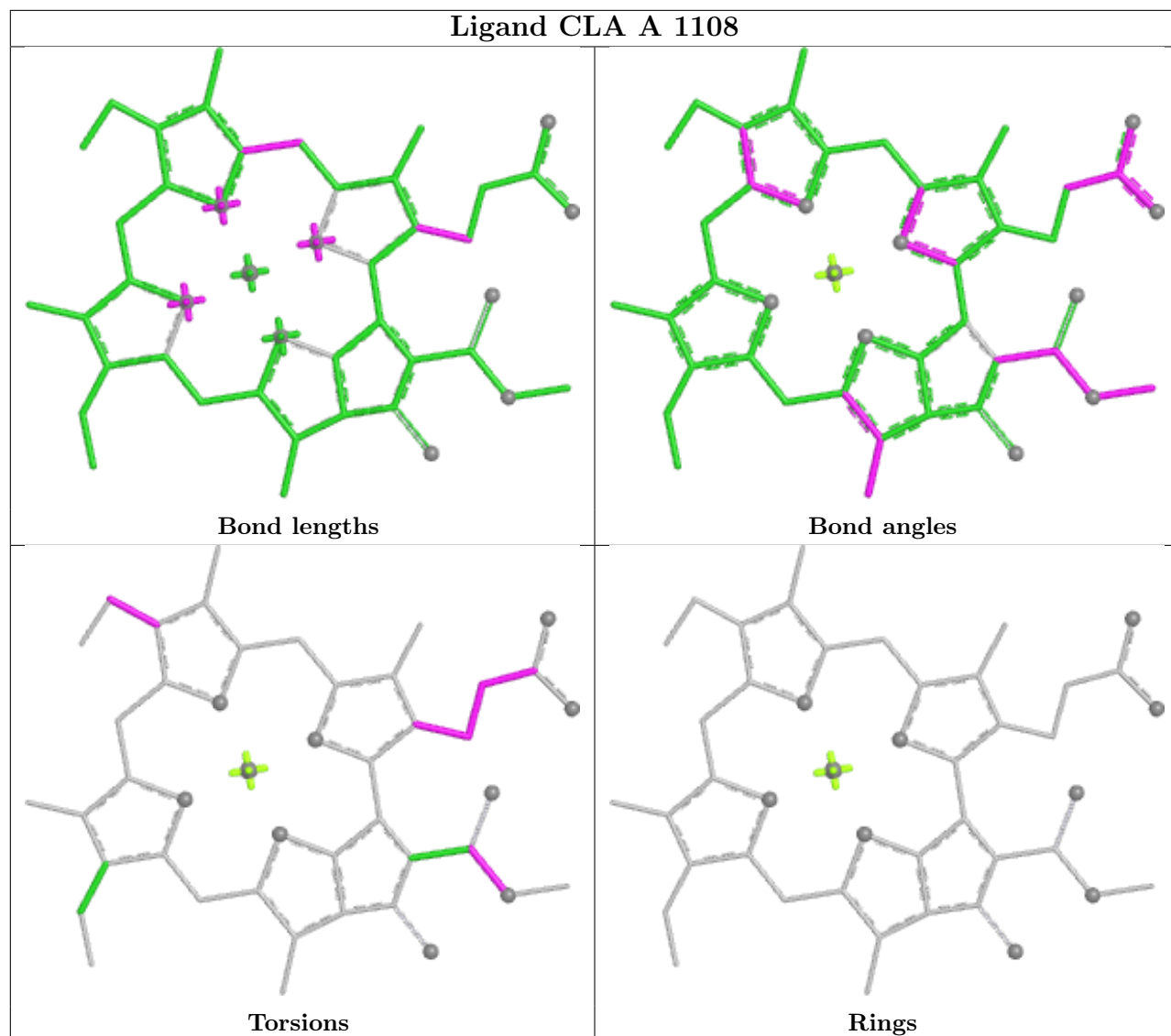


Rings

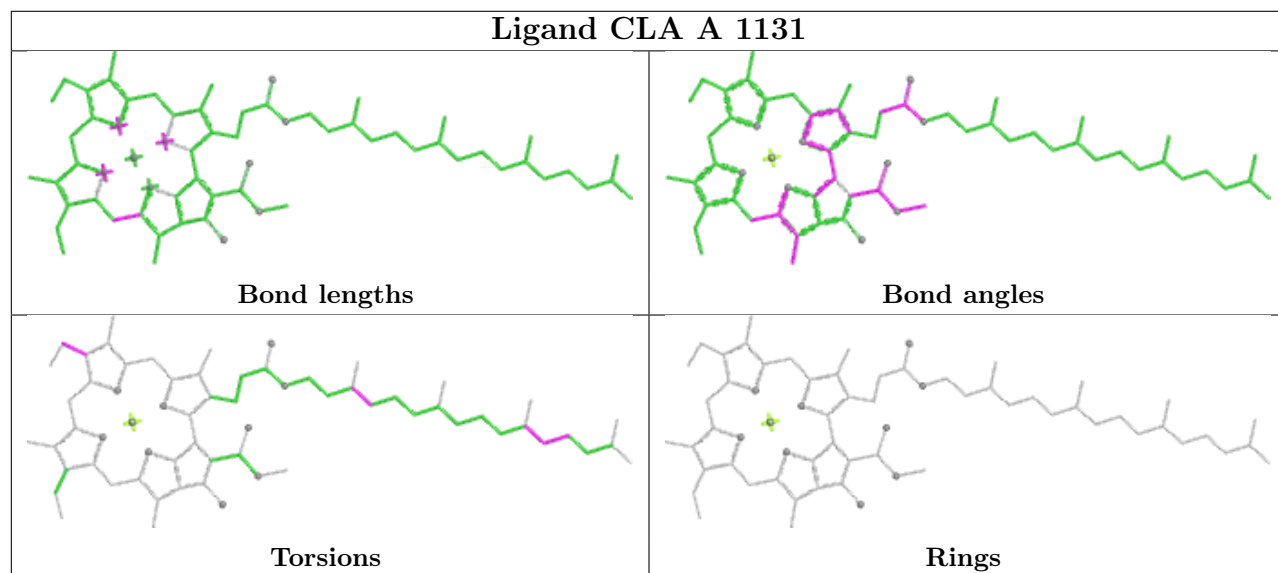
Ligand BCR A 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

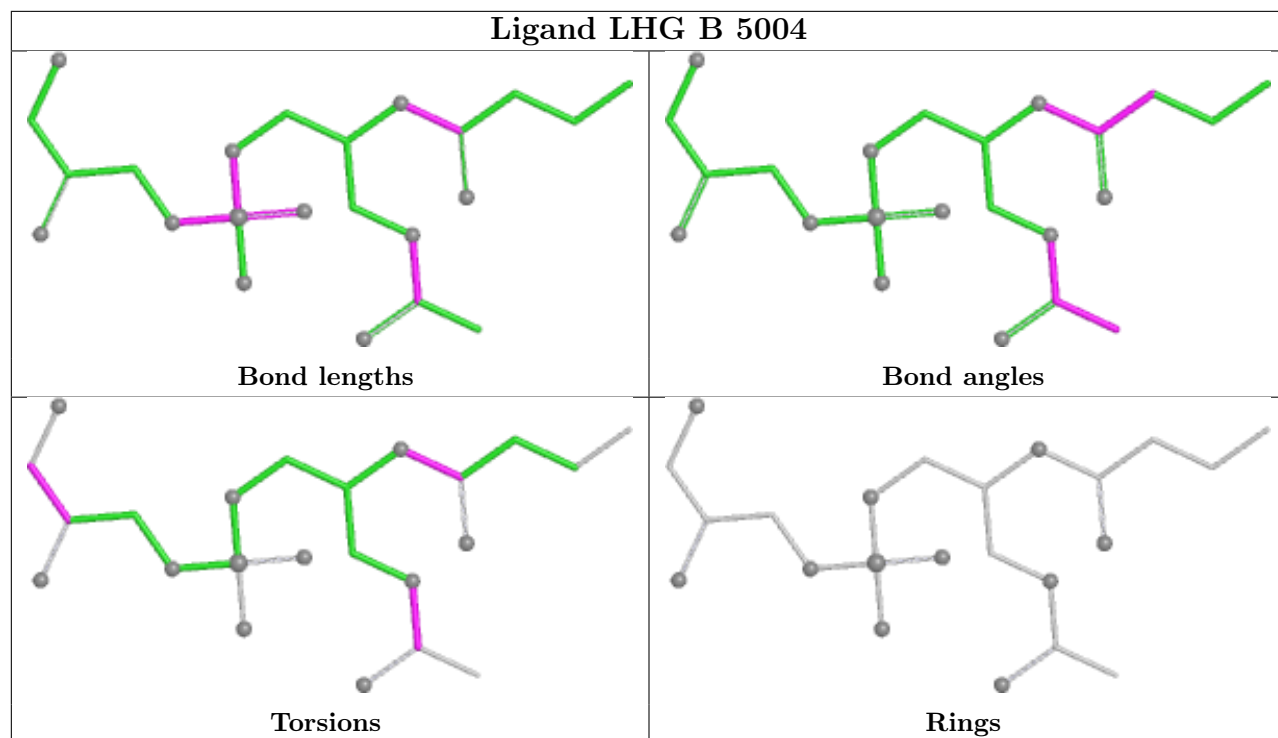
Ligand BCR B 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings

