wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 08:46 AM EDT

PDB ID	:	1W5C
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 (i) 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 (1)) were used in the production of this report:

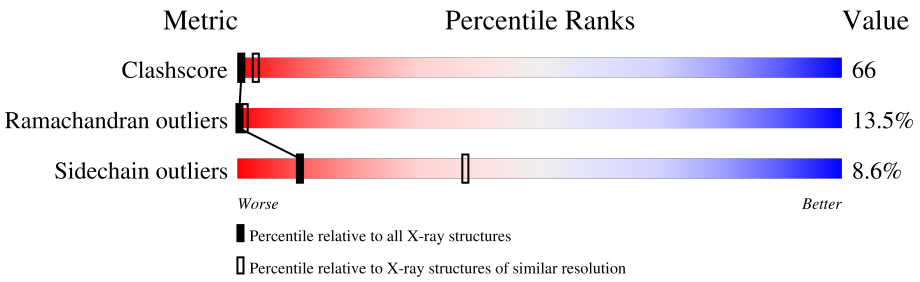
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	23% 54% 13% • 8%
1	G	360	25% 54% 12% • 8%
2	B	510	32% 49% 11% • 6%
2	H	510	32% 49% 11% • 6%
3	C	473	30% 49% 12% • 7%
3	I	473	29% 48% 14% • 7%
4	D	352	24% 59% 14% ••
4	J	352	26% 59% 14% ••

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Mol	Chain	Length	Quality of chain
5	E	84	24% 49% 14% • 10%
5	K	84	23% 49% 15% • 10%
6	F	44	14% 52% 14% 5% 16%
6	L	44	16% 45% 16% 7% 16%
7	O	179	68% 32%
7	P	179	66% 34%
8	S	100	43% 57%
8	U	100	39% 61%
9	T	163	56% 26% • 17%
9	V	163	53% 29% • 17%
10	X	359	52% 48%
10	Y	359	53% 47%

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 (i)

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
			Total	C	N	O	S			
1	A	332	2279	1505	370	390	14	0	0	31
1	G	332	2279	1505	370	390	14	0	0	31

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called UNASSIGNED SUBUNITS.

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

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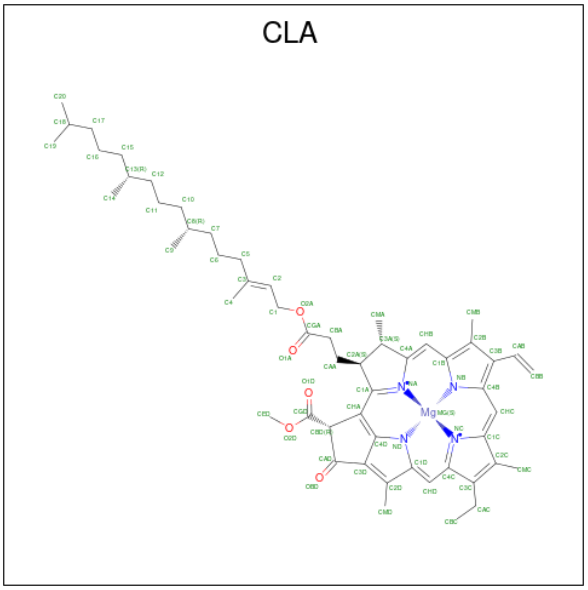
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	Y	359	1791	1073	359	359	0	0	0

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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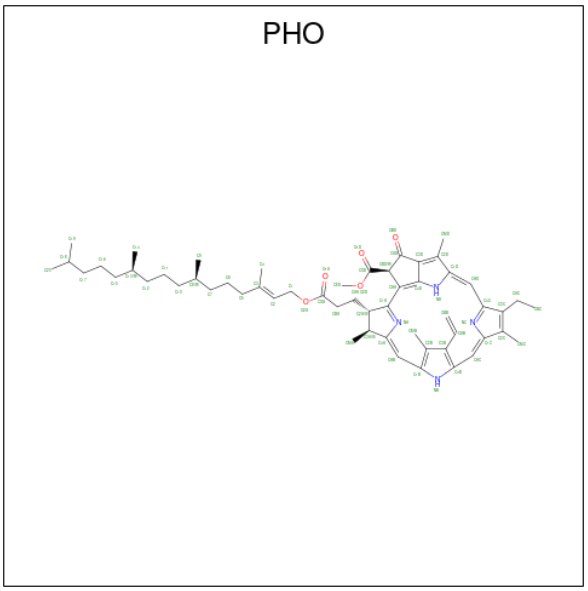
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total C Mg N O 55 45 1 4 5	0	0
11	H	1	Total C Mg N O 65 55 1 4 5	0	0
11	H	1	Total C Mg N O 41 33 1 4 3	0	0
11	I	1	Total C Mg N O 45 35 1 4 5	0	0
11	I	1	Total C Mg N O 47 37 1 4 5	0	0
11	I	1	Total C Mg N 27 22 1 4	0	0
11	I	1	Total C Mg N O 56 46 1 4 5	0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

- Molecule 12 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

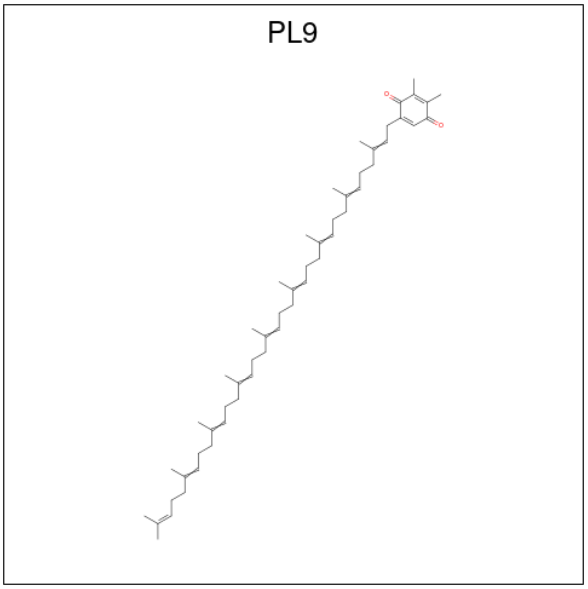
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
13	A	4	4	4	0	0
13	G	4	4	4	0	0

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

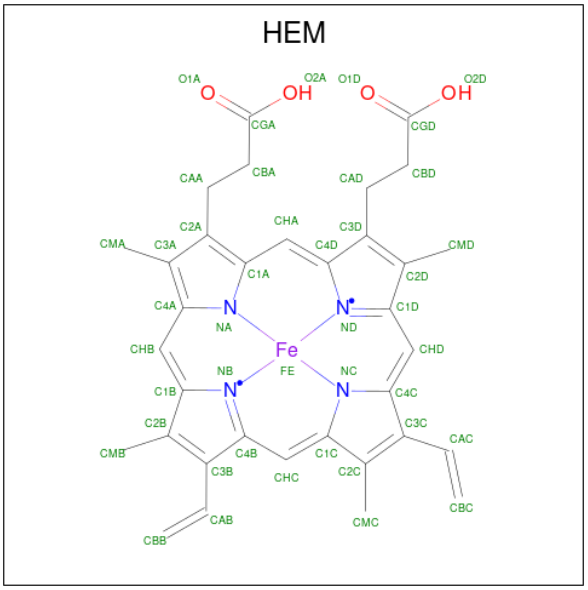
- Molecule 15 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,

3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



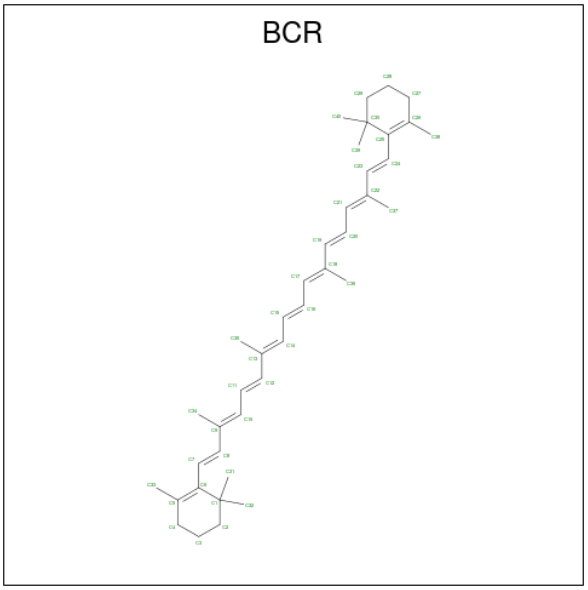
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C 6 6	0	0
15	J	1	Total C 6 6	0	0

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



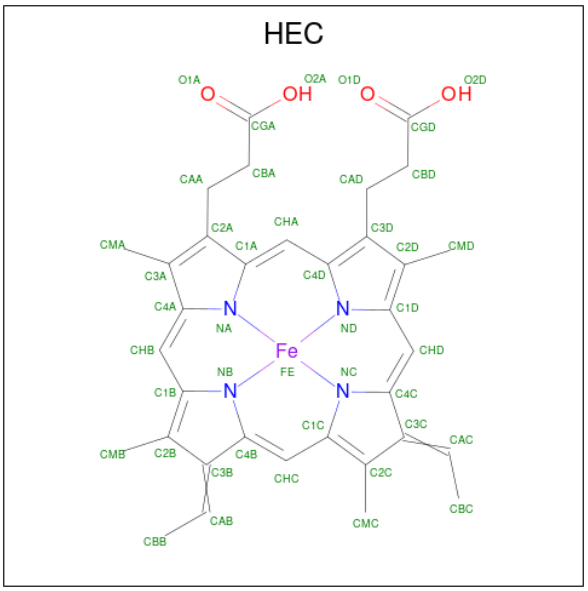
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Fe	N		
16	E	1	25	20	1	4	0	0
			Total	C	Fe	N		
16	L	1	25	20	1	4	0	0

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

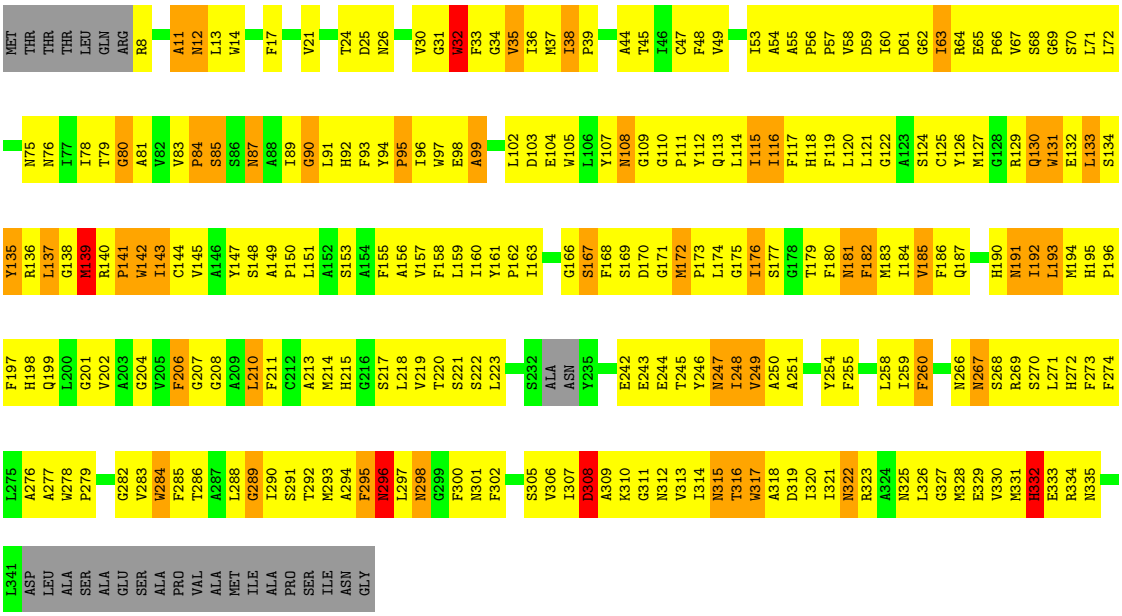
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

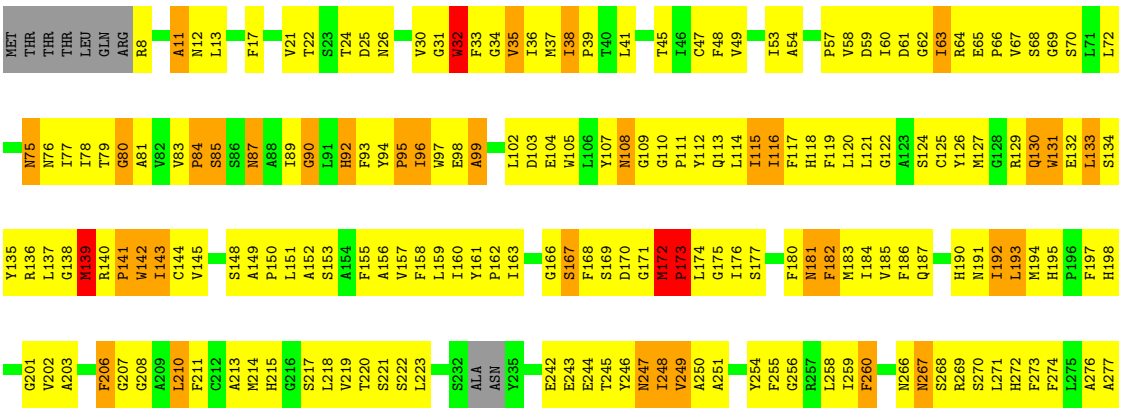
• Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

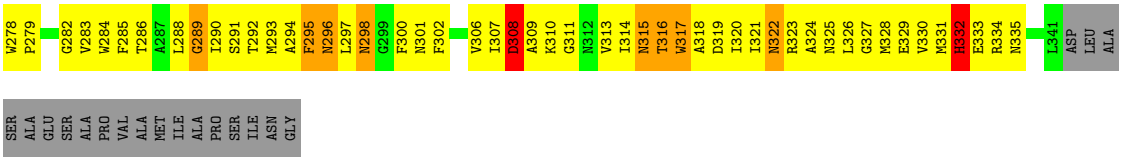
Chain A: 23% 54% 13% • 8%



• Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

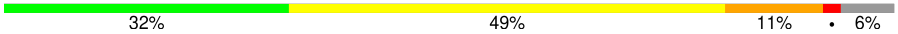
Chain G: 25% 54% 12% • 8%

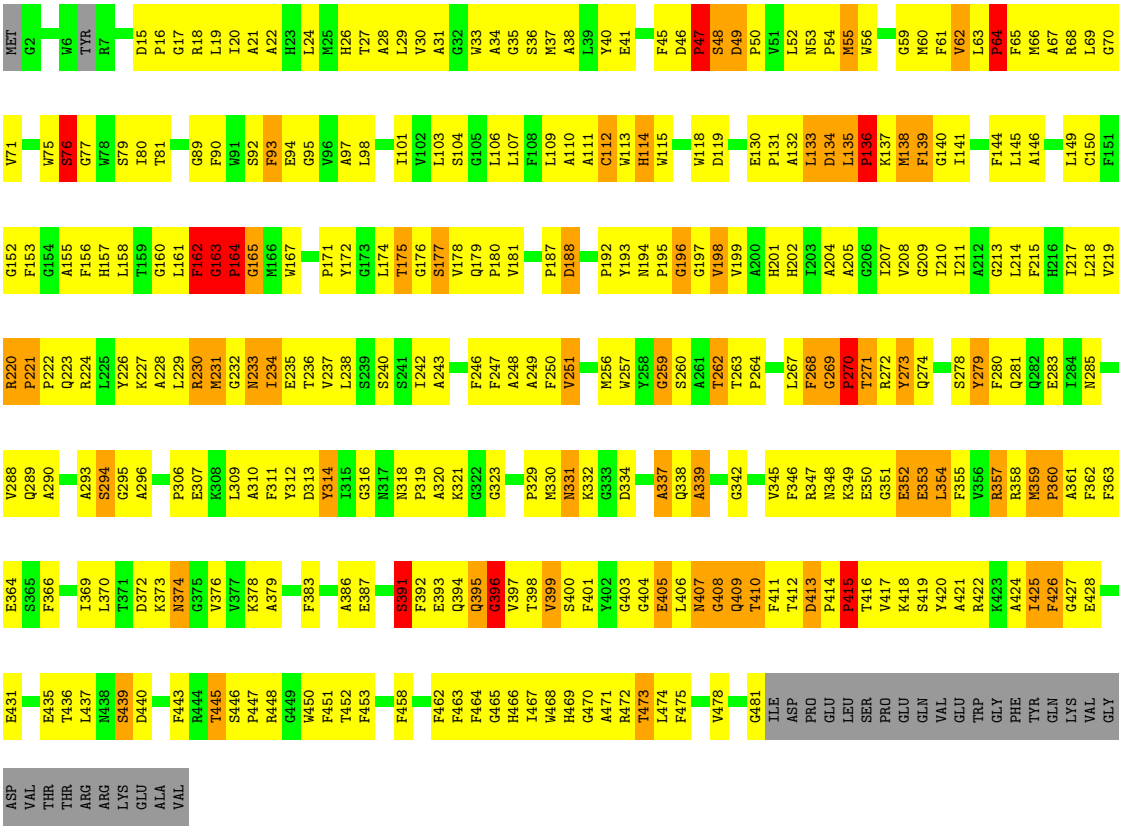




• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN

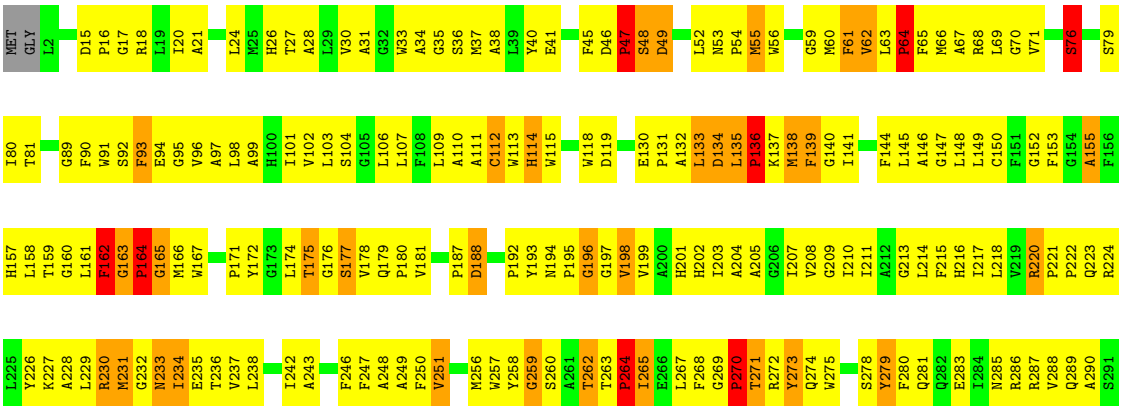
Chain B:

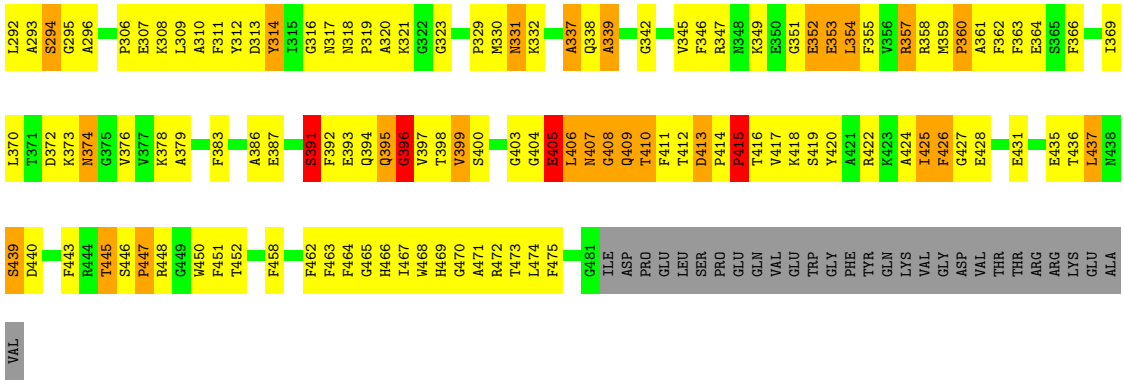




• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN

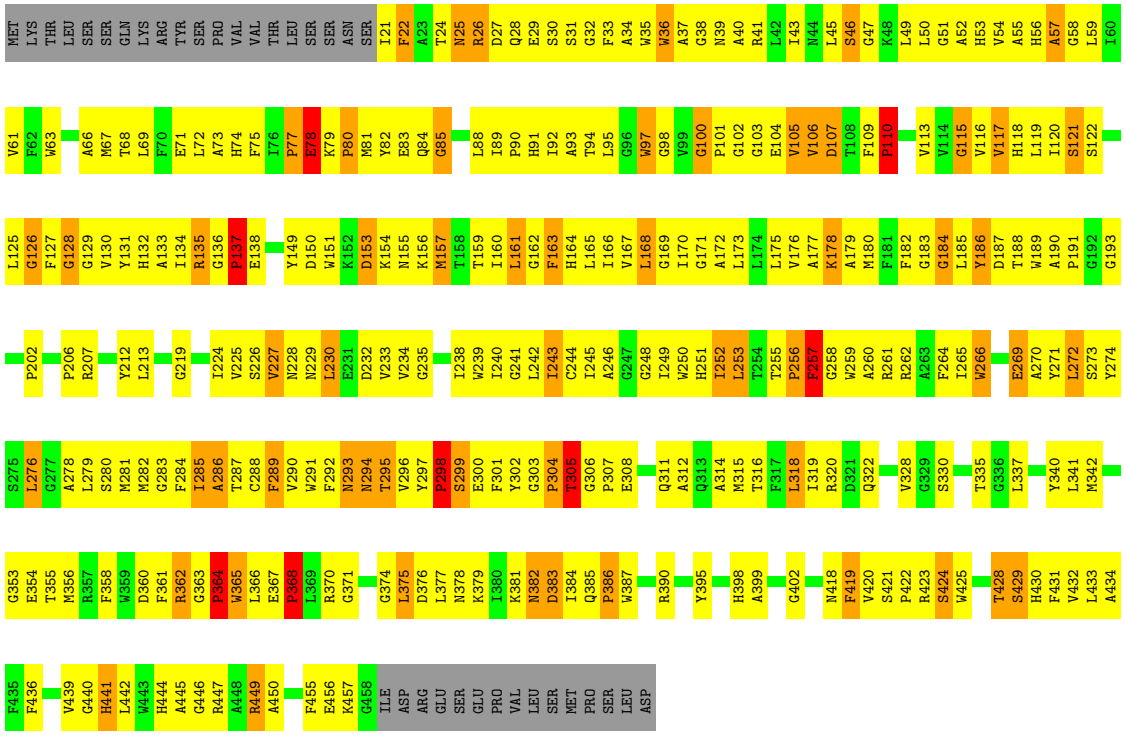
Chain H:





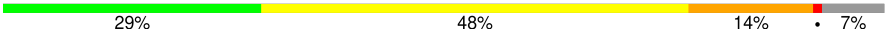
• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

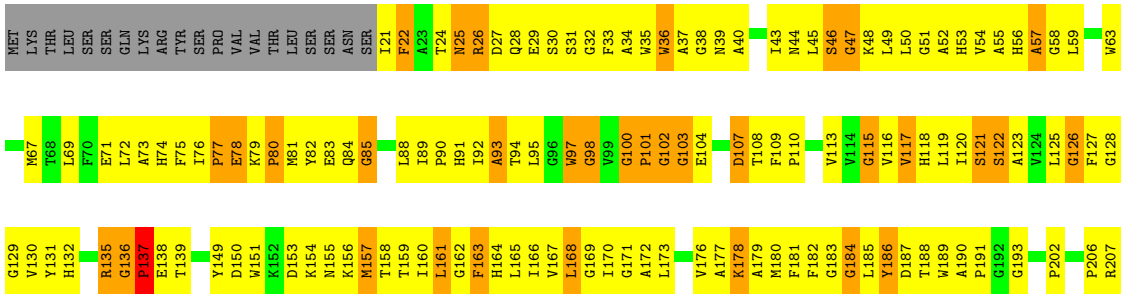
Chain C:

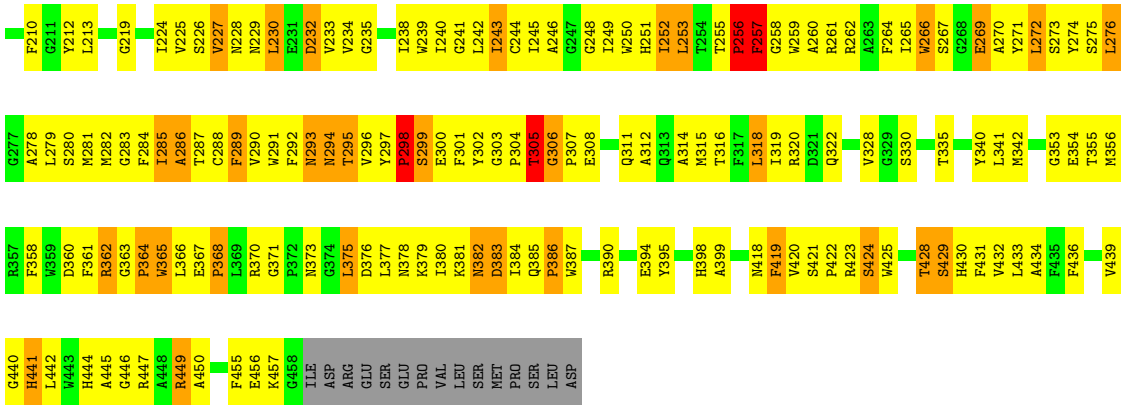


• Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

Chain I:

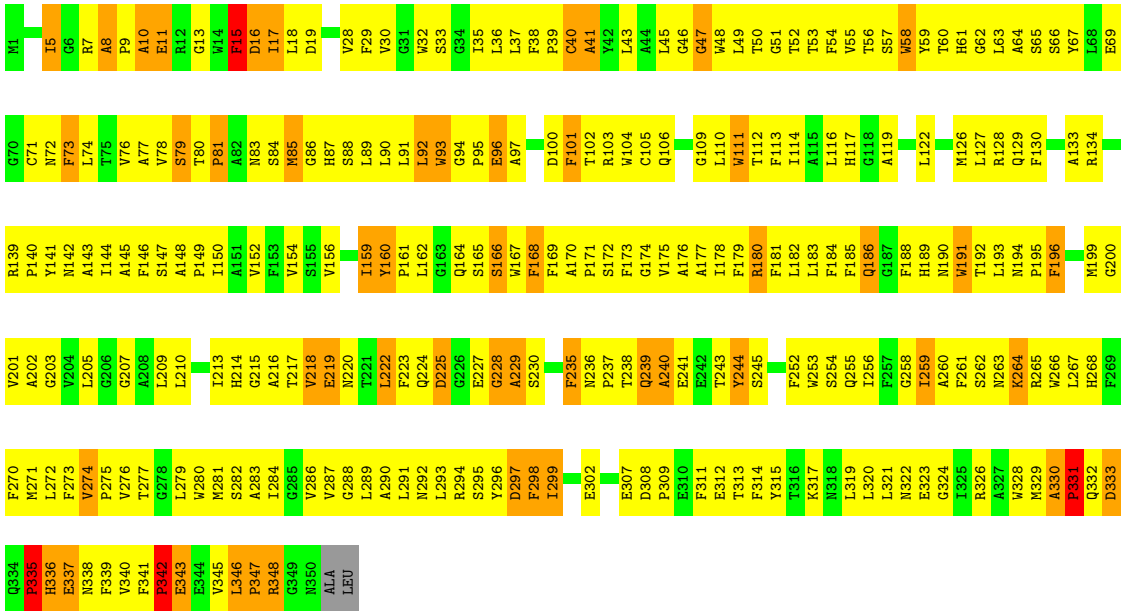






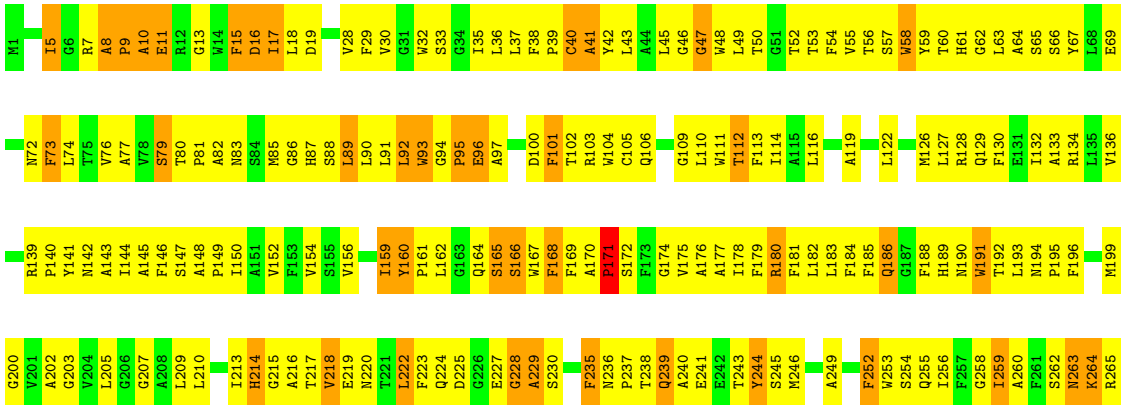
- Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

Chain D: 24% 59% 14% ••



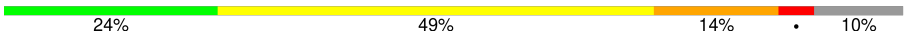
- Molecule 4: PHOTOSYSTEM II REACTION CENTER D2 PROTEIN

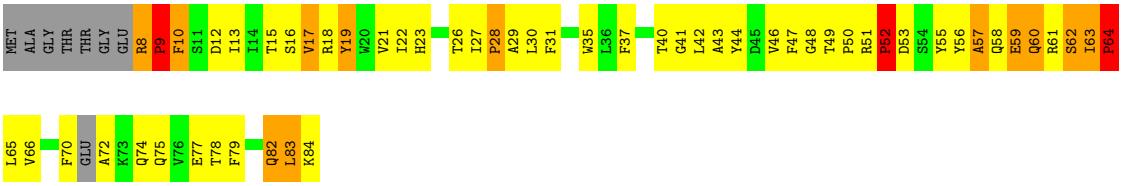
Chain J: 26% 59% 14% ••



• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

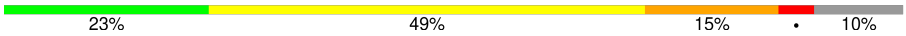
Chain E:





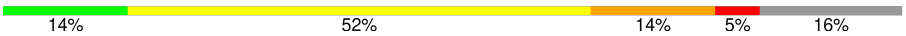
• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

Chain K:



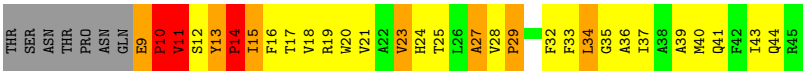
• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

Chain F:



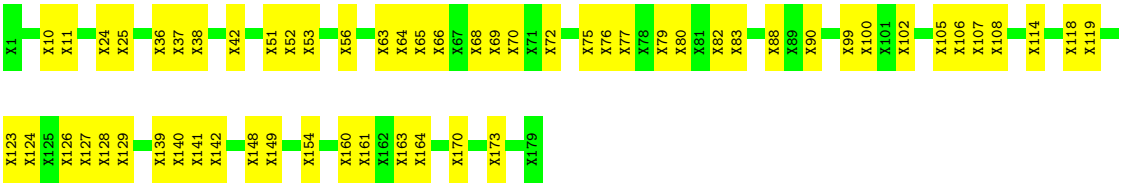
• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

Chain L:



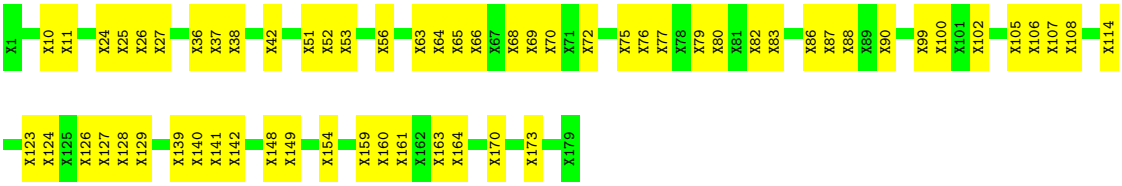
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE

Chain O:



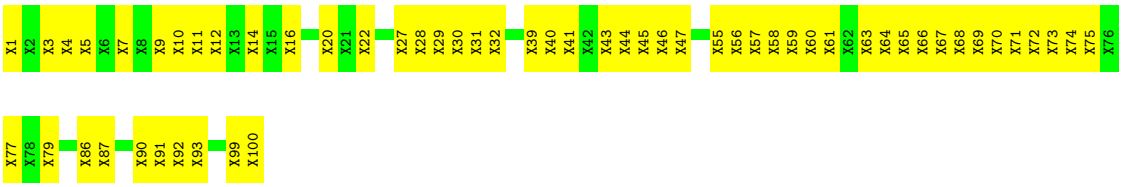
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE

Chain P: 66% 34%



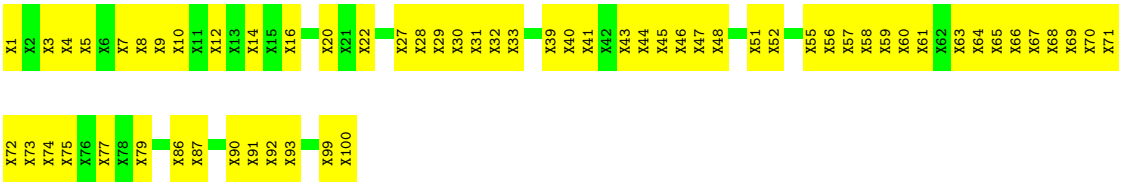
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

Chain S: 43% 57%



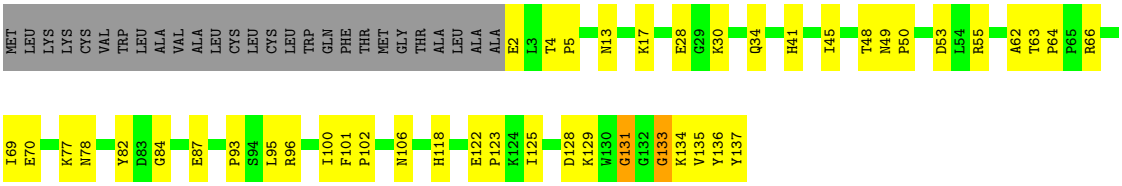
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

Chain U: 39% 61%



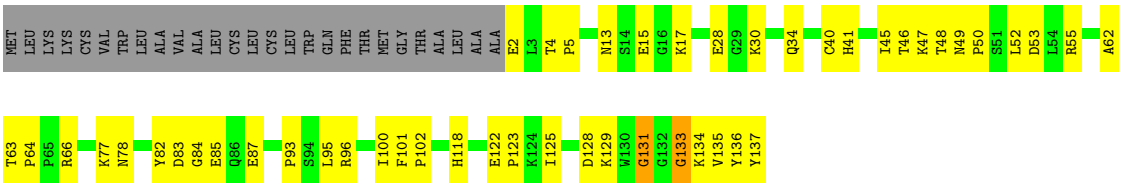
• Molecule 9: CYTOCHROME C-550

Chain T: 56% 26% • 17%



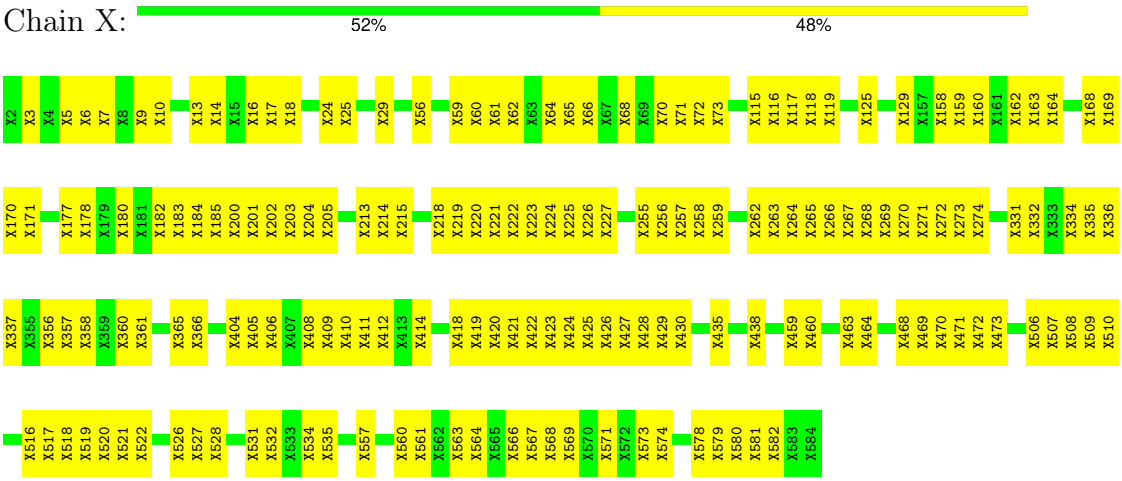
• Molecule 9: CYTOCHROME C-550

Chain V: 53% 29% • 17%



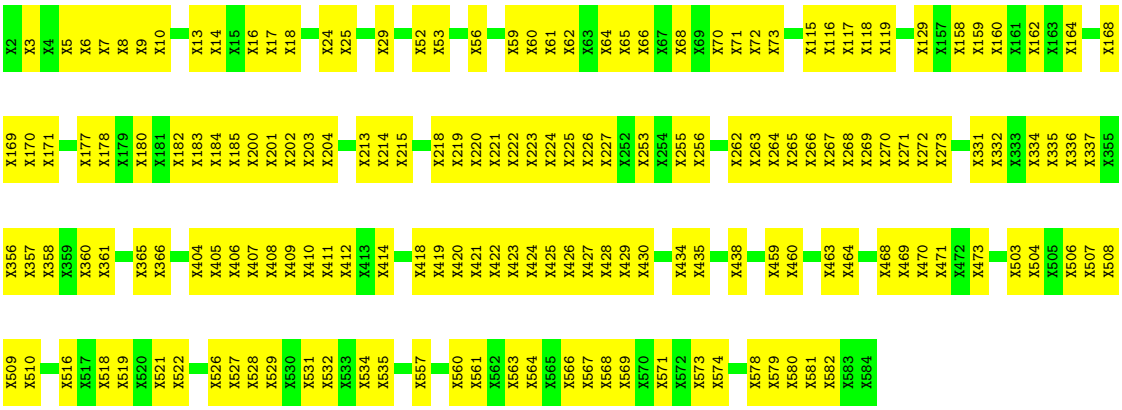
- Molecule 10: UNASSIGNED SUBUNITS

Chain X:



- Molecule 10: UNASSIGNED SUBUNITS

Chain Y:



4 Data and refinement statistics (i)

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: MN, BCR, PL9, CLA, FE2, PHO, 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	0.69	0/2315	0.88	1/3161 (0.0%)
1	G	0.66	0/2315	0.91	2/3161 (0.1%)
2	B	0.69	0/3081	0.98	9/4202 (0.2%)
2	H	0.67	0/3081	0.99	9/4202 (0.2%)
3	C	0.62	0/2806	0.90	3/3822 (0.1%)
3	I	0.62	0/2806	0.89	5/3822 (0.1%)
4	D	0.70	0/2688	0.96	4/3678 (0.1%)
4	J	0.69	0/2688	0.97	5/3678 (0.1%)
5	E	0.62	0/547	0.89	0/751
5	K	0.66	0/547	0.95	1/751 (0.1%)
6	F	0.77	0/307	1.19	4/421 (1.0%)
6	L	0.79	0/307	1.21	4/421 (1.0%)
9	T	0.65	0/1079	0.81	0/1466
9	V	0.69	0/1079	0.81	0/1466
All	All	0.67	0/25646	0.94	47/35002 (0.1%)

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

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	270	PRO	CA-N-CD	-14.97	90.54	111.50
2	B	270	PRO	CA-N-CD	-13.49	92.62	111.50
4	J	171	PRO	CA-N-CD	-11.70	95.12	111.50
2	B	47	PRO	CA-N-CD	-11.20	95.81	111.50
2	B	396	GLY	N-CA-C	-10.89	85.88	113.10

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 (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	2279	0	2113	445	0
1	G	2279	0	2113	452	0
2	B	3053	0	2666	441	0
2	H	3053	0	2666	456	0
3	C	2791	0	2530	447	0
3	I	2791	0	2530	445	0
4	D	2602	0	2383	463	0
4	J	2602	0	2383	473	0
5	E	536	0	480	87	0
5	K	536	0	480	91	0
6	F	297	0	304	56	0
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	59	0
9	V	1058	0	1066	62	0
10	X	1791	0	396	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	1791	0	393	135	0
11	A	222	0	207	37	0
11	B	846	0	774	84	0
11	C	598	0	458	69	0
11	D	115	0	111	19	0
11	G	222	0	207	33	0
11	H	846	0	774	91	0
11	I	598	0	458	69	0
11	J	115	0	111	16	0
12	A	64	0	74	14	0
12	D	54	0	51	4	0
12	G	64	0	74	17	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	3	0
18	V	43	0	31	2	0
All	All	35614	0	28078	4207	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 66.

