wwPDB EM Validation Summary Report

Oct 6, 2024 – 02:49 pm BST

PDB ID	:	8ASP
EMDB ID	:	EMD-15621
Title	:	RCII/PSI complex, focused refinement of PSI
Authors	:	Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.; Sazanov, L.A.; Komenda, J.
Deposited on	:	2022-08-20
Resolution	:	2.90 Å(reported)
Based on initial models	:	5OY0, 2XBG, 6WJ6

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

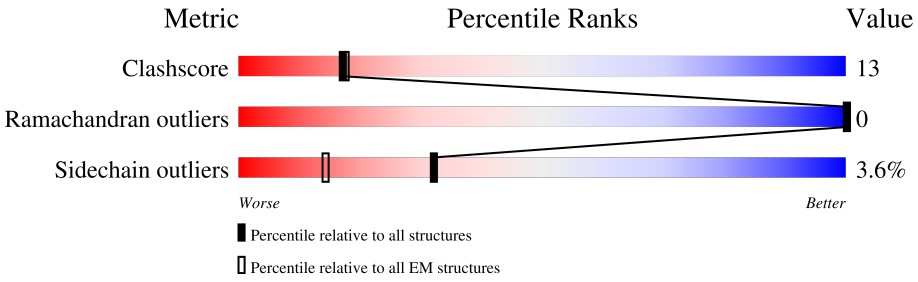
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	751	97%
2	b	731	98%
3	c	81	95%
4	d	141	96%
5	e	74	86% 7% 7%
6	f	165	82% 14%
7	i	40	8% 95% 5%
8	j	40	95% 5%

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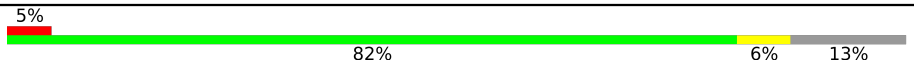
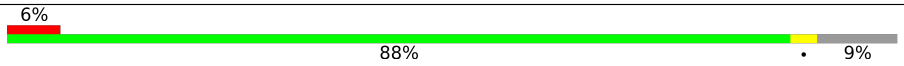
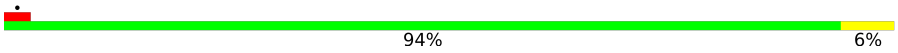
Mol	Chain	Length	Quality of chain
9	k	88	
10	l	157	
11	m	31	

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
12	CL0	a	801	X	-	-	-
13	CLA	a	802	X	-	-	-
13	CLA	a	803	X	-	-	-
13	CLA	a	804	X	-	-	-
13	CLA	a	805	X	-	-	-
13	CLA	a	806	X	-	-	-
13	CLA	a	807	X	-	-	-
13	CLA	a	808	X	-	-	-
13	CLA	a	809	X	-	-	-
13	CLA	a	810	X	-	-	-
13	CLA	a	811	X	-	-	-
13	CLA	a	812	X	-	-	-
13	CLA	a	813	X	-	-	-
13	CLA	a	814	X	-	-	-
13	CLA	a	815	X	-	-	-
13	CLA	a	816	X	-	-	-
13	CLA	a	817	X	-	-	-
13	CLA	a	818	X	-	-	-
13	CLA	a	819	X	-	-	-
13	CLA	a	820	X	-	-	-
13	CLA	a	821	X	-	-	-
13	CLA	a	822	X	-	-	-
13	CLA	a	823	X	-	-	-
13	CLA	a	824	X	-	-	-
13	CLA	a	825	X	-	-	-
13	CLA	a	826	X	-	-	-
13	CLA	a	827	X	-	-	-
13	CLA	a	828	X	-	-	-
13	CLA	a	829	X	-	-	-
13	CLA	a	830	X	-	-	-
13	CLA	a	831	X	-	-	-
13	CLA	a	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	833	X	-	-	-
13	CLA	a	834	X	-	-	-
13	CLA	a	835	X	-	-	-
13	CLA	a	836	X	-	-	-
13	CLA	a	837	X	-	-	-
13	CLA	a	838	X	-	-	-
13	CLA	a	839	X	-	-	-
13	CLA	a	840	X	-	-	-
13	CLA	a	841	X	-	-	-
13	CLA	a	842	X	-	-	-
13	CLA	a	854	X	-	-	-
13	CLA	a	855	X	-	-	-
13	CLA	b	801	X	-	-	-
13	CLA	b	803	X	-	-	-
13	CLA	b	804	X	-	-	-
13	CLA	b	805	X	-	-	-
13	CLA	b	806	X	-	-	-
13	CLA	b	807	X	-	-	-
13	CLA	b	808	X	-	-	-
13	CLA	b	809	X	-	-	-
13	CLA	b	810	X	-	-	-
13	CLA	b	811	X	-	-	-
13	CLA	b	812	X	-	-	-
13	CLA	b	813	X	-	-	-
13	CLA	b	814	X	-	-	-
13	CLA	b	815	X	-	-	-
13	CLA	b	816	X	-	-	-
13	CLA	b	817	X	-	-	-
13	CLA	b	818	X	-	-	-
13	CLA	b	819	X	-	-	-
13	CLA	b	820	X	-	-	-
13	CLA	b	821	X	-	-	-
13	CLA	b	822	X	-	-	-
13	CLA	b	823	X	-	-	-
13	CLA	b	824	X	-	-	-
13	CLA	b	825	X	-	-	-
13	CLA	b	826	X	-	-	-
13	CLA	b	827	X	-	-	-
13	CLA	b	828	X	-	-	-
13	CLA	b	829	X	-	-	-
13	CLA	b	830	X	-	-	-
13	CLA	b	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	832	X	-	-	-
13	CLA	b	833	X	-	-	-
13	CLA	b	834	X	-	-	-
13	CLA	b	835	X	-	-	-
13	CLA	b	836	X	-	-	-
13	CLA	b	837	X	-	-	-
13	CLA	b	838	X	-	-	-
13	CLA	b	839	X	-	-	-
13	CLA	b	840	X	-	-	-
13	CLA	b	841	X	-	-	-
13	CLA	b	842	X	-	-	-
13	CLA	f	201	X	-	-	-
13	CLA	f	203	X	-	-	-
13	CLA	f	204	X	-	-	-
13	CLA	j	103	X	-	-	-
13	CLA	j	104	X	-	-	-
13	CLA	k	4002	X	-	-	-
13	CLA	k	4003	X	-	-	-
13	CLA	k	4004	X	-	-	-
13	CLA	l	1501	X	-	-	-
13	CLA	l	1502	X	-	-	-
13	CLA	l	1503	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 24596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	740	5786	3791	982	986	27	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	729	5770	3798	967	990	15	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	600	369	103	117	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	139	1087	688	188	208	3	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	e	69	538	337	95	106	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	142	1108	715	184	204	5	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	77	Total	C	N	O	S	0	0
			535	350	89	92	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	87	GLY	-	expression tag	UNP P72712
k	88	VAL	-	expression tag	UNP P72712

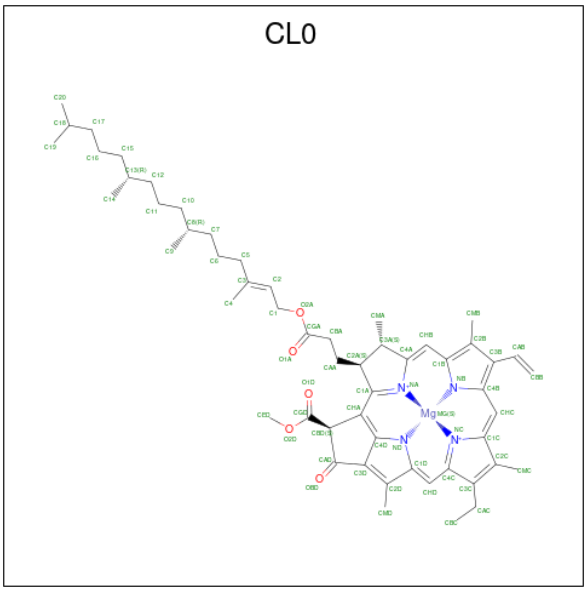
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

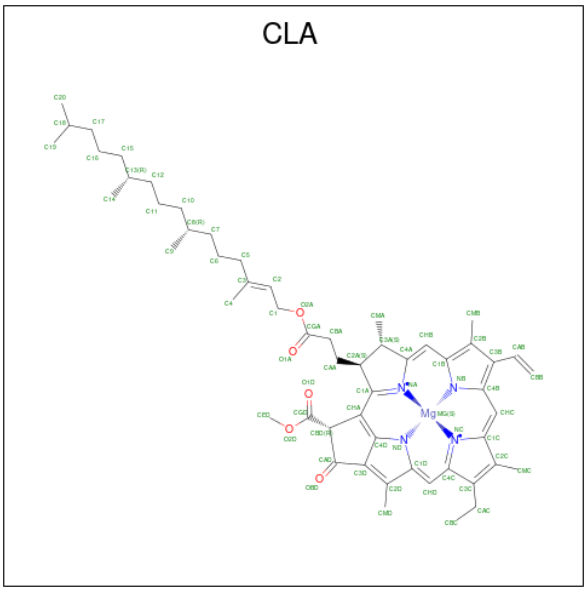
Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms	AltConf
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 51 41 1 4 5	0
13	a	1	Total C Mg N O 53 43 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 52 42 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 47 37 1 4 5	0
13	a	1	Total C Mg N O 46 36 1 4 5	0
13	a	1	Total C Mg N O 46 36 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 65 55 1 4 5	0
13	a	1	Total C Mg N O 60 50 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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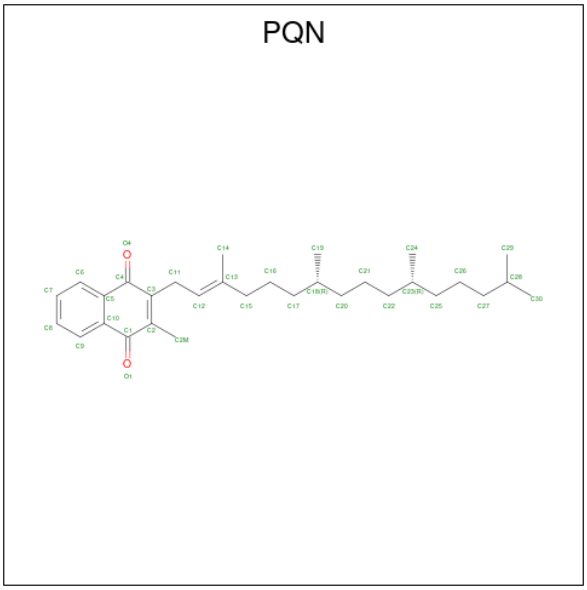
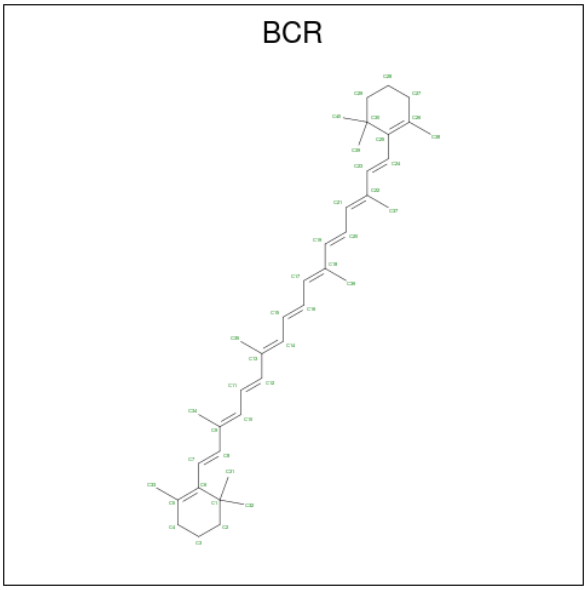
Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 25 25	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	i	1	Total C 40 40	0

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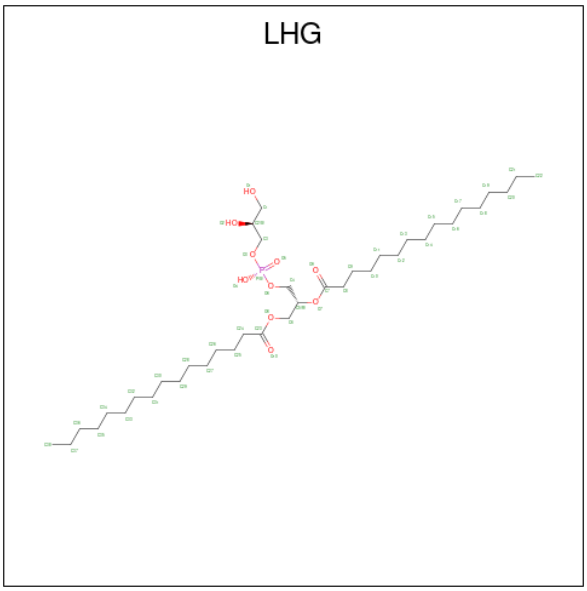
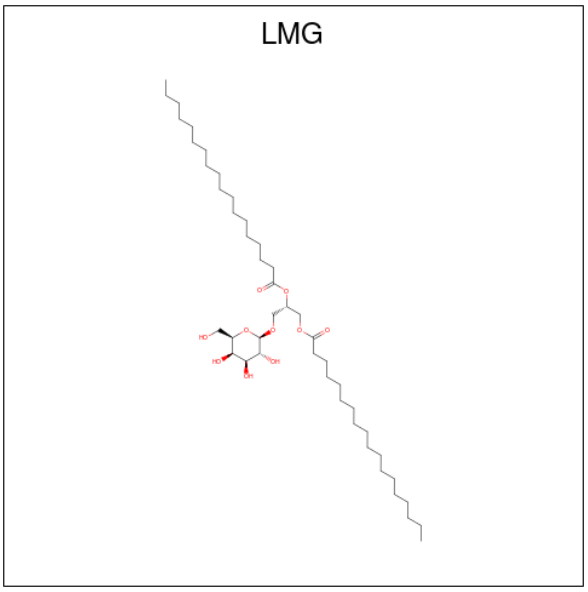
Mol	Chain	Residues	Atoms	AltConf
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	1	Total C 40 40	0
15	k	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



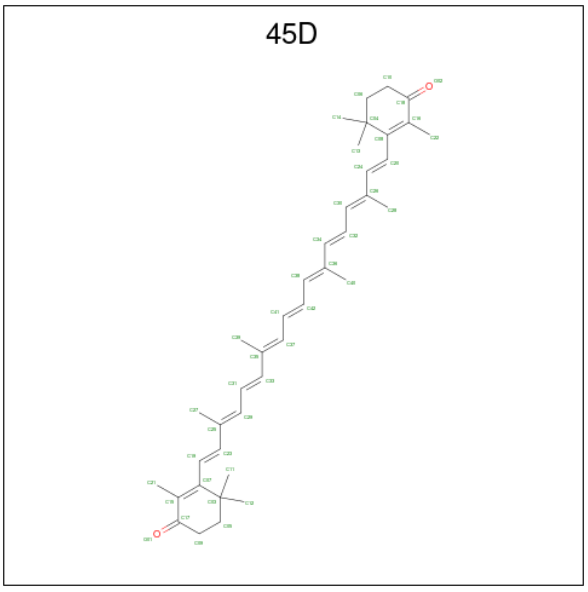
Mol	Chain	Residues	Atoms	AltConf
16	a	1	Total C O P 49 38 10 1	0
16	a	1	Total C O P 49 38 10 1	0
16	a	1	Total C O P 49 38 10 1	0
16	b	1	Total C O P 38 27 10 1	0
16	f	1	Total C O P 49 38 10 1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



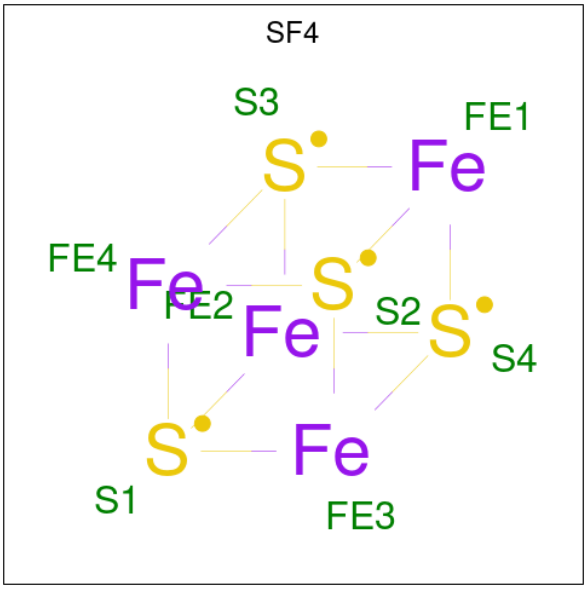
Mol	Chain	Residues	Atoms			AltConf
17	a	1	Total	C	O	0
			50	40	10	
17	a	1	Total	C	O	0
			40	30	10	
17	b	1	Total	C	O	0
			55	45	10	
17	b	1	Total	C	O	0
			55	45	10	

- Molecule 18 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).



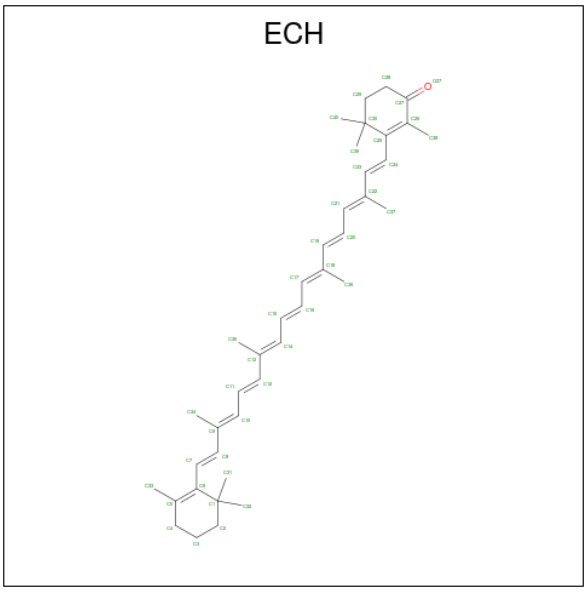
Mol	Chain	Residues	Atoms			AltConf
18	a	1	Total	C	O	0
			42	40	2	

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



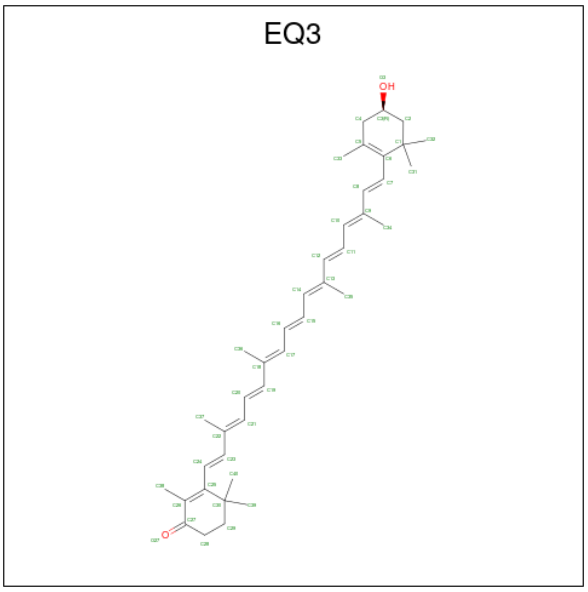
Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	
19	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 20 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



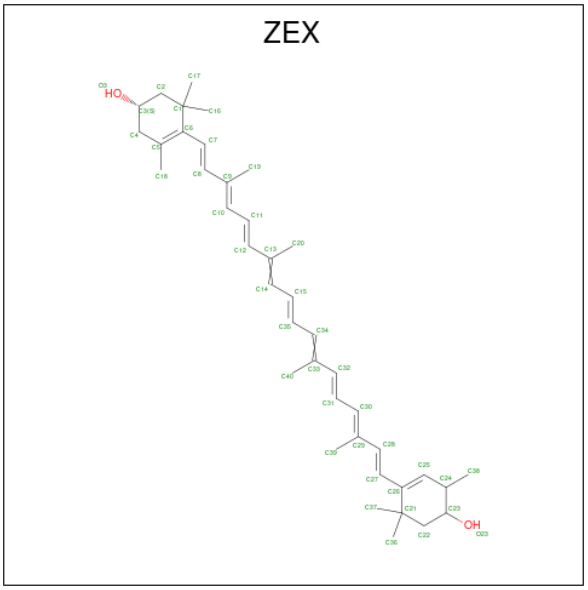
Mol	Chain	Residues	Atoms			AltConf
20	b	1	Total	C	O	0
			41	40	1	
20	m	1	Total	C	O	0
			41	40	1	

- Molecule 21 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: $C_{40}H_{54}O_2$).



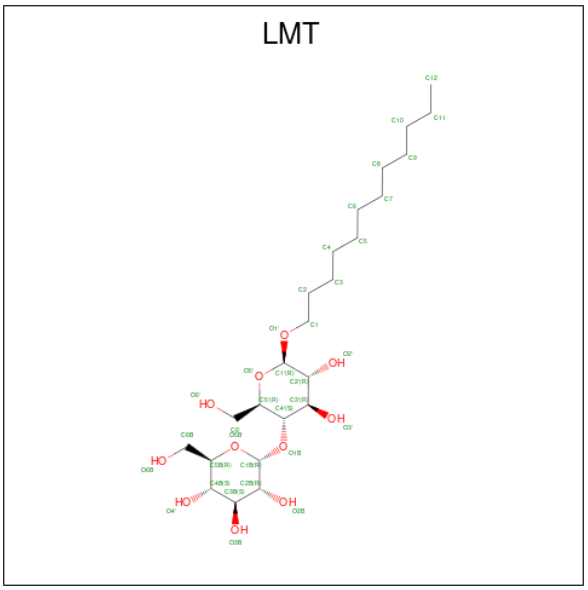
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
22	b	1	Total	C	O	0
			42	40	2	
22	f	1	Total	C	O	0
			42	40	2	

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



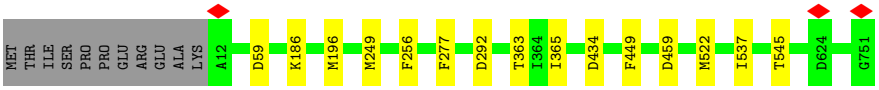
Mol	Chain	Residues	Atoms			AltConf
23	j	1	Total	C	O	0
			35	24	11	

3 Residue-property plots (i)

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

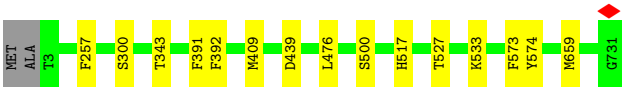
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



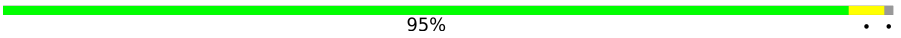
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



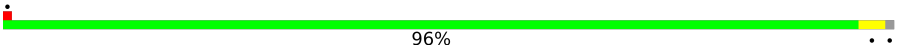
• Molecule 3: Photosystem I iron-sulfur center

Chain c:



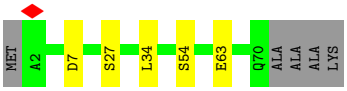
• Molecule 4: Photosystem I reaction center subunit II

Chain d:



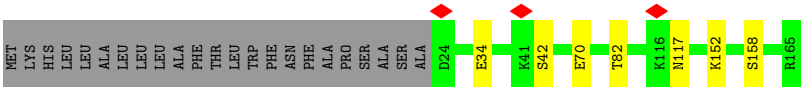
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



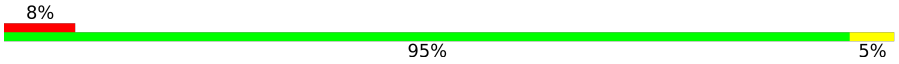
• Molecule 6: Photosystem I reaction center subunit III

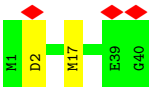
Chain f:



• Molecule 7: Photosystem I reaction center subunit VIII

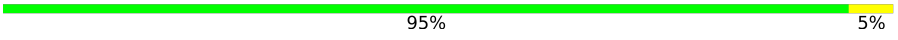
Chain i:

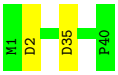




• Molecule 8: Photosystem I reaction center subunit IX

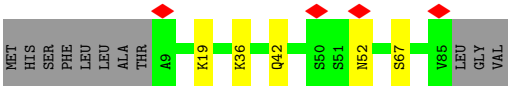
Chain j:





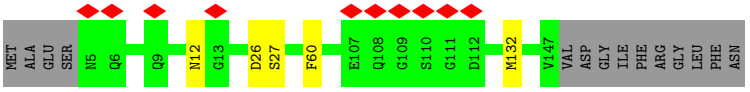
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain k:



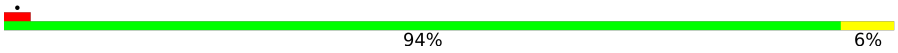
• Molecule 10: Photosystem I reaction center subunit XI

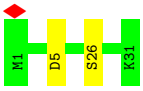
Chain l:



• Molecule 11: Photosystem I reaction center subunit XII

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.526	Depositor
Minimum map value	-0.118	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, ECH, SF4, EQ3, PQN, ZEX, CL0, LHG, CLA, LMG, LMT, 45D

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	0.26	0/5984	0.43	0/8158
2	b	0.26	0/5981	0.43	1/8178 (0.0%)
3	c	0.25	0/610	0.51	0/826
4	d	0.26	0/1111	0.49	0/1497
5	e	0.28	0/547	0.58	0/741
6	f	0.28	0/1138	0.49	0/1546
7	i	0.27	0/322	0.45	0/438
8	j	0.25	0/328	0.45	0/443
9	k	0.26	0/546	0.50	0/741
10	l	0.27	0/1097	0.49	0/1493
11	m	0.27	0/241	0.50	0/326
All	All	0.26	0/17905	0.46	1/24387 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	659	MET	CA-CB-CG	5.75	123.08	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5786	0	5640	0	0
2	b	5770	0	5547	0	0
3	c	600	0	581	0	0
4	d	1087	0	1082	0	0
5	e	538	0	514	0	0
6	f	1108	0	1100	0	0
7	i	311	0	304	0	0
8	j	319	0	328	0	0
9	k	535	0	559	0	0
10	l	1069	0	1044	0	0
11	m	238	0	260	0	0
12	a	65	0	72	0	0
13	a	2637	0	2754	0	0
13	b	2475	0	2528	0	0
13	f	160	0	144	0	0
13	j	101	0	82	0	0
13	k	156	0	138	0	0
13	l	167	0	154	0	0
14	a	33	0	46	0	0
14	b	33	0	46	0	0
15	a	185	0	257	0	0
15	b	200	0	280	0	0
15	f	40	0	56	0	0
15	i	80	0	112	0	0
15	j	80	0	112	0	0
15	k	80	0	112	0	0
16	a	147	0	222	0	0
16	b	38	0	49	0	0
16	f	49	0	74	0	0
17	a	90	0	123	0	0
17	b	110	0	172	0	0
18	a	42	0	52	0	0
19	b	8	0	0	0	0
19	c	16	0	0	0	0
20	b	41	0	54	0	0
20	m	41	0	54	0	0
21	b	42	0	0	0	0
22	b	42	0	56	0	0
22	f	42	0	56	0	0
23	j	35	0	45	0	0
All	All	24596	0	24809	0	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 13.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	738/751 (98%)	717 (97%)	21 (3%)	0	100	100
2	b	727/731 (100%)	705 (97%)	22 (3%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	d	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
5	e	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
6	f	140/165 (85%)	139 (99%)	1 (1%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
9	k	75/88 (85%)	70 (93%)	5 (7%)	0	100	100
10	l	141/157 (90%)	136 (96%)	5 (4%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	2208/2299 (96%)	2144 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	592/603 (98%)	577 (98%)	15 (2%)	42	75
2	b	582/583 (100%)	568 (98%)	14 (2%)	44	76
3	c	68/69 (99%)	65 (96%)	3 (4%)	24	57
4	d	114/116 (98%)	110 (96%)	4 (4%)	31	66
5	e	57/60 (95%)	52 (91%)	5 (9%)	8	26
6	f	119/137 (87%)	112 (94%)	7 (6%)	16	45
7	i	32/32 (100%)	30 (94%)	2 (6%)	15	42
8	j	35/35 (100%)	33 (94%)	2 (6%)	17	47
9	k	54/63 (86%)	49 (91%)	5 (9%)	7	23
10	l	107/118 (91%)	102 (95%)	5 (5%)	22	55
11	m	25/25 (100%)	23 (92%)	2 (8%)	10	30
All	All	1785/1841 (97%)	1721 (96%)	64 (4%)	32	65

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	l	12	ASN
10	l	27	SER
2	b	517	HIS
2	b	500	SER
10	l	60	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	d	7	GLN
6	f	121	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

134 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	CLA	b	820	-	60,68,73	1.53	6 (10%)	70,107,113	1.39	7 (10%)
13	CLA	a	831	-	56,64,73	1.59	6 (10%)	65,102,113	1.46	8 (12%)
13	CLA	b	834	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
13	CLA	b	839	-	50,58,73	1.72	6 (12%)	58,95,113	1.52	7 (12%)
17	LMG	a	852	-	40,40,55	0.83	0	48,48,63	1.24	4 (8%)
13	CLA	a	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
13	CLA	j	103	8	55,63,73	1.62	5 (9%)	64,101,113	1.41	7 (10%)
19	SF4	c	101	3	0,12,12	-	-	-		
13	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
15	BCR	b	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	5 (8%)
14	PQN	b	843	-	34,34,34	0.39	0	42,45,45	0.38	0
15	BCR	k	4001	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	k	4004	9	45,53,73	1.77	5 (11%)	52,89,113	1.70	9 (17%)
13	CLA	a	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
16	LHG	a	851	13	48,48,48	0.59	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	b	825	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	823	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	6 (11%)
13	CLA	a	821	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
13	CLA	a	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	9 (11%)
12	CL0	a	801	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	7 (9%)
13	CLA	b	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
13	CLA	a	820	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	a	805	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	8 (10%)
13	CLA	b	801	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
13	CLA	a	839	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
13	CLA	a	836	1	55,63,73	1.61	6 (10%)	64,101,113	1.47	8 (12%)
13	CLA	a	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
15	BCR	k	4005	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	a	808	1	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
13	CLA	a	812	-	52,60,73	1.68	6 (11%)	60,97,113	1.50	9 (15%)
13	CLA	b	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	840	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	9 (11%)
13	CLA	a	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	8 (10%)
13	CLA	a	823	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
16	LHG	f	206	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
23	LMT	j	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
13	CLA	a	810	-	53,61,73	1.62	7 (13%)	61,98,113	1.51	8 (13%)
13	CLA	b	811	-	56,64,73	1.64	6 (10%)	65,102,113	1.41	7 (10%)
13	CLA	b	814	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
15	BCR	a	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
15	BCR	b	845	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	4 (7%)
13	CLA	a	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
13	CLA	l	1503	-	52,60,73	1.64	6 (11%)	60,97,113	1.55	7 (11%)
13	CLA	a	815	-	46,54,73	1.71	6 (13%)	53,90,113	1.60	6 (11%)
13	CLA	b	817	-	56,64,73	1.55	6 (10%)	65,102,113	1.49	8 (12%)
22	ZEX	b	854	-	42,43,43	1.67	8 (19%)	55,60,60	1.61	12 (21%)
15	BCR	a	848	-	25,25,41	1.16	1 (4%)	33,33,56	1.30	5 (15%)
14	PQN	a	843	-	34,34,34	0.38	0	42,45,45	0.40	0
13	CLA	a	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
15	BCR	b	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	a	854	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	7 (9%)
13	CLA	a	822	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
13	CLA	a	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
13	CLA	a	835	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
13	CLA	a	809	1	51,59,73	1.65	6 (11%)	59,96,113	1.61	7 (11%)
17	LMG	b	852	-	55,55,55	0.78	1 (1%)	63,63,63	1.33	9 (14%)
17	LMG	a	850	-	50,50,55	0.78	0	58,58,63	1.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	819	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
13	CLA	a	803	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	a	855	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	6 (7%)
13	CLA	b	827	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
13	CLA	b	816	-	55,63,73	1.62	6 (10%)	64,101,113	1.42	8 (12%)
13	CLA	a	818	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	7 (9%)
13	CLA	f	204	6	45,53,73	1.80	5 (11%)	52,89,113	1.58	6 (11%)
17	LMG	b	850	-	55,55,55	0.70	0	63,63,63	1.38	8 (12%)
13	CLA	b	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.34	7 (9%)
15	BCR	a	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	a	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	831	-	51,59,73	1.69	5 (9%)	59,96,113	1.49	8 (13%)
15	BCR	b	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	7 (12%)
18	45D	a	856	-	43,43,43	1.73	10 (23%)	54,60,60	1.61	10 (18%)
13	CLA	b	805	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	9 (11%)
13	CLA	a	837	-	51,59,73	1.63	6 (11%)	59,96,113	1.56	7 (11%)
13	CLA	b	826	-	55,63,73	1.59	6 (10%)	64,101,113	1.49	8 (12%)
13	CLA	f	201	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
13	CLA	b	821	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
22	ZEX	f	205	-	42,43,43	1.67	8 (19%)	55,60,60	1.59	11 (20%)
13	CLA	l	1502	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
19	SF4	c	102	3	0,12,12	-	-	-		
13	CLA	b	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
21	EQ3	b	853	-	43,43,43	1.66	9 (20%)	56,60,60	1.54	11 (19%)
13	CLA	b	808	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
20	ECH	m	101	-	42,42,42	1.79	9 (21%)	55,58,58	1.86	13 (23%)
13	CLA	b	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
16	LHG	a	853	-	48,48,48	0.60	0	51,54,54	1.26	6 (11%)
13	CLA	a	824	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	7 (10%)
13	CLA	b	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.54	7 (12%)
13	CLA	a	817	-	65,73,73	1.46	5 (7%)	76,113,113	1.38	8 (10%)
13	CLA	b	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	6 (7%)
13	CLA	k	4002	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
13	CLA	b	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
13	CLA	b	812	-	56,64,73	1.58	6 (10%)	65,102,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	842	16	46,54,73	1.74	5 (10%)	53,90,113	1.58	6 (11%)
13	CLA	b	824	-	57,65,73	1.59	6 (10%)	66,103,113	1.47	8 (12%)
13	CLA	a	816	-	46,54,73	1.75	5 (10%)	53,90,113	1.59	6 (11%)
13	CLA	a	838	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
13	CLA	b	810	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
13	CLA	b	822	-	60,68,73	1.54	5 (8%)	70,107,113	1.44	6 (8%)
13	CLA	j	104	-	46,54,73	1.76	6 (13%)	53,90,113	1.49	6 (11%)
13	CLA	a	819	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
15	BCR	a	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	8 (14%)
13	CLA	a	832	-	60,68,73	1.53	6 (10%)	70,107,113	1.44	9 (12%)
13	CLA	k	4003	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
16	LHG	a	849	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
13	CLA	b	804	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
15	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	a	814	-	47,55,73	1.73	5 (10%)	54,91,113	1.61	8 (14%)
13	CLA	b	807	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
15	BCR	i	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	b	813	-	50,58,73	1.68	6 (12%)	58,95,113	1.52	8 (13%)
13	CLA	b	830	-	65,73,73	1.45	6 (9%)	76,113,113	1.52	8 (10%)
15	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.16	5 (8%)
13	CLA	b	841	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
13	CLA	a	804	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
13	CLA	b	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	7 (9%)
13	CLA	a	830	-	65,73,73	1.46	6 (9%)	76,113,113	1.50	9 (11%)
13	CLA	b	832	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	9 (15%)
16	LHG	b	851	13	37,37,48	0.69	1 (2%)	40,43,54	1.20	3 (7%)
13	CLA	b	809	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
20	ECH	b	846	-	42,42,42	1.74	8 (19%)	55,58,58	2.33	14 (25%)
13	CLA	a	841	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	9 (11%)
13	CLA	a	840	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
13	CLA	f	203	-	50,58,73	1.71	5 (10%)	58,95,113	1.52	8 (13%)
15	BCR	i	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	f	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
15	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	a	811	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	b	818	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	8 (10%)
19	SF4	b	802	2,1	0,12,12	-	-	-		
13	CLA	a	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
13	CLA	a	842	16	45,53,73	1.76	5 (11%)	52,89,113	1.62	7 (13%)
13	CLA	l	1501	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
13	CLA	a	827	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
13	CLA	b	837	-	52,60,73	1.63	6 (11%)	60,97,113	1.59	9 (15%)

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
13	CLA	b	820	-	1/1/14/20	7/31/109/115	-
13	CLA	a	831	-	1/1/13/20	10/27/105/115	-
13	CLA	b	834	-	1/1/15/20	14/37/115/115	-
13	CLA	b	839	-	1/1/12/20	5/19/97/115	-
17	LMG	a	852	-	-	19/35/55/70	0/1/1/1
13	CLA	a	826	-	1/1/15/20	9/37/115/115	-
13	CLA	j	103	8	1/1/13/20	9/25/103/115	-
19	SF4	c	101	3	-	-	0/6/5/5
13	CLA	a	828	-	1/1/15/20	12/37/115/115	-
15	BCR	b	849	-	-	14/29/63/63	0/2/2/2
14	PQN	b	843	-	-	1/23/43/43	0/2/2/2
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	k	4004	9	1/1/11/20	6/13/91/115	-
13	CLA	a	806	-	1/1/15/20	12/37/115/115	-
16	LHG	a	851	13	-	19/53/53/53	-
13	CLA	b	825	-	1/1/15/20	14/37/115/115	-
13	CLA	b	823	-	1/1/11/20	4/15/93/115	-
13	CLA	a	821	-	1/1/15/20	13/37/115/115	-
13	CLA	a	833	-	1/1/15/20	16/37/115/115	-
12	CL0	a	801	-	3/3/20/25	8/37/135/135	-
13	CLA	b	803	-	1/1/15/20	18/37/115/115	-
13	CLA	a	820	-	1/1/15/20	24/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	805	-	1/1/15/20	11/37/115/115	-
13	CLA	b	801	-	1/1/15/20	14/37/115/115	-
13	CLA	a	839	-	1/1/15/20	19/37/115/115	-
13	CLA	a	836	1	1/1/13/20	8/25/103/115	-
13	CLA	a	807	-	1/1/15/20	16/37/115/115	-
15	BCR	k	4005	-	-	4/29/63/63	0/2/2/2
13	CLA	a	808	1	1/1/15/20	13/37/115/115	-
13	CLA	a	812	-	1/1/12/20	8/22/100/115	-
13	CLA	b	835	-	1/1/15/20	19/37/115/115	-
13	CLA	b	840	-	1/1/15/20	16/37/115/115	-
13	CLA	a	825	-	1/1/15/20	13/37/115/115	-
13	CLA	a	823	-	1/1/15/20	18/37/115/115	-
16	LHG	f	206	-	-	20/53/53/53	-
23	LMT	j	102	-	-	15/21/61/61	0/2/2/2
13	CLA	a	810	-	1/1/12/20	10/23/101/115	-
13	CLA	b	811	-	1/1/13/20	9/27/105/115	-
13	CLA	b	814	-	1/1/15/20	16/37/115/115	-
15	BCR	a	847	-	-	10/29/63/63	0/2/2/2
15	BCR	b	845	-	-	5/29/63/63	0/2/2/2
13	CLA	a	834	-	1/1/15/20	15/37/115/115	-
13	CLA	l	1503	-	1/1/12/20	6/22/100/115	-
13	CLA	a	815	-	1/1/11/20	5/15/93/115	-
13	CLA	b	817	-	1/1/13/20	9/27/105/115	-
22	ZEX	b	854	-	-	3/29/67/67	0/2/2/2
15	BCR	a	848	-	-	8/18/35/63	0/1/1/2
14	PQN	a	843	-	-	1/23/43/43	0/2/2/2
13	CLA	a	829	-	1/1/15/20	15/37/115/115	-
15	BCR	b	847	-	-	6/29/63/63	0/2/2/2
13	CLA	a	854	-	1/1/15/20	6/37/115/115	-
13	CLA	a	822	-	1/1/15/20	13/37/115/115	-
13	CLA	a	802	-	1/1/15/20	10/37/115/115	-
13	CLA	a	835	-	1/1/15/20	13/37/115/115	-
13	CLA	a	809	1	1/1/12/20	4/21/99/115	-
17	LMG	b	852	-	-	22/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMG	a	850	-	-	27/45/65/70	0/1/1/1
13	CLA	b	819	-	1/1/15/20	15/37/115/115	-
13	CLA	a	803	-	1/1/15/20	6/37/115/115	-
13	CLA	a	855	-	1/1/15/20	17/37/115/115	-
13	CLA	b	827	-	1/1/15/20	7/37/115/115	-
13	CLA	b	816	-	1/1/13/20	12/25/103/115	-
13	CLA	a	818	-	1/1/15/20	23/37/115/115	-
13	CLA	f	204	6	1/1/11/20	5/13/91/115	-
17	LMG	b	850	-	-	24/50/70/70	0/1/1/1
13	CLA	b	833	-	1/1/15/20	15/37/115/115	-
15	BCR	a	844	-	-	6/29/63/63	0/2/2/2
15	BCR	a	845	-	-	6/29/63/63	0/2/2/2
13	CLA	b	831	-	1/1/12/20	9/21/99/115	-
15	BCR	b	844	-	-	11/29/63/63	0/2/2/2
18	45D	a	856	-	-	4/29/69/69	0/2/2/2
13	CLA	b	805	-	1/1/15/20	12/37/115/115	-
13	CLA	a	837	-	1/1/12/20	5/21/99/115	-
13	CLA	b	826	-	1/1/13/20	6/25/103/115	-
13	CLA	f	201	-	1/1/15/20	18/37/115/115	-
13	CLA	b	821	-	1/1/15/20	11/37/115/115	-
22	ZEX	f	205	-	-	6/29/67/67	0/2/2/2
13	CLA	l	1502	-	1/1/15/20	13/37/115/115	-
19	SF4	c	102	3	-	-	0/6/5/5
13	CLA	b	838	-	1/1/15/20	15/37/115/115	-
21	EQ3	b	853	-	-	2/29/68/68	0/2/2/2
13	CLA	b	808	-	1/1/15/20	15/37/115/115	-
20	ECH	m	101	-	-	6/29/66/66	0/2/2/2
13	CLA	b	828	-	1/1/15/20	15/37/115/115	-
16	LHG	a	853	-	-	30/53/53/53	-
13	CLA	a	824	-	1/1/14/20	11/31/109/115	-
13	CLA	b	836	-	1/1/12/20	9/19/97/115	-
13	CLA	a	817	-	1/1/15/20	12/37/115/115	-
13	CLA	b	829	-	1/1/15/20	10/37/115/115	-
13	CLA	k	4002	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	815	-	1/1/15/20	10/37/115/115	-
13	CLA	b	812	-	1/1/13/20	7/27/105/115	-
13	CLA	b	842	16	1/1/11/20	9/15/93/115	-
13	CLA	b	824	-	1/1/13/20	12/28/106/115	-
13	CLA	a	816	-	1/1/11/20	7/15/93/115	-
13	CLA	a	838	-	1/1/15/20	15/37/115/115	-
13	CLA	b	810	2	1/1/15/20	13/37/115/115	-
13	CLA	b	822	-	1/1/14/20	16/31/109/115	-
13	CLA	j	104	-	1/1/11/20	8/15/93/115	-
13	CLA	a	819	-	1/1/15/20	15/37/115/115	-
15	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	a	832	-	1/1/14/20	14/31/109/115	-
13	CLA	k	4003	-	1/1/11/20	9/15/93/115	-
16	LHG	a	849	-	-	31/53/53/53	-
13	CLA	b	804	-	1/1/15/20	18/37/115/115	-
15	BCR	j	105	-	-	5/29/63/63	0/2/2/2
13	CLA	a	814	-	1/1/11/20	11/16/94/115	-
13	CLA	b	807	-	1/1/15/20	14/37/115/115	-
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
13	CLA	b	813	-	1/1/12/20	7/19/97/115	-
13	CLA	b	830	-	1/1/15/20	16/37/115/115	-
15	BCR	b	848	-	-	8/29/63/63	0/2/2/2
13	CLA	b	841	-	1/1/15/20	16/37/115/115	-
13	CLA	a	804	-	1/1/15/20	12/37/115/115	-
13	CLA	b	806	-	1/1/15/20	12/37/115/115	-
13	CLA	a	830	-	1/1/15/20	12/37/115/115	-
13	CLA	b	832	-	1/1/12/20	5/19/97/115	-
16	LHG	b	851	13	-	25/42/42/53	-
13	CLA	b	809	-	1/1/15/20	5/37/115/115	-
20	ECH	b	846	-	-	10/29/66/66	0/2/2/2
13	CLA	a	841	-	1/1/15/20	13/37/115/115	-
13	CLA	a	840	-	1/1/15/20	18/37/115/115	-
13	CLA	f	203	-	1/1/12/20	4/19/97/115	-
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	f	202	-	-	8/29/63/63	0/2/2/2
15	BCR	j	101	-	-	6/29/63/63	0/2/2/2
13	CLA	a	811	-	1/1/15/20	15/37/115/115	-
13	CLA	b	818	-	1/1/15/20	7/37/115/115	-
19	SF4	b	802	2,1	-	-	0/6/5/5
13	CLA	a	813	-	1/1/15/20	13/37/115/115	-
13	CLA	a	842	16	1/1/11/20	6/13/91/115	-
13	CLA	l	1501	-	1/1/12/20	10/19/97/115	-
13	CLA	a	827	-	1/1/15/20	16/37/115/115	-
13	CLA	b	837	-	1/1/12/20	6/22/100/115	-

The worst 5 of 662 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	811	CLA	C4B-NB	7.94	1.42	1.35
13	b	823	CLA	C4B-NB	7.88	1.42	1.35
13	a	804	CLA	C4B-NB	7.73	1.42	1.35
13	b	839	CLA	C4B-NB	7.72	1.42	1.35
13	b	805	CLA	C4B-NB	7.67	1.42	1.35

The worst 5 of 948 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	846	ECH	C15-C16-C17	8.45	140.79	123.47
13	a	840	CLA	C4A-NA-C1A	7.33	110.00	106.71
13	a	805	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	l	1502	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	b	806	CLA	C4A-NA-C1A	7.06	109.88	106.71

5 of 98 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	a	801	CL0	ND
12	a	801	CL0	NA
12	a	801	CL0	NC
13	a	802	CLA	ND
13	a	803	CLA	ND

5 of 1505 torsion outliers are listed below:

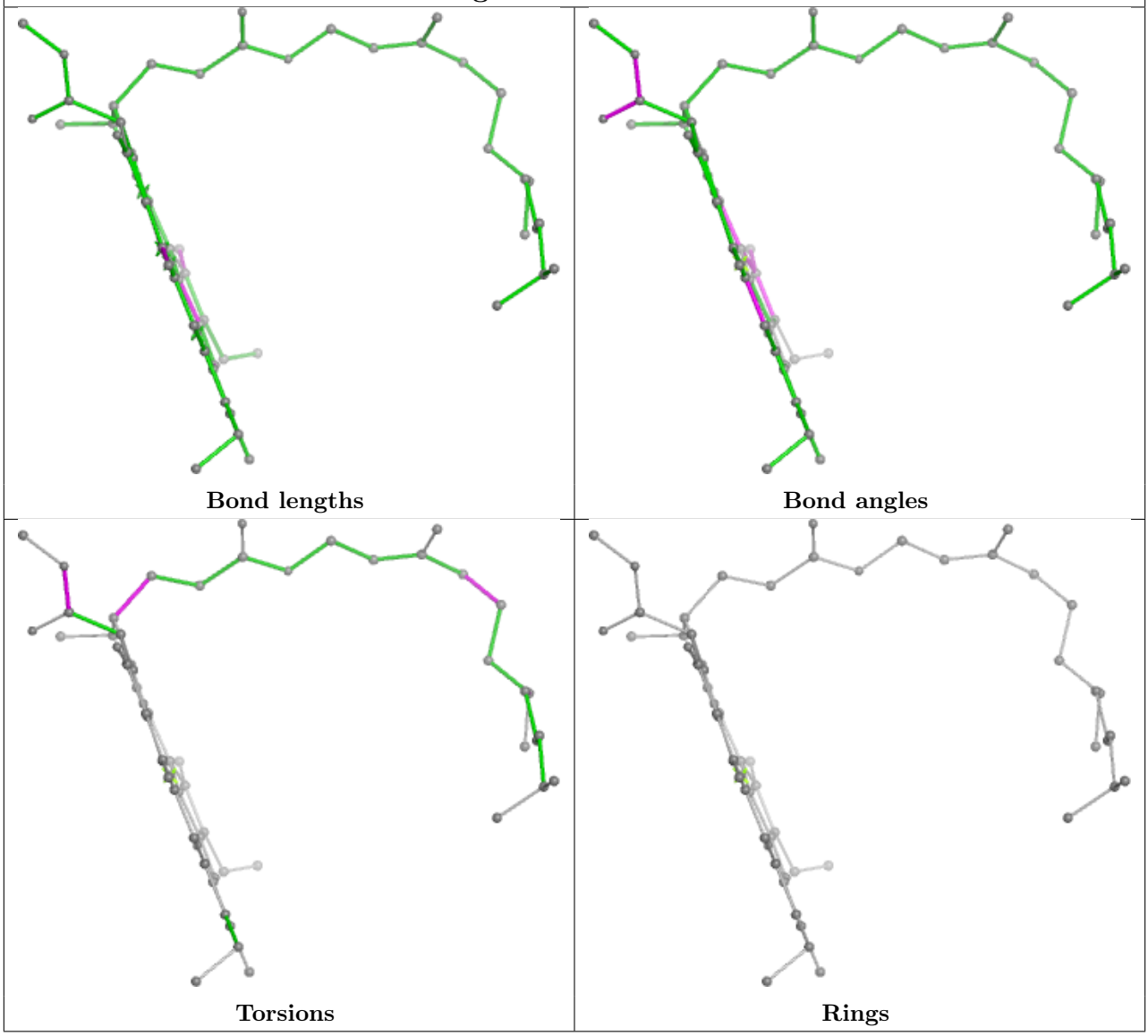
Mol	Chain	Res	Type	Atoms
13	a	802	CLA	CBA-CGA-O2A-C1
13	a	802	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	C3A-C2A-CAA-CBA
13	a	806	CLA	C2-C3-C5-C6

There are no ring outliers.

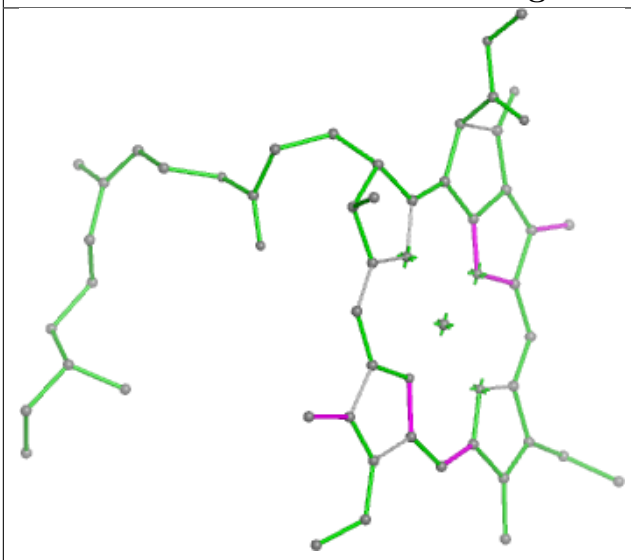
No monomer is involved in short contacts.

