



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:57 PM UTC

PDB ID : 1W5C / pdb_00001w5c
Title : Photosystem II from Thermosynechococcus elongatus
Authors : Biesiadka, J.; Loll, B.; Kern, J.; Irrgang, K.-D.; Saenger, W.
Deposited on : 2004-08-06
Resolution : 3.20 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)	:	2.49

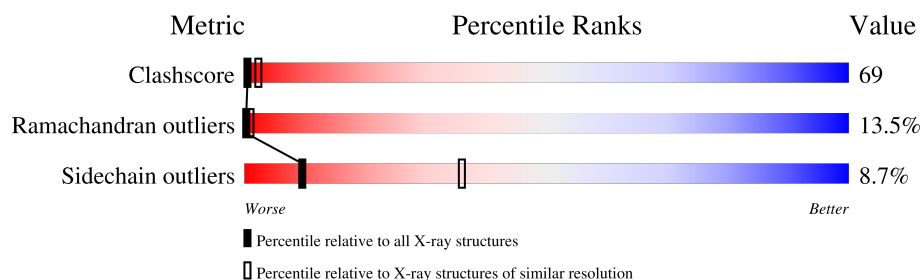
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	360	21% 52% 17% • 8%
1	G	360	22% 51% 16% • 8%
2	B	510	29% 47% 15% • 6%
2	H	510	29% 47% 14% • 6%
3	C	473	25% 47% 18% • 7%
3	I	473	26% 46% 18% • 7%
4	D	352	21% 56% 20% ..
4	J	352	23% 53% 21% ..

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Mol	Chain	Length	Quality of chain
5	E	84	
5	K	84	
6	F	44	
6	L	44	
7	O	179	
7	P	179	
8	S	100	
8	U	100	
9	T	163	
9	V	163	
10	X	359	
10	Y	359	

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
11	CLA	A	1342	X	-	-	-
11	CLA	A	1343	X	-	-	-
11	CLA	A	1344	X	-	-	-
11	CLA	A	1346	X	-	-	-
11	CLA	B	1482	X	-	-	-
11	CLA	B	1483	X	-	-	-
11	CLA	B	1484	X	-	-	-
11	CLA	B	1485	X	-	-	-
11	CLA	B	1486	X	-	-	-
11	CLA	B	1487	X	-	-	-
11	CLA	B	1488	X	-	-	-
11	CLA	B	1489	X	-	-	-
11	CLA	B	1490	X	-	-	-
11	CLA	B	1491	X	-	-	-
11	CLA	B	1492	X	-	-	-
11	CLA	B	1493	X	-	-	-
11	CLA	B	1494	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1495	X	-	-	-
11	CLA	B	1496	X	-	-	-
11	CLA	B	1497	X	-	-	-
11	CLA	C	1459	X	-	-	-
11	CLA	C	1460	X	-	-	-
11	CLA	C	1461	X	-	-	-
11	CLA	C	1462	X	-	-	-
11	CLA	C	1463	X	-	-	-
11	CLA	C	1464	X	-	-	-
11	CLA	C	1465	X	-	-	-
11	CLA	C	1466	X	-	-	-
11	CLA	C	1467	X	-	-	-
11	CLA	C	1468	X	-	-	-
11	CLA	C	1469	X	-	-	-
11	CLA	C	1470	X	-	-	-
11	CLA	C	1471	X	-	-	-
11	CLA	D	1351	X	-	-	-
11	CLA	D	1353	X	-	-	-
11	CLA	G	1342	X	-	-	-
11	CLA	G	1343	X	-	-	-
11	CLA	G	1344	X	-	-	-
11	CLA	G	1346	X	-	-	-
11	CLA	H	1482	X	-	-	-
11	CLA	H	1483	X	-	-	-
11	CLA	H	1484	X	-	-	-
11	CLA	H	1485	X	-	-	-
11	CLA	H	1486	X	-	-	-
11	CLA	H	1487	X	-	-	-
11	CLA	H	1488	X	-	-	-
11	CLA	H	1489	X	-	-	-
11	CLA	H	1490	X	-	-	-
11	CLA	H	1491	X	-	-	-
11	CLA	H	1492	X	-	-	-
11	CLA	H	1493	X	-	-	-
11	CLA	H	1494	X	-	-	-
11	CLA	H	1495	X	-	-	-
11	CLA	H	1496	X	-	-	-
11	CLA	H	1497	X	-	-	-
11	CLA	I	1459	X	-	-	-
11	CLA	I	1460	X	-	-	-
11	CLA	I	1461	X	-	-	-
11	CLA	I	1462	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	I	1463	X	-	-	-
11	CLA	I	1464	X	-	-	-
11	CLA	I	1465	X	-	-	-
11	CLA	I	1466	X	-	-	-
11	CLA	I	1467	X	-	-	-
11	CLA	I	1468	X	-	-	-
11	CLA	I	1469	X	-	-	-
11	CLA	I	1470	X	-	-	-
11	CLA	I	1471	X	-	-	-
11	CLA	J	1351	X	-	-	-
11	CLA	J	1353	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35614 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 Q(B) PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	31
			2279	1505	370	390	14			
1	G	332	Total	C	N	O	S	0	0	31
			2279	1505	370	390	14			

- Molecule 2 is a protein called PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	479	Total	C	N	O	S	0	0	66
			3053	2027	504	510	12			
2	H	479	Total	C	N	O	S	0	0	66
			3053	2027	504	510	12			

- Molecule 3 is a protein called PHOTOSYSTEM II CP43 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	438	Total	C	N	O	S	0	0	73
			2791	1861	467	452	11			
3	I	438	Total	C	N	O	S	0	0	73
			2791	1861	467	452	11			

- Molecule 4 is a protein called PHOTOSYSTEM II REACTION CENTER D2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	350	Total	C	N	O	S	0	0	0
			2602	1719	421	450	12			
4	J	350	Total	C	N	O	S	0	0	0
			2602	1719	421	450	12			

- Molecule 5 is a protein called CYTOCHROME B559 ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	5
			536	354	89	93			
5	K	76	Total	C	N	O	0	0	5
			536	354	89	93			

- Molecule 6 is a protein called CYTOCHROME B559 BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	37	Total	C	N	O	S	0	0	0
			297	202	48	46	1			
6	L	37	Total	C	N	O	S	0	0	0
			297	202	48	46	1			

- Molecule 7 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	179	Total	C	N	O	0	0	3
			883	531	176	176			
7	P	179	Total	C	N	O	0	0	3
			883	531	176	176			

- Molecule 8 is a protein called PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	100	Total	C	N	O	0	0	0
			499	299	100	100			
8	U	100	Total	C	N	O	0	0	0
			499	299	100	100			

- Molecule 9 is a protein called CYTOCHROME C-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	T	136	Total	C	N	O	S	0	0	0
			1058	672	176	206	4			
9	V	136	Total	C	N	O	S	0	0	0
			1058	672	176	206	4			

- Molecule 10 is a protein called UNASSIGNED SUBUNITS.

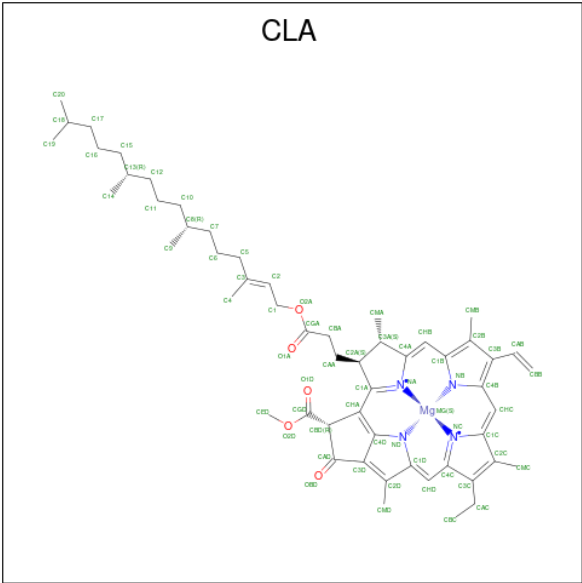
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	X	359	Total	C	N	O	0	0	0
			1791	1073	359	359			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Y	359	Total	C	N	O	0	0	0
			1791	1073	359	359			

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	C	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	C	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	C	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	C	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	C	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		

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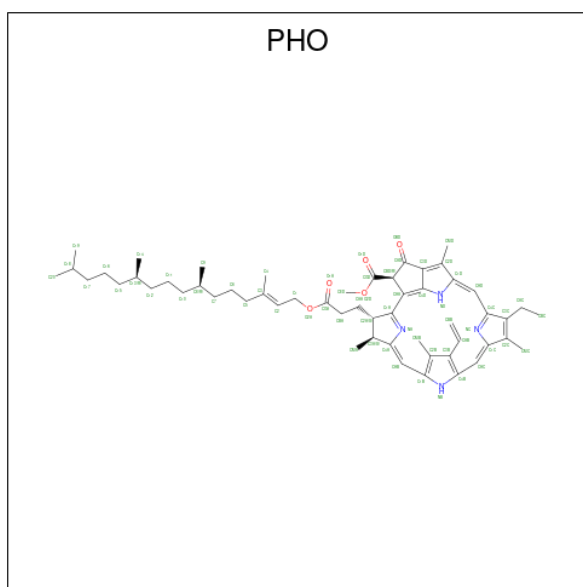
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
11	C	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
11	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	D	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
11	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	G	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
11	G	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	G	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
11	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	H	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
11	H	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	H	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
11	H	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
11	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	H	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
11	H	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	H	1	Total 27	C 22	Mg 1	N 4		0	0
11	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
11	H	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
11	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	H	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	I	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	I	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	I	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	I	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	I	1	Total	C	Mg	N		0	0
			27	22	1	4			
11	I	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	I	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	I	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
11	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			64	55	4	5		
12	D	1	Total	C	N	O	0	0
			54	45	4	5		
12	G	1	Total	C	N	O	0	0
			64	55	4	5		
12	J	1	Total	C	N	O	0	0
			54	45	4	5		

- Molecule 13 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

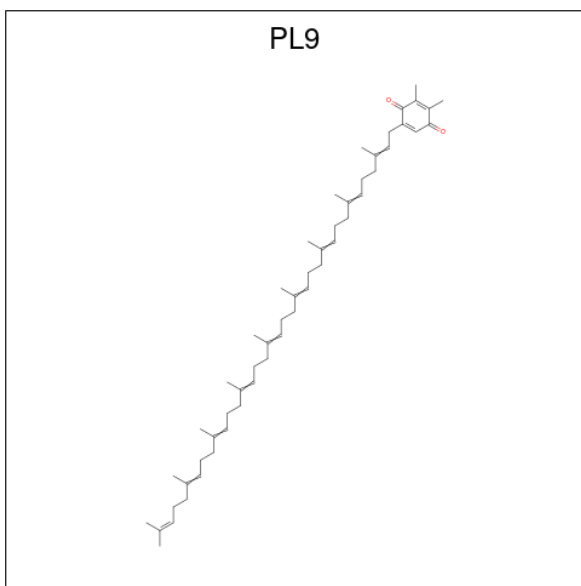
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	Mn	0	0
			4	4		
13	G	4	Total	Mn	0	0
			4	4		

- Molecule 14 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Fe	0	0
			1	1		
14	G	1	Total	Fe	0	0
			1	1		

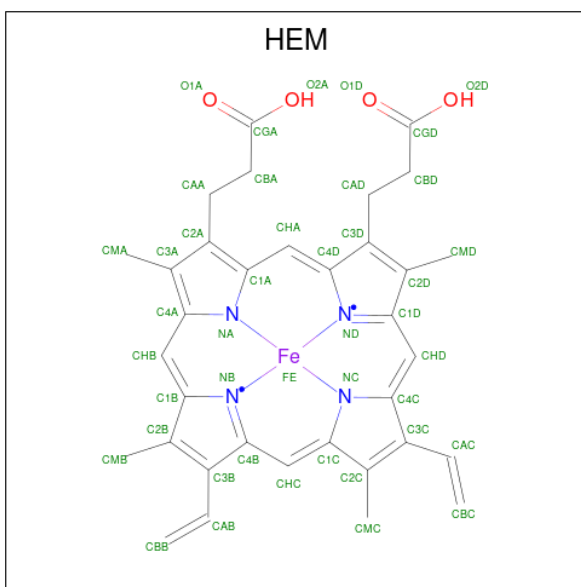
- Molecule 15 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DI

METHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



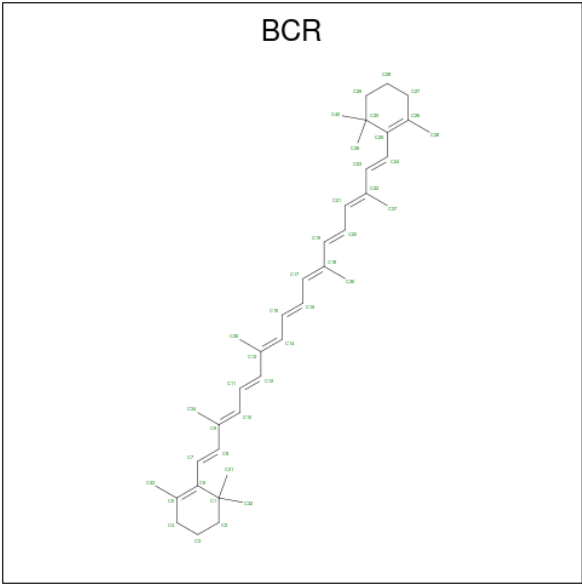
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C 6 6	0	0
15	J	1	Total C 6 6	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



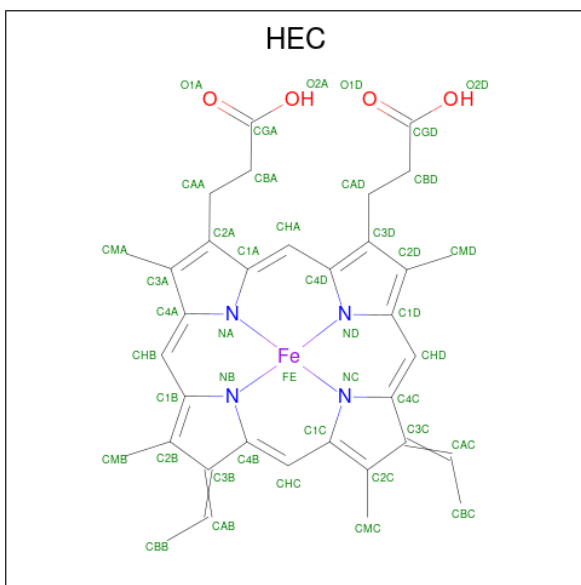
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	E	1	Total	C	Fe	N	0	0
			25	20	1	4		
16	L	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



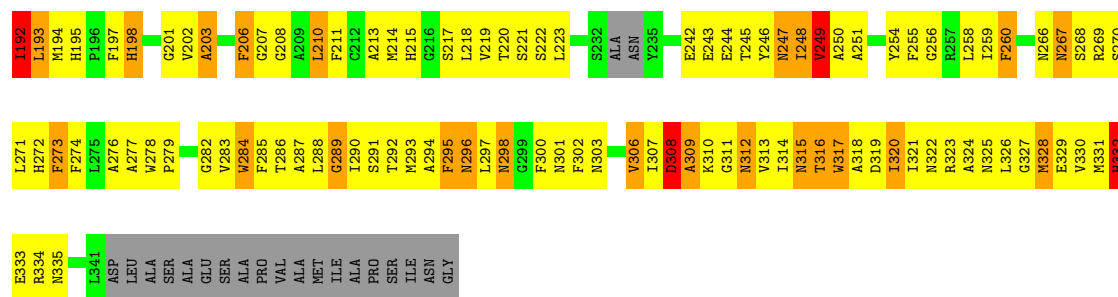
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	1	Total	C	0	0
			40	40		
17	L	1	Total	C	0	0
			40	40		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).

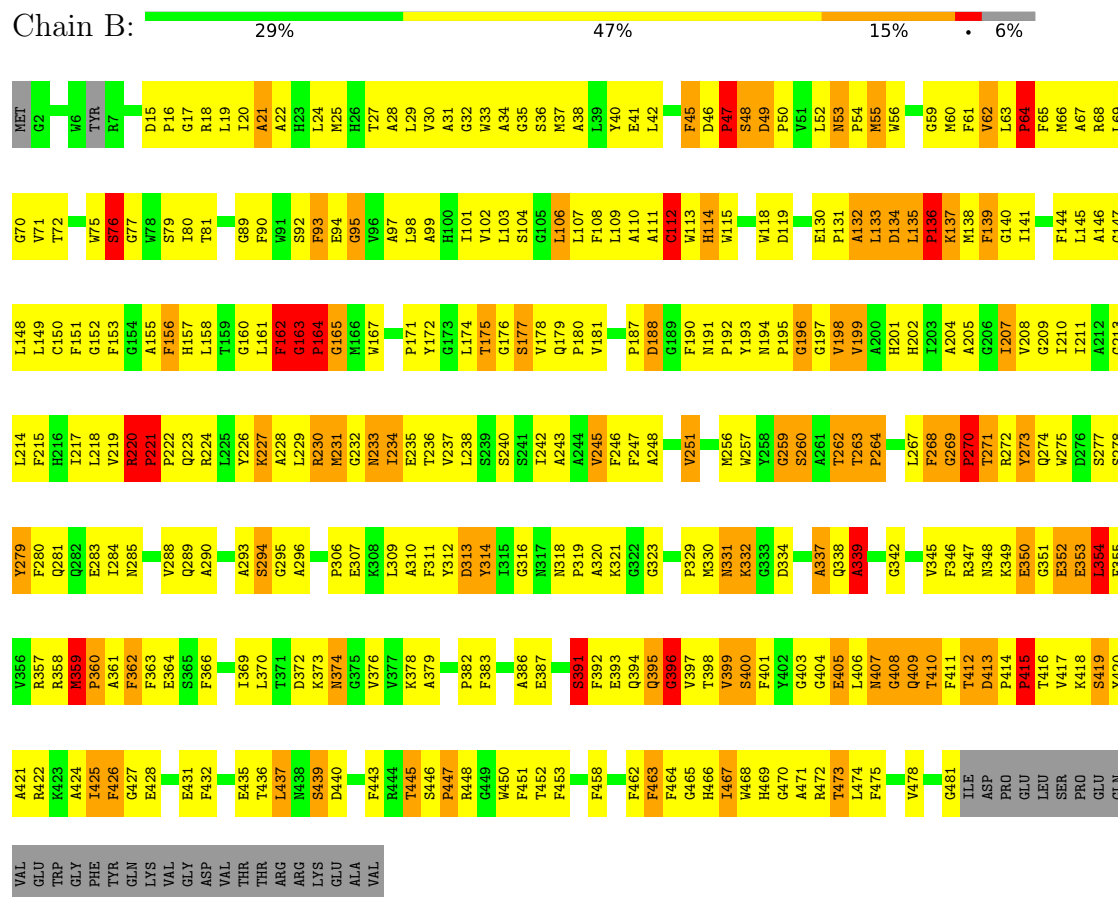


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
18	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



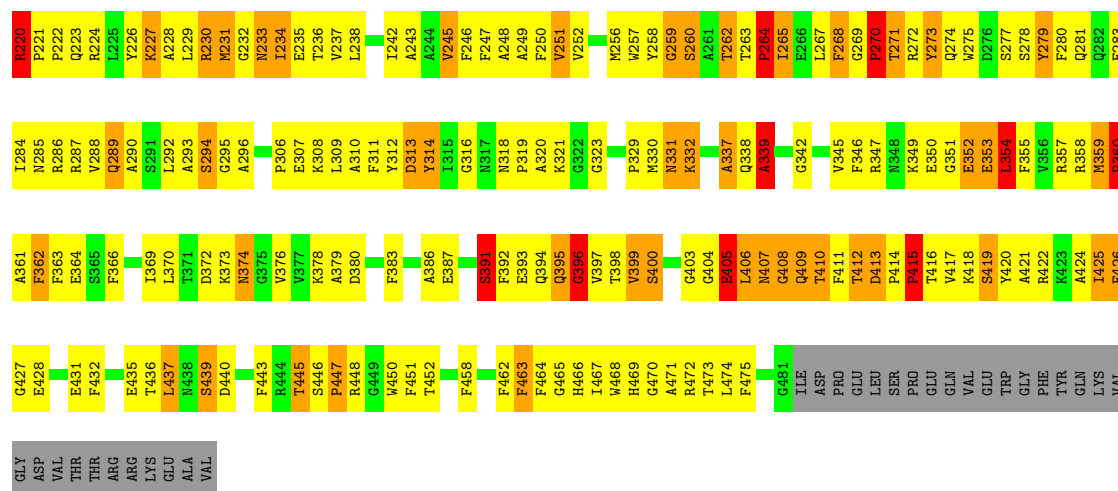


• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN



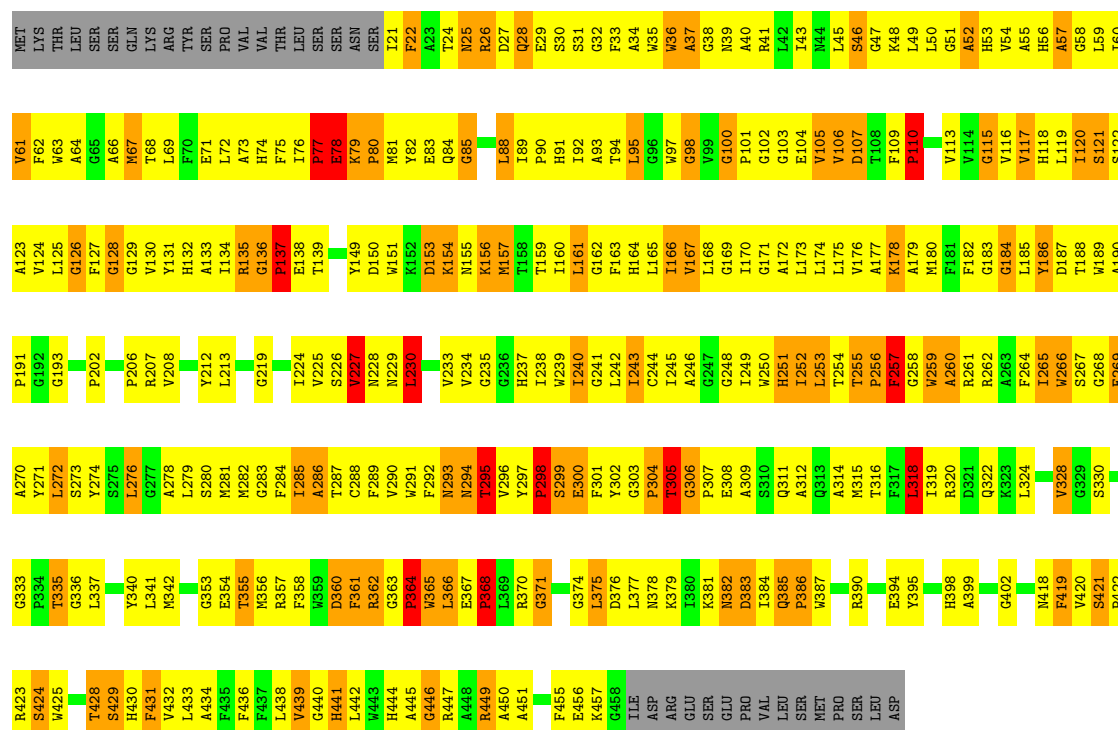
• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN





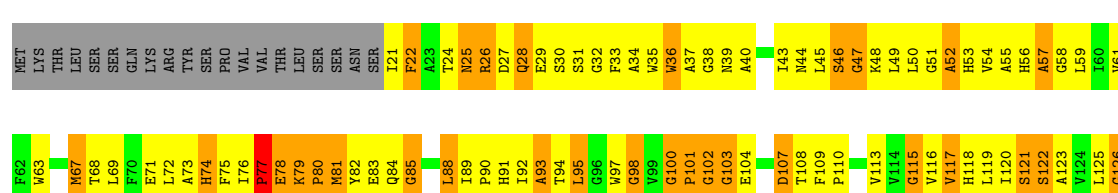
• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

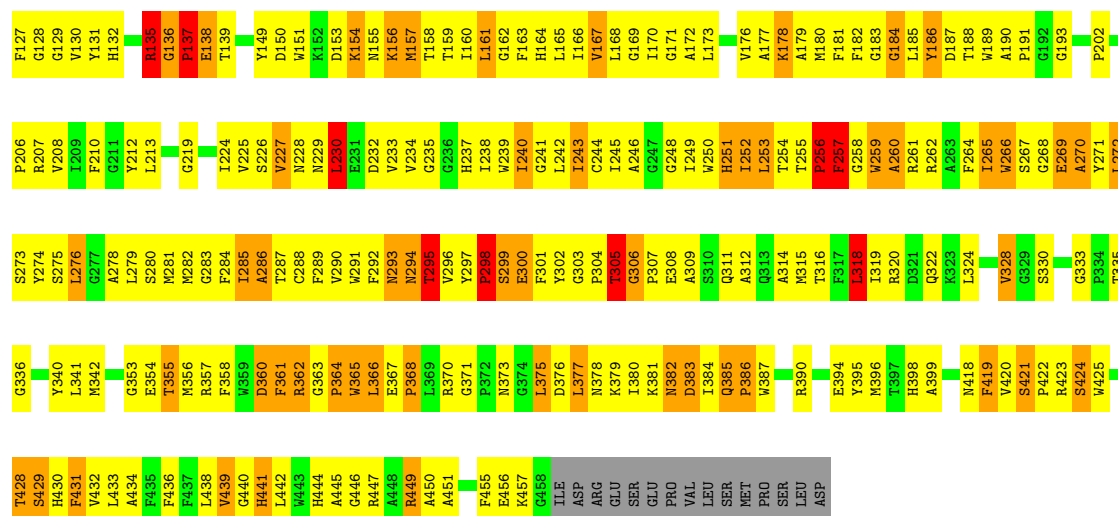
Chain C: 25% 47% 18% 7%



• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

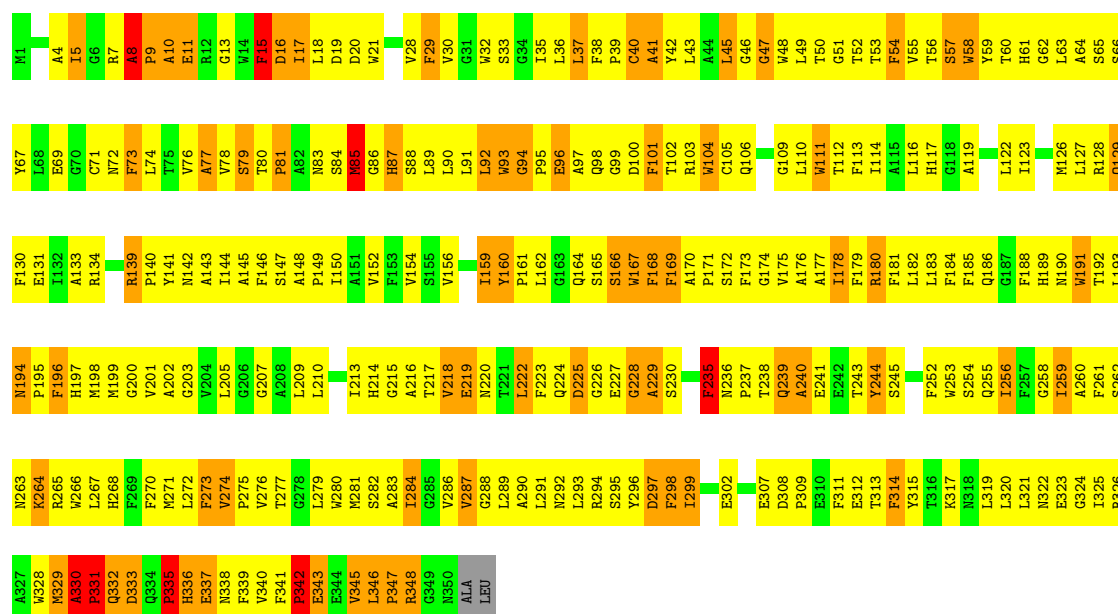
Chain I: 26% 46% 18% 7%





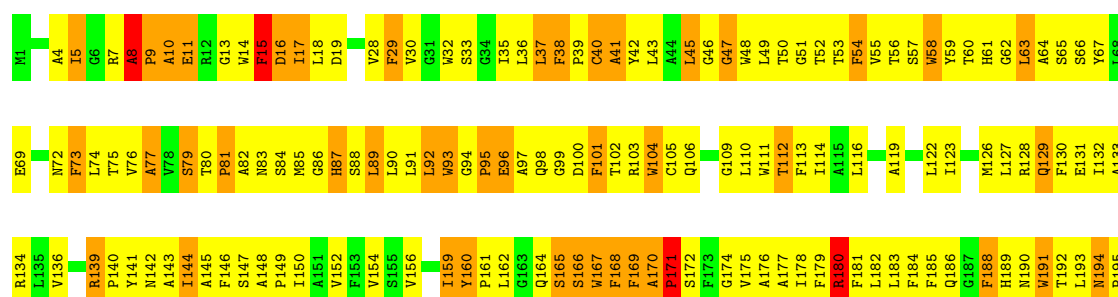
● Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

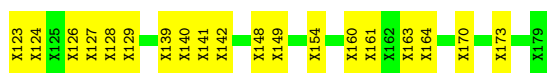
Chain D: 21% 56% 20% ..



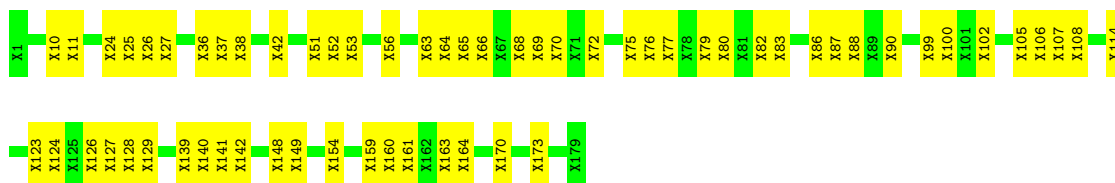
● Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

Chain J: 23% 53% 21% ..

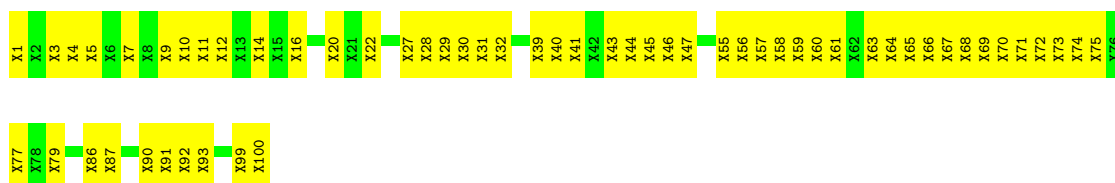




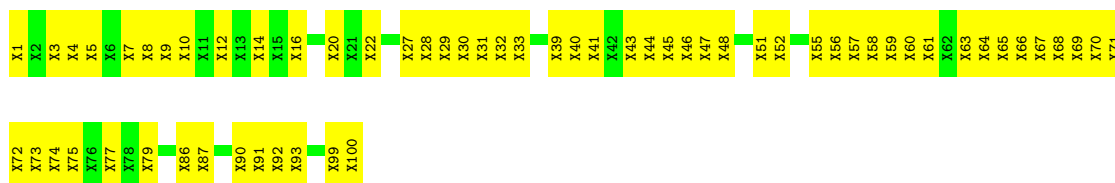
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE



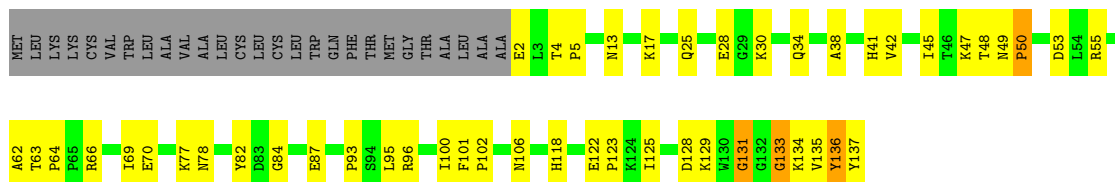
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN



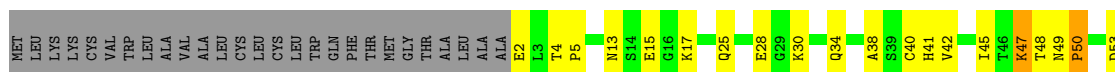
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

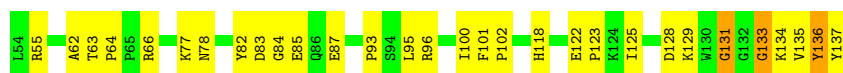


• Molecule 9: CYTOCHROME C-550



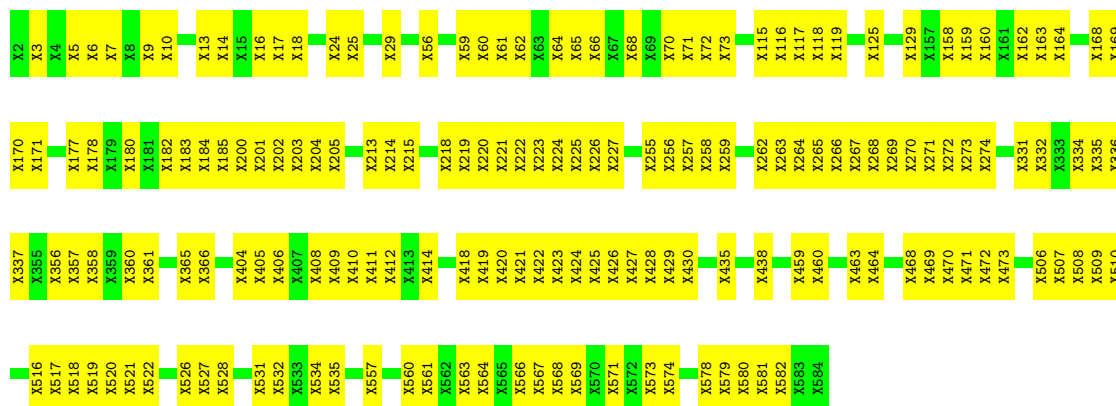
• Molecule 9: CYTOCHROME C-550





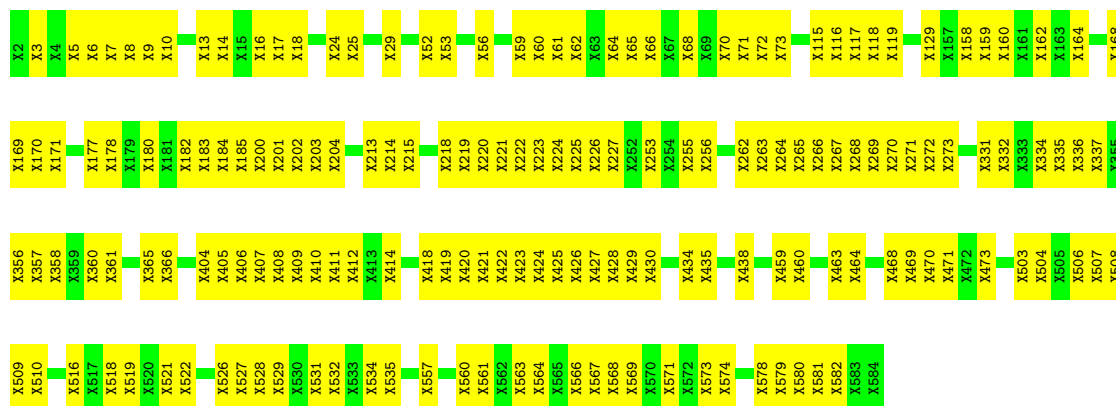
• Molecule 10: UNASSIGNED SUBUNITS

Chain X: 52% 48%



• Molecule 10: UNASSIGNED SUBUNITS

Chain Y: 53% 47%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.52Å 224.61Å 305.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	75.6 (10.00-3.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35614	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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: FE2, CLA, PL9, PHO, BCR, MN, HEM, HEC

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	0.93	1/2315 (0.0%)	1.40	39/3161 (1.2%)
1	G	0.89	1/2315 (0.0%)	1.38	33/3161 (1.0%)
2	B	0.91	0/3081	1.46	55/4202 (1.3%)
2	H	0.86	0/3081	1.48	50/4202 (1.2%)
3	C	0.79	0/2806	1.41	53/3822 (1.4%)
3	I	0.77	0/2806	1.38	43/3822 (1.1%)
4	D	0.95	0/2688	1.42	43/3678 (1.2%)
4	J	0.91	1/2688 (0.0%)	1.43	48/3678 (1.3%)
5	E	0.83	0/547	1.39	6/751 (0.8%)
5	K	0.87	1/547 (0.2%)	1.36	7/751 (0.9%)
6	F	1.02	0/307	1.75	12/421 (2.9%)
6	L	1.00	0/307	1.56	7/421 (1.7%)
9	T	0.85	0/1079	1.14	5/1466 (0.3%)
9	V	0.90	0/1079	1.15	5/1466 (0.3%)
All	All	0.88	4/25646 (0.0%)	1.41	406/35002 (1.2%)

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
1	A	0	1
1	G	0	1
2	B	0	1
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ILE	CA-CB	-5.45	1.48	1.54
1	G	320	ILE	CA-CB	-5.14	1.48	1.54
4	J	339	PHE	CA-C	-5.02	1.46	1.52
5	K	17	VAL	CA-CB	5.02	1.61	1.54

The worst 5 of 406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	270	PRO	CA-N-CD	-15.33	90.54	112.00
2	B	270	PRO	CA-N-CD	-13.84	92.62	112.00
2	B	76	SER	N-CA-C	-13.04	83.02	110.80
2	H	76	SER	N-CA-C	-12.99	83.12	110.80
1	G	83	VAL	CA-C-N	12.20	132.33	119.89

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	HIS	Sidechain
2	B	273	TYR	Sidechain
1	G	332	HIS	Sidechain
2	H	273	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2279	0	2113	471	0
1	G	2279	0	2113	479	0
2	B	3053	0	2666	463	0
2	H	3053	0	2666	479	0
3	C	2791	0	2530	480	0
3	I	2791	0	2530	477	0
4	D	2602	0	2383	490	0
4	J	2602	0	2383	501	0
5	E	536	0	480	89	0
5	K	536	0	480	94	0
6	F	297	0	304	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	297	0	304	62	0
7	O	883	0	221	43	0
7	P	883	0	219	45	0
8	S	499	0	116	50	0
8	U	499	0	115	52	0
9	T	1058	0	1066	61	0
9	V	1058	0	1066	63	0
10	X	1791	0	396	137	0
10	Y	1791	0	393	135	0
11	A	222	0	207	38	0
11	B	846	0	774	74	0
11	C	598	0	458	65	0
11	D	115	0	111	18	0
11	G	222	0	207	33	0
11	H	846	0	774	78	0
11	I	598	0	458	65	0
11	J	115	0	111	16	0
12	A	64	0	74	13	0
12	D	54	0	51	4	0
12	G	64	0	74	16	0
12	J	54	0	51	9	0
13	A	4	0	0	0	0
13	G	4	0	0	0	0
14	A	1	0	0	0	0
14	G	1	0	0	0	0
15	D	6	0	1	1	0
15	J	6	0	1	1	0
16	E	25	0	4	2	0
16	L	25	0	4	2	0
17	F	40	0	56	4	0
17	L	40	0	56	3	0
18	T	43	0	31	2	0
18	V	43	0	31	2	0
All	All	35614	0	28078	4407	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 69.