The worst 5 of 4207 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 (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	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	1
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%)	10	44
9	V	134/163 (82%)	124 (92%)	8 (6%)	2 (2%)	10	44
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 (i)

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%)	201 (93%)	16 (7%)	13	46
1	G	217/291 (75%)	200 (92%)	17 (8%)	12	43
2	B	256/407 (63%)	232 (91%)	24 (9%)	8	33
2	H	256/407 (63%)	229 (90%)	27 (10%)	7	28
3	C	243/374 (65%)	213 (88%)	30 (12%)	4	21
3	I	243/374 (65%)	212 (87%)	31 (13%)	4	20
4	D	239/283 (84%)	223 (93%)	16 (7%)	16	50
4	J	239/283 (84%)	225 (94%)	14 (6%)	19	54
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	19
6	L	31/38 (82%)	26 (84%)	5 (16%)	2	11
9	T	117/138 (85%)	116 (99%)	1 (1%)	78	91
9	V	117/138 (85%)	116 (99%)	1 (1%)	78	91
All	All	2304/3208 (72%)	2106 (91%)	198 (9%)	10	38

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	49	ASP
3	I	108	THR
2	H	102	VAL
2	H	265	ILE
3	I	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	118	HIS

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Mol	Chain	Res	Type
9	T	118	HIS
2	H	289	GLN
9	T	106	ASN
4	J	224	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 monosaccharides 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	1495	-	53,63,73	2.02	12 (22%)	62,101,113	2.14	12 (19%)
11	CLA	H	1483	2	58,68,73	1.96	9 (15%)	68,107,113	1.73	9 (13%)
11	CLA	B	1491	-	28,35,73	2.57	8 (28%)	28,60,113	2.50	3 (10%)
11	CLA	B	1482	-	63,73,73	1.89	12 (19%)	74,113,113	2.00	9 (12%)
11	CLA	I	1471	-	39,49,73	2.68	5 (12%)	46,84,113	2.27	7 (15%)
11	CLA	I	1469	3	39,49,73	2.49	6 (15%)	46,84,113	2.40	7 (15%)
11	CLA	C	1467	3	45,55,73	2.31	7 (15%)	52,91,113	2.10	9 (17%)
11	CLA	A	1346	-	49,59,73	2.03	11 (22%)	56,96,113	2.04	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CLA	B	1490	2	43,53,73	2.89	11 (25%)	50,89,113	2.06	6 (12%)
11	CLA	H	1485	2	45,55,73	1.81	9 (20%)	52,91,113	1.87	7 (13%)
11	CLA	B	1486	2	39,49,73	2.46	8 (20%)	46,84,113	2.29	9 (19%)
11	CLA	J	1353	4	48,58,73	2.09	10 (20%)	56,95,113	1.92	8 (14%)
11	CLA	G	1342	1	63,73,73	1.68	11 (17%)	74,113,113	1.78	11 (14%)
11	CLA	G	1343	-	59,69,73	1.91	10 (16%)	69,108,113	2.01	10 (14%)
11	CLA	J	1351	4	63,73,73	2.56	11 (17%)	74,113,113	2.12	13 (17%)
11	CLA	B	1483	2	58,68,73	2.05	8 (13%)	68,107,113	1.79	9 (13%)
11	CLA	I	1468	3	28,35,73	3.03	9 (32%)	28,60,113	2.45	4 (14%)
11	CLA	H	1494	-	63,73,73	1.94	10 (15%)	74,113,113	1.95	11 (14%)
11	CLA	C	1465	-	63,73,73	1.58	8 (12%)	74,113,113	1.83	12 (16%)
11	CLA	B	1484	-	43,53,73	1.98	8 (18%)	50,89,113	2.05	8 (16%)
11	CLA	I	1470	-	39,49,73	2.37	9 (23%)	46,84,113	2.18	8 (17%)
11	CLA	H	1488	-	63,73,73	1.79	13 (20%)	74,113,113	1.82	9 (12%)
11	CLA	B	1497	2	39,49,73	2.19	11 (28%)	46,84,113	2.22	8 (17%)
11	CLA	H	1487	-	63,73,73	1.75	12 (19%)	74,113,113	1.78	12 (16%)
17	BCR	L	1047	-	41,41,41	1.66	7 (17%)	56,56,56	2.21	22 (39%)
11	CLA	H	1493	-	43,53,73	2.17	9 (20%)	50,89,113	2.25	10 (20%)
11	CLA	C	1461	3	28,35,73	3.14	12 (42%)	28,60,113	2.44	4 (14%)
11	CLA	H	1495	-	53,63,73	2.05	11 (20%)	62,101,113	2.21	12 (19%)
11	CLA	C	1462	-	54,64,73	1.87	12 (22%)	63,102,113	1.87	13 (20%)
11	CLA	A	1343	-	59,69,73	1.87	6 (10%)	69,108,113	1.95	12 (17%)
11	CLA	D	1353	4	48,58,73	2.12	11 (22%)	56,95,113	1.99	10 (17%)
12	PHO	D	1352	-	40,59,69	1.25	5 (12%)	36,87,99	1.78	12 (33%)
11	CLA	I	1459	3	43,53,73	2.18	7 (16%)	50,89,113	2.18	9 (18%)
11	CLA	H	1482	-	63,73,73	2.13	11 (17%)	74,113,113	2.02	11 (14%)
11	CLA	B	1487	-	63,73,73	1.74	12 (19%)	74,113,113	1.78	13 (17%)
18	HEC	T	1138	9	32,50,50	2.05	11 (34%)	30,82,82	2.36	7 (23%)
11	CLA	B	1493	-	43,53,73	2.26	7 (16%)	50,89,113	2.22	9 (18%)
11	CLA	B	1488	-	63,73,73	1.75	12 (19%)	74,113,113	1.84	11 (14%)
17	BCR	F	1046	-	41,41,41	1.71	8 (19%)	56,56,56	2.21	24 (42%)
11	CLA	H	1484	-	43,53,73	1.86	7 (16%)	50,89,113	1.99	8 (16%)
11	CLA	C	1463	3	53,63,73	2.29	11 (20%)	62,101,113	2.06	9 (14%)
11	CLA	C	1471	-	39,49,73	2.47	7 (17%)	46,84,113	2.23	5 (10%)
11	CLA	B	1492	2	63,73,73	1.73	9 (14%)	74,113,113	2.04	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CLA	H	1491	-	28,35,73	2.66	10 (35%)	28,60,113	2.35	3 (10%)
11	CLA	C	1468	3	28,35,73	3.03	11 (39%)	28,60,113	2.53	4 (14%)
11	CLA	C	1470	-	39,49,73	2.44	8 (20%)	46,84,113	2.29	7 (15%)
11	CLA	H	1492	2	63,73,73	1.64	7 (11%)	74,113,113	2.02	12 (16%)
11	CLA	C	1459	3	43,53,73	2.18	9 (20%)	50,89,113	2.01	10 (20%)
16	HEM	E	1085	6,5	22,32,50	2.40	10 (45%)	25,54,82	1.56	3 (12%)
16	HEM	L	1046	6,5	22,32,50	2.20	8 (36%)	25,54,82	1.52	4 (16%)
15	PL9	J	1354	-	6,6,55	1.96	2 (33%)	6,6,69	1.09	0
11	CLA	B	1489	2	48,58,73	2.01	7 (14%)	56,95,113	2.15	10 (17%)
11	CLA	G	1346	-	49,59,73	2.19	10 (20%)	56,96,113	2.01	9 (16%)
11	CLA	I	1465	-	63,73,73	1.68	8 (12%)	74,113,113	1.84	12 (16%)
11	CLA	H	1489	2	48,58,73	1.98	7 (14%)	56,95,113	2.25	9 (16%)
11	CLA	A	1344	-	43,53,73	2.01	7 (16%)	50,89,113	2.13	9 (18%)
12	PHO	G	1345	-	50,69,69	0.94	3 (6%)	48,99,99	1.72	10 (20%)
11	CLA	C	1460	3	45,55,73	2.22	7 (15%)	52,91,113	2.12	9 (17%)
15	PL9	D	1354	-	6,6,55	2.06	2 (33%)	6,6,69	1.06	0
11	CLA	H	1486	2	39,49,73	2.25	8 (20%)	46,84,113	2.19	8 (17%)
11	CLA	C	1464	3	54,64,73	1.83	8 (14%)	63,102,113	2.01	13 (20%)
11	CLA	H	1497	2	39,49,73	2.23	13 (33%)	46,84,113	2.29	8 (17%)
12	PHO	A	1345	-	50,69,69	0.92	3 (6%)	48,99,99	1.70	11 (22%)
11	CLA	B	1496	-	63,73,73	1.89	7 (11%)	74,113,113	1.88	11 (14%)
12	PHO	J	1352	-	40,59,69	1.23	2 (5%)	36,87,99	1.79	11 (30%)
11	CLA	G	1344	-	43,53,73	2.01	7 (16%)	50,89,113	2.11	9 (18%)
11	CLA	H	1496	-	63,73,73	1.97	10 (15%)	74,113,113	1.99	12 (16%)
11	CLA	I	1464	3	54,64,73	1.88	10 (18%)	63,102,113	1.95	12 (19%)
11	CLA	I	1467	3	45,55,73	2.10	4 (8%)	52,91,113	2.08	8 (15%)
11	CLA	A	1342	1	63,73,73	1.64	9 (14%)	74,113,113	1.90	13 (17%)
11	CLA	B	1485	2	45,55,73	1.88	7 (15%)	52,91,113	1.92	7 (13%)
11	CLA	D	1351	4	63,73,73	1.96	10 (15%)	74,113,113	2.05	13 (17%)
11	CLA	I	1463	3	53,63,73	2.28	10 (18%)	62,101,113	2.12	9 (14%)
11	CLA	I	1462	-	54,64,73	1.99	13 (24%)	63,102,113	1.88	13 (20%)
18	HEC	V	1138	9	32,50,50	2.00	7 (21%)	30,82,82	2.37	5 (16%)
11	CLA	I	1460	3	45,55,73	2.05	9 (20%)	52,91,113	2.04	7 (13%)
11	CLA	H	1490	2	43,53,73	2.75	11 (25%)	50,89,113	2.15	7 (14%)
11	CLA	I	1461	3	28,35,73	3.06	13 (46%)	28,60,113	2.37	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CLA	C	1466	3	48,58,73	2.12	10 (20%)	56,95,113	2.14	11 (19%)
11	CLA	B	1494	-	63,73,73	1.95	10 (15%)	74,113,113	1.82	9 (12%)
11	CLA	C	1469	3	39,49,73	2.46	6 (15%)	46,84,113	2.35	7 (15%)
11	CLA	I	1466	3	48,58,73	2.00	8 (16%)	56,95,113	2.13	10 (17%)

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	1495	-	1/1/13/20	9/25/103/115	-
11	CLA	H	1483	2	1/1/14/20	10/31/109/115	-
11	CLA	B	1491	-	1/1/5/20	-	-
11	CLA	B	1482	-	1/1/15/20	9/37/115/115	-
11	CLA	I	1471	-	1/1/10/20	4/8/86/115	-
11	CLA	I	1469	3	1/1/10/20	2/8/86/115	-
11	CLA	C	1467	3	1/1/11/20	6/16/94/115	-
11	CLA	A	1346	-	1/1/12/20	6/21/99/115	-
11	CLA	B	1490	2	1/1/11/20	8/13/91/115	-
11	CLA	H	1485	2	1/1/11/20	7/16/94/115	-
11	CLA	B	1486	2	1/1/10/20	4/8/86/115	-
11	CLA	J	1353	4	1/1/12/20	3/19/97/115	-
11	CLA	G	1342	1	1/1/15/20	3/37/115/115	-
11	CLA	G	1343	-	1/1/14/20	15/33/111/115	-
11	CLA	J	1351	4	1/1/15/20	12/37/115/115	-
11	CLA	B	1483	2	1/1/14/20	10/31/109/115	-
11	CLA	I	1468	3	1/1/5/20	-	-
11	CLA	H	1494	-	1/1/15/20	9/37/115/115	-
11	CLA	C	1465	-	1/1/15/20	15/37/115/115	-
11	CLA	B	1484	-	1/1/11/20	4/13/91/115	-
11	CLA	I	1470	-	1/1/10/20	2/8/86/115	-
11	CLA	H	1488	-	1/1/15/20	13/37/115/115	-
11	CLA	B	1497	2	1/1/10/20	4/8/86/115	-
11	CLA	H	1487	-	1/1/15/20	8/37/115/115	-
17	BCR	L	1047	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	H	1493	-	1/1/11/20	6/13/91/115	-
11	CLA	C	1461	3	1/1/5/20	-	-
11	CLA	H	1495	-	1/1/13/20	9/25/103/115	-
11	CLA	C	1462	-	1/1/13/20	6/27/105/115	-
11	CLA	A	1343	-	1/1/14/20	15/33/111/115	-
11	CLA	D	1353	4	1/1/12/20	3/19/97/115	-
12	PHO	D	1352	-	-	7/25/91/103	0/5/6/6
11	CLA	I	1459	3	1/1/11/20	7/13/91/115	-
11	CLA	H	1482	-	1/1/15/20	11/37/115/115	-
11	CLA	B	1487	-	1/1/15/20	8/37/115/115	-
18	HEC	T	1138	9	-	4/10/54/54	-
11	CLA	B	1493	-	1/1/11/20	6/13/91/115	-
11	CLA	B	1488	-	1/1/15/20	14/37/115/115	-
17	BCR	F	1046	-	-	3/29/63/63	0/2/2/2
11	CLA	H	1484	-	1/1/11/20	4/13/91/115	-
11	CLA	C	1463	3	1/1/13/20	9/25/103/115	-
11	CLA	C	1471	-	1/1/10/20	4/8/86/115	-
11	CLA	B	1492	2	1/1/15/20	13/37/115/115	-
11	CLA	H	1491	-	1/1/5/20	-	-
11	CLA	C	1468	3	1/1/5/20	-	-
11	CLA	C	1470	-	1/1/10/20	2/8/86/115	-
11	CLA	H	1492	2	1/1/15/20	13/37/115/115	-
11	CLA	C	1459	3	1/1/11/20	7/13/91/115	-
15	PL9	J	1354	-	-	-	0/1/1/1
11	CLA	B	1489	2	1/1/12/20	3/19/97/115	-
11	CLA	G	1346	-	1/1/12/20	5/21/99/115	-
11	CLA	I	1465	-	1/1/15/20	14/37/115/115	-
11	CLA	H	1489	2	1/1/12/20	3/19/97/115	-
11	CLA	A	1344	-	1/1/11/20	5/13/91/115	-
12	PHO	G	1345	-	-	12/37/103/103	0/5/6/6
11	CLA	C	1460	3	1/1/11/20	3/16/94/115	-
15	PL9	D	1354	-	-	-	0/1/1/1
11	CLA	H	1486	2	1/1/10/20	4/8/86/115	-
11	CLA	C	1464	3	1/1/13/20	13/27/105/115	-
11	CLA	H	1497	2	1/1/10/20	4/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PHO	A	1345	-	-	10/37/103/103	0/5/6/6
11	CLA	B	1496	-	1/1/15/20	16/37/115/115	-
12	PHO	J	1352	-	-	7/25/91/103	0/5/6/6
11	CLA	G	1344	-	1/1/11/20	5/13/91/115	-
11	CLA	H	1496	-	1/1/15/20	15/37/115/115	-
11	CLA	I	1464	3	1/1/13/20	13/27/105/115	-
11	CLA	I	1467	3	1/1/11/20	7/16/94/115	-
11	CLA	A	1342	1	1/1/15/20	3/37/115/115	-
11	CLA	B	1485	2	1/1/11/20	7/16/94/115	-
11	CLA	D	1351	4	1/1/15/20	11/37/115/115	-
11	CLA	I	1463	3	2/2/13/20	9/25/103/115	-
11	CLA	I	1462	-	1/1/13/20	6/27/105/115	-
18	HEC	V	1138	9	-	5/10/54/54	-
11	CLA	I	1460	3	1/1/11/20	4/16/94/115	-
11	CLA	H	1490	2	1/1/11/20	8/13/91/115	-
11	CLA	I	1461	3	1/1/5/20	-	-
11	CLA	C	1466	3	1/1/12/20	7/19/97/115	-
11	CLA	B	1494	-	1/1/15/20	8/37/115/115	-
11	CLA	C	1469	3	1/1/10/20	2/8/86/115	-
11	CLA	I	1466	3	1/1/12/20	7/19/97/115	-

The worst 5 of 714 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	I	1471	CLA	CHB-C4A	13.48	1.45	1.33
11	B	1490	CLA	CHB-C4A	12.61	1.44	1.33
11	C	1469	CLA	CHB-C4A	12.31	1.44	1.33
11	H	1496	CLA	CHB-C4A	12.18	1.44	1.33

The worst 5 of 754 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 533 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1343	CLA	C1A-C2A-CAA-CBA
11	A	1343	CLA	CBD-CGD-O2D-CED
11	A	1344	CLA	CAD-CBD-CGD-O2D
11	A	1346	CLA	C2-C3-C5-C6
11	A	1346	CLA	C4-C3-C5-C6

There are no ring outliers.

78 monomers are involved in 469 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1495	CLA	3	0
11	H	1483	CLA	4	0
11	B	1491	CLA	3	0
11	B	1482	CLA	1	0
11	I	1471	CLA	5	0
11	I	1469	CLA	5	0
11	C	1467	CLA	8	0
11	A	1346	CLA	7	0
11	B	1490	CLA	3	0
11	H	1485	CLA	6	0
11	B	1486	CLA	13	0
11	J	1353	CLA	5	0
11	G	1342	CLA	19	0
11	G	1343	CLA	4	0
11	J	1351	CLA	11	0
11	B	1483	CLA	5	0
11	H	1494	CLA	3	0
11	C	1465	CLA	5	0
11	B	1484	CLA	7	0
11	I	1470	CLA	4	0
11	H	1488	CLA	13	0
11	B	1497	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	1487	CLA	6	0
17	L	1047	BCR	3	0
11	H	1493	CLA	2	0
11	H	1495	CLA	2	0
11	C	1462	CLA	3	0
11	A	1343	CLA	8	0
11	D	1353	CLA	6	0
12	D	1352	PHO	4	0
11	I	1459	CLA	5	0
11	H	1482	CLA	2	0
11	B	1487	CLA	8	0
18	T	1138	HEC	3	0
11	B	1493	CLA	1	0
11	B	1488	CLA	7	0
17	F	1046	BCR	4	0
11	H	1484	CLA	8	0
11	C	1463	CLA	8	0
11	C	1471	CLA	5	0
11	B	1492	CLA	5	0
11	H	1491	CLA	2	0
11	C	1470	CLA	5	0
11	H	1492	CLA	6	0
11	C	1459	CLA	6	0
16	E	1085	HEM	2	0
16	L	1046	HEM	2	0
15	J	1354	PL9	1	0
11	B	1489	CLA	4	0
11	G	1346	CLA	6	0
11	I	1465	CLA	9	0
11	H	1489	CLA	4	0
11	A	1344	CLA	6	0
12	G	1345	PHO	17	0
11	C	1460	CLA	4	0
15	D	1354	PL9	1	0
11	H	1486	CLA	15	0
11	C	1464	CLA	9	0
11	H	1497	CLA	10	0
12	A	1345	PHO	14	0
11	B	1496	CLA	15	0
12	J	1352	PHO	9	0
11	G	1344	CLA	6	0
11	H	1496	CLA	15	0

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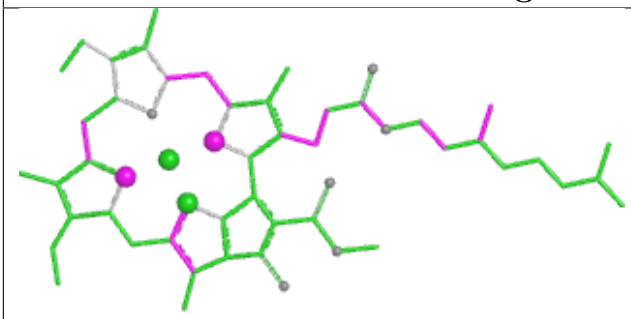
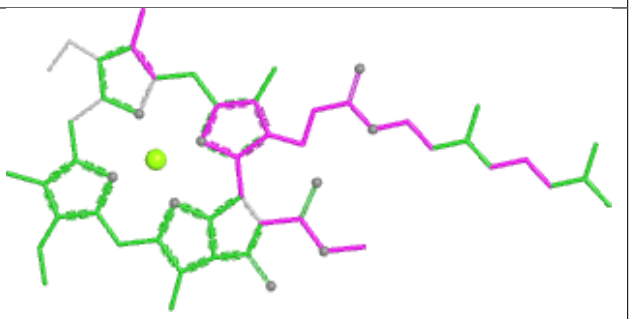
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	1464	CLA	11	0
11	I	1467	CLA	7	0
11	A	1342	CLA	18	0
11	B	1485	CLA	5	0
11	D	1351	CLA	13	0
11	I	1463	CLA	9	0
11	I	1462	CLA	4	0
18	V	1138	HEC	2	0
11	I	1460	CLA	4	0
11	H	1490	CLA	3	0
11	C	1466	CLA	10	0
11	B	1494	CLA	3	0
11	C	1469	CLA	7	0
11	I	1466	CLA	10	0

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 then 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.

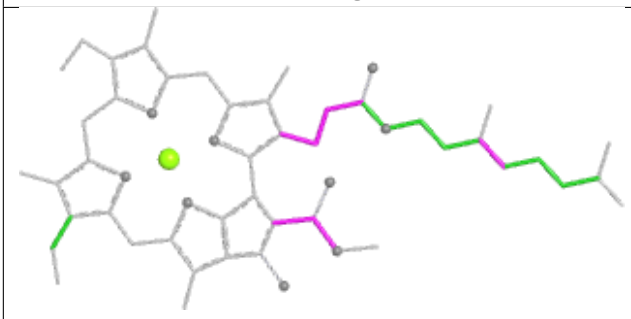
Ligand CLA B 1495



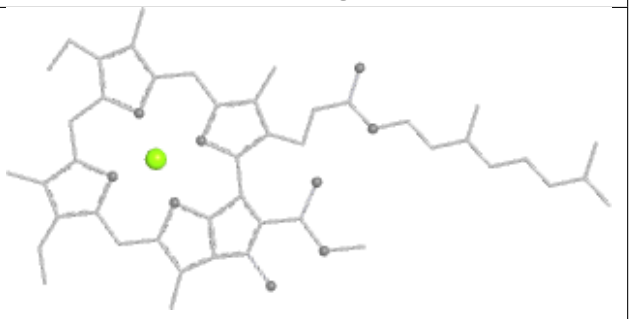
Bond lengths



Bond angles

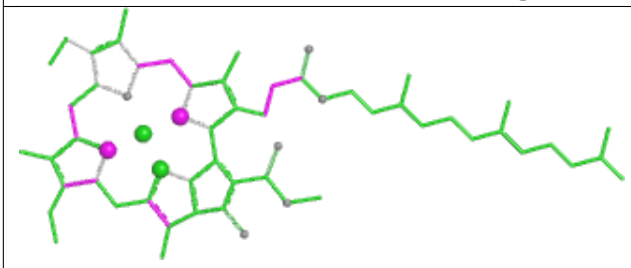


Torsions

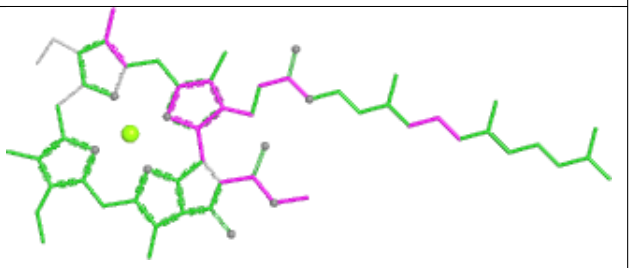


Rings

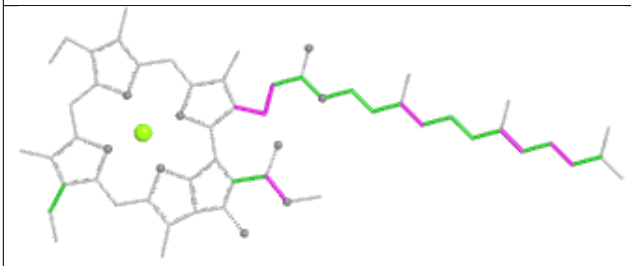
Ligand CLA H 1483



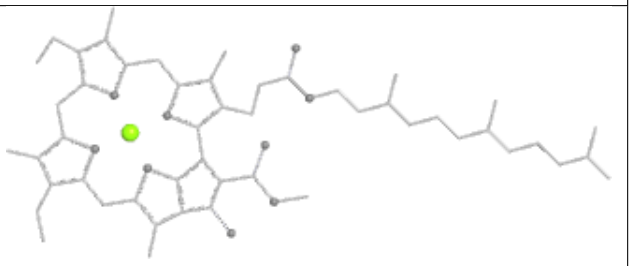
Bond lengths



Bond angles

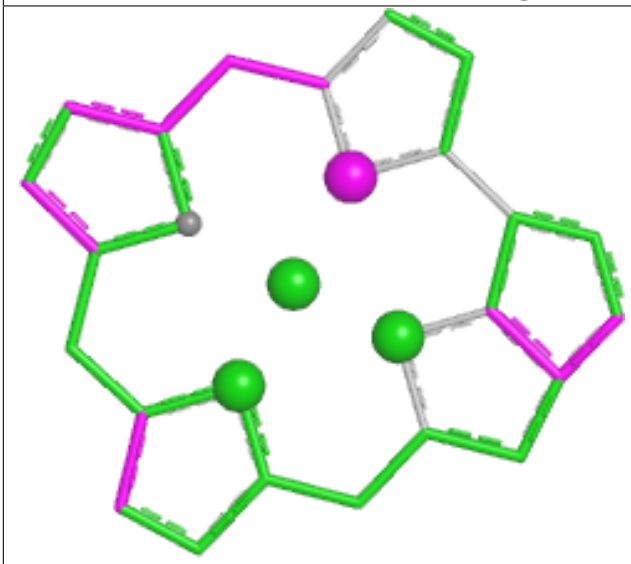


Torsions

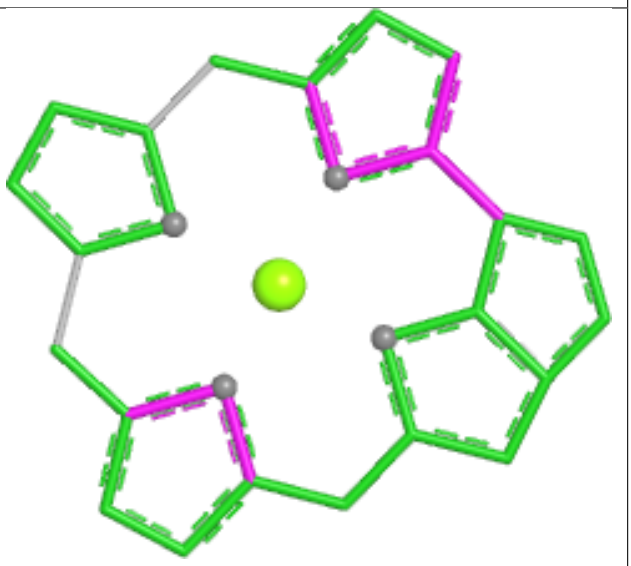


Rings

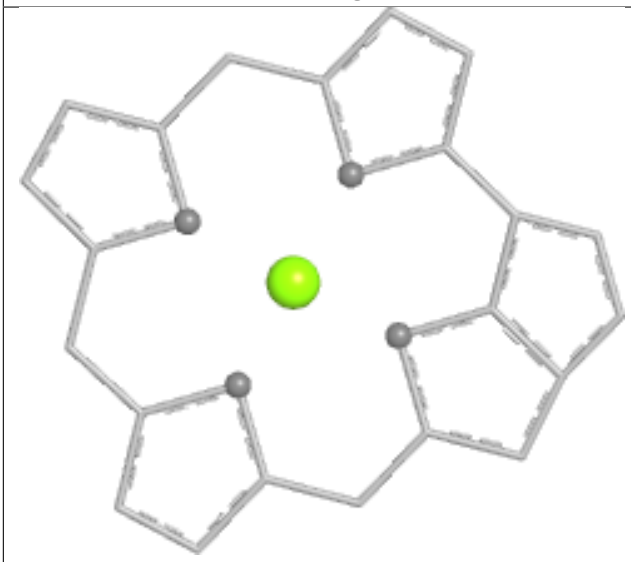
Ligand CLA B 1491



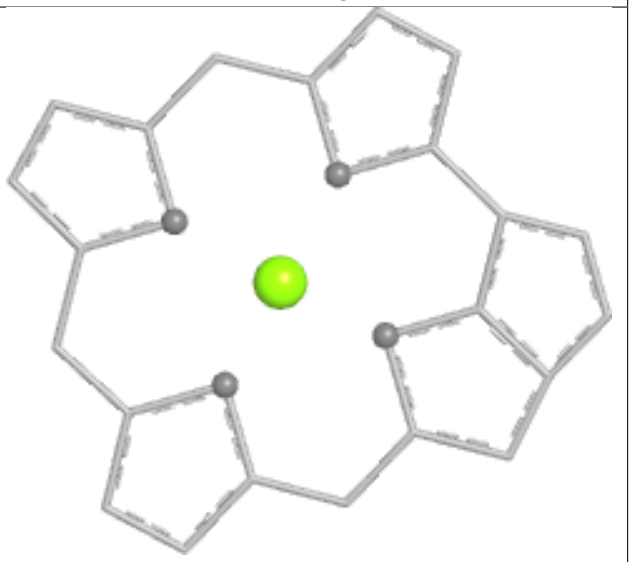
Bond lengths



Bond angles

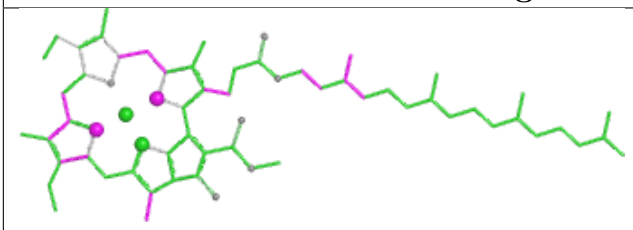


Torsions

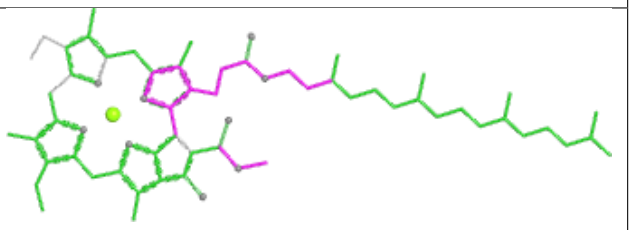


Rings

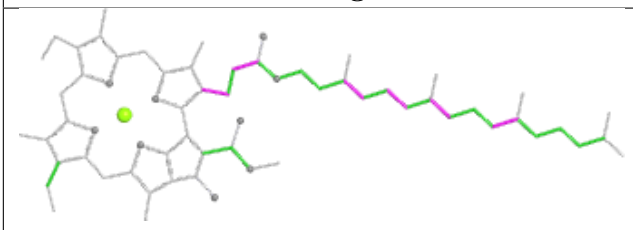
Ligand CLA B 1482



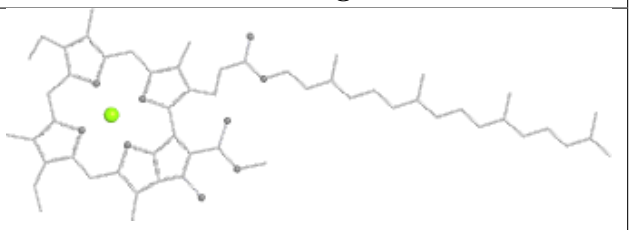
Bond lengths



Bond angles

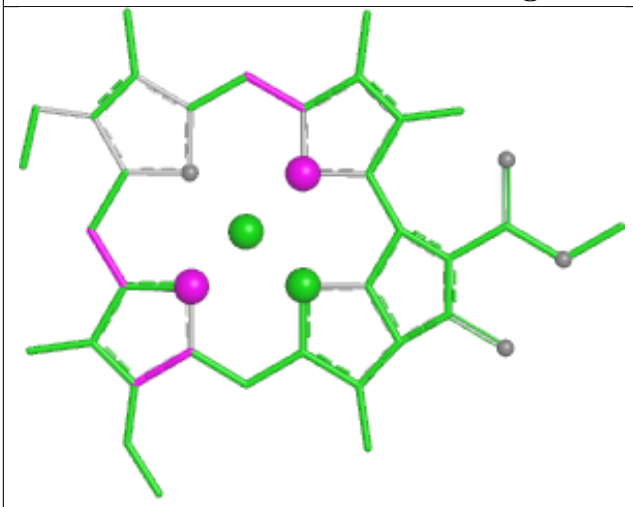


Torsions

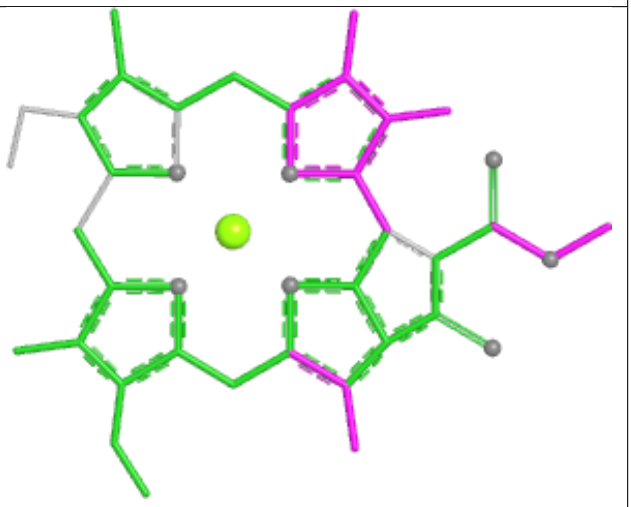


Rings

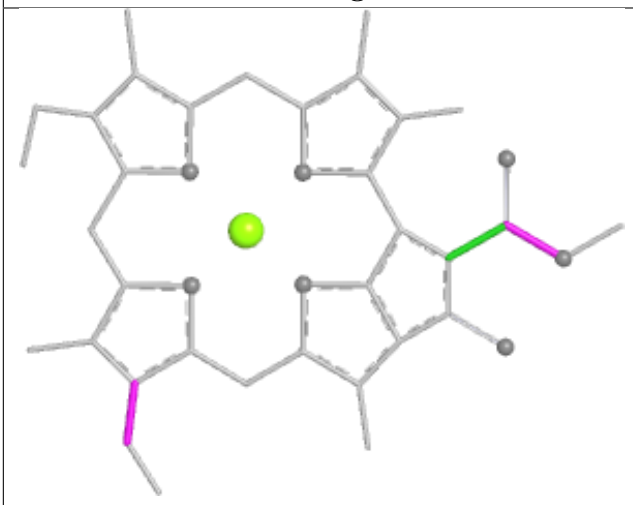
Ligand CLA I 1471



Bond lengths



Bond angles



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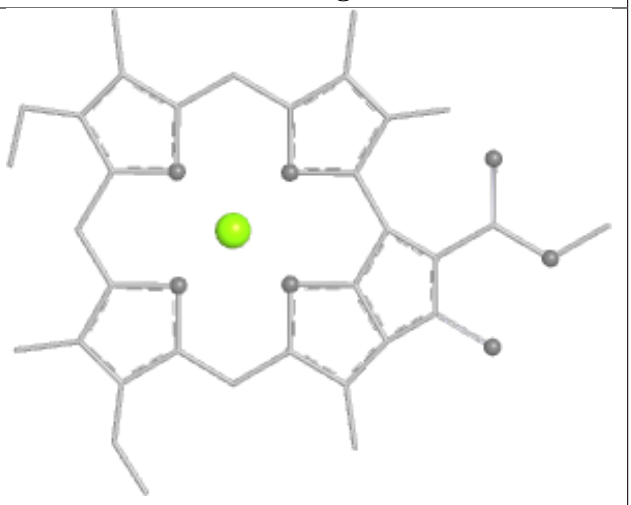
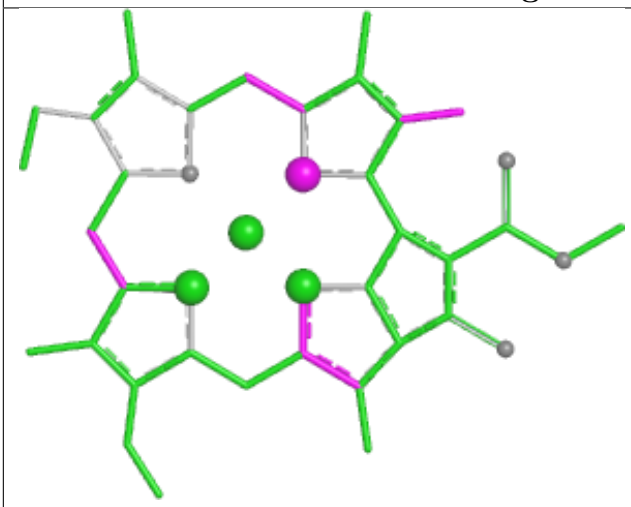


Rings

Ligand CLA I 1469



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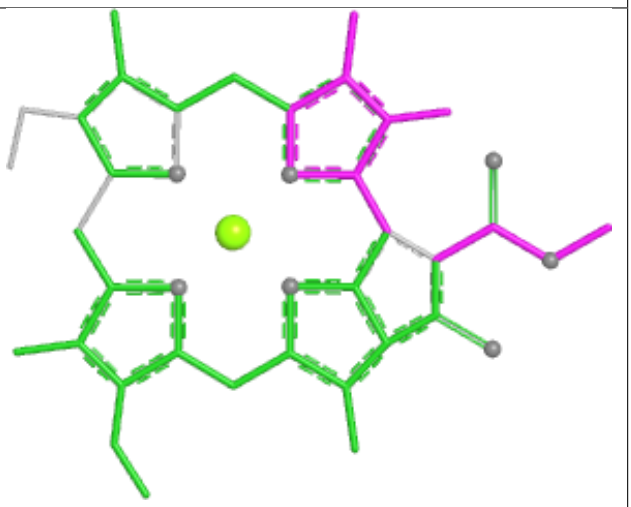
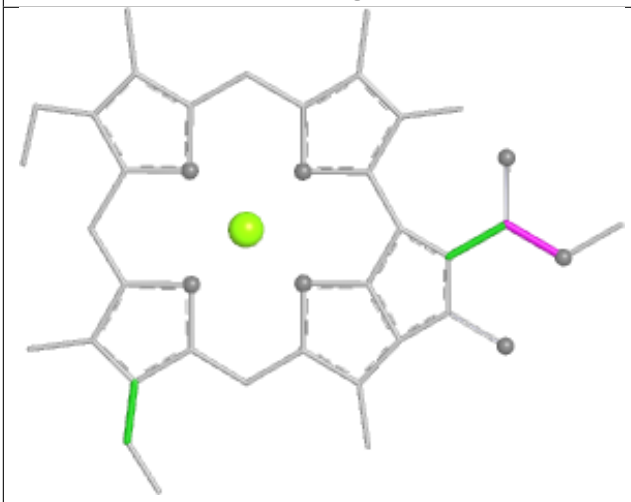