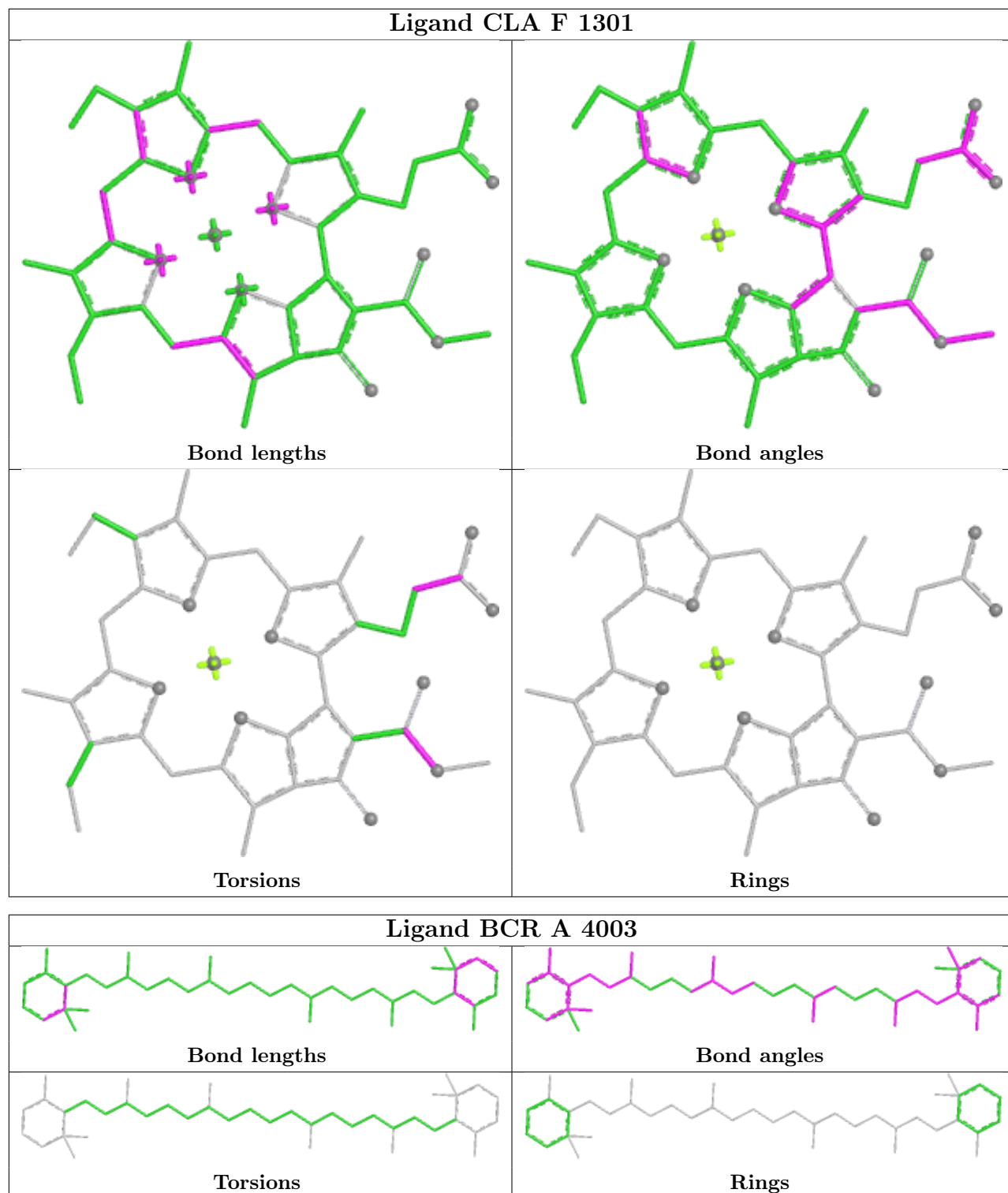
Ligand CLA A 1108



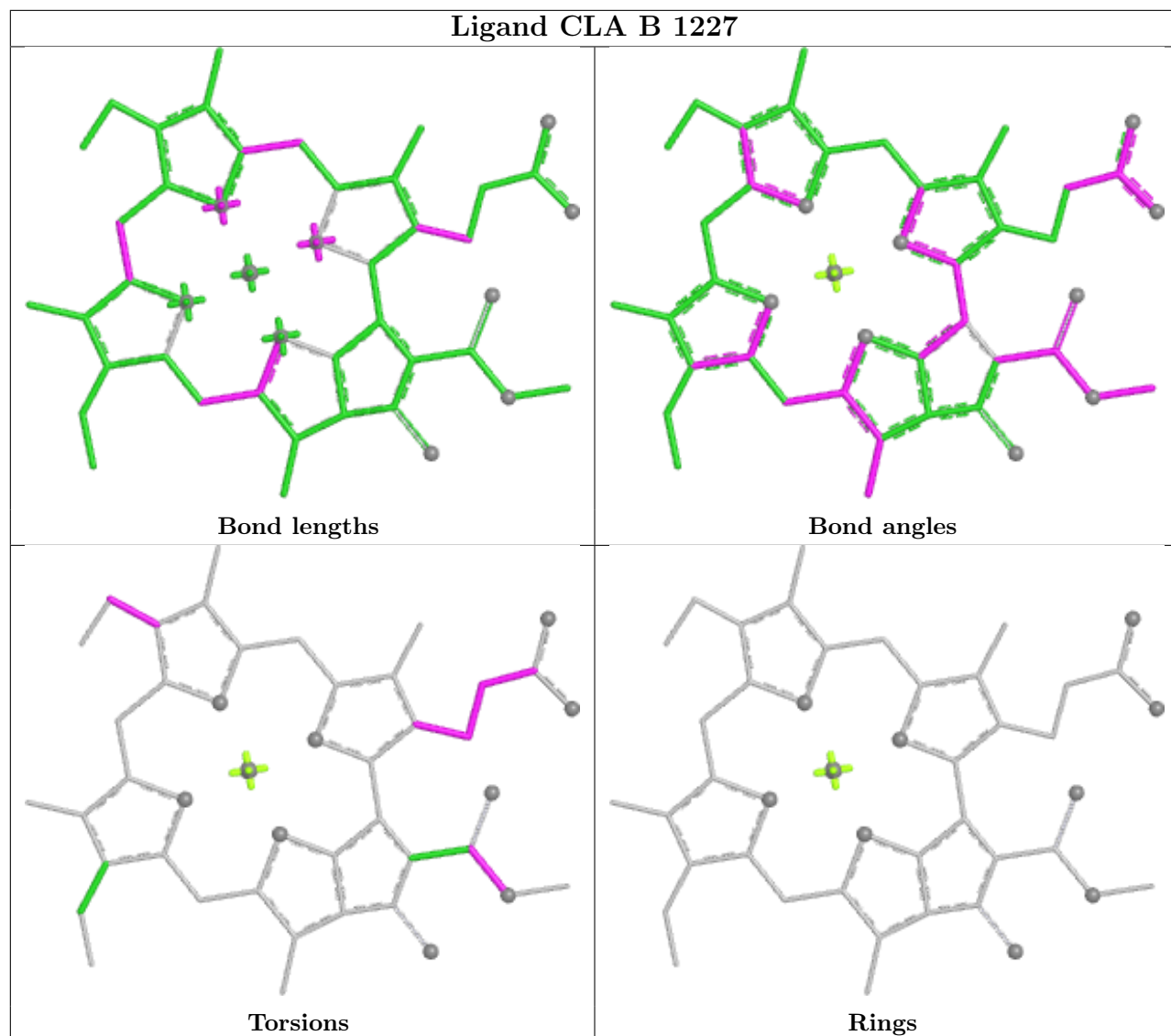
Ligand CLA A 1131