The worst 5 of 4407 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)
4:D:330:ALA:HB1	4:D:331:PRO:CD	1.48	1.42
4:J:330:ALA:HB1	4:J:331:PRO:CD	1.54	1.36
1:G:84:PRO:CG	1:G:173:PRO:HG3	1.56	1.35
4:D:330:ALA:CB	4:D:331:PRO:CD	1.99	1.33
4:J:330:ALA:CB	4:J:331:PRO:CD	2.07	1.28

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	295/360 (82%)	188 (64%)	67 (23%)	40 (14%)	0	1
1	G	295/360 (82%)	184 (62%)	71 (24%)	40 (14%)	0	1
2	B	399/510 (78%)	244 (61%)	94 (24%)	61 (15%)	0	0
2	H	399/510 (78%)	246 (62%)	94 (24%)	59 (15%)	0	1
3	C	353/473 (75%)	205 (58%)	96 (27%)	52 (15%)	0	1
3	I	353/473 (75%)	206 (58%)	99 (28%)	48 (14%)	0	1
4	D	348/352 (99%)	223 (64%)	76 (22%)	49 (14%)	0	1
4	J	348/352 (99%)	222 (64%)	79 (23%)	47 (14%)	0	1
5	E	67/84 (80%)	40 (60%)	13 (19%)	14 (21%)	0	0
5	K	67/84 (80%)	43 (64%)	10 (15%)	14 (21%)	0	0
6	F	35/44 (80%)	24 (69%)	4 (11%)	7 (20%)	0	0
6	L	35/44 (80%)	22 (63%)	6 (17%)	7 (20%)	0	0
9	T	134/163 (82%)	121 (90%)	11 (8%)	2 (2%)	8	37
9	V	134/163 (82%)	124 (92%)	8 (6%)	2 (2%)	8	37
All	All	3262/3972 (82%)	2092 (64%)	728 (22%)	442 (14%)	0	1

5 of 442 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	12	ASN
1	A	63	ILE
1	A	80	GLY
1	A	85	SER

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	217/291 (75%)	202 (93%)	15 (7%)	14	45
1	G	217/291 (75%)	201 (93%)	16 (7%)	13	43
2	B	256/407 (63%)	230 (90%)	26 (10%)	7	29
2	H	256/407 (63%)	227 (89%)	29 (11%)	5	24
3	C	243/374 (65%)	213 (88%)	30 (12%)	4	22
3	I	243/374 (65%)	210 (86%)	33 (14%)	3	18
4	D	239/283 (84%)	224 (94%)	15 (6%)	16	48
4	J	239/283 (84%)	225 (94%)	14 (6%)	18	50
5	E	49/73 (67%)	43 (88%)	6 (12%)	5	22
5	K	49/73 (67%)	43 (88%)	6 (12%)	5	22
6	F	31/38 (82%)	27 (87%)	4 (13%)	4	20
6	L	31/38 (82%)	26 (84%)	5 (16%)	2	13
9	T	117/138 (85%)	116 (99%)	1 (1%)	70	81
9	V	117/138 (85%)	116 (99%)	1 (1%)	70	81
All	All	2304/3208 (72%)	2103 (91%)	201 (9%)	9	36

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	55	MET
3	I	78	GLU
9	T	50	PRO

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Mol	Chain	Res	Type
2	H	114	HIS
2	H	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	129	GLN
4	J	220	ASN
6	L	41	GLN
4	D	164	GLN
4	D	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	$\# Z > 2$
11	CLA	B	1486	2	45,49,73	1.60	7 (15%)	54,84,113	2.10	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	I	1459	3	49,53,73	1.53	7 (14%)	58,89,113	2.05	10 (17%)
11	CLA	G	1342	1	69,73,73	1.48	11 (15%)	82,113,113	1.69	10 (12%)
11	CLA	H	1485	2	51,55,73	1.32	10 (19%)	60,91,113	1.73	6 (10%)
11	CLA	H	1495	-	59,63,73	1.54	10 (16%)	70,101,113	2.09	11 (15%)
11	CLA	D	1353	4	54,58,73	1.53	10 (18%)	64,95,113	1.85	8 (12%)
11	CLA	G	1343	-	65,69,73	1.44	10 (15%)	77,108,113	1.91	10 (12%)
11	CLA	C	1461	3	27,35,73	2.57	13 (48%)	32,60,113	2.33	4 (12%)
11	CLA	I	1468	3	27,35,73	2.24	9 (33%)	32,60,113	2.35	5 (15%)
11	CLA	B	1488	-	69,73,73	1.47	11 (15%)	82,113,113	1.76	11 (13%)
11	CLA	C	1465	-	69,73,73	1.22	6 (8%)	82,113,113	1.75	12 (14%)
18	HEC	T	1138	9	46,50,50	2.11	15 (32%)	58,82,82	2.19	14 (24%)
11	CLA	H	1482	-	69,73,73	1.56	10 (14%)	82,113,113	1.93	10 (12%)
11	CLA	I	1470	-	45,49,73	1.54	9 (20%)	54,84,113	2.03	8 (14%)
11	CLA	B	1496	-	69,73,73	1.23	7 (10%)	82,113,113	1.79	11 (13%)
11	CLA	C	1467	3	51,55,73	1.58	5 (9%)	60,91,113	1.96	9 (15%)
11	CLA	C	1469	3	45,49,73	1.48	7 (15%)	54,84,113	2.20	8 (14%)
12	PHO	J	1352	-	48,59,69	1.75	6 (12%)	43,87,99	2.34	13 (30%)
11	CLA	C	1466	3	54,58,73	1.60	9 (16%)	64,95,113	2.01	11 (17%)
11	CLA	I	1471	-	45,49,73	1.63	6 (13%)	54,84,113	2.12	8 (14%)
11	CLA	I	1460	3	51,55,73	1.56	8 (15%)	60,91,113	1.91	7 (11%)
11	CLA	H	1486	2	45,49,73	1.55	8 (17%)	54,84,113	1.99	6 (11%)
11	CLA	B	1494	-	69,73,73	1.29	11 (15%)	82,113,113	1.74	10 (12%)
12	PHO	D	1352	-	48,59,69	1.75	9 (18%)	43,87,99	2.47	15 (34%)
15	PL9	D	1354	-	6,6,55	2.06	2 (33%)	6,6,69	1.06	0
11	CLA	H	1497	2	45,49,73	1.60	13 (28%)	54,84,113	2.14	8 (14%)
11	CLA	I	1466	3	54,58,73	1.59	8 (14%)	64,95,113	2.01	11 (17%)
11	CLA	J	1353	4	54,58,73	1.51	8 (14%)	64,95,113	1.79	7 (10%)
11	CLA	H	1494	-	69,73,73	1.39	11 (15%)	82,113,113	1.86	11 (13%)
11	CLA	B	1489	2	54,58,73	1.34	5 (9%)	64,95,113	2.02	10 (15%)
11	CLA	B	1493	-	49,53,73	1.62	5 (10%)	58,89,113	2.08	9 (15%)
11	CLA	H	1490	2	49,53,73	2.08	11 (22%)	58,89,113	2.03	7 (12%)
11	CLA	H	1483	2	64,68,73	1.37	8 (12%)	76,107,113	1.64	9 (11%)
11	CLA	H	1488	-	69,73,73	1.51	12 (17%)	82,113,113	1.75	9 (10%)
11	CLA	B	1492	2	69,73,73	1.27	9 (13%)	82,113,113	1.95	13 (15%)
11	CLA	H	1484	-	49,53,73	1.29	6 (12%)	58,89,113	1.83	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	C	1470	-	45,49,73	1.54	6 (13%)	54,84,113	2.13	7 (12%)
11	CLA	A	1344	-	49,53,73	1.60	7 (14%)	58,89,113	1.99	9 (15%)
11	CLA	C	1460	3	51,55,73	1.57	6 (11%)	60,91,113	1.99	9 (15%)
11	CLA	H	1496	-	69,73,73	1.26	10 (14%)	82,113,113	1.90	12 (14%)
11	CLA	A	1346	-	55,59,73	1.60	9 (16%)	64,96,113	1.90	8 (12%)
16	HEM	E	1085	6,5	32,32,50	2.38	13 (40%)	30,54,82	1.61	4 (13%)
11	CLA	C	1464	3	60,64,73	1.37	7 (11%)	71,102,113	1.90	13 (18%)
11	CLA	B	1483	2	64,68,73	1.45	8 (12%)	76,107,113	1.70	9 (11%)
11	CLA	C	1462	-	60,64,73	1.61	14 (23%)	71,102,113	1.76	12 (16%)
11	CLA	I	1462	-	60,64,73	1.69	14 (23%)	71,102,113	1.77	12 (16%)
11	CLA	C	1471	-	45,49,73	1.60	8 (17%)	54,84,113	2.09	5 (9%)
11	CLA	C	1463	3	59,63,73	1.72	9 (15%)	70,101,113	1.96	9 (12%)
11	CLA	I	1463	3	59,63,73	1.76	7 (11%)	70,101,113	2.01	9 (12%)
15	PL9	J	1354	-	6,6,55	1.96	2 (33%)	6,6,69	1.09	0
18	HEC	V	1138	9	46,50,50	2.10	15 (32%)	58,82,82	2.21	12 (20%)
11	CLA	C	1468	3	27,35,73	2.22	9 (33%)	32,60,113	2.43	5 (15%)
17	BCR	F	1046	-	41,41,41	1.71	8 (19%)	56,56,56	2.21	24 (42%)
16	HEM	L	1046	6,5	32,32,50	2.31	13 (40%)	30,54,82	1.60	5 (16%)
11	CLA	G	1344	-	49,53,73	1.52	6 (12%)	58,89,113	1.98	9 (15%)
11	CLA	B	1487	-	69,73,73	1.62	12 (17%)	82,113,113	1.70	12 (14%)
11	CLA	J	1351	4	69,73,73	2.17	11 (15%)	82,113,113	2.05	13 (15%)
11	CLA	B	1495	-	59,63,73	1.49	10 (16%)	70,101,113	2.03	12 (17%)
11	CLA	I	1467	3	51,55,73	1.37	4 (7%)	60,91,113	1.94	8 (13%)
11	CLA	B	1491	-	27,35,73	2.11	7 (25%)	32,60,113	2.38	4 (12%)
17	BCR	L	1047	-	41,41,41	1.66	7 (17%)	56,56,56	2.21	22 (39%)
11	CLA	B	1485	2	51,55,73	1.33	6 (11%)	60,91,113	1.78	7 (11%)
11	CLA	A	1343	-	65,69,73	1.29	6 (9%)	77,108,113	1.84	11 (14%)
11	CLA	A	1342	1	69,73,73	1.35	7 (10%)	82,113,113	1.81	12 (14%)
11	CLA	I	1461	3	27,35,73	2.48	13 (48%)	32,60,113	2.29	4 (12%)
11	CLA	H	1492	2	69,73,73	1.22	5 (7%)	82,113,113	1.94	12 (14%)
11	CLA	B	1490	2	49,53,73	2.10	11 (22%)	58,89,113	1.94	6 (10%)
11	CLA	I	1464	3	60,64,73	1.39	9 (15%)	71,102,113	1.84	12 (16%)
11	CLA	H	1493	-	49,53,73	1.63	6 (12%)	58,89,113	2.11	10 (17%)
11	CLA	B	1497	2	45,49,73	1.50	9 (20%)	54,84,113	2.07	8 (14%)
12	PHO	G	1345	-	58,69,69	1.55	8 (13%)	55,99,99	2.12	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1482	-	69,73,73	1.42	12 (17%)	82,113,113	1.91	9 (10%)
11	CLA	G	1346	-	55,59,73	1.60	8 (14%)	64,96,113	1.85	7 (10%)
11	CLA	I	1465	-	69,73,73	1.23	8 (11%)	82,113,113	1.76	12 (14%)
11	CLA	D	1351	4	69,73,73	1.65	10 (14%)	82,113,113	1.98	13 (15%)
11	CLA	C	1459	3	49,53,73	1.51	10 (20%)	58,89,113	1.89	10 (17%)
11	CLA	B	1484	-	49,53,73	1.36	6 (12%)	58,89,113	1.90	6 (10%)
11	CLA	I	1469	3	45,49,73	1.62	7 (15%)	54,84,113	2.25	8 (14%)
11	CLA	H	1487	-	69,73,73	1.63	12 (17%)	82,113,113	1.70	11 (13%)
11	CLA	H	1489	2	54,58,73	1.44	4 (7%)	64,95,113	2.11	8 (12%)
12	PHO	A	1345	-	58,69,69	1.55	6 (10%)	55,99,99	2.14	16 (29%)
11	CLA	H	1491	-	27,35,73	2.17	9 (33%)	32,60,113	2.26	4 (12%)

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
11	CLA	B	1486	2	1/1/10/20	4/10/86/115	-
11	CLA	I	1459	3	1/1/11/20	9/15/91/115	-
11	CLA	G	1342	1	1/1/15/20	5/39/115/115	-
11	CLA	H	1485	2	1/1/11/20	9/18/94/115	-
11	CLA	H	1495	-	1/1/13/20	11/27/103/115	-
11	CLA	D	1353	4	1/1/12/20	5/21/97/115	-
11	CLA	G	1343	-	1/1/14/20	17/35/111/115	-
11	CLA	C	1461	3	1/1/5/20	-	-
11	CLA	I	1468	3	1/1/5/20	-	-
11	CLA	B	1488	-	1/1/15/20	16/39/115/115	-
11	CLA	C	1465	-	1/1/15/20	17/39/115/115	-
18	HEC	T	1138	9	-	8/14/54/54	-
11	CLA	H	1482	-	1/1/15/20	13/39/115/115	-
11	CLA	I	1470	-	1/1/10/20	4/10/86/115	-
11	CLA	B	1496	-	1/1/15/20	18/39/115/115	-
11	CLA	C	1467	3	1/1/11/20	6/18/94/115	-
11	CLA	C	1469	3	1/1/10/20	4/10/86/115	-
12	PHO	J	1352	-	-	7/25/91/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	C	1466	3	1/1/12/20	9/21/97/115	-
11	CLA	I	1471	-	1/1/10/20	6/10/86/115	-
11	CLA	I	1460	3	1/1/11/20	4/18/94/115	-
11	CLA	H	1486	2	1/1/10/20	4/10/86/115	-
11	CLA	B	1494	-	1/1/15/20	10/39/115/115	-
12	PHO	D	1352	-	-	7/25/91/103	0/5/6/6
15	PL9	D	1354	-	-	-	0/1/1/1
11	CLA	H	1497	2	1/1/10/20	4/10/86/115	-
11	CLA	I	1466	3	1/1/12/20	9/21/97/115	-
11	CLA	J	1353	4	1/1/12/20	5/21/97/115	-
11	CLA	H	1494	-	1/1/15/20	11/39/115/115	-
11	CLA	B	1489	2	1/1/12/20	3/21/97/115	-
11	CLA	B	1493	-	1/1/11/20	8/15/91/115	-
11	CLA	H	1490	2	1/1/11/20	10/15/91/115	-
11	CLA	H	1483	2	1/1/14/20	12/33/109/115	-
11	CLA	H	1488	-	1/1/15/20	15/39/115/115	-
11	CLA	B	1492	2	1/1/15/20	15/39/115/115	-
11	CLA	H	1484	-	1/1/11/20	6/15/91/115	-
11	CLA	C	1470	-	1/1/10/20	4/10/86/115	-
11	CLA	A	1344	-	1/1/11/20	7/15/91/115	-
11	CLA	C	1460	3	1/1/11/20	4/18/94/115	-
11	CLA	H	1496	-	1/1/15/20	17/39/115/115	-
11	CLA	A	1346	-	1/1/12/20	6/23/99/115	-
11	CLA	C	1464	3	1/1/13/20	15/29/105/115	-
11	CLA	B	1483	2	1/1/14/20	12/33/109/115	-
11	CLA	C	1462	-	1/1/13/20	8/29/105/115	-
11	CLA	I	1462	-	1/1/13/20	8/29/105/115	-
11	CLA	C	1471	-	1/1/10/20	6/10/86/115	-
11	CLA	C	1463	3	1/1/13/20	11/27/103/115	-
11	CLA	I	1463	3	2/2/13/20	11/27/103/115	-
15	PL9	J	1354	-	-	-	0/1/1/1
18	HEC	V	1138	9	-	8/14/54/54	-
11	CLA	C	1468	3	1/1/5/20	-	-
17	BCR	F	1046	-	-	3/29/63/63	0/2/2/2
11	CLA	G	1344	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1487	-	1/1/15/20	10/39/115/115	-
11	CLA	J	1351	4	1/1/15/20	12/39/115/115	-
11	CLA	B	1495	-	1/1/13/20	11/27/103/115	-
11	CLA	I	1467	3	1/1/11/20	7/18/94/115	-
11	CLA	B	1491	-	1/1/5/20	-	-
17	BCR	L	1047	-	-	3/29/63/63	0/2/2/2
11	CLA	B	1485	2	1/1/11/20	9/18/94/115	-
11	CLA	A	1343	-	1/1/14/20	17/35/111/115	-
11	CLA	A	1342	1	1/1/15/20	5/39/115/115	-
11	CLA	I	1461	3	1/1/5/20	-	-
11	CLA	H	1492	2	1/1/15/20	15/39/115/115	-
11	CLA	B	1490	2	1/1/11/20	10/15/91/115	-
11	CLA	I	1464	3	1/1/13/20	15/29/105/115	-
11	CLA	H	1493	-	1/1/11/20	7/15/91/115	-
11	CLA	B	1497	2	1/1/10/20	4/10/86/115	-
12	PHO	G	1345	-	-	13/37/103/103	0/5/6/6
11	CLA	B	1482	-	1/1/15/20	11/39/115/115	-
11	CLA	G	1346	-	1/1/12/20	5/23/99/115	-
11	CLA	I	1465	-	1/1/15/20	16/39/115/115	-
11	CLA	D	1351	4	1/1/15/20	11/39/115/115	-
11	CLA	C	1459	3	1/1/11/20	9/15/91/115	-
11	CLA	B	1484	-	1/1/11/20	6/15/91/115	-
11	CLA	I	1469	3	1/1/10/20	4/10/86/115	-
11	CLA	H	1487	-	1/1/15/20	10/39/115/115	-
11	CLA	H	1489	2	1/1/12/20	3/21/97/115	-
12	PHO	A	1345	-	-	10/37/103/103	0/5/6/6
11	CLA	H	1491	-	1/1/5/20	-	-

The worst 5 of 706 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1351	CLA	MG-NA	13.61	2.38	2.06
11	H	1490	CLA	MG-NA	9.48	2.28	2.06
11	B	1490	CLA	MG-NA	9.35	2.28	2.06
11	I	1463	CLA	MG-NA	9.33	2.28	2.06
11	C	1461	CLA	MG-NA	8.23	2.25	2.06

The worst 5 of 769 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	1469	CLA	C4A-NA-C1A	13.40	112.79	106.68
11	C	1469	CLA	C4A-NA-C1A	13.11	112.66	106.68
11	H	1495	CLA	C4A-NA-C1A	12.76	112.50	106.68
11	I	1463	CLA	C4A-NA-C1A	12.62	112.44	106.68
11	H	1496	CLA	C4A-NA-C1A	12.56	112.41	106.68

5 of 71 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1342	CLA	ND
11	A	1343	CLA	ND
11	A	1344	CLA	ND
11	A	1346	CLA	ND
11	B	1482	CLA	ND

5 of 641 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1343	CLA	C1A-C2A-CAA-CBA
11	A	1343	CLA	C2B-C3B-CAB-CBB
11	A	1343	CLA	C4B-C3B-CAB-CBB
11	A	1343	CLA	CBD-CGD-O2D-CED
11	A	1344	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

77 monomers are involved in 435 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1486	CLA	10	0
11	I	1459	CLA	3	0
11	G	1342	CLA	18	0
11	H	1485	CLA	5	0
11	H	1495	CLA	2	0
11	D	1353	CLA	6	0
11	G	1343	CLA	7	0
11	B	1488	CLA	7	0
11	C	1465	CLA	5	0
18	T	1138	HEC	2	0
11	H	1482	CLA	2	0
11	I	1470	CLA	3	0
11	B	1496	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1467	CLA	7	0
11	C	1469	CLA	6	0
12	J	1352	PHO	9	0
11	C	1466	CLA	10	0
11	I	1471	CLA	5	0
11	I	1460	CLA	3	0
11	H	1486	CLA	12	0
11	B	1494	CLA	2	0
12	D	1352	PHO	4	0
15	D	1354	PL9	1	0
11	H	1497	CLA	8	0
11	I	1466	CLA	10	0
11	J	1353	CLA	5	0
11	H	1494	CLA	2	0
11	B	1489	CLA	4	0
11	H	1490	CLA	1	0
11	H	1483	CLA	3	0
11	H	1488	CLA	14	0
11	B	1492	CLA	5	0
11	H	1484	CLA	7	0
11	C	1470	CLA	3	0
11	A	1344	CLA	5	0
11	C	1460	CLA	4	0
11	H	1496	CLA	12	0
11	A	1346	CLA	5	0
16	E	1085	HEM	2	0
11	C	1464	CLA	8	0
11	B	1483	CLA	4	0
11	C	1462	CLA	4	0
11	I	1462	CLA	4	0
11	C	1471	CLA	5	0
11	C	1463	CLA	9	0
11	I	1463	CLA	10	0
15	J	1354	PL9	1	0
18	V	1138	HEC	2	0
17	F	1046	BCR	4	0
16	L	1046	HEM	2	0
11	G	1344	CLA	5	0
11	B	1487	CLA	7	0
11	J	1351	CLA	11	0
11	B	1495	CLA	3	0
11	I	1467	CLA	7	0

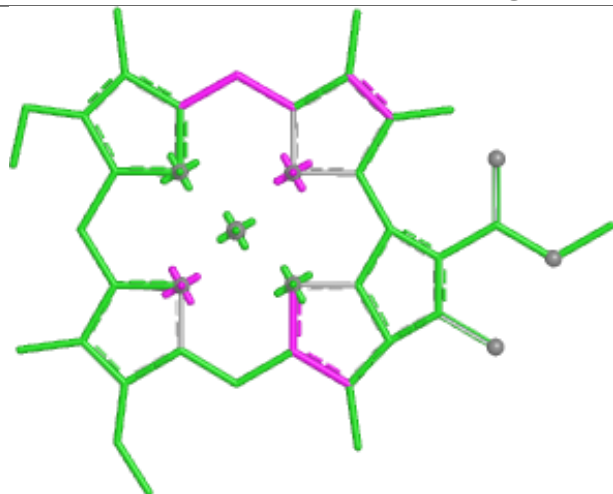
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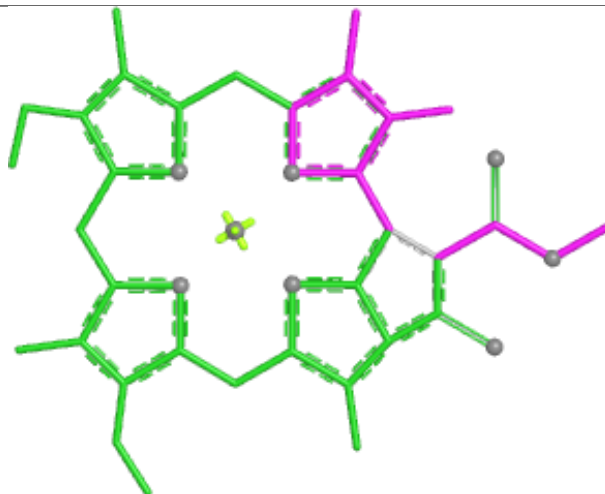
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1491	CLA	3	0
17	L	1047	BCR	3	0
11	B	1485	CLA	4	0
11	A	1343	CLA	12	0
11	A	1342	CLA	17	0
11	H	1492	CLA	6	0
11	B	1490	CLA	3	0
11	I	1464	CLA	9	0
11	H	1493	CLA	1	0
11	B	1497	CLA	9	0
12	G	1345	PHO	16	0
11	B	1482	CLA	1	0
11	G	1346	CLA	4	0
11	I	1465	CLA	9	0
11	D	1351	CLA	12	0
11	C	1459	CLA	4	0
11	B	1484	CLA	7	0
11	I	1469	CLA	4	0
11	H	1487	CLA	5	0
11	H	1489	CLA	4	0
12	A	1345	PHO	13	0
11	H	1491	CLA	2	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.