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

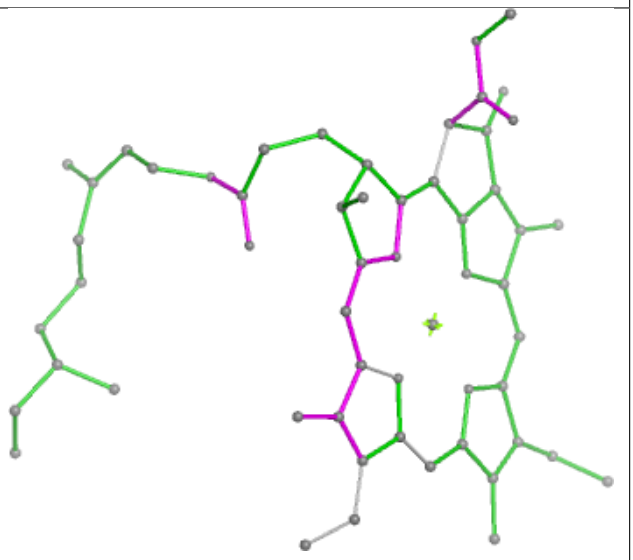
Ligand CLA b 820



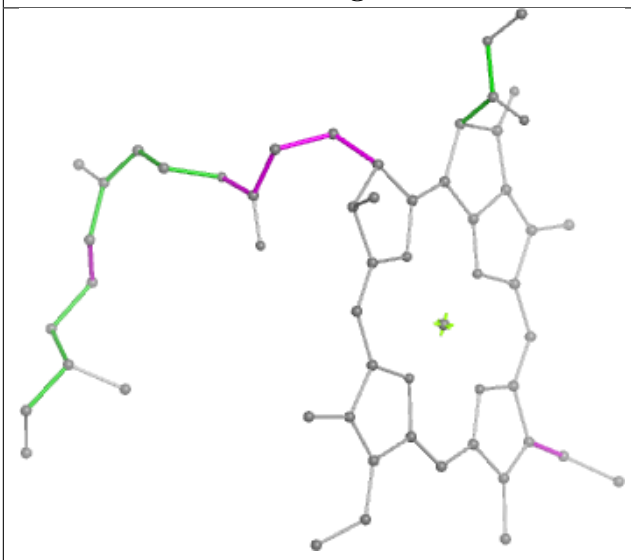
Ligand CLA a 831



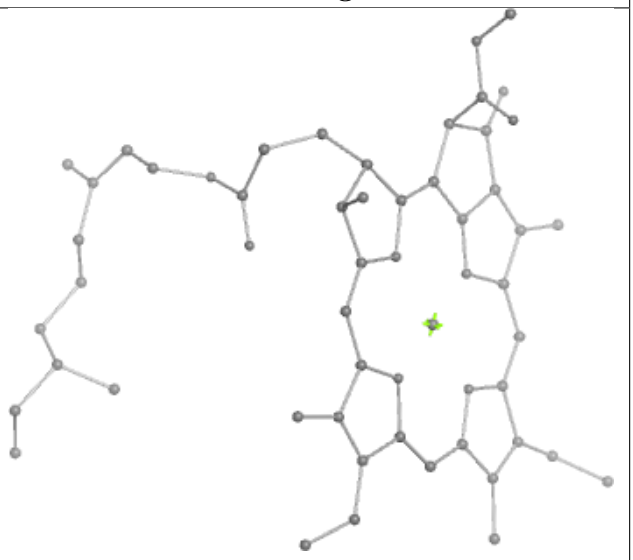
Bond lengths



Bond angles

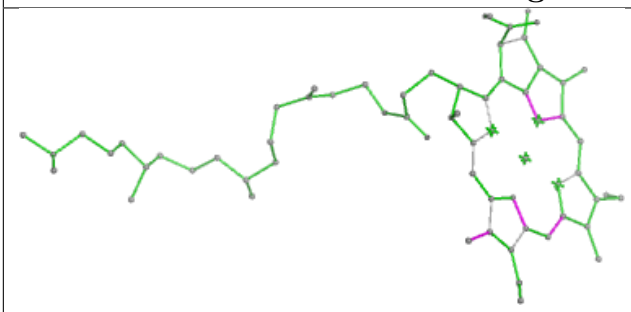


Torsions

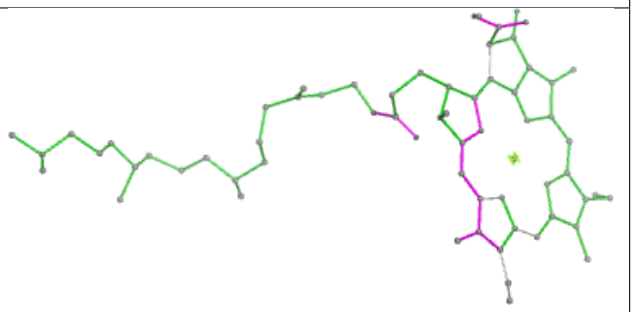


Rings

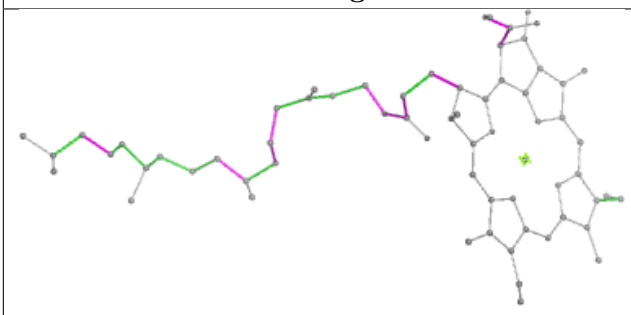
Ligand CLA b 834



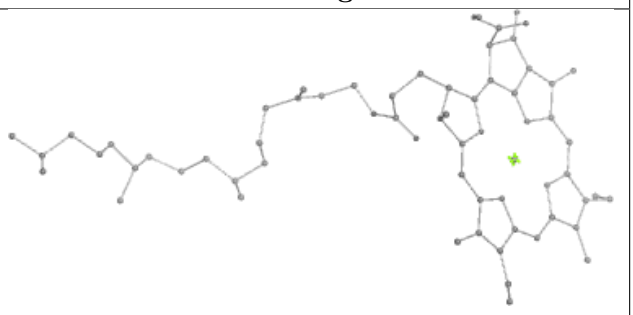
Bond lengths



Bond angles

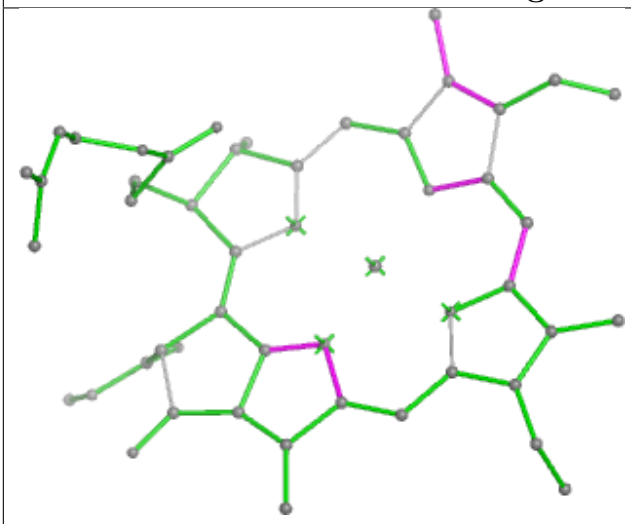


Torsions

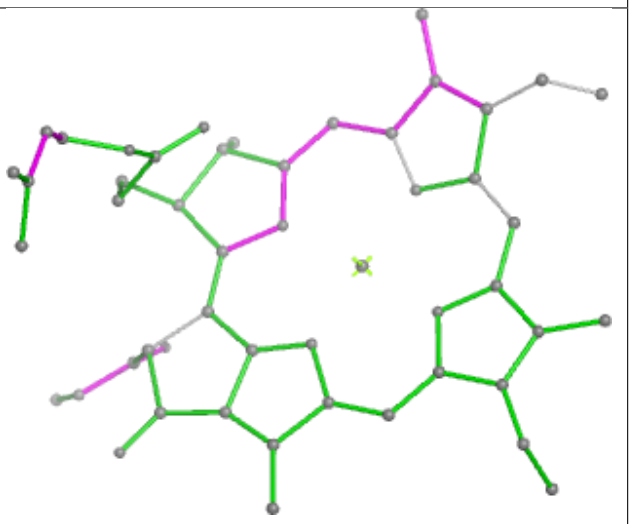


Rings

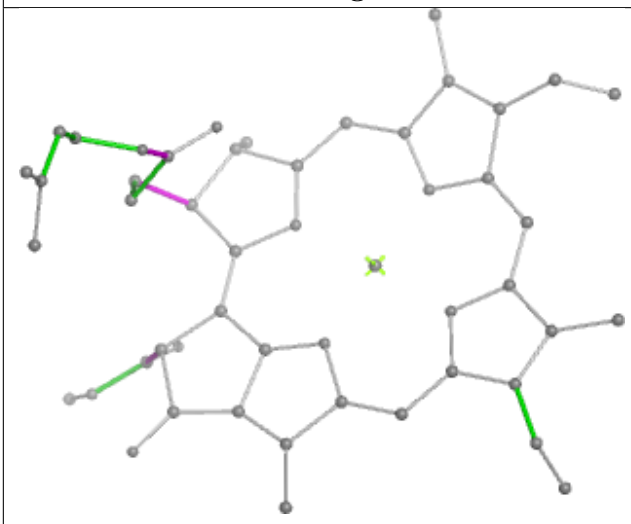
Ligand CLA b 839



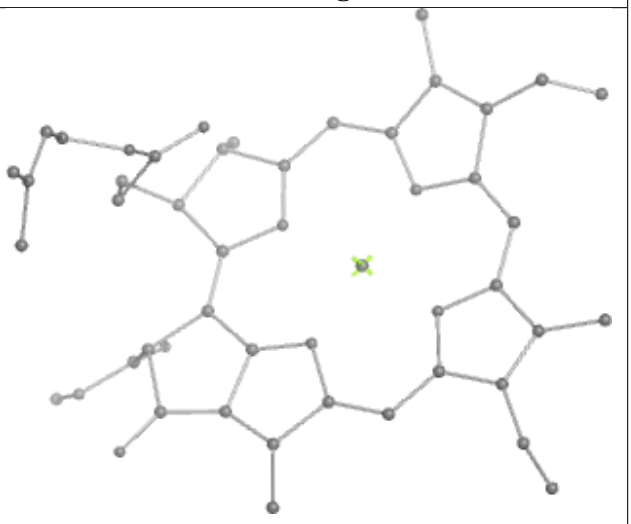
Bond lengths



Bond angles

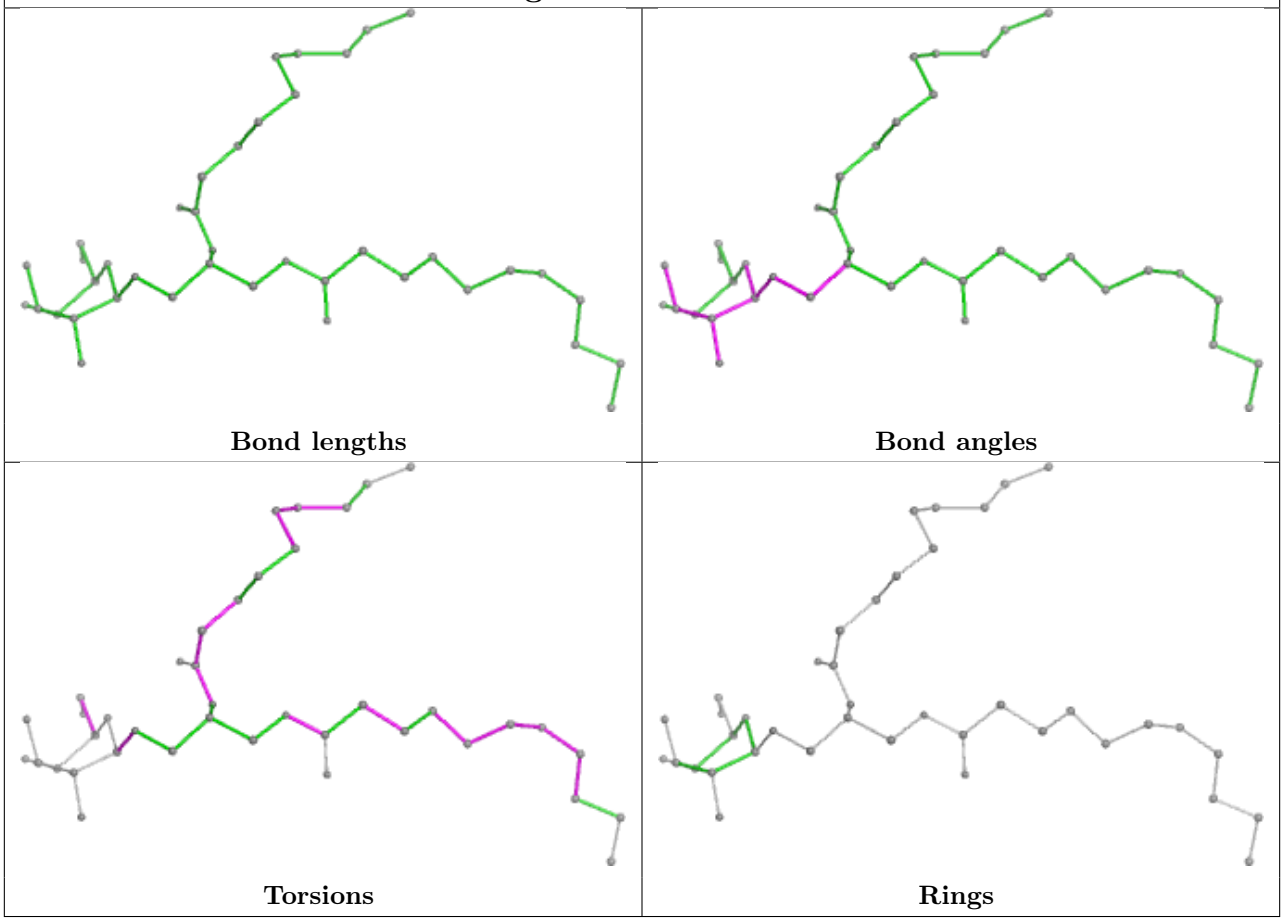


Torsions

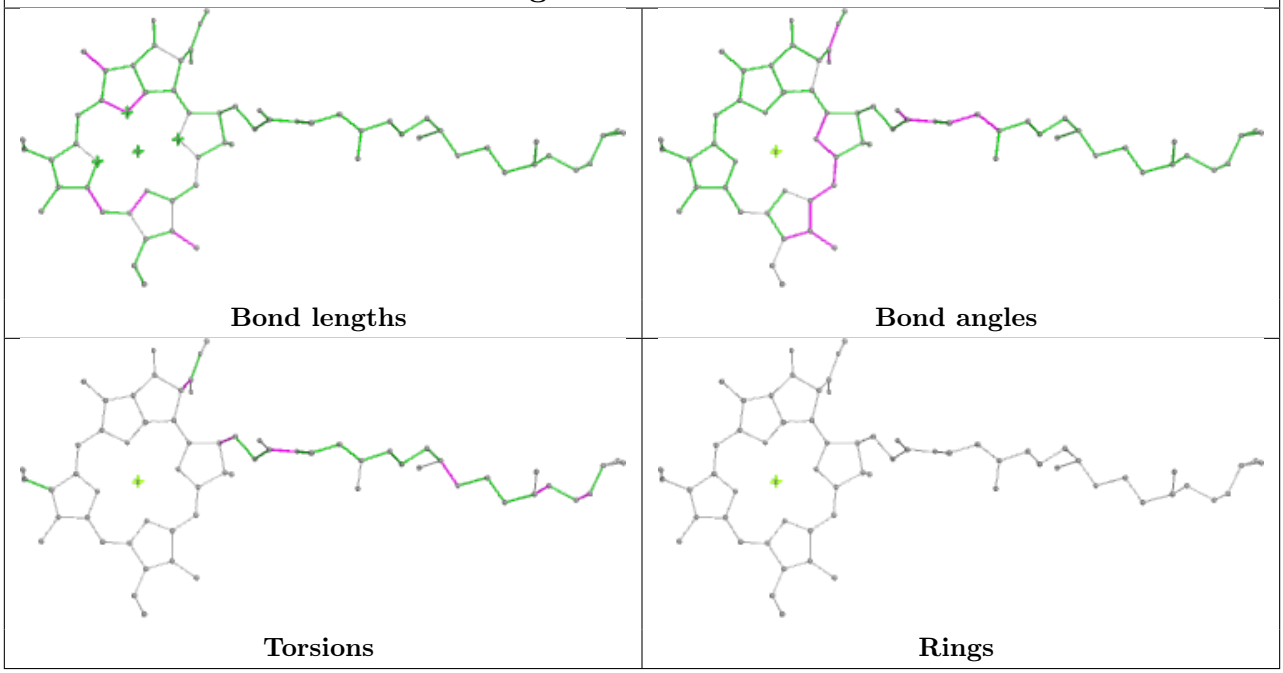


Rings

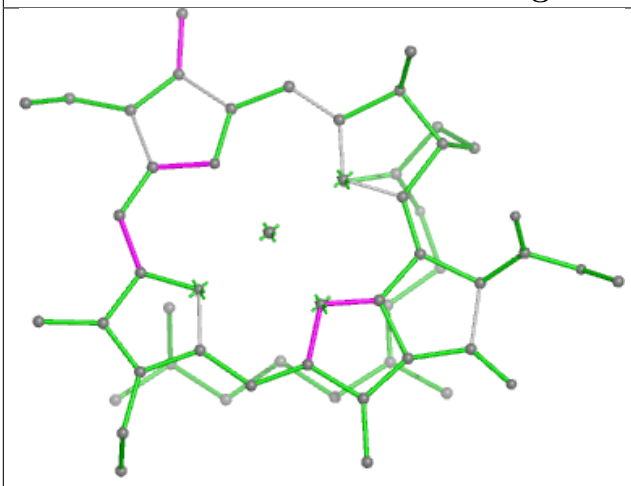
Ligand LMG a 852



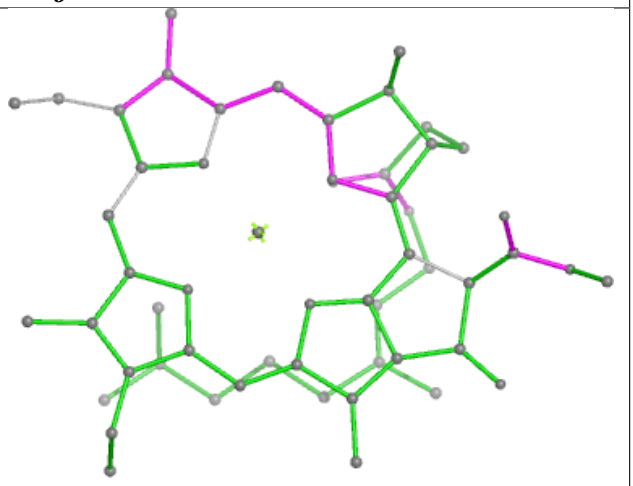
Ligand CLA a 826



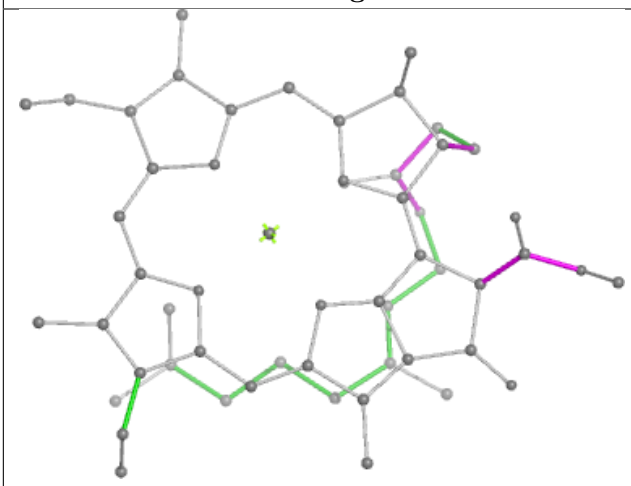
Ligand CLA j 103



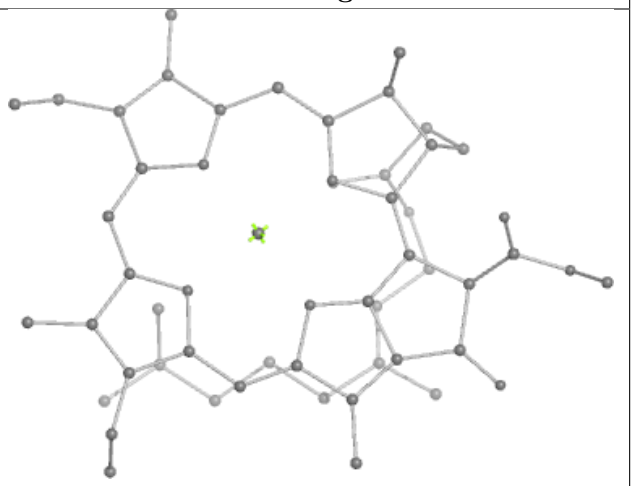
Bond lengths



Bond angles

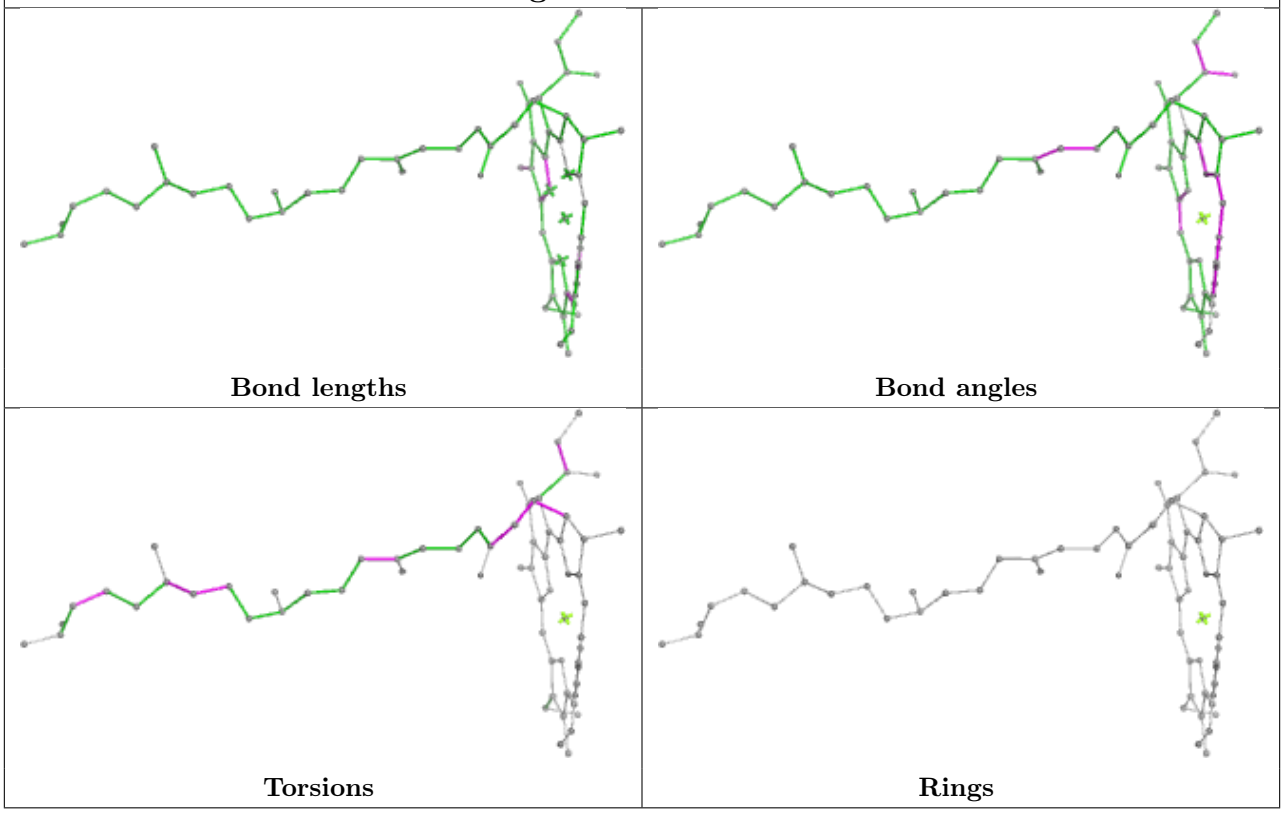


Torsions



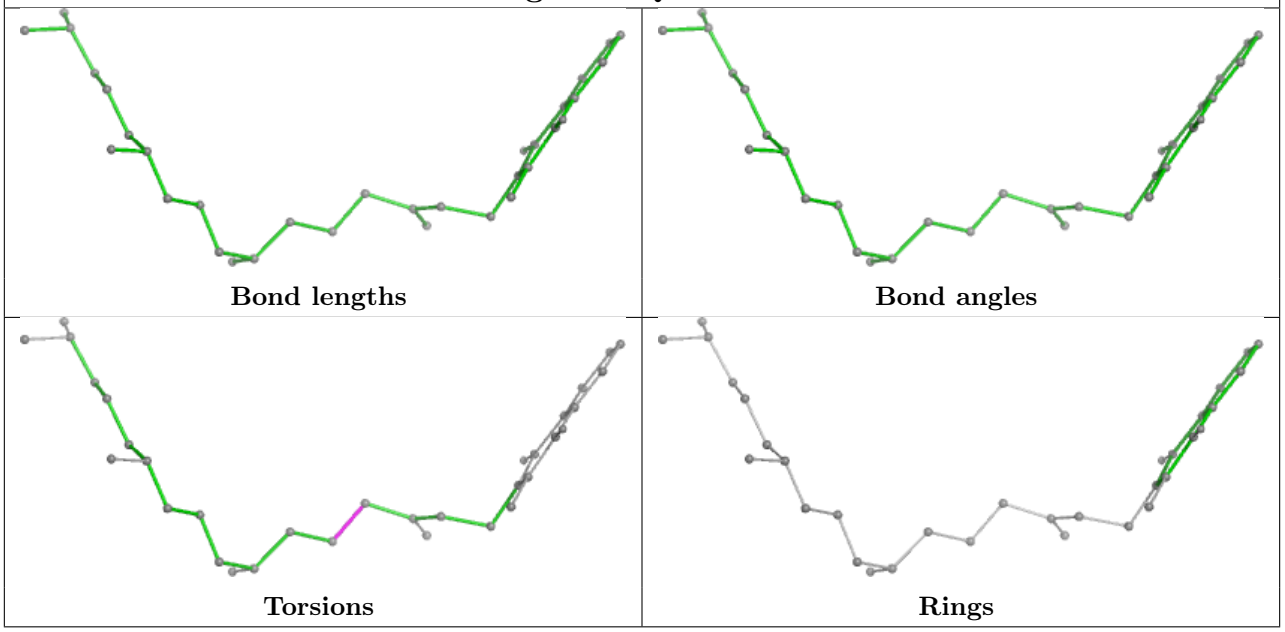
Rings

Ligand CLA a 828

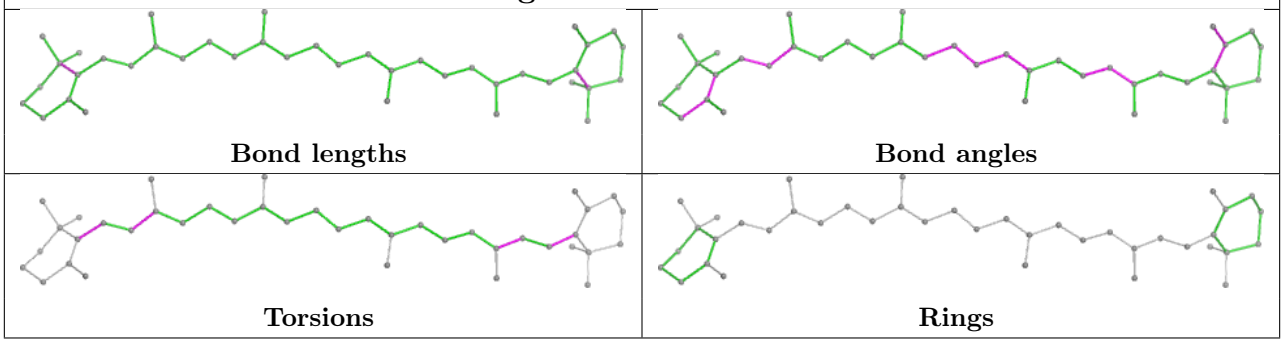


Ligand BCR b 849

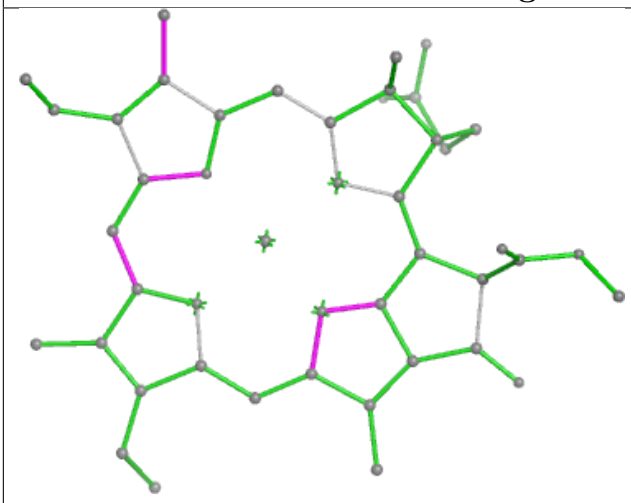
Ligand PQN b 843



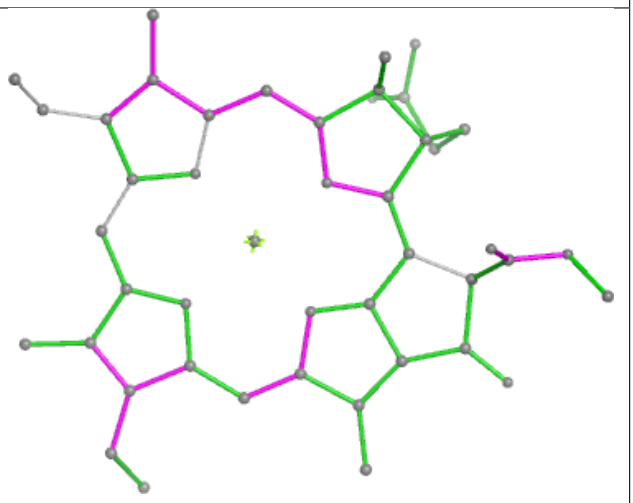
Ligand BCR k 4001



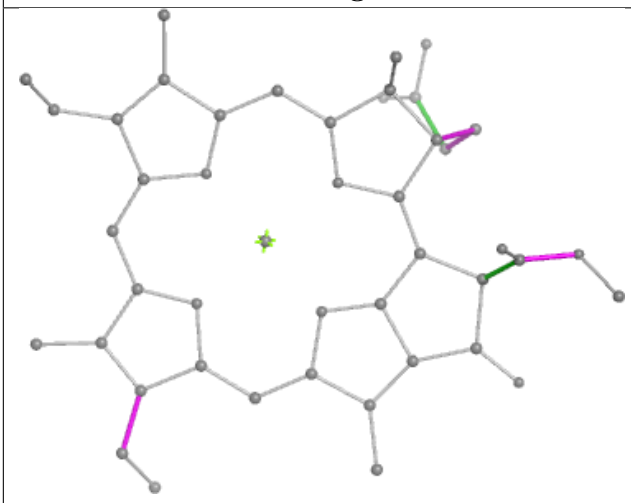
Ligand CLA k 4004



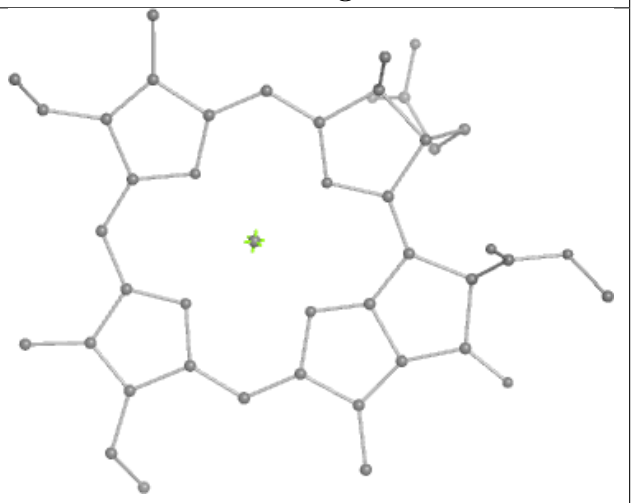
Bond lengths



Bond angles

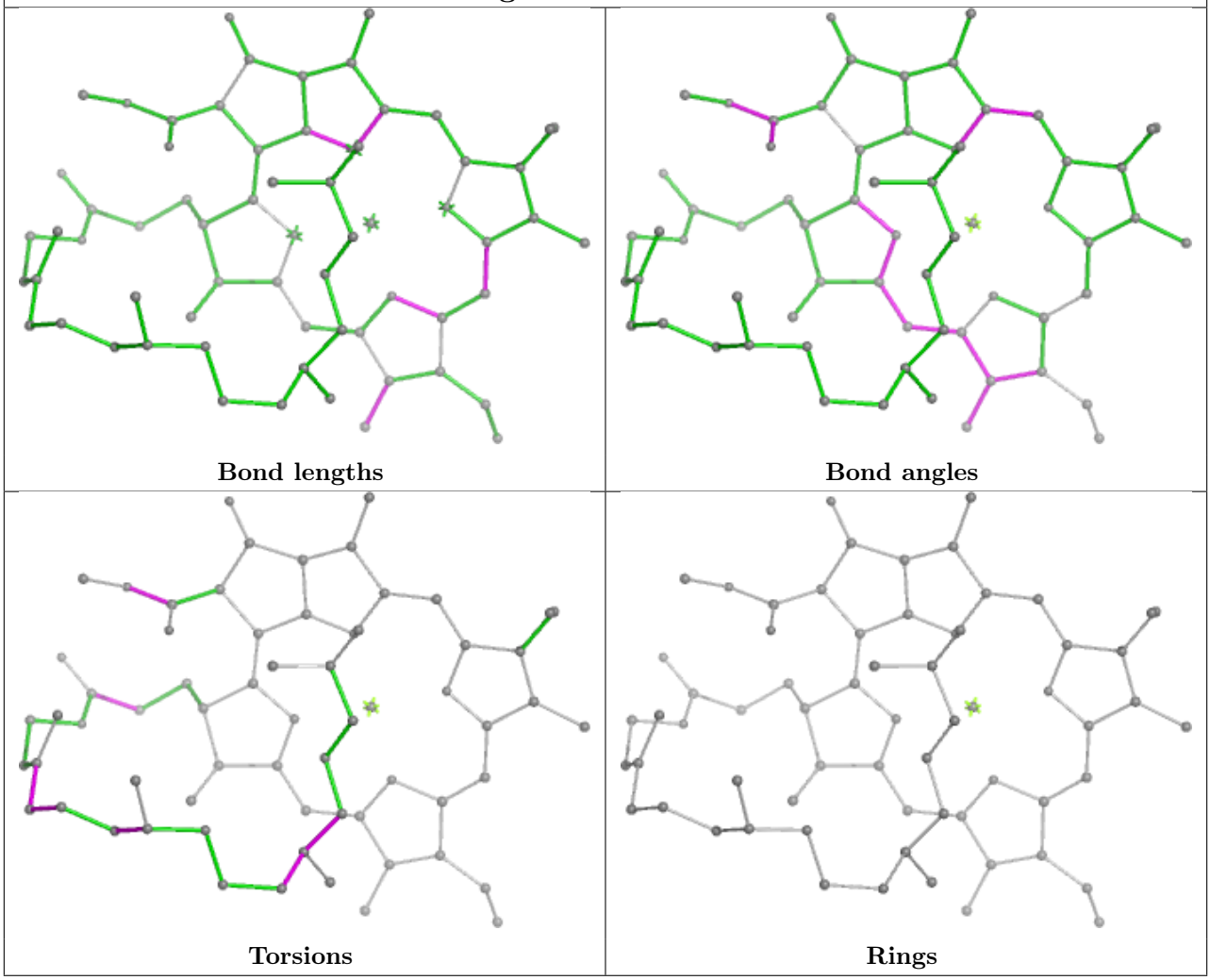


Torsions

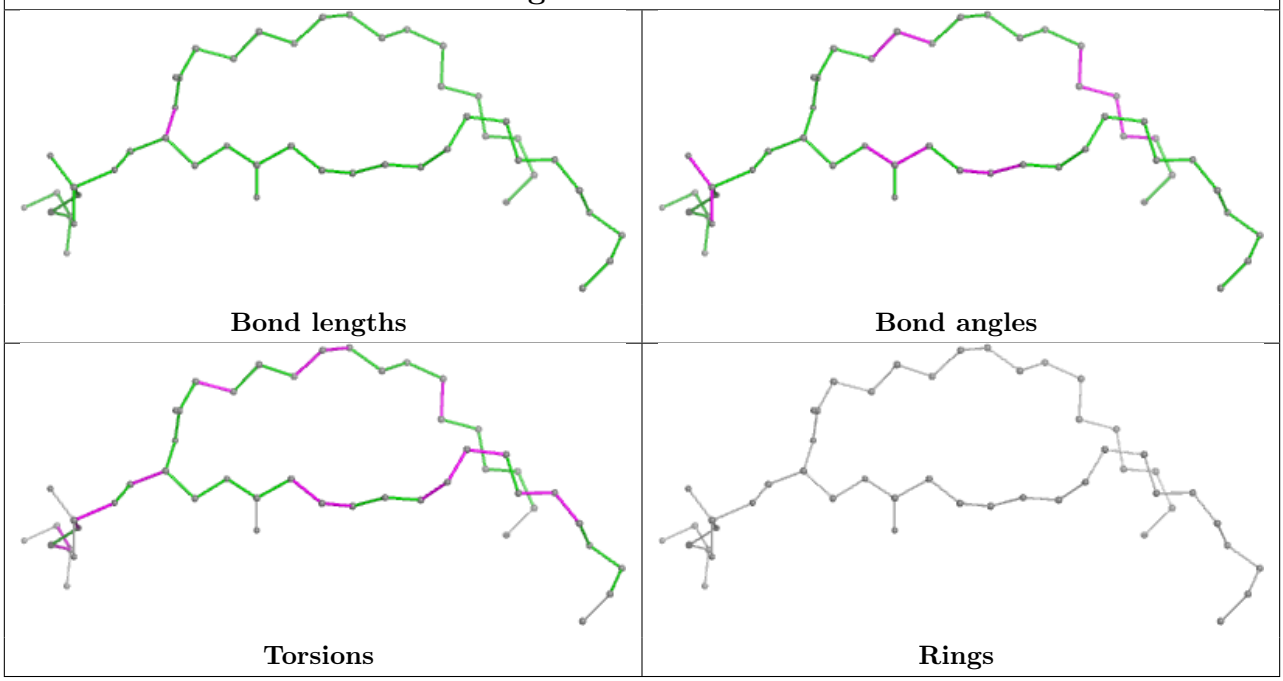


Rings

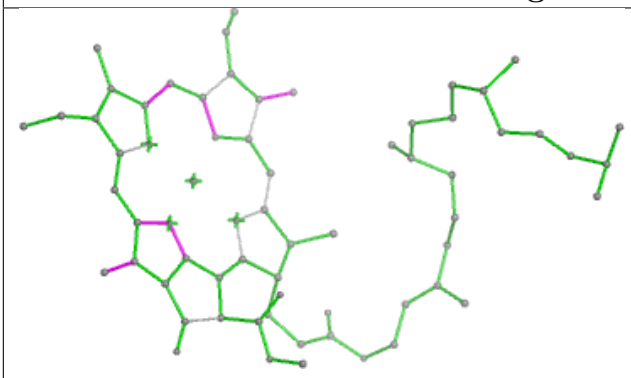
Ligand CLA a 806



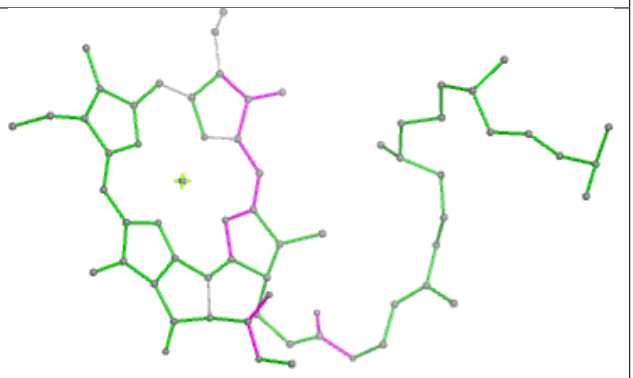
Ligand LHG a 851



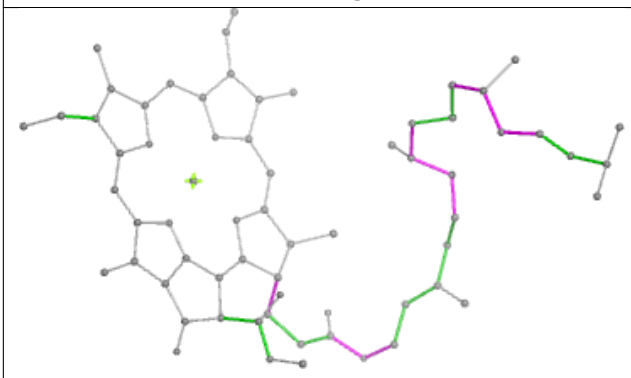
Ligand CLA b 825



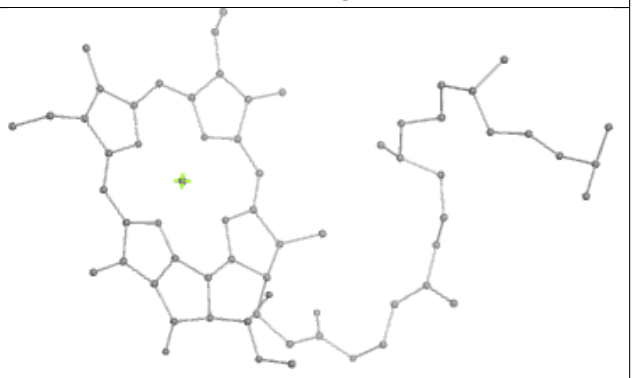
Bond lengths



Bond angles

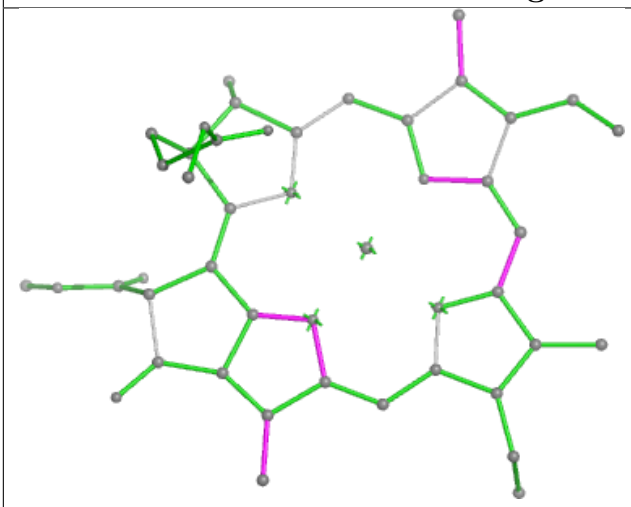


Torsions

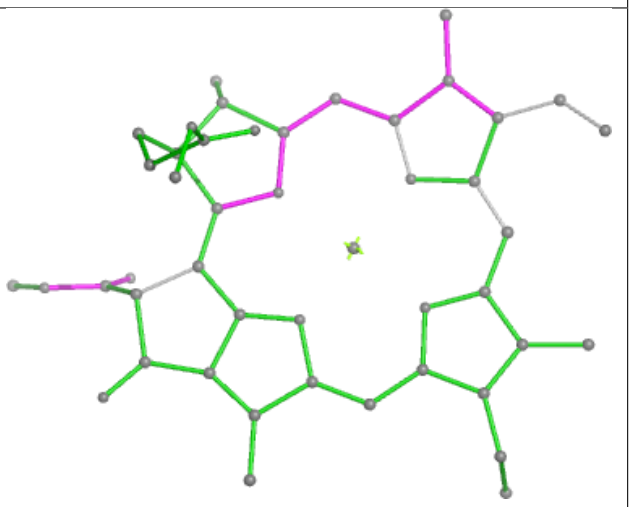


Rings

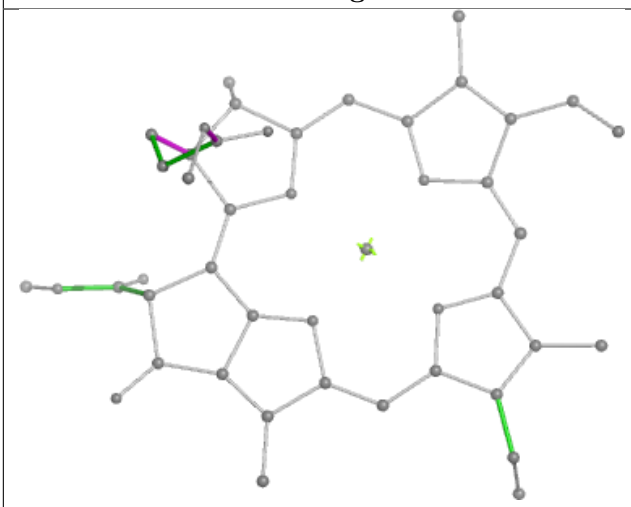
Ligand CLA b 823



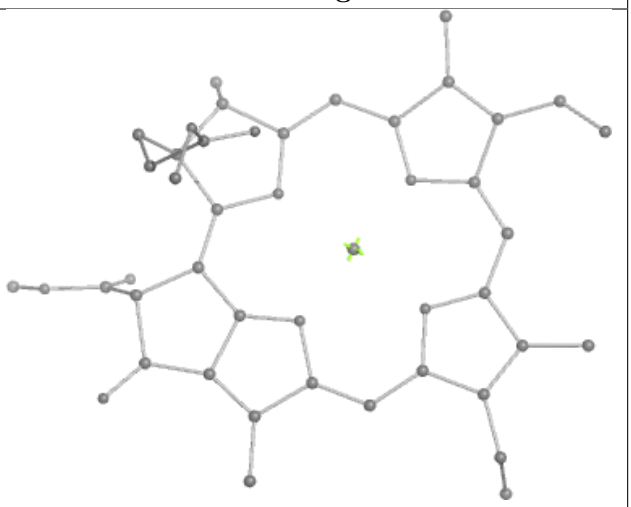
Bond lengths



Bond angles

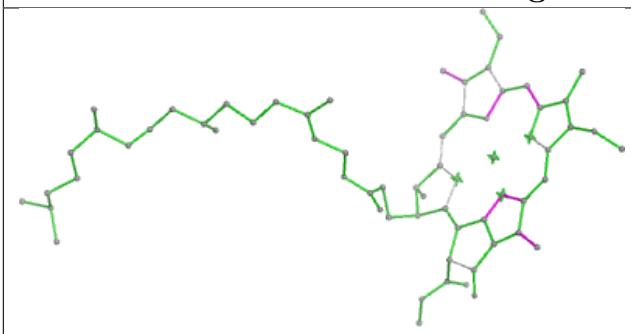


Torsions

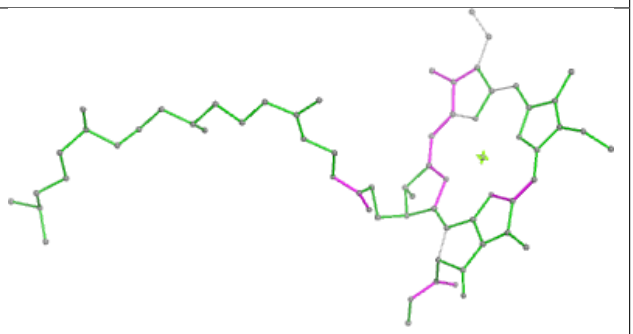


Rings

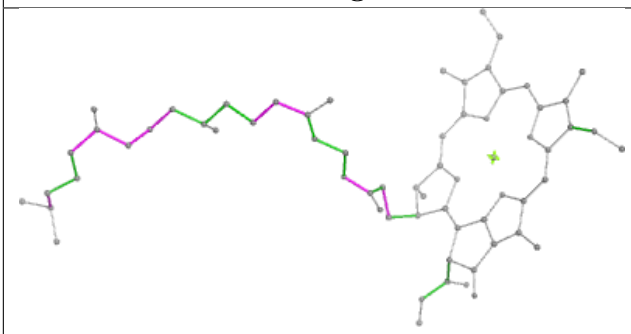
Ligand CLA a 821



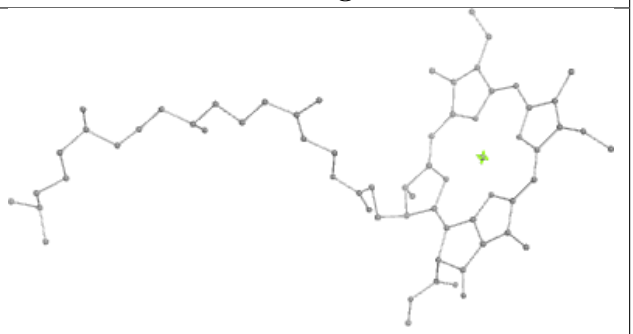
Bond lengths



Bond angles

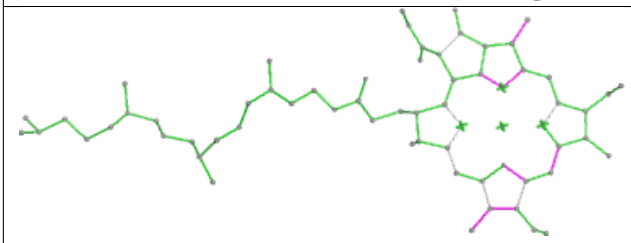


Torsions

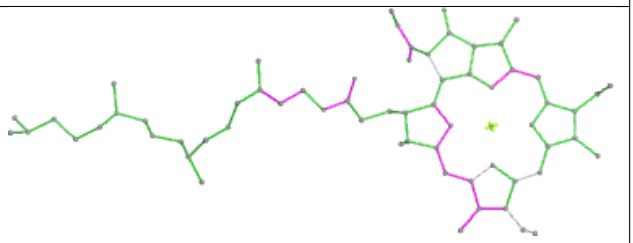


Rings

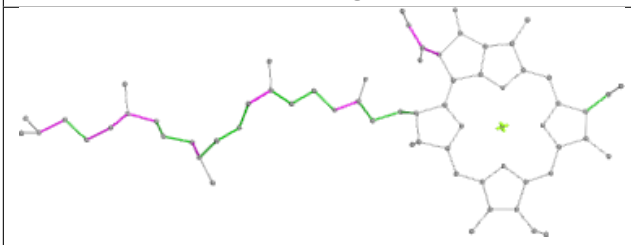
Ligand CLA a 833



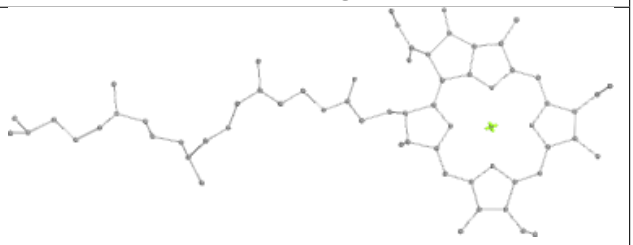
Bond lengths



Bond angles

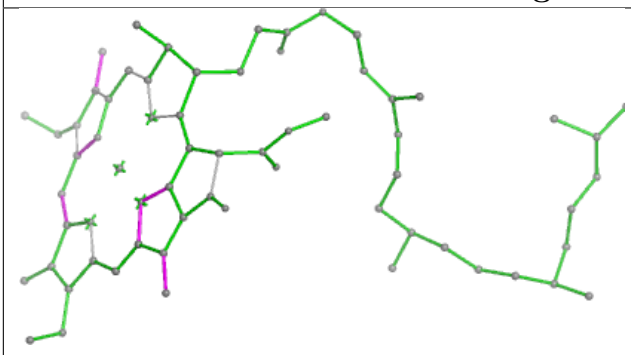


Torsions

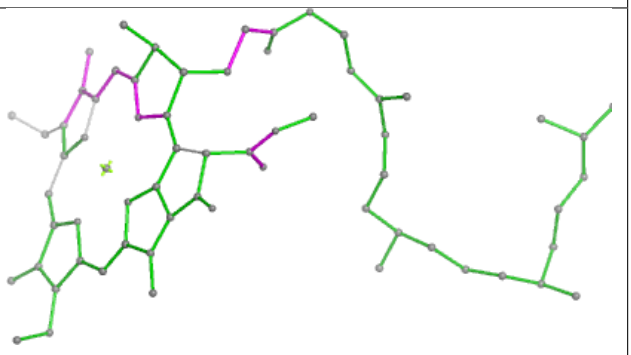


Rings

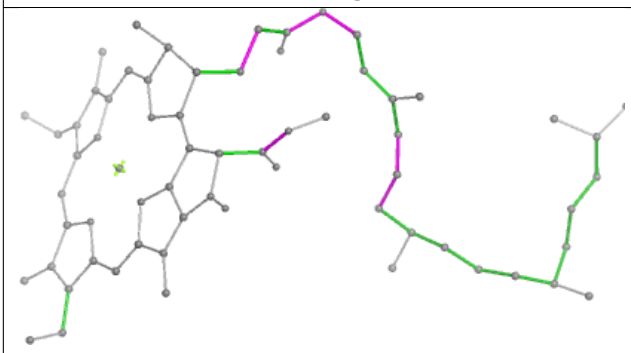
Ligand CL0 a 801



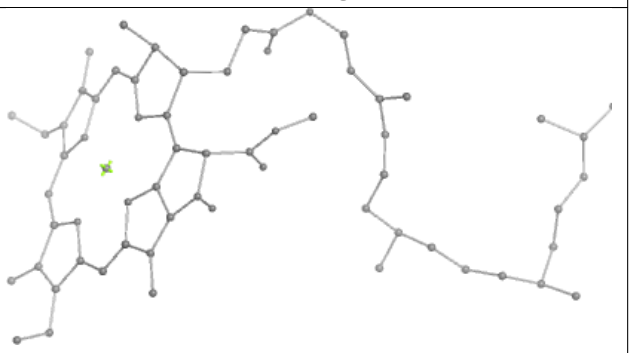
Bond lengths



Bond angles

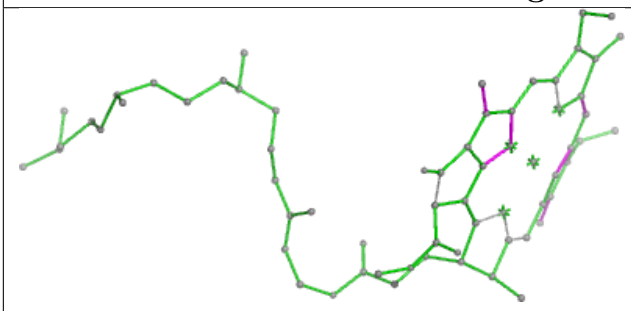


Torsions



Rings

Ligand CLA b 803



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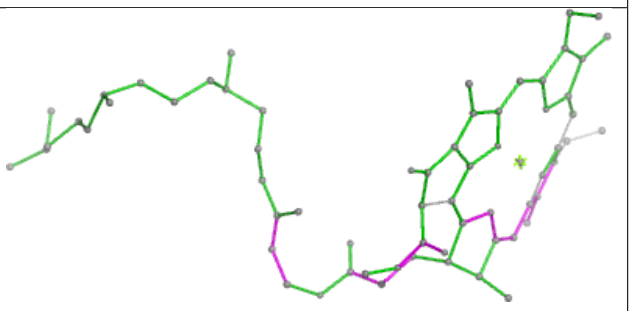
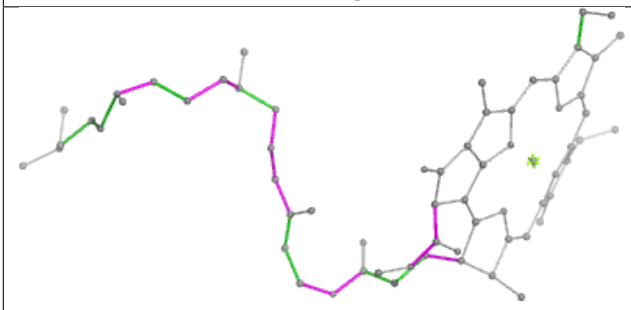
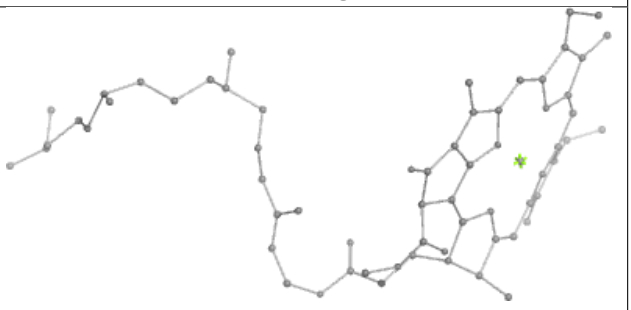


Bond angles

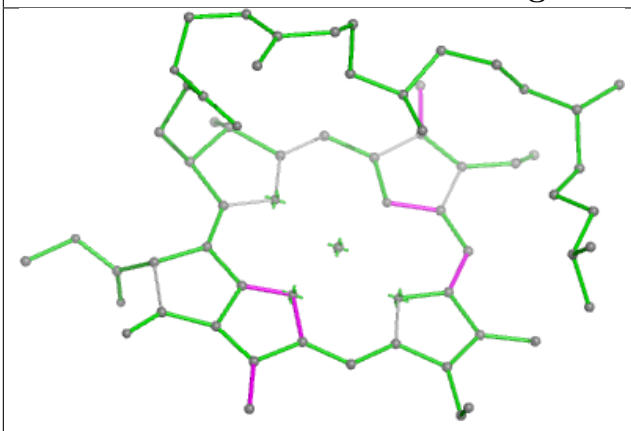


Torsions

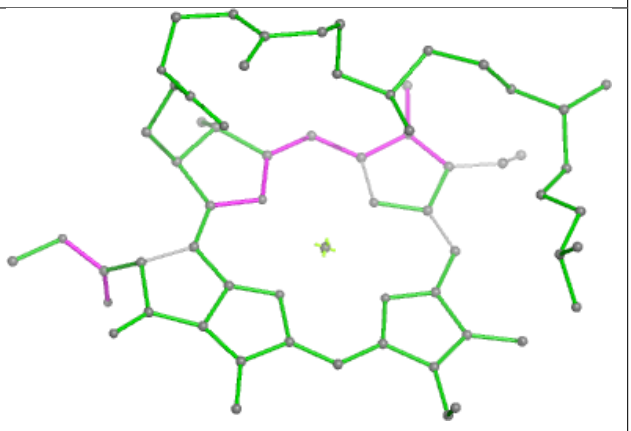


Rings

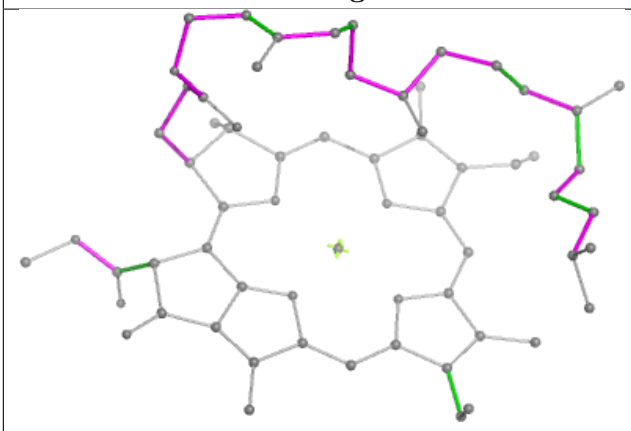
Ligand CLA a 820



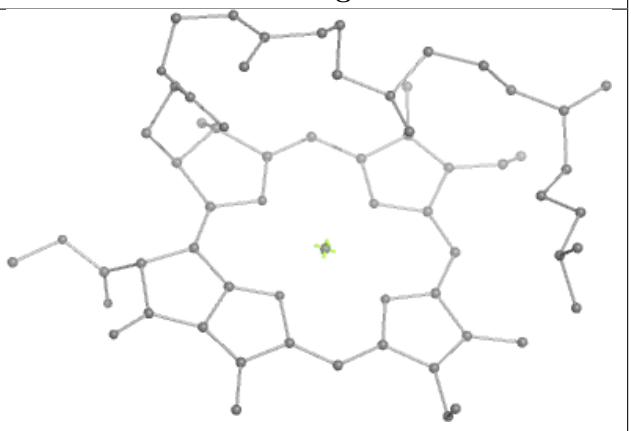
Bond lengths



Bond angles

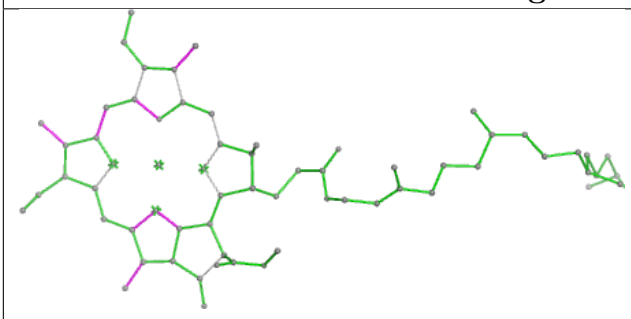


Torsions

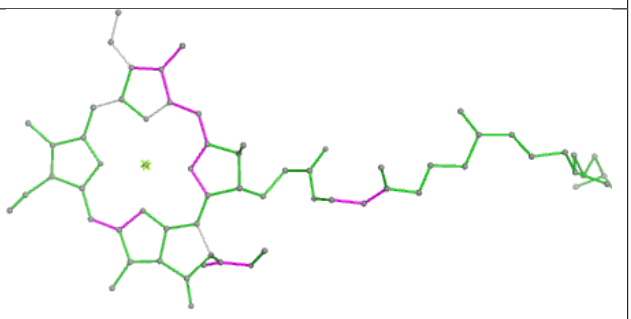


Rings

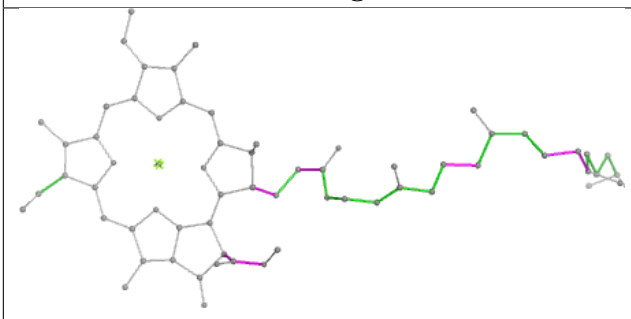
Ligand CLA a 805



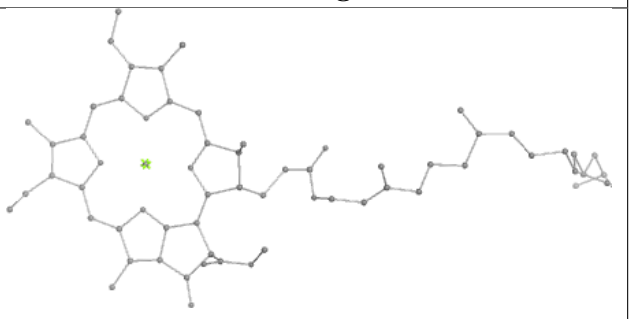
Bond lengths



Bond angles

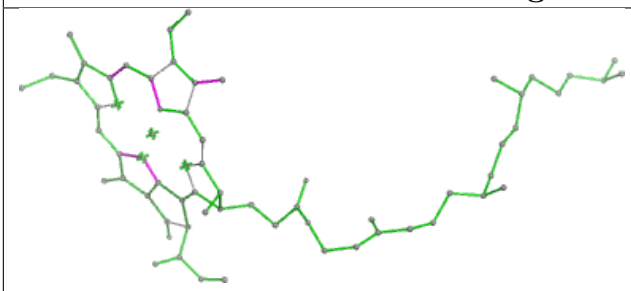


Torsions

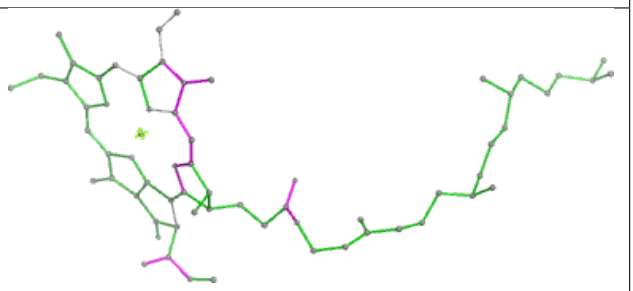


Rings

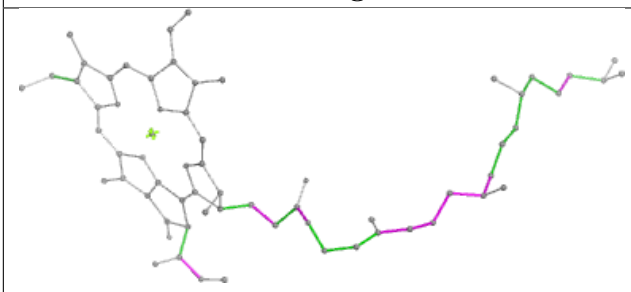
Ligand CLA b 801



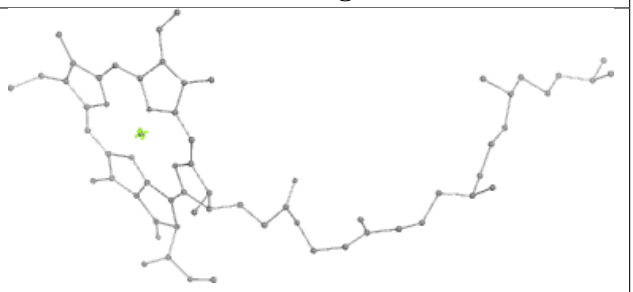
Bond lengths



Bond angles

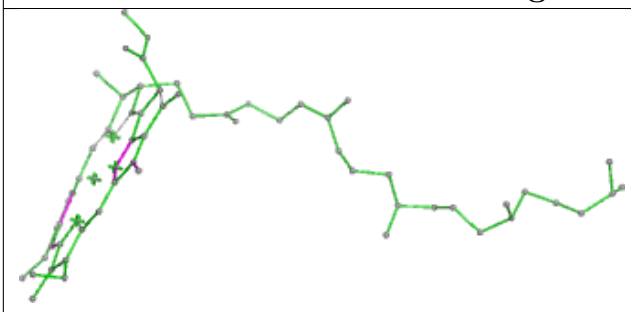


Torsions



Rings

Ligand CLA a 839



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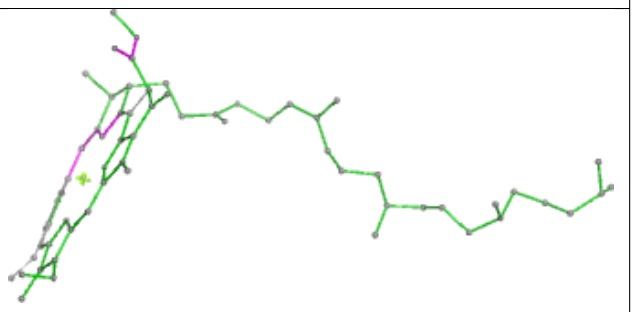
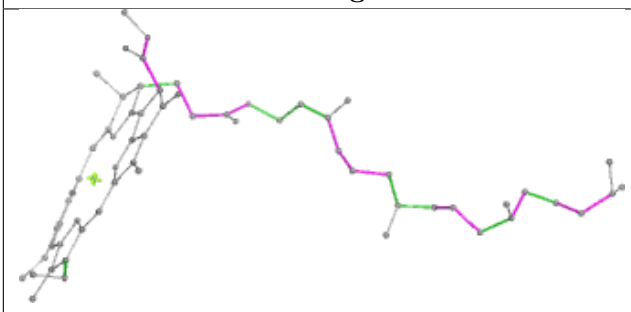
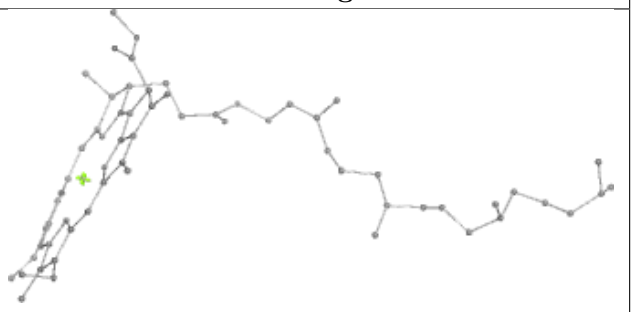