Bond angles



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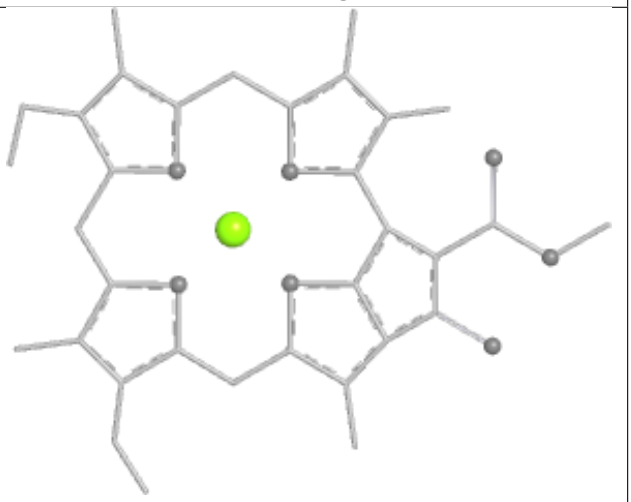
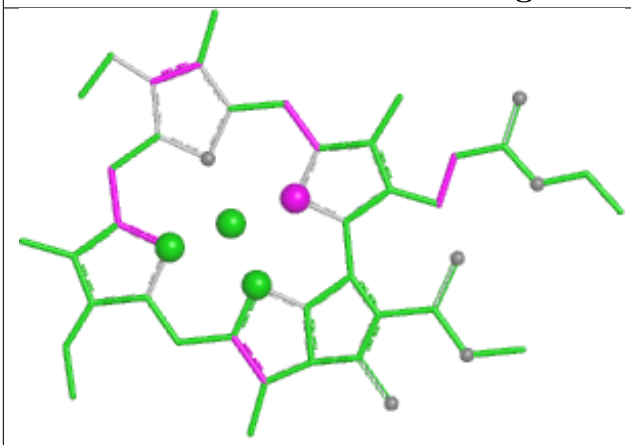


Rings

Ligand CLA C 1467



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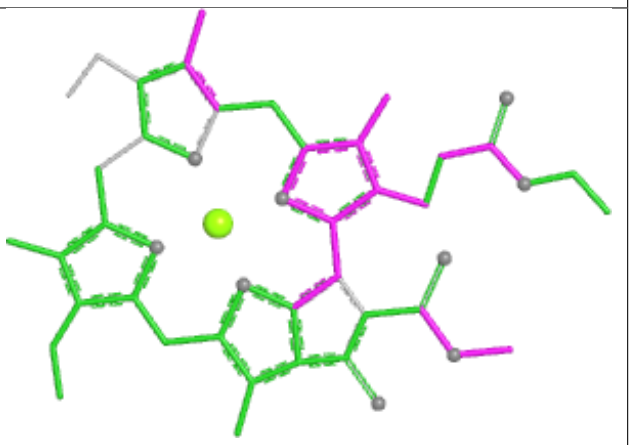
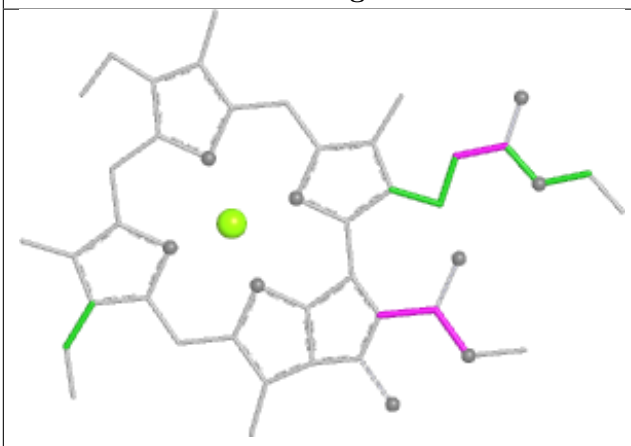


Bond angles



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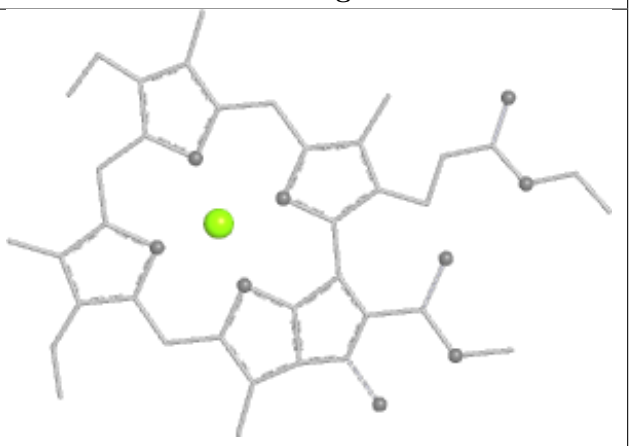
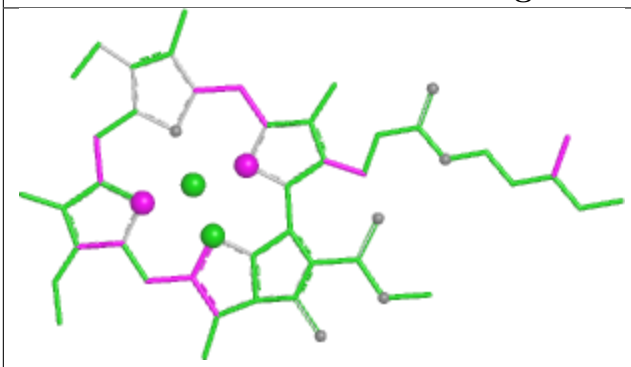


Rings

Ligand CLA A 1346



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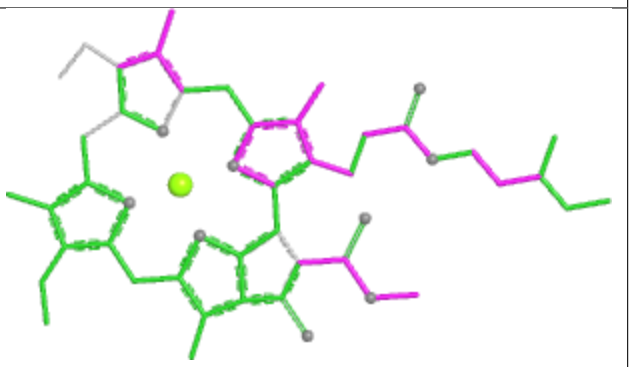
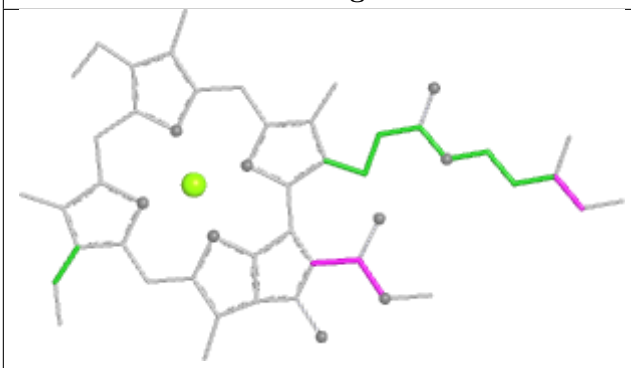
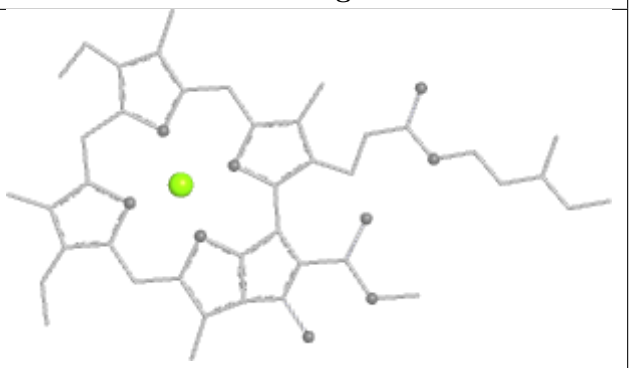


Bond angles

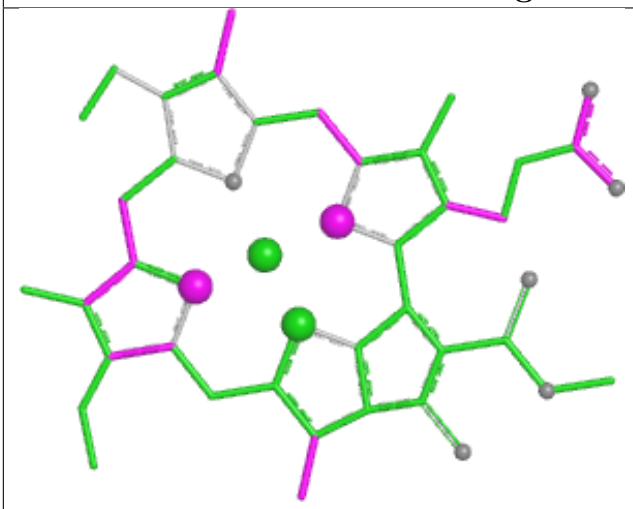


Torsions



Rings

Ligand CLA B 1490



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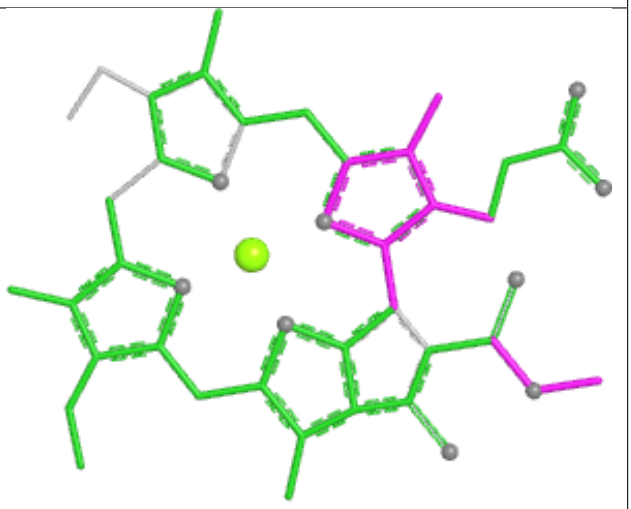
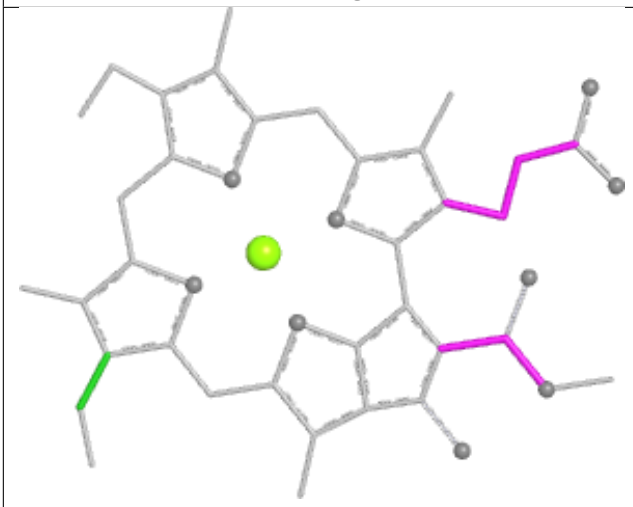


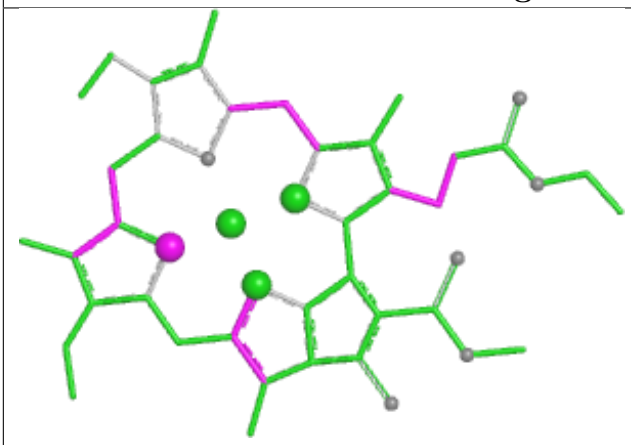
Bond angles



Torsions

Rings

Ligand CLA H 1485



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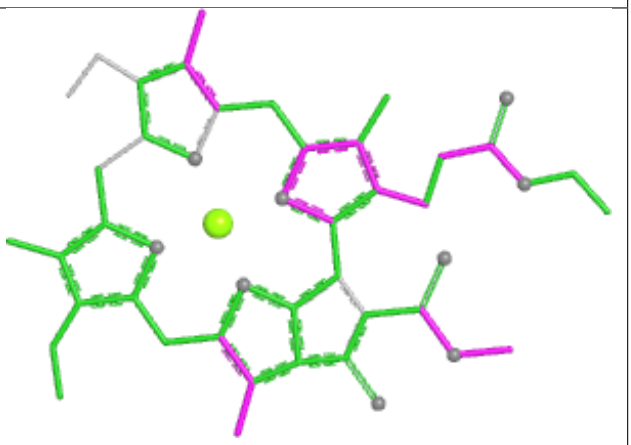

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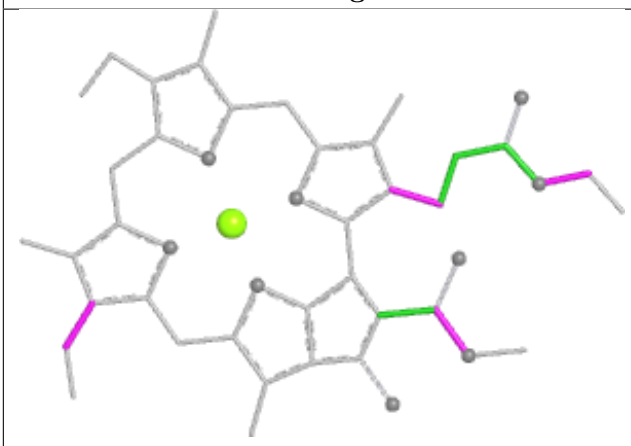
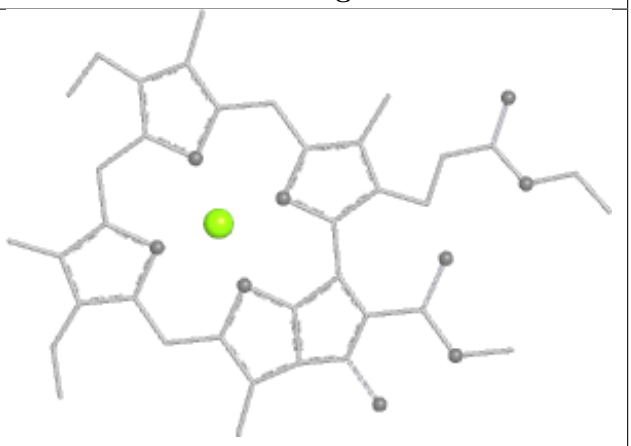
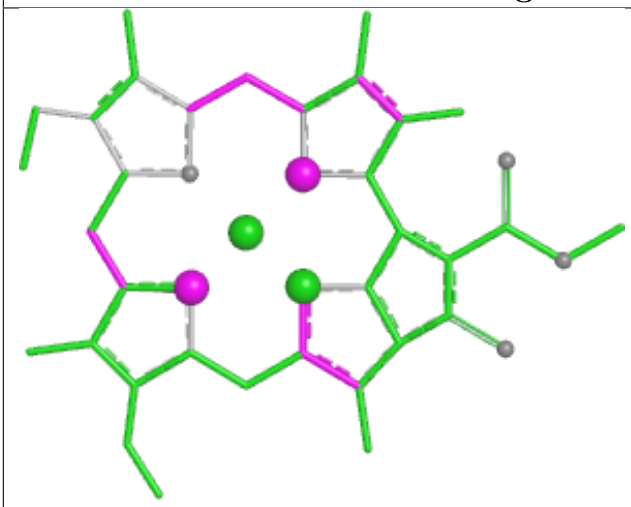


Torsions



Rings

Ligand CLA B 1486



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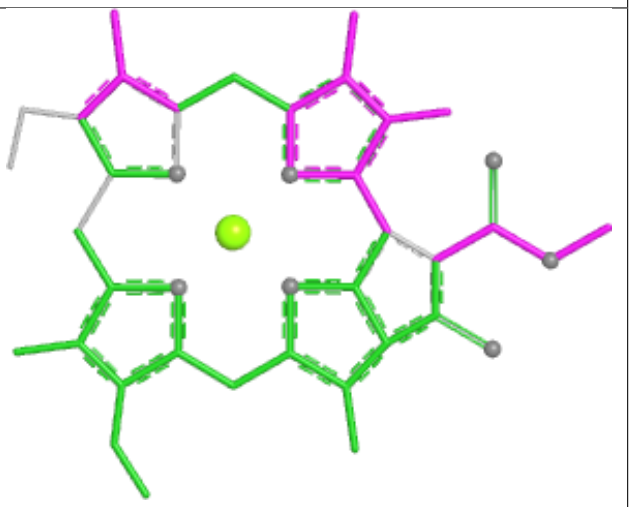
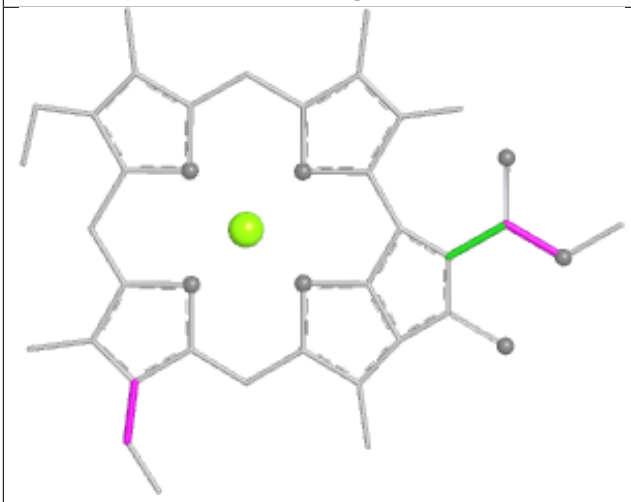
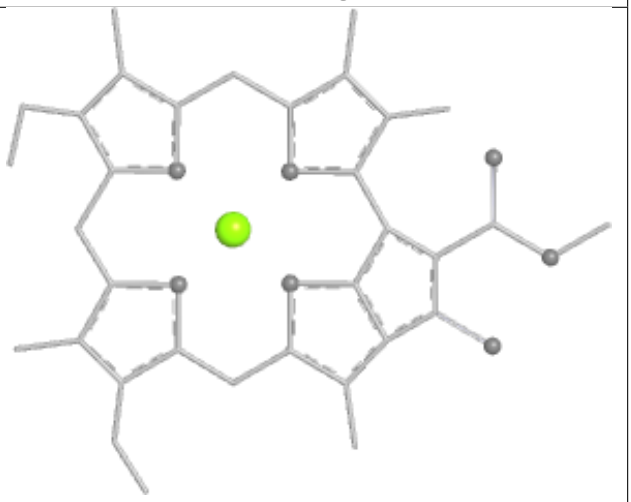


Bond angles

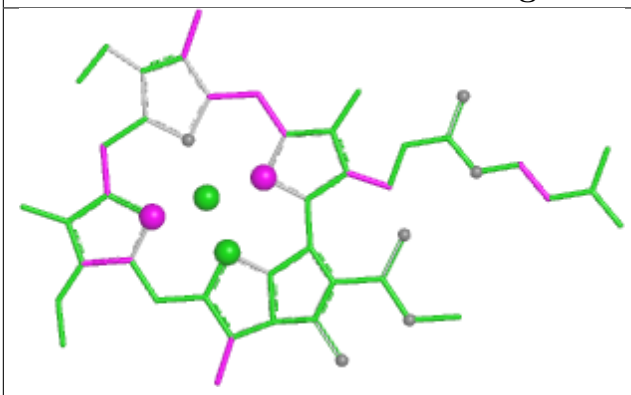


Torsions



Rings

Ligand CLA J 1353



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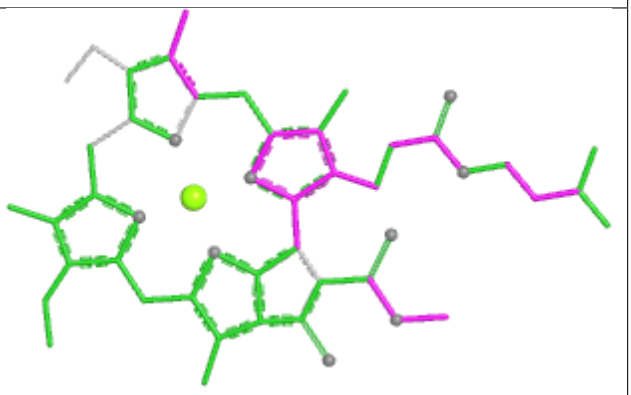
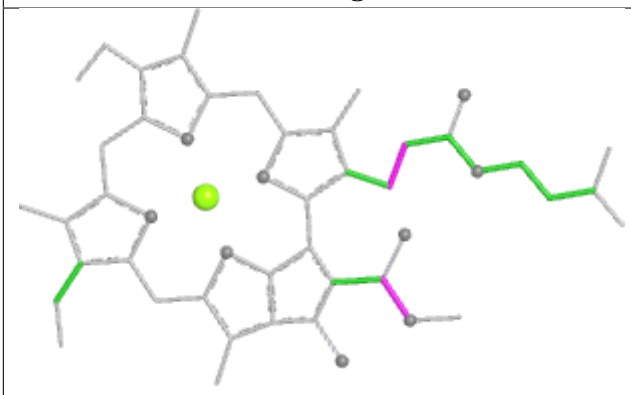
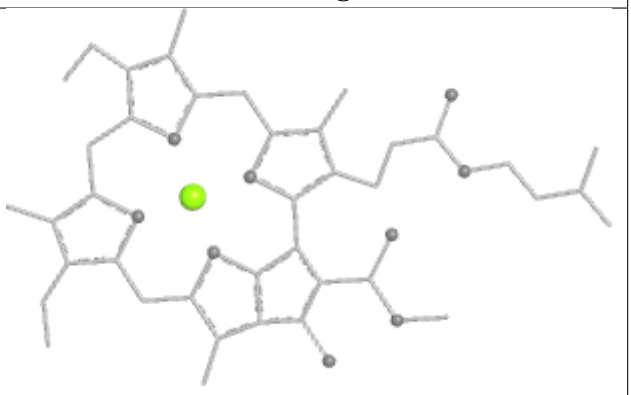


Bond angles

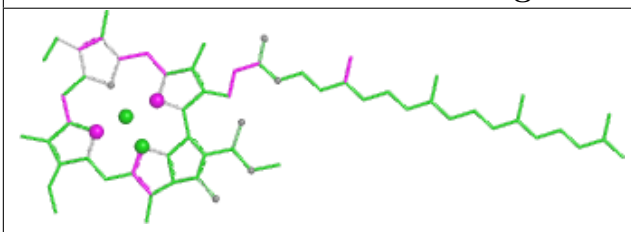


Torsions



Rings

Ligand CLA G 1342



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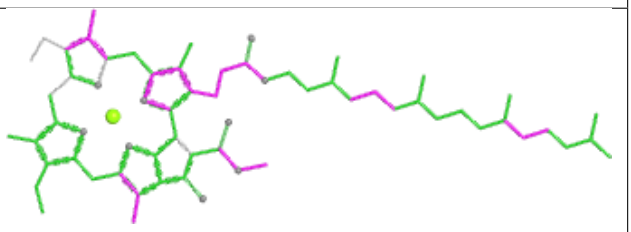
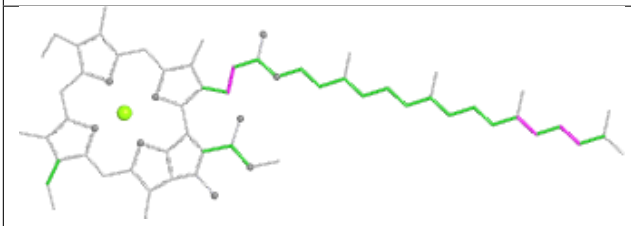


Bond angles



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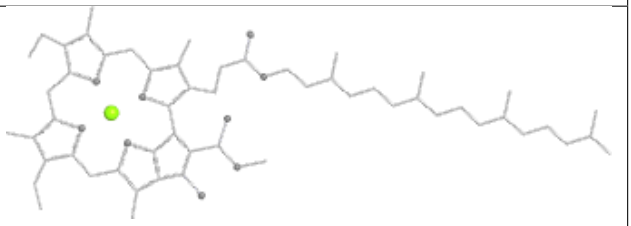
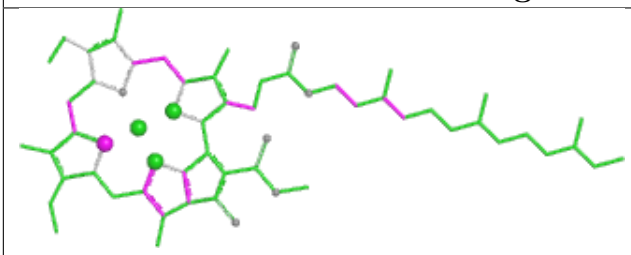
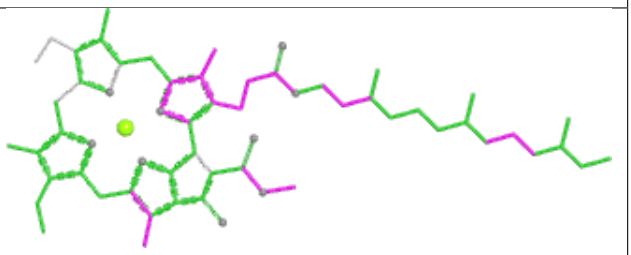
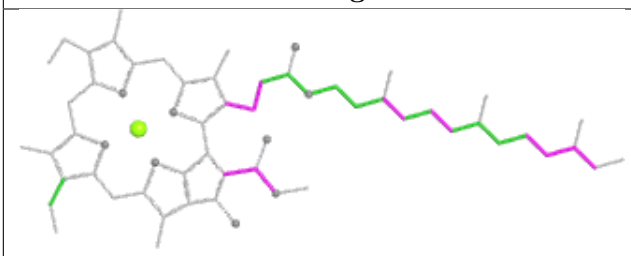
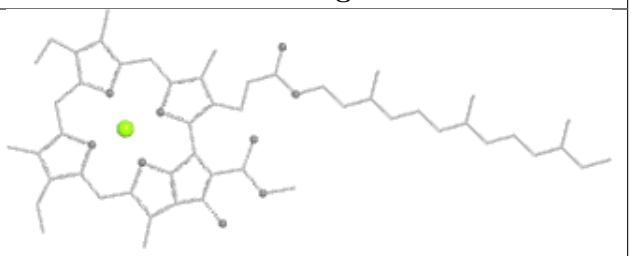
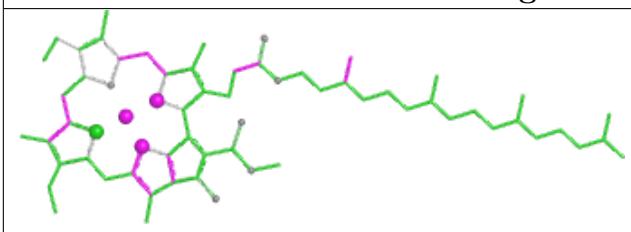
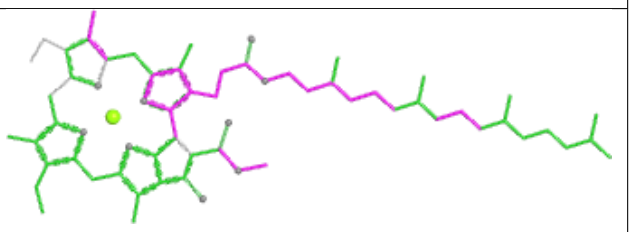
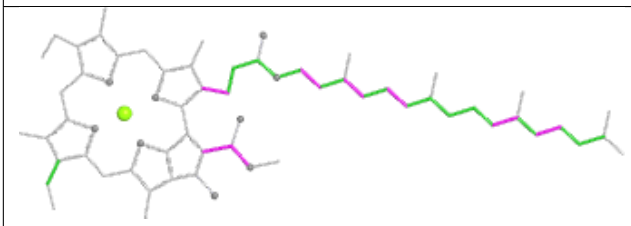
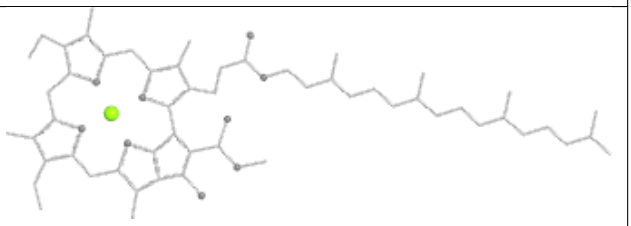


Rings

Ligand CLA G 1343	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 1351	
 Bond lengths	 Bond angles
 Torsions	 Rings

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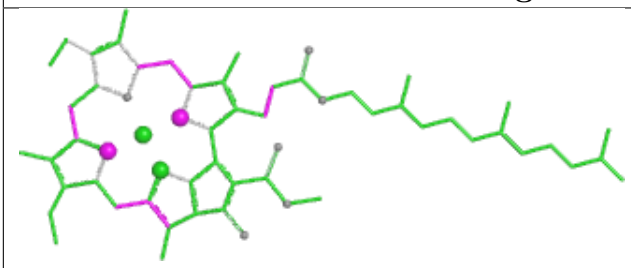
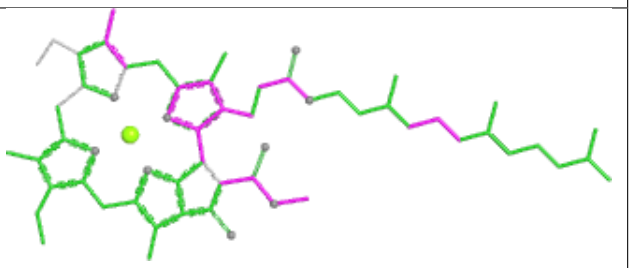
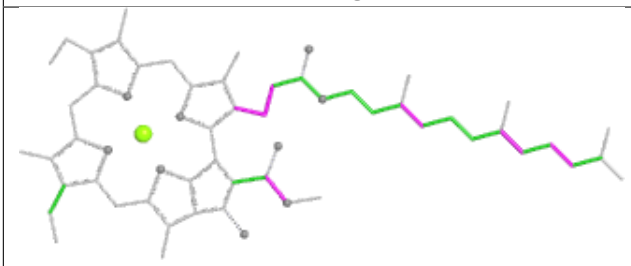
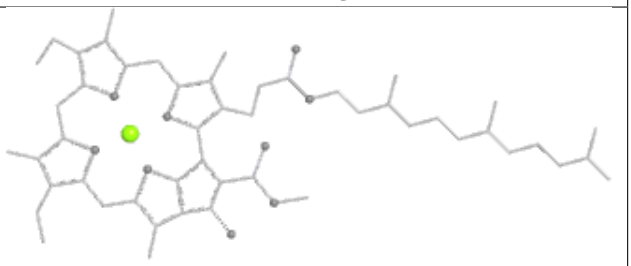
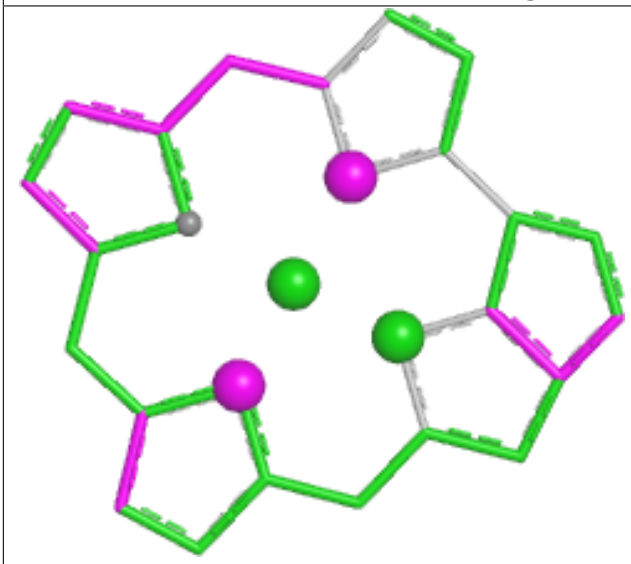
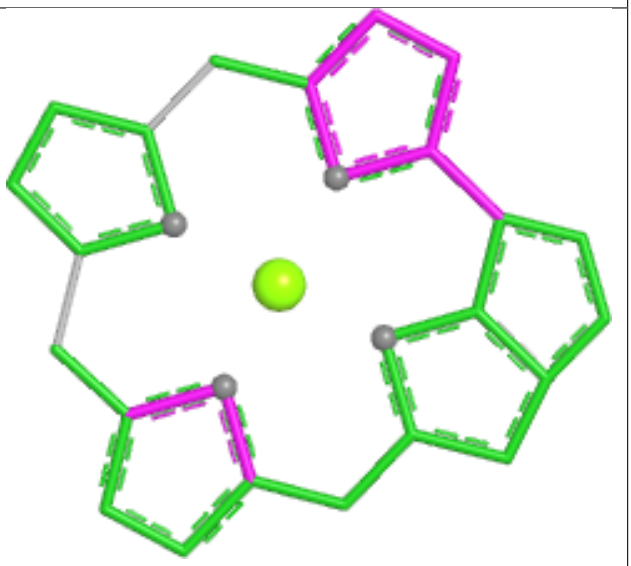
 Bond lengths	 Bond angles
 Torsions	 Rings

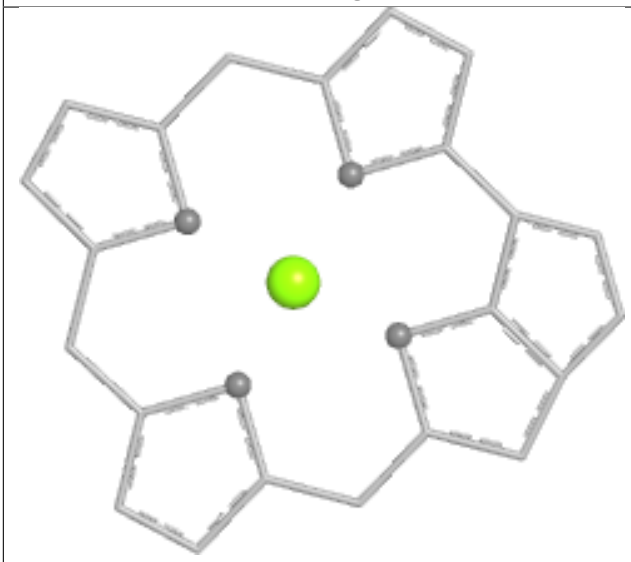
Ligand CLA I 1468



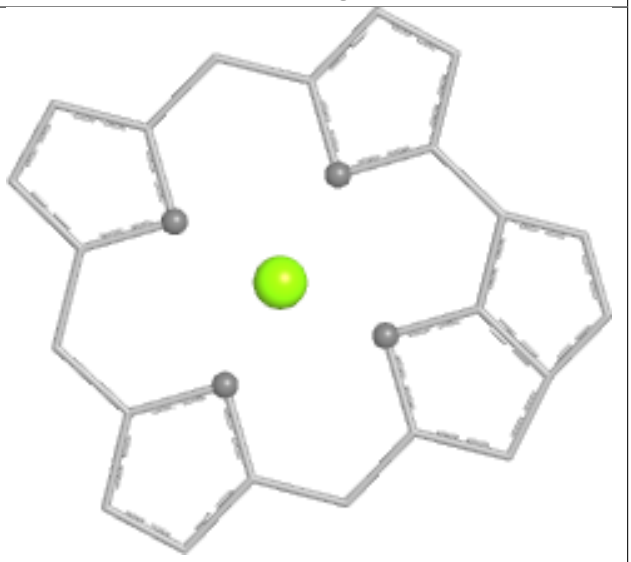
Bond lengths



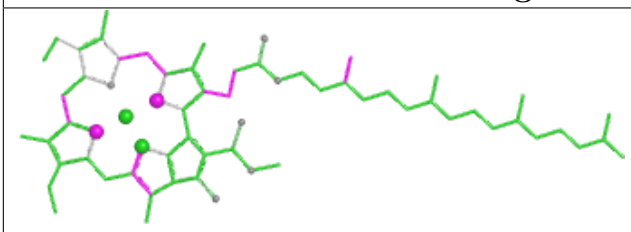
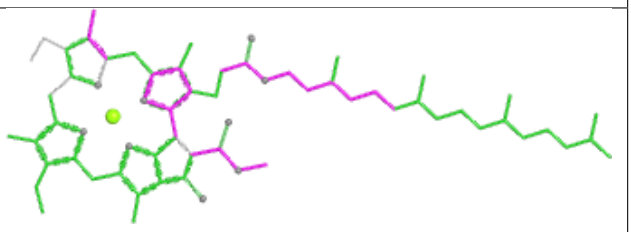
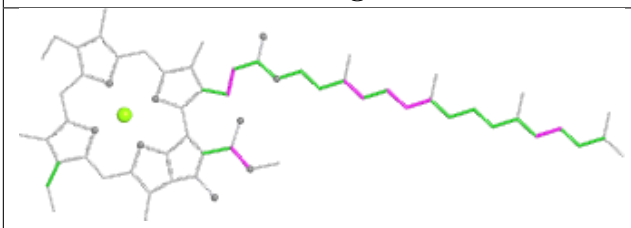
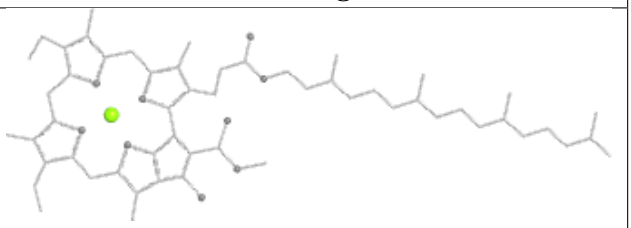
Bond angles