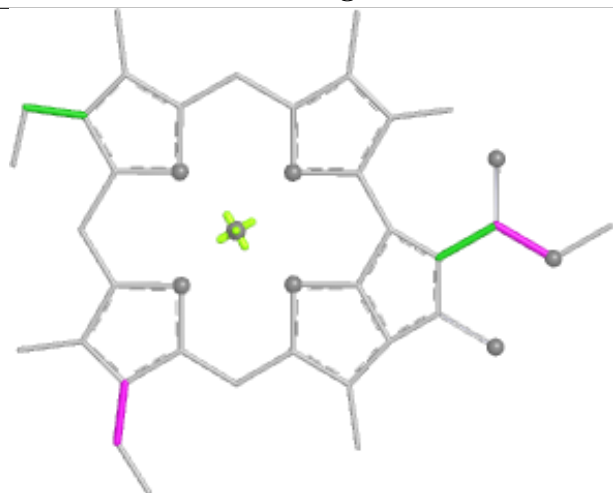
Ligand CLA B 1486



Bond lengths



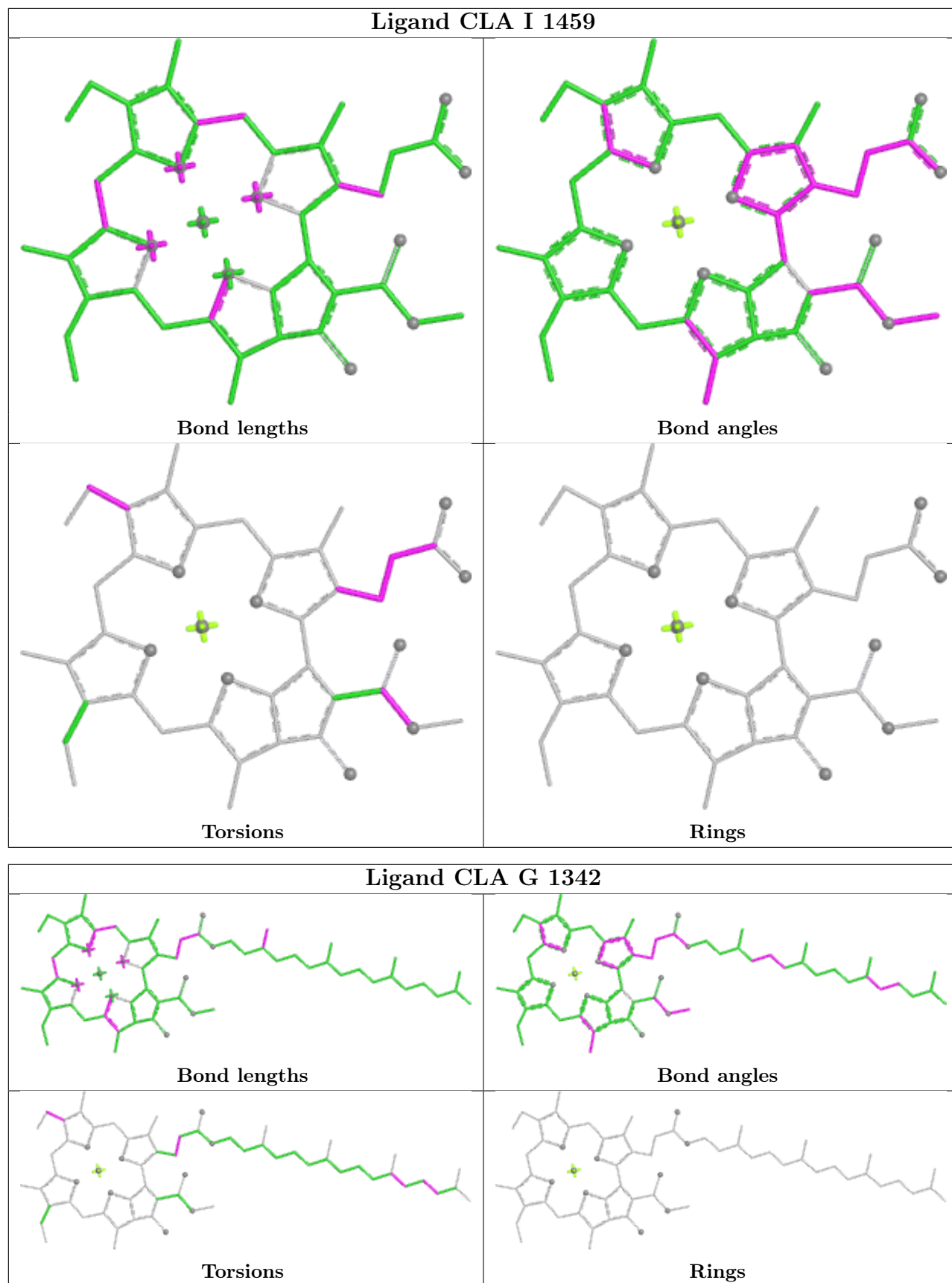
Bond angles



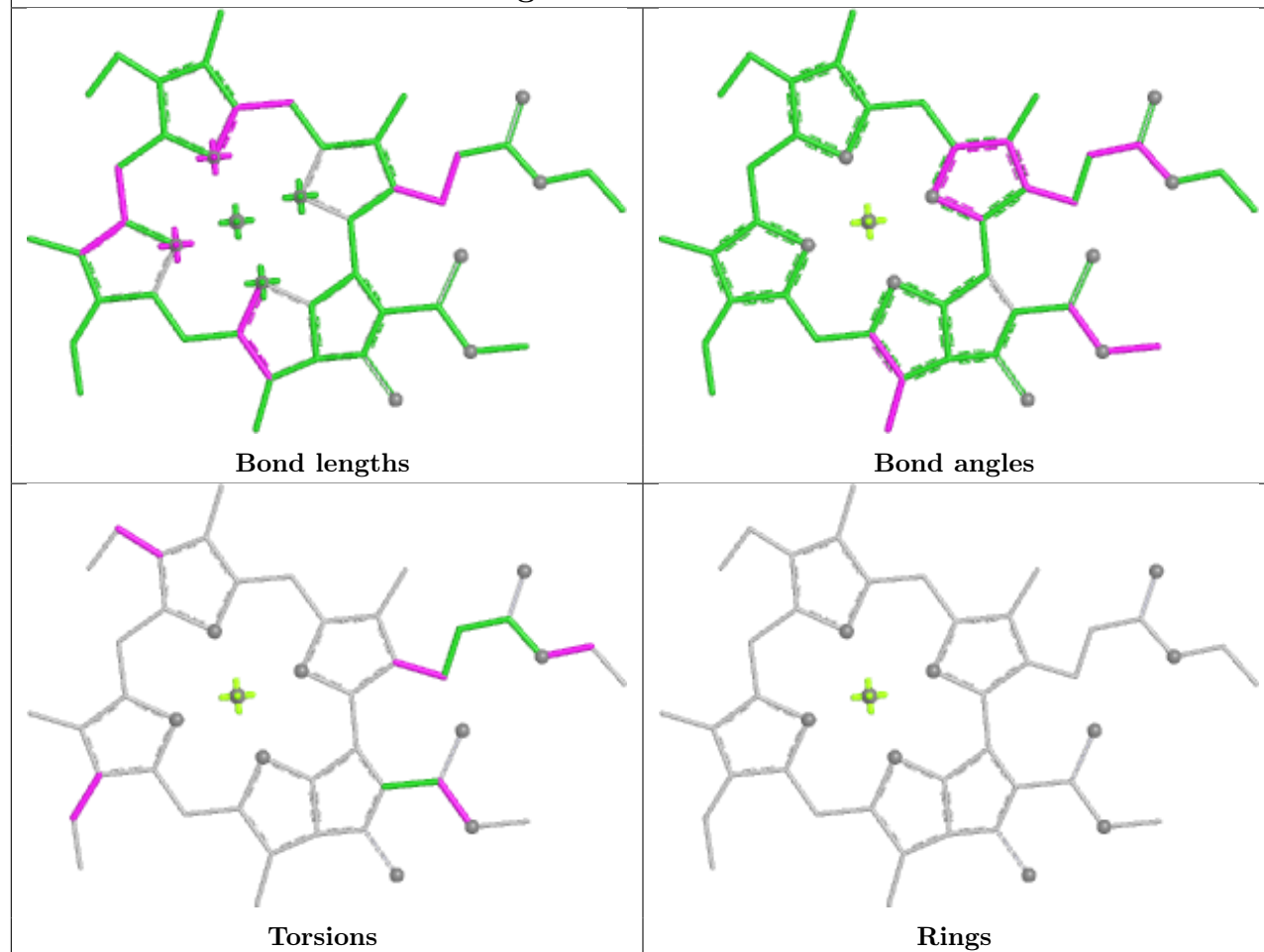
Torsions



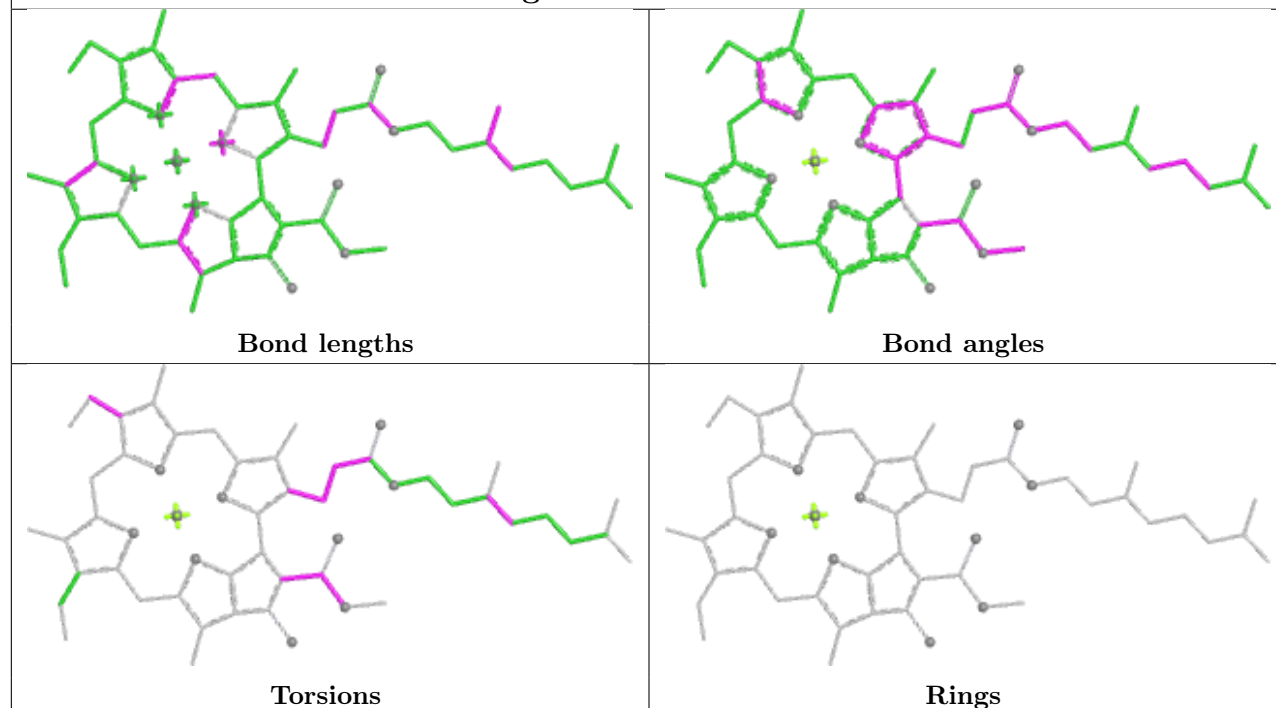
Rings



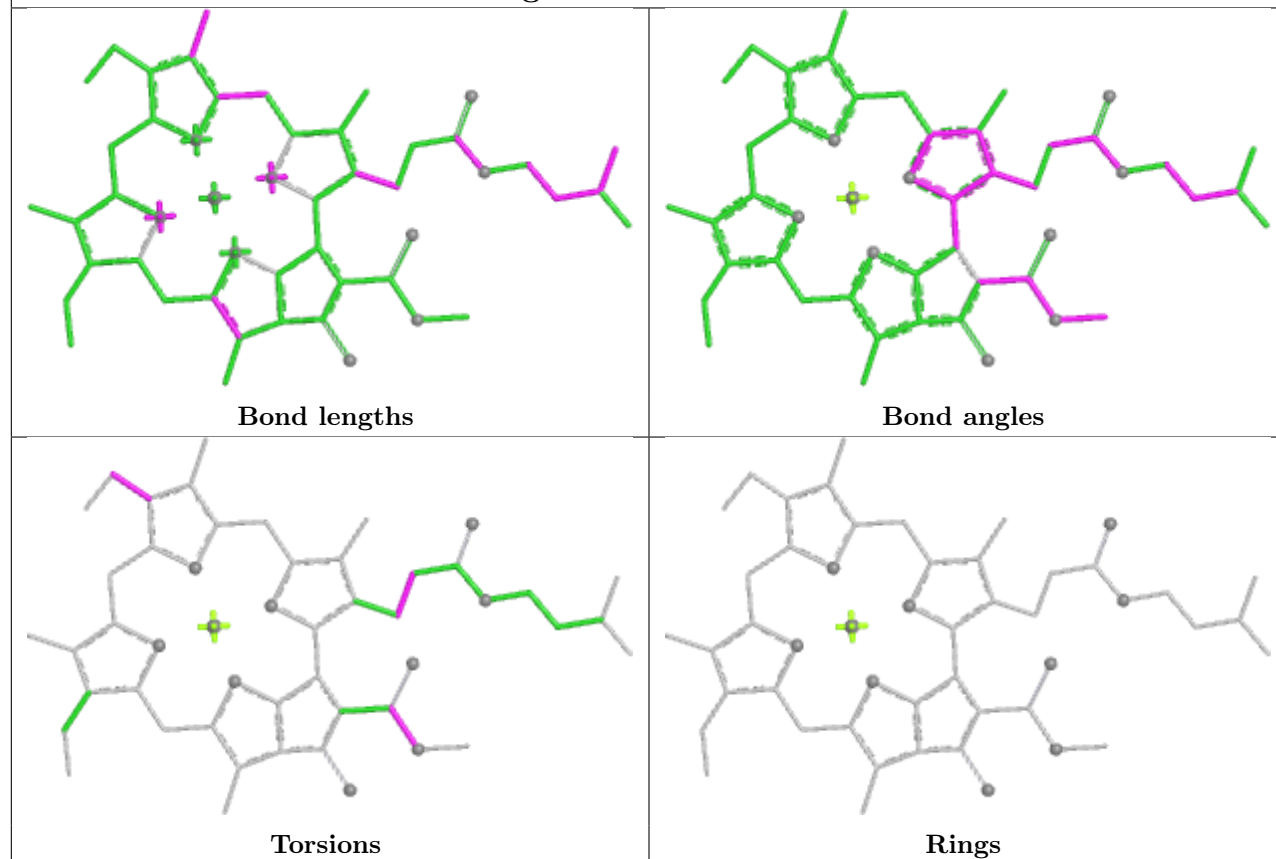
Ligand CLA H 1485



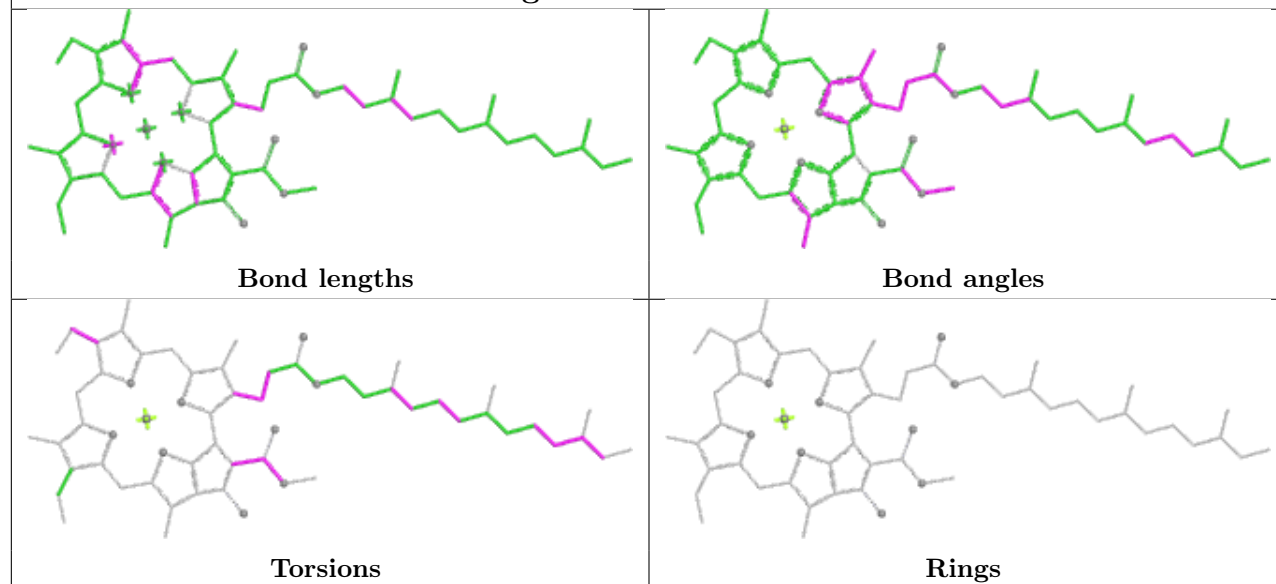
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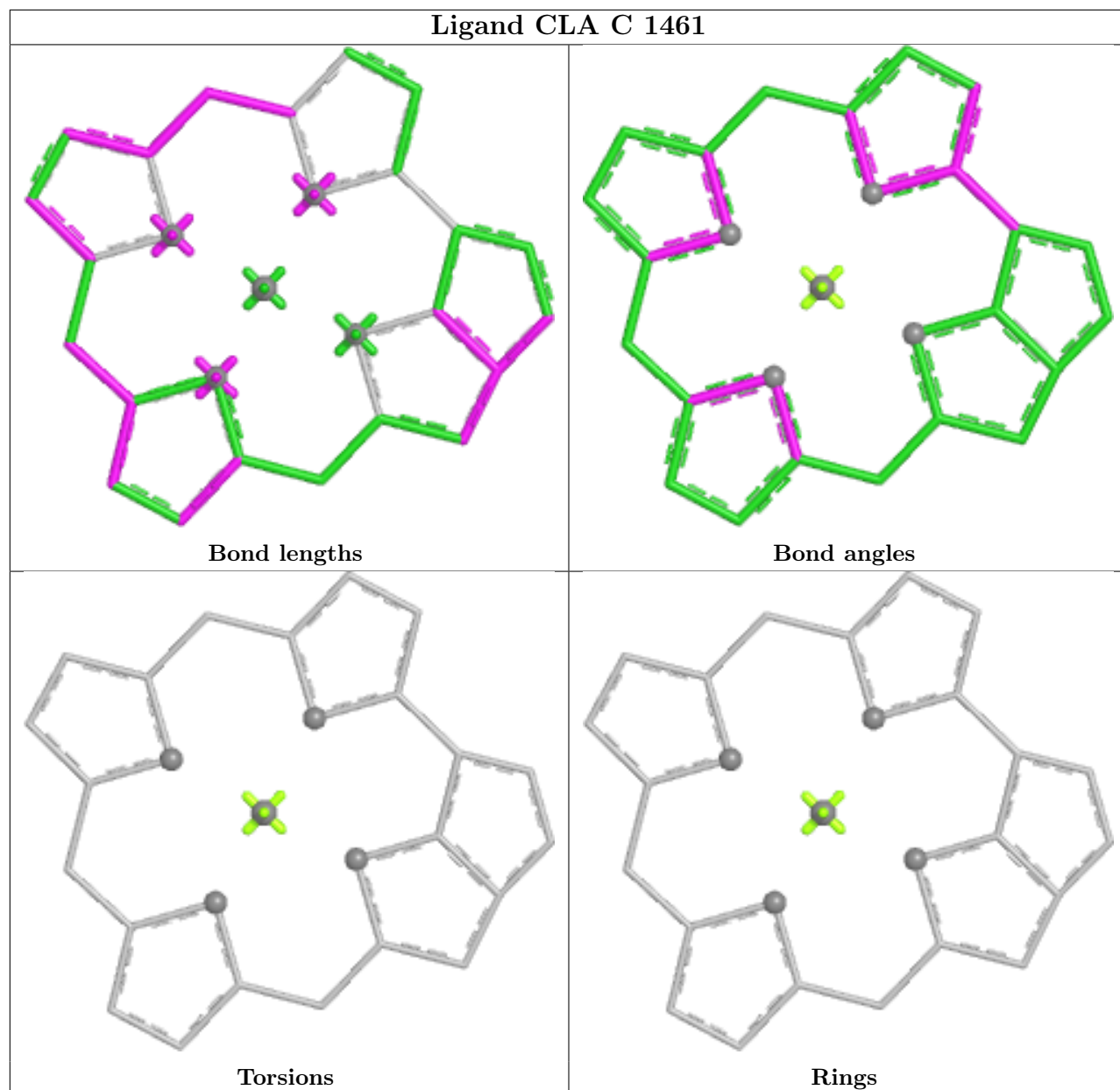
Ligand CLA D 1353



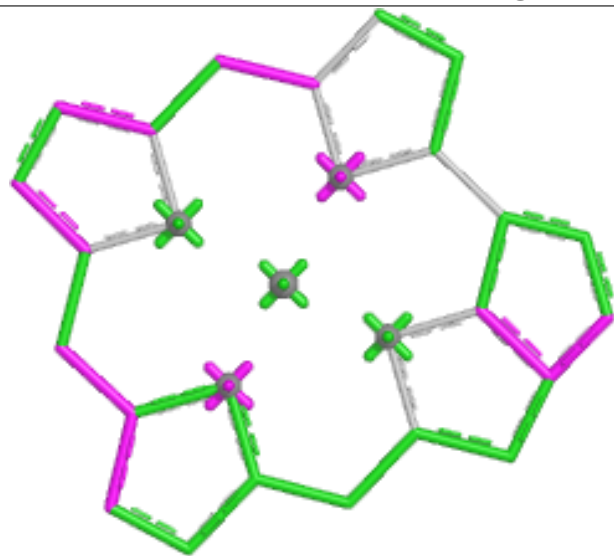
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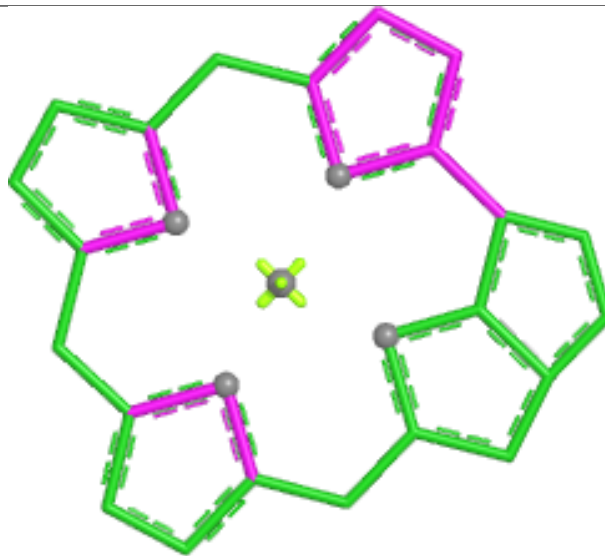
Ligand CLA C 1461



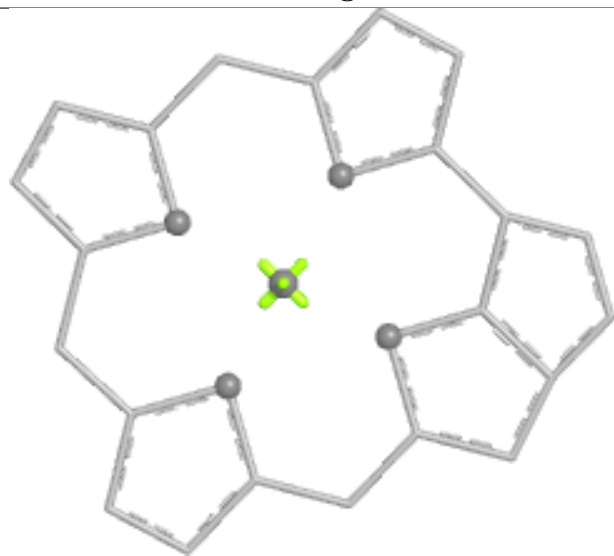
Ligand CLA I 1468



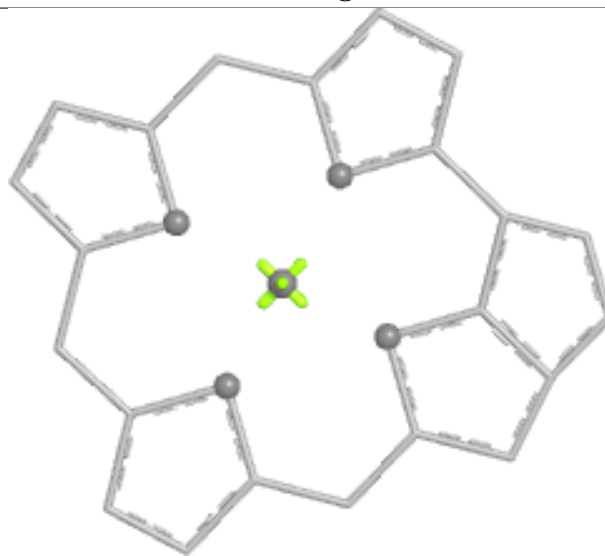
Bond lengths



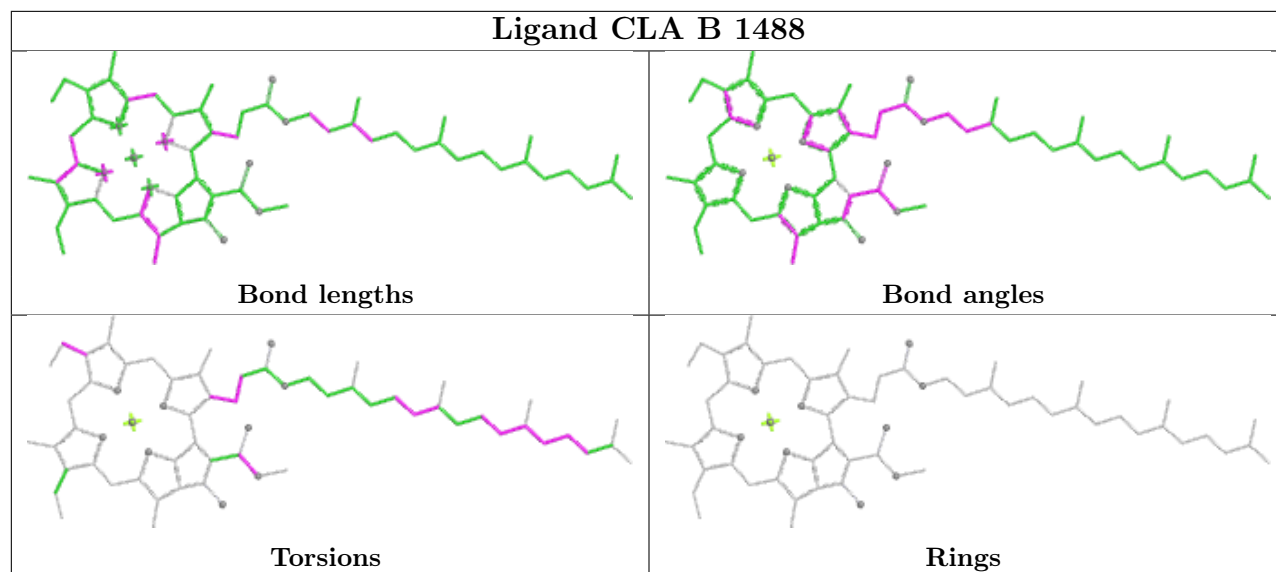
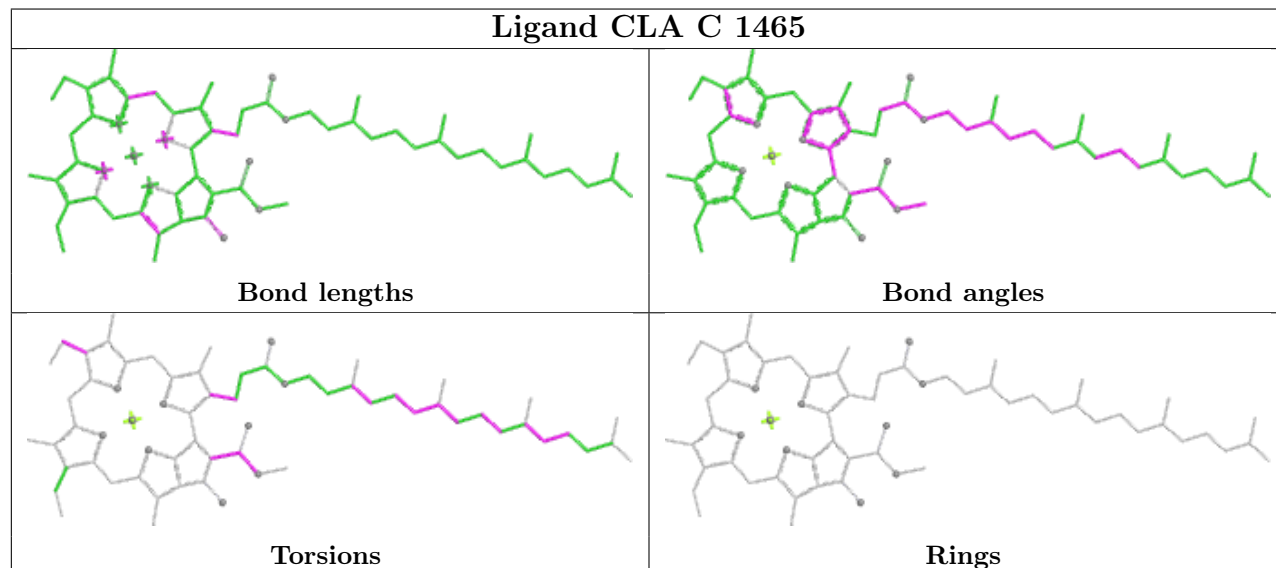
Bond angles