Bond angles

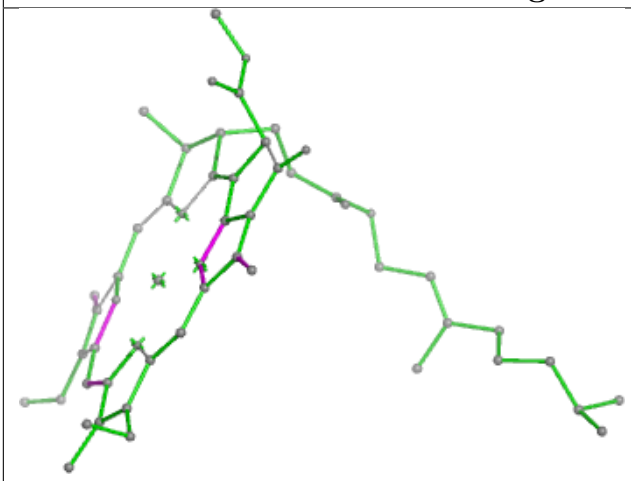


Torsions

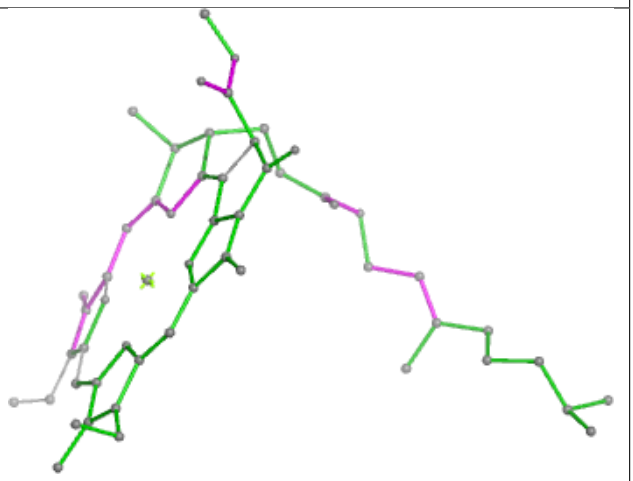


Rings

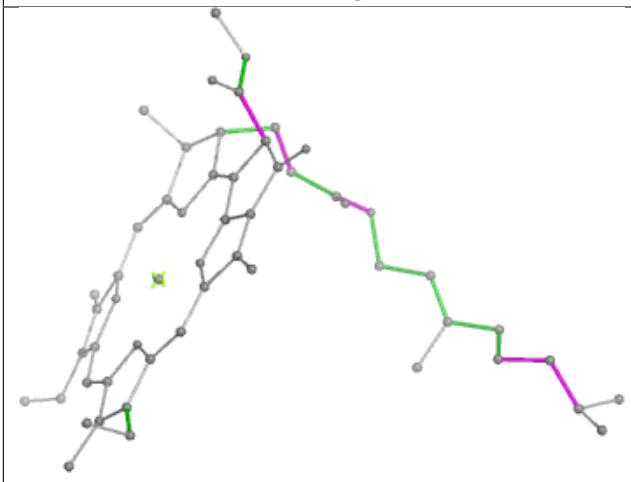
Ligand CLA a 836



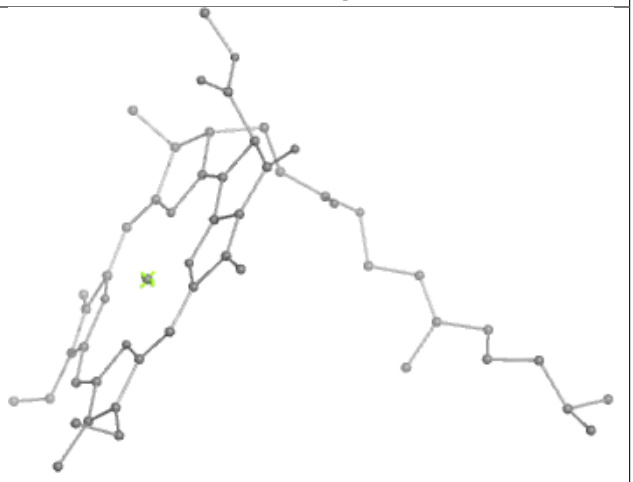
Bond lengths



Bond angles

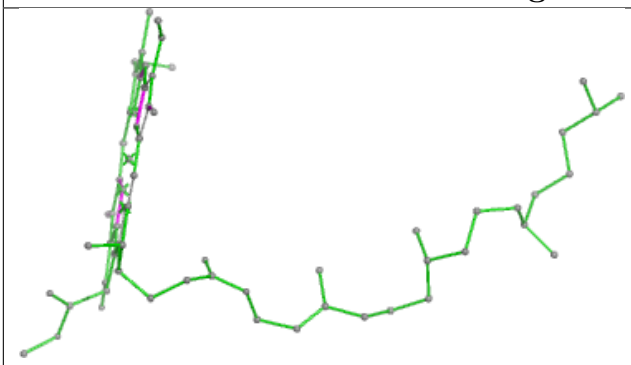


Torsions

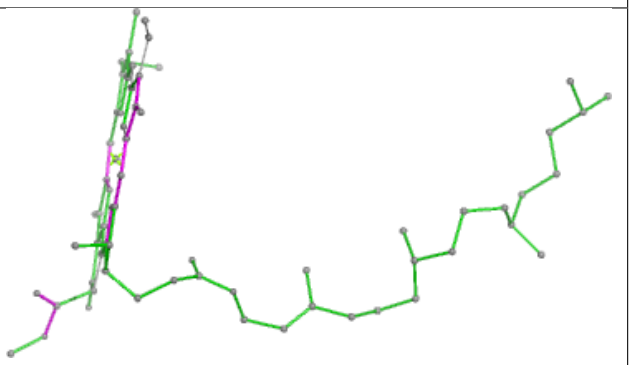


Rings

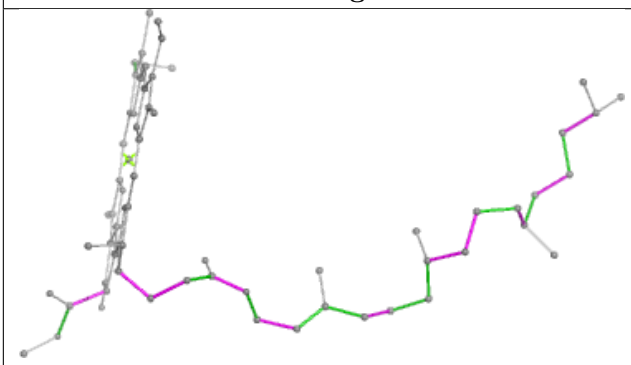
Ligand CLA a 807



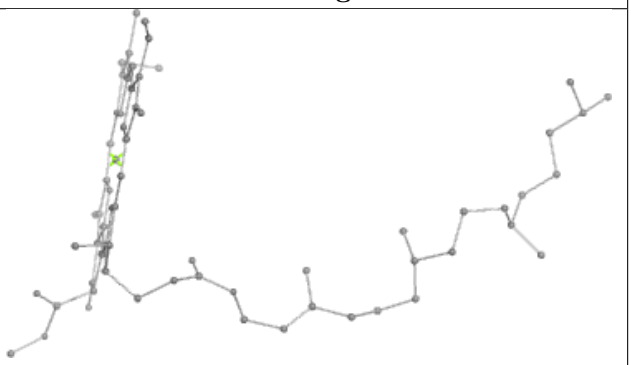
Bond lengths



Bond angles

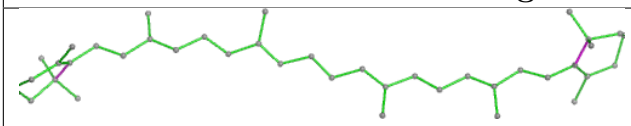


Torsions

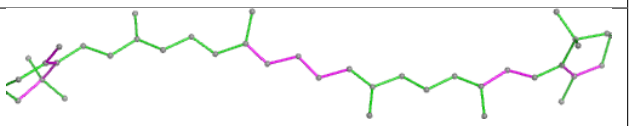


Rings

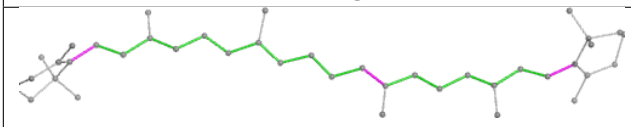
Ligand BCR k 4005



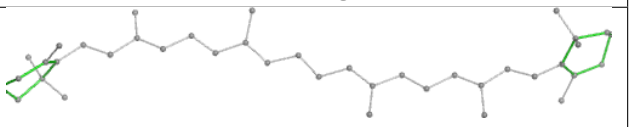
Bond lengths



Bond angles

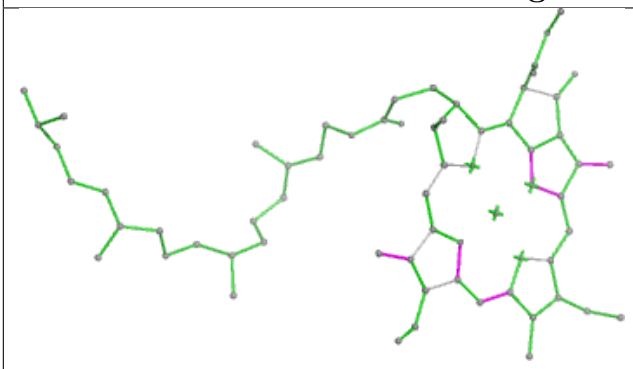


Torsions

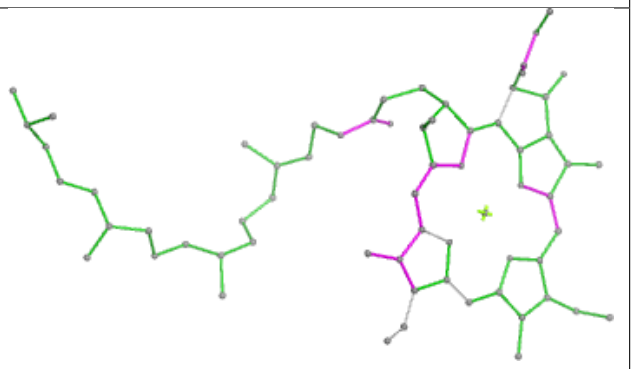


Rings

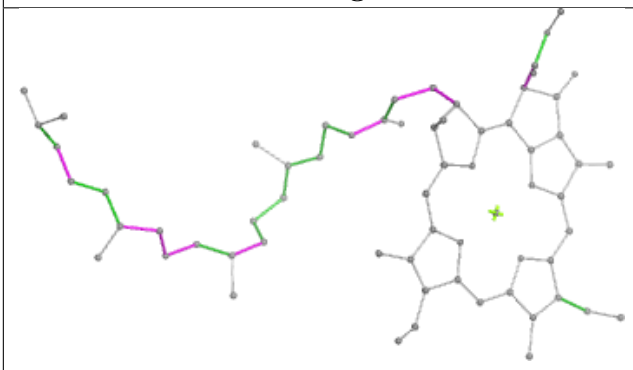
Ligand CLA a 808



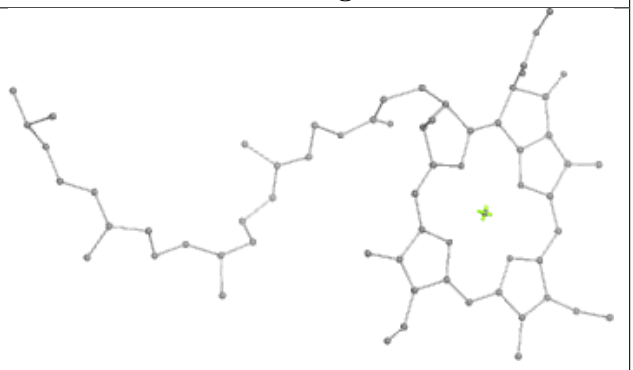
Bond lengths



Bond angles

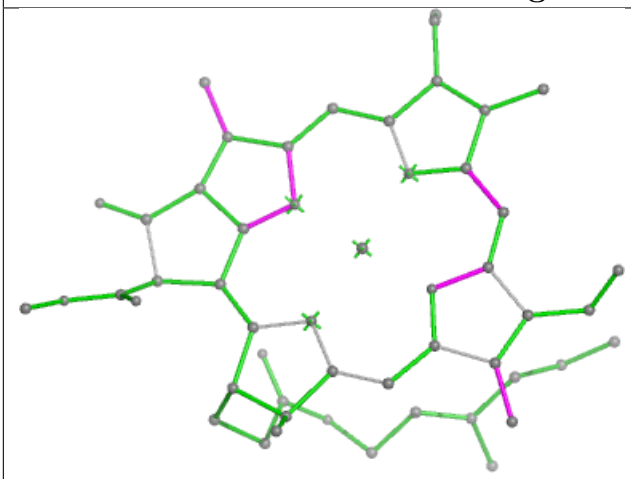


Torsions

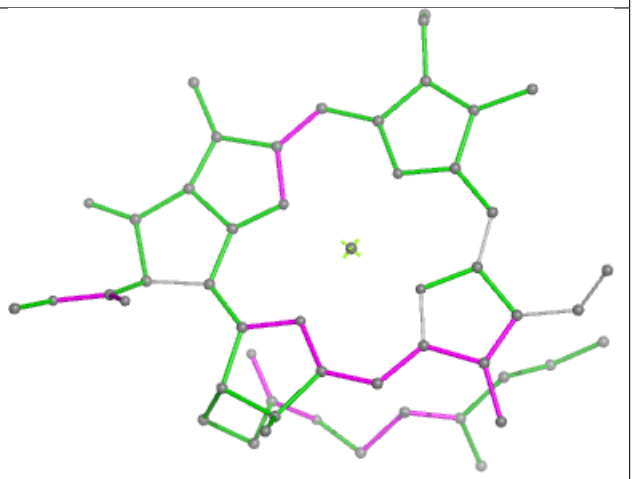


Rings

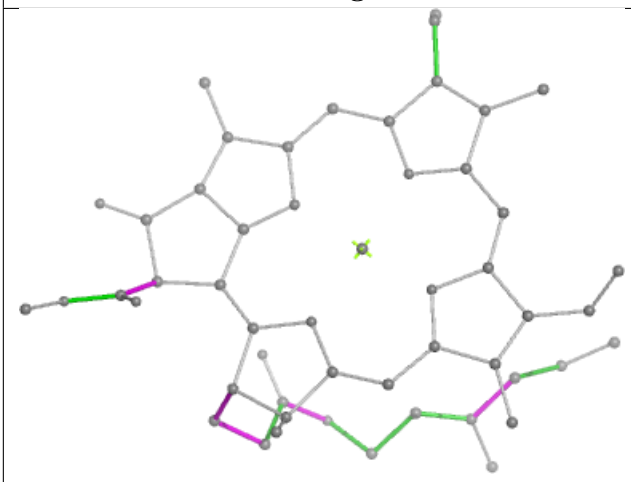
Ligand CLA a 812



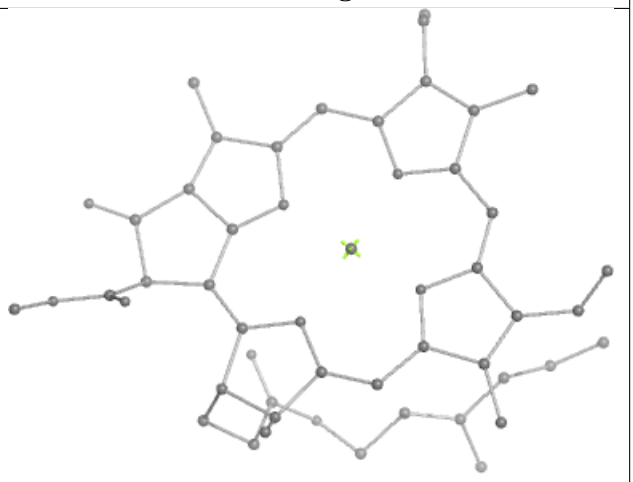
Bond lengths



Bond angles

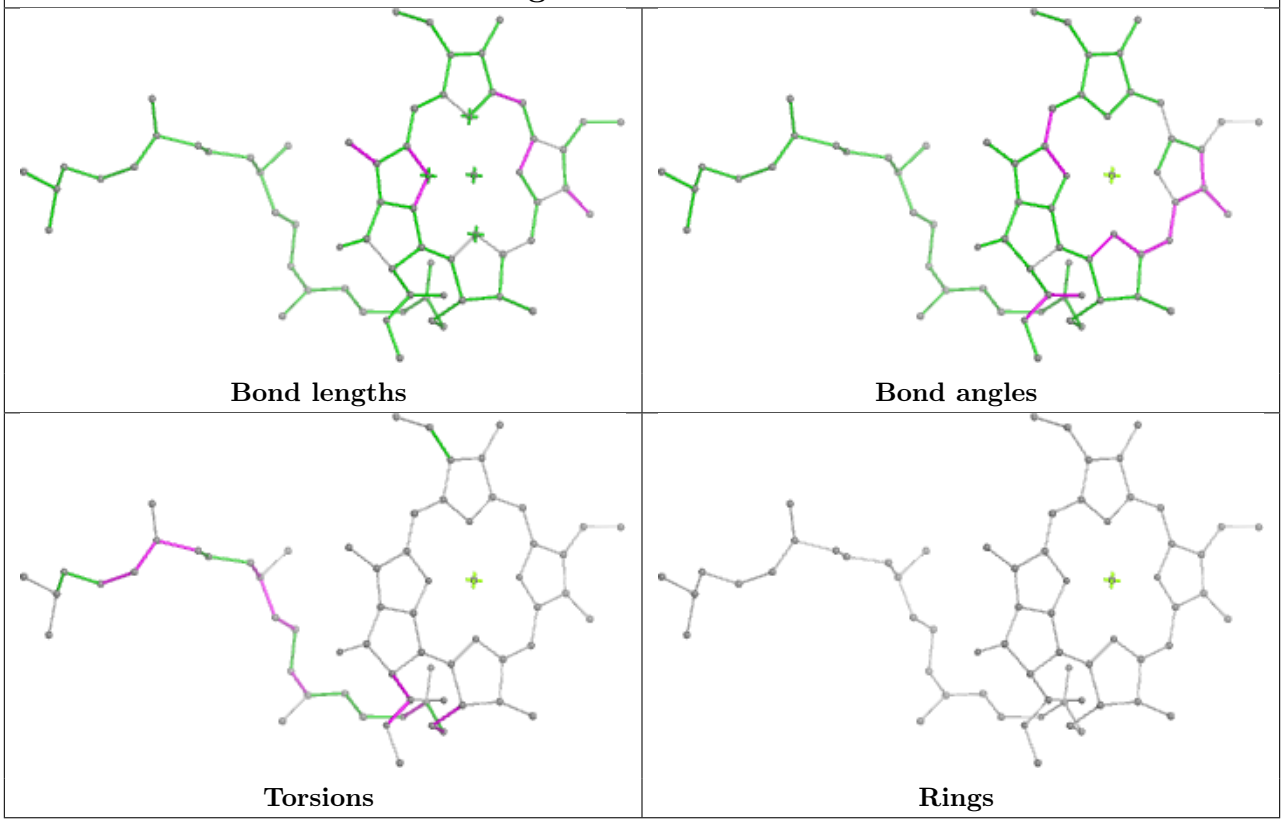


Torsions

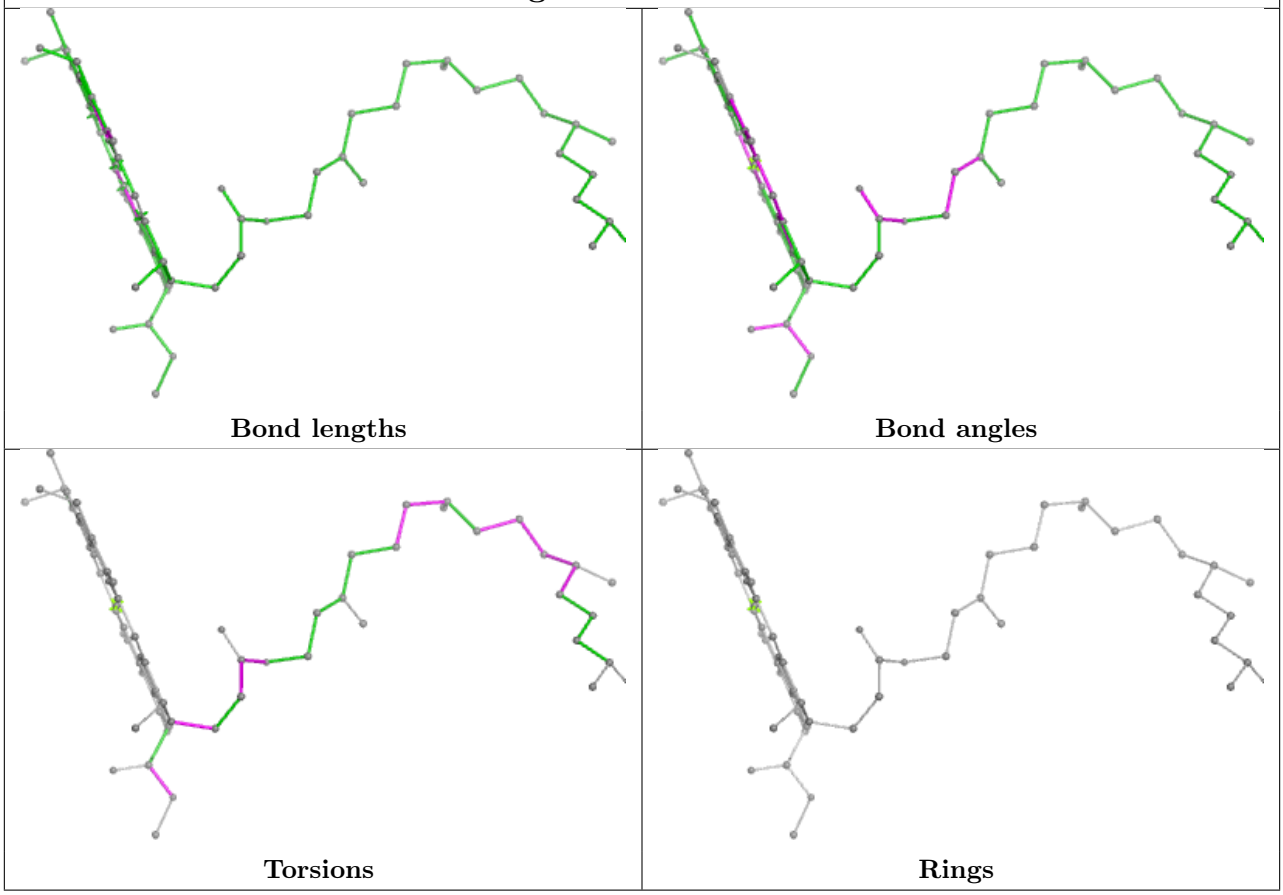


Rings

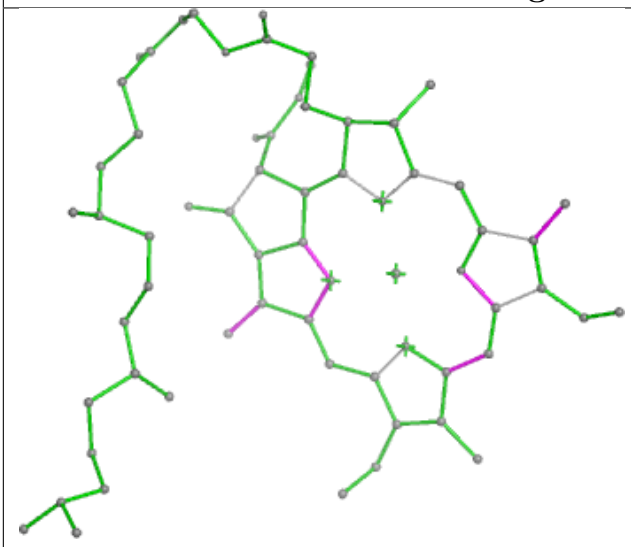
Ligand CLA b 835



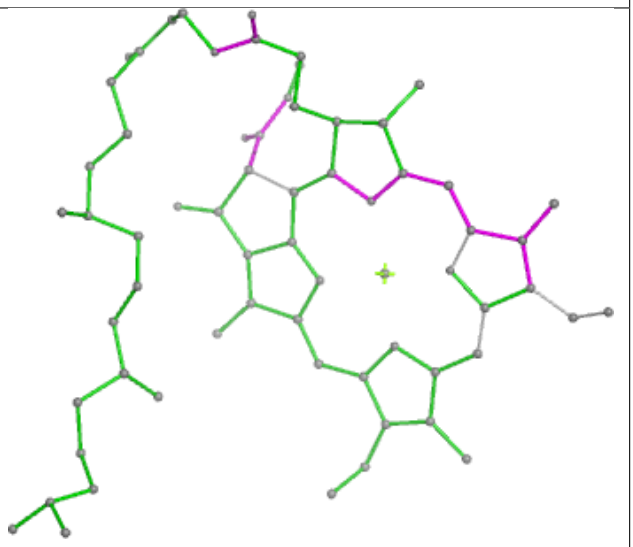
Ligand CLA b 840



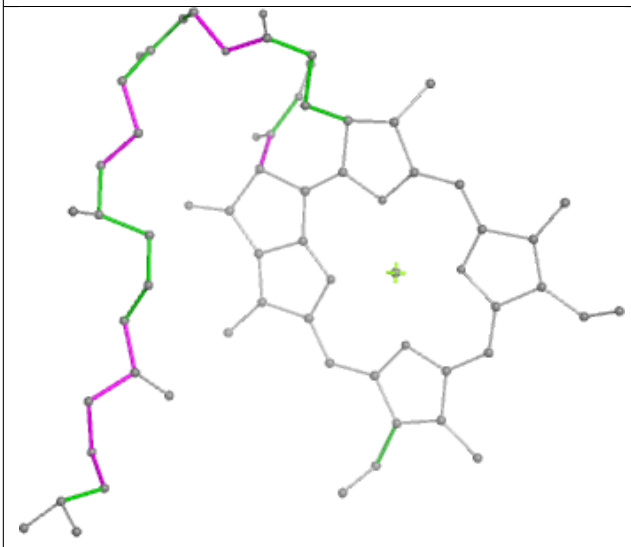
Ligand CLA a 825



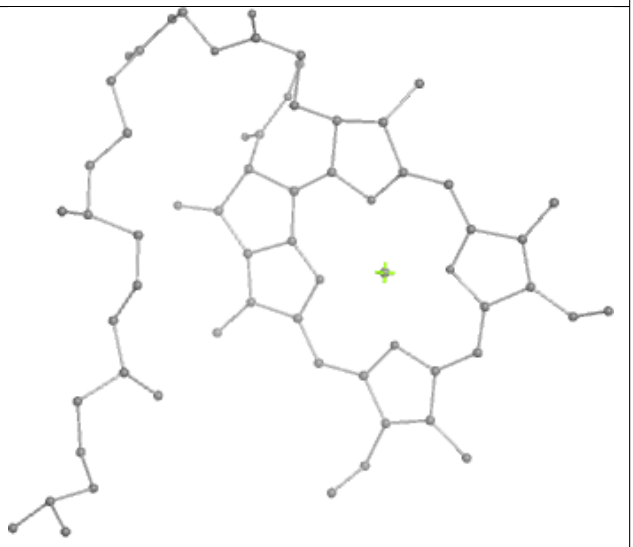
Bond lengths



Bond angles

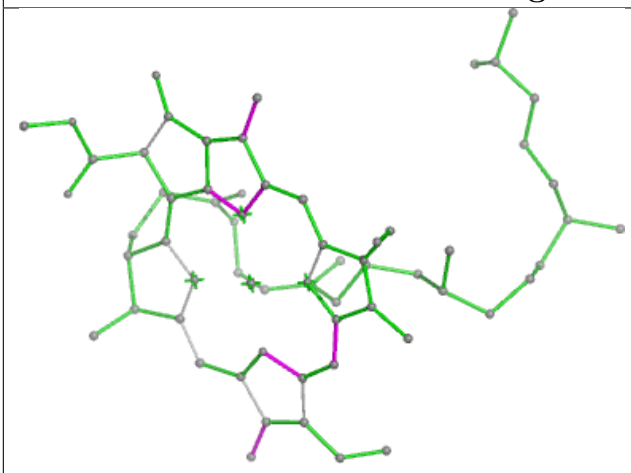


Torsions

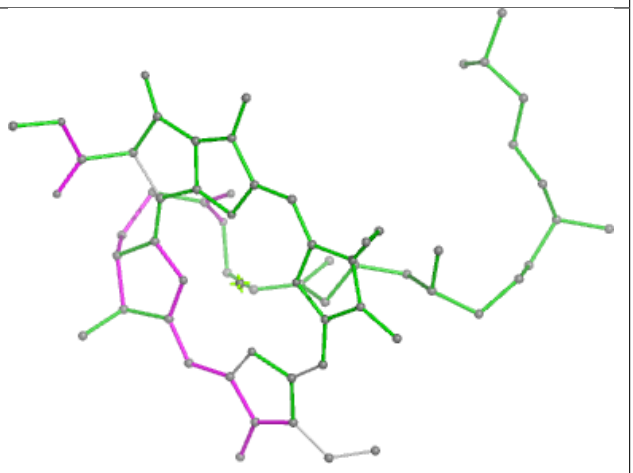


Rings

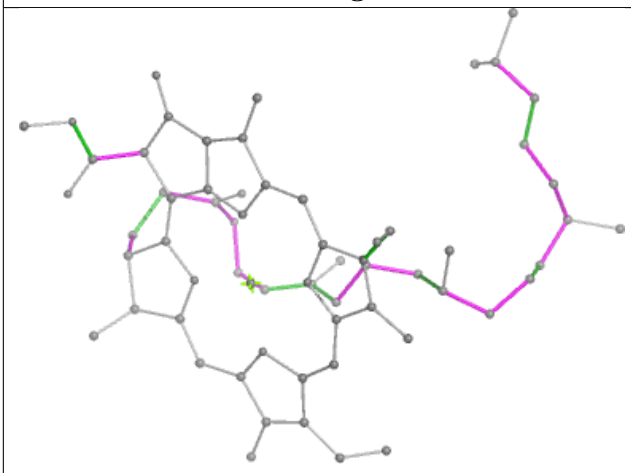
Ligand CLA a 823



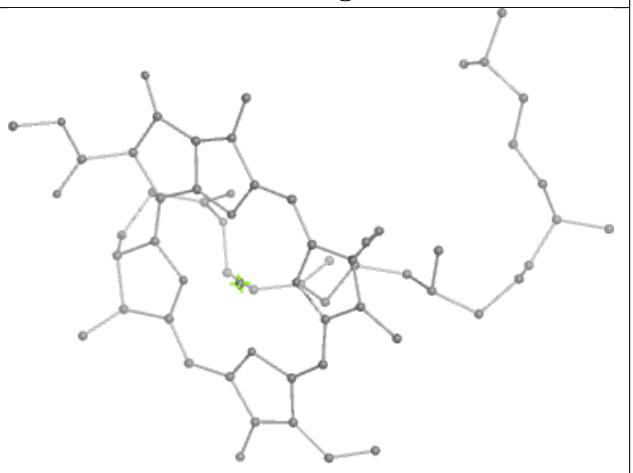
Bond lengths



Bond angles

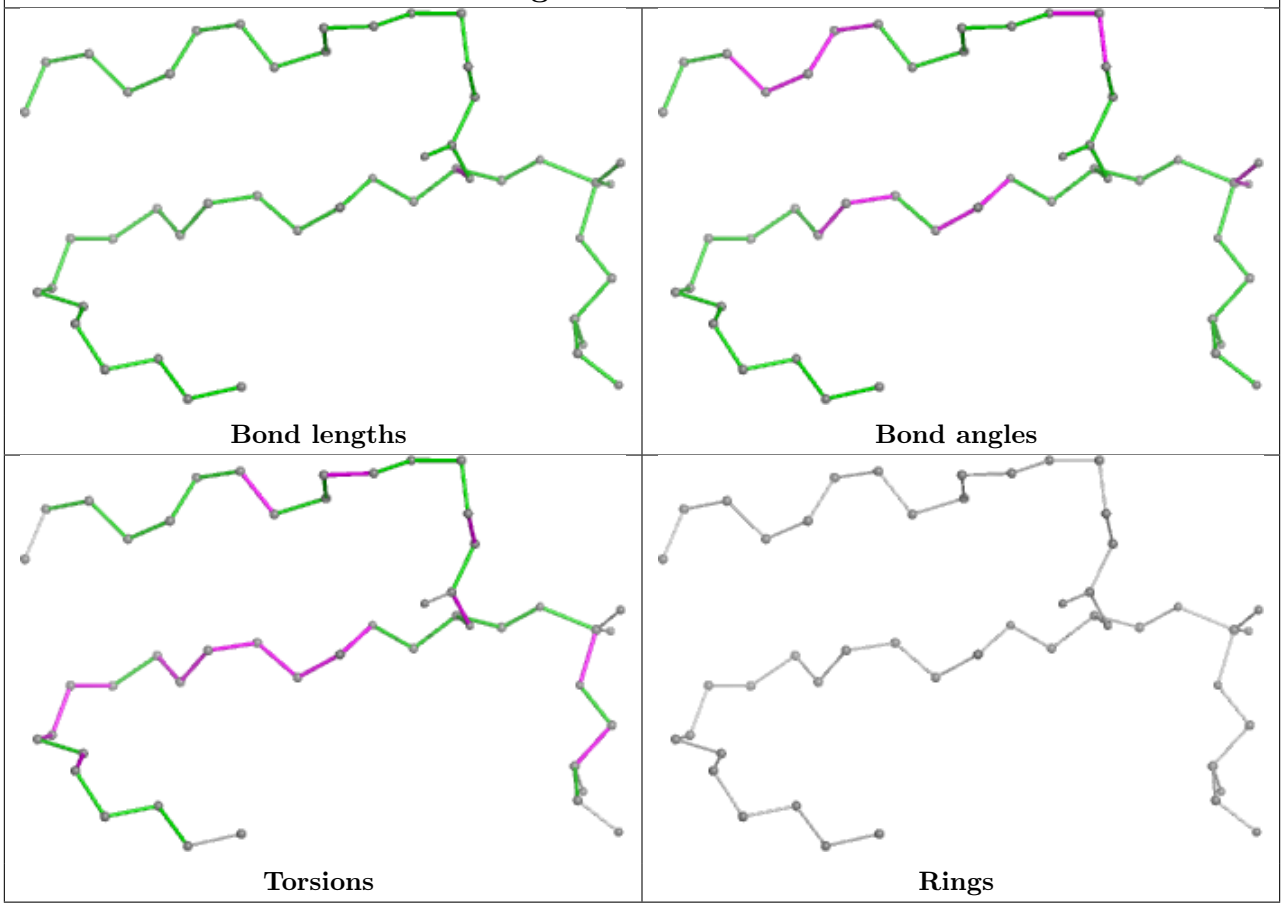


Torsions

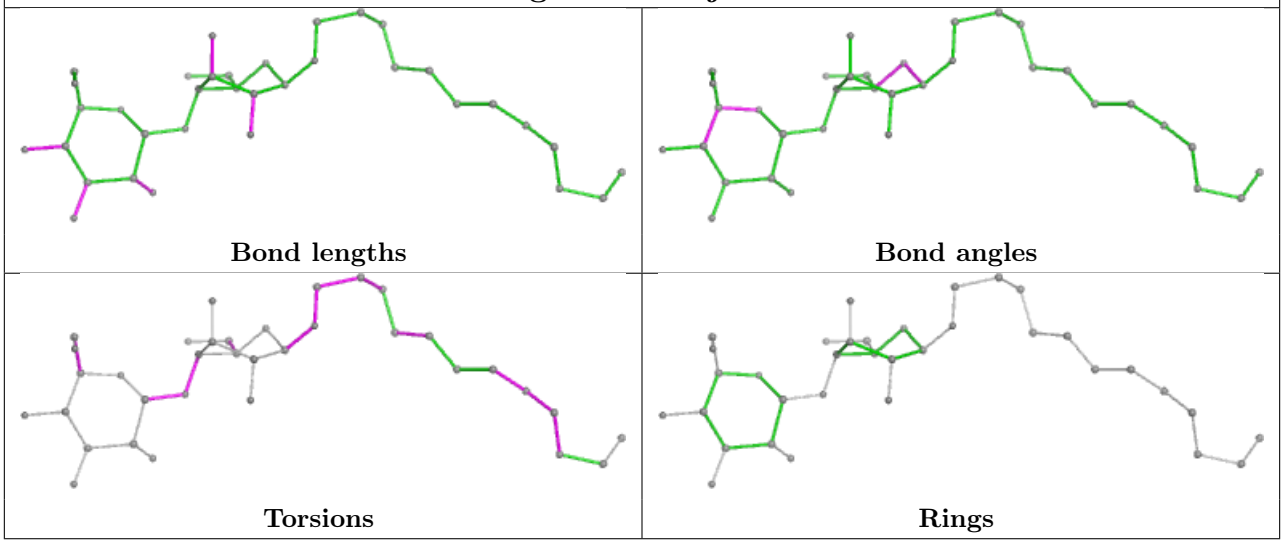


Rings

Ligand LHG f 206



Ligand LMT j 102



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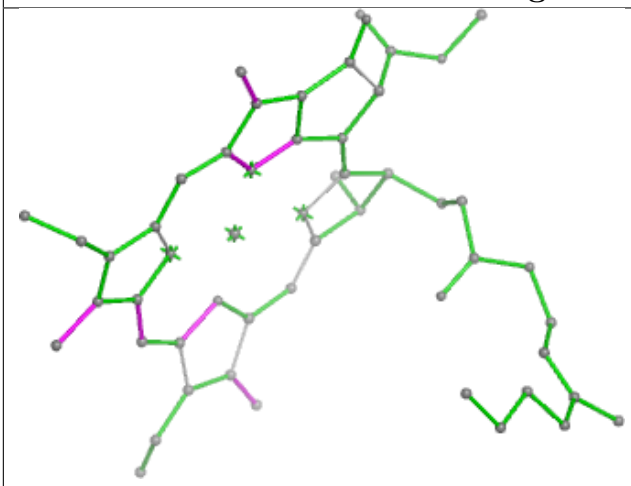
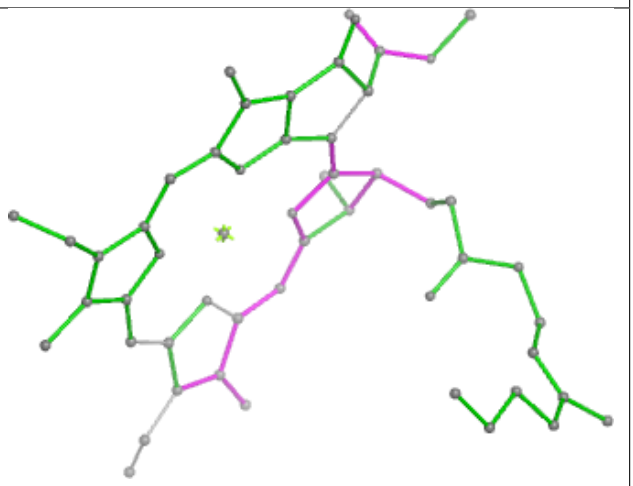
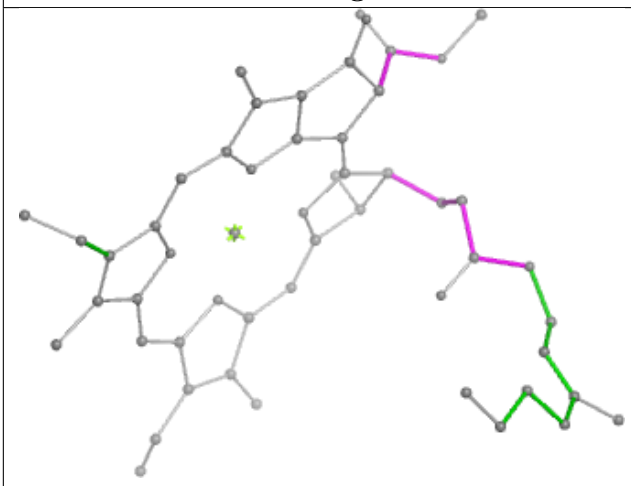


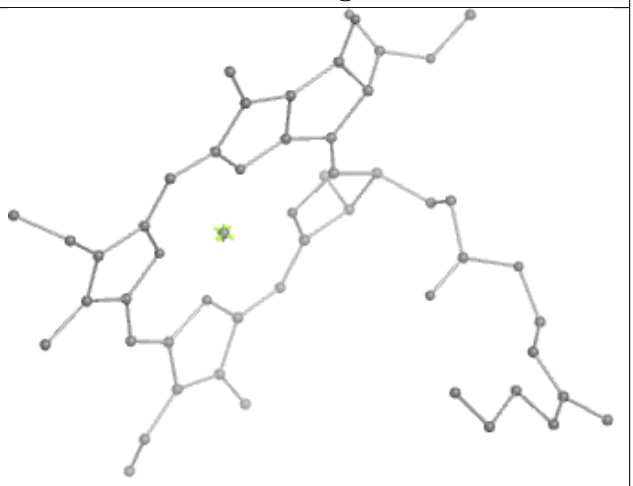
Bond lengths



Bond angles

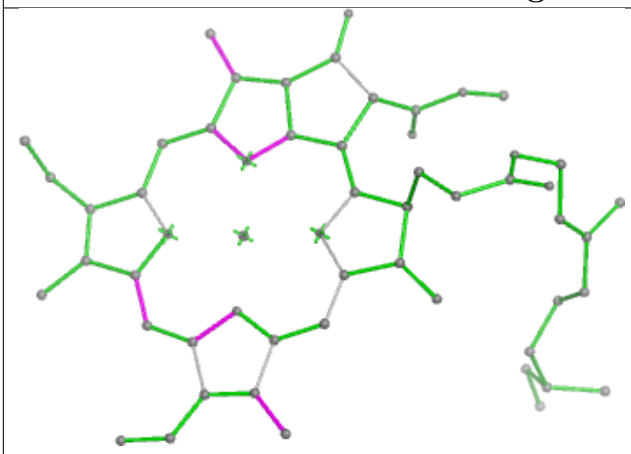


Torsions

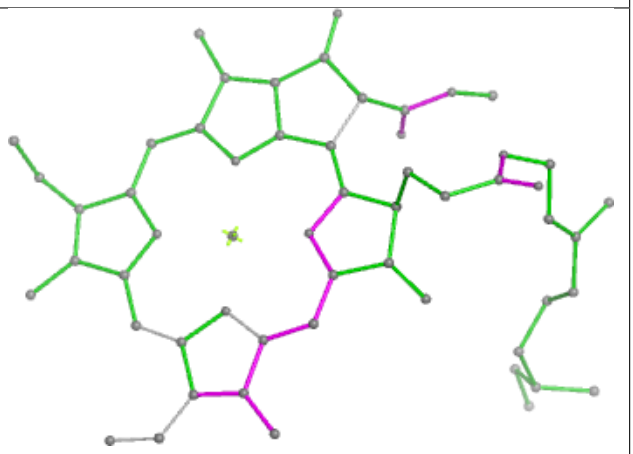


Rings

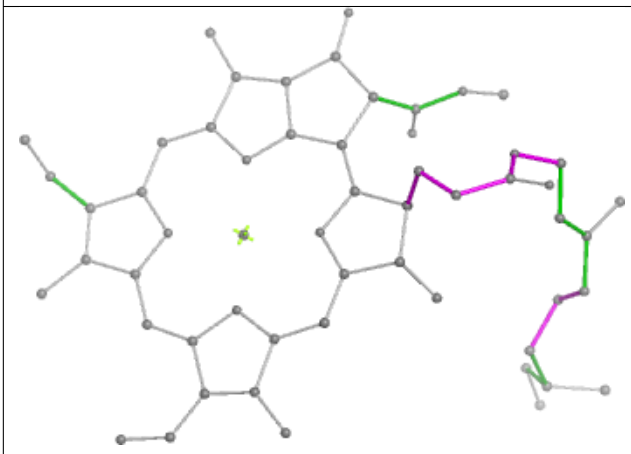
Ligand CLA b 811



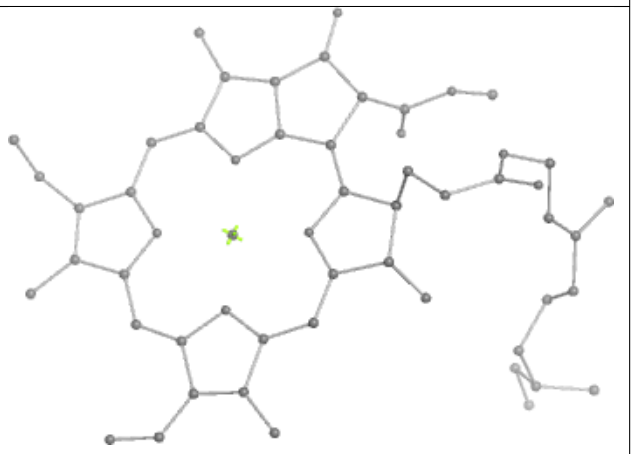
Bond lengths



Bond angles

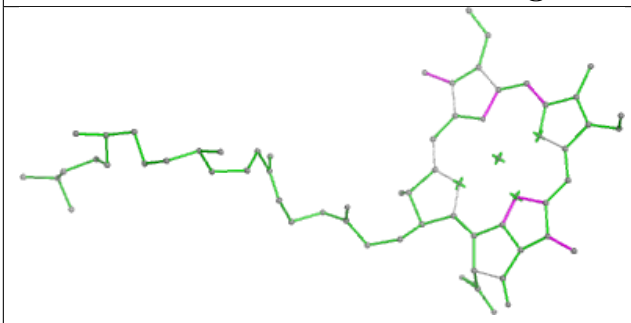


Torsions

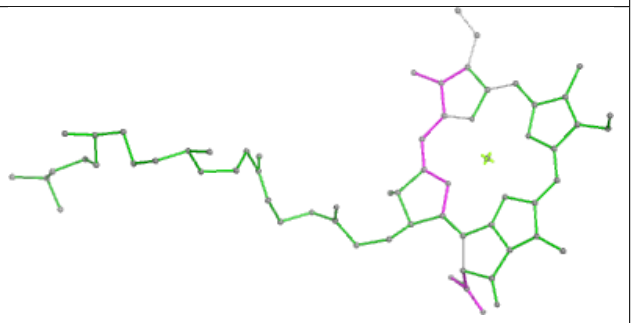


Rings

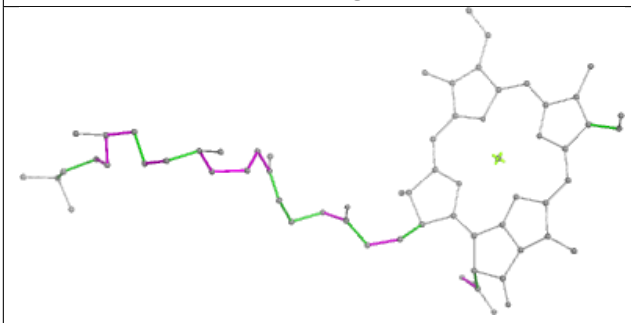
Ligand CLA b 814



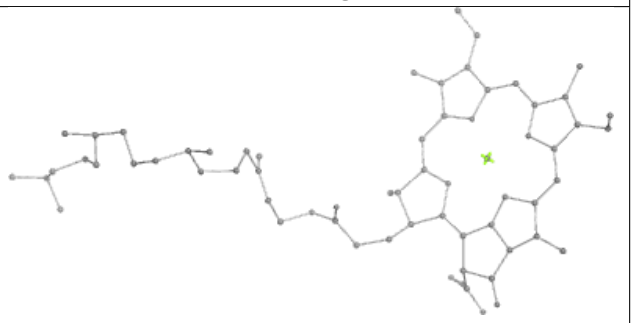
Bond lengths



Bond angles

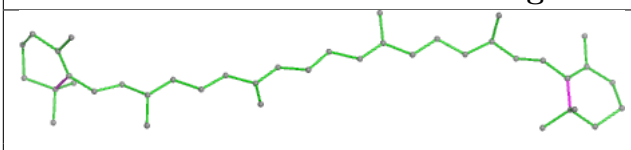


Torsions

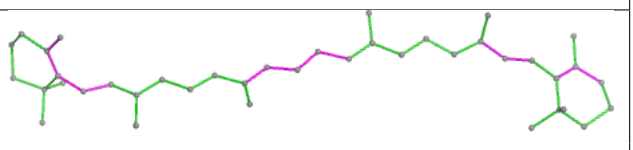


Rings

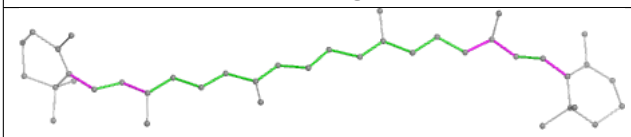
Ligand BCR a 847



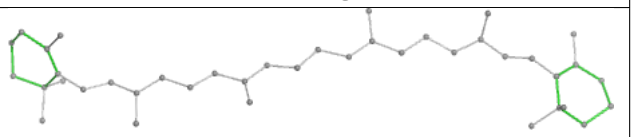
Bond lengths



Bond angles

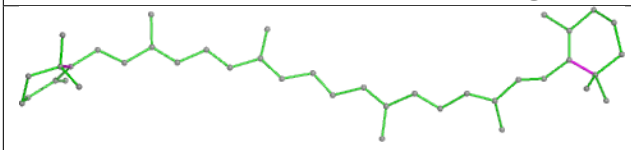


Torsions

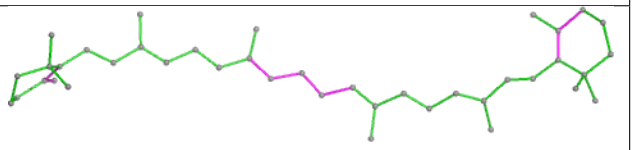


Rings

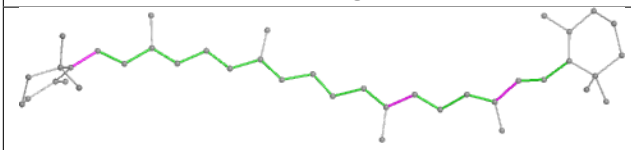
Ligand BCR b 845



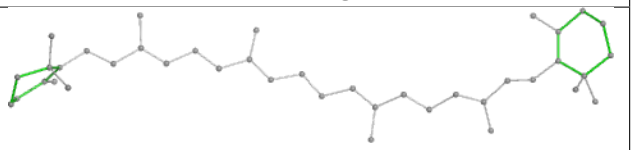
Bond lengths



Bond angles

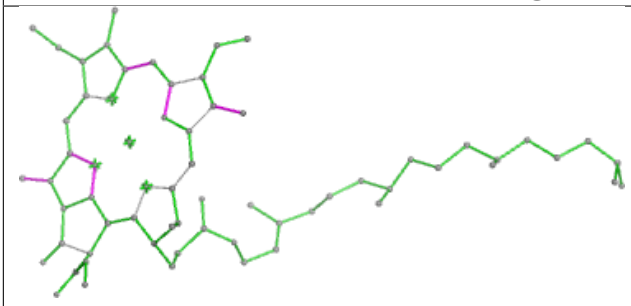


Torsions

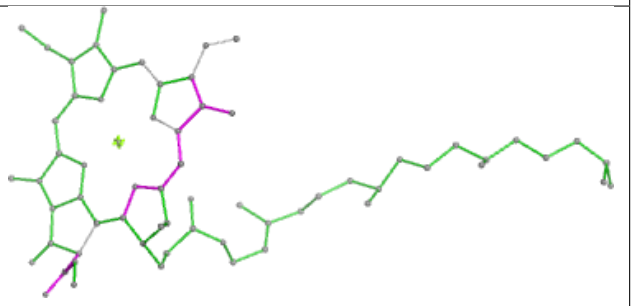


Rings

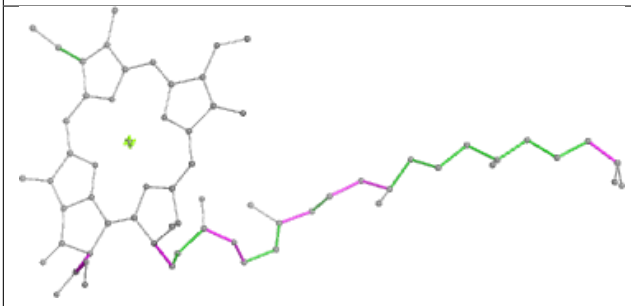
Ligand CLA a 834



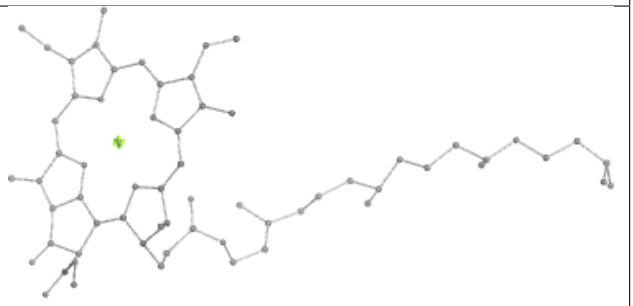
Bond lengths



Bond angles

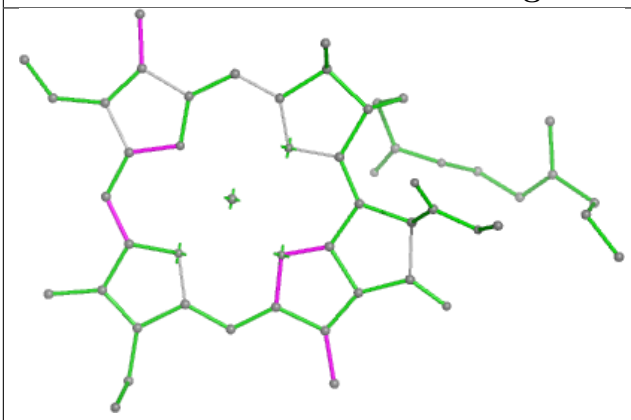


Torsions



Rings

Ligand CLA l 1503



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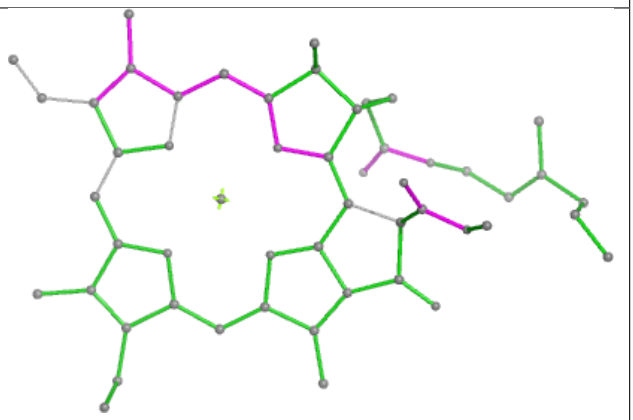
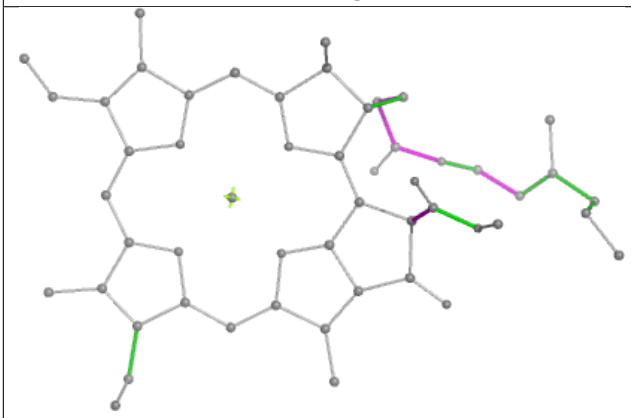
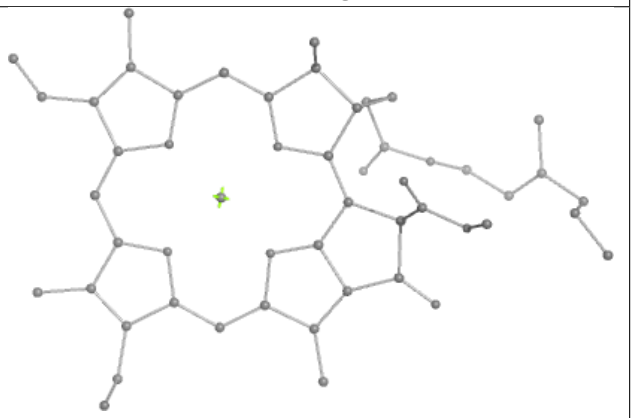


Bond angles

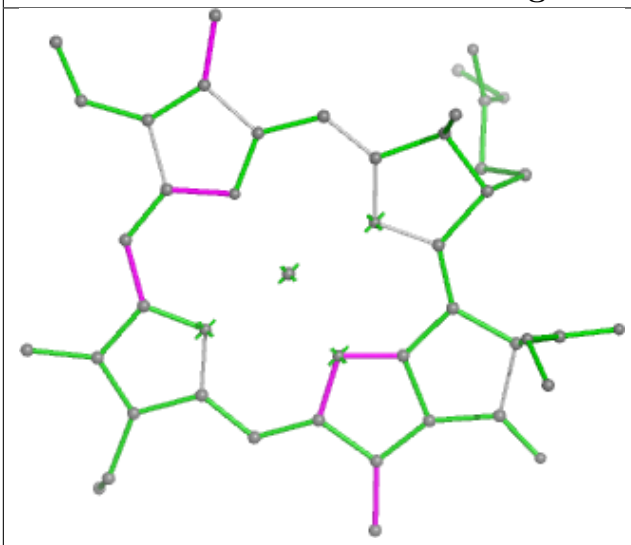


Torsions

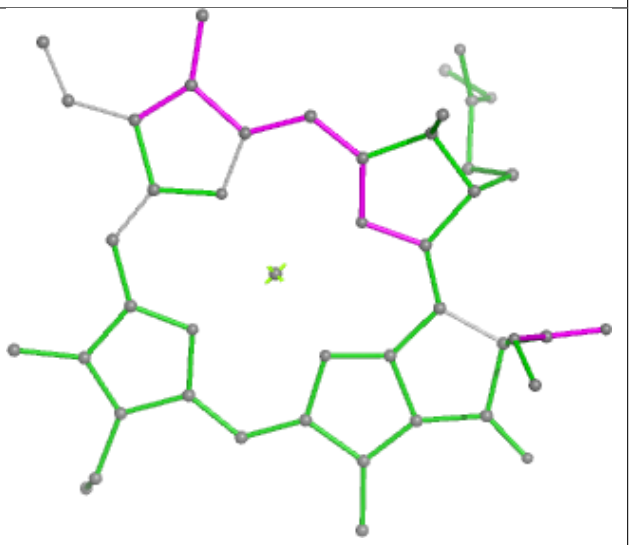


Rings

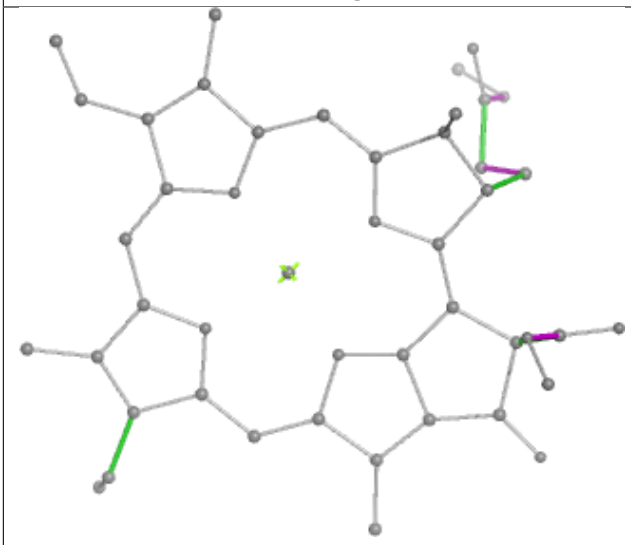
Ligand CLA a 815



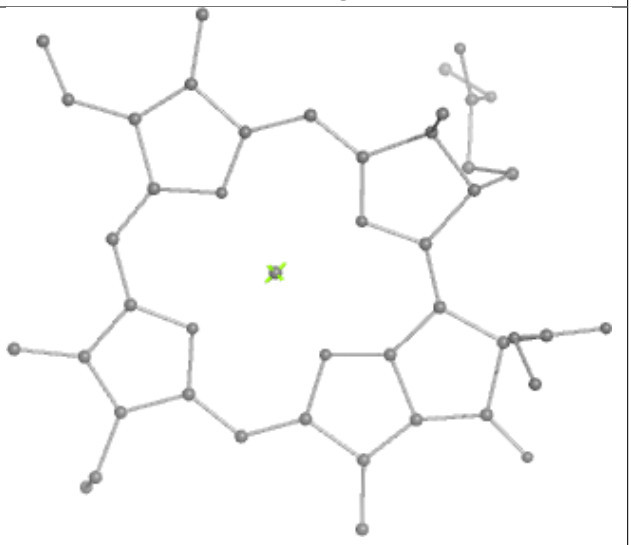
Bond lengths



Bond angles

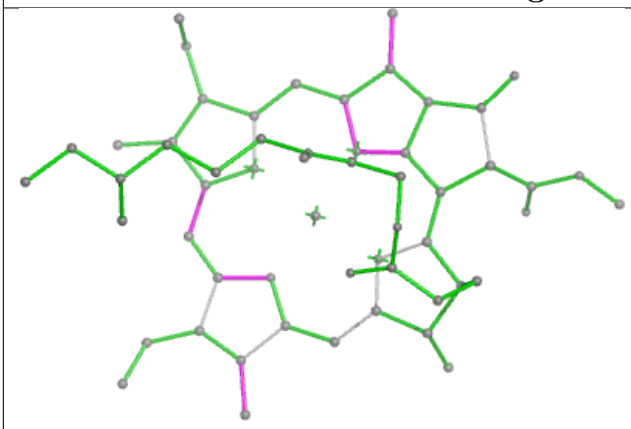


Torsions



Rings

Ligand CLA b 817



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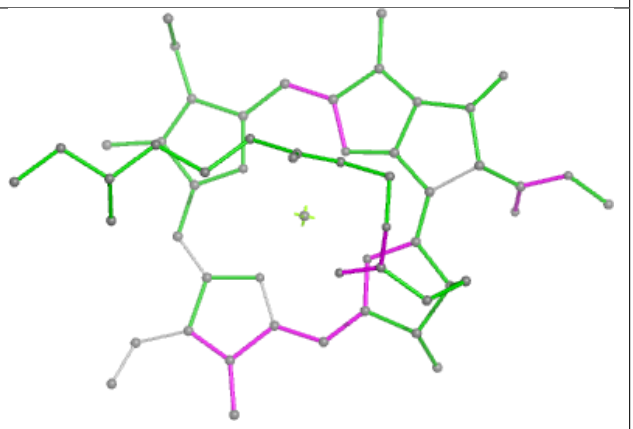
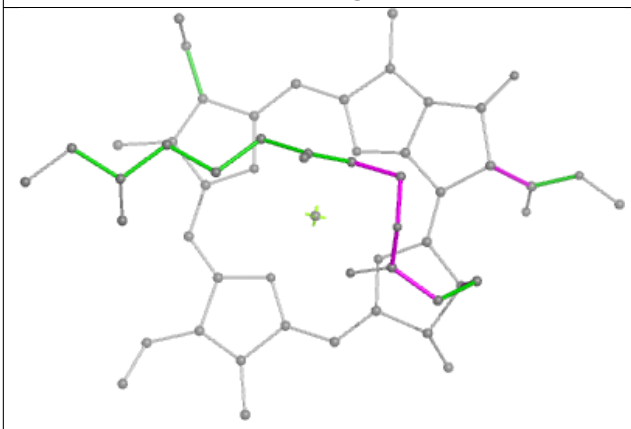
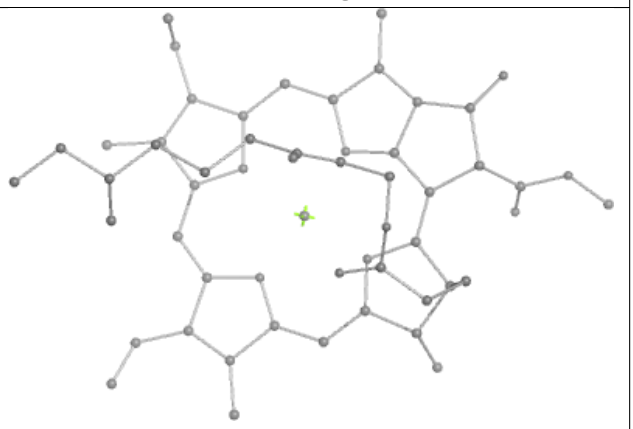