Torsions



Rings

Ligand CLA H 1494	
 Bond lengths	 Bond angles
 Torsions	 Rings

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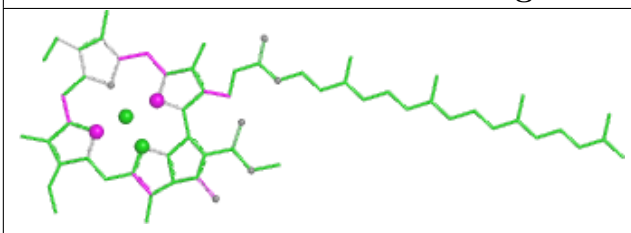
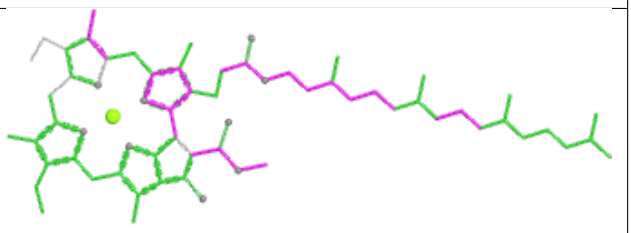
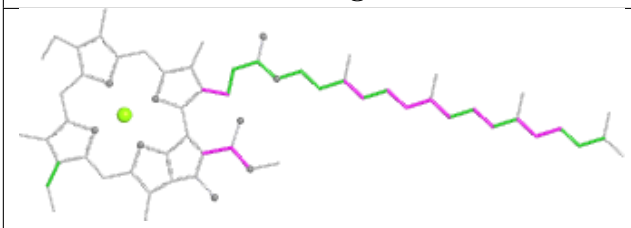
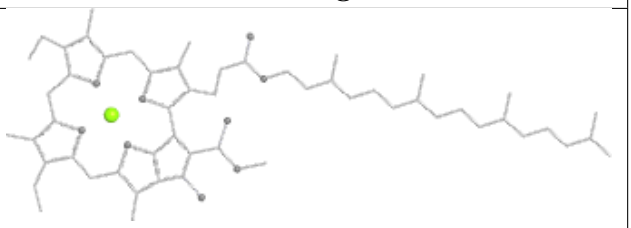
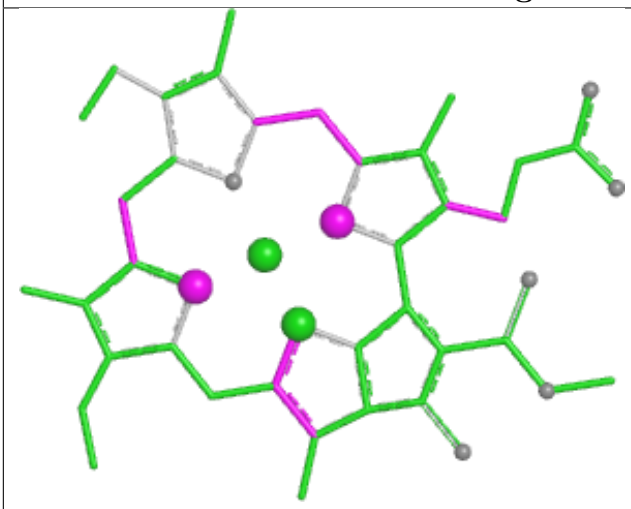
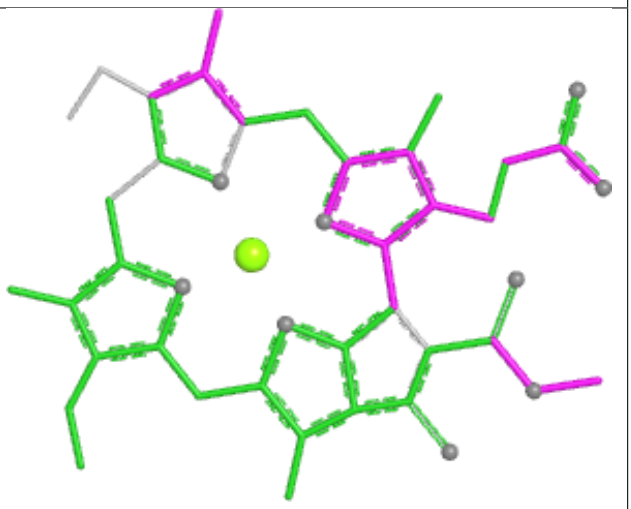
 Bond lengths	 Bond angles
 Torsions	 Rings

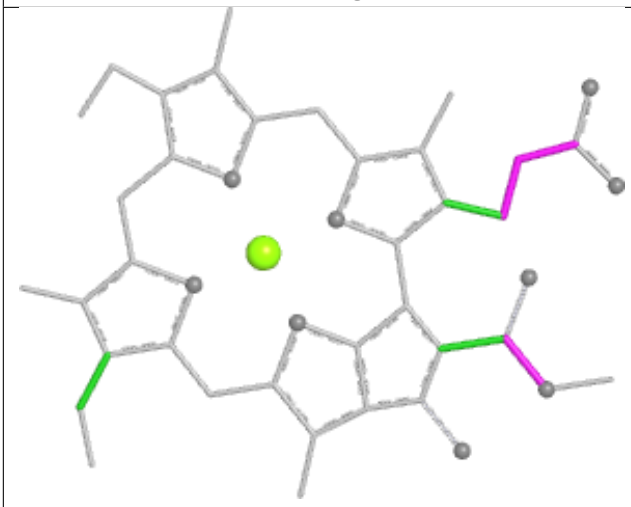
Ligand CLA B 1484



Bond lengths



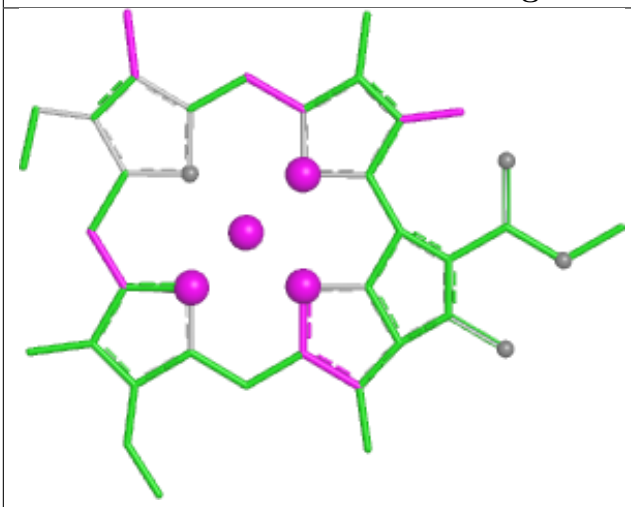
Bond angles



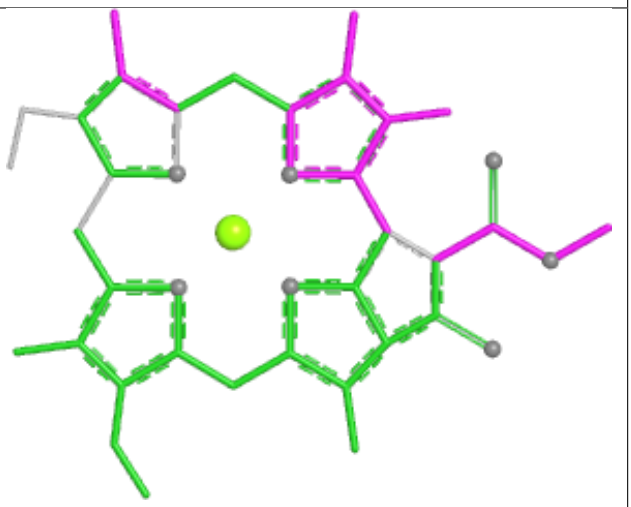
Torsions

Rings

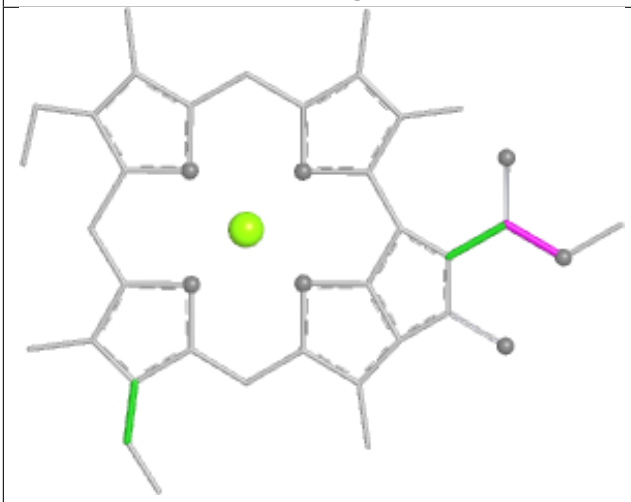
Ligand CLA I 1470



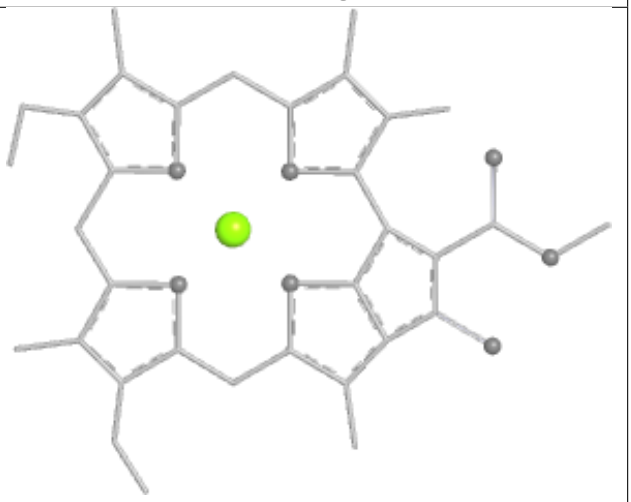
Bond lengths



Bond angles

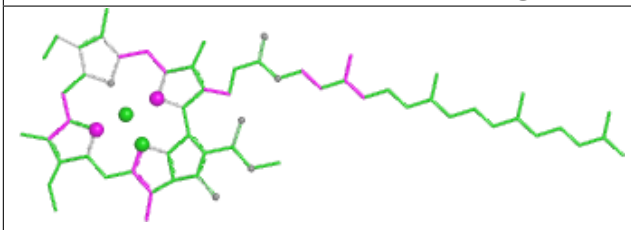


Torsions



Rings

Ligand CLA H 1488



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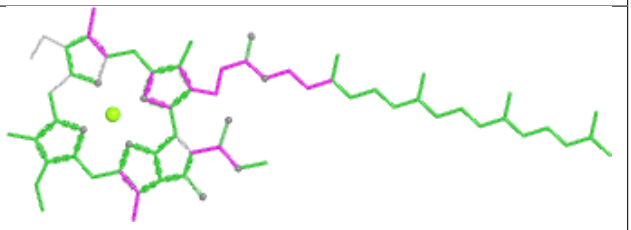

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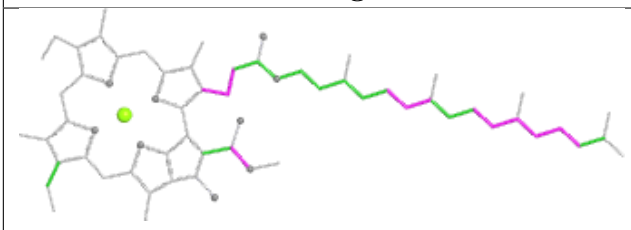
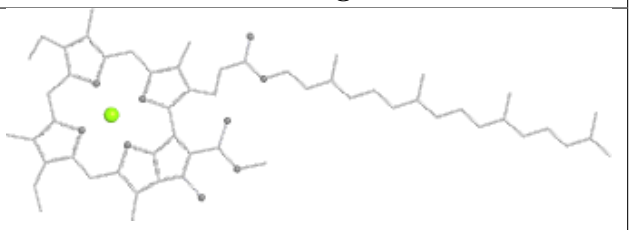
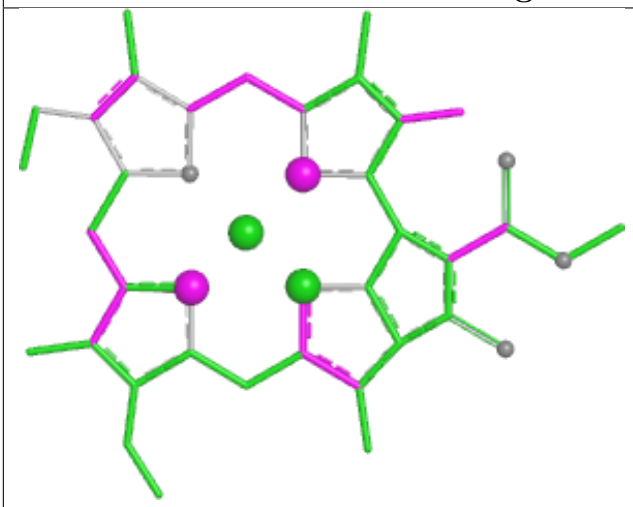


Torsions



Rings

Ligand CLA B 1497



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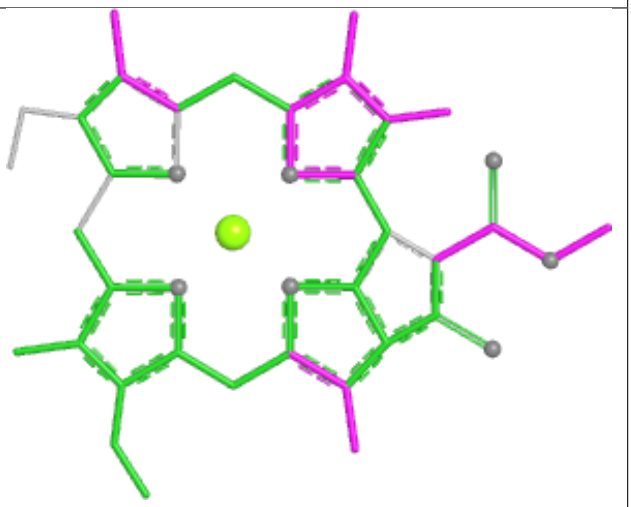

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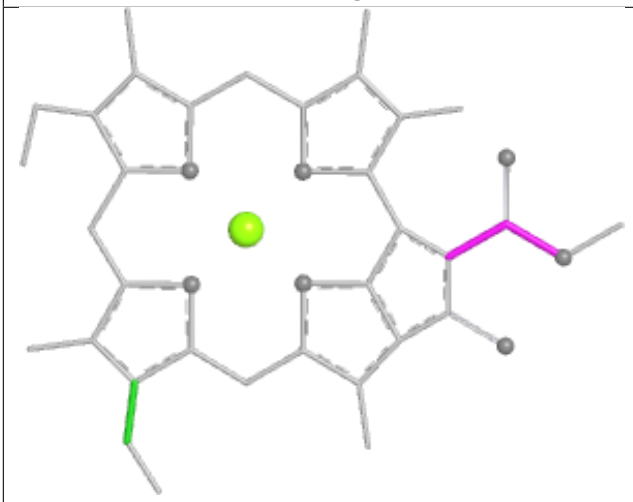
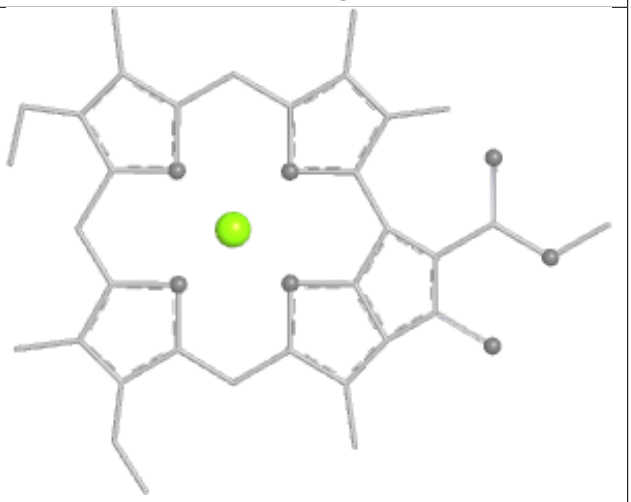
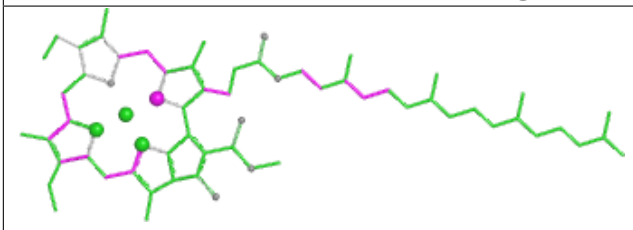


Torsions



Rings

Ligand CLA H 1487



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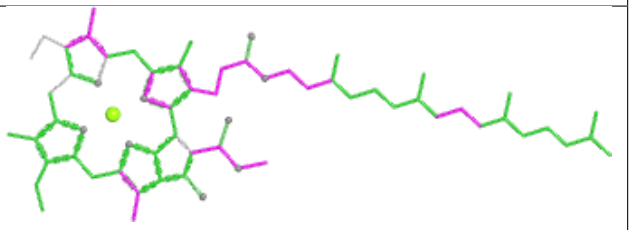
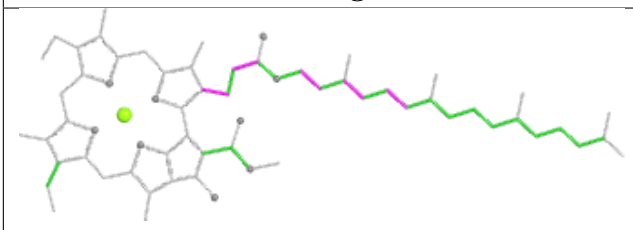


Bond angles



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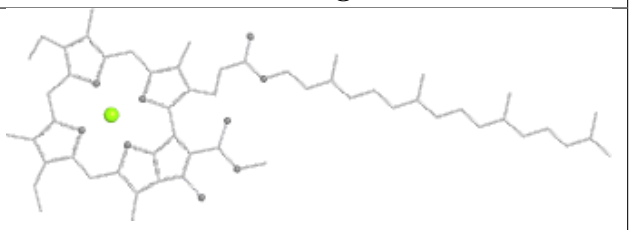
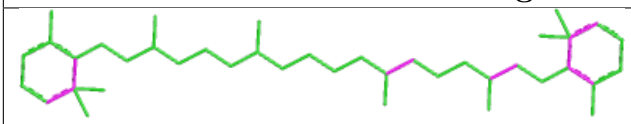


Rings

Ligand BCR L 1047



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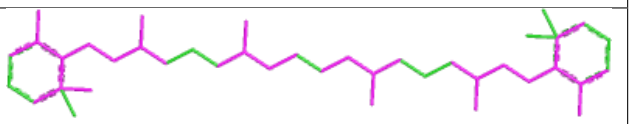
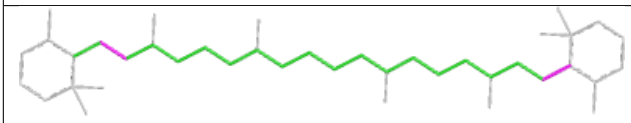
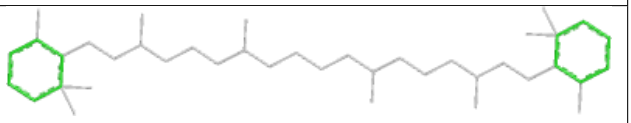


Bond angles

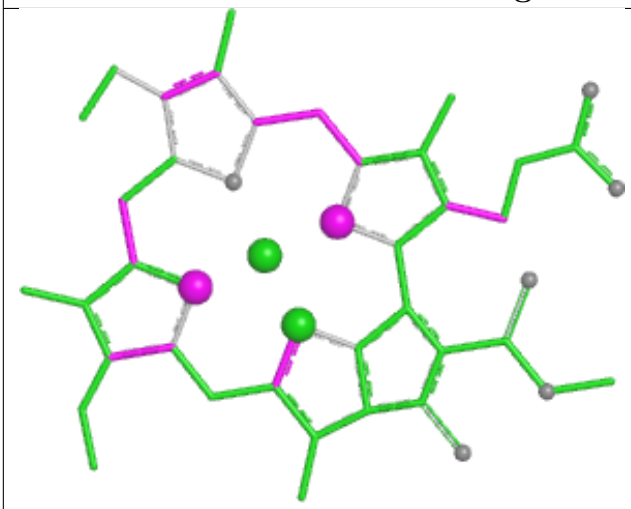


Torsions



Rings

Ligand CLA H 1493



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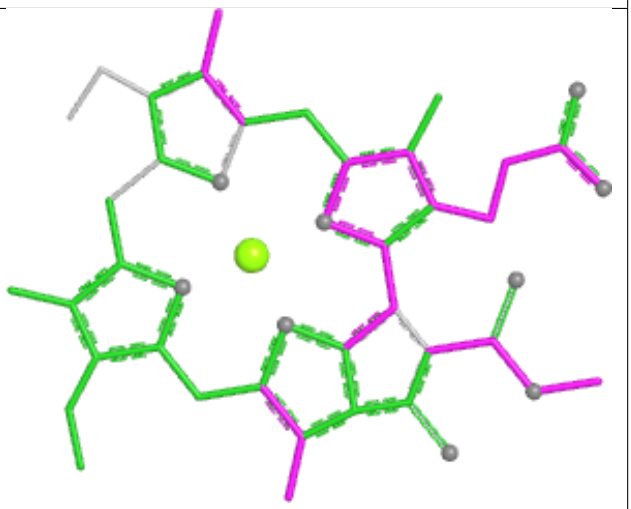
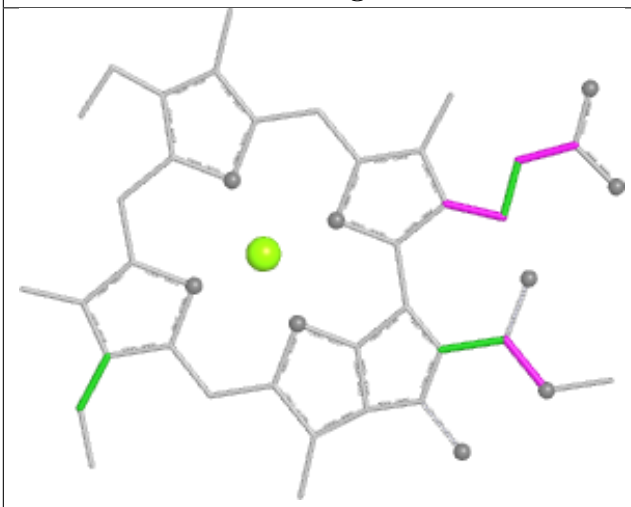
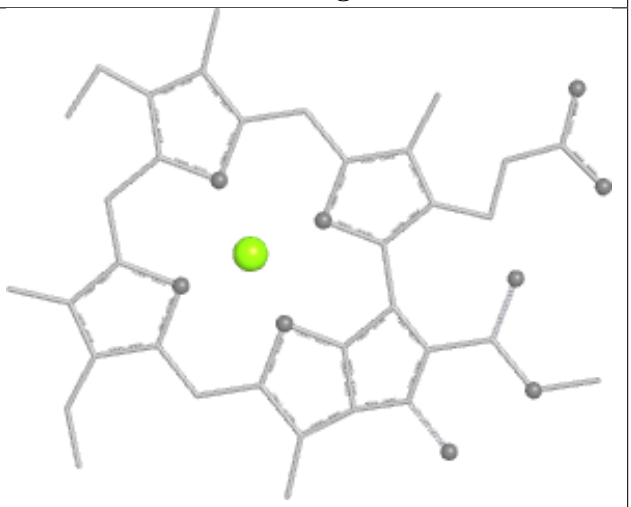


Bond angles

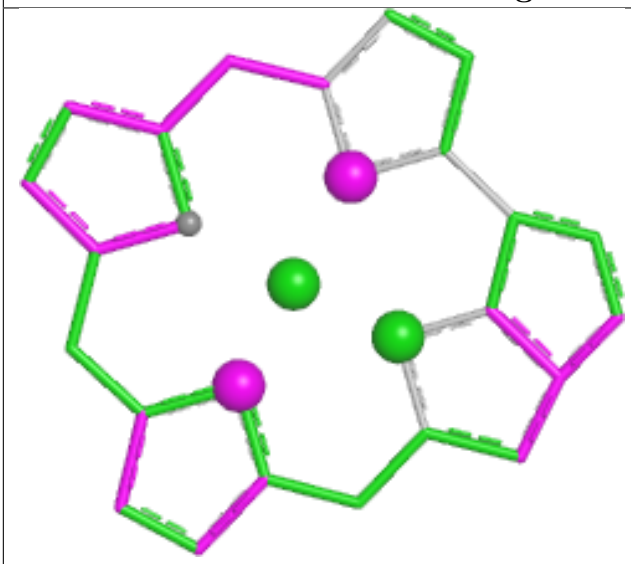


Torsions



Rings

Ligand CLA C 1461



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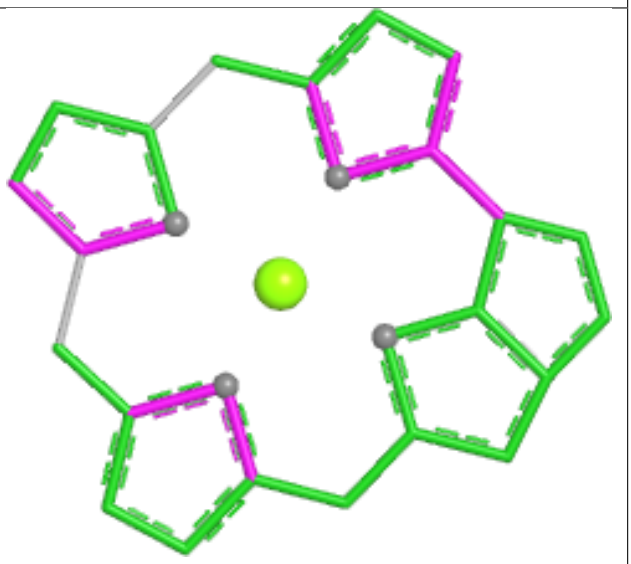
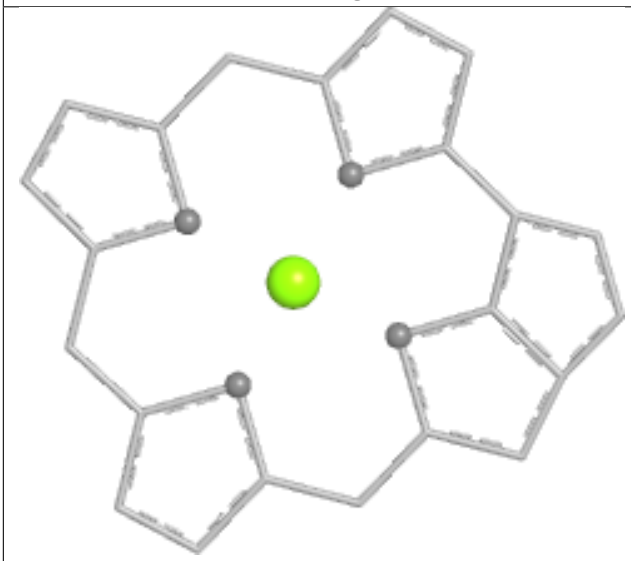
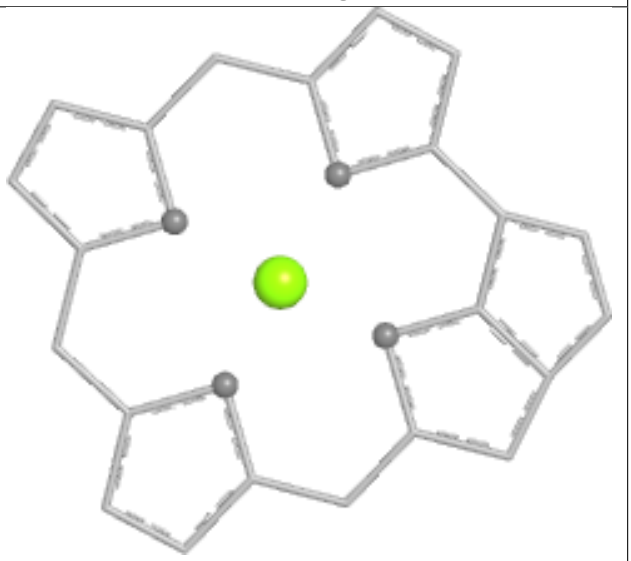


Bond angles

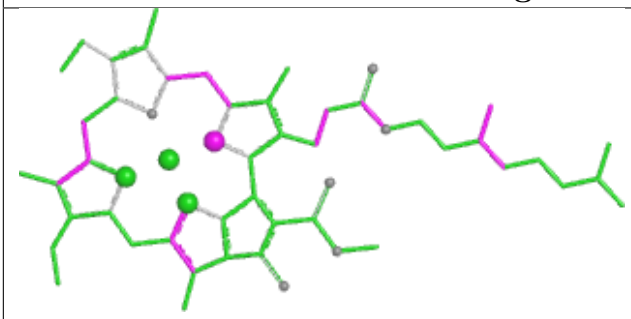


Torsions

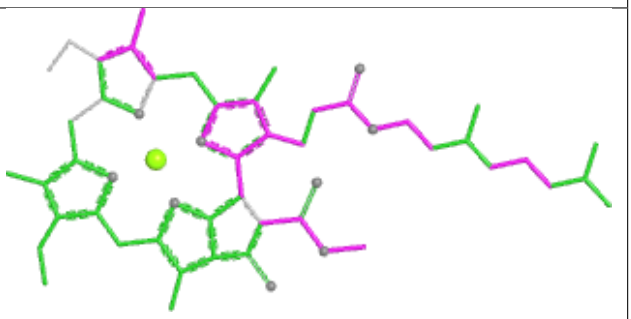


Rings

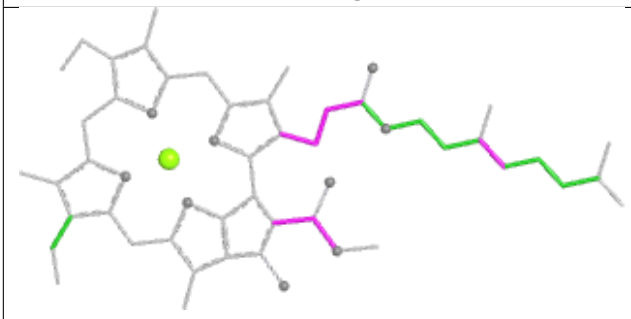
Ligand CLA H 1495



Bond lengths



Bond angles



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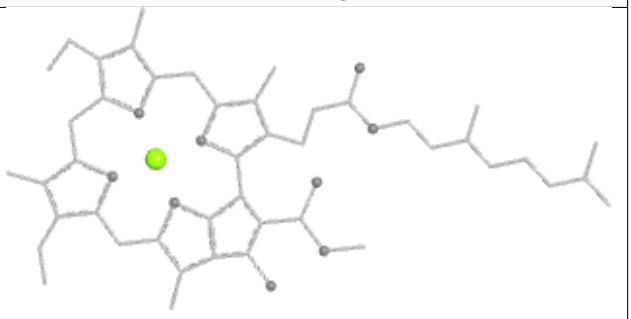
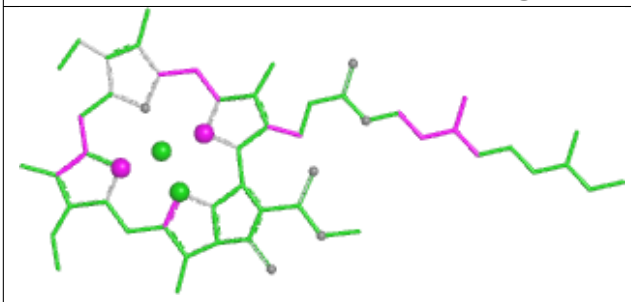


Rings

Ligand CLA C 1462



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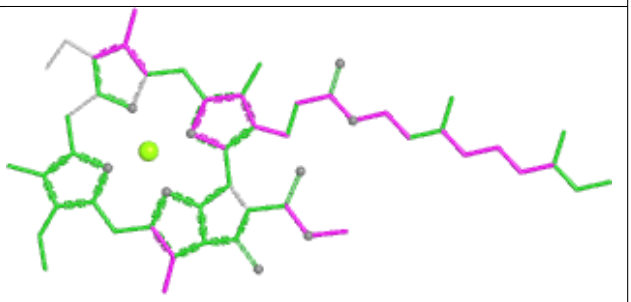

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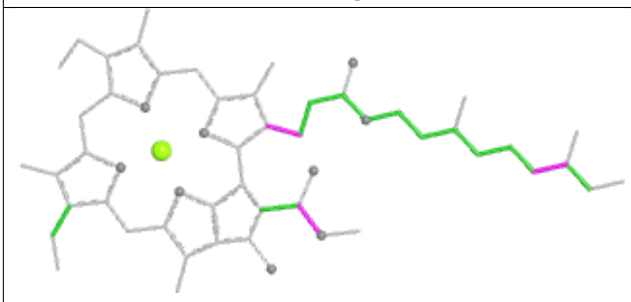

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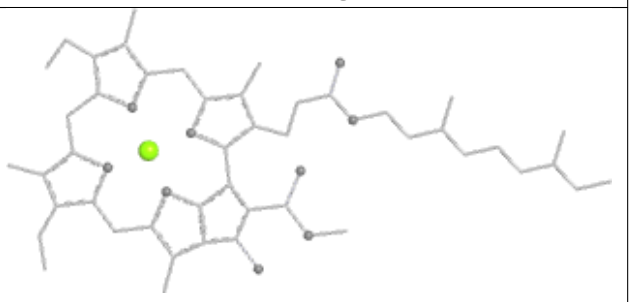
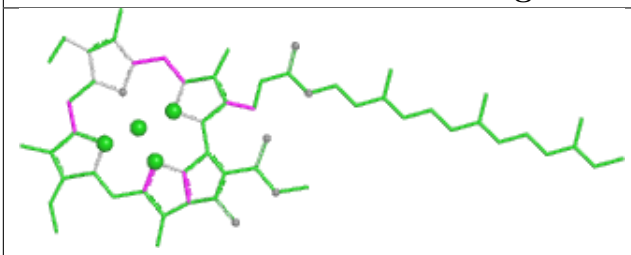


Rings

Ligand CLA A 1343



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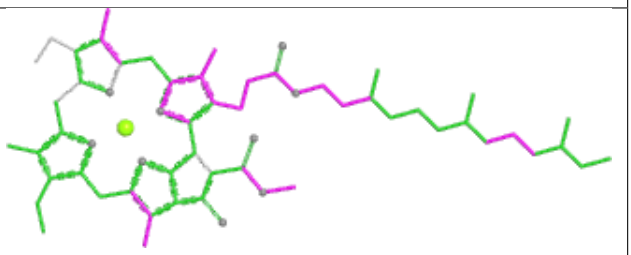
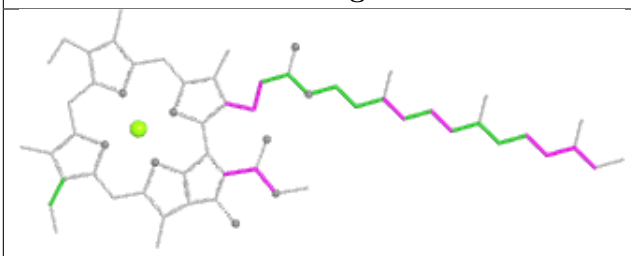
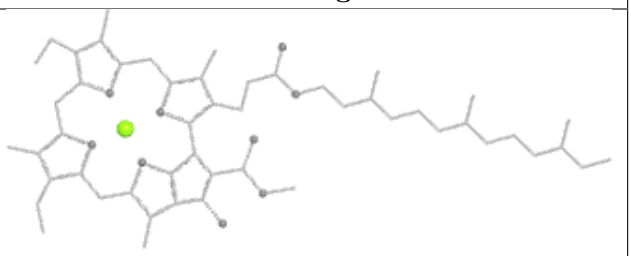


Bond angles



Torsions



Rings

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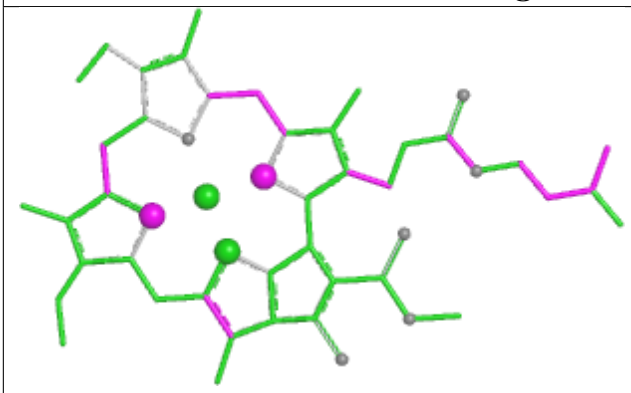

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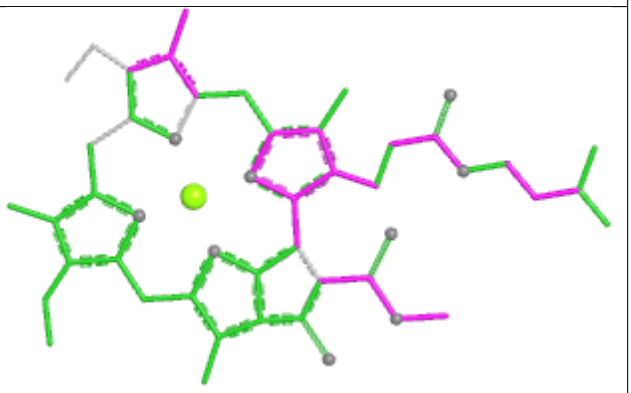
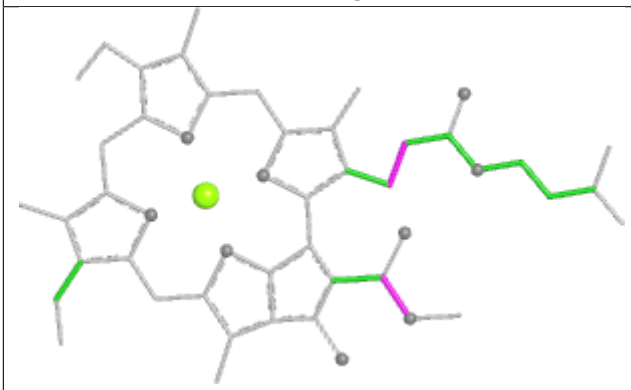


Bond angles



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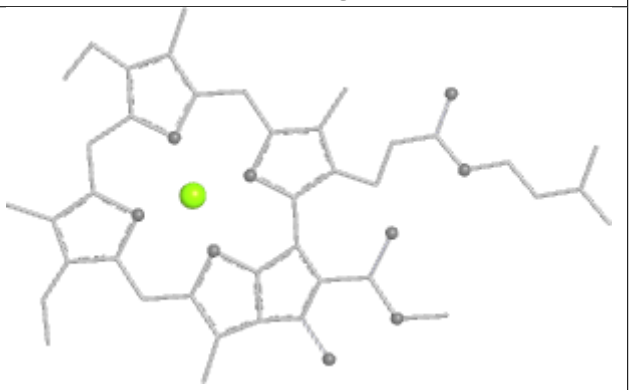
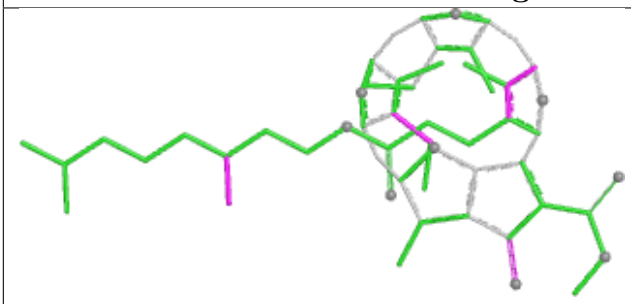
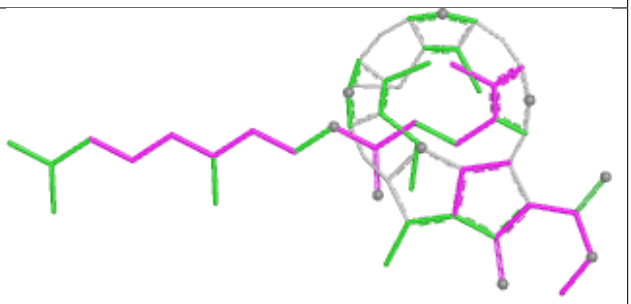
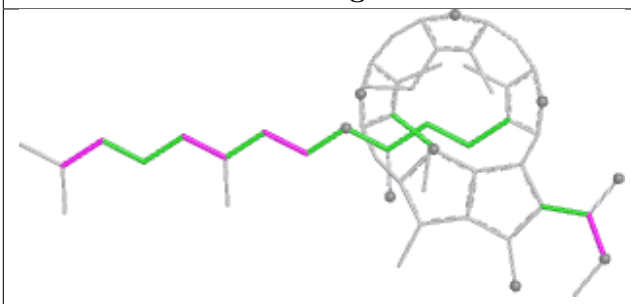
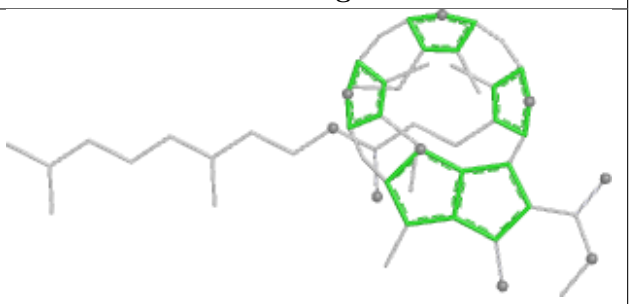
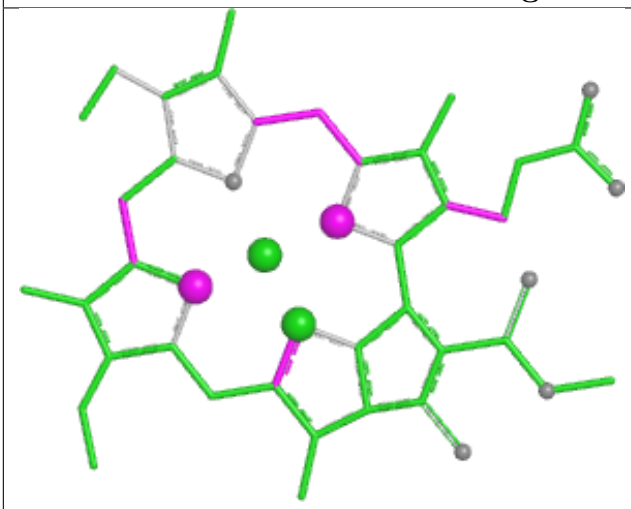