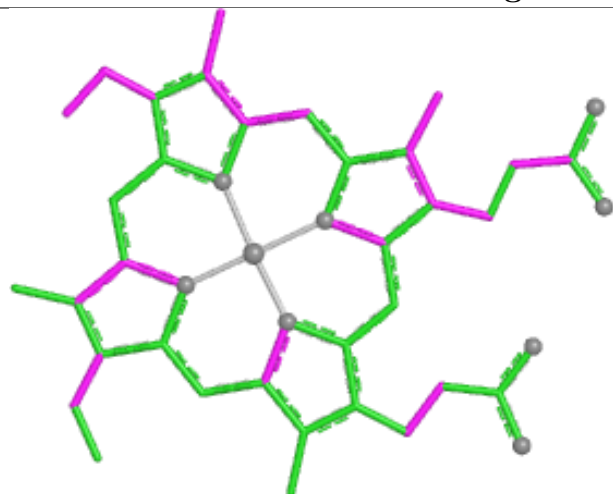
Torsions



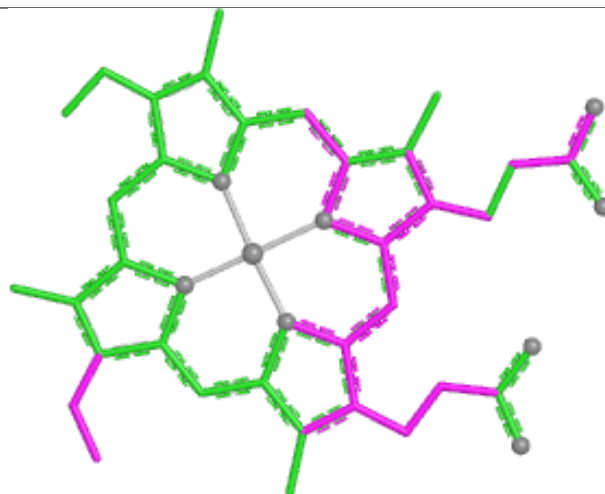
Rings

Ligand CLA B 1488**Ligand CLA C 1465**

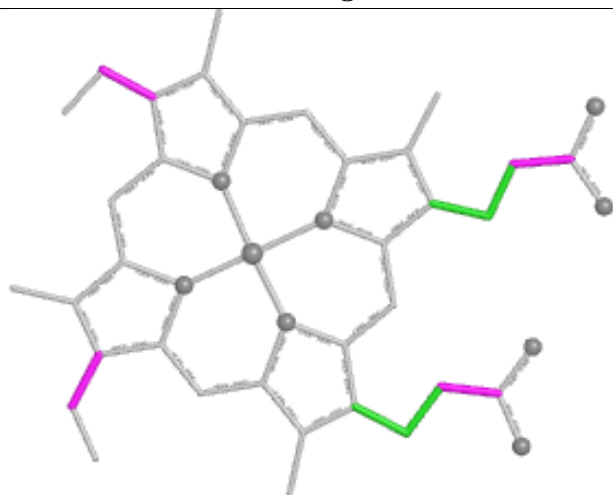
Ligand HEC T 1138



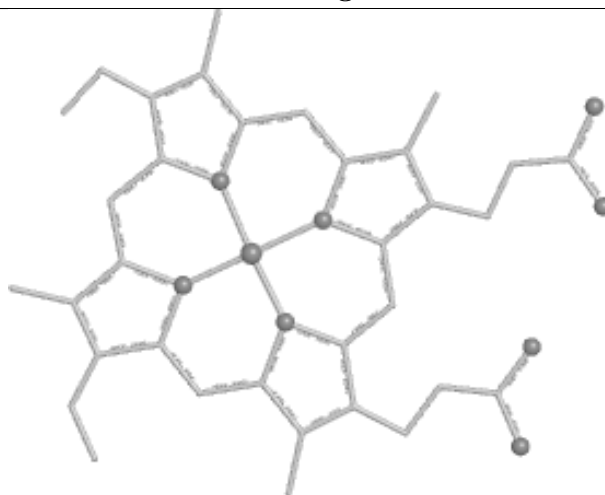
Bond lengths



Bond angles

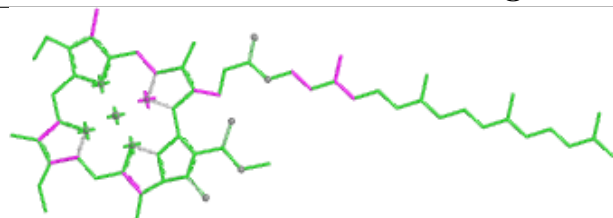


Torsions

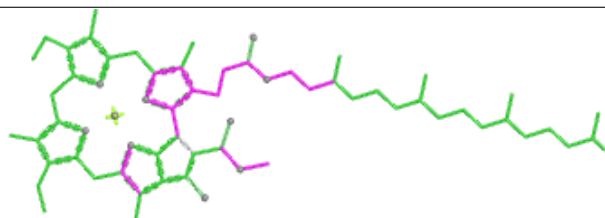


Rings

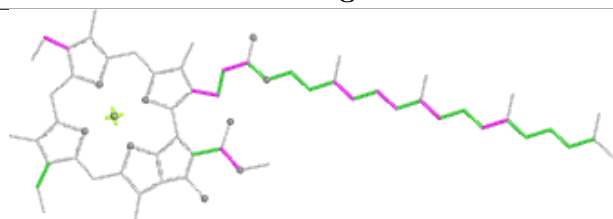
Ligand CLA H 1482



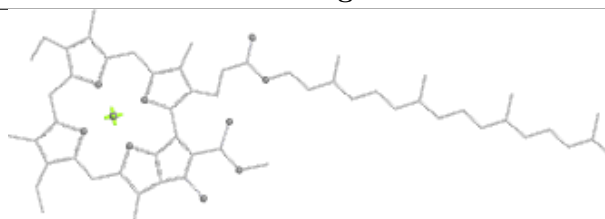
Bond lengths



Bond angles

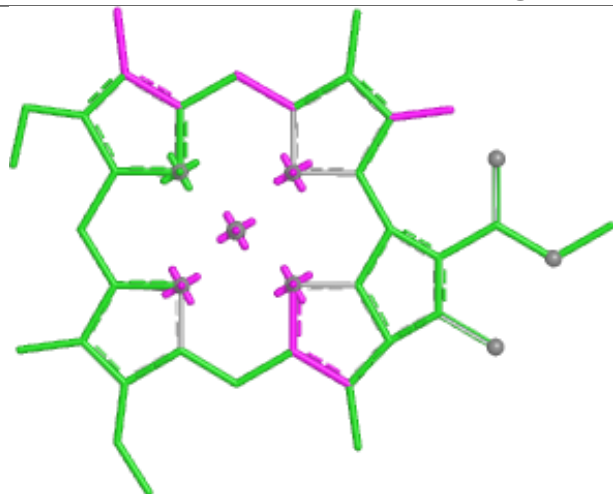


Torsions

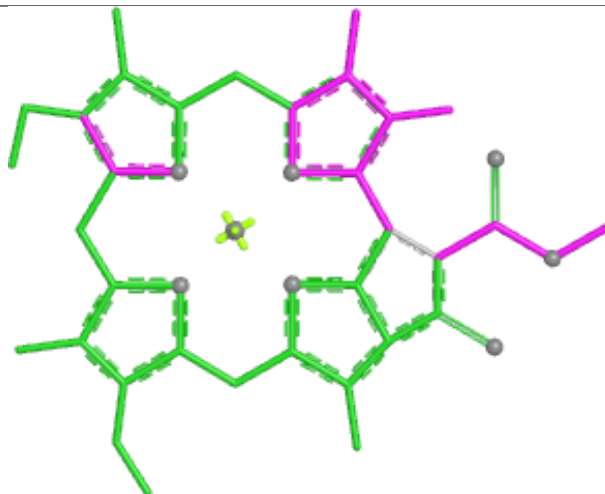


Rings

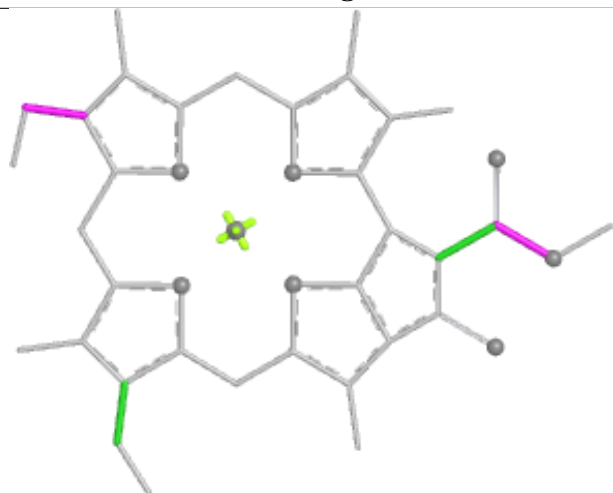
Ligand CLA I 1470



Bond lengths



Bond angles

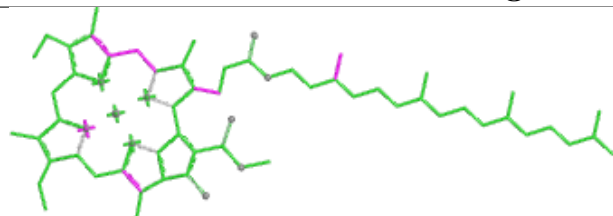


Torsions

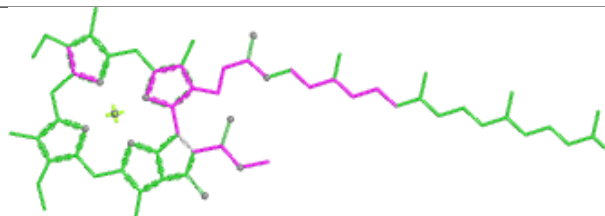


Rings

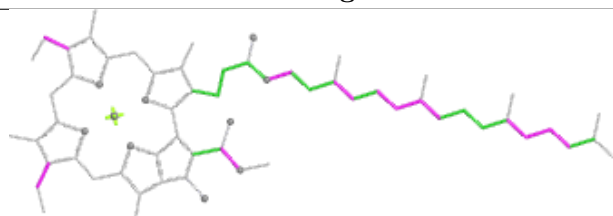
Ligand CLA B 1496



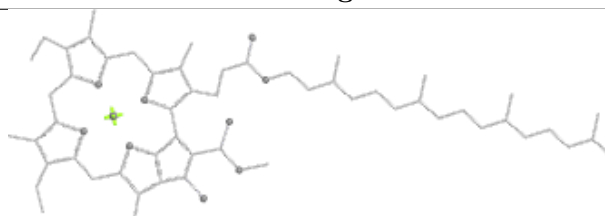
Bond lengths



Bond angles

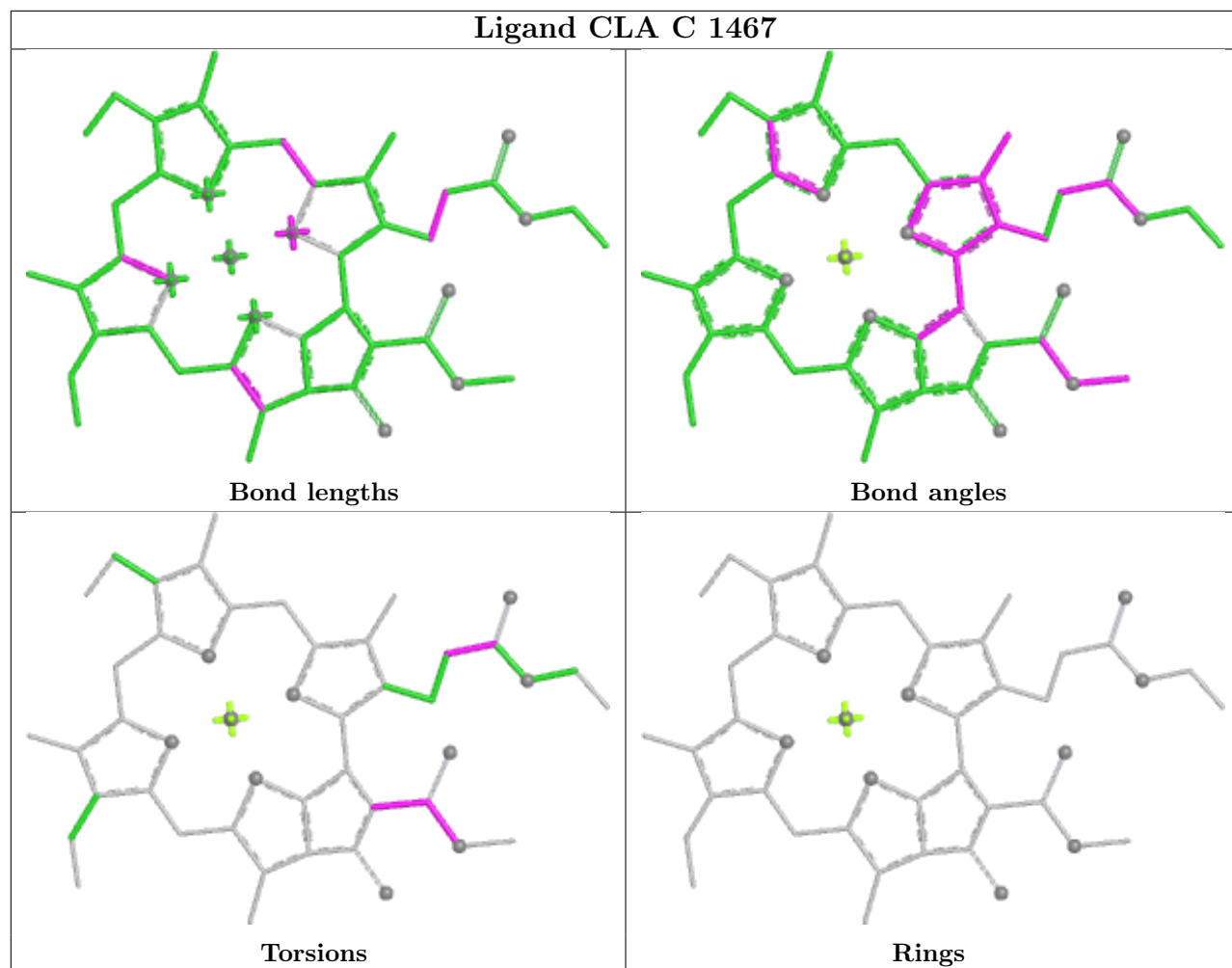


Torsions

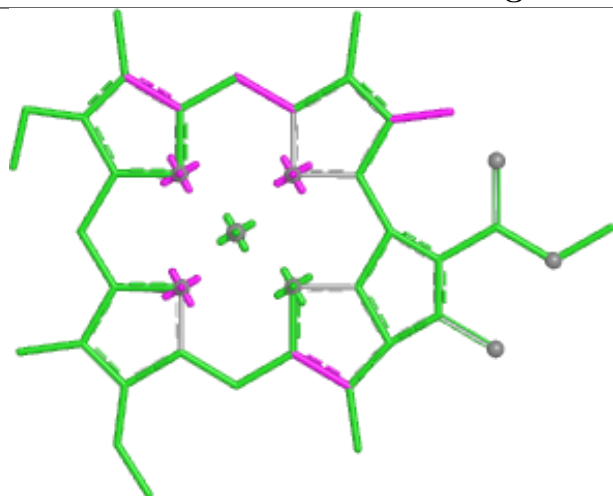


Rings

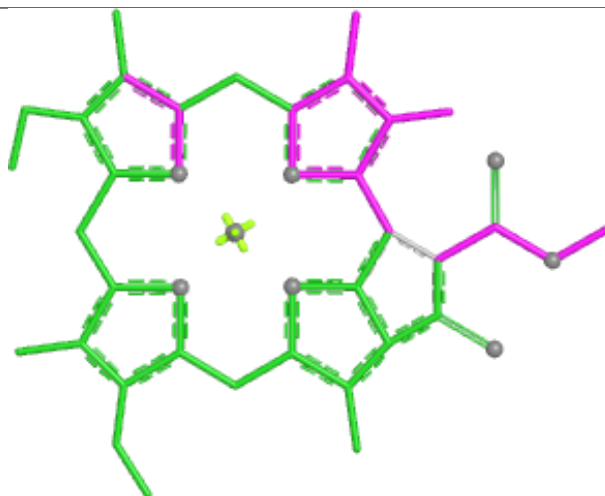
Ligand CLA C 1467



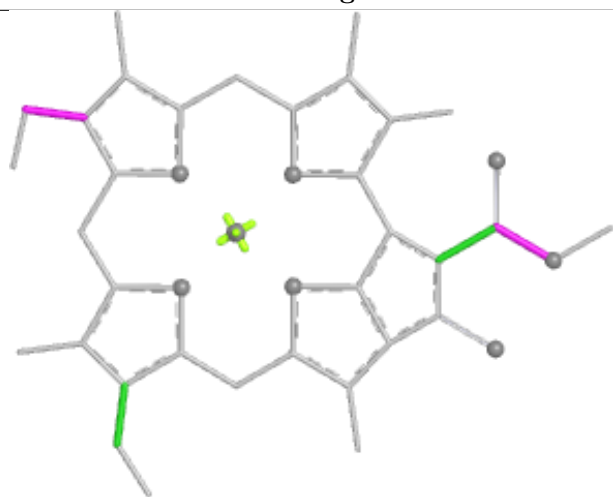
Ligand CLA C 1469



Bond lengths



Bond angles

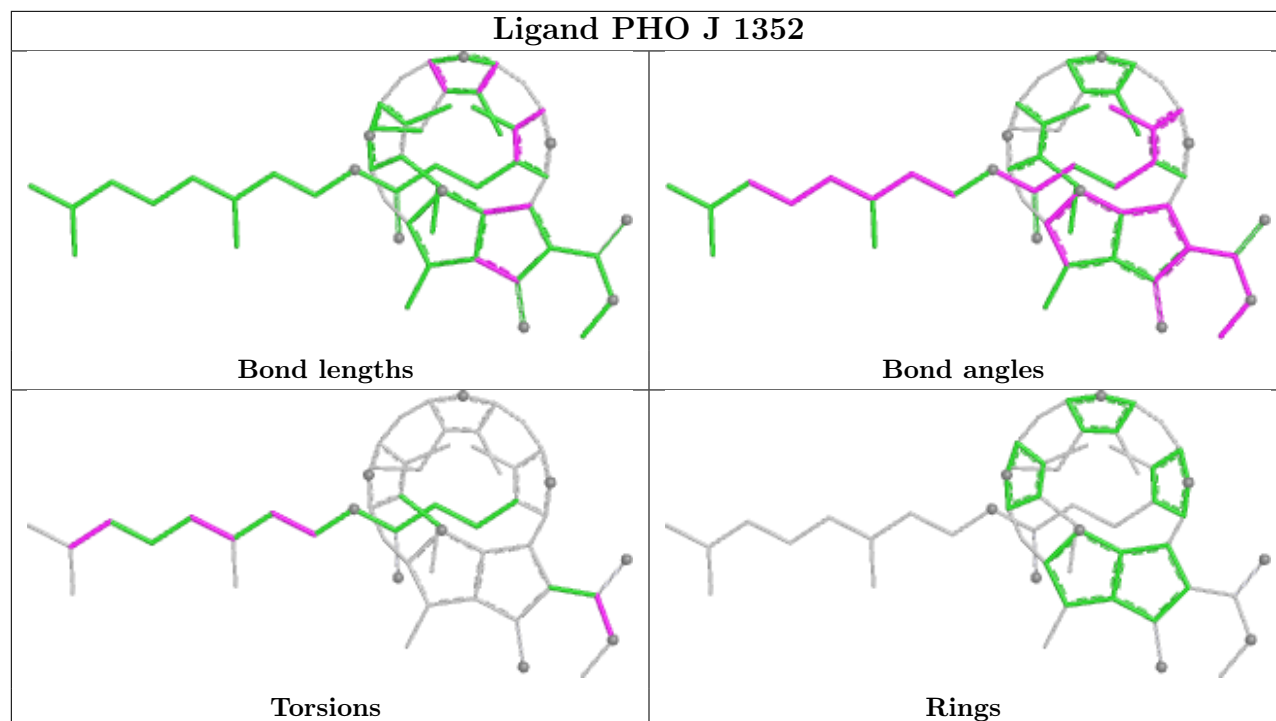


Torsions

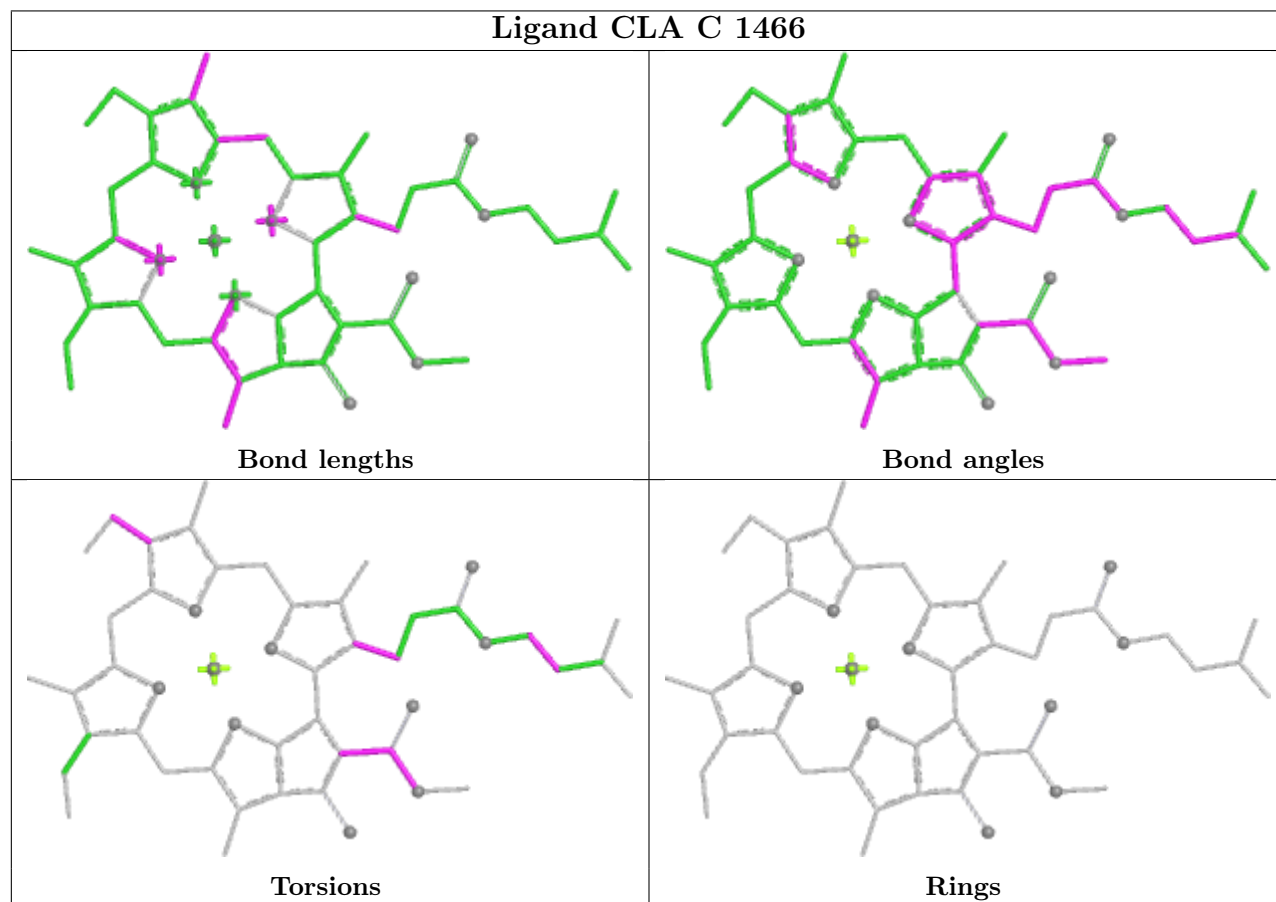


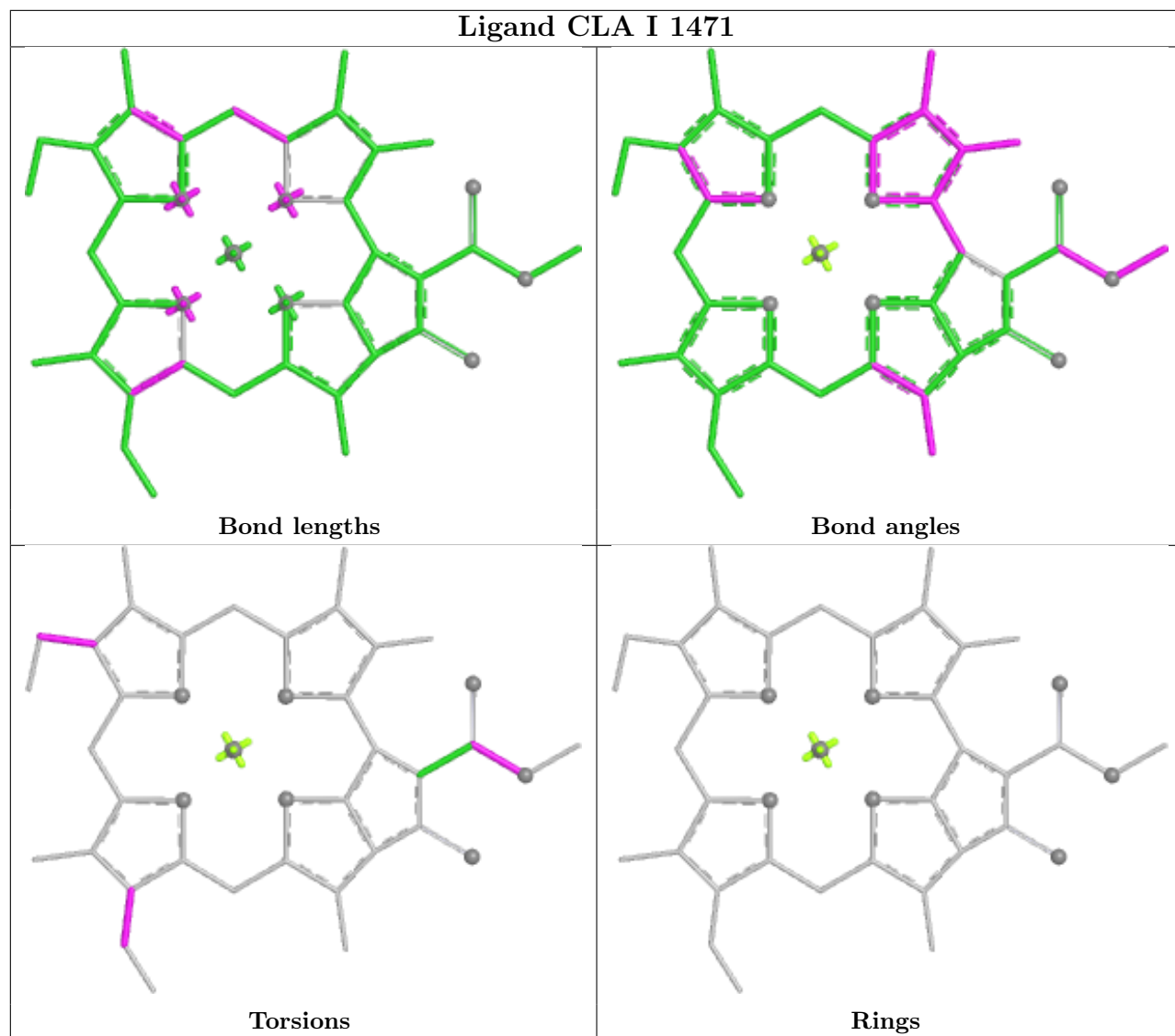
Rings

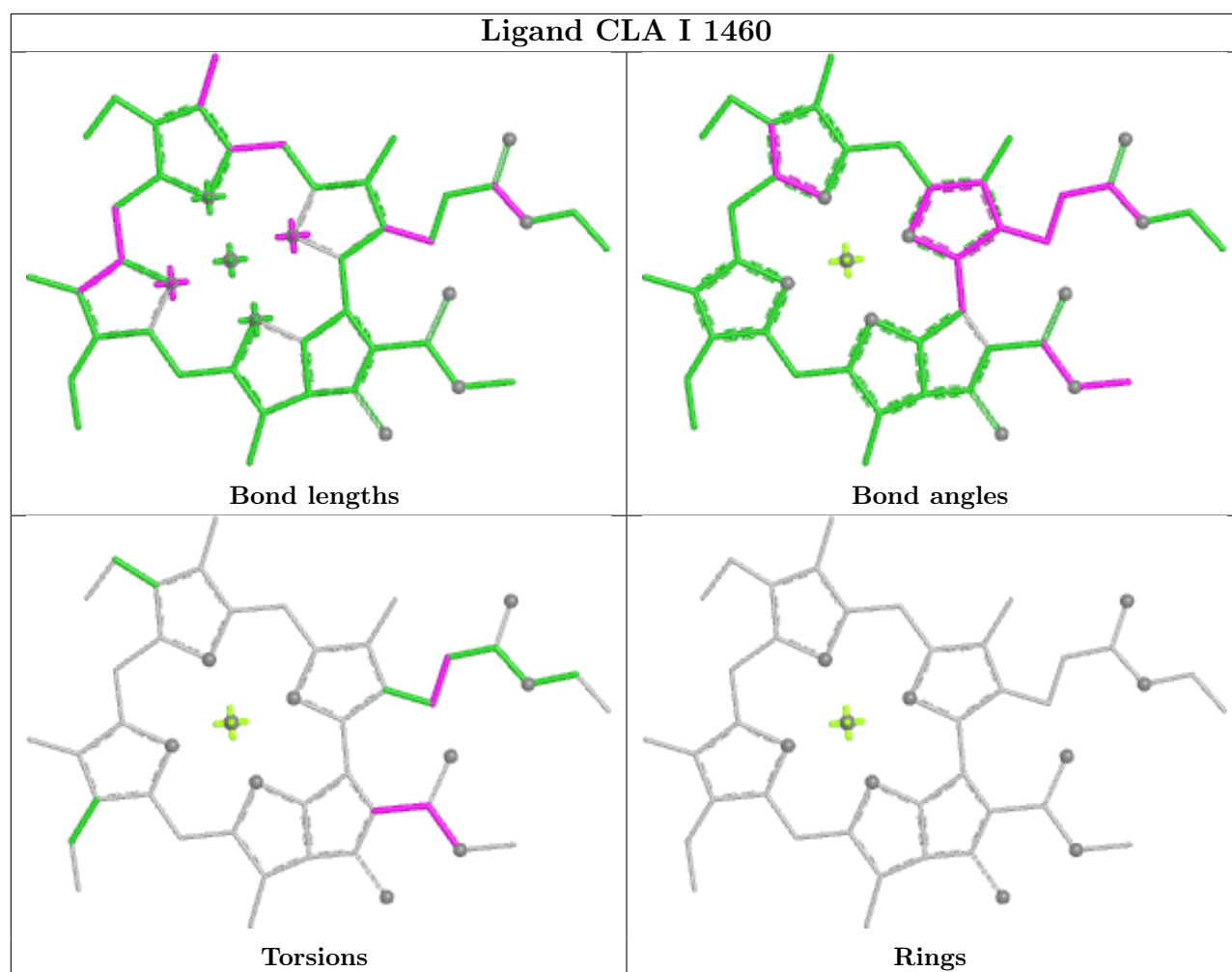
Ligand PHO J 1352



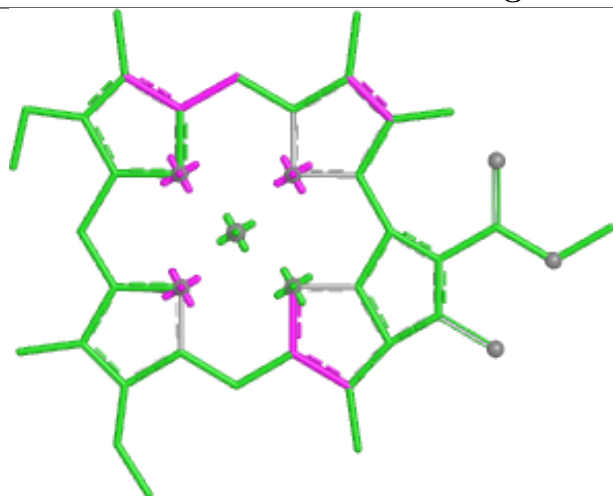
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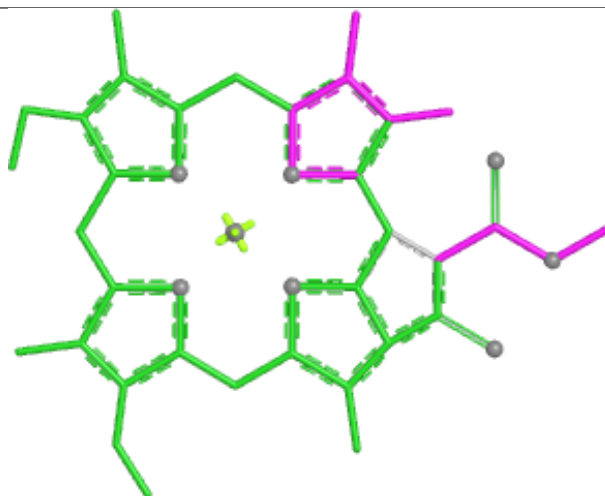