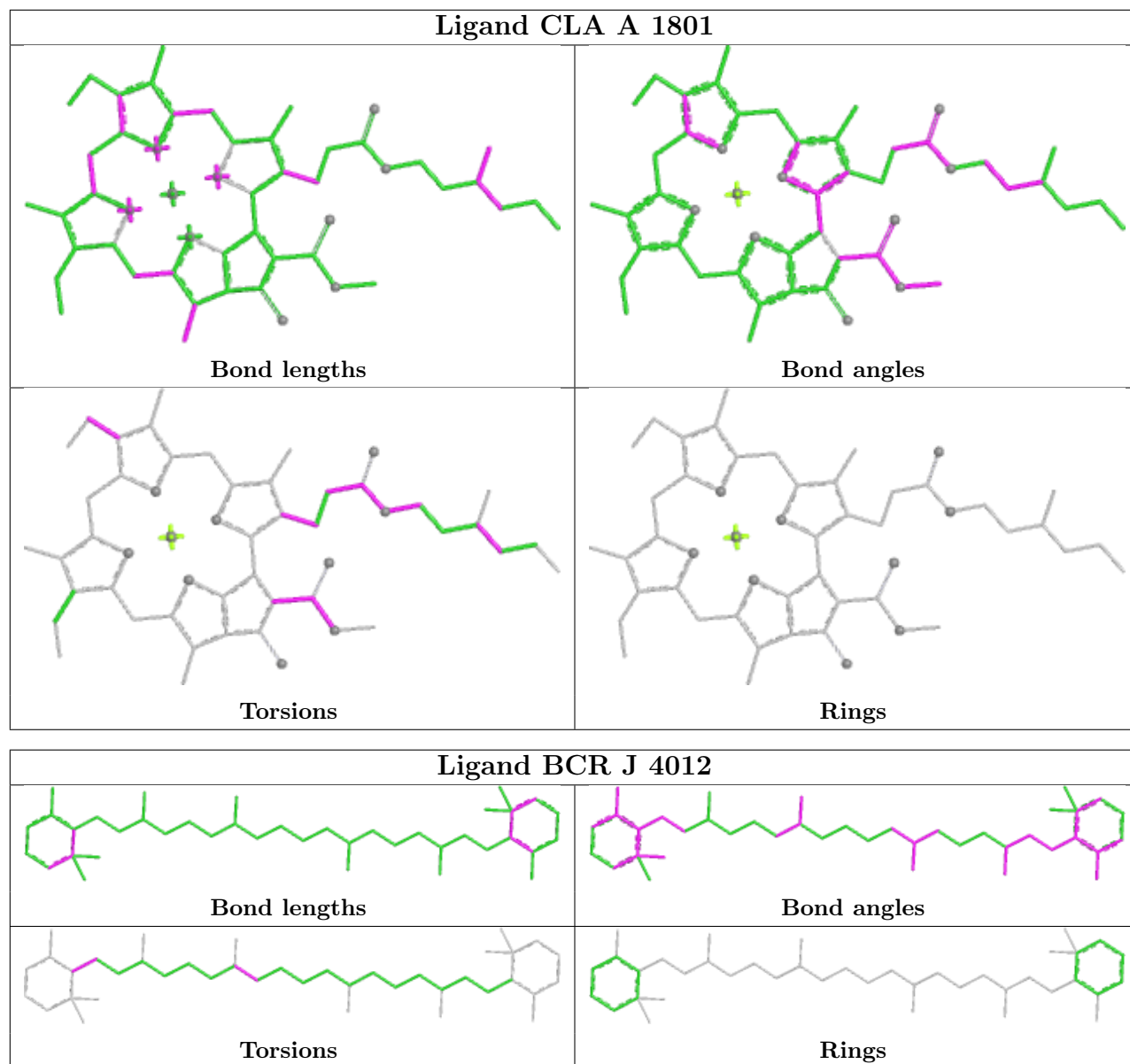


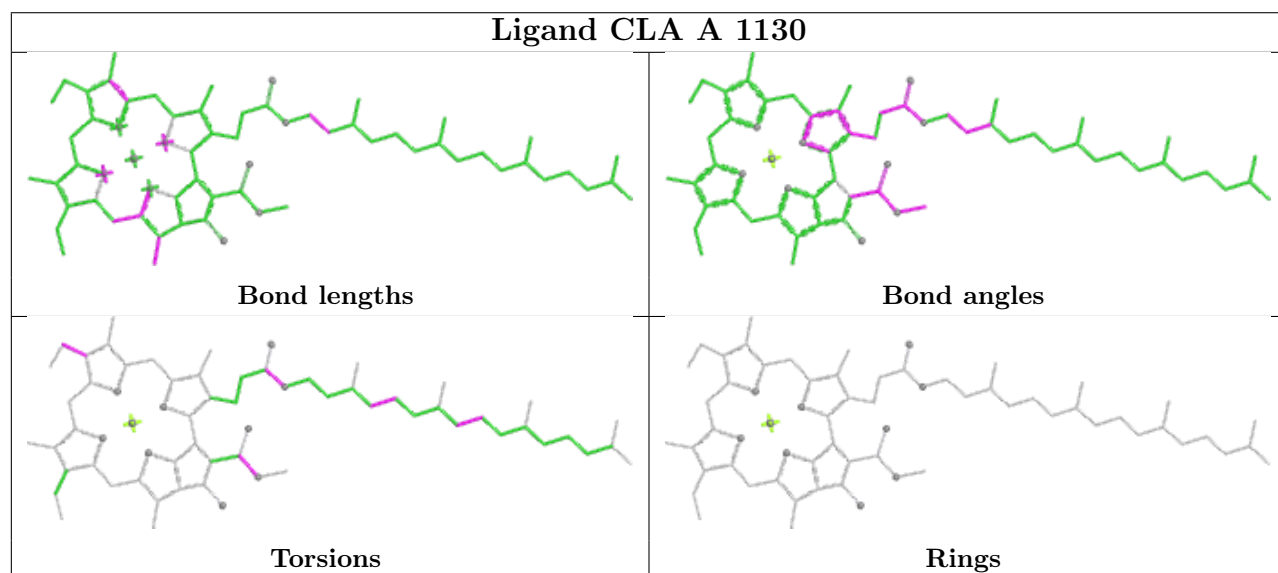
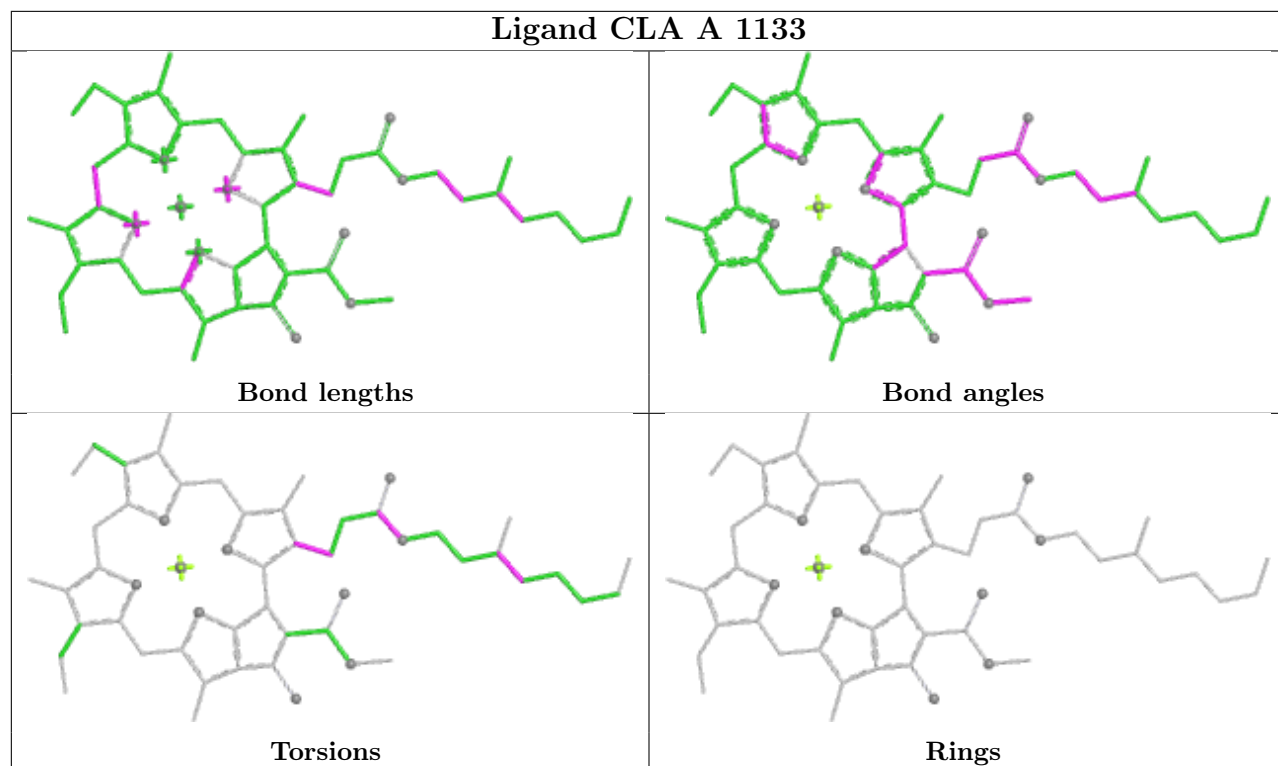