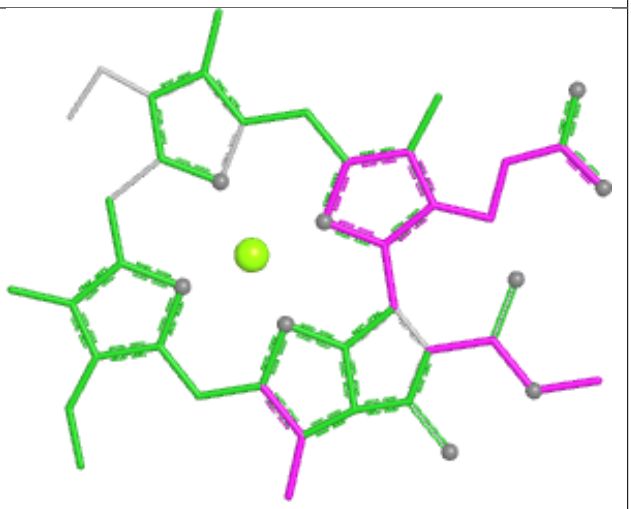
Rings

Ligand PHO D 1352	
 Bond lengths	 Bond angles
 Torsions	 Rings

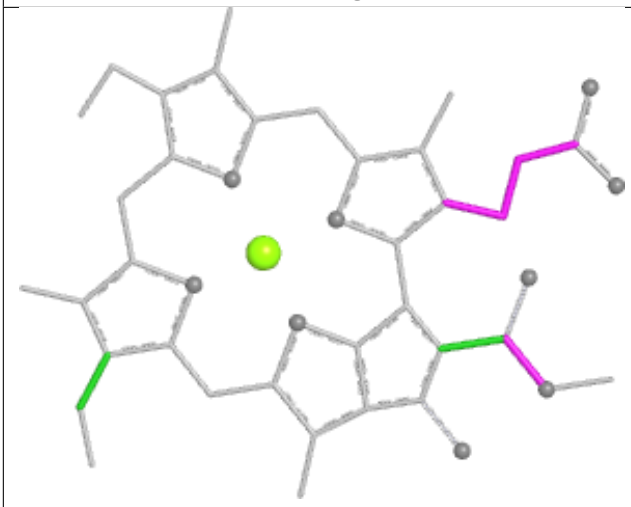
Ligand CLA I 1459



Bond lengths



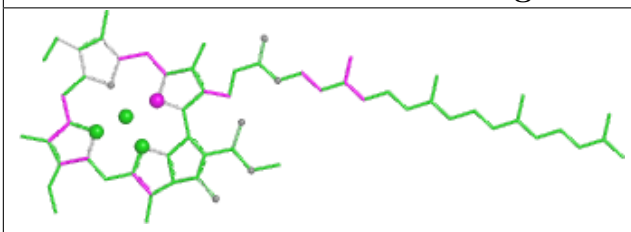
Bond angles



Torsions

Rings

Ligand CLA H 1482



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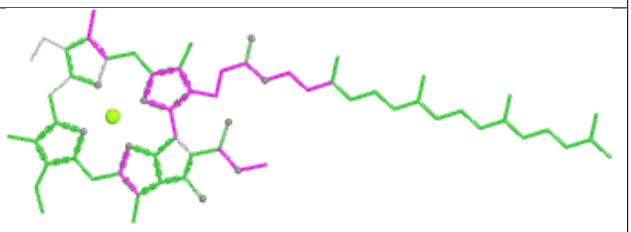
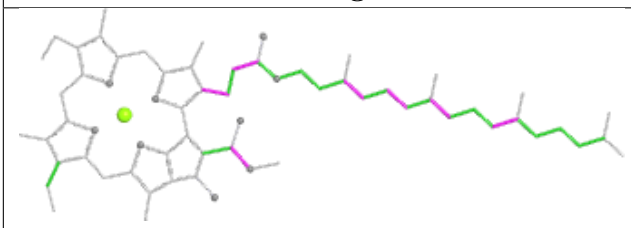


Bond angles



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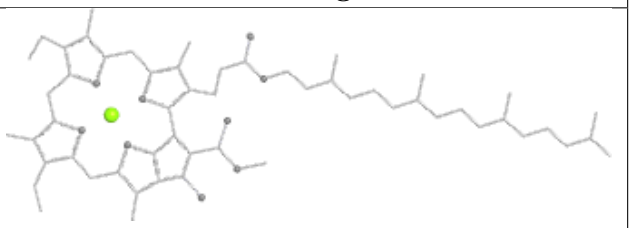
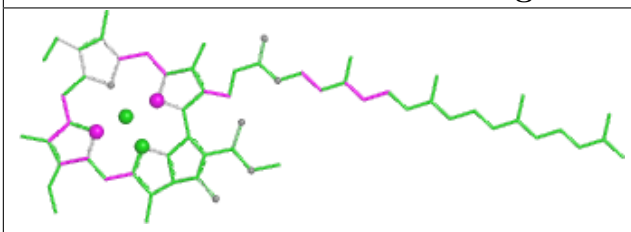


Rings

Ligand CLA B 1487



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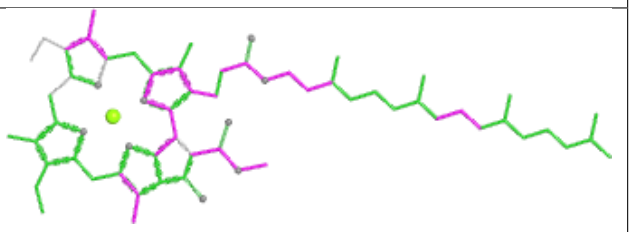
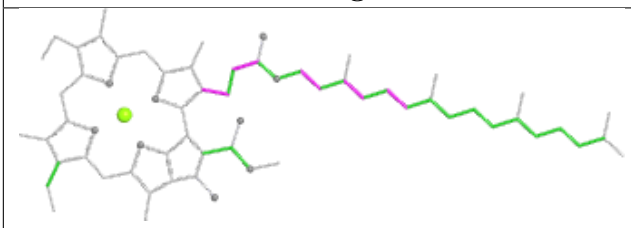


Bond angles



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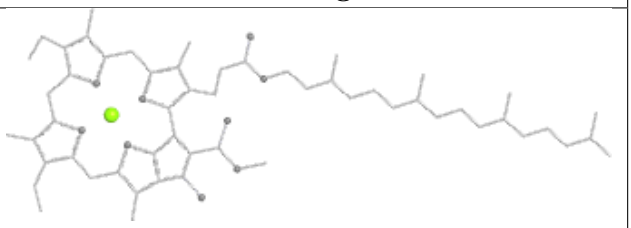
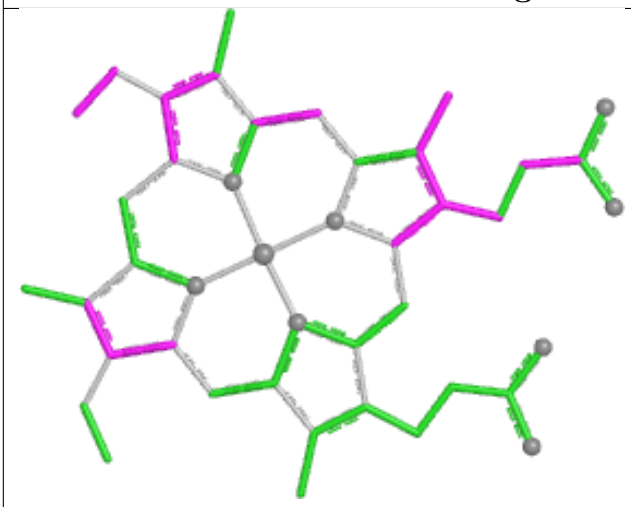


Rings

Ligand HEC T 1138



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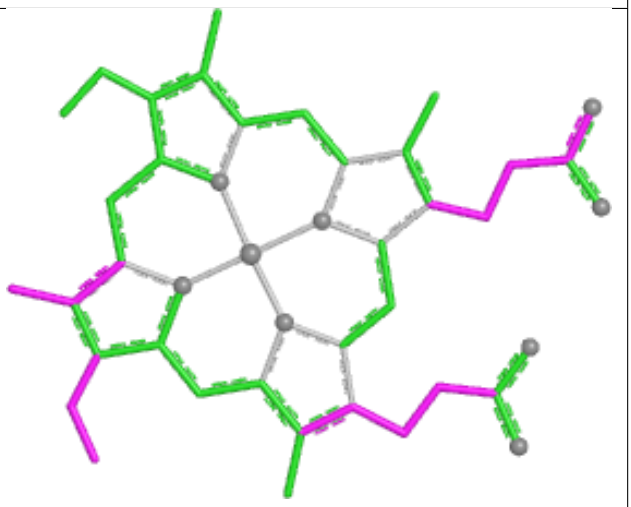

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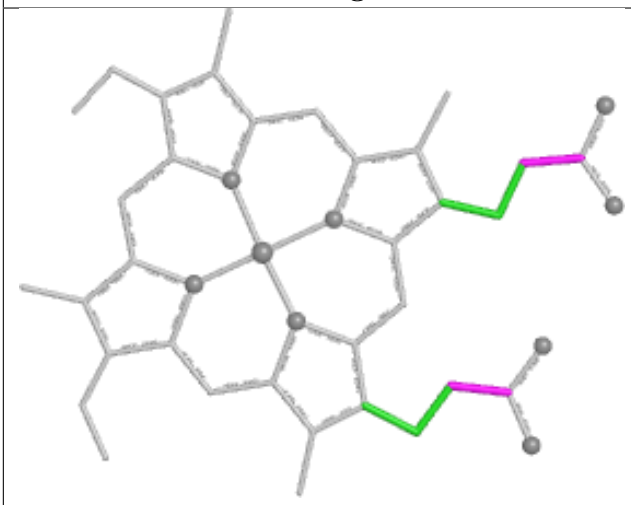

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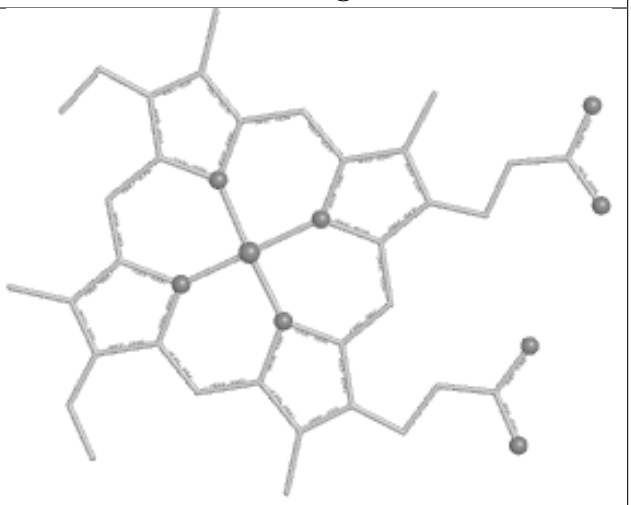
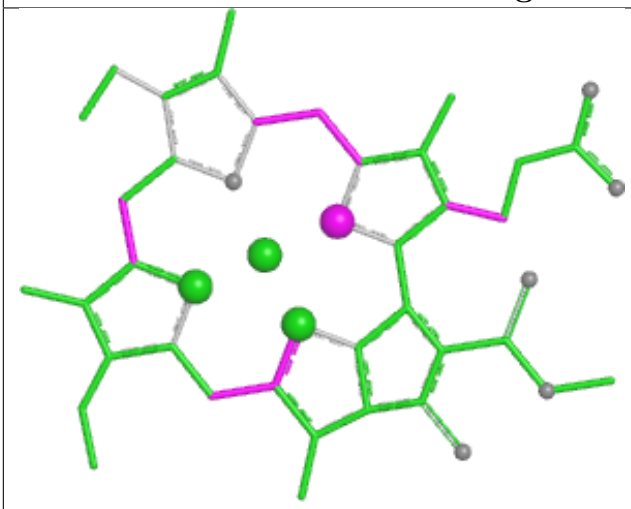


Rings

Ligand CLA B 1493



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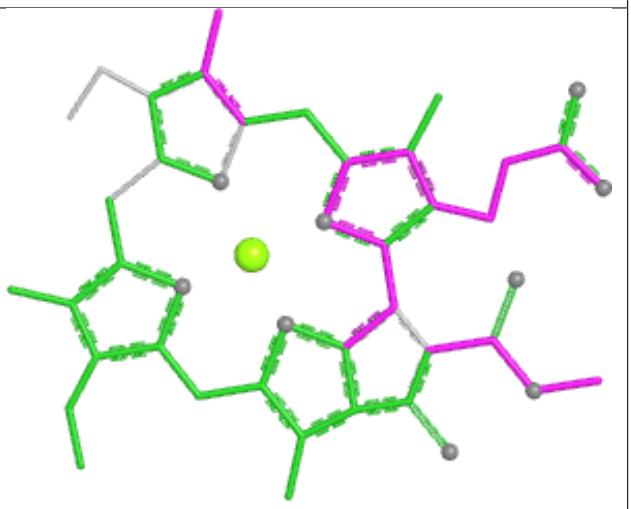
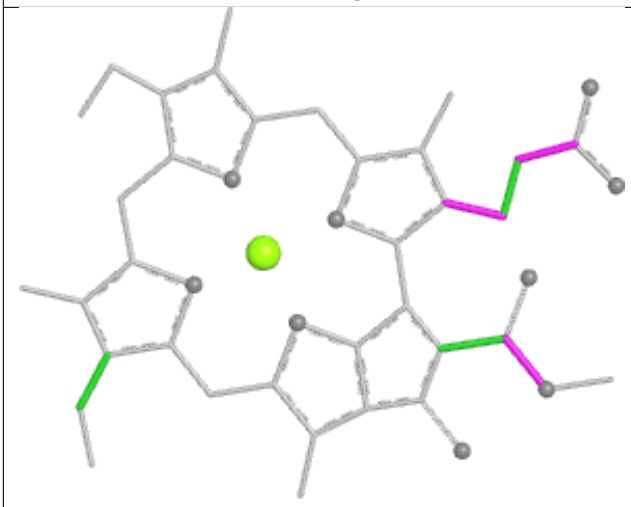


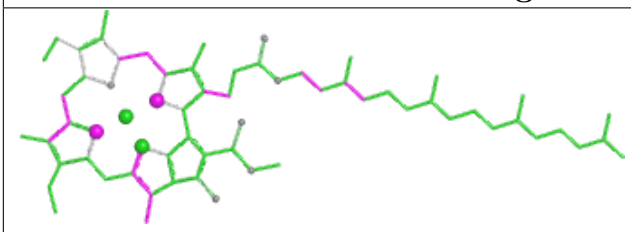
Bond angles



Torsions

Rings

Ligand CLA B 1488



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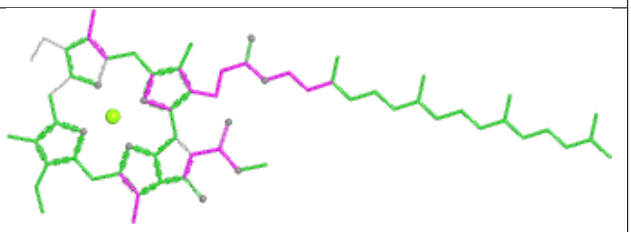
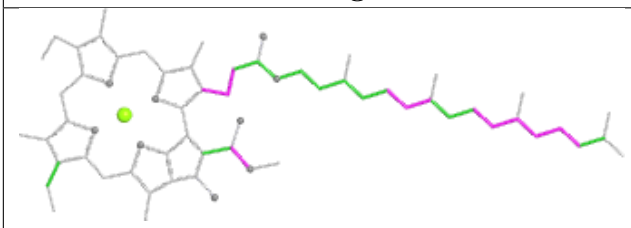


Bond angles



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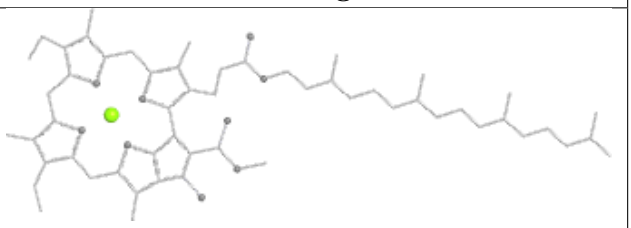
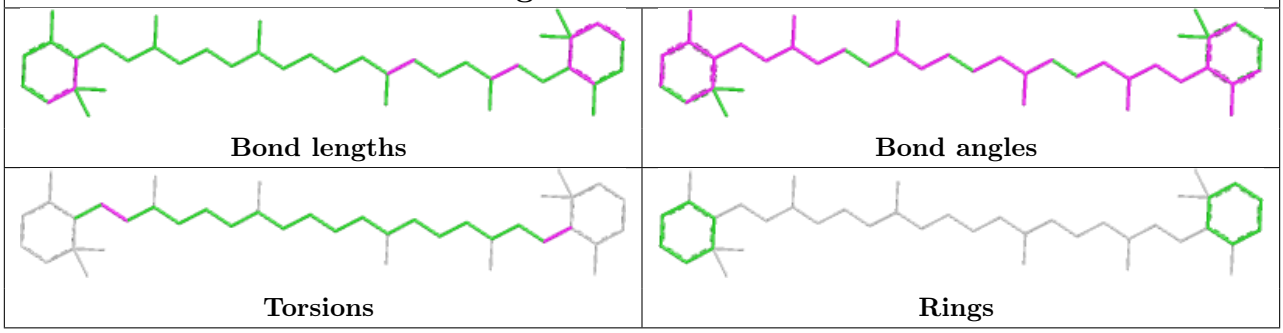
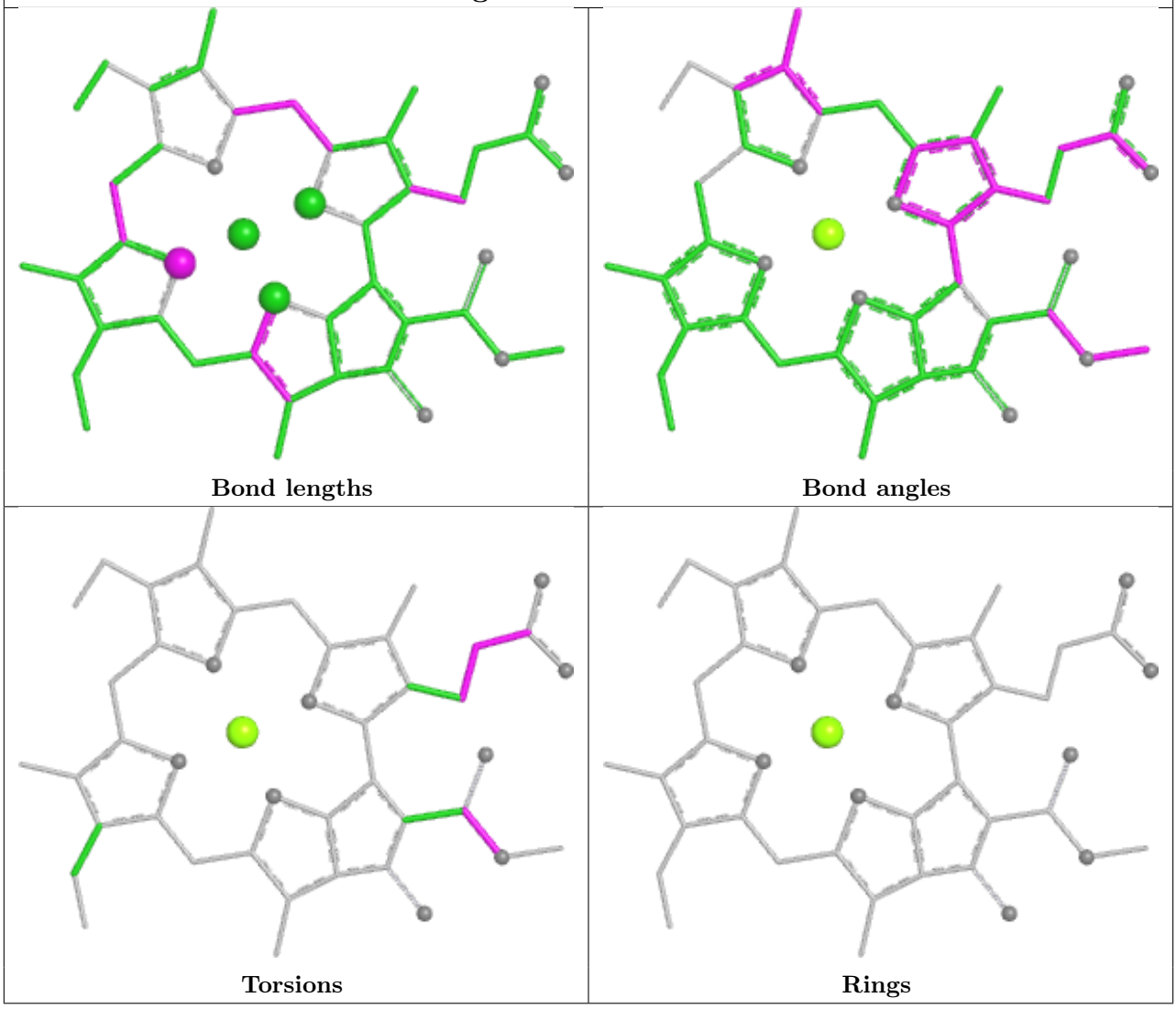


Rings

Ligand BCR F 1046



Ligand CLA H 1484



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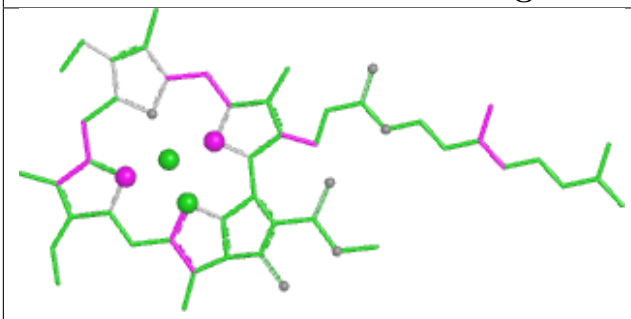
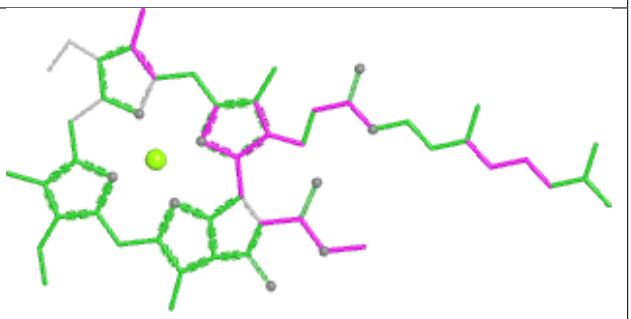
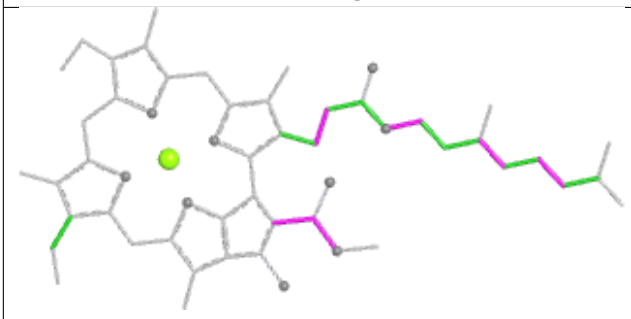
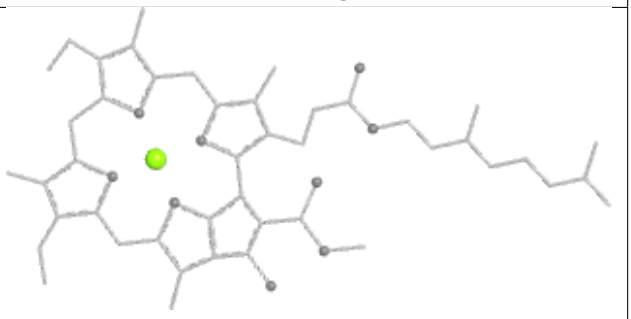
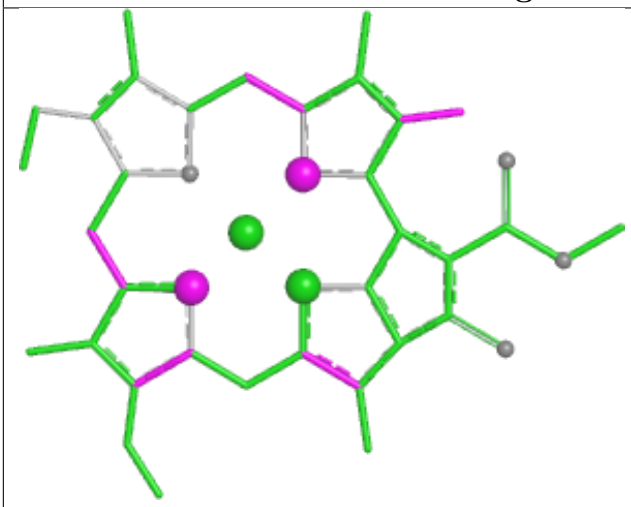
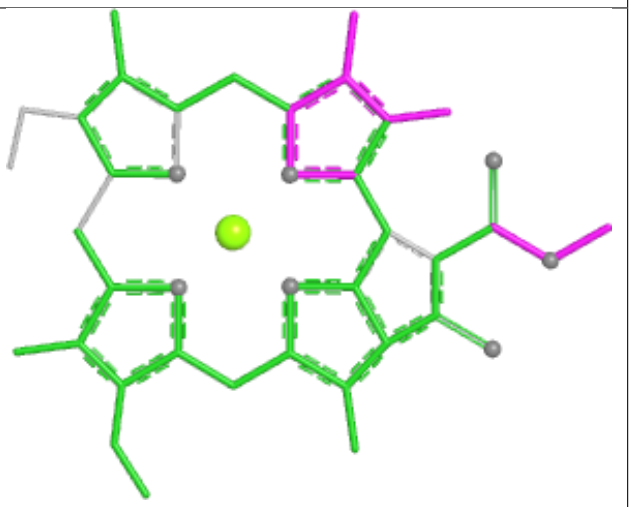
 Bond lengths	 Bond angles
 Torsions	 Rings

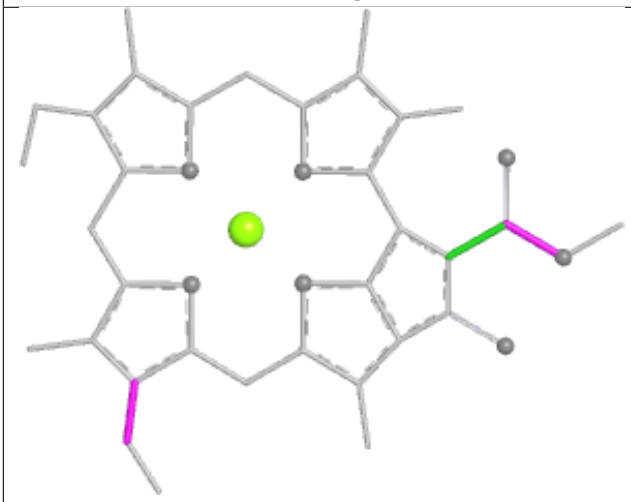
Ligand CLA C 1471



Bond lengths



Bond angles



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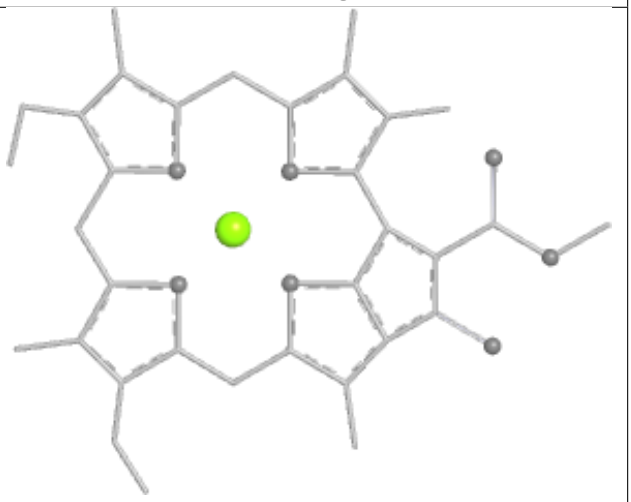
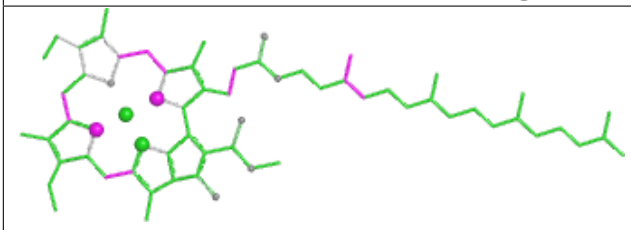
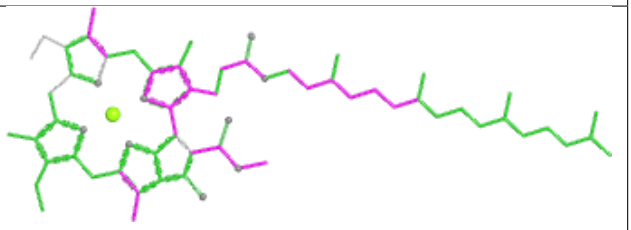


Rings

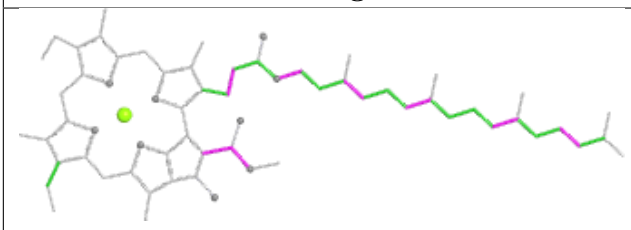
Ligand CLA B 1492



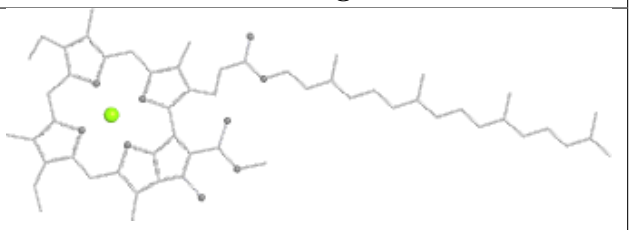
Bond lengths



Bond angles

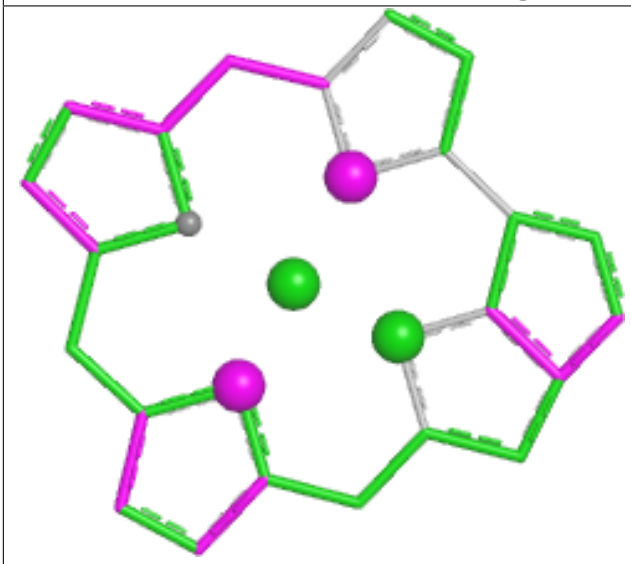


Torsions



Rings

Ligand CLA H 1491



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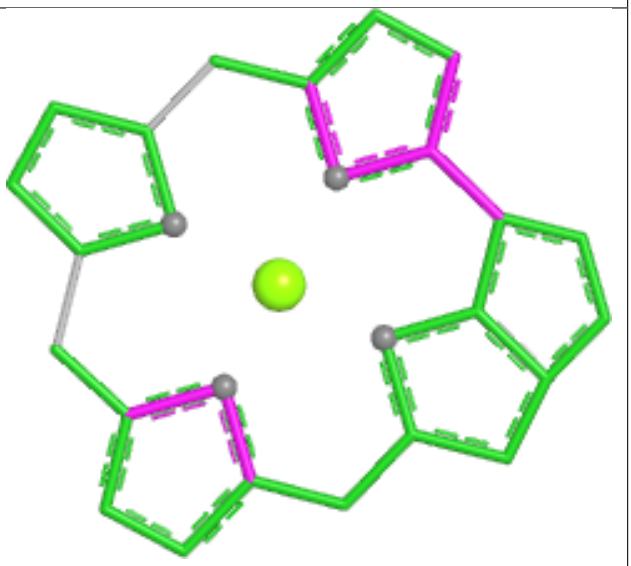
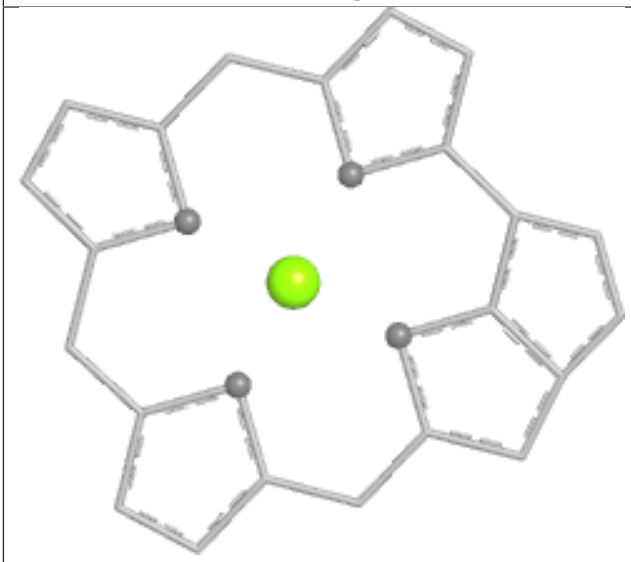


Bond angles



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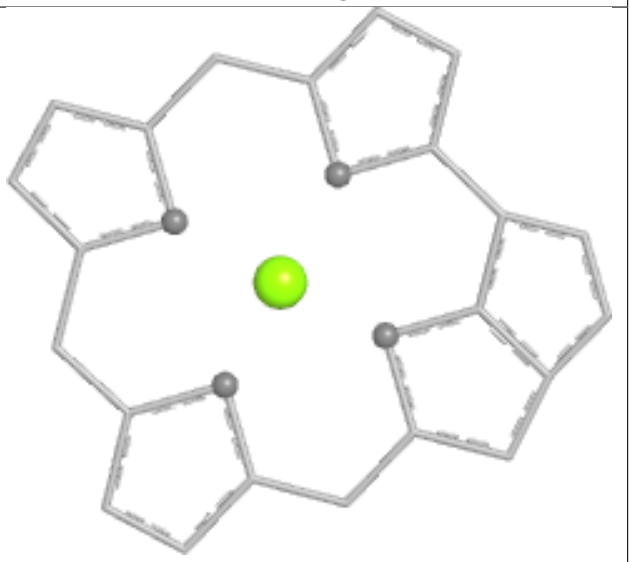
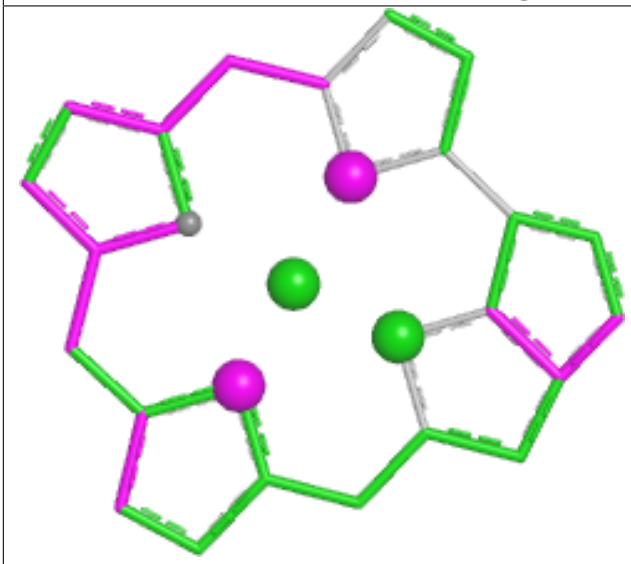


Rings

Ligand CLA C 1468



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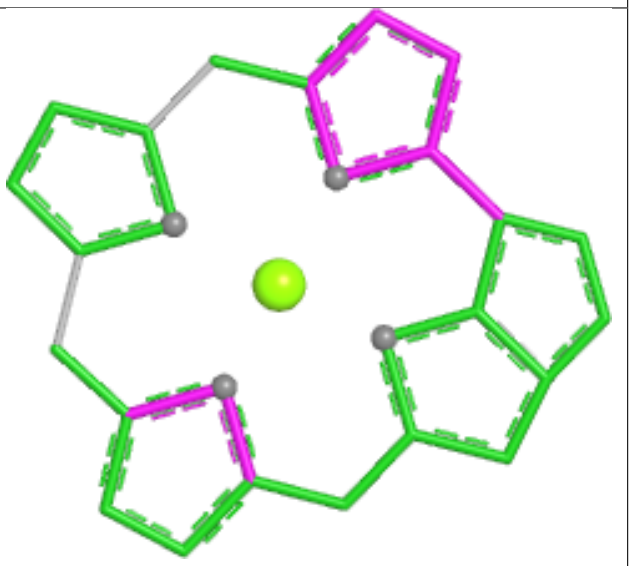
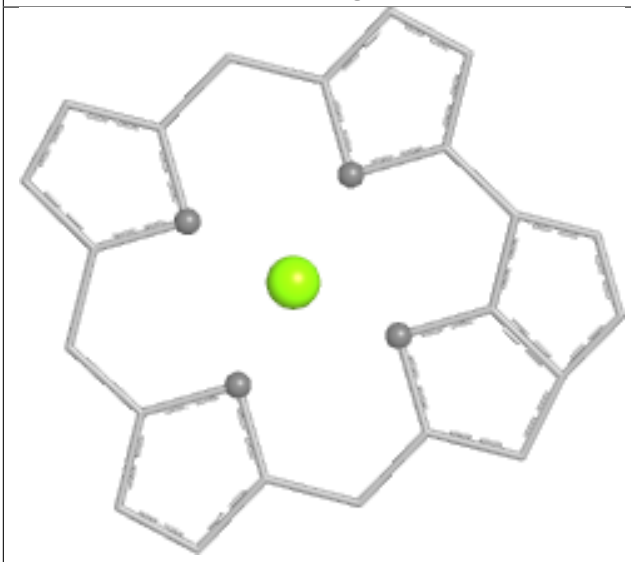


Bond angles



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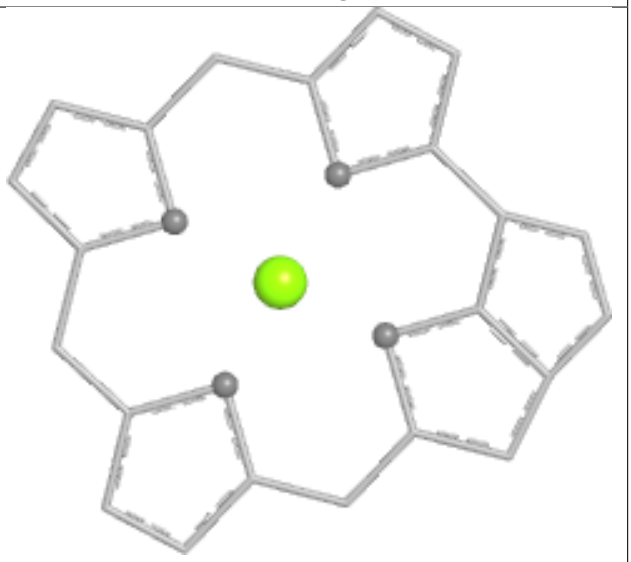
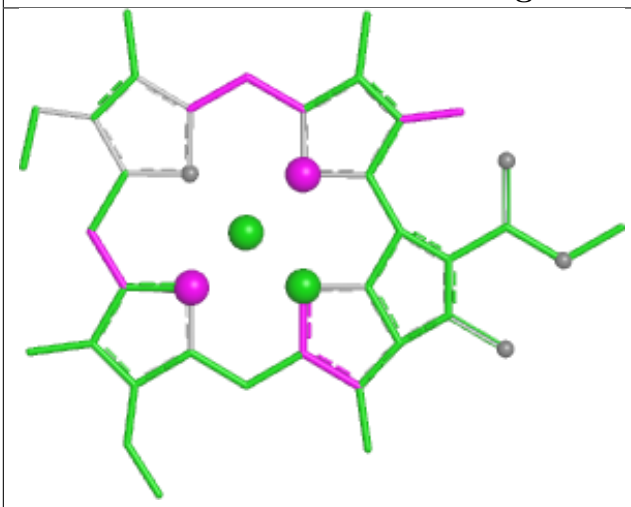