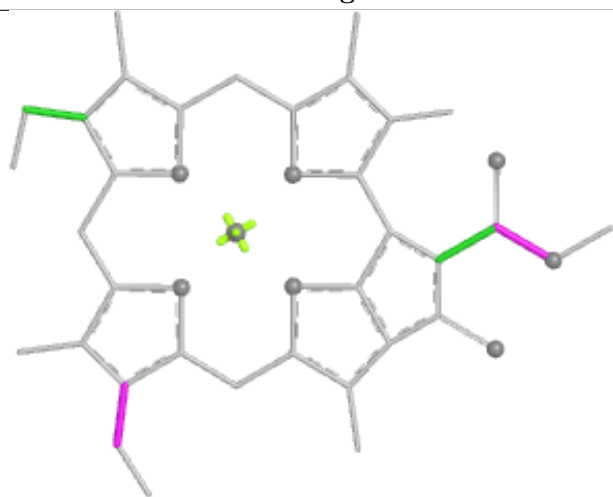
Ligand CLA H 1486



Bond lengths



Bond angles

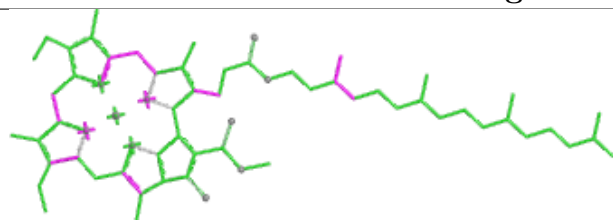


Torsions

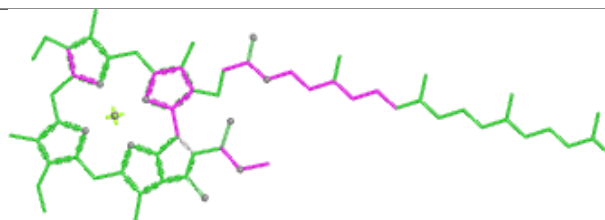


Rings

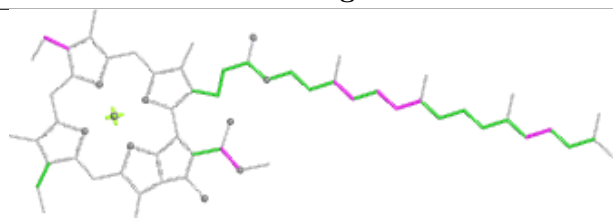
Ligand CLA B 1494



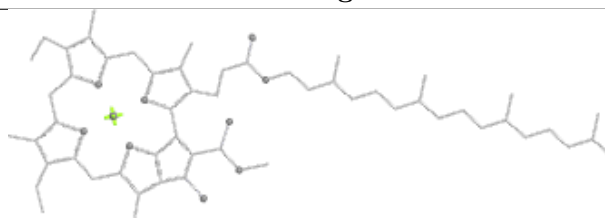
Bond lengths



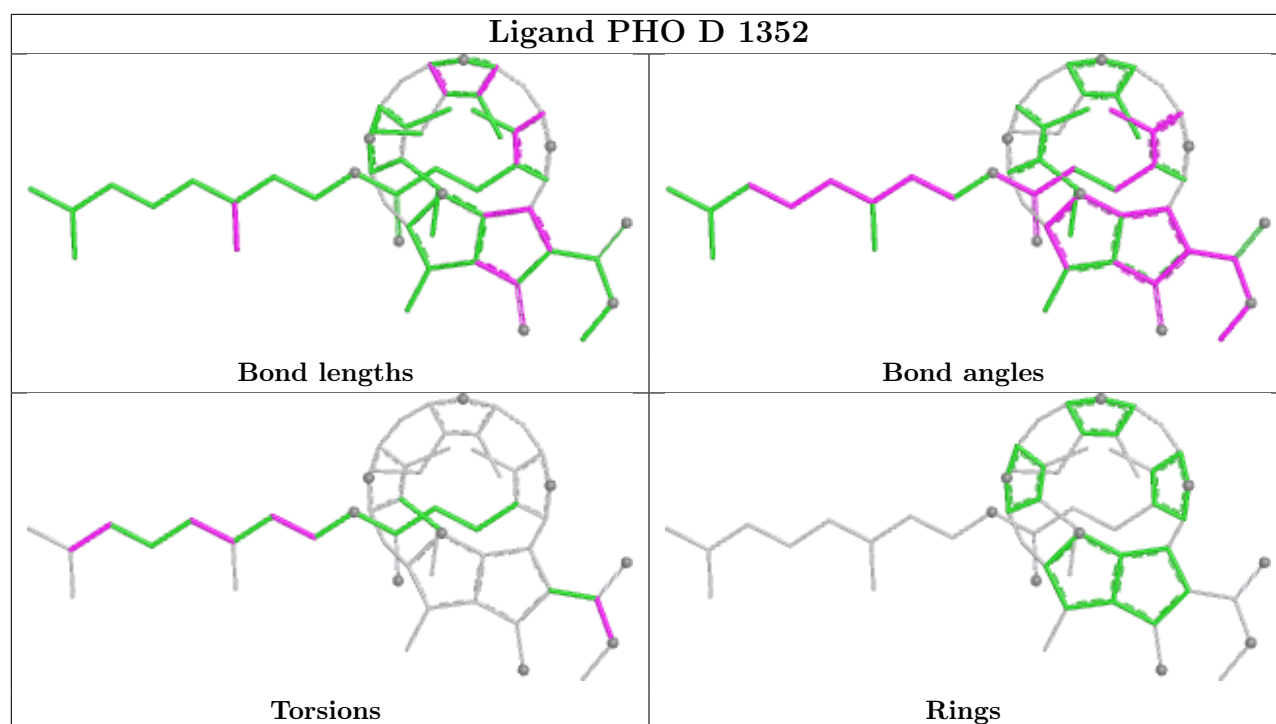
Bond angles

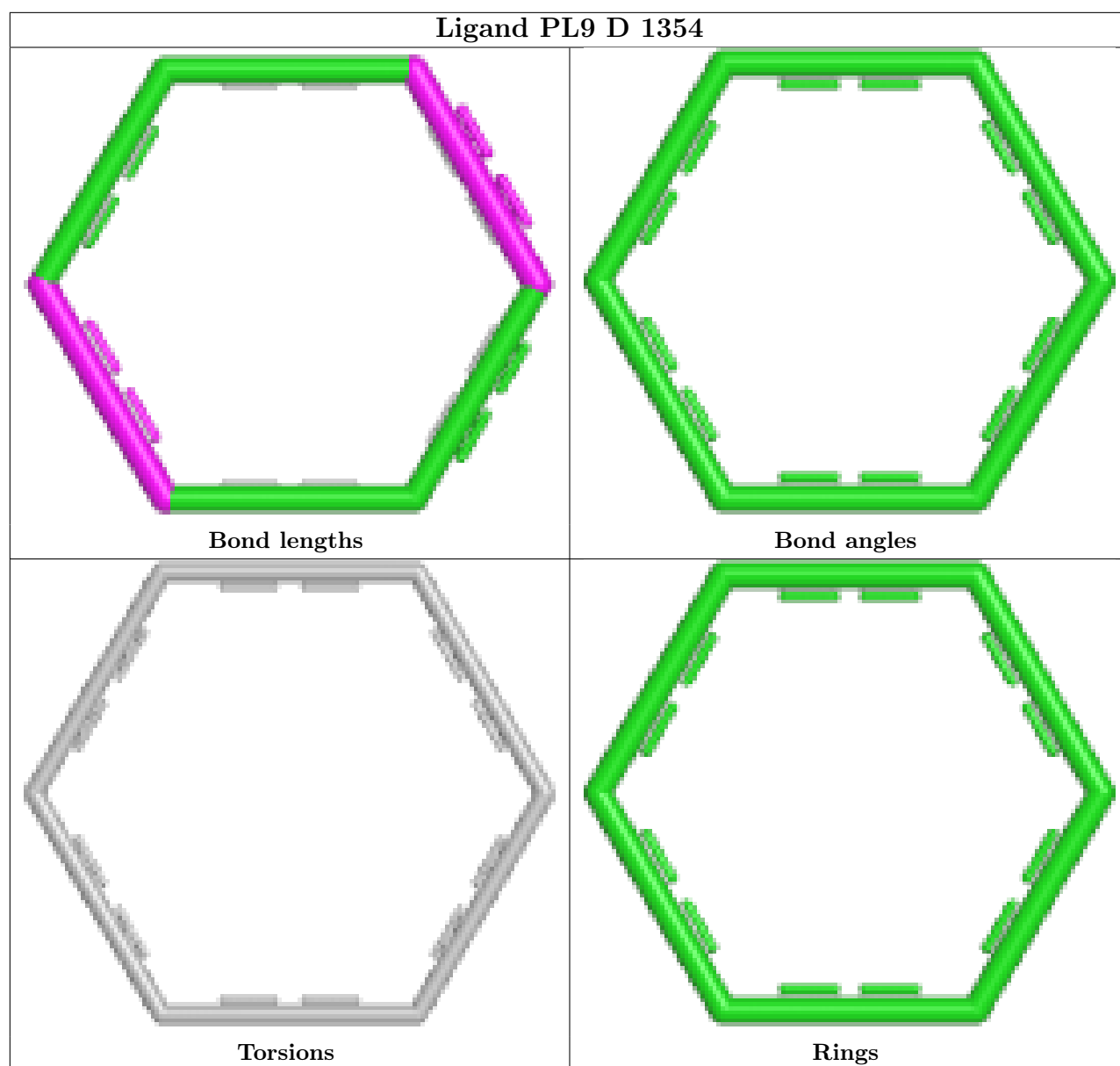


Torsions

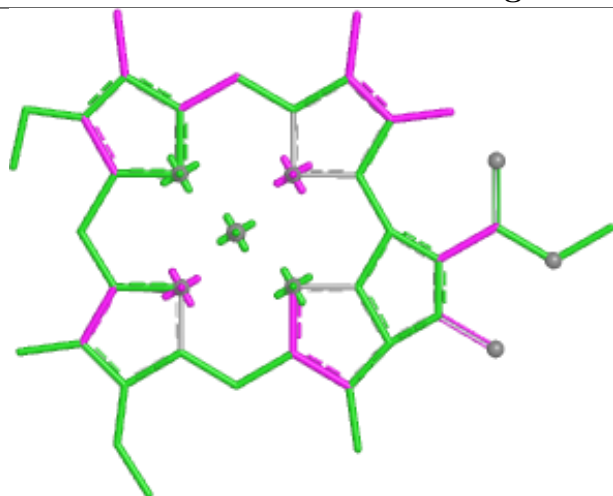


Rings

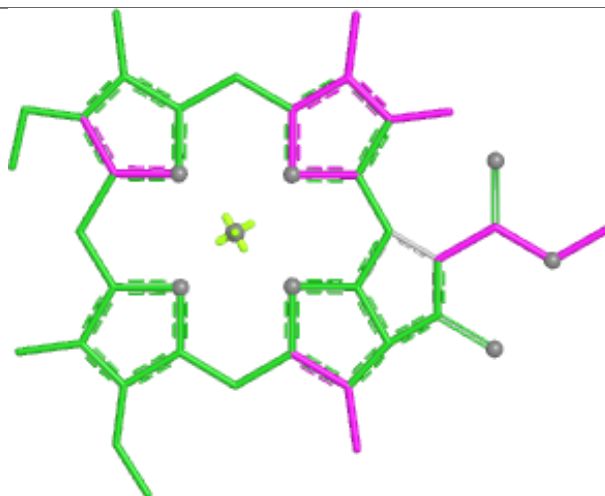




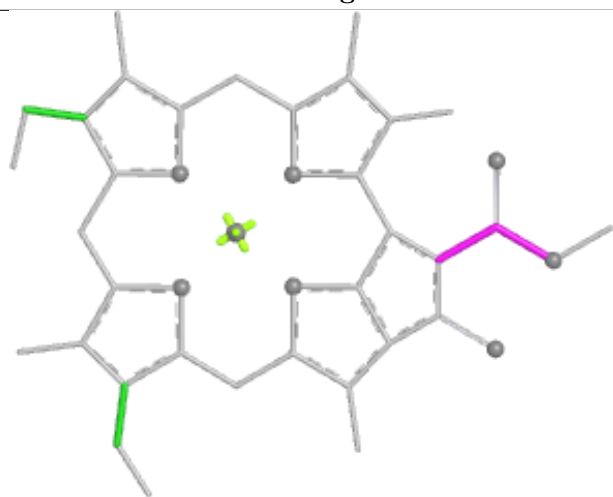
Ligand CLA H 1497



Bond lengths



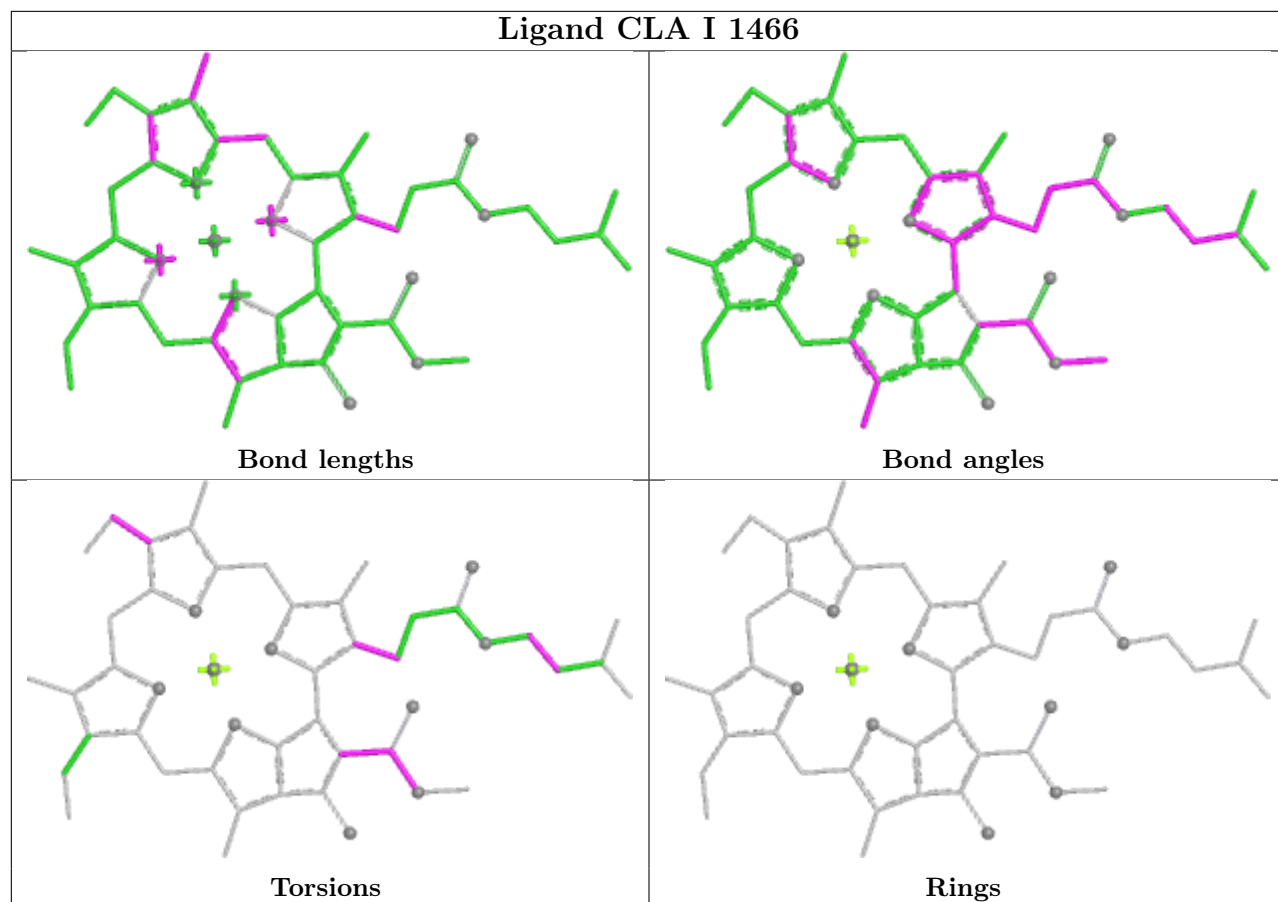
Bond angles

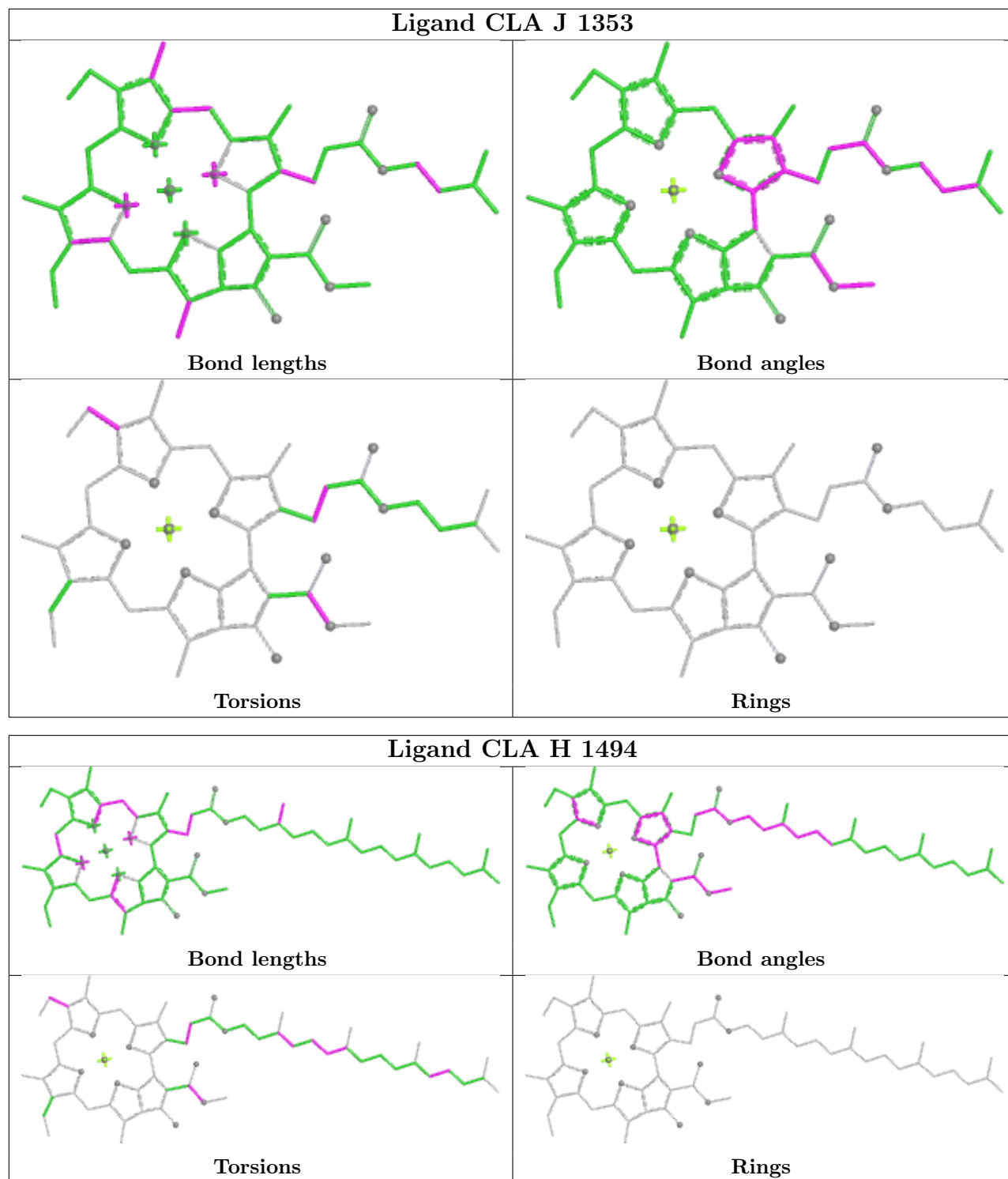


Torsions

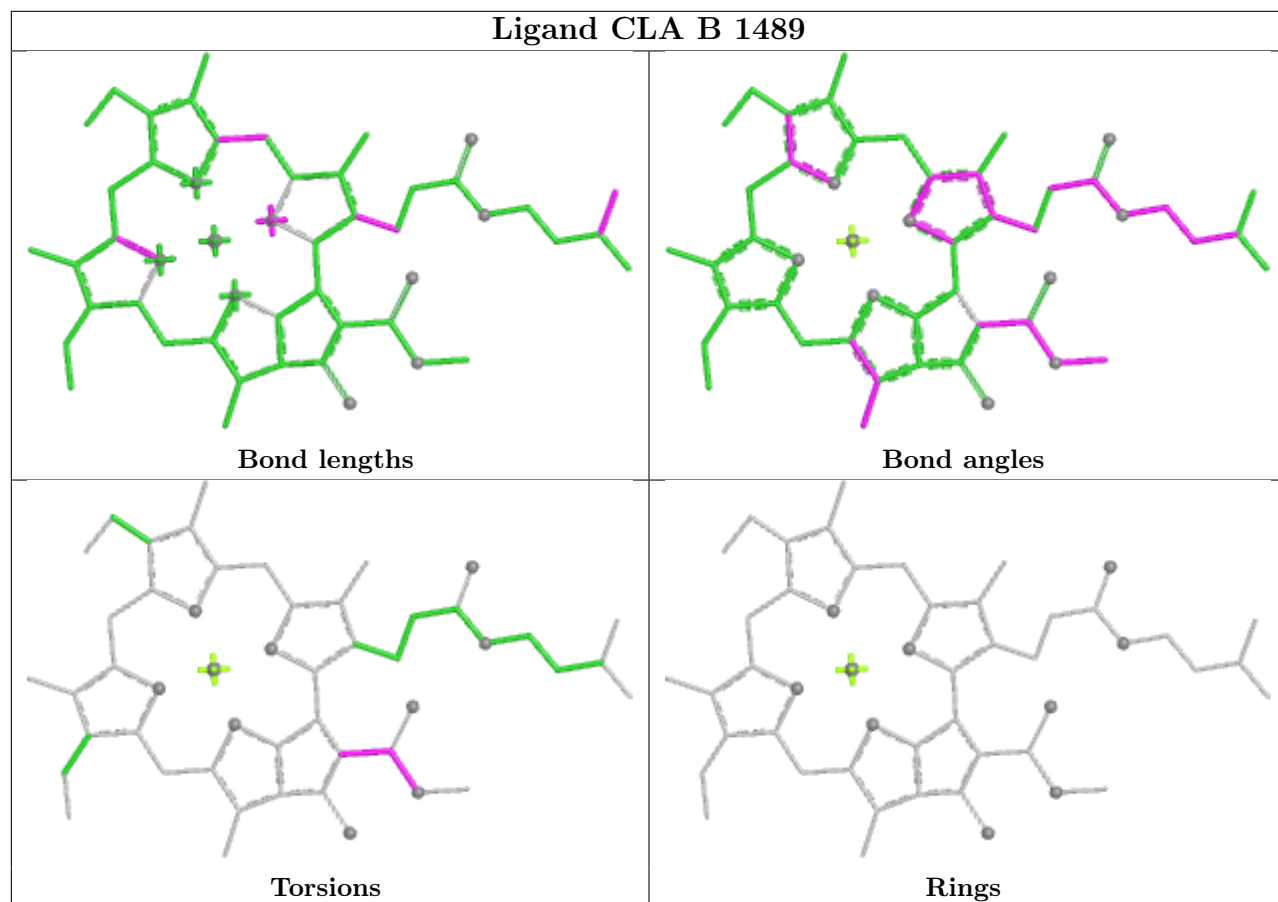


Rings

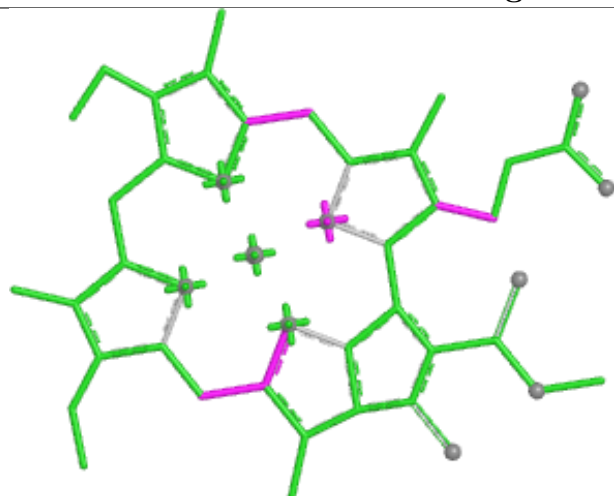




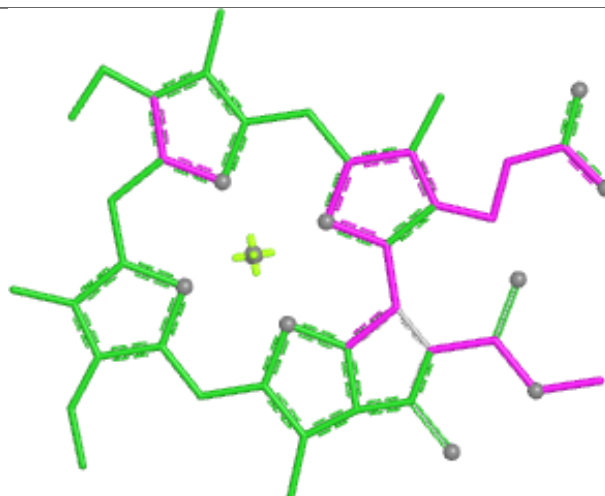
Ligand CLA B 1489



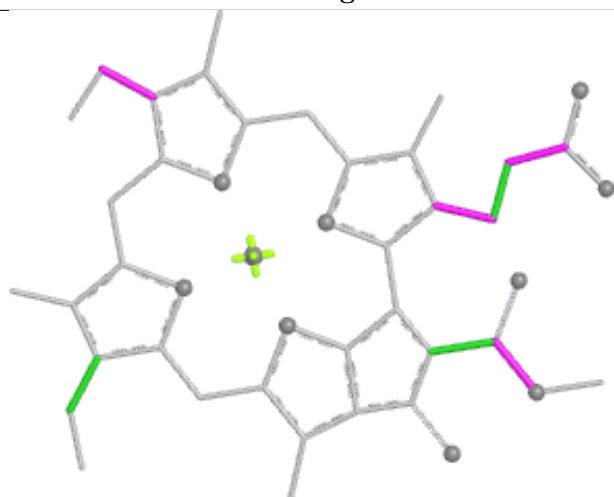
Ligand CLA B 1493



Bond lengths



Bond angles

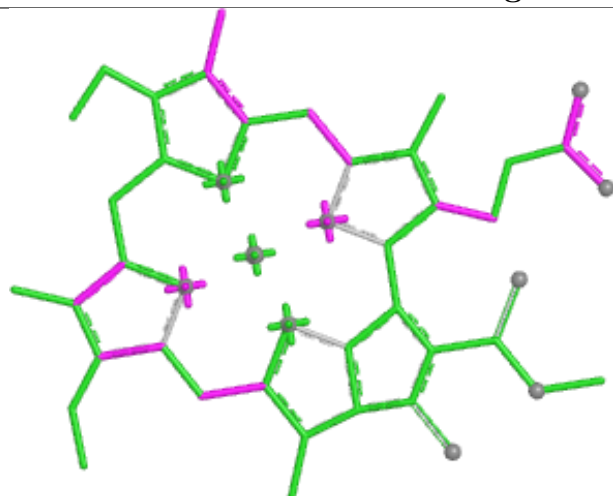


Torsions

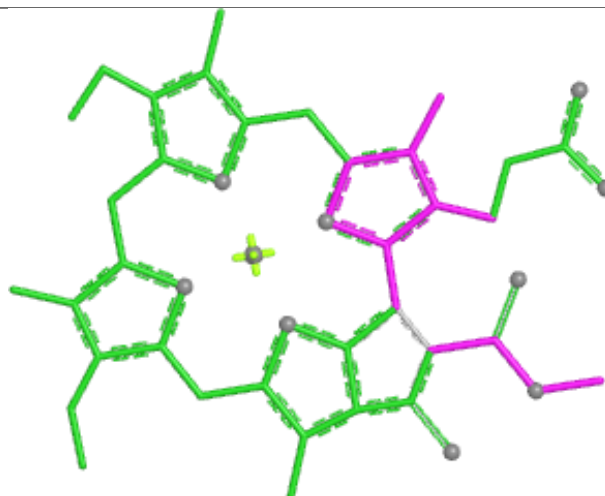


Rings

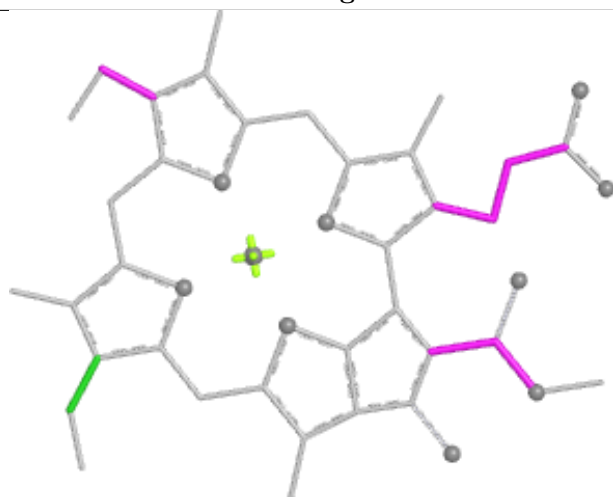
Ligand CLA H 1490



Bond lengths



Bond angles

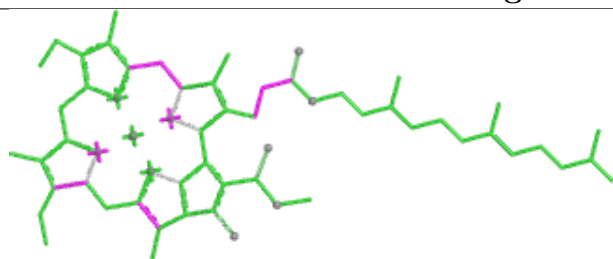


Torsions

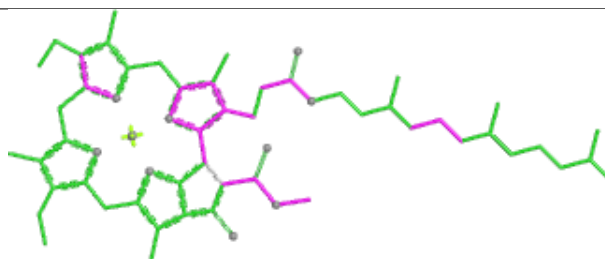


Rings

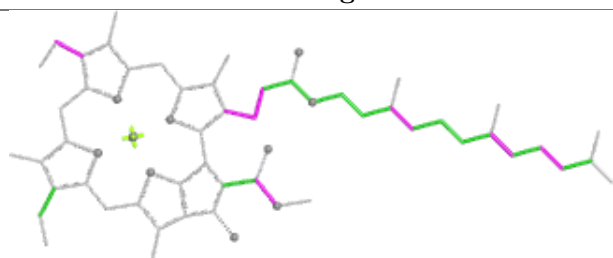
Ligand CLA H 1483



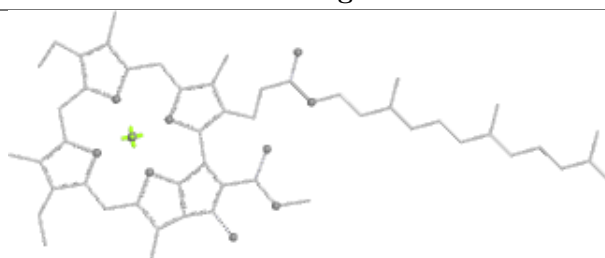
Bond lengths



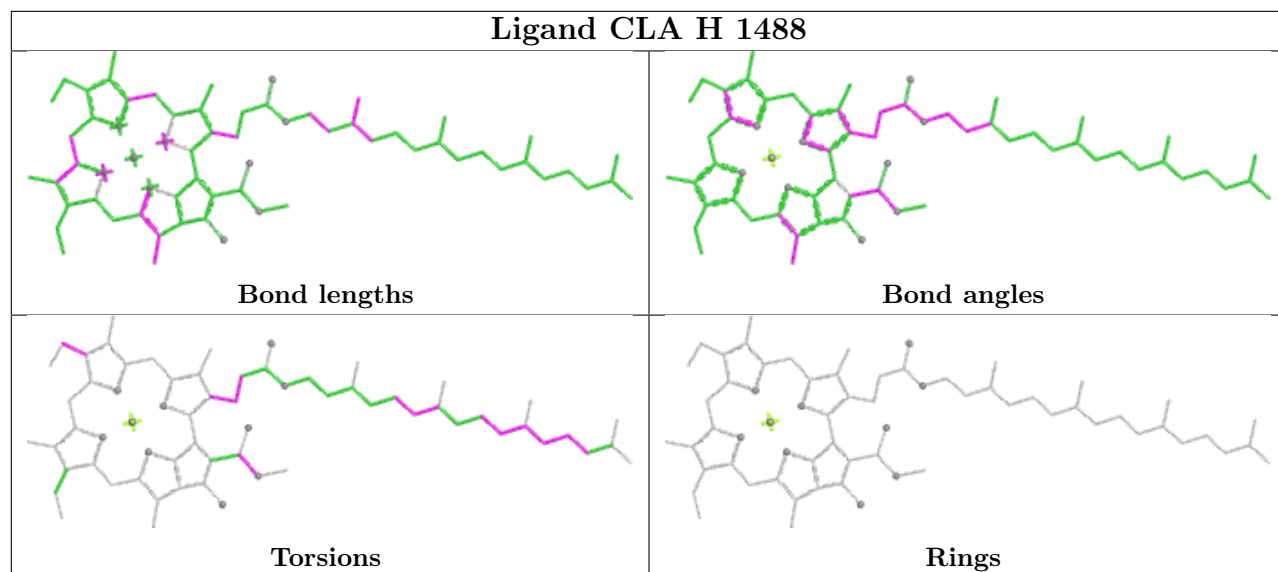
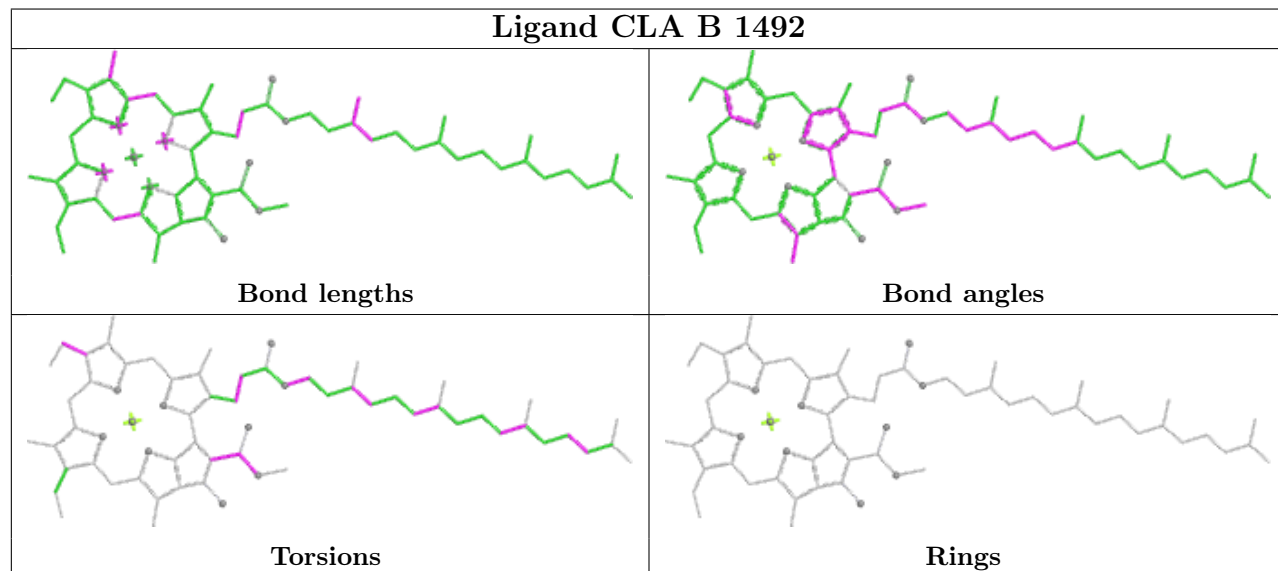
Bond angles