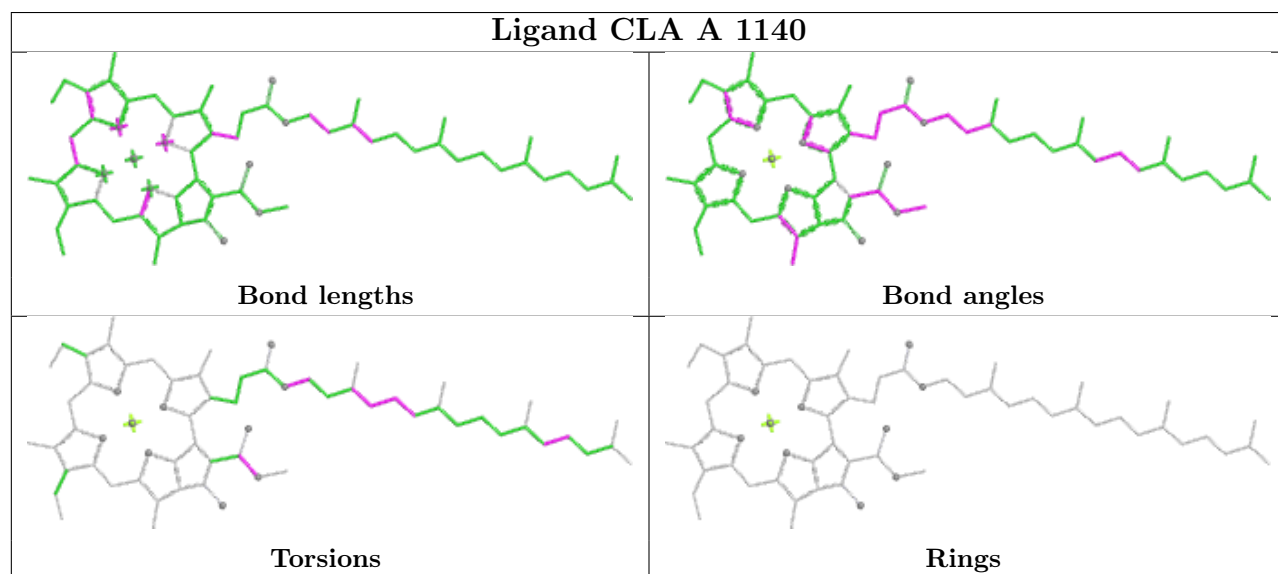
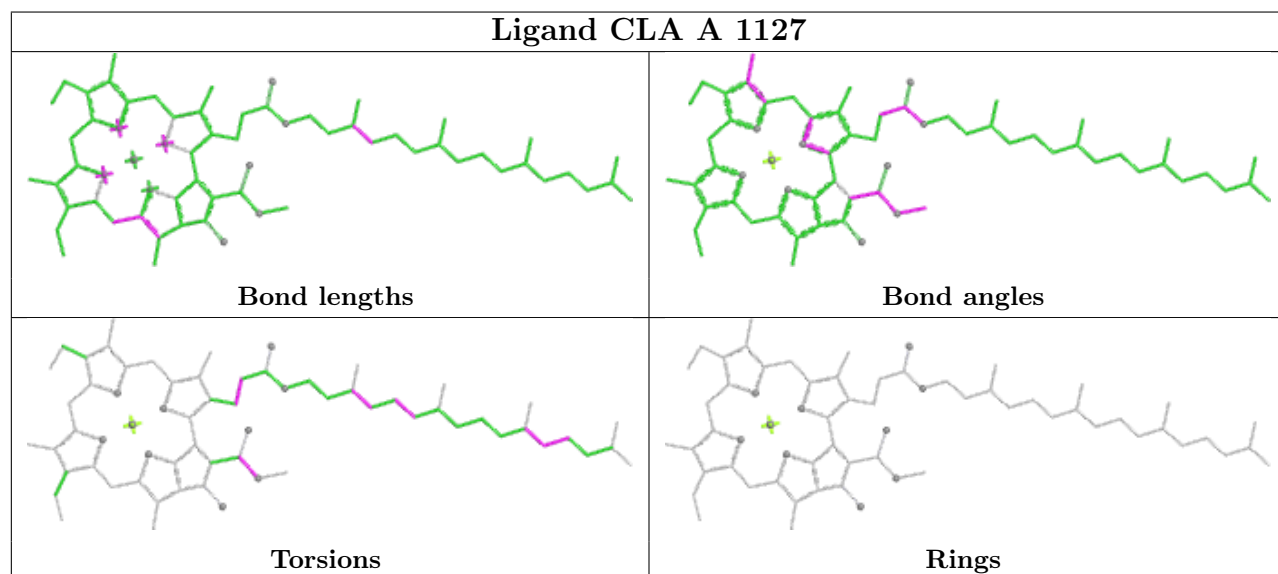
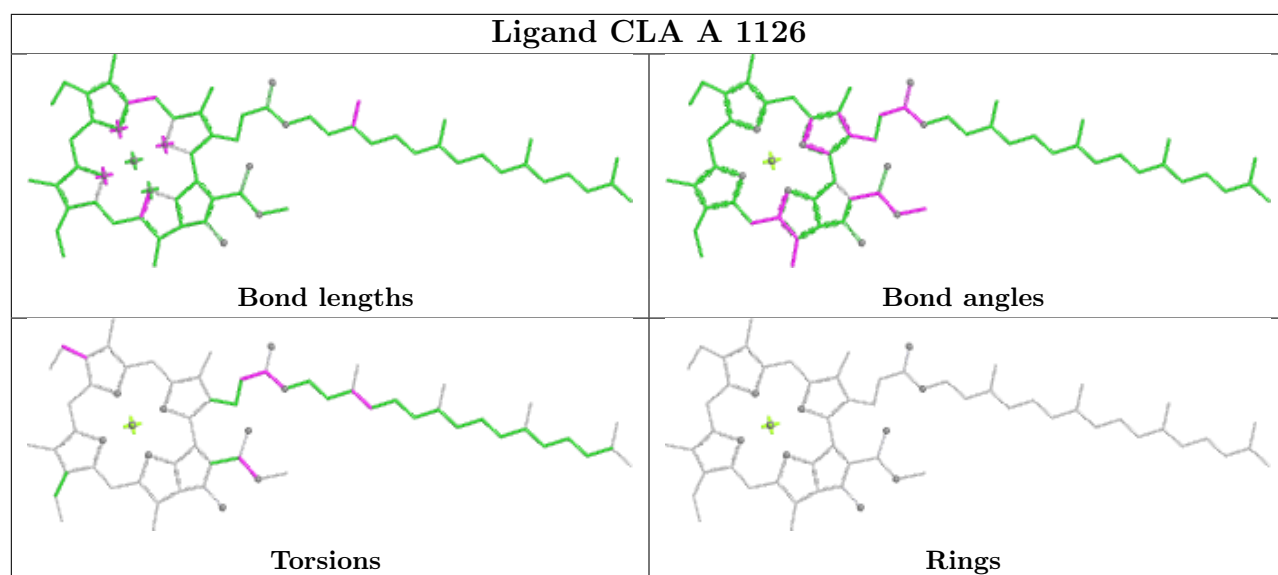