Bond angles

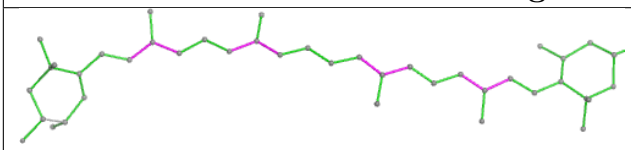


Torsions

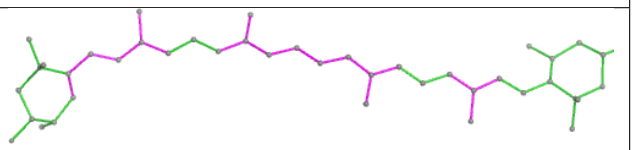


Rings

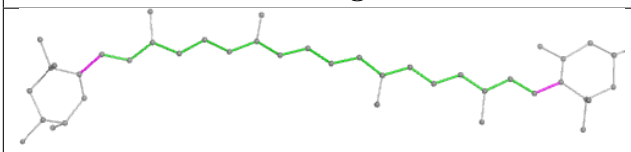
Ligand ZEX b 854



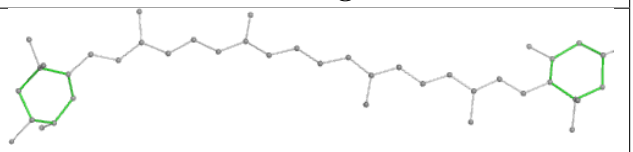
Bond lengths



Bond angles

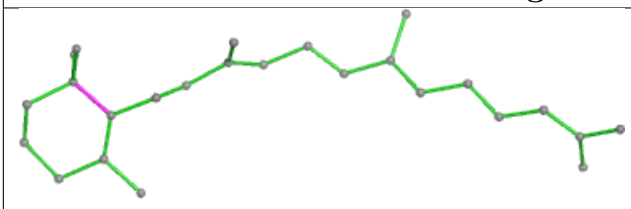


Torsions

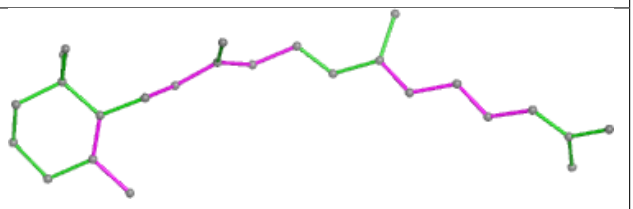


Rings

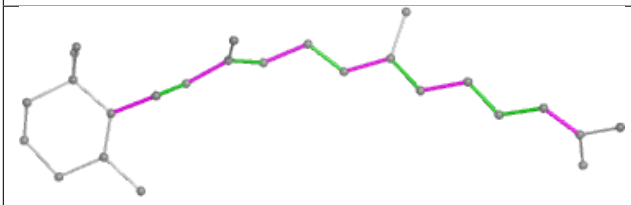
Ligand BCR a 848



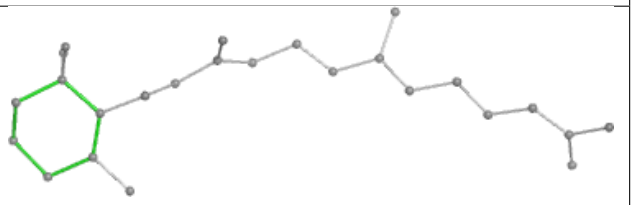
Bond lengths



Bond angles

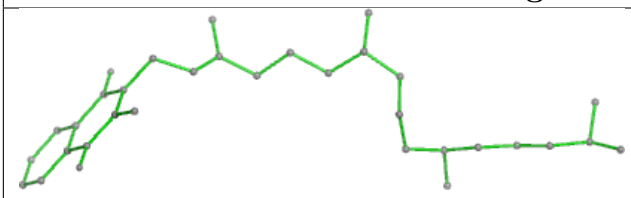


Torsions

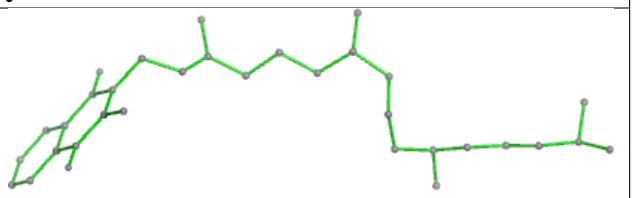


Rings

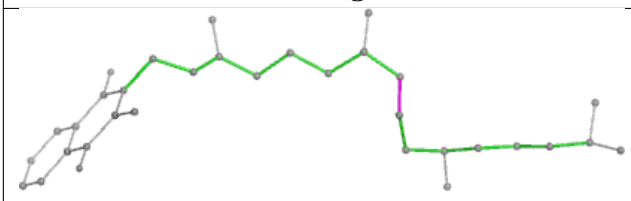
Ligand PQN a 843



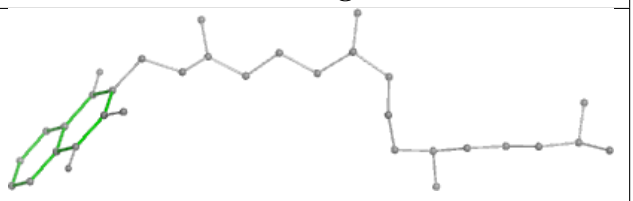
Bond lengths



Bond angles

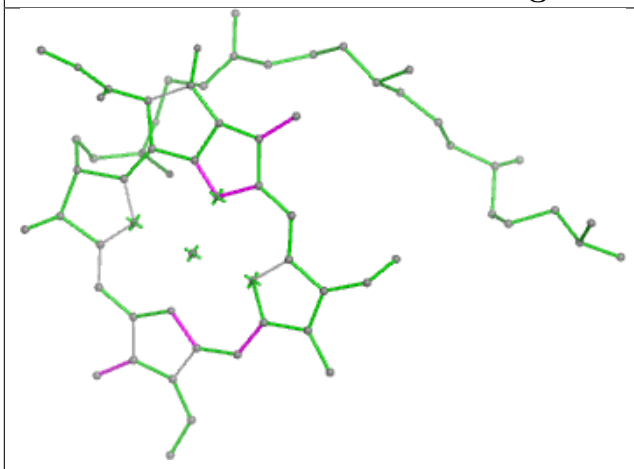


Torsions

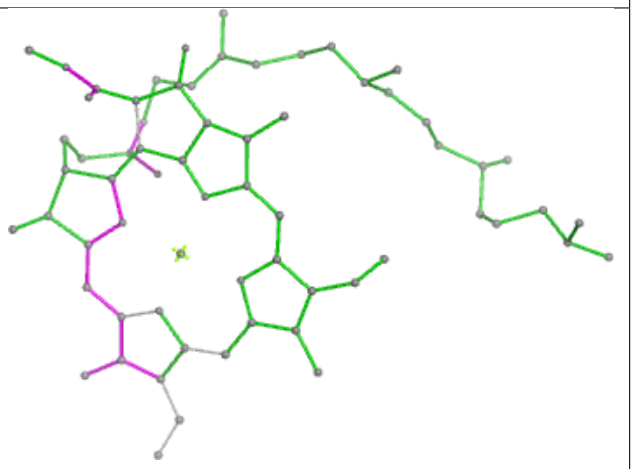


Rings

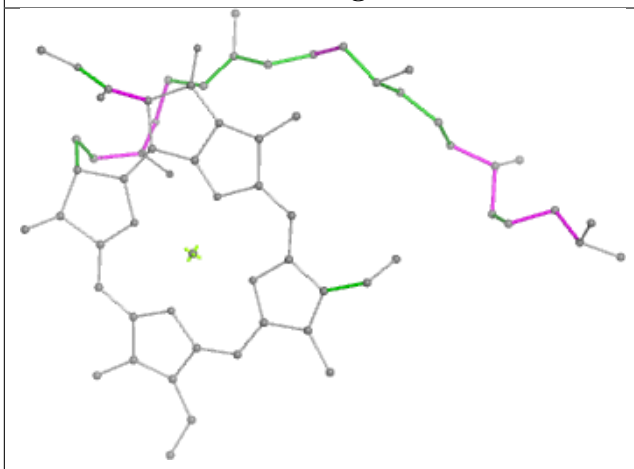
Ligand CLA a 829



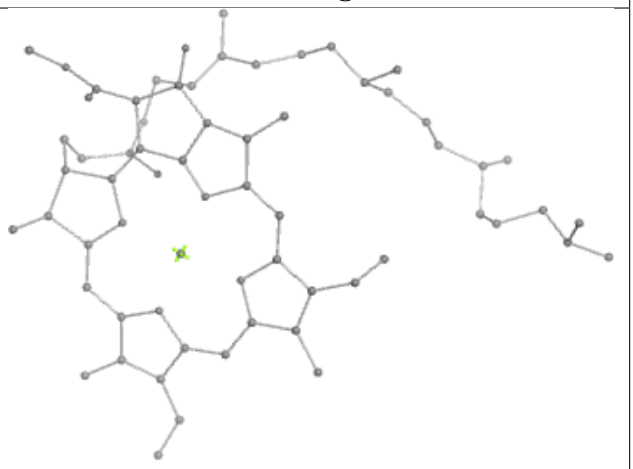
Bond lengths



Bond angles

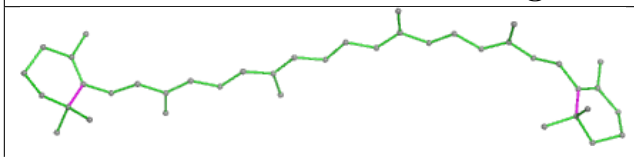


Torsions

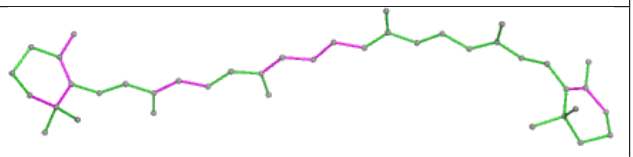


Rings

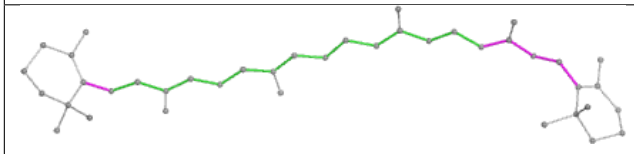
Ligand BCR b 847



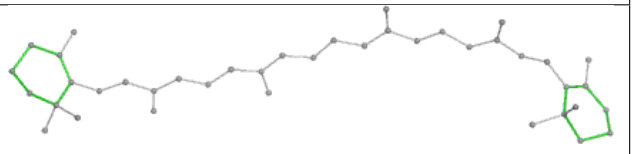
Bond lengths



Bond angles

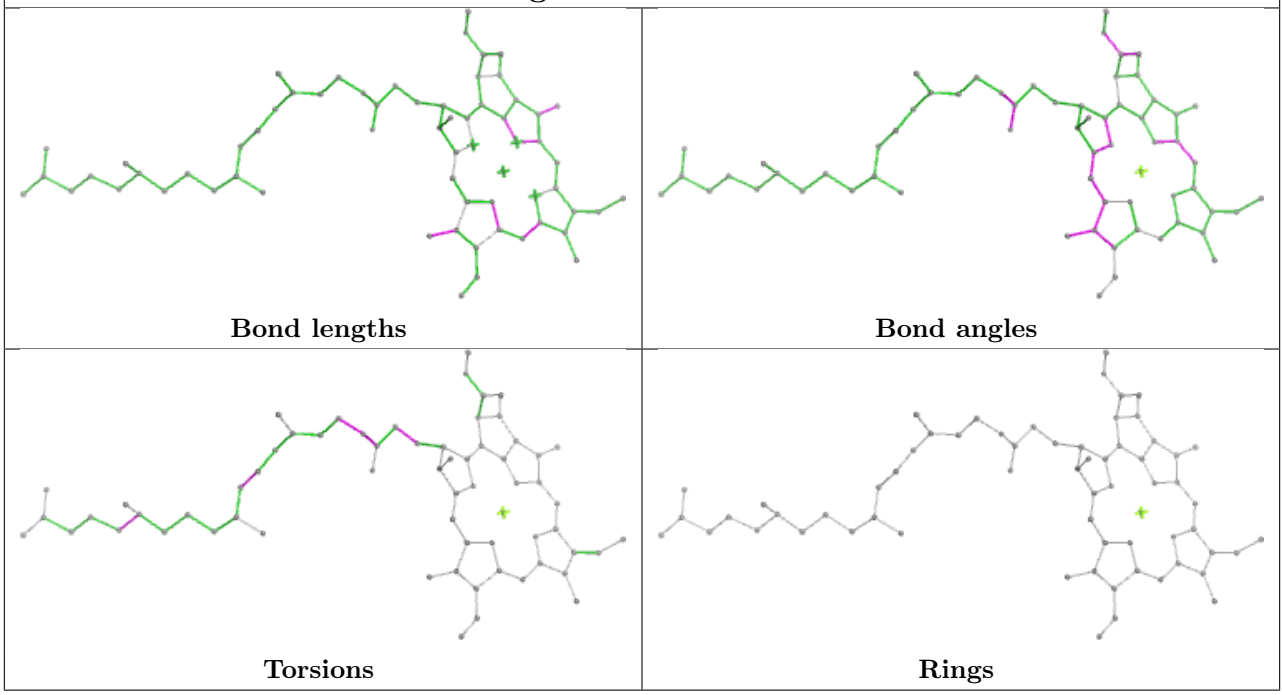


Torsions

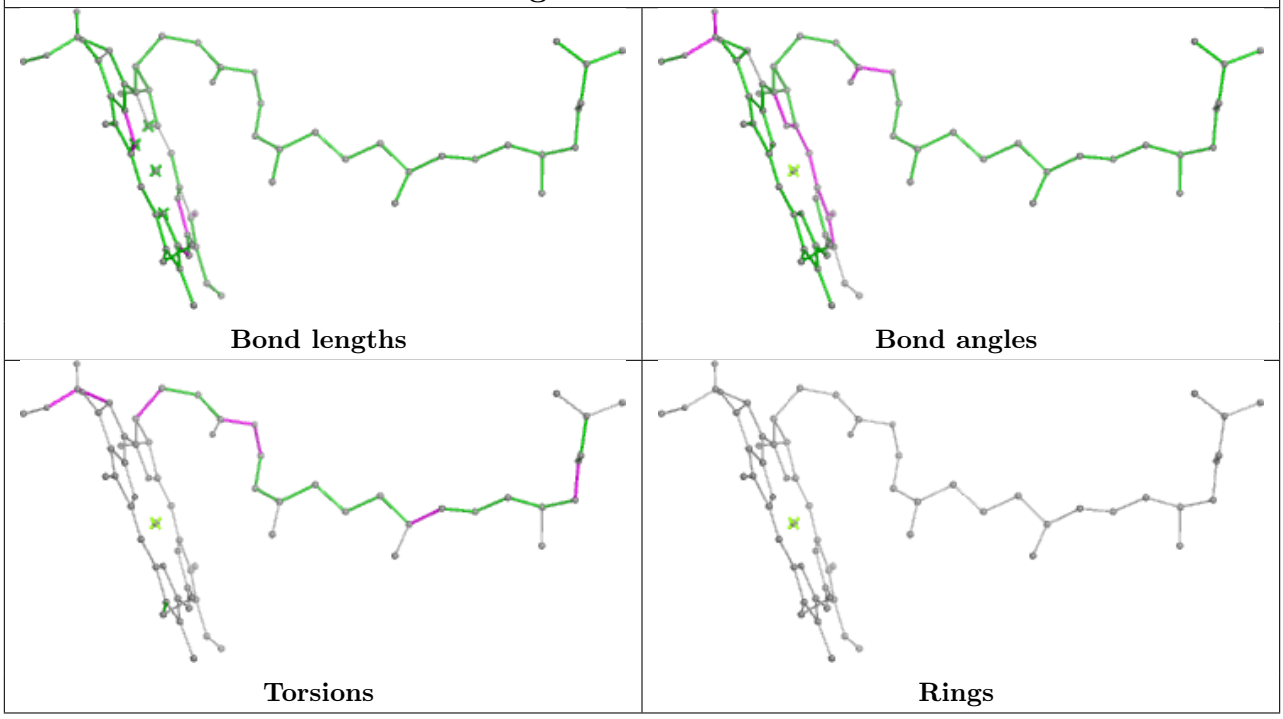


Rings

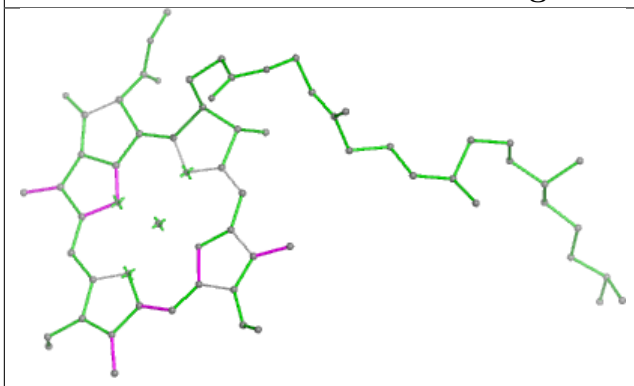
Ligand CLA a 854



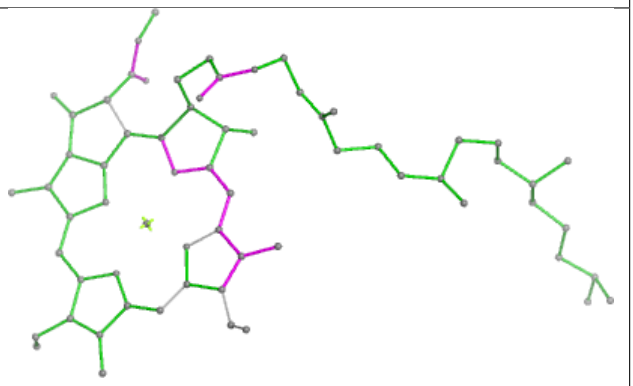
Ligand CLA a 822



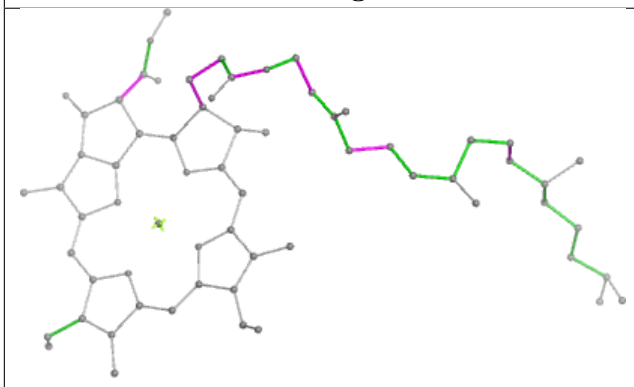
Ligand CLA a 802



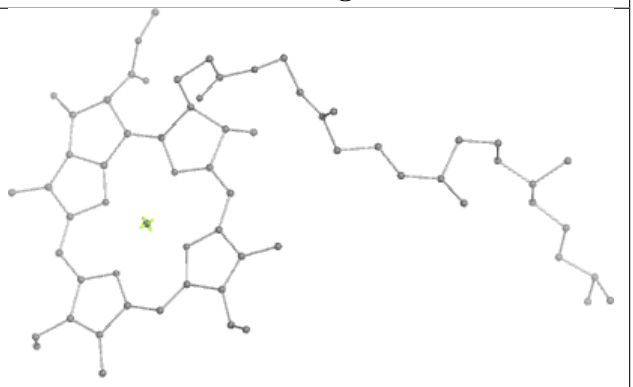
Bond lengths



Bond angles

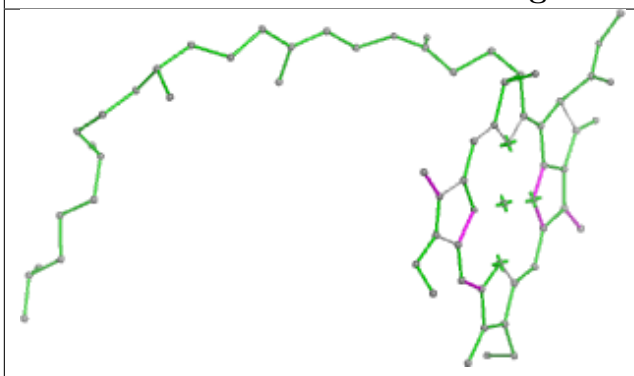


Torsions

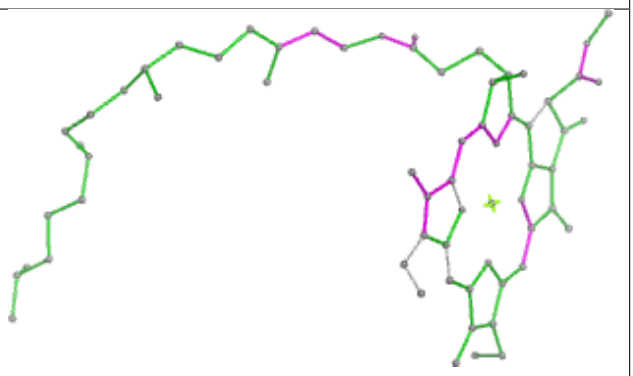


Rings

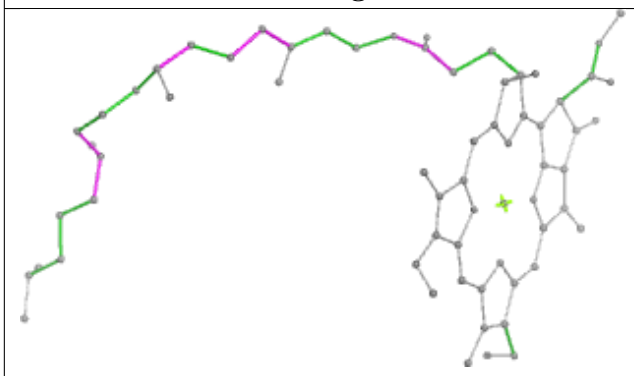
Ligand CLA a 835



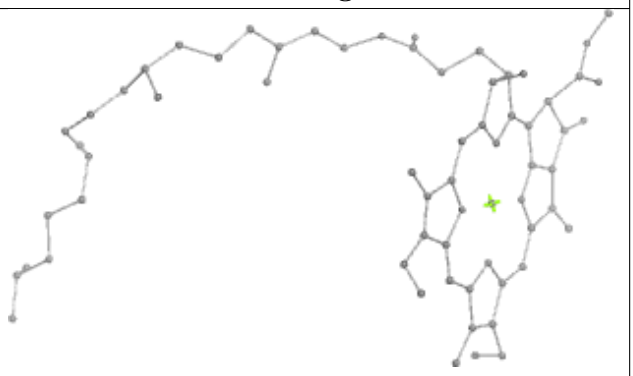
Bond lengths



Bond angles

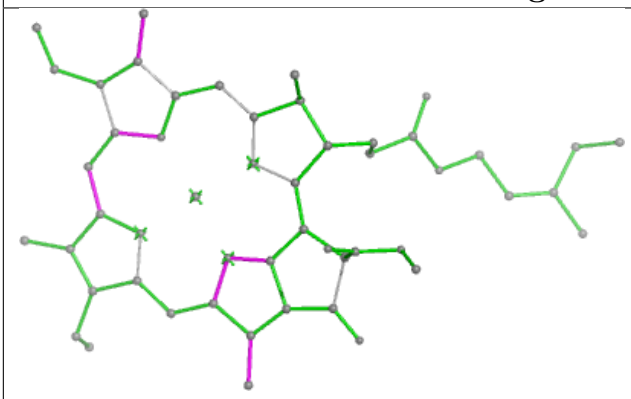


Torsions

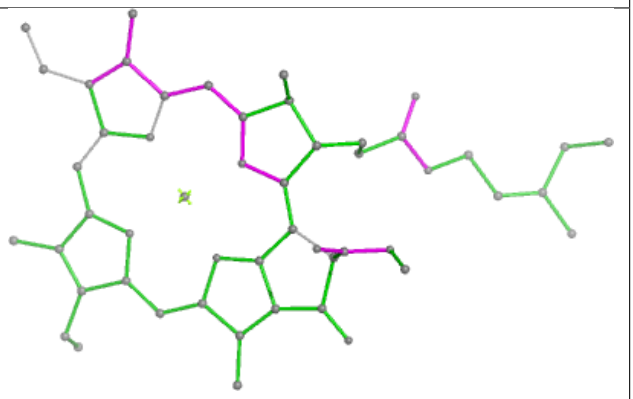


Rings

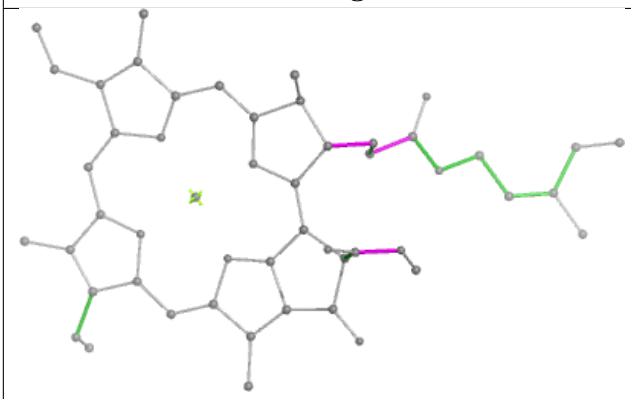
Ligand CLA a 809



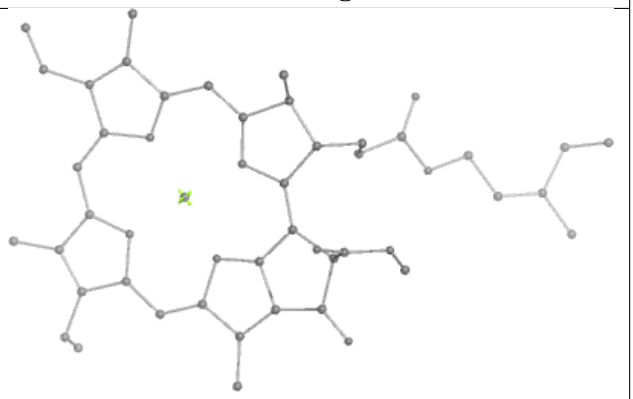
Bond lengths



Bond angles

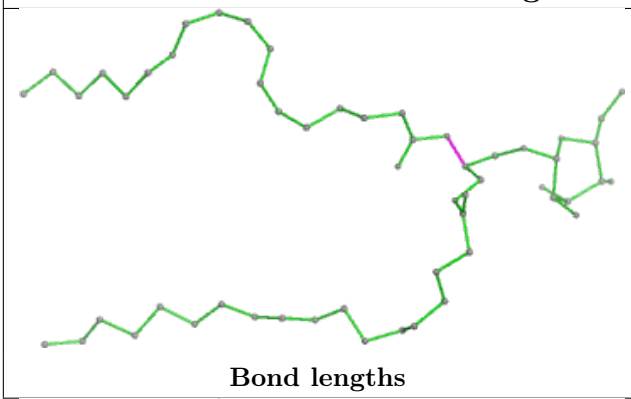


Torsions

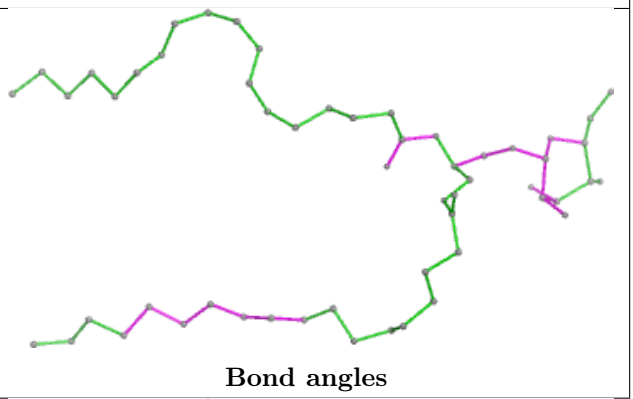


Rings

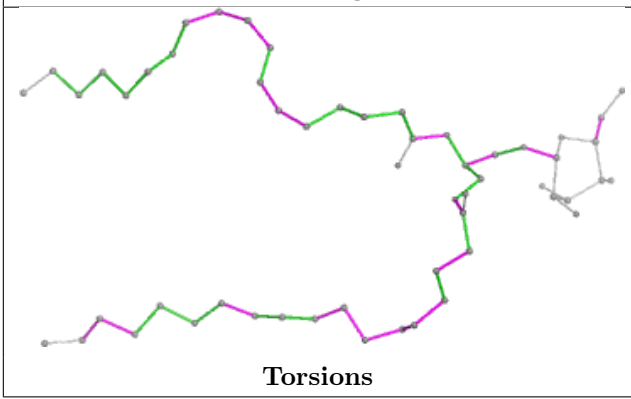
Ligand LMG b 852



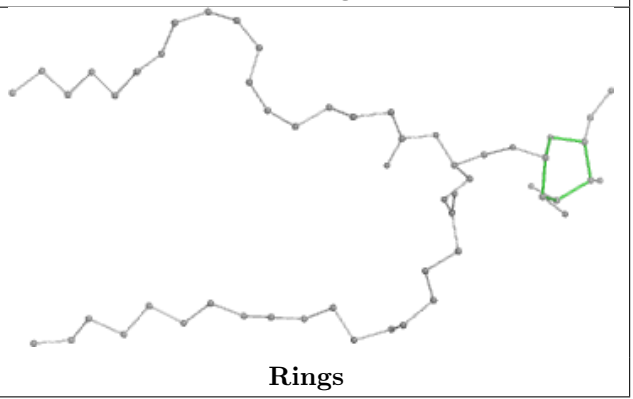
Bond lengths



Bond angles

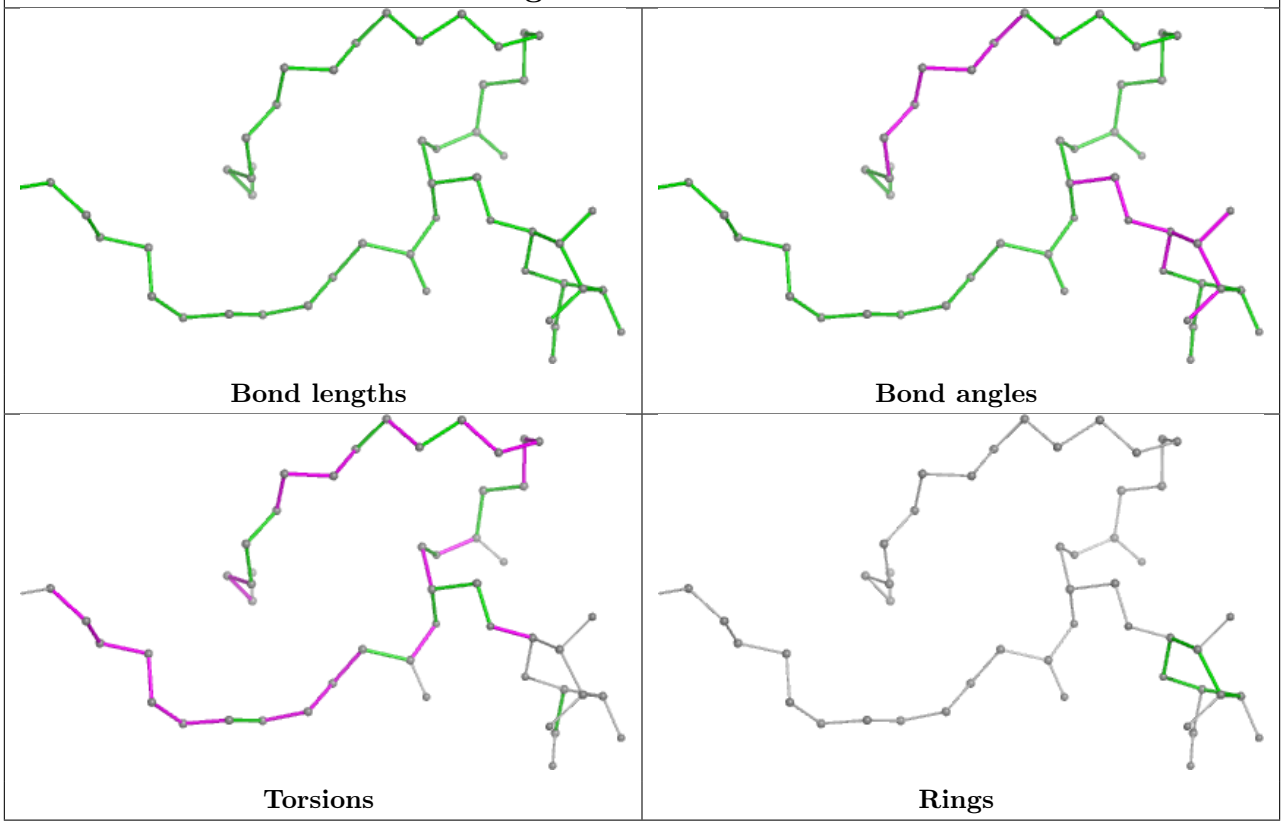


Torsions

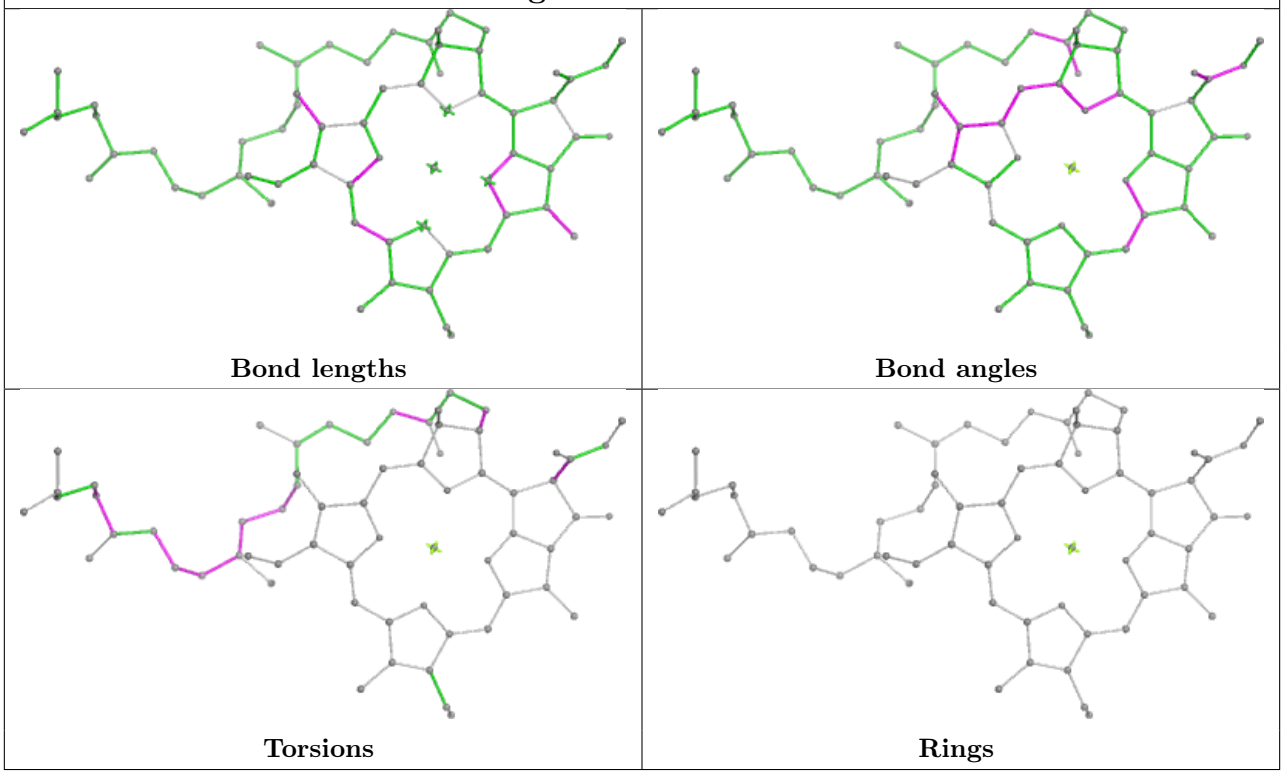


Rings

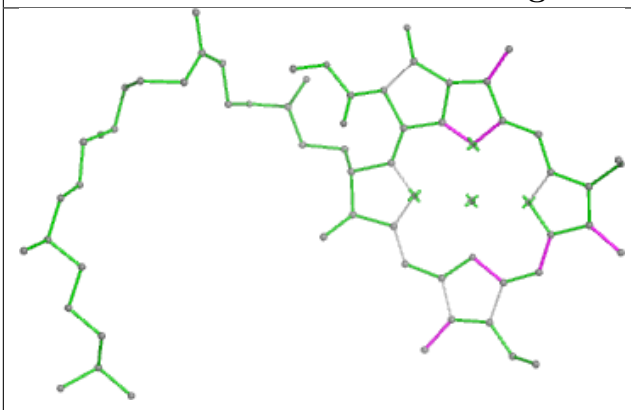
Ligand LMG a 850



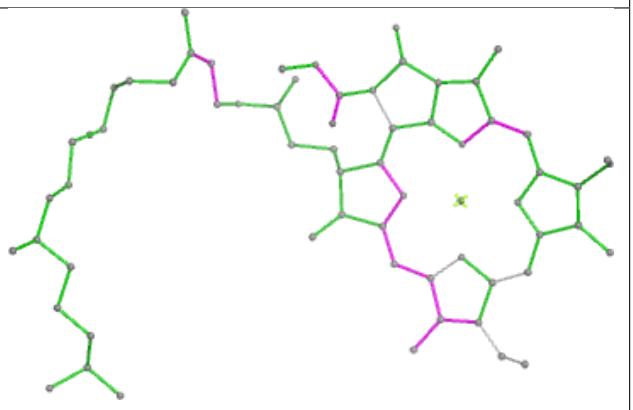
Ligand CLA b 819



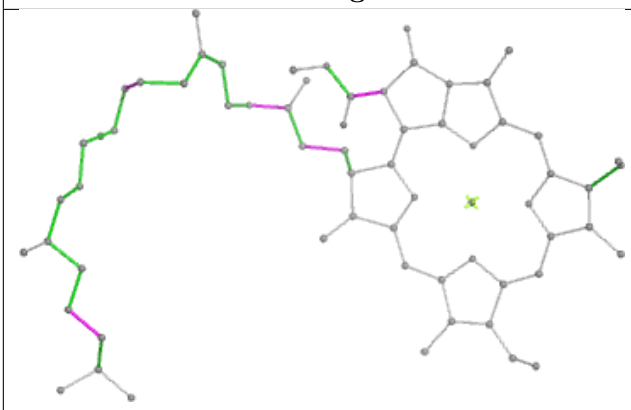
Ligand CLA a 803



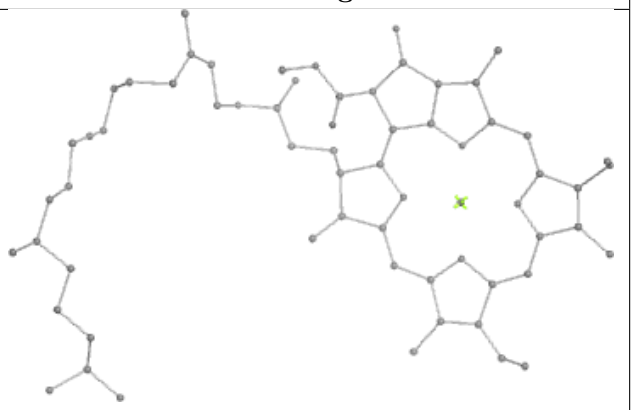
Bond lengths



Bond angles

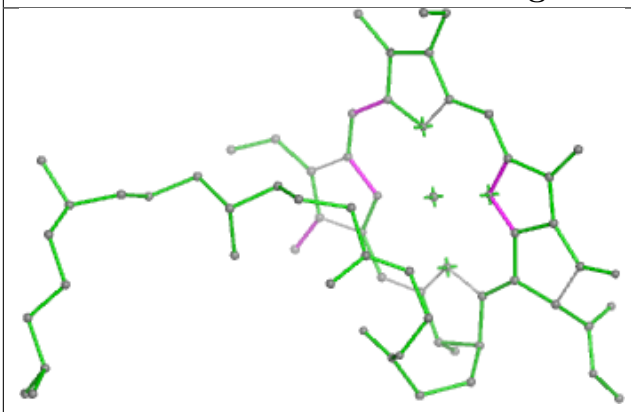


Torsions

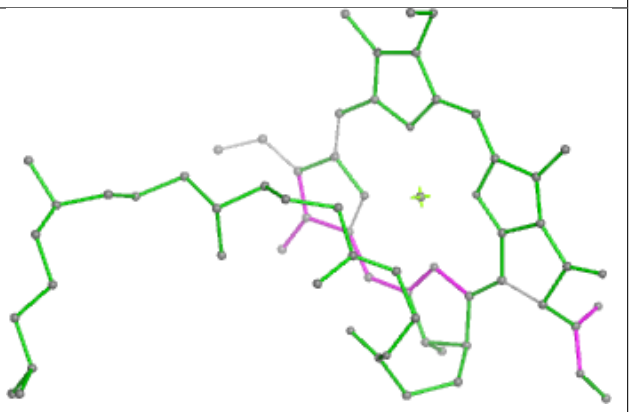


Rings

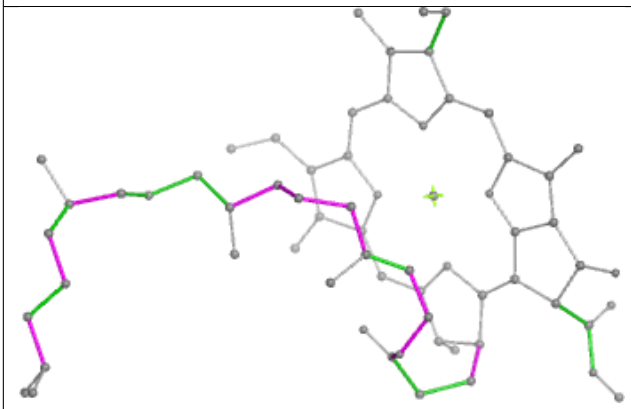
Ligand CLA a 855



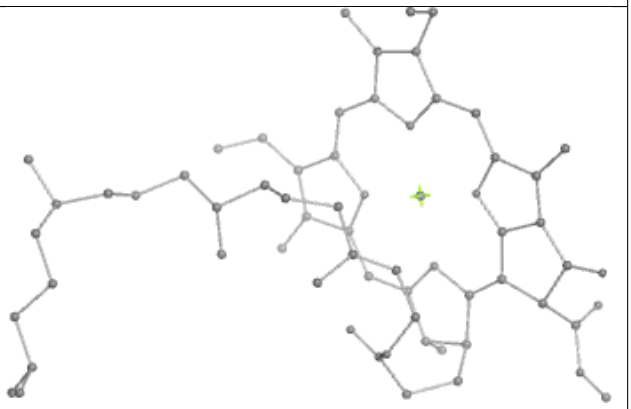
Bond lengths



Bond angles

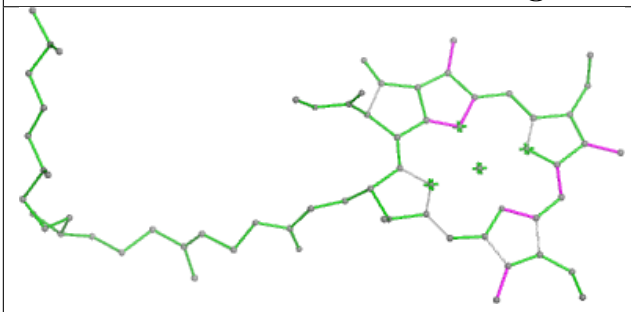


Torsions

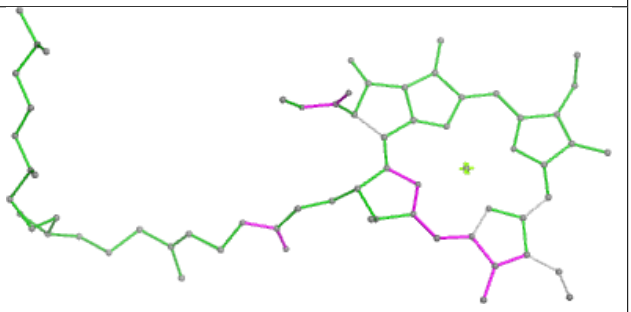


Rings

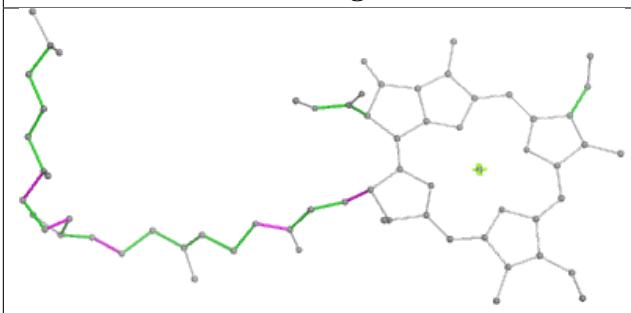
Ligand CLA b 827



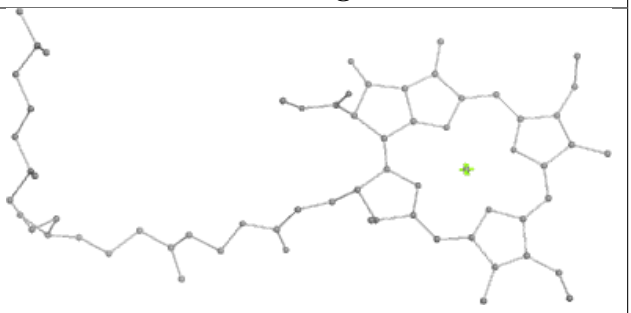
Bond lengths



Bond angles

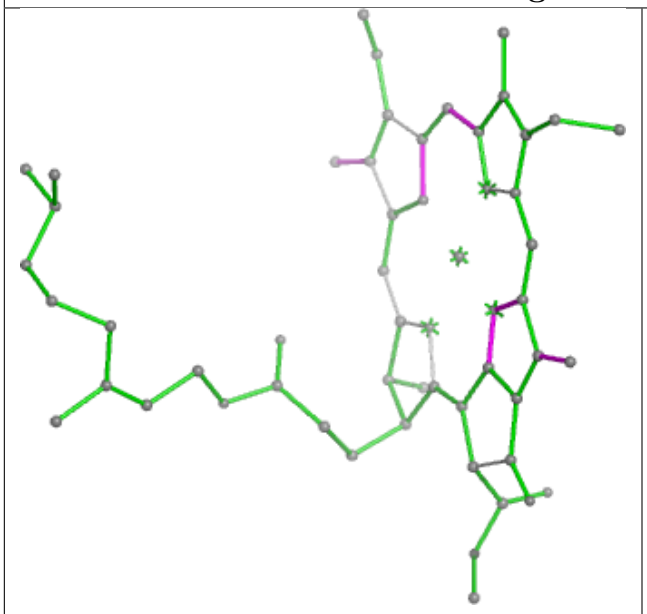


Torsions

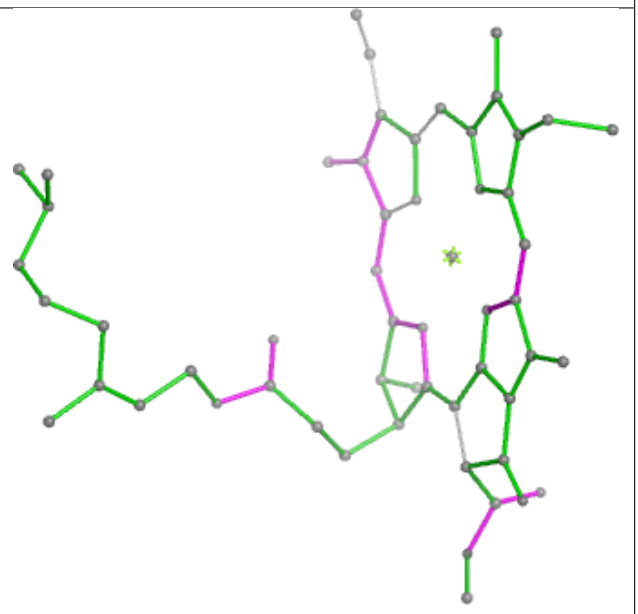


Rings

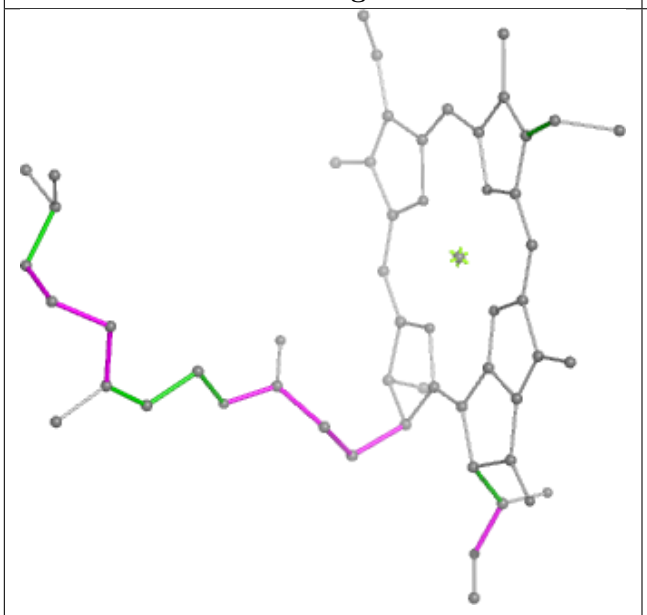
Ligand CLA b 816



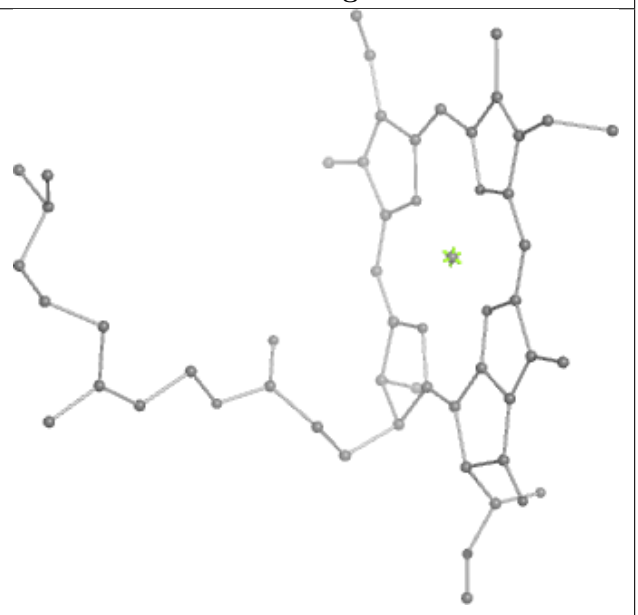