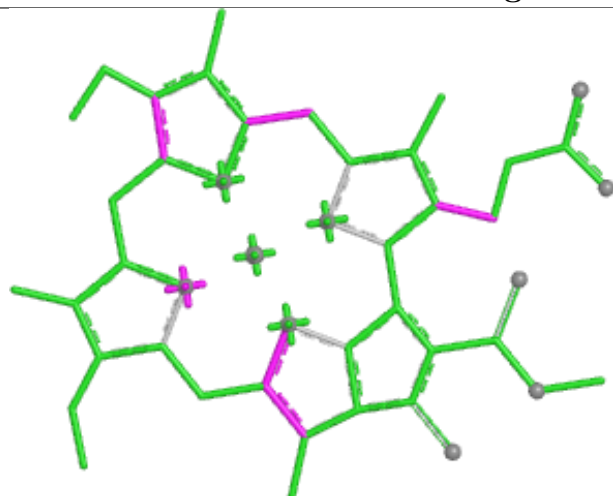
Torsions



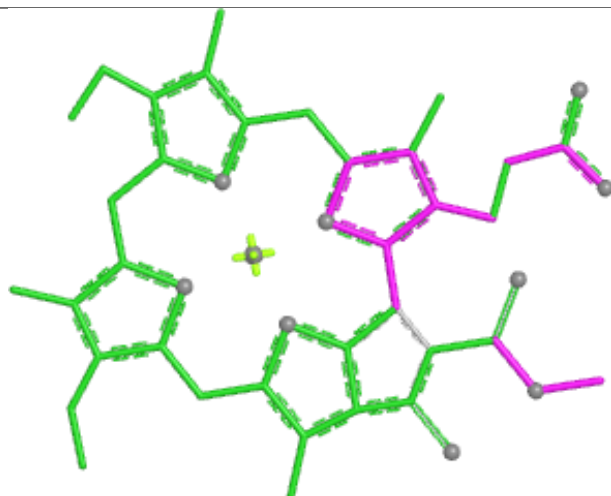
Rings

Ligand CLA H 1488**Ligand CLA B 1492**

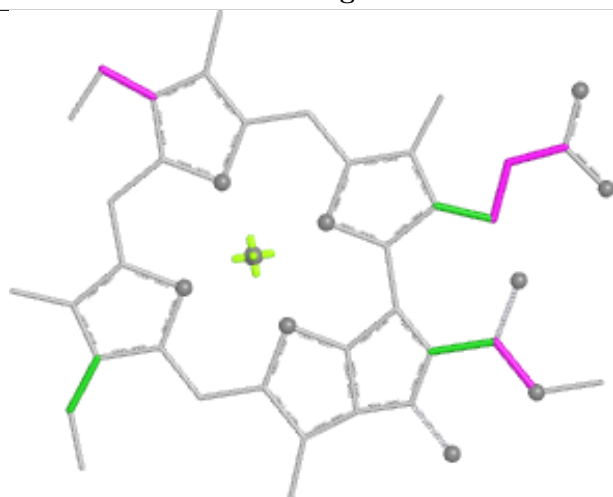
Ligand CLA H 1484



Bond lengths



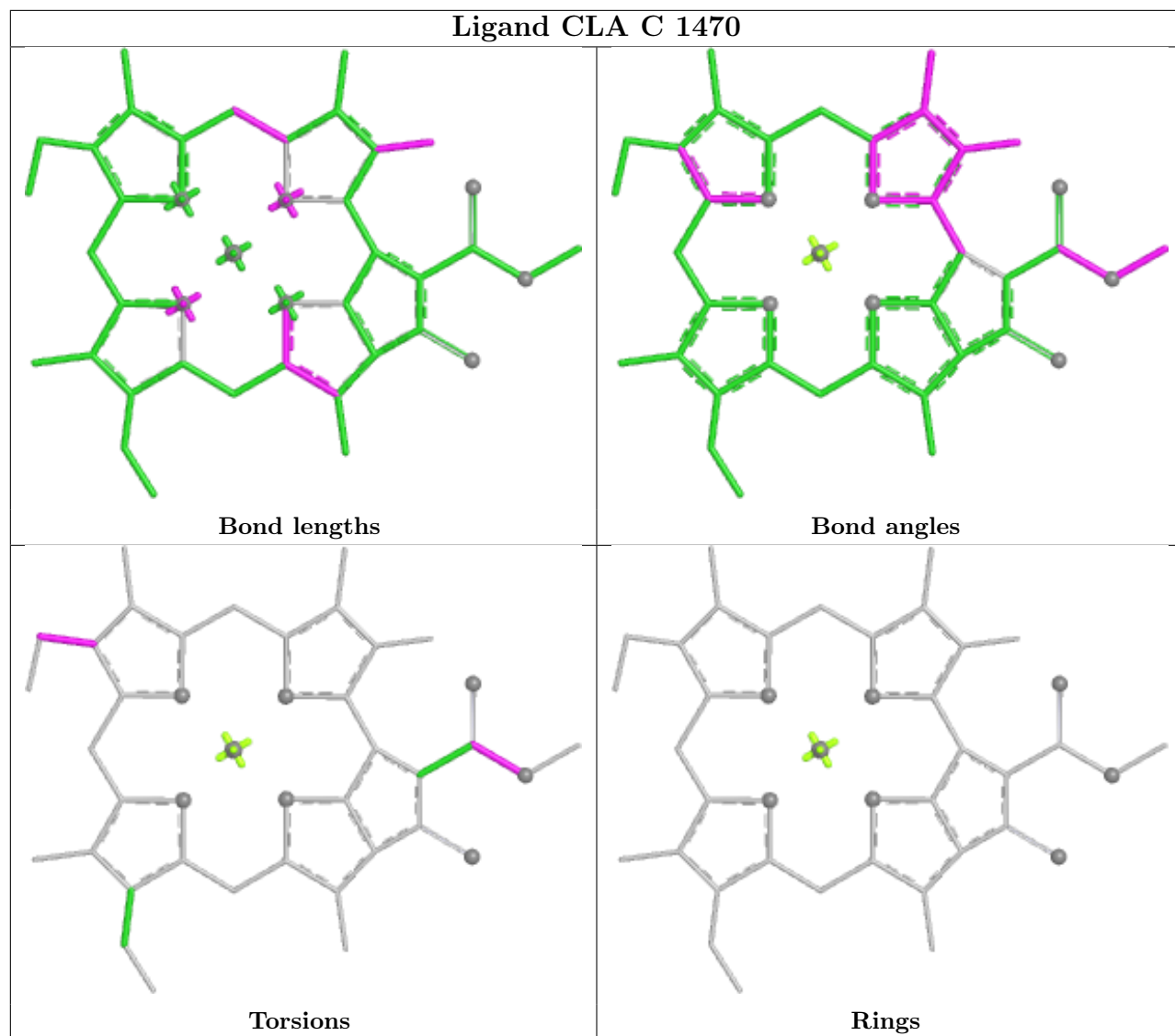
Bond angles



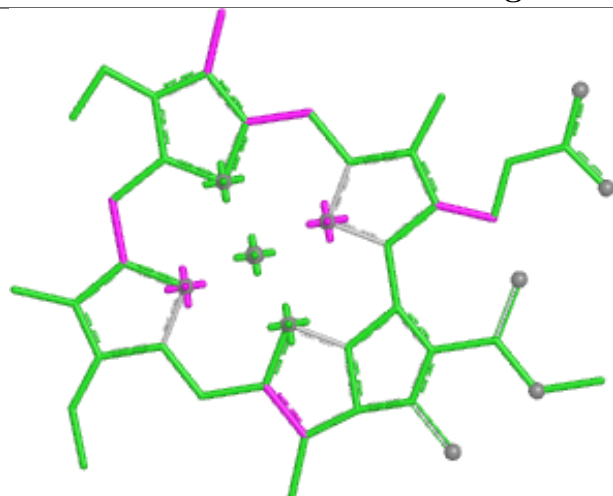
Torsions



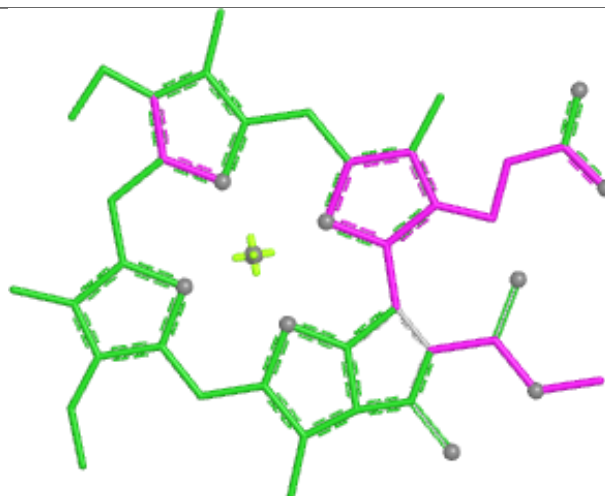
Rings



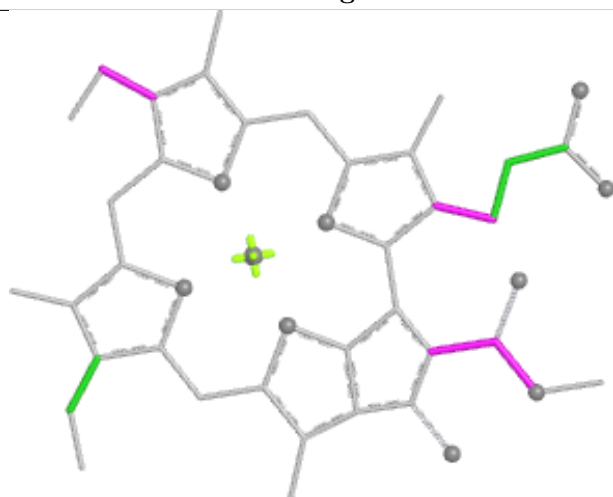
Ligand CLA A 1344



Bond lengths



Bond angles

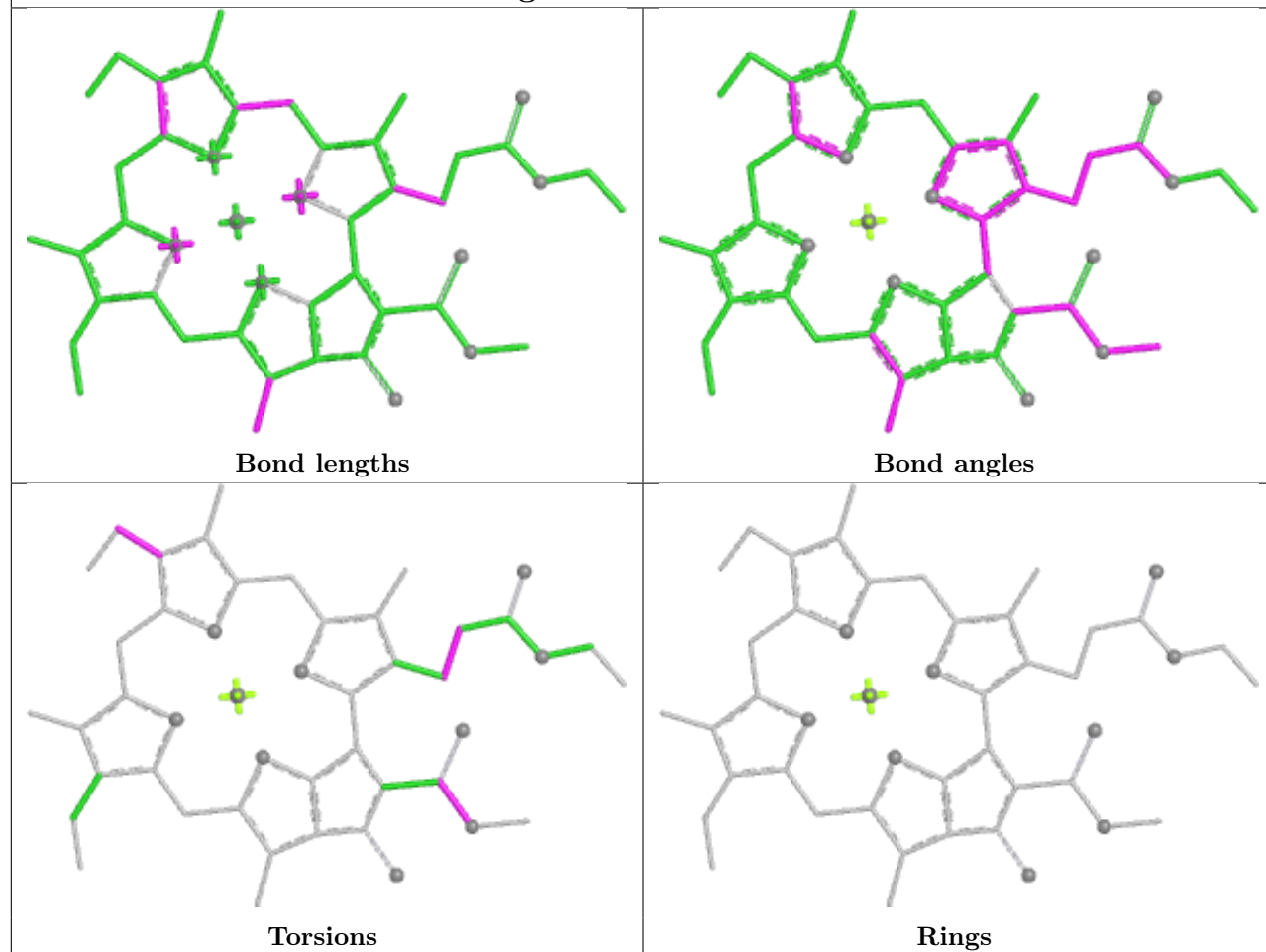


Torsions

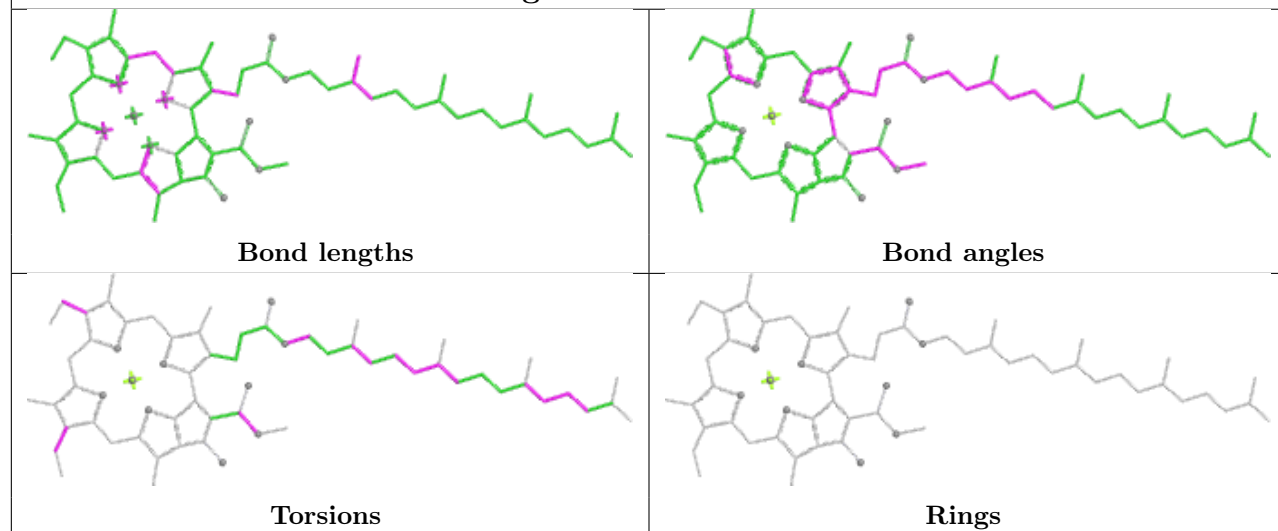


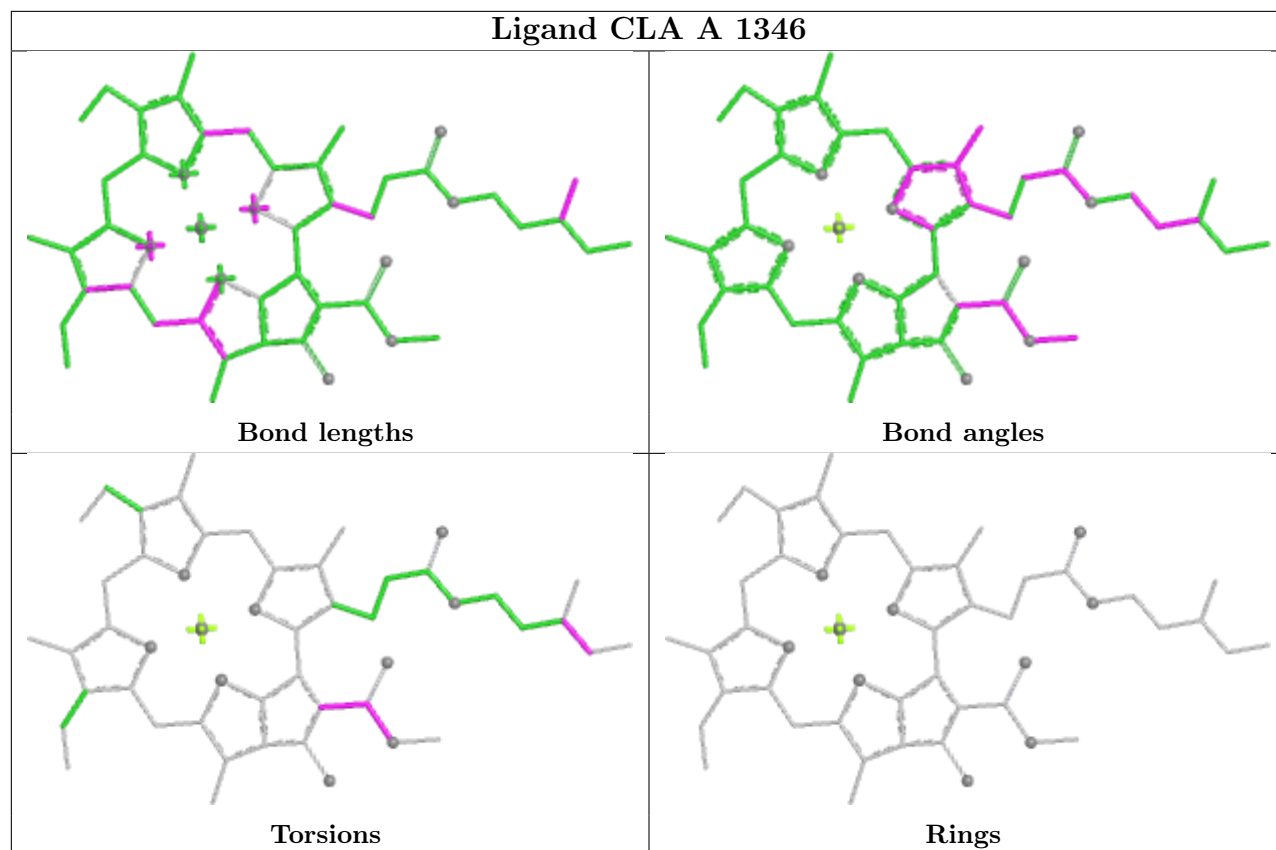
Rings

Ligand CLA C 1460

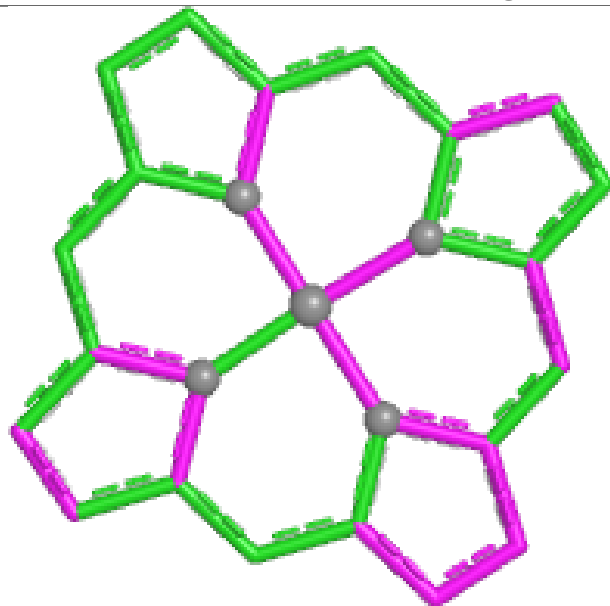


Ligand CLA H 1496

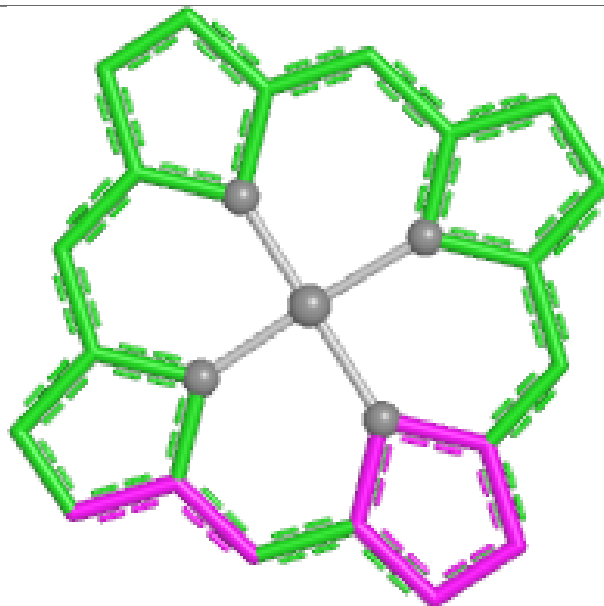




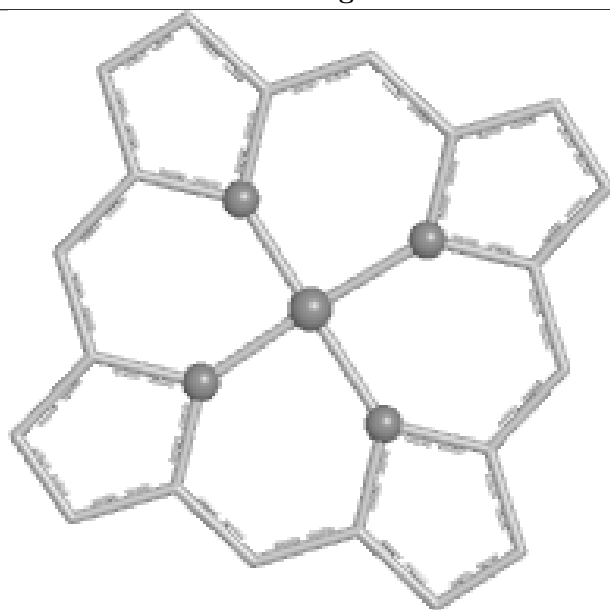
Ligand HEM E 1085



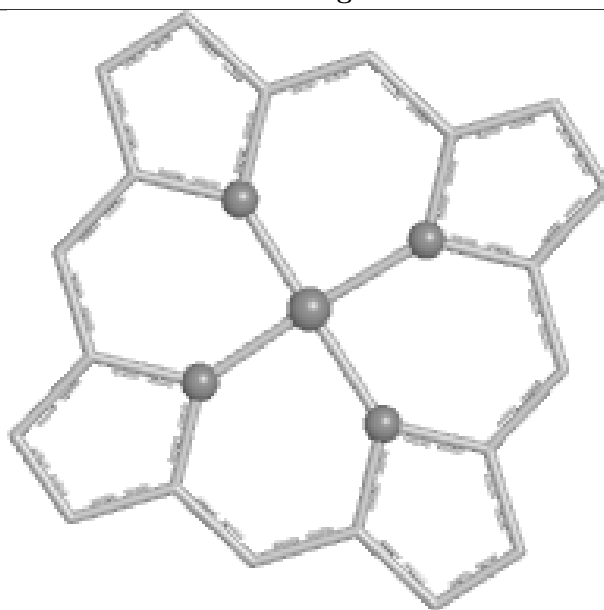
Bond lengths



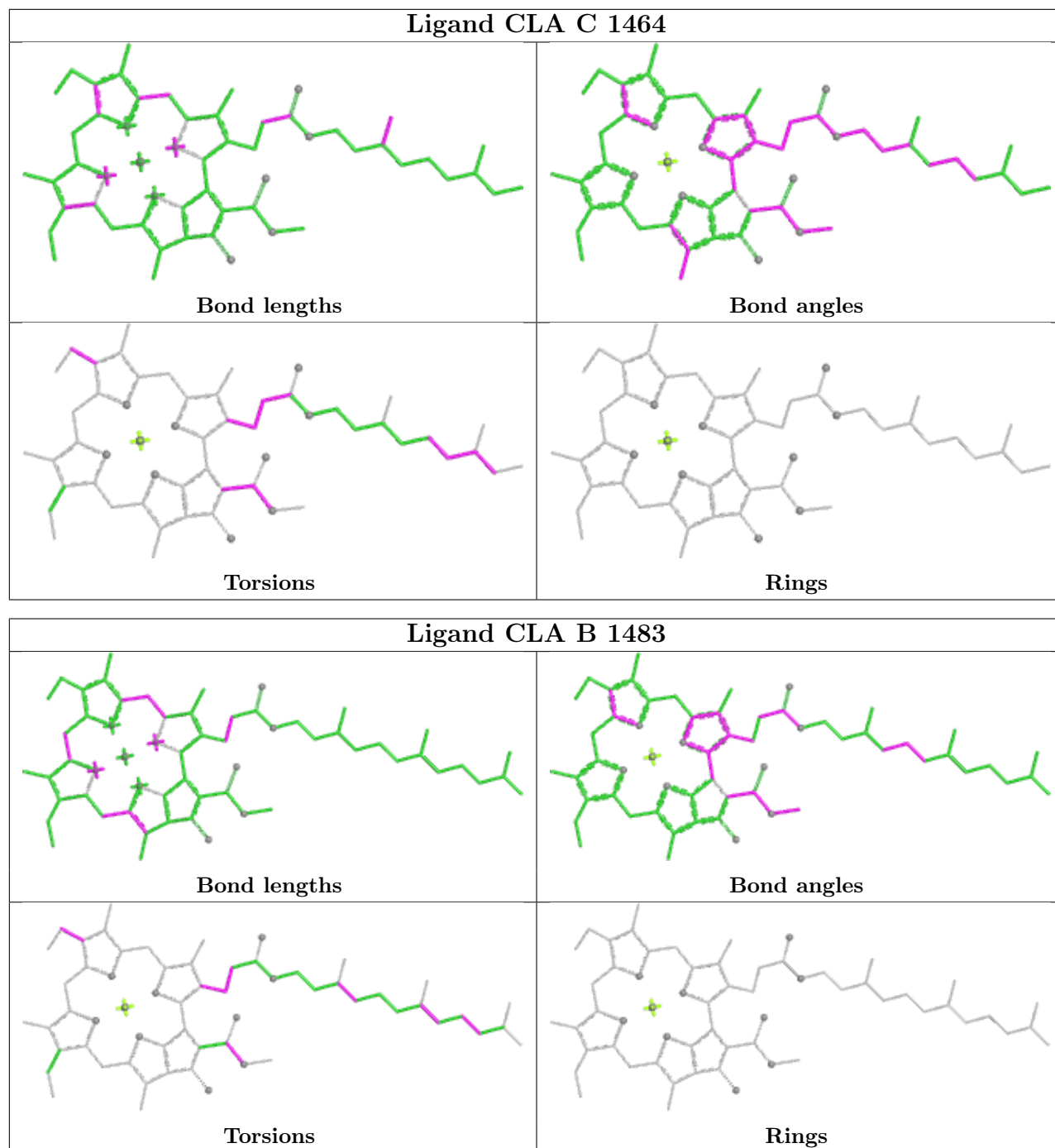
Bond angles



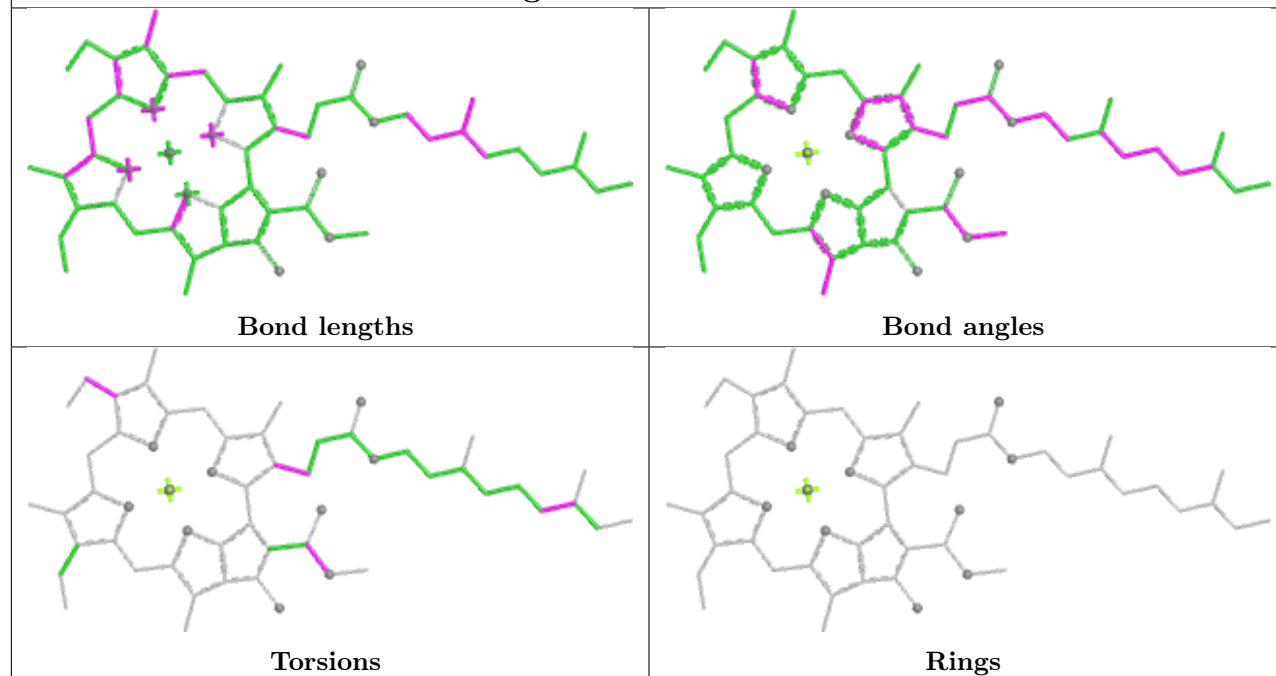
Torsions



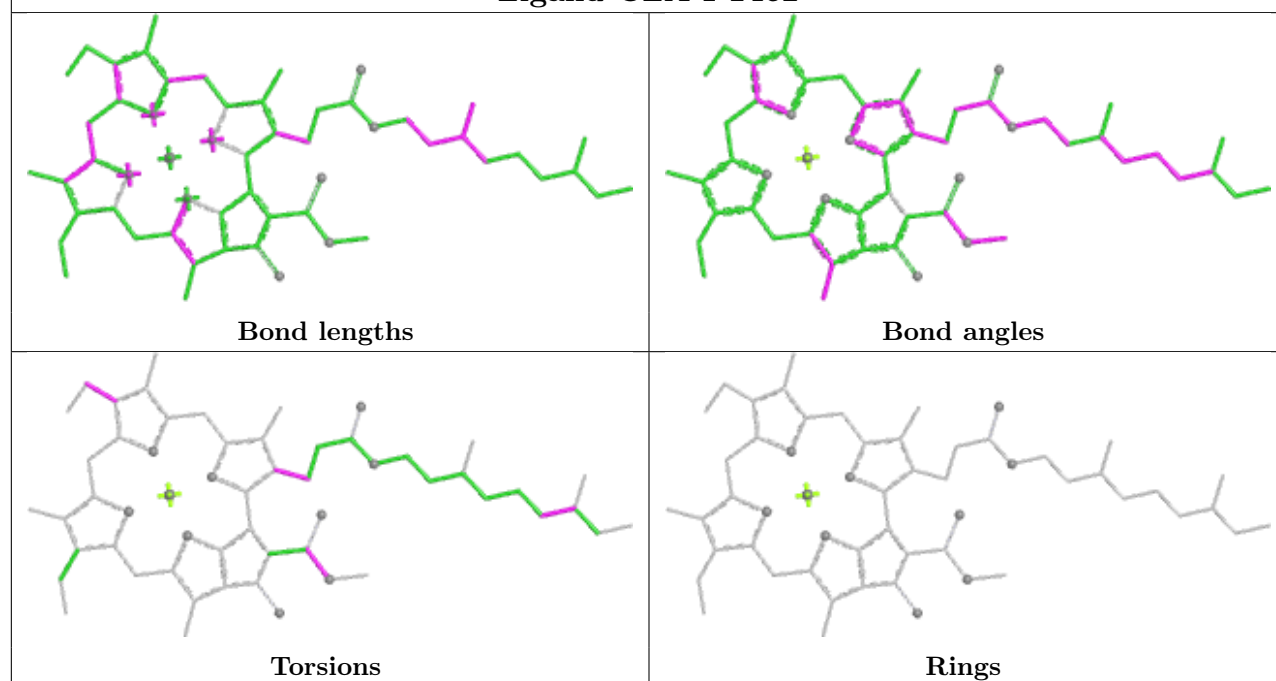
Rings



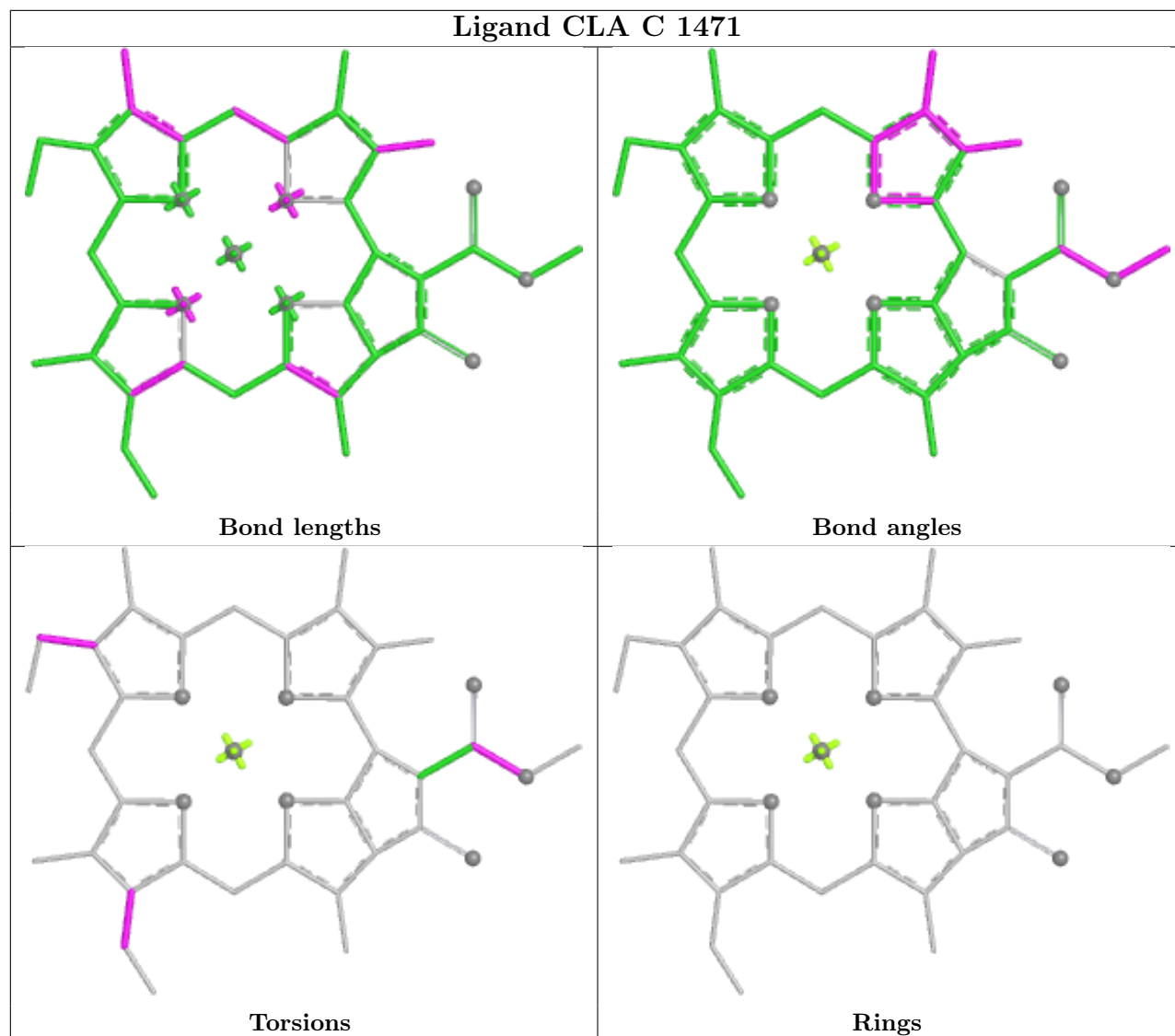
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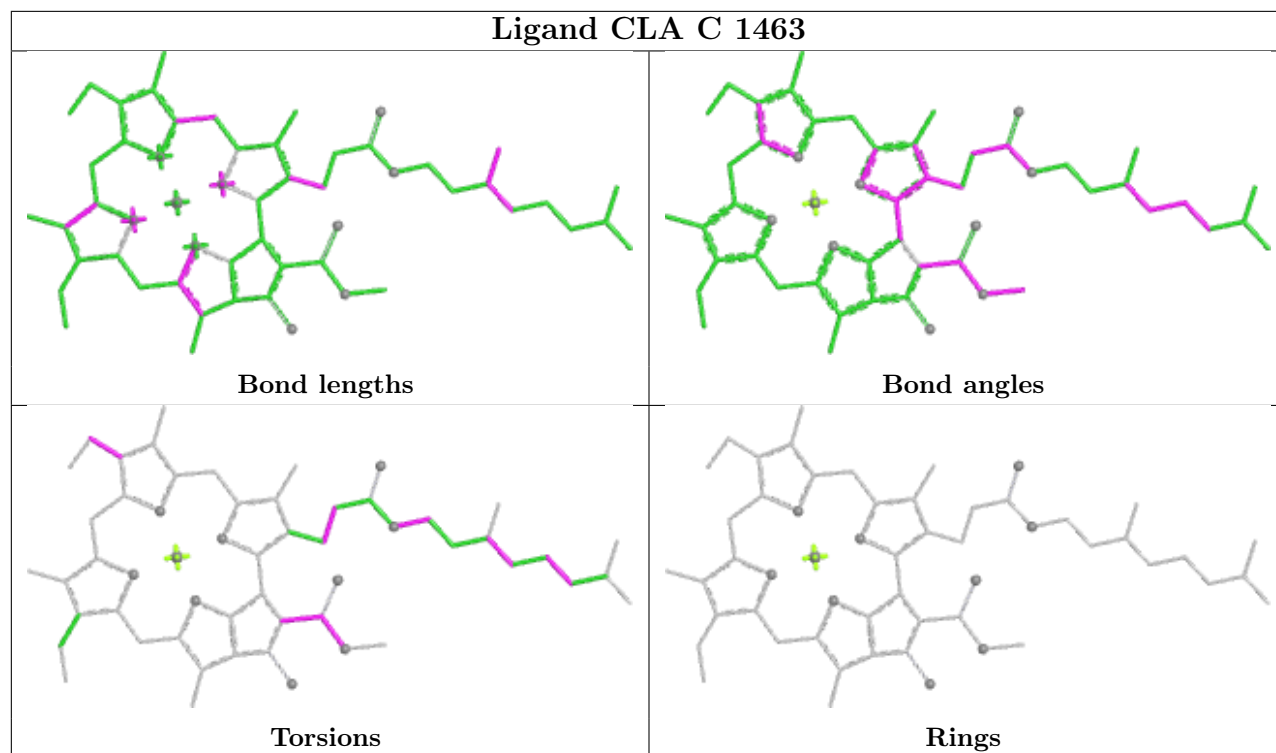
Ligand CLA I 1462



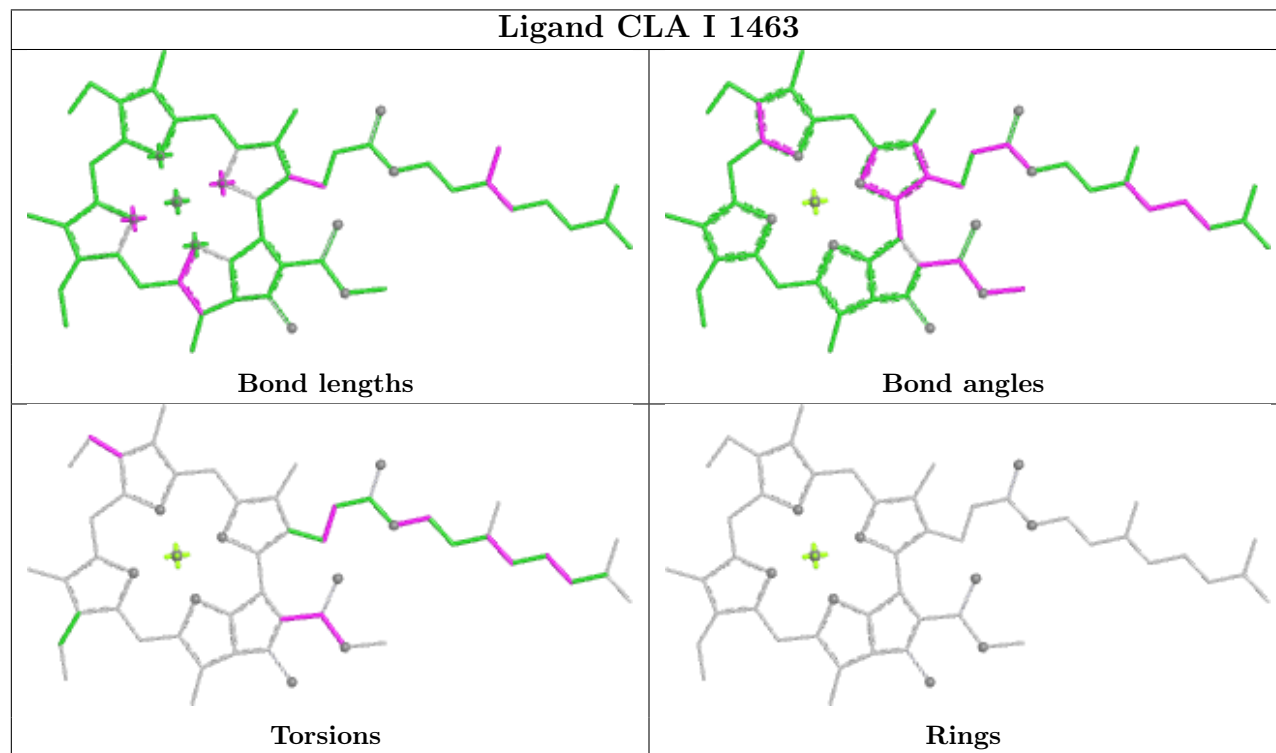
Ligand CLA C 1471

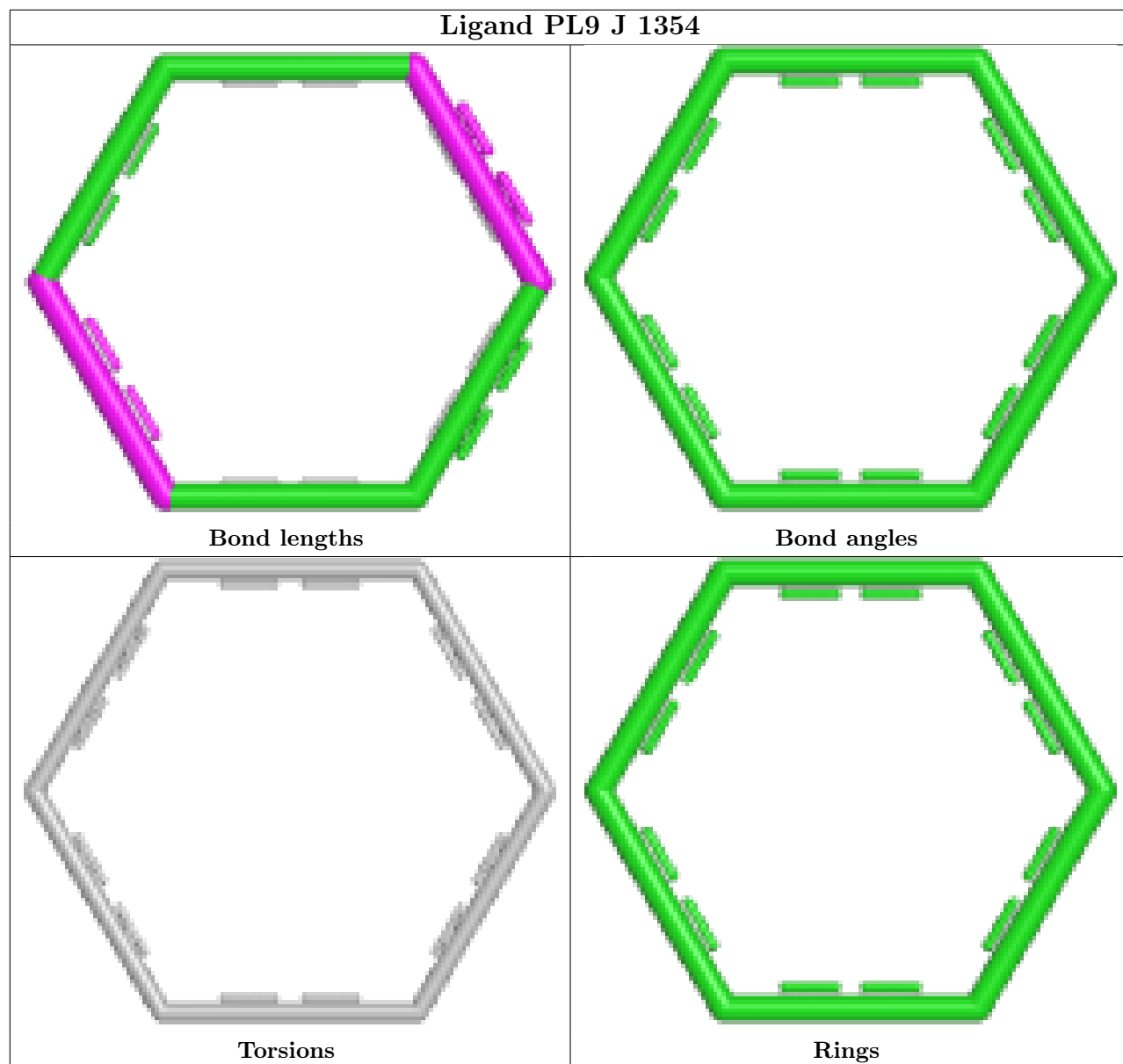


Ligand CLA C 1463

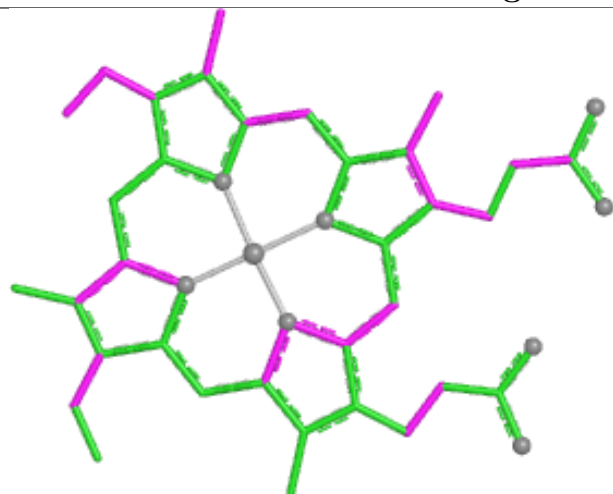


Ligand CLA I 1463

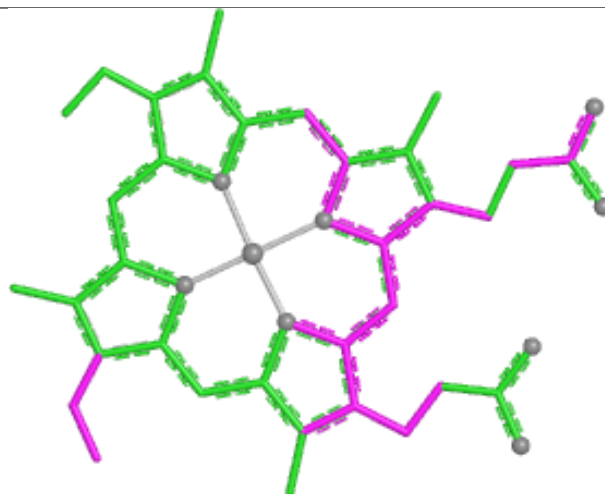




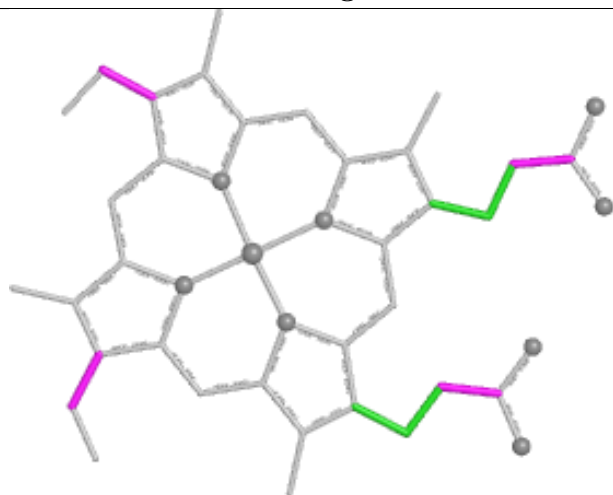
Ligand HEC V 1138



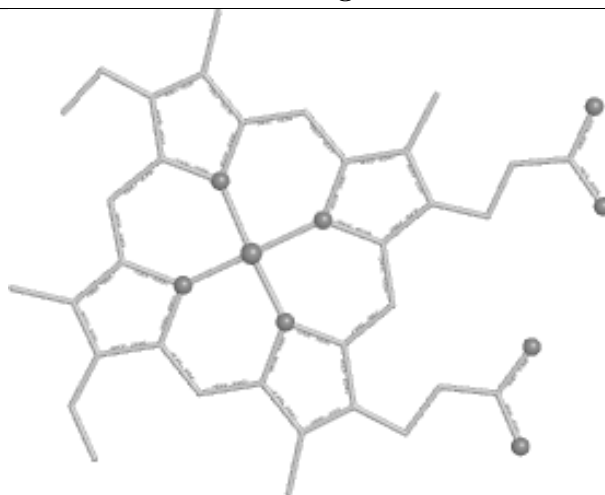
Bond lengths



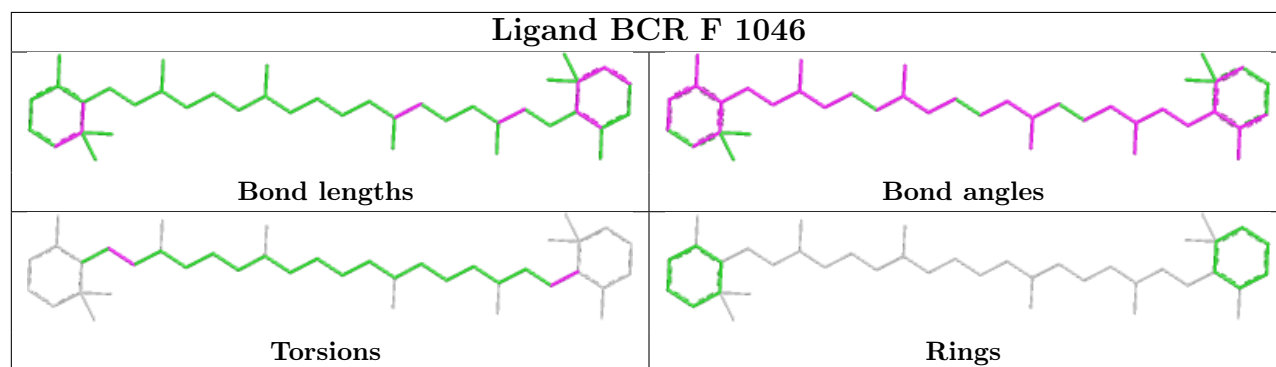
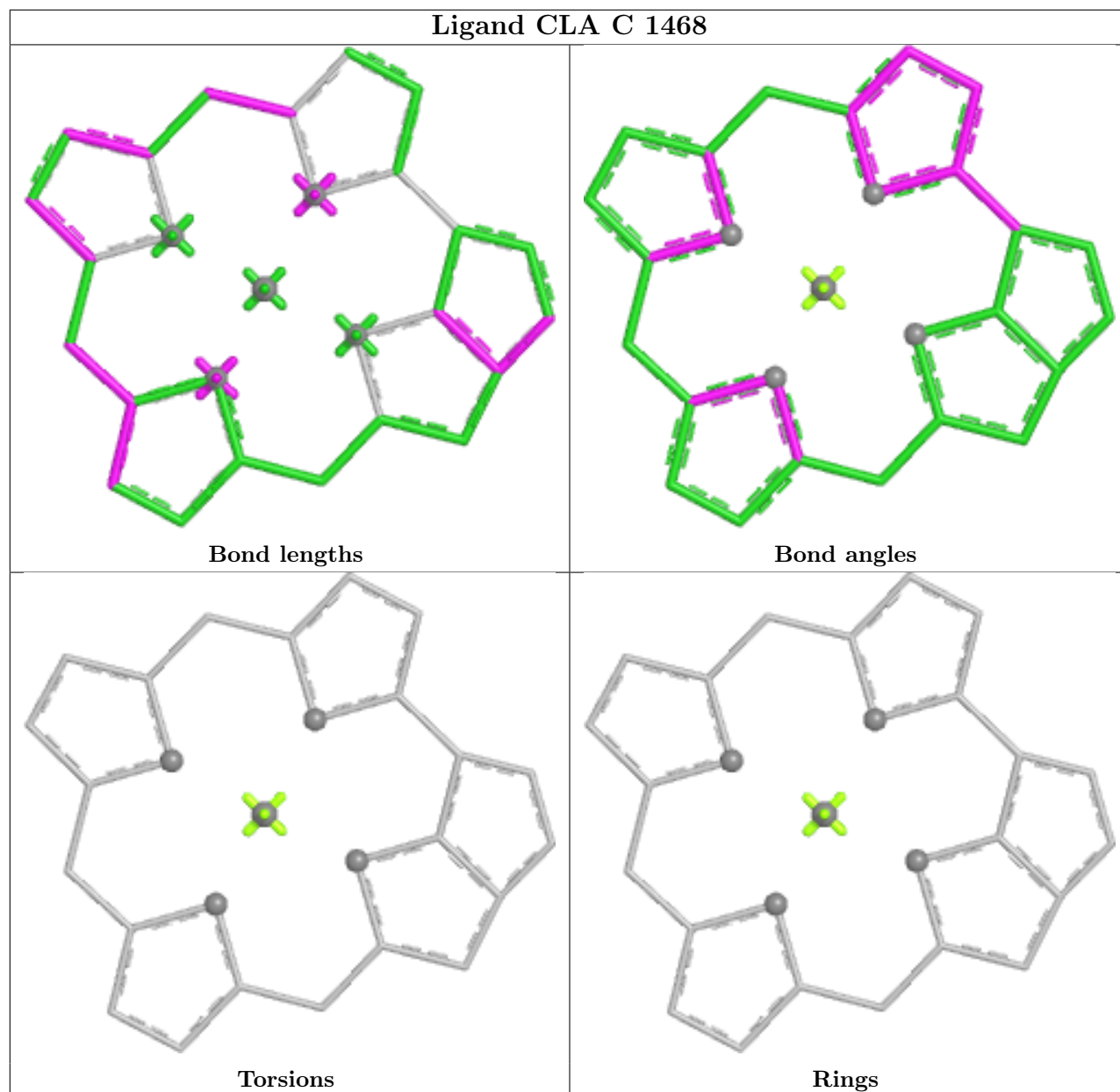
Bond angles