Ligand CLA B 1227

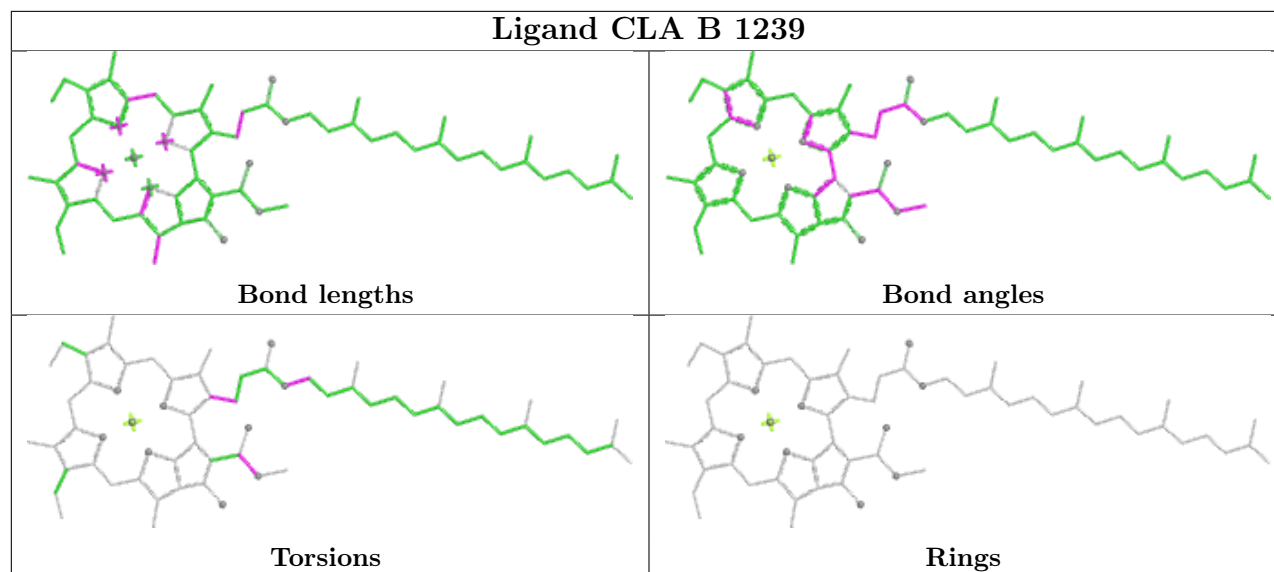




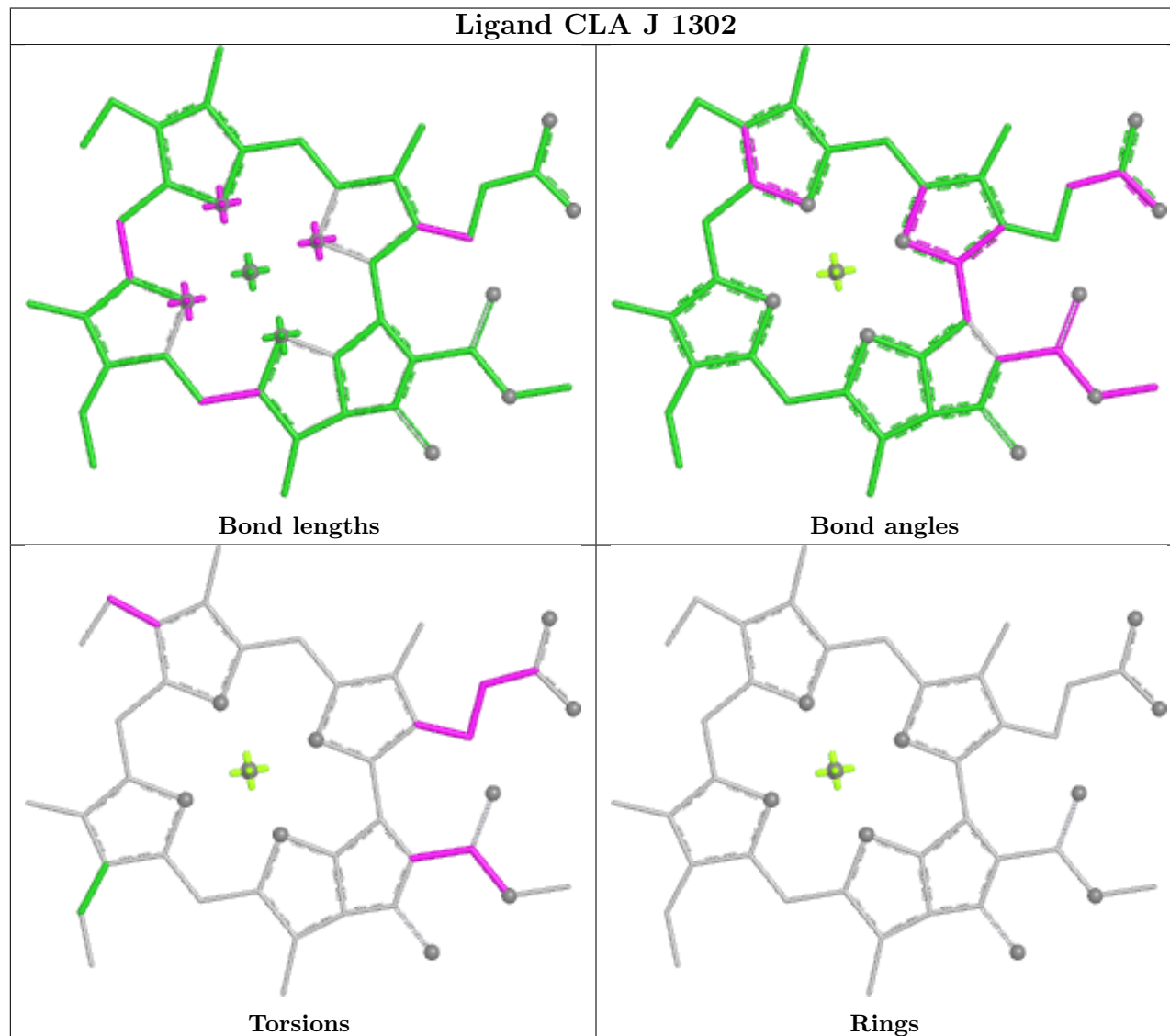


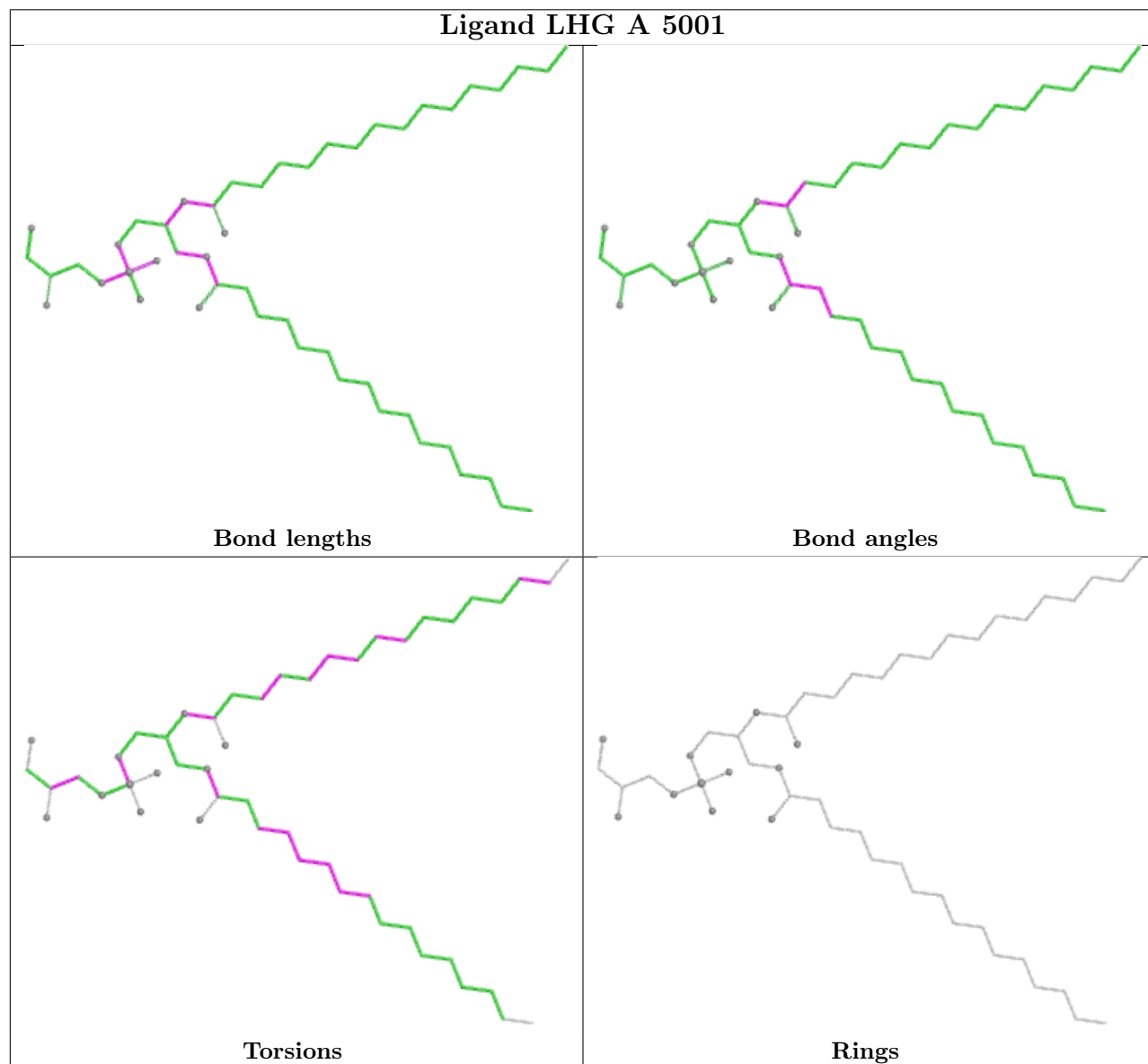