Bond lengths



Bond angles

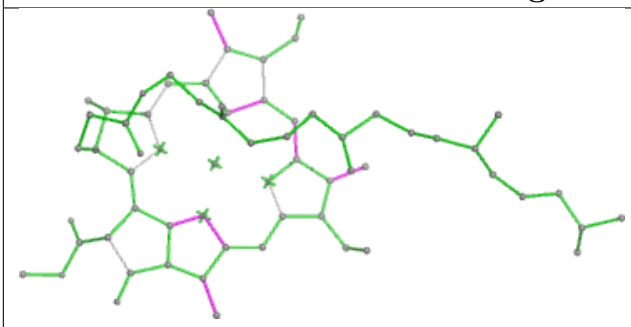


Torsions

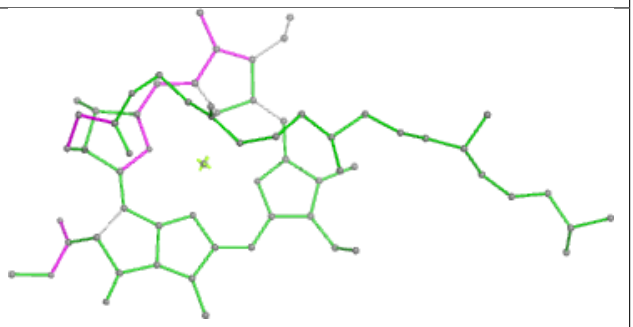


Rings

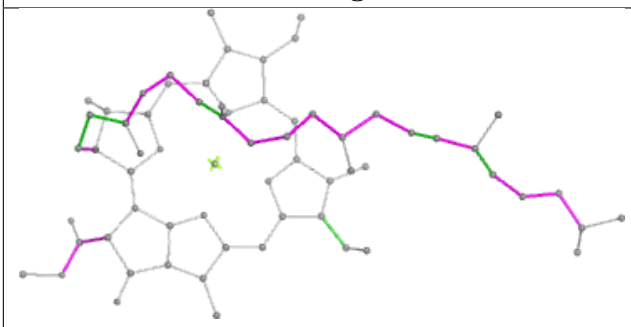
Ligand CLA a 818



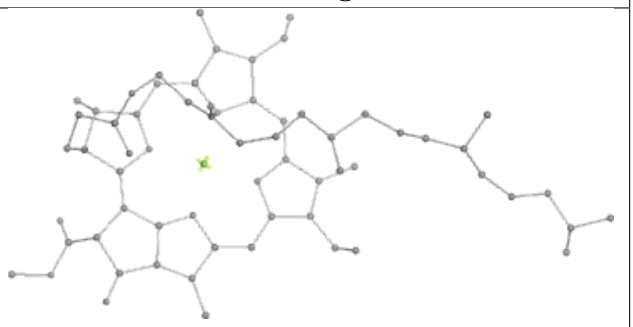
Bond lengths



Bond angles

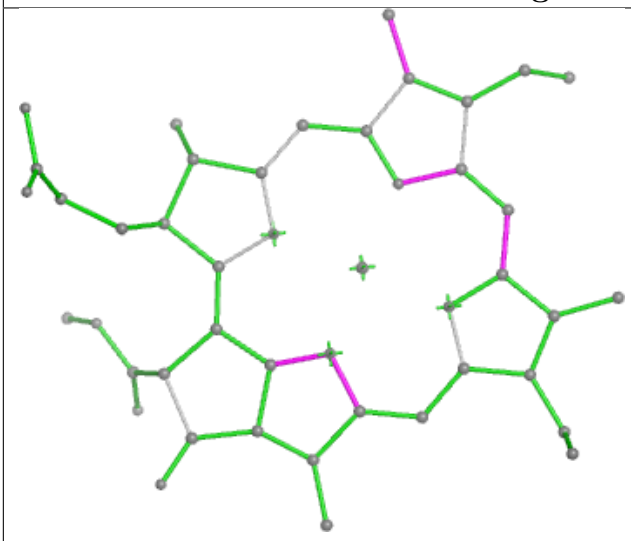


Torsions

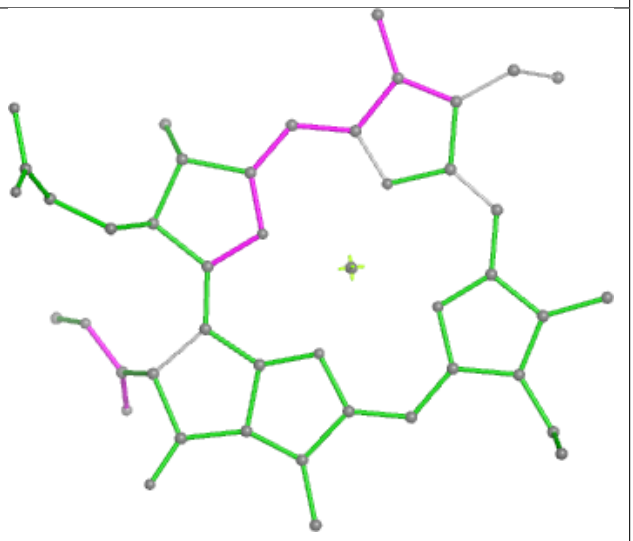


Rings

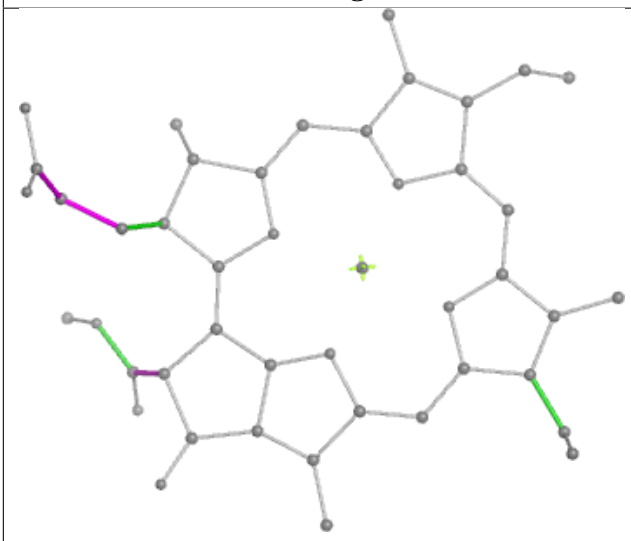
Ligand CLA f 204



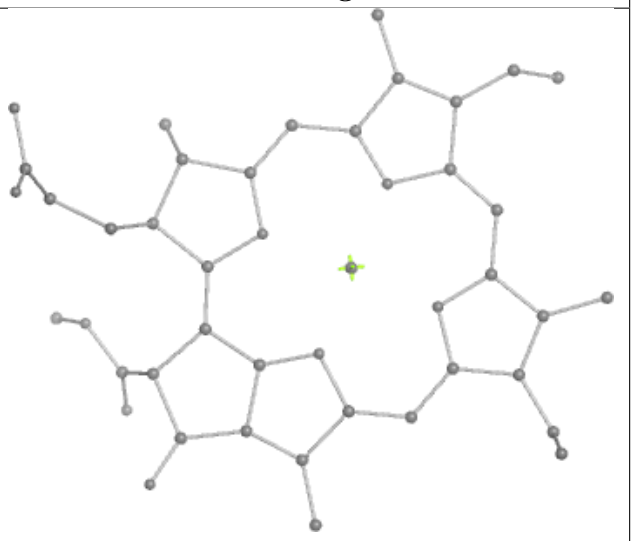
Bond lengths



Bond angles

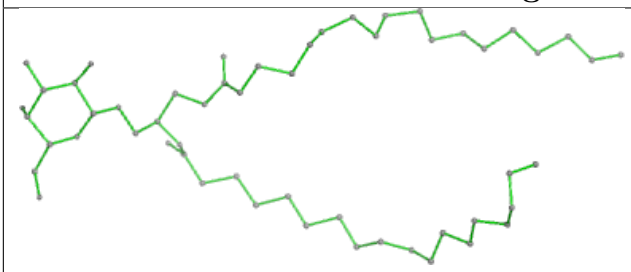


Torsions

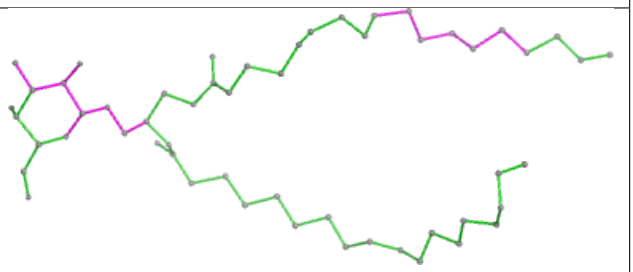


Rings

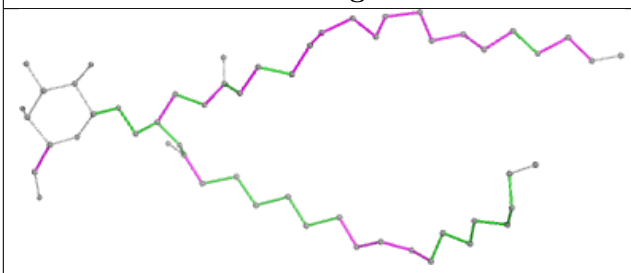
Ligand LMG b 850



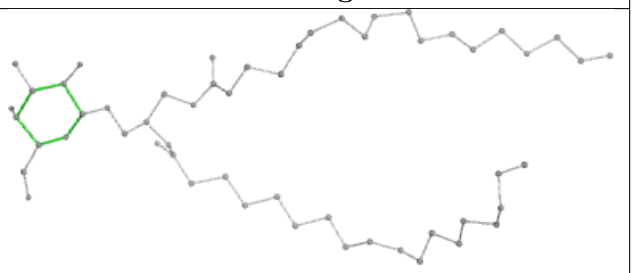
Bond lengths



Bond angles

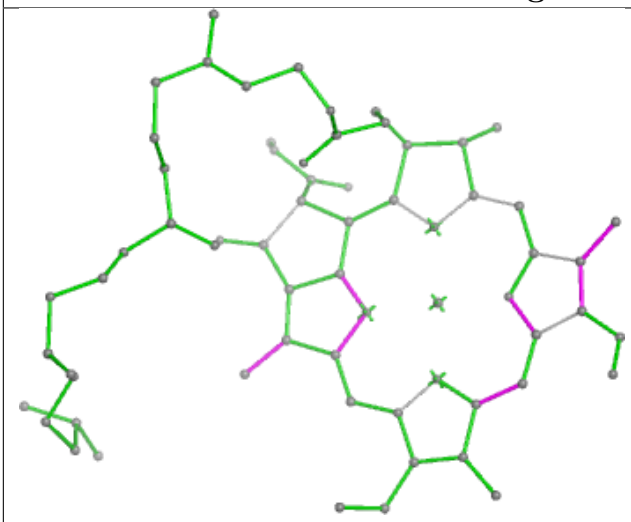


Torsions

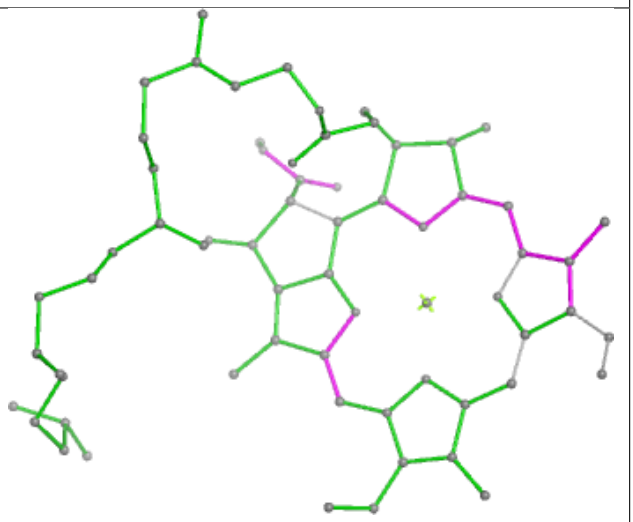


Rings

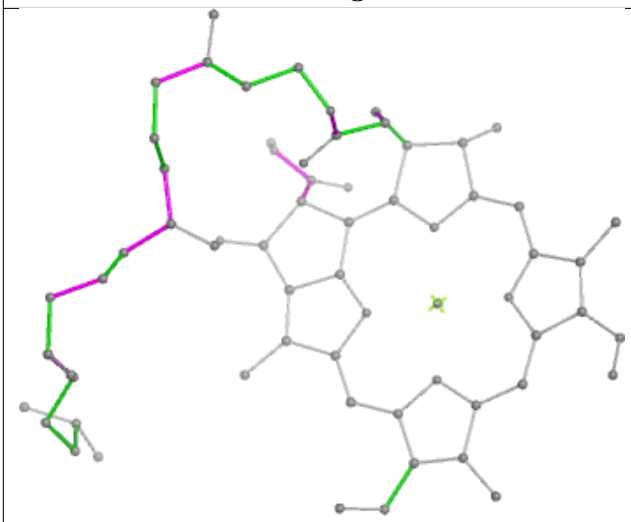
Ligand CLA b 833



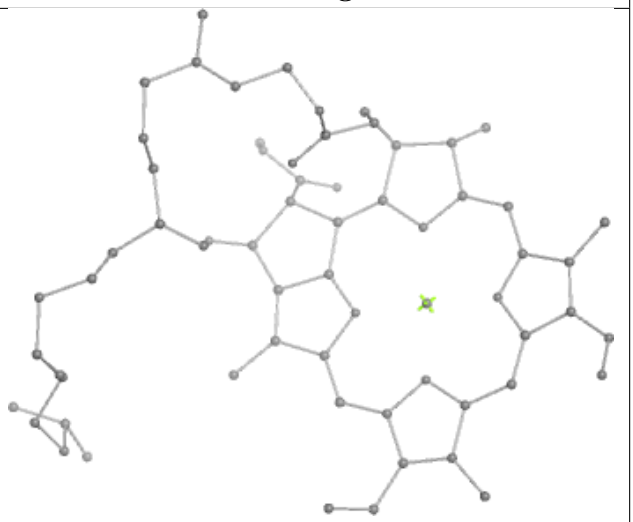
Bond lengths



Bond angles

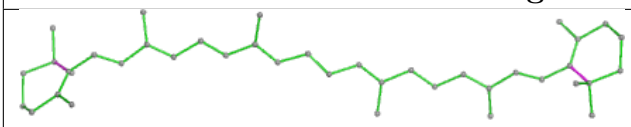


Torsions



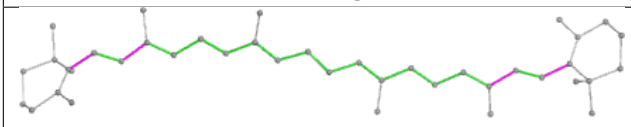
Rings

Ligand BCR a 844



Bond lengths

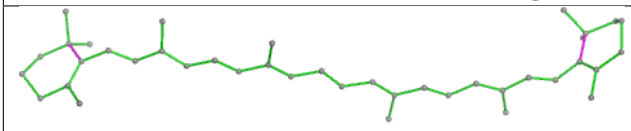
Bond angles



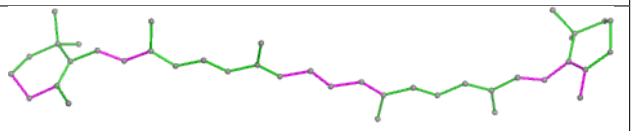
Torsions

Rings

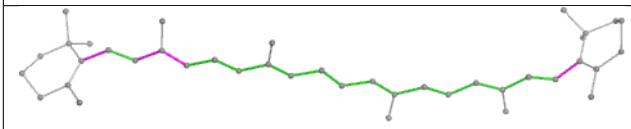
Ligand BCR a 845



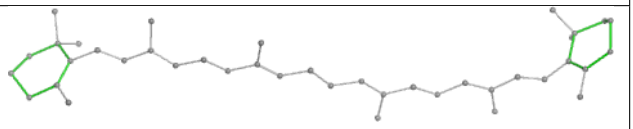
Bond lengths



Bond angles

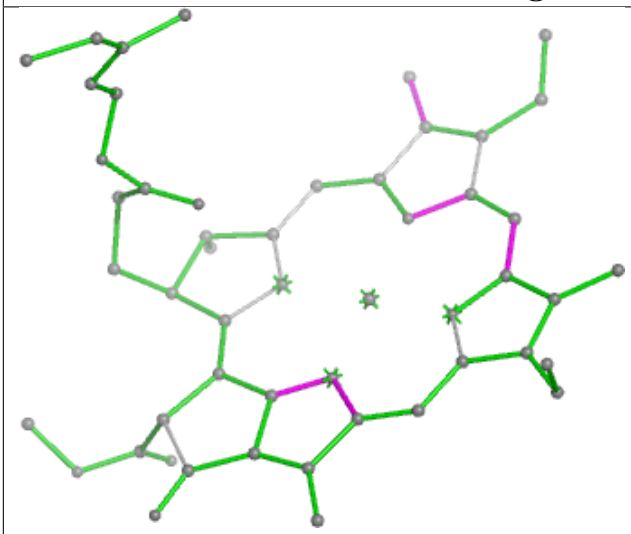


Torsions

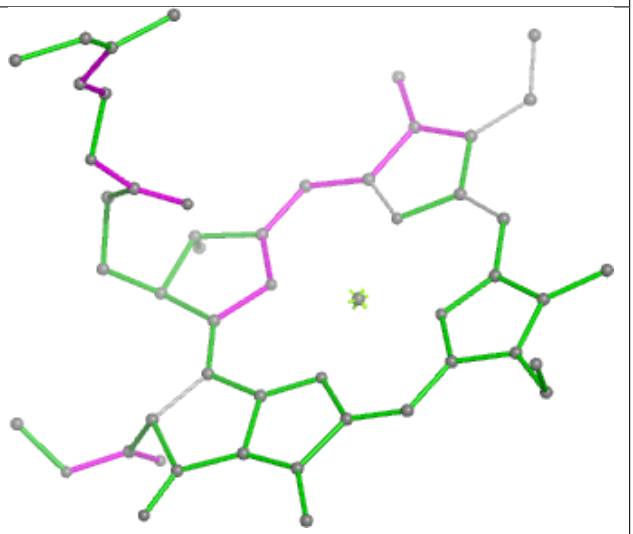


Rings

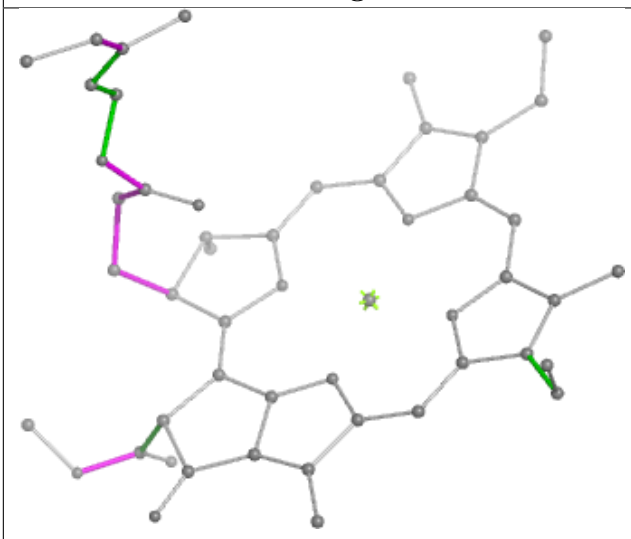
Ligand CLA b 831



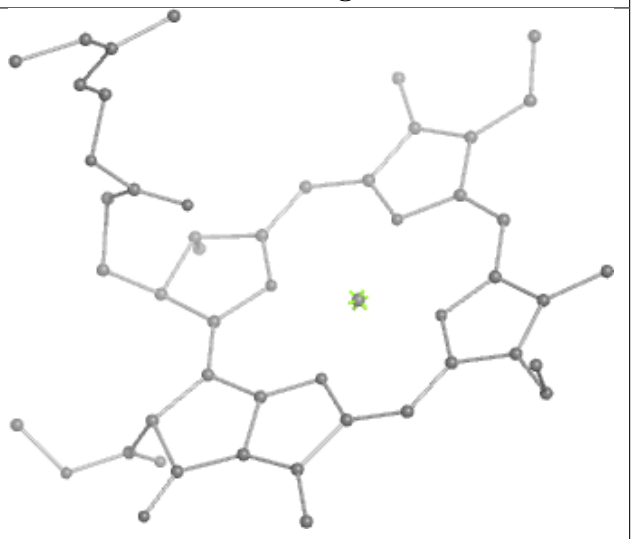
Bond lengths



Bond angles

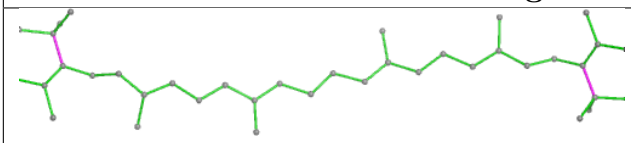


Torsions

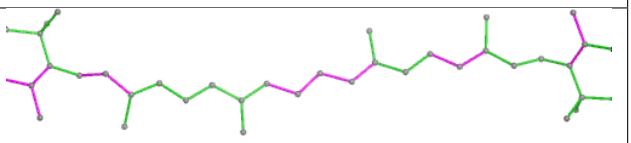


Rings

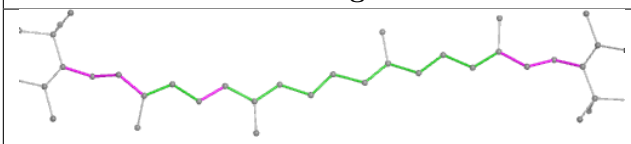
Ligand BCR b 844



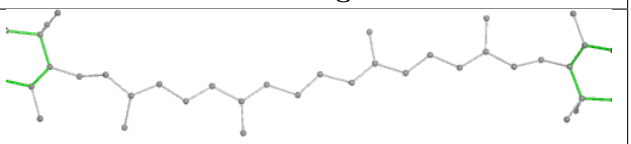
Bond lengths



Bond angles

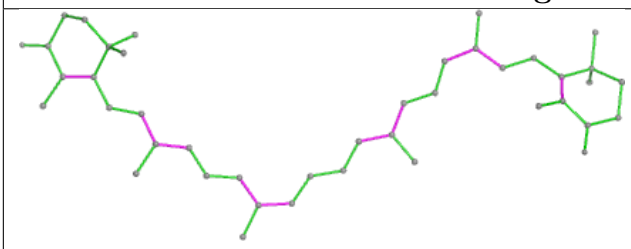


Torsions

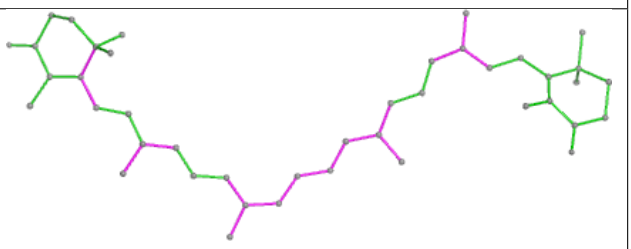


Rings

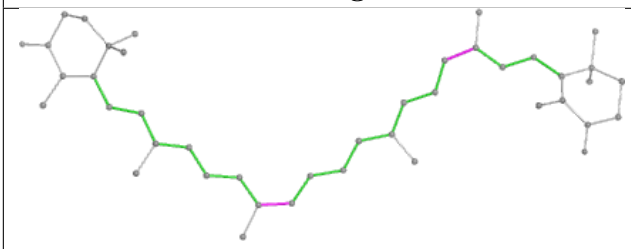
Ligand 45D a 856



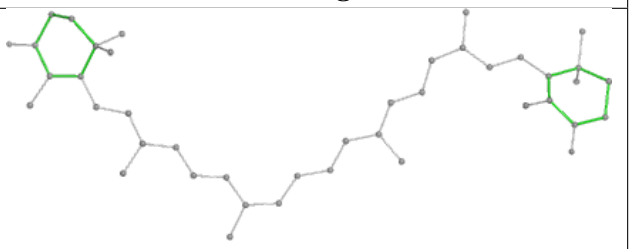
Bond lengths



Bond angles

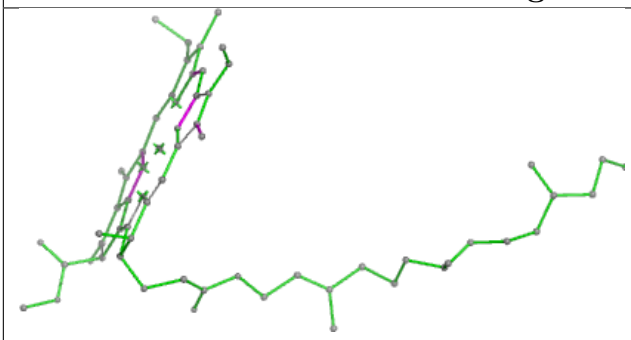


Torsions

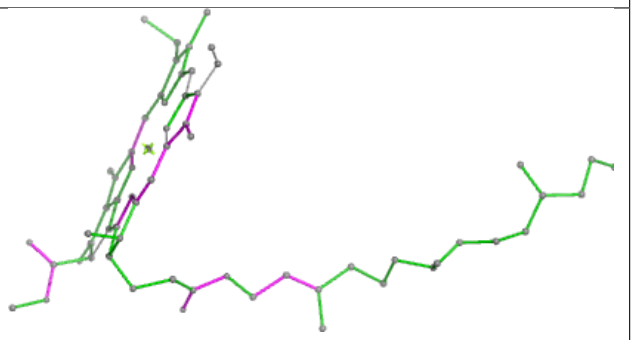


Rings

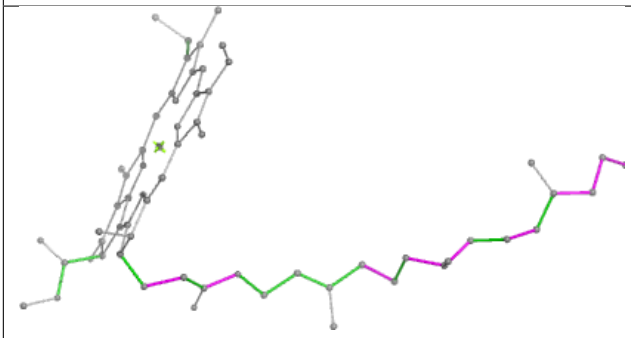
Ligand CLA b 805



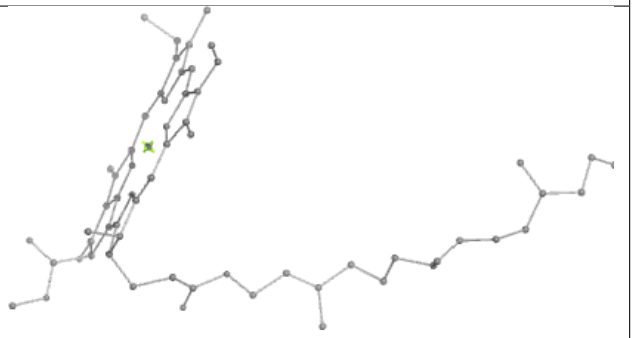
Bond lengths



Bond angles

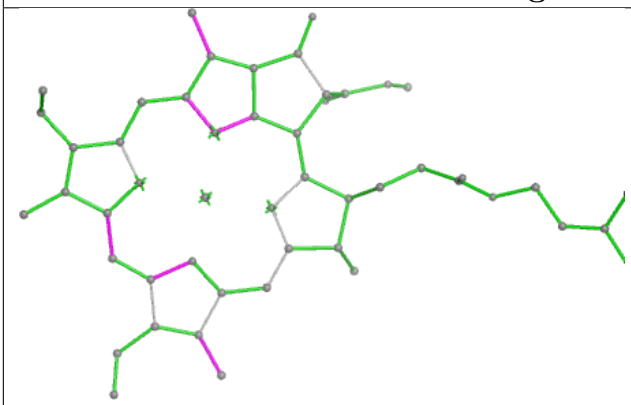


Torsions

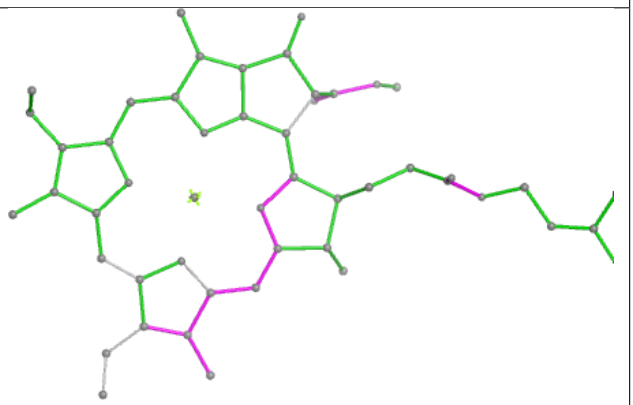


Rings

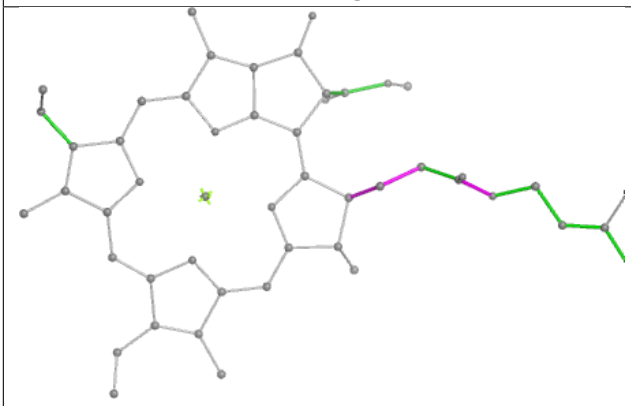
Ligand CLA a 837



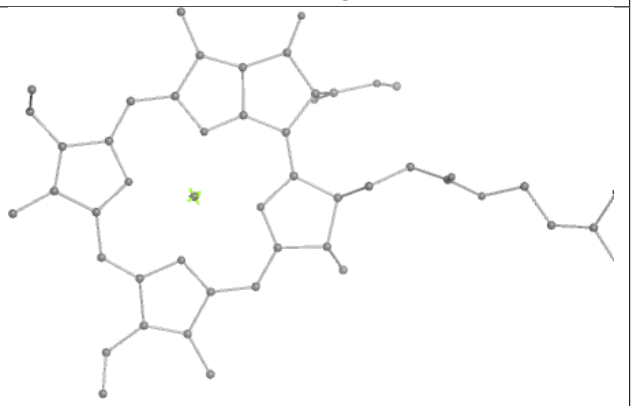
Bond lengths



Bond angles

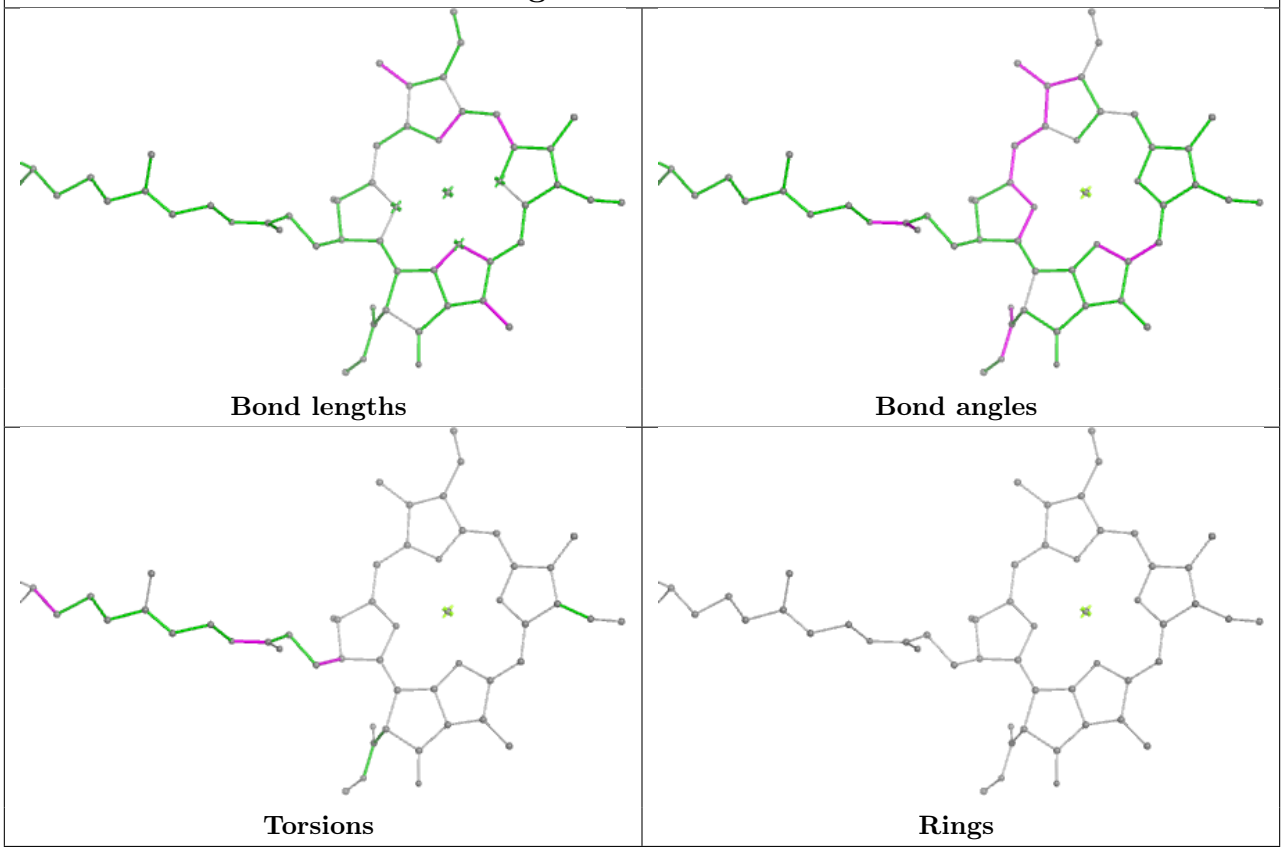


Torsions

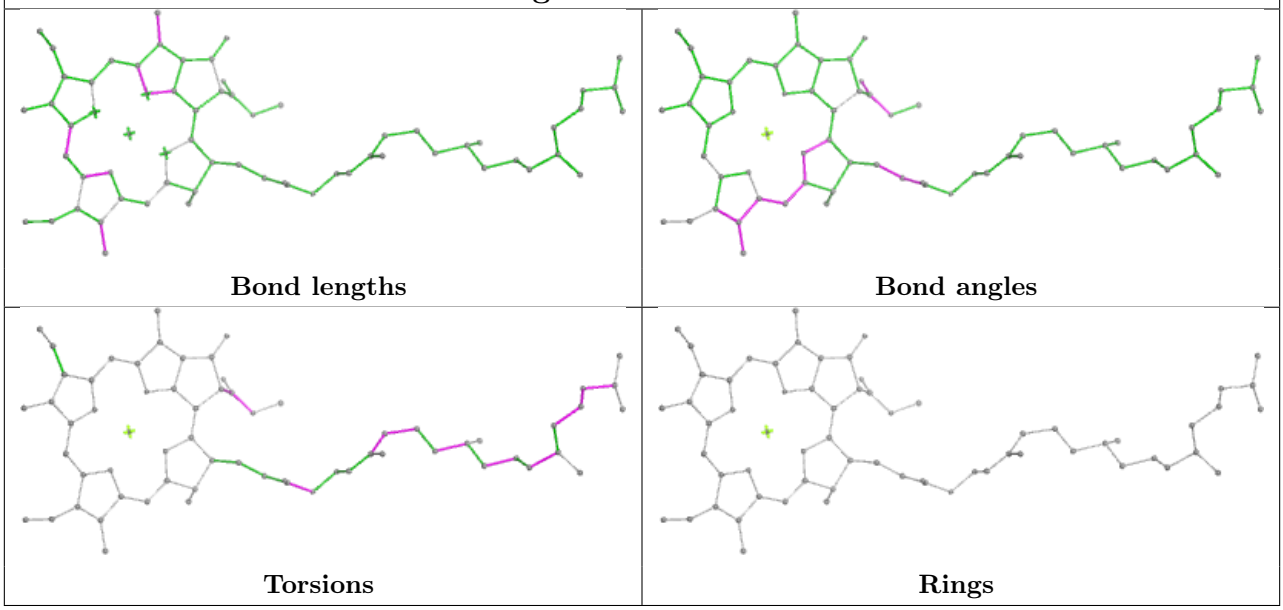


Rings

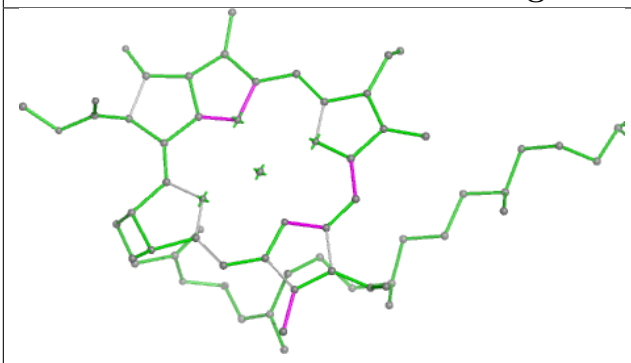
Ligand CLA b 826



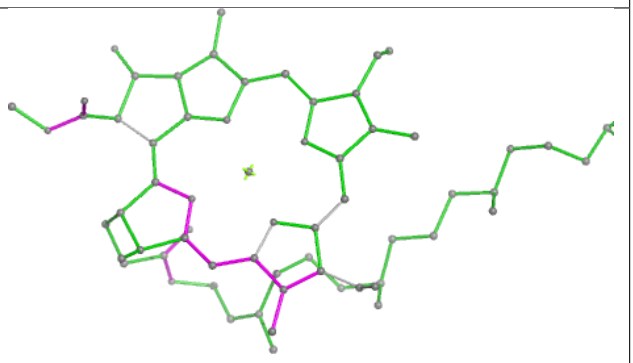
Ligand CLA f 201



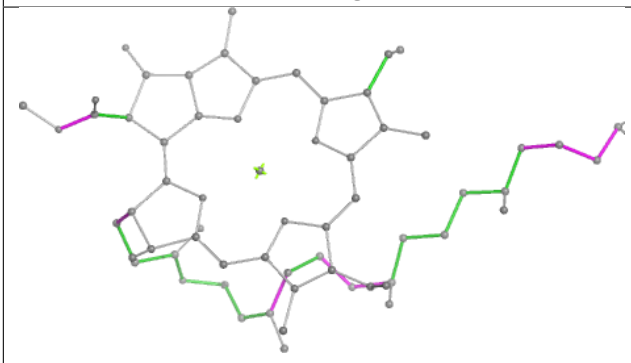
Ligand CLA b 821



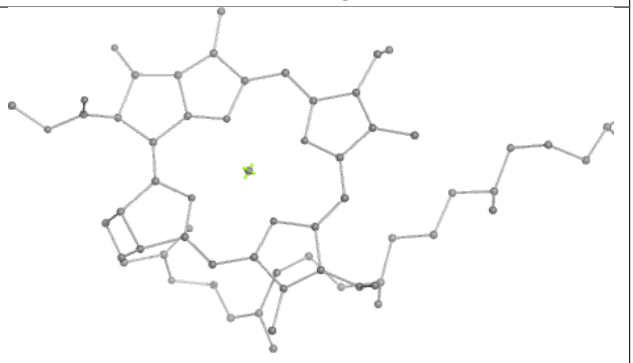
Bond lengths



Bond angles

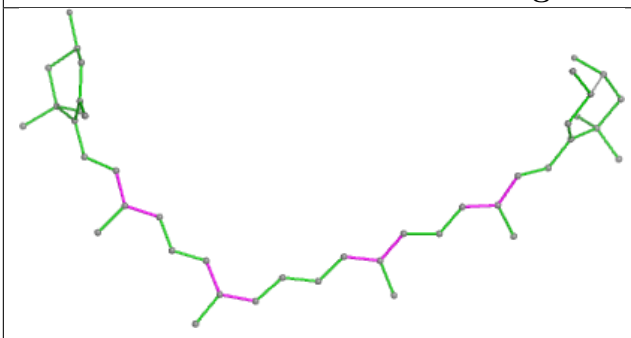


Torsions

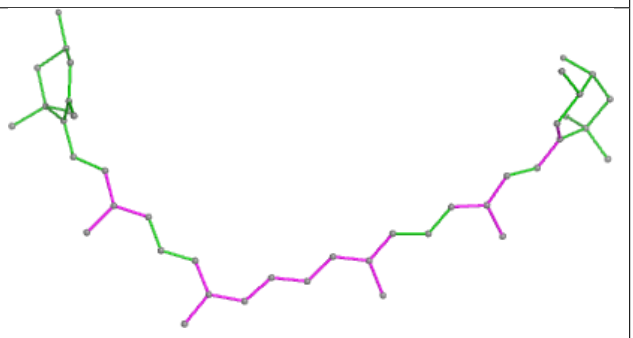


Rings

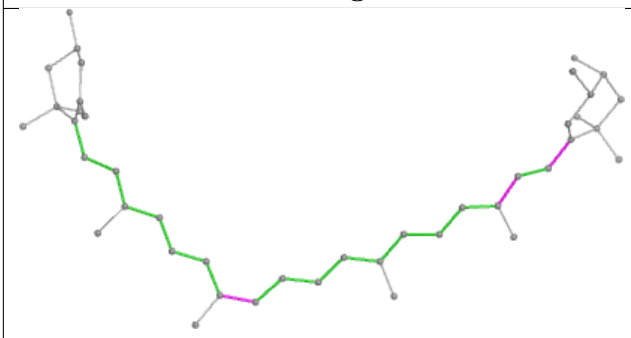
Ligand ZEX f 205



Bond lengths



Bond angles



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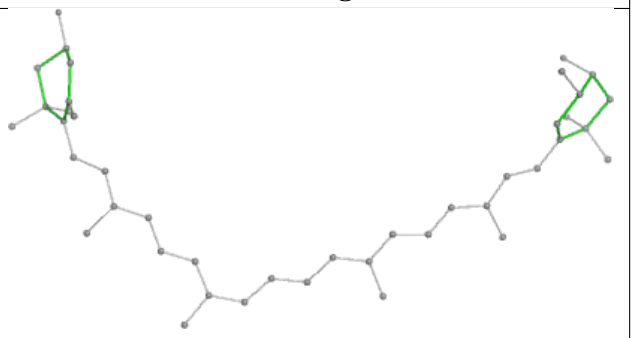
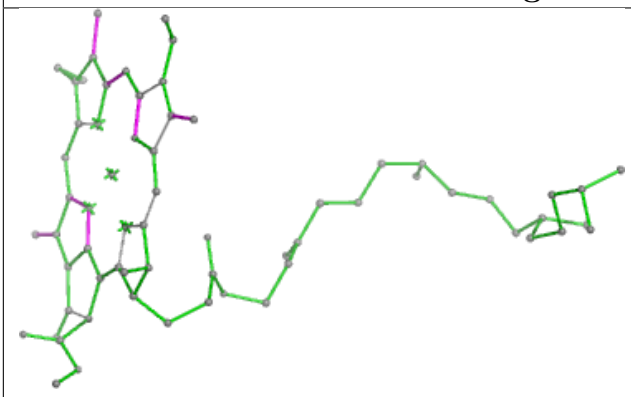
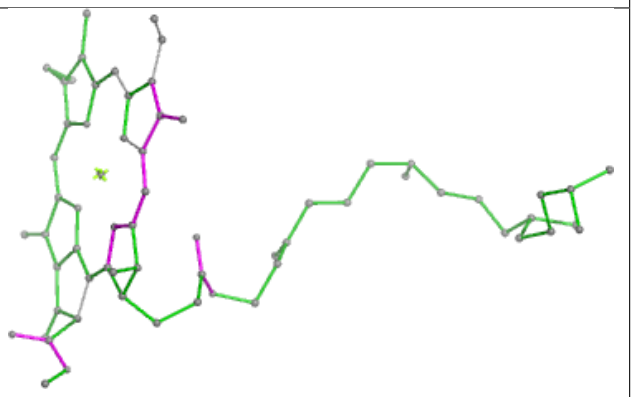