Rings

Ligand CLA C 1470



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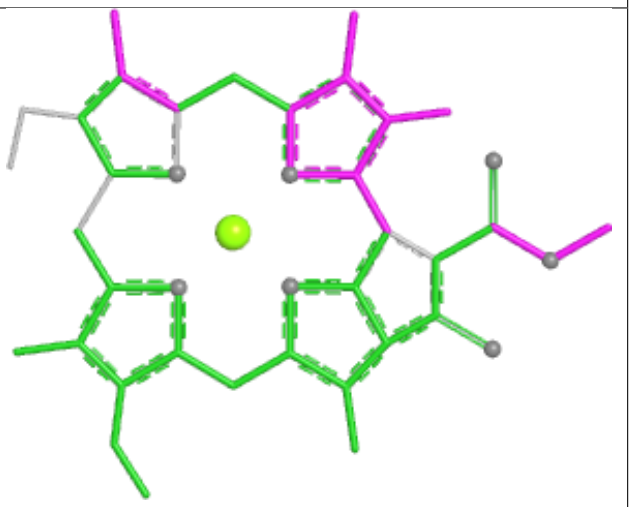

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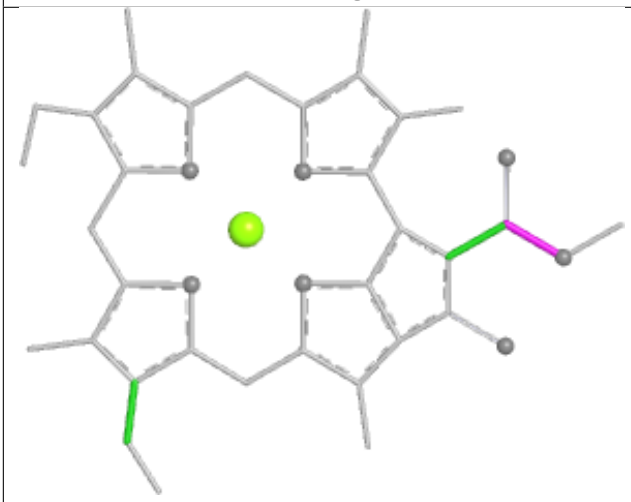

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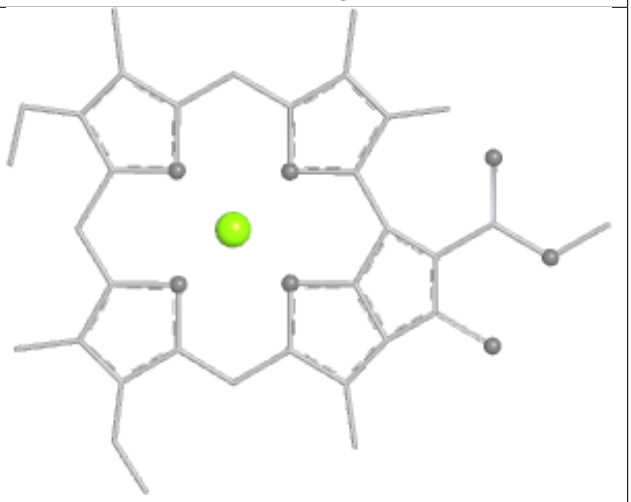
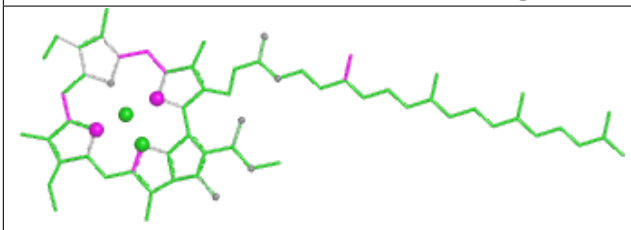


Rings

Ligand CLA H 1492



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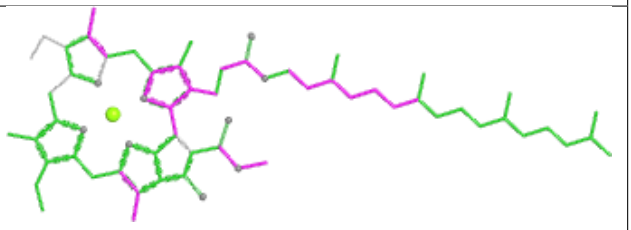

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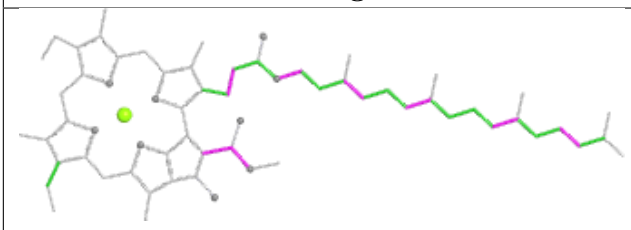

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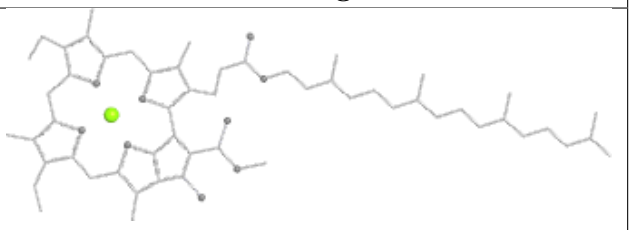
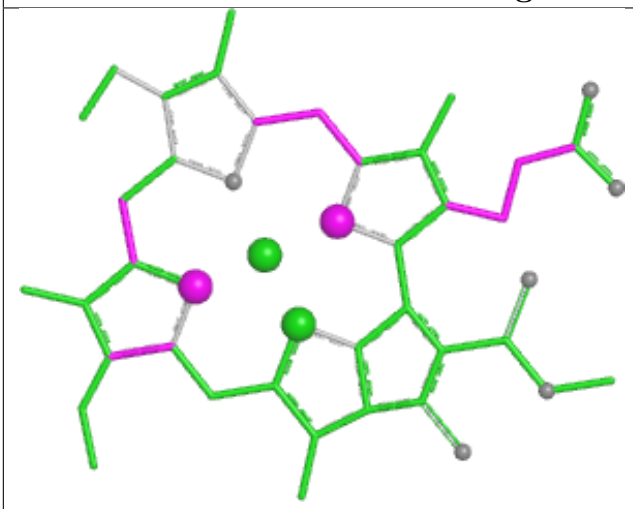


Rings

Ligand CLA C 1459



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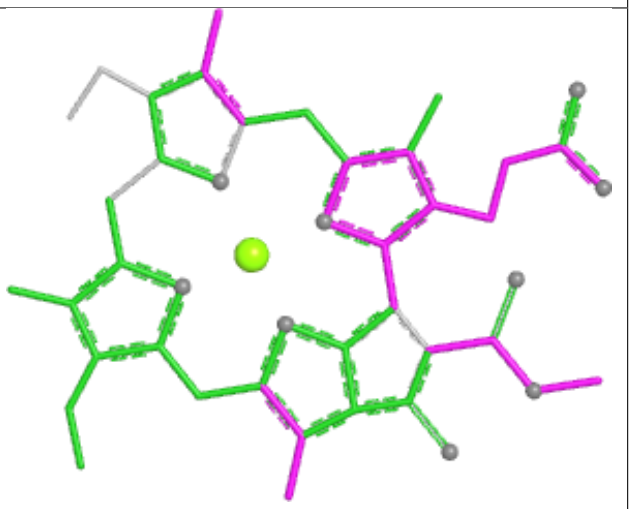
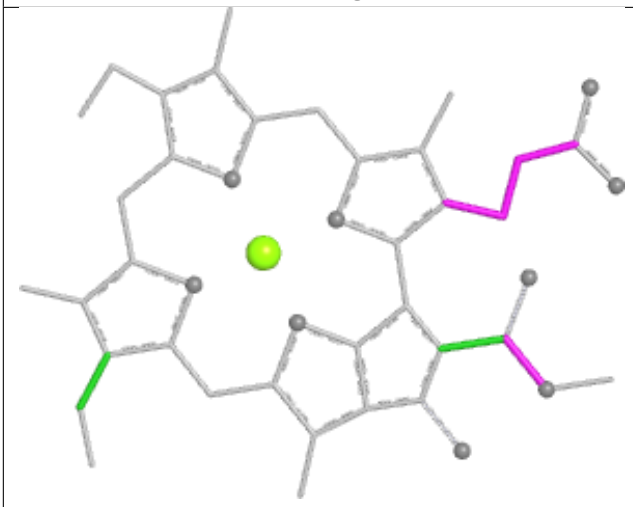


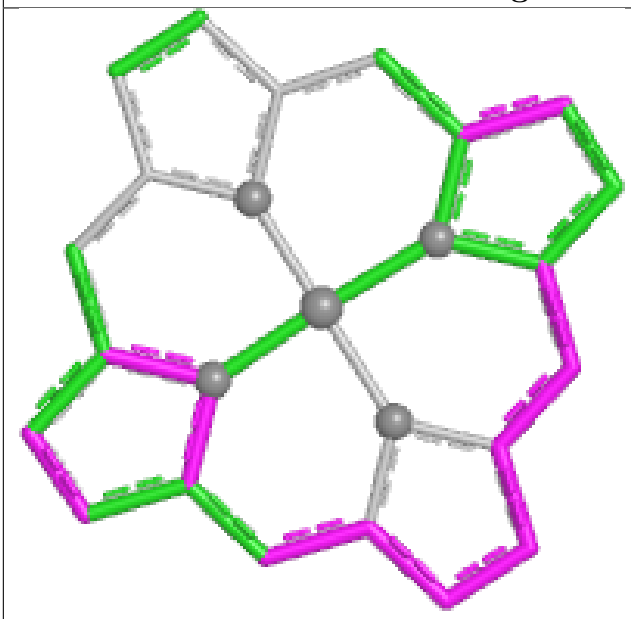
Bond angles



Torsions

Rings

Ligand HEM E 1085



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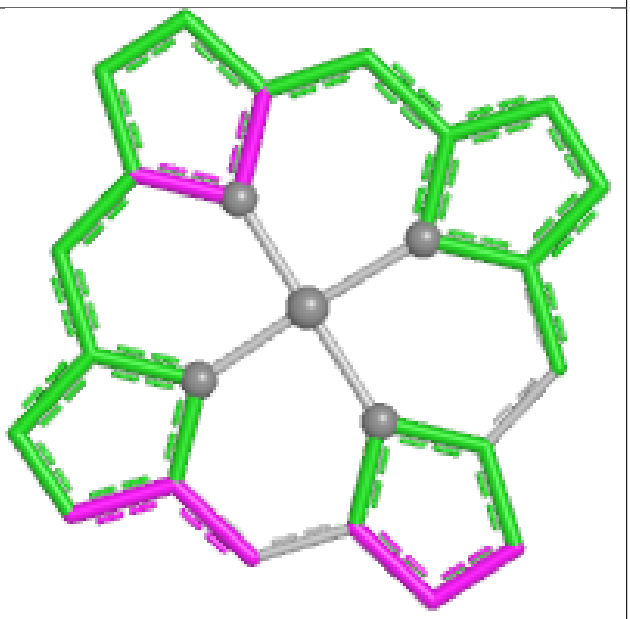

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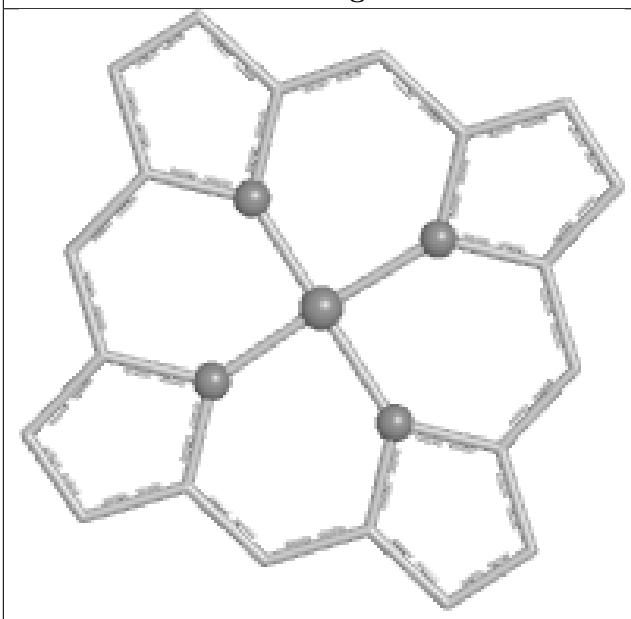
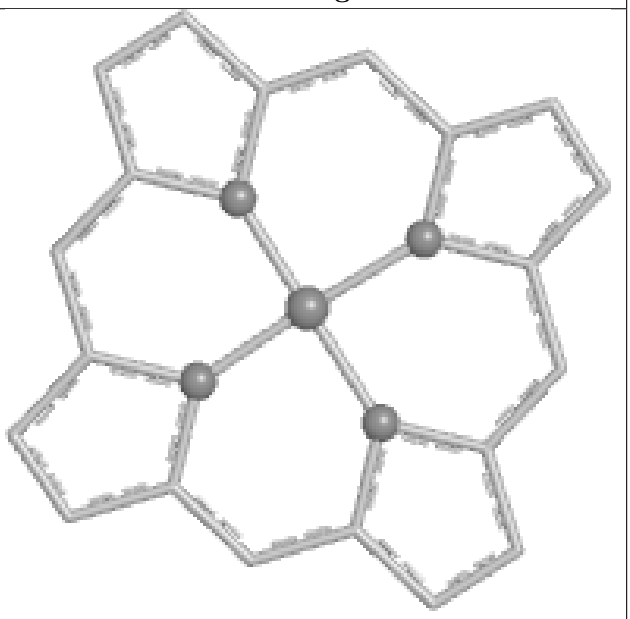
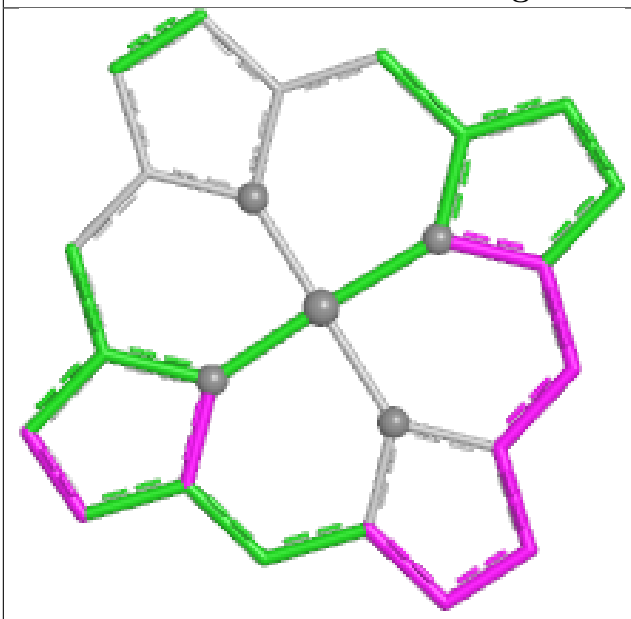


Torsions



Rings

Ligand HEM L 1046



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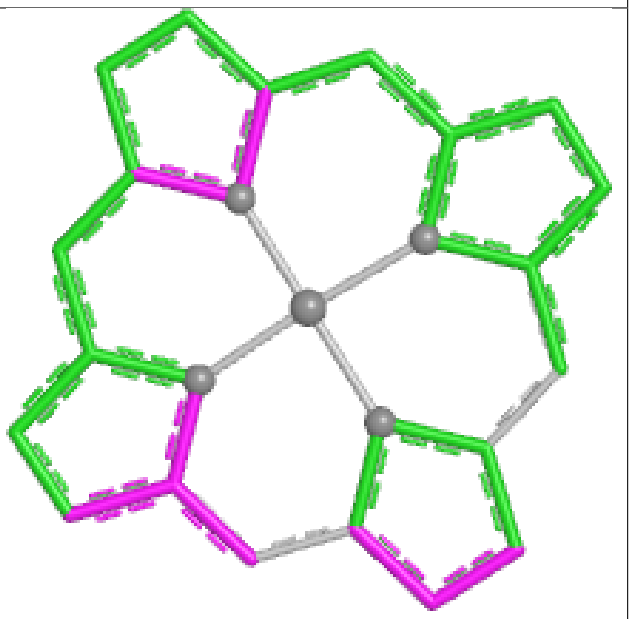
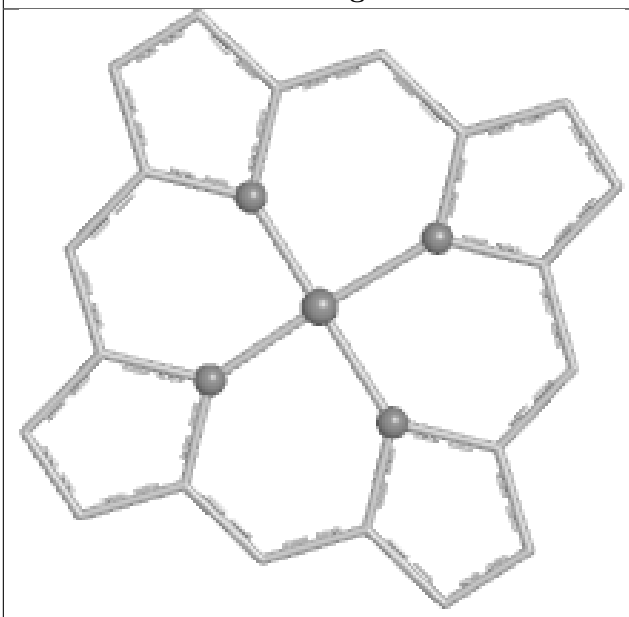


Bond angles



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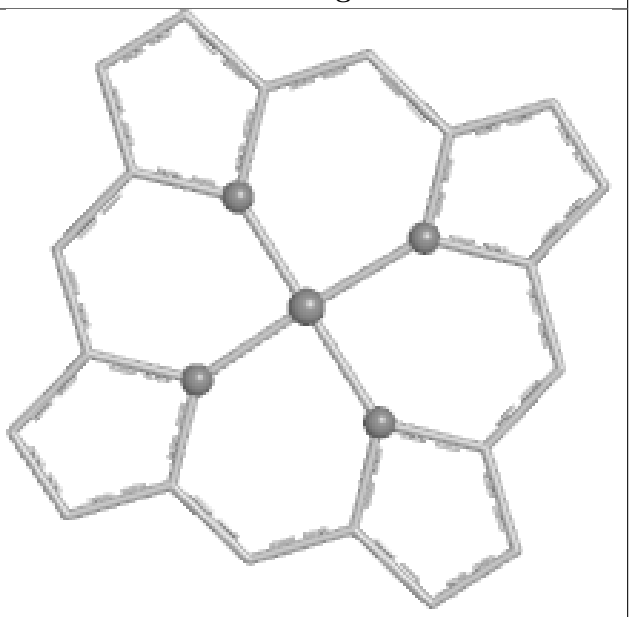
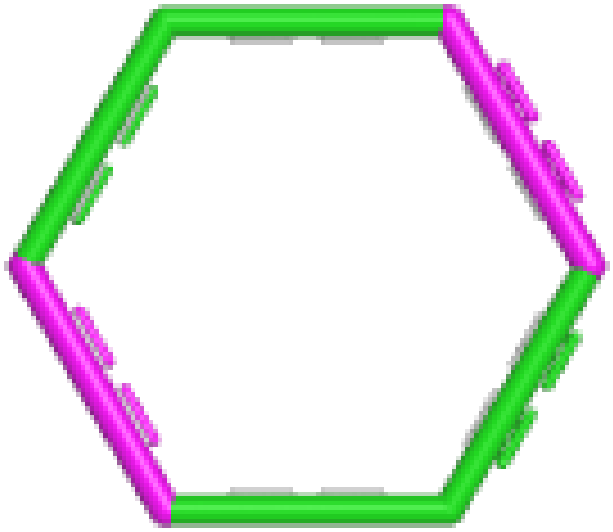


Rings

Ligand PL9 J 1354



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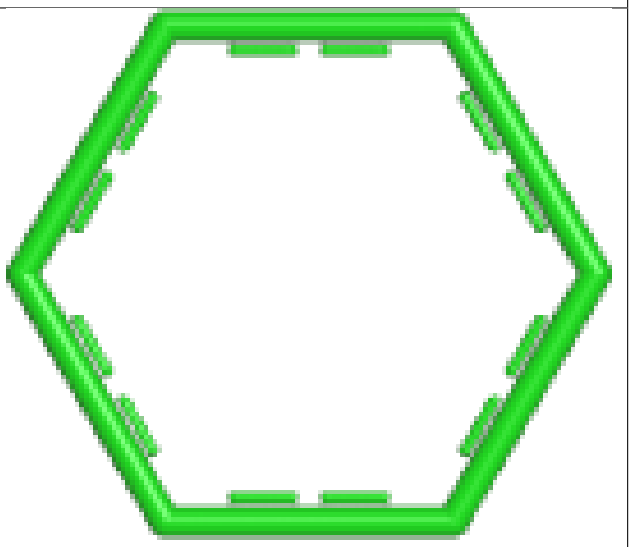

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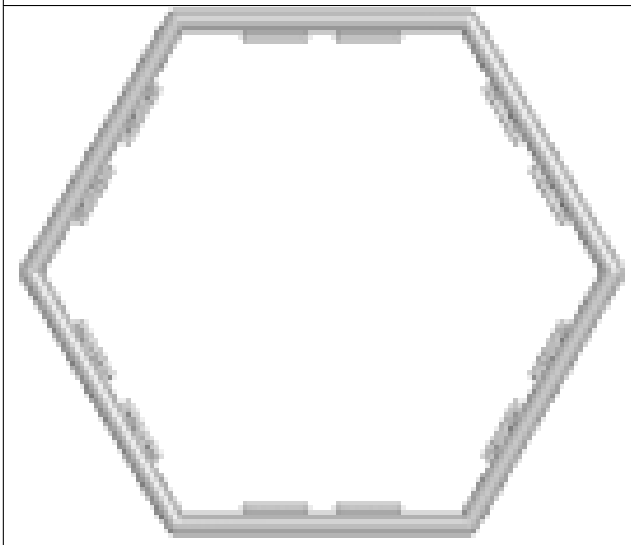
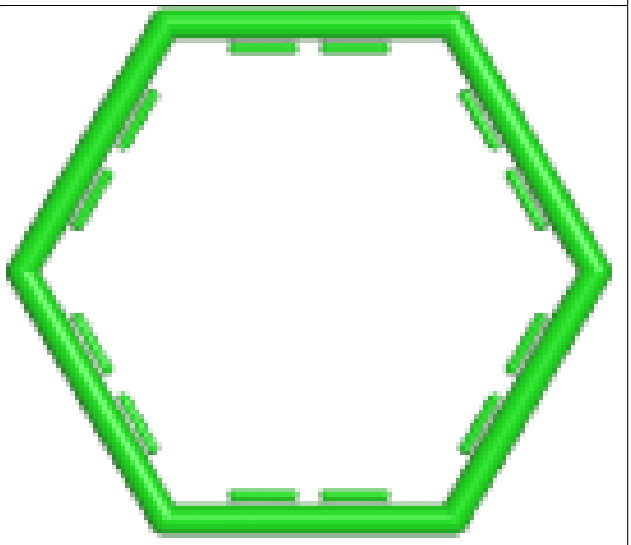
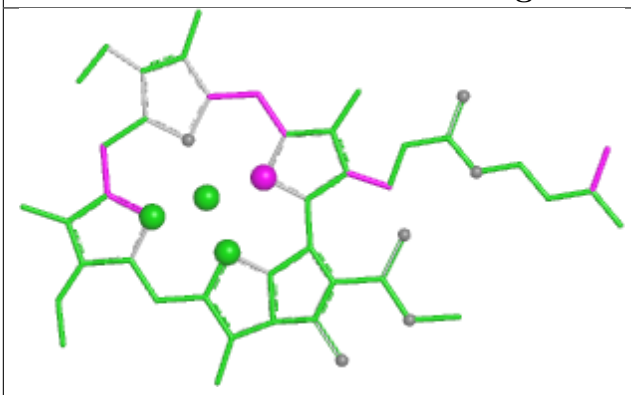


Torsions



Rings

Ligand CLA B 1489



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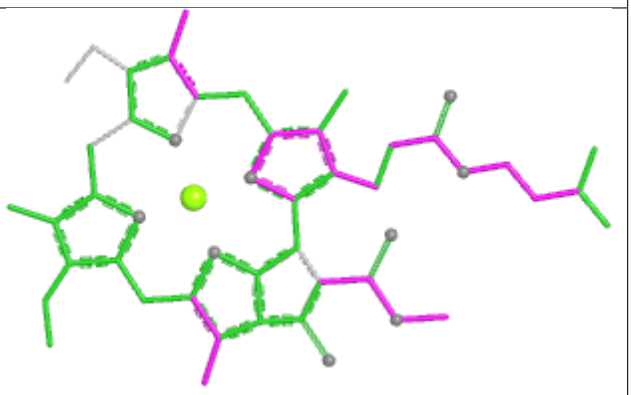

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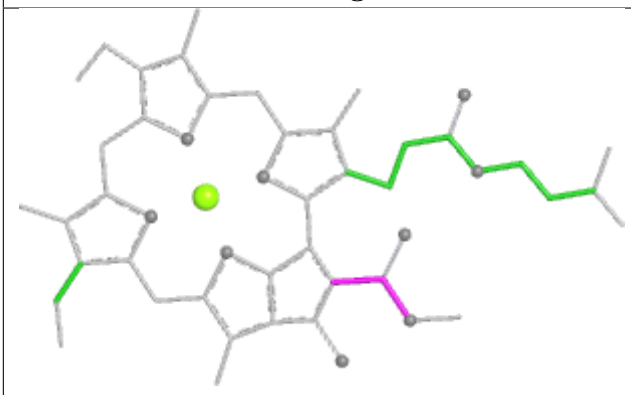

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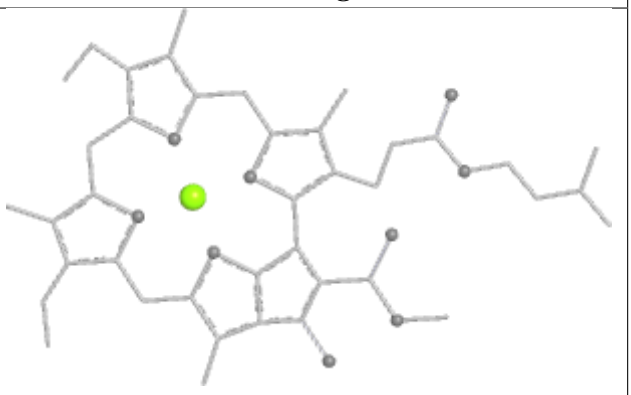
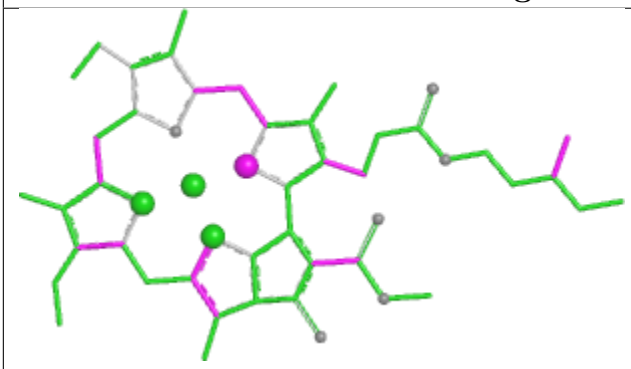


Rings

Ligand CLA G 1346



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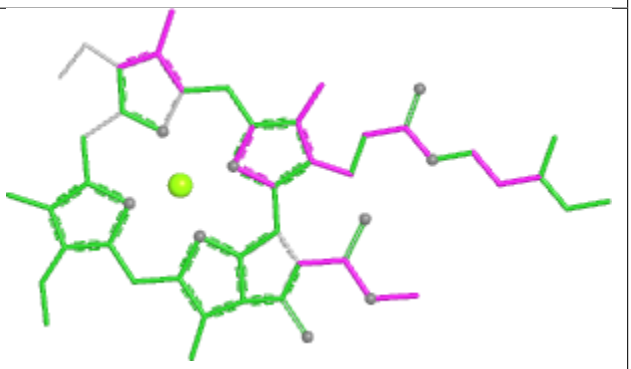

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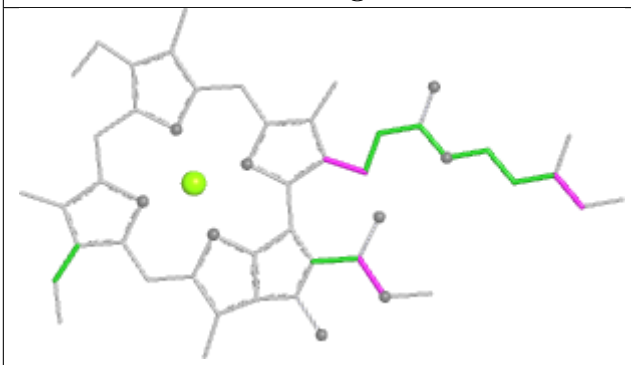

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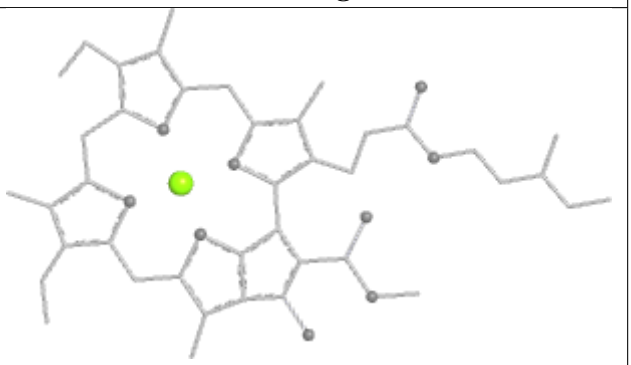
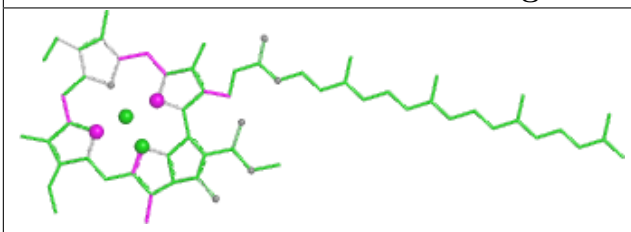


Rings

Ligand CLA I 1465



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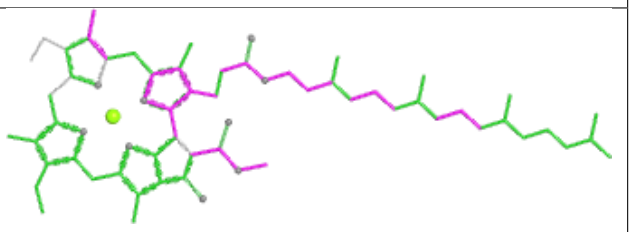
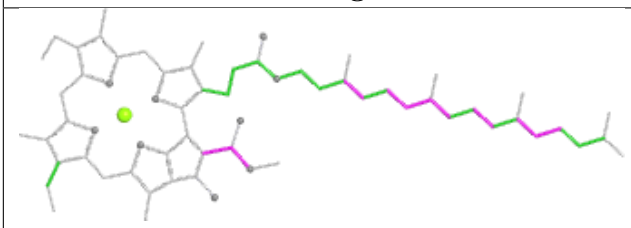


Bond angles



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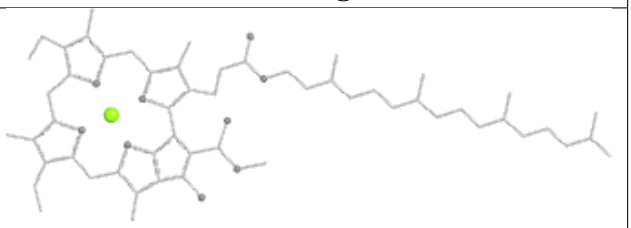
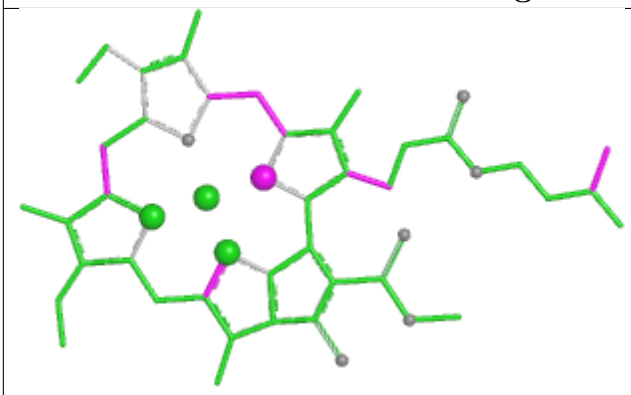


Rings

Ligand CLA H 1489



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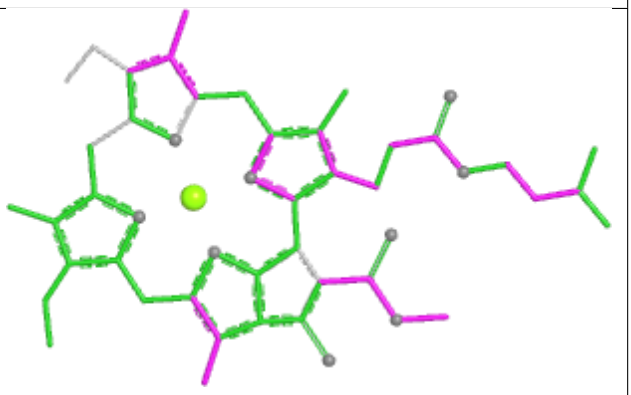
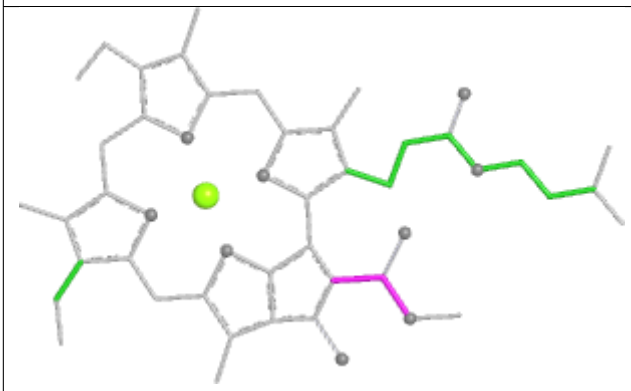


Bond angles



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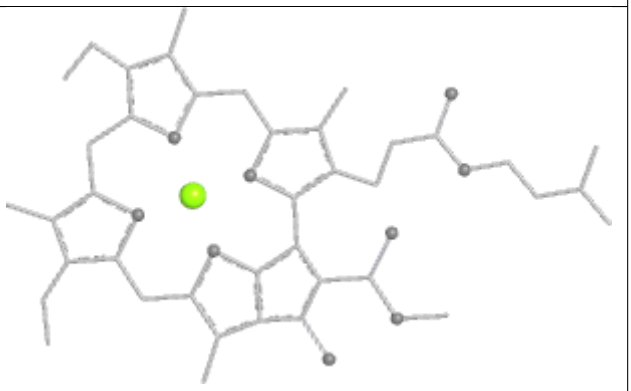

Rings

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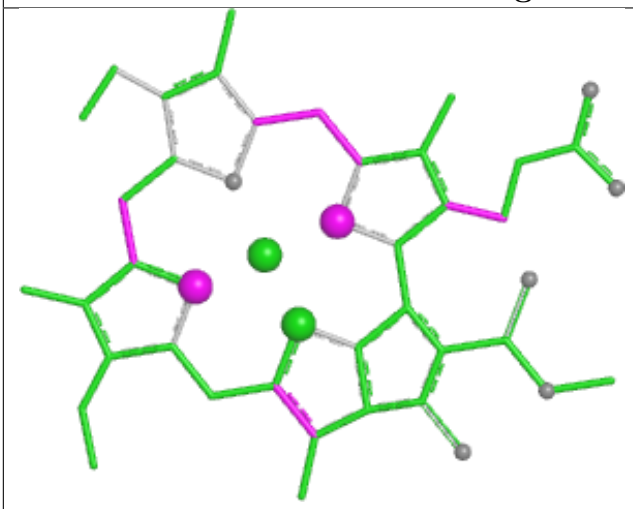

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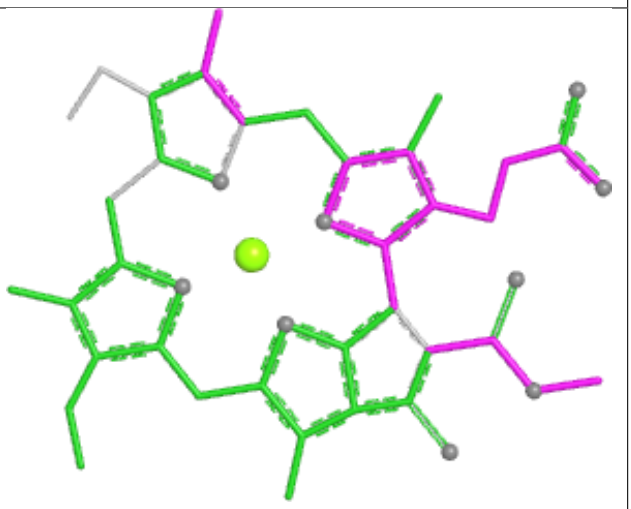
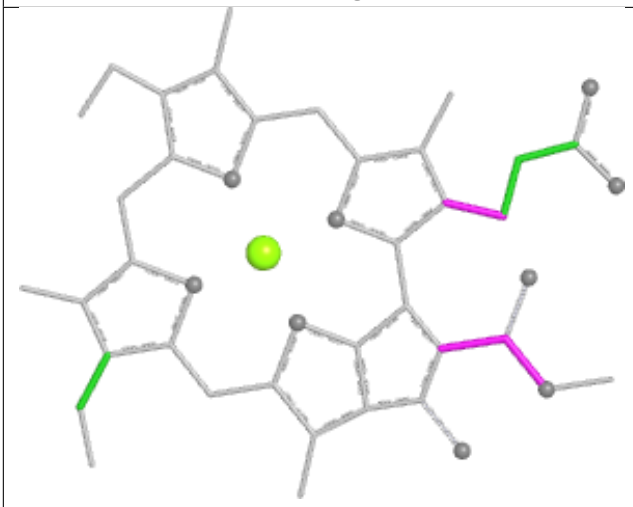