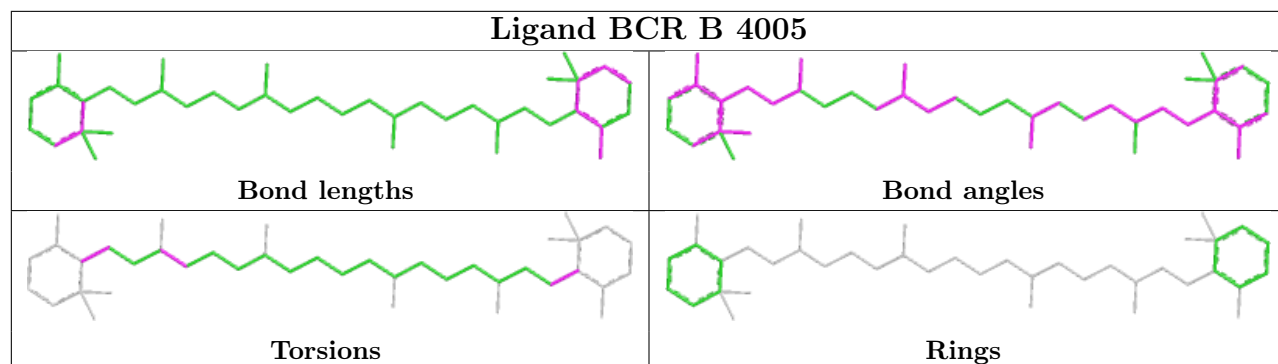


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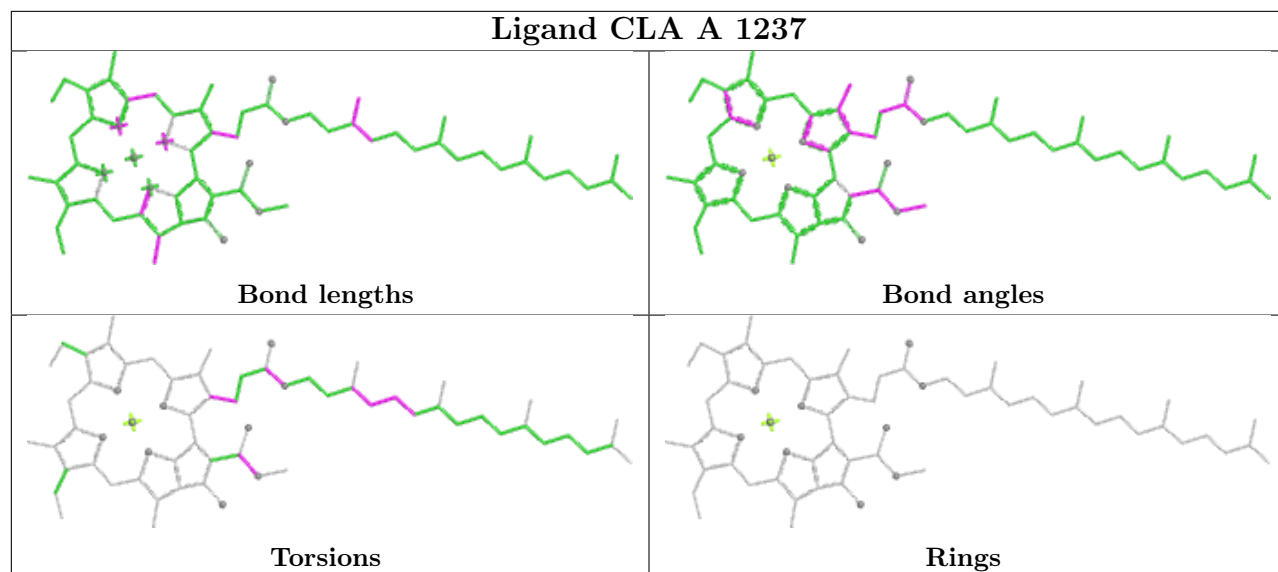