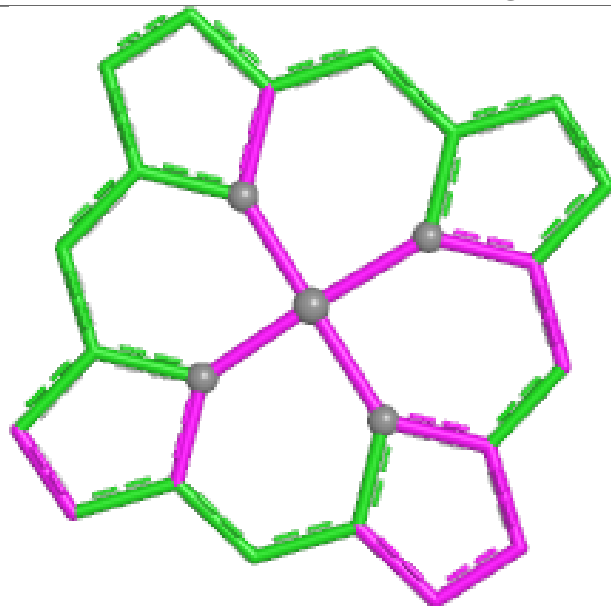
Torsions



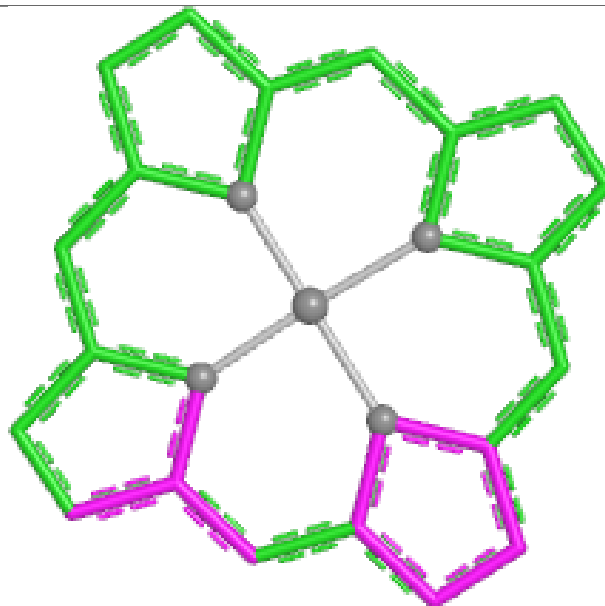
Rings



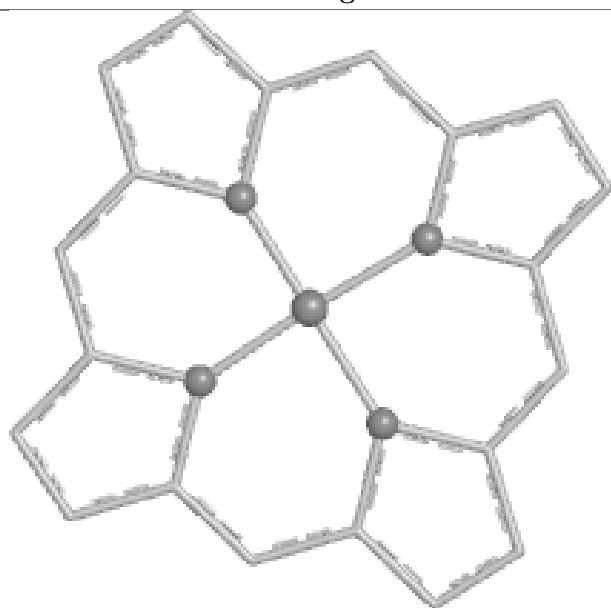
Ligand HEM L 1046



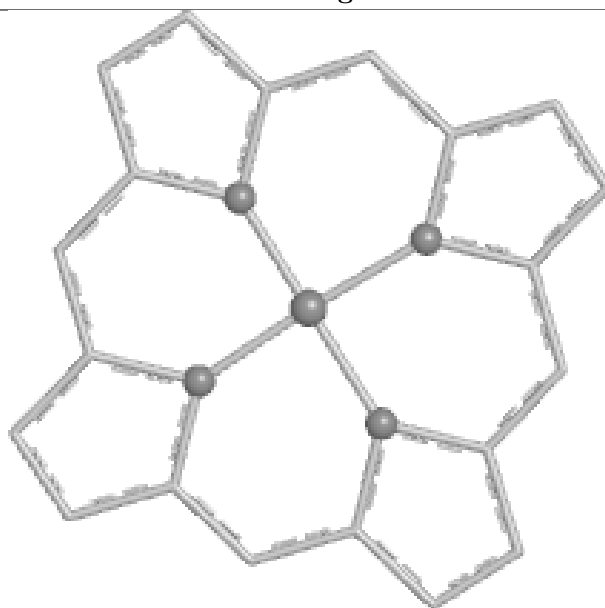
Bond lengths



Bond angles

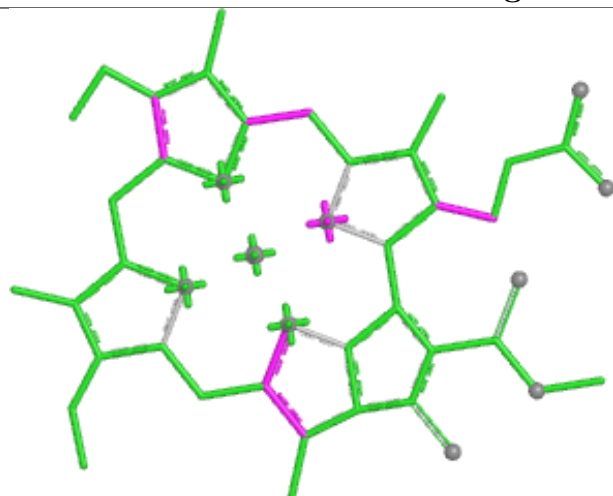


Torsions

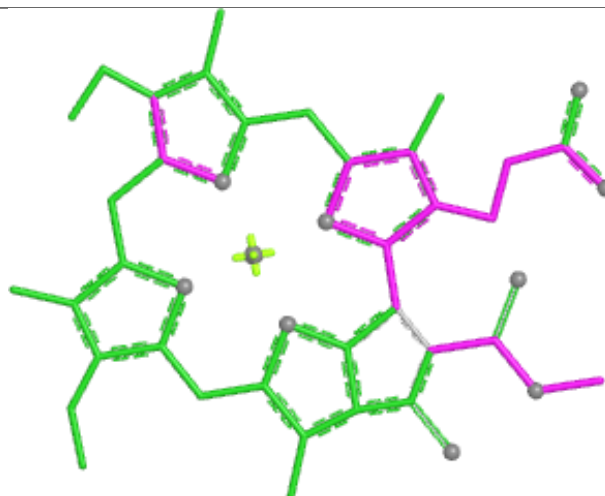


Rings

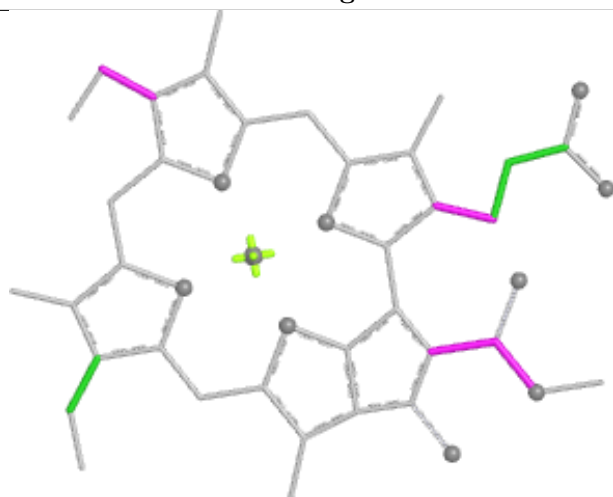
Ligand CLA G 1344



Bond lengths



Bond angles

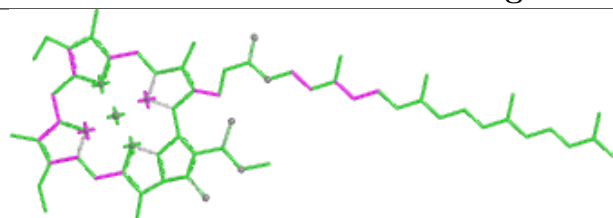


Torsions

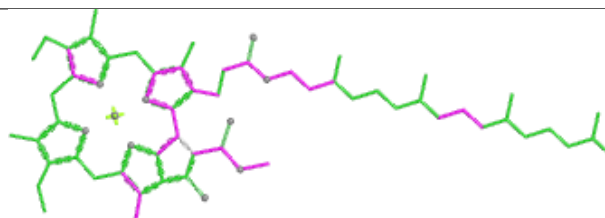


Rings

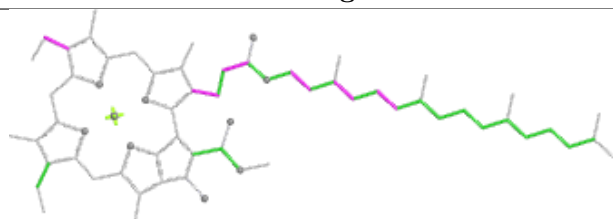
Ligand CLA B 1487



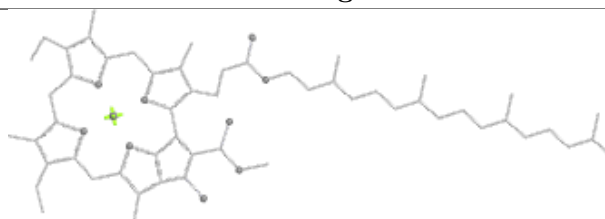
Bond lengths



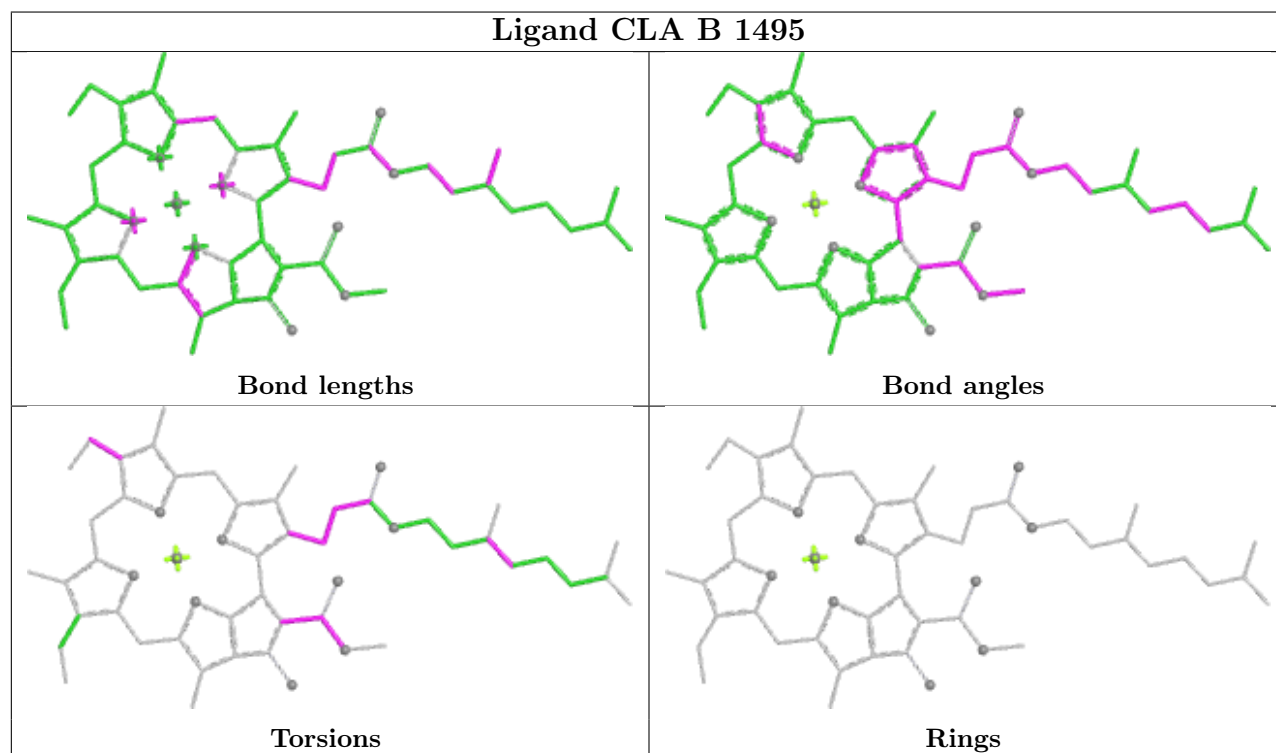
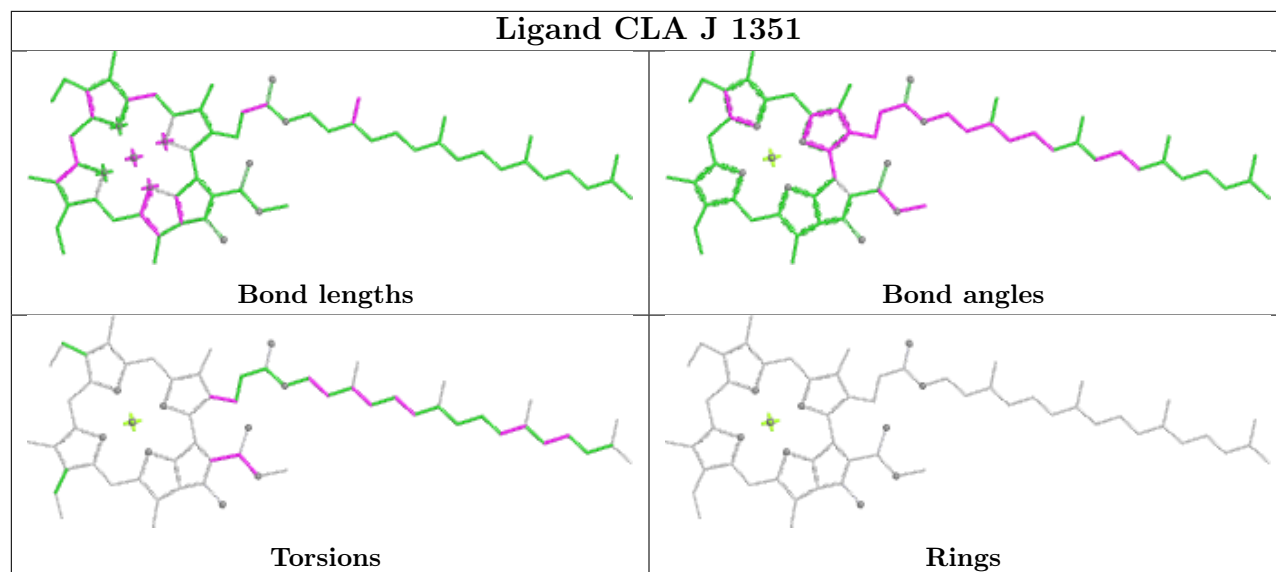
Bond angles

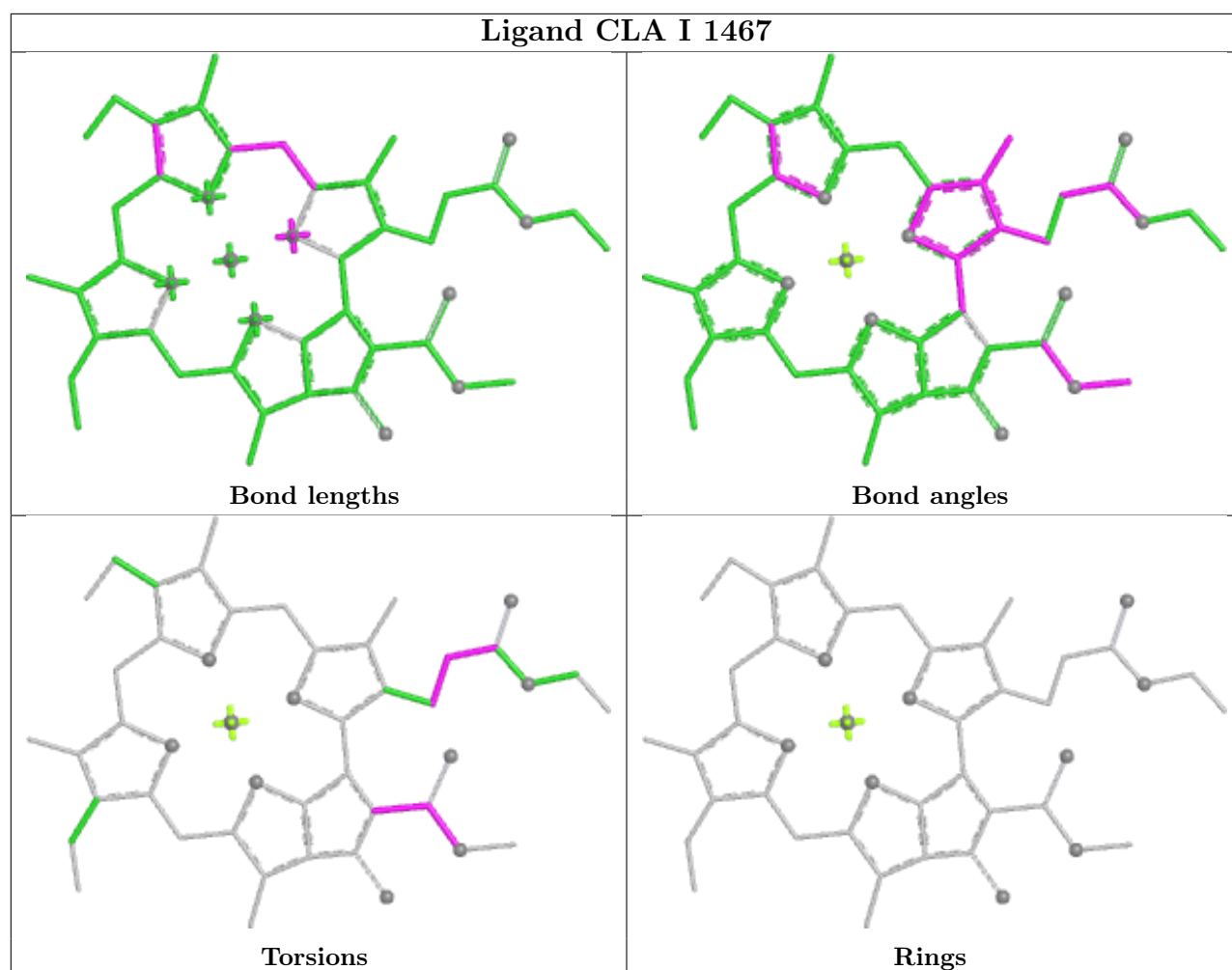


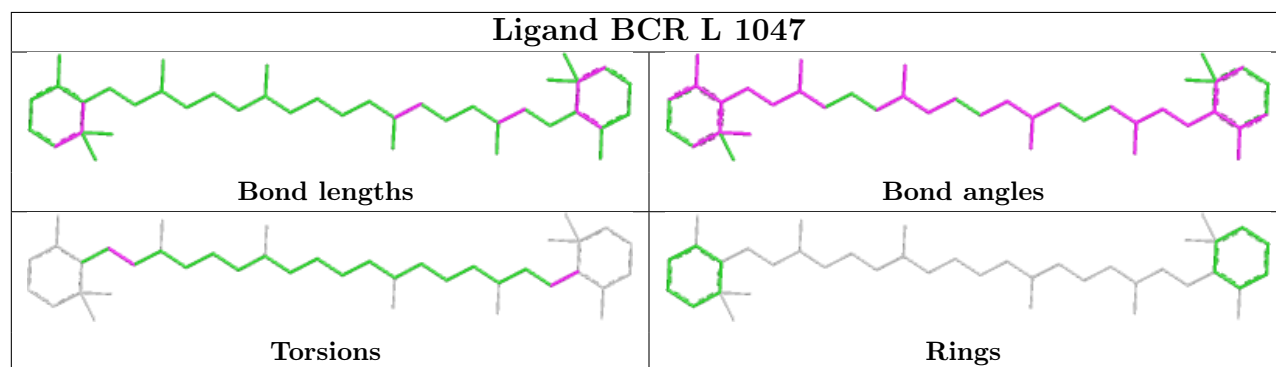
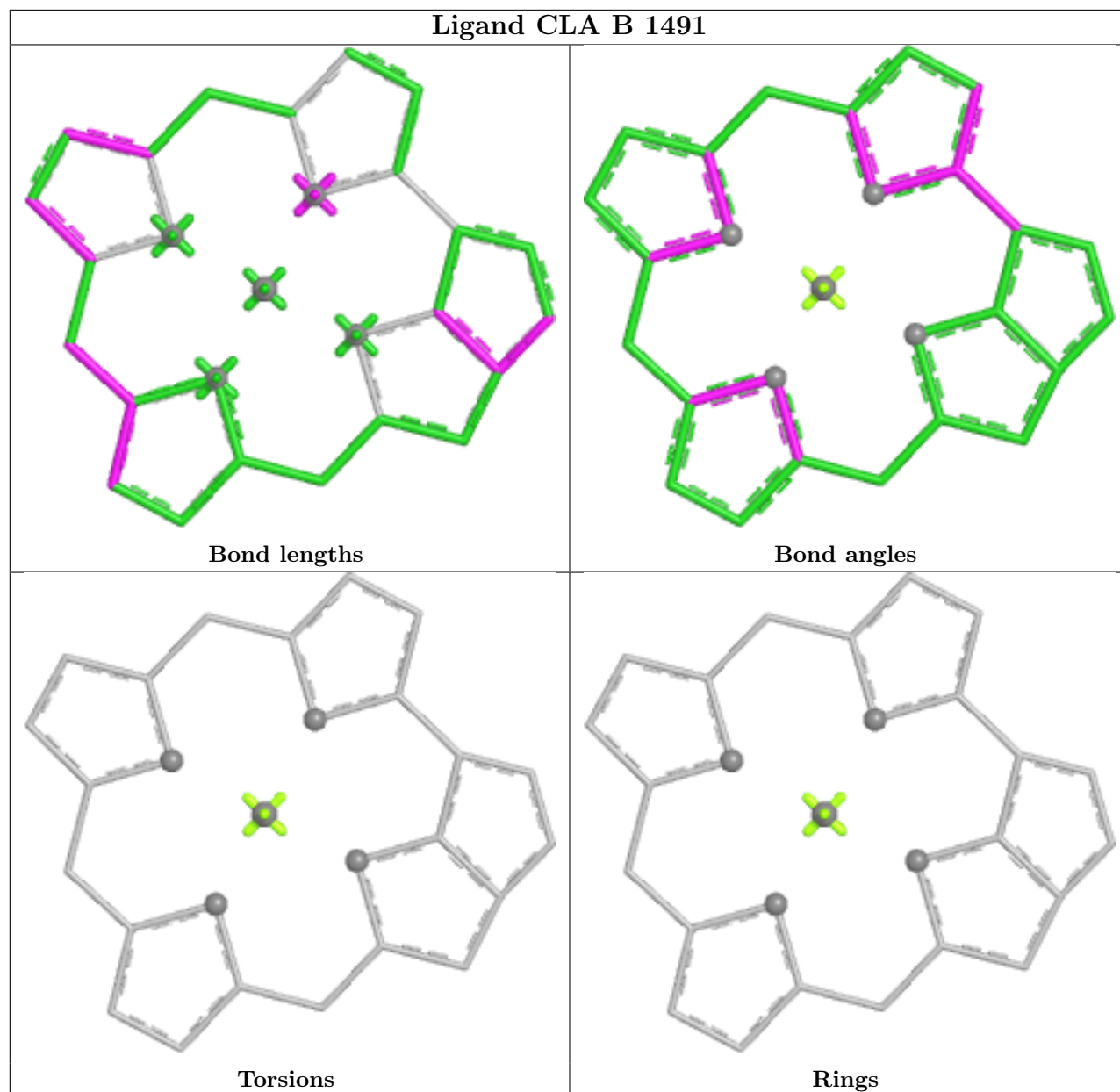
Torsions



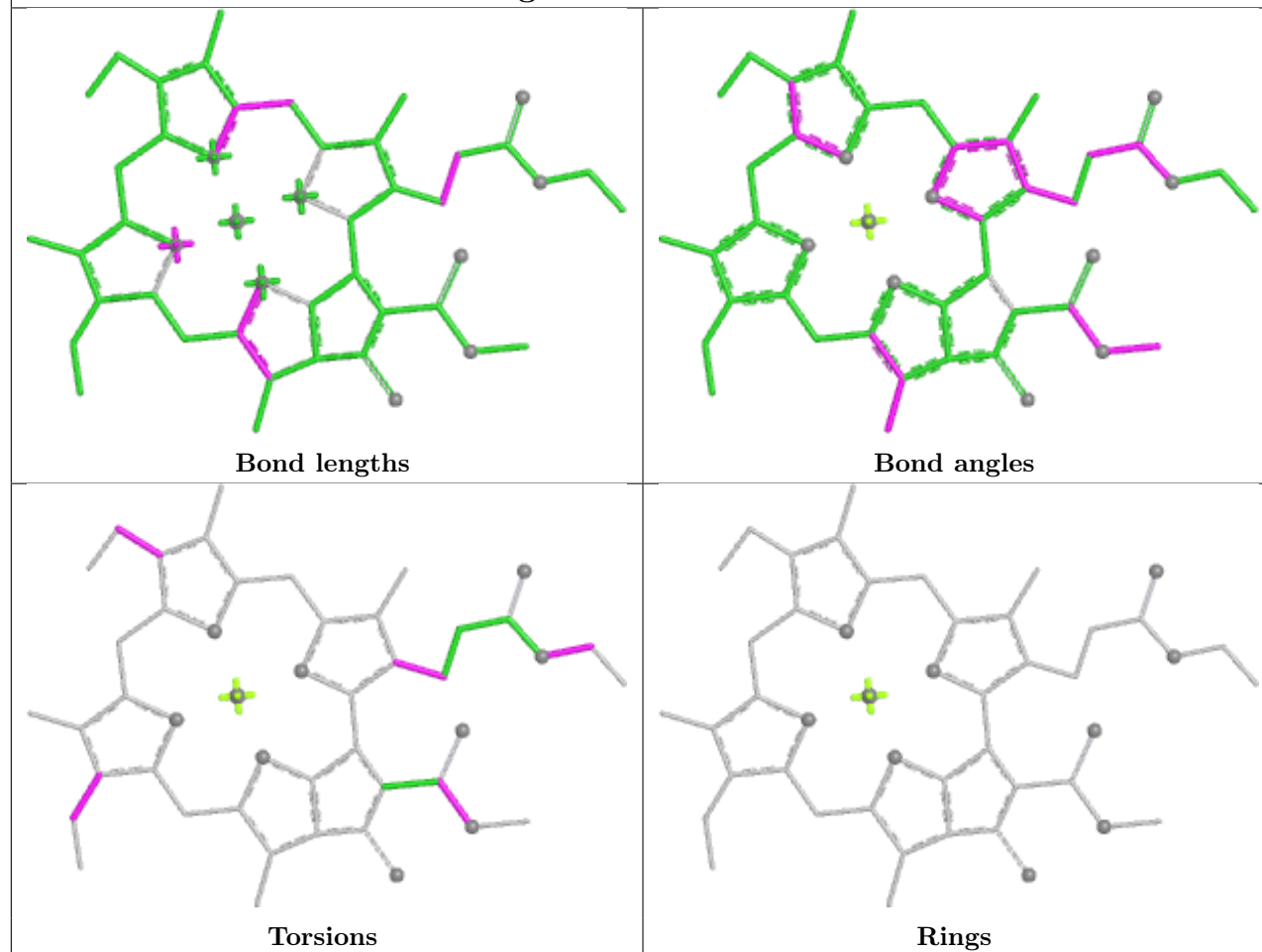
Rings



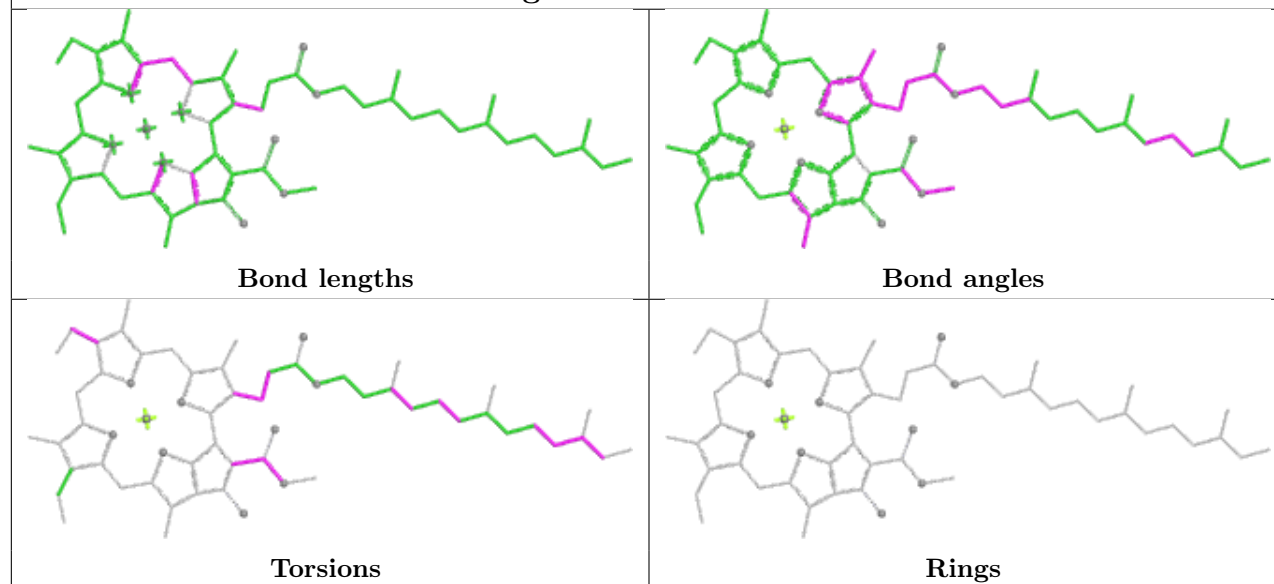


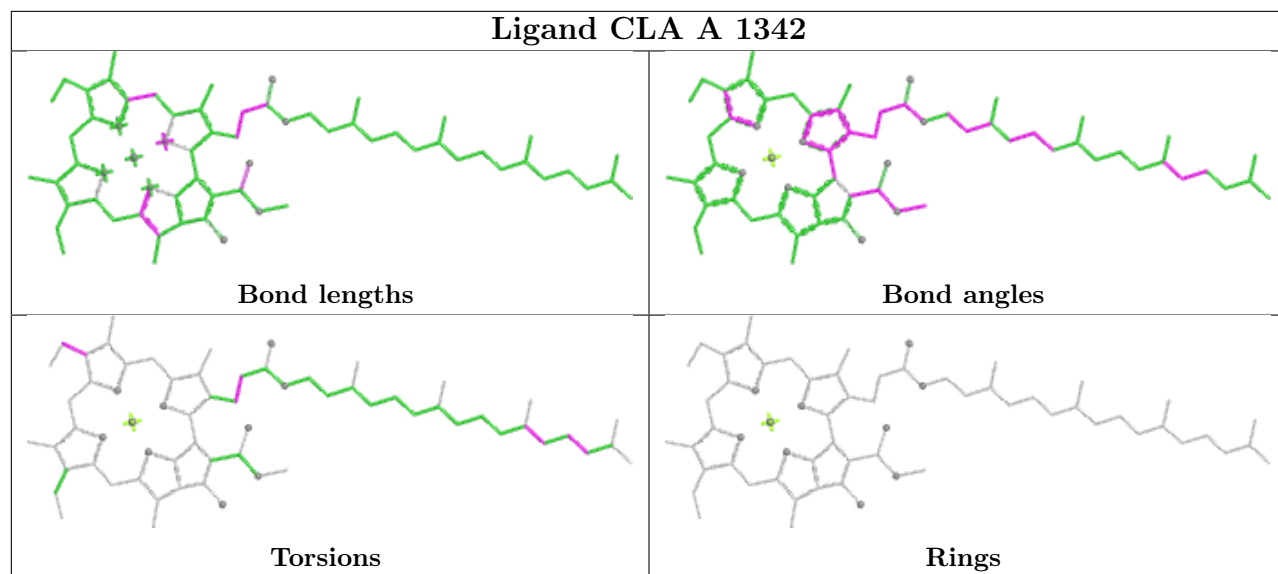


Ligand CLA B 1485

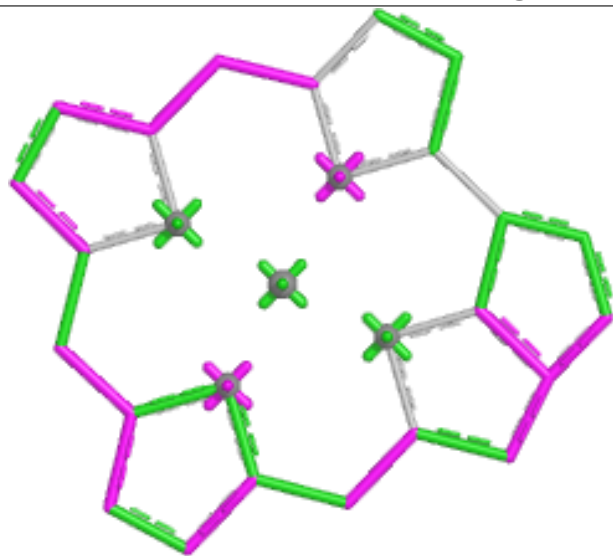


Ligand CLA A 1343

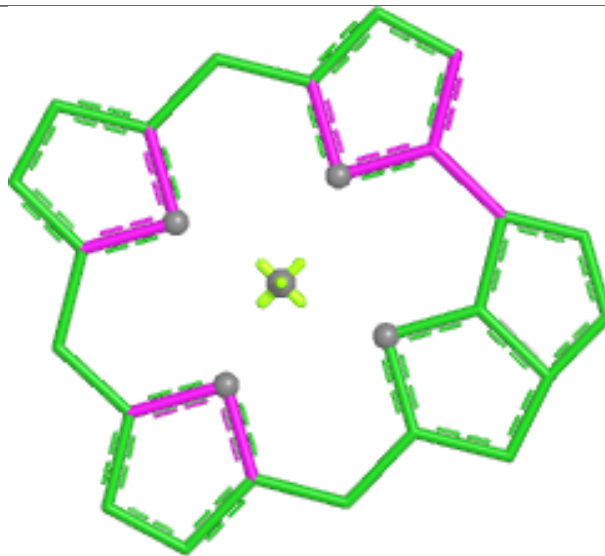




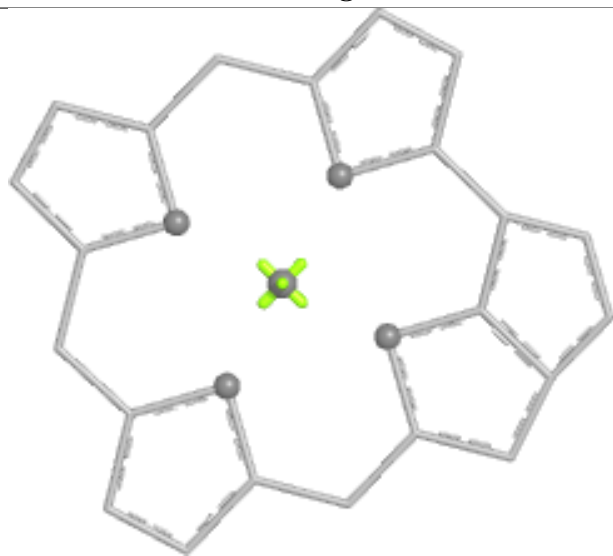
Ligand CLA I 1461



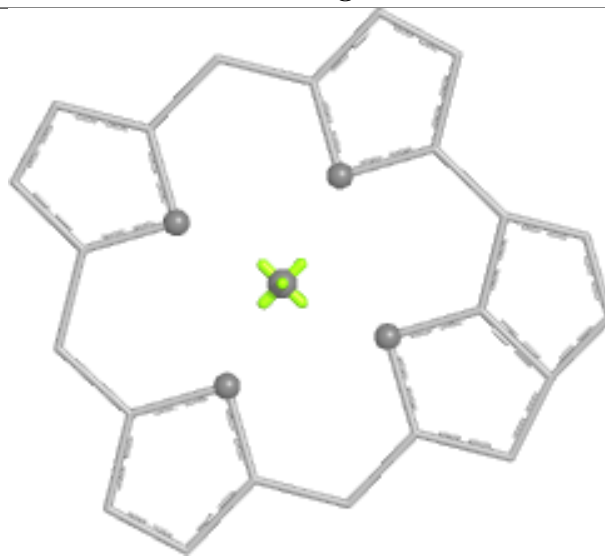
Bond lengths



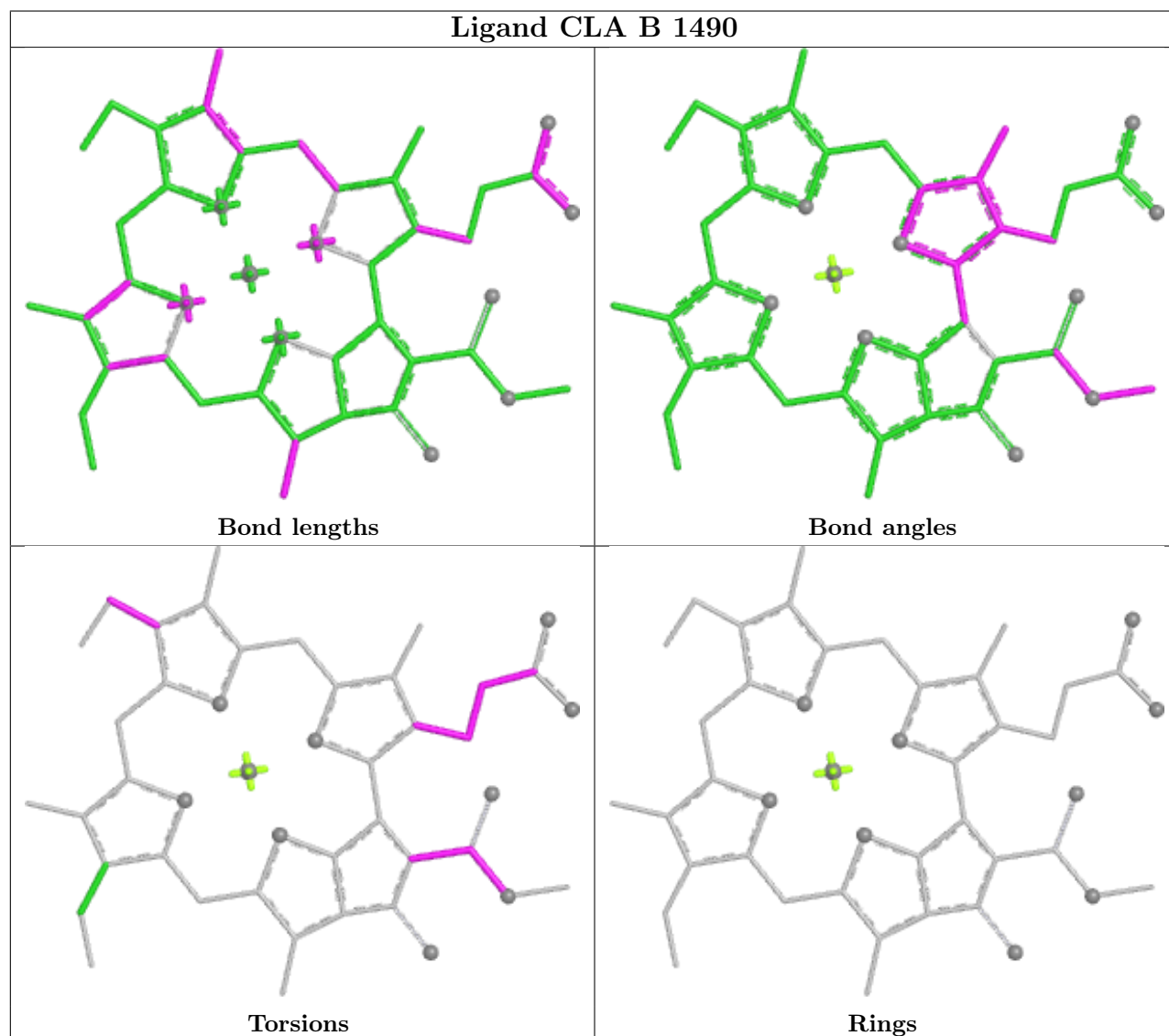
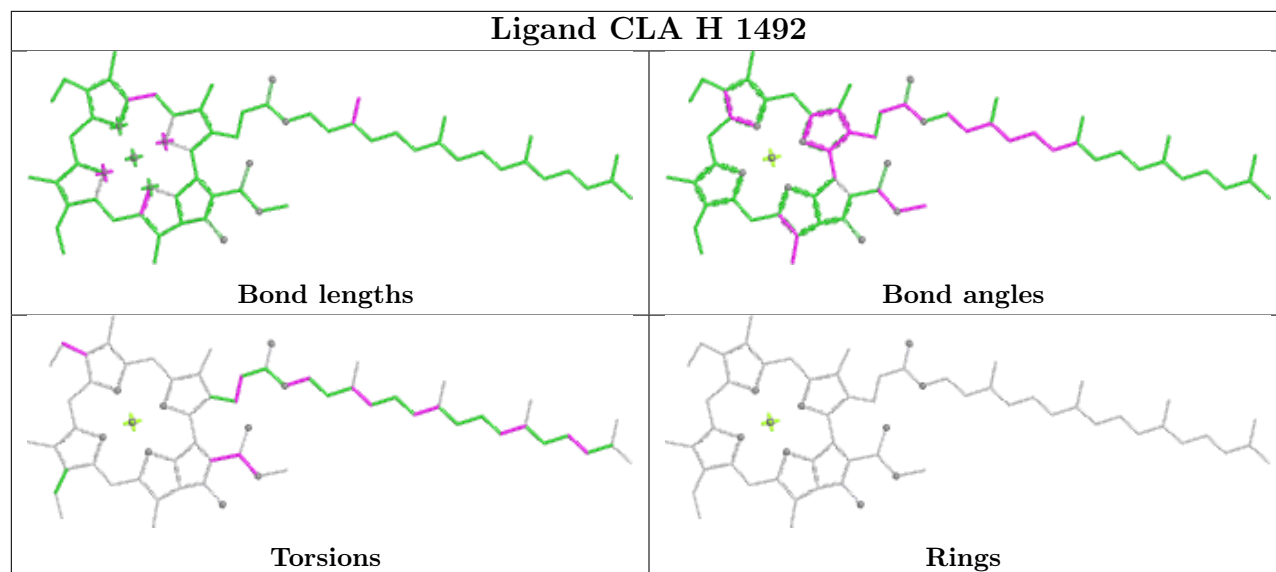
Bond angles