Rings

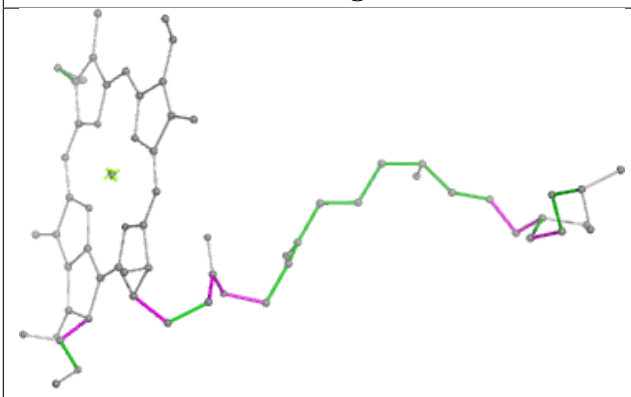
Ligand CLA l 1502



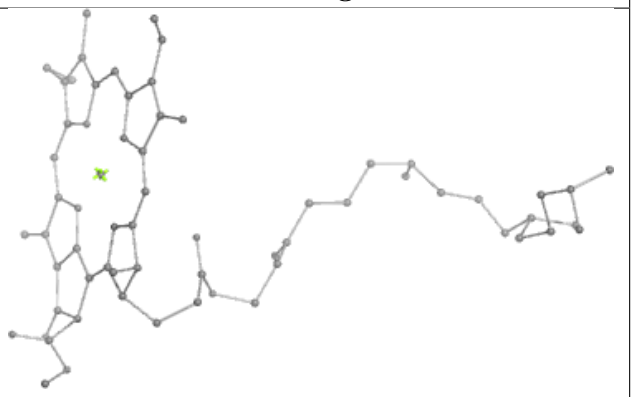
Bond lengths



Bond angles

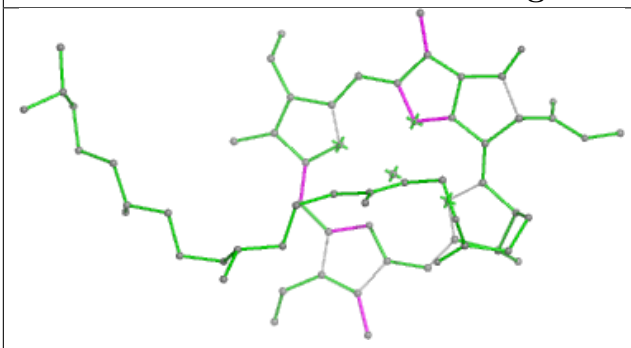


Torsions

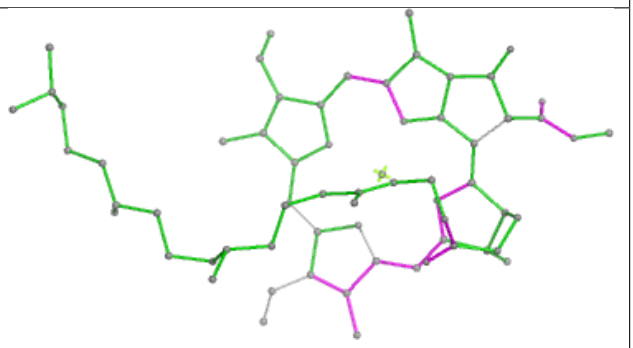


Rings

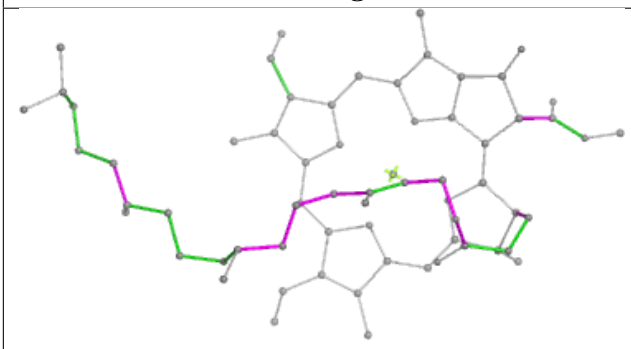
Ligand CLA b 838



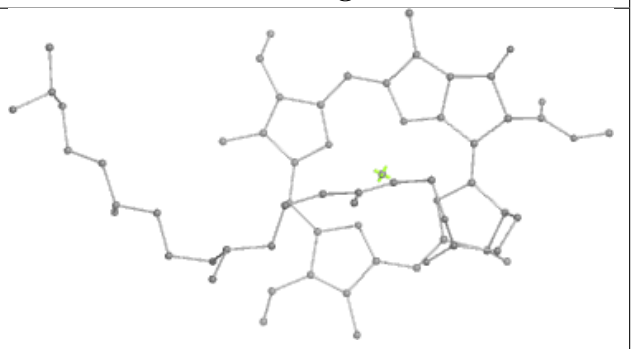
Bond lengths



Bond angles

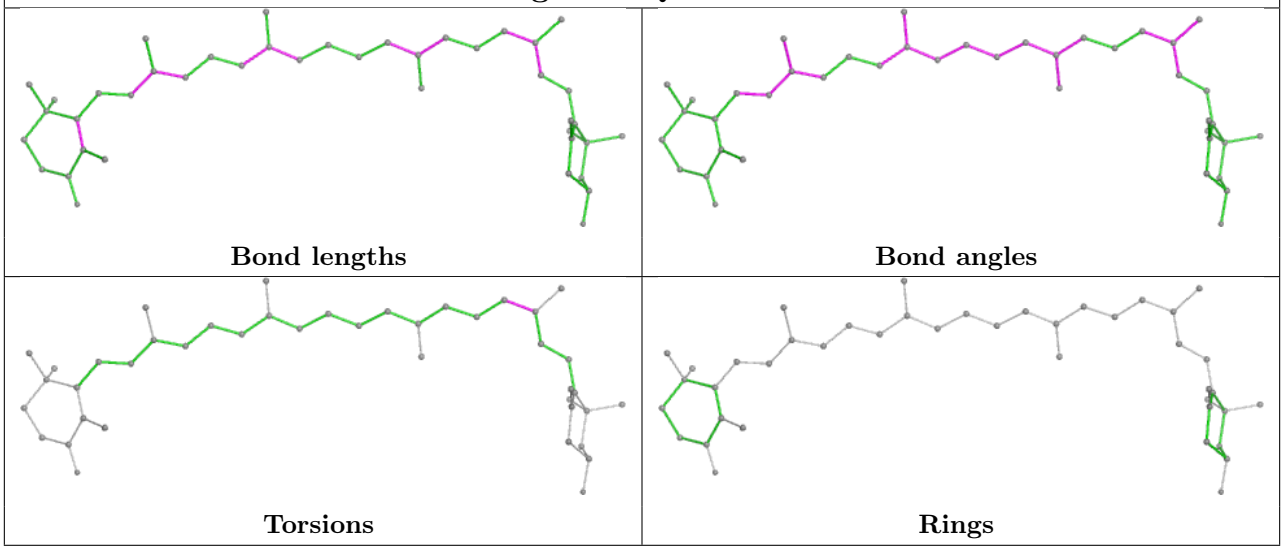


Torsions

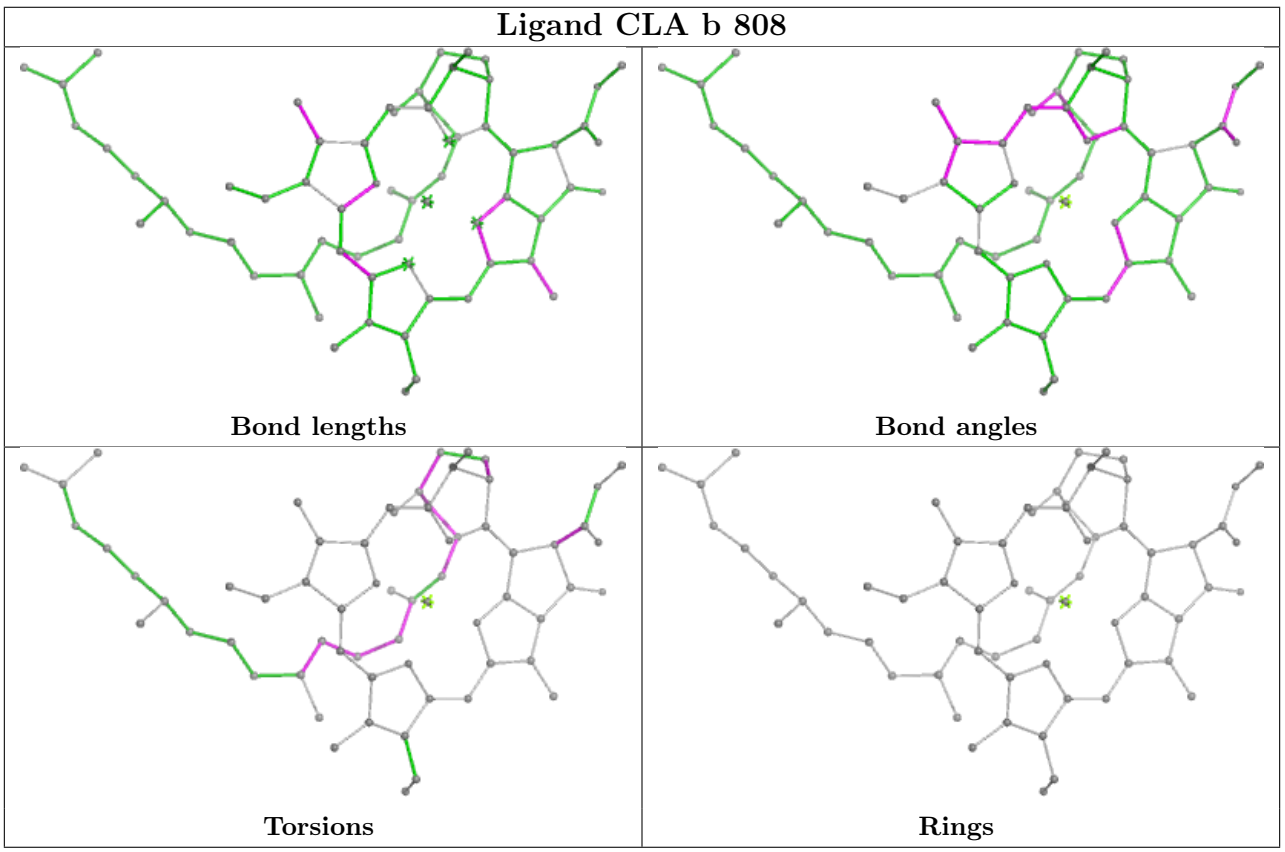


Rings

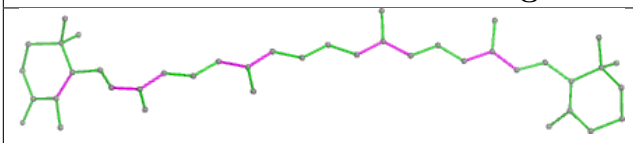
Ligand EQ3 b 853



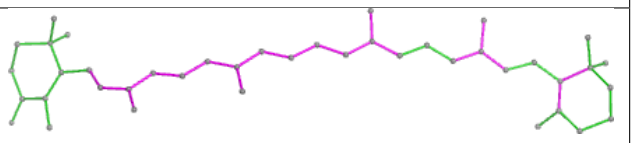
Ligand CLA b 808



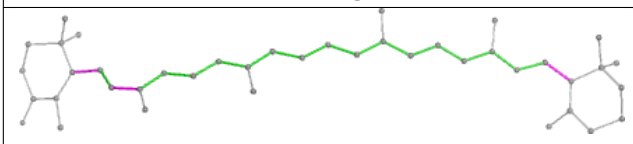
Ligand ECH m 101



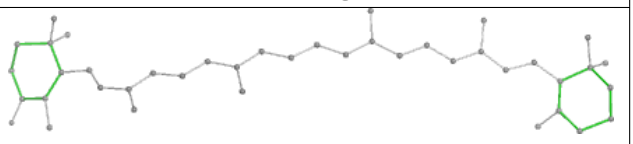
Bond lengths



Bond angles

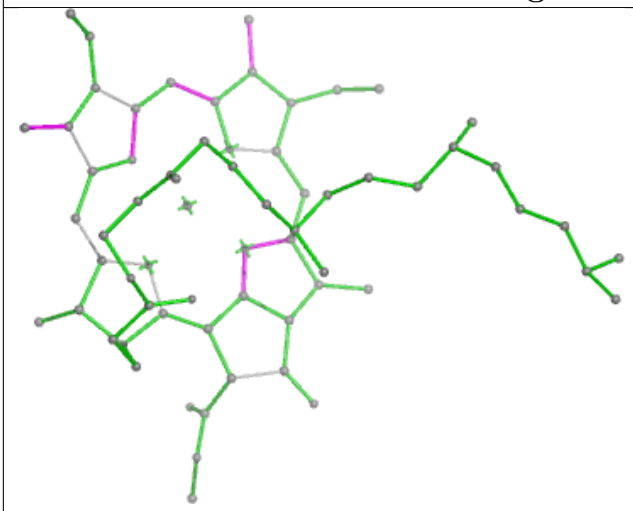


Torsions

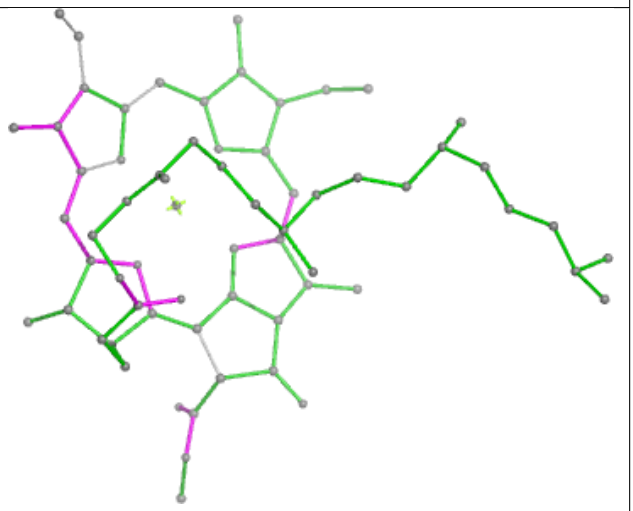


Rings

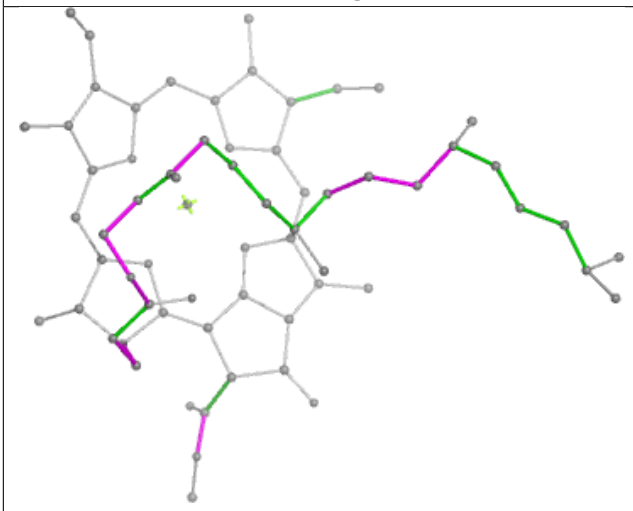
Ligand CLA b 828



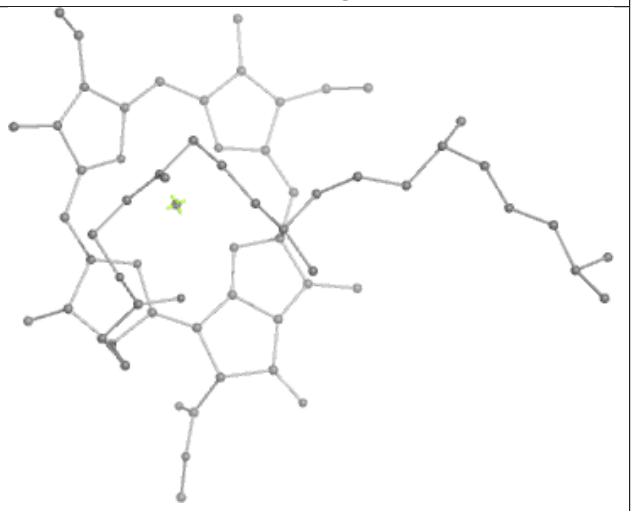
Bond lengths



Bond angles

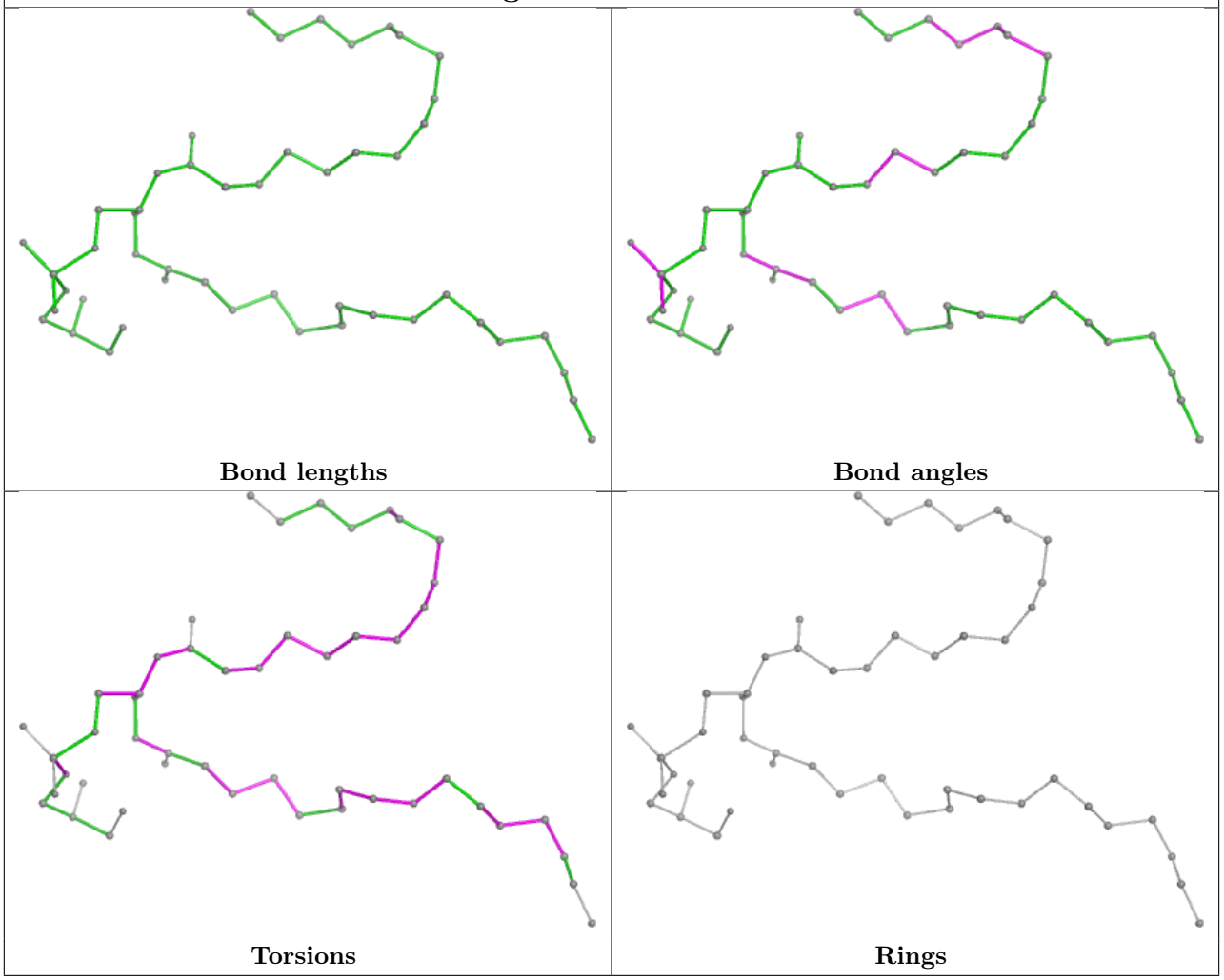


Torsions

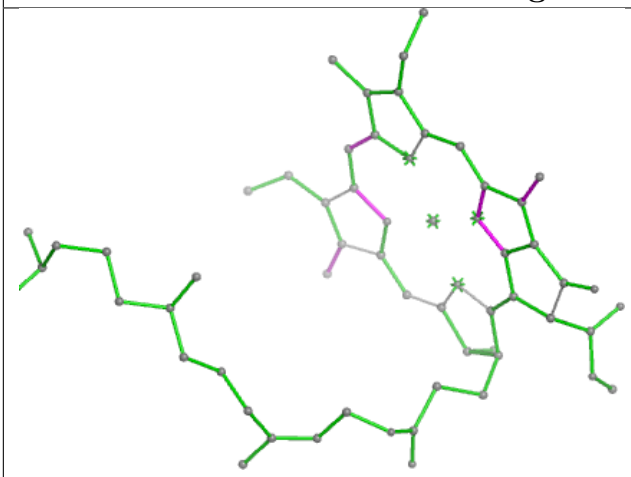


Rings

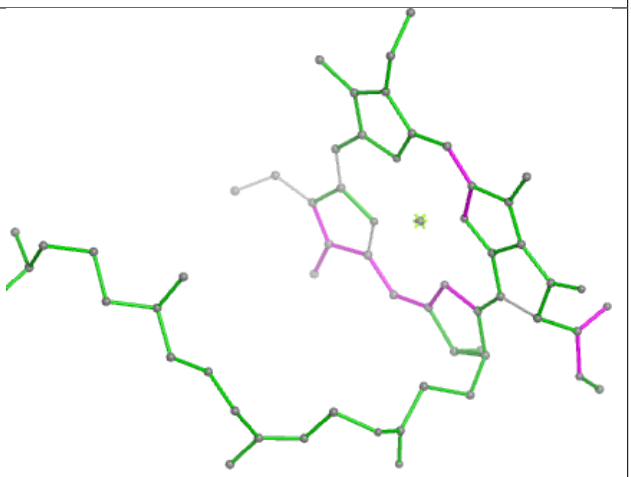
Ligand LHG a 853



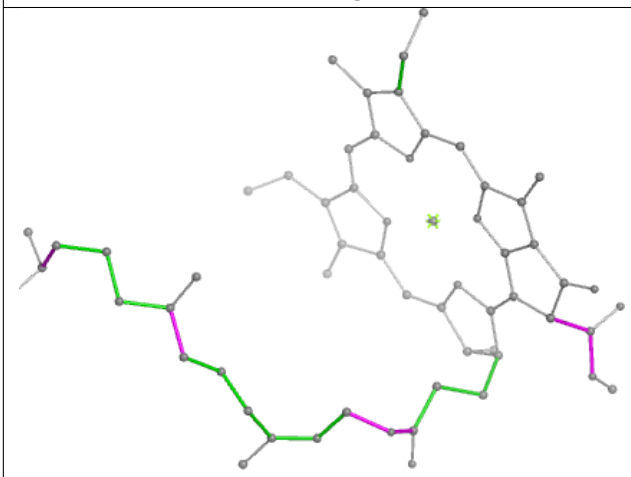
Ligand CLA a 824



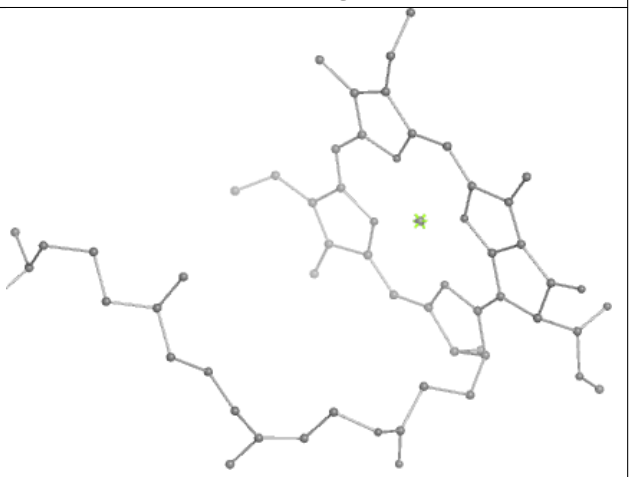
Bond lengths



Bond angles

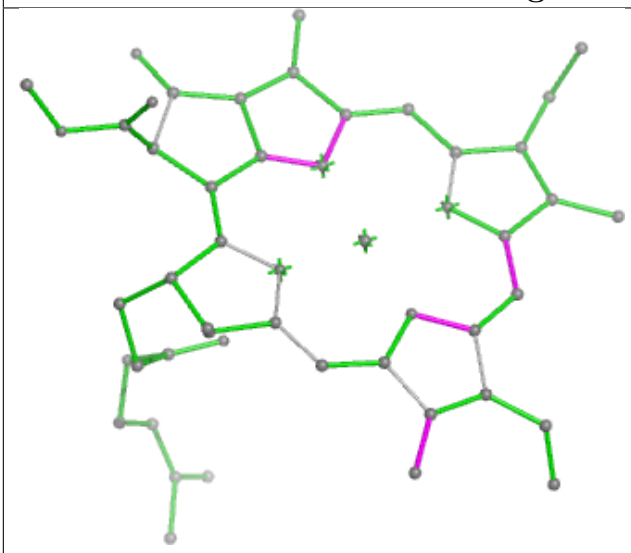


Torsions

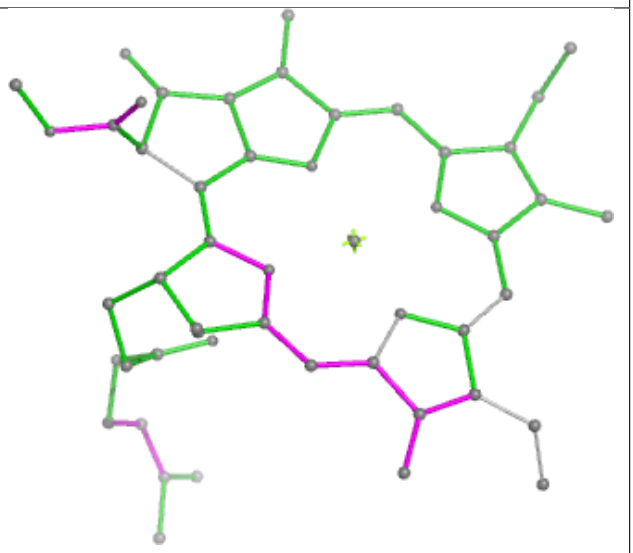


Rings

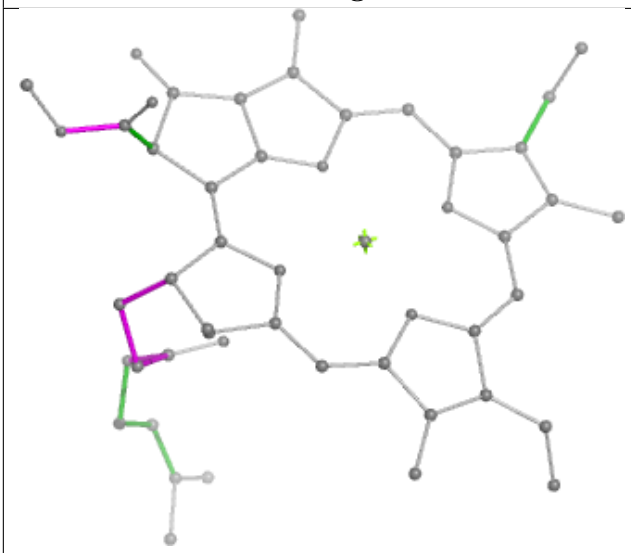
Ligand CLA b 836



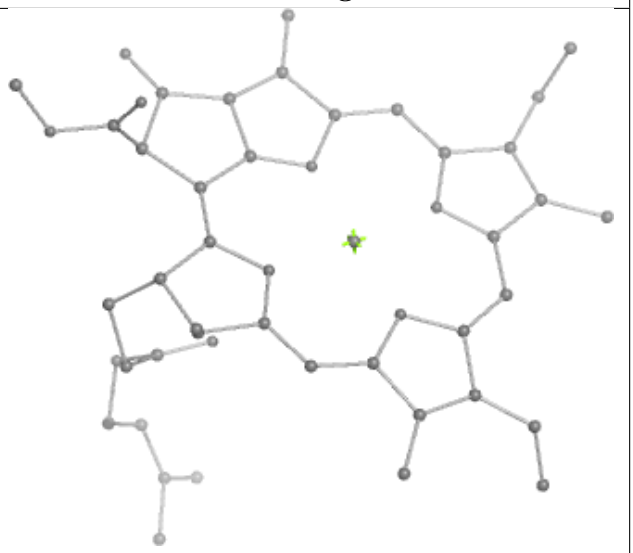
Bond lengths



Bond angles

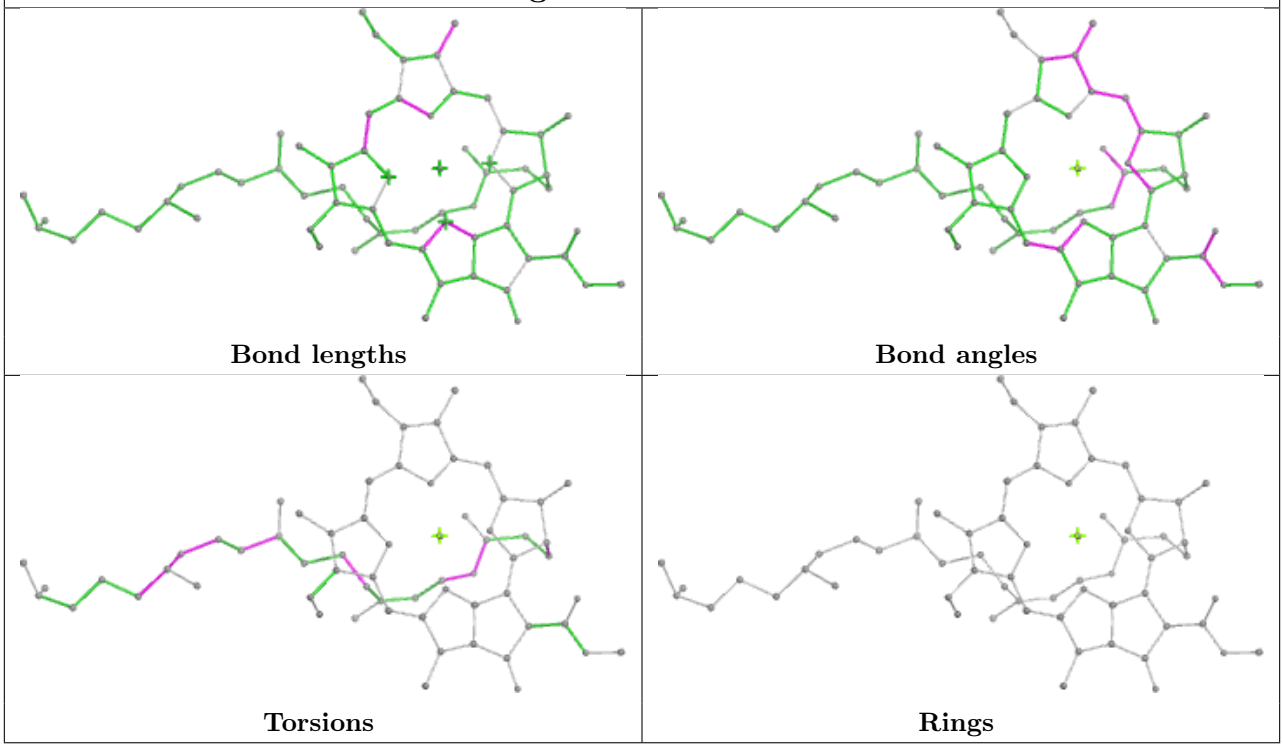


Torsions

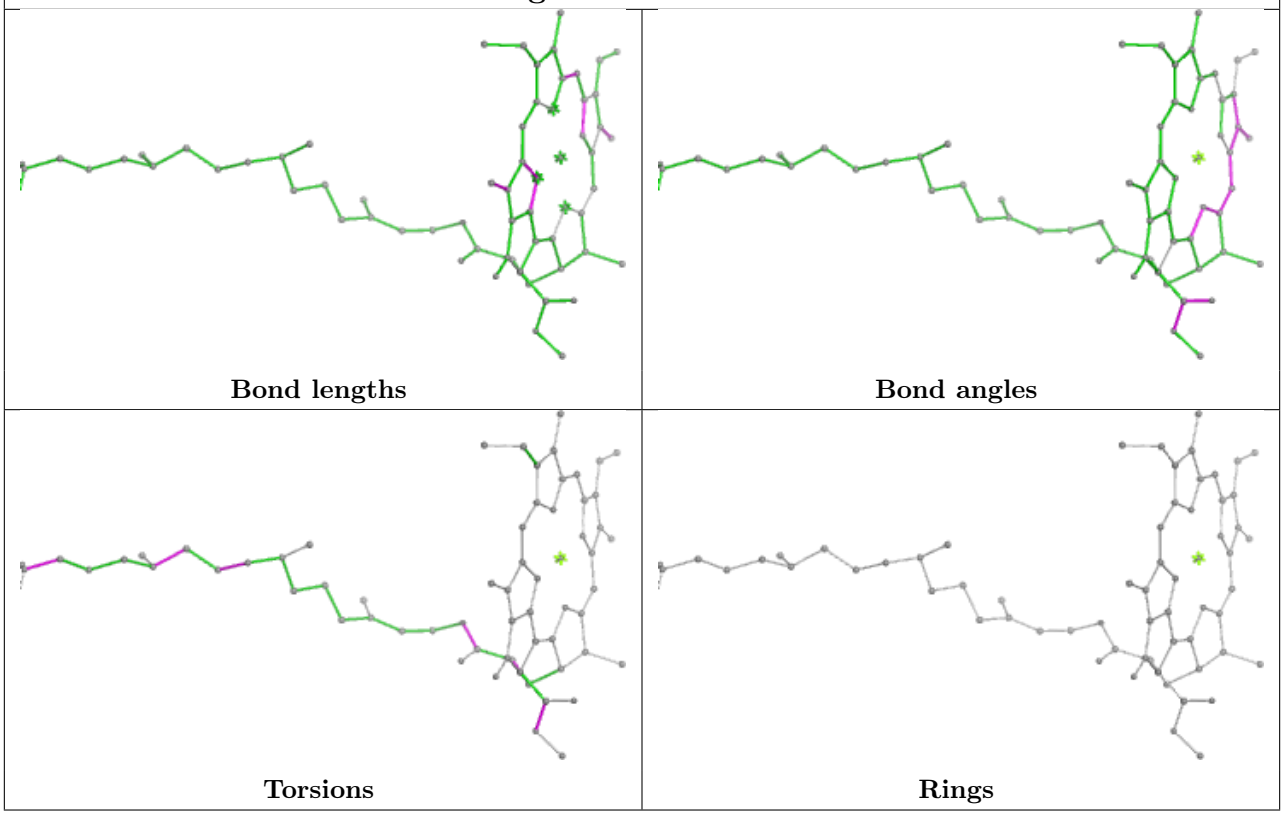


Rings

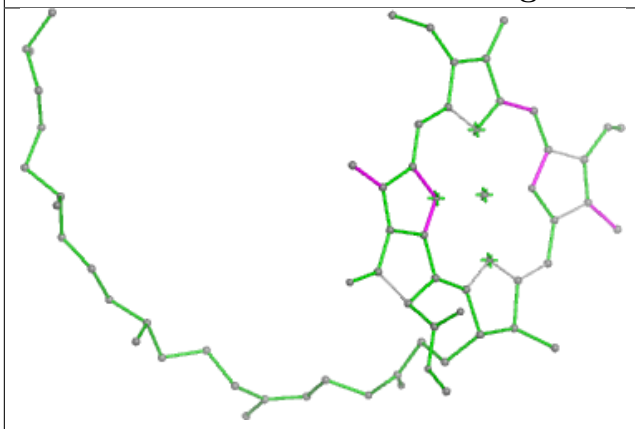
Ligand CLA a 817



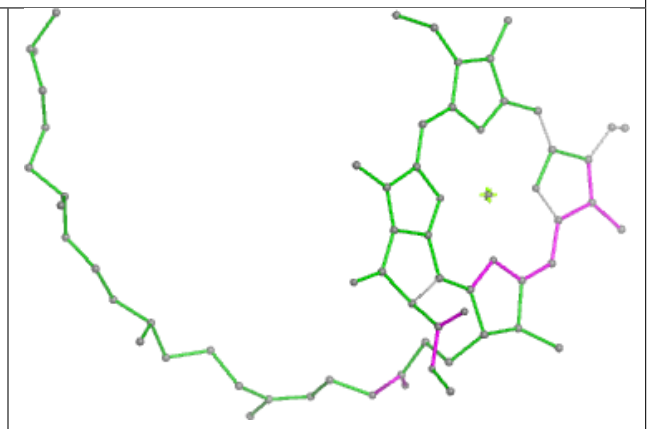
Ligand CLA b 829



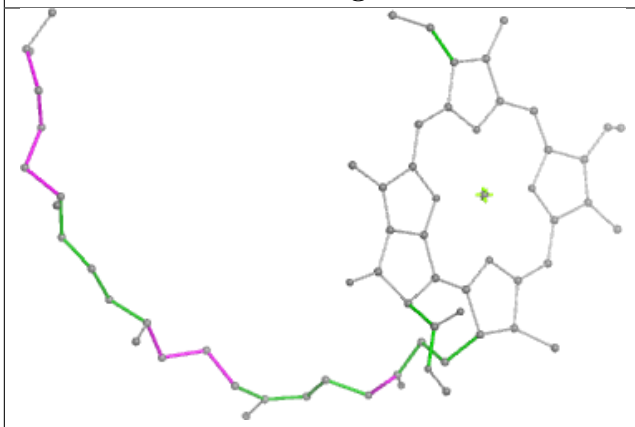
Ligand CLA k 4002



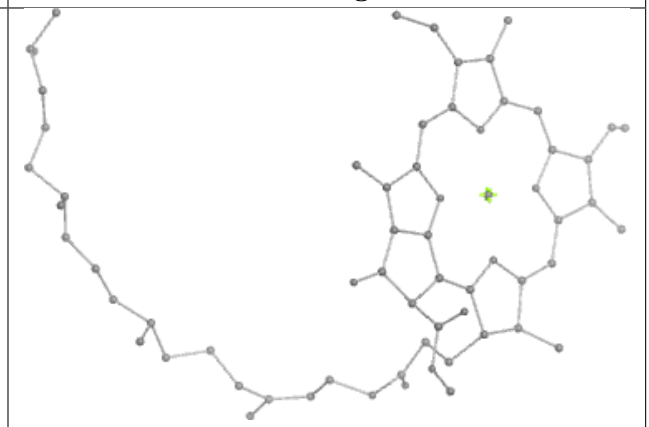
Bond lengths



Bond angles

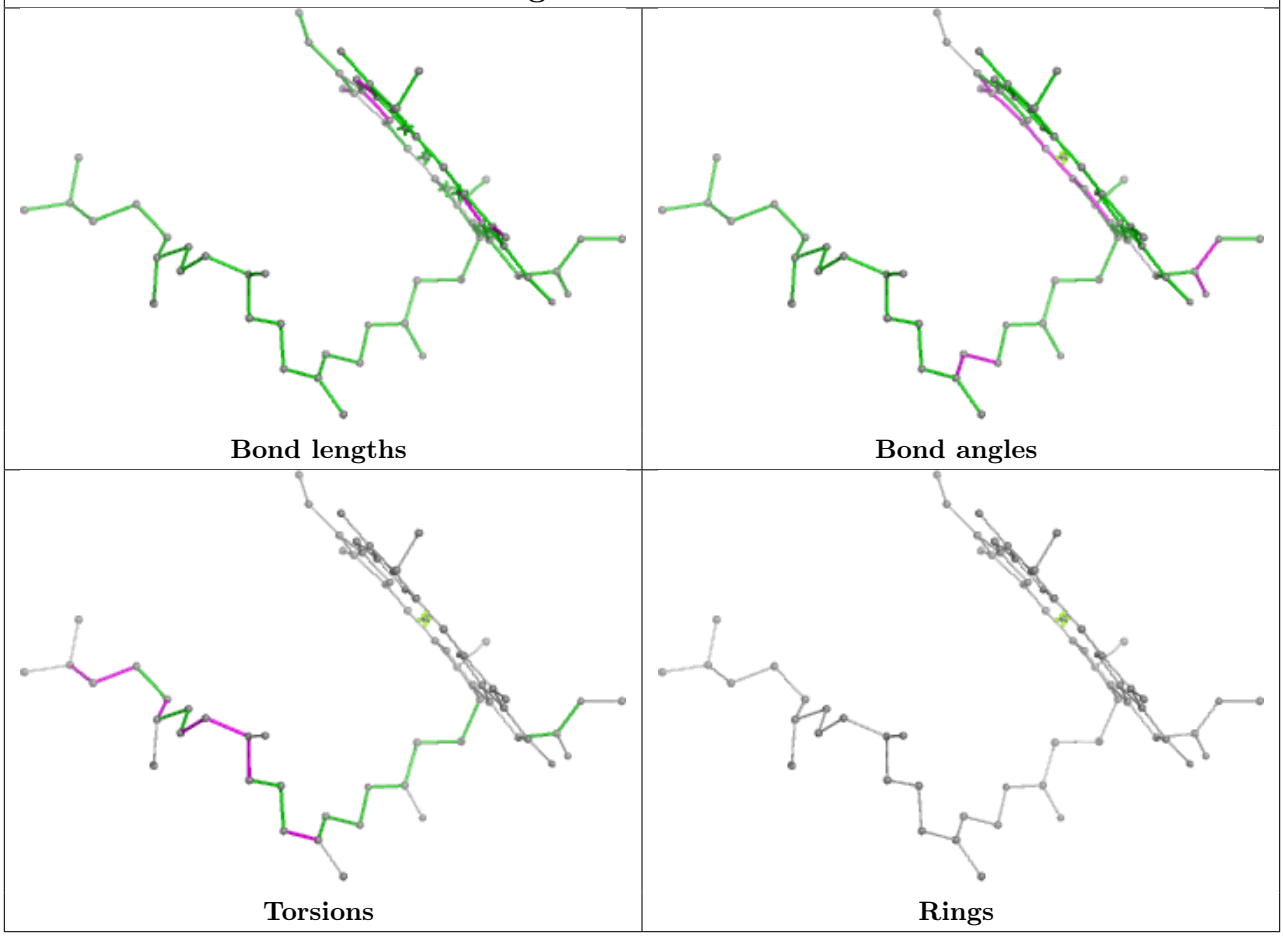


Torsions

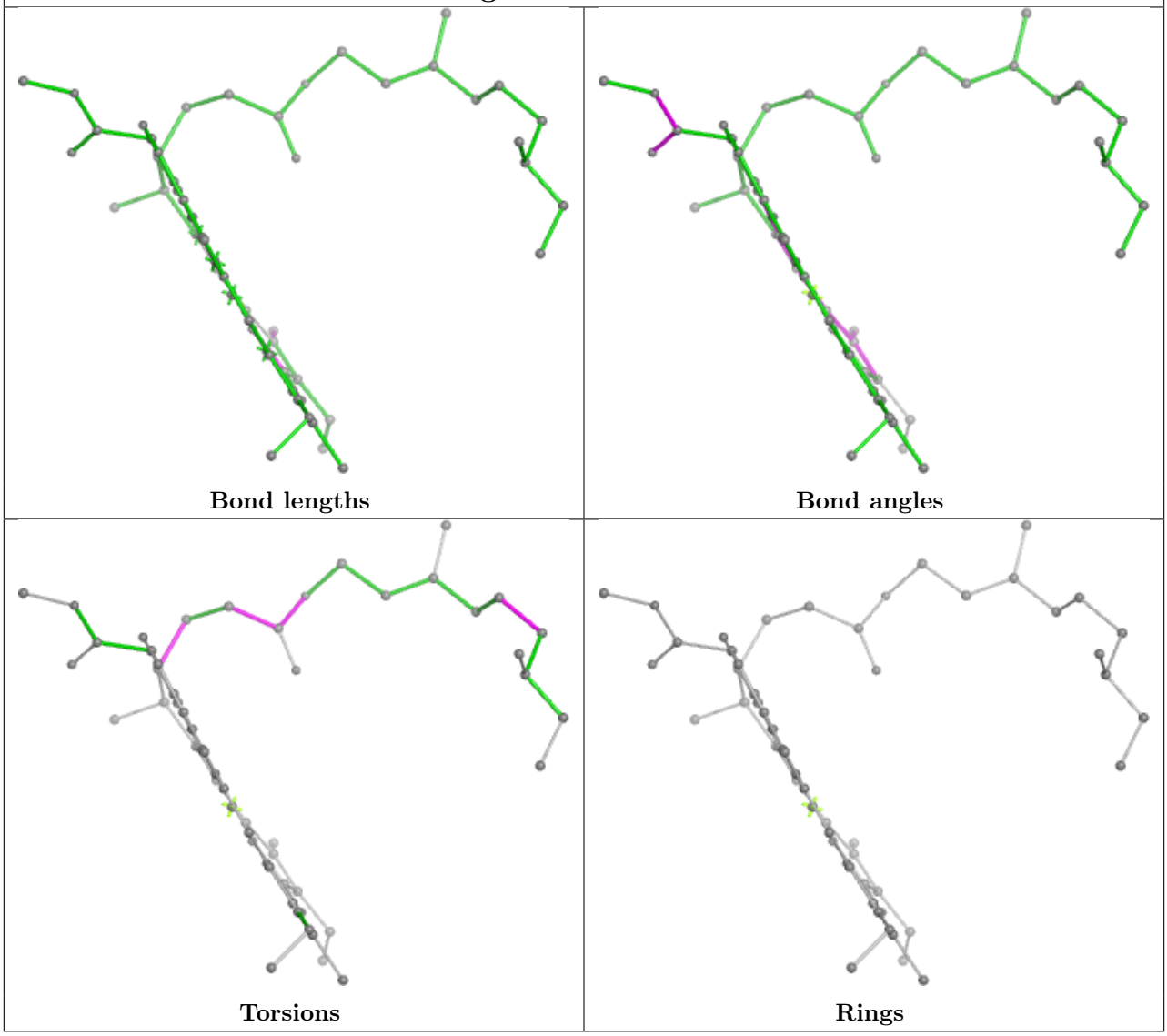


Rings

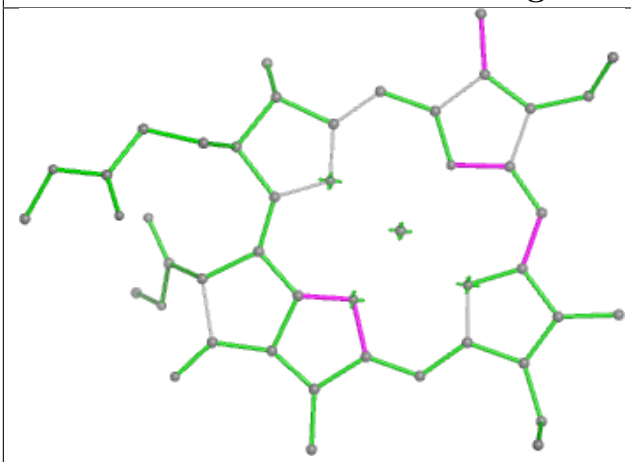
Ligand CLA b 815



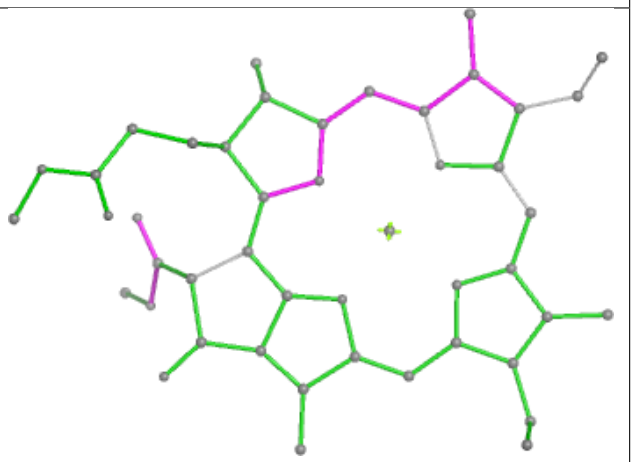
Ligand CLA b 812



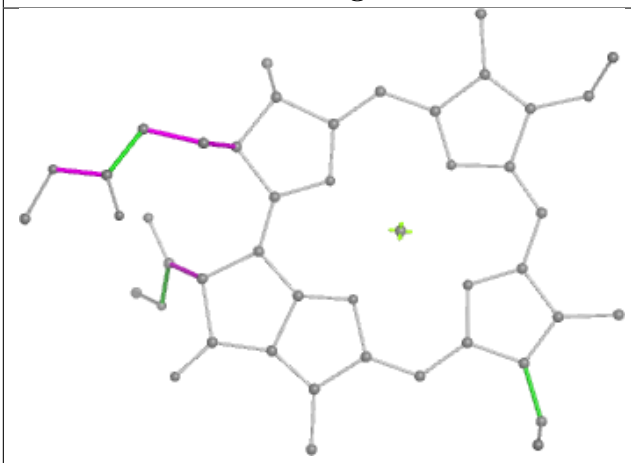
Ligand CLA b 842



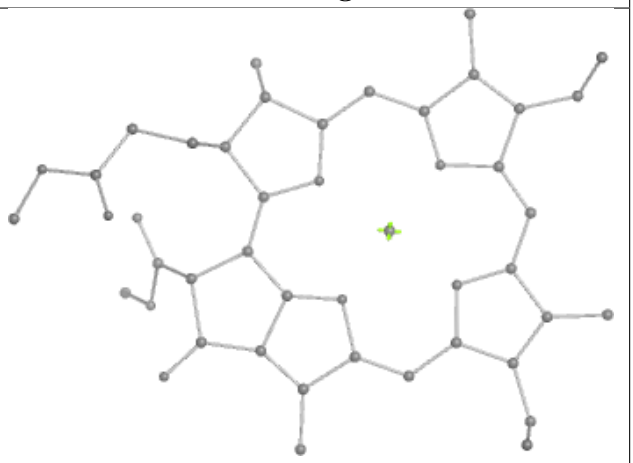
Bond lengths



Bond angles

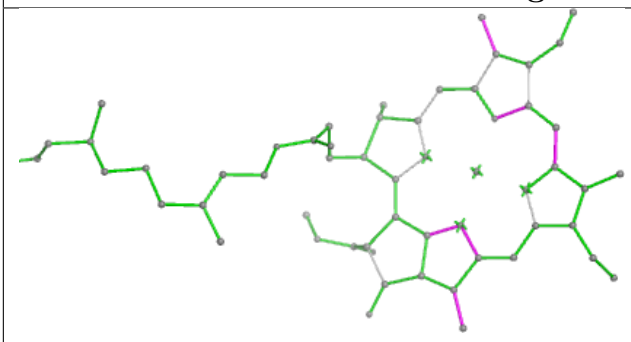


Torsions

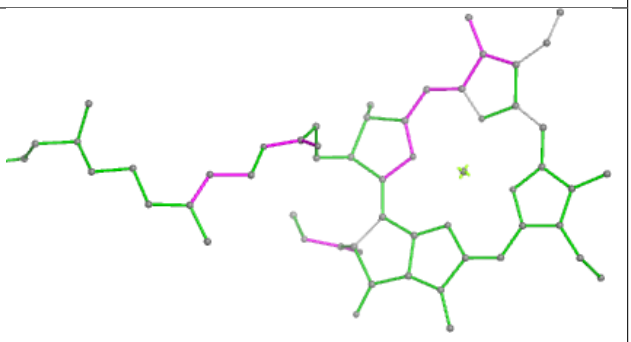


Rings

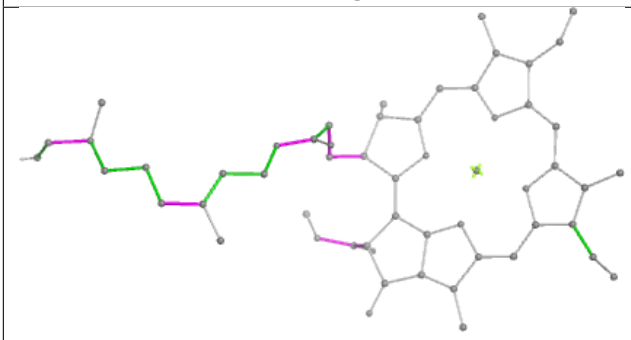
Ligand CLA b 824



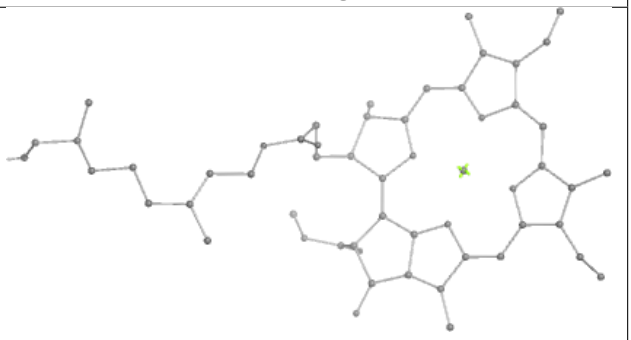
Bond lengths



Bond angles

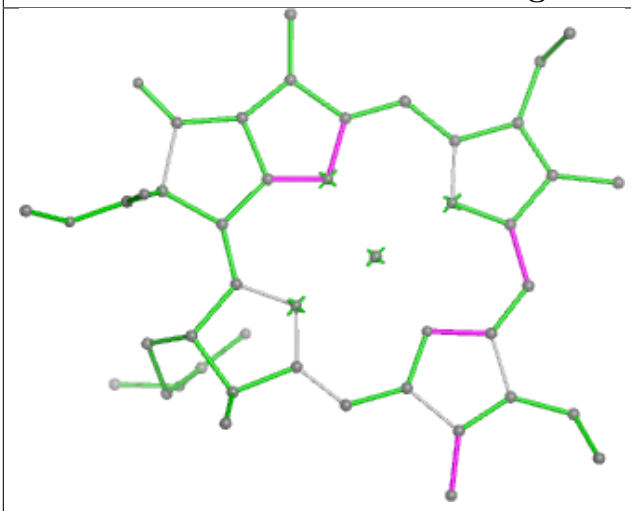


Torsions

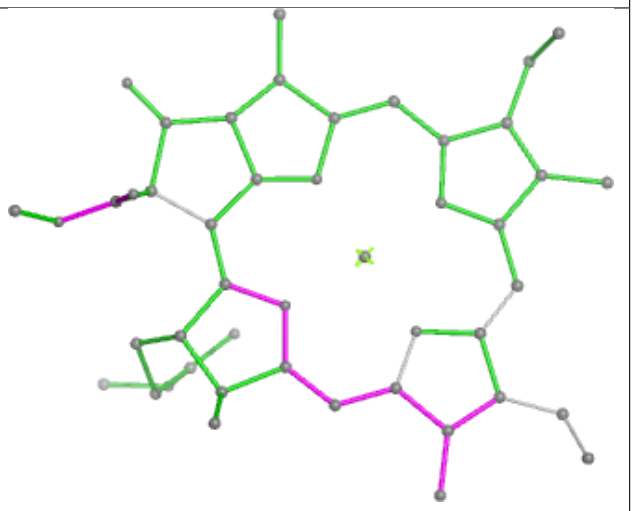


Rings

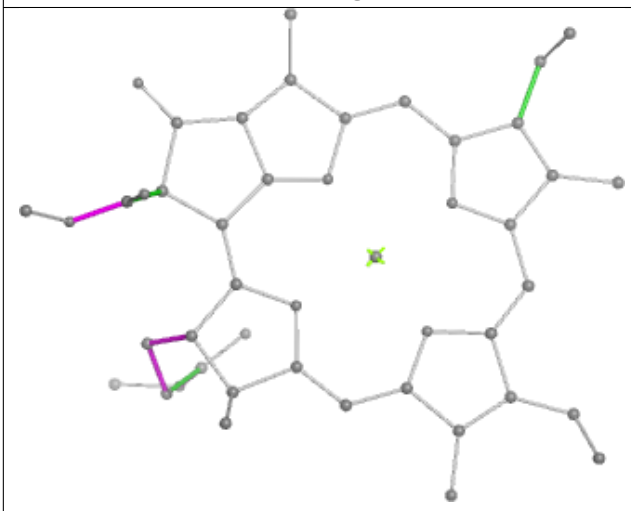
Ligand CLA a 816



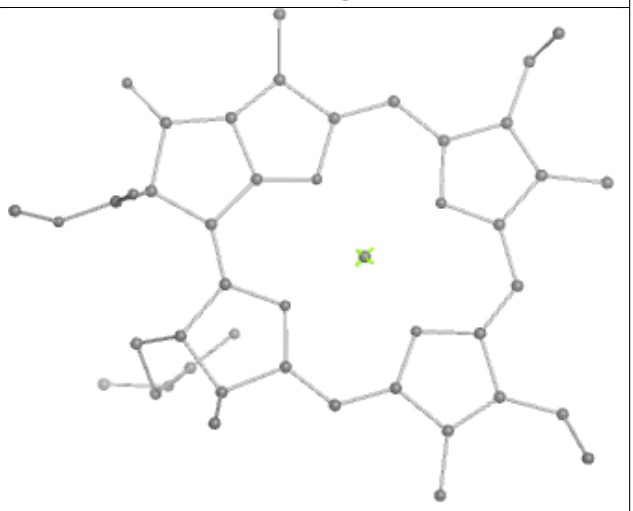
Bond lengths



Bond angles

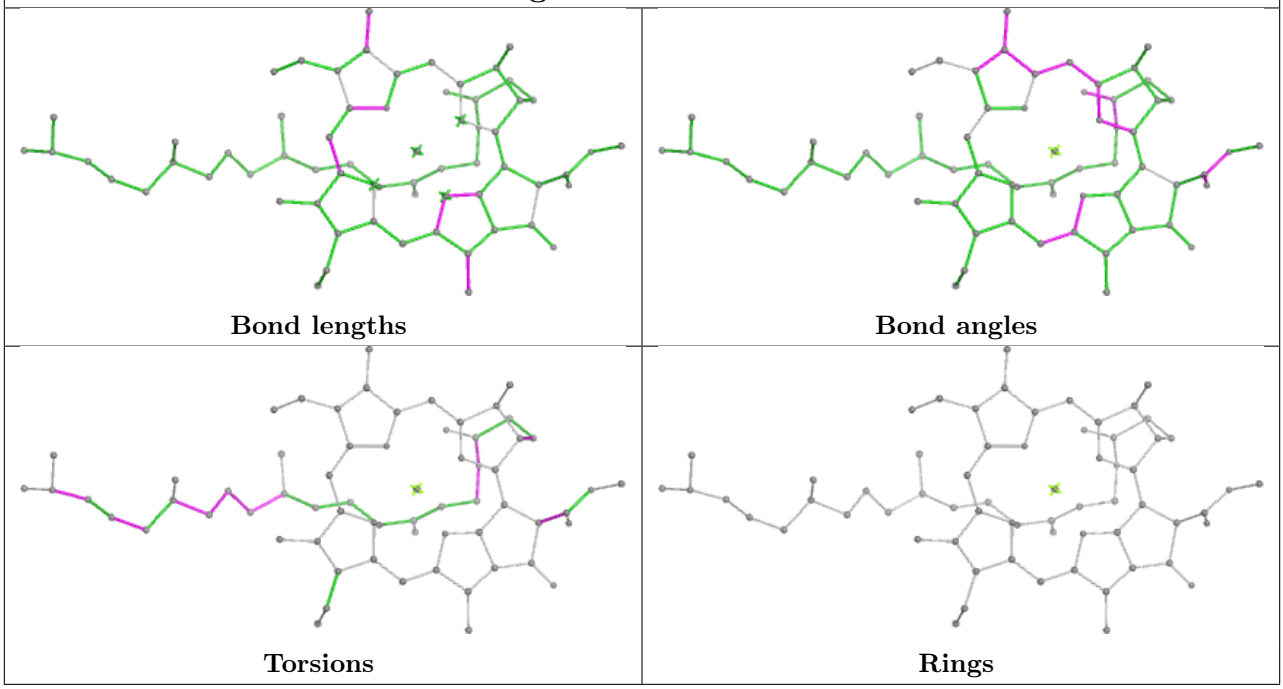


Torsions

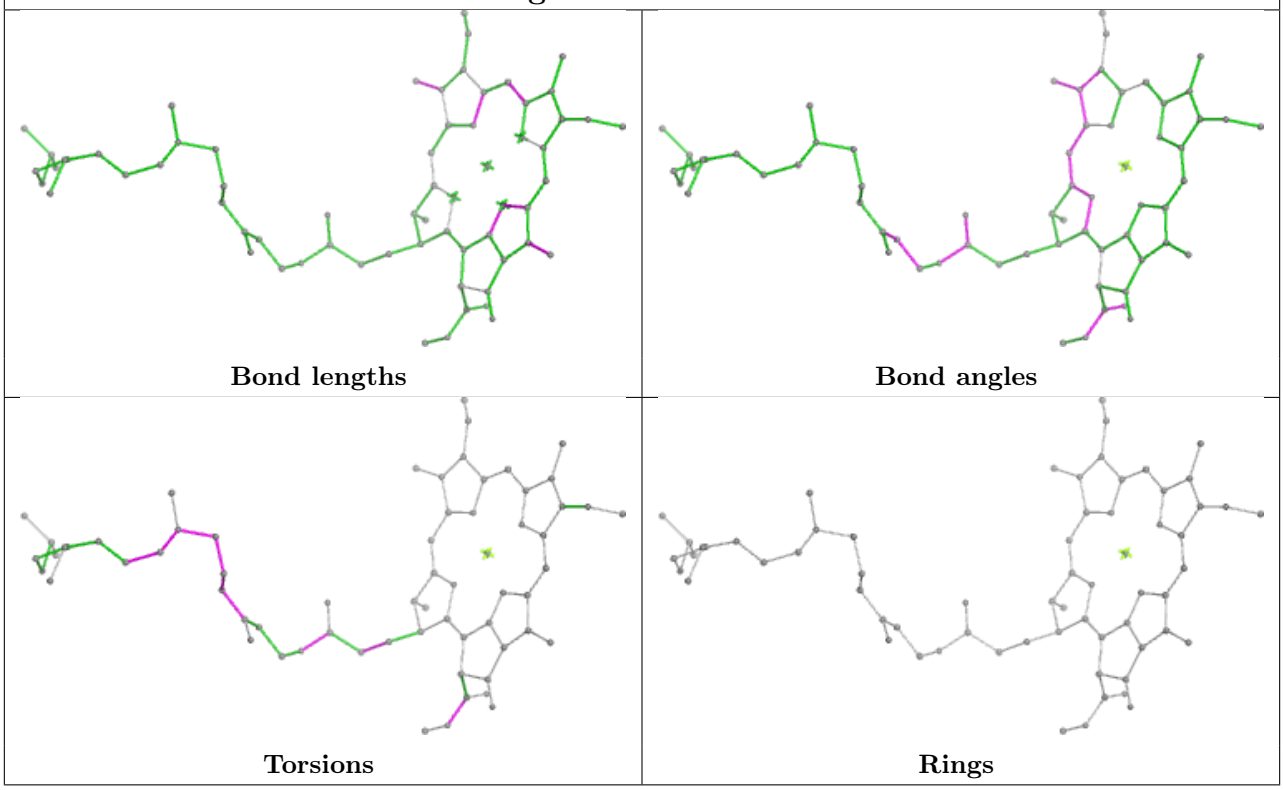


Rings

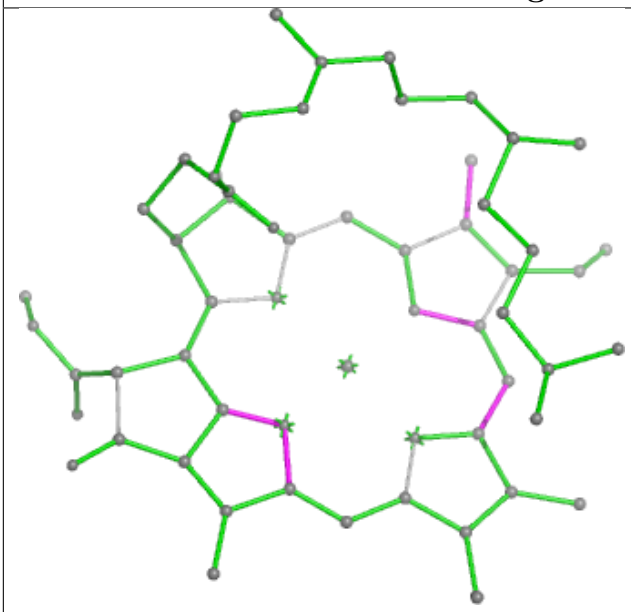
Ligand CLA a 838



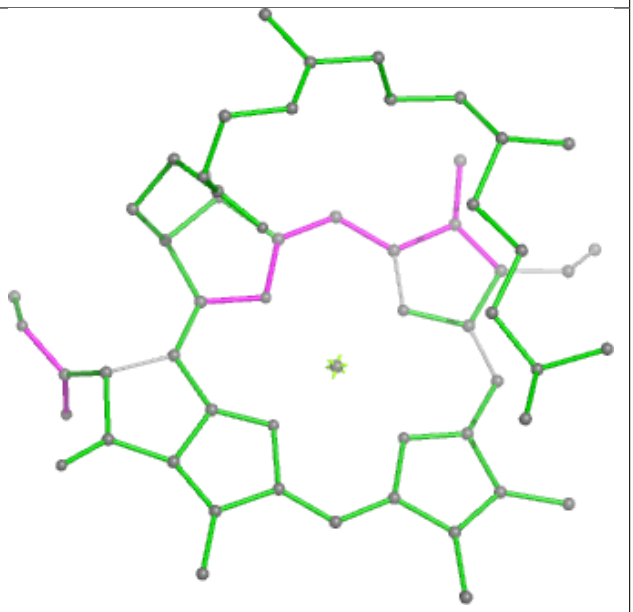
Ligand CLA b 810



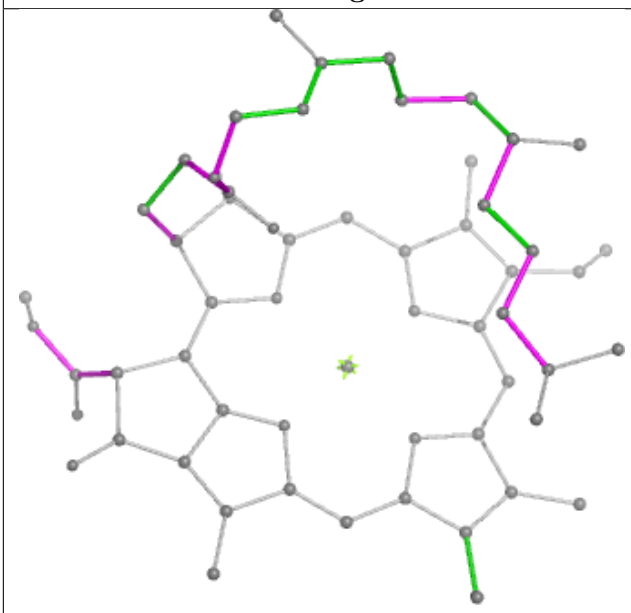
Ligand CLA b 822



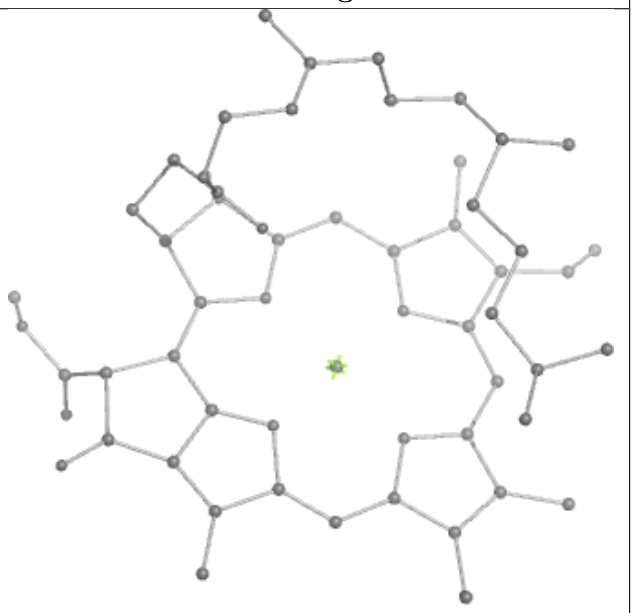
Bond lengths



Bond angles

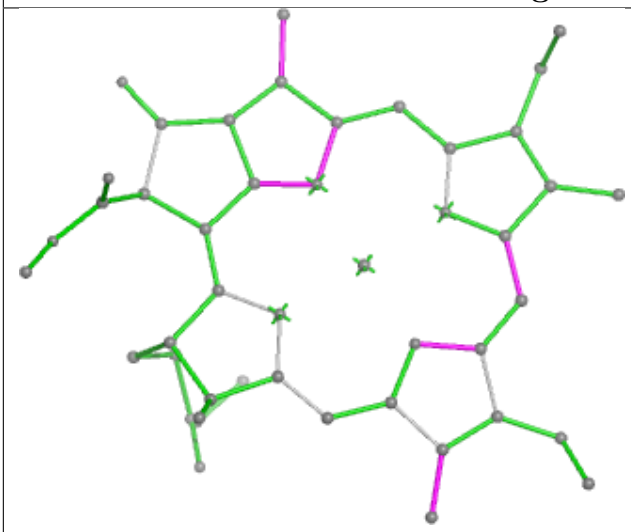


Torsions

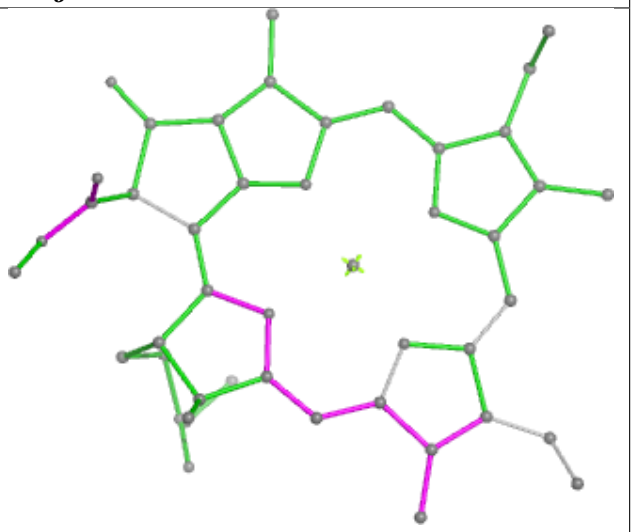


Rings

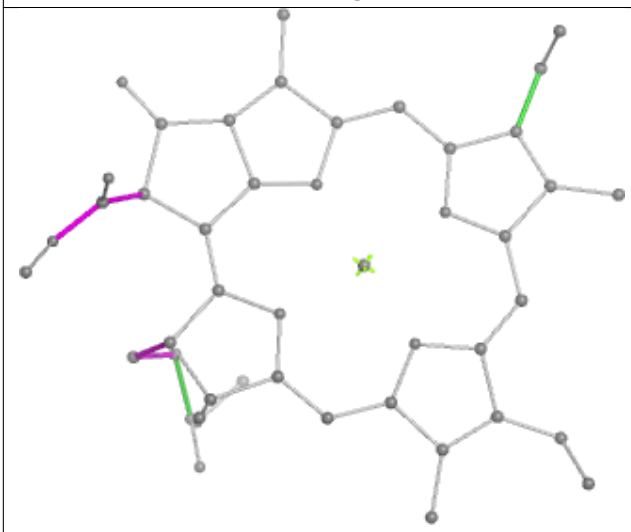
Ligand CLA j 104



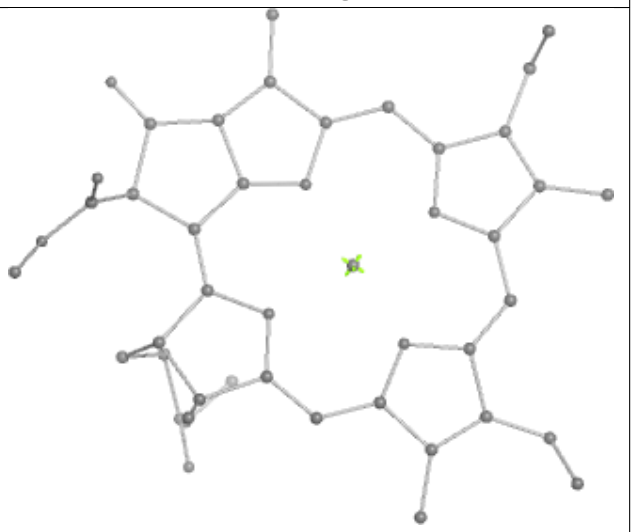
Bond lengths



Bond angles

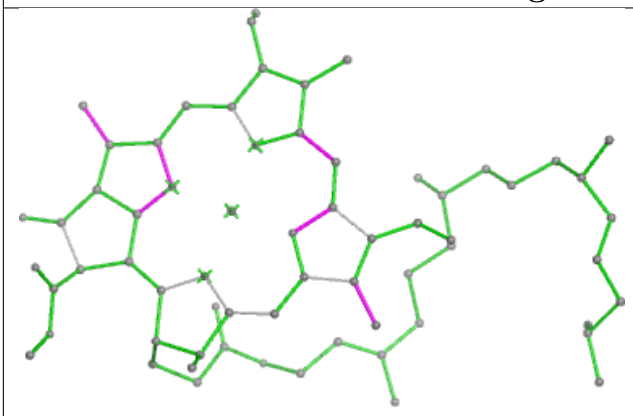


Torsions

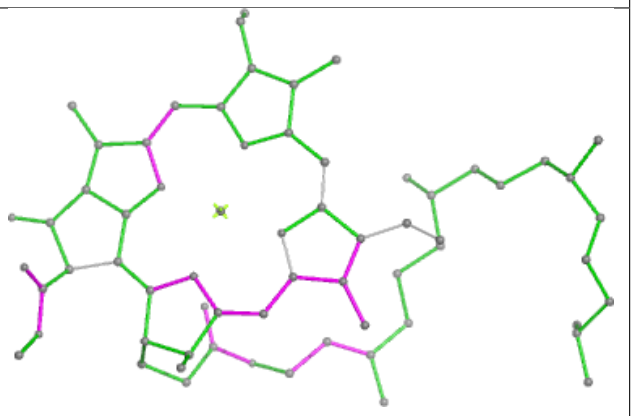


Rings

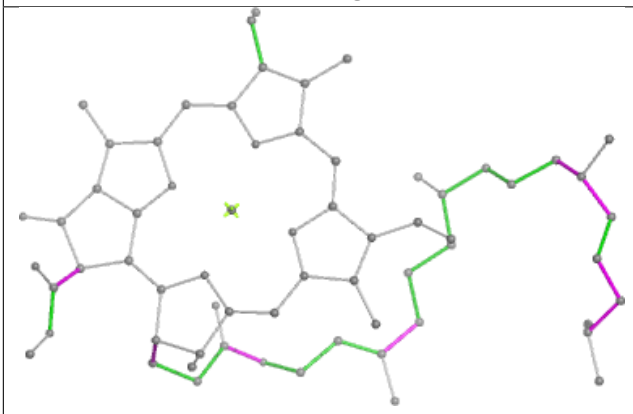
Ligand CLA a 819



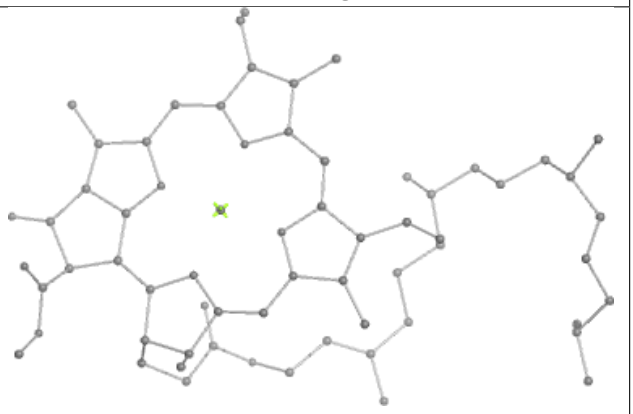
Bond lengths



Bond angles

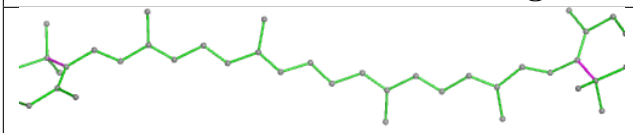


Torsions



Rings

Ligand BCR a 846



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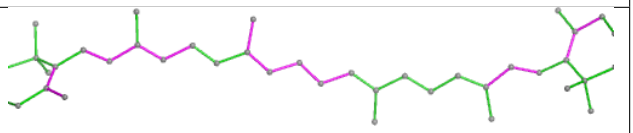
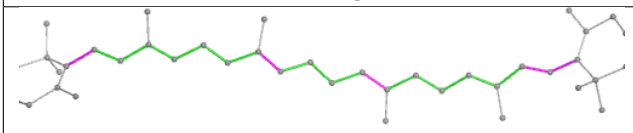
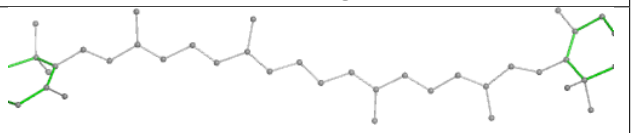