Ligand CLA J 1302

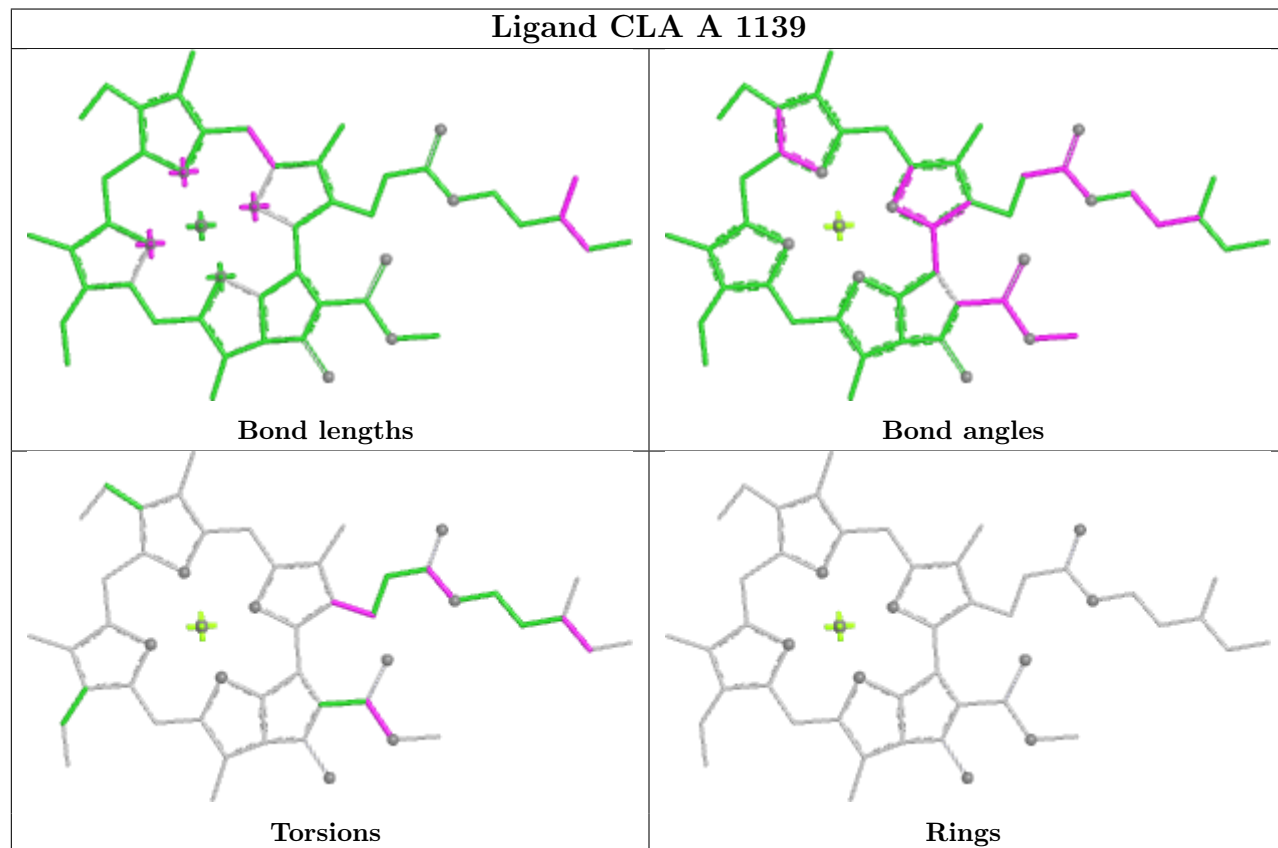


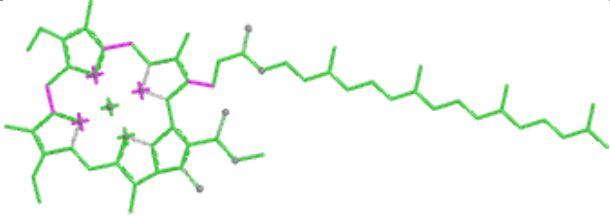
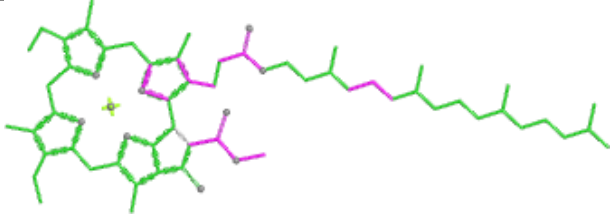
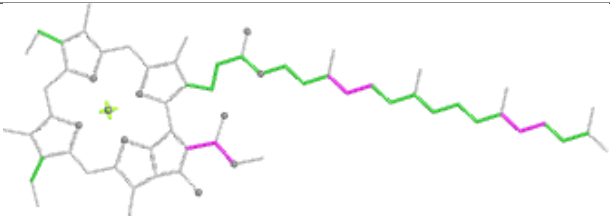
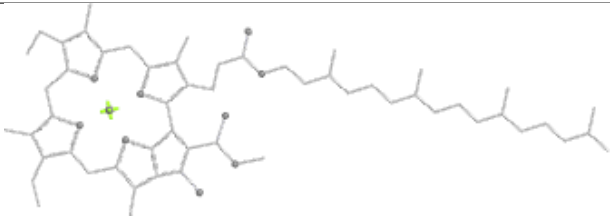
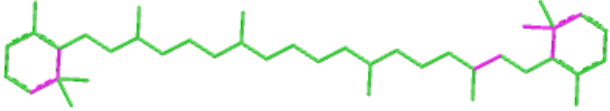
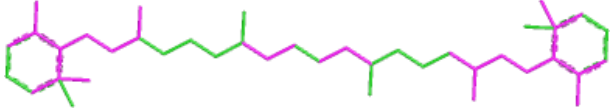
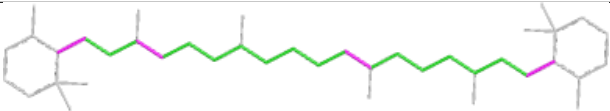
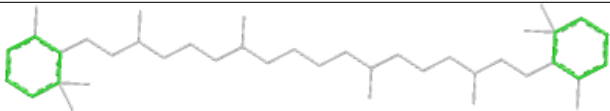