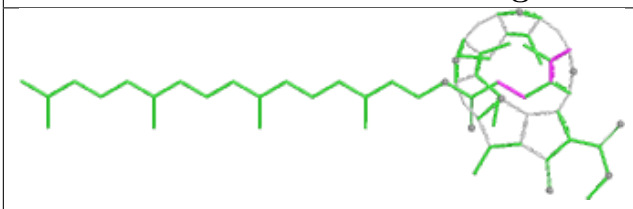
Bond angles



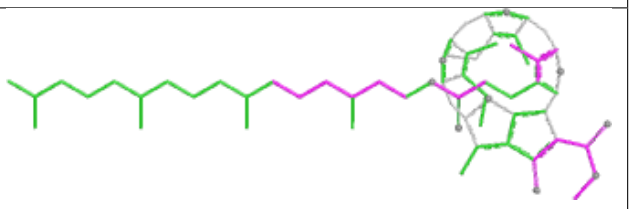
Torsions

Rings

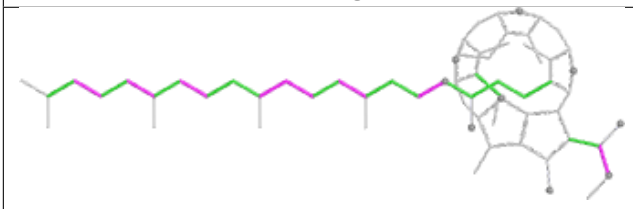
Ligand PHO G 1345



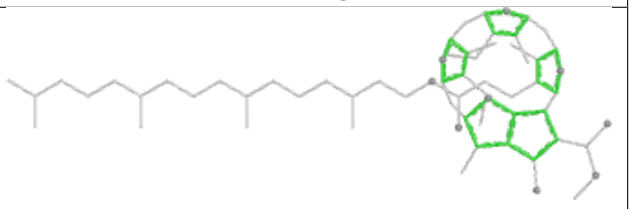
Bond lengths



Bond angles

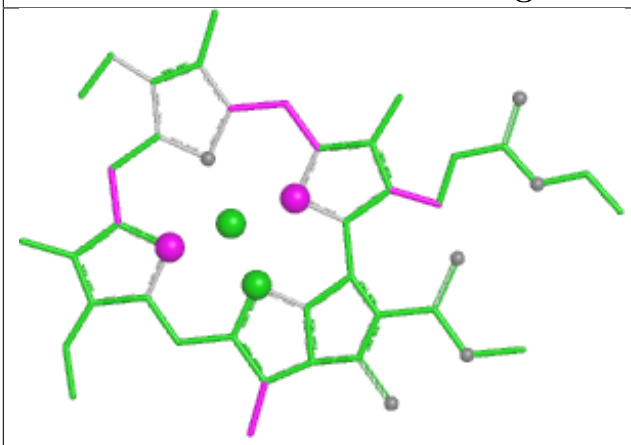


Torsions



Rings

Ligand CLA C 1460



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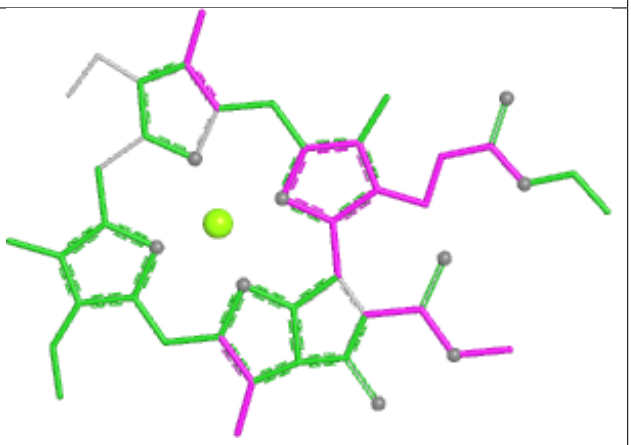
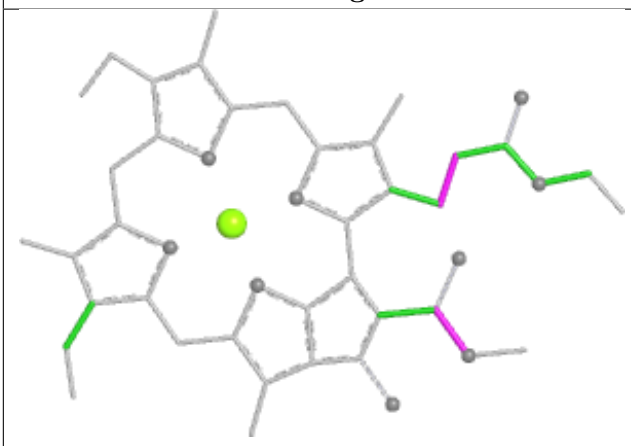
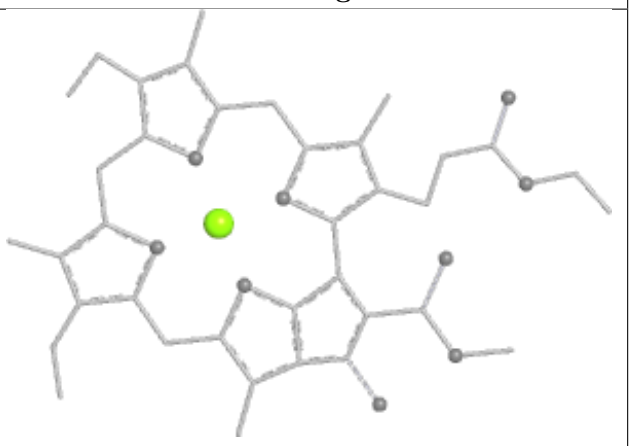


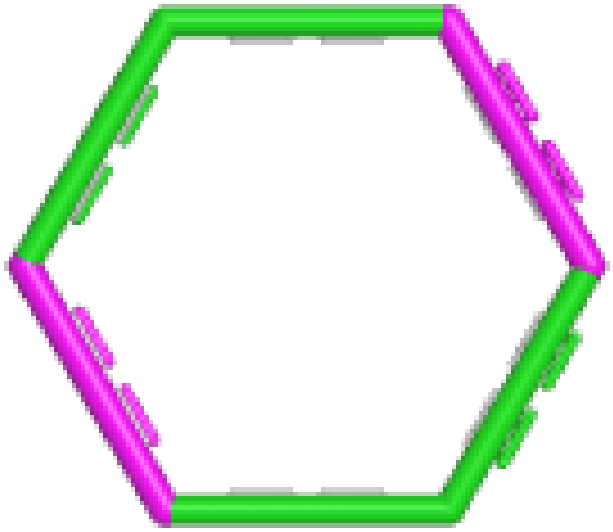
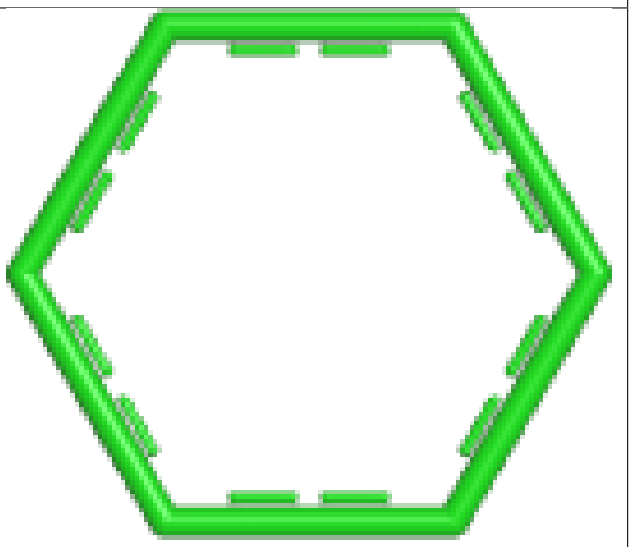
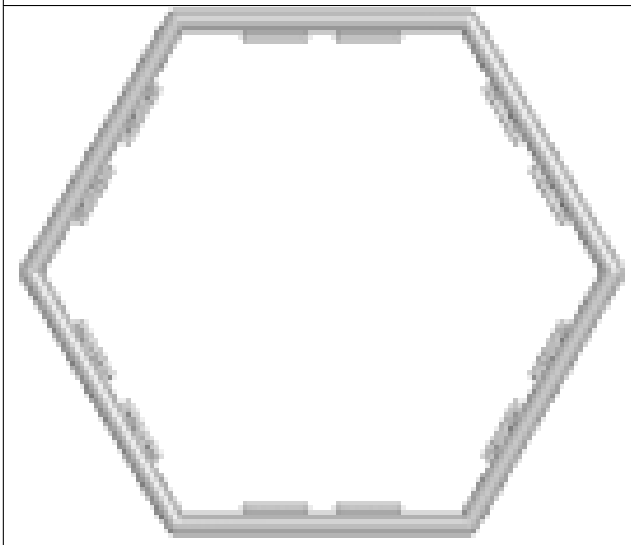
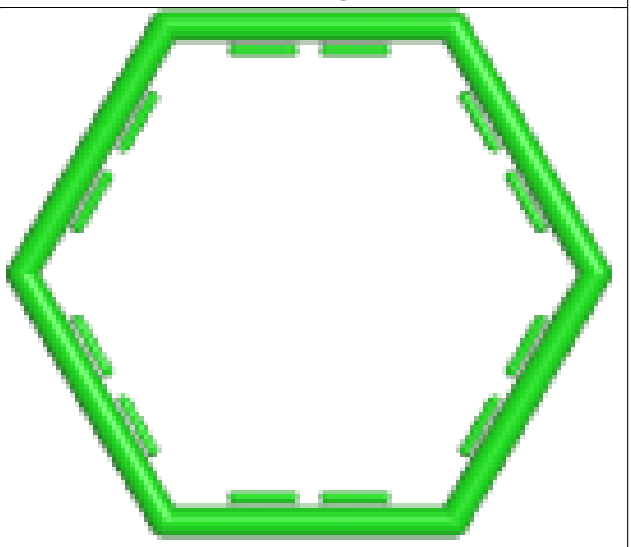
Bond angles



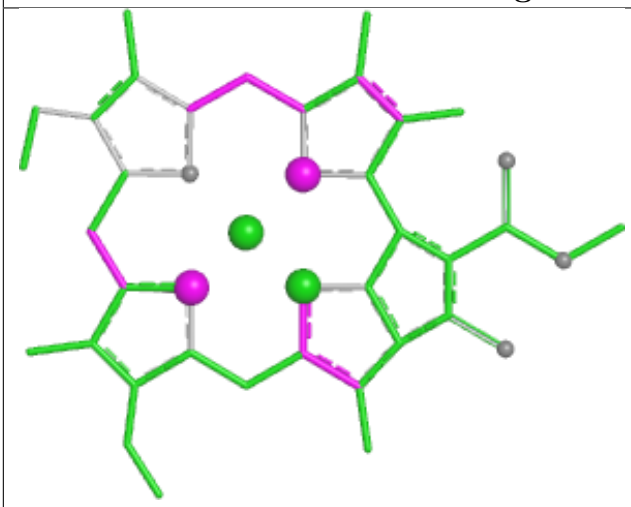
Torsions



Rings

Ligand PL9 D 1354	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA H 1486



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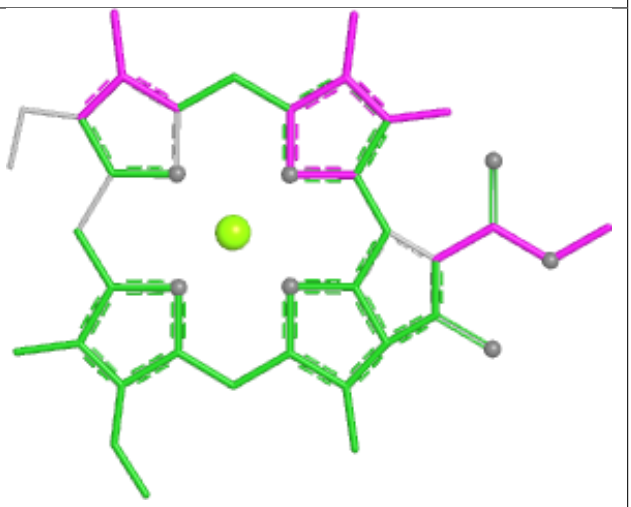
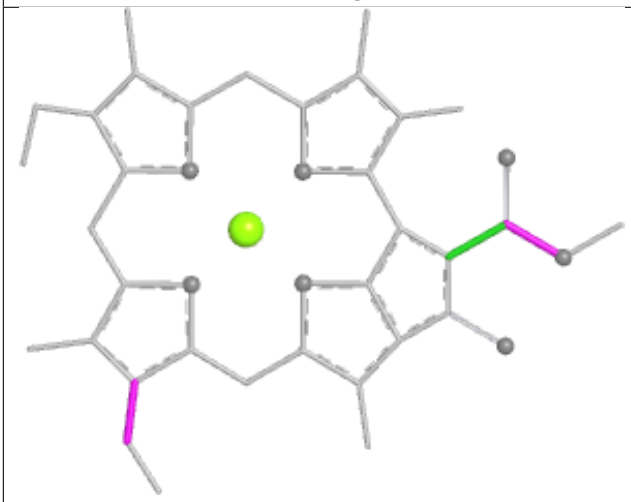
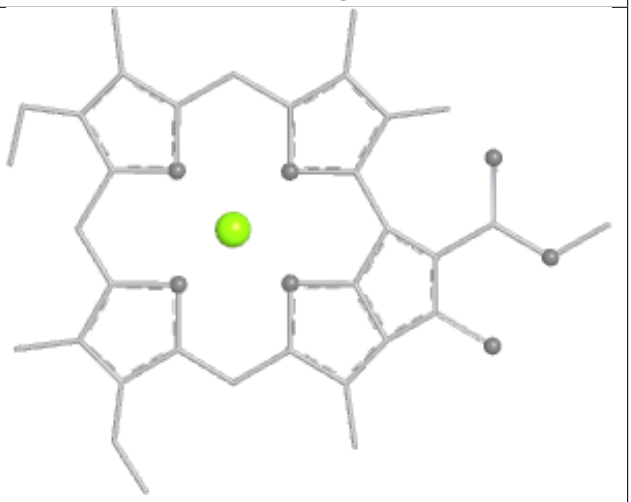


Bond angles



Torsions



Rings

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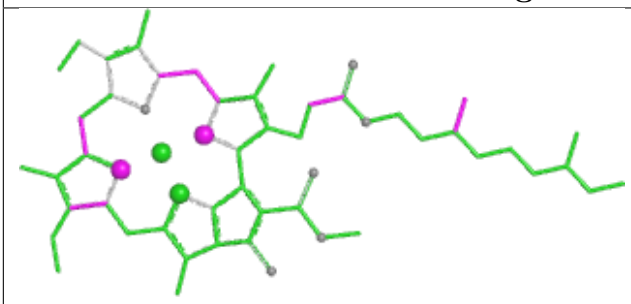
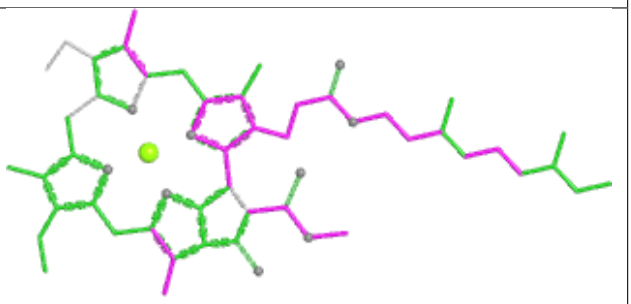
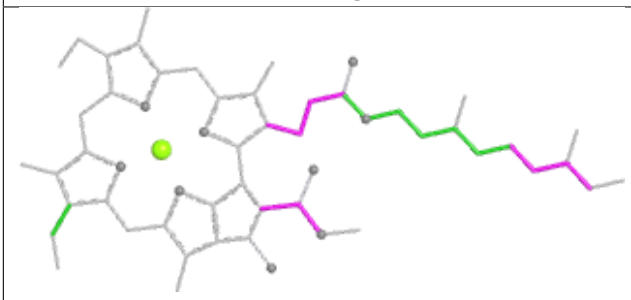
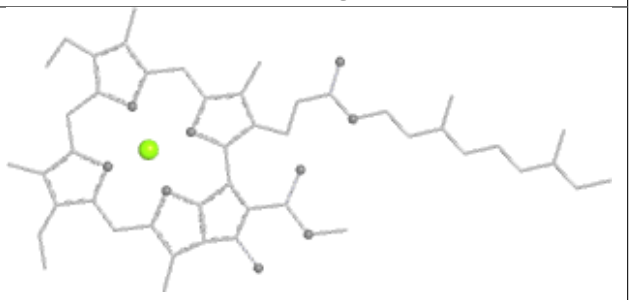
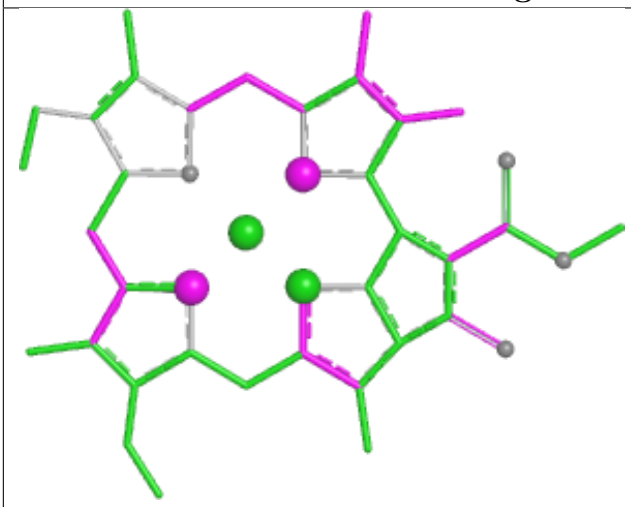
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1497



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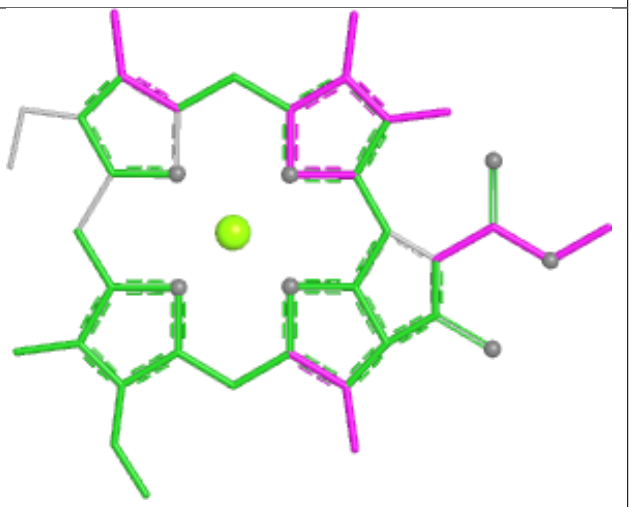
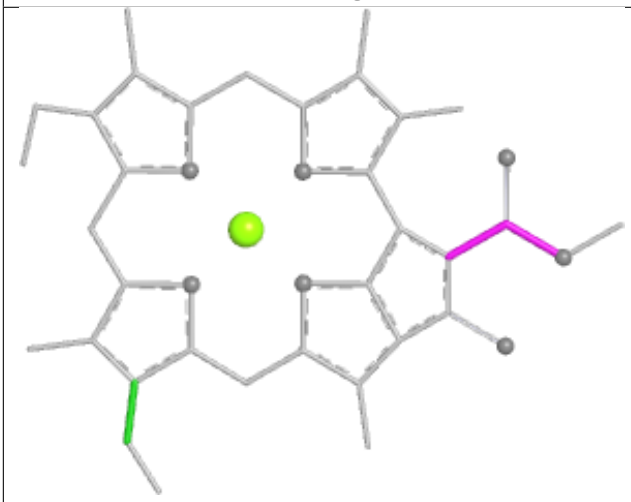
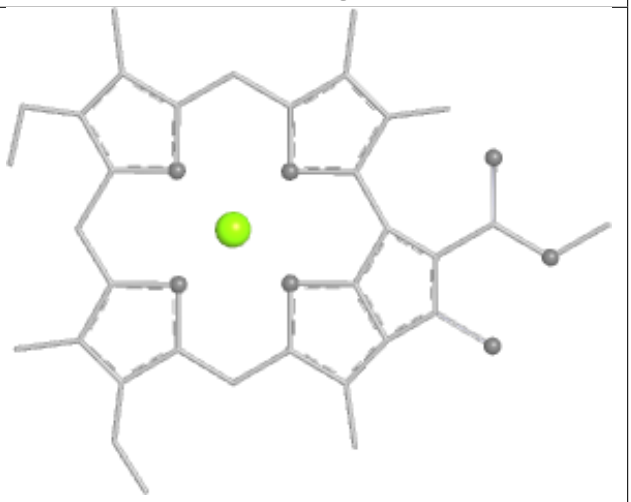


Bond angles

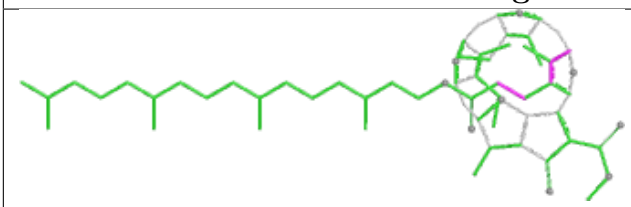


Torsions



Rings

Ligand PHO A 1345



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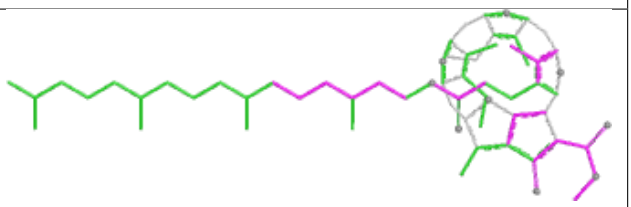
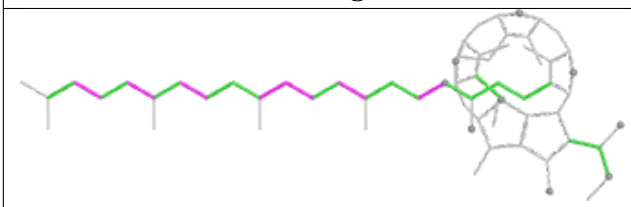


Bond angles



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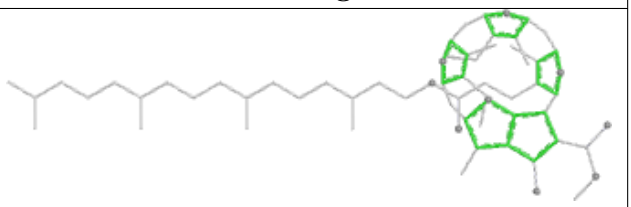
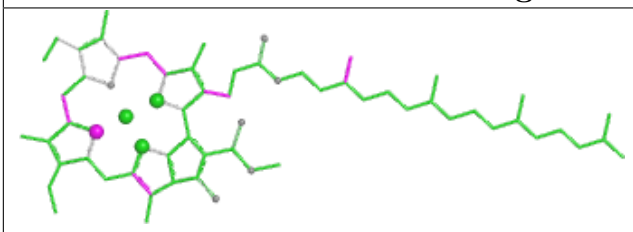


Rings

Ligand CLA B 1496



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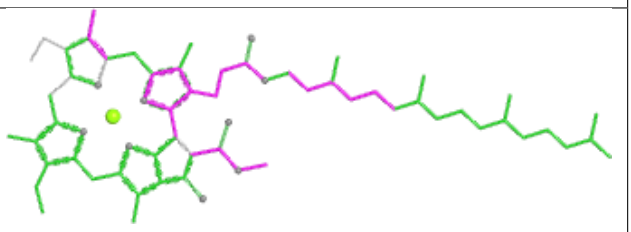
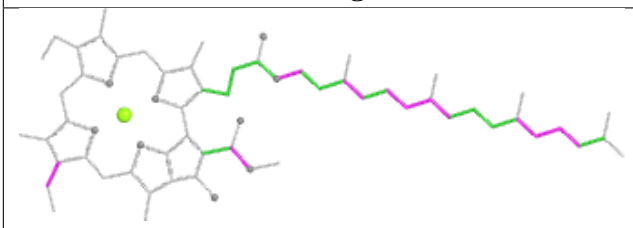


Bond angles



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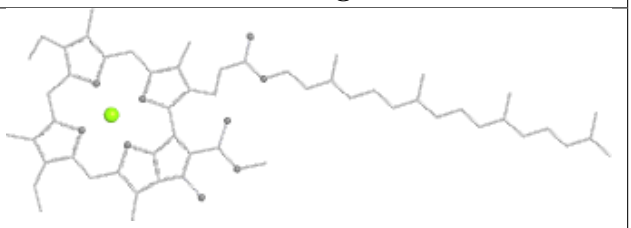
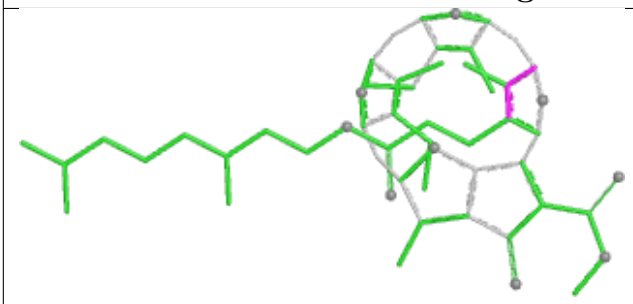


Rings

Ligand PHO J 1352



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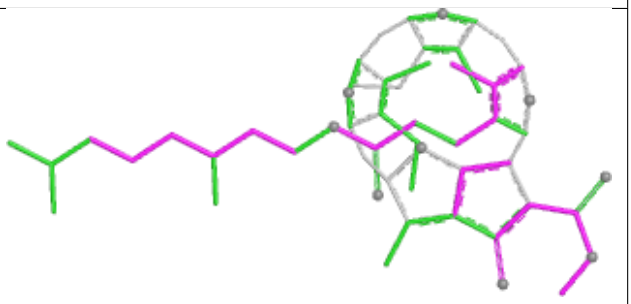
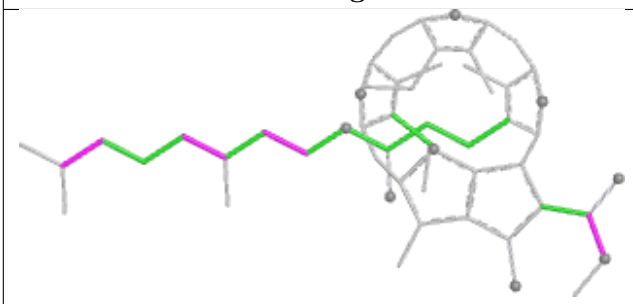


Bond angles



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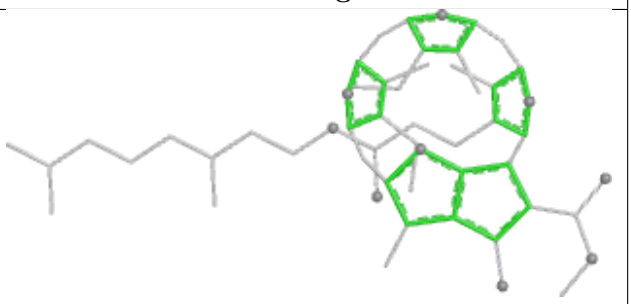
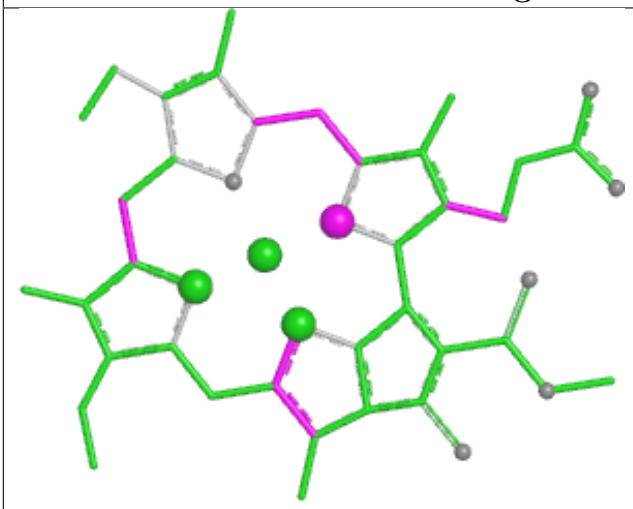


Rings

Ligand CLA G 1344



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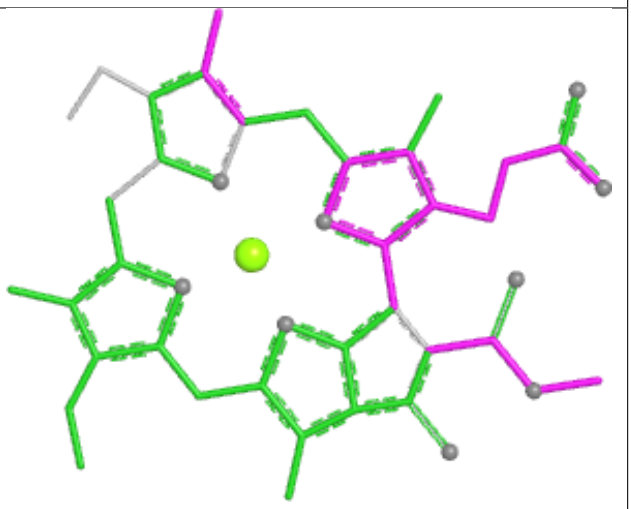
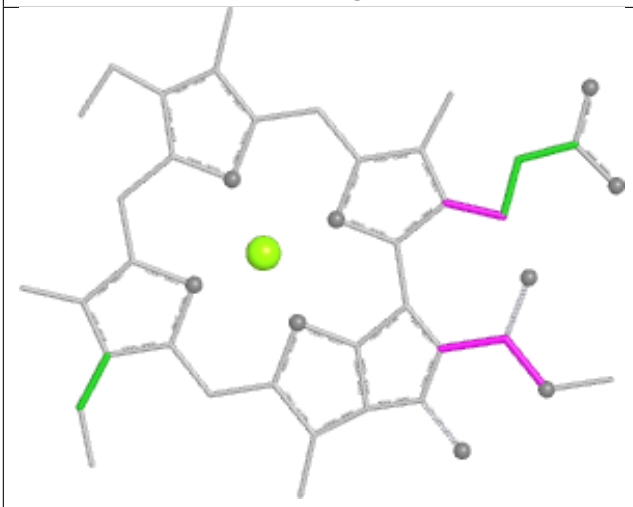


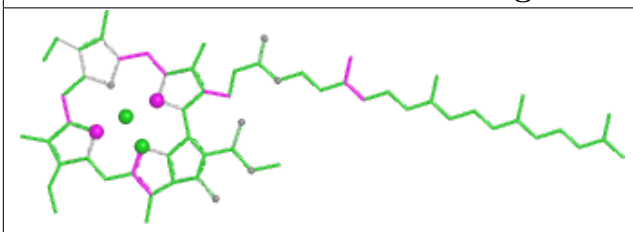
Bond angles



Torsions

Rings

Ligand CLA H 1496



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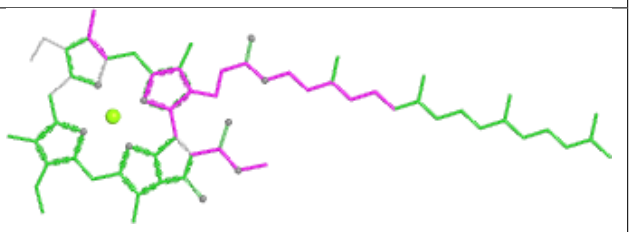

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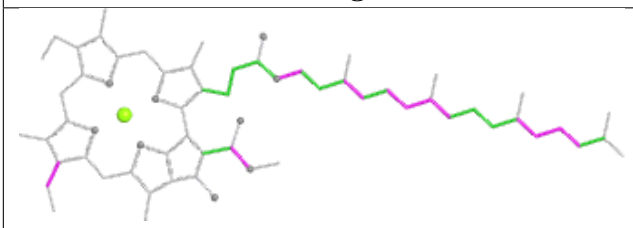
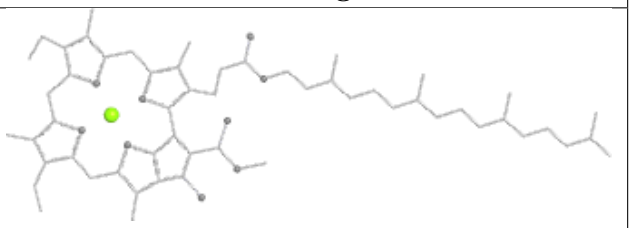
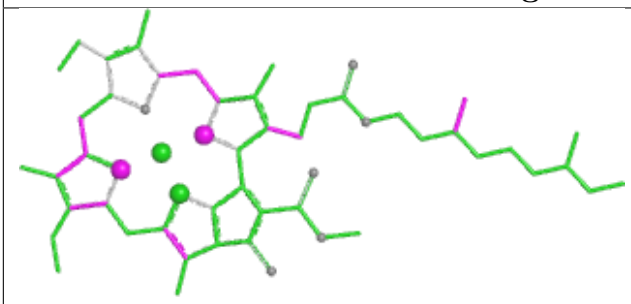


Torsions



Rings

Ligand CLA I 1464



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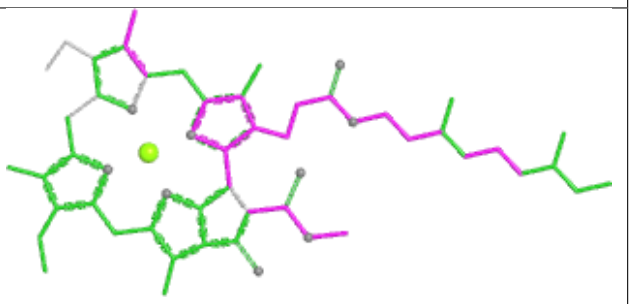

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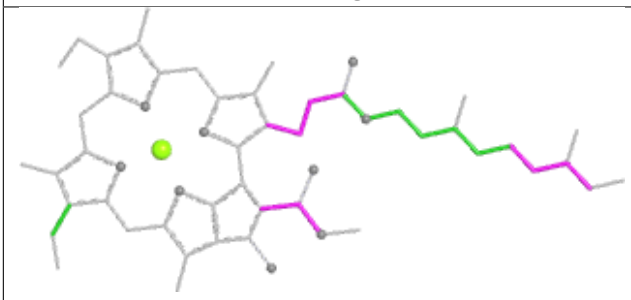
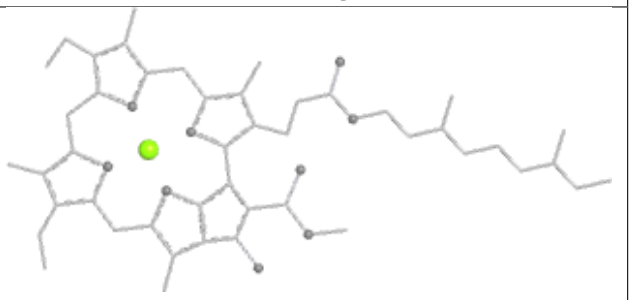
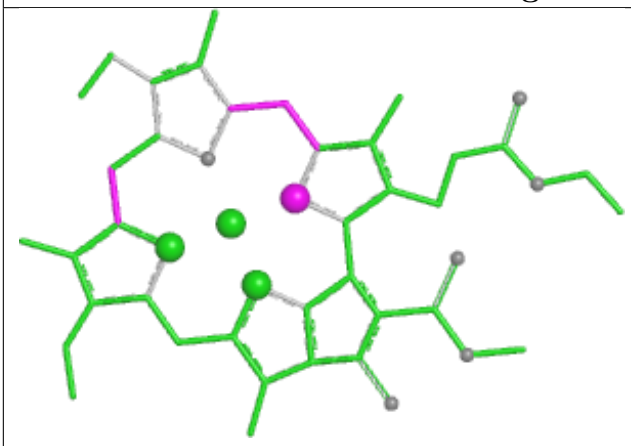


Torsions



Rings

Ligand CLA I 1467



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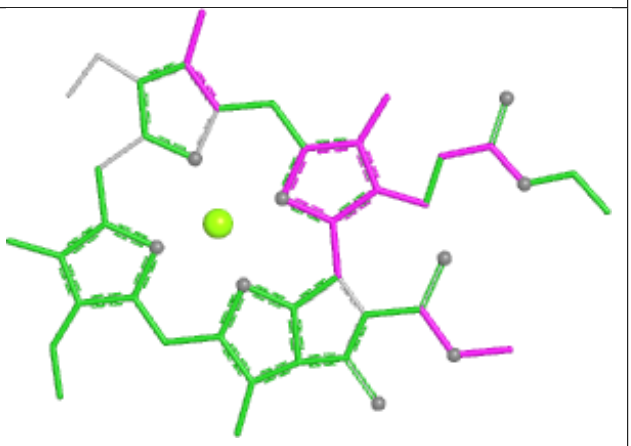
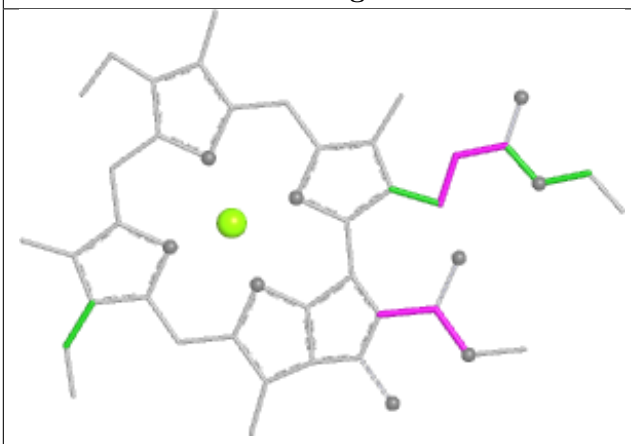


Bond angles



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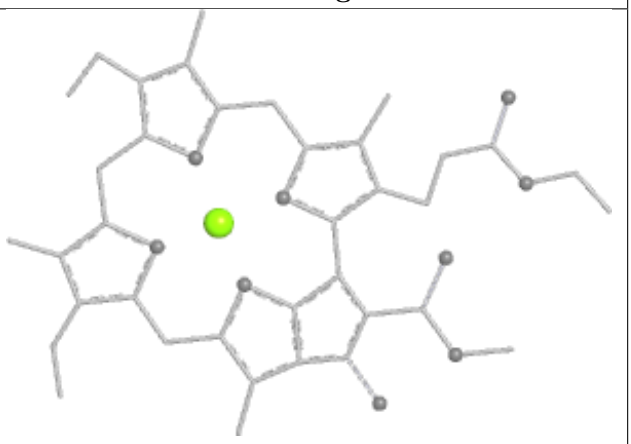
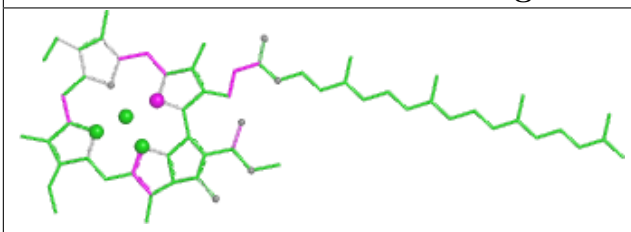


Rings

Ligand CLA A 1342



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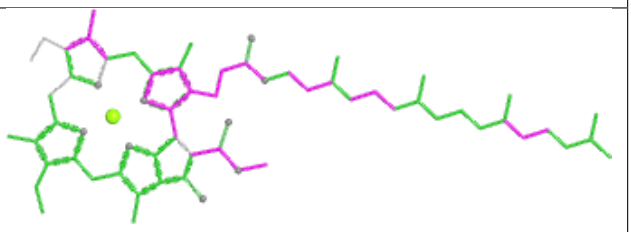
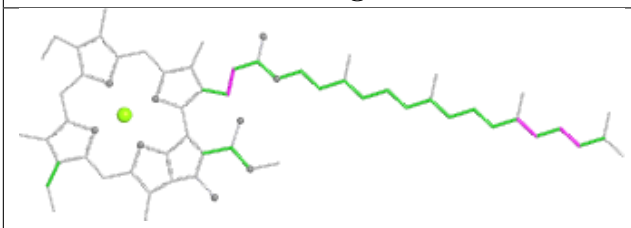
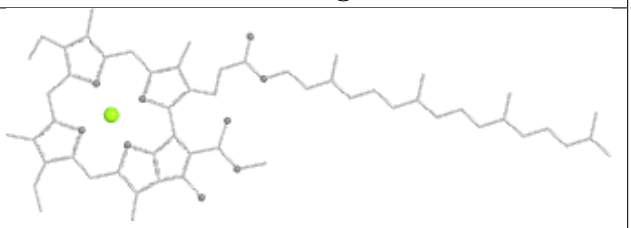