Bond angles

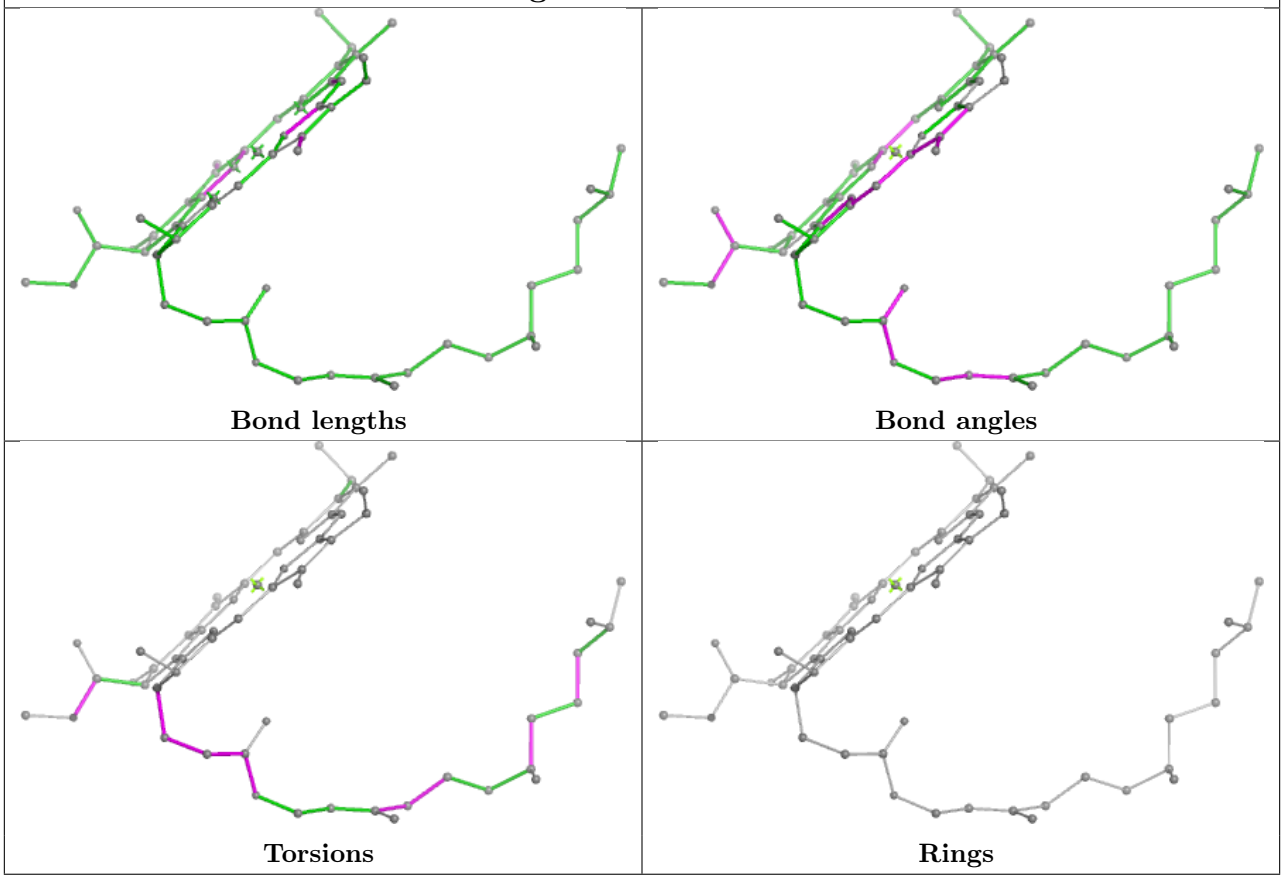


Torsions

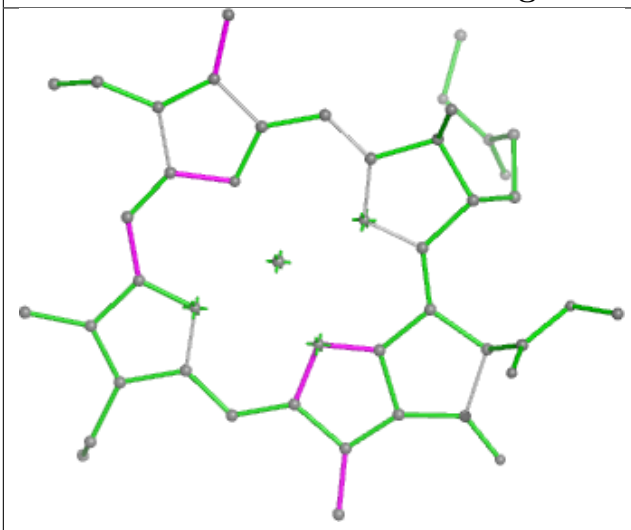


Rings

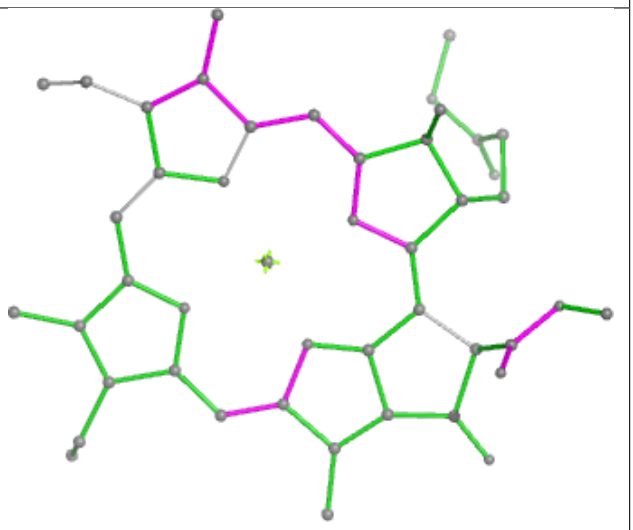
Ligand CLA a 832



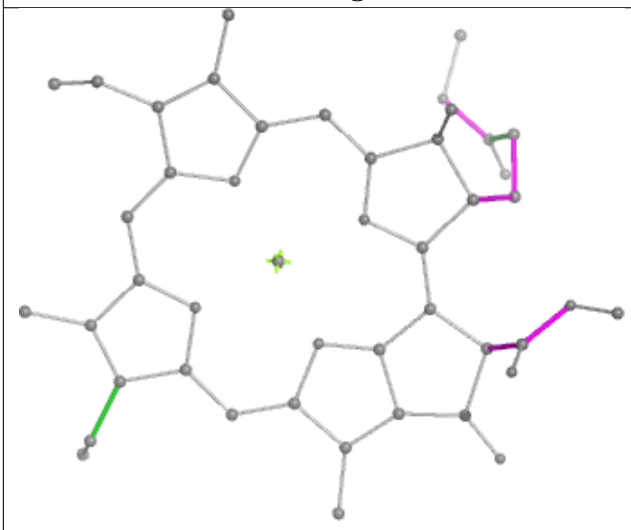
Ligand CLA k 4003



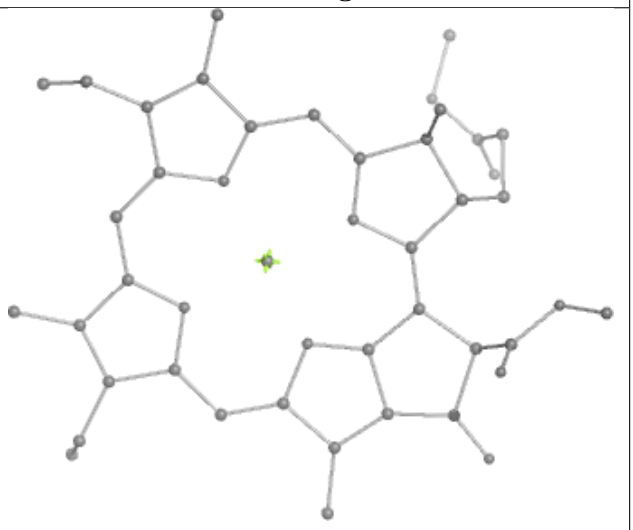
Bond lengths



Bond angles

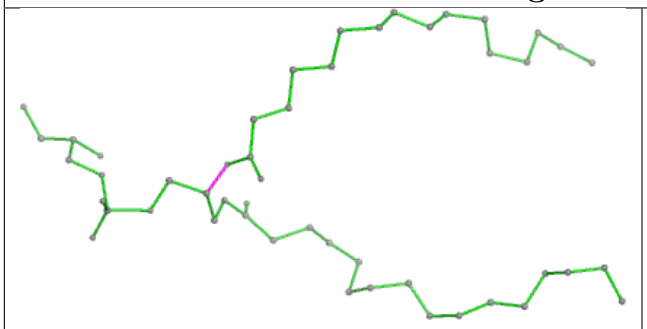


Torsions

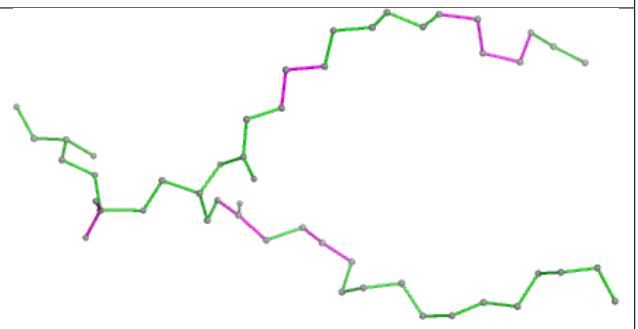


Rings

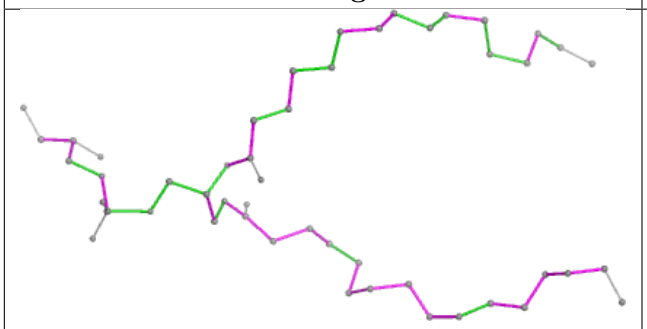
Ligand LHG a 849



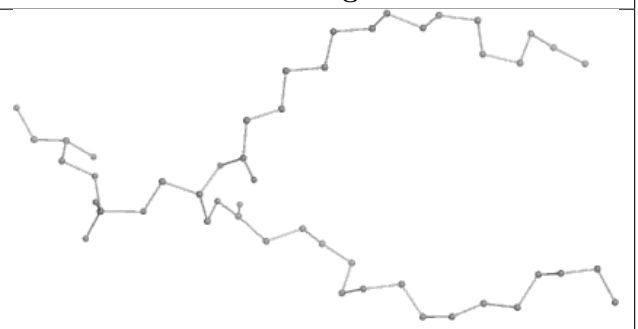
Bond lengths



Bond angles

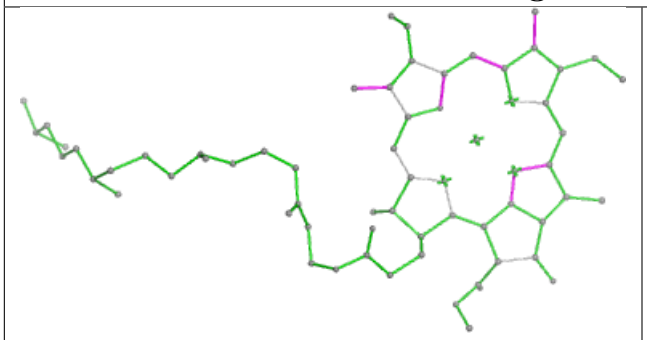


Torsions

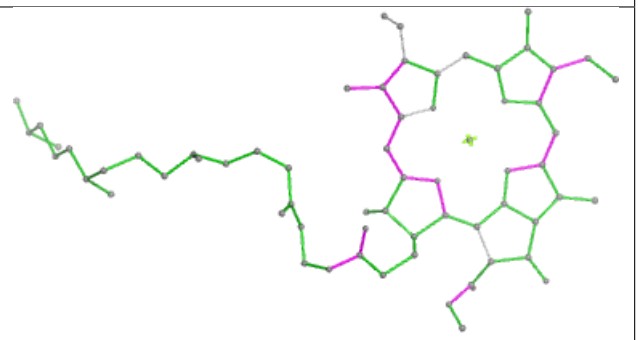


Rings

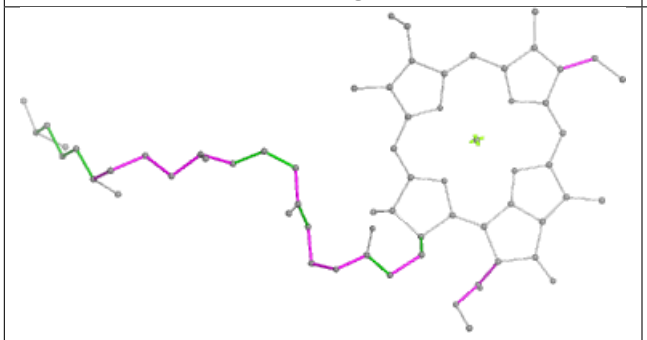
Ligand CLA b 804



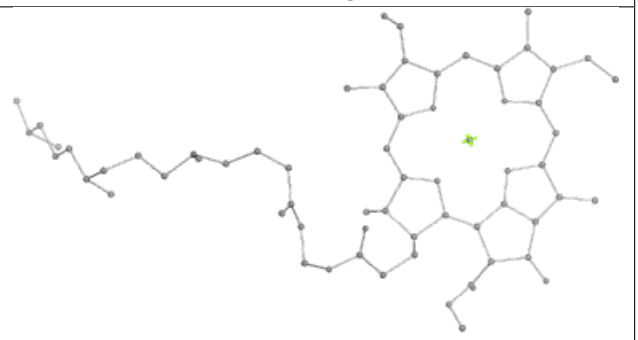
Bond lengths



Bond angles

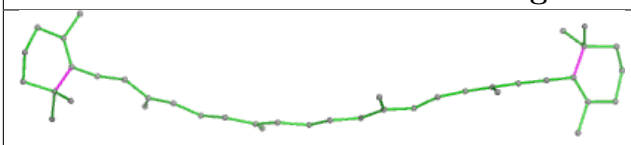


Torsions

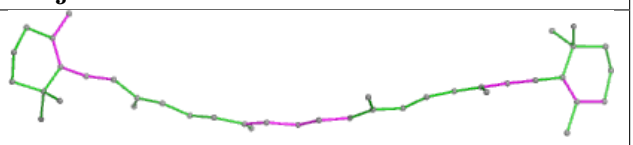


Rings

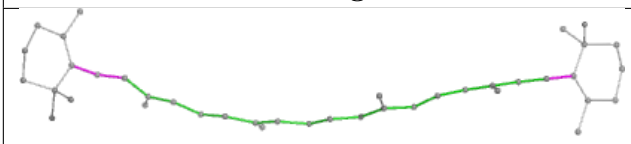
Ligand BCR j 105



Bond lengths



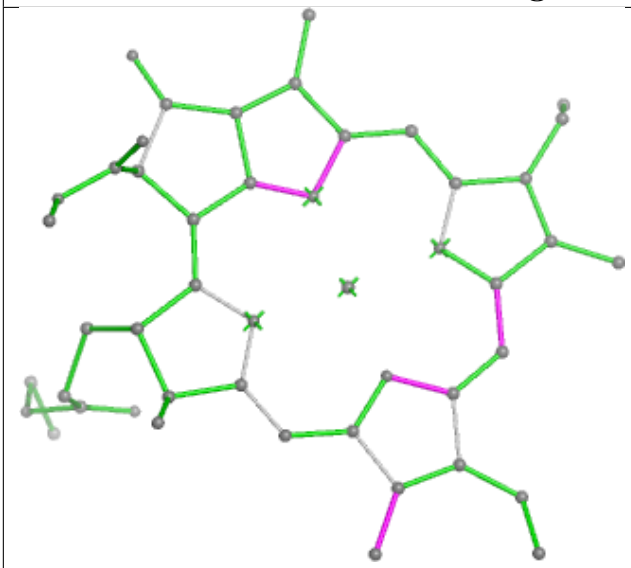
Bond angles



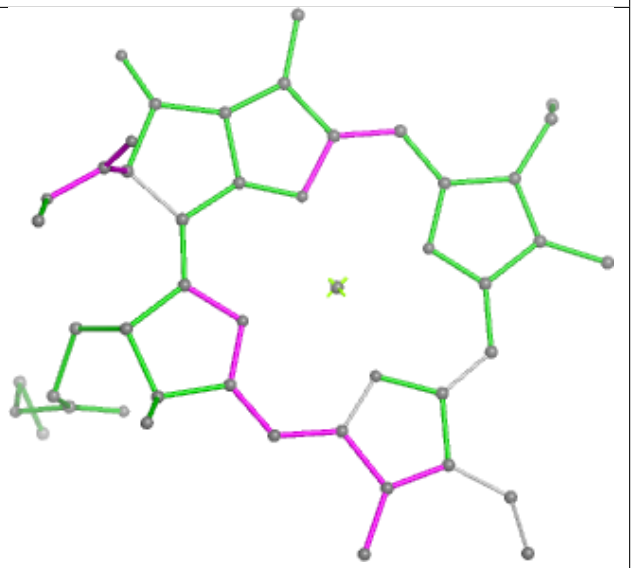
Torsions

Rings

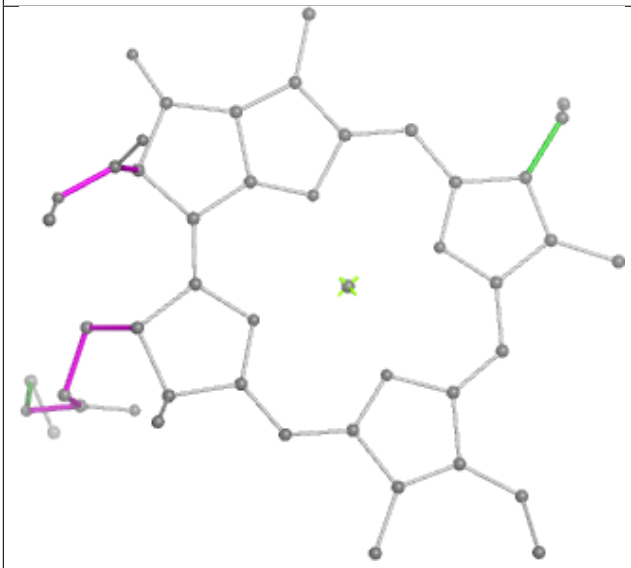
Ligand CLA a 814



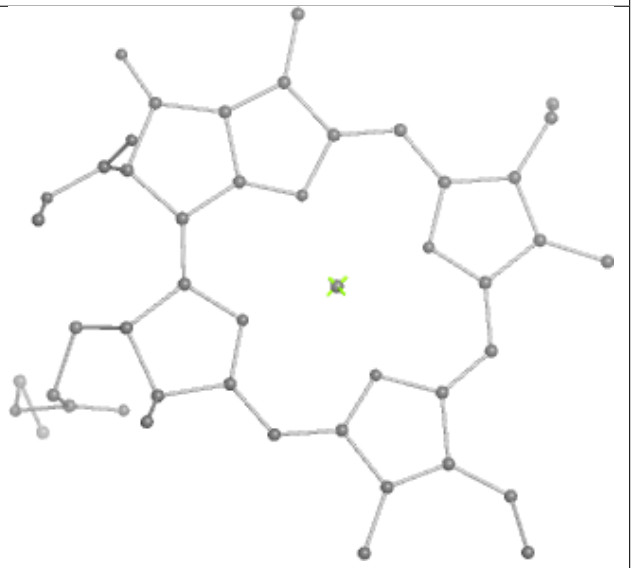
Bond lengths



Bond angles

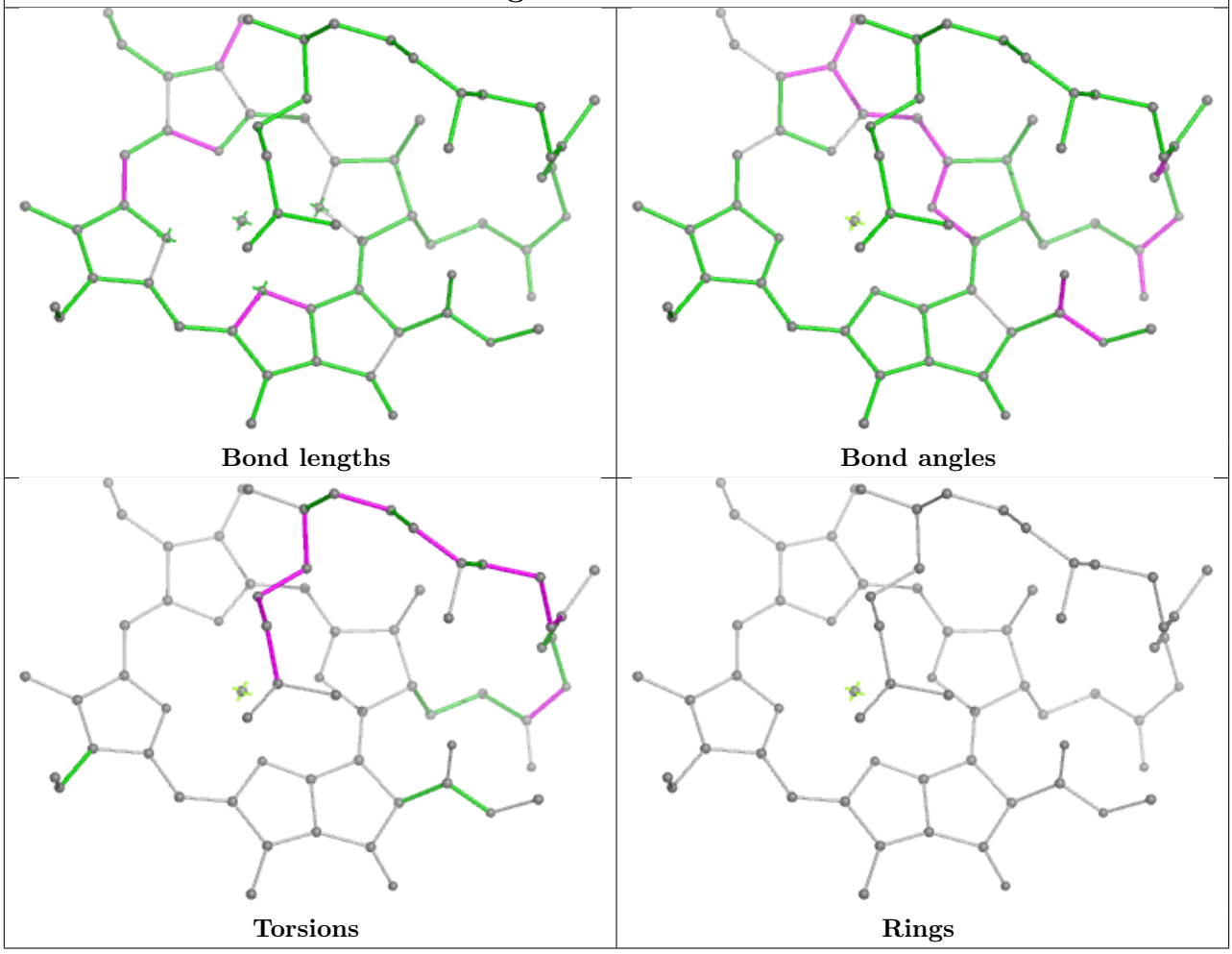


Torsions

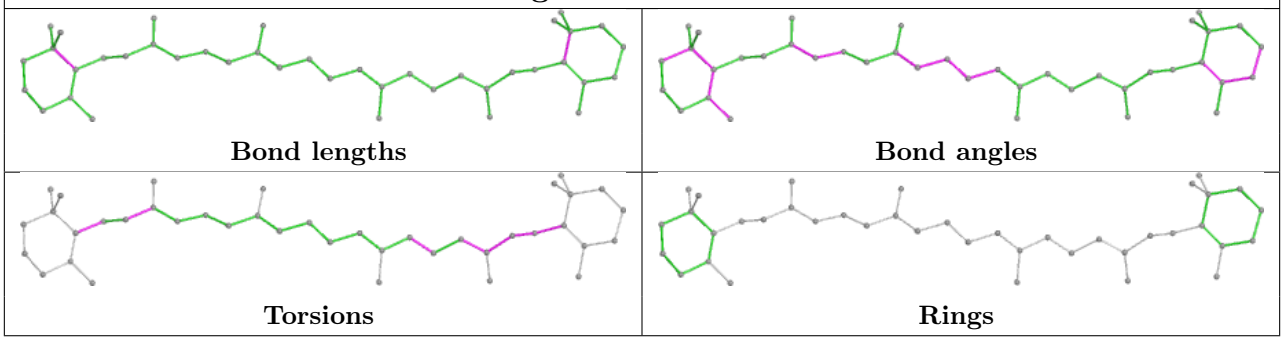


Rings

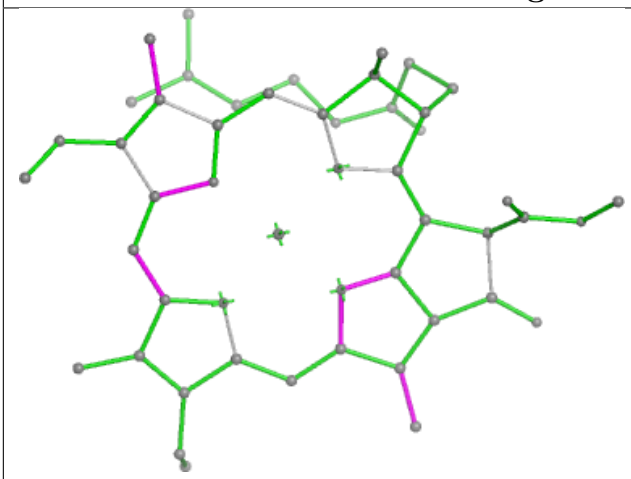
Ligand CLA b 807



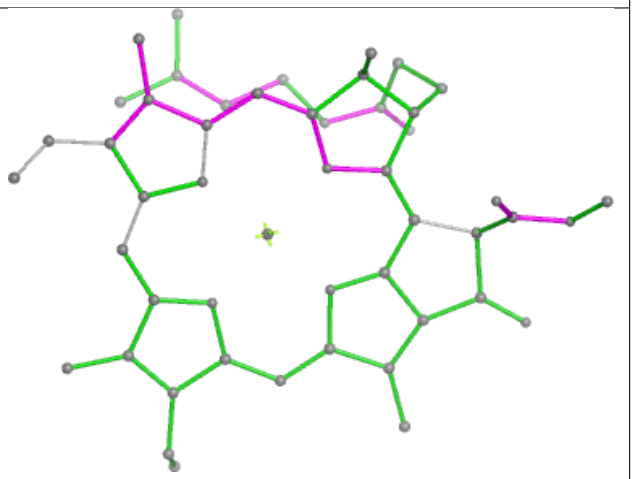
Ligand BCR i 102



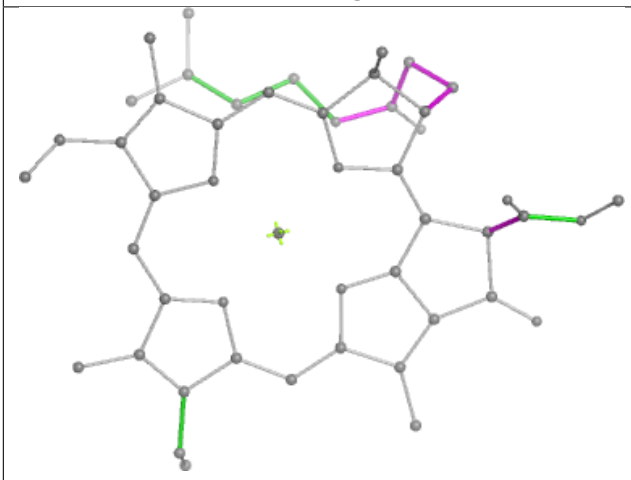
Ligand CLA b 813



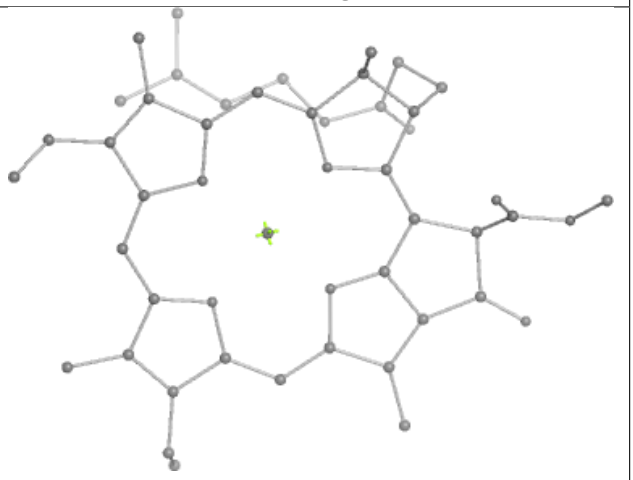
Bond lengths



Bond angles

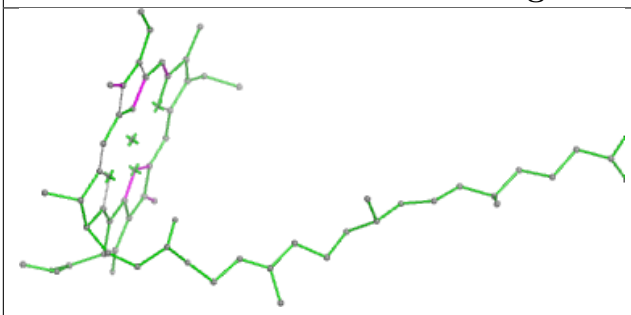


Torsions

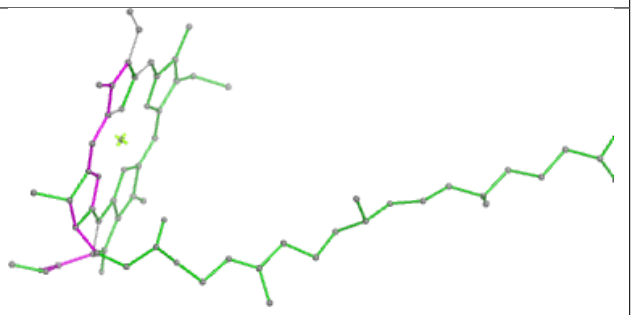


Rings

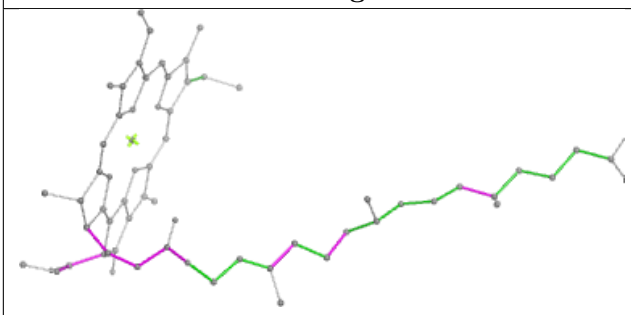
Ligand CLA b 830



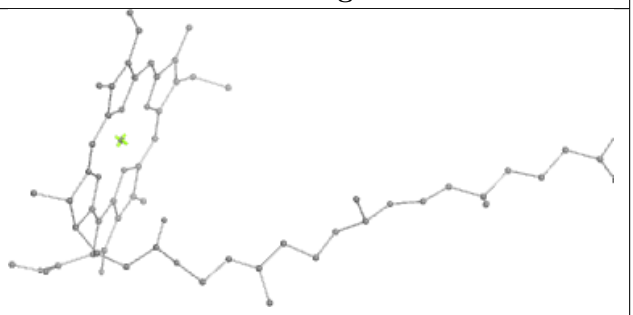
Bond lengths



Bond angles

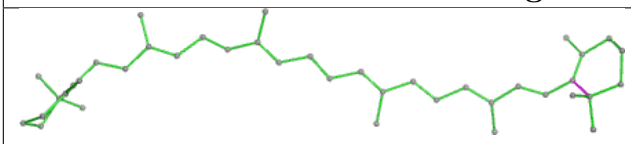


Torsions

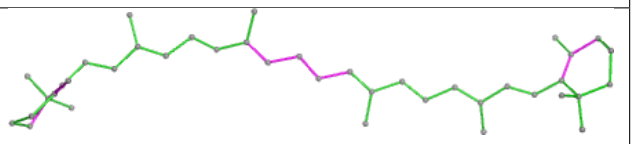


Rings

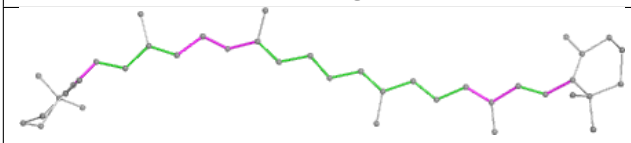
Ligand BCR b 848



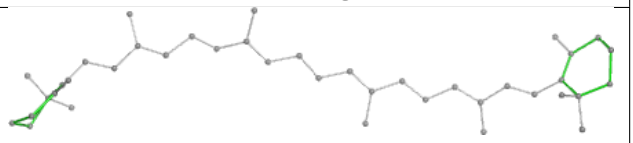
Bond lengths



Bond angles

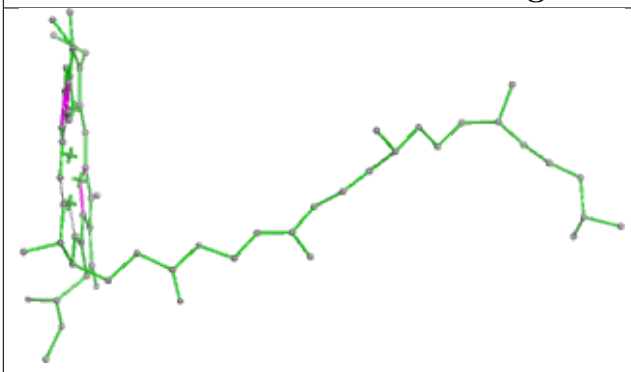


Torsions

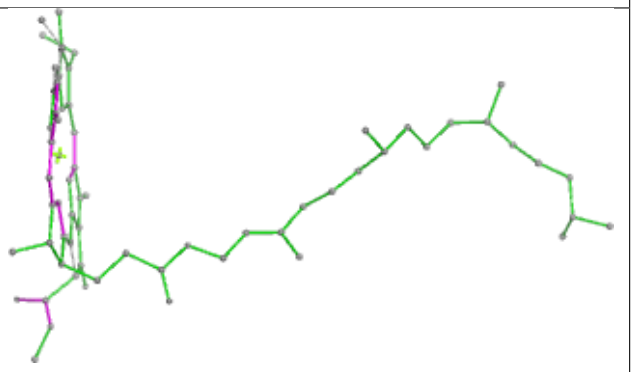


Rings

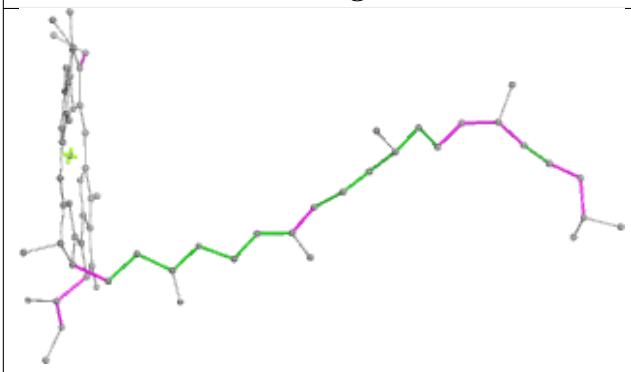
Ligand CLA b 841



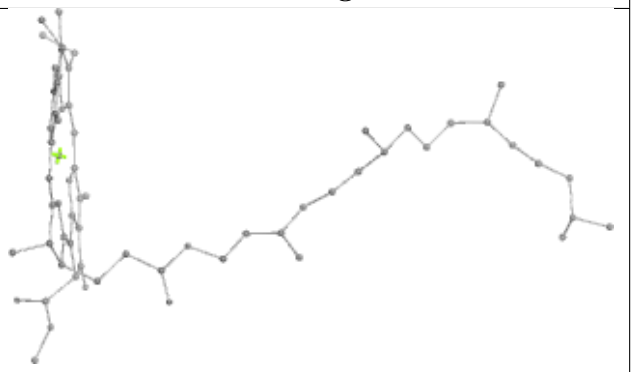
Bond lengths



Bond angles

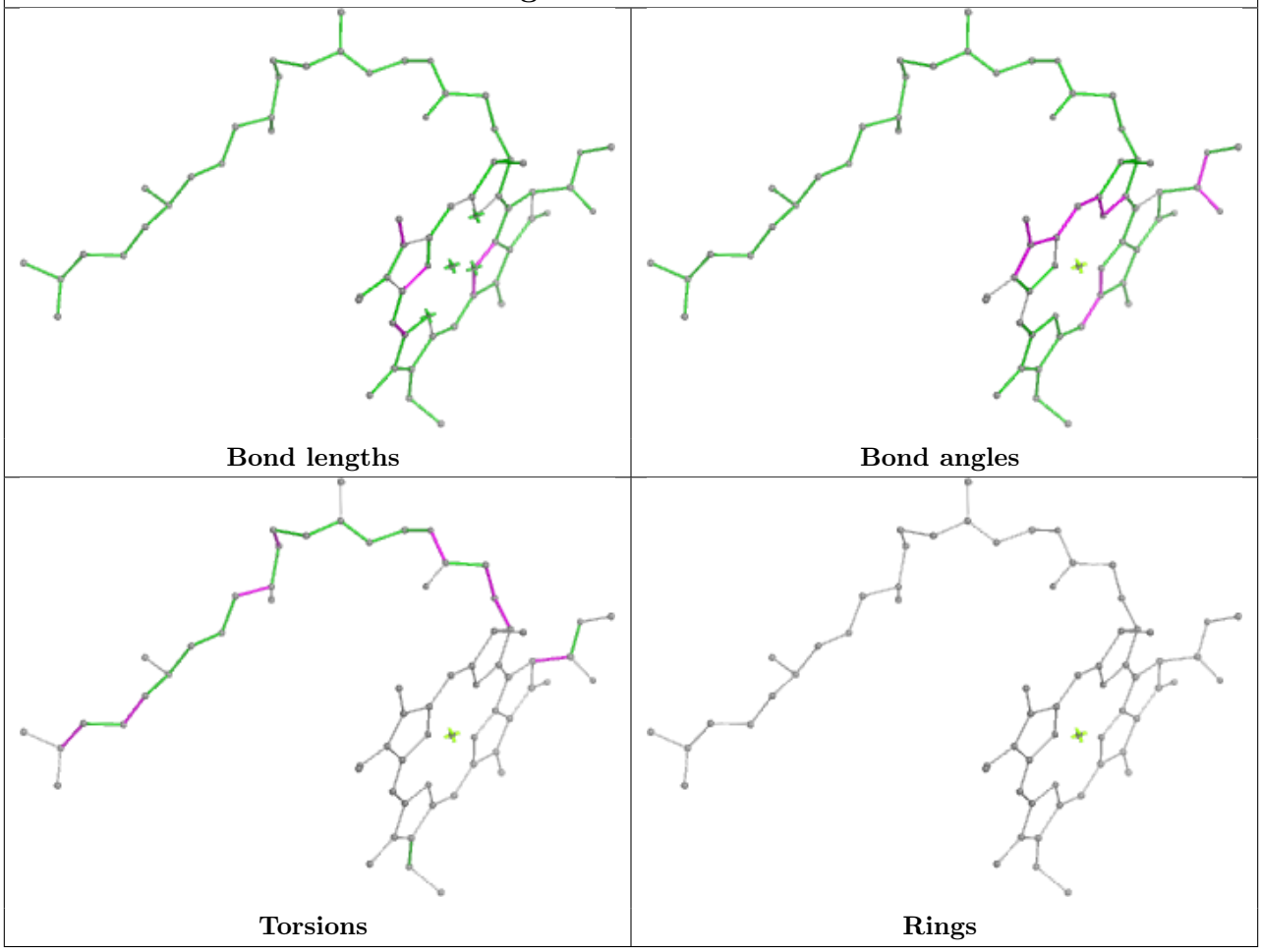


Torsions

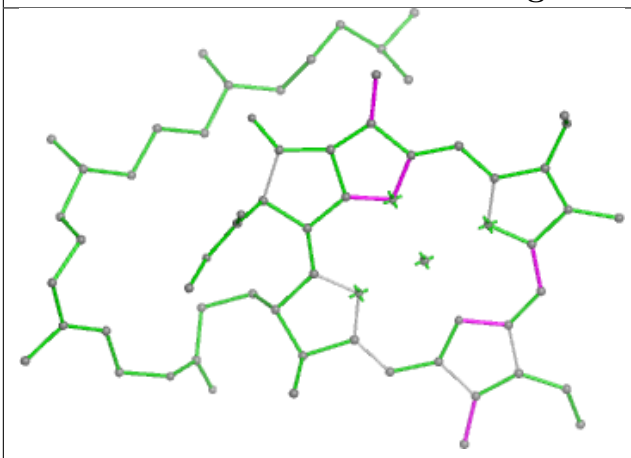


Rings

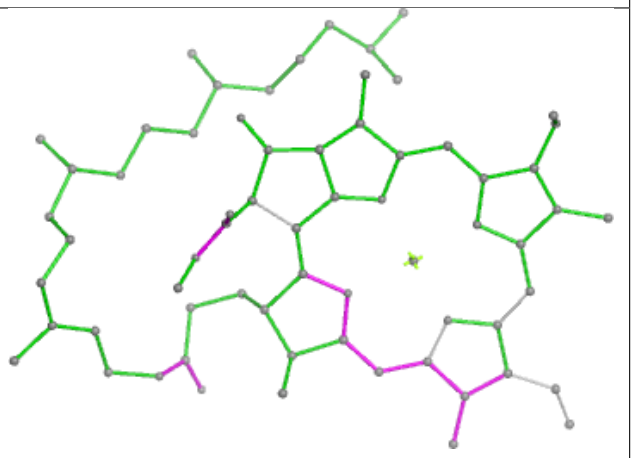
Ligand CLA a 804



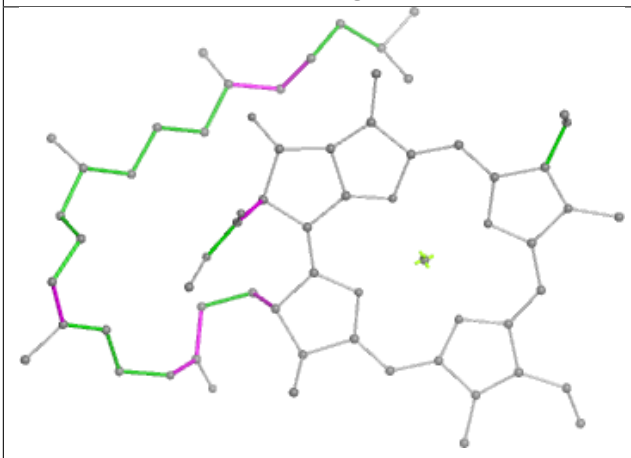
Ligand CLA b 806



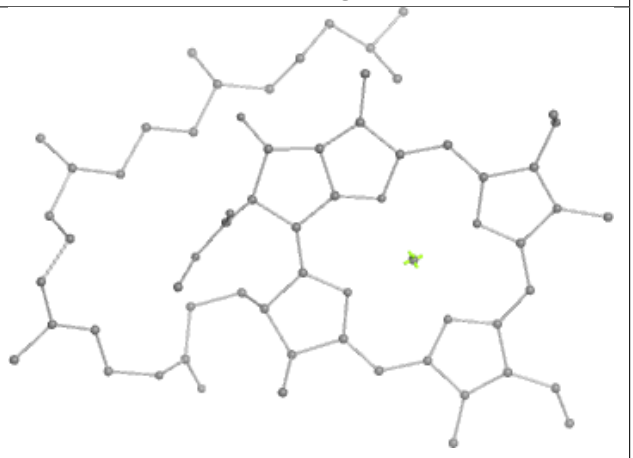
Bond lengths



Bond angles

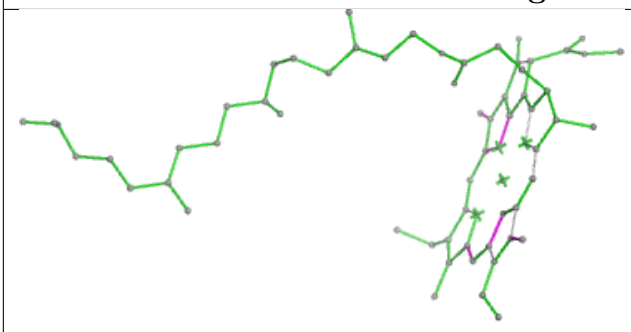


Torsions

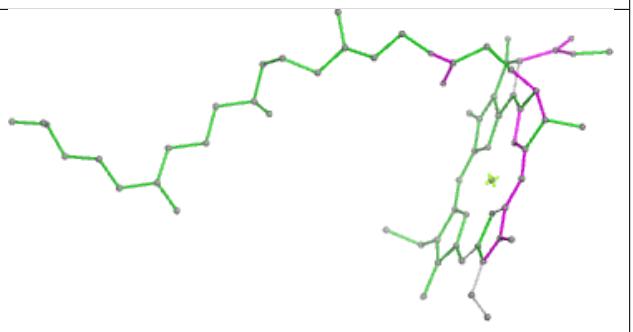


Rings

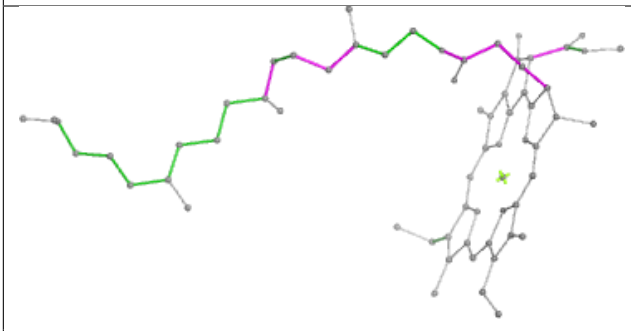
Ligand CLA a 830



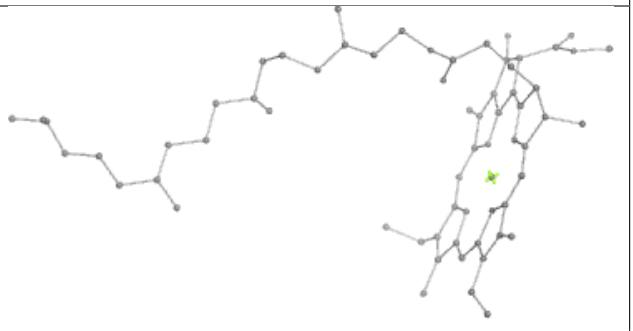
Bond lengths



Bond angles

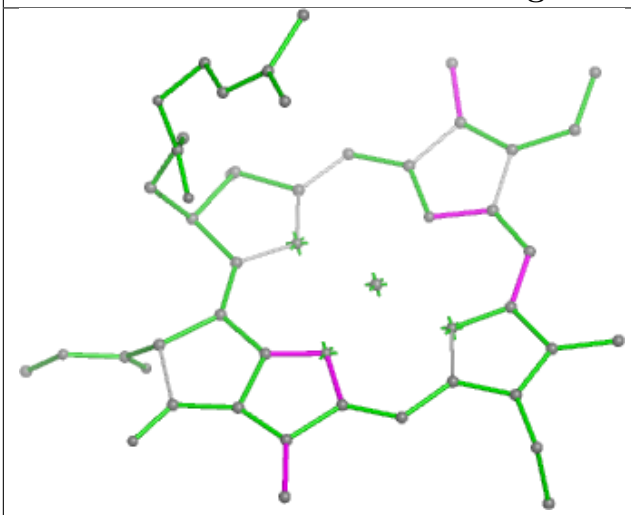


Torsions

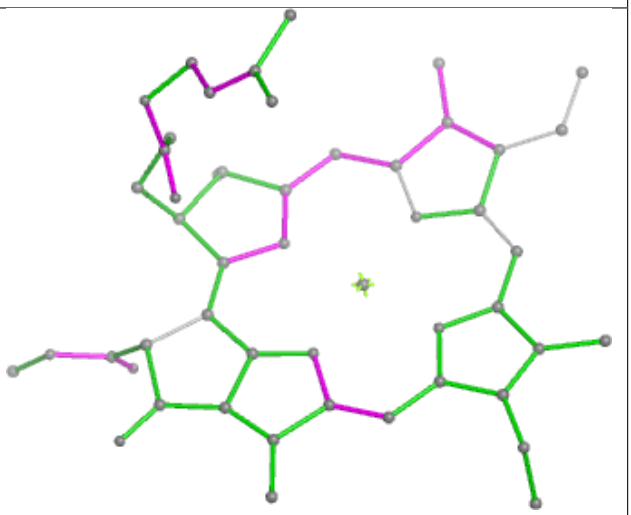


Rings

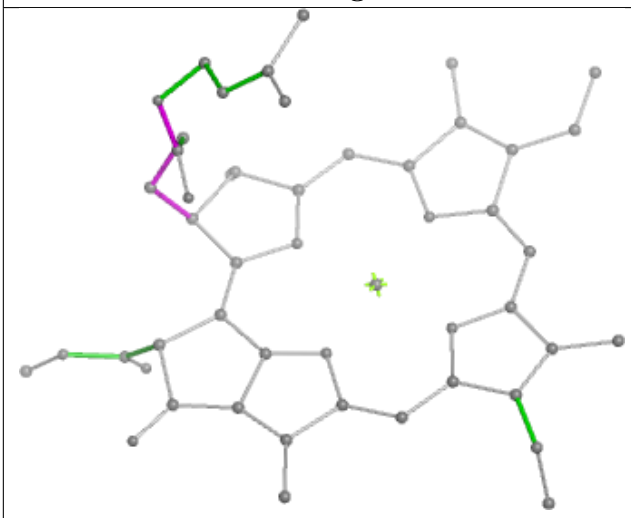
Ligand CLA b 832



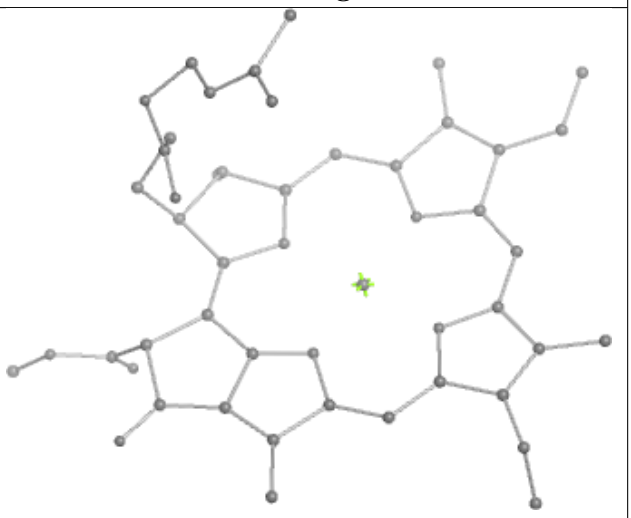
Bond lengths



Bond angles

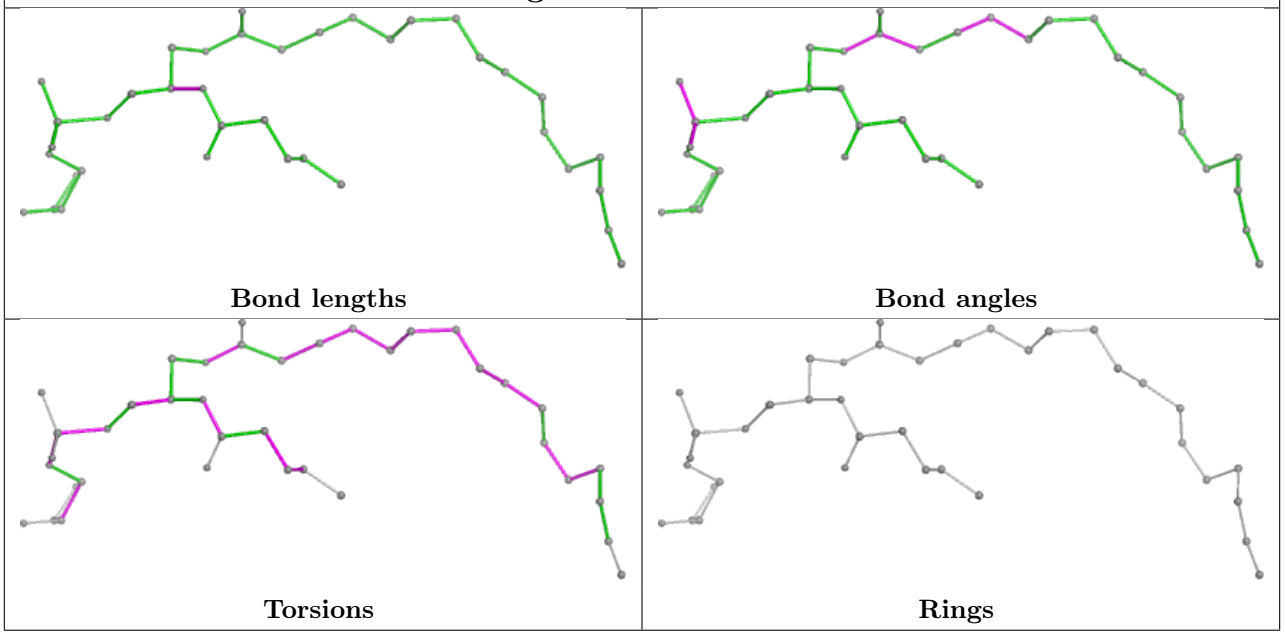


Torsions

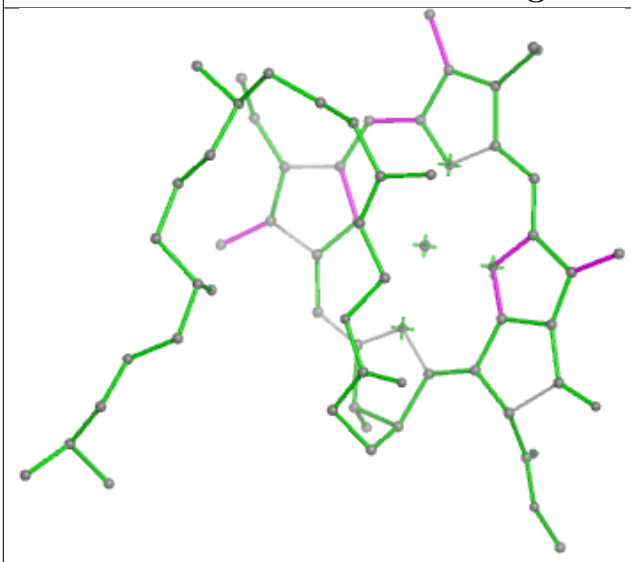


Rings

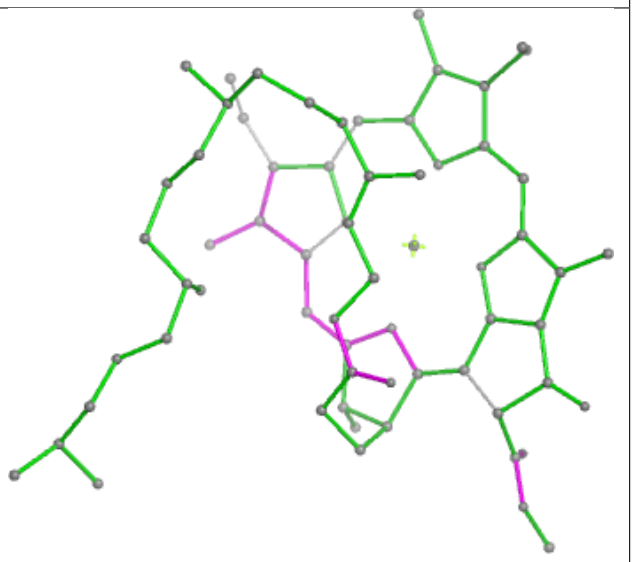
Ligand LHG b 851



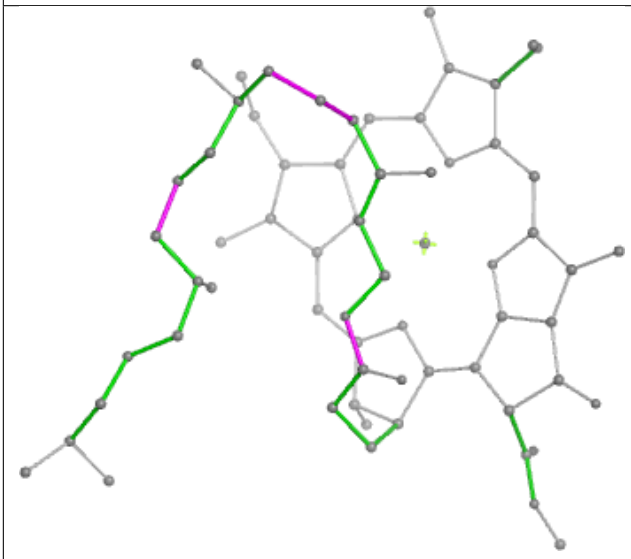
Ligand CLA b 809



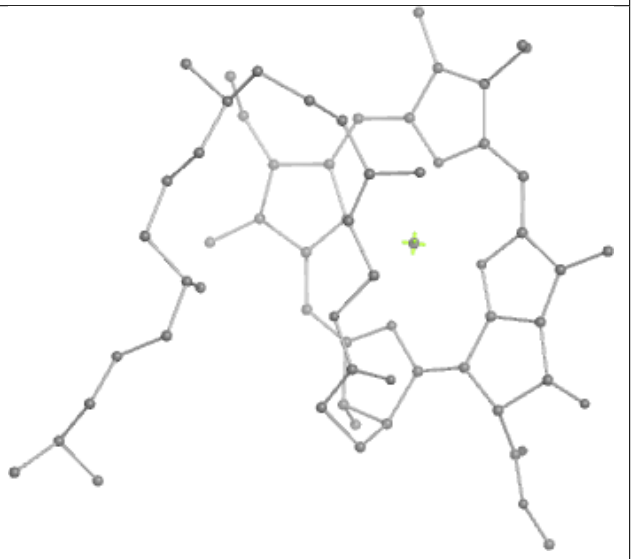
Bond lengths



Bond angles

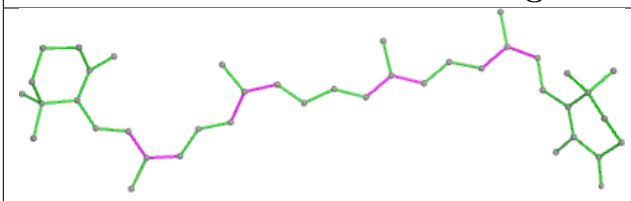


Torsions

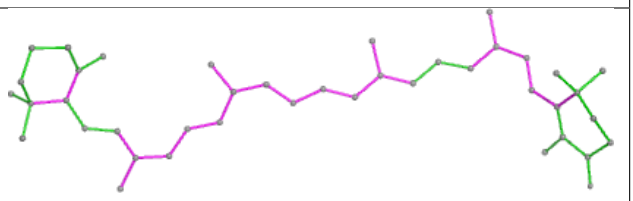


Rings

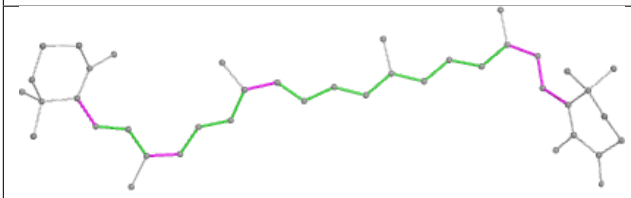
Ligand ECH b 846



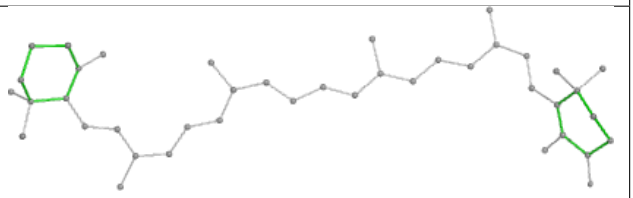
Bond lengths



Bond angles

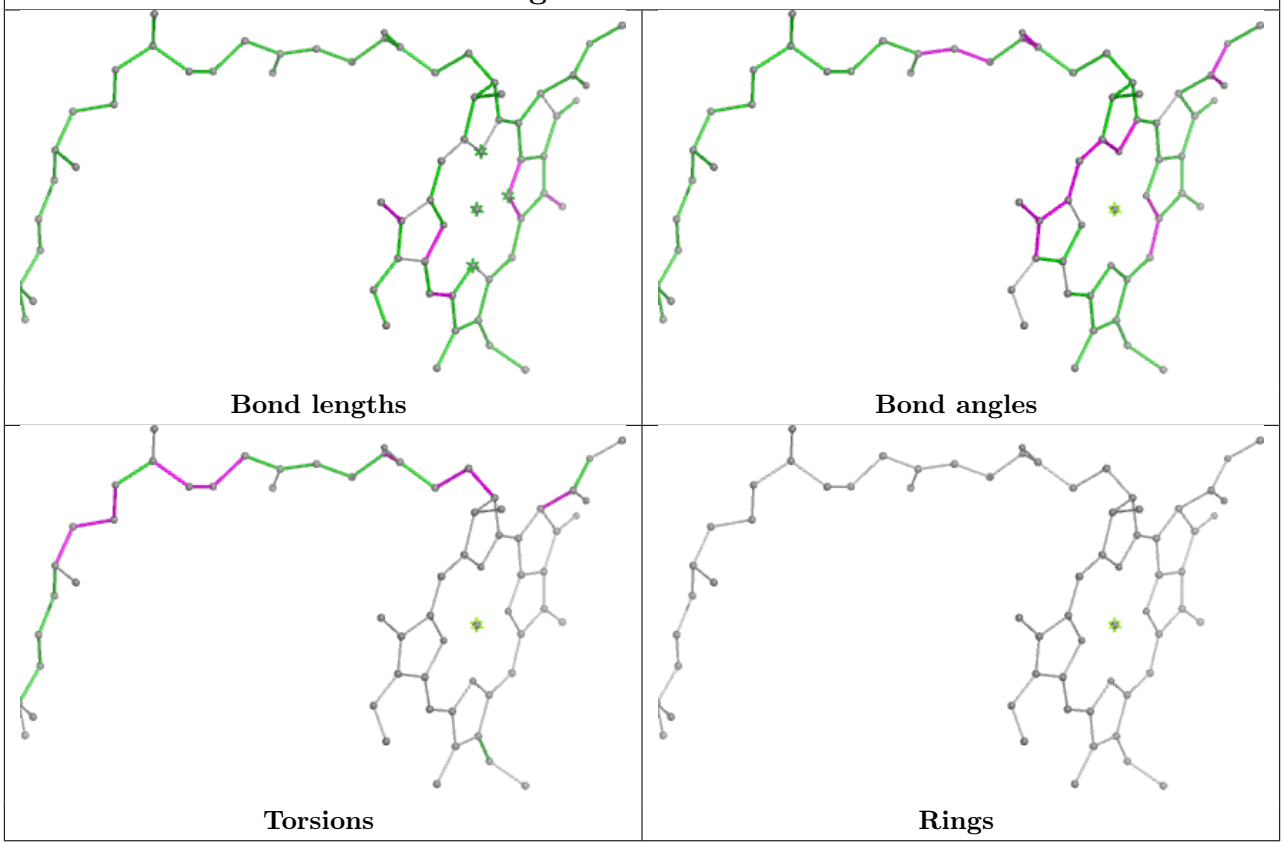


Torsions

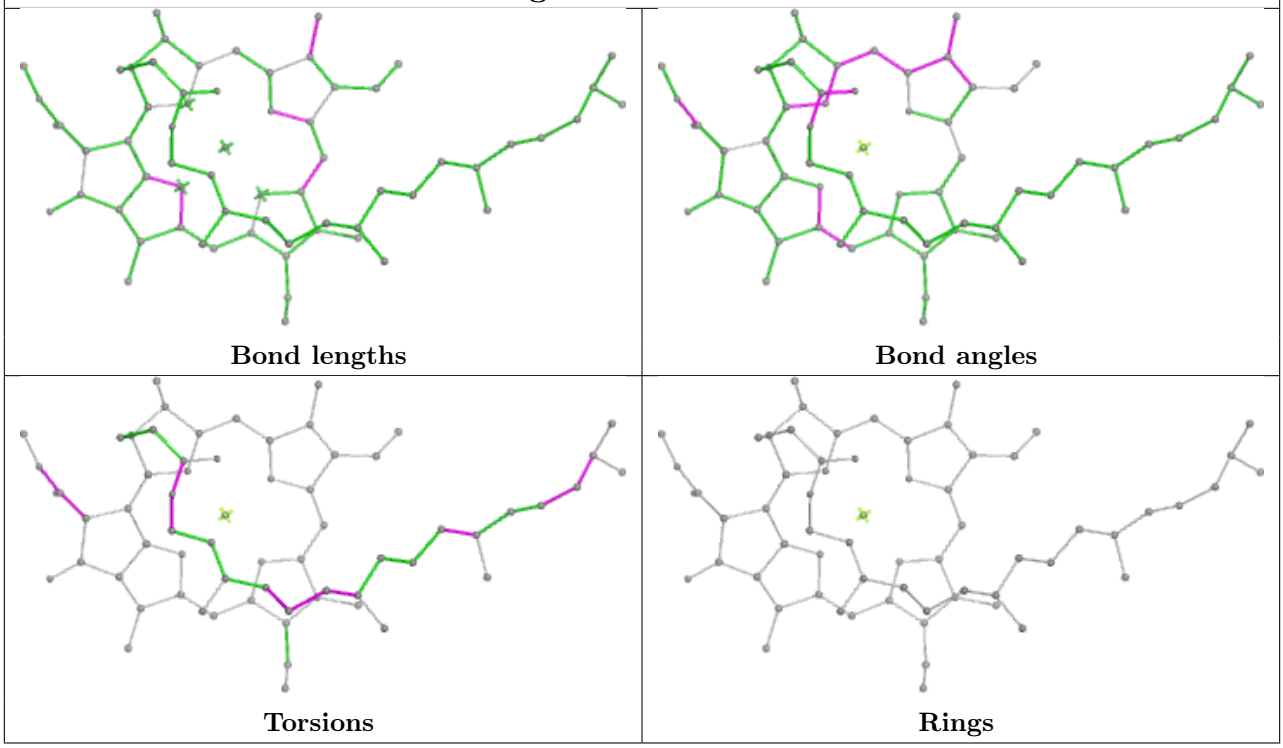


Rings

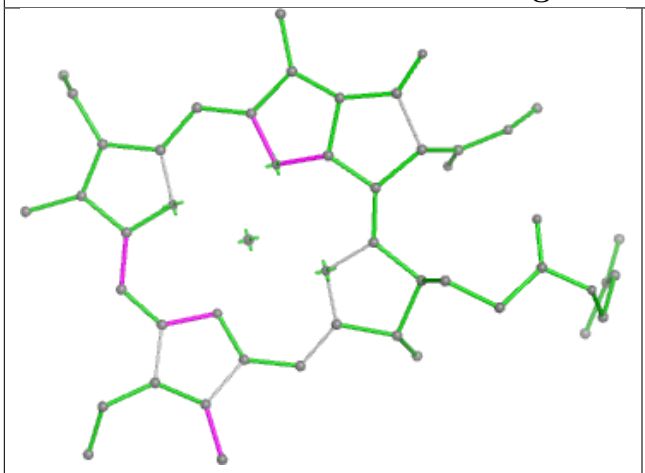
Ligand CLA a 841



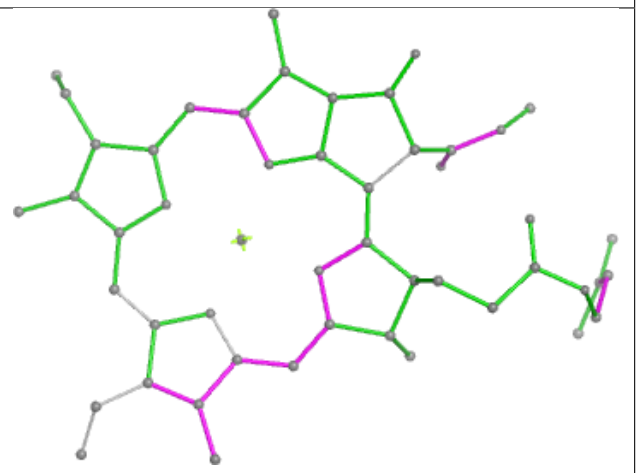
Ligand CLA a 840



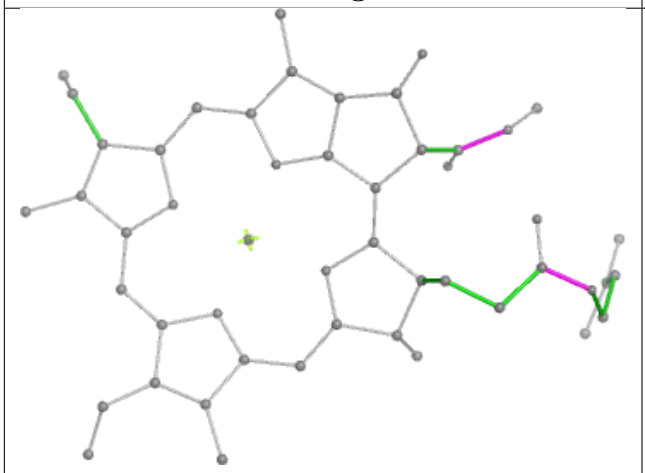
Ligand CLA f 203



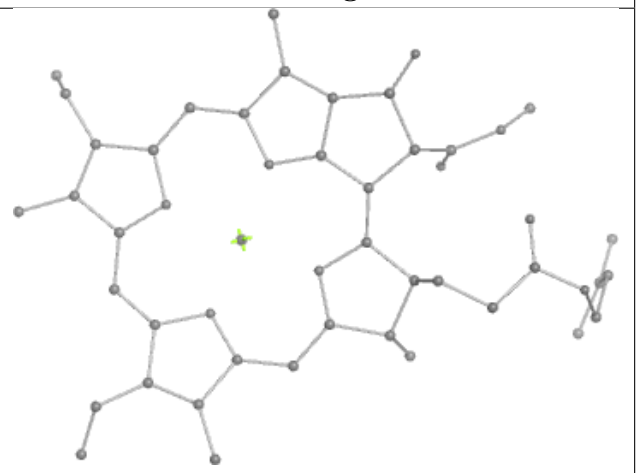
Bond lengths



Bond angles

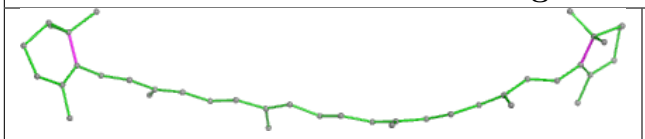


Torsions

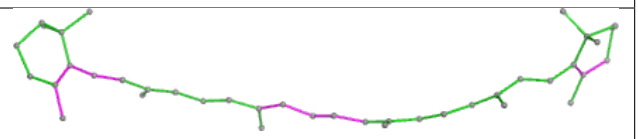


Rings

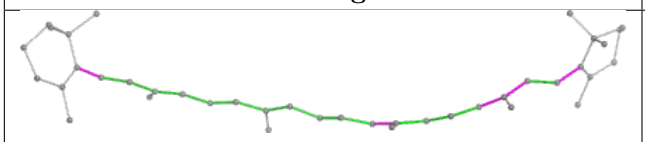
Ligand BCR i 101



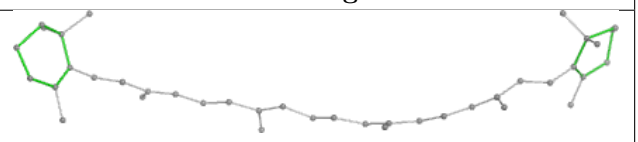
Bond lengths



Bond angles

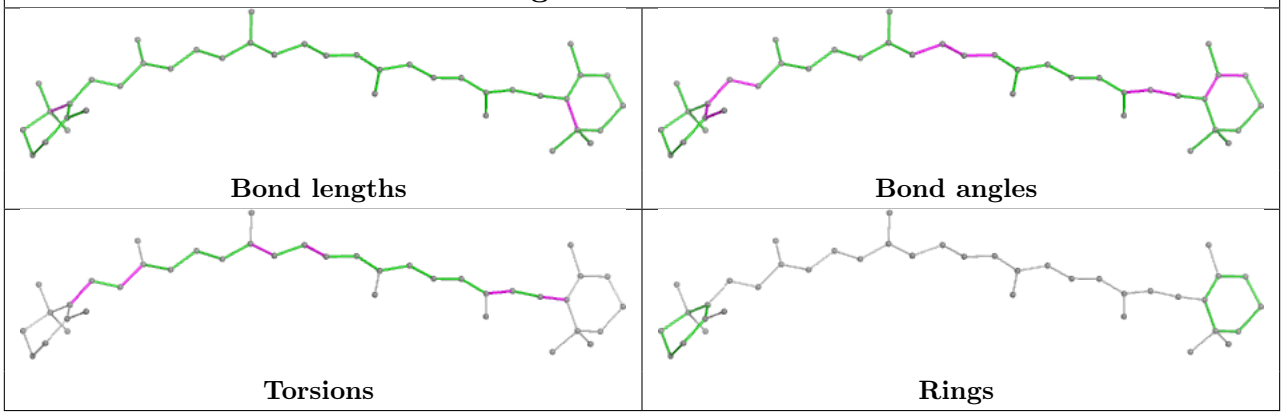


Torsions

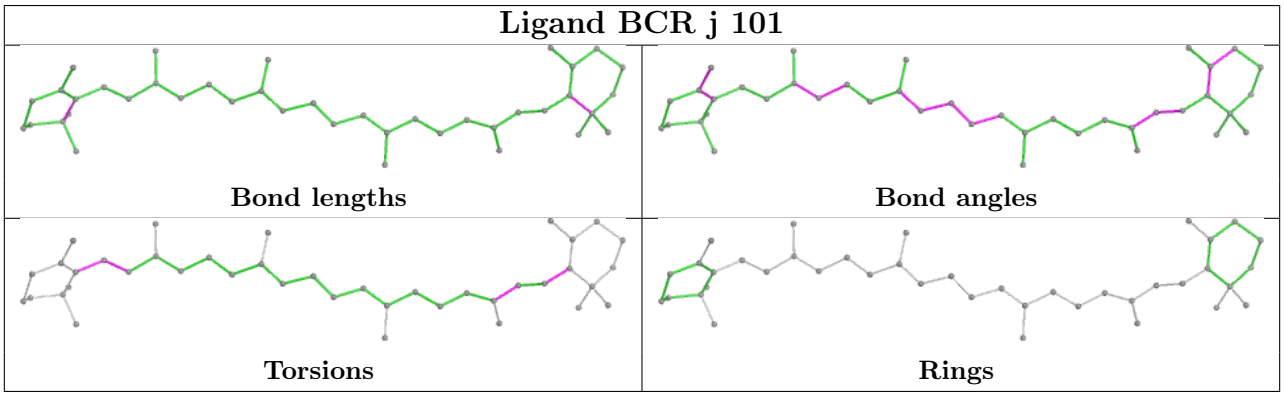


Rings

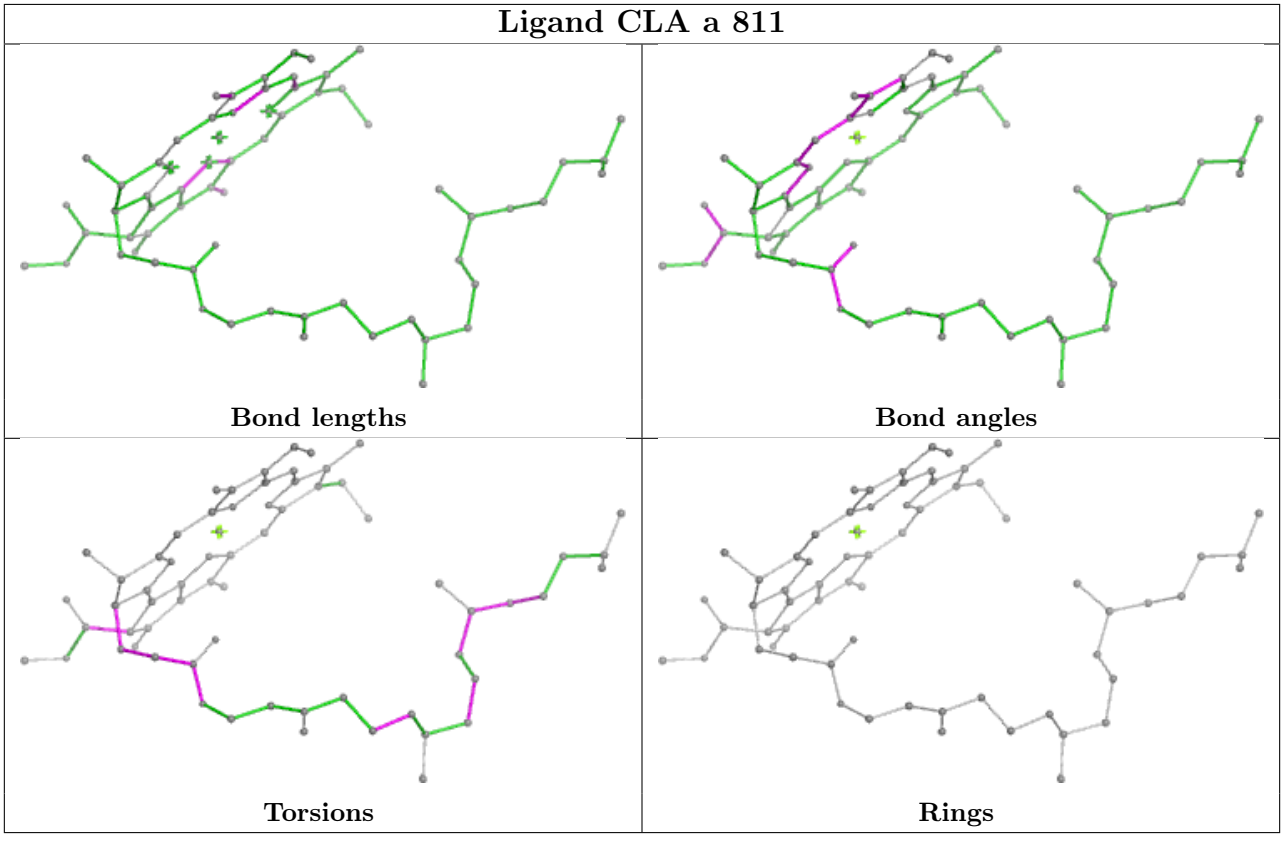
Ligand BCR f 202



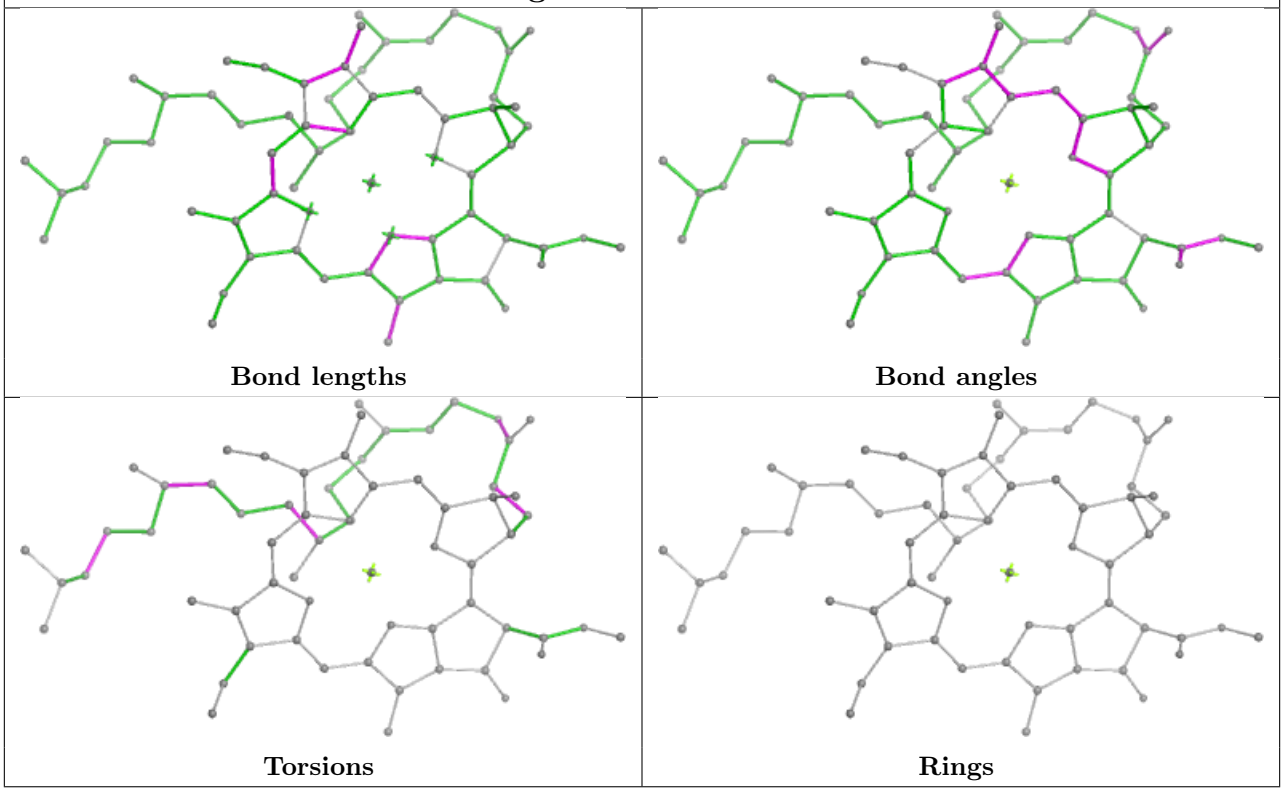
Ligand BCR j 101



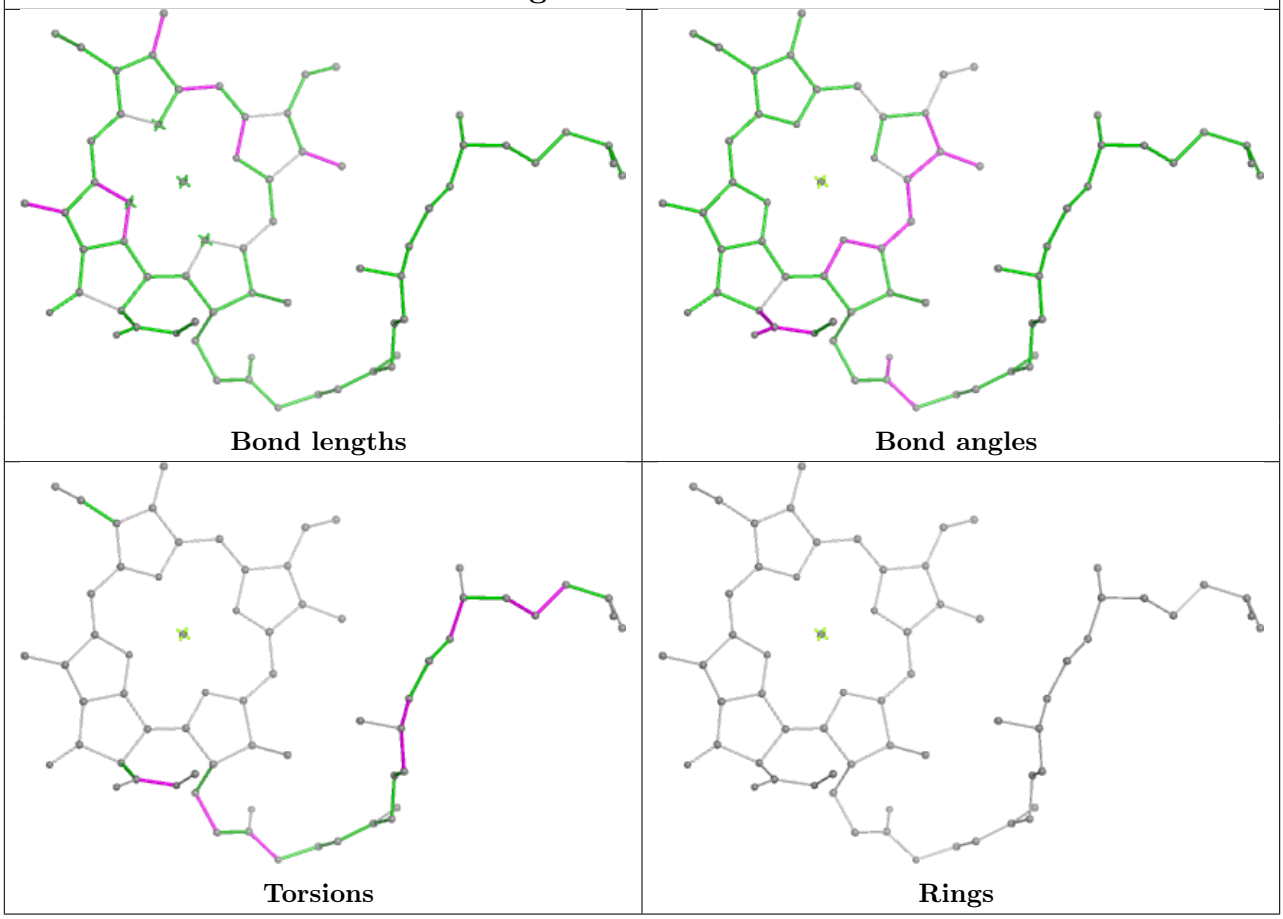