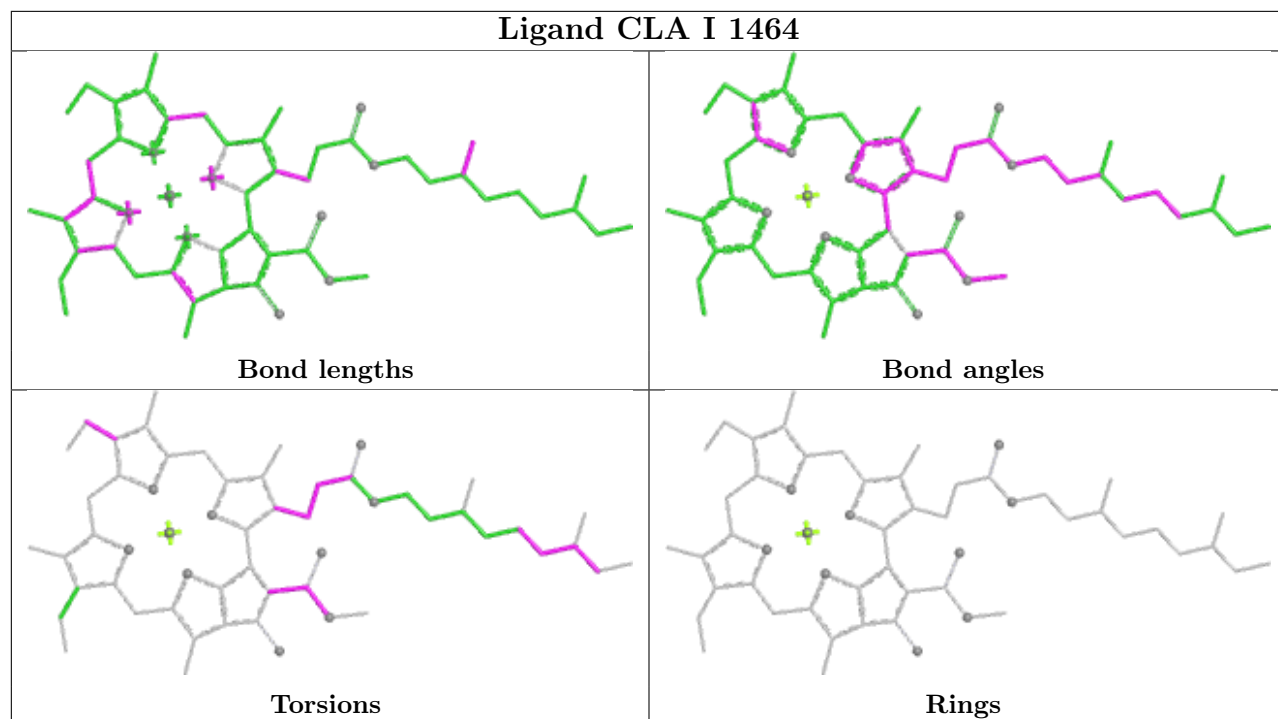


Torsions

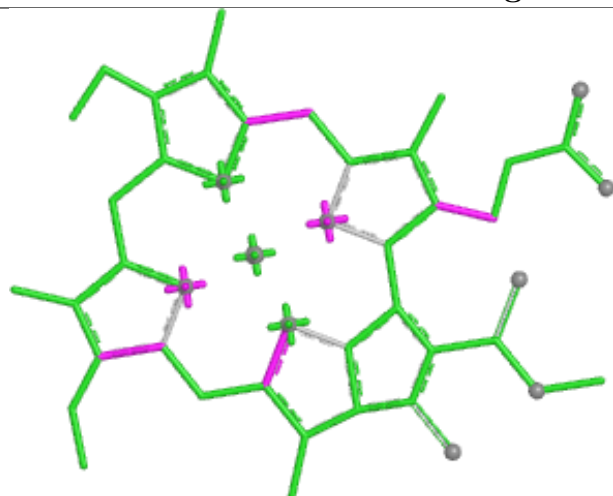


Rings

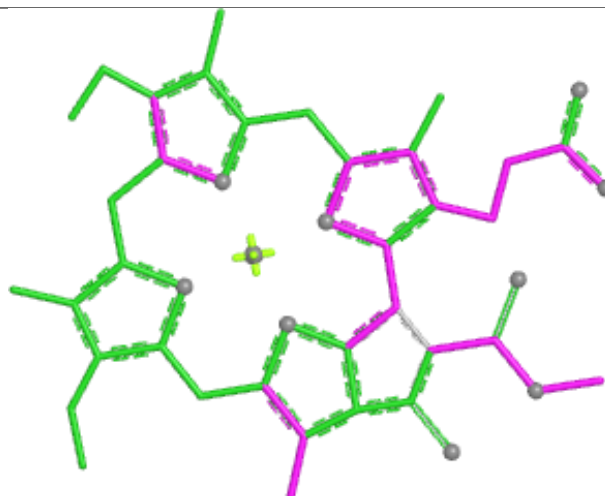




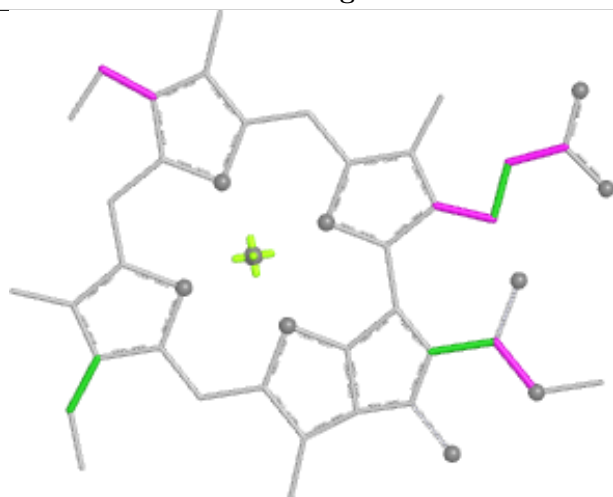
Ligand CLA H 1493



Bond lengths



Bond angles

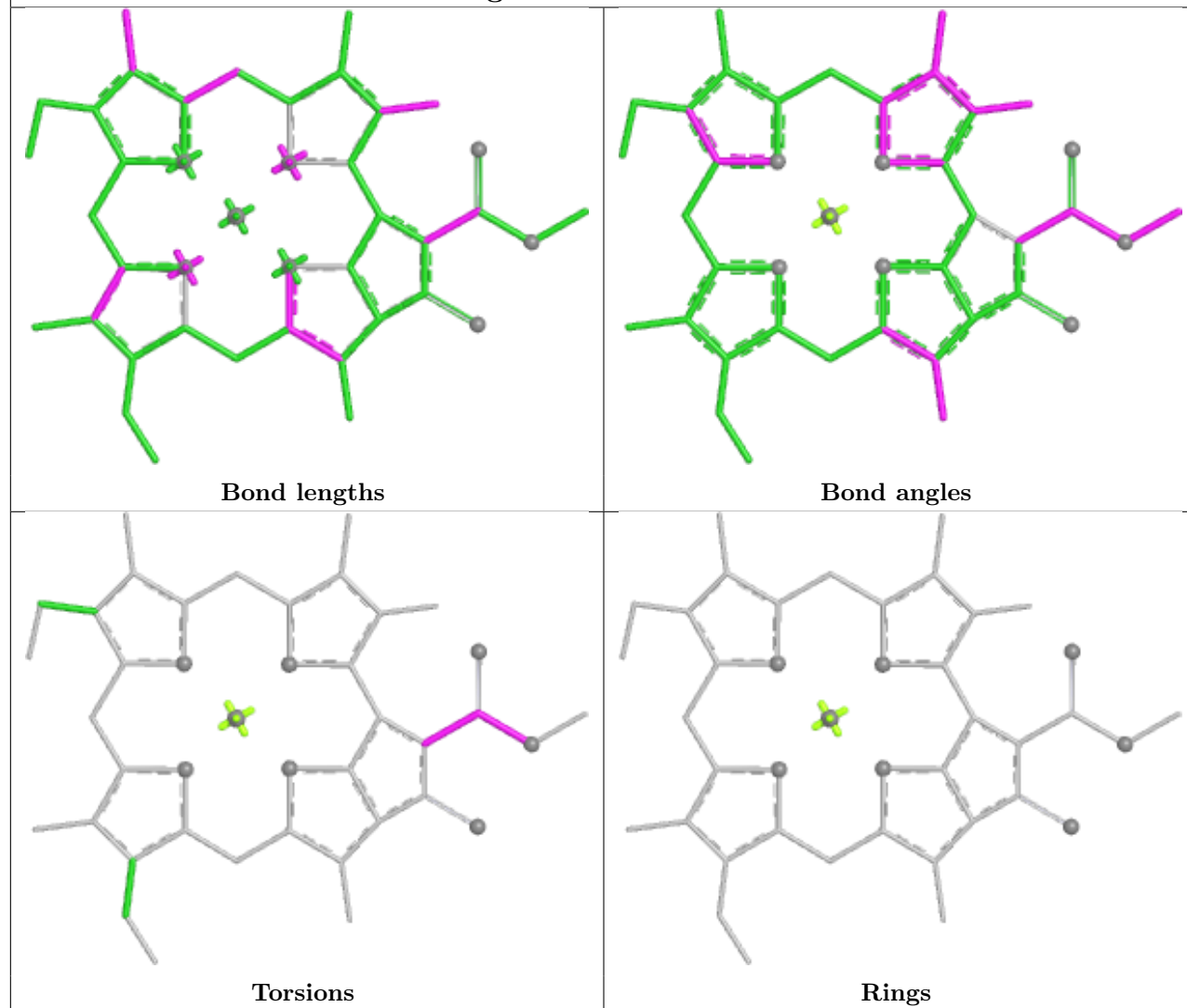


Torsions

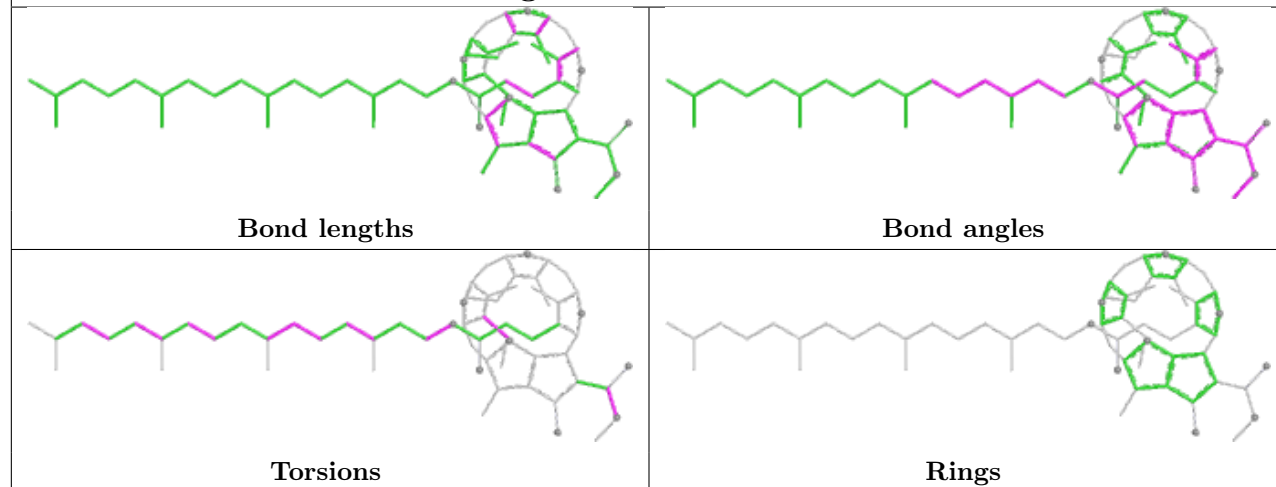


Rings

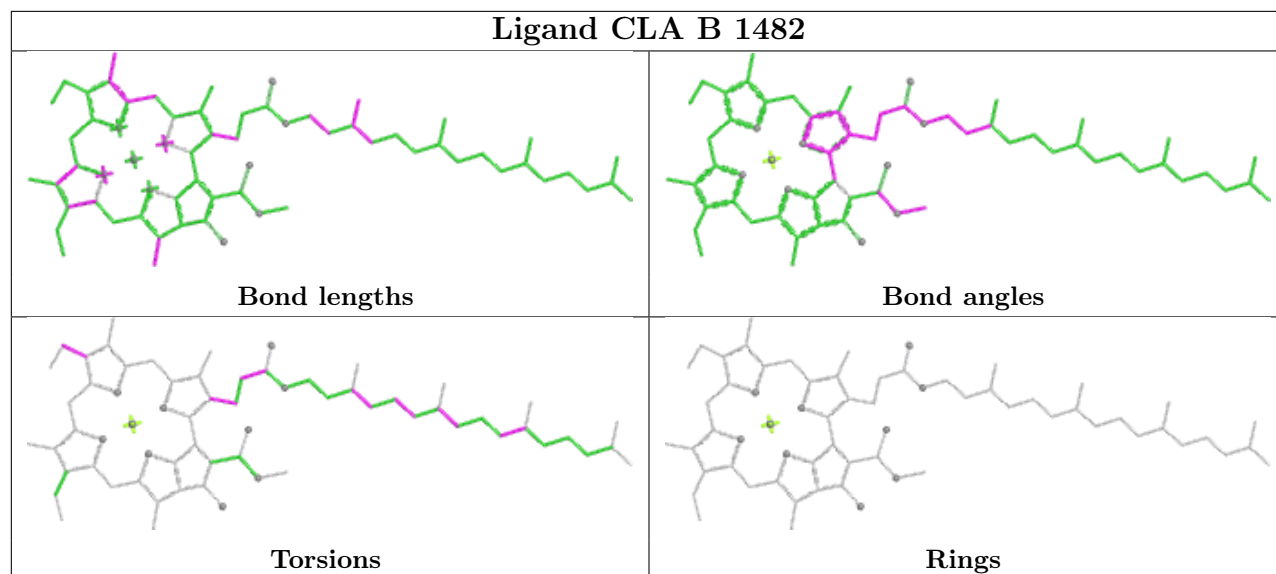
Ligand CLA B 1497



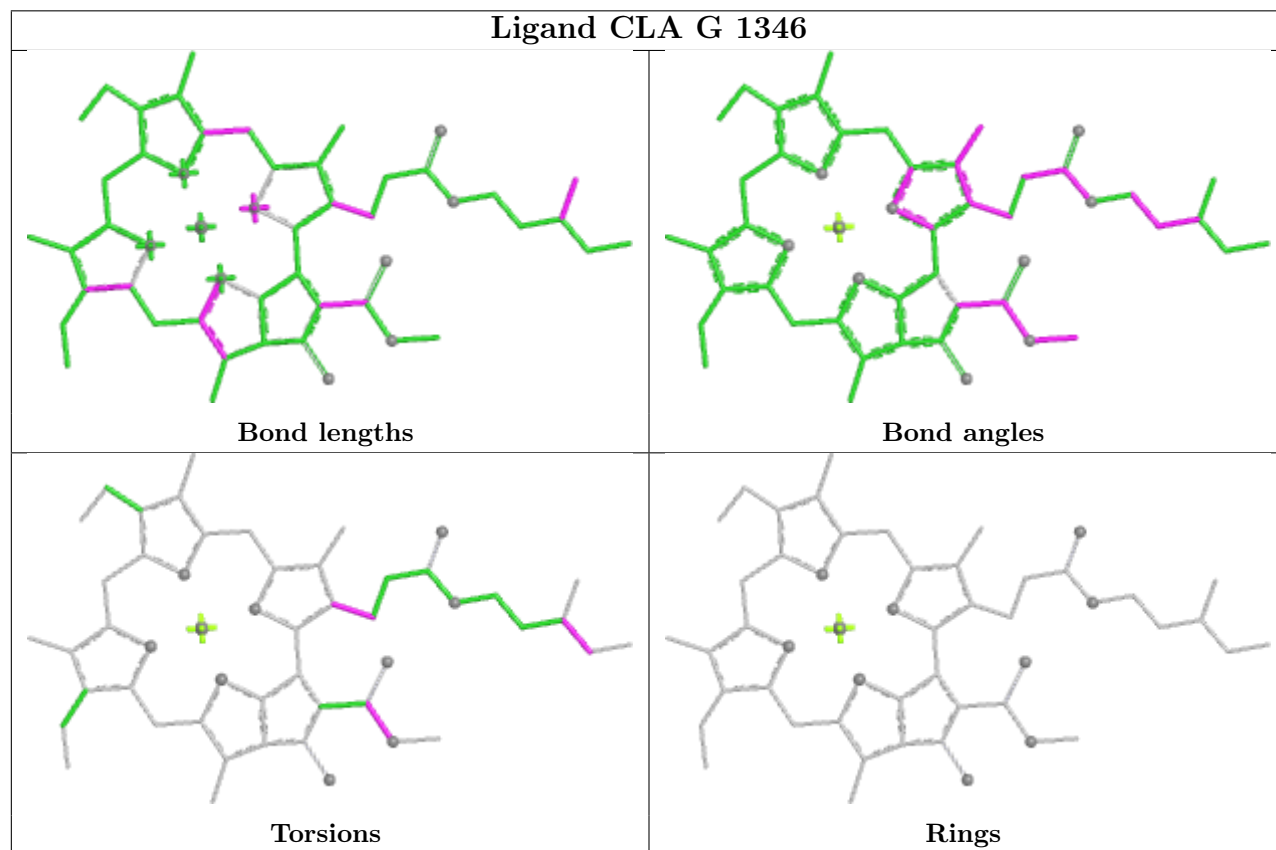
Ligand PHO G 1345

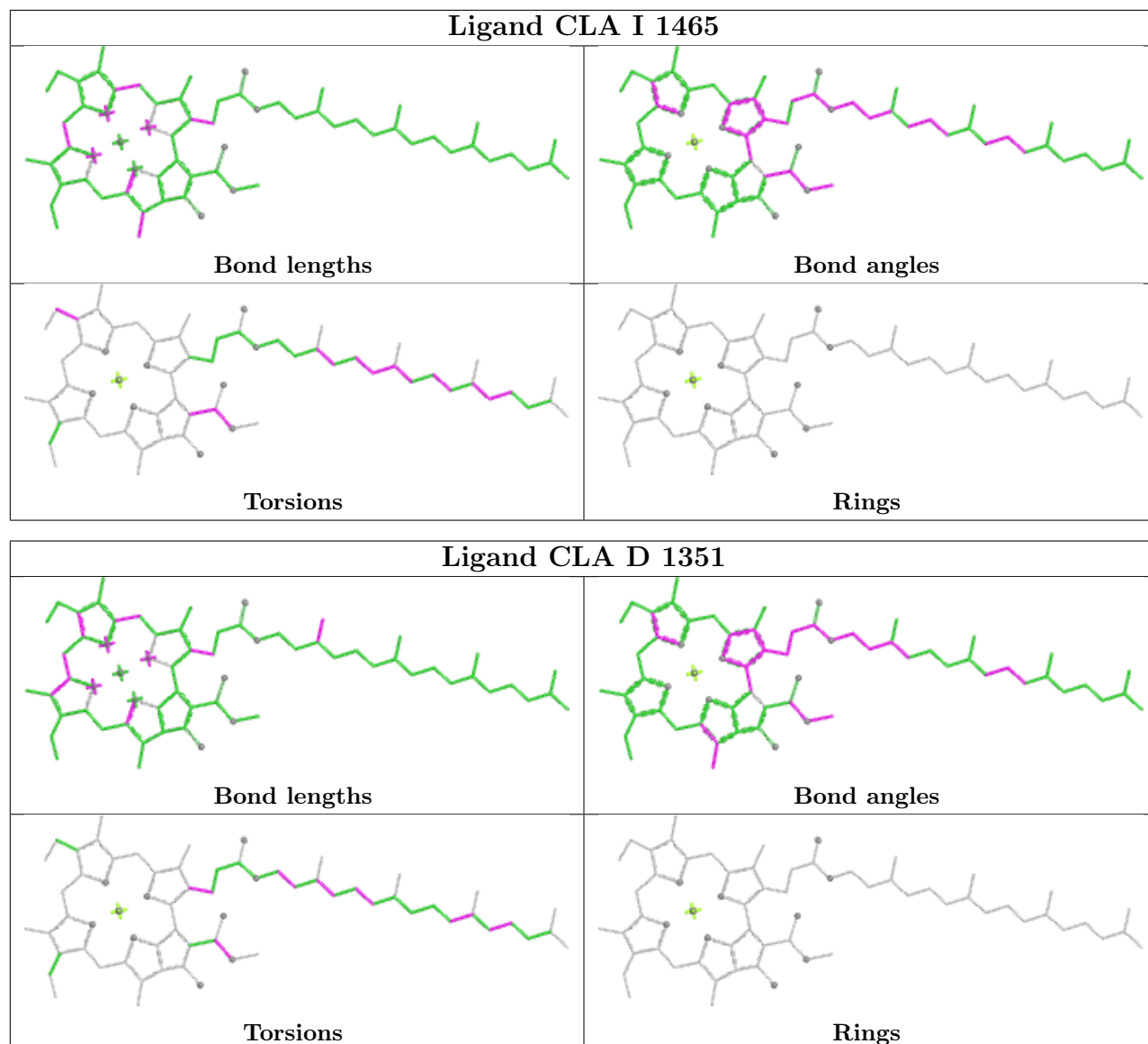


Ligand CLA B 1482

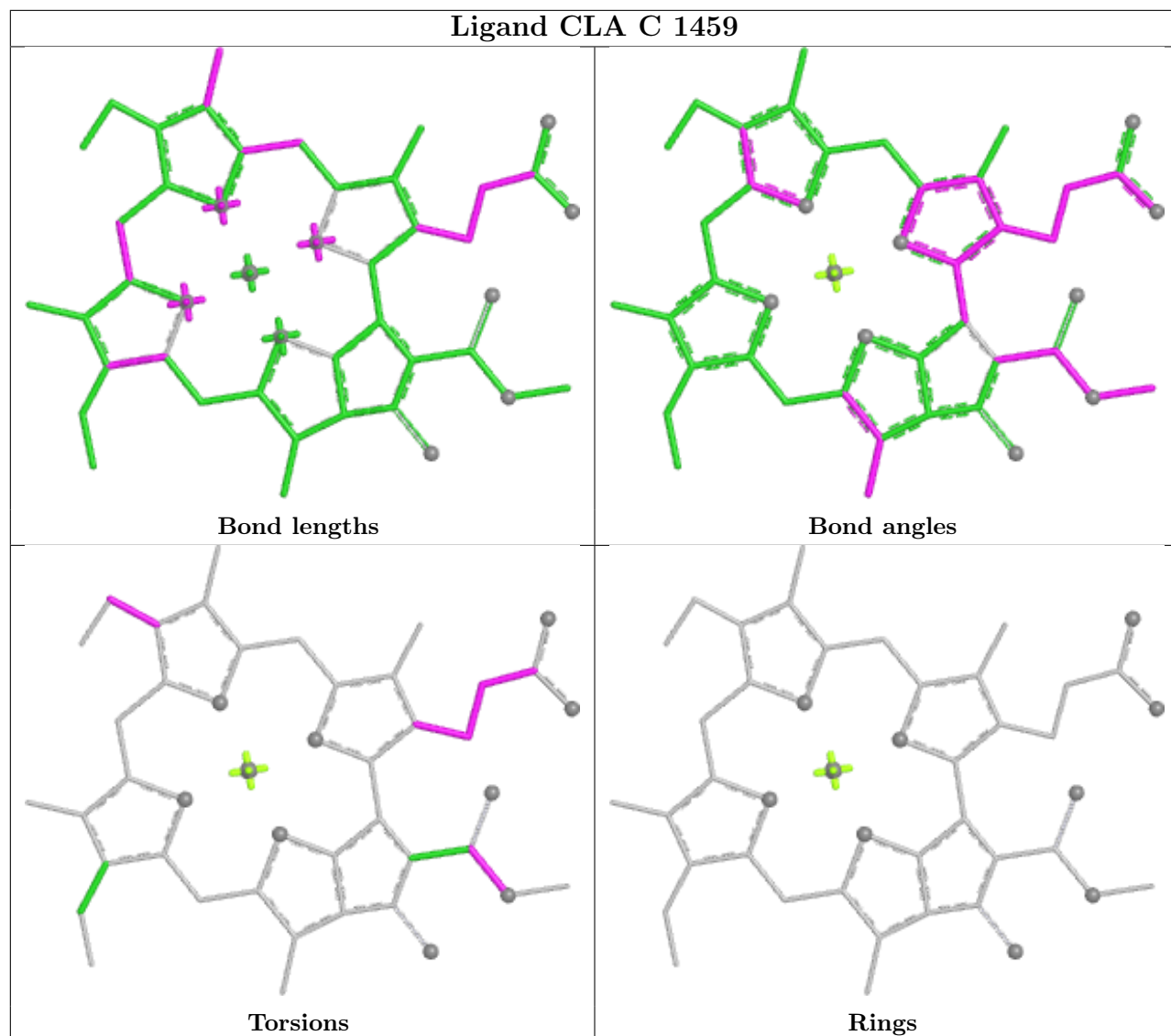


Ligand CLA G 1346

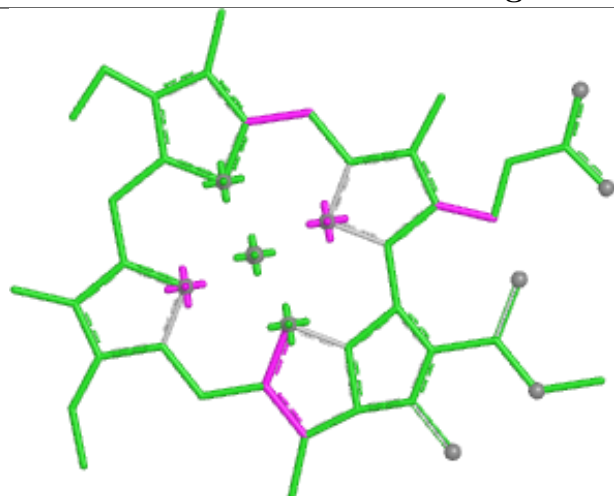




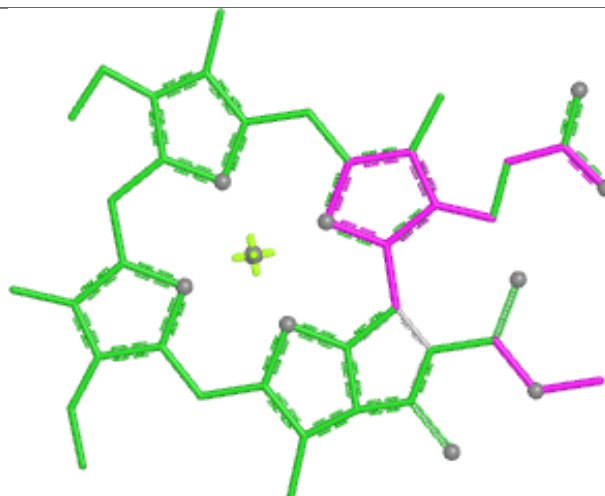
Ligand CLA C 1459



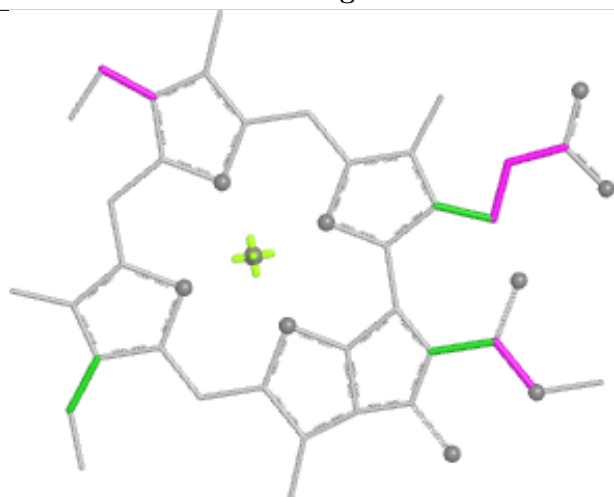
Ligand CLA B 1484



Bond lengths



Bond angles

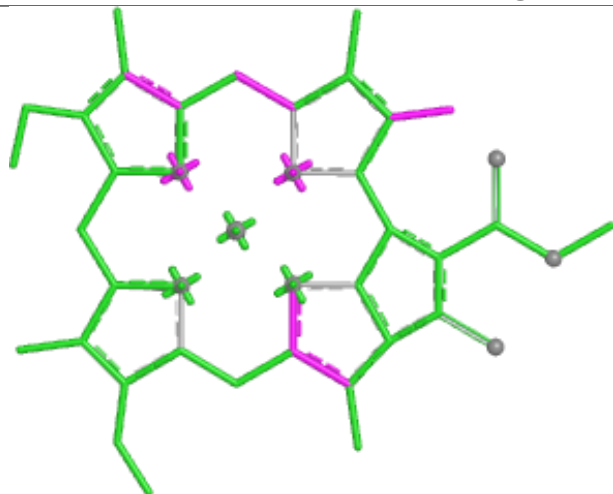


Torsions

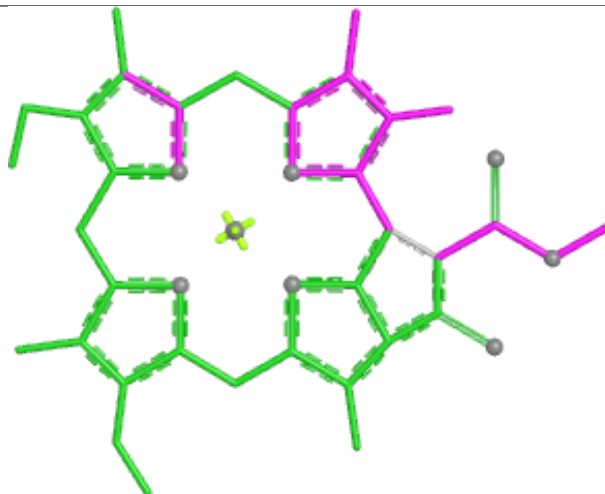


Rings

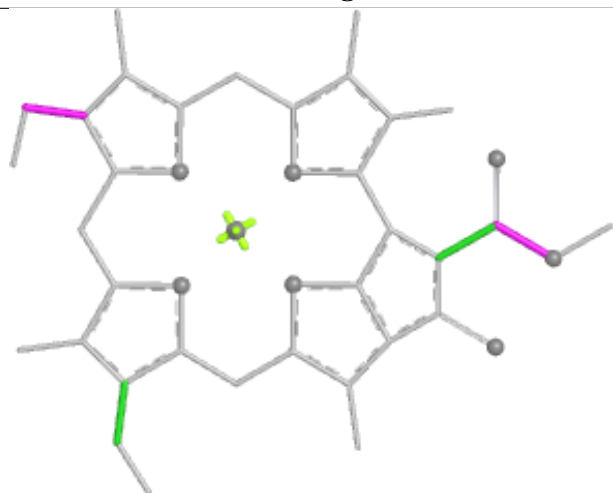
Ligand CLA I 1469



Bond lengths



Bond angles

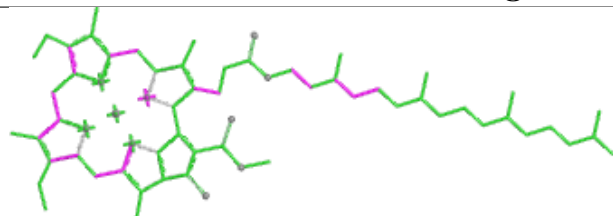


Torsions

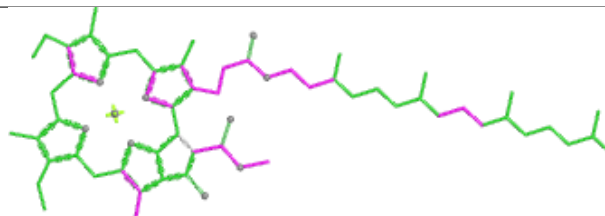


Rings

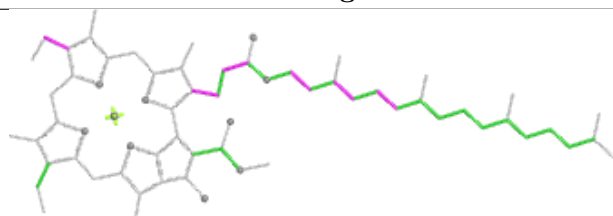
Ligand CLA H 1487



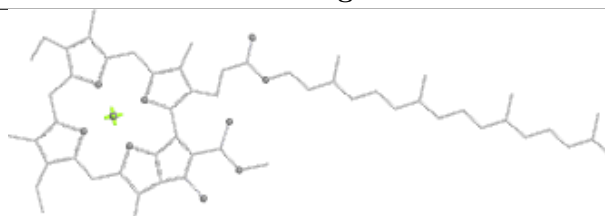
Bond lengths



Bond angles

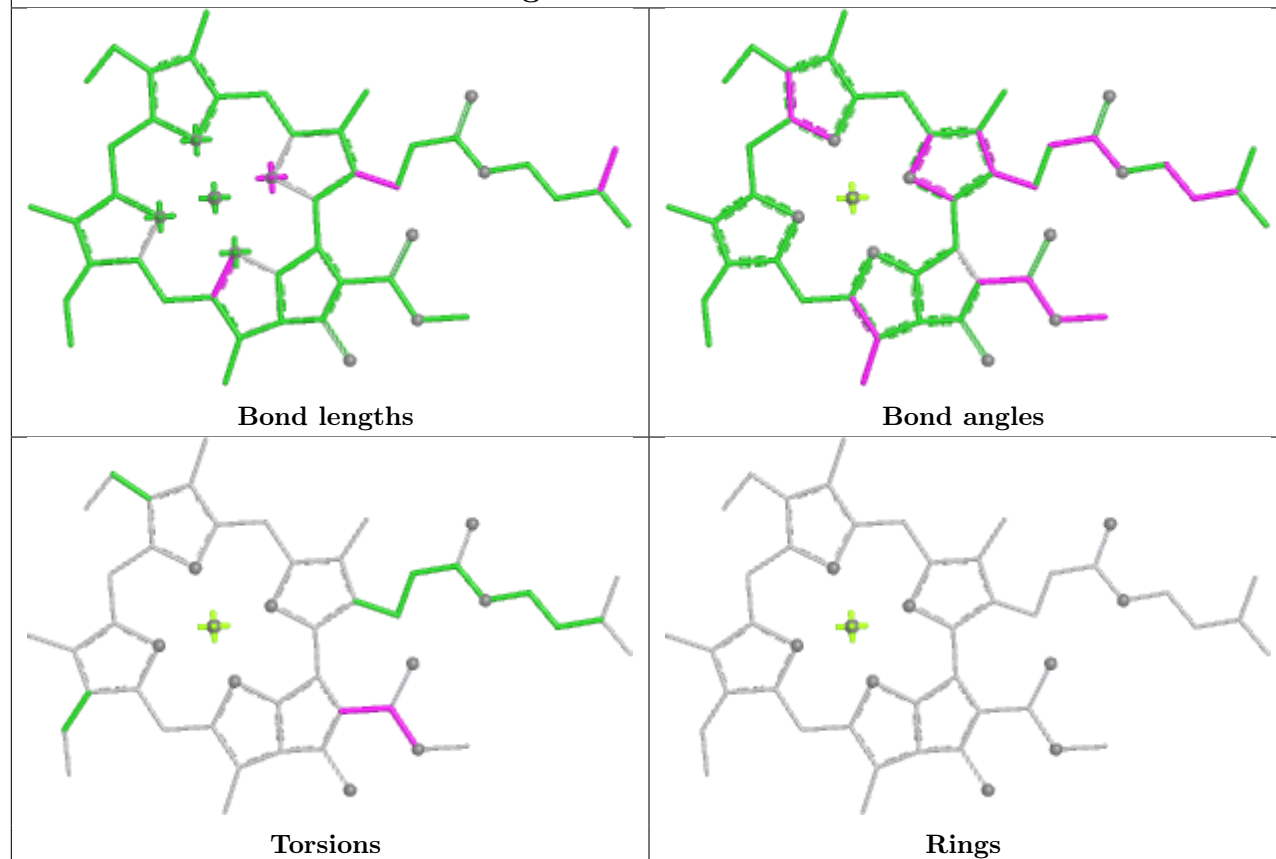


Torsions

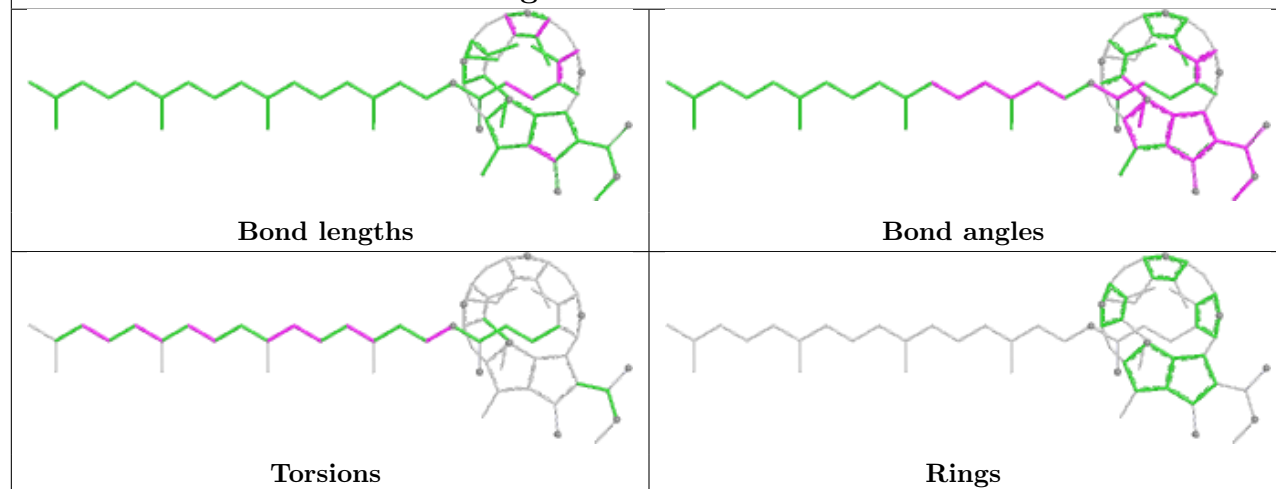


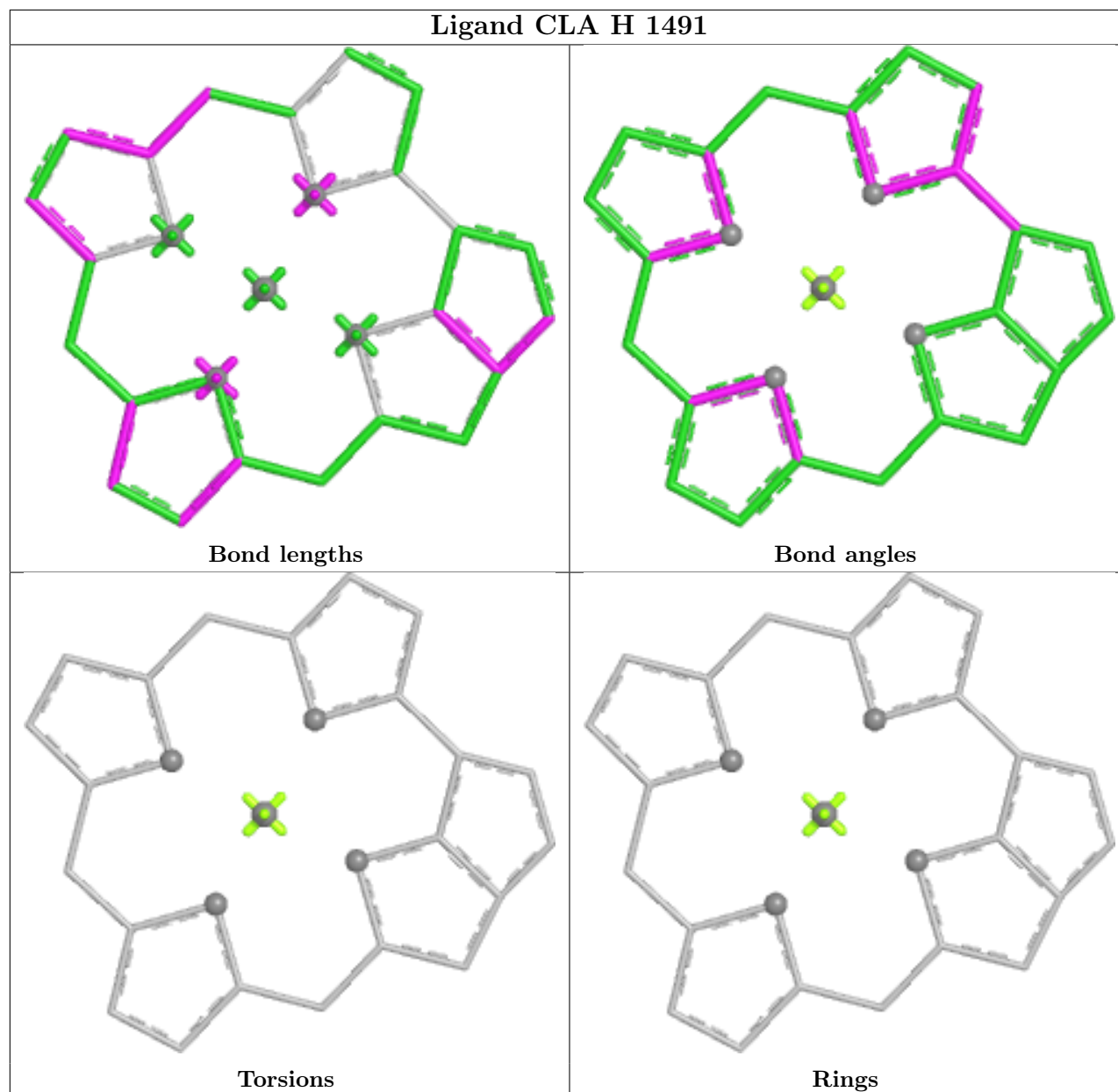
Rings

Ligand CLA H 1489



Ligand PHO A 1345





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	Y	11
10	X	11

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
7	O	5
7	P	5

The worst 5 of 32 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	185:UNK	C	200:UNK	N	108.56
1	X	185:UNK	C	200:UNK	N	108.51
1	X	374:UNK	C	400:UNK	N	87.82
1	Y	374:UNK	C	400:UNK	N	87.78
1	X	475:UNK	C	501:UNK	N	66.94

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.