Bond angles

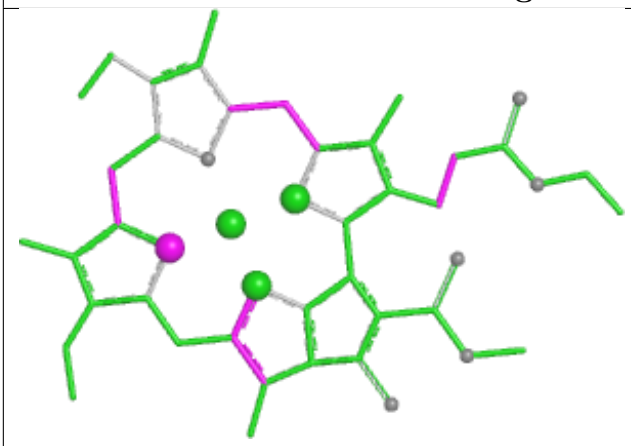


Torsions

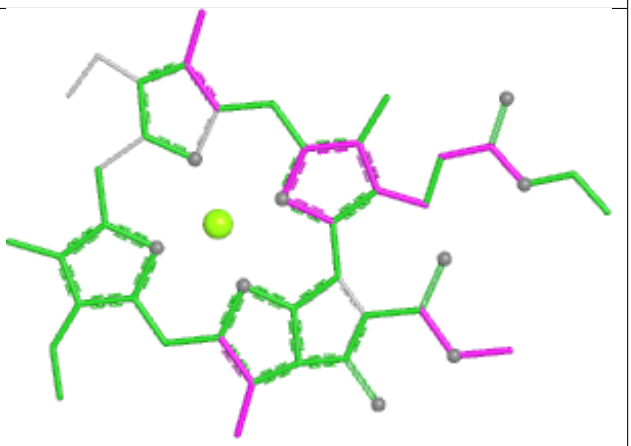


Rings

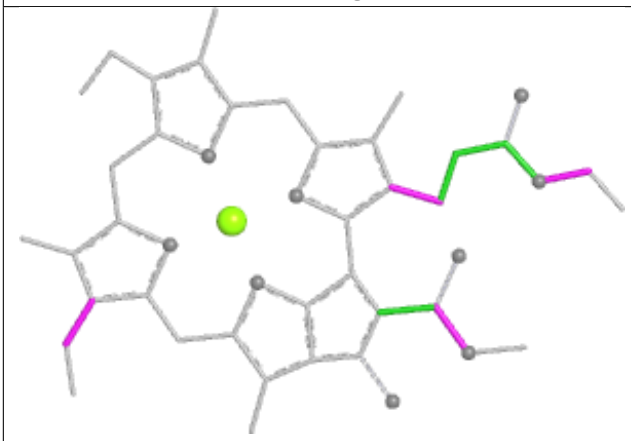
Ligand CLA B 1485



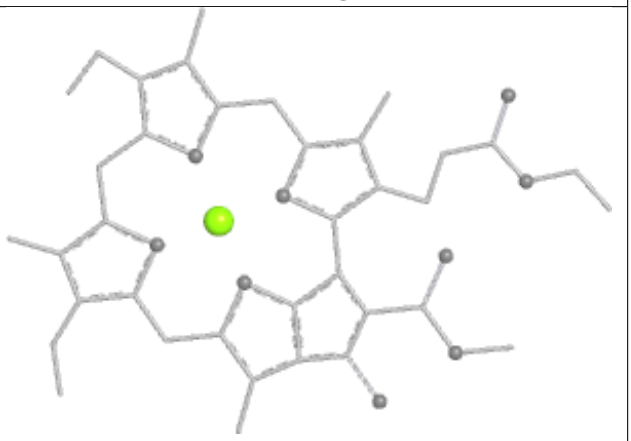
Bond lengths



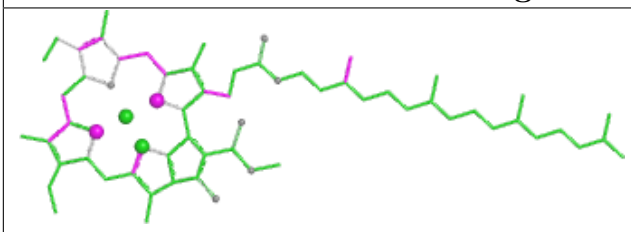
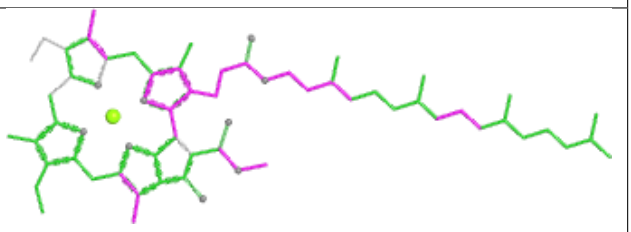
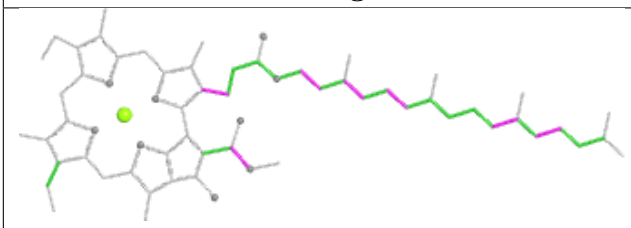
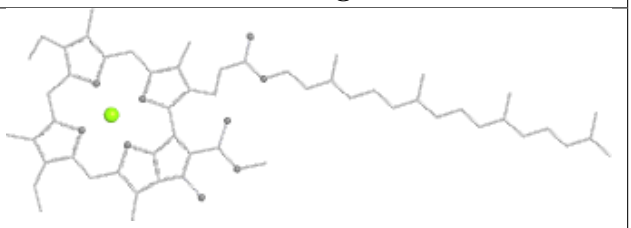
Bond angles

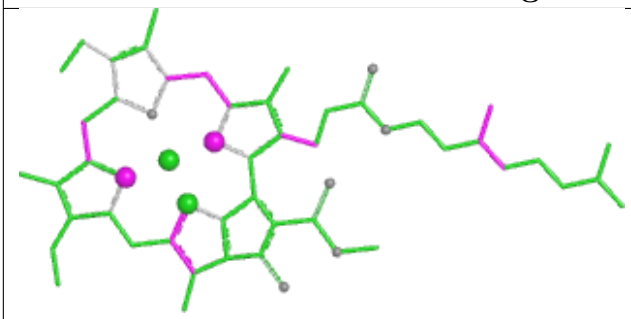
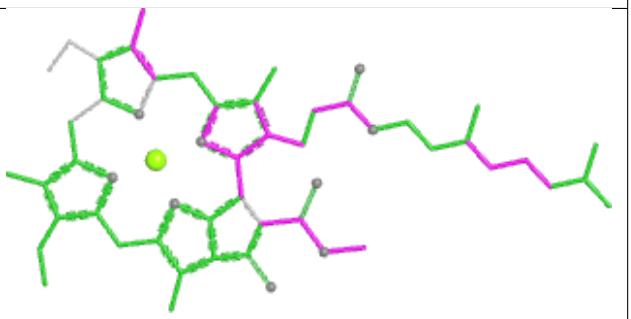
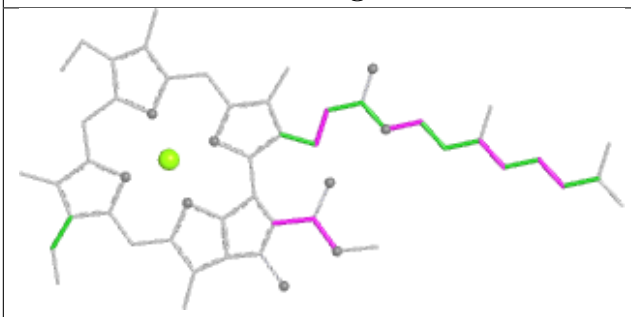
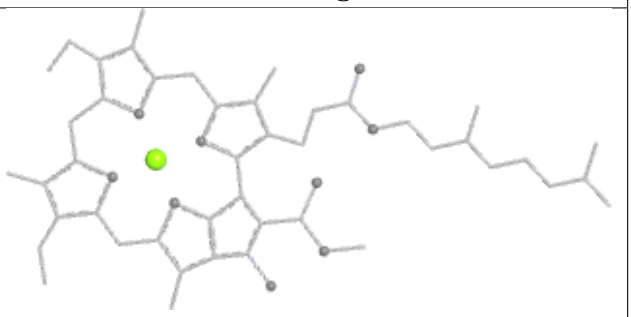


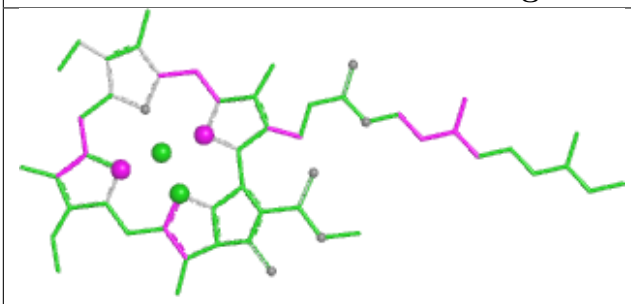
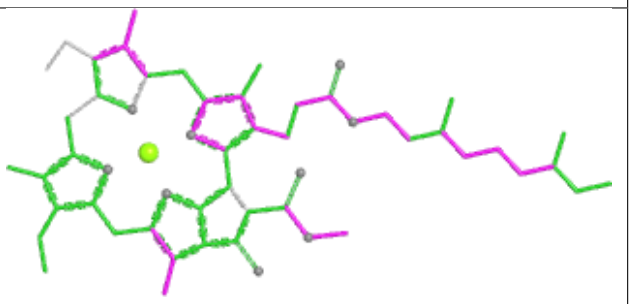
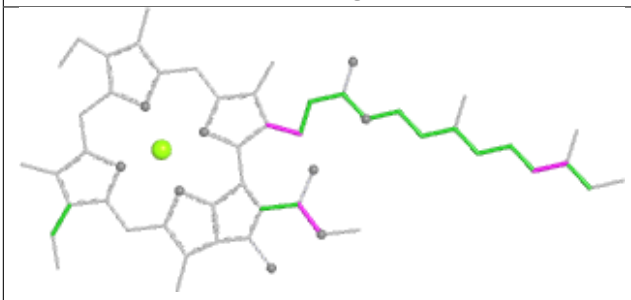
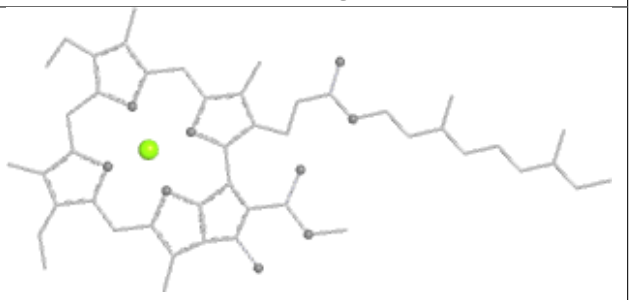
Torsions



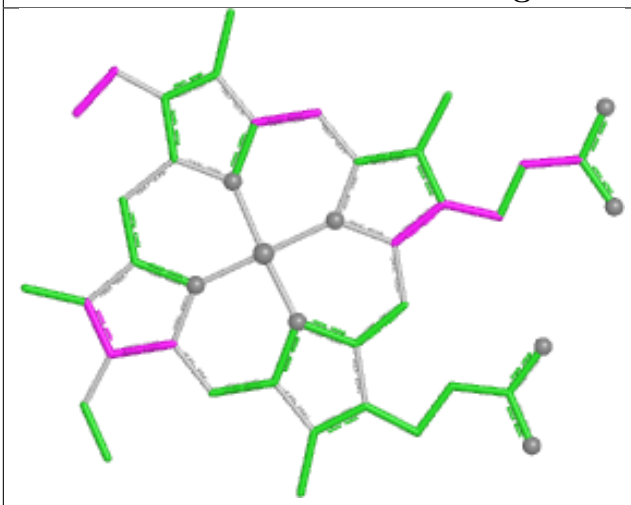
Rings

Ligand CLA D 1351	
 Bond lengths	 Bond angles
 Torsions	 Rings

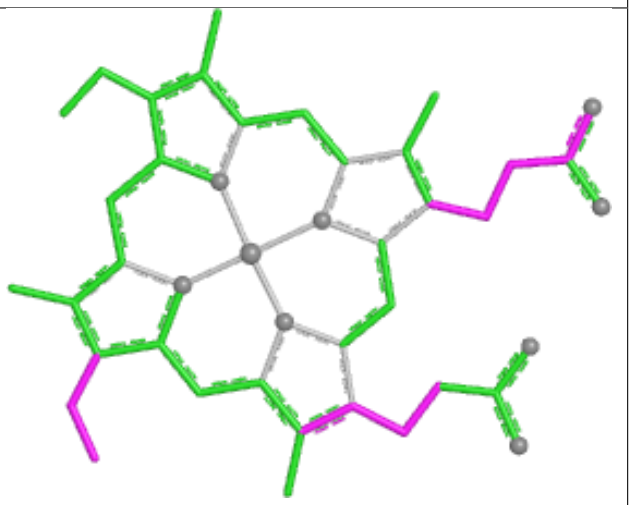
Ligand CLA I 1463	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA I 1462	
 Bond lengths	 Bond angles
 Torsions	 Rings

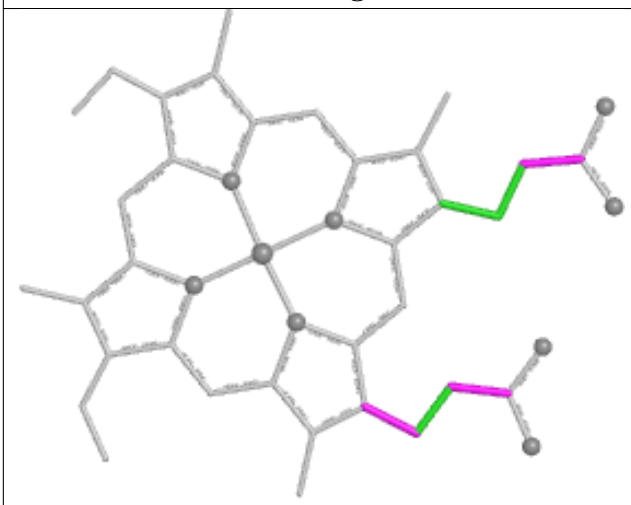
Ligand HEC V 1138



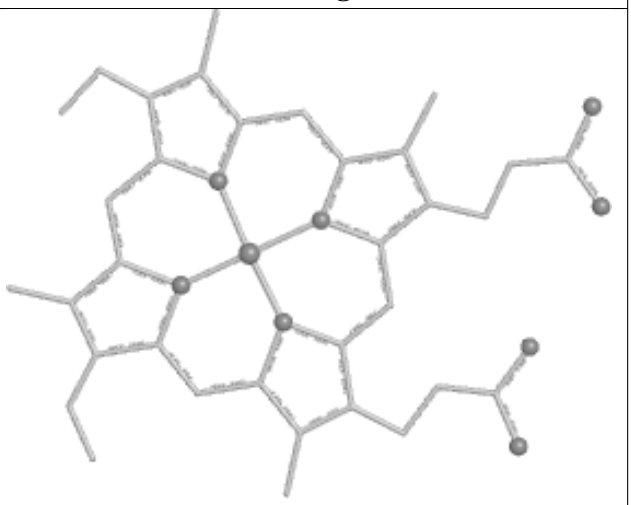
Bond lengths



Bond angles

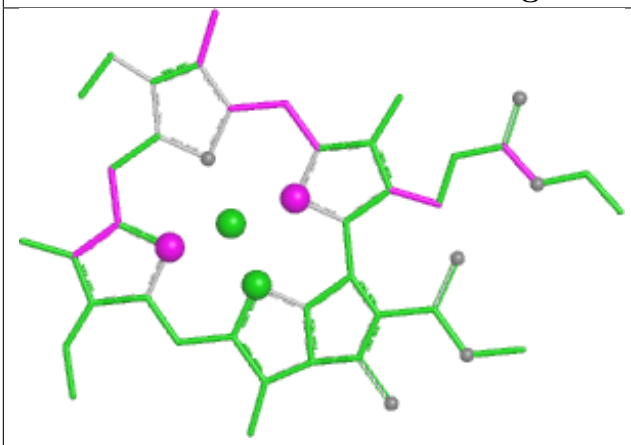


Torsions

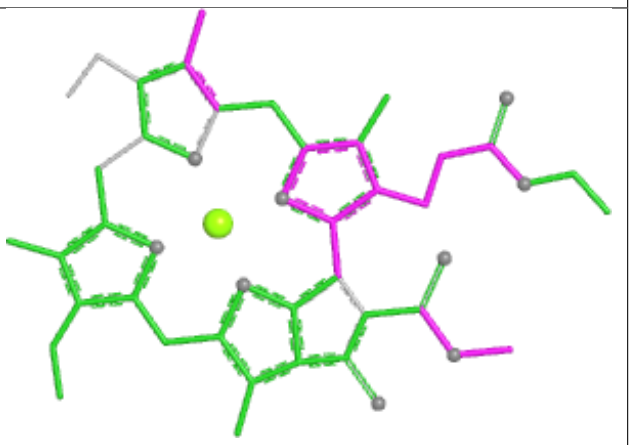


Rings

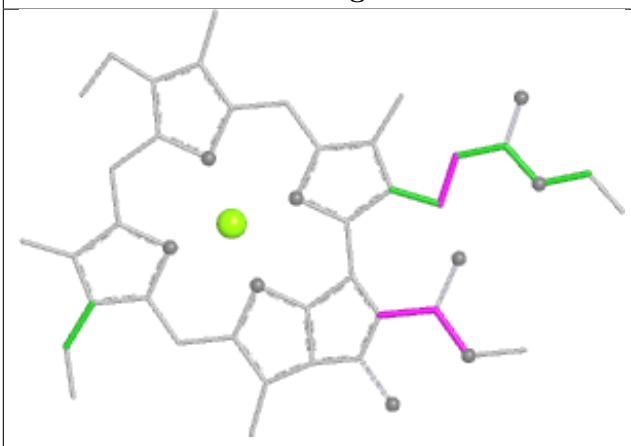
Ligand CLA I 1460



Bond lengths



Bond angles



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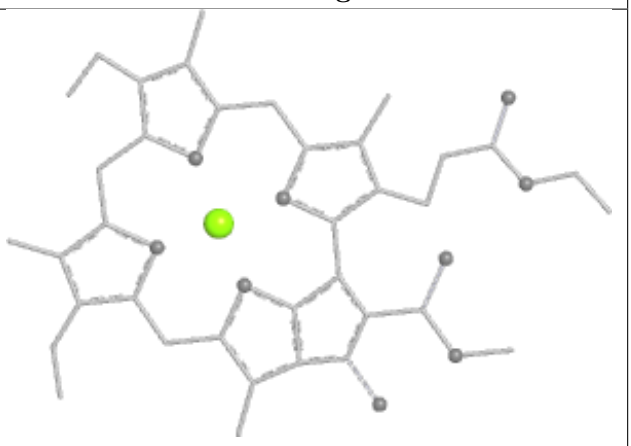
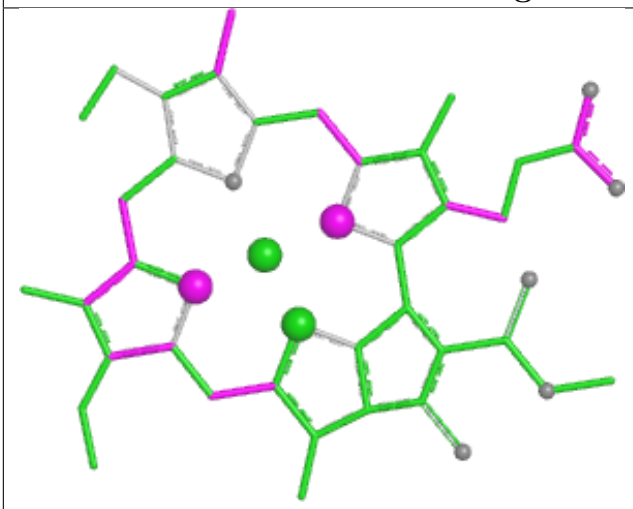
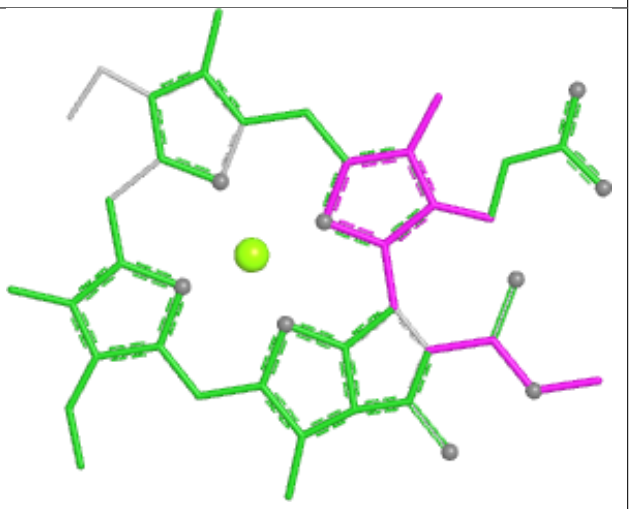


Rings

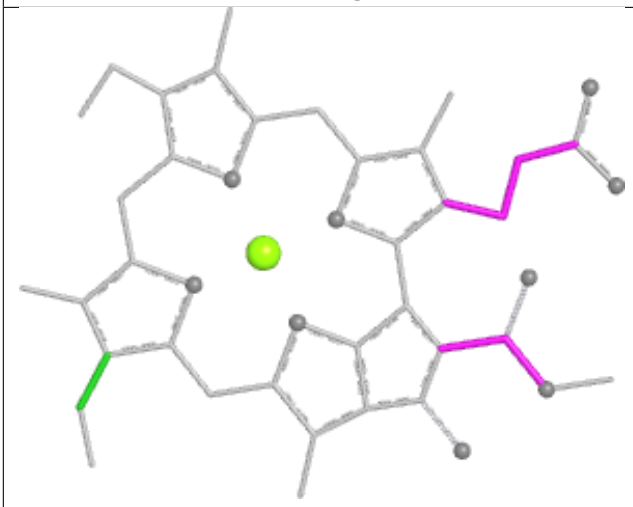
Ligand CLA H 1490



Bond lengths



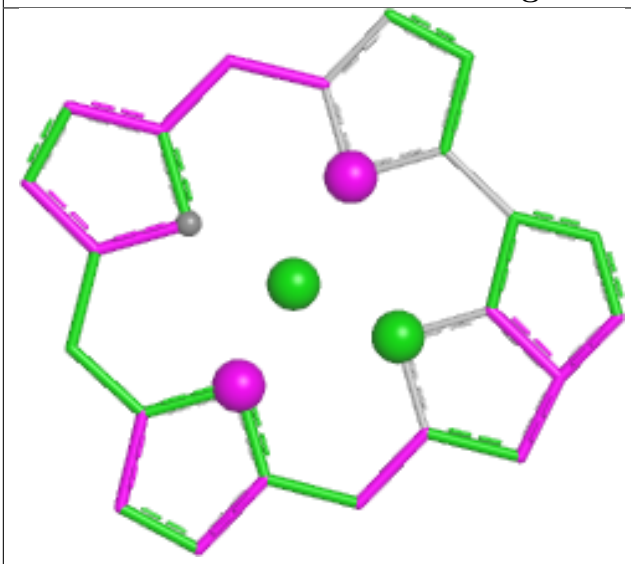
Bond angles



Torsions

Rings

Ligand CLA I 1461



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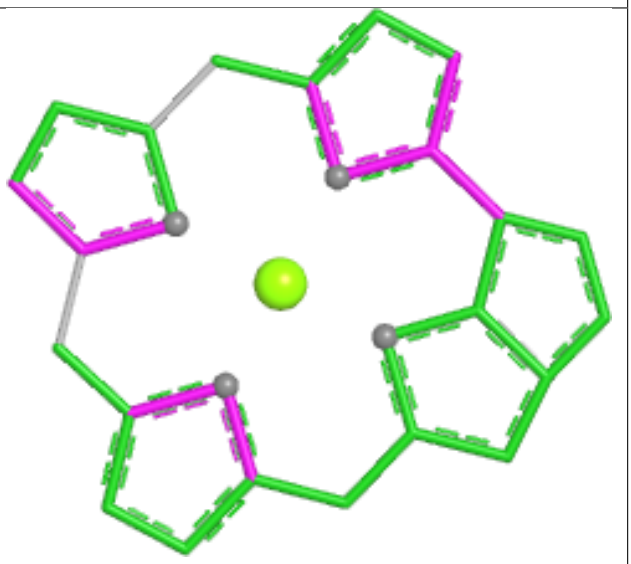

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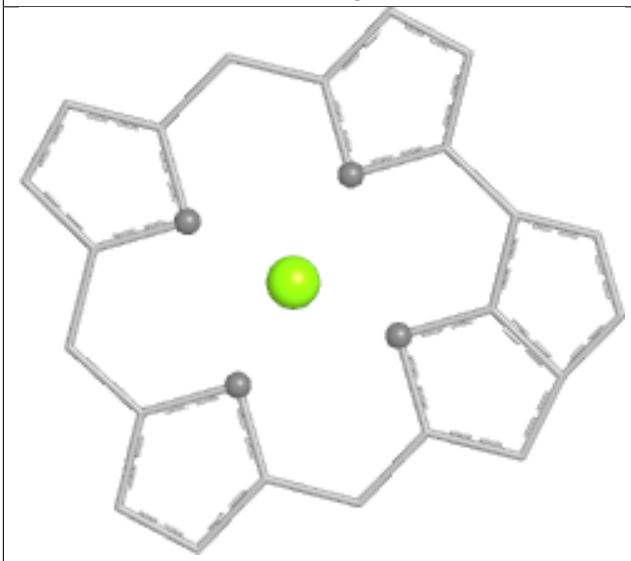
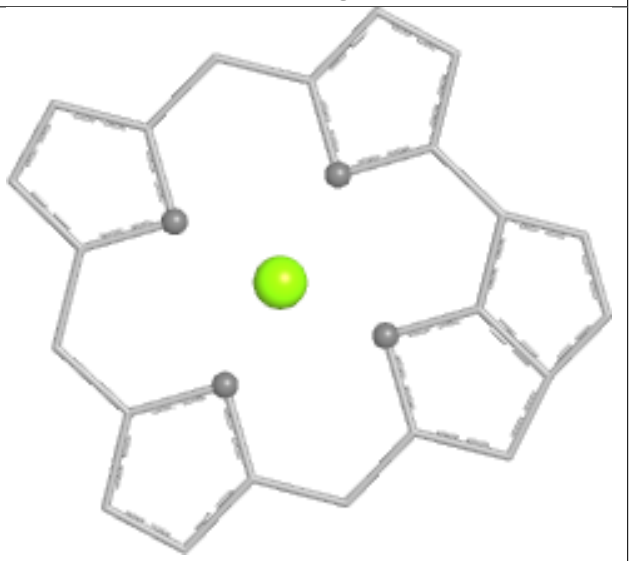
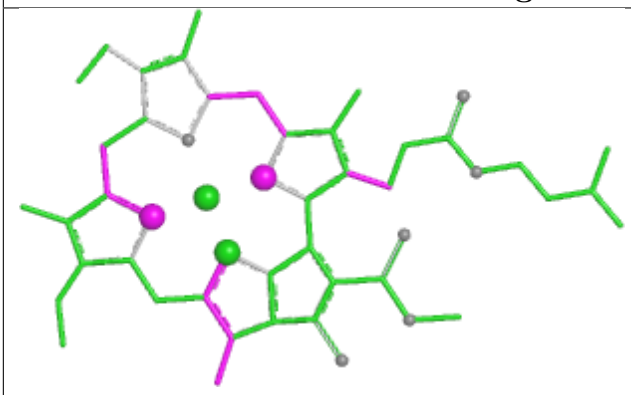


Torsions



Rings

Ligand CLA C 1466



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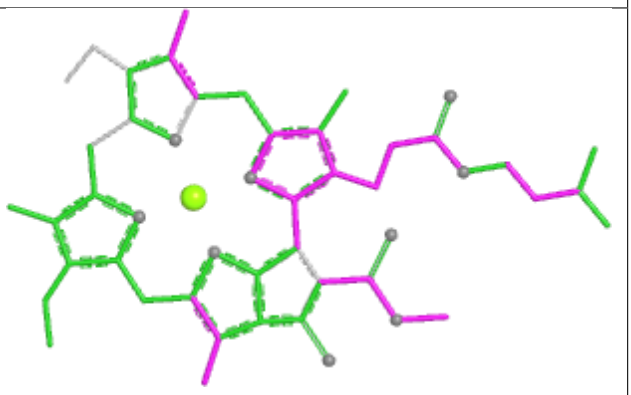

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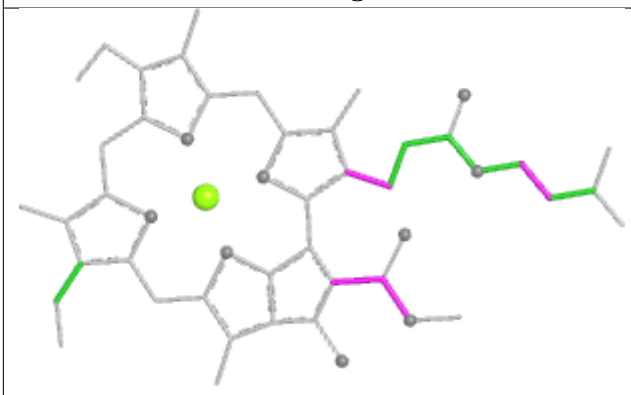

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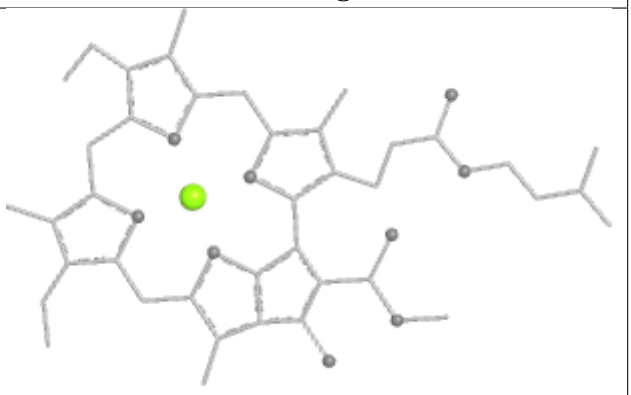
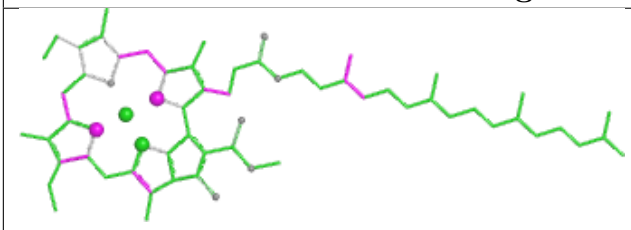


Rings

Ligand CLA B 1494



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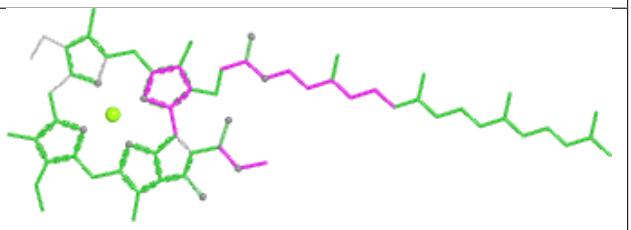

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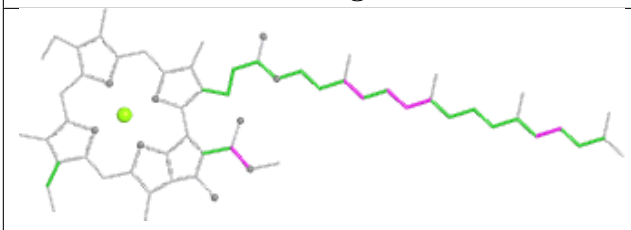

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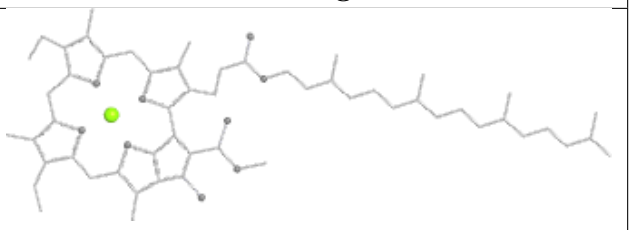
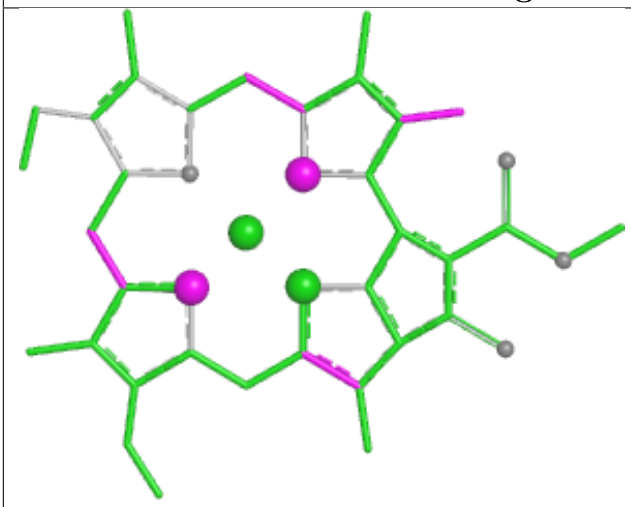


Rings

Ligand CLA C 1469



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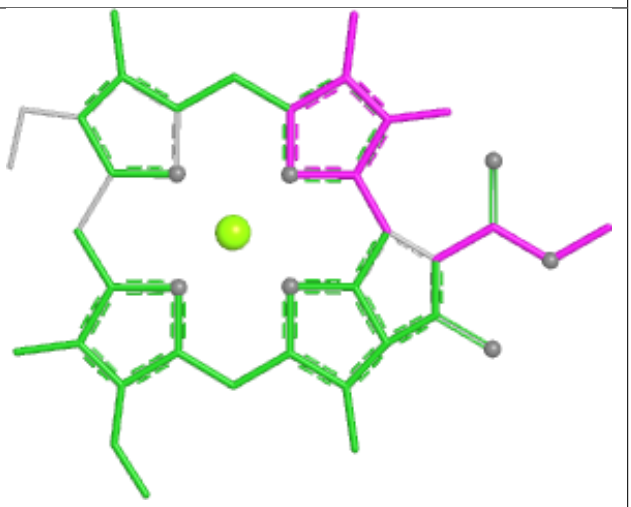
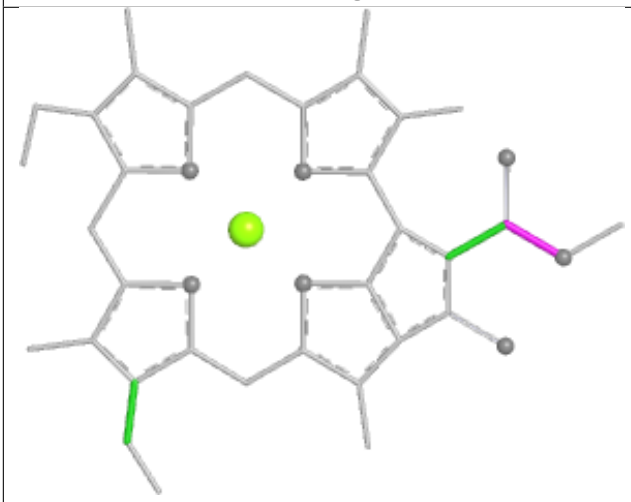
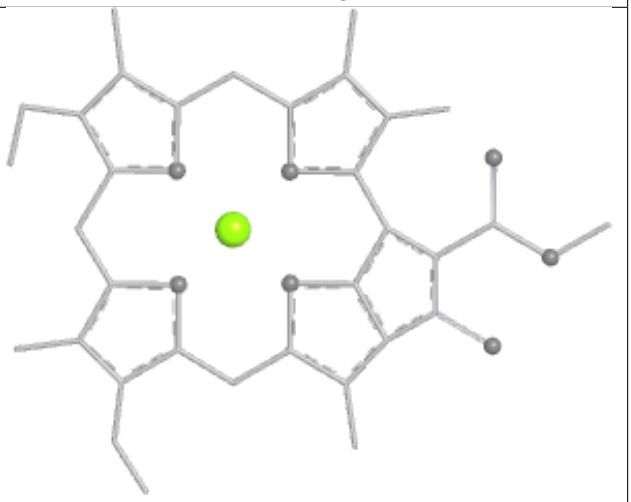


Bond angles

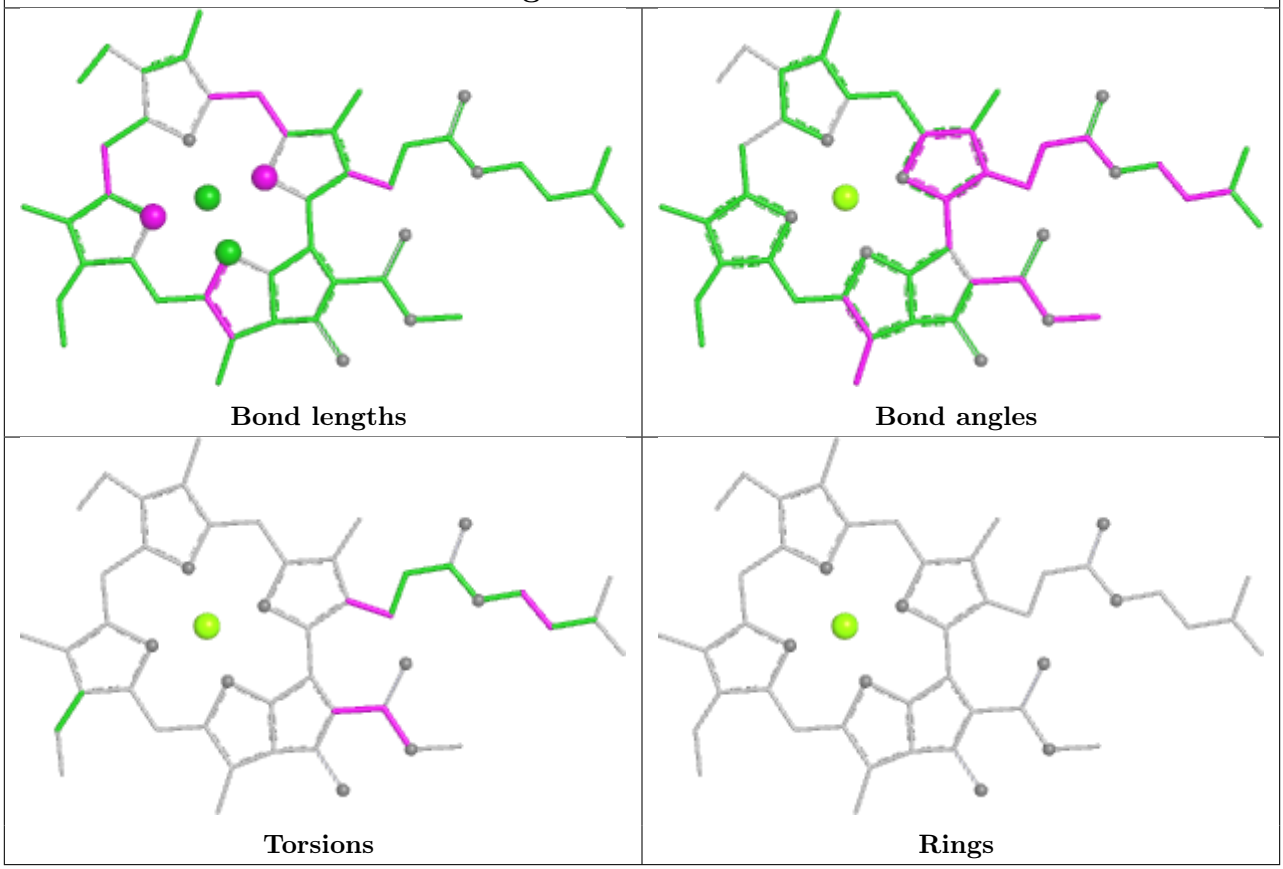


Torsions



Rings

Ligand CLA I 1466



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
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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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.