Ligand CLA a 811



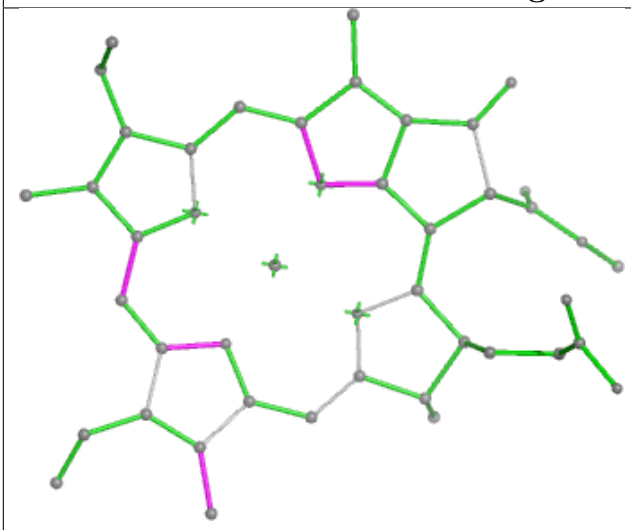
Ligand CLA b 818



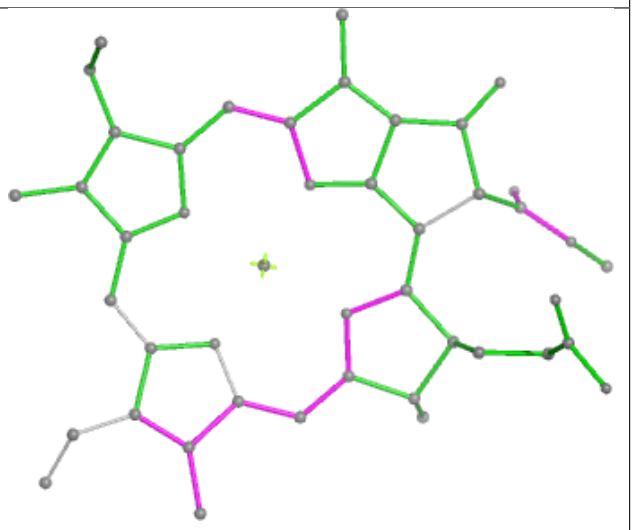
Ligand CLA a 813



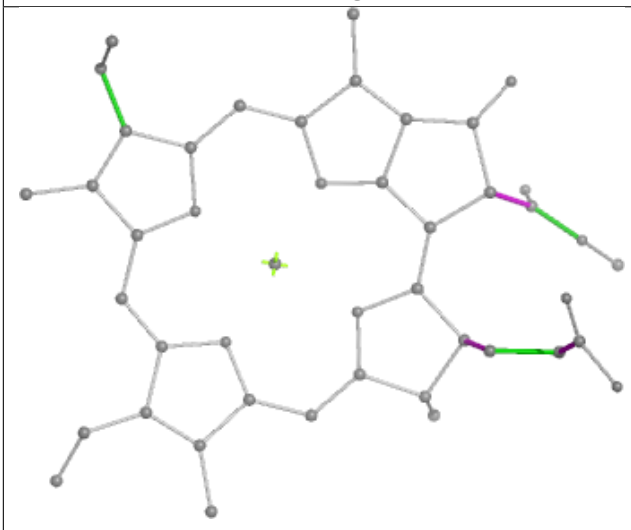
Ligand CLA a 842



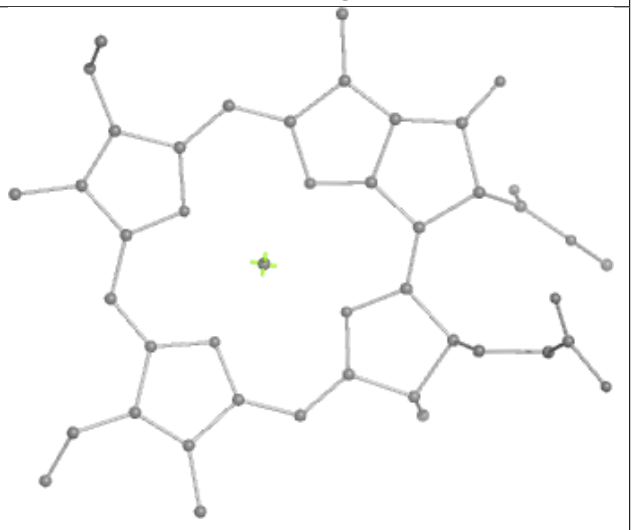
Bond lengths



Bond angles

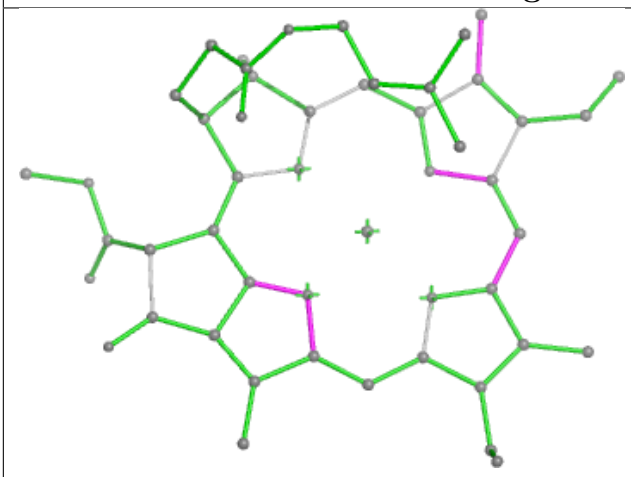


Torsions

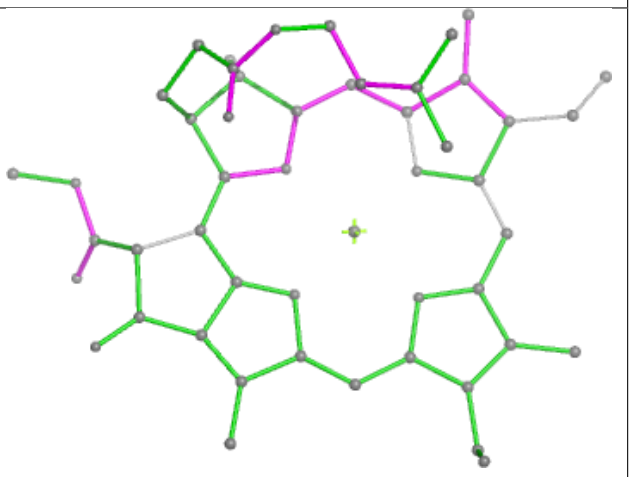


Rings

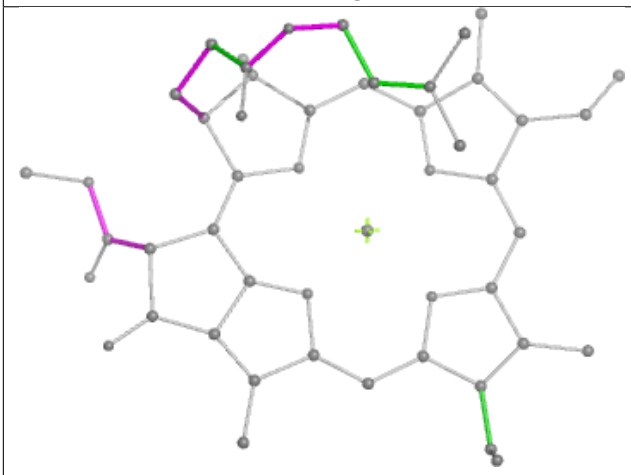
Ligand CLA l 1501



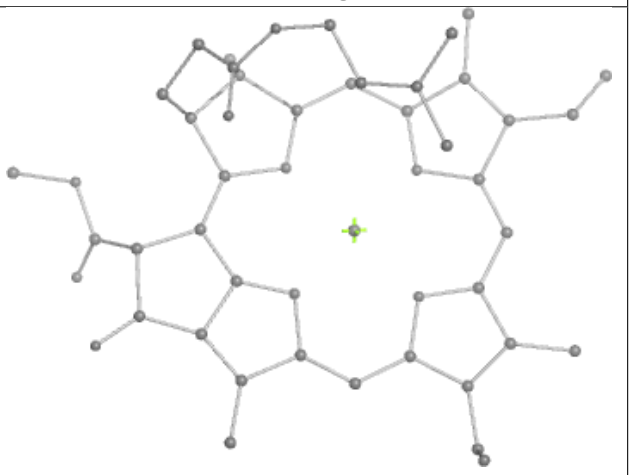
Bond lengths



Bond angles

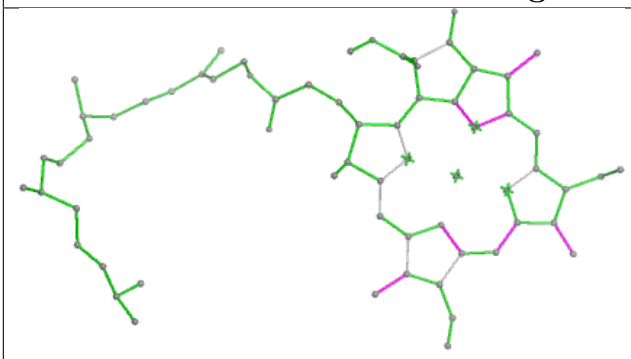


Torsions

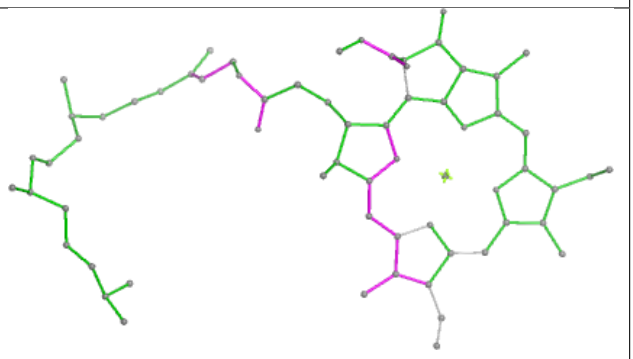


Rings

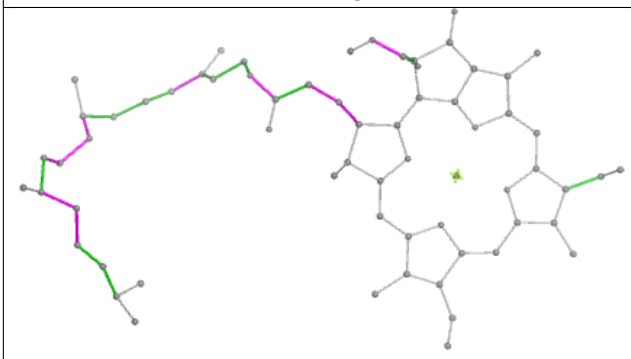
Ligand CLA a 827



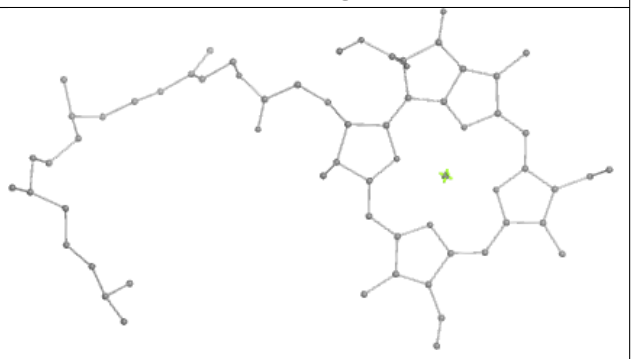
Bond lengths



Bond angles

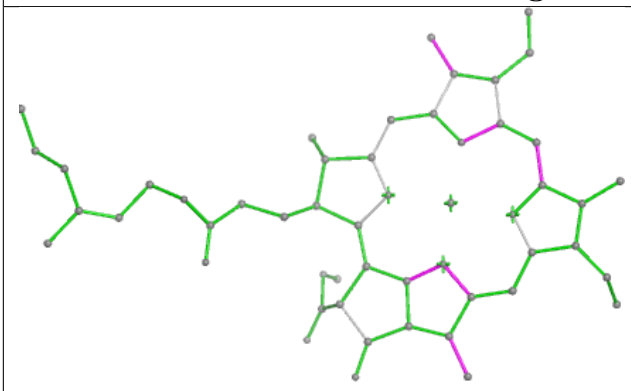


Torsions

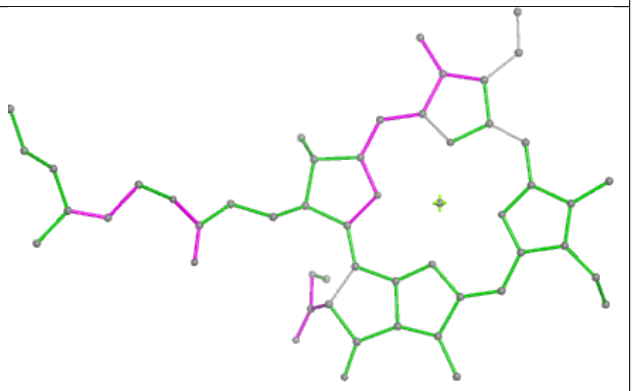


Rings

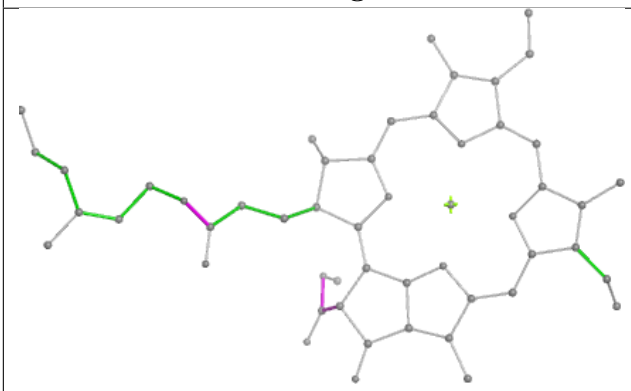
Ligand CLA b 837



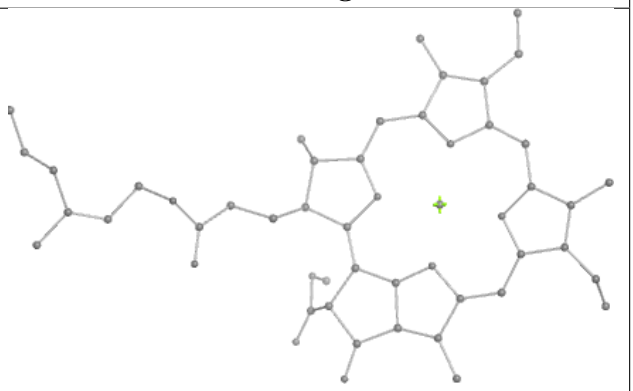
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

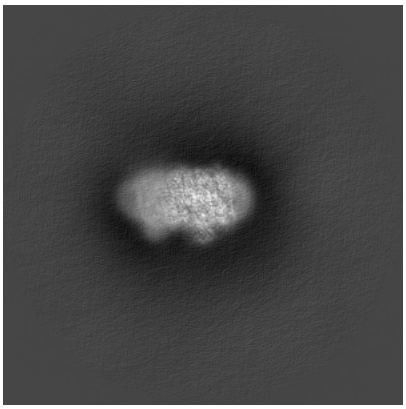
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15621. These allow visual inspection of the internal detail of the map and identification of artifacts.

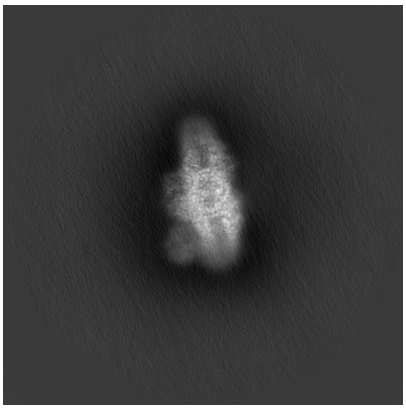
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

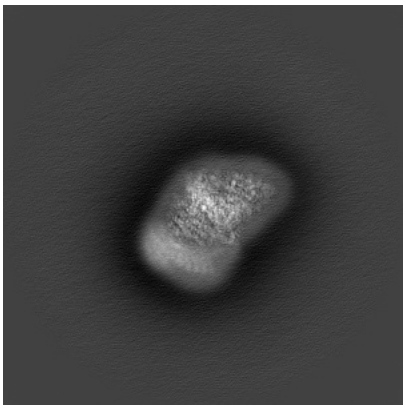
6.1.1 Primary map



X

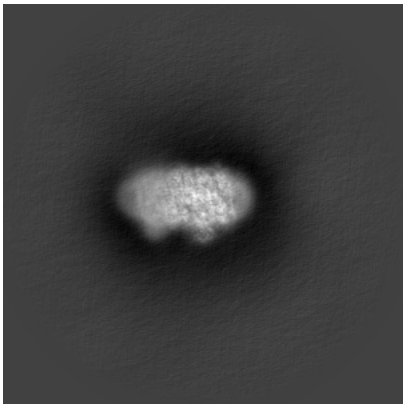


Y

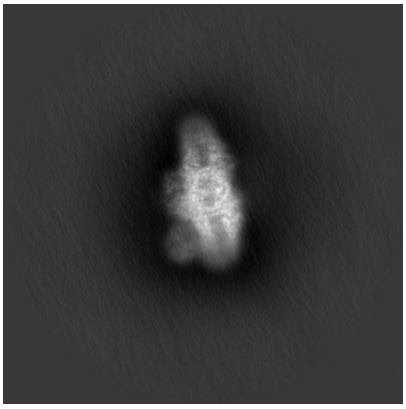


Z

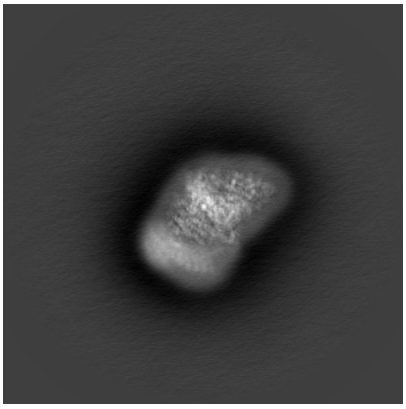
6.1.2 Raw map



X



Y

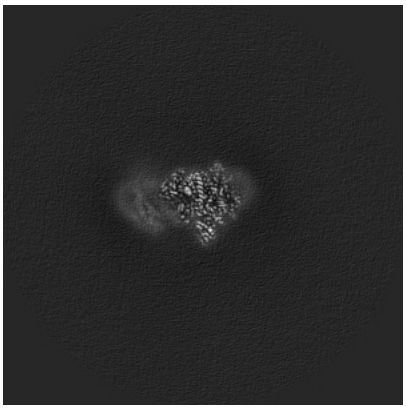


Z

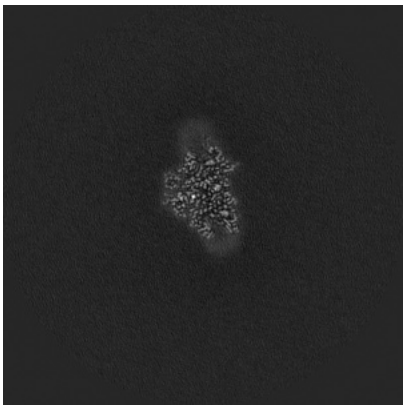
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

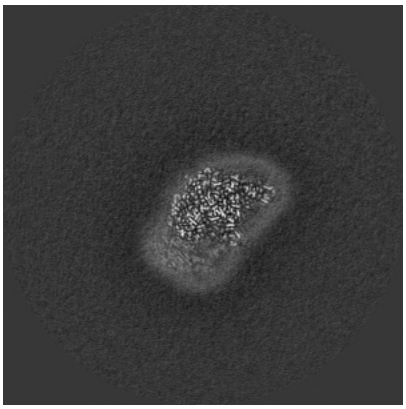
6.2.1 Primary map



X Index: 200

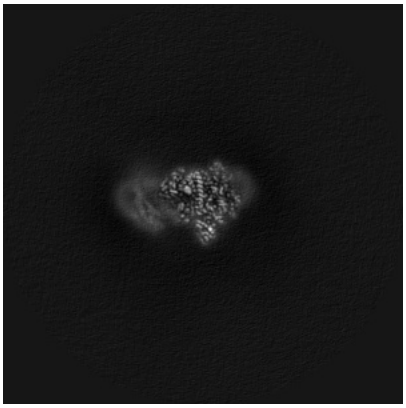


Y Index: 200

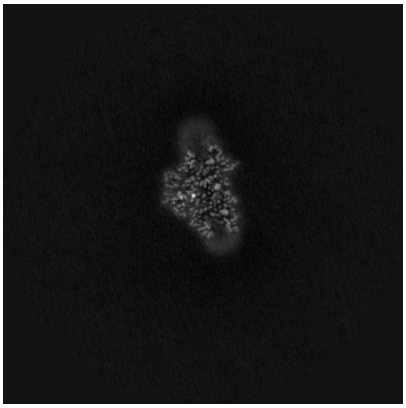


Z Index: 200

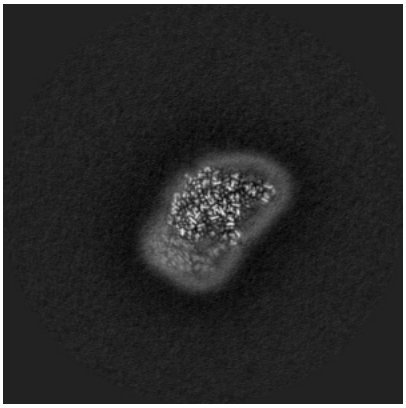
6.2.2 Raw map



X Index: 200



Y Index: 200

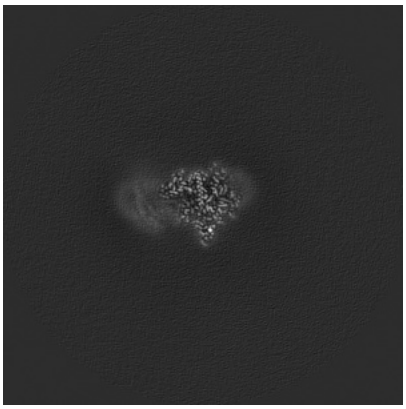


Z Index: 200

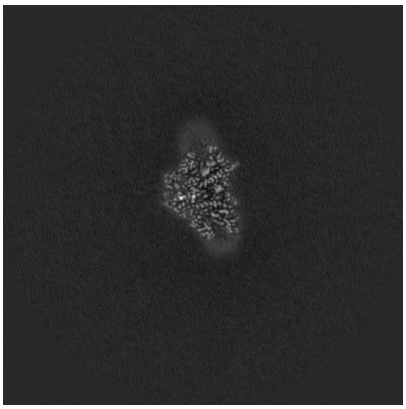
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

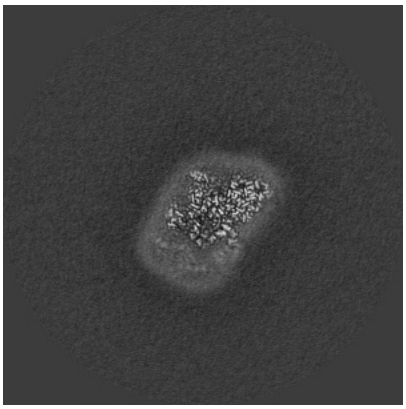
6.3.1 Primary map



X Index: 201

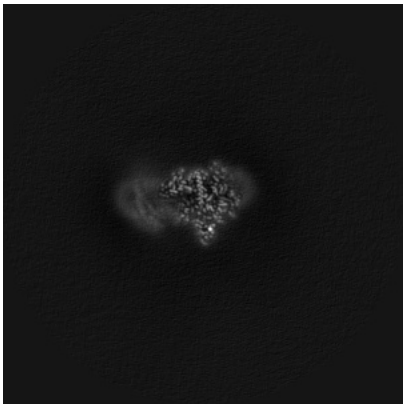


Y Index: 199

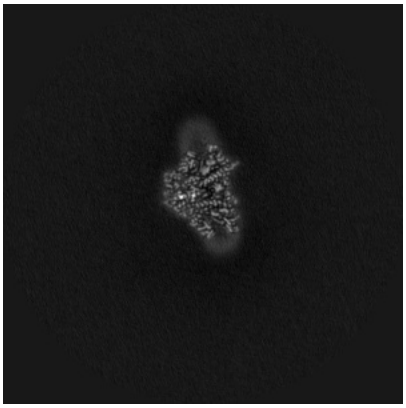


Z Index: 209

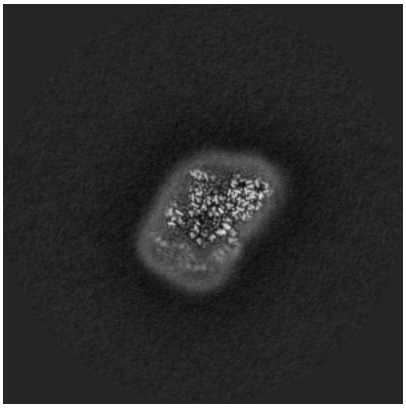
6.3.2 Raw map



X Index: 201



Y Index: 199

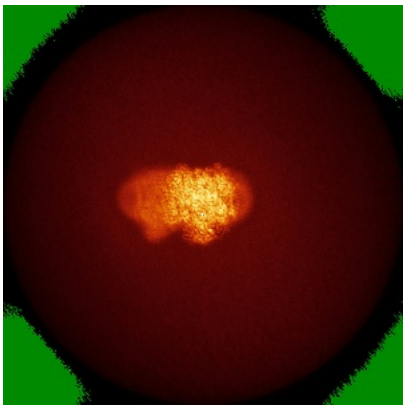


Z Index: 209

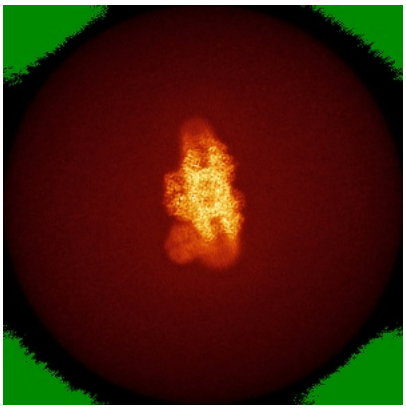
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

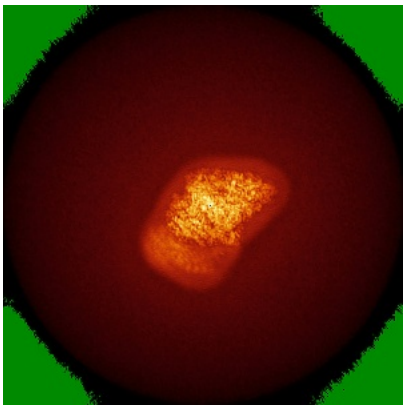
6.4.1 Primary map



X

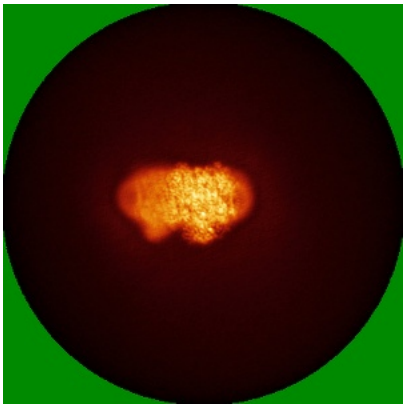


Y

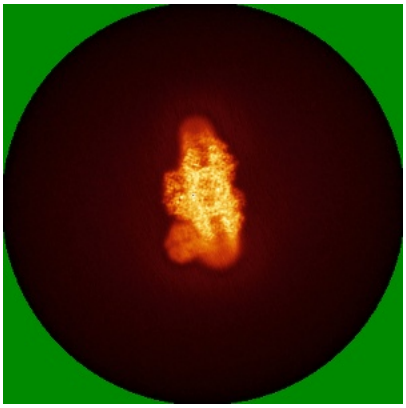


Z

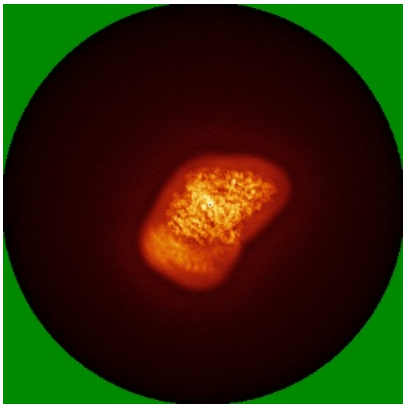
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

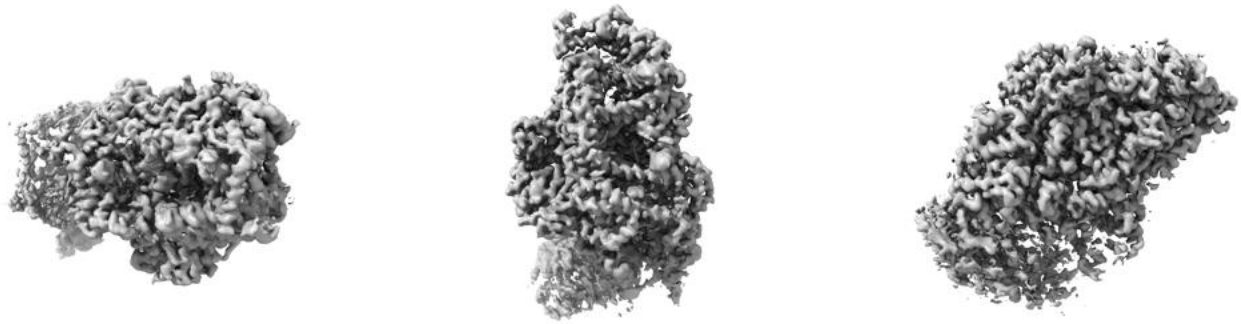
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

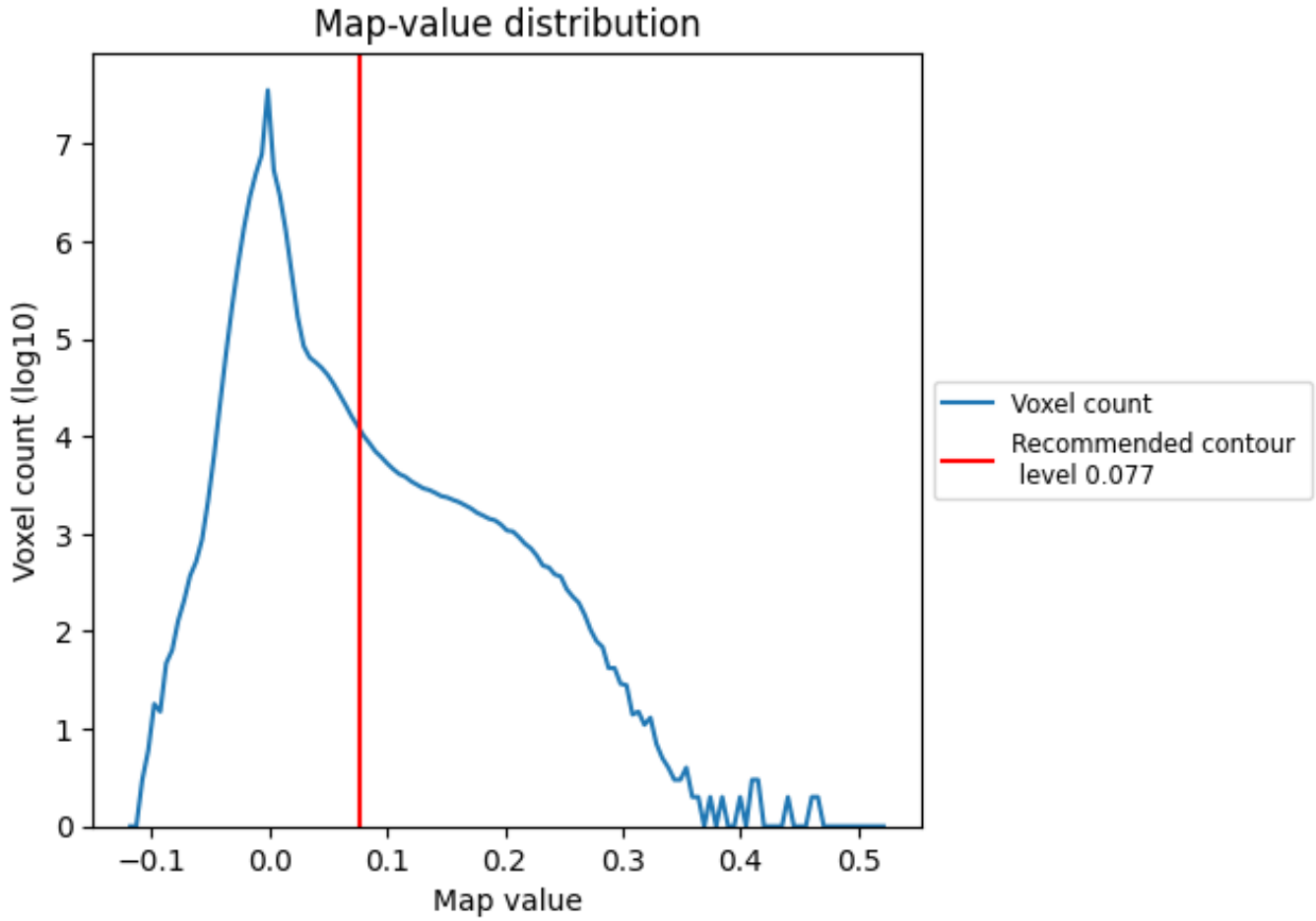
6.6 Mask visualisation (i)

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

7 Map analysis

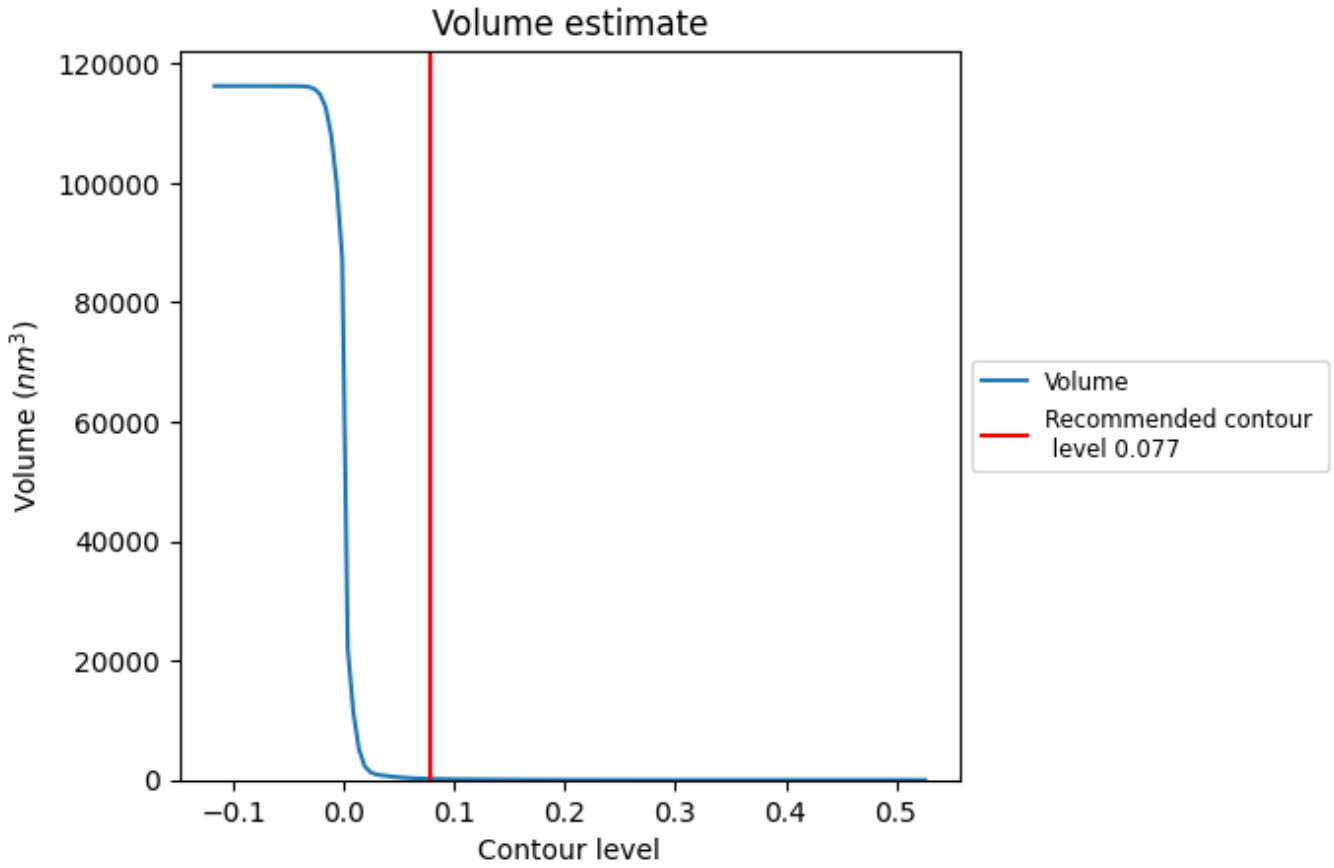
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

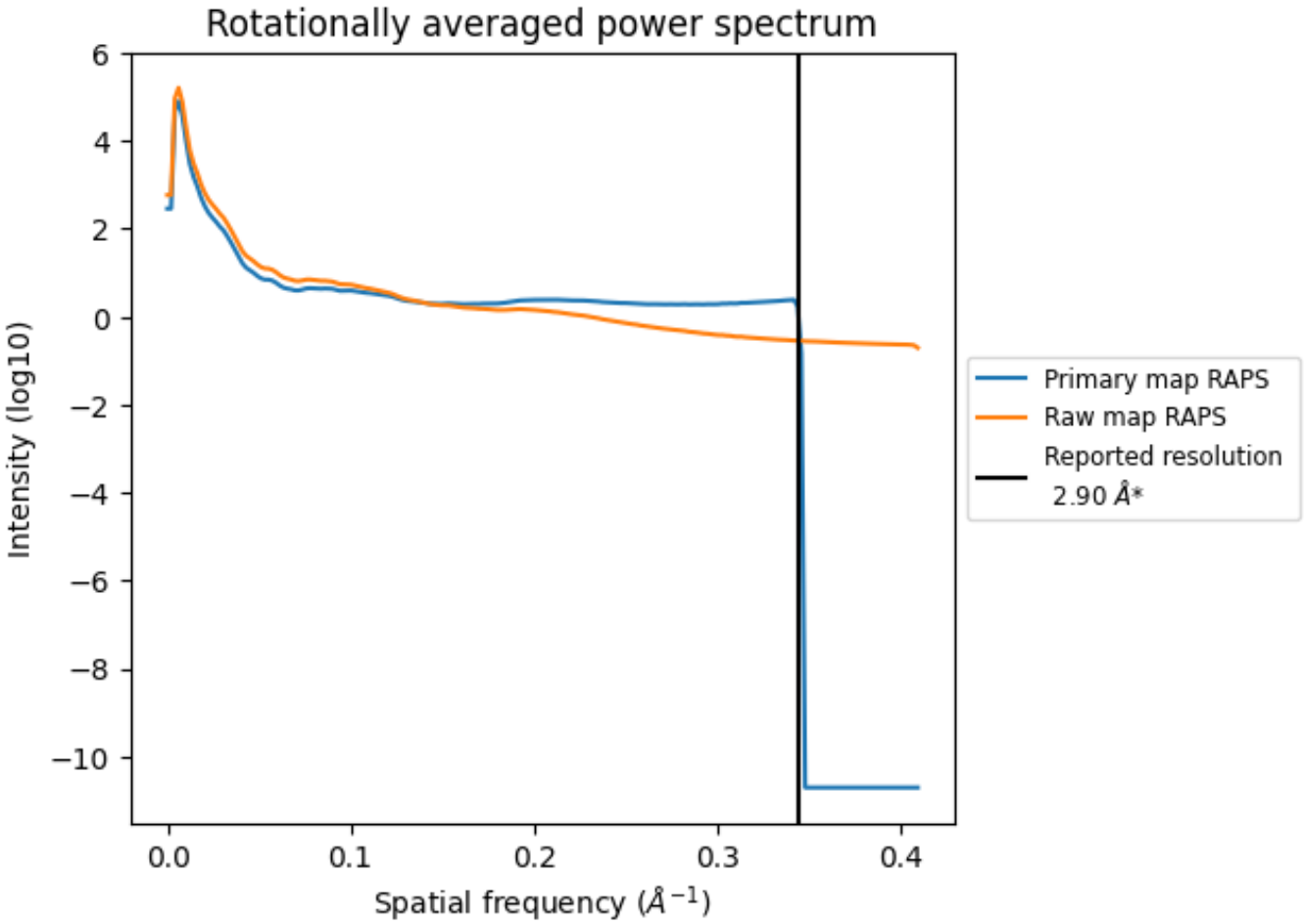
7.2 Volume estimate



The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 165 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

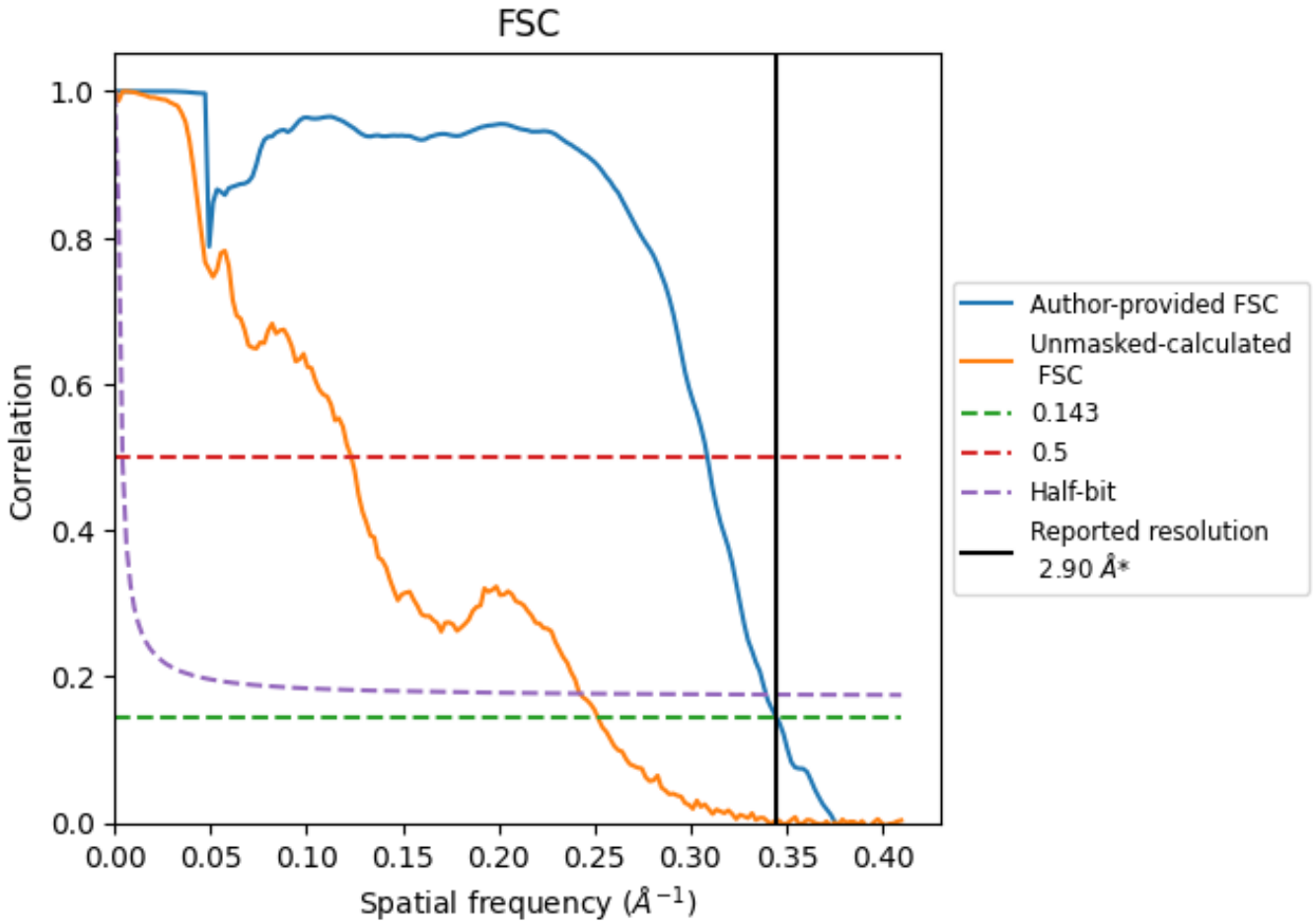


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

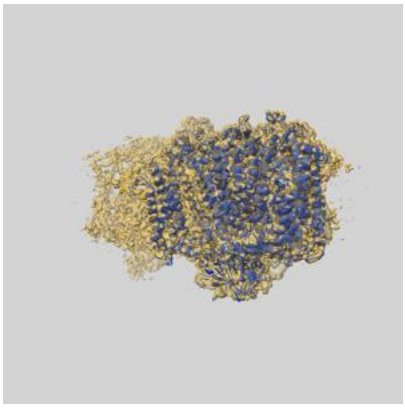
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.24	2.95
Unmasked-calculated*	3.97	8.12	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.9 by more than 10 %

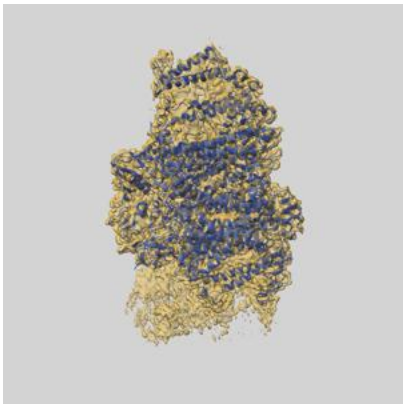
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15621 and PDB model 8ASP. Per-residue inclusion information can be found in section 3 on page 21.

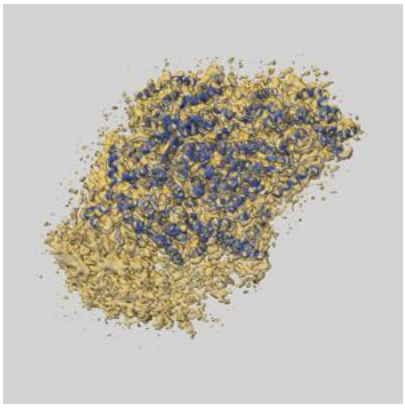
9.1 Map-model overlay



X



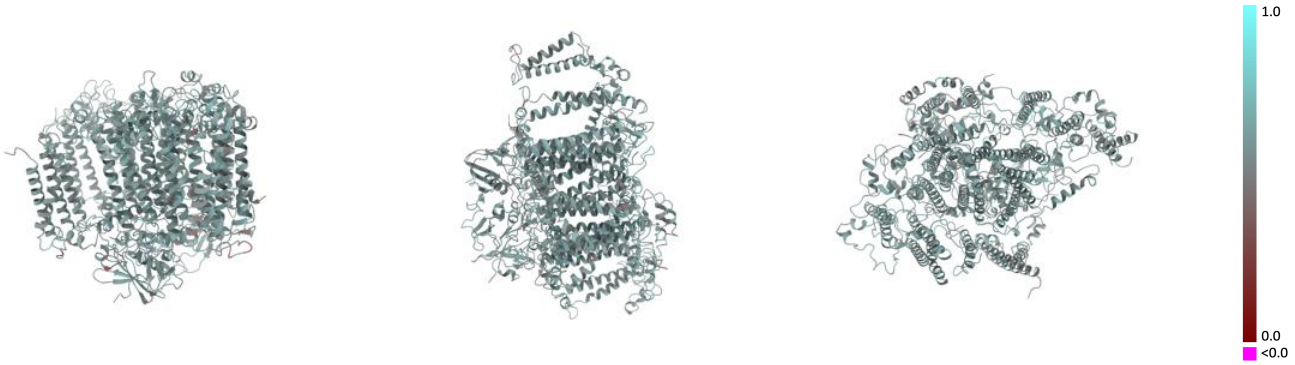
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

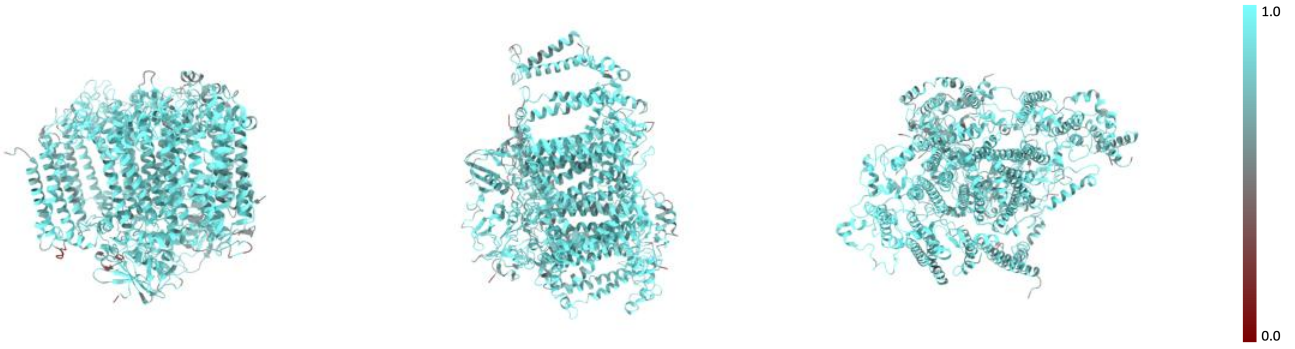
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

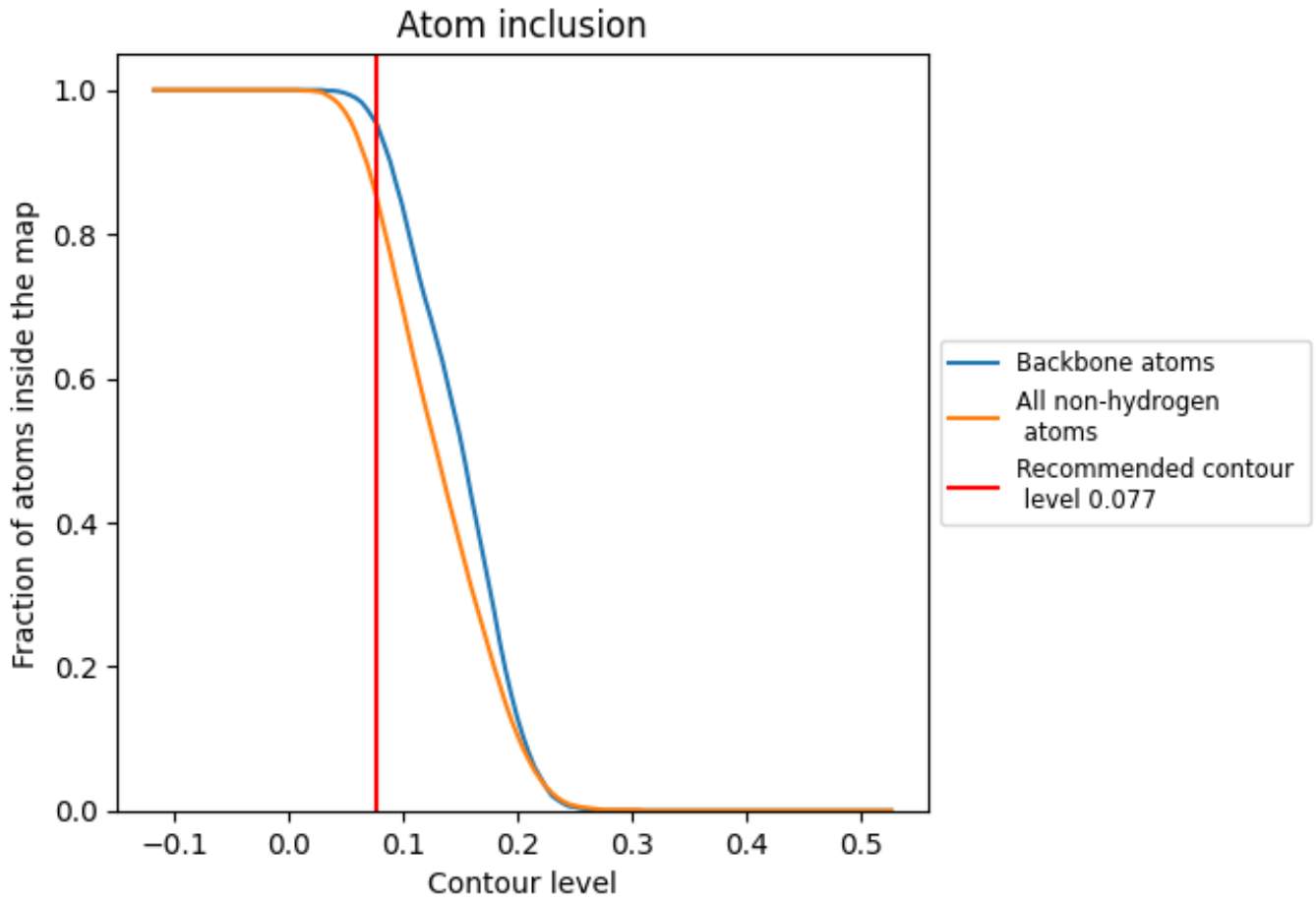
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.077).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5710
a	0.8670	0.5810
b	0.8770	0.5800
c	0.9450	0.5740
d	0.8630	0.5670
e	0.8160	0.5560
f	0.7640	0.5490
i	0.8350	0.5750
j	0.6760	0.5200
k	0.7140	0.5370
l	0.7420	0.5220
m	0.7970	0.5590