Ligand CLA A 1237

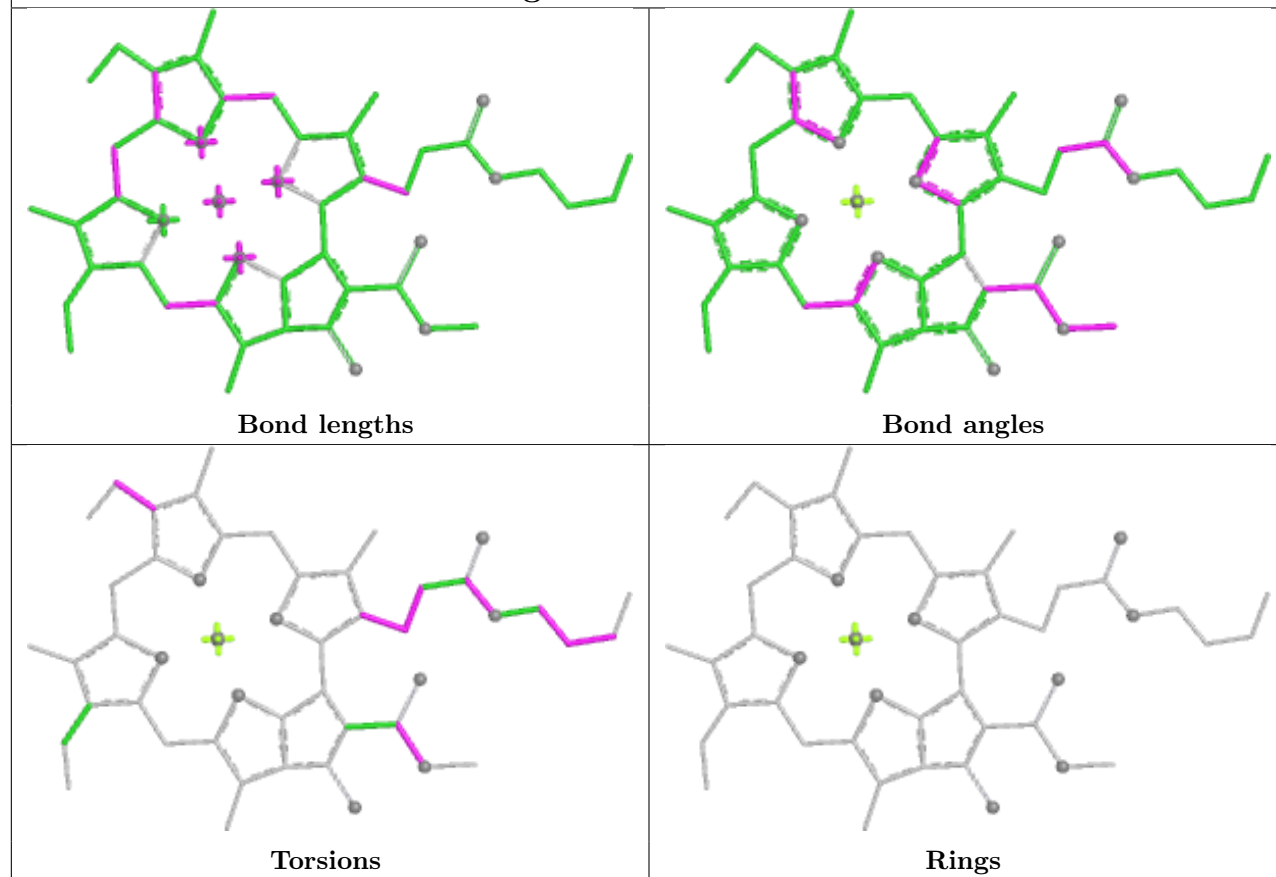


Ligand CLA A 1139

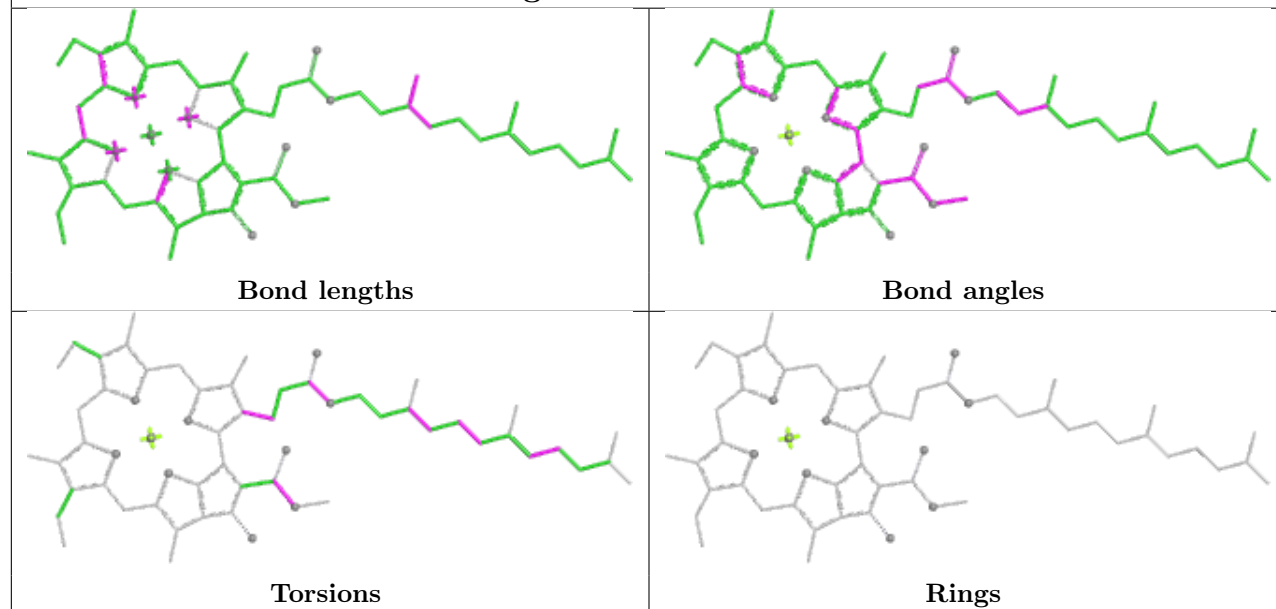


Ligand CLA B 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4011	
 Bond lengths	 Bond angles
 Torsions	 Rings

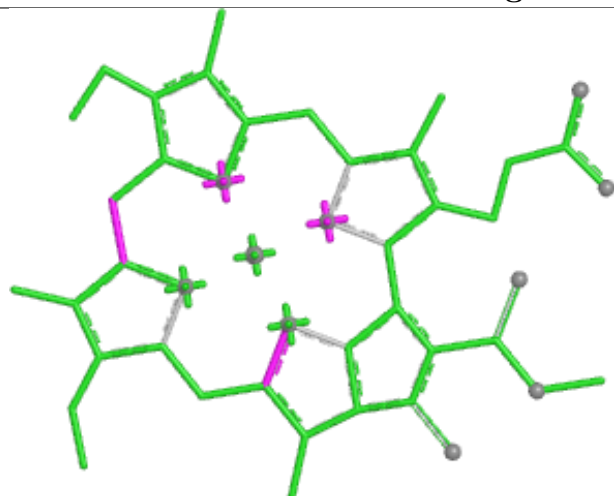
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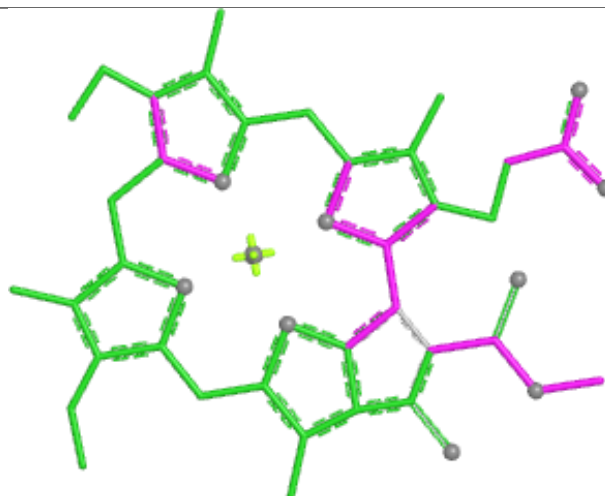
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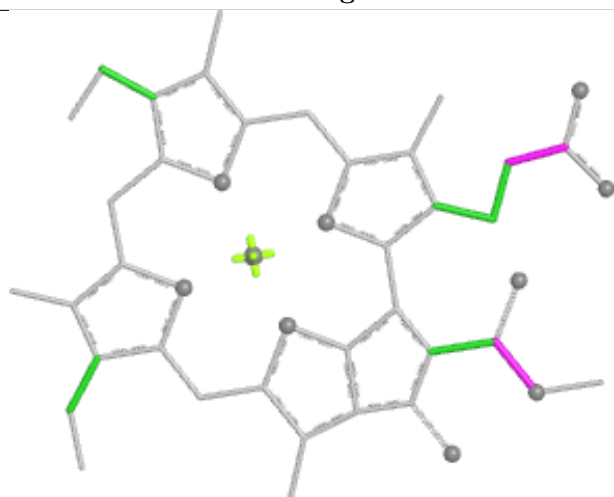
Ligand CLA B 1233



Bond lengths



Bond angles

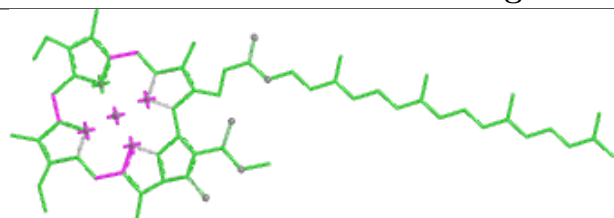


Torsions

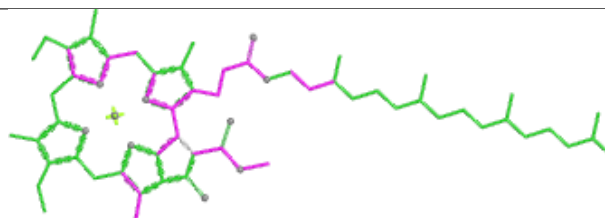


Rings

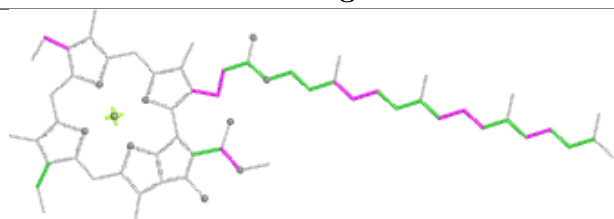
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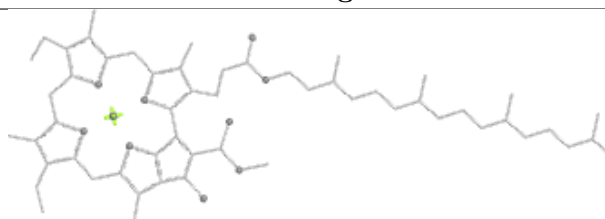
Bond lengths



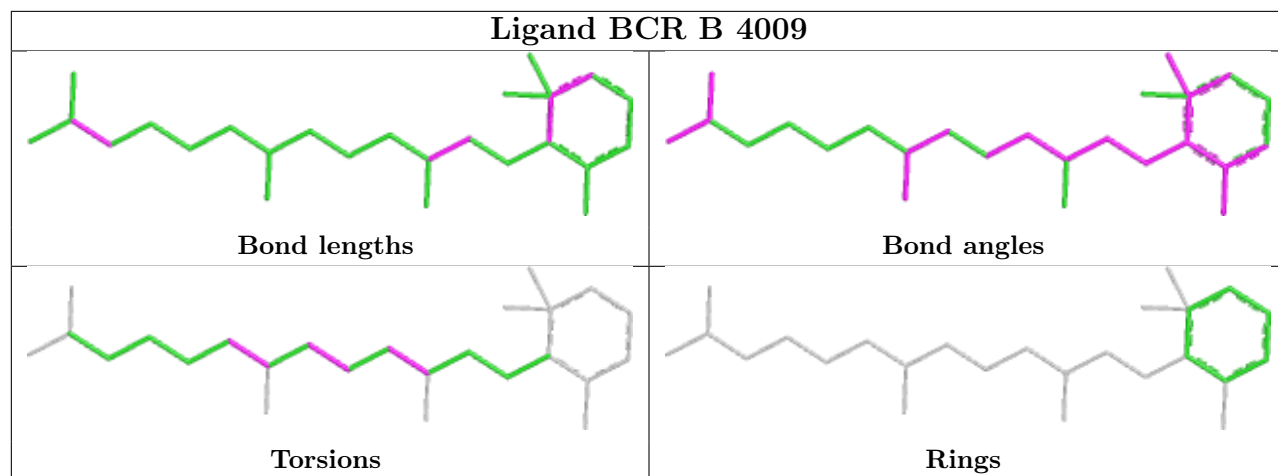
Bond angles



Torsions



Rings



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 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.